OXC Scenario Results

Online Resource 2

Article: A computational framework for posterior probability vectors over discrete pharmacokinetic states

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Summary across sensitivity scenarios

One reference scenario and 82 sensitivity scenarios.

Unavailable denotes missing or excluded values. Valid-output counts refer to the five formal runs; pilot and historical attempts are retained under Run times and numerical checks.

Definitions and comparison rules: Online Resource 1, Section 5.

Virtual-patient comparisons use archived web-displayed probabilities without renormalization and matched visible input settings. Noncomparable web outputs are listed separately. A displayed zero need not be an exact posterior zero.

Archived virtual-patient curve panels retain their source axis labels; the monitored analyte in the OXC scenarios is MHD.

Scenario map



Filled indicators: available outputs; slashes: qualified outputs; crosses: failed computations; open indicators: undetermined coverage; dash: no corresponding MC setting. R stability flags are retained but do not alone exclude a complete posterior output.

Scenario index

Reference scenario

Scenario	Change from reference	Page
C003	Reference scenario.	6

Structural parameters

Scenario	Change from reference	Page
C001	CL_p: 1.68 to 0.84.	8
C002	CL_p: 1.68 to 1.344.	10
C004	CL_p: 1.68 to 2.016.	12
C005	CL_p: 1.68 to 3.36.	14
C006	V_p: 14.7 to 7.35.	16
C007	V_p: 14.7 to 11.76.	18
C008	V_p: 14.7 to 17.64.	20
C009	V_p: 14.7 to 29.4.	22
C010	ka: 0.83 to 0.415.	24
C011	ka: 0.83 to 0.664.	26
C012	ka: 0.83 to 0.996.	28
C013	ka: 0.83 to 1.66.	30
C014	BW: 25 to 12.5.	32
C015	BW: 25 to 20.	34
C016	BW: 25 to 30.	36
C017	BW: 25 to 50.	38

Variability

Scenario	Change from reference	Page
C018	Clearance IIV: CV 0.01000000002%.	40
C019	Clearance IIV: CV 2.775%.	42
C020	Clearance IIV: CV 5.55%.	44
C021	Clearance IIV: CV 8.325%.	46
C022	Clearance IIV: CV 16.65%.	48
C023	Clearance IIV: CV 22.2%.	50
C024	Clearance IIV: CV 33.3%.	52
C025	Clearance IIV: CV 44.4%.	54
C026	Additive residual SD: 1e-06 mg/L.	56
C027	Additive residual SD: 0.748 mg/L.	58
C028	Additive residual SD: 1.496 mg/L.	60
C029	Additive residual SD: 2.244 mg/L.	62
C030	Additive residual SD: 4.488 mg/L.	64
C031	Additive residual SD: 5.984 mg/L.	66
C032	Additive residual SD: 8.976 mg/L.	68
C033	Additive residual SD: 11.968 mg/L.	70

Actual dosing histories

Scenario	Change from reference	Page
C034	Observation generated from 300 mg at 0 h and 300 mg at 12 h; candidate histories unchanged.	72
C035	Observation generated from 150 mg at 0 h and 300 mg at 12 h; candidate histories unchanged.	74
C036	Observation generated from 600 mg at 0 h and 300 mg at 12 h; candidate histories unchanged.	76
C037	Observation generated from 300 mg at 0 h and 150 mg at 12 h; candidate histories unchanged.	78
C038	Observation generated from 300 mg at 0 h and 600 mg at 12 h; candidate histories unchanged.	80
C039	Observation generated from 300 mg at -4 h and 300 mg at 12 h; candidate histories unchanged.	82
C040	Observation generated from 300 mg at -2 h and 300 mg at 12 h; candidate histories unchanged.	84
C041	Observation generated from 300 mg at 2 h and 300 mg at 12 h; candidate histories unchanged.	86
C042	Observation generated from 300 mg at 4 h and 300 mg at 12 h; candidate histories unchanged.	88
C043	Observation generated from 300 mg at 0 h and 300 mg at 8 h; candidate histories unchanged.	90
C044	Observation generated from 300 mg at 0 h and 300 mg at 10 h; candidate histories unchanged.	92
C045	Observation generated from 300 mg at 0 h and 300 mg at 14 h; candidate histories unchanged.	94
C046	Observation generated from 300 mg at 0 h and 300 mg at 16 h; candidate histories unchanged.	96

Observation records

Scenario	Change from reference	Page
C047	Observation times: 16 h.	98
C048	Observation times: 18 h.	100
C049	Observation times: 20 h.	102
C050	Observation times: 22 h.	104
C051	Observation times: 26 h.	106
C052	Observation times: 28 h.	108
C053	Observation times: 30 h.	110
C054	Observation times: 32 h.	112
C055	Observation times: 0, 24 h.	114
C056	Observation times: 18, 24 h.	116
C057	Observation times: 24, 30 h.	118
C058	Observation times: 0, 24, 30 h.	120
C059	Observation times: 18, 24, 30 h.	122

Prior probabilities

Scenario	Change from reference	Page
C060	Independent per-dose prior probability: 0.1.	124
C061	Independent per-dose prior probability: 0.3.	126
C062	Independent per-dose prior probability: 0.7.	128
C063	Independent per-dose prior probability: 0.8.	130
C064	Independent per-dose prior probability: 0.9.	132

Candidate states

Scenario	Change from reference	Page
C065	Remove state omega_00.	134
C066	Remove state omega_01.	136
C067	Remove state omega_10.	138
C068	Remove state omega_11.	140
C069	Add one candidate history.	142
C070	Candidate dose events: 150 mg at 0 h; 300 mg at 12 h.	144
C071	Candidate dose events: 600 mg at 0 h; 300 mg at 12 h.	146
C072	Candidate dose events: 300 mg at 0 h; 150 mg at 12 h.	148
C073	Candidate dose events: 300 mg at 0 h; 600 mg at 12 h.	150
C074	Candidate dose events: 300 mg at -4 h; 300 mg at 12 h.	152
C075	Candidate dose events: 300 mg at -2 h; 300 mg at 12 h.	154
C076	Candidate dose events: 300 mg at 2 h; 300 mg at 12 h.	156
C077	Candidate dose events: 300 mg at 4 h; 300 mg at 12 h.	158
C078	Candidate dose events: 300 mg at 0 h; 300 mg at 8 h.	160
C079	Candidate dose events: 300 mg at 0 h; 300 mg at 10 h.	162
C080	Candidate dose events: 300 mg at 0 h; 300 mg at 14 h.	164
C081	Candidate dose events: 300 mg at 0 h; 300 mg at 16 h.	166
C082	Candidate dose times: 12 h; 2 candidate states.	168
C083	Candidate dose times: -12, 0, 12 h; 8 candidate states.	170

Scenario results

OXC C003: Reference scenario

Body weight 25 kg; scheduled oral doses of 300 mg at 0 h and 12 h; observed concentration of 12 mg/L at 24 h. Each of the four candidate dosing histories had a prior probability of 0.25.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

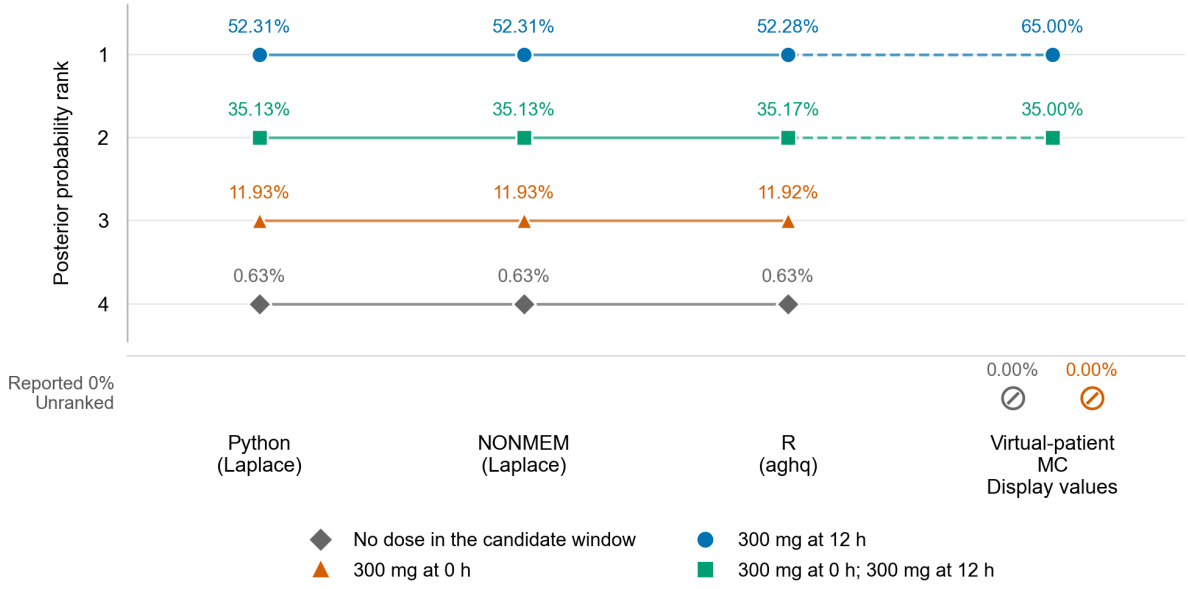
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.04004×10^{-8}	1.04004×10^{-8}	1.42054×10^{-8}	7.71641×10^{-9}
Python vs R aghq	3.47167×10^{-4}	3.47167×10^{-4}	4.43153×10^{-4}	2.94282×10^{-4}
NONMEM vs R aghq	3.47158×10^{-4}	3.47158×10^{-4}	4.43139×10^{-4}	2.94276×10^{-4}
Python vs Virtual patient	0.126927	0.126927	0.174302	0.257363
NONMEM vs Virtual patient	0.126927	0.126927	0.174302	0.257363
R aghq vs Virtual patient	0.127197	0.127197	0.174471	0.257318

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



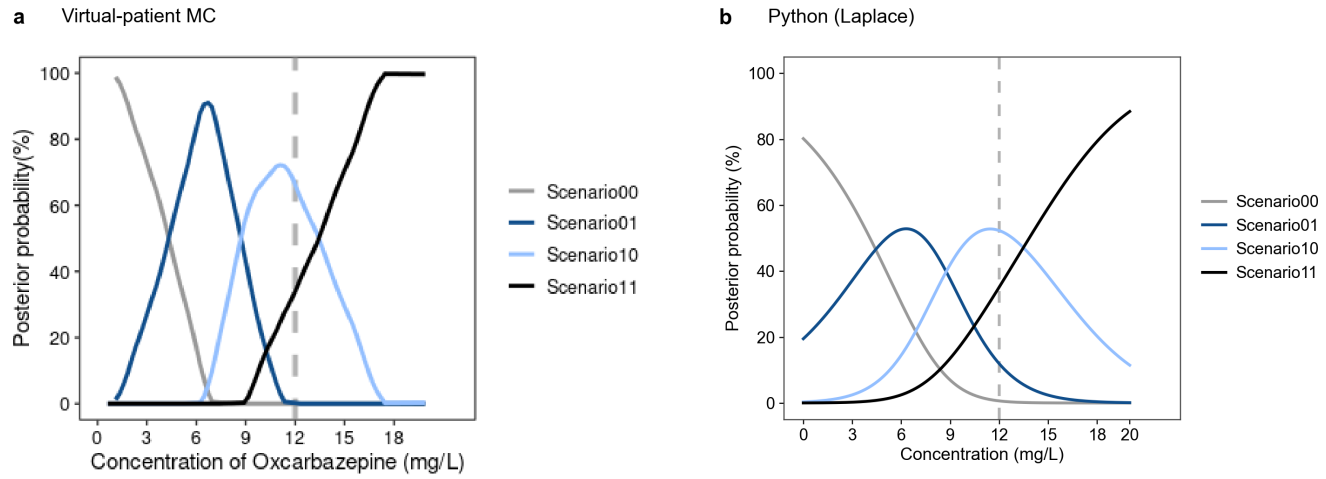
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00629656	0.00629656	0.00626151	0
ω_{01}: 300 mg at 0 h	0.25	0.11928606	0.11928606	0.11924385	0
ω_{10}: 300 mg at 12 h	0.25	0.52307289	0.52307288	0.52280298	0.65
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.35134449	0.35134450	0.35169166	0.35

Method	P_{max}	G	H_N
Python Laplace	0.523073	0.171728	0.715584
NONMEM Laplace	0.523073	0.171728	0.715584
R aghq	0.522803	0.171111	0.715527
Virtual patient (displayed)	0.65	0.3	0.467034

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C001: Structural parameters

CL_p: 1.68 to 0.84.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

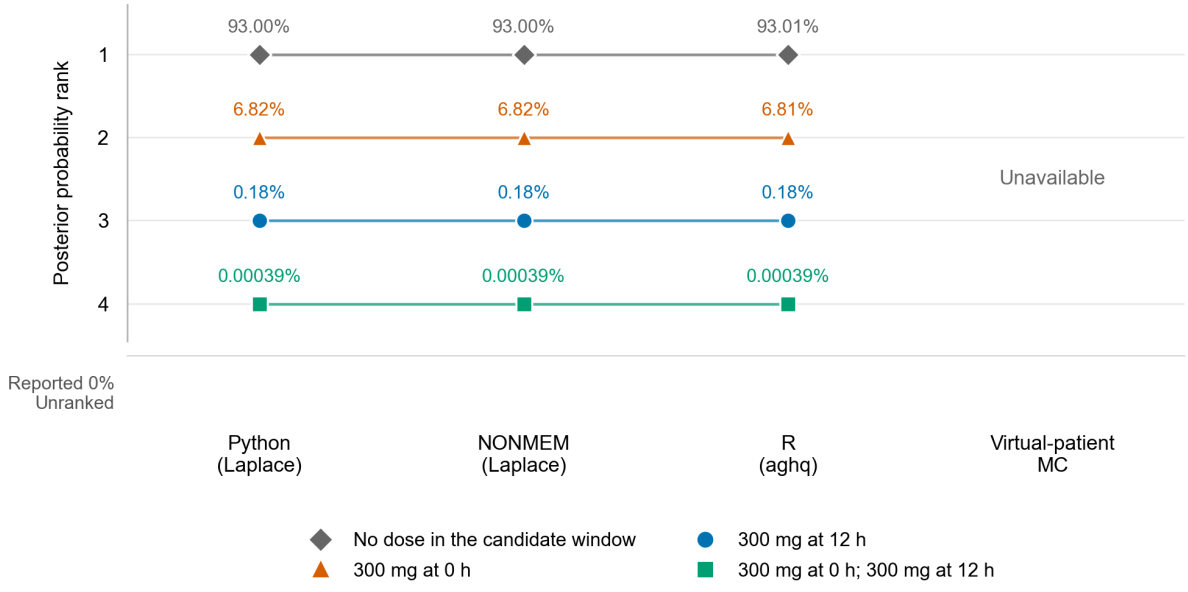
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	5.11647×10^{-10}	5.11647×10^{-10}	6.96232×10^{-10}	7.92125×10^{-10}
Python vs R aghq	5.65709×10^{-5}	5.65709×10^{-5}	7.78386×10^{-5}	7.97620×10^{-5}
NONMEM vs R aghq	5.65714×10^{-5}	5.65714×10^{-5}	7.78393×10^{-5}	7.97625×10^{-5}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.92999733	0.92999733	0.93005390
ω_{01}: 300 mg at 0 h	0.25	0.06819419	0.06819419	0.06814082
ω_{10}: 300 mg at 12 h	0.25	0.00180455	0.00180455	0.00180135
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.00000393	0.00000393	0.00000393

Method	P_{max}	G	H_N
Python Laplace	0.929997	0.861803	0.189044
NONMEM Laplace	0.929997	0.861803	0.189044
R aghq	0.930054	0.861913	0.188929

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C002: Structural parameters

CL_p: 1.68 to 1.344.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

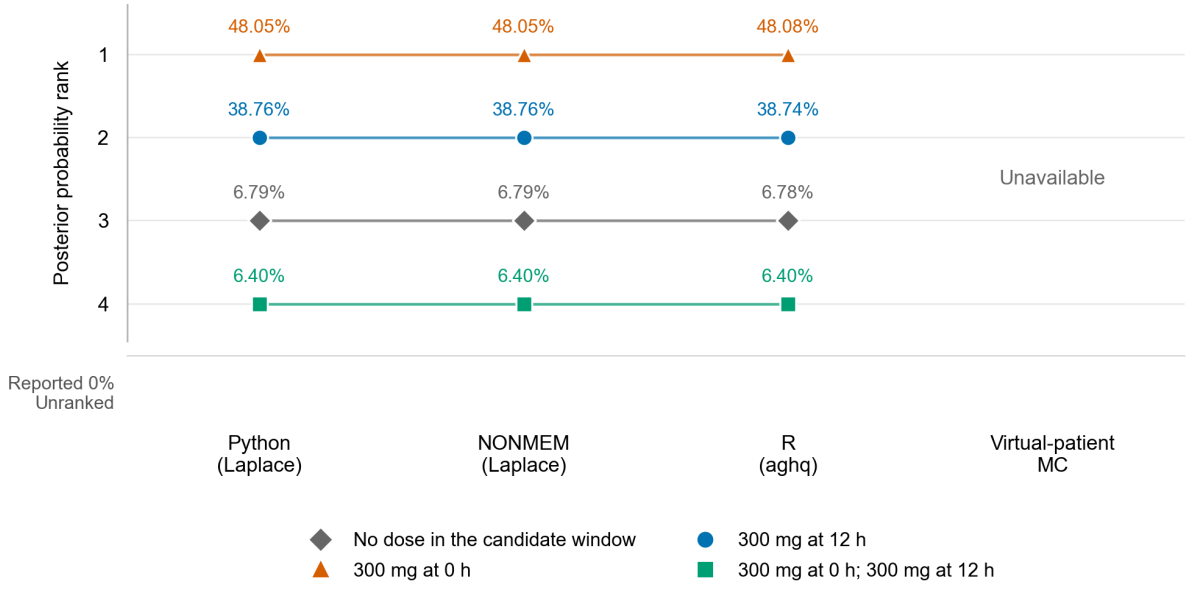
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	3.48478×10^{-9}	3.48478×10^{-9}	4.23636×10^{-9}	2.50425×10^{-9}
Python vs R aghq	3.44849×10^{-4}	3.81447×10^{-4}	4.42680×10^{-4}	3.05281×10^{-4}
NONMEM vs R aghq	3.44846×10^{-4}	3.81445×10^{-4}	4.42676×10^{-4}	3.05279×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.06794884	0.06794884	0.06779656
ω_{01}: 300 mg at 0 h	0.25	0.48046120	0.48046120	0.48080605
ω_{10}: 300 mg at 12 h	0.25	0.38761699	0.38761699	0.38738783
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.06397297	0.06397297	0.06400957

Method	P_{max}	G	H_N
Python Laplace	0.480461	0.092844	0.777711
NONMEM Laplace	0.480461	0.092844	0.777711
R aghq	0.480806	0.093418	0.777514

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C004: Structural parameters

CL_p: 1.68 to 2.016.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

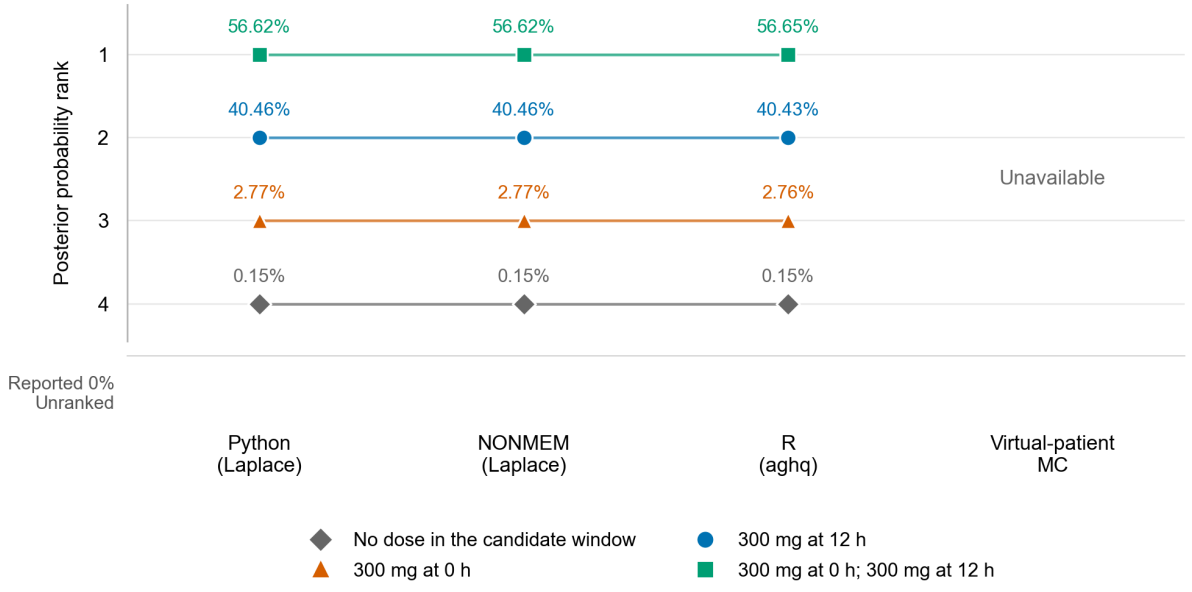
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	4.17968×10^{-9}	4.19311×10^{-9}	5.90828×10^{-9}	3.04459×10^{-9}
Python vs R aghq	3.30607×10^{-4}	3.30607×10^{-4}	4.27113×10^{-4}	2.55315×10^{-4}
NONMEM vs R aghq	3.30611×10^{-4}	3.30611×10^{-4}	4.27119×10^{-4}	2.55318×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00153953	0.00153953	0.00153508
ω_{01}: 300 mg at 0 h	0.25	0.02770027	0.02770027	0.02763699
ω_{10}: 300 mg at 12 h	0.25	0.40457861	0.40457862	0.40431574
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.56618158	0.56618158	0.56651219

Method	P_{max}	G	H_N
Python Laplace	0.566182	0.161603	0.575265
NONMEM Laplace	0.566182	0.161603	0.575265
R aghq	0.566512	0.162196	0.575044

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C005: Structural parameters

CL_p: 1.68 to 3.36.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

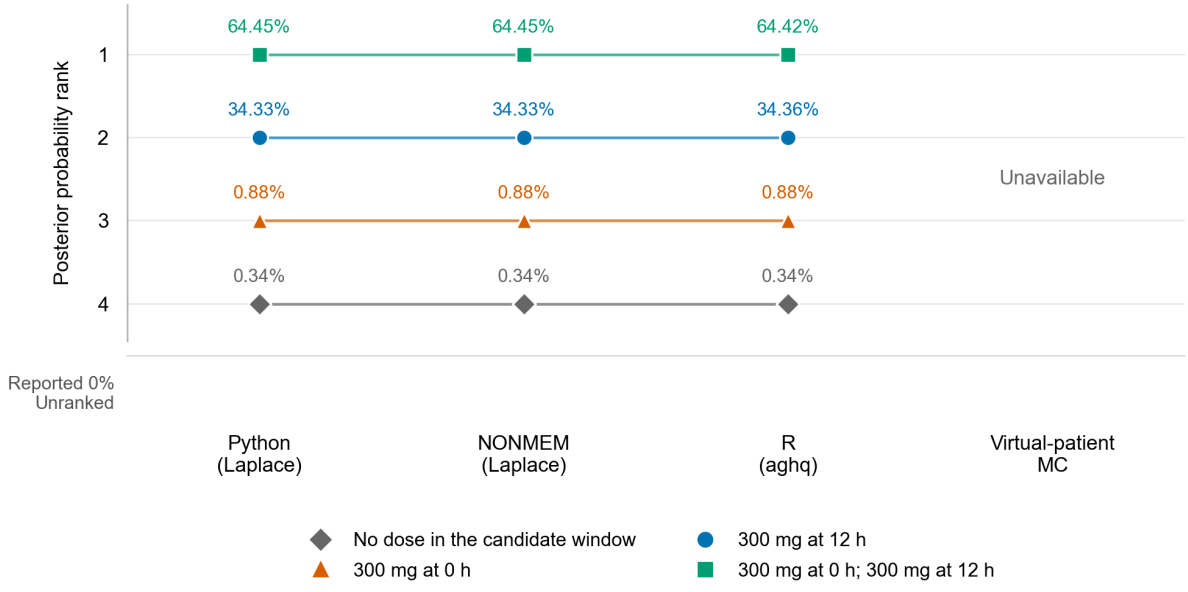
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	7.06476×10^{-11}	7.06476×10^{-11}	8.99255×10^{-11}	2.68434×10^{-10}
Python vs R aghq	2.34953×10^{-4}	2.34953×10^{-4}	3.27723×10^{-4}	1.76332×10^{-4}
NONMEM vs R aghq	2.34954×10^{-4}	2.34954×10^{-4}	3.27723×10^{-4}	1.76332×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00339268	0.00339268	0.00339884
ω_{01}: 300 mg at 0 h	0.25	0.00879625	0.00879625	0.00879665
ω_{10}: 300 mg at 12 h	0.25	0.34334044	0.34334044	0.34356883
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.64447063	0.64447063	0.64423568

Method	P_{max}	G	H_N
Python Laplace	0.644471	0.301130	0.512952
NONMEM Laplace	0.644471	0.301130	0.512952
R aghq	0.644236	0.300667	0.513080

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C006: Structural parameters

V_p: 14.7 to 7.35.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

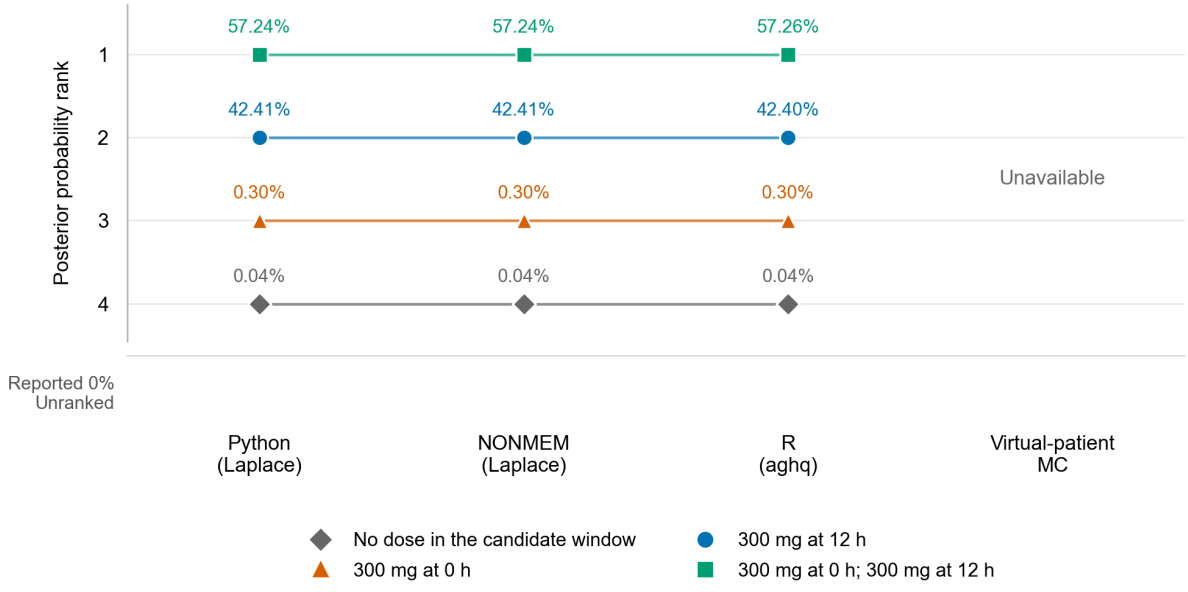
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	5.22023×10^{-10}	5.22023×10^{-10}	7.20848×10^{-10}	3.94604×10^{-10}
Python vs R aghq	1.38682×10^{-4}	1.39528×10^{-4}	1.83905×10^{-4}	1.61465×10^{-4}
NONMEM vs R aghq	1.38681×10^{-4}	1.39527×10^{-4}	1.83904×10^{-4}	1.61465×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00042100	0.00042100	0.00042184
ω_{01}: 300 mg at 0 h	0.25	0.00301529	0.00301529	0.00299479
ω_{10}: 300 mg at 12 h	0.25	0.42413637	0.42413637	0.42401734
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.57242735	0.57242735	0.57256603

Method	P_{max}	G	H_N
Python Laplace	0.572427	0.148291	0.507753
NONMEM Laplace	0.572427	0.148291	0.507753
R aghq	0.572566	0.148549	0.507654

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C007: Structural parameters

V_p: 14.7 to 11.76.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

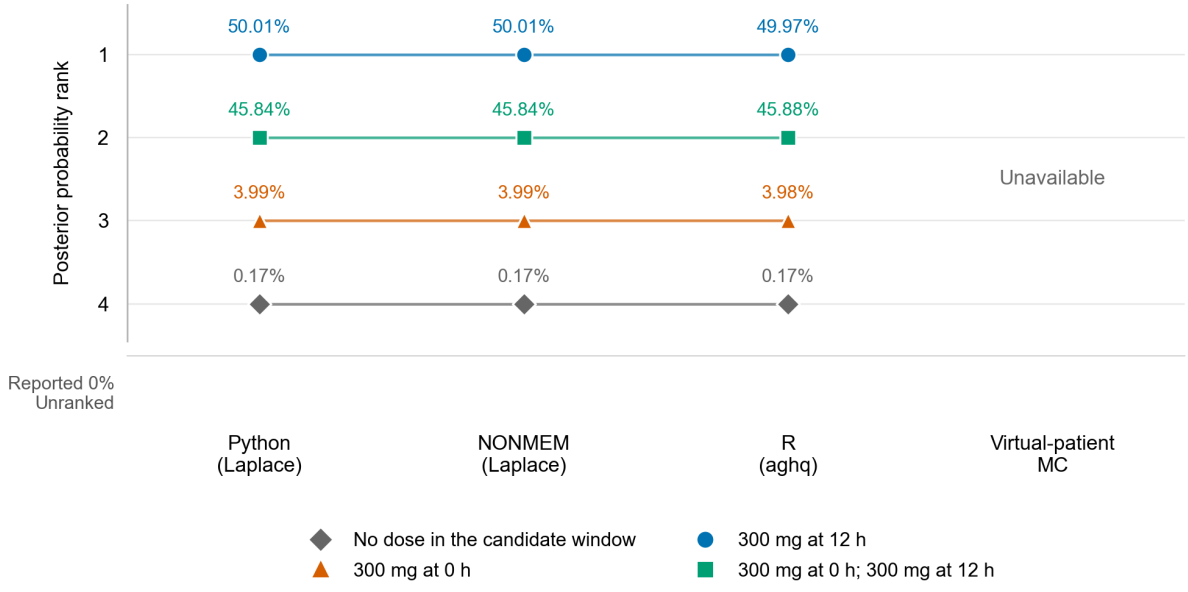
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	5.22140×10^{-10}	5.22140×10^{-10}	6.51018×10^{-10}	4.36151×10^{-10}
Python vs R aghq	4.16323×10^{-4}	4.16323×10^{-4}	5.32524×10^{-4}	3.19767×10^{-4}
NONMEM vs R aghq	4.16323×10^{-4}	4.16323×10^{-4}	5.32524×10^{-4}	3.19767×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00167237	0.00167237	0.00166413
ω_{01}: 300 mg at 0 h	0.25	0.03989253	0.03989253	0.03980451
ω_{10}: 300 mg at 12 h	0.25	0.50005043	0.50005044	0.49973037
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.45838467	0.45838467	0.45880099

Method	P_{max}	G	H_N
Python Laplace	0.500050	0.041666	0.608333
NONMEM Laplace	0.500050	0.041666	0.608333
R aghq	0.499730	0.040929	0.608164

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C008: Structural parameters

V_p: 14.7 to 17.64.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

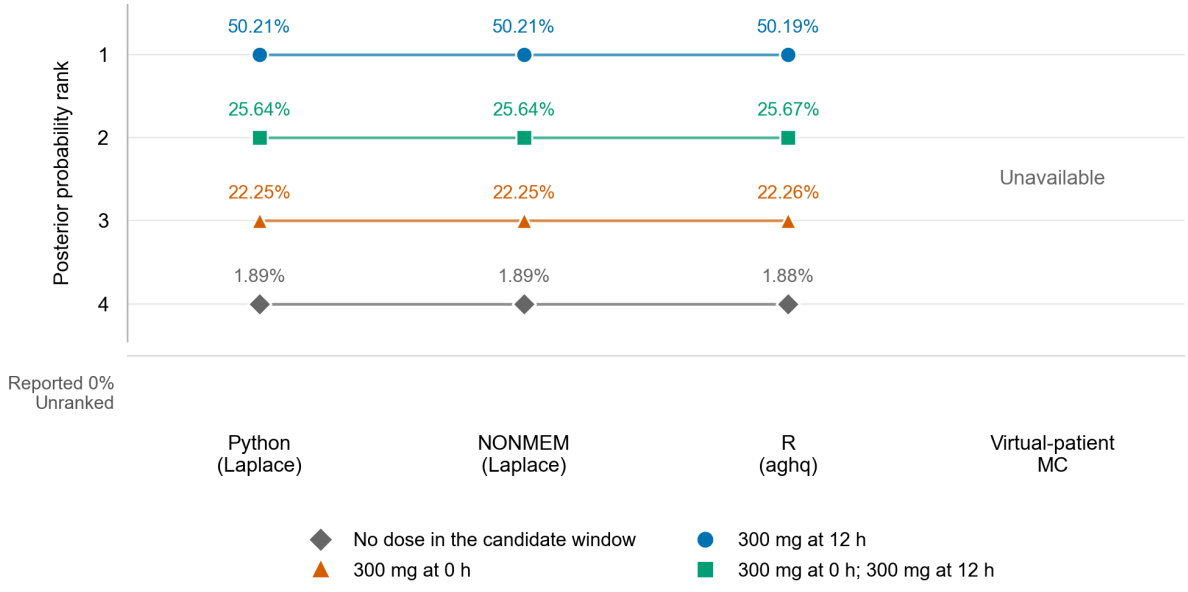
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.68856×10^{-9}	1.68856×10^{-9}	2.17646×10^{-9}	1.57182×10^{-9}
Python vs R aghq	2.20717×10^{-4}	2.75124×10^{-4}	3.15096×10^{-4}	2.57837×10^{-4}
NONMEM vs R aghq	2.20719×10^{-4}	2.75124×10^{-4}	3.15097×10^{-4}	2.57838×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.01889659	0.01889659	0.01882889
ω_{01}: 300 mg at 0 h	0.25	0.22252693	0.22252694	0.22258134
ω_{10}: 300 mg at 12 h	0.25	0.50214352	0.50214352	0.50193609
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.25643295	0.25643295	0.25665367

Method	P_{max}	G	H_N
Python Laplace	0.502144	0.245711	0.796567
NONMEM Laplace	0.502144	0.245711	0.796567
R aghq	0.501936	0.245282	0.796546

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C009: Structural parameters

V_p: 14.7 to 29.4.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

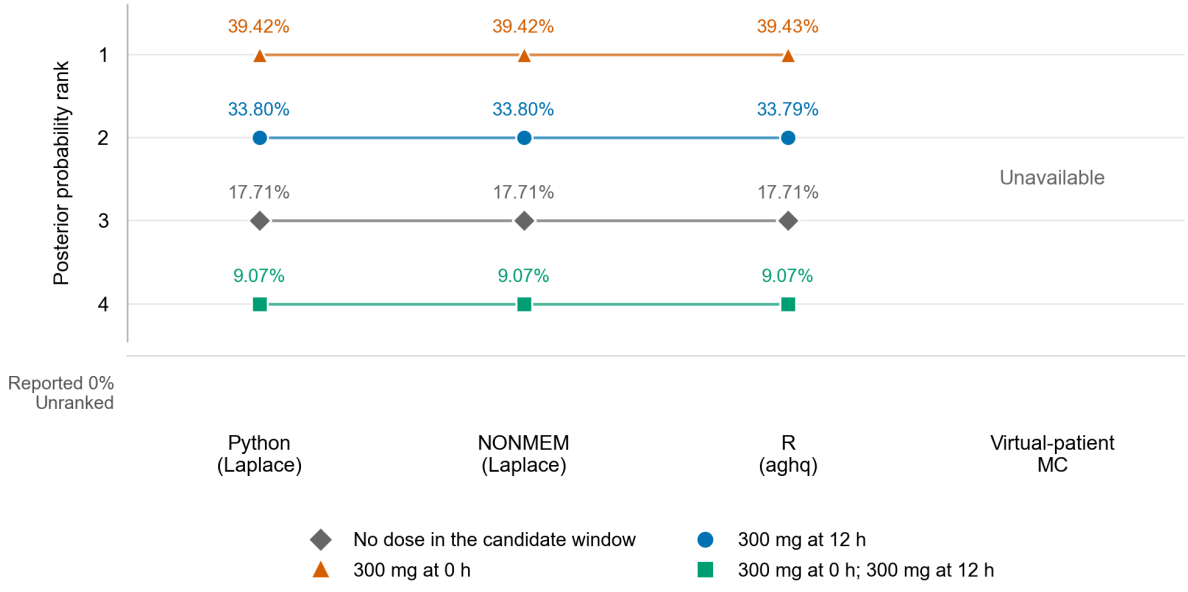
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	5.43599×10^{-9}	5.43599×10^{-9}	6.40633×10^{-9}	4.56779×10^{-9}
Python vs R aghq	1.11061×10^{-4}	1.36358×10^{-4}	1.49237×10^{-4}	9.88847×10^{-5}
NONMEM vs R aghq	1.11067×10^{-4}	1.36361×10^{-4}	1.49242×10^{-4}	9.88872×10^{-5}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.17712018	0.17712019	0.17705233
ω_{01}: 300 mg at 0 h	0.25	0.39418117	0.39418116	0.39429223
ω_{10}: 300 mg at 12 h	0.25	0.33799782	0.33799782	0.33792931
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.09070083	0.09070083	0.09072612

Method	P_{max}	G	H_N
Python Laplace	0.394181	0.056183	0.907364
NONMEM Laplace	0.394181	0.056183	0.907364
R aghq	0.394292	0.056363	0.907344

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C010: Structural parameters

ka: 0.83 to 0.415.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

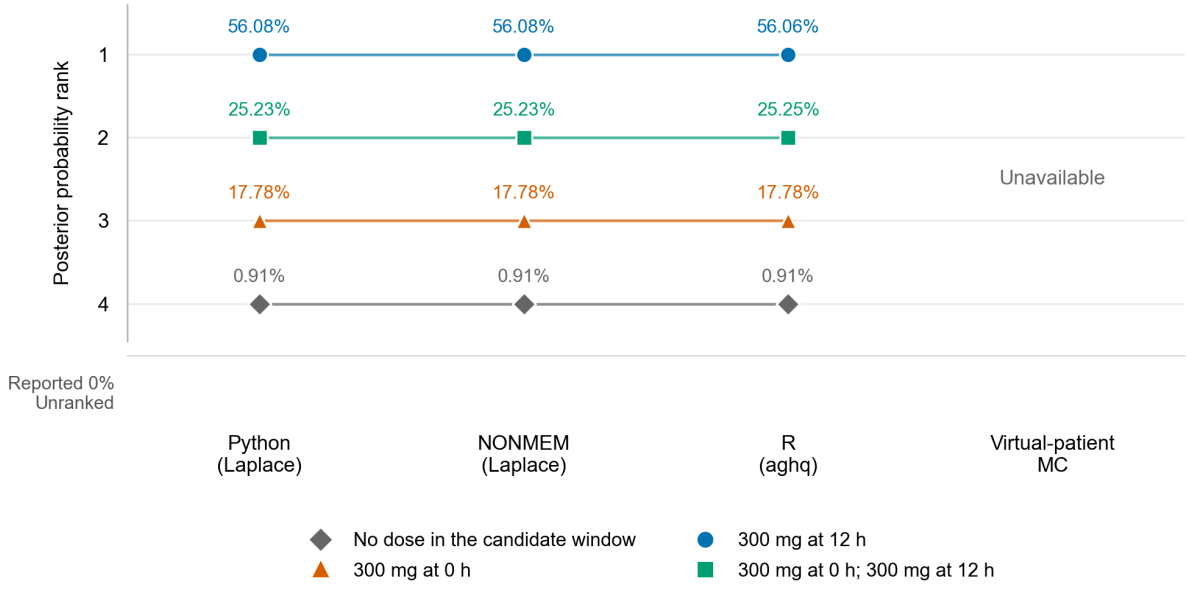
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	2.76747×10^{-9}	2.80746×10^{-9}	3.61176×10^{-9}	2.27255×10^{-9}
Python vs R aghq	2.56861×10^{-4}	2.62257×10^{-4}	3.38937×10^{-4}	2.68699×10^{-4}
NONMEM vs R aghq	2.56859×10^{-4}	2.62255×10^{-4}	3.38934×10^{-4}	2.68698×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00913199	0.00913199	0.00908596
ω_{01}: 300 mg at 0 h	0.25	0.17781176	0.17781176	0.17781716
ω_{10}: 300 mg at 12 h	0.25	0.56078371	0.56078371	0.56056749
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.25227254	0.25227254	0.25252940

Method	P_{max}	G	H_N
Python Laplace	0.560784	0.308511	0.737058
NONMEM Laplace	0.560784	0.308511	0.737058
R aghq	0.560567	0.308038	0.737074

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C011: Structural parameters

ka: 0.83 to 0.664.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

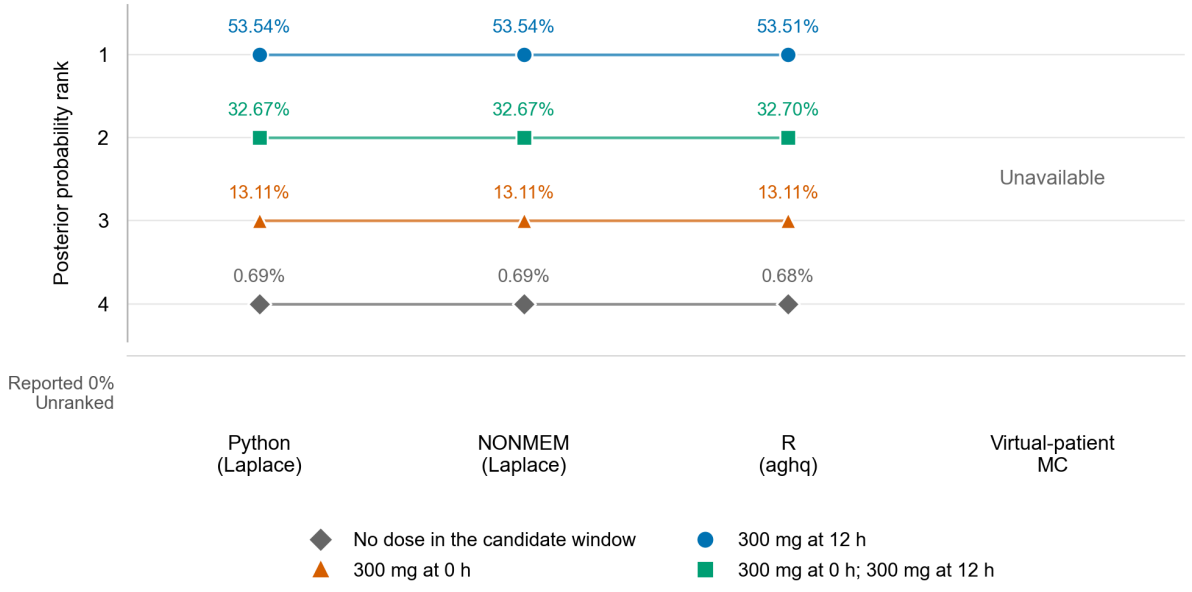
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	2.70879×10^{-9}	2.70879×10^{-9}	3.70229×10^{-9}	2.19049×10^{-9}
Python vs R aghq	3.26238×10^{-4}	3.26238×10^{-4}	4.18029×10^{-4}	2.87379×10^{-4}
NONMEM vs R aghq	3.26240×10^{-4}	3.26240×10^{-4}	4.18033×10^{-4}	2.87381×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00685453	0.00685454	0.00681719
ω_{01}: 300 mg at 0 h	0.25	0.13108951	0.13108951	0.13105730
ω_{10}: 300 mg at 12 h	0.25	0.53536280	0.53536280	0.53510612
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.32669315	0.32669315	0.32701939

Method	P_{max}	G	H_N
Python Laplace	0.535363	0.208670	0.721705
NONMEM Laplace	0.535363	0.208670	0.721705
R aghq	0.535106	0.208087	0.721671

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C012: Structural parameters

ka: 0.83 to 0.996.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

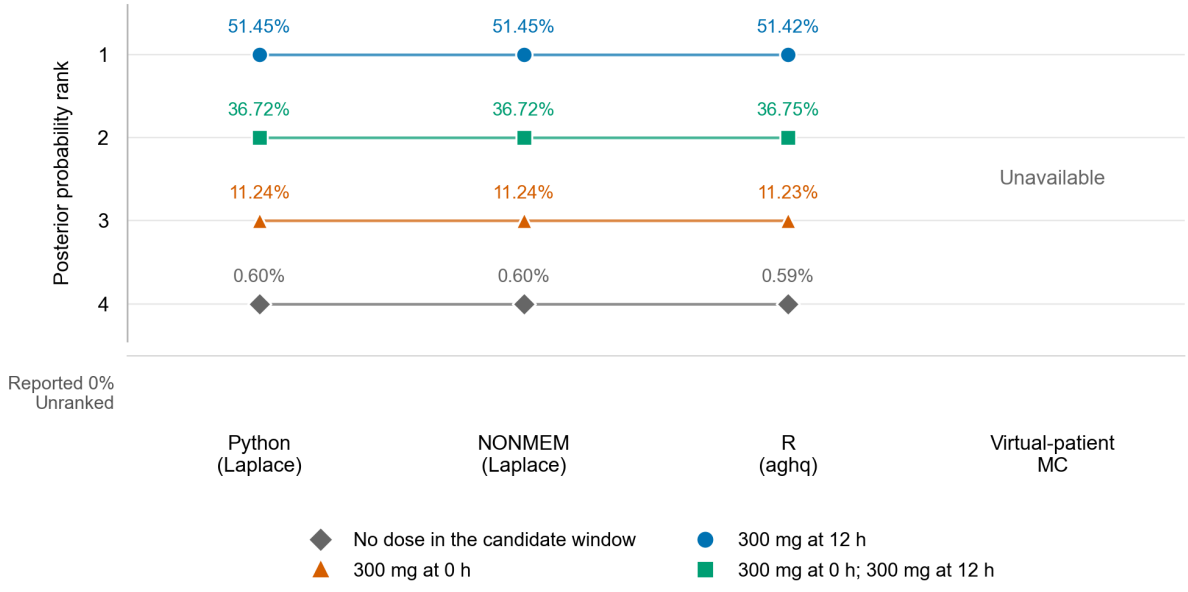
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	7.98166×10^{-9}	7.98166×10^{-9}	1.05019×10^{-8}	5.70349×10^{-9}
Python vs R aghq	3.60042×10^{-4}	3.60042×10^{-4}	4.58756×10^{-4}	2.98849×10^{-4}
NONMEM vs R aghq	3.60036×10^{-4}	3.60036×10^{-4}	4.58746×10^{-4}	2.98845×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00597292	0.00597292	0.00593923
ω_{01}: 300 mg at 0 h	0.25	0.11235889	0.11235889	0.11231068
ω_{10}: 300 mg at 12 h	0.25	0.51448593	0.51448593	0.51420778
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.36718226	0.36718226	0.36754230

Method	P_{max}	G	H_N
Python Laplace	0.514486	0.147304	0.711254
NONMEM Laplace	0.514486	0.147304	0.711254
R aghq	0.514208	0.146665	0.711180

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C013: Structural parameters

ka: 0.83 to 1.66.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

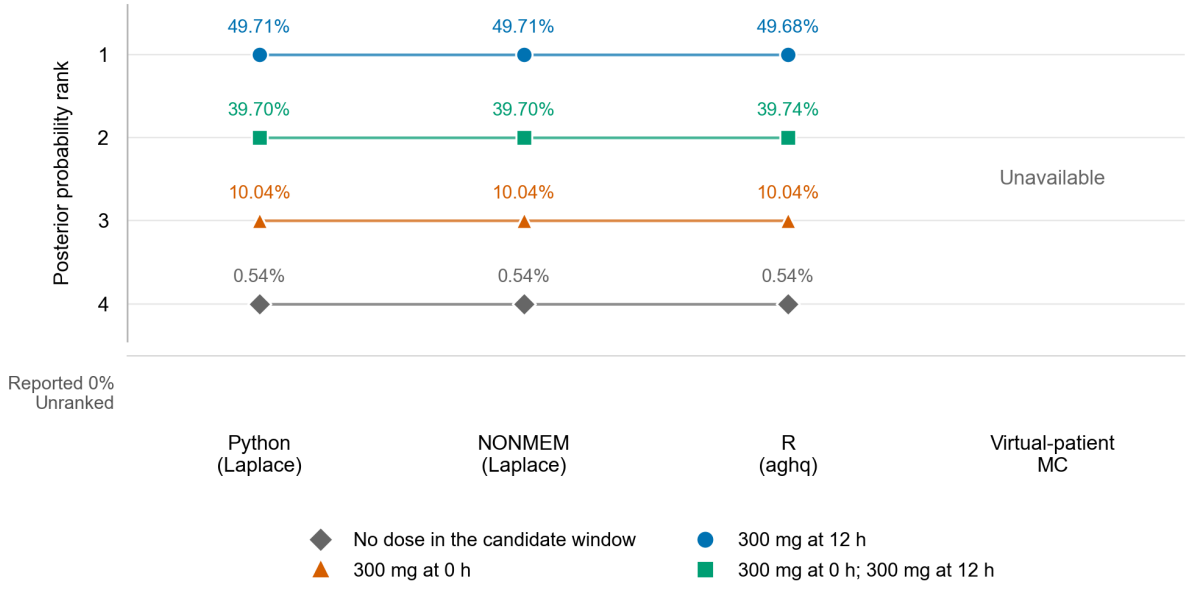
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	6.31305×10^{-9}	6.33276×10^{-9}	8.27480×10^{-9}	4.48988×10^{-9}
Python vs R aghq	3.83010×10^{-4}	3.83010×10^{-4}	4.86791×10^{-4}	3.07672×10^{-4}
NONMEM vs R aghq	3.83016×10^{-4}	3.83016×10^{-4}	4.86798×10^{-4}	3.07675×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00542375	0.00542375	0.00539247
ω_{01}: 300 mg at 0 h	0.25	0.10043522	0.10043522	0.10037647
ω_{10}: 300 mg at 12 h	0.25	0.49710077	0.49710078	0.49680779
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.39704026	0.39704025	0.39742327

Method	P_{max}	G	H_N
Python Laplace	0.497101	0.100061	0.702108
NONMEM Laplace	0.497101	0.100061	0.702108
R aghq	0.496808	0.099385	0.702000

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C014: Structural parameters

BW: 25 to 12.5.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

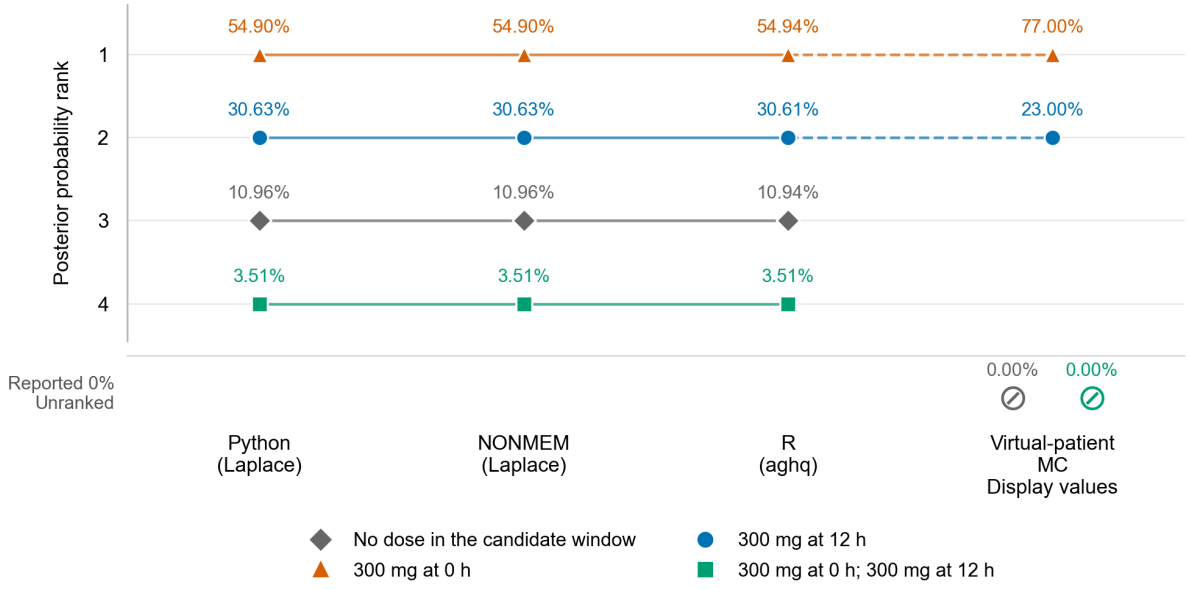
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	4.15456×10^{-9}	4.87391×10^{-9}	5.76404×10^{-9}	4.96974×10^{-9}
Python vs R aghq	3.66230×10^{-4}	3.77867×10^{-4}	4.55348×10^{-4}	2.82101×10^{-4}
NONMEM vs R aghq	3.66235×10^{-4}	3.77870×10^{-4}	4.55352×10^{-4}	2.82104×10^{-4}
Python vs Virtual patient	0.220959	0.220959	0.260548	0.290473
NONMEM vs Virtual patient	0.220959	0.220959	0.260548	0.290473
R aghq vs Virtual patient	0.220592	0.220592	0.260107	0.290263

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



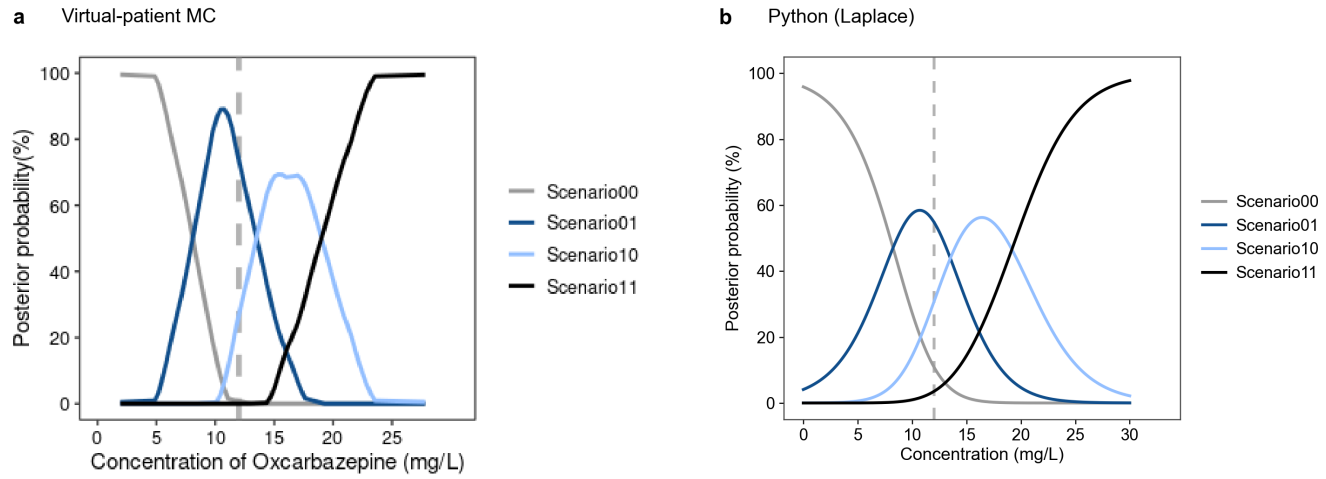
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.10959398	0.10959398	0.10943411	0
ω_{01}: 300 mg at 0 h	0.25	0.54904149	0.54904148	0.54940772	0.77
ω_{10}: 300 mg at 12 h	0.25	0.30630350	0.30630350	0.30608550	0.23
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.03506104	0.03506104	0.03507268	0

Method	P_{max}	G	H_N
Python Laplace	0.549041	0.242738	0.758420
NONMEM Laplace	0.549041	0.242738	0.758420
R aghq	0.549408	0.243322	0.758166
Virtual patient (displayed)	0.77	0.54	0.389006

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C015: Structural parameters

BW: 25 to 20.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

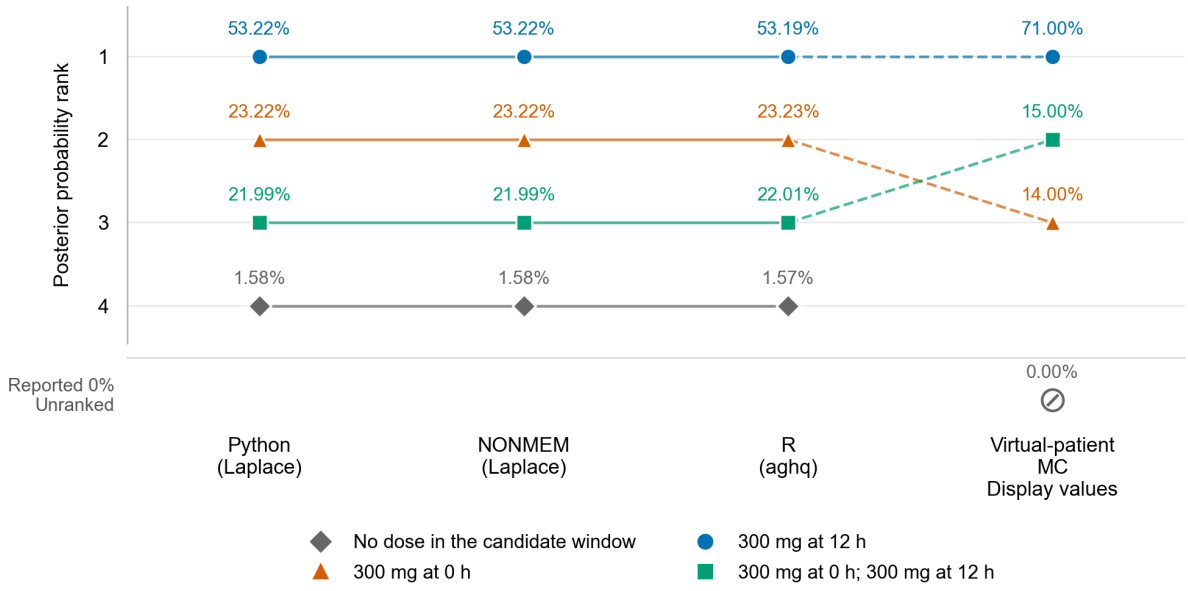
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	3.03517×10^{-9}	3.20934×10^{-9}	4.08314×10^{-9}	2.53230×10^{-9}
Python vs R aghq	2.29398×10^{-4}	3.04526×10^{-4}	3.37582×10^{-4}	2.97777×10^{-4}
NONMEM vs R aghq	2.29395×10^{-4}	3.04523×10^{-4}	3.37579×10^{-4}	2.97776×10^{-4}
Python vs Virtual patient	0.177829	0.177829	0.212731	0.152996
NONMEM vs Virtual patient	0.177829	0.177829	0.212731	0.152996
R aghq vs Virtual patient	0.178059	0.178059	0.213026	0.153025

