

Supplementary Information for BEAM-1: A Biophysics-Informed Multiscale Mathematical Framework for CNS Pharmaceutical Permeability

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July 2026

Overview of Supplementary Material

The following is supplementary information for the research paper: *BEAM-1: A Biophysics-Informed Multiscale Mathematical Framework for CNS Pharmaceutical Permeability*. The structure of this document consists of tables from each ordered section of the main paper labeled numerically. For convenience, all tables, pseudocode, and images from the original paper have been reproduced along with supplementary tables not included in the main paper. Please contact nithik.bioresearch@gmail.com for clarification or questions.

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Table S1: Physical Constants and Parameters for BBB Framework

Parameter Name	Value	Units
Blood-Brain Barrier Thickness (x)	200	nm
Standard Extracellular Temperature (T)	310	K
Blood-Brain Barrier Viscosity (η)	0.004	Pa·s
Concentration Traveled (dC)	1	mol/m ³
Boltzmann Constant (k_B)	1.3806×10^{-23}	m ² · kg · s ⁻² · K ⁻¹

Table S2: Physicochemical Properties of the 25 FDA-Approved Medications

#	Name	Formula	MW (Da)	WPC/OPC	Polarity	HBA	HBD
0	Levodopa	C ₉ H ₁₁ NO ₄	197.19	-2.7	Polar	5	4
1	Carbidopa	C ₁₀ H ₁₄ N ₂ O ₄	226.23	-2.2	Polar	6	5
2	Levetiracetam	C ₈ H ₁₄ N ₂ O ₂	170.21	-0.3	Slightly Polar	2	1
3	Gabapentin	C ₉ H ₁₇ NO ₂	171.24	-1.1	Polar	3	2
4	Phenobarbital	C ₁₂ H ₁₂ N ₂ O ₃	232.23	1.5	Nonpolar	3	2
5	Phenytoin	C ₁₅ H ₁₂ N ₂ O ₂	252.27	2.5	Nonpolar	2	2
6	Diazepam	C ₁₆ H ₁₃ ClN ₂ O	284.74	3.0	Nonpolar	2	0
7	Buspirone	C ₂₁ H ₃₁ N ₅ O ₂	385.50	2.6	Nonpolar	6	0
8	Ceftriaxone	C ₁₈ H ₁₈ N ₈ O ₇ S ₃	554.60	-1.3	Polar	13	4
9	Vancomycin	C ₆₆ H ₇₅ Cl ₂ N ₉ O ₂₄	1449.20	-2.6	Polar	26	19
10	Fluconazole	C ₁₃ H ₁₂ F ₂ N ₆ O	306.27	0.4	Slightly Nonpolar	7	1
11	Temozolomide	C ₆ H ₆ N ₆ O ₂	194.15	-1.1	Polar	5	1
12	Lomustine	C ₉ H ₁₆ ClN ₃ O ₂	233.69	2.8	Nonpolar	3	1
13	Methotrexate	C ₂₀ H ₂₂ N ₈ O ₅	454.40	-1.8	Polar	12	5
14	Carmustine	C ₅ H ₉ Cl ₂ N ₃ O ₂	214.05	1.5	Nonpolar	3	1
15	Etoposide	C ₂₉ H ₃₂ O ₁₃	588.60	0.6	Slightly Nonpolar	13	3
16	Vorafenib	C ₁₄ H ₁₃ ClF ₆ N ₆	414.74	5.3	Nonpolar	12	2
17	Tovorafenib	C ₁₇ H ₁₂ Cl ₂ F ₃ N ₇ O ₂ S	506.30	3.0	Nonpolar	11	3
18	Dexamethasone	C ₂₂ H ₂₉ FO ₅	392.50	1.9	Nonpolar	6	3
19	Metronidazole	C ₆ H ₉ N ₃ O ₃	171.15	0.0	Slightly Nonpolar	4	1
20	Doxorubicin	C ₂₇ H ₂₉ NO ₁₁	543.50	1.3	Nonpolar	12	6
21	Paclitaxel	C ₄₇ H ₅₁ NO ₁₄	853.90	2.5	Nonpolar	14	4
22	Erlotinib	C ₂₂ H ₂₃ N ₃ O ₄	393.40	3.3	Nonpolar	7	1
23	Loperamide	C ₂₉ H ₃₃ ClN ₂ O ₂	477.00	5.0	Nonpolar	3	1
24	Gefitinib	C ₂₂ H ₂₄ ClFN ₄ O ₃	446.90	4.1	Nonpolar	8	1

