

Supplementary Material

Investigating the Antimicrobial Efficacy of Cannabinoids and Their Derivatives Against *Neisseria Gonorrhoeae* by Computational Analysis

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Supplementary Table:

Supplementary Table S1: Protein-Ligand Interactions.

Protein	Hydrophobic Interactions					Hydrogen Bonds						
	Residue	AA	Distance	Ligand Atom	Protein Atom	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Donor Atom	Acceptor Atom
1,3-Benzenediol, 2-[3-methyl-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl-, (1R-trans)-	134A	TYR	3.78	3131	1182	331A	PHE	3.02	3.74	132.19	3125 [O3]	3072 [O2]
	134A	TYR	3.99	3130	1184							
	164A	ARG	3.77	3116	1463							
	213A	ASP	3.9	3119	1925							
	331A	PHE	3.71	3111	3074							

	331A	PHE	3.57	3110	3073							
	331A	PHE	3.73	3131	3077							
	331A	PHE	3.46	3128	3075							
	145A	ARG	3.59	3134	1279	164A	ARG	2.27	3.17	145.48	1458 [Nam]	3121 [O3]
	147A	TYR	3.35	3119	1306	214A	THR	2.22	2.9	128.17	1936 [O3]	3121 [O3]
	147A	TYR	3.84	3134	1308	214A	THR	2.48	2.9	106.12	3121 [O3]	1936 [O3]
Ferruginene C	164A	ARG	3.71	3110	1463	332A	THR	3.28	4.09	142.37	3130 [O3]	3084 [O2]
	166A	ARG	3.3	3109	1496	334A	SER	2.03	2.95	147.54	3097 [Nam]	3130 [O3]
	331A	PHE	3.63	3119	3079							
	331A	PHE	3.44	3117	3078							
	331A	PHE	3.8	3114	3076							
Dronabinol	164A	ARG	3.38	3111	1462	331A	PHE	2.14	3.04	152.73	3129 [O3]	3072 [O2]
	331A	PHE	3.74	3114	3073							
Cannabinolic acid A (CBNA)	331A	PHE	3.72	3127	3076	147A	TYR	3.14	3.9	135.16	3133 [O3]	1311 [O3]
	331A	PHE	3.63	3129	3073	164A	ARG	2.43	3.18	129.7	1458 [Nam]	3133 [O3]
	134A	TYR	3.49	3130	1184	146A	SER	2.94	3.84	147.89	1292 [Nam]	3107 [O3]
Cannabigerolic acid (CBGA)	147A	TYR	3.92	3118	1308	332A	THR	1.85	2.68	139.57	3134 [O3]	3084 [O2]
	164A	ARG	3.9	3123	1463	334A	SER	2.62	3	104.47	3102 [O3]	3133[O3]
	331A	PHE	3.59	3112	3073							
	331A	PHE	3.59	3128	3075							

Supplementary Figure S1 (A-E):