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



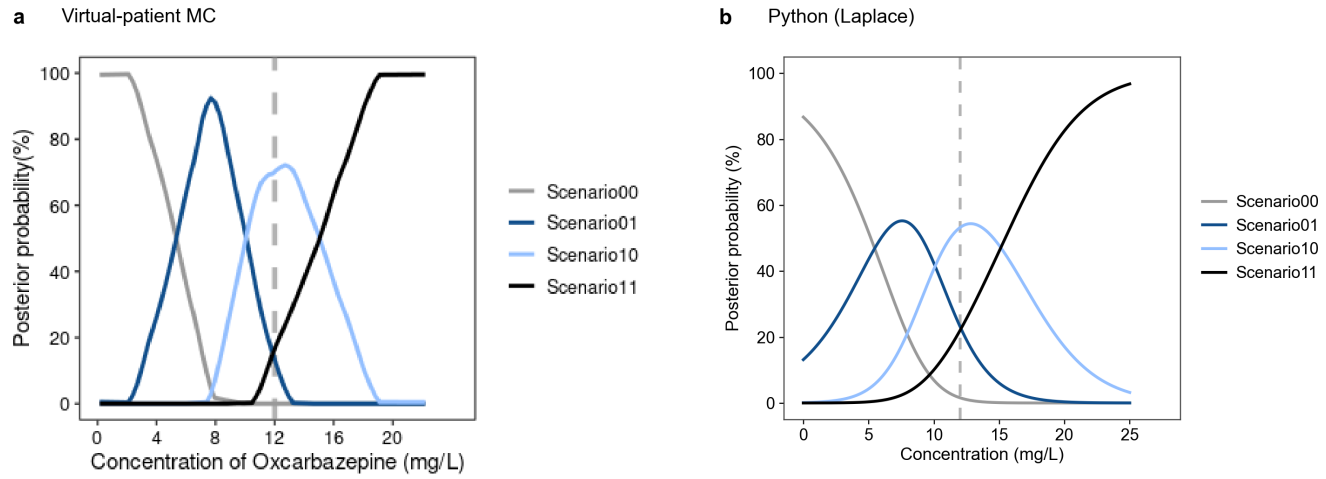
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.01576094	0.01576094	0.01568581	0
ω_{01}: 300 mg at 0 h	0.25	0.23220558	0.23220559	0.23228956	0.14
ω_{10}: 300 mg at 12 h	0.25	0.53217072	0.53217071	0.53194132	0.71
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.21986276	0.21986276	0.22008331	0.15

Method	P_{max}	G	H_N
Python Laplace	0.532171	0.299965	0.774142
NONMEM Laplace	0.532171	0.299965	0.774142
R aghq	0.531941	0.299652	0.774142
Virtual patient (displayed)	0.71	0.56	0.579236

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C016: Structural parameters

BW: 25 to 30.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

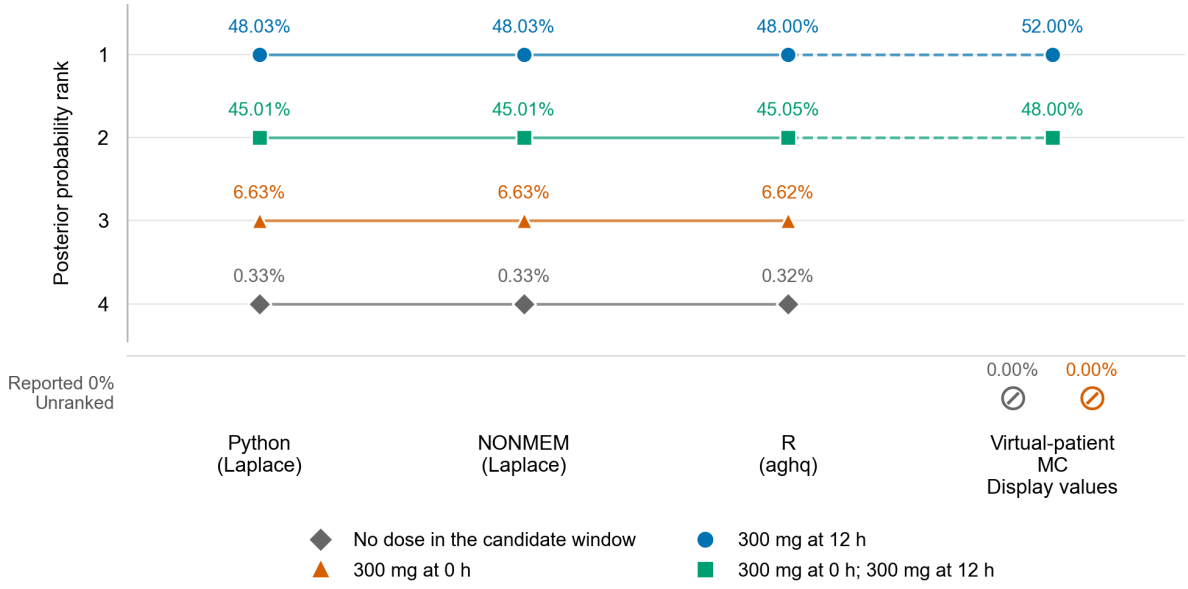
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.78688×10^{-9}	1.78688×10^{-9}	2.22937×10^{-9}	1.36959×10^{-9}
Python vs R aghq	3.85947×10^{-4}	3.85947×10^{-4}	4.91618×10^{-4}	2.91788×10^{-4}
NONMEM vs R aghq	3.85946×10^{-4}	3.85946×10^{-4}	4.91616×10^{-4}	2.91788×10^{-4}
Python vs Virtual patient	0.066294	0.069560	0.082903	0.188185
NONMEM vs Virtual patient	0.066294	0.069560	0.082903	0.188185
R aghq vs Virtual patient	0.066220	0.069469	0.082847	0.188063

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



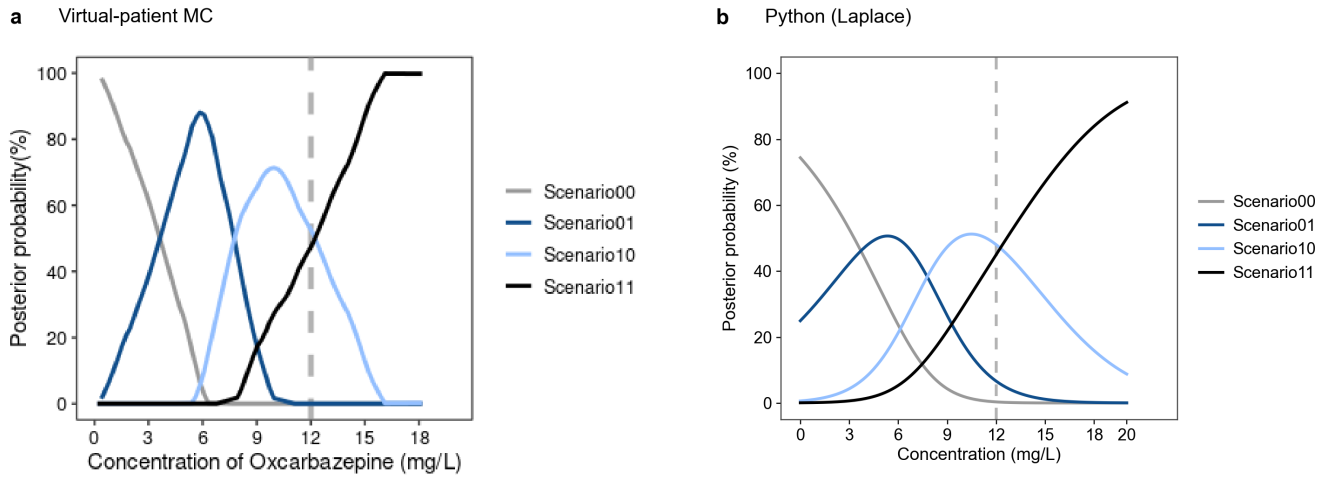
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00326578	0.00326578	0.00324907	0
ω_{01}: 300 mg at 0 h	0.25	0.06629396	0.06629396	0.06621953	0
ω_{10}: 300 mg at 12 h	0.25	0.48031491	0.48031491	0.48002010	0.52
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.45012535	0.45012536	0.45051130	0.48

Method	P_{max}	G	H_N
Python Laplace	0.480315	0.030190	0.656511
NONMEM Laplace	0.480315	0.030190	0.656511
R aghq	0.480020	0.029509	0.656362
Virtual patient (displayed)	0.52	0.04	0.499423

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C017: Structural parameters

BW: 25 to 50.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

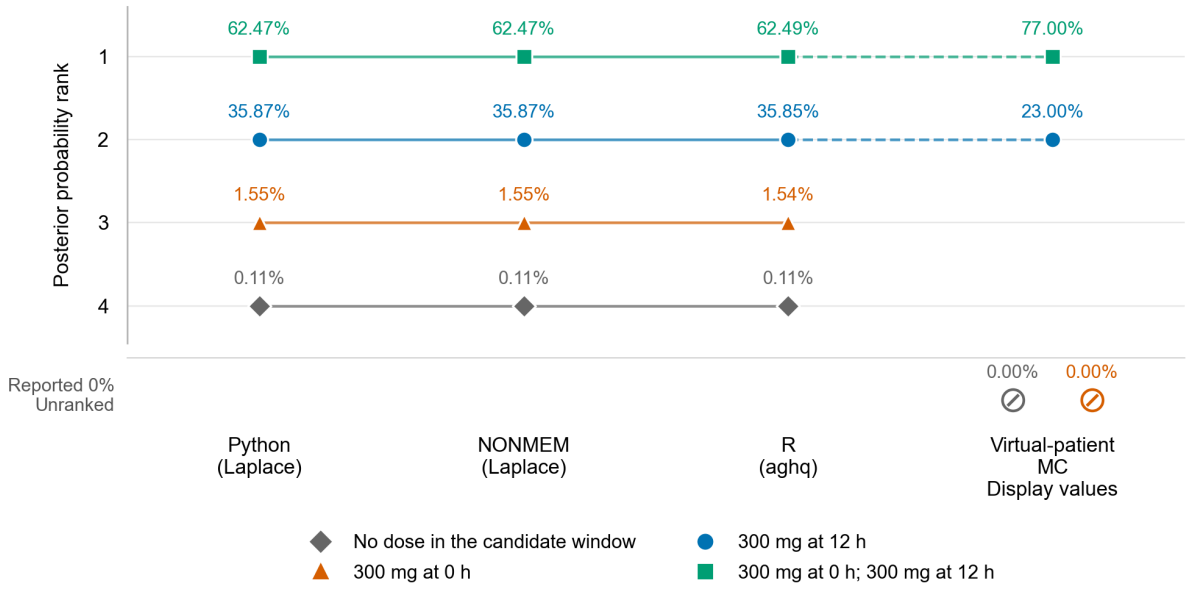
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	8.28924×10^{-11}	1.07344×10^{-10}	1.16194×10^{-10}	2.90961×10^{-10}
Python vs R aghq	2.31520×10^{-4}	2.31520×10^{-4}	3.00588×10^{-4}	1.96308×10^{-4}
NONMEM vs R aghq	2.31520×10^{-4}	2.31520×10^{-4}	3.00588×10^{-4}	1.96308×10^{-4}
Python vs Virtual patient	0.145314	0.145314	0.194738	0.138635
NONMEM vs Virtual patient	0.145314	0.145314	0.194738	0.138635
R aghq vs Virtual patient	0.145082	0.145082	0.194439	0.138440

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



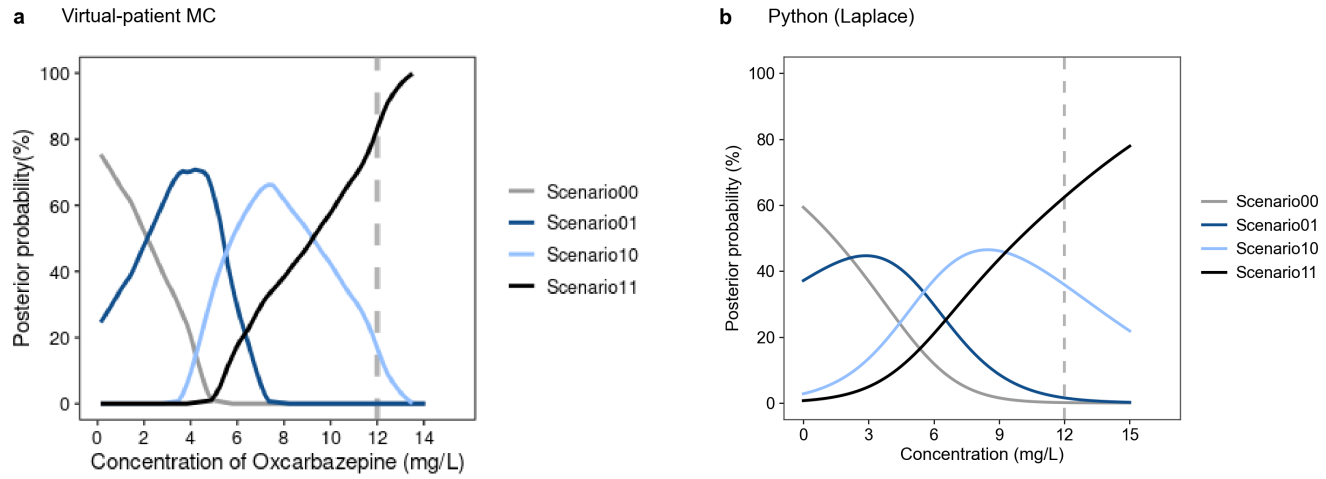
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00111297	0.00111297	0.00111195	0
ω_{01}: 300 mg at 0 h	0.25	0.01549352	0.01549352	0.01544964	0
ω_{10}: 300 mg at 12 h	0.25	0.35870747	0.35870747	0.35852086	0.23
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.62468604	0.62468604	0.62491756	0.77

Method	P_{max}	G	H_N
Python Laplace	0.624686	0.265979	0.529338
NONMEM Laplace	0.624686	0.265979	0.529338
R aghq	0.624918	0.266397	0.529142
Virtual patient (displayed)	0.77	0.54	0.389006

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C018: Variability

Clearance IIV: CV 0.01000000002%.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

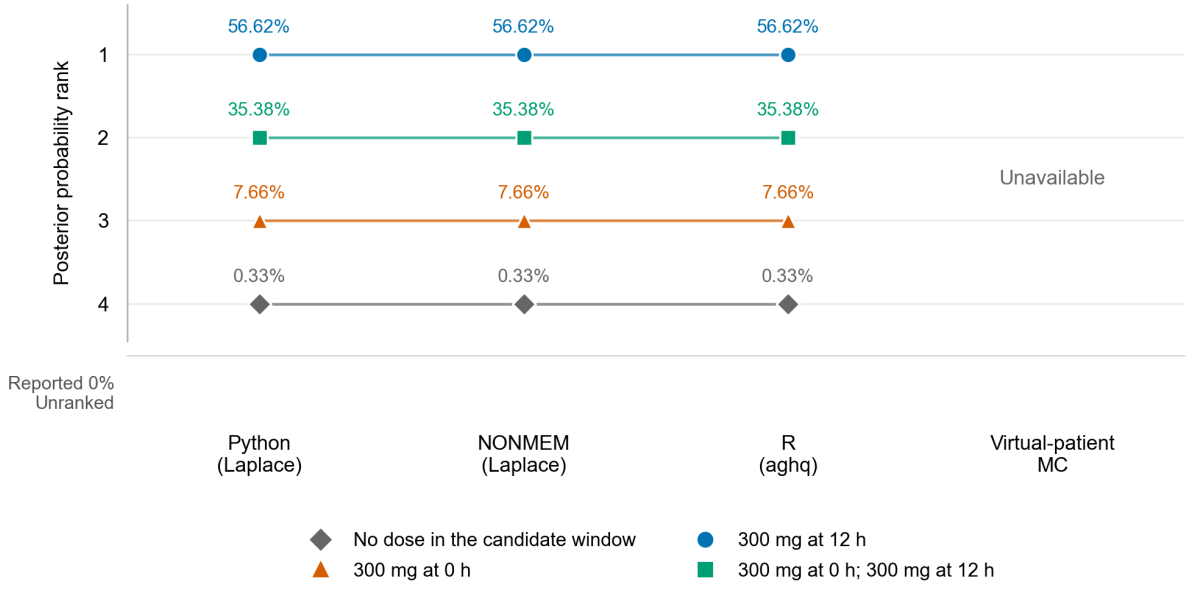
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.66783×10^{-11}	1.66783×10^{-11}	2.05691×10^{-11}	1.35264×10^{-11}
Python vs R aghq	5.20695×10^{-14}	5.20621×10^{-14}	6.77207×10^{-14}	3.72248×10^{-14}
NONMEM vs R aghq	1.67207×10^{-11}	1.67207×10^{-11}	2.06273×10^{-11}	1.35468×10^{-11}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00333592	0.00333592	0.00333592
ω_{01}: 300 mg at 0 h	0.25	0.07664445	0.07664445	0.07664445
ω_{10}: 300 mg at 12 h	0.25	0.56622934	0.56622934	0.56622934
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.35379028	0.35379028	0.35379028

Method	P_{max}	G	H_N
Python Laplace	0.566229	0.212439	0.653212
NONMEM Laplace	0.566229	0.212439	0.653212
R aghq	0.566229	0.212439	0.653212

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C019: Variability

Clearance IIV: CV 2.775%.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

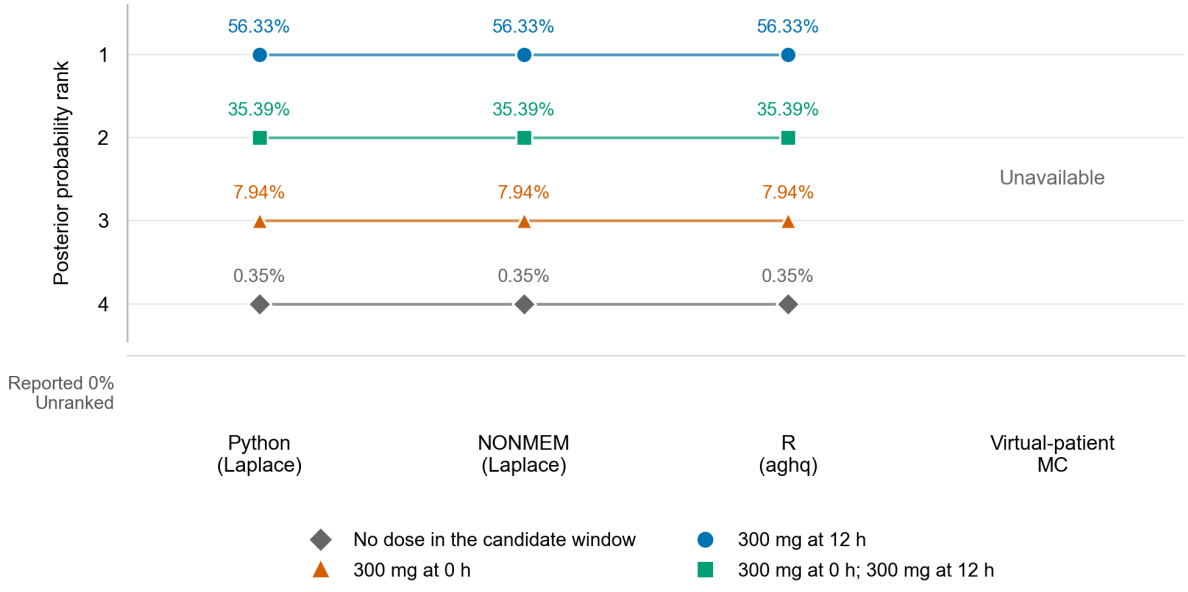
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	4.90791×10^{-10}	4.90791×10^{-10}	6.19939×10^{-10}	3.75576×10^{-10}
Python vs R aghq	7.25479×10^{-7}	7.42674×10^{-7}	9.05625×10^{-7}	5.70039×10^{-7}
NONMEM vs R aghq	7.25833×10^{-7}	7.43032×10^{-7}	9.06122×10^{-7}	5.70183×10^{-7}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00345972	0.00345972	0.00345973
ω_{01}: 300 mg at 0 h	0.25	0.07939166	0.07939166	0.07939139
ω_{10}: 300 mg at 12 h	0.25	0.56325021	0.56325021	0.56325093
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.35389841	0.35389841	0.35389795

Method	P_{max}	G	H_N
Python Laplace	0.563250	0.209352	0.657628
NONMEM Laplace	0.563250	0.209352	0.657628
R aghq	0.563251	0.209353	0.657628

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C020: Variability

Clearance IIV: CV 5.55%.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

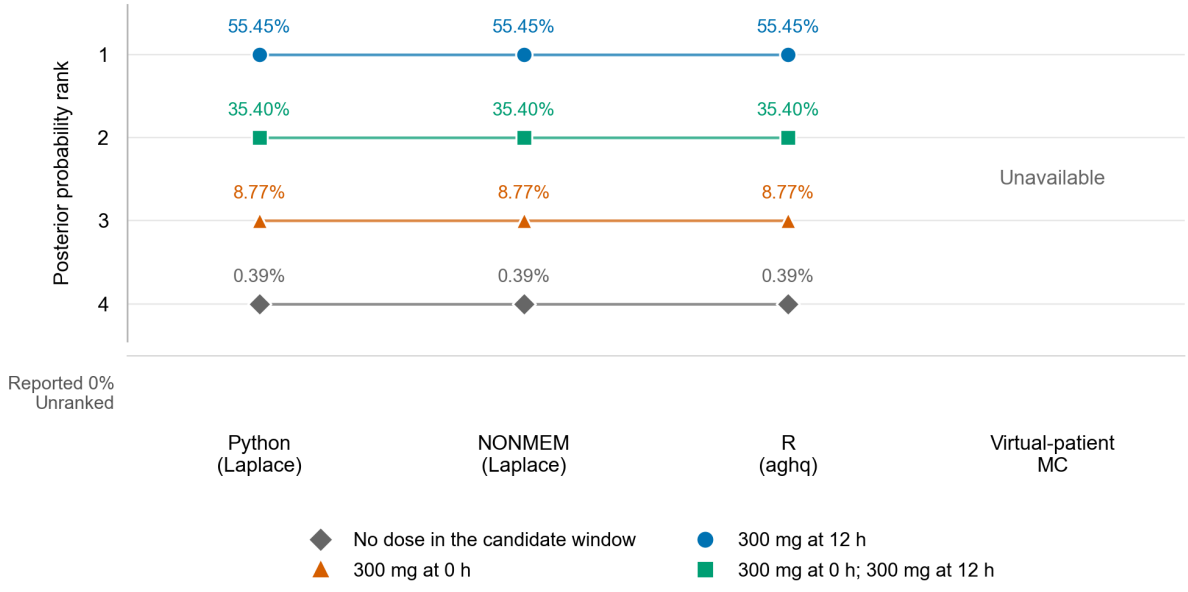
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	6.98998×10^{-10}	6.98998×10^{-10}	9.20933×10^{-10}	5.20537×10^{-10}
Python vs R aghq	1.53733×10^{-5}	1.53733×10^{-5}	1.88670×10^{-5}	1.45599×10^{-5}
NONMEM vs R aghq	1.53740×10^{-5}	1.53740×10^{-5}	1.88678×10^{-5}	1.45603×10^{-5}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00387029	0.00387029	0.00387007
ω_{01}: 300 mg at 0 h	0.25	0.08771262	0.08771262	0.08770349
ω_{10}: 300 mg at 12 h	0.25	0.55445654	0.55445654	0.55445051
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.35396056	0.35396055	0.35397593

Method	P_{max}	G	H_N
Python Laplace	0.554457	0.200496	0.670547
NONMEM Laplace	0.554457	0.200496	0.670547
R aghq	0.554451	0.200475	0.670539

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C021: Variability

Clearance IIV: CV 8.325%.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

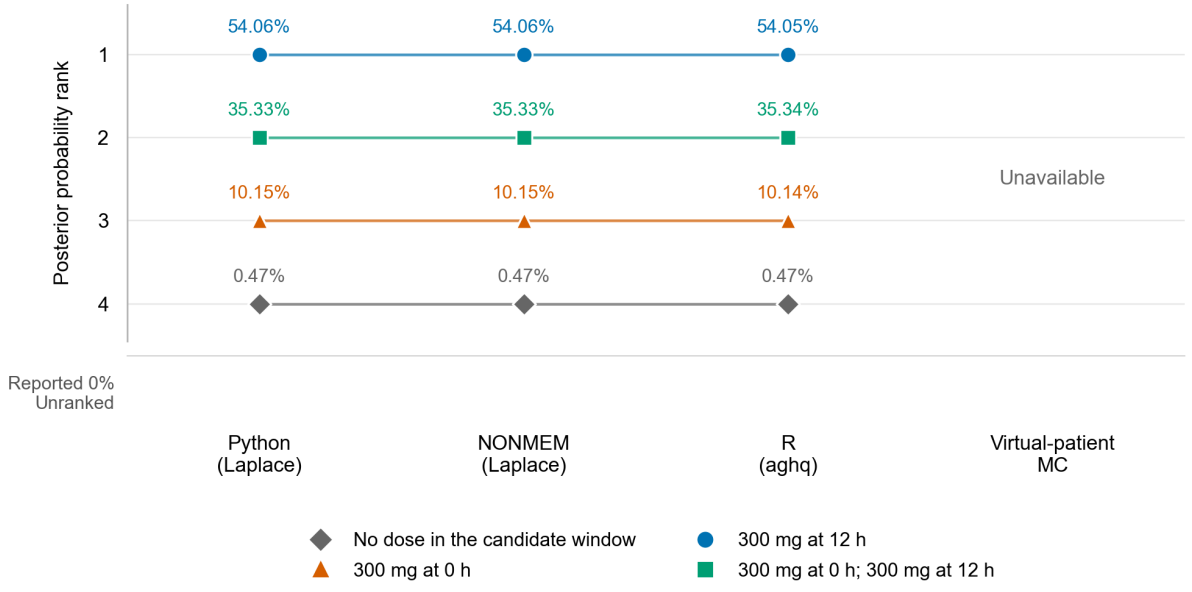
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	3.06435×10^{-9}	3.07432×10^{-9}	3.95636×10^{-9}	2.28255×10^{-9}
Python vs R aghq	1.28630×10^{-4}	1.28630×10^{-4}	1.56596×10^{-4}	1.03918×10^{-4}
NONMEM vs R aghq	1.28633×10^{-4}	1.28633×10^{-4}	1.56600×10^{-4}	1.03920×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00470990	0.00470990	0.00470457
ω_{01}: 300 mg at 0 h	0.25	0.10145273	0.10145273	0.10140426
ω_{10}: 300 mg at 12 h	0.25	0.54055124	0.54055125	0.54047642
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.35328612	0.35328612	0.35341475

Method	P_{max}	G	H_N
Python Laplace	0.540551	0.187265	0.690684
NONMEM Laplace	0.540551	0.187265	0.690684
R aghq	0.540476	0.187062	0.690647

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C022: Variability

Clearance IIV: CV 16.65%.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

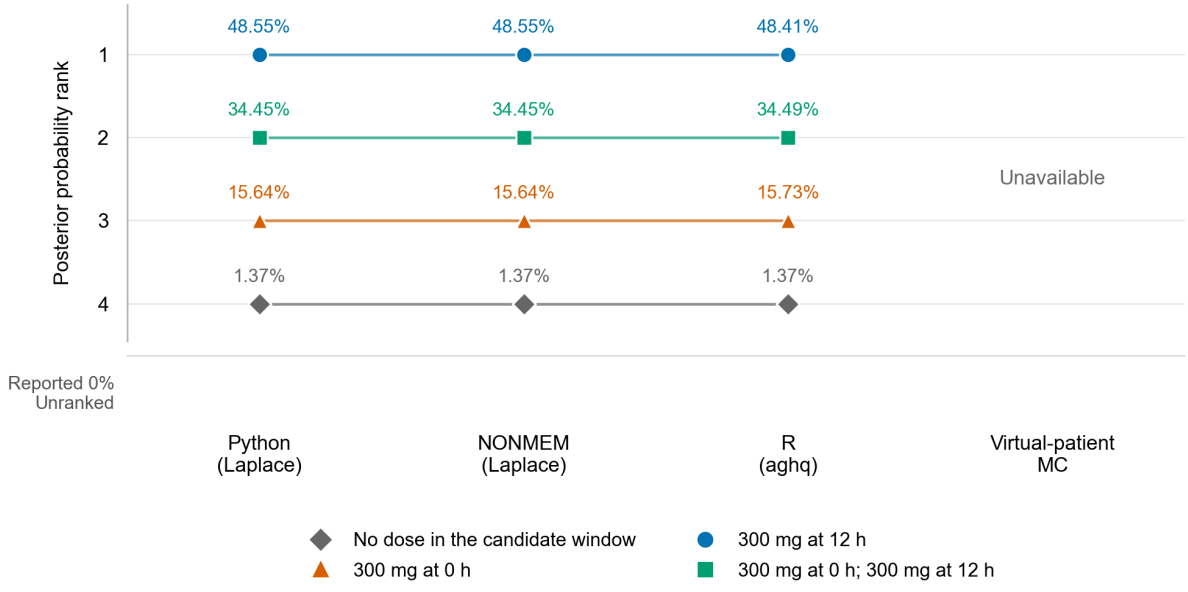
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.56620×10^{-9}	1.56620×10^{-9}	1.94086×10^{-9}	1.17164×10^{-9}
Python vs R aghq	1.30726×10^{-3}	1.30726×10^{-3}	1.63717×10^{-3}	1.08036×10^{-3}
NONMEM vs R aghq	1.30726×10^{-3}	1.30726×10^{-3}	1.63717×10^{-3}	1.08036×10^{-3}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.01365588	0.01365588	0.01368706
ω_{01}: 300 mg at 0 h	0.25	0.15636518	0.15636518	0.15728273
ω_{10}: 300 mg at 12 h	0.25	0.48545472	0.48545473	0.48414747
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.34452421	0.34452421	0.34488274

Method	P_{max}	G	H_N
Python Laplace	0.485455	0.140931	0.769478
NONMEM Laplace	0.485455	0.140931	0.769478
R aghq	0.484147	0.139265	0.770393

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C023: Variability

Clearance IIV: CV 22.2%.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

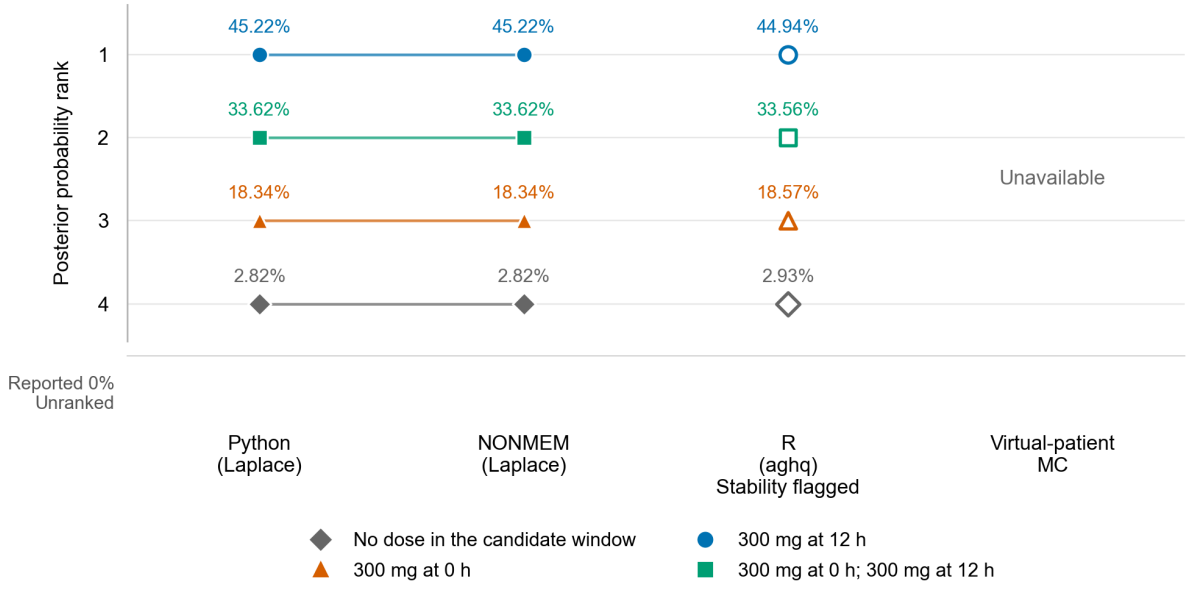
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	2.35737×10^{-9}	2.43408×10^{-9}	3.12957×10^{-9}	2.38649×10^{-9}
Python vs R aghq	2.82954×10^{-3}	3.45453×10^{-3}	3.87096×10^{-3}	3.44291×10^{-3}
NONMEM vs R aghq	2.82954×10^{-3}	3.45454×10^{-3}	3.87096×10^{-3}	3.44292×10^{-3}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks. Hollow R markers denote outputs with unmet quadrature stability checks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.02817110	0.02817110	0.02934137
ω_{01}: 300 mg at 0 h	0.25	0.18340010	0.18340009	0.18568436
ω_{10}: 300 mg at 12 h	0.25	0.45219906	0.45219906	0.44936952
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.33622975	0.33622975	0.33560476

Method	P_{max}	G	H_N
Python Laplace	0.452199	0.115969	0.820154
NONMEM Laplace	0.452199	0.115969	0.820154
R aghq	0.449370	0.113765	0.823816

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C024: Variability

Clearance IIV: CV 33.3%.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

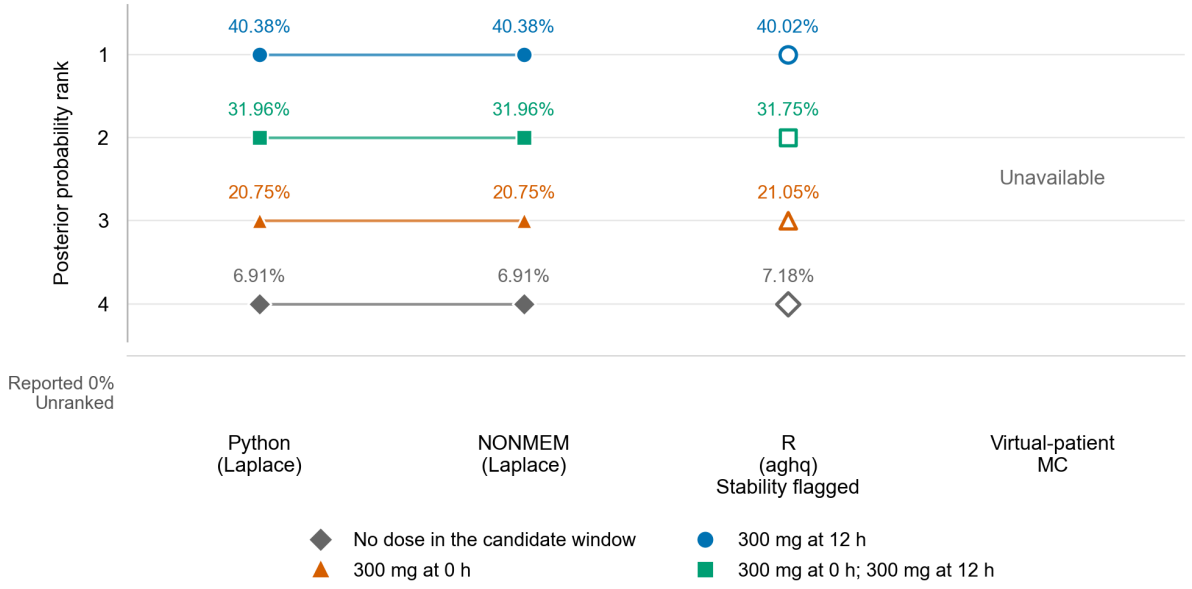
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.67199×10^{-8}	1.67199×10^{-8}	1.99449×10^{-8}	1.20851×10^{-8}
Python vs R aghq	3.62111×10^{-3}	5.70662×10^{-3}	5.81041×10^{-3}	4.95126×10^{-3}
NONMEM vs R aghq	3.62110×10^{-3}	5.70662×10^{-3}	5.81040×10^{-3}	4.95125×10^{-3}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks. Hollow R markers denote outputs with unmet quadrature stability checks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.06906194	0.06906194	0.07182504
ω_{01}: 300 mg at 0 h	0.25	0.20753331	0.20753331	0.21047683
ω_{10}: 300 mg at 12 h	0.25	0.40378648	0.40378646	0.40016537
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.31961828	0.31961829	0.31753277

Method	P_{max}	G	H_N
Python Laplace	0.403786	0.084168	0.895676
NONMEM Laplace	0.403786	0.084168	0.895676
R aghq	0.400165	0.082633	0.900187

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C025: Variability

Clearance IIV: CV 44.4%.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

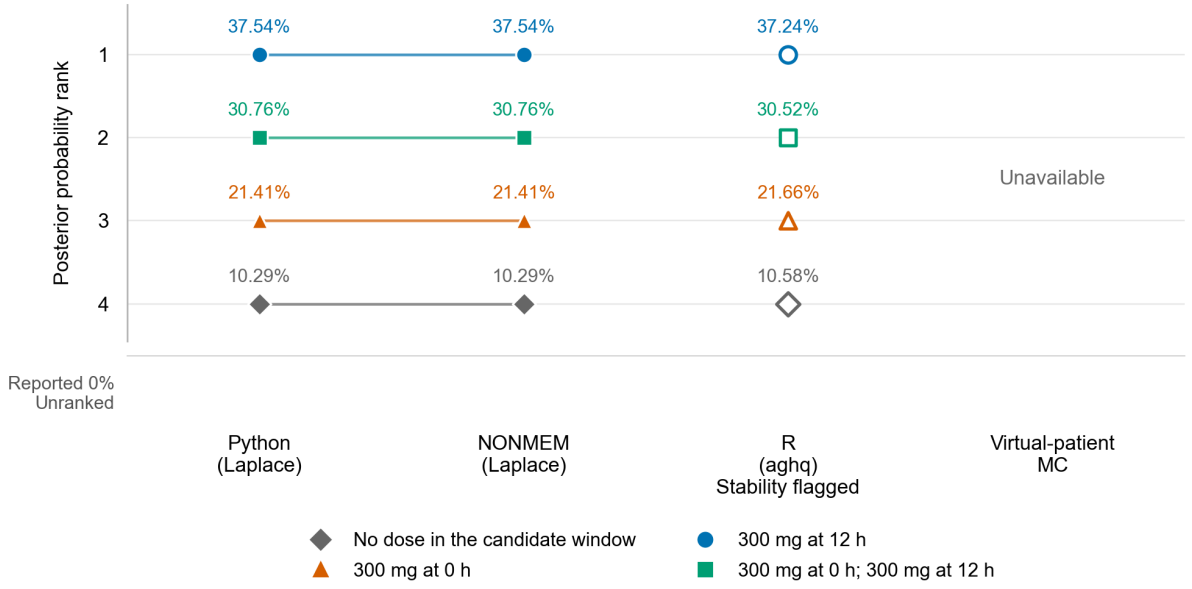
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	7.12166×10^{-9}	9.86181×10^{-9}	1.03887×10^{-8}	7.20386×10^{-9}
Python vs R aghq	2.96571×10^{-3}	5.39179×10^{-3}	5.41540×10^{-3}	4.37505×10^{-3}
NONMEM vs R aghq	2.96572×10^{-3}	5.39179×10^{-3}	5.41540×10^{-3}	4.37505×10^{-3}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks. Hollow R markers denote outputs with unmet quadrature stability checks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.10291296	0.10291296	0.10584287
ω_{01}: 300 mg at 0 h	0.25	0.21409216	0.21409215	0.21655404
ω_{10}: 300 mg at 12 h	0.25	0.37540173	0.37540174	0.37243602
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.30759315	0.30759314	0.30516707

Method	P_{max}	G	H_N
Python Laplace	0.375402	0.067809	0.933748
NONMEM Laplace	0.375402	0.067809	0.933748
R aghq	0.372436	0.067269	0.937077

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C026: Variability

Additive residual SD: 1e-06 mg/L.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	0/5	Unavailable

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	Unavailable	Unavailable	Unavailable	Unavailable

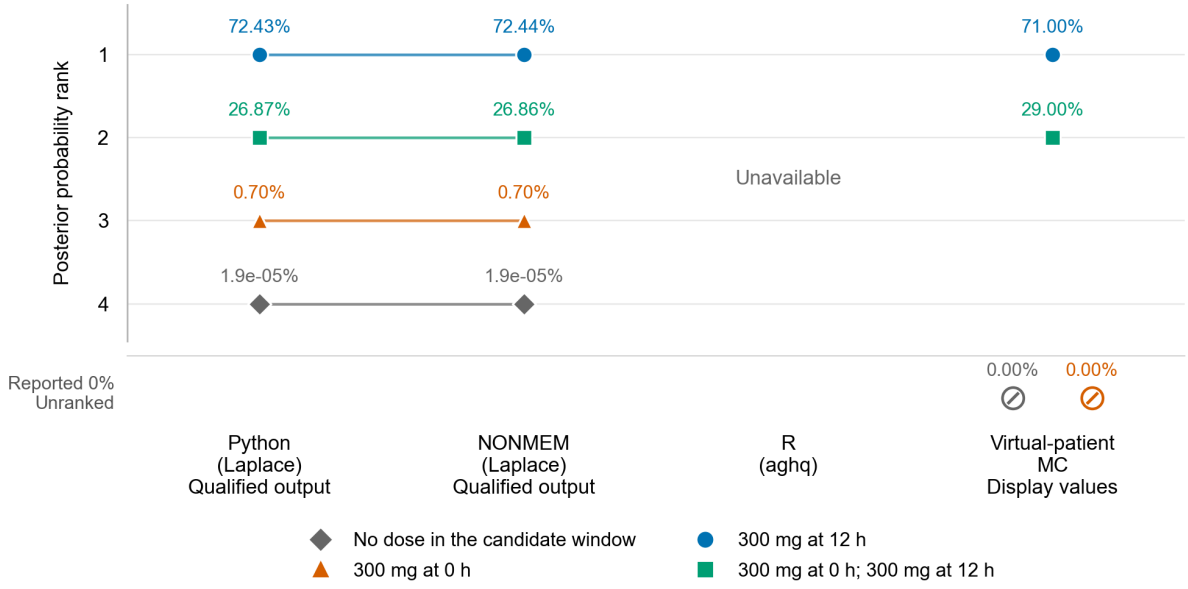
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.18987×10^{-4}	1.18987×10^{-4}	1.67028×10^{-4}	9.49449×10^{-5}
Python vs R aghq	Unavailable	Unavailable	Unavailable	Unavailable
NONMEM vs R aghq	Unavailable	Unavailable	Unavailable	Unavailable
Python vs Virtual patient	0.021269	0.021269	0.026559	0.061038
NONMEM vs Virtual patient	0.021388	0.021388	0.026718	0.061069
R aghq vs Virtual patient	Unavailable	Unavailable	Unavailable	Unavailable

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



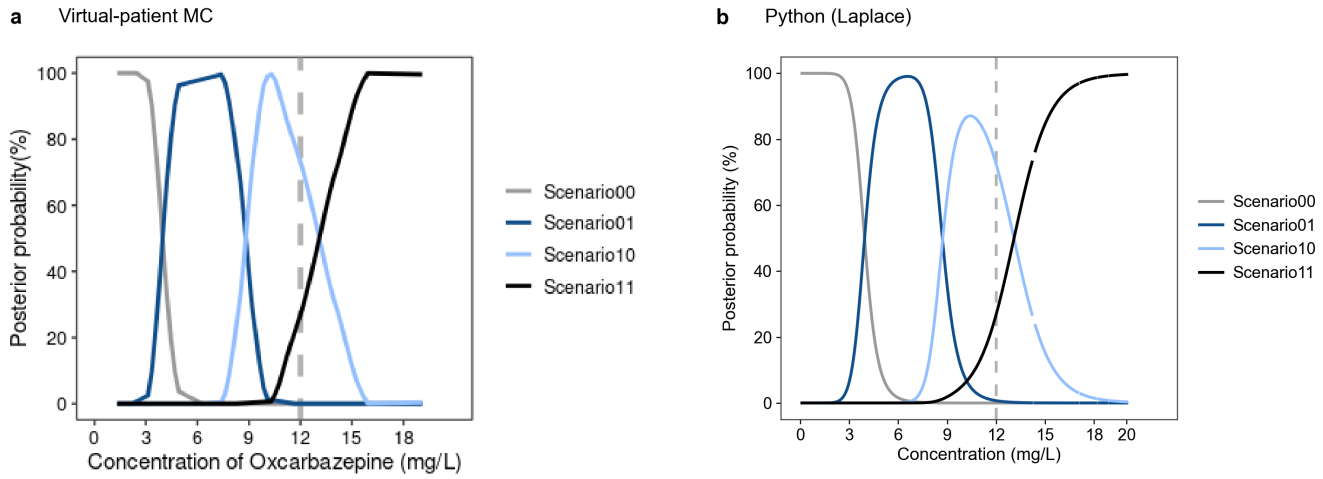
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00000019	0.00000019	Unavailable	0
ω_{01}: 300 mg at 0 h	0.25	0.00697489	0.00697667	Unavailable	0
ω_{10}: 300 mg at 12 h	0.25	0.72429431	0.72441151	Unavailable	0.71
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.26873061	0.26861162	Unavailable	0.29

Method	P_{max}	G	H_N
Python Laplace	0.724294	0.455564	0.448236
NONMEM Laplace	0.724412	0.455800	0.448157
R aghq	Unavailable	Unavailable	Unavailable
Virtual patient (displayed)	0.71	0.42	0.434361

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C027: Variability

Additive residual SD: 0.748 mg/L.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

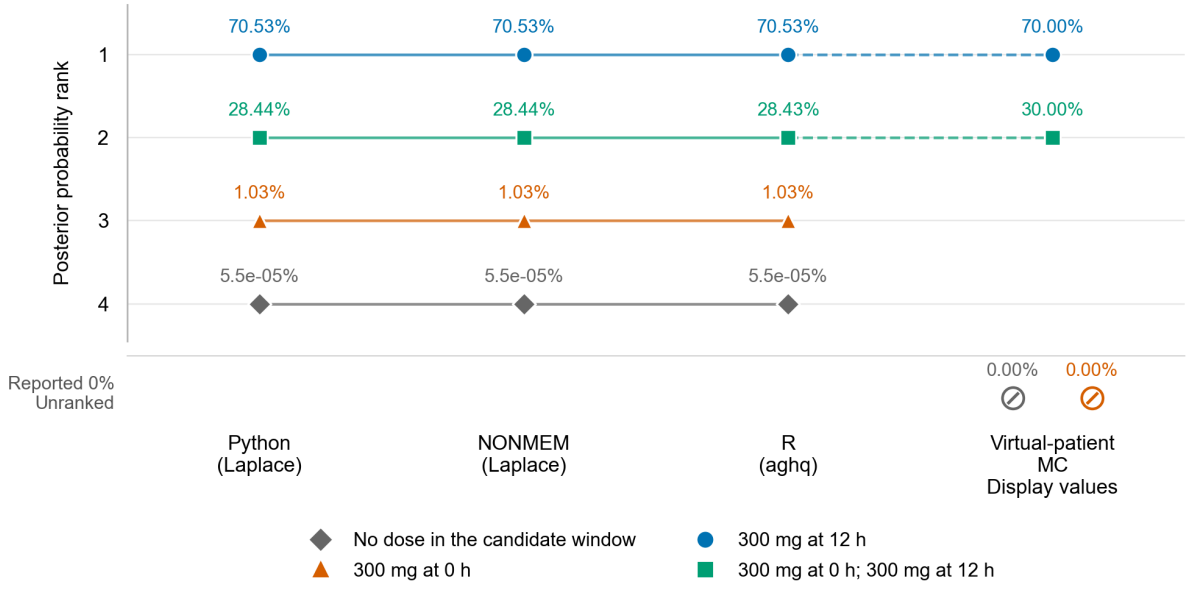
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	9.48944×10^{-9}	9.48944×10^{-9}	1.32941×10^{-8}	7.43871×10^{-9}
Python vs R aghq	3.70198×10^{-5}	3.70198×10^{-5}	4.75289×10^{-5}	4.00877×10^{-5}
NONMEM vs R aghq	3.70103×10^{-5}	3.70103×10^{-5}	4.75159×10^{-5}	4.00823×10^{-5}
Python vs Virtual patient	0.015619	0.015619	0.019456	0.072599
NONMEM vs Virtual patient	0.015619	0.015619	0.019457	0.072599
R aghq vs Virtual patient	0.015656	0.015656	0.019498	0.072632

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



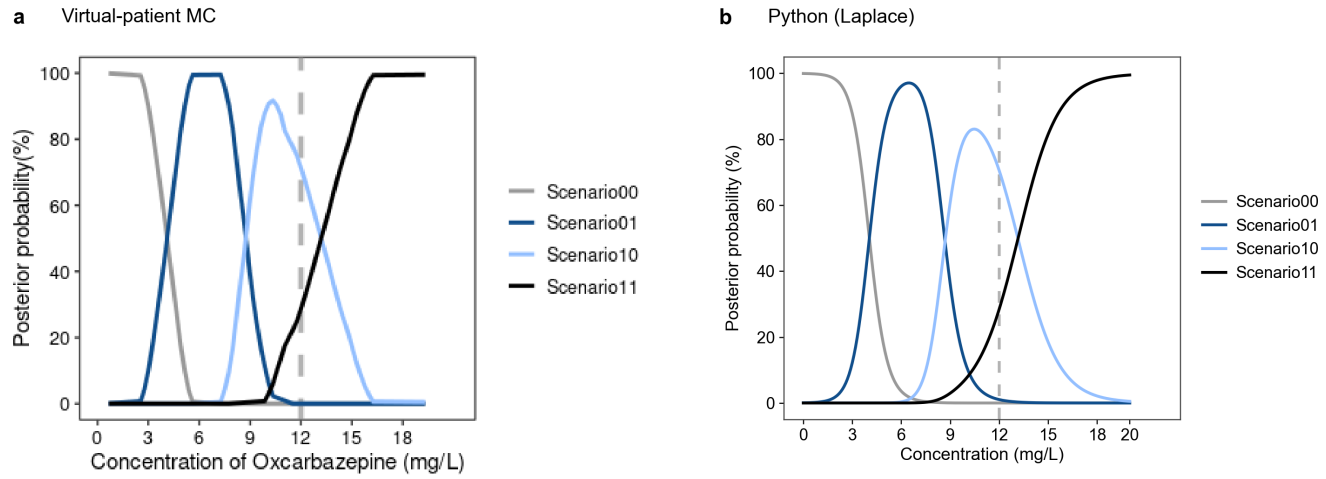
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00000055	0.00000055	0.00000055	0
ω_{01}: 300 mg at 0 h	0.25	0.01032206	0.01032207	0.01033049	0
ω_{10}: 300 mg at 12 h	0.25	0.70529652	0.70529652	0.70532511	0.7
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.28438087	0.28438086	0.28434385	0.3

Method	P_{max}	G	H_N
Python Laplace	0.705297	0.420916	0.469635
NONMEM Laplace	0.705297	0.420916	0.469635
R aghq	0.705325	0.420981	0.469637
Virtual patient (displayed)	0.7	0.4	0.440645

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

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Run times and numerical checks

OXC C028: Variability

Additive residual SD: 1.496 mg/L.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

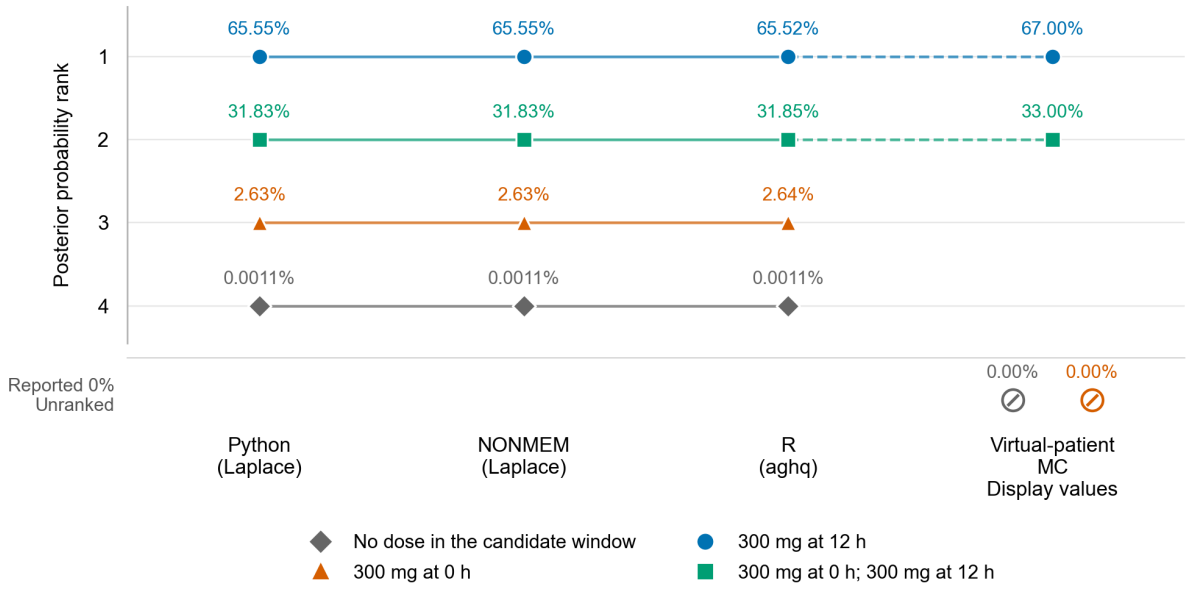
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.14591×10^{-9}	1.14591×10^{-9}	1.48174×10^{-9}	9.69660×10^{-10}
Python vs R aghq	3.05342×10^{-4}	3.05342×10^{-4}	3.78266×10^{-4}	3.03881×10^{-4}
NONMEM vs R aghq	3.05341×10^{-4}	3.05341×10^{-4}	3.78265×10^{-4}	3.03881×10^{-4}
Python vs Virtual patient	0.026261	0.026272	0.032229	0.115018
NONMEM vs Virtual patient	0.026261	0.026272	0.032229	0.115018
R aghq vs Virtual patient	0.026373	0.026385	0.032390	0.115262

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



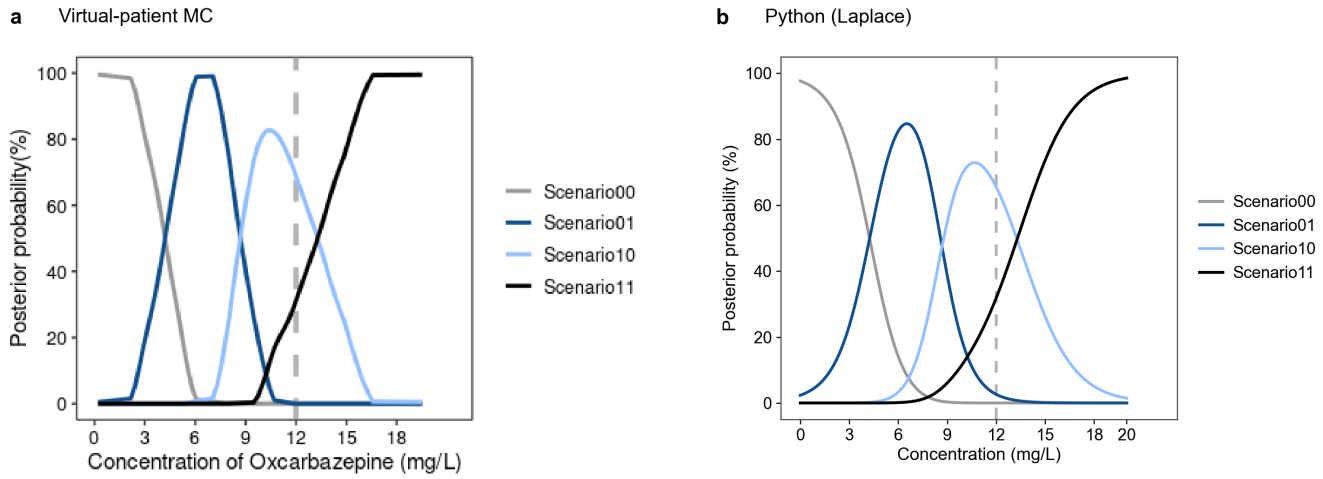
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00001130	0.00001130	0.00001144	0
ω_{01}: 300 mg at 0 h	0.25	0.02626110	0.02626110	0.02637324	0
ω_{10}: 300 mg at 12 h	0.25	0.65545552	0.65545552	0.65515018	0.67
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.31827207	0.31827207	0.31846514	0.33

Method	P_{max}	G	H_N
Python Laplace	0.655456	0.337183	0.531607
NONMEM Laplace	0.655456	0.337183	0.531607
R aghq	0.655150	0.336685	0.531969
Virtual patient (displayed)	0.67	0.34	0.457463

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

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Run times and numerical checks

OXC C029: Variability

Additive residual SD: 2.244 mg/L.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

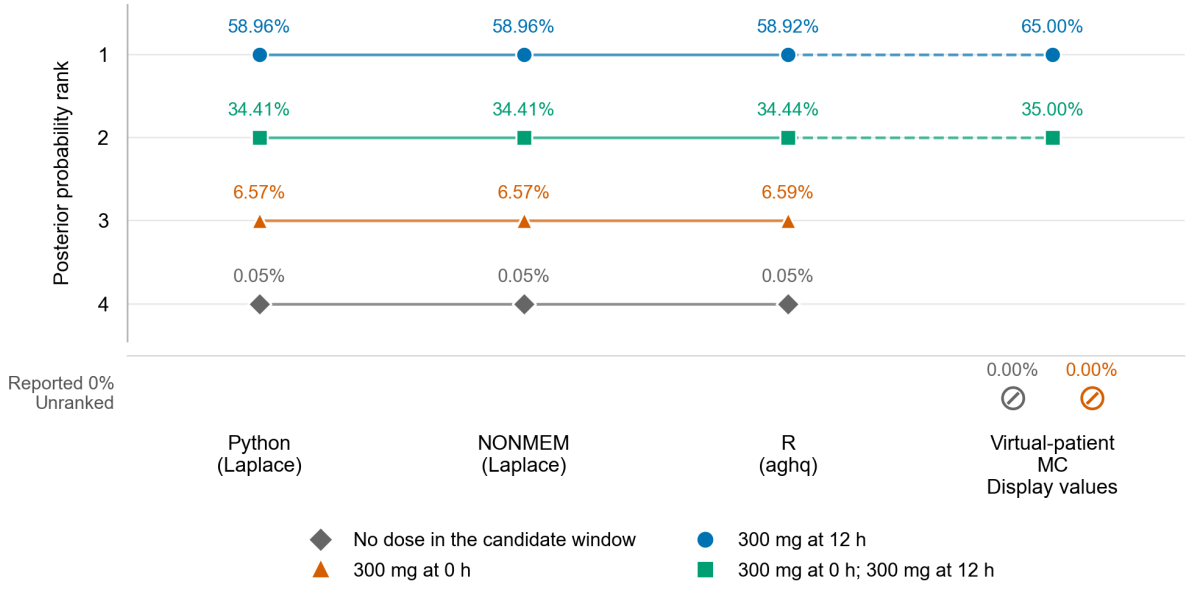
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.77761×10^{-9}	1.77761×10^{-9}	2.17720×10^{-9}	1.66314×10^{-9}
Python vs R aghq	4.70374×10^{-4}	4.72710×10^{-4}	5.94649×10^{-4}	3.52472×10^{-4}
NONMEM vs R aghq	4.70375×10^{-4}	4.72711×10^{-4}	5.94650×10^{-4}	3.52472×10^{-4}
Python vs Virtual patient	0.065749	0.066258	0.089454	0.184057
NONMEM vs Virtual patient	0.065749	0.066258	0.089454	0.184057
R aghq vs Virtual patient	0.065883	0.066391	0.089849	0.184265

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



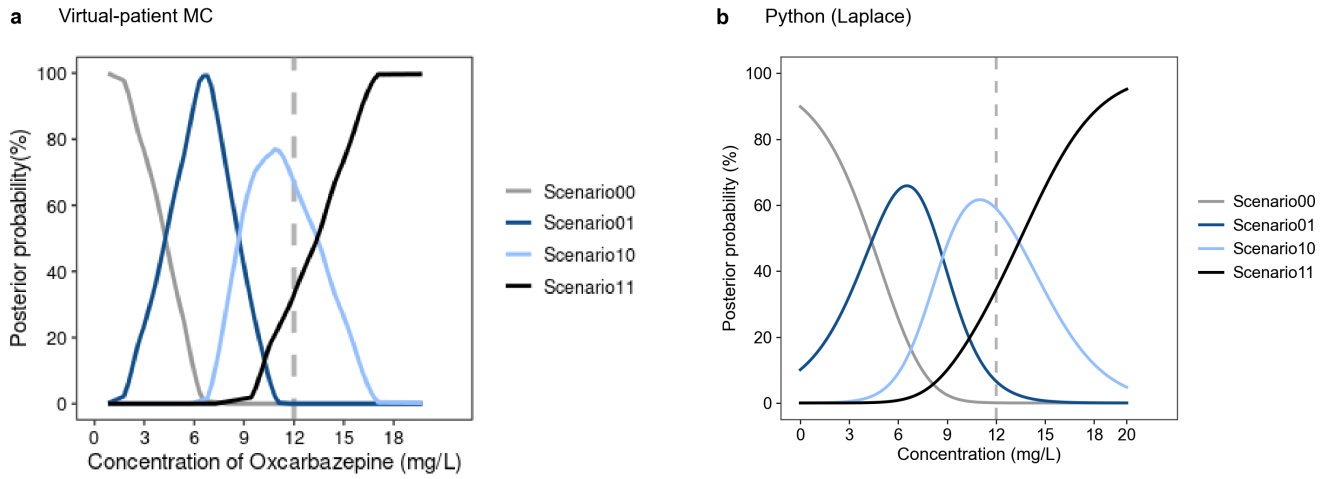
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00050986	0.00050986	0.00050752	0
ω_{01}: 300 mg at 0 h	0.25	0.06574854	0.06574854	0.06588335	0
ω_{10}: 300 mg at 12 h	0.25	0.58963326	0.58963327	0.58916289	0.65
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.34410834	0.34410833	0.34444624	0.35