Algorithm S1 Polarity Categorization based on XlogP

```

1: procedure CLASSIFYPOLARITY( $XlogP$ )
2:   if  $XlogP < -1$  then
3:     return "Polar"
4:   else if  $XlogP > 1$  then
5:     return "Nonpolar"
6:   else if  $-1 \leq XlogP \leq 0$  then
7:     return "Slightly Polar"
8:   else if  $0 \leq XlogP \leq 1$  then
9:     return "Slightly Nonpolar"
10:  end if
11: end procedure

```

Table S3: Calculated Chemical Transport Properties

#	Name	Radii	$D_{constant}$	MW	#	Name	Radii	$D_{constant}$	MW
0	Levodopa	2.698	2.104	197.19	13	Methotrexate	3.607	1.574	454.40
1	Carbidopa	2.830	2.006	226.23	14	Carmustine	2.647	2.145	214.05
2	Levetiracetam	2.677	2.121	170.21	15	Etoposide	3.806	1.491	588.60
3	Gabapentin	2.660	2.134	171.24	16	Vorasidenib	3.246	1.749	414.74
4	Phenobarbital	2.993	1.897	232.23	17	Tovorafenib	3.535	1.606	506.30
5	Phenytoin	3.132	1.812	252.27	18	Dexamethasone	3.432	1.654	392.50
6	Diazepam	3.267	1.738	284.74	19	Metronidazole	2.579	2.201	171.15
7	Buspirone	3.610	1.572	385.50	20	Doxorubicin	3.747	1.515	543.50
8	Ceftriaxone	3.761	1.509	554.60	21	Paclitaxel	4.428	1.282	853.90
9	Vancomycin	5.160	1.100	1449.2	22	Erlotinib	3.535	1.606	393.40
10	Fluconazole	3.038	1.869	306.27	23	Loperamide	3.834	1.481	477.00
11	Temozolomide	2.601	2.182	194.15	24	Gefitinib	3.640	1.559	446.90
12	Lomustine	2.861	1.984	233.69					

Spherical Radii and Diffusion Constants are scaled by 10^{-10} . For all compounds, $\beta_{constant} = 1$.

Table S4: Model Coefficients of Transformed Temporal Quadratic

$$f(t) = \alpha t^2 + \rho t + \epsilon$$

#	Name	J-Mag	α	ρ	#	Name	J-Mag	α	ρ
0	Levodopa	0.0010	-10.52	1.05	13	Methotrexate	0.0008	-7.87	0.79
1	Carbidopa	0.0010	-10.03	1.00	14	Carmustine	0.0011	-10.72	1.07
2	Levetiracetam	0.0011	-10.60	1.06	15	Etoposide	0.0007	-7.46	0.75
3	Gabapentin	0.0011	-10.67	1.07	16	Vorasidenib	0.0009	-8.74	0.87
4	Phenobarbital	0.0009	-9.48	0.95	17	Tovorafenib	0.0008	-8.03	0.80
5	Phenytoin	0.0009	-9.06	0.91	18	Dexamethasone	0.0008	-8.27	0.83
6	Diazepam	0.0009	-8.69	0.87	19	Metronidazole	0.0011	-11.01	1.10
7	Buspirone	0.0008	-7.86	0.79	20	Doxorubicin	0.0008	-7.58	0.76
8	Ceftriaxone	0.0008	-7.55	0.75	21	Paclitaxel	0.0006	-6.41	0.64
9	Vancomycin	0.0006	-5.50	0.55	22	Erlotinib	0.0008	-8.03	0.80
10	Fluconazole	0.0009	-9.34	0.93	23	Loperamide	0.0007	-7.40	0.74
11	Temozolomide	0.0011	-10.91	1.09	24	Gefitinib	0.0008	-7.80	0.78
12	Lomustine	0.0010	-9.92	0.99					

ρ values are scaled by 10^{-12} . All ϵ Brownian constants = 20.