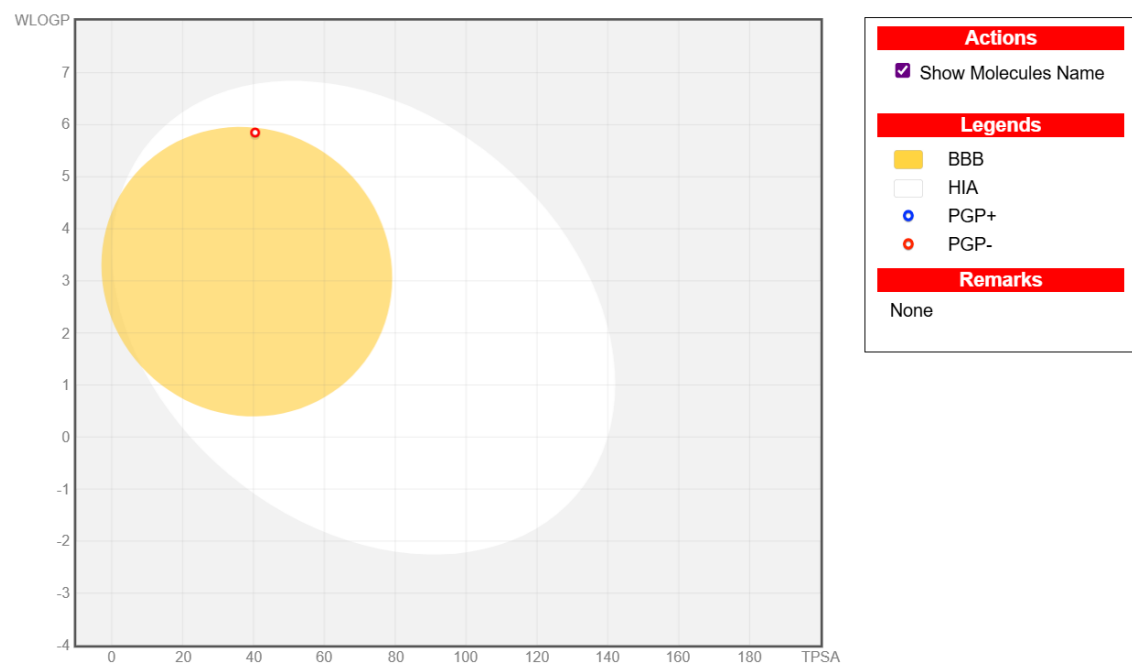


Figure S1A: BOILED-Egg analysis indicates that 1,3-Benzenediol, 2-[3-methyl-6-(1-methylethenyl)-2-cyclohex-en-1-yl]-5-pentyl-, (1R-trans)- exhibits high predicted gastrointestinal absorption, effective blood–brain barrier penetration, and is not a substrate of P-glycoprotein.

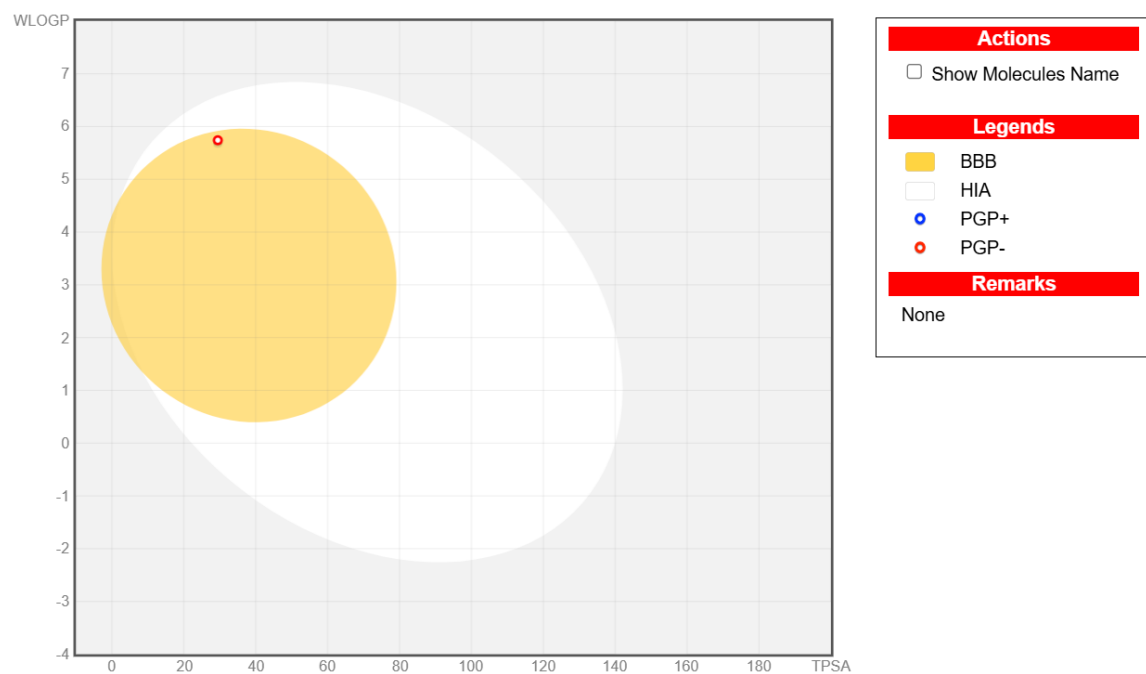


Figure S1B: BOILED-Egg analysis indicates that dronabinol exhibits high predicted gastrointestinal absorption, effective blood–brain barrier penetration, and is not a substrate of P-glycoprotein.