Method	P_{max}	G	H_N
Python Laplace	0.589633	0.245525	0.621368
NONMEM Laplace	0.589633	0.245525	0.621368
R aghq	0.589163	0.244717	0.621700
Virtual patient (displayed)	0.65	0.3	0.467034

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

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Run times and numerical checks

OXC C030: Variability

Additive residual SD: 4.488 mg/L.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

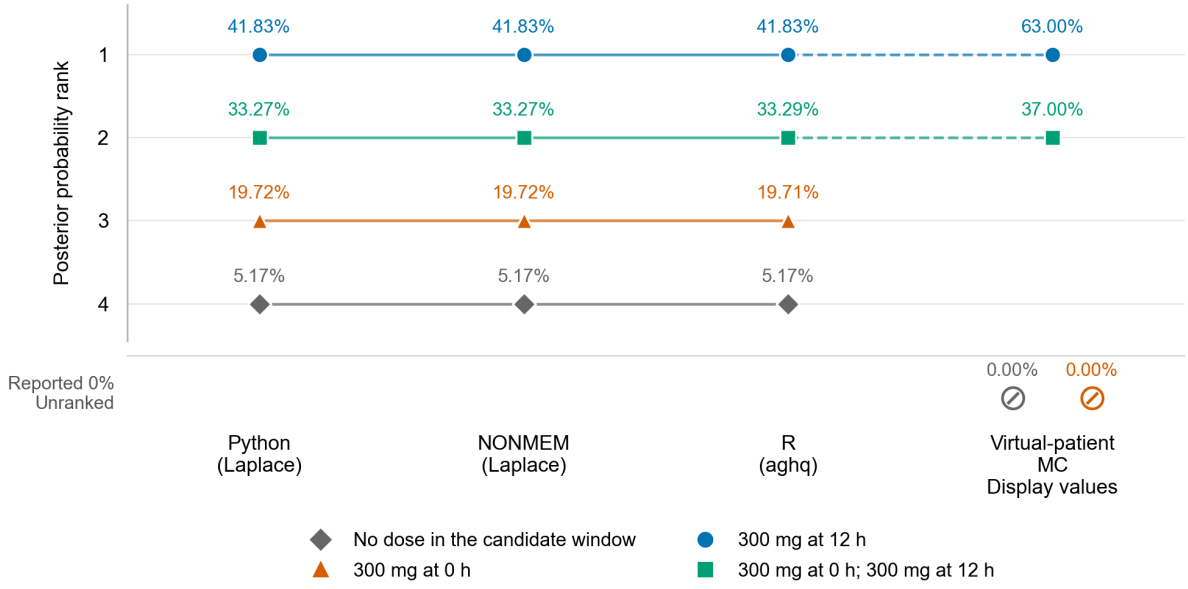
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.54781×10^{-9}	1.54781×10^{-9}	1.86382×10^{-9}	1.37574×10^{-9}
Python vs R aghq	1.96992×10^{-4}	1.96992×10^{-4}	2.39315×10^{-4}	1.77598×10^{-4}
NONMEM vs R aghq	1.96991×10^{-4}	1.96991×10^{-4}	2.39314×10^{-4}	1.77597×10^{-4}
Python vs Virtual patient	0.211690	0.248973	0.296275	0.368483
NONMEM vs Virtual patient	0.211690	0.248973	0.296275	0.368483
R aghq vs Virtual patient	0.211709	0.248795	0.296173	0.368358

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



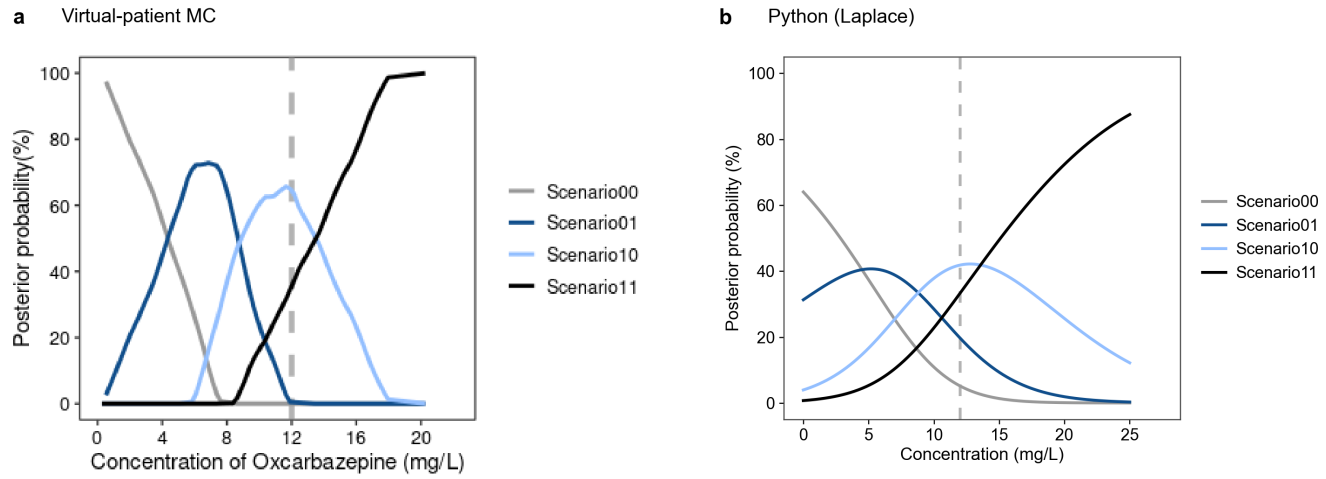
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.05174472	0.05174472	0.05168977	0
ω_{01}: 300 mg at 0 h	0.25	0.19722816	0.19722816	0.19710538	0
ω_{10}: 300 mg at 12 h	0.25	0.41831013	0.41831013	0.41829087	0.63
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.33271699	0.33271699	0.33291398	0.37

Method	P_{max}	G	H_N
Python Laplace	0.418310	0.085593	0.868597
NONMEM Laplace	0.418310	0.085593	0.868597
R aghq	0.418291	0.085377	0.868480
Virtual patient (displayed)	0.63	0.26	0.475336

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

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Run times and numerical checks

OXC C031: Variability

Additive residual SD: 5.984 mg/L.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

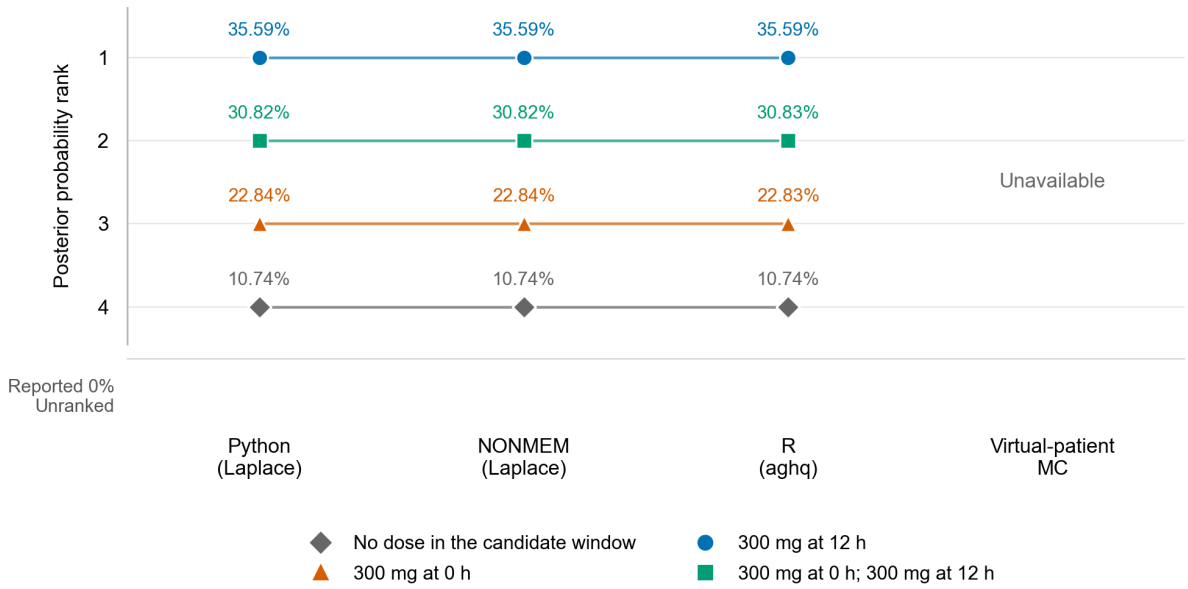
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	2.22001×10^{-9}	2.22001×10^{-9}	2.59843×10^{-9}	1.69794×10^{-9}
Python vs R aghq	7.76619×10^{-5}	9.11410×10^{-5}	1.09746×10^{-4}	7.66226×10^{-5}
NONMEM vs R aghq	7.76614×10^{-5}	9.11426×10^{-5}	1.09747×10^{-4}	7.66232×10^{-5}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.10744615	0.10744616	0.10742955
ω_{01}: 300 mg at 0 h	0.25	0.22842153	0.22842153	0.22834699
ω_{10}: 300 mg at 12 h	0.25	0.35591518	0.35591518	0.35592866
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.30821713	0.30821714	0.30829480

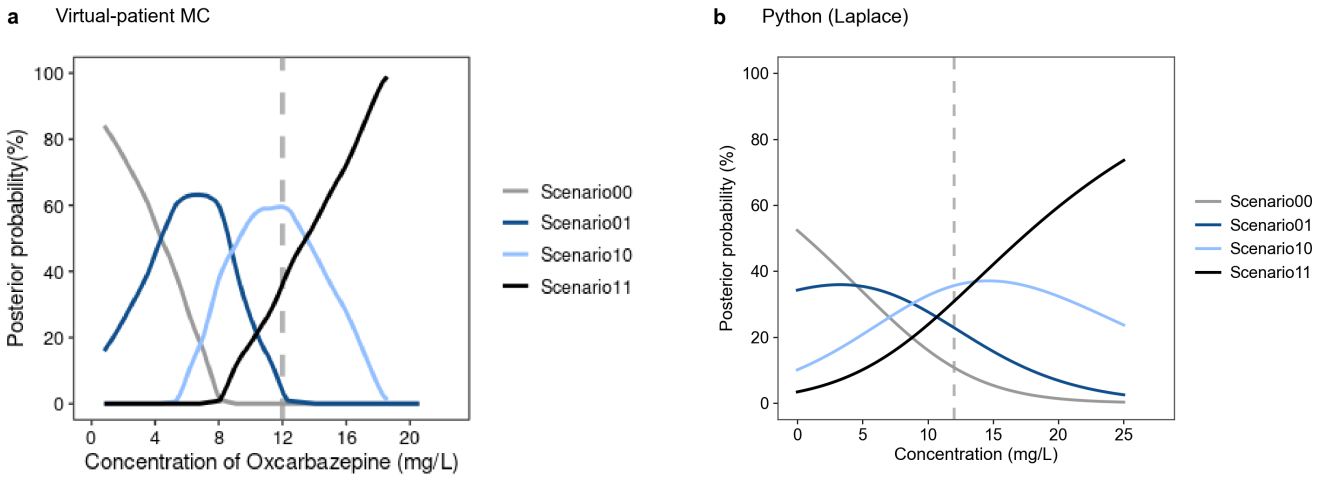
Method	P_{max}	G	H_N
Python Laplace	0.355915	0.047698	0.943093
NONMEM Laplace	0.355915	0.047698	0.943093
R aghq	0.355929	0.047634	0.943063

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

External web output

The displayed total is 99.00%; the web output is excluded from comparisons.

Web state	Candidate dosing history	Reported probability (%)
Scenario00	No dose in the candidate window	0.00
Scenario01	300 mg at 0 h	2.00
Scenario10	300 mg at 12 h	60.00
Scenario11	300 mg at 0 h; 300 mg at 12 h	37.00



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

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Run times and numerical checks

OXC C032: Variability

Additive residual SD: 8.976 mg/L.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

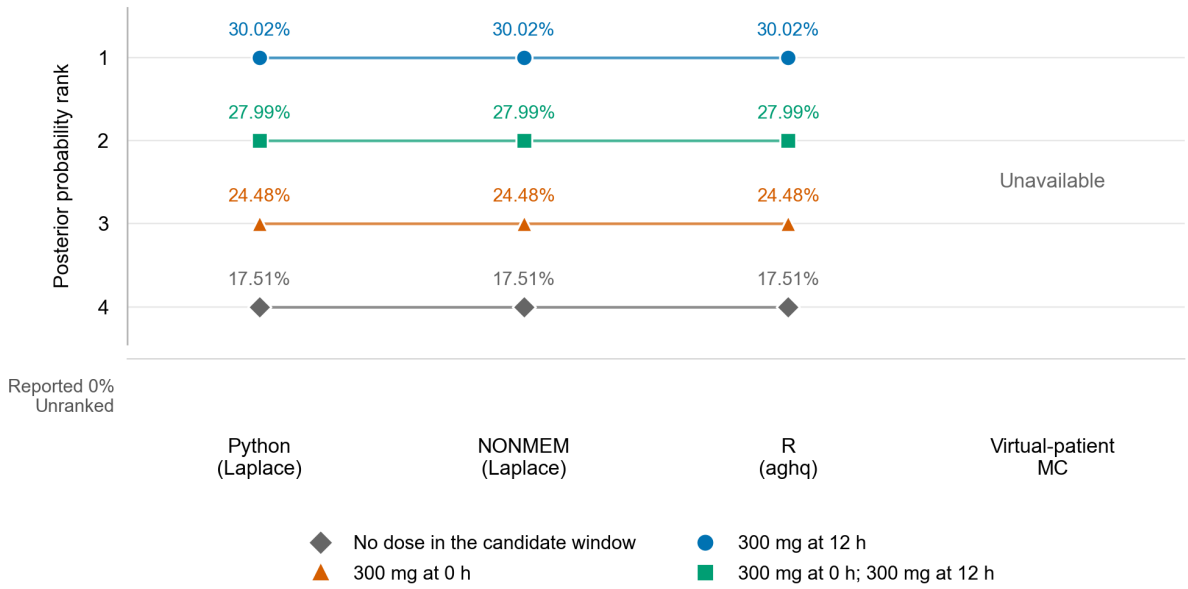
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.17379×10^{-9}	1.17379×10^{-9}	1.40603×10^{-9}	1.01058×10^{-9}
Python vs R aghq	2.82583×10^{-5}	2.82583×10^{-5}	3.32592×10^{-5}	2.44094×10^{-5}
NONMEM vs R aghq	2.82571×10^{-5}	2.82571×10^{-5}	3.32578×10^{-5}	2.44084×10^{-5}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.17510720	0.17510720	0.17512131
ω_{01}: 300 mg at 0 h	0.25	0.24480860	0.24480860	0.24478034
ω_{10}: 300 mg at 12 h	0.25	0.30017508	0.30017508	0.30018422
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.27990912	0.27990912	0.27991413

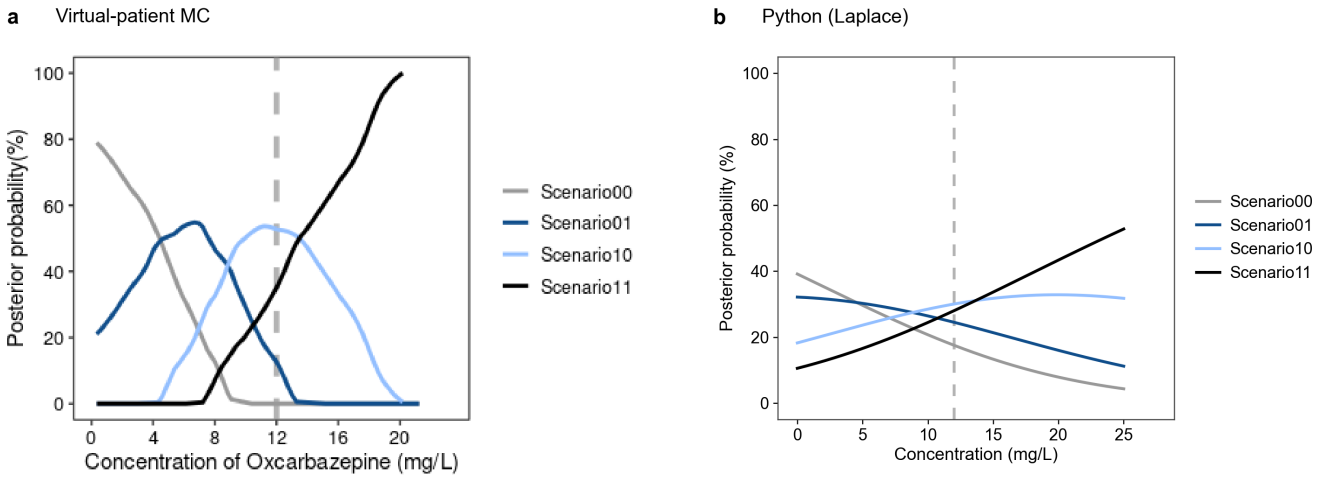
Method	P_{max}	G	H_N
Python Laplace	0.300175	0.020266	0.986260
NONMEM Laplace	0.300175	0.020266	0.986260
R aghq	0.300184	0.020270	0.986261

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

External web output

The displayed total is 101.00%; the web output is excluded from comparisons.

Web state	Candidate dosing history	Reported probability (%)
Scenario00	No dose in the candidate window	0.00
Scenario01	300 mg at 0 h	12.00
Scenario10	300 mg at 12 h	53.00
Scenario11	300 mg at 0 h; 300 mg at 12 h	36.00



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

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Run times and numerical checks

OXC C033: Variability

Additive residual SD: 11.968 mg/L.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

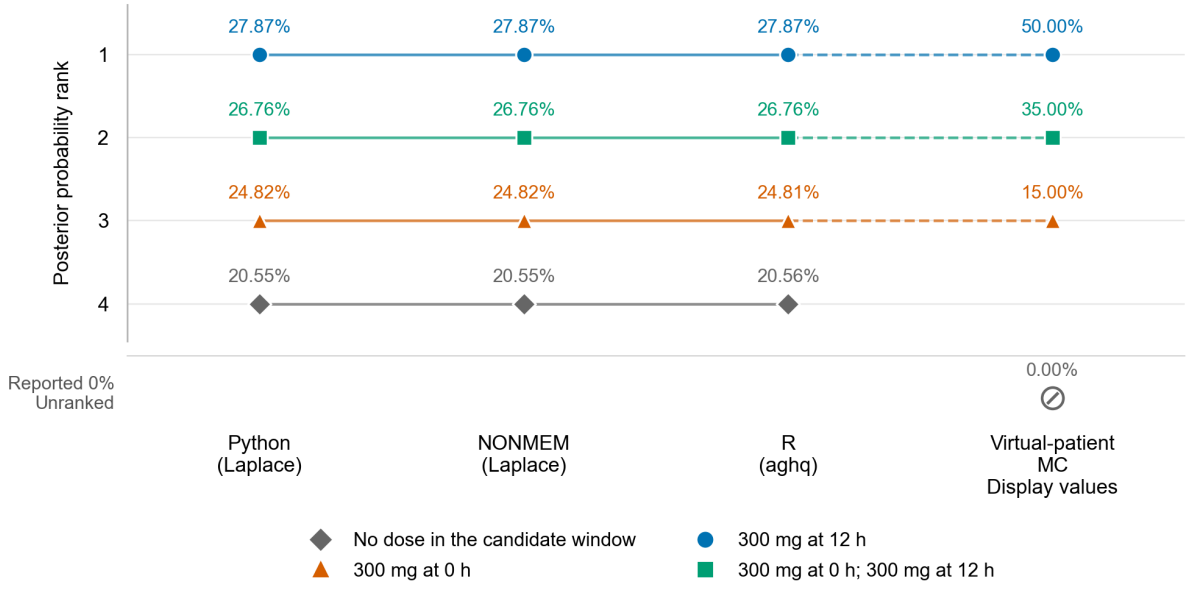
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	4.86371×10^{-10}	4.86371×10^{-10}	5.63693×10^{-10}	3.89857×10^{-10}
Python vs R aghq	1.53187×10^{-5}	2.02688×10^{-5}	2.22969×10^{-5}	1.64987×10^{-5}
NONMEM vs R aghq	1.53185×10^{-5}	2.02685×10^{-5}	2.22967×10^{-5}	1.64985×10^{-5}
Python vs Virtual patient	0.221303	0.303710	0.328104	0.357401
NONMEM vs Virtual patient	0.221303	0.303710	0.328104	0.357401
R aghq vs Virtual patient	0.221298	0.303711	0.328107	0.357409

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



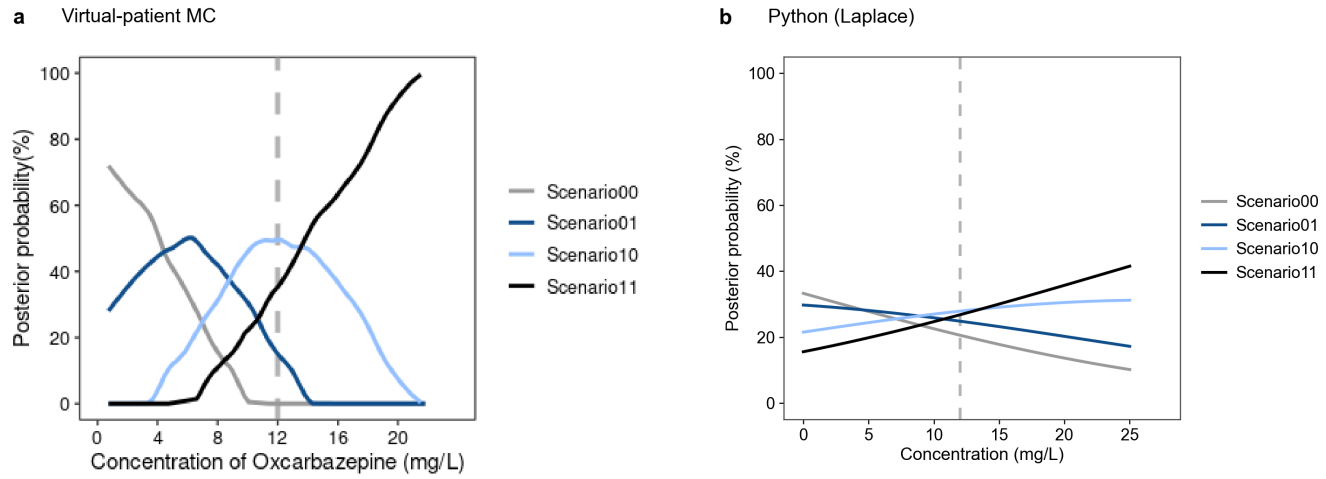
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.20554932	0.20554932	0.20556464	0
ω_{01}: 300 mg at 0 h	0.25	0.24816094	0.24816095	0.24814677	0.15
ω_{10}: 300 mg at 12 h	0.25	0.27869697	0.27869697	0.27870192	0.5
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.26759276	0.26759276	0.26758666	0.35

Method	P_{max}	G	H_N
Python Laplace	0.278697	0.011104	0.995377
NONMEM Laplace	0.278697	0.011104	0.995377
R aghq	0.278702	0.011115	0.995379
Virtual patient (displayed)	0.5	0.15	0.720323

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C034: Actual dosing histories

Observation generated from 300 mg at 0 h and 300 mg at 12 h; candidate histories unchanged.

Observations: 14.9680494 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

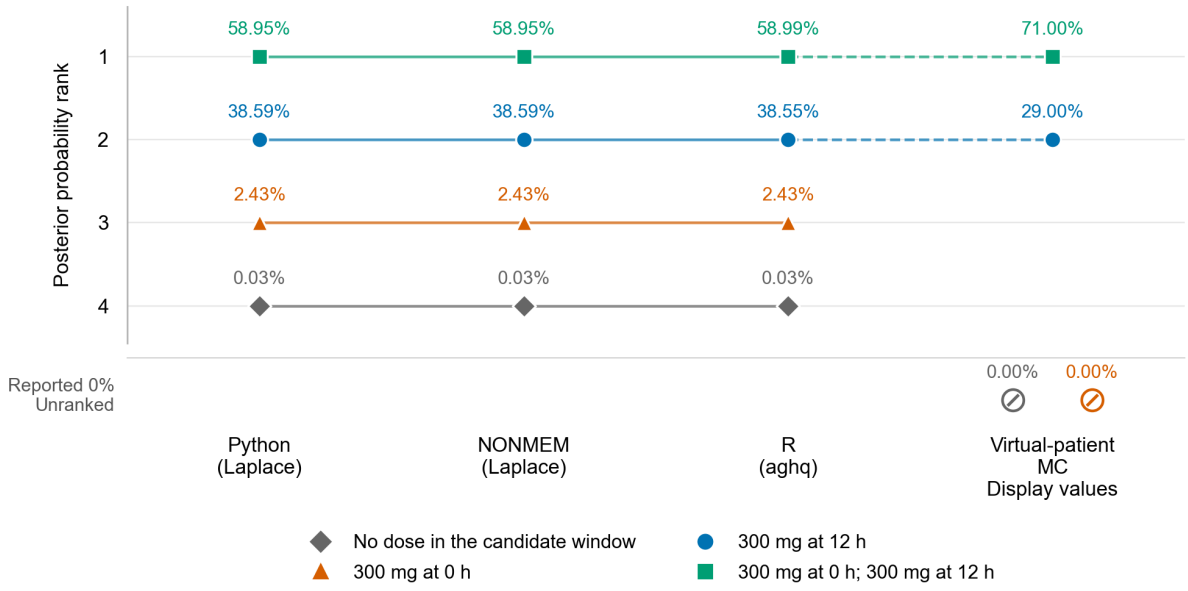
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	4.07135×10^{-9}	4.07135×10^{-9}	5.50132×10^{-9}	3.00820×10^{-9}
Python vs R aghq	4.26217×10^{-4}	4.26217×10^{-4}	5.96222×10^{-4}	3.12415×10^{-4}
NONMEM vs R aghq	4.26221×10^{-4}	4.26221×10^{-4}	5.96228×10^{-4}	3.12418×10^{-4}
Python vs Virtual patient	0.120537	0.120537	0.155958	0.136095
NONMEM vs Virtual patient	0.120537	0.120537	0.155958	0.136095
R aghq vs Virtual patient	0.120111	0.120111	0.155371	0.135900

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



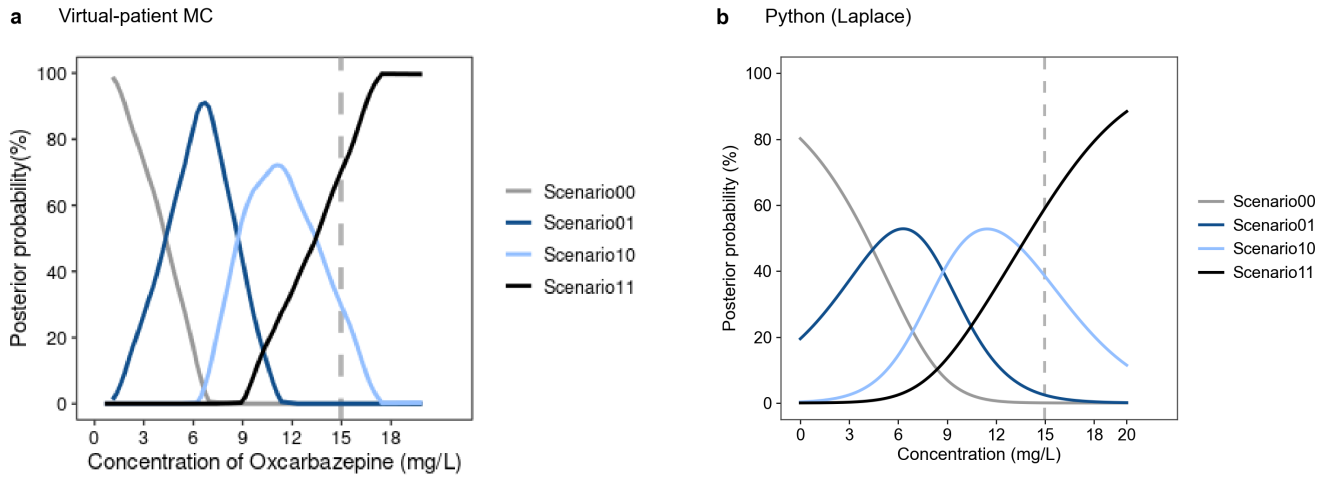
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00032499	0.00032499	0.00032242	0
ω_{01}: 300 mg at 0 h	0.25	0.02427322	0.02427322	0.02426643	0
ω_{10}: 300 mg at 12 h	0.25	0.38593890	0.38593891	0.38552205	0.29
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.58946288	0.58946288	0.58988910	0.71

Method	P_{max}	G	H_N
Python Laplace	0.589463	0.203524	0.556785
NONMEM Laplace	0.589463	0.203524	0.556785
R aghq	0.589889	0.204367	0.556627
Virtual patient (displayed)	0.71	0.42	0.434361

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

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Run times and numerical checks

OXC C035: Actual dosing histories

Observation generated from 150 mg at 0 h and 300 mg at 12 h; candidate histories unchanged.

Observations: 13.17213692 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

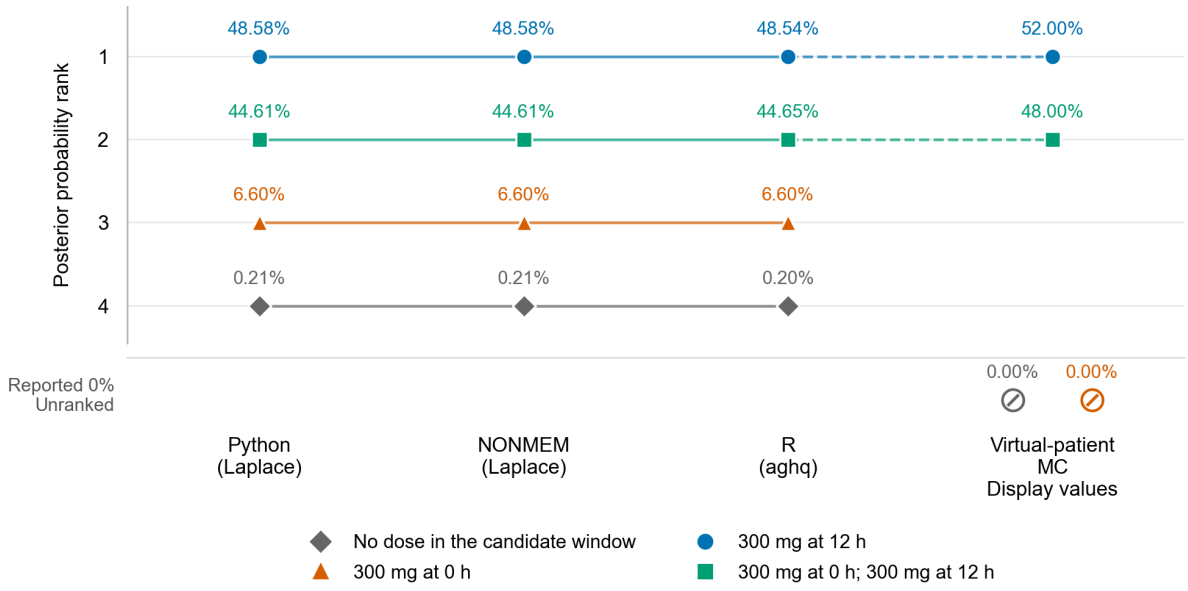
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	2.83231×10^{-9}	2.83231×10^{-9}	3.46829×10^{-9}	2.71533×10^{-9}
Python vs R aghq	3.94140×10^{-4}	3.94140×10^{-4}	5.32451×10^{-4}	2.96850×10^{-4}
NONMEM vs R aghq	3.94137×10^{-4}	3.94137×10^{-4}	5.32448×10^{-4}	2.96848×10^{-4}
Python vs Virtual patient	0.066026	0.068085	0.081740	0.186128
NONMEM vs Virtual patient	0.066026	0.068085	0.081740	0.186128
R aghq vs Virtual patient	0.066002	0.068048	0.081708	0.186075

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



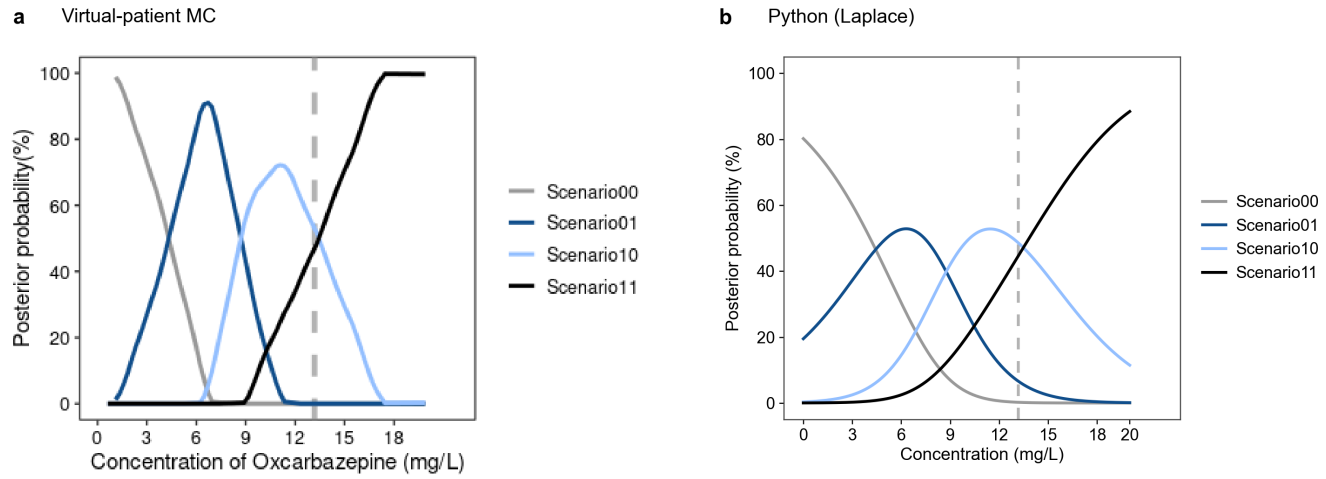
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00205957	0.00205957	0.00204629	0
ω_{01}: 300 mg at 0 h	0.25	0.06602578	0.06602578	0.06600186	0
ω_{10}: 300 mg at 12 h	0.25	0.48580591	0.48580591	0.48544897	0.52
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.44610874	0.44610874	0.44650288	0.48

Method	P_{max}	G	H_N
Python Laplace	0.485806	0.039697	0.651376
NONMEM Laplace	0.485806	0.039697	0.651376
R aghq	0.485449	0.038946	0.651313
Virtual patient (displayed)	0.52	0.04	0.499423

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

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Run times and numerical checks

OXC C036: Actual dosing histories

Observation generated from 600 mg at 0 h and 300 mg at 12 h; candidate histories unchanged.

Observations: 18.55987435 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

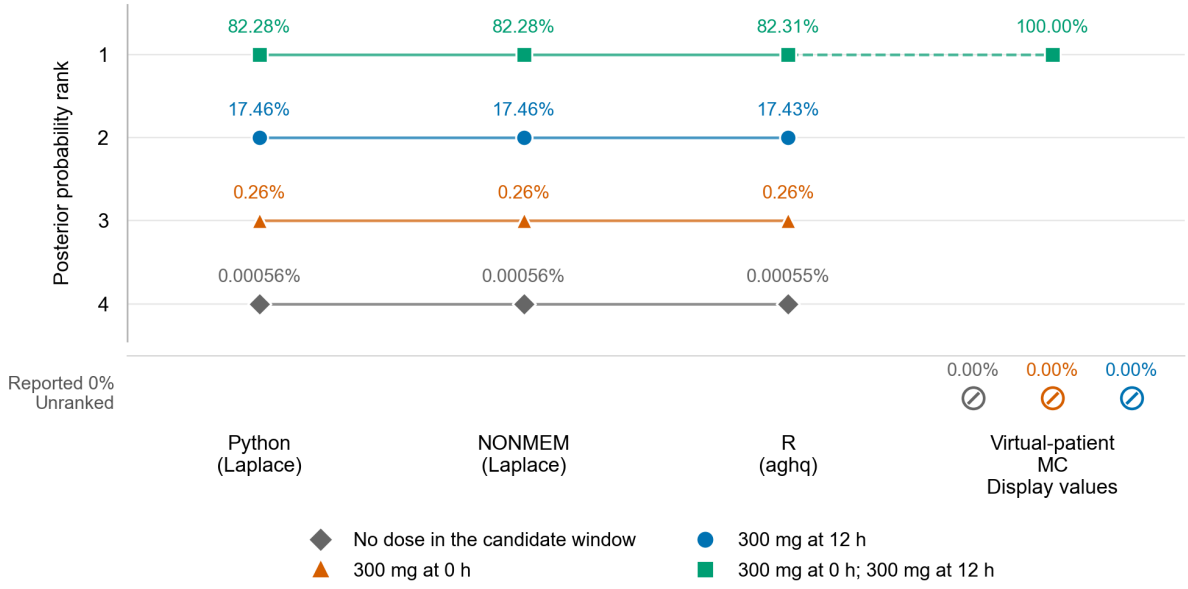
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	4.10789×10^{-9}	4.10789×10^{-9}	5.75105×10^{-9}	3.80675×10^{-9}
Python vs R aghq	3.13972×10^{-4}	3.14030×10^{-4}	4.43548×10^{-4}	2.92655×10^{-4}
NONMEM vs R aghq	3.13968×10^{-4}	3.14026×10^{-4}	4.43542×10^{-4}	2.92651×10^{-4}
Python vs Virtual patient	0.177228	0.177228	0.248805	0.304848
NONMEM vs Virtual patient	0.177228	0.177228	0.248805	0.304848
R aghq vs Virtual patient	0.176915	0.176915	0.248362	0.304565

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



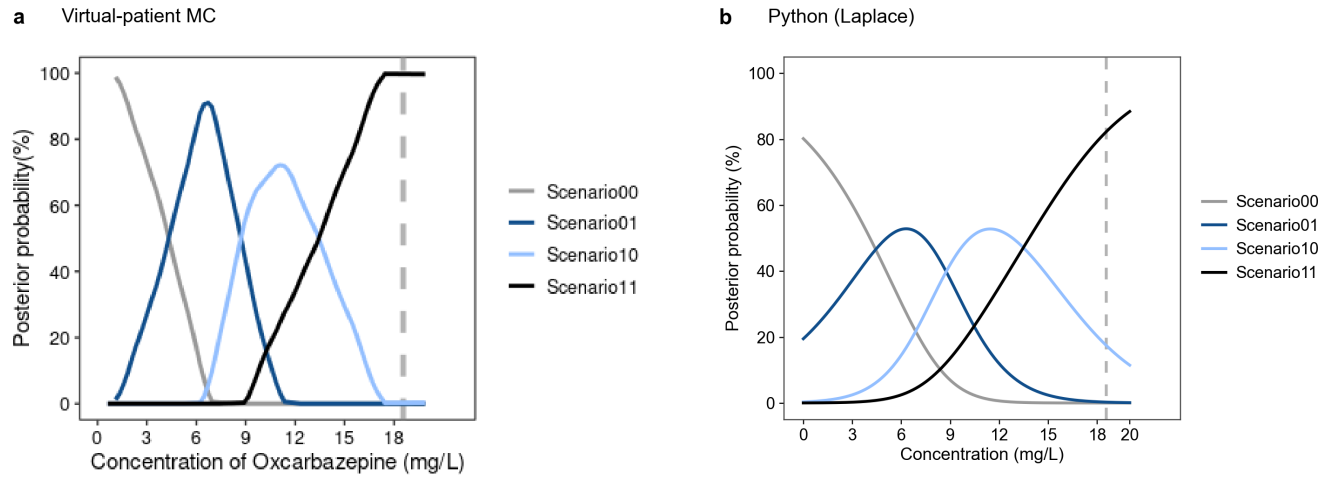
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00000560	0.00000560	0.00000554	0
ω_{01}: 300 mg at 0 h	0.25	0.00261630	0.00261630	0.00261703	0
ω_{10}: 300 mg at 12 h	0.25	0.17460641	0.17460640	0.17429243	0
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.82277170	0.82277170	0.82308500	1

Method	P_{max}	G	H_N
Python Laplace	0.822772	0.648165	0.346863
NONMEM Laplace	0.822772	0.648165	0.346863
R aghq	0.823085	0.648793	0.346514
Virtual patient (displayed)	1	1	0

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

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Run times and numerical checks

OXC C037: Actual dosing histories

Observation generated from 300 mg at 0 h and 150 mg at 12 h; candidate histories unchanged.

Observations: 10.47594498 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

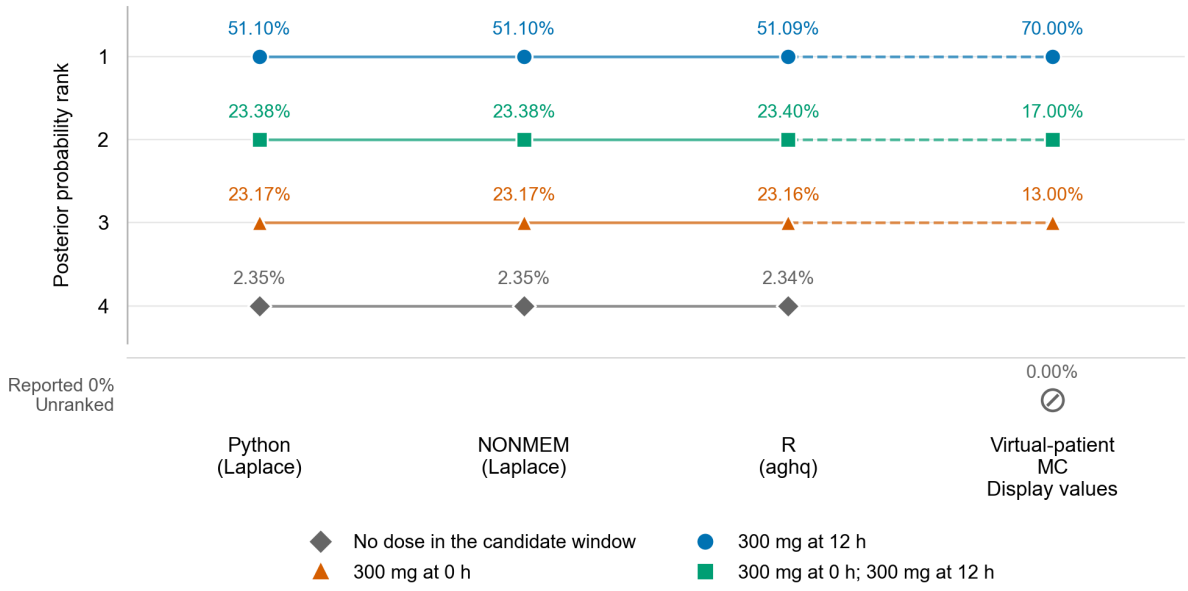
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	3.05572×10^{-9}	3.05572×10^{-9}	3.71176×10^{-9}	2.18113×10^{-9}
Python vs R aghq	2.70460×10^{-4}	2.70460×10^{-4}	3.14782×10^{-4}	3.21481×10^{-4}
NONMEM vs R aghq	2.70462×10^{-4}	2.70462×10^{-4}	3.14785×10^{-4}	3.21481×10^{-4}
Python vs Virtual patient	0.188951	0.188951	0.225073	0.170292
NONMEM vs Virtual patient	0.188951	0.188951	0.225073	0.170292
R aghq vs Virtual patient	0.189057	0.189057	0.225202	0.170201

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



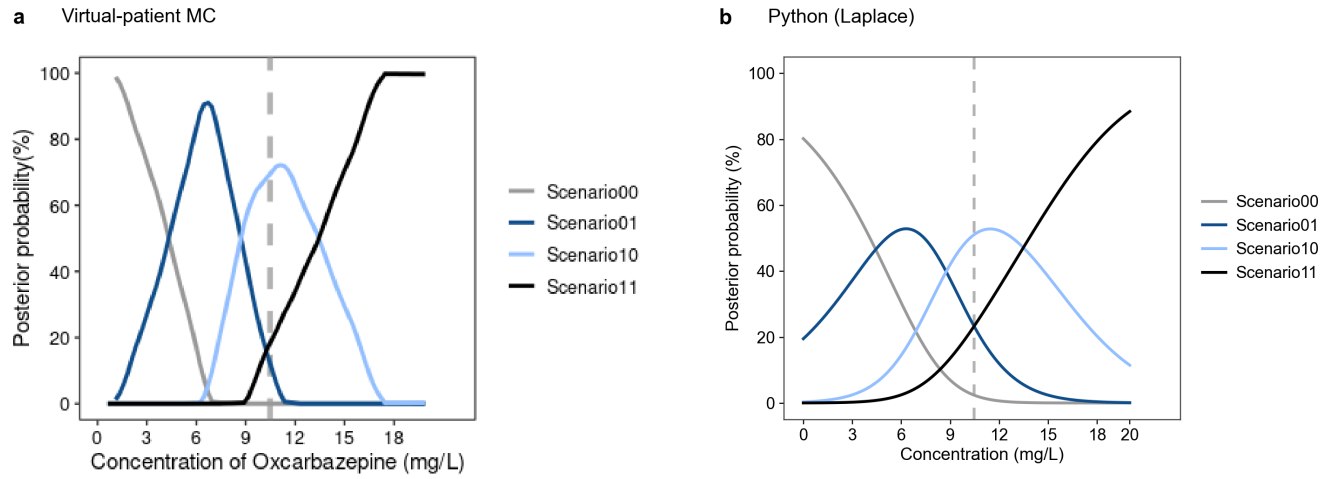
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.02351714	0.02351714	0.02341131	0
ω_{01}: 300 mg at 0 h	0.25	0.23166714	0.23166714	0.23160919	0.13
ω_{10}: 300 mg at 12 h	0.25	0.51104939	0.51104940	0.51094271	0.7
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.23376632	0.23376632	0.23403678	0.17

Method	P_{max}	G	H_N
Python Laplace	0.511049	0.277283	0.800564
NONMEM Laplace	0.511049	0.277283	0.800564
R aghq	0.510943	0.276906	0.800449
Virtual patient (displayed)	0.7	0.53	0.588716

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C038: Actual dosing histories

Observation generated from 300 mg at 0 h and 600 mg at 12 h; candidate histories unchanged.

Observations: 23.95225822 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

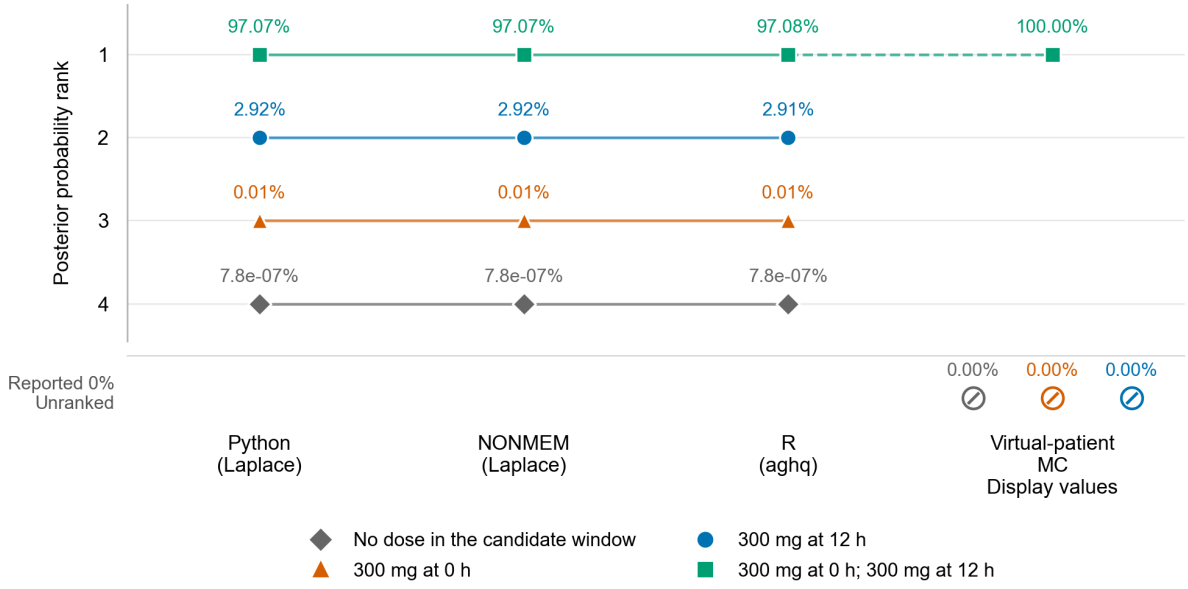
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.21408×10^{-10}	1.21409×10^{-10}	1.71218×10^{-10}	2.55169×10^{-10}
Python vs R aghq	7.09186×10^{-5}	7.09186×10^{-5}	1.00178×10^{-4}	1.49178×10^{-4}
NONMEM vs R aghq	7.09184×10^{-5}	7.09185×10^{-5}	1.00178×10^{-4}	1.49177×10^{-4}
Python vs Virtual patient	0.029264	0.029264	0.041334	0.121412
NONMEM vs Virtual patient	0.029264	0.029264	0.041334	0.121412
R aghq vs Virtual patient	0.029194	0.029194	0.041233	0.121264

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



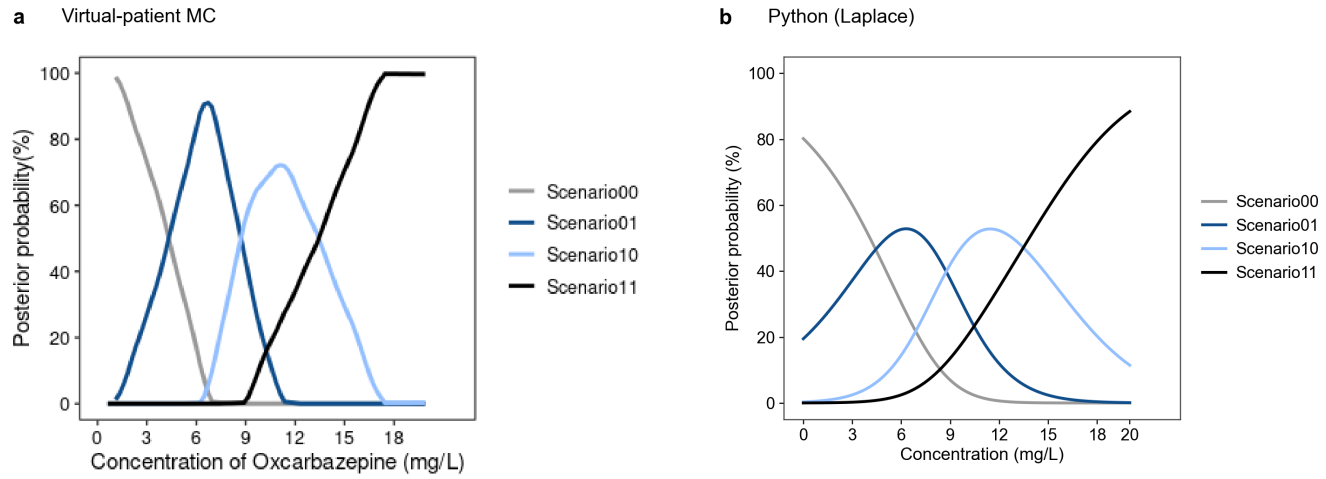
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	7.82064×10^{-9}	7.82064×10^{-9}	7.79742×10^{-9}	0
ω_{01}: 300 mg at 0 h	0.25	0.00007418	0.00007418	0.00007434	0
ω_{10}: 300 mg at 12 h	0.25	0.02919007	0.02919007	0.02911915	0
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.97073574	0.97073574	0.97080649	1

Method	P_{max}	G	H_N
Python Laplace	0.970736	0.941546	0.095718
NONMEM Laplace	0.970736	0.941546	0.095718
R aghq	0.970806	0.941687	0.095540
Virtual patient (displayed)	1	1	0

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C039: Actual dosing histories

Observation generated from 300 mg at -4 h and 300 mg at 12 h; candidate histories unchanged.

Observations: 14.02214317 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

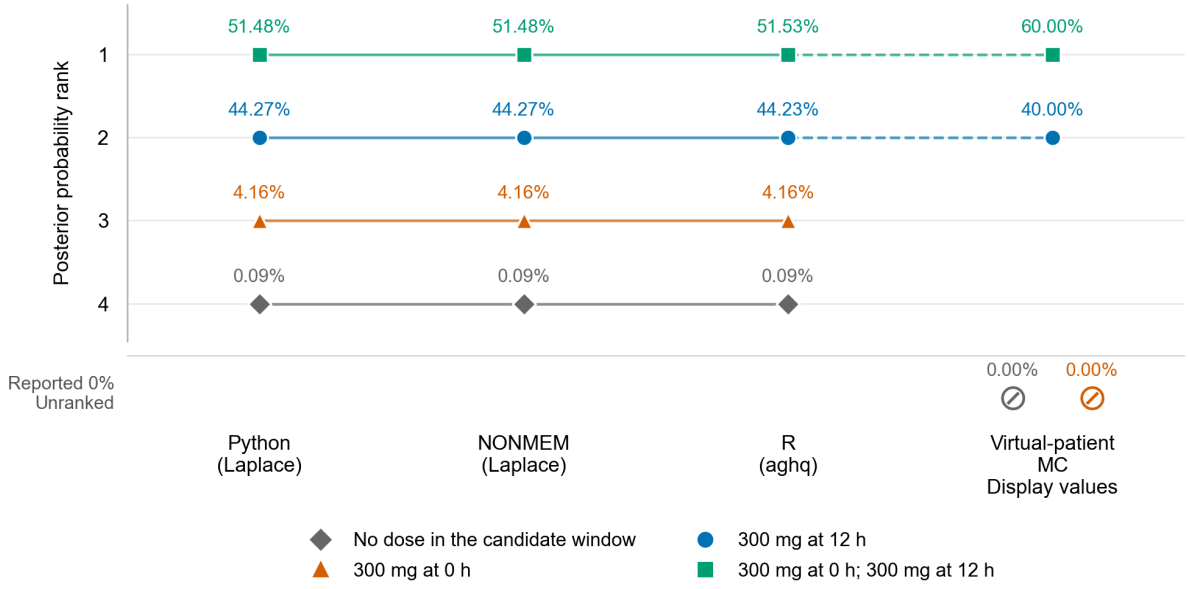
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	3.21208×10^{-10}	3.21207×10^{-10}	4.36158×10^{-10}	5.41743×10^{-10}
Python vs R aghq	4.16604×10^{-4}	4.16604×10^{-4}	5.75217×10^{-4}	3.04399×10^{-4}
NONMEM vs R aghq	4.16604×10^{-4}	4.16604×10^{-4}	5.75218×10^{-4}	3.04399×10^{-4}
Python vs Virtual patient	0.085159	0.085159	0.103949	0.153030
NONMEM vs Virtual patient	0.085159	0.085159	0.103949	0.153030
R aghq vs Virtual patient	0.084743	0.084743	0.103439	0.152911

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



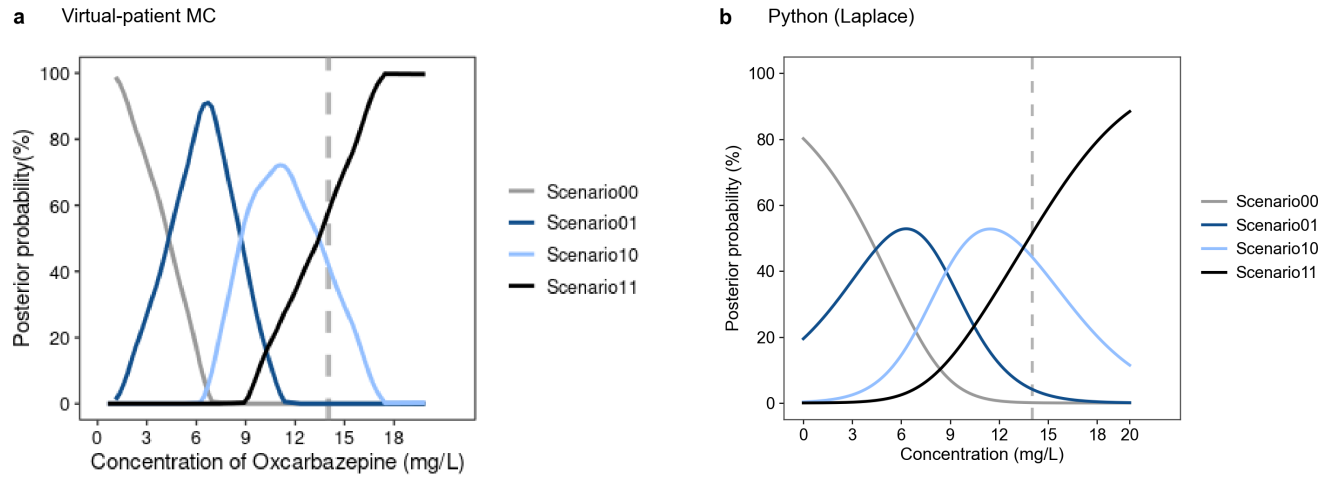
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00087531	0.00087531	0.00086908	0
ω_{01}: 300 mg at 0 h	0.25	0.04162298	0.04162298	0.04160895	0
ω_{10}: 300 mg at 12 h	0.25	0.44266100	0.44266100	0.44226466	0.4
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.51484070	0.51484070	0.51525731	0.6

Method	P_{max}	G	H_N
Python Laplace	0.514841	0.072180	0.606679
NONMEM Laplace	0.514841	0.072180	0.606679
R aghq	0.515257	0.072993	0.606581
Virtual patient (displayed)	0.6	0.2	0.485475

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C040: Actual dosing histories

Observation generated from 300 mg at -2 h and 300 mg at 12 h; candidate histories unchanged.