Table S5: Calculated Molecular Diffused Area for Compounds

#	Name	Area	#	Name	Area
0	Levodopa	9.5617	13	Methotrexate	9.6722
1	Carbidopa	9.5822	14	Carmustine	9.5532
2	Levetiracetam	9.5582	15	Etoposide	9.6893
3	Gabapentin	9.5554	16	Vorasidenib	9.6357
4	Phenobarbital	9.6049	17	Tovorafenib	9.6655
5	Phenytoin	9.6224	18	Dexamethasone	9.6554
6	Diazepam	9.6380	19	Metronidazole	9.5414
7	Buspirone	9.6724	20	Doxorubicin	9.6844
8	Ceftriaxone	9.6855	21	Paclitaxel	9.7329
9	Vancomycin	9.7708	22	Erlotinib	9.6654
10	Fluconazole	9.6107	23	Loperamide	9.6916
11	Temozolomide	9.5454	24	Gefitinib	9.6751
12	Lomustine	9.5867			

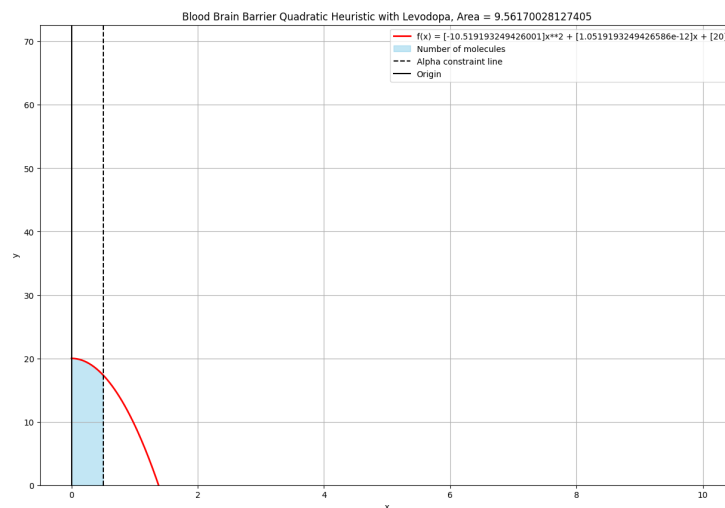


Figure S1: Area Graph of Levodopa Molecule after $\lambda = 0.5$

Table S6: Min-Max Normalized Transport Parameters

#	Name	J-Mag	Area	MW	#	Name	J-Mag	Area	MW
0	Levodopa	.9114	.0886	.0211	13	Methotrexate	.4300	.5700	.2222
1	Carbidopa	.8223	.1777	.0438	14	Carmustine	.9485	.0515	.0343
2	Levetiracetam	.9268	.0732	.0000	15	Etoposide	.3553	.6447	.3271
3	Gabapentin	.9388	.0612	.0008	16	Vorasidenib	.5889	.4111	.1912
4	Phenobarbital	.7233	.2767	.0485	17	Tovorafenib	.4592	.5408	.2628
5	Phenytoin	.6468	.3532	.0642	18	Dexamethasone	.5030	.4970	.1738
6	Diazepam	.5789	.4211	.0895	19	Metronidazole	1.000	.0000	.0007
7	Buspirone	.4288	.5712	.1683	20	Doxorubicin	.3769	.6231	.2919
8	Ceftriaxone	.3717	.6283	.3005	21	Paclitaxel	.1653	.8347	.5346
9	Vancomycin	.0000	1.000	1.000	22	Erlotinib	.4593	.5407	.1745
10	Fluconazole	.6979	.3021	.1064	23	Loperamide	.3455	.6545	.2399
11	Temozolomide	.9826	.0174	.0187	24	Gefitinib	.4171	.5829	.2163
12	Lomustine	.8026	.1974	.0496					

