BIOINFORMATION

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Supplementary material:

Methodology:

Docking the ligand molecule with BDNF

Eintra is the internal energy of the ligand:	$E_{intra} = \sum_{i \in ligand} \sum_{j \in protein} E_{PLP}(r_{ij}) + \sum_{flexible\ bonds} A[1-\cos(m.\theta - \theta_0)] + E_{clash}$

Table 1: Cavities and Highest binding energies of Omega-3 PUFA (ligand)

S.No	Omega-3 PUFA(Ligand)	Cavity	Binding Energy (kcal/mol)
1	(5Z,7E,9E,14Z,17Z)-Eicosapentaenoicacid(5282061)	cavity_2	-160.226
2	11,14,17,-Eicosatrienoic acid(5312529)	cavity_1	-159.692
3	12-Hydroxy-5,8,10,14-Eicosatetraenoic acid(5312983)	cavity_1	-175.795
4	15-Hydroperoxy-5,8,11,14,17-Eicosapentaenoic acid(6438853)	cavity_1	-168.305
5	18-Hydroxy-5,8,11,14-Eicosatetraenoic acid(6442778)	cavity_1	-155.303
6	Alpha-linolenic acid(860)	cavity_1	-155.405
7	Docosahexaenoic acid(445580)	cavity_4	-171.42
8	Docosapentaenoic acid (5497182)	cavity_1	-164.931
9	Eicosapentaenoic acid(446284)	cavity_1	-162.239
10	Stearidonic acid(5312508)	cavity_1	-153.456

Table 2: Cavities and Highest binding energies of Omega-6 PUFA (Ligand)

S.No	Omega-6 PUFAS(Ligand)	Cavity	Binding Energy (kcal/mol)
1.	7,10,13,16-Docosapentaenoic acid-4(5282848)	cavity_1	-164.87
2.	8,11,14-Eicosatrienoc acid(5280581)	cavity_2	-148.456
3.	Arachidonic acid(444899)	cavity_3	-158.436
4.	Docosa-4,7,10,13,16- pentaenoic acid_(5282848)	cavity _1	-170.703
5.	Gamma-Linolenic acid (5280933)	cavity_1	-150.726
6.	Linoleic acid(5280934)	cavity_1	-154.523

Table 3: Cavities and Highest binding energies of Metabolites (Ligand)

S.No	Metabolite (Ligand)	Cavity	Binding Energy (kcal/mol)
1	LXA_4(5280914)	cav_1	-202.888
2	NPD (16042541)	cav_1	-183.325
3	HDHA (24875301)	Cav_1	-182.36