Observations: 14.45902787 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

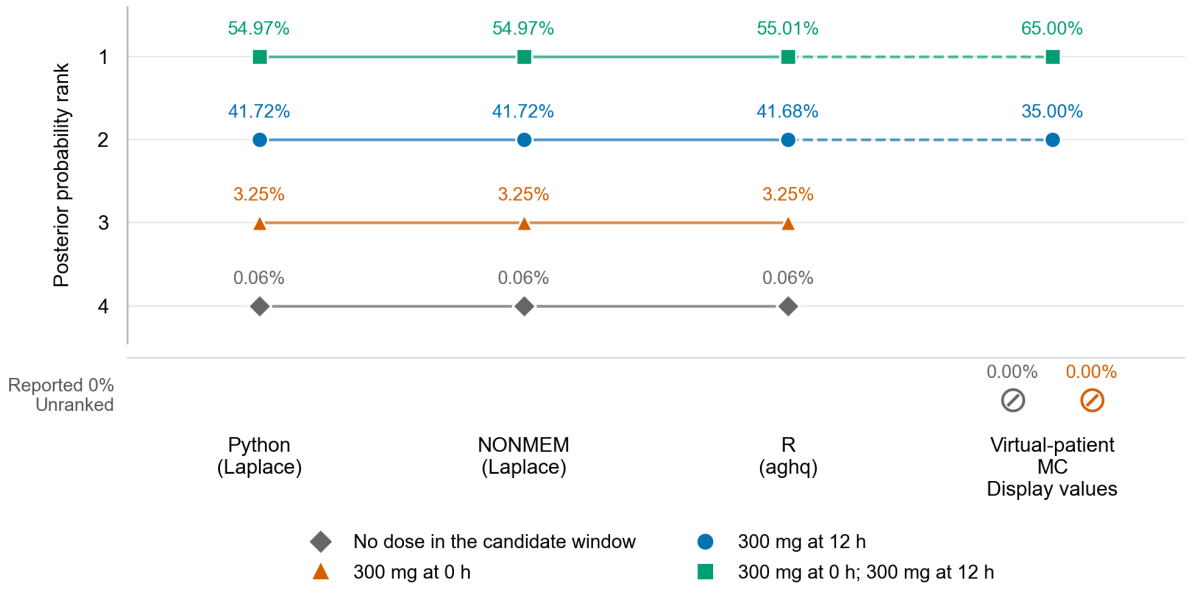
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	4.18857×10^{-9}	4.18857×10^{-9}	5.65443×10^{-9}	3.02534×10^{-9}
Python vs R aghq	4.23224×10^{-4}	4.23224×10^{-4}	5.88536×10^{-4}	3.08419×10^{-4}
NONMEM vs R aghq	4.23228×10^{-4}	4.23228×10^{-4}	5.88542×10^{-4}	3.08422×10^{-4}
Python vs Virtual patient	0.100339	0.100339	0.125092	0.141878
NONMEM vs Virtual patient	0.100339	0.100339	0.125092	0.141878
R aghq vs Virtual patient	0.099915	0.099915	0.124530	0.141727

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



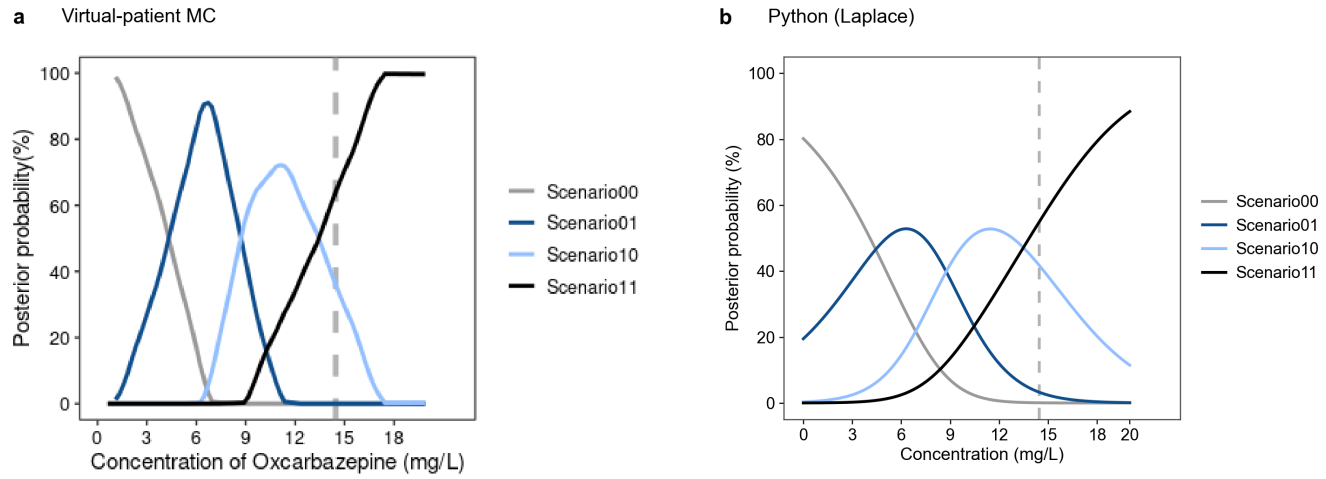
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00055654	0.00055654	0.00055238	0
ω_{01}: 300 mg at 0 h	0.25	0.03254684	0.03254684	0.03253660	0
ω_{10}: 300 mg at 12 h	0.25	0.41723519	0.41723520	0.41682637	0.35
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.54966143	0.54966142	0.55008465	0.65

Method	P_{max}	G	H_N
Python Laplace	0.549661	0.132426	0.583786
NONMEM Laplace	0.549661	0.132426	0.583786
R aghq	0.550085	0.133258	0.583663
Virtual patient (displayed)	0.65	0.3	0.467034

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C041: Actual dosing histories

Observation generated from 300 mg at 2 h and 300 mg at 12 h; candidate histories unchanged.

Observations: 15.56111858 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

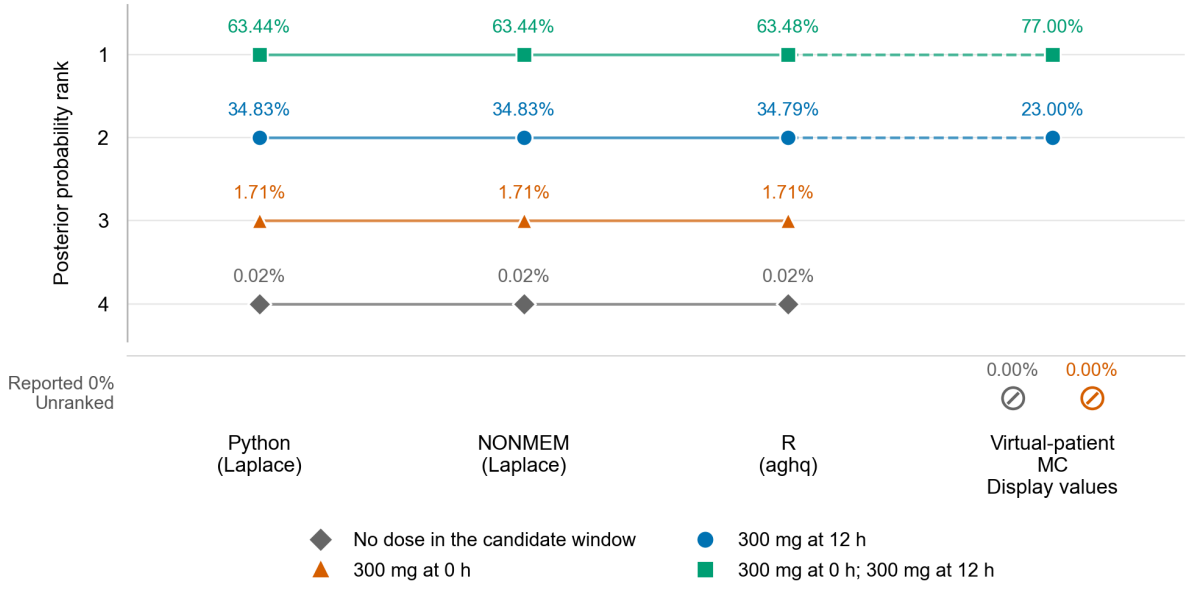
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	5.64404×10^{-10}	5.64404×10^{-10}	7.51536×10^{-10}	4.35862×10^{-10}
Python vs R aghq	4.23019×10^{-4}	4.23019×10^{-4}	5.94499×10^{-4}	3.15466×10^{-4}
NONMEM vs R aghq	4.23018×10^{-4}	4.23018×10^{-4}	5.94498×10^{-4}	3.15466×10^{-4}
Python vs Virtual patient	0.135606	0.135606	0.180787	0.134300
NONMEM vs Virtual patient	0.135606	0.135606	0.180787	0.134300
R aghq vs Virtual patient	0.135183	0.135183	0.180196	0.134064

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



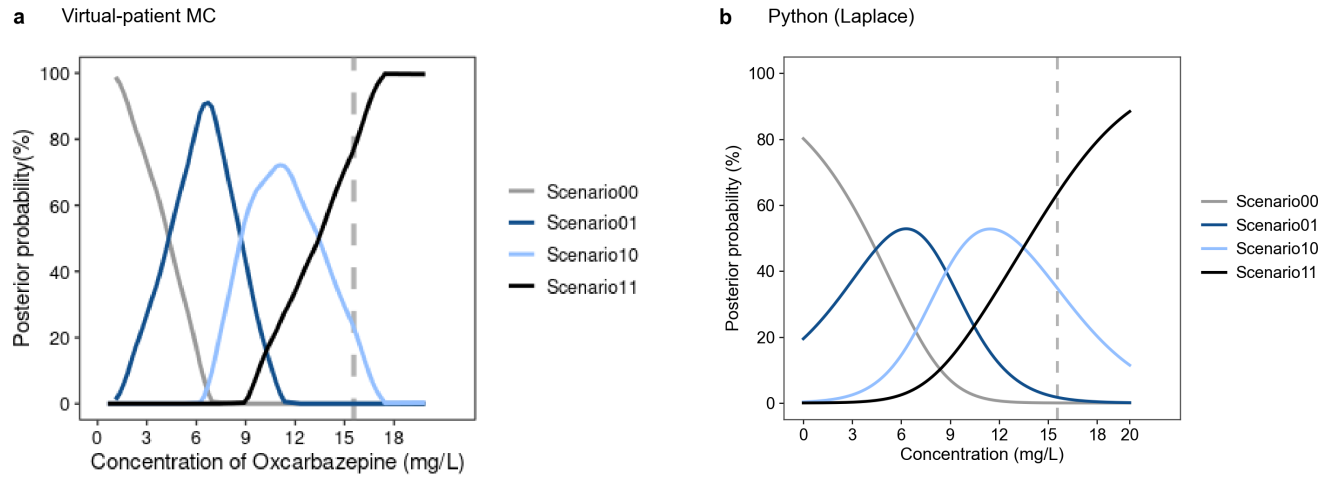
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00017137	0.00017137	0.00016993	0
ω_{01}: 300 mg at 0 h	0.25	0.01710411	0.01710411	0.01710022	0
ω_{10}: 300 mg at 12 h	0.25	0.34833081	0.34833081	0.34791312	0.23
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.63439371	0.63439371	0.63481673	0.77

Method	P_{max}	G	H_N
Python Laplace	0.634394	0.286063	0.524511
NONMEM Laplace	0.634394	0.286063	0.524511
R aghq	0.634817	0.286904	0.524312
Virtual patient (displayed)	0.77	0.54	0.389006

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

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Run times and numerical checks

OXC C042: Actual dosing histories

Observation generated from 300 mg at 4 h and 300 mg at 12 h; candidate histories unchanged.

Observations: 16.25211237 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

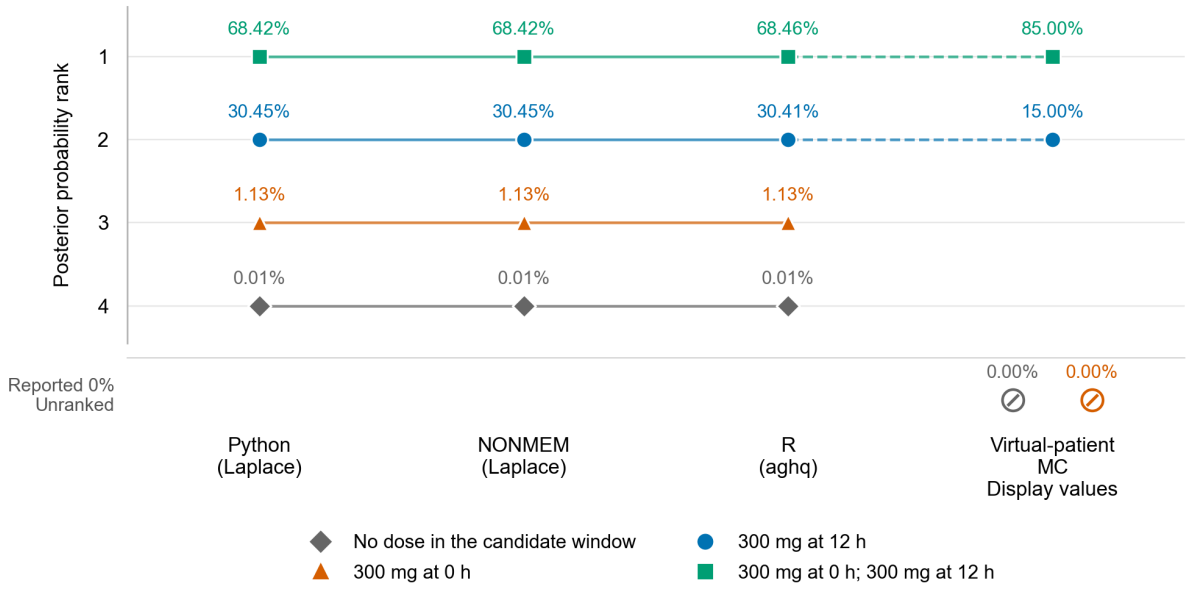
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.37387×10^{-9}	1.37387×10^{-9}	1.87137×10^{-9}	1.09359×10^{-9}
Python vs R aghq	4.10311×10^{-4}	4.10311×10^{-4}	5.78588×10^{-4}	3.16142×10^{-4}
NONMEM vs R aghq	4.10310×10^{-4}	4.10310×10^{-4}	5.78586×10^{-4}	3.16141×10^{-4}
Python vs Virtual patient	0.165829	0.165829	0.226920	0.153934
NONMEM vs Virtual patient	0.165829	0.165829	0.226920	0.153934
R aghq vs Virtual patient	0.165419	0.165419	0.226343	0.153656

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



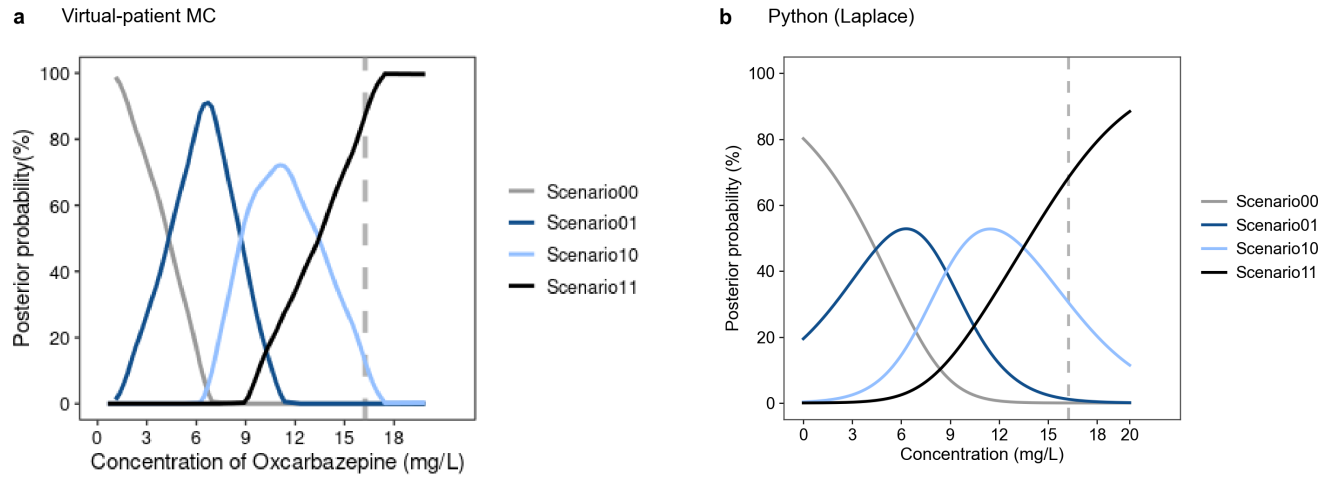
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00007995	0.00007995	0.00007923	0
ω_{01}: 300 mg at 0 h	0.25	0.01126038	0.01126038	0.01125872	0
ω_{10}: 300 mg at 12 h	0.25	0.30448868	0.30448867	0.30408075	0.15
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.68417099	0.68417099	0.68458130	0.85

Method	P_{max}	G	H_N
Python Laplace	0.684171	0.379682	0.485483
NONMEM Laplace	0.684171	0.379682	0.485483
R aghq	0.684581	0.380501	0.485235
Virtual patient (displayed)	0.85	0.7	0.304920

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

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Run times and numerical checks

OXC C043: Actual dosing histories

Observation generated from 300 mg at 0 h and 300 mg at 8 h; candidate histories unchanged.

Observations: 12.60280411 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

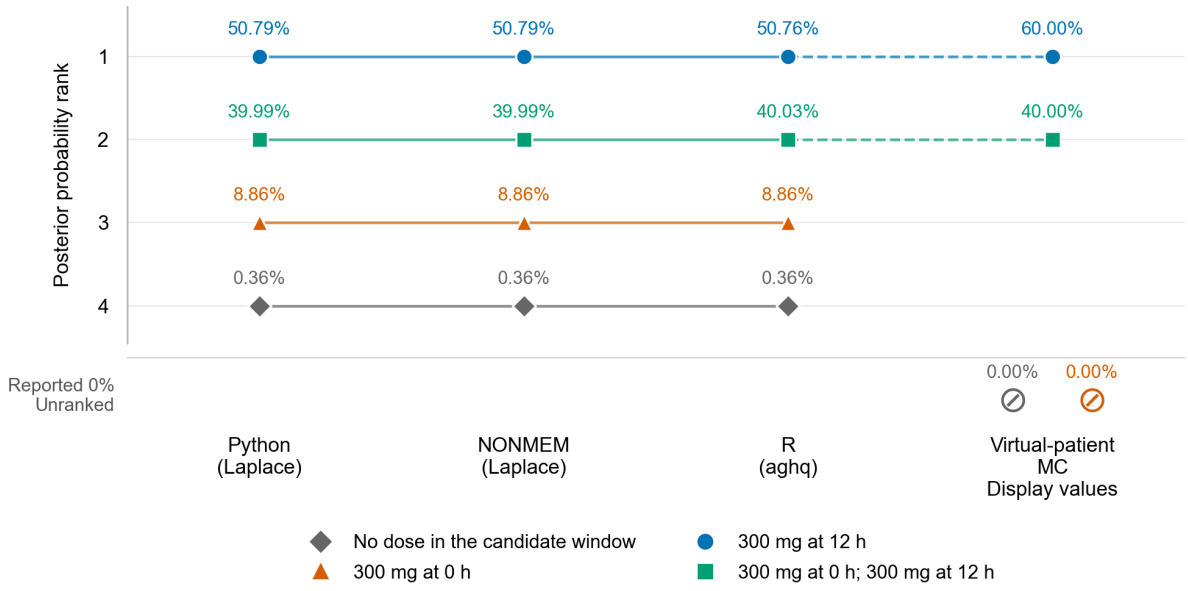
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	6.07326×10^{-9}	6.07326×10^{-9}	8.19611×10^{-9}	7.83975×10^{-9}
Python vs R aghq	3.73208×10^{-4}	3.73208×10^{-4}	4.92725×10^{-4}	2.93800×10^{-4}
NONMEM vs R aghq	3.73202×10^{-4}	3.73202×10^{-4}	4.92721×10^{-4}	2.93797×10^{-4}
Python vs Virtual patient	0.092120	0.092218	0.127890	0.219152
NONMEM vs Virtual patient	0.092120	0.092218	0.127890	0.219152
R aghq vs Virtual patient	0.092439	0.092439	0.128098	0.219122

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



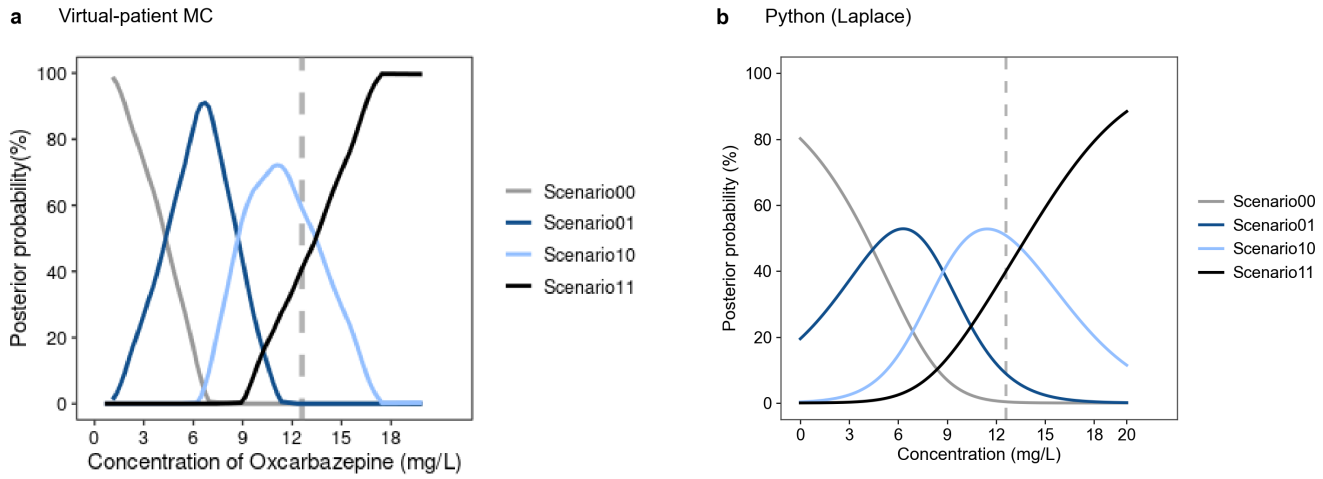
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00357897	0.00357897	0.00355745	0
ω_{01}: 300 mg at 0 h	0.25	0.08863945	0.08863945	0.08860711	0
ω_{10}: 300 mg at 12 h	0.25	0.50788006	0.50788006	0.50756071	0.6
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.39990152	0.39990152	0.40027473	0.4

Method	P_{max}	G	H_N
Python Laplace	0.507880	0.107979	0.682082
NONMEM Laplace	0.507880	0.107979	0.682082
R aghq	0.507561	0.107286	0.682029
Virtual patient (displayed)	0.6	0.2	0.485475

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

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Run times and numerical checks

OXC C044: Actual dosing histories

Observation generated from 300 mg at 0 h and 300 mg at 10 h; candidate histories unchanged.

Observations: 13.69554667 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

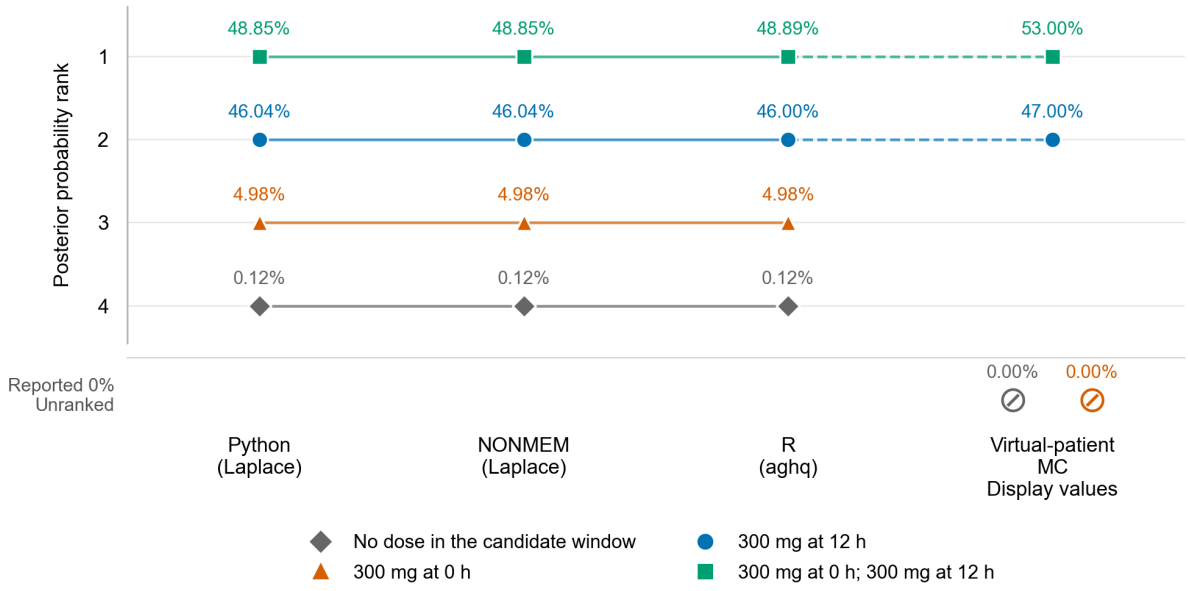
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.89441×10^{-9}	1.89524×10^{-9}	2.67421×10^{-9}	3.15732×10^{-9}
Python vs R aghq	4.09378×10^{-4}	4.09378×10^{-4}	5.61328×10^{-4}	3.01314×10^{-4}
NONMEM vs R aghq	4.09378×10^{-4}	4.09378×10^{-4}	5.61329×10^{-4}	3.01314×10^{-4}
Python vs Virtual patient	0.049837	0.051058	0.065548	0.161171
NONMEM vs Virtual patient	0.049837	0.051058	0.065548	0.161171
R aghq vs Virtual patient	0.049820	0.051032	0.065334	0.161110

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



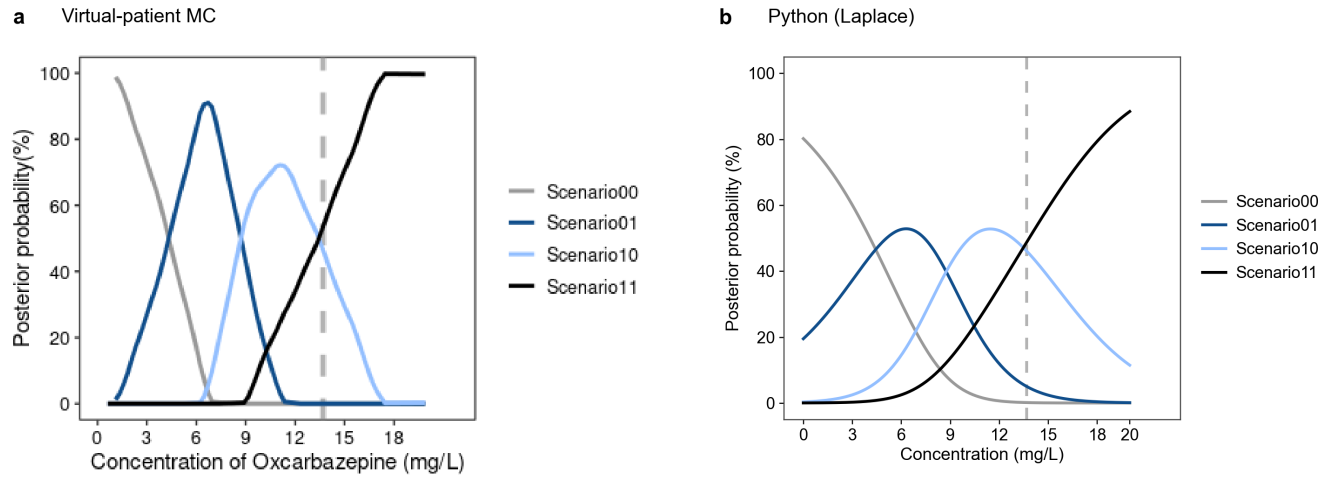
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00122105	0.00122105	0.00121267	0
ω_{01}: 300 mg at 0 h	0.25	0.04983702	0.04983702	0.04981959	0
ω_{10}: 300 mg at 12 h	0.25	0.46040561	0.46040561	0.46002204	0.47
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.48853632	0.48853632	0.48894570	0.53

Method	P_{max}	G	H_N
Python Laplace	0.488536	0.028131	0.623766
NONMEM Laplace	0.488536	0.028131	0.623766
R aghq	0.488946	0.028924	0.623684
Virtual patient (displayed)	0.53	0.06	0.498701

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

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Run times and numerical checks

OXC C045: Actual dosing histories

Observation generated from 300 mg at 0 h and 300 mg at 14 h; candidate histories unchanged.

Observations: 16.44714155 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

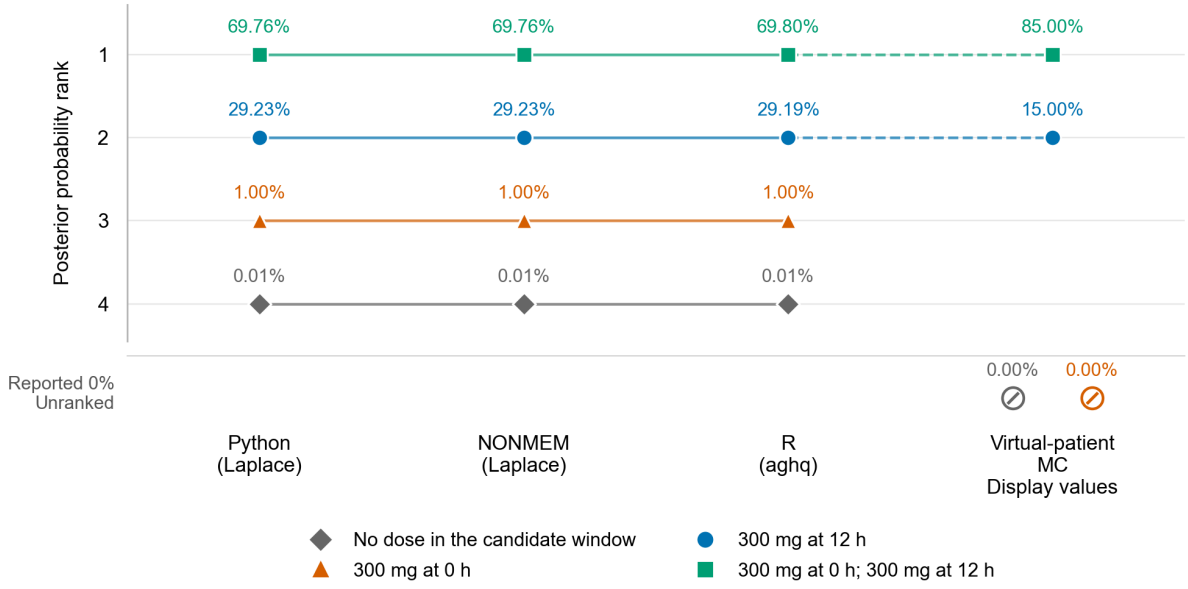
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	3.58591×10^{-9}	3.58591×10^{-9}	4.96782×10^{-9}	2.76277×10^{-9}
Python vs R aghq	4.05069×10^{-4}	4.05069×10^{-4}	5.71581×10^{-4}	3.15702×10^{-4}
NONMEM vs R aghq	4.05072×10^{-4}	4.05072×10^{-4}	5.71586×10^{-4}	3.15705×10^{-4}
Python vs Virtual patient	0.152373	0.152373	0.208739	0.143342
NONMEM vs Virtual patient	0.152373	0.152373	0.208739	0.143342
R aghq vs Virtual patient	0.151968	0.151968	0.208168	0.143066

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



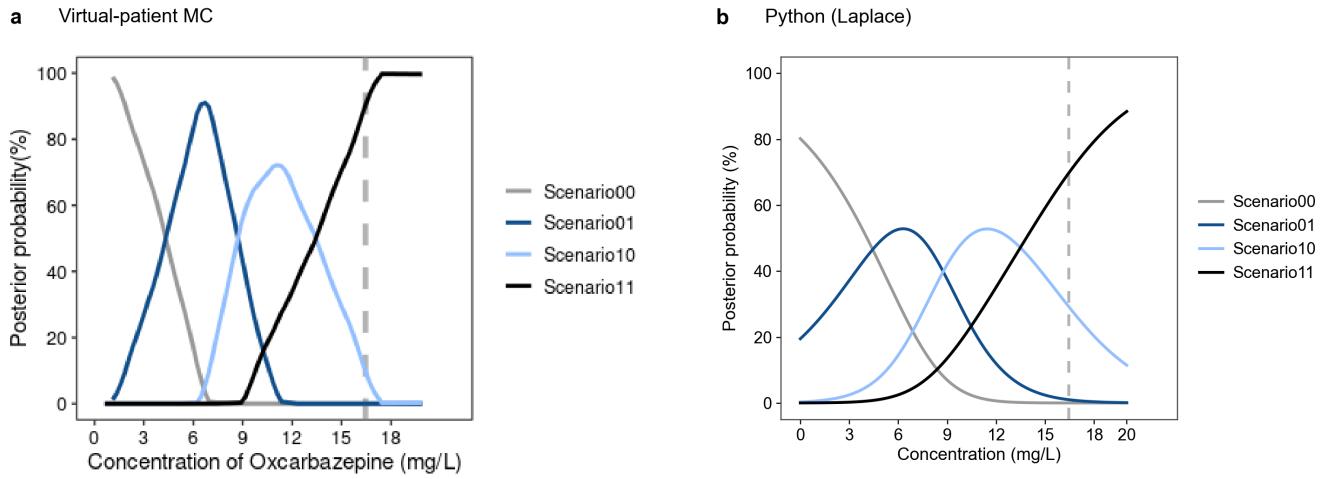
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00006427	0.00006427	0.00006369	0
ω_{01}: 300 mg at 0 h	0.25	0.00998906	0.00998906	0.00998784	0
ω_{10}: 300 mg at 12 h	0.25	0.29231929	0.29231929	0.29191602	0.15
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.69762738	0.69762738	0.69803245	0.85

Method	P_{max}	G	H_N
Python Laplace	0.697627	0.405308	0.474180
NONMEM Laplace	0.697627	0.405308	0.474180
R aghq	0.698032	0.406116	0.473919
Virtual patient (displayed)	0.85	0.7	0.304920

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C046: Actual dosing histories

Observation generated from 300 mg at 0 h and 300 mg at 16 h; candidate histories unchanged.

Observations: 18.1519344 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

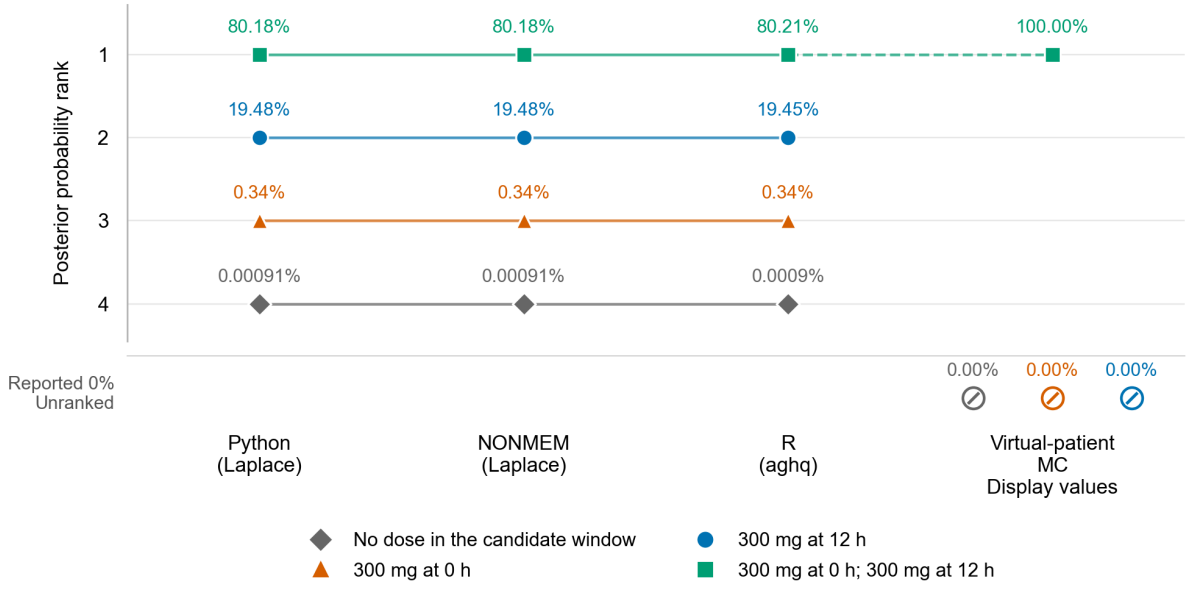
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	3.45178×10^{-9}	3.45178×10^{-9}	4.82866×10^{-9}	3.06296×10^{-9}
Python vs R aghq	3.35195×10^{-4}	3.35288×10^{-4}	4.73660×10^{-4}	2.99585×10^{-4}
NONMEM vs R aghq	3.35191×10^{-4}	3.35284×10^{-4}	4.73655×10^{-4}	2.99582×10^{-4}
Python vs Virtual patient	0.198212	0.198212	0.277931	0.323379
NONMEM vs Virtual patient	0.198212	0.198212	0.277931	0.323379
R aghq vs Virtual patient	0.197877	0.197877	0.277457	0.323090

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



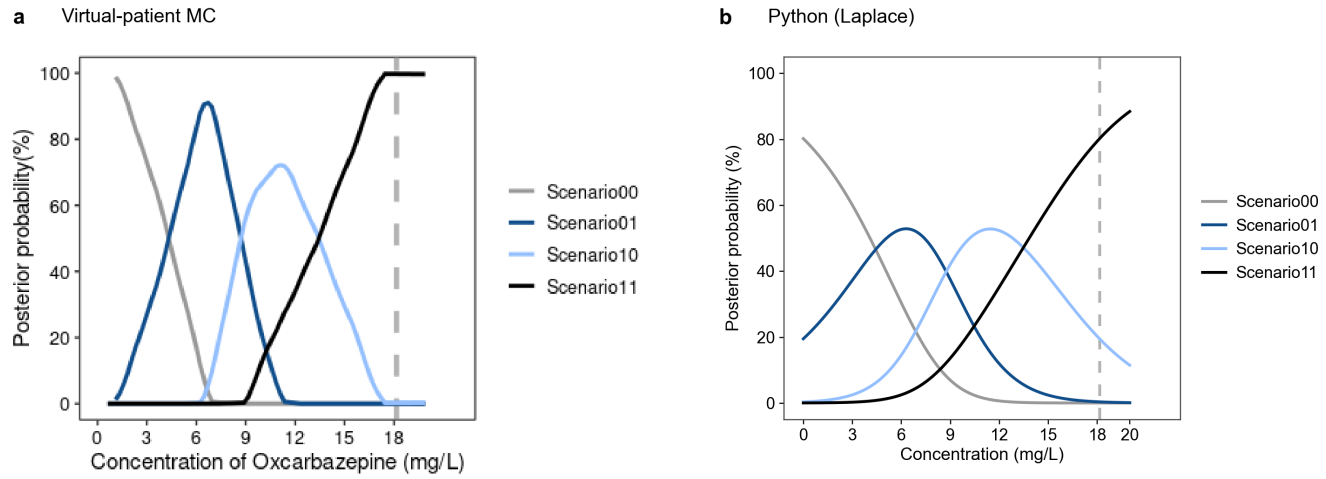
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00000906	0.00000906	0.00000897	0
ω_{01}: 300 mg at 0 h	0.25	0.00340614	0.00340614	0.00340677	0
ω_{10}: 300 mg at 12 h	0.25	0.19479677	0.19479676	0.19446157	0
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.80178803	0.80178804	0.80212269	1

Method	P_{max}	G	H_N
Python Laplace	0.801788	0.606991	0.371661
NONMEM Laplace	0.801788	0.606991	0.371661
R aghq	0.802123	0.607661	0.371320
Virtual patient (displayed)	1	1	0

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C047: Observation records

Observation times: 16 h.

Observations: 21.25843942 mg/L at 16 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

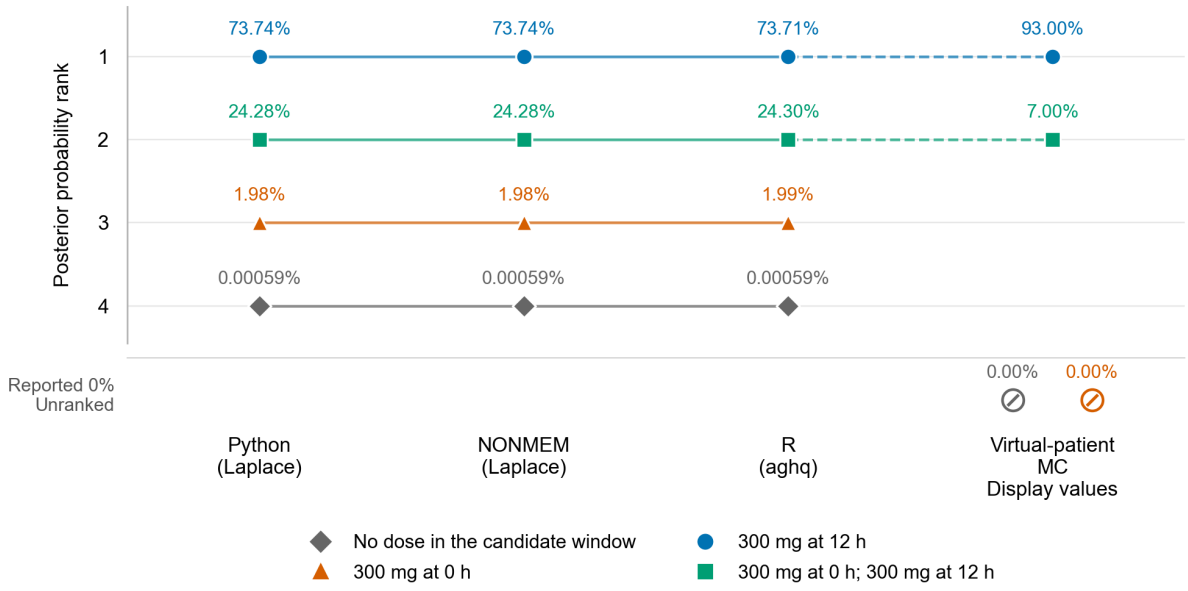
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	6.59243×10^{-10}	6.59243×10^{-10}	8.87858×10^{-10}	5.31916×10^{-10}
Python vs R aghq	3.05823×10^{-4}	3.05823×10^{-4}	4.05666×10^{-4}	2.50957×10^{-4}
NONMEM vs R aghq	3.05822×10^{-4}	3.05822×10^{-4}	4.05665×10^{-4}	2.50956×10^{-4}
Python vs Virtual patient	0.192590	0.192590	0.259480	0.203757
NONMEM vs Virtual patient	0.192590	0.192590	0.259480	0.203757
R aghq vs Virtual patient	0.192896	0.192896	0.259886	0.204005

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



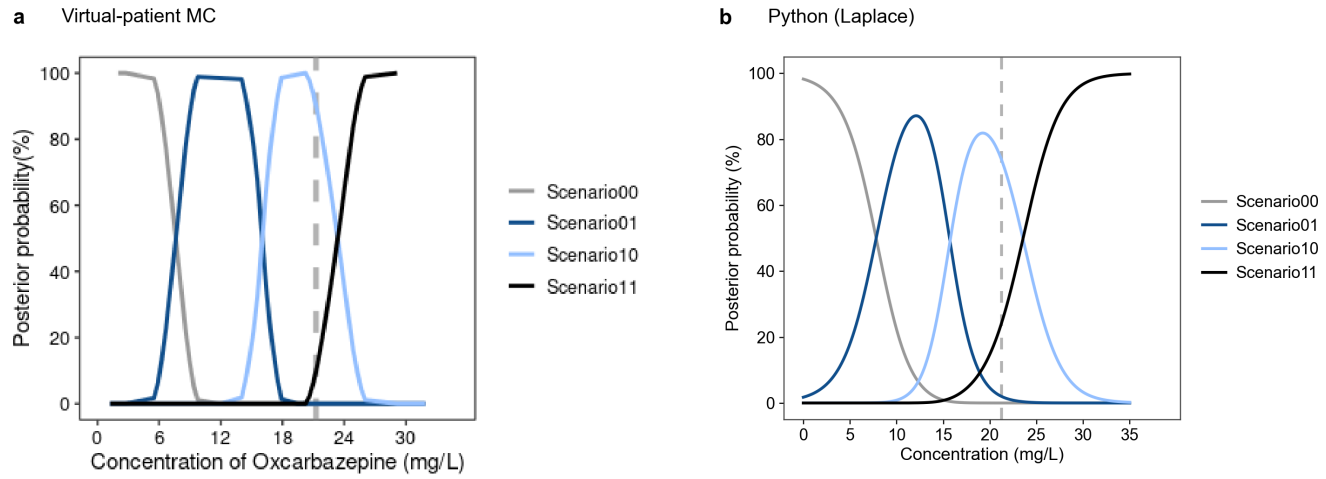
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00000593	0.00000593	0.00000594	0
ω_{01}: 300 mg at 0 h	0.25	0.01982437	0.01982437	0.01986710	0
ω_{10}: 300 mg at 12 h	0.25	0.73740976	0.73740976	0.73710393	0.93
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.24275994	0.24275994	0.24302302	0.07

Method	P_{max}	G	H_N
Python Laplace	0.737410	0.494650	0.466058
NONMEM Laplace	0.737410	0.494650	0.466058
R aghq	0.737104	0.494081	0.466381
Virtual patient (displayed)	0.93	0.86	0.182962

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C048: Observation records

Observation times: 18 h.

Observations: 18.81848437 mg/L at 18 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

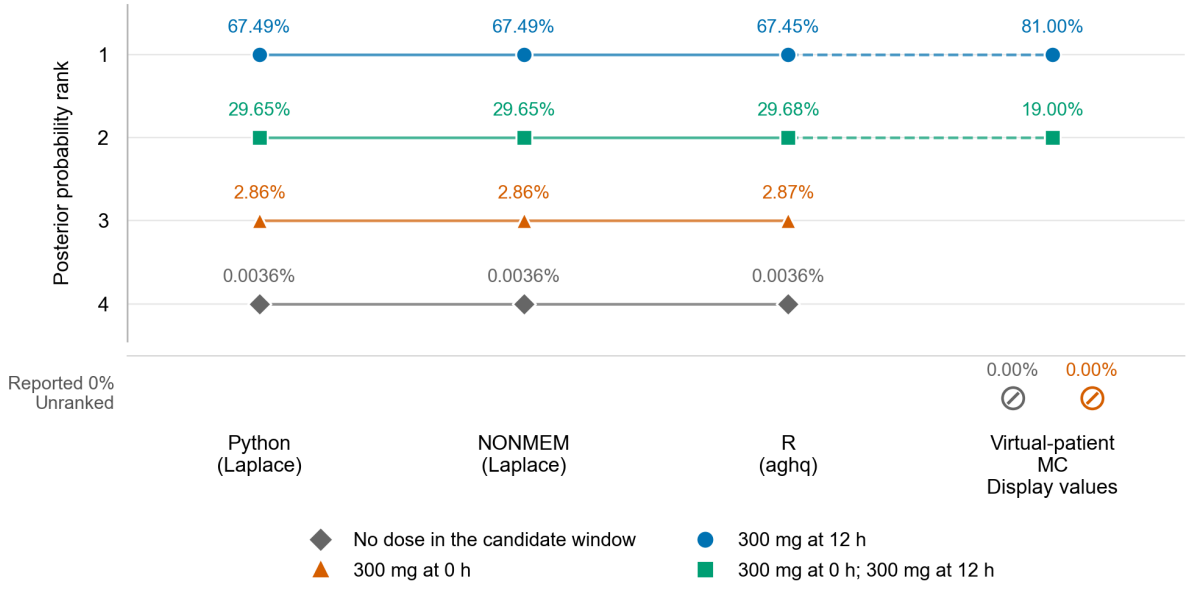
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	7.42145×10^{-9}	7.42145×10^{-9}	1.01323×10^{-8}	5.60678×10^{-9}
Python vs R aghq	3.44484×10^{-4}	3.44538×10^{-4}	4.55468×10^{-4}	2.63920×10^{-4}
NONMEM vs R aghq	3.44491×10^{-4}	3.44546×10^{-4}	4.55478×10^{-4}	2.63926×10^{-4}
Python vs Virtual patient	0.135113	0.135113	0.174381	0.152646
NONMEM vs Virtual patient	0.135113	0.135113	0.174381	0.152646
R aghq vs Virtual patient	0.135458	0.135458	0.174836	0.152879

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



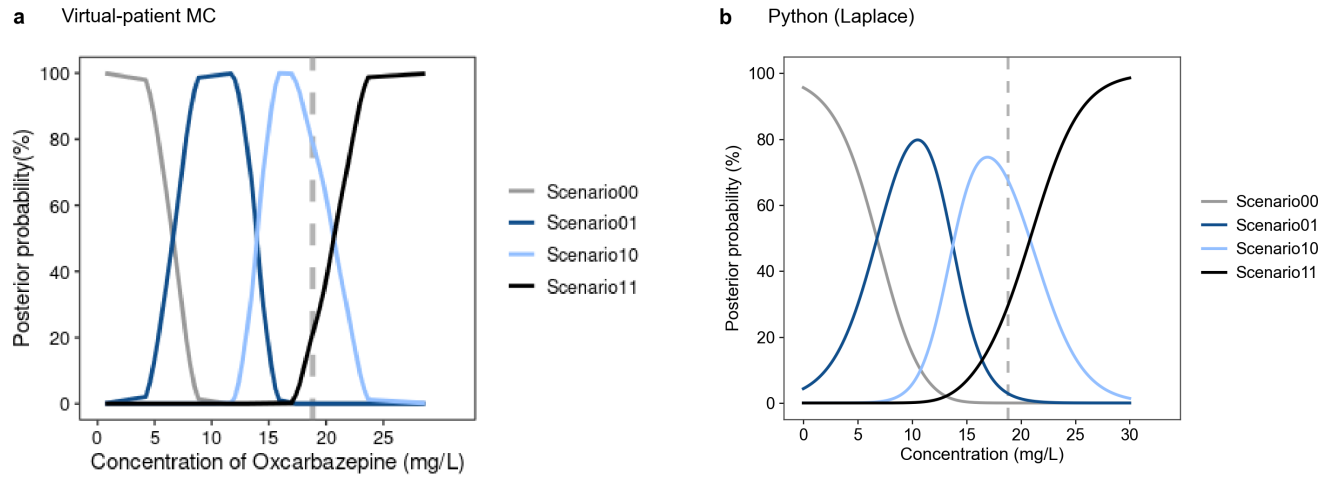
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00003633	0.00003633	0.00003628	0
ω_{01}: 300 mg at 0 h	0.25	0.02861239	0.02861239	0.02866336	0
ω_{10}: 300 mg at 12 h	0.25	0.67488686	0.67488687	0.67454238	0.81
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.29646441	0.29646441	0.29675799	0.19

Method	P_{max}	G	H_N
Python Laplace	0.674887	0.378422	0.525054
NONMEM Laplace	0.674887	0.378422	0.525054
R aghq	0.674542	0.377784	0.525344
Virtual patient (displayed)	0.81	0.62	0.350736

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C049: Observation records

Observation times: 20 h.

Observations: 16.26048751 mg/L at 20 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

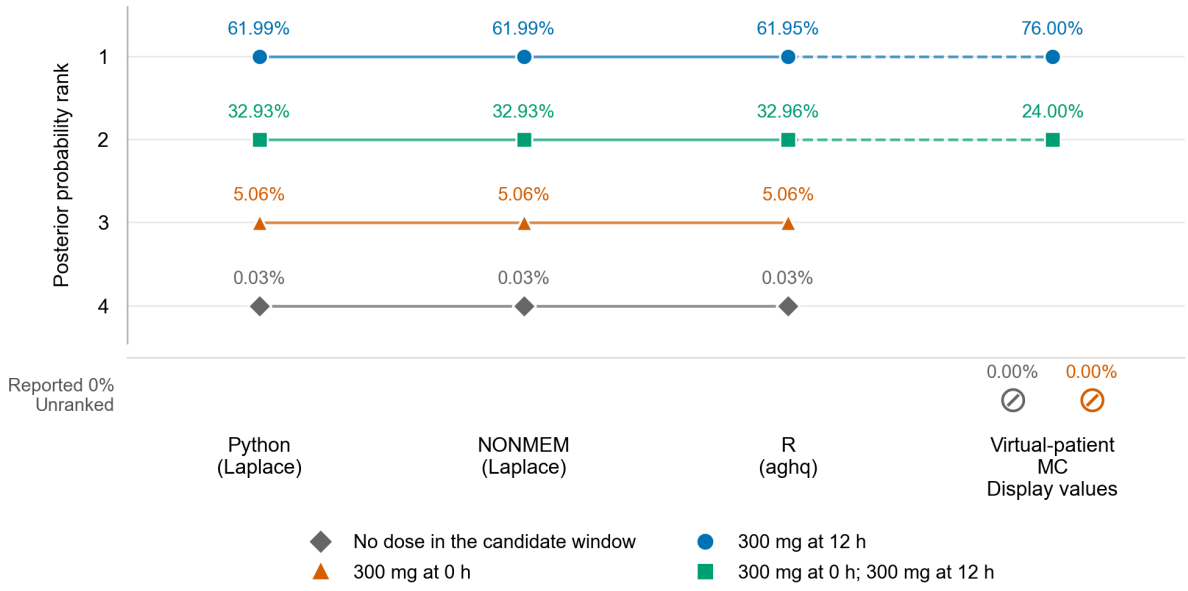
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	6.38791×10^{-9}	6.38791×10^{-9}	8.41434×10^{-9}	4.65939×10^{-9}
Python vs R aghq	3.62157×10^{-4}	3.63449×10^{-4}	4.77580×10^{-4}	2.66225×10^{-4}
NONMEM vs R aghq	3.62151×10^{-4}	3.63442×10^{-4}	4.77572×10^{-4}	2.66221×10^{-4}
Python vs Virtual patient	0.140137	0.140137	0.173692	0.180302
NONMEM vs Virtual patient	0.140137	0.140137	0.173692	0.180302
R aghq vs Virtual patient	0.140500	0.140500	0.174158	0.180495

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



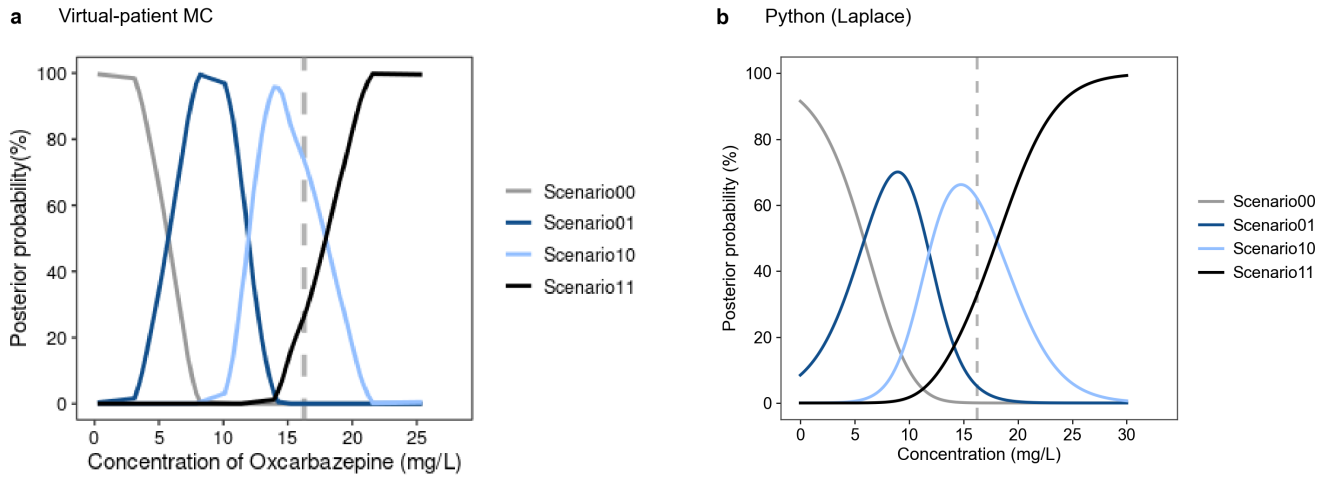
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00028447	0.00028447	0.00028318	0
ω_{01}: 300 mg at 0 h	0.25	0.05055055	0.05055055	0.05060803	0
ω_{10}: 300 mg at 12 h	0.25	0.61986261	0.61986261	0.61950046	0.76
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.32930236	0.32930237	0.32960834	0.24

Method	P_{max}	G	H_N
Python Laplace	0.619863	0.290560	0.588216
NONMEM Laplace	0.619863	0.290560	0.588216
R aghq	0.619500	0.289892	0.588453
Virtual patient (displayed)	0.76	0.52	0.397520

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C050: Observation records

Observation times: 22 h.

Observations: 13.97681045 mg/L at 22 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

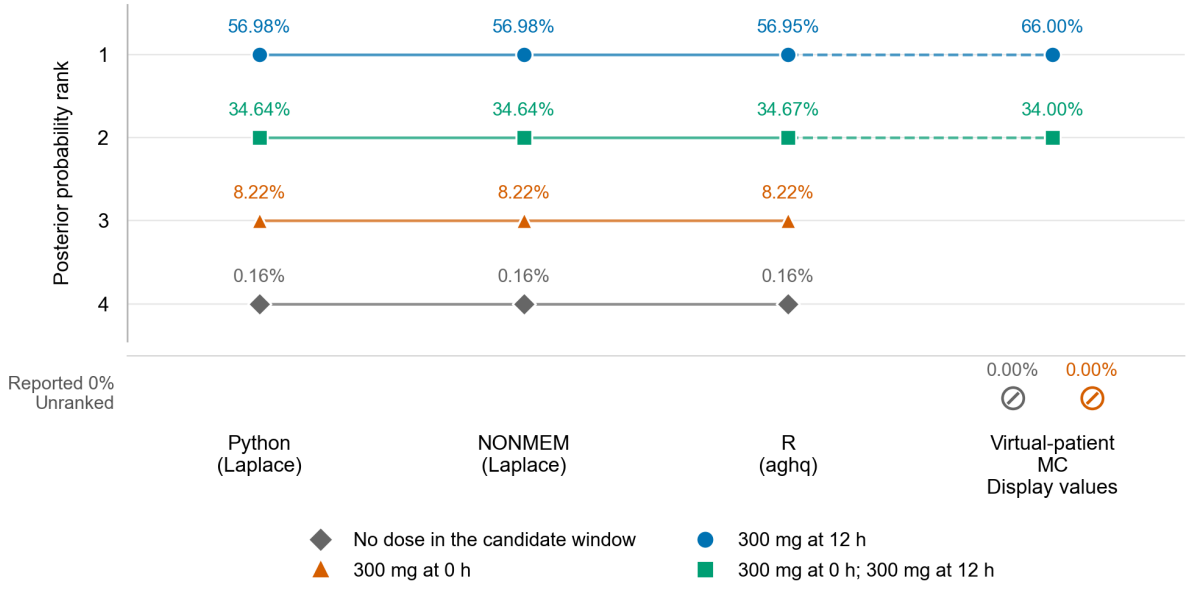
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	2.92512×10^{-9}	2.98999×10^{-9}	3.61138×10^{-9}	2.48123×10^{-9}
Python vs R aghq	3.40462×10^{-4}	3.49811×10^{-4}	4.67712×10^{-4}	2.65287×10^{-4}
NONMEM vs R aghq	3.40459×10^{-4}	3.49808×10^{-4}	4.67709×10^{-4}	2.65285×10^{-4}
Python vs Virtual patient	0.090190	0.090190	0.122193	0.208729
NONMEM vs Virtual patient	0.090190	0.090190	0.122193	0.208729
R aghq vs Virtual patient	0.090530	0.090530	0.122482	0.208789

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



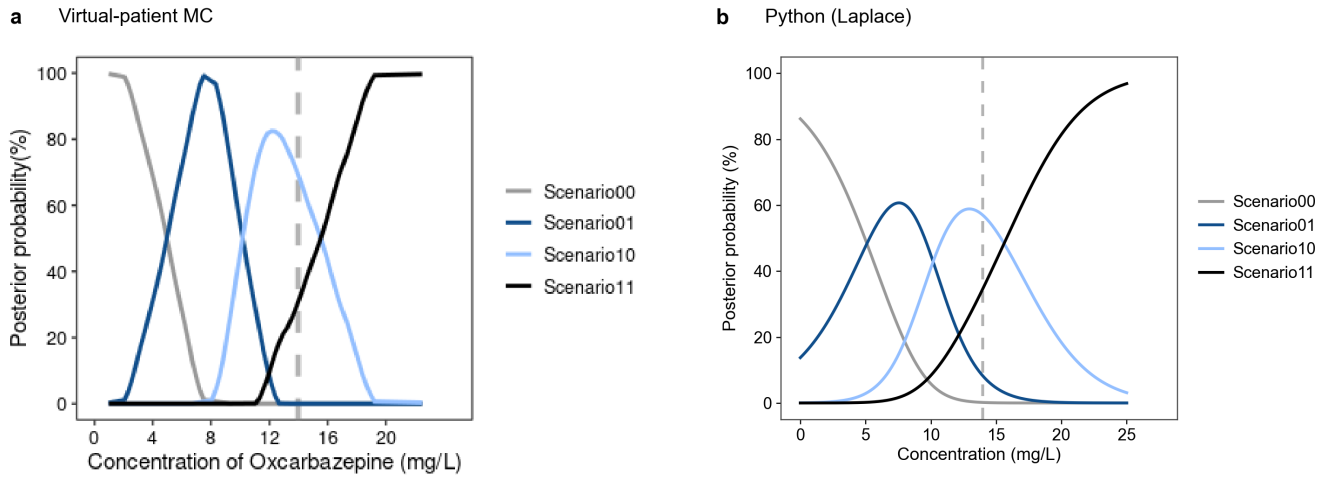
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.00161538	0.00161538	0.00160603	0
ω_{01}: 300 mg at 0 h	0.25	0.08217855	0.08217856	0.08220929	0
ω_{10}: 300 mg at 12 h	0.25	0.56981025	0.56981024	0.56946979	0.66
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.34639582	0.34639582	0.34671489	0.34

Method	P_{max}	G	H_N
Python Laplace	0.569810	0.223414	0.651714
NONMEM Laplace	0.569810	0.223414	0.651714
R aghq	0.569470	0.222755	0.651832
Virtual patient (displayed)	0.66	0.32	0.462409

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

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Run times and numerical checks

OXC C051: Observation records

Observation times: 26 h.