Table S7: Overall nDPI Score Distributions through H(x) function

#	Chemical Name	Value	#	Chemical Name	Value
0	Levodopa	5.2186	13	Methotrexate	3.4035
1	Carbidopa	4.8341	14	Carmustine	5.0904
2	Levetiracetam	4.8331	15	Etoposide	2.8479
3	Gabapentin	5.0191	16	Vorasidenib	4.5716
4	Phenobarbital	4.4003	17	Tovorafenib	3.6769
5	Phenytoin	4.3440	18	Dexamethasone	3.6898
6	Diazepam	4.2091	19	Metronidazole	4.9953
7	Buspirone	3.6047	20	Doxorubicin	3.0800
8	Ceftriaxone	3.0557	21	Paclitaxel	2.4289
9	Vancomycin	1.4866	22	Erlotinib	3.8222
10	Fluconazole	4.0588	23	Loperamide	3.7359
11	Temozolomide	5.1326	24	Gefitinib	3.8047
12	Lomustine	4.8826			

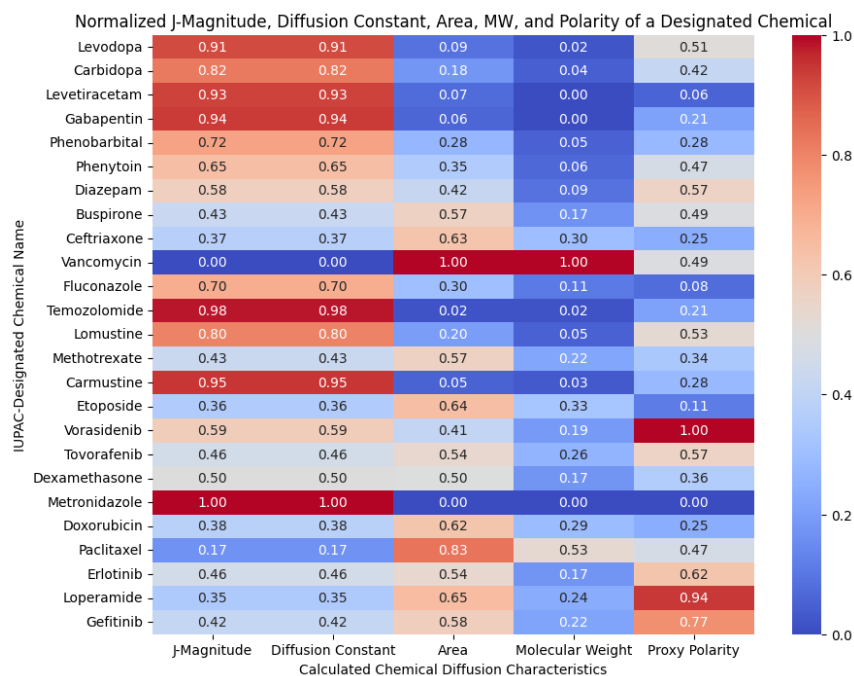


Figure S2: Visual representation of the heat map distribution.