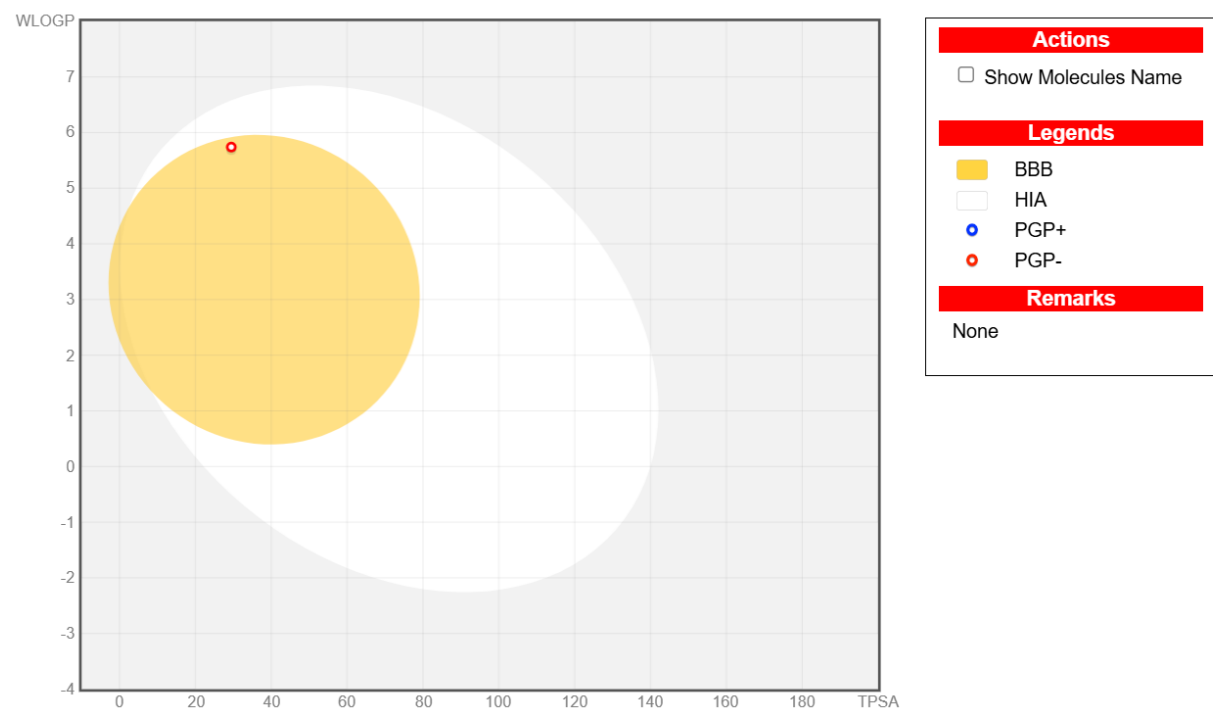


Figure S1C: BOILED-Egg analysis indicates that CBNA exhibits high predicted gastrointestinal absorption, effective blood–brain barrier penetration, and is not a substrate of P-glycoprotein.