Observations: 10.30014823 mg/L at 26 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

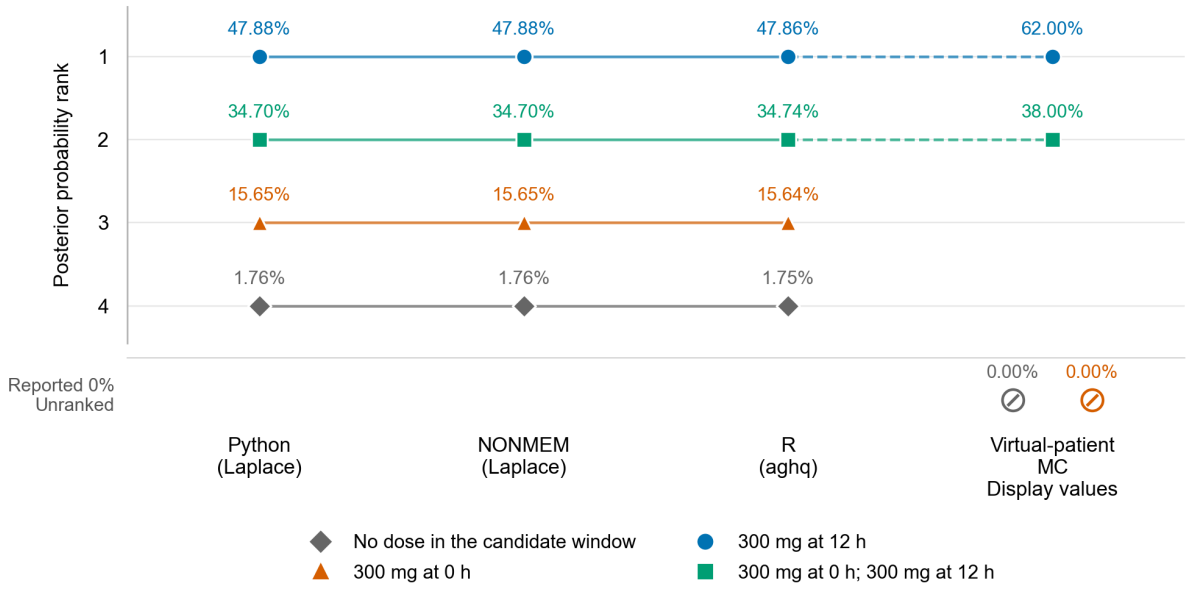
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.49482×10^{-9}	1.49482×10^{-9}	1.79220×10^{-9}	1.26713×10^{-9}
Python vs R aghq	3.88413×10^{-4}	3.88413×10^{-4}	4.52585×10^{-4}	3.53079×10^{-4}
NONMEM vs R aghq	3.88415×10^{-4}	3.88415×10^{-4}	4.52586×10^{-4}	3.53081×10^{-4}
Python vs Virtual patient	0.156527	0.174154	0.214091	0.303324
NONMEM vs Virtual patient	0.156527	0.174154	0.214091	0.303324
R aghq vs Virtual patient	0.156383	0.173928	0.214027	0.303142

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



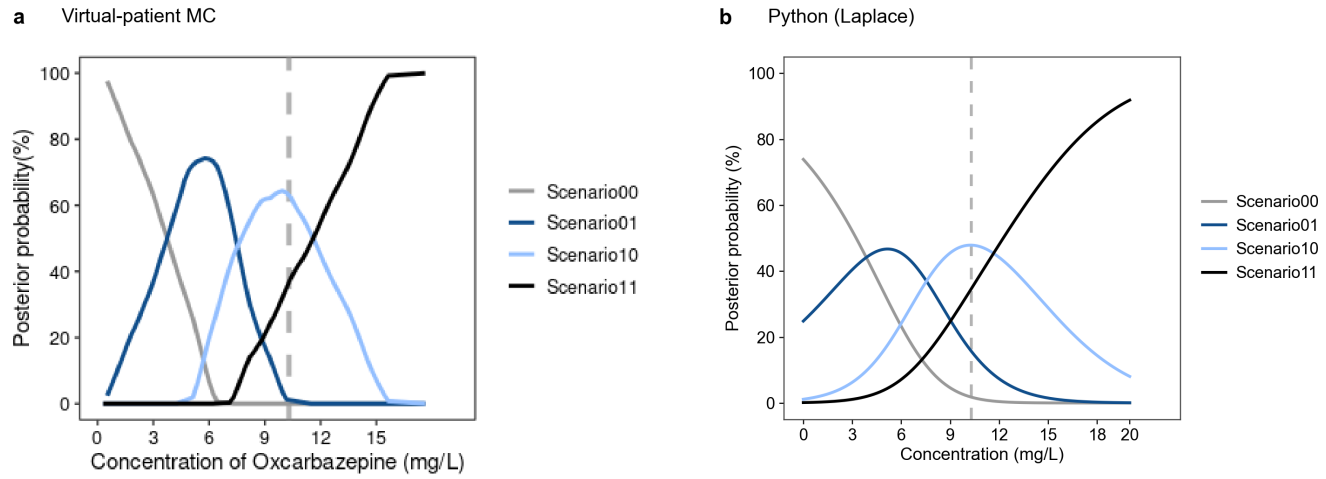
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.01762690	0.01762690	0.01754577	0
ω_{01}: 300 mg at 0 h	0.25	0.15652694	0.15652695	0.15638265	0
ω_{10}: 300 mg at 12 h	0.25	0.47879867	0.47879867	0.47863568	0.62
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.34704749	0.34704748	0.34743590	0.38

Method	P_{max}	G	H_N
Python Laplace	0.478799	0.131751	0.780042
NONMEM Laplace	0.478799	0.131751	0.780042
R aghq	0.478636	0.131200	0.779822
Virtual patient (displayed)	0.62	0.24	0.479021

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C052: Observation records

Observation times: 28 h.

Observations: 8.840587609 mg/L at 28 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

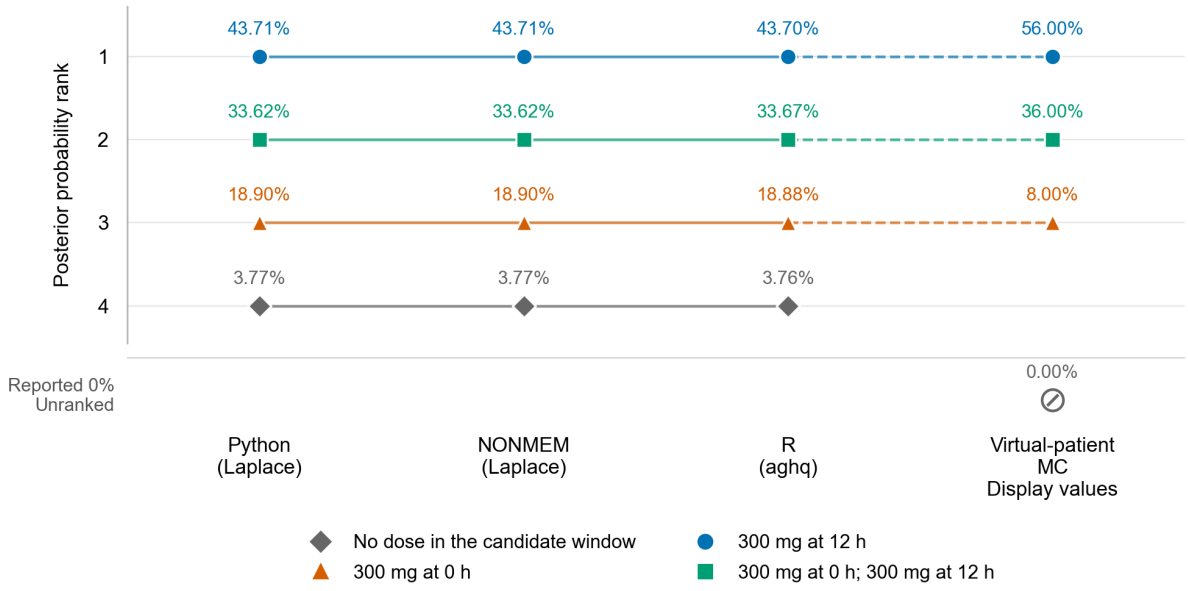
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	2.24922×10^{-9}	2.82366×10^{-9}	3.09448×10^{-9}	2.22775×10^{-9}
Python vs R aghq	4.22326×10^{-4}	4.22326×10^{-4}	5.05950×10^{-4}	4.00560×10^{-4}
NONMEM vs R aghq	4.22325×10^{-4}	4.22325×10^{-4}	5.05949×10^{-4}	4.00560×10^{-4}
Python vs Virtual patient	0.122923	0.146691	0.170228	0.185435
NONMEM vs Virtual patient	0.122923	0.146691	0.170228	0.185435
R aghq vs Virtual patient	0.122976	0.146321	0.170024	0.185138

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



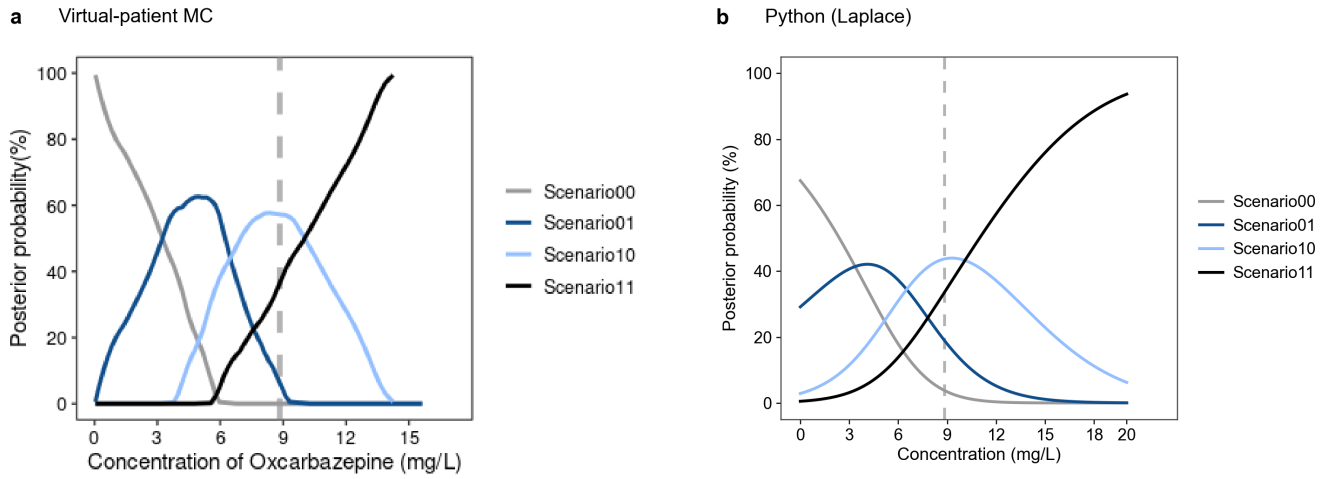
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.03768521	0.03768521	0.03755685	0
ω_{01}: 300 mg at 0 h	0.25	0.18900584	0.18900584	0.18876415	0.08
ω_{10}: 300 mg at 12 h	0.25	0.43707674	0.43707674	0.43702447	0.56
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.33623220	0.33623220	0.33665453	0.36

Method	P_{max}	G	H_N
Python Laplace	0.437077	0.100845	0.841562
NONMEM Laplace	0.437077	0.100845	0.841562
R aghq	0.437024	0.100370	0.841268
Virtual patient (displayed)	0.56	0.2	0.645282

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C053: Observation records

Observation times: 30 h.

Observations: 7.587755822 mg/L at 30 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

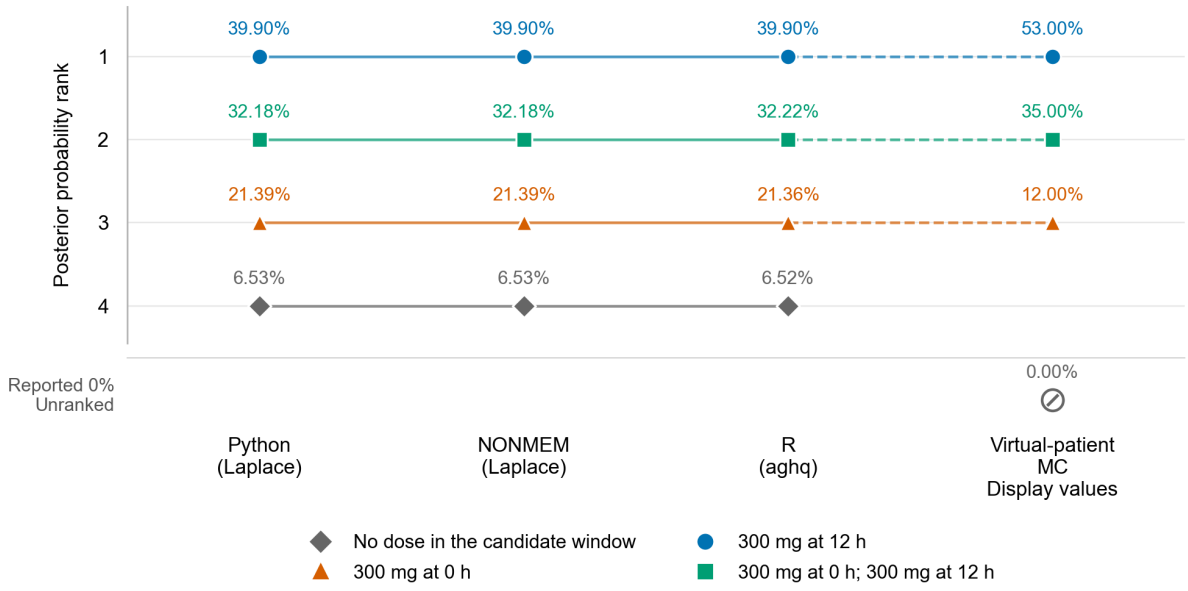
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.12164×10^{-9}	1.21841×10^{-9}	1.44133×10^{-9}	9.21948×10^{-10}
Python vs R aghq	4.25326×10^{-4}	4.55880×10^{-4}	5.46591×10^{-4}	4.09596×10^{-4}
NONMEM vs R aghq	4.25325×10^{-4}	4.55881×10^{-4}	5.46591×10^{-4}	4.09596×10^{-4}
Python vs Virtual patient	0.131034	0.159214	0.176204	0.210548
NONMEM vs Virtual patient	0.131034	0.159214	0.176204	0.210548
R aghq vs Virtual patient	0.131003	0.158758	0.175895	0.210254

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



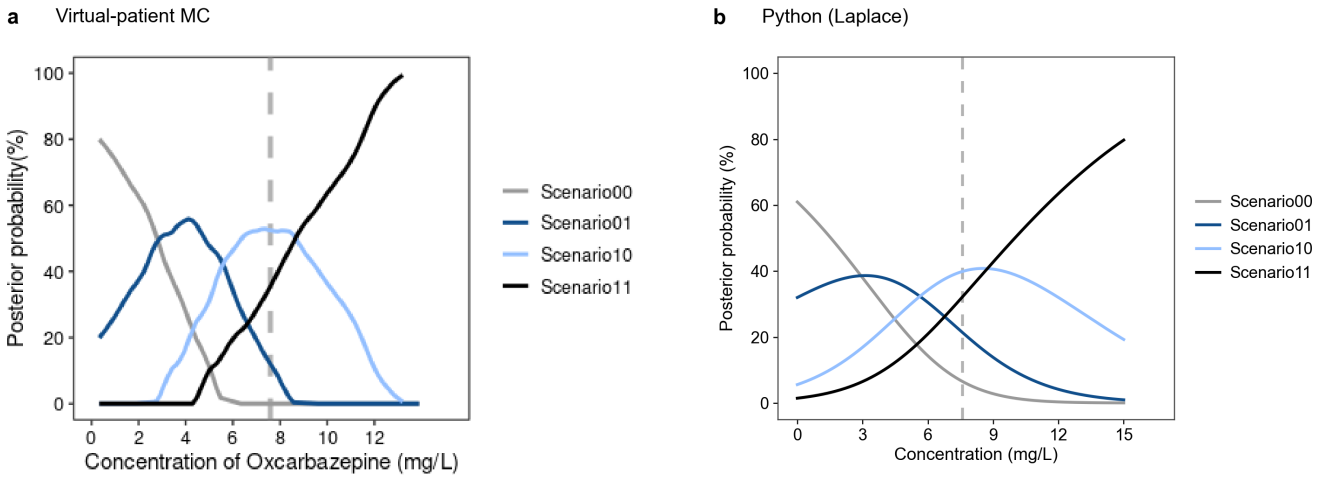
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.06530342	0.06530342	0.06515614	0
ω_{01}: 300 mg at 0 h	0.25	0.21391075	0.21391075	0.21360215	0.12
ω_{10}: 300 mg at 12 h	0.25	0.39896617	0.39896617	0.39899673	0.53
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.32181966	0.32181966	0.32224499	0.35

Method	P_{max}	G	H_N
Python Laplace	0.398966	0.077147	0.894150
NONMEM Laplace	0.398966	0.077147	0.894150
R aghq	0.398997	0.076752	0.893885
Virtual patient (displayed)	0.53	0.18	0.691307

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C054: Observation records

Observation times: 32 h.

Observations: 6.512449298 mg/L at 32 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

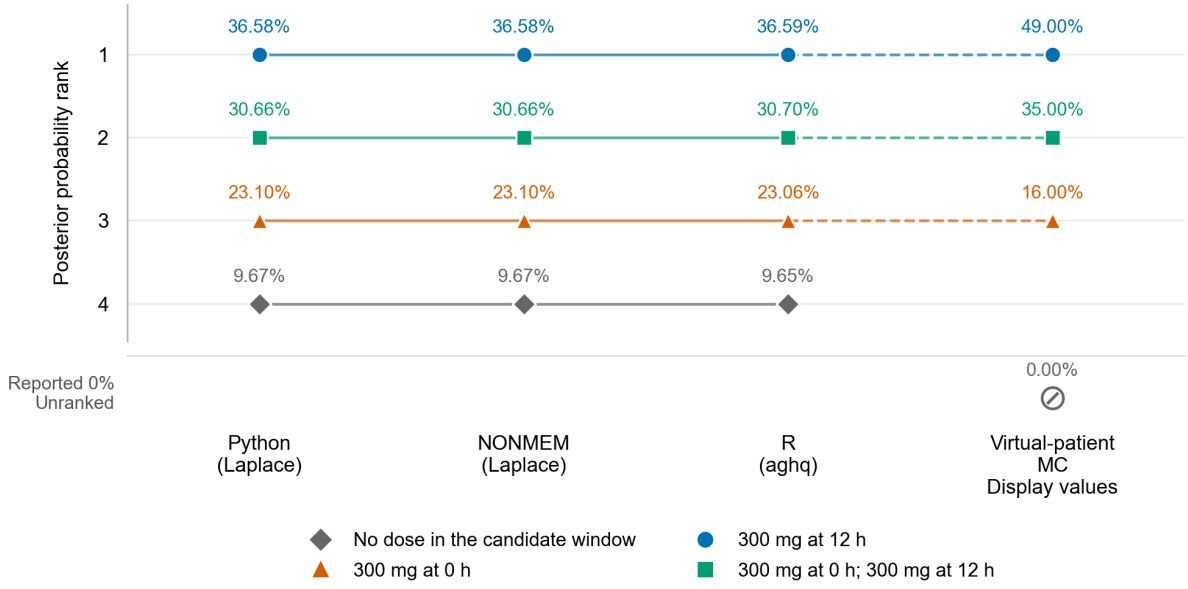
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	2.42814×10^{-9}	2.82118×10^{-9}	3.23263×10^{-9}	2.03210×10^{-9}
Python vs R aghq	3.87664×10^{-4}	4.60619×10^{-4}	5.33509×10^{-4}	3.79938×10^{-4}
NONMEM vs R aghq	3.87666×10^{-4}	4.60618×10^{-4}	5.33509×10^{-4}	3.79938×10^{-4}
Python vs Virtual patient	0.124222	0.167633	0.178033	0.238385
NONMEM vs Virtual patient	0.124222	0.167633	0.178033	0.238385
R aghq vs Virtual patient	0.124149	0.167172	0.177687	0.238156

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



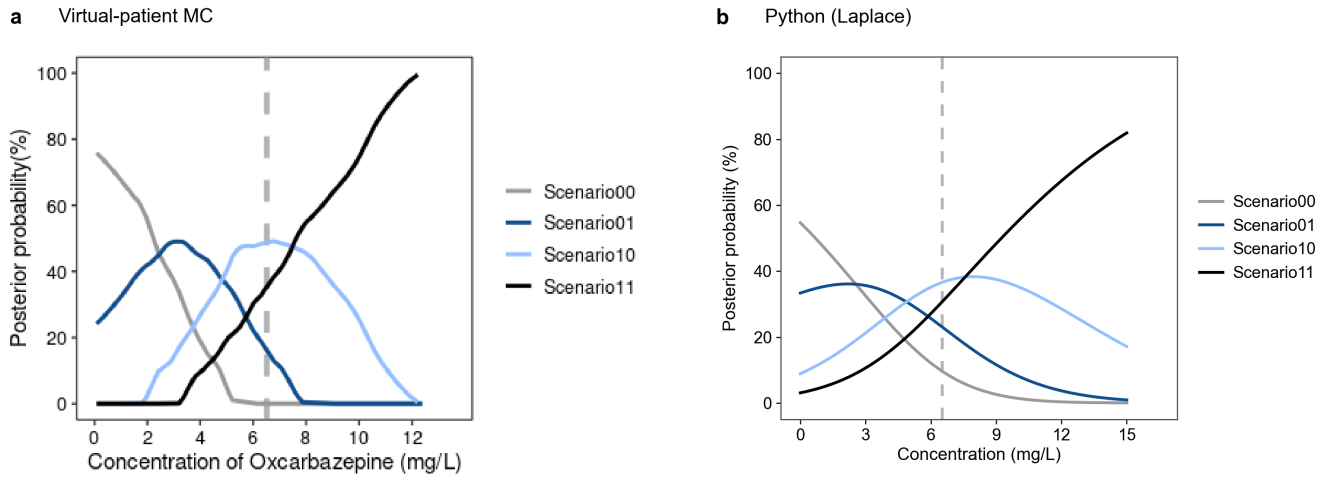
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.25	0.09665800	0.09665800	0.09653479	0
ω_{01}: 300 mg at 0 h	0.25	0.23097474	0.23097474	0.23063733	0.16
ω_{10}: 300 mg at 12 h	0.25	0.36577827	0.36577828	0.36585123	0.49
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.30658899	0.30658899	0.30697666	0.35

Method	P_{max}	G	H_N
Python Laplace	0.365778	0.059189	0.933905
NONMEM Laplace	0.365778	0.059189	0.933905
R aghq	0.365851	0.058875	0.933724
Virtual patient (displayed)	0.49	0.14	0.728700

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C055: Observation records

Observation times: 0, 24 h.

Observations: 15.78877014 mg/L at 0 h; 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

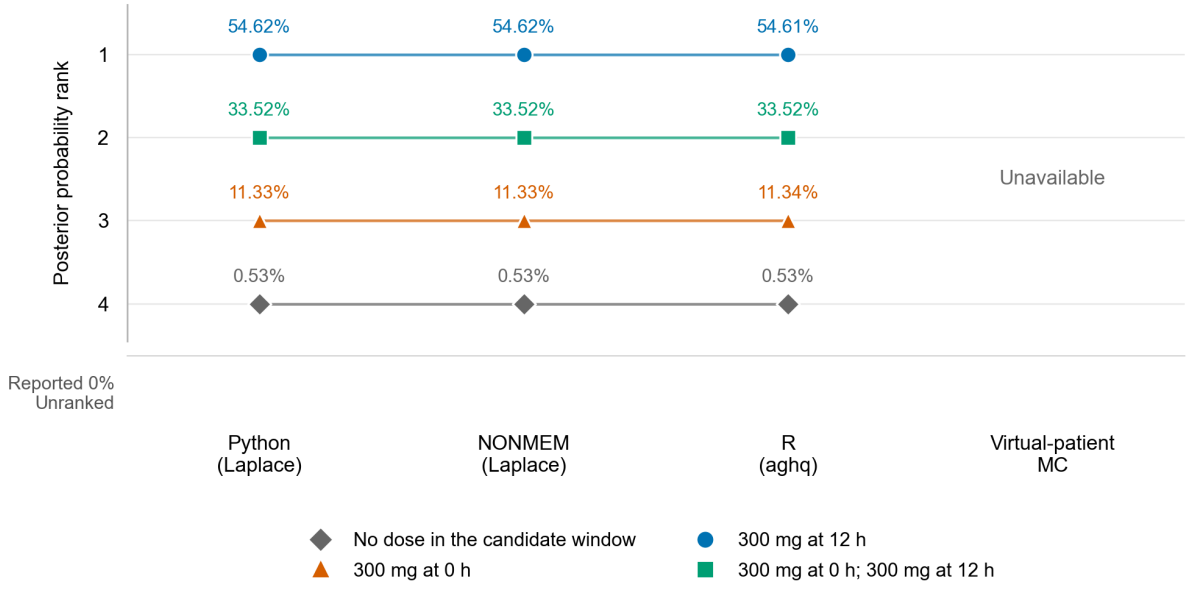
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	8.33038×10^{-9}	8.44695×10^{-9}	1.16438×10^{-8}	6.43685×10^{-9}
Python vs R aghq	1.58333×10^{-4}	1.63401×10^{-4}	1.97227×10^{-4}	1.21371×10^{-4}
NONMEM vs R aghq	1.58325×10^{-4}	1.63393×10^{-4}	1.97217×10^{-4}	1.21367×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00531559	0.00531559	0.00531052
ω_{01}: 300 mg at 0 h	0.25	0.11332053	0.11332053	0.11338717
ω_{10}: 300 mg at 12 h	0.25	0.54621261	0.54621260	0.54605428
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.33515127	0.33515128	0.33524803

Method	P_{max}	G	H_N
Python Laplace	0.546213	0.211061	0.700642
NONMEM Laplace	0.546213	0.211061	0.700642
R aghq	0.546054	0.210806	0.700735

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C056: Observation records

Observation times: 18, 24 h.

Observations: 18.81848437 mg/L at 18 h; 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

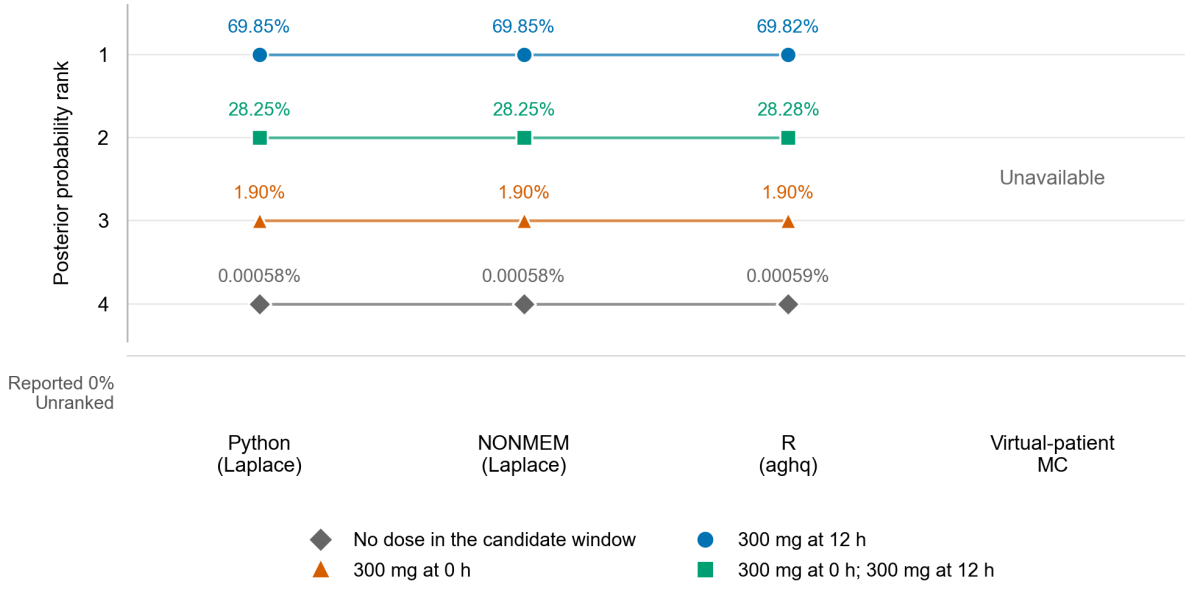
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	2.35742×10^{-9}	2.35742×10^{-9}	3.25059×10^{-9}	1.81756×10^{-9}
Python vs R aghq	3.47339×10^{-4}	3.47339×10^{-4}	4.51263×10^{-4}	2.93277×10^{-4}
NONMEM vs R aghq	3.47336×10^{-4}	3.47336×10^{-4}	4.51260×10^{-4}	2.93275×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00000581	0.00000581	0.00000586
ω_{01}: 300 mg at 0 h	0.25	0.01896598	0.01896598	0.01903311
ω_{10}: 300 mg at 12 h	0.25	0.69854847	0.69854847	0.69820113
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.28247974	0.28247974	0.28275990

Method	P_{max}	G	H_N
Python Laplace	0.698548	0.416069	0.492661
NONMEM Laplace	0.698548	0.416069	0.492661
R aghq	0.698201	0.415441	0.493019

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C057: Observation records

Observation times: 24, 30 h.

Observations: 12 mg/L at 24 h; 7.587755822 mg/L at 30 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

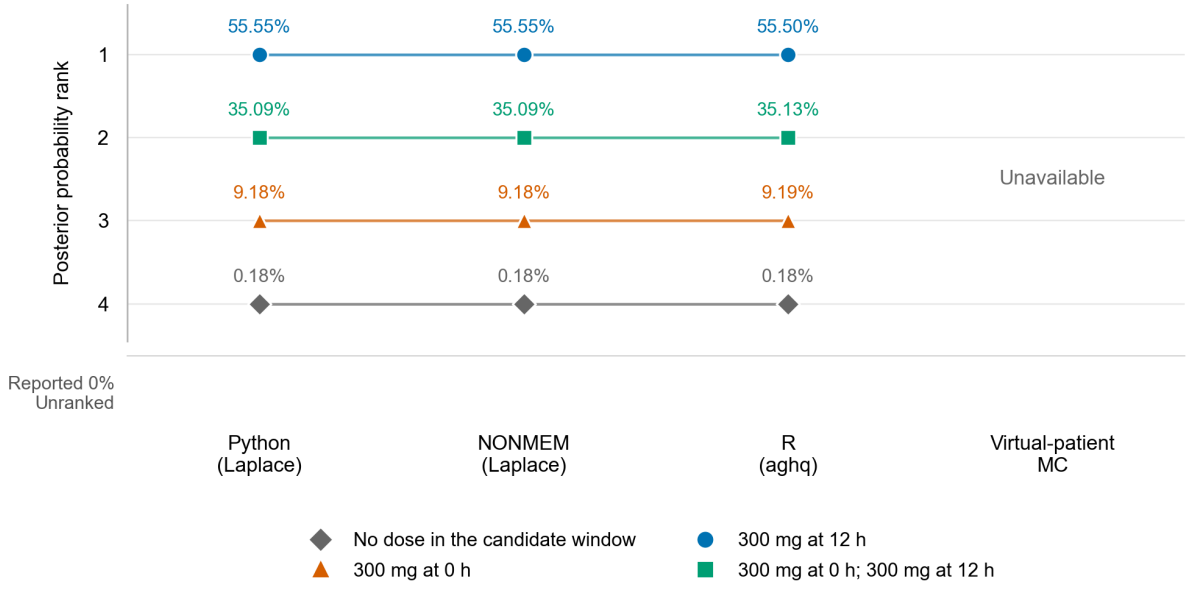
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	6.69986×10^{-9}	6.69986×10^{-9}	9.18599×10^{-9}	5.01068×10^{-9}
Python vs R aghq	4.62410×10^{-4}	4.77494×10^{-4}	6.01396×10^{-4}	3.58415×10^{-4}
NONMEM vs R aghq	4.62416×10^{-4}	4.77500×10^{-4}	6.01405×10^{-4}	3.58419×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00180671	0.00180671	0.00179162
ω_{01}: 300 mg at 0 h	0.25	0.09179102	0.09179102	0.09190010
ω_{10}: 300 mg at 12 h	0.25	0.55551032	0.55551033	0.55504791
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.35089195	0.35089195	0.35126037

Method	P_{max}	G	H_N
Python Laplace	0.555510	0.204618	0.667015
NONMEM Laplace	0.555510	0.204618	0.667015
R aghq	0.555048	0.203788	0.667216

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C058: Observation records

Observation times: 0, 24, 30 h.

Observations: 15.78877014 mg/L at 0 h; 12 mg/L at 24 h; 7.587755822 mg/L at 30 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

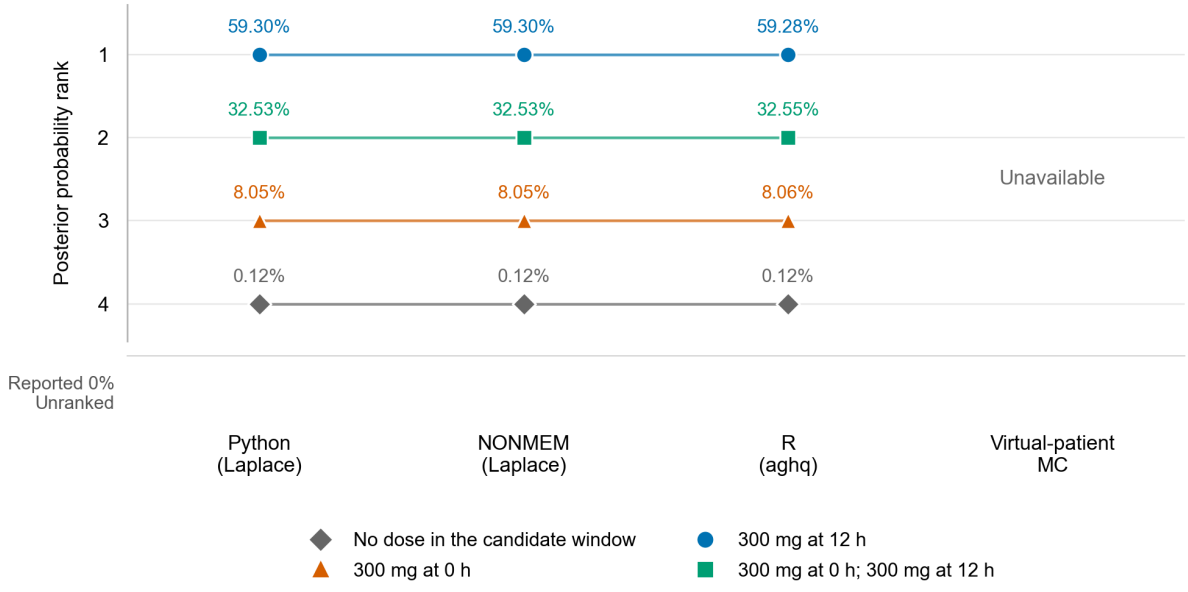
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	8.51488×10^{-9}	8.51488×10^{-9}	1.06837×10^{-8}	8.51262×10^{-9}
Python vs R aghq	2.11734×10^{-4}	2.13234×10^{-4}	2.61203×10^{-4}	1.66788×10^{-4}
NONMEM vs R aghq	2.11726×10^{-4}	2.13226×10^{-4}	2.61193×10^{-4}	1.66780×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00117235	0.00117235	0.00117085
ω_{01}: 300 mg at 0 h	0.25	0.08049602	0.08049602	0.08058448
ω_{10}: 300 mg at 12 h	0.25	0.59299563	0.59299562	0.59278390
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.32533600	0.32533600	0.32546077

Method	P_{max}	G	H_N
Python Laplace	0.592996	0.267660	0.639060
NONMEM Laplace	0.592996	0.267660	0.639060
R aghq	0.592784	0.267323	0.639234

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C059: Observation records

Observation times: 18, 24, 30 h.

Observations: 18.81848437 mg/L at 18 h; 12 mg/L at 24 h; 7.587755822 mg/L at 30 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

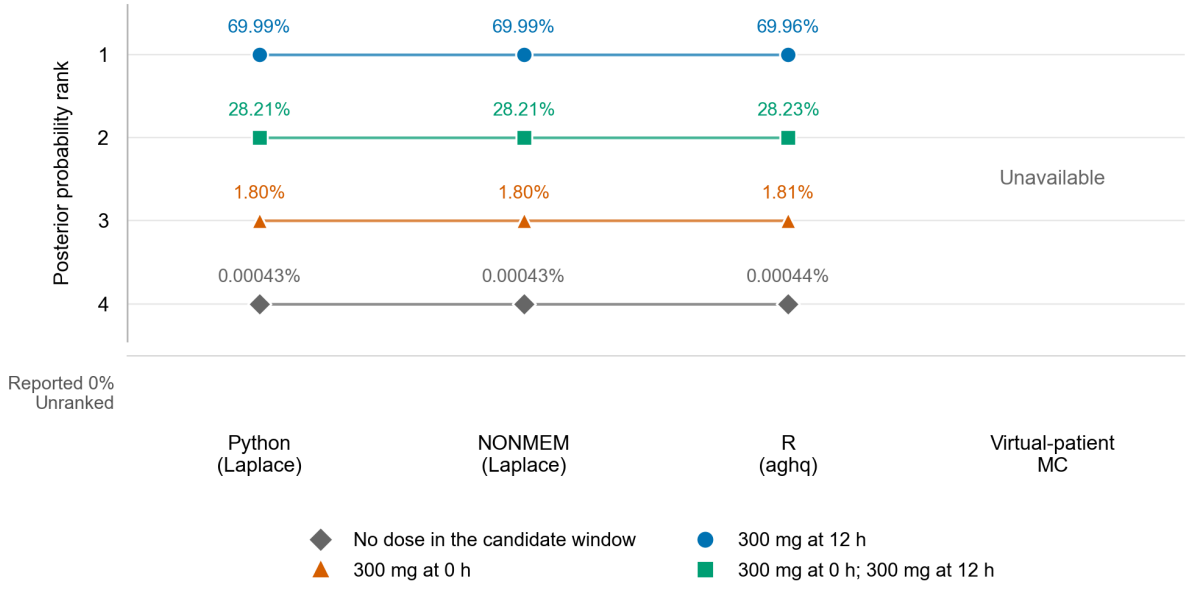
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	2.21076×10^{-9}	2.21076×10^{-9}	2.73745×10^{-9}	2.68024×10^{-9}
Python vs R aghq	3.03074×10^{-4}	3.03074×10^{-4}	3.88108×10^{-4}	2.74837×10^{-4}
NONMEM vs R aghq	3.03073×10^{-4}	3.03073×10^{-4}	3.88106×10^{-4}	2.74837×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00000433	0.00000433	0.00000438
ω_{01}: 300 mg at 0 h	0.25	0.01798646	0.01798646	0.01805778
ω_{10}: 300 mg at 12 h	0.25	0.69993144	0.69993144	0.69962837
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.25	0.28207776	0.28207777	0.28230947

Method	P_{max}	G	H_N
Python Laplace	0.699931	0.417854	0.489818
NONMEM Laplace	0.699931	0.417854	0.489818
R aghq	0.699628	0.417319	0.490158

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C060: Prior probabilities

Independent per-dose prior probability: 0.1.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

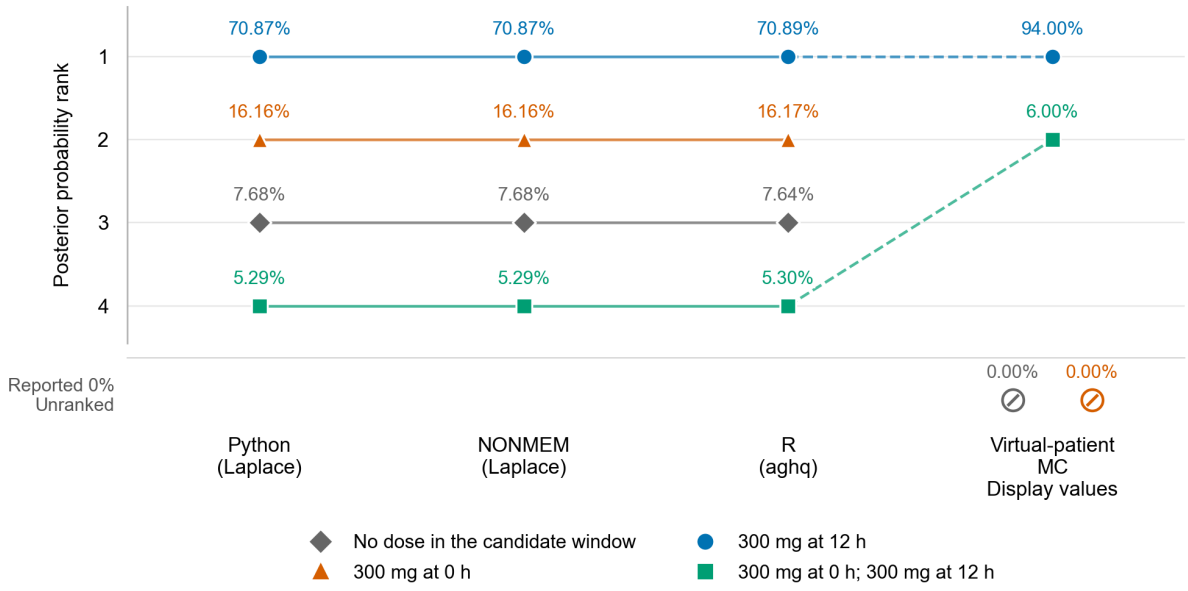
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	5.93264×10^{-9}	5.93264×10^{-9}	6.97677×10^{-9}	4.92434×10^{-9}
Python vs R aghq	3.66472×10^{-4}	3.66472×10^{-4}	4.34087×10^{-4}	5.01327×10^{-4}
NONMEM vs R aghq	3.66473×10^{-4}	3.66473×10^{-4}	4.34089×10^{-4}	5.01328×10^{-4}
Python vs Virtual patient	0.231293	0.238400	0.292512	0.357021
NONMEM vs Virtual patient	0.231293	0.238400	0.292512	0.357021
R aghq vs Virtual patient	0.231093	0.238106	0.292295	0.356789

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



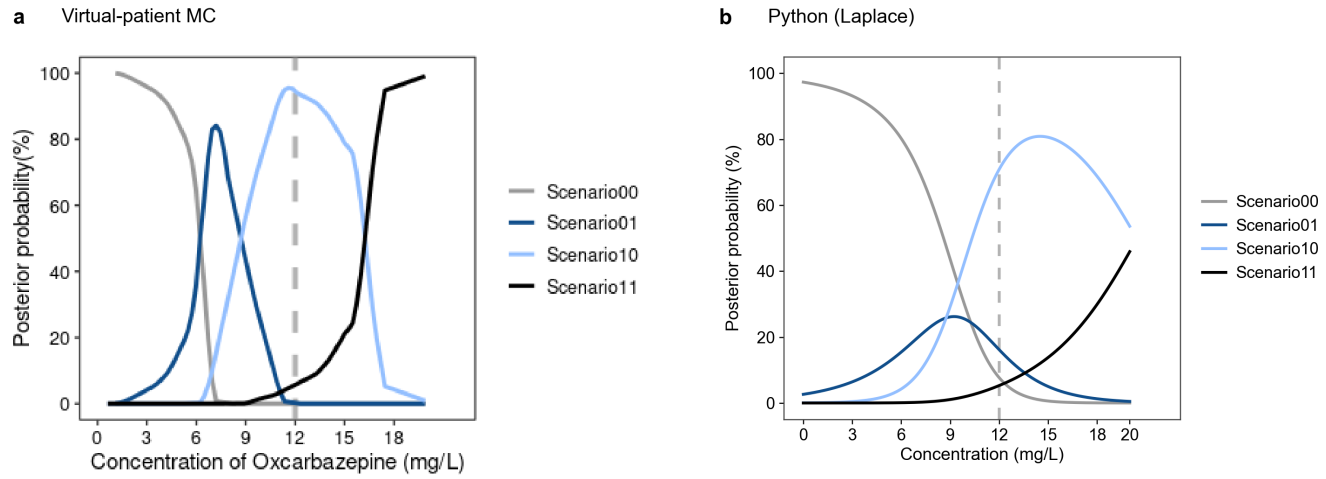
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.81	0.07678042	0.07678042	0.07641395	0
ω_{01}: 300 mg at 0 h	0.09	0.16161972	0.16161972	0.16169157	0
ω_{10}: 300 mg at 12 h	0.09	0.70870721	0.70870721	0.70890728	0.94
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.01	0.05289264	0.05289265	0.05298720	0.06

Method	P_{max}	G	H_N
Python Laplace	0.708707	0.547087	0.642813
NONMEM Laplace	0.708707	0.547087	0.642813
R aghq	0.708907	0.547216	0.642479
Virtual patient (displayed)	0.94	0.88	0.163722

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C061: Prior probabilities

Independent per-dose prior probability: 0.3.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

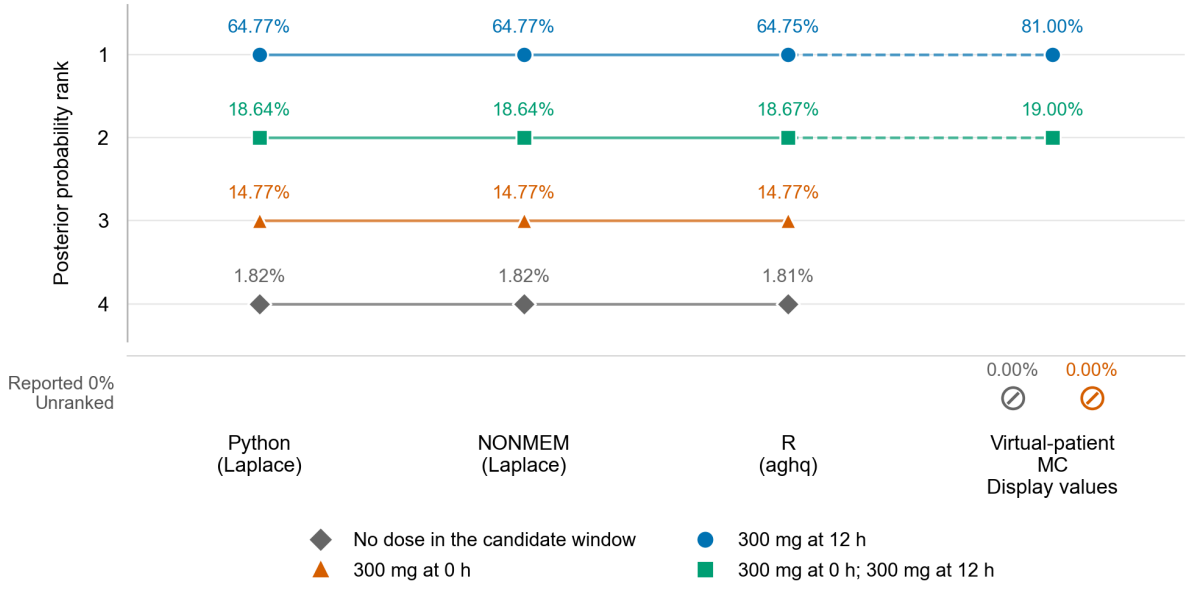
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	8.46734×10^{-9}	8.46734×10^{-9}	1.07819×10^{-8}	6.67112×10^{-9}
Python vs R aghq	2.40886×10^{-4}	2.40886×10^{-4}	2.93612×10^{-4}	3.25257×10^{-4}
NONMEM vs R aghq	2.40879×10^{-4}	2.40879×10^{-4}	2.93603×10^{-4}	3.25253×10^{-4}
Python vs Virtual patient	0.162334	0.165891	0.220252	0.295783
NONMEM vs Virtual patient	0.162334	0.165891	0.220252	0.295783
R aghq vs Virtual patient	0.162471	0.165788	0.220337	0.295708

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



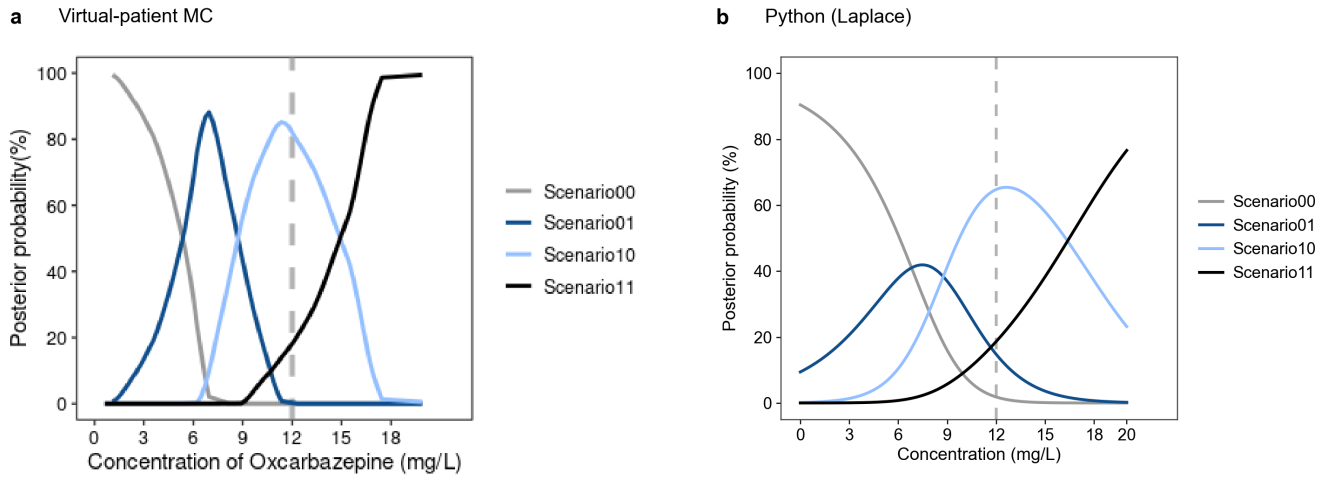
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.49	0.01819153	0.01819153	0.01809575	0
ω_{01}: 300 mg at 0 h	0.21	0.14769942	0.14769943	0.14769199	0
ω_{10}: 300 mg at 12 h	0.21	0.64766631	0.64766630	0.64752865	0.81
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.09	0.18644273	0.18644274	0.18668362	0.19

Method	P_{max}	G	H_N
Python Laplace	0.647666	0.461224	0.685182
NONMEM Laplace	0.647666	0.461224	0.685182
R aghq	0.647529	0.460845	0.685144
Virtual patient (displayed)	0.81	0.62	0.350736

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C062: Prior probabilities

Independent per-dose prior probability: 0.7.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

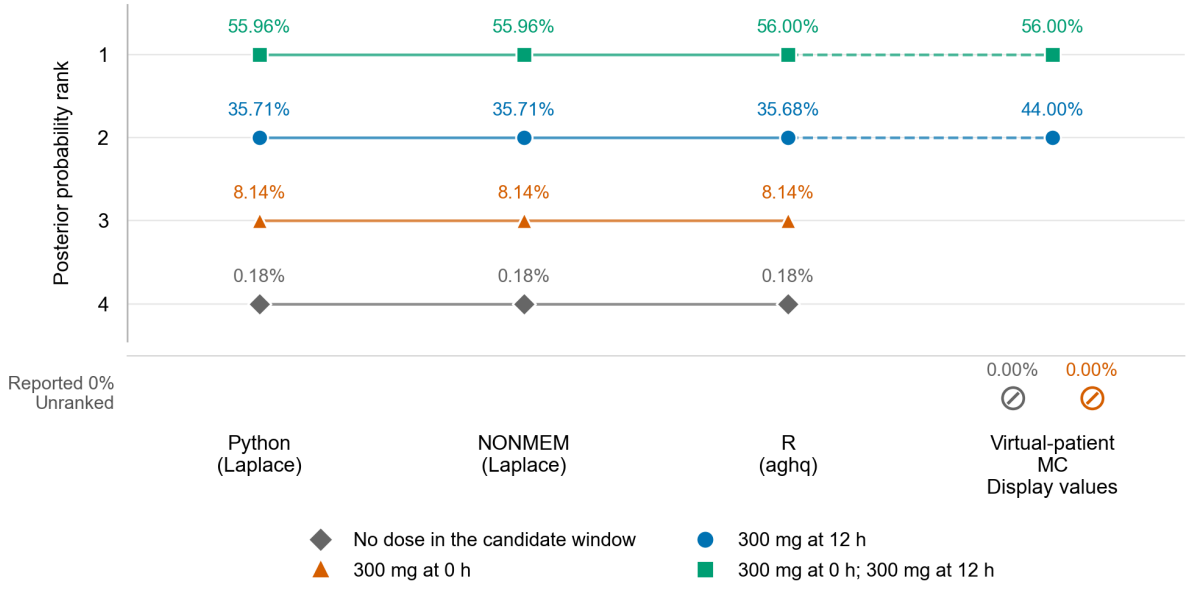
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.04549×10^{-8}	1.04549×10^{-8}	1.46317×10^{-8}	7.82026×10^{-9}
Python vs R aghq	3.68372×10^{-4}	3.68372×10^{-4}	4.79624×10^{-4}	2.73847×10^{-4}
NONMEM vs R aghq	3.68362×10^{-4}	3.68362×10^{-4}	4.79609×10^{-4}	2.73840×10^{-4}
Python vs Virtual patient	0.082920	0.083274	0.116234	0.209283
NONMEM vs Virtual patient	0.082920	0.083274	0.116234	0.209283
R aghq vs Virtual patient	0.083222	0.083222	0.116410	0.209243

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



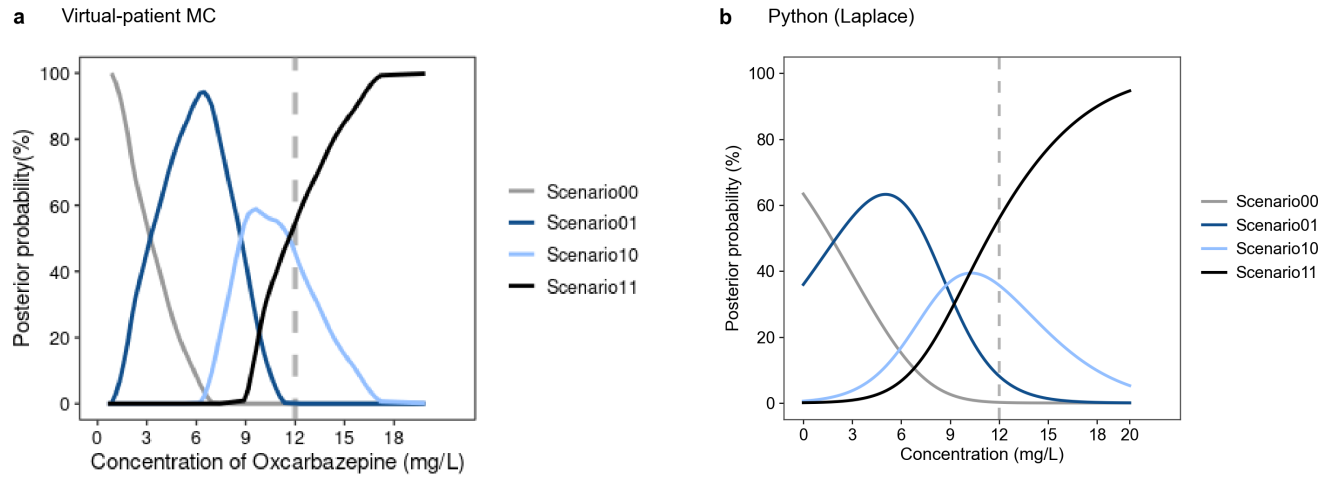
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.09	0.00184217	0.00184217	0.00183131	0
ω_{01}: 300 mg at 0 h	0.21	0.08143164	0.08143164	0.08137600	0
ω_{10}: 300 mg at 12 h	0.21	0.35708015	0.35708014	0.35677828	0.44
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.49	0.55964604	0.55964605	0.56001441	0.56

Method	P_{max}	G	H_N
Python Laplace	0.559646	0.202566	0.655269
NONMEM Laplace	0.559646	0.202566	0.655269
R aghq	0.560014	0.203236	0.655049
Virtual patient (displayed)	0.56	0.12	0.494794

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C063: Prior probabilities

Independent per-dose prior probability: 0.8.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

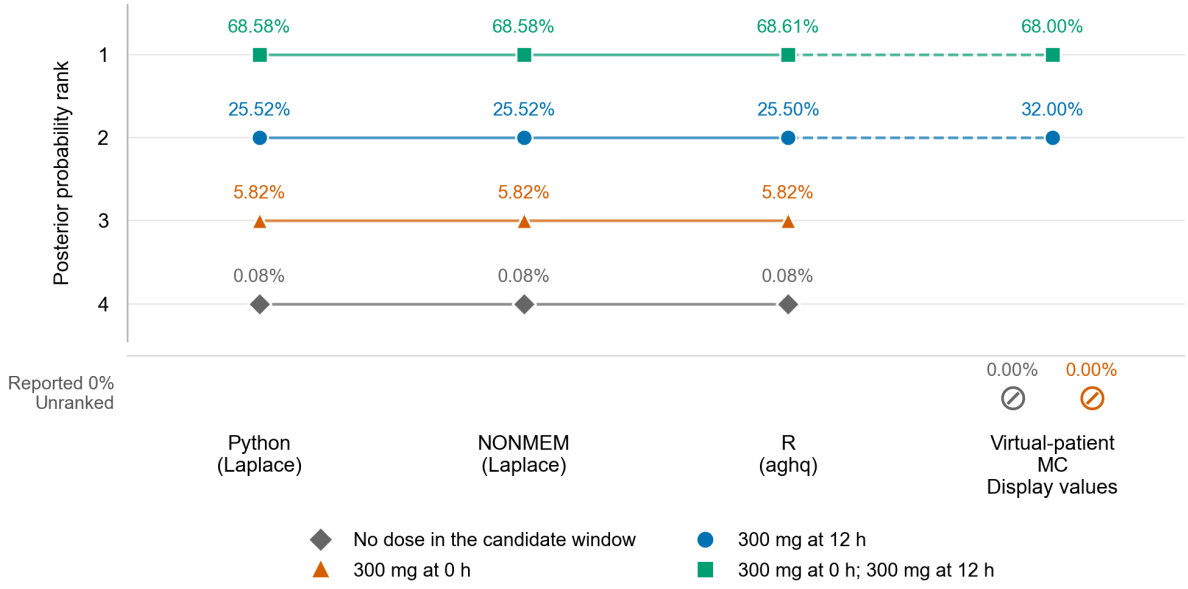
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	9.14780×10^{-9}	9.14780×10^{-9}	1.26181×10^{-8}	7.25324×10^{-9}
Python vs R aghq	3.20135×10^{-4}	3.20135×10^{-4}	4.18440×10^{-4}	2.49206×10^{-4}
NONMEM vs R aghq	3.20126×10^{-4}	3.20126×10^{-4}	4.18427×10^{-4}	2.49199×10^{-4}
Python vs Virtual patient	0.064757	0.064757	0.087267	0.176981
NONMEM vs Virtual patient	0.064757	0.064757	0.087267	0.176981
R aghq vs Virtual patient	0.065021	0.065021	0.087452	0.176950