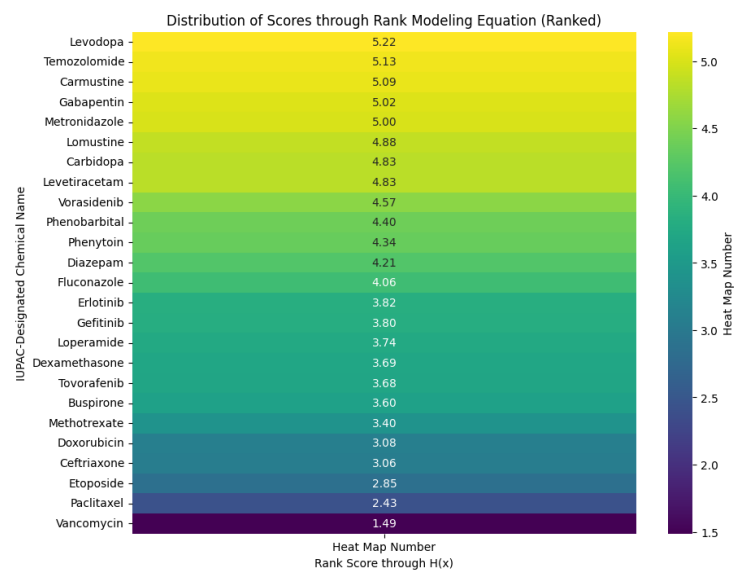


Figure S3: Overall nDPI-Scale Scores

Table S8: Canonical SMILES Notation for the 25 FDA-Approved Medications

#	Name	SMILES
0	Levodopa	<chem>C1=CC(=C(C=C1CC(C(=O)O)N)O)O</chem>
1	Carbidopa	<chem>CC(CN)(C(=O)O)NN.O</chem>
2	Levetiracetam	<chem>CCC(C(=O)N)N1CCCC1=O</chem>
3	Gabapentin	<chem>C1CCC(CC1)(CC(=O)O)CN</chem>
4	Phenobarbital	<chem>CCC1(C(=O)NC(=O)NC1=O)C2=CC=CC=C2</chem>
5	Phenytoin	<chem>C1=CC=C(C=C1)C2(C(=O)NC(=O)N2)C3=CC=CC=C3</chem>
6	Diazepam	<chem>CN1C(=O)CN=C(C2=CC=CC=C21)C3=CC=CC=C3Cl</chem>
7	Buspirone	<chem>C1CC(=O)N(C(=O)C1)CCCCN2CCN(CC2)C3=NC=CC=N3</chem>
8	Ceftriaxone	<chem>CON=C(C1=CSC(=N1)N)C(=O)NC2C3N(C2=O)C(=C(CS3)CS C4=NC(=O)C(=O)NN4C)C(=O)O</chem>
9	Vancomycin	<chem>CC1C(C(CC(O1)OC2C(C(C(OC2OC3=C4C=C5C=C3OC6=C(C =C(C=C6)C(C(C(=O)NC(C(=O)NC5C(=O)NC7C(=O)NC(C8= CC(=C(C=C8C9=C(C=CC(=C9)C(C(C(=O)N7)NC(=O)C(C(C 1=CC(=C(O4)C=C1)Cl)O)NC(=O)C(CC(=O)N)NC(=O)C(CC1 =CC=C(C=C1)O)NC)O)O)Cl)CO)C(=O)O)NC(=O)C)O)N)C O)O</chem>
10	Fluconazole	<chem>C1=CC(=C(C=C1F)F)C(CN2C=NC=N2)(CN3C=NC=N3)O</chem>
11	Temozolomide	<chem>CN1C(=O)N2C=NC(=C2N=N1)C(=O)N</chem>
12	Lomustine	<chem>C1CCC(CC1)NC(=O)N(CCC1)N=O</chem>
13	Methotrexate	<chem>CN(CC1=CN=C2C(=N1)C(=NC(=N2)N)N)C3=CC=C(C=C3)C (=O)NC(CCC(=O)O)C(=O)O</chem>
14	Carmustine	<chem>C(CCl)NC(=O)N(CCC1)N=O</chem>
15	Etoposide	<chem>CC1OC2COC3C(C2C(O1)O)OCC4=CC5=C(C=C34)OCO5</chem>
16	Vorasidenib	<chem>C1=CC(=CC=C1F)C2=NC(=NC(=N2)N3CCC(CC3)F)NC4=C C=CC(=C4Cl)F</chem>
17	Tovorafenib	<chem>CN1C=C(C2=CC=CC=C21)C3=NC(=C(N=C3)N)C4=NN(C5= CC=CC=C54)S(=O)(=O)C</chem>
18	Dexamethasone	<chem>CC1CC2C3CCC4=CC(=O)C=CC4(C3(C(CC2(C1(C(=O)CO)O) C)O)F)C</chem>
19	Metronidazole	<chem>CC1=NC=C(N1CCO)[N+](=O)[O-]</chem>
20	Doxorubicin	<chem>CC1C(C(CC(O1)OC2CC(CC3=C2C(=C4C(=C3O)C(=O)C5=C(C4=O)C=CC=C5OC)O)(C(=O)CO)O)N)O</chem>
21	Paclitaxel	<chem>CC1=C2C(C(=O)C3(C(CC4C(C3C(C(C2(C)C)(CC1OC(=O)C(C (C5=CC=CC=C5)NC(=O)C6=CC=CC=C6)O)O)OC(=O)C7=C C=CC=C7)(CO4)OC(=O)C)O)C)OC(=O)C</chem>
22	Erlotinib	<chem>COCCOC1=C(C=C2C(=C1)C(=NC=N2)NC3=CC=CC(=C3)C #C)OCCOC</chem>
23	Loperamide	<chem>CCC1(CCN(CC1)CCC(C2=CC=CC=C2)(C3=CC=CC=C3)O)C (=O)N(C)C</chem>
24	Gefitinib	<chem>COC1=CC2=C(C(C=C1OCCCN3CCOCC3)N=CN=C2NC4=CC(= C(C=C4)F)Cl</chem>

