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

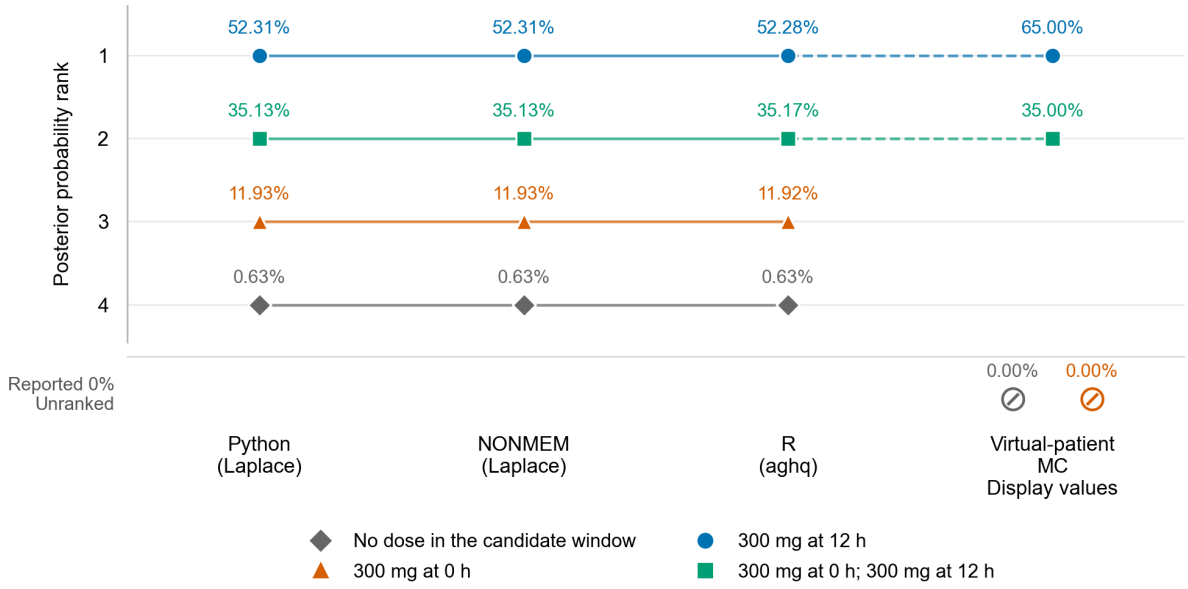
SD, sample standard deviation; raw, before normalization; norm., after normalization. Maxima are taken across candidate states.

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.



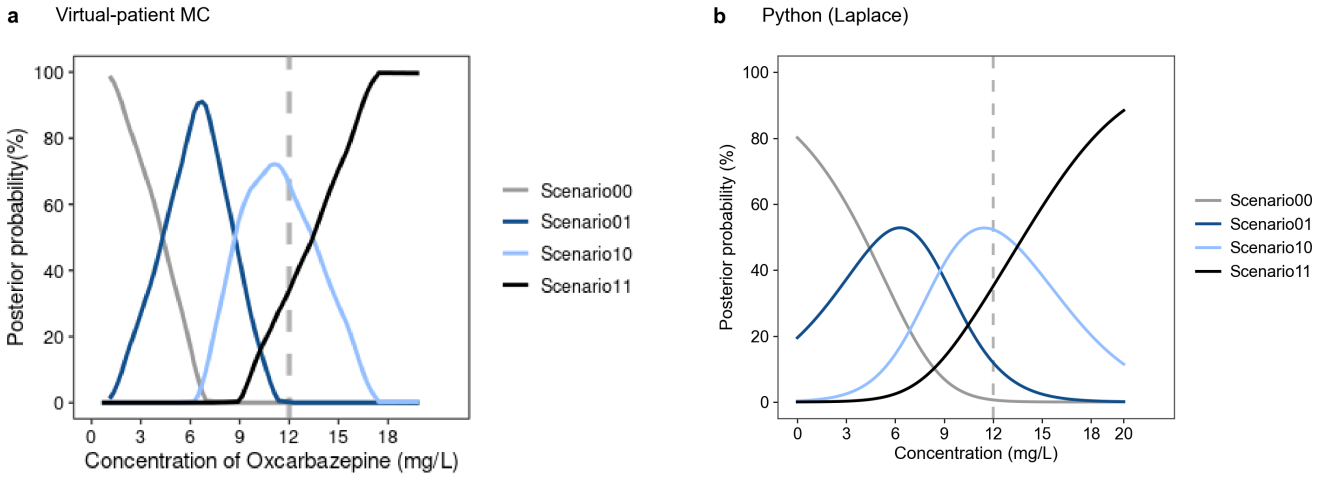
Candidate-state rankings. Slashed circles denote reported zeros, shown without ranks.

Posterior probability summaries

Candidate state and dosing history	Python Laplace	NONMEM Laplace	R aghq	Virtual patient
ω_{00}: Neither dose taken	0.00629656	0.00629656	0.00626151	0
ω_{01}: 0 h dose only	0.11928606	0.11928606	0.11924385	0
ω_{10}: 12 h dose only	0.52307289	0.52307288	0.52280298	0.65
ω_{11}: Both doses taken	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	0.30	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 12 mg/L. Panel (a) retains the source axis label; the observed analyte is MHD. Source for (a): virtual-patient Dashboard.