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



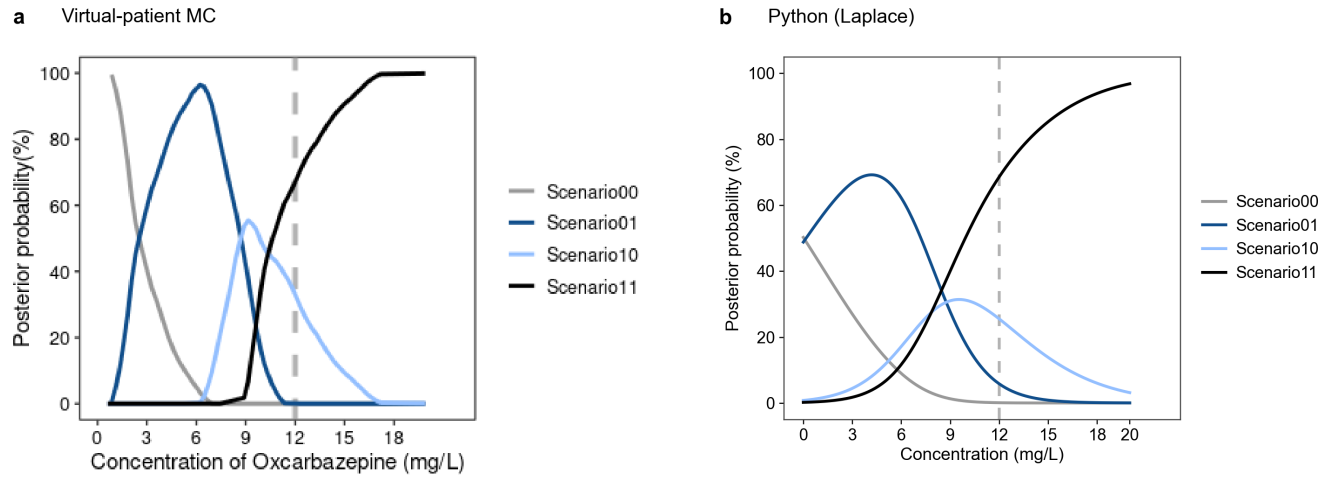
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.04	0.00076813	0.00076813	0.00076346	0
ω_{01}: 300 mg at 0 h	0.16	0.05820788	0.05820788	0.05815699	0
ω_{10}: 300 mg at 12 h	0.16	0.25524329	0.25524328	0.25497872	0.32
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.64	0.68578070	0.68578071	0.68610083	0.68

Method	P_{max}	G	H_N
Python Laplace	0.685781	0.430537	0.561393
NONMEM Laplace	0.685781	0.430537	0.561393
R aghq	0.686101	0.431122	0.561090
Virtual patient (displayed)	0.68	0.36	0.452191

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C064: Prior probabilities

Independent per-dose prior probability: 0.9.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

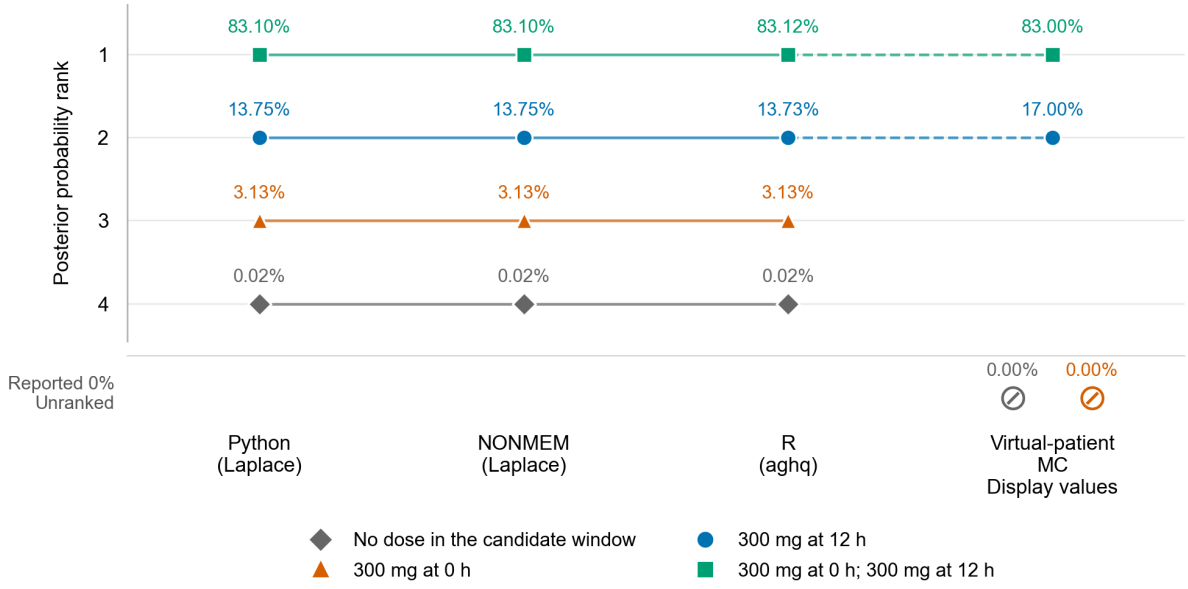
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	5.96498×10^{-9}	5.96498×10^{-9}	8.13987×10^{-9}	5.81827×10^{-9}
Python vs R aghq	2.07626×10^{-4}	2.07626×10^{-4}	2.71946×10^{-4}	1.97655×10^{-4}
NONMEM vs R aghq	2.07620×10^{-4}	2.07620×10^{-4}	2.71938×10^{-4}	1.97649×10^{-4}
Python vs Virtual patient	0.032536	0.032536	0.045192	0.128955
NONMEM vs Virtual patient	0.032536	0.032536	0.045192	0.128955
R aghq vs Virtual patient	0.032708	0.032708	0.045298	0.128925

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



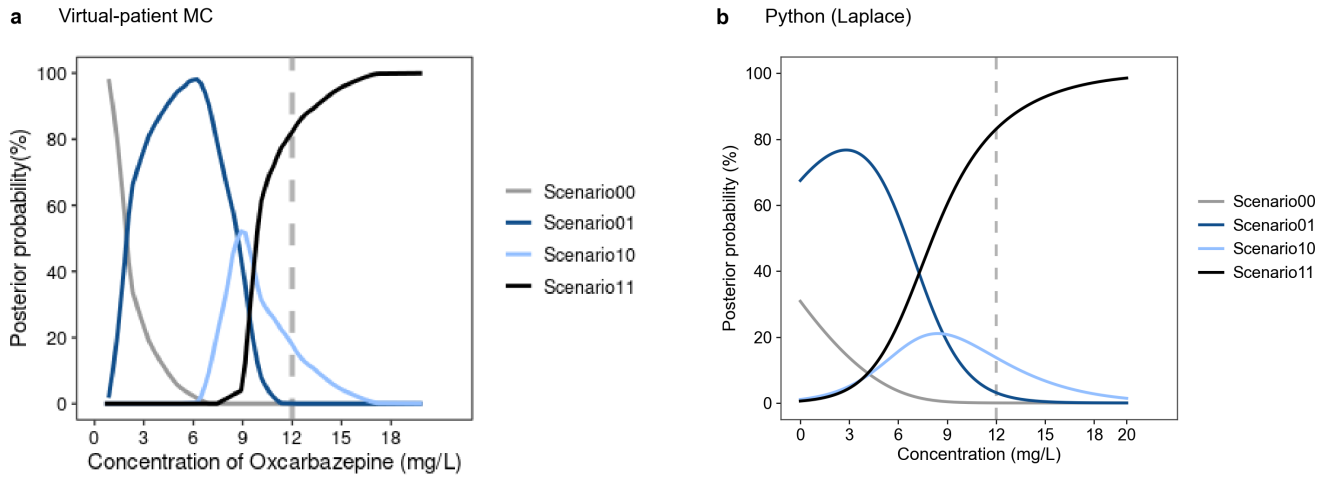
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: No dose in the candidate window	0.01	0.00018386	0.00018386	0.00018270	0
ω_{01}: 300 mg at 0 h	0.09	0.03134851	0.03134851	0.03131430	0
ω_{10}: 300 mg at 12 h	0.09	0.13746413	0.13746413	0.13729187	0.17
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.81	0.83100350	0.83100350	0.83121112	0.83

Method	P_{max}	G	H_N
Python Laplace	0.831003	0.693539	0.387182
NONMEM Laplace	0.831004	0.693539	0.387182
R aghq	0.831211	0.693919	0.386870
Virtual patient (displayed)	0.83	0.66	0.328852

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C065: Candidate states

Remove state omega_00.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	3
NONMEM Laplace	5/5	3
R aghq	5/5	3

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

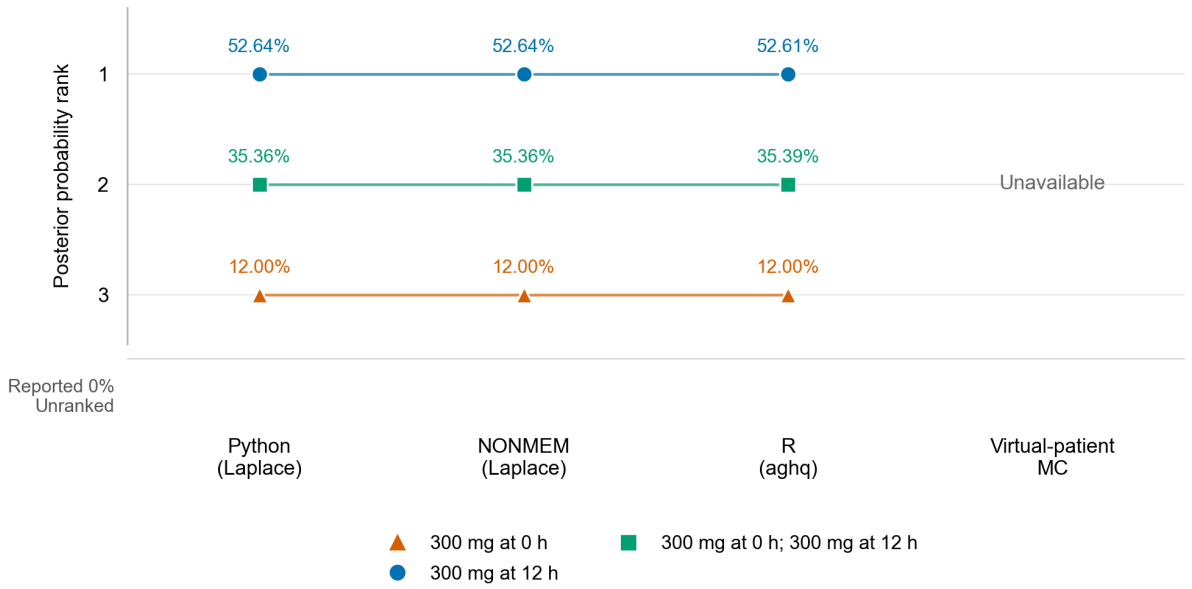
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.04611×10^{-8}	1.04611×10^{-8}	1.42940×10^{-8}	7.74070×10^{-9}
Python vs R aghq	3.36882×10^{-4}	3.36882×10^{-4}	4.47071×10^{-4}	2.49753×10^{-4}
NONMEM vs R aghq	3.36873×10^{-4}	3.36873×10^{-4}	4.47057×10^{-4}	2.49745×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{01}: 300 mg at 0 h	0.3333333333	0.12004191	0.12004191	0.11999521
ω_{10}: 300 mg at 12 h	0.3333333333	0.52638732	0.52638731	0.52609714
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.3333333333	0.35357077	0.35357078	0.35390765

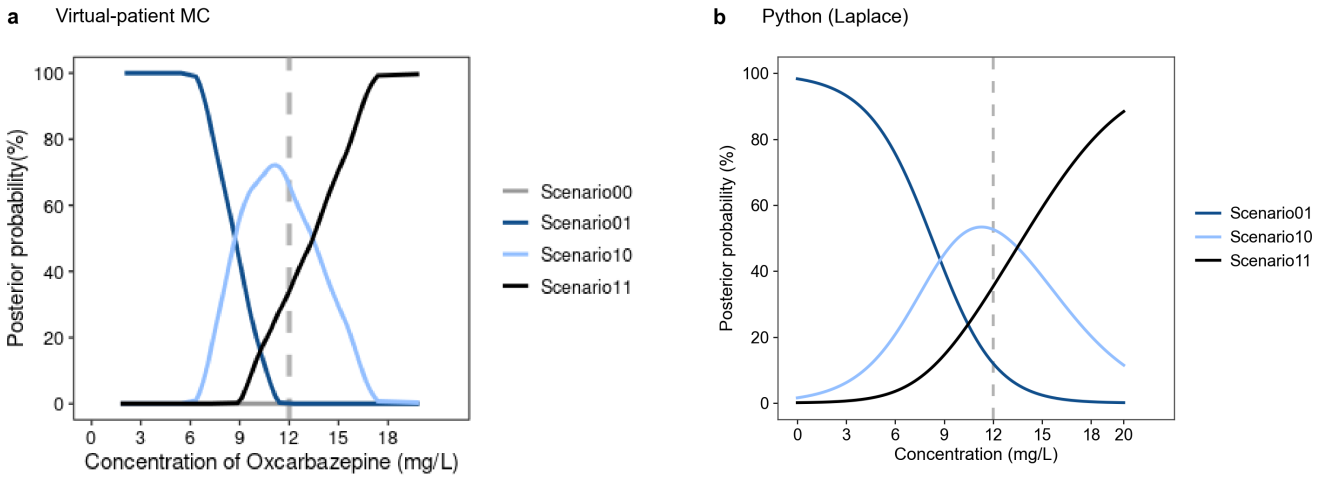
Method	P_{max}	G	H_N
Python Laplace	0.526387	0.172817	0.873710
NONMEM Laplace	0.526387	0.172817	0.873710
R aghq	0.526097	0.172189	0.873769

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

External web output

Four web states cannot be aligned to the three-state candidate set; the web output is excluded from comparisons.

Web state	Candidate dosing history	Reported probability (%)
Scenario00	No dose in the candidate window	0.00
Scenario01	300 mg at 0 h	0.00
Scenario10	300 mg at 12 h	65.00
Scenario11	300 mg at 0 h; 300 mg at 12 h	35.00



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C066: Candidate states

Remove state omega_01.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	3
NONMEM Laplace	5/5	3
R aghq	5/5	3

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

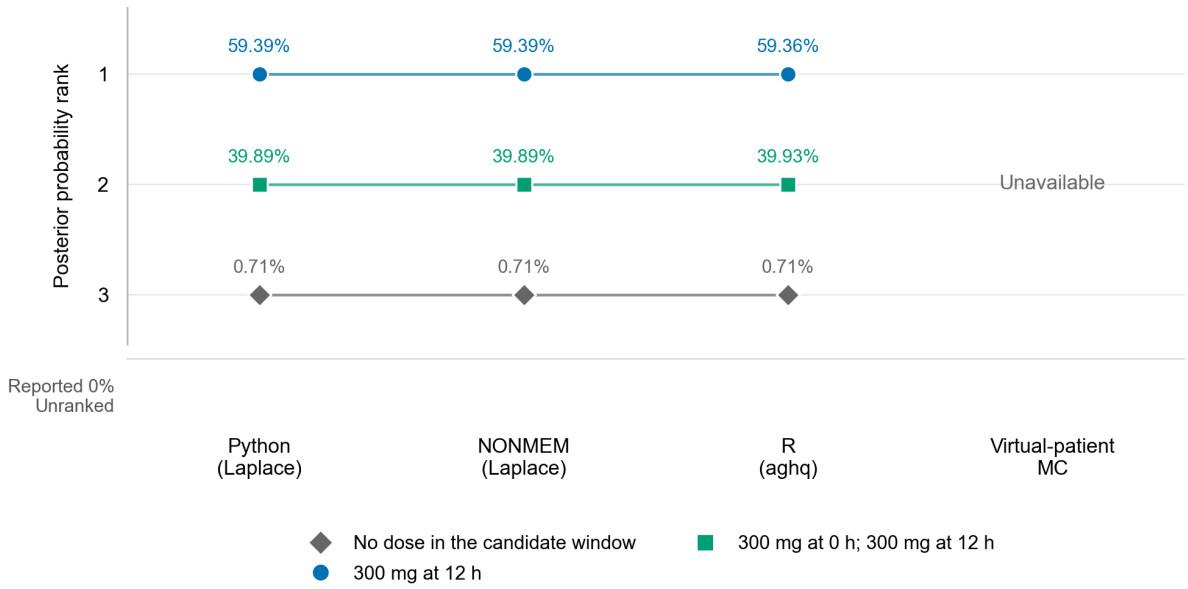
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.13079×10^{-8}	1.13079×10^{-8}	1.59797×10^{-8}	8.17689×10^{-9}
Python vs R aghq	3.75052×10^{-4}	3.75052×10^{-4}	5.04420×10^{-4}	3.09713×10^{-4}
NONMEM vs R aghq	3.75041×10^{-4}	3.75041×10^{-4}	5.04404×10^{-4}	3.09706×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.3333333333	0.00714938	0.00714938	0.00710924
ω_{10}: 300 mg at 12 h	0.3333333333	0.59391917	0.59391915	0.59358426
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.3333333333	0.39893145	0.39893146	0.39930650

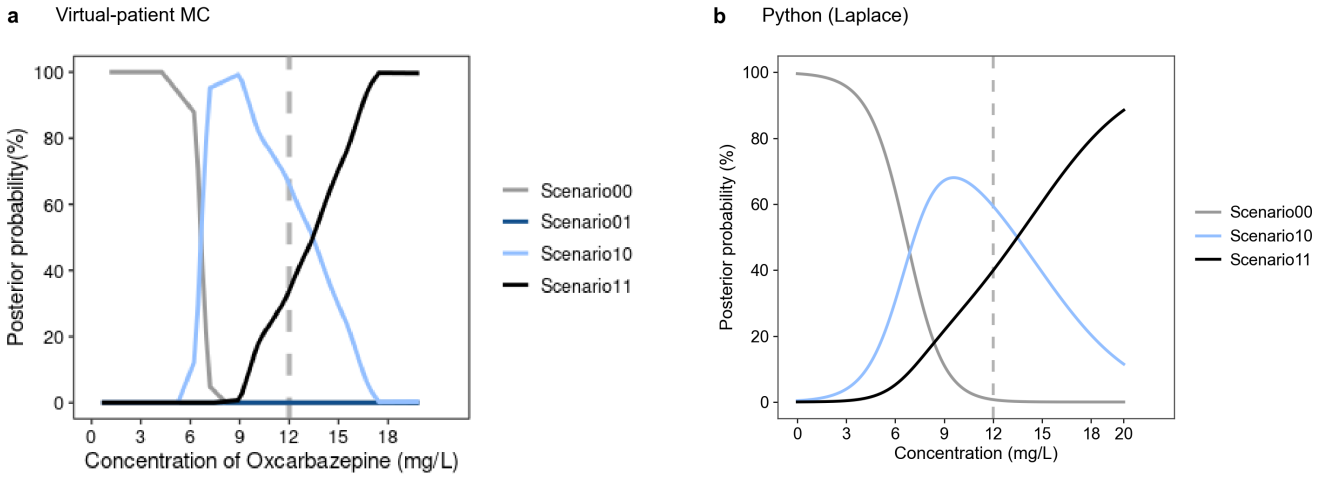
Method	P_{max}	G	H_N
Python Laplace	0.593919	0.194988	0.647514
NONMEM Laplace	0.593919	0.194988	0.647514
R aghq	0.593584	0.194278	0.647488

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

External web output

Four web states cannot be aligned to the three-state candidate set; the web output is excluded from comparisons.

Web state	Candidate dosing history	Reported probability (%)
Scenario00	No dose in the candidate window	0.00
Scenario01	300 mg at 0 h	0.00
Scenario10	300 mg at 12 h	65.00
Scenario11	300 mg at 0 h; 300 mg at 12 h	35.00



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C067: Candidate states

Remove state omega_10.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	3
NONMEM Laplace	5/5	3
R aghq	5/5	3

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

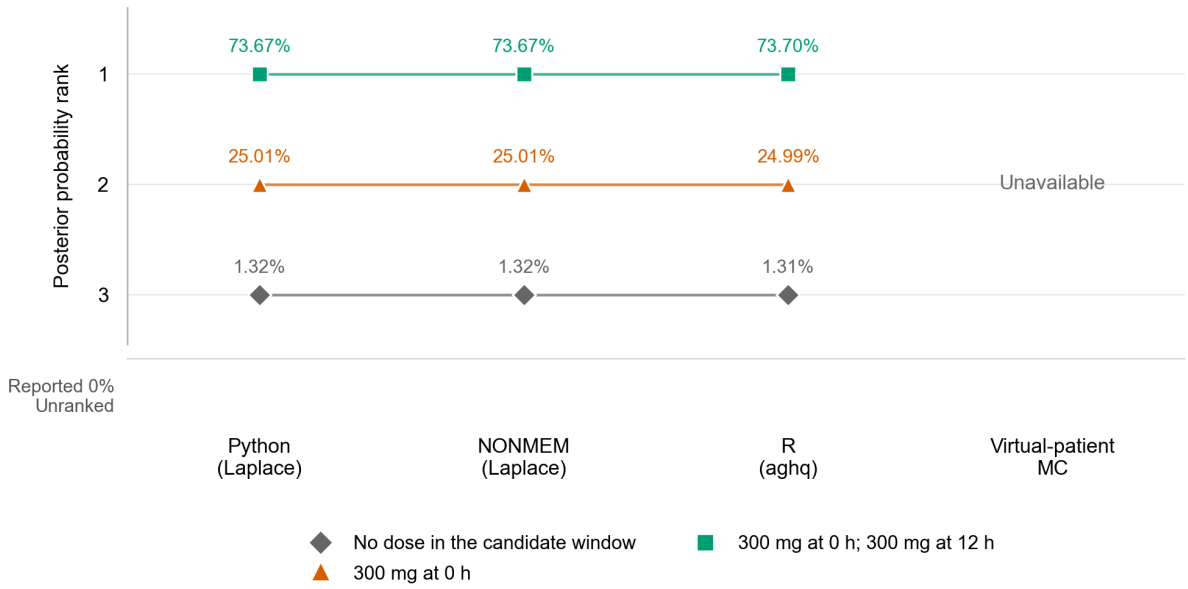
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	4.16331×10^{-9}	4.16331×10^{-9}	5.70820×10^{-9}	3.34716×10^{-9}
Python vs R aghq	3.10841×10^{-4}	3.10841×10^{-4}	3.95008×10^{-4}	3.24067×10^{-4}
NONMEM vs R aghq	3.10837×10^{-4}	3.10837×10^{-4}	3.95003×10^{-4}	3.24064×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.3333333333	0.01320235	0.01320235	0.01312143
ω_{01}: 300 mg at 0 h	0.3333333333	0.25011382	0.25011382	0.24988391
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.3333333333	0.73668383	0.73668383	0.73699467

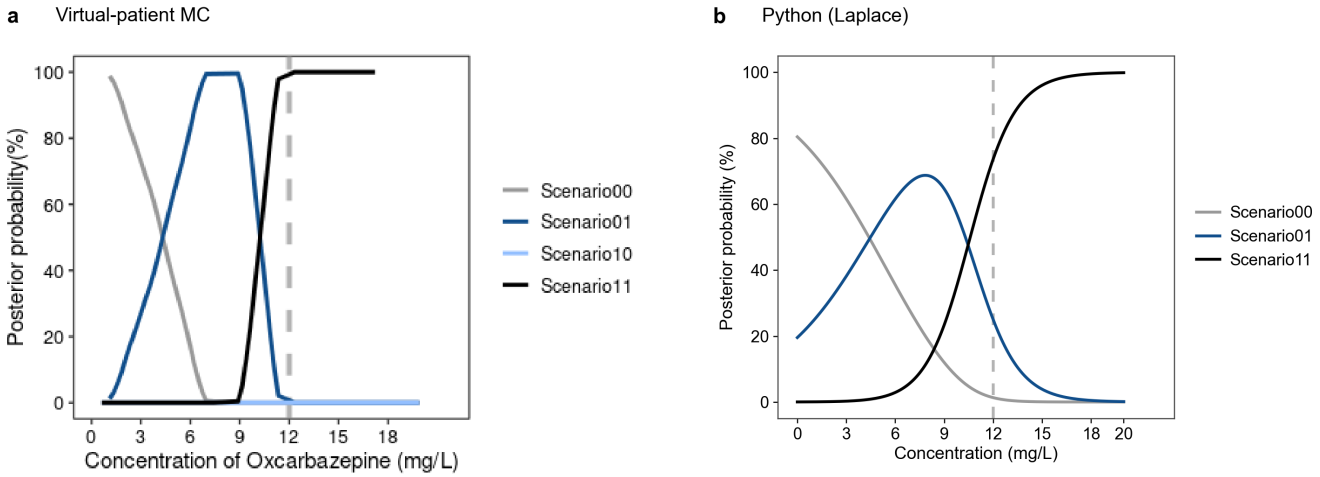
Method	P_{max}	G	H_N
Python Laplace	0.736684	0.486570	0.572428
NONMEM Laplace	0.736684	0.486570	0.572428
R aghq	0.736995	0.487111	0.571906

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

External web output

Four web states cannot be aligned to the three-state candidate set; the web output is excluded from comparisons.

Web state	Candidate dosing history	Reported probability (%)
Scenario00	No dose in the candidate window	0.00
Scenario01	300 mg at 0 h	0.00
Scenario10	300 mg at 12 h	0.00
Scenario11	300 mg at 0 h; 300 mg at 12 h	100.00



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C068: Candidate states

Remove state omega_11.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	3
NONMEM Laplace	5/5	3
R aghq	5/5	3

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

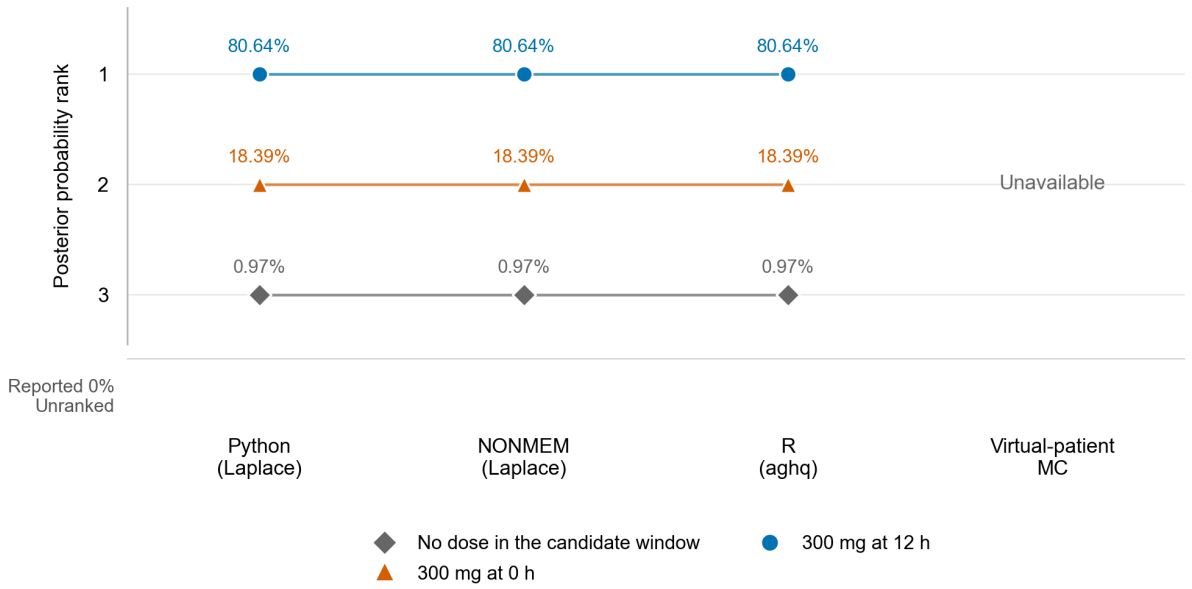
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	4.04034×10^{-9}	4.04034×10^{-9}	5.60450×10^{-9}	3.61875×10^{-9}
Python vs R aghq	4.88726×10^{-5}	4.88726×10^{-5}	6.11761×10^{-5}	1.77847×10^{-4}
NONMEM vs R aghq	4.88728×10^{-5}	4.88728×10^{-5}	6.11752×10^{-5}	1.77847×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.3333333333	0.00970709	0.00970709	0.00965822
ω_{01}: 300 mg at 0 h	0.3333333333	0.18389740	0.18389740	0.18393077
ω_{10}: 300 mg at 12 h	0.3333333333	0.80639551	0.80639550	0.80641101

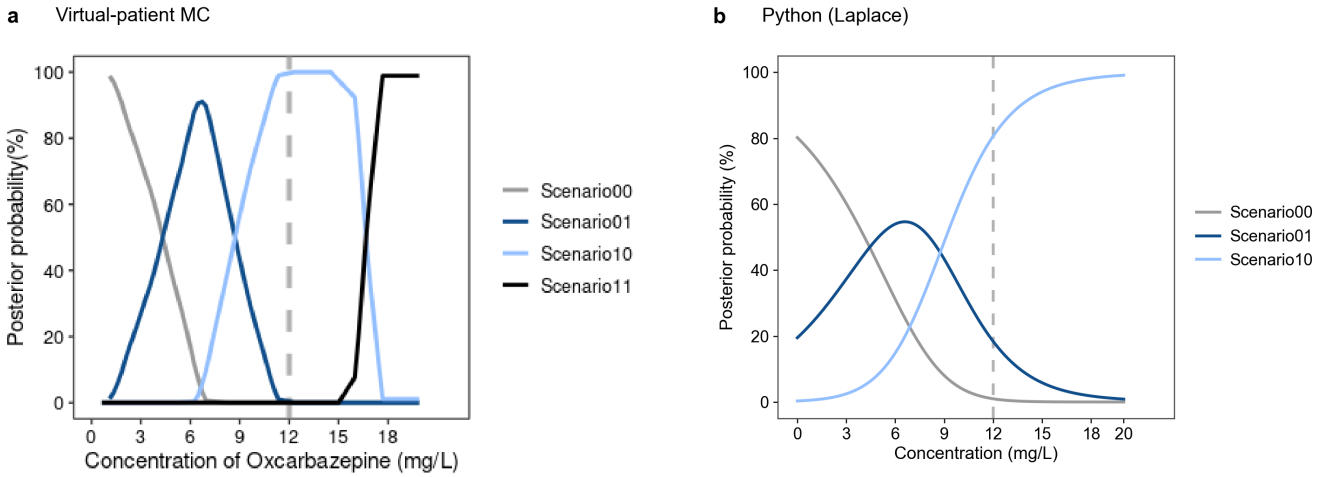
Method	P_{max}	G	H_N
Python Laplace	0.806396	0.622498	0.482354
NONMEM Laplace	0.806396	0.622498	0.482354
R aghq	0.806411	0.622480	0.482202

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

External web output

Four web states cannot be aligned to the three-state candidate set; the web output is excluded from comparisons.

Web state	Candidate dosing history	Reported probability (%)
Scenario00	No dose in the candidate window	0.00
Scenario01	300 mg at 0 h	0.00
Scenario10	300 mg at 12 h	100.00
Scenario11	300 mg at 0 h; 300 mg at 12 h	0.00



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

OXC C069: Candidate states

Add one candidate history.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	5
NONMEM Laplace	5/5	5
R aghq	5/5	5

Repeatability

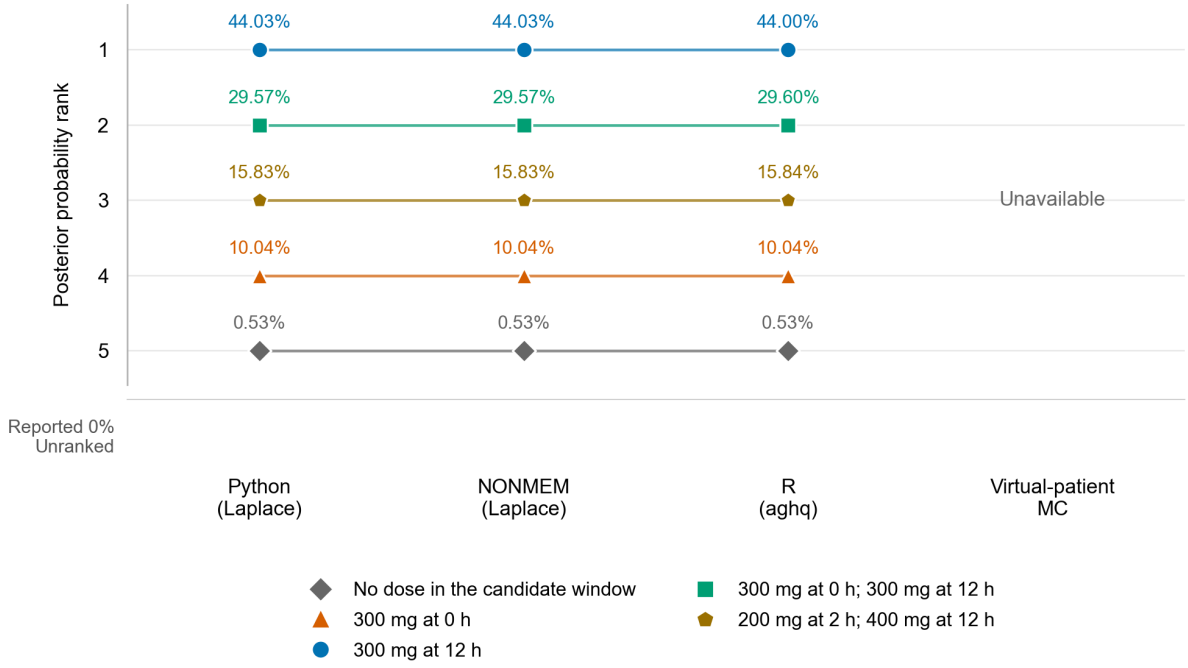
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	5.09817×10^{-9}	5.09817×10^{-9}	6.10706×10^{-9}	3.87092×10^{-9}
Python vs R aghq	2.87429×10^{-4}	3.66925×10^{-4}	4.03218×10^{-4}	2.92139×10^{-4}
NONMEM vs R aghq	2.87424×10^{-4}	3.66921×10^{-4}	4.03213×10^{-4}	2.92137×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.2	0.00529999	0.00530000	0.00526977
ω_{01}: 300 mg at 0 h	0.2	0.10040649	0.10040650	0.10035723
ω_{10}: 300 mg at 12 h	0.2	0.44028543	0.44028542	0.43999800
ω_{11}: 300 mg at 0 h; 300 mg at 12 h	0.2	0.29573672	0.29573672	0.29598841
omega_add: 200 mg at 2 h; 400 mg at 12 h	0.2	0.15827136	0.15827136	0.15838659

Method	P_{max}	G	H_N
Python Laplace	0.440285	0.144549	0.790211
NONMEM Laplace	0.440285	0.144549	0.790211
R aghq	0.439998	0.144010	0.790218

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C070: Candidate states

Candidate dose events: 150 mg at 0 h; 300 mg at 12 h.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

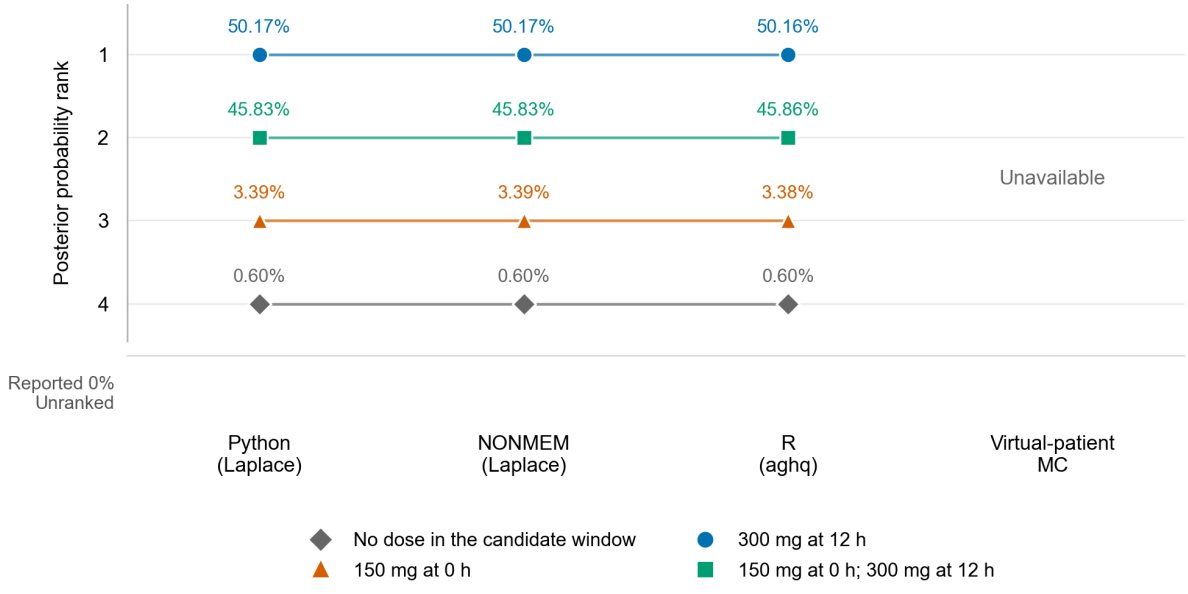
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	6.78122×10^{-9}	6.78122×10^{-9}	9.24659×10^{-9}	4.79765×10^{-9}
Python vs R aghq	2.49652×10^{-4}	2.49652×10^{-4}	2.97818×10^{-4}	2.58190×10^{-4}
NONMEM vs R aghq	2.49645×10^{-4}	2.49645×10^{-4}	2.97810×10^{-4}	2.58188×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00603987	0.00603987	0.00600770
ω_{01}: 150 mg at 0 h	0.25	0.03389037	0.03389037	0.03381067
ω_{10}: 300 mg at 12 h	0.25	0.50174905	0.50174904	0.50161127
ω_{11}: 150 mg at 0 h; 300 mg at 12 h	0.25	0.45832071	0.45832071	0.45857036

Method	P_{max}	G	H_N
Python Laplace	0.501749	0.043428	0.612551
NONMEM Laplace	0.501749	0.043428	0.612551
R aghq	0.501611	0.043041	0.612309

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C071: Candidate states

Candidate dose events: 600 mg at 0 h; 300 mg at 12 h.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

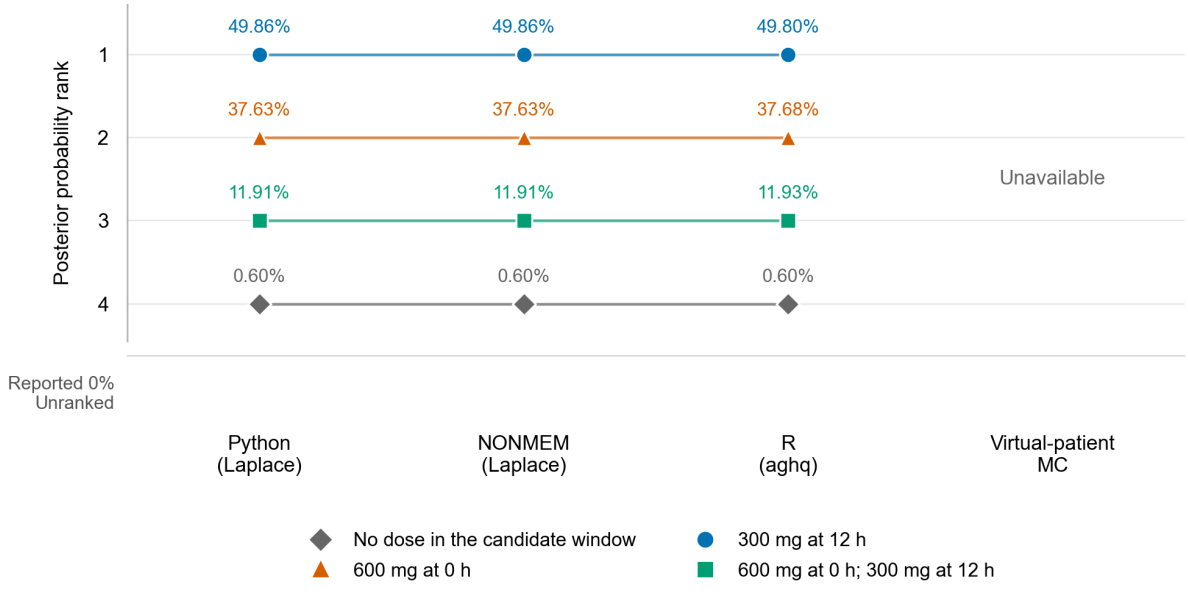
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	6.54008×10^{-9}	6.54008×10^{-9}	8.69086×10^{-9}	4.70601×10^{-9}
Python vs R aghq	6.13514×10^{-4}	6.51195×10^{-4}	8.05514×10^{-4}	4.80649×10^{-4}
NONMEM vs R aghq	6.13508×10^{-4}	6.51188×10^{-4}	8.05505×10^{-4}	4.80645×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00600185	0.00600185	0.00596417
ω_{01}: 600 mg at 0 h	0.25	0.37631087	0.37631087	0.37680823
ω_{10}: 300 mg at 12 h	0.25	0.49859038	0.49859037	0.49797687
ω_{11}: 600 mg at 0 h; 300 mg at 12 h	0.25	0.11909690	0.11909690	0.11925074

Method	P_{max}	G	H_N
Python Laplace	0.498590	0.122280	0.720560
NONMEM Laplace	0.498590	0.122280	0.720560
R aghq	0.497977	0.121169	0.720699

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C072: Candidate states

Candidate dose events: 300 mg at 0 h; 150 mg at 12 h.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

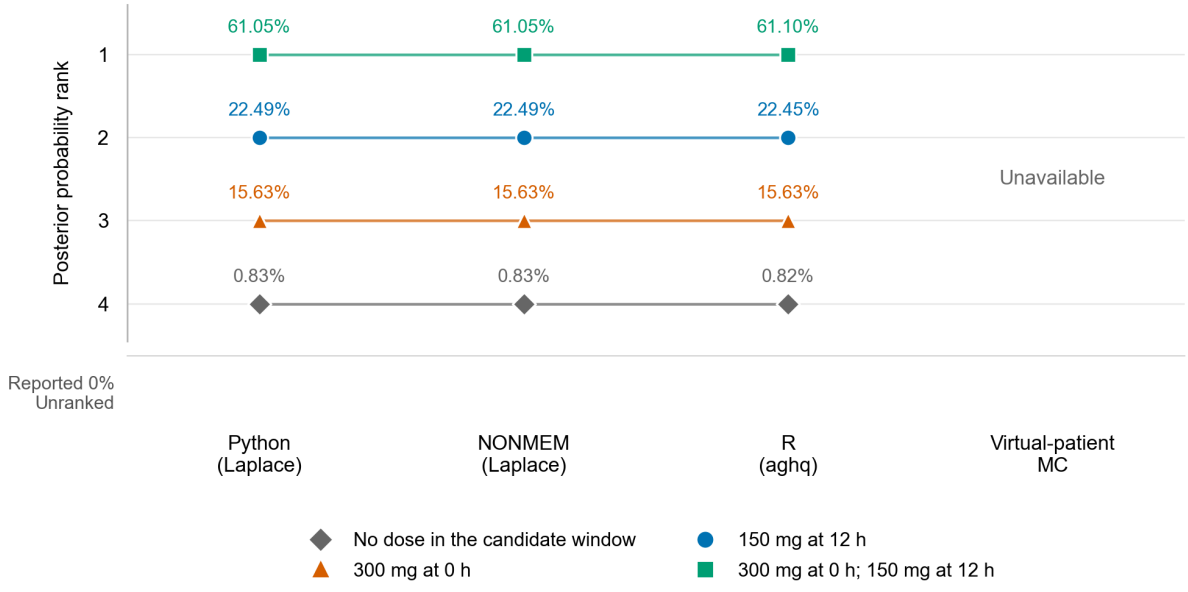
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.16374×10^{-9}	1.16374×10^{-9}	1.46397×10^{-9}	8.79282×10^{-10}
Python vs R aghq	4.63774×10^{-4}	4.63774×10^{-4}	6.14741×10^{-4}	4.03802×10^{-4}
NONMEM vs R aghq	4.63773×10^{-4}	4.63773×10^{-4}	6.14740×10^{-4}	4.03801×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00825070	0.00825070	0.00820666
ω_{01}: 300 mg at 0 h	0.25	0.15630645	0.15630645	0.15628735
ω_{10}: 150 mg at 12 h	0.25	0.22490733	0.22490733	0.22450669
ω_{11}: 300 mg at 0 h; 150 mg at 12 h	0.25	0.61053552	0.61053552	0.61099929

Method	P_{max}	G	H_N
Python Laplace	0.610536	0.385628	0.697185
NONMEM Laplace	0.610536	0.385628	0.697185
R aghq	0.610999	0.386493	0.696741

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C073: Candidate states

Candidate dose events: 300 mg at 0 h; 600 mg at 12 h.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

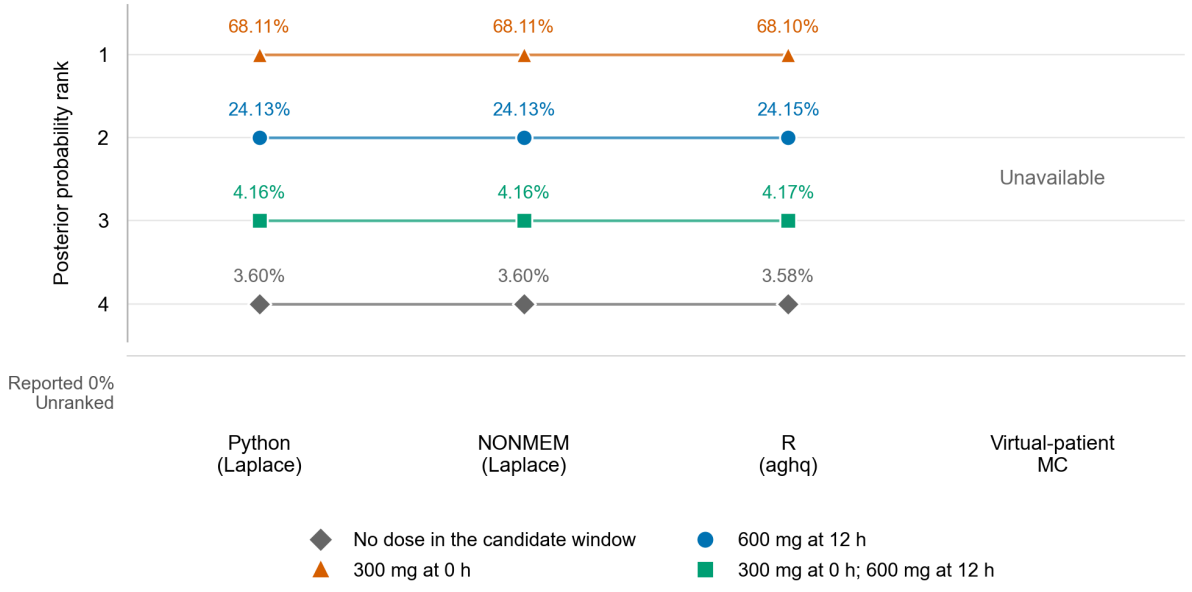
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	5.69961×10^{-9}	5.69961×10^{-9}	7.61764×10^{-9}	4.72138×10^{-9}
Python vs R aghq	2.13409×10^{-4}	2.85525×10^{-4}	3.10537×10^{-4}	4.12088×10^{-4}
NONMEM vs R aghq	2.13404×10^{-4}	2.85520×10^{-4}	3.10531×10^{-4}	4.12085×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.03595265	0.03595265	0.03576026
ω_{01}: 300 mg at 0 h	0.25	0.68111006	0.68111005	0.68101693
ω_{10}: 600 mg at 12 h	0.25	0.24131090	0.24131090	0.24152431
ω_{11}: 300 mg at 0 h; 600 mg at 12 h	0.25	0.04162639	0.04162639	0.04169850

Method	P_{max}	G	H_N
Python Laplace	0.681110	0.439799	0.617853
NONMEM Laplace	0.681110	0.439799	0.617853
R aghq	0.681017	0.439493	0.617749

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C074: Candidate states

Candidate dose events: 300 mg at -4 h; 300 mg at 12 h.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

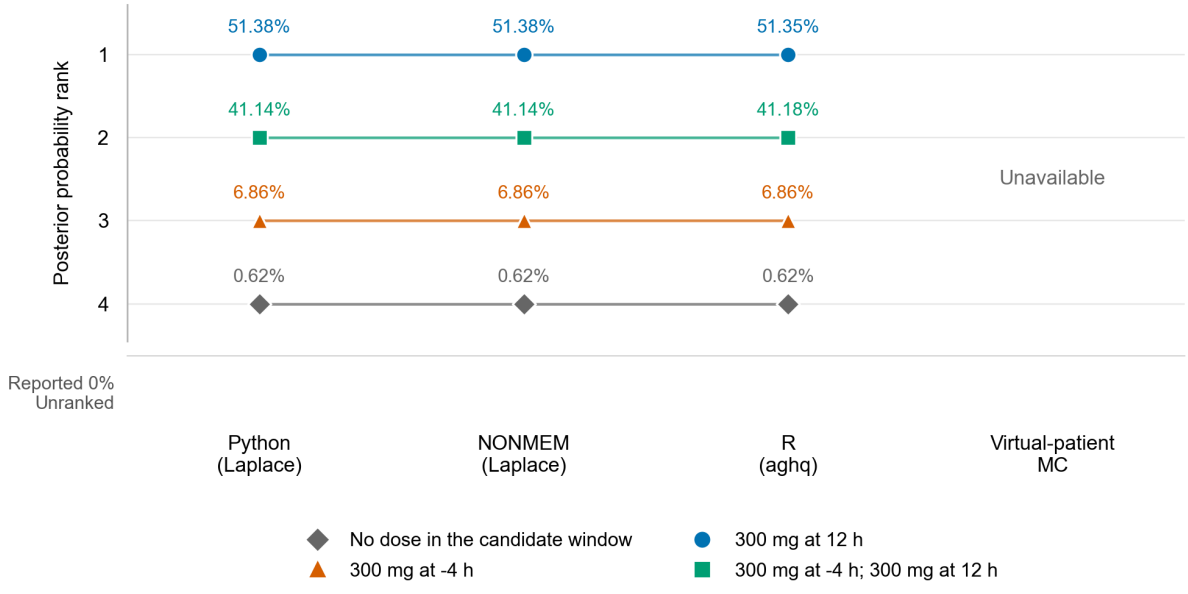
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.48270×10^{-9}	1.52513×10^{-9}	1.98107×10^{-9}	1.09972×10^{-9}
Python vs R aghq	3.50816×10^{-4}	3.50816×10^{-4}	4.45504×10^{-4}	2.88428×10^{-4}
NONMEM vs R aghq	3.50815×10^{-4}	3.50815×10^{-4}	4.45502×10^{-4}	2.88427×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00618501	0.00618501	0.00615054
ω_{01}: 300 mg at -4 h	0.25	0.06860421	0.06860421	0.06855598
ω_{10}: 300 mg at 12 h	0.25	0.51380590	0.51380590	0.51353778
ω_{11}: 300 mg at -4 h; 300 mg at 12 h	0.25	0.41140488	0.41140488	0.41175570

Method	P_{max}	G	H_N
Python Laplace	0.513806	0.102401	0.665675
NONMEM Laplace	0.513806	0.102401	0.665675
R aghq	0.513538	0.101782	0.665551

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C075: Candidate states

Candidate dose events: 300 mg at -2 h; 300 mg at 12 h.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

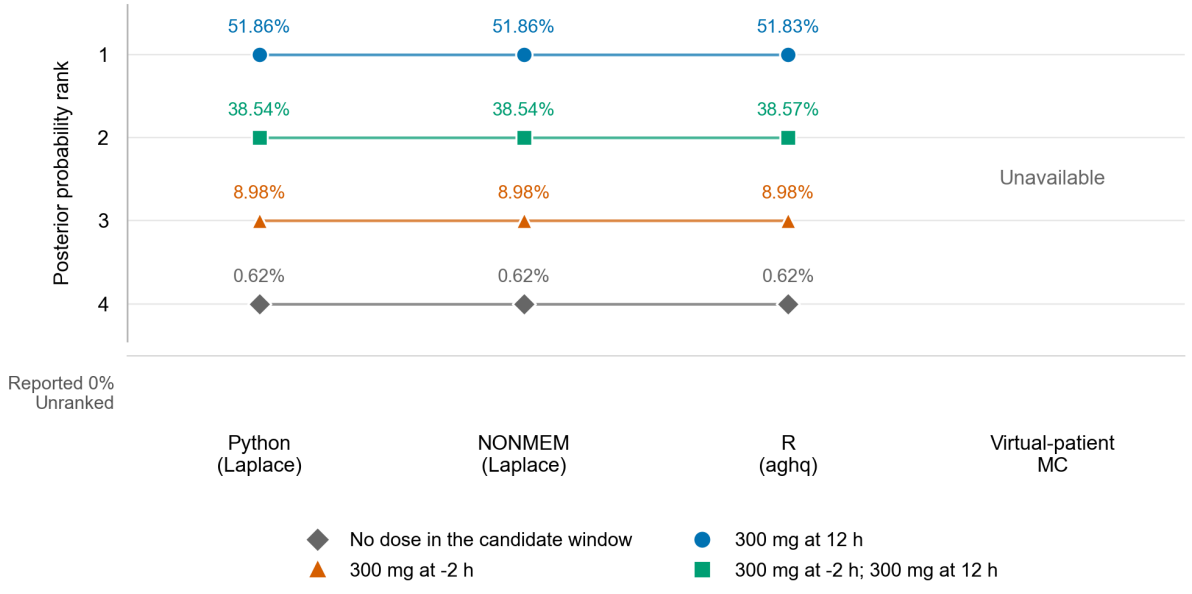
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.44039×10^{-9}	1.45777×10^{-9}	1.84740×10^{-9}	1.79633×10^{-9}
Python vs R aghq	3.55208×10^{-4}	3.55208×10^{-4}	4.52764×10^{-4}	2.93902×10^{-4}
NONMEM vs R aghq	3.55208×10^{-4}	3.55208×10^{-4}	4.52764×10^{-4}	2.93902×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00624232	0.00624232	0.00620748
ω_{01}: 300 mg at -2 h	0.25	0.08981178	0.08981178	0.08976625
ω_{10}: 300 mg at 12 h	0.25	0.51856726	0.51856726	0.51829243
ω_{11}: 300 mg at -2 h; 300 mg at 12 h	0.25	0.38537863	0.38537863	0.38573384

Method	P_{max}	G	H_N
Python Laplace	0.518567	0.133189	0.689712
NONMEM Laplace	0.518567	0.133189	0.689712
R aghq	0.518292	0.132559	0.689619

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C076: Candidate states

Candidate dose events: 300 mg at 2 h; 300 mg at 12 h.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

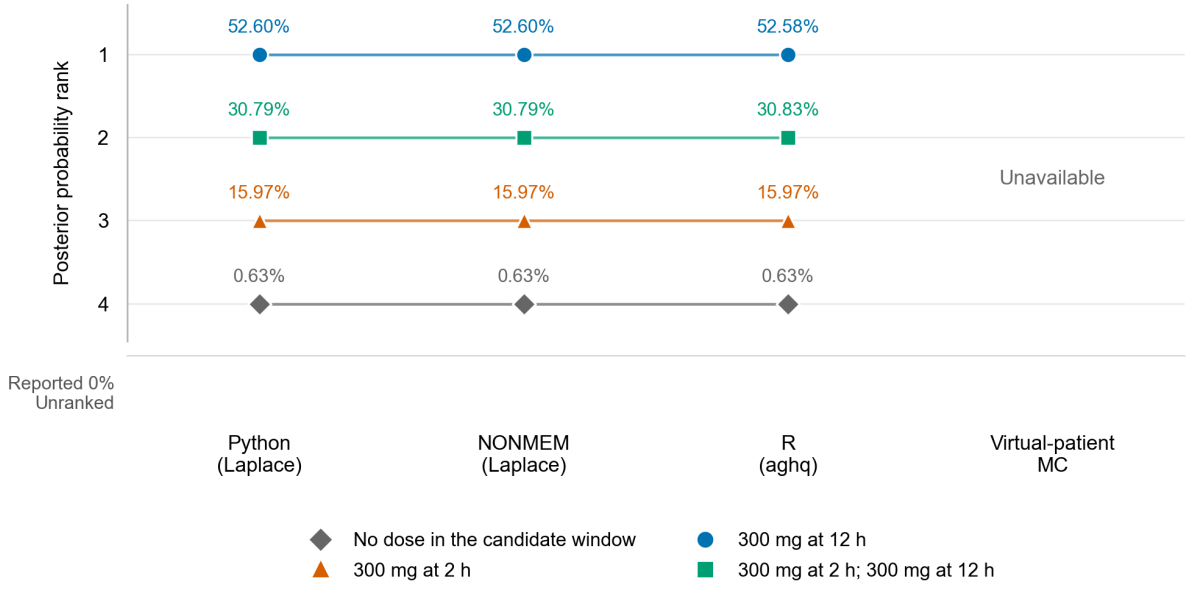
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	3.53145×10^{-9}	3.57167×10^{-9}	4.93665×10^{-9}	2.79838×10^{-9}
Python vs R aghq	3.23788×10^{-4}	3.23788×10^{-4}	4.12885×10^{-4}	2.87892×10^{-4}
NONMEM vs R aghq	3.23792×10^{-4}	3.23792×10^{-4}	4.12890×10^{-4}	2.87894×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00633187	0.00633187	0.00629687
ω_{01}: 300 mg at 2 h	0.25	0.15971586	0.15971586	0.15967804
ω_{10}: 300 mg at 12 h	0.25	0.52600634	0.52600635	0.52575539
ω_{11}: 300 mg at 2 h; 300 mg at 12 h	0.25	0.30794592	0.30794592	0.30826971

Method	P_{max}	G	H_N
Python Laplace	0.526006	0.218060	0.739862
NONMEM Laplace	0.526006	0.218060	0.739862
R aghq	0.525755	0.217486	0.739842

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C077: Candidate states

Candidate dose events: 300 mg at 4 h; 300 mg at 12 h.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

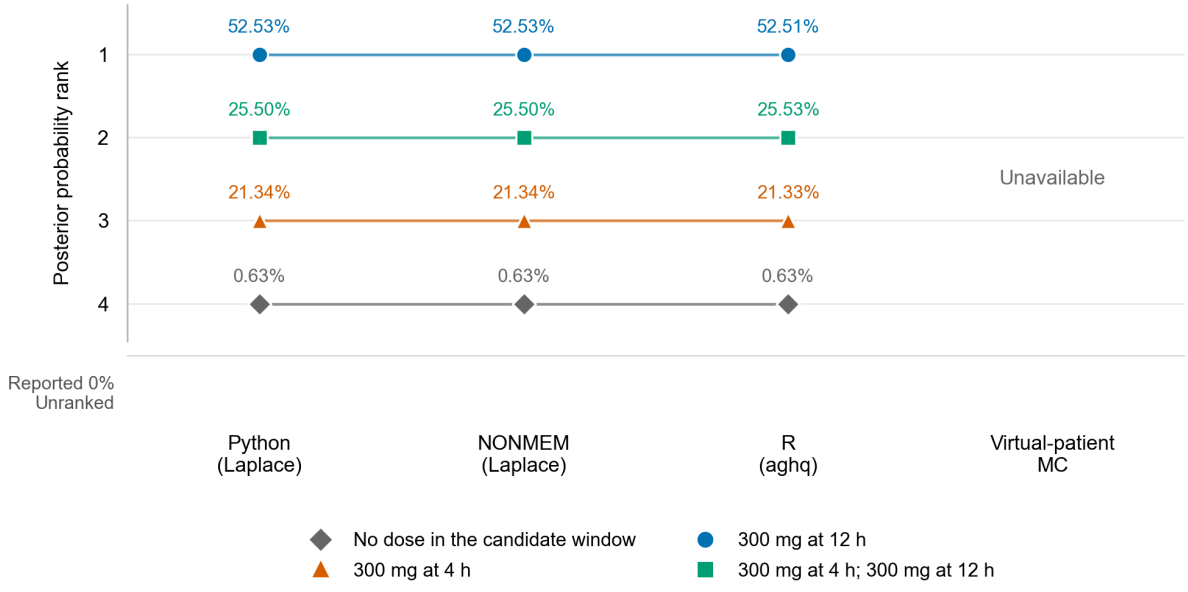
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	3.41154×10^{-9}	3.41154×10^{-9}	4.16632×10^{-9}	2.90682×10^{-9}
Python vs R aghq	2.83044×10^{-4}	2.83044×10^{-4}	3.59570×10^{-4}	2.73296×10^{-4}
NONMEM vs R aghq	2.83047×10^{-4}	2.83047×10^{-4}	3.59573×10^{-4}	2.73298×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00632359	0.00632359	0.00628904
ω_{01}: 300 mg at 4 h	0.25	0.21338103	0.21338103	0.21334927
ω_{10}: 300 mg at 12 h	0.25	0.52531840	0.52531841	0.52510167
ω_{11}: 300 mg at 4 h; 300 mg at 12 h	0.25	0.25497698	0.25497698	0.25526002

Method	P_{max}	G	H_N
Python Laplace	0.525318	0.270341	0.756149
NONMEM Laplace	0.525318	0.270341	0.756149
R aghq	0.525102	0.269842	0.756165