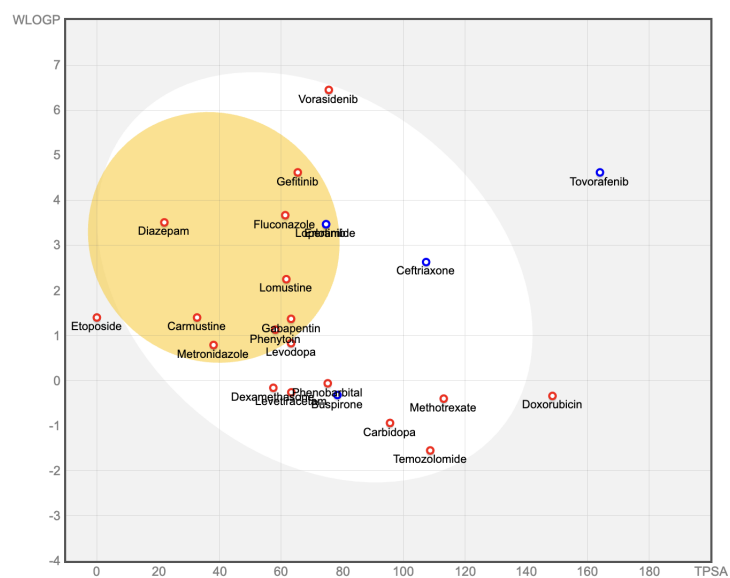


Figure S4: BOILED-Egg Throughput

Table S9: BBB+/BBB- Boiled Egg Test Results Summary

Rank	BBB+/BBB- Boiled Egg Test
1: Levodopa	No
2: Temozolomide	No
3: Carmustine	Yes
4: Gabapentin	Yes
5: Metronidazole	Yes
6: Lomustine	Yes
7: Carbidopa	No
8: Levetiracetam	No
9: Vorasidenib	No
10: Phenobarbital	No
11: Phenytoin	Yes
12: Diazepam	Yes
13: Flucanazole	Yes
14: Erlotinib	Yes
15: Gefitinib	Yes
16: Loperamide	Yes
17: Dexamethasone	No
18: Tovorafenib	No
19: Buspirone	No
20: Methotrexate	No
21: Doxorubicin	No
22: Ceftriaxone	No
23: Etoposide	Yes
24: Paclitaxel	No
25: Vancomycin	No

Table S10: H(x) Score and B3DB BBB+/BBB- Classification for 19 Drugs

Drug	H(x)	BBB+/BBB-	Drug	H(x)	BBB+/BBB-
Levodopa	5.2186	BBB+	Fluconazole	4.0588	BBB+
Carbidopa	4.8341	BBB-	Temozolomide	5.1326	BBB+
Levetiracetam	4.8331	BBB+	Lomustine	4.8826	BBB+
Gabapentin	5.0191	BBB+	Methotrexate	3.4035	BBB-
Phenobarbital	4.4003	BBB+	Etoposide	2.8479	BBB-
Phenytoin	4.3440	BBB+	Dexamethasone	3.6898	BBB+
Diazepam	4.2091	BBB+	Metronidazole	4.9953	BBB+
Buspirone	3.6047	BBB+	Doxorubicin	3.0800	BBB-
Ceftriaxone	3.0557	BBB-	Gefitinib	3.8047	BBB+
Vancomycin	1.4866	BBB-			