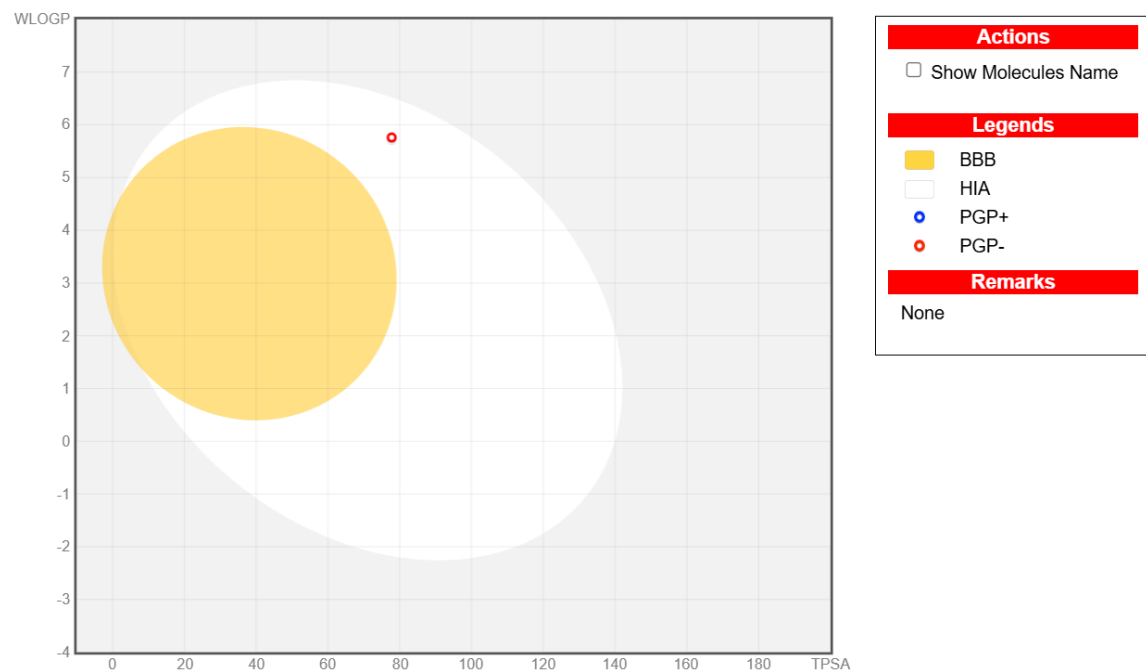


Figure S1D: BOILED-Egg analysis indicates that Cannabigerolic acid (CBGA) exhibits high predicted gastrointestinal absorption, is unlikely to cross the blood–brain barrier, and is not a substrate of P-glycoprotein.

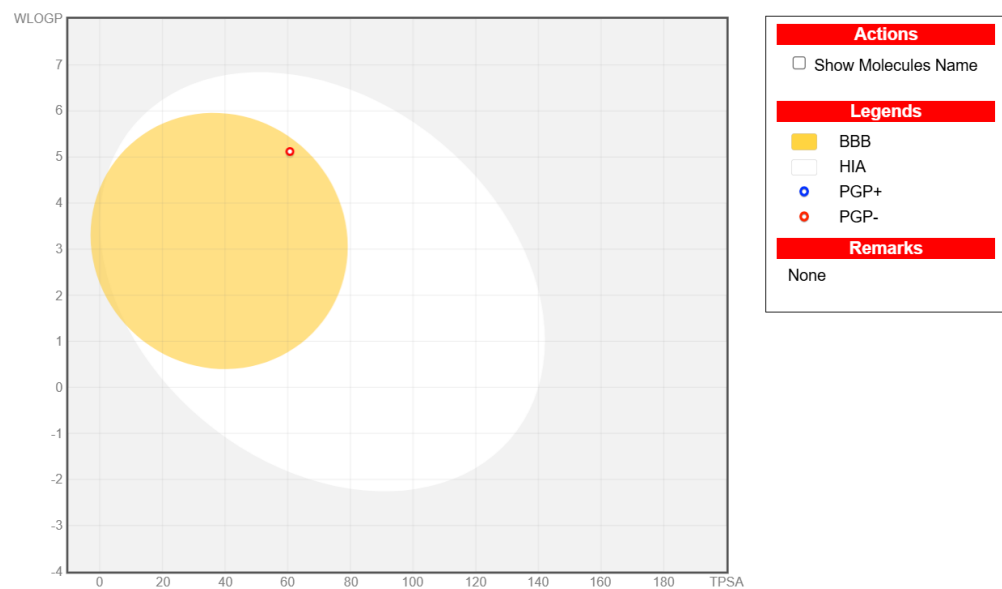


Figure S1E: BOILED-Egg analysis indicates that Ferruginene C exhibits high predicted gastrointestinal absorption, limited blood–brain barrier penetration, and is not a substrate of P-glycoprotein.