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C078: Candidate states

Candidate dose events: 300 mg at 0 h; 300 mg at 8 h.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

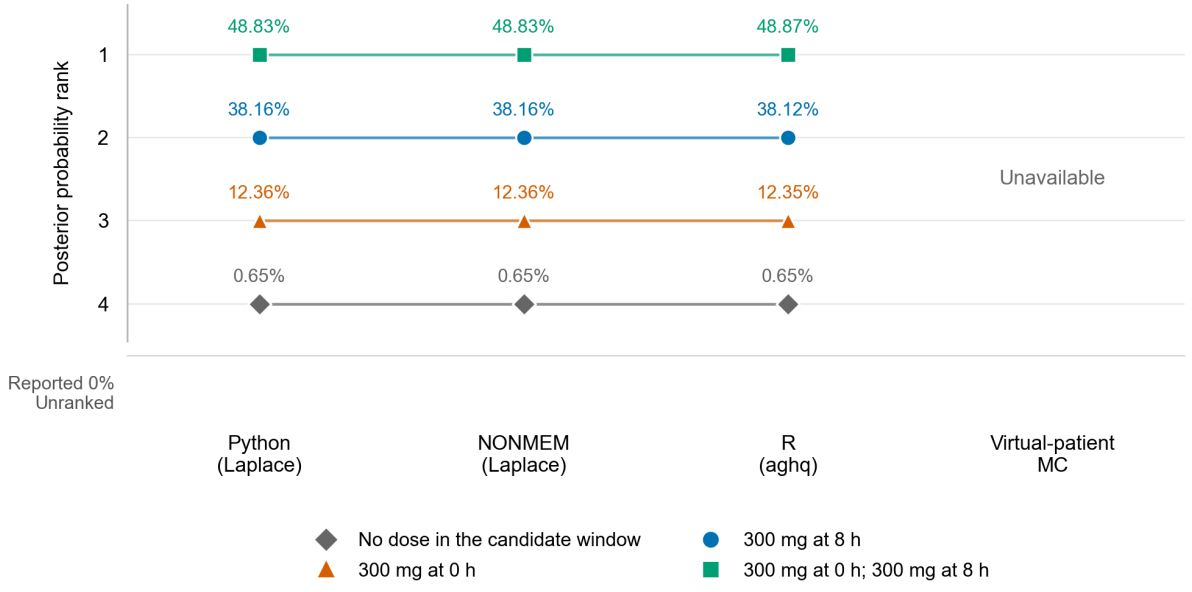
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	3.47204×10^{-9}	3.48304×10^{-9}	4.26275×10^{-9}	2.60868×10^{-9}
Python vs R aghq	4.63047×10^{-4}	4.63047×10^{-4}	5.72923×10^{-4}	3.59644×10^{-4}
NONMEM vs R aghq	4.63051×10^{-4}	4.63051×10^{-4}	5.72928×10^{-4}	3.59646×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00652580	0.00652580	0.00648623
ω_{01}: 300 mg at 0 h	0.25	0.12362891	0.12362891	0.12352346
ω_{10}: 300 mg at 8 h	0.25	0.38156629	0.38156629	0.38124825
ω_{11}: 300 mg at 0 h; 300 mg at 8 h	0.25	0.48827901	0.48827900	0.48874205

Method	P_{max}	G	H_N
Python Laplace	0.488279	0.106713	0.727796
NONMEM Laplace	0.488279	0.106713	0.727796
R aghq	0.488742	0.107494	0.727512

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C079: Candidate states

Candidate dose events: 300 mg at 0 h; 300 mg at 10 h.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

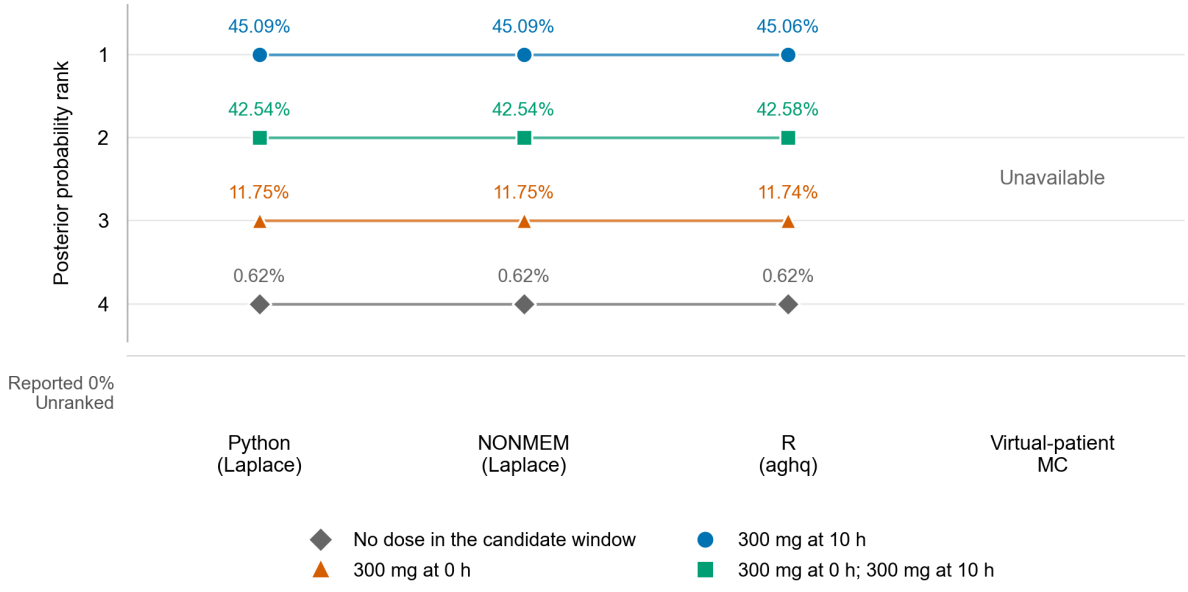
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	1.38280×10^{-9}	1.46358×10^{-9}	1.72908×10^{-9}	1.57224×10^{-9}
Python vs R aghq	4.12426×10^{-4}	4.12426×10^{-4}	5.18979×10^{-4}	3.27891×10^{-4}
NONMEM vs R aghq	4.12427×10^{-4}	4.12427×10^{-4}	5.18979×10^{-4}	3.27891×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00620069	0.00620069	0.00616459
ω_{01}: 300 mg at 0 h	0.25	0.11746990	0.11746990	0.11739820
ω_{10}: 300 mg at 10 h	0.25	0.45090797	0.45090797	0.45060334
ω_{11}: 300 mg at 0 h; 300 mg at 10 h	0.25	0.42542144	0.42542144	0.42583387

Method	P_{max}	G	H_N
Python Laplace	0.450908	0.025487	0.725554
NONMEM Laplace	0.450908	0.025487	0.725554
R aghq	0.450603	0.024769	0.725389

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C080: Candidate states

Candidate dose events: 300 mg at 0 h; 300 mg at 14 h.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

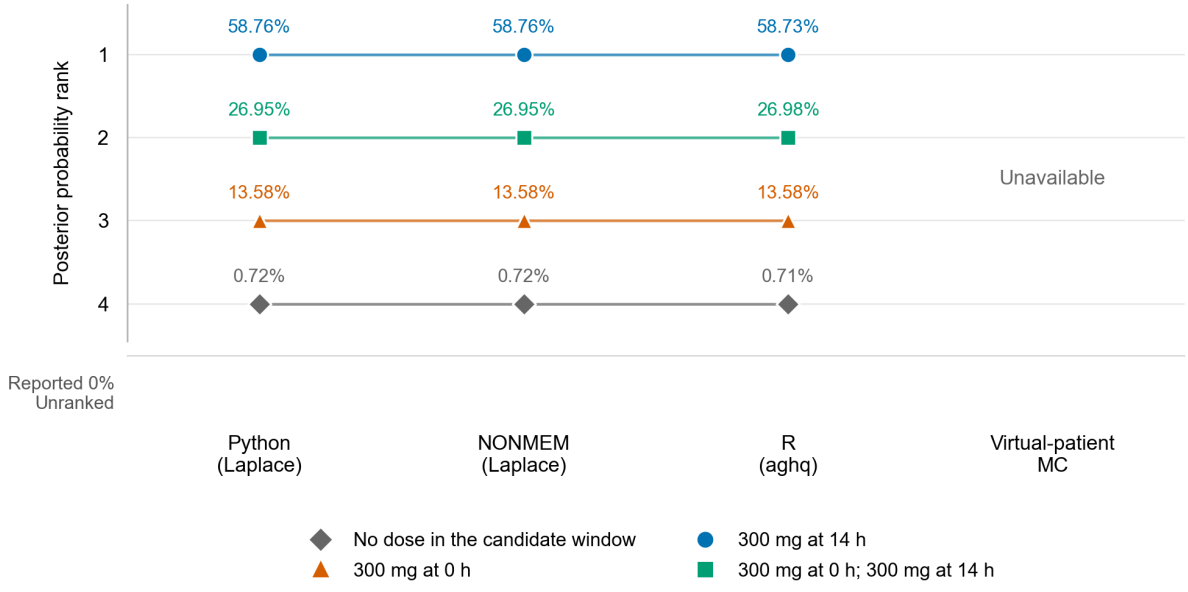
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	7.88086×10^{-9}	7.88086×10^{-9}	1.07427×10^{-8}	6.37197×10^{-9}
Python vs R aghq	2.66956×10^{-4}	2.66956×10^{-4}	3.44471×10^{-4}	2.61614×10^{-4}
NONMEM vs R aghq	2.66964×10^{-4}	2.66964×10^{-4}	3.44482×10^{-4}	2.61619×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00716681	0.00716681	0.00712865
ω_{01}: 300 mg at 0 h	0.25	0.13577269	0.13577269	0.13575771
ω_{10}: 300 mg at 14 h	0.25	0.58755185	0.58755186	0.58733804
ω_{11}: 300 mg at 0 h; 300 mg at 14 h	0.25	0.26950865	0.26950864	0.26977560

Method	P_{max}	G	H_N
Python Laplace	0.587552	0.318043	0.701382
NONMEM Laplace	0.587552	0.318043	0.701382
R aghq	0.587338	0.317562	0.701394

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C081: Candidate states

Candidate dose events: 300 mg at 0 h; 300 mg at 16 h.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	4
NONMEM Laplace	5/5	4
R aghq	5/5	4

Repeatability

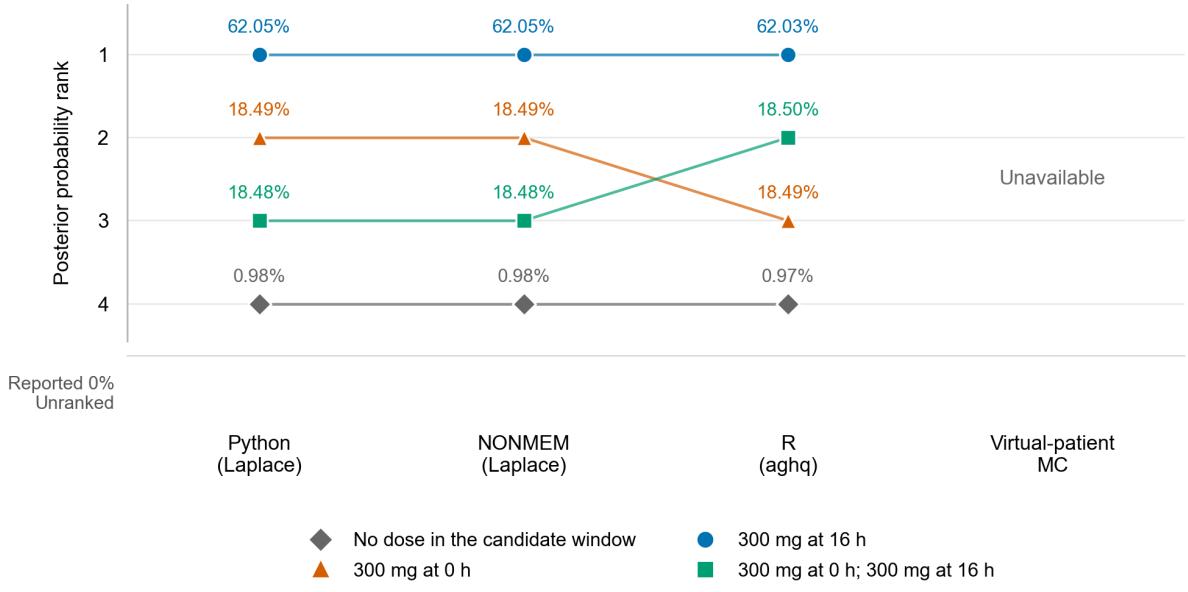
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	4.95454×10^{-9}	4.95863×10^{-9}	6.42980×10^{-9}	4.03718×10^{-9}
Python vs R aghq	1.77755×10^{-4}	1.93020×10^{-4}	2.34020×10^{-4}	2.40544×10^{-4}
NONMEM vs R aghq	1.77754×10^{-4}	1.93015×10^{-4}	2.34016×10^{-4}	2.40543×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{00}: No dose in the candidate window	0.25	0.00976079	0.00976079	0.00971068
ω_{01}: 300 mg at 0 h	0.25	0.18491461	0.18491462	0.18492988
ω_{10}: 300 mg at 16 h	0.25	0.62048294	0.62048293	0.62034002
ω_{11}: 300 mg at 0 h; 300 mg at 16 h	0.25	0.18484166	0.18484166	0.18501941

Method	P_{max}	G	H_N
Python Laplace	0.620483	0.435568	0.696451
NONMEM Laplace	0.620483	0.435568	0.696451
R aghq	0.620340	0.435321	0.696470

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C082: Candidate states

Candidate dose times: 12 h; 2 candidate states.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	2
NONMEM Laplace	5/5	2
R aghq	5/5	2

Repeatability

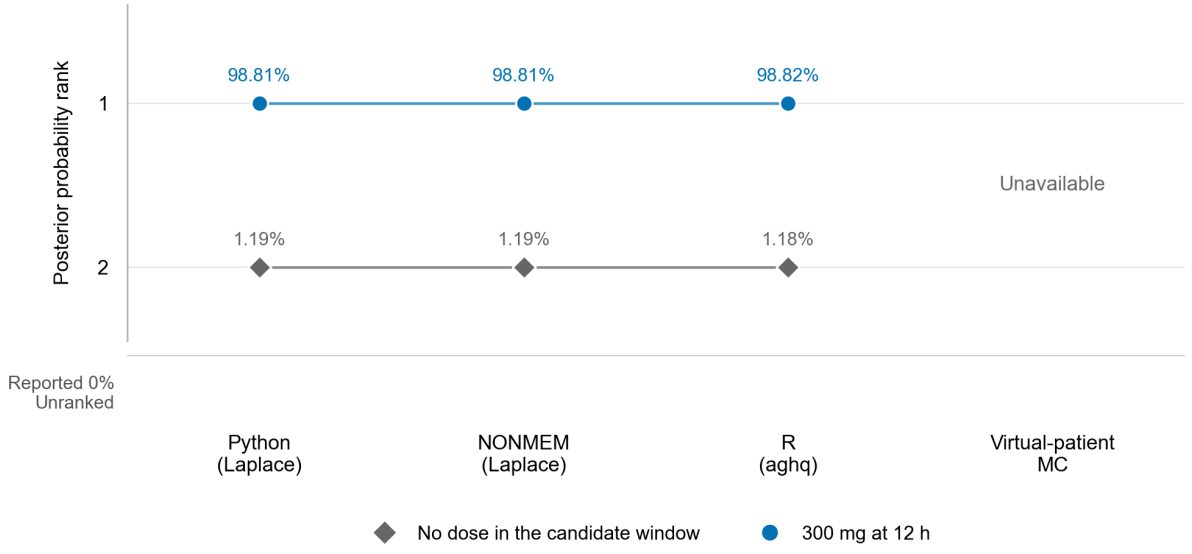
Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	4.45783×10^{-10}	4.45783×10^{-10}	6.30433×10^{-10}	1.45380×10^{-9}
Python vs R aghq	5.94014×10^{-5}	5.94014×10^{-5}	8.40063×10^{-5}	1.93961×10^{-4}
NONMEM vs R aghq	5.94019×10^{-5}	5.94019×10^{-5}	8.40070×10^{-5}	1.93963×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_0: No dose in the candidate window	0.5	0.01189445	0.01189445	0.01183505
ω_1: 300 mg at 12 h	0.5	0.98810555	0.98810555	0.98816495

Method	P_{max}	G	H_N
Python Laplace	0.988106	0.976211	0.093106
NONMEM Laplace	0.988106	0.976211	0.093106
R aghq	0.988165	0.976330	0.092727

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

Run times and numerical checks

OXC C083: Candidate states

Candidate dose times: -12, 0, 12 h; 8 candidate states.

Observations: 12 mg/L at 24 h.

Output availability

Computational route	Valid outputs/runs	States/run
Python Laplace	5/5	8
NONMEM Laplace	5/5	8
R aghq	5/5	8

Repeatability

Method	Max SD (raw)	Max range (raw)	Max SD (norm.)	Max range (norm.)
Python Laplace	0	0	0	0
NONMEM Laplace	0	0	0	0
R aghq	0	0	0	0

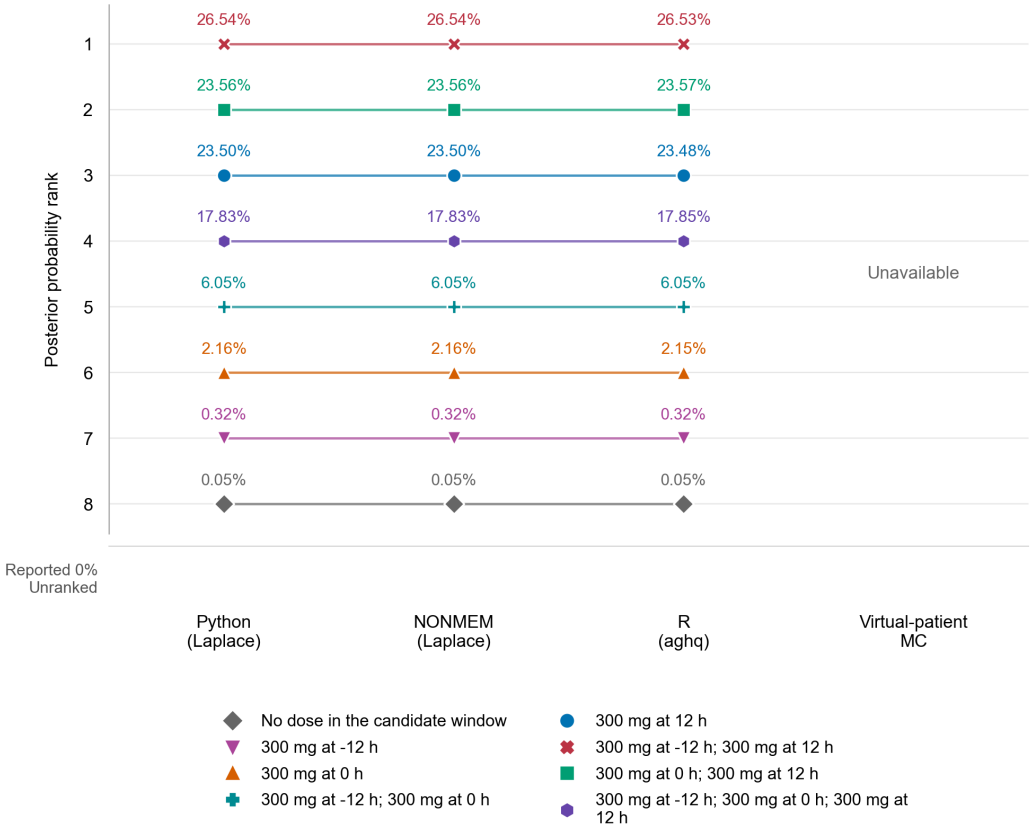
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

The virtual patient approach had only a single web record; repeatability was not evaluated.

Cross-method agreement

Method pair	d_∞	TV	d_2	d_H
Python vs NONMEM	5.20300×10^{-9}	8.32152×10^{-9}	8.32685×10^{-9}	6.30439×10^{-9}
Python vs R aghq	2.11168×10^{-4}	3.33101×10^{-4}	3.16544×10^{-4}	2.86850×10^{-4}
NONMEM vs R aghq	2.11163×10^{-4}	3.33099×10^{-4}	3.16543×10^{-4}	2.86848×10^{-4}

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.



Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Prior	Python Laplace	NONMEM Laplace	R aghq
ω_{000}: No dose in the candidate window	0.125	0.00045698	0.00045698	0.00045605
ω_{001}: 300 mg at -12 h	0.125	0.00319497	0.00319497	0.00317780
ω_{010}: 300 mg at 0 h	0.125	0.02157643	0.02157643	0.02153256
ω_{011}: 300 mg at -12 h; 300 mg at 0 h	0.125	0.06052750	0.06052750	0.06051796
ω_{100}: 300 mg at 12 h	0.125	0.23496606	0.23496606	0.23478937
ω_{101}: 300 mg at -12 h; 300 mg at 12 h	0.125	0.26541489	0.26541488	0.26532998
ω_{110}: 300 mg at 0 h; 300 mg at 12 h	0.125	0.23558581	0.23558581	0.23570774
ω_{111}: 300 mg at -12 h; 300 mg at 0 h; 300 mg at 12 h	0.125	0.17827737	0.17827737	0.17848854

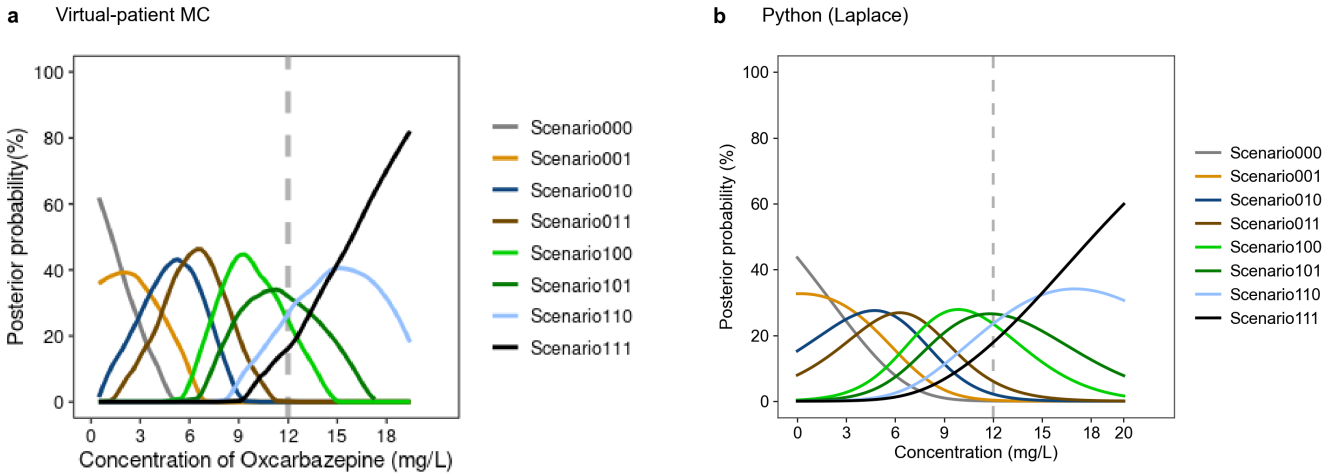
Method	P_{max}	G	H_N
Python Laplace	0.265415	0.029829	0.776543
NONMEM Laplace	0.265415	0.029829	0.776543
R aghq	0.265330	0.029622	0.776481

P_{max}, maximum probability; G, top-two probability gap; H_N, normalized entropy.

External web output

The displayed total is 99.00%; the web output is excluded from comparisons.

Web state	Candidate dosing history	Reported probability (%)
Scenario000	No dose in the candidate window	0.00
Scenario001	300 mg at -12 h	0.00
Scenario010	300 mg at 0 h	0.00
Scenario100	300 mg at 12 h	23.00
Scenario011	300 mg at -12 h; 300 mg at 0 h	0.00
Scenario101	300 mg at -12 h; 300 mg at 12 h	31.00
Scenario110	300 mg at 0 h; 300 mg at 12 h	28.00
Scenario111	300 mg at -12 h; 300 mg at 0 h; 300 mg at 12 h	17.00



Concentration-dependent posterior probabilities: (a) archived virtual-patient Monte Carlo display; (b) Python Laplace. Dashed lines mark the scenario observation.

Scan probabilities | Diagnostics | MC source.

Run times and numerical checks

Run times and numerical checks

Times are wall-clock times. Formal, pilot and historical runs retain their recorded status.

OXC C003

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.609
Python-Laplace	Formal 2	valid	2.859
Python-Laplace	Formal 3	valid	3.157
Python-Laplace	Formal 4	valid	2.829
Python-Laplace	Formal 5	valid	2.781
Python-Laplace	Pilot 1	valid	3
NONMEM-Laplace	Formal 1	valid	1.391
NONMEM-Laplace	Formal 2	valid	1.438
NONMEM-Laplace	Formal 3	valid	1.375
NONMEM-Laplace	Formal 4	valid	1.391
NONMEM-Laplace	Formal 5	valid	1.406
R aghq	Formal 1	valid	2.562
R aghq	Formal 2	valid	2.843
R aghq	Formal 3	valid	2.765
R aghq	Formal 4	valid	2.859
R aghq	Formal 5	valid	2.828
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C001

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.828
Python-Laplace	Formal 2	valid	2.969
Python-Laplace	Formal 3	valid	3.078
Python-Laplace	Formal 4	valid	3
Python-Laplace	Formal 5	valid	3.187
Python-Laplace	Pilot 1	valid	3.266
NONMEM-Laplace	Formal 1	valid	1.437
NONMEM-Laplace	Formal 2	valid	1.407
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.406
NONMEM-Laplace	Formal 5	valid	1.406
R aghq	Formal 1	valid	2.719
R aghq	Formal 2	valid	3.062
R aghq	Formal 3	valid	2.954
R aghq	Formal 4	valid	2.922
R aghq	Formal 5	valid	2.953
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C002

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.672
Python-Laplace	Formal 2	valid	2.938
Python-Laplace	Formal 3	valid	2.985
Python-Laplace	Formal 4	valid	2.969
Python-Laplace	Formal 5	valid	3.187
Python-Laplace	Pilot 1	valid	3.125
NONMEM-Laplace	Formal 1	valid	1.391
NONMEM-Laplace	Formal 2	valid	1.391
NONMEM-Laplace	Formal 3	valid	1.453
NONMEM-Laplace	Formal 4	valid	1.39
NONMEM-Laplace	Formal 5	valid	1.391
R aghq	Formal 1	valid	2.593
R aghq	Formal 2	valid	2.954
R aghq	Formal 3	valid	2.813
R aghq	Formal 4	valid	3.187
R aghq	Formal 5	valid	2.812
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C004

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.625
Python-Laplace	Formal 2	valid	2.891
Python-Laplace	Formal 3	valid	2.735
Python-Laplace	Formal 4	valid	3.078
Python-Laplace	Formal 5	valid	2.953
Python-Laplace	Pilot 1	valid	3.078
NONMEM-Laplace	Formal 1	valid	1.391
NONMEM-Laplace	Formal 2	valid	1.391
NONMEM-Laplace	Formal 3	valid	1.359
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.391
R aghq	Formal 1	valid	2.609
R aghq	Formal 2	valid	2.812
R aghq	Formal 3	valid	2.782
R aghq	Formal 4	valid	2.953
R aghq	Formal 5	valid	2.797
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C005

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.579
Python-Laplace	Formal 2	valid	2.875
Python-Laplace	Formal 3	valid	2.656
Python-Laplace	Formal 4	valid	3.063
Python-Laplace	Formal 5	valid	3.094
Python-Laplace	Pilot 1	valid	3.188
NONMEM-Laplace	Formal 1	valid	1.391
NONMEM-Laplace	Formal 2	valid	1.391
NONMEM-Laplace	Formal 3	valid	1.391
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.407
R aghq	Formal 1	valid	2.563
R aghq	Formal 2	valid	2.75
R aghq	Formal 3	valid	2.75
R aghq	Formal 4	valid	2.906
R aghq	Formal 5	valid	2.797
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C006

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.735
Python-Laplace	Formal 2	valid	2.907
Python-Laplace	Formal 3	valid	2.672
Python-Laplace	Formal 4	valid	3.266
Python-Laplace	Formal 5	valid	2.969
Python-Laplace	Pilot 1	valid	3.188
NONMEM-Laplace	Formal 1	valid	1.391
NONMEM-Laplace	Formal 2	valid	1.375
NONMEM-Laplace	Formal 3	valid	1.39
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.406
R aghq	Formal 1	valid	2.625
R aghq	Formal 2	valid	2.843
R aghq	Formal 3	valid	2.797
R aghq	Formal 4	valid	2.812
R aghq	Formal 5	valid	2.812
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C007

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.734
Python-Laplace	Formal 2	valid	3.063
Python-Laplace	Formal 3	valid	2.719
Python-Laplace	Formal 4	valid	3.282
Python-Laplace	Formal 5	valid	3.109
Python-Laplace	Pilot 1	valid	3.281
NONMEM-Laplace	Formal 1	valid	1.438
NONMEM-Laplace	Formal 2	valid	1.391
NONMEM-Laplace	Formal 3	valid	1.453
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.375
R aghq	Formal 1	valid	2.547
R aghq	Formal 2	valid	2.75
R aghq	Formal 3	valid	2.828
R aghq	Formal 4	valid	2.828
R aghq	Formal 5	valid	3
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C008

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.672
Python-Laplace	Formal 2	valid	2.828
Python-Laplace	Formal 3	valid	2.782
Python-Laplace	Formal 4	valid	2.906
Python-Laplace	Formal 5	valid	2.937
Python-Laplace	Pilot 1	valid	3.11
NONMEM-Laplace	Formal 1	valid	1.375
NONMEM-Laplace	Formal 2	valid	1.407
NONMEM-Laplace	Formal 3	valid	1.375
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.375
R aghq	Formal 1	valid	2.546
R aghq	Formal 2	valid	2.797
R aghq	Formal 3	valid	2.813
R aghq	Formal 4	valid	2.875
R aghq	Formal 5	valid	2.766
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C009

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.672
Python-Laplace	Formal 2	valid	2.844
Python-Laplace	Formal 3	valid	2.781
Python-Laplace	Formal 4	valid	2.797
Python-Laplace	Formal 5	valid	2.922
Python-Laplace	Pilot 1	valid	3.141
NONMEM-Laplace	Formal 1	valid	1.375
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.375
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.406
R aghq	Formal 1	valid	2.579
R aghq	Formal 2	valid	2.781
R aghq	Formal 3	valid	2.969
R aghq	Formal 4	valid	2.859
R aghq	Formal 5	valid	2.812
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C010

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.609
Python-Laplace	Formal 2	valid	2.813
Python-Laplace	Formal 3	valid	2.844
Python-Laplace	Formal 4	valid	3.094
Python-Laplace	Formal 5	valid	2.86
Python-Laplace	Pilot 1	valid	3.079
NONMEM-Laplace	Formal 1	valid	1.344
NONMEM-Laplace	Formal 2	valid	1.406
NONMEM-Laplace	Formal 3	valid	1.422
NONMEM-Laplace	Formal 4	valid	1.359
NONMEM-Laplace	Formal 5	valid	1.39
R aghq	Formal 1	valid	2.531
R aghq	Formal 2	valid	2.812
R aghq	Formal 3	valid	2.828
R aghq	Formal 4	valid	2.734
R aghq	Formal 5	valid	2.828
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C011

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.625
Python-Laplace	Formal 2	valid	2.813
Python-Laplace	Formal 3	valid	2.907
Python-Laplace	Formal 4	valid	3.047
Python-Laplace	Formal 5	valid	2.891
Python-Laplace	Pilot 1	valid	3.093
NONMEM-Laplace	Formal 1	valid	1.391
NONMEM-Laplace	Formal 2	valid	1.39
NONMEM-Laplace	Formal 3	valid	1.391
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.375
R aghq	Formal 1	valid	2.547
R aghq	Formal 2	valid	2.937
R aghq	Formal 3	valid	2.797
R aghq	Formal 4	valid	2.828
R aghq	Formal 5	valid	2.812
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C012

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.735
Python-Laplace	Formal 2	valid	3.062
Python-Laplace	Formal 3	valid	3.078
Python-Laplace	Formal 4	valid	2.969
Python-Laplace	Formal 5	valid	2.875
Python-Laplace	Pilot 1	valid	3.188
NONMEM-Laplace	Formal 1	valid	1.36
NONMEM-Laplace	Formal 2	valid	1.406
NONMEM-Laplace	Formal 3	valid	1.375
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.39
R aghq	Formal 1	valid	2.547
R aghq	Formal 2	valid	2.844
R aghq	Formal 3	valid	2.812
R aghq	Formal 4	valid	2.766
R aghq	Formal 5	valid	2.782
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C013

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.797
Python-Laplace	Formal 2	valid	3.078
Python-Laplace	Formal 3	valid	3.062
Python-Laplace	Formal 4	valid	2.922
Python-Laplace	Formal 5	valid	2.969
Python-Laplace	Pilot 1	valid	3.313
NONMEM-Laplace	Formal 1	valid	1.407
NONMEM-Laplace	Formal 2	valid	1.391
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.359
NONMEM-Laplace	Formal 5	valid	1.406
R aghq	Formal 1	valid	2.578
R aghq	Formal 2	valid	2.875
R aghq	Formal 3	valid	2.875
R aghq	Formal 4	valid	2.813
R aghq	Formal 5	valid	2.875
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C014

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.703
Python-Laplace	Formal 2	valid	3.282
Python-Laplace	Formal 3	valid	3.031
Python-Laplace	Formal 4	valid	2.938
Python-Laplace	Formal 5	valid	3.343
Python-Laplace	Pilot 1	valid	3.297
NONMEM-Laplace	Formal 1	valid	1.422
NONMEM-Laplace	Formal 2	valid	1.391
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.406
R aghq	Formal 1	valid	2.656
R aghq	Formal 2	valid	2.891
R aghq	Formal 3	valid	2.844
R aghq	Formal 4	valid	2.812
R aghq	Formal 5	valid	2.875
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C015

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.687
Python-Laplace	Formal 2	valid	3.375
Python-Laplace	Formal 3	valid	3.031
Python-Laplace	Formal 4	valid	2.969
Python-Laplace	Formal 5	valid	3.329
Python-Laplace	Pilot 1	valid	3.328
NONMEM-Laplace	Formal 1	valid	1.485
NONMEM-Laplace	Formal 2	valid	1.375
NONMEM-Laplace	Formal 3	valid	1.39
NONMEM-Laplace	Formal 4	valid	1.391
NONMEM-Laplace	Formal 5	valid	1.375
R aghq	Formal 1	valid	2.64
R aghq	Formal 2	valid	2.922
R aghq	Formal 3	valid	2.797
R aghq	Formal 4	valid	2.812
R aghq	Formal 5	valid	2.812
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C016

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.813
Python-Laplace	Formal 2	valid	2.954
Python-Laplace	Formal 3	valid	3.281
Python-Laplace	Formal 4	valid	3.219
Python-Laplace	Formal 5	valid	2.984
Python-Laplace	Pilot 1	valid	3.031
NONMEM-Laplace	Formal 1	valid	1.438
NONMEM-Laplace	Formal 2	valid	1.375
NONMEM-Laplace	Formal 3	valid	1.359
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.406
R aghq	Formal 1	valid	2.61
R aghq	Formal 2	valid	2.875
R aghq	Formal 3	valid	2.796
R aghq	Formal 4	valid	2.766
R aghq	Formal 5	valid	2.75
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C017

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.781
Python-Laplace	Formal 2	valid	2.891
Python-Laplace	Formal 3	valid	3.313
Python-Laplace	Formal 4	valid	3.188
Python-Laplace	Formal 5	valid	3.016
Python-Laplace	Pilot 1	valid	2.968
NONMEM-Laplace	Formal 1	valid	1.453
NONMEM-Laplace	Formal 2	valid	1.391
NONMEM-Laplace	Formal 3	valid	1.375
NONMEM-Laplace	Formal 4	valid	1.391
NONMEM-Laplace	Formal 5	valid	1.407
R aghq	Formal 1	valid	2.609
R aghq	Formal 2	valid	2.843
R aghq	Formal 3	valid	2.781
R aghq	Formal 4	valid	3.063
R aghq	Formal 5	valid	2.703
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C018

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.547
Python-Laplace	Formal 2	valid	2.609
Python-Laplace	Formal 3	valid	2.735
Python-Laplace	Formal 4	valid	2.703
Python-Laplace	Formal 5	valid	2.797
Python-Laplace	Pilot 1	valid	2.656
NONMEM-Laplace	Formal 1	valid	1.406
NONMEM-Laplace	Formal 2	valid	1.391
NONMEM-Laplace	Formal 3	valid	1.328
NONMEM-Laplace	Formal 4	valid	1.344
NONMEM-Laplace	Formal 5	valid	1.343
R aghq	Formal 1	valid	2.532
R aghq	Formal 2	valid	2.75
R aghq	Formal 3	valid	2.672
R aghq	Formal 4	valid	2.86
R aghq	Formal 5	valid	2.625
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C019

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.609
Python-Laplace	Formal 2	valid	2.765
Python-Laplace	Formal 3	valid	2.86
Python-Laplace	Formal 4	valid	2.938
Python-Laplace	Formal 5	valid	2.797
Python-Laplace	Pilot 1	valid	2.703
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.344
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.703
R aghq	Formal 2	valid	2.781
R aghq	Formal 3	valid	2.766
R aghq	Formal 4	valid	2.829
R aghq	Formal 5	valid	2.641
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C020

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.578
Python-Laplace	Formal 2	valid	2.75
Python-Laplace	Formal 3	valid	2.937
Python-Laplace	Formal 4	valid	2.813
Python-Laplace	Formal 5	valid	2.813
Python-Laplace	Pilot 1	valid	2.89
NONMEM-Laplace	Formal 1	valid	1.375
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.343
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.625
R aghq	Formal 2	valid	2.797
R aghq	Formal 3	valid	2.812
R aghq	Formal 4	valid	2.797
R aghq	Formal 5	valid	2.687
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C021

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.64
Python-Laplace	Formal 2	valid	2.89
Python-Laplace	Formal 3	valid	3.047
Python-Laplace	Formal 4	valid	2.937
Python-Laplace	Formal 5	valid	2.859
Python-Laplace	Pilot 1	valid	2.954
NONMEM-Laplace	Formal 1	valid	1.375
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.344
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.641
R aghq	Formal 2	valid	2.86
R aghq	Formal 3	valid	2.86
R aghq	Formal 4	valid	2.953
R aghq	Formal 5	valid	2.703
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C022

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.75
Python-Laplace	Formal 2	valid	3.094
Python-Laplace	Formal 3	valid	3.313
Python-Laplace	Formal 4	valid	3.015
Python-Laplace	Formal 5	valid	2.984
Python-Laplace	Pilot 1	valid	3.516
NONMEM-Laplace	Formal 1	valid	1.375
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.343
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.703
R aghq	Formal 2	valid	2.907
R aghq	Formal 3	valid	2.938
R aghq	Formal 4	valid	2.937
R aghq	Formal 5	valid	2.766
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C023

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.781
Python-Laplace	Formal 2	valid	3.296
Python-Laplace	Formal 3	valid	3.547
Python-Laplace	Formal 4	valid	3.046
Python-Laplace	Formal 5	valid	3.062
Python-Laplace	Pilot 1	valid	3.547
NONMEM-Laplace	Formal 1	valid	1.375
NONMEM-Laplace	Formal 2	valid	1.328
NONMEM-Laplace	Formal 3	valid	1.266
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.375
R aghq	Formal 1	qualified	2.687
R aghq	Formal 2	qualified	2.969
R aghq	Formal 3	qualified	2.875
R aghq	Formal 4	qualified	2.922
R aghq	Formal 5	qualified	2.781
Virtual-patient MC	Unavailable	Unavailable	Unavailable

R aghq: the quadrature stability check failed; five complete outputs are included.

Flagged Numerical Checks

The following checks did not meet their stated criteria.

Method	Run	State	Check	Value	Unit	Criterion
R aghq	r_aghq/OXC/C023/formal_parallel_20261022/r01; r_aghq/OXC/C023/formal_parallel_20261022/r02; r_aghq/OXC/C023/formal_parallel_20261022/r03; r_aghq/OXC/C023/formal_parallel_20261022/r04; r_aghq/OXC/C023/formal_parallel_20261022/r05	omega_00	candidate_log_integral_stability	No		Both last two log-integral changes <= 1e-6; order sensitivity, not error certification
R aghq	r_aghq/OXC/C023/formal_parallel_20261022/r01; r_aghq/OXC/C023/formal_parallel_20261022/r02; r_aghq/OXC/C023/formal_parallel_20261022/r03; r_aghq/OXC/C023/formal_parallel_20261022/r04; r_aghq/OXC/C023/formal_parallel_20261022/r05	omega_00	log_integral_change_to_order_31	1.621386246e-05		Recorded absolute log-integral change <= 1e-6
R aghq	r_aghq/OXC/C023/formal_parallel_20261022/r01; r_aghq/OXC/C023/formal_parallel_20261022/r02; r_aghq/OXC/C023/formal_parallel_20261022/r03; r_aghq/OXC/C023/formal_parallel_20261022/r04; r_aghq/OXC/C023/formal_parallel_20261022/r05	omega_01	candidate_log_integral_stability	No		Both last two log-integral changes <= 1e-6; order sensitivity, not error certification
R aghq	r_aghq/OXC/C023/formal_parallel_20261022/r01; r_aghq/OXC/C023/formal_parallel_20261022/r02; r_aghq/OXC/C023/formal_parallel_20261022/r03; r_aghq/OXC/C023/formal_parallel_20261022/r04; r_aghq/OXC/C023/formal_parallel_20261022/r05	omega_01	log_integral_change_to_order_31	1.044066024e-06		Recorded absolute log-integral change <= 1e-6
R aghq	r_aghq/OXC/C023/formal_parallel_20261022/r01; r_aghq/OXC/C023/formal_parallel_20261022/r02; r_aghq/OXC/C023/formal_parallel_20261022/r03; r_aghq/OXC/C023/formal_parallel_20261022/r04; r_aghq/OXC/C023/formal_parallel_20261022/r05	All states	stability_passed	No		All candidate log-integral and posterior last-two-change criteria pass

Statewise repeatability and numerical-check records.

OXC C024

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.828
Python-Laplace	Formal 2	valid	3.516
Python-Laplace	Formal 3	valid	3.375
Python-Laplace	Formal 4	valid	3.282
Python-Laplace	Formal 5	valid	3.172
Python-Laplace	Pilot 1	valid	3.5
NONMEM-Laplace	Formal 1	valid	1.36
NONMEM-Laplace	Formal 2	valid	1.328
NONMEM-Laplace	Formal 3	valid	1.343
NONMEM-Laplace	Formal 4	valid	1.344
NONMEM-Laplace	Formal 5	valid	1.36
R aghq	Formal 1	qualified	2.719
R aghq	Formal 2	qualified	2.938
R aghq	Formal 3	qualified	2.875
R aghq	Formal 4	qualified	2.969
R aghq	Formal 5	qualified	2.812
Virtual-patient MC	Unavailable	Unavailable	Unavailable

R aghq: the quadrature stability check failed; five complete outputs are included.

Flagged Numerical Checks

The following checks did not meet their stated criteria.

Method	Run	State	Check	Value	Unit	Criterion
R aghq	r_aghq/OXC/C024/formal_parallel_20261022/r01; r_aghq/OXC/C024/formal_parallel_20261022/r02; r_aghq/OXC/C024/formal_parallel_20261022/r03; r_aghq/OXC/C024/formal_parallel_20261022/r04; r_aghq/OXC/C024/formal_parallel_20261022/r05	omega_00	candidate_log_integral_stability	No		Both last two log-integral changes <= 1e-6; order sensitivity, not error certification
R aghq	r_aghq/OXC/C024/formal_parallel_20261022/r01; r_aghq/OXC/C024/formal_parallel_20261022/r02; r_aghq/OXC/C024/formal_parallel_20261022/r03; r_aghq/OXC/C024/formal_parallel_20261022/r04; r_aghq/OXC/C024/formal_parallel_20261022/r05	omega_00	log_integral_change_to_order_31	0.0006133590921		Recorded absolute log-integral change <= 1e-6
R aghq	r_aghq/OXC/C024/formal_parallel_20261022/r01; r_aghq/OXC/C024/formal_parallel_20261022/r02; r_aghq/OXC/C024/formal_parallel_20261022/r03; r_aghq/OXC/C024/formal_parallel_20261022/r04; r_aghq/OXC/C024/formal_parallel_20261022/r05	omega_00	log_integral_change_to_order_61	2.097598343e-05		Recorded absolute log-integral change <= 1e-6
R aghq	r_aghq/OXC/C024/formal_parallel_20261022/r01; r_aghq/OXC/C024/formal_parallel_20261022/r02; r_aghq/OXC/C024/formal_parallel_20261022/r03; r_aghq/OXC/C024/formal_parallel_20261022/r04; r_aghq/OXC/C024/formal_parallel_20261022/r05	omega_01	candidate_log_integral_stability	No		Both last two log-integral changes <= 1e-6; order sensitivity, not error certification
R aghq	r_aghq/OXC/C024/formal_parallel_20261022/r01; r_aghq/OXC/C024/formal_parallel_20261022/r02; r_aghq/OXC/C024/formal_parallel_20261022/r03; r_aghq/OXC/C024/formal_parallel_20261022/r04; r_aghq/OXC/C024/formal_parallel_20261022/r05	omega_01	log_integral_change_to_order_31	5.279786764e-05		Recorded absolute log-integral change <= 1e-6

Method	Run	State	Check	Value	Unit	Criterion
R aghq	r_aghq/OXC/C024/formal_parallel_20261022/r01; r_aghq/OXC/C024/formal_parallel_20261022/r02; r_aghq/OXC/C024/formal_parallel_20261022/r03; r_aghq/OXC/C024/formal_parallel_20261022/r04; r_aghq/OXC/C024/formal_parallel_20261022/r05	All states	posterior_change_to_order_31	4.006660452e-05		Recorded maximum statewise absolute change <= 1e-6
R aghq	r_aghq/OXC/C024/formal_parallel_20261022/r01; r_aghq/OXC/C024/formal_parallel_20261022/r02; r_aghq/OXC/C024/formal_parallel_20261022/r03; r_aghq/OXC/C024/formal_parallel_20261022/r04; r_aghq/OXC/C024/formal_parallel_20261022/r05	All states	posterior_change_to_order_61	1.391928094e-06		Recorded maximum statewise absolute change <= 1e-6
R aghq	r_aghq/OXC/C024/formal_parallel_20261022/r01; r_aghq/OXC/C024/formal_parallel_20261022/r02; r_aghq/OXC/C024/formal_parallel_20261022/r03; r_aghq/OXC/C024/formal_parallel_20261022/r04; r_aghq/OXC/C024/formal_parallel_20261022/r05	All states	stability_passed	No		All candidate log-integral and posterior last-two-change criteria pass

Statewise repeatability and numerical-check records.

OXC C025

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.922
Python-Laplace	Formal 2	valid	3.36
Python-Laplace	Formal 3	valid	3.281
Python-Laplace	Formal 4	valid	3.234
Python-Laplace	Formal 5	valid	3.266
Python-Laplace	Pilot 1	valid	3.5
NONMEM-Laplace	Formal 1	valid	1.375
NONMEM-Laplace	Formal 2	valid	1.343
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	qualified	2.734
R aghq	Formal 2	qualified	2.875
R aghq	Formal 3	qualified	2.953
R aghq	Formal 4	qualified	3.187
R aghq	Formal 5	qualified	2.813
Virtual-patient MC	Unavailable	Unavailable	Unavailable

R aghq: the quadrature stability check failed; five complete outputs are included.

Flagged Numerical Checks

The following checks did not meet their stated criteria.

Method	Run	State	Check	Value	Unit	Criterion
R aghq	r_aghq/OXC/C025/formal_parallel_20261022/r01; r_aghq/OXC/C025/formal_parallel_20261022/r02; r_aghq/OXC/C025/formal_parallel_20261022/r03; r_aghq/OXC/C025/formal_parallel_20261022/r04; r_aghq/OXC/C025/formal_parallel_20261022/r05	omega_00	candidate_log_integral_stability	No		Both last two log-integral changes <= 1e-6; order sensitivity, not error certification
R aghq	r_aghq/OXC/C025/formal_parallel_20261022/r01; r_aghq/OXC/C025/formal_parallel_20261022/r02; r_aghq/OXC/C025/formal_parallel_20261022/r03; r_aghq/OXC/C025/formal_parallel_20261022/r04; r_aghq/OXC/C025/formal_parallel_20261022/r05	omega_00	log_integral_change_to_order_31	0.0009292963094		Recorded absolute log-integral change <= 1e-6
R aghq	r_aghq/OXC/C025/formal_parallel_20261022/r01; r_aghq/OXC/C025/formal_parallel_20261022/r02; r_aghq/OXC/C025/formal_parallel_20261022/r03; r_aghq/OXC/C025/formal_parallel_20261022/r04; r_aghq/OXC/C025/formal_parallel_20261022/r05	omega_00	log_integral_change_to_order_61	0.0001298170726		Recorded absolute log-integral change <= 1e-6
R aghq	r_aghq/OXC/C025/formal_parallel_20261022/r01; r_aghq/OXC/C025/formal_parallel_20261022/r02; r_aghq/OXC/C025/formal_parallel_20261022/r03; r_aghq/OXC/C025/formal_parallel_20261022/r04; r_aghq/OXC/C025/formal_parallel_20261022/r05	omega_01	candidate_log_integral_stability	No		Both last two log-integral changes <= 1e-6; order sensitivity, not error certification
R aghq	r_aghq/OXC/C025/formal_parallel_20261022/r01; r_aghq/OXC/C025/formal_parallel_20261022/r02; r_aghq/OXC/C025/formal_parallel_20261022/r03; r_aghq/OXC/C025/formal_parallel_20261022/r04; r_aghq/OXC/C025/formal_parallel_20261022/r05	omega_01	log_integral_change_to_order_31	0.0001820748898		Recorded absolute log-integral change <= 1e-6

Method	Run	State	Check	Value	Unit	Criterion
R aghq	r_aghq/OXC/C025/formal_parallel_20261022/r01; r_aghq/OXC/C025/formal_parallel_20261022/r02; r_aghq/OXC/C025/formal_parallel_20261022/r03; r_aghq/OXC/C025/formal_parallel_20261022/r04; r_aghq/OXC/C025/formal_parallel_20261022/r05	omega_01	log_integral_change_to_order_61	8.398039801e-06		Recorded absolute log-integral change <= 1e-6
R aghq	r_aghq/OXC/C025/formal_parallel_20261022/r01; r_aghq/OXC/C025/formal_parallel_20261022/r02; r_aghq/OXC/C025/formal_parallel_20261022/r03; r_aghq/OXC/C025/formal_parallel_20261022/r04; r_aghq/OXC/C025/formal_parallel_20261022/r05	omega_10	candidate_log_integral_stability	No		Both last two log-integral changes <= 1e-6; order sensitivity, not error certification
R aghq	r_aghq/OXC/C025/formal_parallel_20261022/r01; r_aghq/OXC/C025/formal_parallel_20261022/r02; r_aghq/OXC/C025/formal_parallel_20261022/r03; r_aghq/OXC/C025/formal_parallel_20261022/r04; r_aghq/OXC/C025/formal_parallel_20261022/r05	omega_10	log_integral_change_to_order_31	4.302836518e-06		Recorded absolute log-integral change <= 1e-6
R aghq	r_aghq/OXC/C025/formal_parallel_20261022/r01; r_aghq/OXC/C025/formal_parallel_20261022/r02; r_aghq/OXC/C025/formal_parallel_20261022/r03; r_aghq/OXC/C025/formal_parallel_20261022/r04; r_aghq/OXC/C025/formal_parallel_20261022/r05	omega_11	candidate_log_integral_stability	No		Both last two log-integral changes <= 1e-6; order sensitivity, not error certification
R aghq	r_aghq/OXC/C025/formal_parallel_20261022/r01; r_aghq/OXC/C025/formal_parallel_20261022/r02; r_aghq/OXC/C025/formal_parallel_20261022/r03; r_aghq/OXC/C025/formal_parallel_20261022/r04; r_aghq/OXC/C025/formal_parallel_20261022/r05	omega_11	log_integral_change_to_order_31	6.818145192e-06		Recorded absolute log-integral change <= 1e-6
R aghq	r_aghq/OXC/C025/formal_parallel_20261022/r01; r_aghq/OXC/C025/formal_parallel_20261022/r02; r_aghq/OXC/C025/formal_parallel_20261022/r03; r_aghq/OXC/C025/formal_parallel_20261022/r04; r_aghq/OXC/C025/formal_parallel_20261022/r05	All states	posterior_change_to_order_31	8.334856767e-05		Recorded maximum statewise absolute change <= 1e-6
R aghq	r_aghq/OXC/C025/formal_parallel_20261022/r01; r_aghq/OXC/C025/formal_parallel_20261022/r02; r_aghq/OXC/C025/formal_parallel_20261022/r03; r_aghq/OXC/C025/formal_parallel_20261022/r04; r_aghq/OXC/C025/formal_parallel_20261022/r05	All states	posterior_change_to_order_61	1.209166854e-05		Recorded maximum statewise absolute change <= 1e-6
R aghq	r_aghq/OXC/C025/formal_parallel_20261022/r01; r_aghq/OXC/C025/formal_parallel_20261022/r02; r_aghq/OXC/C025/formal_parallel_20261022/r03; r_aghq/OXC/C025/formal_parallel_20261022/r04; r_aghq/OXC/C025/formal_parallel_20261022/r05	All states	stability_passed	No		All candidate log-integral and posterior last-two-change criteria pass

Statewise repeatability and numerical-check records.

OXC C026

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	3.797
Python-Laplace	Formal 2	valid	3.781
Python-Laplace	Formal 3	valid	3.641
Python-Laplace	Formal 4	valid	3.765
Python-Laplace	Formal 5	valid	3.829
Python-Laplace	Pilot 1	valid	4.375
NONMEM-Laplace	Formal 1	valid	1.422
NONMEM-Laplace	Formal 2	valid	1.375
NONMEM-Laplace	Formal 3	valid	1.359
NONMEM-Laplace	Formal 4	valid	1.359
NONMEM-Laplace	Formal 5	valid	1.359
R aghq	Formal 1	failed	1.813
R aghq	Formal 2	failed	1.969
R aghq	Formal 3	failed	1.953
R aghq	Formal 4	failed	1.969
R aghq	Formal 5	failed	1.954
Virtual-patient MC	Archived web capture	reported	Unavailable

The Python-Laplace output used accepted precision recovery; optimizer convergence was not established.

The current NONMEM output does not resolve the earlier stationarity warning for this scenario.

R aghq: all five attempts failed; no posterior vector was available.

Flagged Numerical Checks

The following checks did not meet their stated criteria.

Method	Run	State	Check	Value	Unit	Criterion
R aghq	r_aghq/OXC/C026/formal_parallel_20261022/r01; r_aghq/OXC/C026/formal_parallel_20261022/r02; r_aghq/OXC/C026/formal_parallel_20261022/r03; r_aghq/OXC/C026/formal_parallel_20261022/r04; r_aghq/OXC/C026/formal_parallel_20261022/r05	All states	output_available	No		Source success and complete finite probability vector
R aghq	r_aghq/OXC/C026/formal_parallel_20261022/r01; r_aghq/OXC/C026/formal_parallel_20261022/r02; r_aghq/OXC/C026/formal_parallel_20261022/r03; r_aghq/OXC/C026/formal_parallel_20261022/r04; r_aghq/OXC/C026/formal_parallel_20261022/r05	omega_00	candidate_execution_success	failed		Source candidate status is success
R aghq	r_aghq/OXC/C026/formal_parallel_20261022/r01; r_aghq/OXC/C026/formal_parallel_20261022/r02; r_aghq/OXC/C026/formal_parallel_20261022/r03; r_aghq/OXC/C026/formal_parallel_20261022/r04; r_aghq/OXC/C026/formal_parallel_20261022/r05	omega_01	candidate_execution_success	failed		Source candidate status is success
R aghq	r_aghq/OXC/C026/formal_parallel_20261022/r01; r_aghq/OXC/C026/formal_parallel_20261022/r02; r_aghq/OXC/C026/formal_parallel_20261022/r03; r_aghq/OXC/C026/formal_parallel_20261022/r04; r_aghq/OXC/C026/formal_parallel_20261022/r05	omega_10	candidate_execution_success	failed		Source candidate status is success
R aghq	r_aghq/OXC/C026/formal_parallel_20261022/r01; r_aghq/OXC/C026/formal_parallel_20261022/r02; r_aghq/OXC/C026/formal_parallel_20261022/r03; r_aghq/OXC/C026/formal_parallel_20261022/r04; r_aghq/OXC/C026/formal_parallel_20261022/r05	omega_11	candidate_execution_success	failed		Source candidate status is success

Statewise repeatability and numerical-check records.

OXC C027

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.89
Python-Laplace	Formal 2	valid	3.093
Python-Laplace	Formal 3	valid	2.859
Python-Laplace	Formal 4	valid	3.062
Python-Laplace	Formal 5	valid	3.109
Python-Laplace	Pilot 1	valid	3.578
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.359
NONMEM-Laplace	Formal 3	valid	1.328
NONMEM-Laplace	Formal 4	valid	1.344
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.765
R aghq	Formal 2	valid	2.969
R aghq	Formal 3	valid	2.938
R aghq	Formal 4	valid	3
R aghq	Formal 5	valid	2.859
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C028

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.89
Python-Laplace	Formal 2	valid	3.25
Python-Laplace	Formal 3	valid	2.984
Python-Laplace	Formal 4	valid	3.203
Python-Laplace	Formal 5	valid	3.469
Python-Laplace	Pilot 1	valid	3.546
NONMEM-Laplace	Formal 1	valid	1.391
NONMEM-Laplace	Formal 2	valid	1.36
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.344
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.735
R aghq	Formal 2	valid	2.89
R aghq	Formal 3	valid	2.922
R aghq	Formal 4	valid	2.859
R aghq	Formal 5	valid	2.844
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C029

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.75
Python-Laplace	Formal 2	valid	3.156
Python-Laplace	Formal 3	valid	2.891
Python-Laplace	Formal 4	valid	3.094
Python-Laplace	Formal 5	valid	3.344
Python-Laplace	Pilot 1	valid	3.391
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.343
NONMEM-Laplace	Formal 3	valid	1.281
NONMEM-Laplace	Formal 4	valid	1.359
NONMEM-Laplace	Formal 5	valid	1.343
R aghq	Formal 1	valid	2.719
R aghq	Formal 2	valid	2.844
R aghq	Formal 3	valid	2.843
R aghq	Formal 4	valid	2.859
R aghq	Formal 5	valid	2.828
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C030

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.578
Python-Laplace	Formal 2	valid	3
Python-Laplace	Formal 3	valid	2.968
Python-Laplace	Formal 4	valid	2.891
Python-Laplace	Formal 5	valid	2.844
Python-Laplace	Pilot 1	valid	3.015
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.328
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.328
R aghq	Formal 1	valid	2.765
R aghq	Formal 2	valid	2.765
R aghq	Formal 3	valid	2.75
R aghq	Formal 4	valid	2.891
R aghq	Formal 5	valid	2.782
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C031

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.515
Python-Laplace	Formal 2	valid	2.984
Python-Laplace	Formal 3	valid	2.922
Python-Laplace	Formal 4	valid	2.922
Python-Laplace	Formal 5	valid	2.75
Python-Laplace	Pilot 1	valid	2.953
NONMEM-Laplace	Formal 1	valid	1.344
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.344
NONMEM-Laplace	Formal 5	valid	1.328
R aghq	Formal 1	valid	2.594
R aghq	Formal 2	valid	2.797
R aghq	Formal 3	valid	2.781
R aghq	Formal 4	valid	2.969
R aghq	Formal 5	valid	2.844
Virtual-patient MC	Archived web capture	not_assessed	Unavailable

Statewise repeatability and numerical-check records.

OXC C032

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.5
Python-Laplace	Formal 2	valid	2.703
Python-Laplace	Formal 3	valid	2.781
Python-Laplace	Formal 4	valid	2.765
Python-Laplace	Formal 5	valid	2.797
Python-Laplace	Pilot 1	valid	2.796
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.36
NONMEM-Laplace	Formal 3	valid	1.313
NONMEM-Laplace	Formal 4	valid	1.344
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.594
R aghq	Formal 2	valid	2.89
R aghq	Formal 3	valid	2.735
R aghq	Formal 4	valid	2.782
R aghq	Formal 5	valid	2.75
Virtual-patient MC	Archived web capture	not_assessed	Unavailable

Statewise repeatability and numerical-check records.

OXC C033

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.375
Python-Laplace	Formal 2	valid	2.64
Python-Laplace	Formal 3	valid	2.656
Python-Laplace	Formal 4	valid	2.688
Python-Laplace	Formal 5	valid	2.781
Python-Laplace	Pilot 1	valid	2.797
NONMEM-Laplace	Formal 1	valid	1.375
NONMEM-Laplace	Formal 2	valid	1.36
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.343
NONMEM-Laplace	Formal 5	valid	1.329
R aghq	Formal 1	valid	2.609
R aghq	Formal 2	valid	2.75
R aghq	Formal 3	valid	2.797
R aghq	Formal 4	valid	2.766
R aghq	Formal 5	valid	2.703
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C034

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.562
Python-Laplace	Formal 2	valid	2.828
Python-Laplace	Formal 3	valid	2.828
Python-Laplace	Formal 4	valid	2.734
Python-Laplace	Formal 5	valid	3.031
Python-Laplace	Pilot 1	valid	2.953
NONMEM-Laplace	Formal 1	valid	1.375
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.328
NONMEM-Laplace	Formal 4	valid	1.344
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.594
R aghq	Formal 2	valid	2.75
R aghq	Formal 3	valid	2.829
R aghq	Formal 4	valid	2.75
R aghq	Formal 5	valid	2.734
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C035

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.64
Python-Laplace	Formal 2	valid	2.813
Python-Laplace	Formal 3	valid	2.922
Python-Laplace	Formal 4	valid	2.859
Python-Laplace	Formal 5	valid	3.016
Python-Laplace	Pilot 1	valid	2.985
NONMEM-Laplace	Formal 1	valid	1.344
NONMEM-Laplace	Formal 2	valid	1.343
NONMEM-Laplace	Formal 3	valid	1.343
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.672
R aghq	Formal 2	valid	2.891
R aghq	Formal 3	valid	2.765
R aghq	Formal 4	valid	2.922
R aghq	Formal 5	valid	2.75
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C036

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.719
Python-Laplace	Formal 2	valid	2.875
Python-Laplace	Formal 3	valid	3.094
Python-Laplace	Formal 4	valid	3.016
Python-Laplace	Formal 5	valid	3.219
Python-Laplace	Pilot 1	valid	3
NONMEM-Laplace	Formal 1	valid	1.36
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.313
NONMEM-Laplace	Formal 5	valid	1.359
R aghq	Formal 1	valid	2.703
R aghq	Formal 2	valid	3.031
R aghq	Formal 3	valid	2.984
R aghq	Formal 4	valid	2.907
R aghq	Formal 5	valid	2.797
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C037

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.688
Python-Laplace	Formal 2	valid	2.844
Python-Laplace	Formal 3	valid	2.984
Python-Laplace	Formal 4	valid	2.907
Python-Laplace	Formal 5	valid	3.015
Python-Laplace	Pilot 1	valid	2.969
NONMEM-Laplace	Formal 1	valid	1.328
NONMEM-Laplace	Formal 2	valid	1.329
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.329
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.64
R aghq	Formal 2	valid	2.875
R aghq	Formal 3	valid	2.891
R aghq	Formal 4	valid	2.969
R aghq	Formal 5	valid	2.875
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C038

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.766
Python-Laplace	Formal 2	valid	3
Python-Laplace	Formal 3	valid	3.157
Python-Laplace	Formal 4	valid	3
Python-Laplace	Formal 5	valid	3.062
Python-Laplace	Pilot 1	valid	3.203
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.359
NONMEM-Laplace	Formal 4	valid	1.344
NONMEM-Laplace	Formal 5	valid	1.328
R aghq	Formal 1	valid	2.985
R aghq	Formal 2	valid	2.828
R aghq	Formal 3	valid	2.922
R aghq	Formal 4	valid	3.046
R aghq	Formal 5	valid	2.906
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C039

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.687
Python-Laplace	Formal 2	valid	2.938
Python-Laplace	Formal 3	valid	2.906
Python-Laplace	Formal 4	valid	2.829
Python-Laplace	Formal 5	valid	2.906
Python-Laplace	Pilot 1	valid	3.11
NONMEM-Laplace	Formal 1	valid	1.375
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.765
R aghq	Formal 2	valid	2.907
R aghq	Formal 3	valid	2.813
R aghq	Formal 4	valid	2.907
R aghq	Formal 5	valid	2.859
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C040

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.672
Python-Laplace	Formal 2	valid	2.922
Python-Laplace	Formal 3	valid	2.985
Python-Laplace	Formal 4	valid	2.86
Python-Laplace	Formal 5	valid	2.938
Python-Laplace	Pilot 1	valid	3
NONMEM-Laplace	Formal 1	valid	1.344
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.359
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.688
R aghq	Formal 2	valid	2.828
R aghq	Formal 3	valid	2.812
R aghq	Formal 4	valid	2.875
R aghq	Formal 5	valid	2.828
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C041

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.672
Python-Laplace	Formal 2	valid	3.031
Python-Laplace	Formal 3	valid	3.047
Python-Laplace	Formal 4	valid	2.954
Python-Laplace	Formal 5	valid	2.985
Python-Laplace	Pilot 1	valid	3.093
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.359
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.344
NONMEM-Laplace	Formal 5	valid	1.329
R aghq	Formal 1	valid	2.672
R aghq	Formal 2	valid	2.86
R aghq	Formal 3	valid	2.86
R aghq	Formal 4	valid	2.86
R aghq	Formal 5	valid	2.813
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C042

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.687
Python-Laplace	Formal 2	valid	3.047
Python-Laplace	Formal 3	valid	3.063
Python-Laplace	Formal 4	valid	3.218
Python-Laplace	Formal 5	valid	3.11
Python-Laplace	Pilot 1	valid	3.187
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.329
R aghq	Formal 1	valid	2.688
R aghq	Formal 2	valid	2.797
R aghq	Formal 3	valid	2.797
R aghq	Formal 4	valid	2.844
R aghq	Formal 5	valid	2.875
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C043

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.609
Python-Laplace	Formal 2	valid	3.062
Python-Laplace	Formal 3	valid	2.891
Python-Laplace	Formal 4	valid	3.141
Python-Laplace	Formal 5	valid	3.094
Python-Laplace	Pilot 1	valid	3.078
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.328
NONMEM-Laplace	Formal 3	valid	1.359
NONMEM-Laplace	Formal 4	valid	1.359
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.687
R aghq	Formal 2	valid	2.968
R aghq	Formal 3	valid	2.797
R aghq	Formal 4	valid	2.859
R aghq	Formal 5	valid	2.969
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C044

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.641
Python-Laplace	Formal 2	valid	2.953
Python-Laplace	Formal 3	valid	2.875
Python-Laplace	Formal 4	valid	2.844
Python-Laplace	Formal 5	valid	3.062
Python-Laplace	Pilot 1	valid	3.062
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.343
NONMEM-Laplace	Formal 3	valid	1.312
NONMEM-Laplace	Formal 4	valid	1.359
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.688
R aghq	Formal 2	valid	2.797
R aghq	Formal 3	valid	2.812
R aghq	Formal 4	valid	2.938
R aghq	Formal 5	valid	2.828
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C045

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.687
Python-Laplace	Formal 2	valid	3.032
Python-Laplace	Formal 3	valid	2.875
Python-Laplace	Formal 4	valid	2.969
Python-Laplace	Formal 5	valid	3.156
Python-Laplace	Pilot 1	valid	3.141
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.313
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.672
R aghq	Formal 2	valid	2.828
R aghq	Formal 3	valid	2.812
R aghq	Formal 4	valid	2.922
R aghq	Formal 5	valid	2.843
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C046

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.672
Python-Laplace	Formal 2	valid	2.891
Python-Laplace	Formal 3	valid	2.781
Python-Laplace	Formal 4	valid	2.875
Python-Laplace	Formal 5	valid	2.875
Python-Laplace	Pilot 1	valid	3.016
NONMEM-Laplace	Formal 1	valid	1.344
NONMEM-Laplace	Formal 2	valid	1.343
NONMEM-Laplace	Formal 3	valid	1.359
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.328
R aghq	Formal 1	valid	2.906
R aghq	Formal 2	valid	2.812
R aghq	Formal 3	valid	2.875
R aghq	Formal 4	valid	2.859
R aghq	Formal 5	valid	2.797
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C047

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.657
Python-Laplace	Formal 2	valid	3.141
Python-Laplace	Formal 3	valid	3.094
Python-Laplace	Formal 4	valid	3.094
Python-Laplace	Formal 5	valid	2.781
Python-Laplace	Pilot 1	valid	3.375
NONMEM-Laplace	Formal 1	valid	1.407
NONMEM-Laplace	Formal 2	valid	1.375
NONMEM-Laplace	Formal 3	valid	1.375
NONMEM-Laplace	Formal 4	valid	1.312
NONMEM-Laplace	Formal 5	valid	1.329
R aghq	Formal 1	valid	2.797
R aghq	Formal 2	valid	2.765
R aghq	Formal 3	valid	2.875
R aghq	Formal 4	valid	2.969
R aghq	Formal 5	valid	2.781
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C048

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.703
Python-Laplace	Formal 2	valid	3.031
Python-Laplace	Formal 3	valid	3
Python-Laplace	Formal 4	valid	3.172
Python-Laplace	Formal 5	valid	2.812
Python-Laplace	Pilot 1	valid	3.281
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.343
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.797
R aghq	Formal 2	valid	2.843
R aghq	Formal 3	valid	2.891
R aghq	Formal 4	valid	2.953
R aghq	Formal 5	valid	2.703
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C049

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.593
Python-Laplace	Formal 2	valid	3.078
Python-Laplace	Formal 3	valid	2.969
Python-Laplace	Formal 4	valid	3.297
Python-Laplace	Formal 5	valid	2.922
Python-Laplace	Pilot 1	valid	3.109
NONMEM-Laplace	Formal 1	valid	1.343
NONMEM-Laplace	Formal 2	valid	1.313
NONMEM-Laplace	Formal 3	valid	1.343
NONMEM-Laplace	Formal 4	valid	1.344
NONMEM-Laplace	Formal 5	valid	1.328
R aghq	Formal 1	valid	2.718
R aghq	Formal 2	valid	2.844
R aghq	Formal 3	valid	2.86
R aghq	Formal 4	valid	3.172
R aghq	Formal 5	valid	2.704
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C050

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.61
Python-Laplace	Formal 2	valid	3.062
Python-Laplace	Formal 3	valid	2.86
Python-Laplace	Formal 4	valid	3.219
Python-Laplace	Formal 5	valid	3
Python-Laplace	Pilot 1	valid	2.907
NONMEM-Laplace	Formal 1	valid	1.343
NONMEM-Laplace	Formal 2	valid	1.328
NONMEM-Laplace	Formal 3	valid	1.36
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.625
R aghq	Formal 2	valid	2.781
R aghq	Formal 3	valid	2.828
R aghq	Formal 4	valid	2.859
R aghq	Formal 5	valid	2.656
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C051

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.641
Python-Laplace	Formal 2	valid	3.047
Python-Laplace	Formal 3	valid	2.797
Python-Laplace	Formal 4	valid	2.937
Python-Laplace	Formal 5	valid	3.187
Python-Laplace	Pilot 1	valid	3.156
NONMEM-Laplace	Formal 1	valid	1.36
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.343
NONMEM-Laplace	Formal 4	valid	1.312
NONMEM-Laplace	Formal 5	valid	1.312
R aghq	Formal 1	valid	2.609
R aghq	Formal 2	valid	2.797
R aghq	Formal 3	valid	2.813
R aghq	Formal 4	valid	2.844
R aghq	Formal 5	valid	2.656
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C052

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.593
Python-Laplace	Formal 2	valid	3.156
Python-Laplace	Formal 3	valid	2.844
Python-Laplace	Formal 4	valid	2.907
Python-Laplace	Formal 5	valid	3.141
Python-Laplace	Pilot 1	valid	3.219
NONMEM-Laplace	Formal 1	valid	1.375
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.328
NONMEM-Laplace	Formal 4	valid	1.313
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.625
R aghq	Formal 2	valid	2.766
R aghq	Formal 3	valid	2.969
R aghq	Formal 4	valid	2.782
R aghq	Formal 5	valid	2.719
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C053

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.609
Python-Laplace	Formal 2	valid	3.078
Python-Laplace	Formal 3	valid	3.015
Python-Laplace	Formal 4	valid	2.953
Python-Laplace	Formal 5	valid	2.89
Python-Laplace	Pilot 1	valid	3.047
NONMEM-Laplace	Formal 1	valid	1.344
NONMEM-Laplace	Formal 2	valid	1.328
NONMEM-Laplace	Formal 3	valid	1.328
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.328
R aghq	Formal 1	valid	2.61
R aghq	Formal 2	valid	2.796
R aghq	Formal 3	valid	2.829
R aghq	Formal 4	valid	2.796
R aghq	Formal 5	valid	2.719
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C054

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.593
Python-Laplace	Formal 2	valid	3.062
Python-Laplace	Formal 3	valid	2.828
Python-Laplace	Formal 4	valid	2.922
Python-Laplace	Formal 5	valid	2.875
Python-Laplace	Pilot 1	valid	3.016
NONMEM-Laplace	Formal 1	valid	1.36
NONMEM-Laplace	Formal 2	valid	1.328
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.343
NONMEM-Laplace	Formal 5	valid	1.343
R aghq	Formal 1	valid	2.594
R aghq	Formal 2	valid	2.781
R aghq	Formal 3	valid	2.797
R aghq	Formal 4	valid	2.813
R aghq	Formal 5	valid	2.703
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C055

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.765
Python-Laplace	Formal 2	valid	3.219
Python-Laplace	Formal 3	valid	3.047
Python-Laplace	Formal 4	valid	3.25
Python-Laplace	Formal 5	valid	3.235
Python-Laplace	Pilot 1	valid	3.25
NONMEM-Laplace	Formal 1	valid	1.344
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.312
NONMEM-Laplace	Formal 5	valid	1.328
R aghq	Formal 1	valid	2.703
R aghq	Formal 2	valid	2.844
R aghq	Formal 3	valid	2.922
R aghq	Formal 4	valid	2.937
R aghq	Formal 5	valid	2.844
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C056

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.797
Python-Laplace	Formal 2	valid	3.235
Python-Laplace	Formal 3	valid	3.172
Python-Laplace	Formal 4	valid	3.281
Python-Laplace	Formal 5	valid	3.422
Python-Laplace	Pilot 1	valid	3.375
NONMEM-Laplace	Formal 1	valid	1.36
NONMEM-Laplace	Formal 2	valid	1.313
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.312
NONMEM-Laplace	Formal 5	valid	1.328
R aghq	Formal 1	valid	2.735
R aghq	Formal 2	valid	2.922
R aghq	Formal 3	valid	2.984
R aghq	Formal 4	valid	3.016
R aghq	Formal 5	valid	2.922
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C057

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.781
Python-Laplace	Formal 2	valid	3.078
Python-Laplace	Formal 3	valid	3.11
Python-Laplace	Formal 4	valid	3.032
Python-Laplace	Formal 5	valid	3.047
Python-Laplace	Pilot 1	valid	3.25
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.343
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.671
R aghq	Formal 2	valid	2.953
R aghq	Formal 3	valid	2.953
R aghq	Formal 4	valid	2.938
R aghq	Formal 5	valid	2.969
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C058

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.781
Python-Laplace	Formal 2	valid	3.031
Python-Laplace	Formal 3	valid	3
Python-Laplace	Formal 4	valid	3.141
Python-Laplace	Formal 5	valid	3.047
Python-Laplace	Pilot 1	valid	3.219
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.343
NONMEM-Laplace	Formal 3	valid	1.328
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.343
R aghq	Formal 1	valid	2.766
R aghq	Formal 2	valid	2.969
R aghq	Formal 3	valid	2.984
R aghq	Formal 4	valid	2.985
R aghq	Formal 5	valid	2.921
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C059

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.953
Python-Laplace	Formal 2	valid	3.016
Python-Laplace	Formal 3	valid	3.093
Python-Laplace	Formal 4	valid	3.094
Python-Laplace	Formal 5	valid	3.625
Python-Laplace	Pilot 1	valid	3.359
NONMEM-Laplace	Formal 1	valid	1.36
NONMEM-Laplace	Formal 2	valid	1.328
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.344
R aghq	Formal 1	valid	2.813
R aghq	Formal 2	valid	3
R aghq	Formal 3	valid	3.062
R aghq	Formal 4	valid	3.094
R aghq	Formal 5	valid	2.938
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C060

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.546
Python-Laplace	Formal 2	valid	2.844
Python-Laplace	Formal 3	valid	2.937
Python-Laplace	Formal 4	valid	2.953
Python-Laplace	Formal 5	valid	3.078
Python-Laplace	Pilot 1	valid	2.985
NONMEM-Laplace	Formal 1	valid	1.39
NONMEM-Laplace	Formal 2	valid	1.407
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.343
NONMEM-Laplace	Formal 5	valid	1.343
R aghq	Formal 1	valid	2.609
R aghq	Formal 2	valid	2.766
R aghq	Formal 3	valid	2.938
R aghq	Formal 4	valid	2.875
R aghq	Formal 5	valid	2.719
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C061

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.578
Python-Laplace	Formal 2	valid	2.969
Python-Laplace	Formal 3	valid	2.812
Python-Laplace	Formal 4	valid	2.844
Python-Laplace	Formal 5	valid	3
Python-Laplace	Pilot 1	valid	2.953
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.344
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.344
NONMEM-Laplace	Formal 5	valid	1.313
R aghq	Formal 1	valid	2.562
R aghq	Formal 2	valid	2.766
R aghq	Formal 3	valid	2.875
R aghq	Formal 4	valid	2.844
R aghq	Formal 5	valid	2.781
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C062

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.563
Python-Laplace	Formal 2	valid	2.968
Python-Laplace	Formal 3	valid	3.171
Python-Laplace	Formal 4	valid	2.922
Python-Laplace	Formal 5	valid	2.953
Python-Laplace	Pilot 1	valid	2.922
NONMEM-Laplace	Formal 1	valid	1.36
NONMEM-Laplace	Formal 2	valid	1.36
NONMEM-Laplace	Formal 3	valid	1.343
NONMEM-Laplace	Formal 4	valid	1.344
NONMEM-Laplace	Formal 5	valid	1.313
R aghq	Formal 1	valid	2.562
R aghq	Formal 2	valid	2.813
R aghq	Formal 3	valid	2.875
R aghq	Formal 4	valid	2.796
R aghq	Formal 5	valid	2.891
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C063

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.562
Python-Laplace	Formal 2	valid	2.969
Python-Laplace	Formal 3	valid	3.032
Python-Laplace	Formal 4	valid	2.843
Python-Laplace	Formal 5	valid	3.032
Python-Laplace	Pilot 1	valid	3.047
NONMEM-Laplace	Formal 1	valid	1.36
NONMEM-Laplace	Formal 2	valid	1.391
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.328
R aghq	Formal 1	valid	2.593
R aghq	Formal 2	valid	2.828
R aghq	Formal 3	valid	2.891
R aghq	Formal 4	valid	2.86
R aghq	Formal 5	valid	2.718
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C064

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.656
Python-Laplace	Formal 2	valid	2.828
Python-Laplace	Formal 3	valid	2.797
Python-Laplace	Formal 4	valid	2.703
Python-Laplace	Formal 5	valid	2.89
Python-Laplace	Pilot 1	valid	2.938
NONMEM-Laplace	Formal 1	valid	1.36
NONMEM-Laplace	Formal 2	valid	1.359
NONMEM-Laplace	Formal 3	valid	1.312
NONMEM-Laplace	Formal 4	valid	1.312
NONMEM-Laplace	Formal 5	valid	1.328
R aghq	Formal 1	valid	2.61
R aghq	Formal 2	valid	3.047
R aghq	Formal 3	valid	2.968
R aghq	Formal 4	valid	2.937
R aghq	Formal 5	valid	2.766
Virtual-patient MC	Archived web capture	reported	Unavailable

Statewise repeatability and numerical-check records.

OXC C065

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.406
Python-Laplace	Formal 2	valid	2.671
Python-Laplace	Formal 3	valid	2.672
Python-Laplace	Formal 4	valid	2.906
Python-Laplace	Formal 5	valid	2.531
Python-Laplace	Pilot 1	valid	2.75
NONMEM-Laplace	Formal 1	valid	1.375
NONMEM-Laplace	Formal 2	valid	1.359
NONMEM-Laplace	Formal 3	valid	1.344
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.297
R aghq	Formal 1	valid	2.5
R aghq	Formal 2	valid	2.641
R aghq	Formal 3	valid	2.703
R aghq	Formal 4	valid	2.657
R aghq	Formal 5	valid	2.437
Virtual-patient MC	Archived web capture	not_assessed	Unavailable

Statewise repeatability and numerical-check records.

OXC C066

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.328
Python-Laplace	Formal 2	valid	2.672
Python-Laplace	Formal 3	valid	2.688
Python-Laplace	Formal 4	valid	2.828
Python-Laplace	Formal 5	valid	2.484
Python-Laplace	Pilot 1	valid	2.687
NONMEM-Laplace	Formal 1	valid	1.344
NONMEM-Laplace	Formal 2	valid	1.297
NONMEM-Laplace	Formal 3	valid	1.343
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.328
R aghq	Formal 1	valid	2.422
R aghq	Formal 2	valid	2.61
R aghq	Formal 3	valid	2.609
R aghq	Formal 4	valid	2.563
R aghq	Formal 5	valid	2.344
Virtual-patient MC	Archived web capture	not_assessed	Unavailable

Statewise repeatability and numerical-check records.

OXC C067

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.469
Python-Laplace	Formal 2	valid	2.859
Python-Laplace	Formal 3	valid	2.609
Python-Laplace	Formal 4	valid	2.812
Python-Laplace	Formal 5	valid	2.469
Python-Laplace	Pilot 1	valid	2.562
NONMEM-Laplace	Formal 1	valid	1.313
NONMEM-Laplace	Formal 2	valid	1.328
NONMEM-Laplace	Formal 3	valid	1.328
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.297
R aghq	Formal 1	valid	2.687
R aghq	Formal 2	valid	2.625
R aghq	Formal 3	valid	2.719
R aghq	Formal 4	valid	2.531
R aghq	Formal 5	valid	2.359
Virtual-patient MC	Archived web capture	not_assessed	Unavailable

Statewise repeatability and numerical-check records.

OXC C068

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.375
Python-Laplace	Formal 2	valid	2.828
Python-Laplace	Formal 3	valid	2.531
Python-Laplace	Formal 4	valid	2.734
Python-Laplace	Formal 5	valid	2.406
Python-Laplace	Pilot 1	valid	2.593
NONMEM-Laplace	Formal 1	valid	1.297
NONMEM-Laplace	Formal 2	valid	1.266
NONMEM-Laplace	Formal 3	valid	1.375
NONMEM-Laplace	Formal 4	valid	1.312
NONMEM-Laplace	Formal 5	valid	1.391
R aghq	Formal 1	valid	2.547
R aghq	Formal 2	valid	2.594
R aghq	Formal 3	valid	2.703
R aghq	Formal 4	valid	2.547
R aghq	Formal 5	valid	2.328
Virtual-patient MC	Archived web capture	not_assessed	Unavailable

Statewise repeatability and numerical-check records.

OXC C069

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.922
Python-Laplace	Formal 2	valid	3.281
Python-Laplace	Formal 3	valid	3.266
Python-Laplace	Formal 4	valid	3.187
Python-Laplace	Formal 5	valid	3
Python-Laplace	Pilot 1	valid	3.219
NONMEM-Laplace	Formal 1	valid	1.344
NONMEM-Laplace	Formal 2	valid	1.359
NONMEM-Laplace	Formal 3	valid	1.375
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.359
R aghq	Formal 1	valid	3.219
R aghq	Formal 2	valid	3.234
R aghq	Formal 3	valid	3.094
R aghq	Formal 4	valid	3.125
R aghq	Formal 5	valid	2.938
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C070

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.609
Python-Laplace	Formal 2	valid	3
Python-Laplace	Formal 3	valid	2.859
Python-Laplace	Formal 4	valid	2.875
Python-Laplace	Formal 5	valid	2.704
Python-Laplace	Pilot 1	valid	2.906
NONMEM-Laplace	Formal 1	valid	1.36
NONMEM-Laplace	Formal 2	valid	1.359
NONMEM-Laplace	Formal 3	valid	1.422
NONMEM-Laplace	Formal 4	valid	1.407
NONMEM-Laplace	Formal 5	valid	1.39
R aghq	Formal 1	valid	2.875
R aghq	Formal 2	valid	3.062
R aghq	Formal 3	valid	2.843
R aghq	Formal 4	valid	2.813
R aghq	Formal 5	valid	2.656
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C071

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.75
Python-Laplace	Formal 2	valid	2.922
Python-Laplace	Formal 3	valid	3.047
Python-Laplace	Formal 4	valid	2.906
Python-Laplace	Formal 5	valid	2.734
Python-Laplace	Pilot 1	valid	3.062
NONMEM-Laplace	Formal 1	valid	1.36
NONMEM-Laplace	Formal 2	valid	1.36
NONMEM-Laplace	Formal 3	valid	1.422
NONMEM-Laplace	Formal 4	valid	1.344
NONMEM-Laplace	Formal 5	valid	1.359
R aghq	Formal 1	valid	2.813
R aghq	Formal 2	valid	3
R aghq	Formal 3	valid	2.766
R aghq	Formal 4	valid	2.812
R aghq	Formal 5	valid	2.781
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C072

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.812
Python-Laplace	Formal 2	valid	2.875
Python-Laplace	Formal 3	valid	3.063
Python-Laplace	Formal 4	valid	3.031
Python-Laplace	Formal 5	valid	2.781
Python-Laplace	Pilot 1	valid	3.141
NONMEM-Laplace	Formal 1	valid	1.391
NONMEM-Laplace	Formal 2	valid	1.375
NONMEM-Laplace	Formal 3	valid	1.422
NONMEM-Laplace	Formal 4	valid	1.36
NONMEM-Laplace	Formal 5	valid	1.375
R aghq	Formal 1	valid	2.765
R aghq	Formal 2	valid	2.969
R aghq	Formal 3	valid	2.828
R aghq	Formal 4	valid	2.797
R aghq	Formal 5	valid	2.687
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C073

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.656
Python-Laplace	Formal 2	valid	2.735
Python-Laplace	Formal 3	valid	3.218
Python-Laplace	Formal 4	valid	3.015
Python-Laplace	Formal 5	valid	2.844
Python-Laplace	Pilot 1	valid	2.938
NONMEM-Laplace	Formal 1	valid	1.375
NONMEM-Laplace	Formal 2	valid	1.36
NONMEM-Laplace	Formal 3	valid	1.406
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.359
R aghq	Formal 1	valid	2.844
R aghq	Formal 2	valid	3.11
R aghq	Formal 3	valid	2.969
R aghq	Formal 4	valid	2.844
R aghq	Formal 5	valid	2.719
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C074

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.531
Python-Laplace	Formal 2	valid	2.625
Python-Laplace	Formal 3	valid	3.234
Python-Laplace	Formal 4	valid	2.953
Python-Laplace	Formal 5	valid	2.797
Python-Laplace	Pilot 1	valid	2.75
NONMEM-Laplace	Formal 1	valid	1.375
NONMEM-Laplace	Formal 2	valid	1.375
NONMEM-Laplace	Formal 3	valid	1.375
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.375
R aghq	Formal 1	valid	2.781
R aghq	Formal 2	valid	2.765
R aghq	Formal 3	valid	2.828
R aghq	Formal 4	valid	2.813
R aghq	Formal 5	valid	2.562
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C075

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.563
Python-Laplace	Formal 2	valid	3.375
Python-Laplace	Formal 3	valid	3.046
Python-Laplace	Formal 4	valid	3.063
Python-Laplace	Formal 5	valid	2.781
Python-Laplace	Pilot 1	valid	3.016
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.375
NONMEM-Laplace	Formal 3	valid	1.422
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.359
R aghq	Formal 1	valid	2.859
R aghq	Formal 2	valid	2.75
R aghq	Formal 3	valid	2.859
R aghq	Formal 4	valid	2.782
R aghq	Formal 5	valid	2.578
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C076

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.578
Python-Laplace	Formal 2	valid	3.422
Python-Laplace	Formal 3	valid	3.016
Python-Laplace	Formal 4	valid	2.969
Python-Laplace	Formal 5	valid	2.765
Python-Laplace	Pilot 1	valid	2.875
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.375
NONMEM-Laplace	Formal 3	valid	1.375
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.375
R aghq	Formal 1	valid	2.797
R aghq	Formal 2	valid	2.797
R aghq	Formal 3	valid	2.922
R aghq	Formal 4	valid	2.797
R aghq	Formal 5	valid	2.579
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C077

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.797
Python-Laplace	Formal 2	valid	3.171
Python-Laplace	Formal 3	valid	3.125
Python-Laplace	Formal 4	valid	2.844
Python-Laplace	Formal 5	valid	2.953
Python-Laplace	Pilot 1	valid	3.015
NONMEM-Laplace	Formal 1	valid	1.375
NONMEM-Laplace	Formal 2	valid	1.375
NONMEM-Laplace	Formal 3	valid	1.375
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.39
R aghq	Formal 1	valid	2.781
R aghq	Formal 2	valid	2.781
R aghq	Formal 3	valid	3.094
R aghq	Formal 4	valid	2.828
R aghq	Formal 5	valid	2.734
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C078

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.829
Python-Laplace	Formal 2	valid	3.157
Python-Laplace	Formal 3	valid	3.015
Python-Laplace	Formal 4	valid	2.891
Python-Laplace	Formal 5	valid	3.094
Python-Laplace	Pilot 1	valid	2.984
NONMEM-Laplace	Formal 1	valid	1.359
NONMEM-Laplace	Formal 2	valid	1.39
NONMEM-Laplace	Formal 3	valid	1.39
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.375
R aghq	Formal 1	valid	2.796
R aghq	Formal 2	valid	2.75
R aghq	Formal 3	valid	3.14
R aghq	Formal 4	valid	2.797
R aghq	Formal 5	valid	2.593
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C079

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	3.219
Python-Laplace	Formal 2	valid	5.437
Python-Laplace	Formal 3	valid	3.125
Python-Laplace	Formal 4	valid	2.828
Python-Laplace	Formal 5	valid	3.078
Python-Laplace	Pilot 1	valid	2.75
NONMEM-Laplace	Formal 1	valid	1.36
NONMEM-Laplace	Formal 2	valid	1.375
NONMEM-Laplace	Formal 3	valid	1.422
NONMEM-Laplace	Formal 4	valid	1.391
NONMEM-Laplace	Formal 5	valid	1.375
R aghq	Formal 1	valid	2.828
R aghq	Formal 2	valid	2.765
R aghq	Formal 3	valid	3
R aghq	Formal 4	valid	2.797
R aghq	Formal 5	valid	2.563
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C080

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.984
Python-Laplace	Formal 2	valid	5.39
Python-Laplace	Formal 3	valid	3
Python-Laplace	Formal 4	valid	2.875
Python-Laplace	Formal 5	valid	2.907
Python-Laplace	Pilot 1	valid	2.671
NONMEM-Laplace	Formal 1	valid	1.375
NONMEM-Laplace	Formal 2	valid	1.359
NONMEM-Laplace	Formal 3	valid	1.391
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.407
R aghq	Formal 1	valid	2.813
R aghq	Formal 2	valid	2.781
R aghq	Formal 3	valid	2.906
R aghq	Formal 4	valid	2.906
R aghq	Formal 5	valid	2.625
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C081

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.984
Python-Laplace	Formal 2	valid	3.078
Python-Laplace	Formal 3	valid	3.047
Python-Laplace	Formal 4	valid	2.906
Python-Laplace	Formal 5	valid	2.922
Python-Laplace	Pilot 1	valid	2.609
NONMEM-Laplace	Formal 1	valid	1.391
NONMEM-Laplace	Formal 2	valid	1.375
NONMEM-Laplace	Formal 3	valid	1.391
NONMEM-Laplace	Formal 4	valid	1.375
NONMEM-Laplace	Formal 5	valid	1.375
R aghq	Formal 1	valid	2.812
R aghq	Formal 2	valid	2.797
R aghq	Formal 3	valid	3
R aghq	Formal 4	valid	2.984
R aghq	Formal 5	valid	2.594
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C082

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	2.359
Python-Laplace	Formal 2	valid	2.297
Python-Laplace	Formal 3	valid	2.375
Python-Laplace	Formal 4	valid	2.281
Python-Laplace	Formal 5	valid	2.406
Python-Laplace	Pilot 1	valid	2.062
NONMEM-Laplace	Formal 1	valid	1.312
NONMEM-Laplace	Formal 2	valid	1.297
NONMEM-Laplace	Formal 3	valid	1.328
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.328
R aghq	Formal 1	valid	2.281
R aghq	Formal 2	valid	2.281
R aghq	Formal 3	valid	2.266
R aghq	Formal 4	valid	2.422
R aghq	Formal 5	valid	2.125
Virtual-patient MC	Unavailable	Unavailable	Unavailable

Statewise repeatability and numerical-check records.

OXC C083

Scenario results

Method	Run	Run status	Time (s)
Python-Laplace	Formal 1	valid	4.015
Python-Laplace	Formal 2	valid	4.359
Python-Laplace	Formal 3	valid	4.188
Python-Laplace	Formal 4	valid	3.781
Python-Laplace	Formal 5	valid	3.891
Python-Laplace	Pilot 1	valid	3.937
NONMEM-Laplace	Formal 1	valid	1.312
NONMEM-Laplace	Formal 2	valid	1.313
NONMEM-Laplace	Formal 3	valid	1.359
NONMEM-Laplace	Formal 4	valid	1.328
NONMEM-Laplace	Formal 5	valid	1.313
R aghq	Formal 1	valid	4.172
R aghq	Formal 2	valid	3.828
R aghq	Formal 3	valid	3.921
R aghq	Formal 4	valid	3.891
R aghq	Formal 5	valid	3.547
Virtual-patient MC	Archived web capture	not_assessed	Unavailable

Statewise repeatability and numerical-check records.

R aghq comparison records

R aghq comparisons by scenario. Scope labels are retained; comparison rules are in Online Resource 1, Section 5.

Reference Scenario

Scenario	Compared with R aghq	Scope	d-infinity	TV	d2	dH
C003	Python-Laplace	Included	0.0003471672017	0.0003471672017	0.0004431526171	0.0002942823017
C003	NONMEM-Laplace	Included	0.0003471575543	0.0003471575543	0.0004431387964	0.0002942761087
C003	Virtual-patient MC	Accepted	0.127197018	0.127197018	0.1744713341	0.2573183006

Sensitivity Scenarios

Scenario	Compared with R aghq	Scope	d-infinity	TV	d2	dH
C001	Python-Laplace	Included	5.657089806e-05	5.657089806e-05	7.783861267e-05	7.976196461e-05
C001	NONMEM-Laplace	Included	5.657136843e-05	5.657136843e-05	7.783930364e-05	7.976252257e-05
C002	Python-Laplace	Included	0.0003448493095	0.000381447358	0.0004426803842	0.0003052812781
C002	NONMEM-Laplace	Included	0.0003448458247	0.0003814445598	0.0004426763745	0.0003052793606
C004	Python-Laplace	Included	0.0003306065639	0.0003306065639	0.0004271134193	0.0002553149824
C004	NONMEM-Laplace	Included	0.0003306107436	0.0003306107436	0.0004271192228	0.0002553175151
C005	Python-Laplace	Included	0.0002349534852	0.0002349534852	0.0003277225657	0.0001763323143
C005	NONMEM-Laplace	Included	0.0002349535015	0.0002349535015	0.0003277225404	0.0001763322943
C006	Python-Laplace	Included	0.0001386817944	0.0001395278875	0.000183904792	0.0001614652608
C006	NONMEM-Laplace	Included	0.0001386812724	0.0001395273685	0.0001839040745	0.0001614649418
C007	Python-Laplace	Included	0.0004163226658	0.0004163226658	0.0005325237652	0.0003197665099
C007	NONMEM-Laplace	Included	0.000416323017	0.000416323017	0.000532524326	0.0003197666134
C008	Python-Laplace	Included	0.0002207168194	0.000275123995	0.0003150962203	0.0002578370978
C008	NONMEM-Laplace	Included	0.000220718508	0.0002751243375	0.0003150973591	0.0002578378401
C009	Python-Laplace	Included	0.0001110613646	0.0001363581847	0.0001492365562	9.888469611e-05
C009	NONMEM-Laplace	Included	0.0001110668006	0.0001363613128	0.000149241636	9.888715859e-05
C010	Python-Laplace	Included	0.0002568614027	0.0002622570875	0.0003389371191	0.0002686993373
C010	NONMEM-Laplace	Included	0.0002568586352	0.0002622548742	0.0003389335986	0.0002686977243
C011	Python-Laplace	Included	0.0003262377669	0.0003262377669	0.000418029221	0.0002873787334
C011	NONMEM-Laplace	Included	0.0003262404757	0.0003262404757	0.0004180328979	0.0002873808342
C012	Python-Laplace	Included	0.0003600424498	0.0003600424498	0.0004587560234	0.0002988491838
C012	NONMEM-Laplace	Included	0.0003600357316	0.0003600357316	0.0004587460422	0.0002988449842
C013	Python-Laplace	Included	0.0003830102643	0.0003830102643	0.000486790625	0.0003076718279
C013	NONMEM-Laplace	Included	0.0003830155001	0.0003830155001	0.0004867984131	0.0003076751769
C014	Python-Laplace	Included	0.0003662304851	0.0003778671008	0.0004553479673	0.0002821010616
C014	NONMEM-Laplace	Included	0.0003662346396	0.0003778701542	0.0004553522608	0.00028210434
C014	Virtual-patient MC	Accepted	0.2205922831	0.2205922831	0.2601074304	0.2902625841
C015	Python-Laplace	Included	0.0002293979806	0.0003045263429	0.0003375817181	0.0002977770469
C015	NONMEM-Laplace	Included	0.0002293949454	0.0003045231335	0.0003375786012	0.000297775517
C015	Virtual-patient MC	Accepted	0.1780586808	0.1780586808	0.2130257529	0.1530250707
C016	Python-Laplace	Included	0.0003859468814	0.0003859468814	0.0004916175838	0.000291788177
C016	NONMEM-Laplace	Included	0.0003859456837	0.0003859456837	0.0004916156607	0.0002917875573
C016	Virtual-patient MC	Accepted	0.06621953462	0.06946860234	0.08284660074	0.1880631285
C017	Python-Laplace	Included	0.0002315197198	0.0002315197198	0.0003005875267	0.0001963082334
C017	NONMEM-Laplace	Included	0.0002315197851	0.0002315197851	0.0003005876224	0.0001963082148
C017	Virtual-patient MC	Accepted	0.1450824446	0.1450824446	0.1944388184	0.1384404954
C018	Python-Laplace	Included	5.206945985e-14	5.206208728e-14	6.772065595e-14	3.72247675e-14
C018	NONMEM-Laplace	Included	1.67206804e-11	1.672068452e-11	2.062733669e-11	1.354684551e-11
C019	Python-Laplace	Included	7.254785513e-07	7.426738277e-07	9.05625452e-07	5.700388045e-07
C019	NONMEM-Laplace	Included	7.258334241e-07	7.430323284e-07	9.061217108e-07	5.701834266e-07
C020	Python-Laplace	Included	1.537331935e-05	1.537331935e-05	1.886695072e-05	1.455994468e-05
C020	NONMEM-Laplace	Included	1.537401834e-05	1.537401834e-05	1.886775381e-05	1.456034982e-05
C021	Python-Laplace	Included	0.0001286298891	0.0001286298891	0.0001565959981	0.0001039175974
C021	NONMEM-Laplace	Included	0.0001286329534	0.0001286329534	0.0001565998727	0.0001039197074
C022	Python-Laplace	Included	0.001307255619	0.001307255619	0.001637170475	0.001080361191
C022	NONMEM-Laplace	Included	0.001307257185	0.001307257185	0.001637172145	0.001080362068
C023	Python-Laplace	Included	0.002829539776	0.003454533216	0.003870955226	0.003442914284
C023	NONMEM-Laplace	Included	0.002829541789	0.003454535153	0.003870957949	0.003442915172
C024	Python-Laplace	Included	0.003621113695	0.005706622797	0.005810409589	0.004951258713
C024	NONMEM-Laplace	Included	0.003621096975	0.005706615461	0.005810398895	0.004951252314
C025	Python-Laplace	Included	0.002965710874	0.005391788986	0.005415395849	0.004375049262
C025	NONMEM-Laplace	Included	0.002965717996	0.005391791909	0.00541539896	0.004375049566

Scenario	Compared with R aghq	Scope	d-infinity	TV	d2	dH
C027	Python-Laplace	Included	3.701980904e-05	3.701980904e-05	4.752890366e-05	4.008774189e-05
C027	NONMEM-Laplace	Included	3.701031959e-05	3.701031959e-05	4.751588059e-05	4.008225324e-05
C027	Virtual-patient MC	Accepted	0.01565615103	0.01565615103	0.01949848441	0.07263231079
C028	Python-Laplace	Included	0.000305342149	0.000305342149	0.0003782659064	0.0003038812307
C028	NONMEM-Laplace	Included	0.0003053412399	0.0003053412399	0.0003782646578	0.0003038811867
C028	Virtual-patient MC	Accepted	0.02637324028	0.02638467887	0.03239009227	0.115261626
C029	Python-Laplace	Included	0.000470373616	0.0004727103439	0.0005946487502	0.000352471777
C029	NONMEM-Laplace	Included	0.0004703745219	0.0004727112499	0.0005946502793	0.000352472019
C029	Virtual-patient MC	Accepted	0.06588335169	0.06639087252	0.08984916104	0.1842652852
C030	Python-Laplace	Included	0.0001969915708	0.0001969915708	0.0002393148803	0.0001775981067
C030	NONMEM-Laplace	Included	0.000196990973	0.000196990973	0.0002393136867	0.0001775972874
C030	Virtual-patient MC	Accepted	0.2117091263	0.2487951463	0.2961730728	0.3683576549
C031	Python-Laplace	Included	7.766194545e-05	9.11409872e-05	0.0001097461617	7.662258397e-05
C031	NONMEM-Laplace	Included	7.766138122e-05	9.114264299e-05	0.0001097468594	7.662321131e-05
C032	Python-Laplace	Included	2.825830711e-05	2.825830711e-05	3.325915391e-05	2.440936073e-05
C032	NONMEM-Laplace	Included	2.825713331e-05	2.825713331e-05	3.325777439e-05	2.44083672e-05
C033	Python-Laplace	Included	1.531868728e-05	2.026884767e-05	2.229691721e-05	1.649869371e-05
C033	NONMEM-Laplace	Included	1.531852578e-05	2.026848953e-05	2.229671106e-05	1.649854756e-05
C033	Virtual-patient MC	Accepted	0.221298077	0.3037114154	0.3281073118	0.357408612
C034	Python-Laplace	Included	0.0004262171859	0.0004262171859	0.0005962223638	0.0003124148489
C034	NONMEM-Laplace	Included	0.0004262208664	0.0004262208664	0.000596227837	0.0003124175863
C034	Virtual-patient MC	Accepted	0.1201108988	0.1201108988	0.1553706969	0.1359000745
C035	Python-Laplace	Included	0.0003941401896	0.0003941401896	0.0005324506503	0.0002968502364
C035	NONMEM-Laplace	Included	0.0003941373572	0.0003941373572	0.0005324476553	0.0002968484999
C035	Virtual-patient MC	Accepted	0.06600185822	0.06804815305	0.08170840561	0.1860748667
C036	Python-Laplace	Included	0.0003139715769	0.0003140300289	0.0004435478456	0.0002926550766
C036	NONMEM-Laplace	Included	0.0003139675529	0.0003140260047	0.0004435420957	0.0002926513259
C036	Virtual-patient MC	Accepted	0.1769150047	0.1769150047	0.2483618742	0.3045647412
C037	Python-Laplace	Included	0.0002704603766	0.0002704603766	0.0003147823864	0.0003214805449
C037	NONMEM-Laplace	Included	0.0002704621243	0.0002704621243	0.0003147846617	0.0003214812212
C037	Virtual-patient MC	Accepted	0.1890572929	0.1890572929	0.2252018822	0.1702008683
C038	Python-Laplace	Included	7.091856864e-05	7.091859185e-05	0.000100177739	0.0001491776365
C038	NONMEM-Laplace	Included	7.091844791e-05	7.091847113e-05	0.0001001775678	0.0001491773844
C038	Virtual-patient MC	Accepted	0.02919350509	0.02919350509	0.04123337649	0.1212636348
C039	Python-Laplace	Included	0.0004166037645	0.0004166037645	0.0005752172766	0.0003043987748
C039	NONMEM-Laplace	Included	0.0004166040857	0.0004166040857	0.0005752175298	0.0003043989515
C039	Virtual-patient MC	Accepted	0.08474269231	0.08474269231	0.1034392841	0.1529106856
C040	Python-Laplace	Included	0.0004232243687	0.0004232243687	0.0005885359017	0.0003084194562
C040	NONMEM-Laplace	Included	0.0004232281464	0.0004232281464	0.0005885415209	0.0003084222035
C040	Virtual-patient MC	Accepted	0.09991534843	0.09991534843	0.1245302219	0.1417267247
C041	Python-Laplace	Included	0.0004230185363	0.0004230185363	0.0005944986869	0.0003154662582
C041	NONMEM-Laplace	Included	0.0004230179719	0.0004230179719	0.0005944979398	0.0003154658617
C041	Virtual-patient MC	Accepted	0.1351832728	0.1351832728	0.1801956372	0.1340642419
C042	Python-Laplace	Included	0.000410311294	0.000410311294	0.0005785880505	0.0003161417515
C042	NONMEM-Laplace	Included	0.0004103100279	0.0004103100279	0.0005785861843	0.0003161407337
C042	Virtual-patient MC	Accepted	0.1654186988	0.1654186988	0.2263426335	0.1536562334
C043	Python-Laplace	Included	0.0003732077804	0.0003732077804	0.0004927249624	0.0002937995372
C043	NONMEM-Laplace	Included	0.0003732023088	0.0003732023088	0.000492720805	0.0002937966003
C043	Virtual-patient MC	Accepted	0.09243929244	0.09243929244	0.1280975171	0.2191220443
C044	Python-Laplace	Included	0.0004093775321	0.0004093775321	0.0005613276361	0.000301314033
C044	NONMEM-Laplace	Included	0.0004093775243	0.0004093775243	0.0005613288613	0.0003013144055
C044	Virtual-patient MC	Accepted	0.04981958778	0.05103225988	0.06533358394	0.1611104922
C045	Python-Laplace	Included	0.0004050685808	0.0004050685808	0.0005715812955	0.0003157024124
C045	NONMEM-Laplace	Included	0.0004050721667	0.0004050721667	0.0005715862604	0.0003157051242

Scenario	Compared with R aghq	Scope	d-infinity	TV	d2	dH
C045	Virtual-patient MC	Accepted	0.1519675483	0.1519675483	0.208168331	0.1430664167
C046	Python-Laplace	Included	0.0003351948093	0.0003352877401	0.0004736595381	0.0002995850355
C046	NONMEM-Laplace	Included	0.0003351914336	0.0003352843642	0.0004736547105	0.0002995820148
C046	Virtual-patient MC	Accepted	0.1978773071	0.1978773071	0.2774569118	0.32308973
C047	Python-Laplace	Included	0.0003058230322	0.0003058230322	0.0004056663024	0.0002509569742
C047	NONMEM-Laplace	Included	0.000305822373	0.000305822373	0.000405665415	0.0002509564458
C047	Virtual-patient MC	Accepted	0.1928960655	0.1928960655	0.2598856643	0.2040052383
C048	Python-Laplace	Included	0.0003444838357	0.0003445384656	0.0004554682319	0.0002639201362
C048	NONMEM-Laplace	Included	0.0003444912571	0.000344545887	0.0004554783383	0.0002639256143
C048	Virtual-patient MC	Accepted	0.135457622	0.135457622	0.1748359928	0.1528792004
C049	Python-Laplace	Included	0.0003621572941	0.0003634487328	0.0004775800878	0.0002662251519
C049	NONMEM-Laplace	Included	0.0003621509061	0.0003634423521	0.0004775716735	0.0002662205344
C049	Virtual-patient MC	Accepted	0.1404995449	0.1404995449	0.1741580572	0.1804954624
C050	Python-Laplace	Included	0.0003404621489	0.0003498111861	0.0004677119588	0.0002652870269
C050	NONMEM-Laplace	Included	0.0003404592238	0.0003498081962	0.0004677086633	0.0002652850944
C050	Virtual-patient MC	Accepted	0.09053021454	0.09053021454	0.1224816584	0.2087890275
C051	Python-Laplace	Included	0.000388413081	0.000388413081	0.0004525845084	0.0003530794576
C051	NONMEM-Laplace	Included	0.0003884145759	0.0003884145758	0.0004525862666	0.0003530806392
C051	Virtual-patient MC	Accepted	0.1563826469	0.1739284195	0.214027282	0.3031422755
C052	Python-Laplace	Included	0.0004223264468	0.0004223264468	0.0005059496554	0.0004005602298
C052	NONMEM-Laplace	Included	0.0004223253515	0.0004223253515	0.0005059491886	0.0004005597955
C052	Virtual-patient MC	Accepted	0.1229755292	0.1463210001	0.1700239644	0.1851378847
C053	Python-Laplace	Included	0.0004253256457	0.0004558800455	0.0005465907871	0.0004095960946
C053	NONMEM-Laplace	Included	0.0004253252205	0.0004558807419	0.0005465909407	0.0004095962321
C053	Virtual-patient MC	Accepted	0.1310032731	0.158758288	0.1758945227	0.2102535343
C054	Python-Laplace	Included	0.0003876636316	0.0004606190548	0.0005335088727	0.0003799380622
C054	NONMEM-Laplace	Included	0.0003876655005	0.0004606184956	0.0005335093871	0.0003799383871
C054	Virtual-patient MC	Accepted	0.1241487711	0.1671721152	0.177686586	0.2381564088
C055	Python-Laplace	Included	0.0001583334345	0.0001634012747	0.0001972274712	0.0001213712081
C055	NONMEM-Laplace	Included	0.0001583253063	0.0001633932631	0.0001972169699	0.0001213666123
C056	Python-Laplace	Included	0.0003473388507	0.0003473388507	0.0004512634729	0.0002932766249
C056	NONMEM-Laplace	Included	0.0003473364933	0.0003473364933	0.0004512602528	0.0002932749957
C057	Python-Laplace	Included	0.000462409772	0.0004774937745	0.0006013957188	0.0003584152972
C057	NONMEM-Laplace	Included	0.0004624160434	0.0004775000714	0.0006014045728	0.0003584194783
C058	Python-Laplace	Included	0.0002117342521	0.0002132339944	0.0002612029437	0.0001667878764
C058	NONMEM-Laplace	Included	0.0002117257372	0.0002132255156	0.0002611928153	0.0001667800188
C059	Python-Laplace	Included	0.0003030742716	0.0003030742716	0.0003881083205	0.0002748365917
C059	NONMEM-Laplace	Included	0.0003030728809	0.0003030728809	0.0003881060653	0.0002748369702
C060	Python-Laplace	Included	0.0003664720454	0.0003664720454	0.0004340865719	0.0005013272922
C060	NONMEM-Laplace	Included	0.0003664730492	0.0003664730492	0.0004340892301	0.0005013276697
C060	Virtual-patient MC	Accepted	0.2310927207	0.2381055248	0.2922948542	0.3567894226
C061	Python-Laplace	Included	0.0002408858501	0.0002408858501	0.0002936117688	0.0003252568187
C061	NONMEM-Laplace	Included	0.000240879461	0.000240879461	0.0002936026555	0.0003252533015
C061	Virtual-patient MC	Accepted	0.1624713532	0.1657877339	0.2203368294	0.2957076388
C062	Python-Laplace	Included	0.0003683722319	0.0003683722319	0.0004796235481	0.0002738467965
C062	NONMEM-Laplace	Included	0.000368361777	0.000368361777	0.0004796090527	0.0002738396052
C062	Virtual-patient MC	Accepted	0.08322172269	0.08322172269	0.1164098918	0.2092431549
C063	Python-Laplace	Included	0.0003201346546	0.0003201346546	0.0004184396353	0.0002492060067
C063	NONMEM-Laplace	Included	0.0003201255068	0.0003201255068	0.0004184270934	0.0002491991207
C063	Virtual-patient MC	Accepted	0.06502127577	0.06502127577	0.08745172607	0.1769496404
C064	Python-Laplace	Included	0.0002076262042	0.0002076262042	0.0002719458917	0.0001976547577
C064	NONMEM-Laplace	Included	0.0002076202392	0.0002076202392	0.0002719377848	0.0001976491206
C064	Virtual-patient MC	Accepted	0.03270812851	0.03270812851	0.04529798622	0.1289246531
C065	Python-Laplace	Included	0.0003368823376	0.0003368823376	0.0004470711233	0.0002497525967

Scenario	Compared with R aghq	Scope	d-infinity	TV	d2	dH
C065	NONMEM-Laplace	Included	0.0003368726256	0.0003368726256	0.0004470570934	0.0002497452257
C066	Python-Laplace	Included	0.0003750520192	0.0003750520192	0.0005044199357	0.0003097132223
C066	NONMEM-Laplace	Included	0.0003750407285	0.0003750407285	0.0005044040342	0.0003097064043
C067	Python-Laplace	Included	0.0003108407847	0.0003108407847	0.0003950084239	0.0003240670757
C067	NONMEM-Laplace	Included	0.0003108366214	0.0003108366214	0.0003950028253	0.0003240643835
C068	Python-Laplace	Included	4.887263709e-05	4.887263709e-05	6.117614541e-05	0.0001778467708
C068	NONMEM-Laplace	Included	4.887279662e-05	4.887279662e-05	6.117517974e-05	0.0001778468957
C069	Python-Laplace	Included	0.0002874293397	0.000366924761	0.0004032183123	0.0002921389619
C069	NONMEM-Laplace	Included	0.0002874242415	0.0003669214797	0.0004032129797	0.0002921370597
C070	Python-Laplace	Included	0.0002496516845	0.0002496516845	0.000297818168	0.0002581902946
C070	NONMEM-Laplace	Included	0.0002496454158	0.0002496454158	0.0002978099056	0.0002581883932
C071	Python-Laplace	Included	0.0006135141207	0.0006511945466	0.0008055135778	0.0004806493231
C071	NONMEM-Laplace	Included	0.0006135075806	0.0006511880565	0.0008055049443	0.0004806450877
C072	Python-Laplace	Included	0.0004637738683	0.0004637738683	0.000614741183	0.0004038022456
C072	NONMEM-Laplace	Included	0.0004637727046	0.0004637727046	0.0006147397416	0.0004038014083
C073	Python-Laplace	Included	0.0002134092942	0.0002855254238	0.0003105365688	0.0004120876089
C073	NONMEM-Laplace	Included	0.0002134035946	0.0002855199606	0.0003105309298	0.0004120852915
C074	Python-Laplace	Included	0.0003508160169	0.0003508160169	0.0004455038687	0.0002884275235
C074	NONMEM-Laplace	Included	0.0003508145342	0.0003508145342	0.0004455019014	0.0002884267151
C075	Python-Laplace	Included	0.0003552076051	0.0003552076051	0.0004527640995	0.0002939018612
C075	NONMEM-Laplace	Included	0.0003552079629	0.0003552079629	0.0004527638588	0.0002939021054
C076	Python-Laplace	Included	0.0003237883897	0.0003237883897	0.0004128848344	0.0002878920199
C076	NONMEM-Laplace	Included	0.0003237918368	0.0003237918368	0.0004128896761	0.0002878944086
C077	Python-Laplace	Included	0.000283043634	0.000283043634	0.0003595696779	0.0002732958589
C077	NONMEM-Laplace	Included	0.0002830470456	0.0002830470456	0.0003595733942	0.0002732981621
C078	Python-Laplace	Included	0.0004630471808	0.0004630471808	0.0005729233768	0.0003596435358
C078	NONMEM-Laplace	Included	0.0004630506529	0.0004630506529	0.0005729275281	0.0003596456767
C079	Python-Laplace	Included	0.0004124263735	0.0004124263735	0.0005189785205	0.0003278905523
C079	NONMEM-Laplace	Included	0.0004124271002	0.0004124271002	0.000518978862	0.0003278911323
C080	Python-Laplace	Included	0.000266955782	0.000266955782	0.0003444708548	0.0002616137885
C080	NONMEM-Laplace	Included	0.0002669636629	0.0002669636629	0.0003444815186	0.0002616191474
C081	Python-Laplace	Included	0.0001777553218	0.0001930201126	0.0002340202648	0.0002405439708
C081	NONMEM-Laplace	Included	0.0001777543426	0.000193015154	0.000234016235	0.000240542707
C082	Python-Laplace	Included	5.940143943e-05	5.940143943e-05	8.400632127e-05	0.0001939611615
C082	NONMEM-Laplace	Included	5.940188522e-05	5.940188522e-05	8.400695171e-05	0.0001939626153
C083	Python-Laplace	Included	0.0002111684131	0.000333100908	0.0003165444696	0.0002868497379
C083	NONMEM-Laplace	Included	0.0002111634679	0.0003330990814	0.0003165425783	0.0002868482988

Summary across sensitivity scenarios

Output availability

Method	Scenarios with five valid outputs	No-output scenarios
Python Laplace	82/82	None
NONMEM Laplace	82/82	None
R aghq	81/82	C026

Cross-method agreement

NONMEM vs R aghq

Metric	n	Median	P95	Maximum	Scenario
d_∞	81	3.30611×10^{-4}	6.13508×10^{-4}	3.62110×10^{-3}	C024
TV	81	3.35284×10^{-4}	6.51188×10^{-4}	5.70662×10^{-3}	C024
d_2	81	4.34089×10^{-4}	8.05505×10^{-4}	5.81040×10^{-3}	C024
d_H	81	2.91788×10^{-4}	5.01328×10^{-4}	4.95125×10^{-3}	C024

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.

Python vs NONMEM

Metric	n	Median	P95	Maximum	Scenario
d_∞	82	3.06003×10^{-9}	1.04066×10^{-8}	1.18987×10^{-4}	C026
TV	82	3.14183×10^{-9}	1.04252×10^{-8}	1.18987×10^{-4}	C026
d_2	82	4.01975×10^{-9}	1.42440×10^{-8}	1.67028×10^{-4}	C026
d_H	82	2.64446×10^{-9}	7.83878×10^{-9}	9.49449×10^{-5}	C026

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.

Python vs R aghq

Metric	n	Median	P95	Maximum	Scenario
d_∞	81	3.30607×10^{-4}	6.13514×10^{-4}	3.62111×10^{-3}	C024
TV	81	3.35288×10^{-4}	6.51195×10^{-4}	5.70662×10^{-3}	C024
d_2	81	4.34087×10^{-4}	8.05514×10^{-4}	5.81041×10^{-3}	C024
d_H	81	2.91788×10^{-4}	5.01327×10^{-4}	4.95126×10^{-3}	C024

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.

Virtual-patient comparisons

NONMEM vs Virtual patient

Metric	n	Median	P95	Maximum	Scenario
d_∞	36	0.127628	0.221045	0.231293	C060
TV	36	0.137872	0.241043	0.303710	C033
d_2	36	0.174037	0.293453	0.328104	C033
d_H	36	0.182179	0.357116	0.368483	C030

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.

Python vs Virtual patient

Metric	n	Median	P95	Maximum	Scenario
d_∞	36	0.127628	0.221045	0.231293	C060
TV	36	0.137872	0.241043	0.303710	C033
d_2	36	0.174037	0.293453	0.328104	C033
d_H	36	0.182179	0.357116	0.368483	C030

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.

R aghq vs Virtual patient

Metric	n	Median	P95	Maximum	Scenario
d_∞	35	0.131003	0.220804	0.231093	C060
TV	35	0.140500	0.241312	0.303711	C033
d_2	35	0.174836	0.293458	0.328107	C033
d_H	35	0.184265	0.356975	0.368358	C030

d_∞, maximum absolute probability difference; TV, total variation; d_2, Euclidean distance; d_H, Hellinger distance.

P95 uses linear interpolation (R type 7). Virtual-patient comparisons use archived display values under matched visible settings.