Journal of Applied Pharmaceutical Science

Available online at: https://japsonline.com

Computational simulations of microalgae-derived bioactive compounds as a novel inhibitor against B-Raf V600E driven melanoma

Fiddy Semba Prasetiya[1,2]*, Wanda Destiarani[3], Irene Retno Cahya Prihastaningtyas[2], Mochamad Untung Kurnia Agung[2], Muhammad Yusuf[3,4]

[1]Research Center for Biosystematics and Evolution, Research Organization for Life Sciences and Environment, National Research and Innovation Agency (BRIN), Cibinong, Indonesia.

[2]Marine Science Department, Faculty of Fisheries and Marine Sciences, Universitas Padjadjaran, Sumedang, Indonesia.

[3]Research Center for Molecular Biotechnology and Bioinformatics, Universitas Padjadjaran, Bandung, Indonesia.

[4]Department of Chemistry, Faculty of Mathematics and Natural Science, Universitas Padjadjaran, Sumedang, Indonesia.

doi: http://doi.org/10.7324/JAPS.2023.10012

Supplementary Material

Table S1. Database of anticancer melanoma candidates from microalgae.

No	Name of molecules	Molecular weight (g/mol)	Species	3D Structure and PubChem ID	Canonical SMILES
1	Butanoic acid	88.11	*Haematococcus pluvialis*	https://pubchem.ncbi.nlm.nih.gov/compound/264#section=3D-Conformer	CCCC(=O)O
2	Cyanovirin-N	93.08	*Nostoc ellipsosporum*	https://pubchem.ncbi.nlm.nih.gov/compound/69245#section=3D-Conformer	C1=COC(=C1)C#N
3	Phenolic	94.11	*Haslea ostrearia*	https://pubchem.ncbi.nlm.nih.gov/compound/996#section=3D-Conformer	C1=CC=C(C=C1)O
4	Vetivenol	220.35	*Asparagopsis taxiformis*	https://pubchem.ncbi.nlm.nih.gov/compound/3085365#section=3D-Conformer	CC1CC(C=C(C12CCC(=C(C)C)C2)C)O

5	Palmitic acid	256.42	*Spirulina platensis*	https://pubchem.ncbi.nlm.nih.gov/compound/985#section=3D-Conformer	CCCCCCCCCCCCCCCC(=O)O
6	Hexadecanoid acid	256.42	*Dunaliella salina*	https://pubchem.ncbi.nlm.nih.gov/compound/985#section=3D-Conformer	CCCCCCCCCCCCCCCC(=O)O
7	Dienoestrol	266.3	*Takayama helix*	https://pubchem.ncbi.nlm.nih.gov/compound/667476#section=3D-Conformer	CC=C(C1=CC=C(C=C1)O)C(=CC)C2=CC=C(C=C2)O
8	Neophytadiene	278.52	*Spirulina platensis*	https://pubchem.ncbi.nlm.nih.gov/compound/10446#section=3D-Conformer	CC(C)CCCC(C)CCCC(C)CCCC(=C)C=C
9	Linoleic acid	280.4	*Spirulina platensis*	https://pubchem.ncbi.nlm.nih.gov/compound/5280450#section=3D-Conformer	CCCCCC=CCC=CCCCCCCCC(=O)O
10	Oleic acid	282.46	*Chlorella vulgaris*	https://pubchem.ncbi.nlm.nih.gov/compound/445639#section=3D-Conformer	CCCCCCCCC=CCCCCCCCC(=O)O
11	9,12,15-octadecatrienoic acid methyl ester	292.5	*Dunaliella salina*	https://pubchem.ncbi.nlm.nih.gov/compound/5367462#section=3D-Conformer	CCC=CCC=CCC=CCCCCCCCC(=O)OC
12	Phytol	296.53	*Spirulina platensis*	https://pubchem.ncbi.nlm.nih.gov/compound/5280435#section=3D-Conformer	CC(C)CCCC(C)CCCC(C)CCCC(=CCO)C
13	Eicosapentaenoic acid (EPA)	302.45	*Phaeodactylum tricornutum*	https://pubchem.ncbi.nlm.nih.gov/compound/446284#section=3D-Conformer	CCC=CCC=CCC=CCC=CCC=CCCCC(=O)O
14	Docosahexaenoic acid (DHA)	328.49	*Spirulina platensis*	https://pubchem.ncbi.nlm.nih.gov/compound/445580#section=3D-Conformer	CCC=CCC=CCC=CCC=CCC=CCC=CCCC(=O)O
15	Cholesta-5,7-dien-3β-ol	384.6	*Crypthecodinium cohnii*	https://pubchem.ncbi.nlm.nih.gov/compound/20056519#section=3D-Conformer	CC(C)CCCC(C)C1CCC2C1(CCC3C2=CC=C4C3(CCC(C4)O)C)C
16	Cholesta-5,24-dien-3β-ol	384.6	*Nitzschia closterium*	https://pubchem.ncbi.nlm.nih.gov/compound/6432322#section=2D-Structure	CC(CCC=C(C)C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C
17	Lathosterol	386.7	*Schizochytrium* sp.	https://pubchem.ncbi.nlm.nih.gov/compound/65728#section=3D-Conformer	CC(C)CCCC(C)C1CCC2C1(CCC3C2=CCC4C3(CCC(C4)O)C)C
18	Ergosterol	396.65	*Chlorella vulgaris*	https://pubchem.ncbi.nlm.nih.gov/compound/444679#section=3D-Conformer	CC(C)C(C)C=CC(C)C1CCC2C1(CCC3C2=CC=C4C3(CCC(C4)O)C)C
19	Crinosterol	398.7	*Bigelowiella natans*	https://pubchem.ncbi.nlm.nih.gov/compound/5283660#section=3D-Conformer	CC(C)C(C)C=CC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C
20	Brassicasterol	398.7	*Olisthodiscus luteus*	https://pubchem.ncbi.nlm.nih.gov/compound/5281327#section=3D-Conformer	C[C@H](/C=C/[C@H](C)C(C)C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C
21	24-Methylenecholesterol	398.7	*Schizochytrium aggregatum*	https://pubchem.ncbi.nlm.nih.gov/compound/92113#section=3D-Conformer	CC(C)C(=C)CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C
22	7-Oxocholesterol	400.64	*Chlorella vulgaris*	https://pubchem.ncbi.nlm.nih.gov/compound/91474#section=3D-Conformer	CC(C)CCCC(C)C1CCC2C1(CCC3C2C(=O)C=C4C3(CCC(C4)O)C)C
23	Campesterol	400.7	*Cyanophora paradoxa*	https://pubchem.ncbi.nlm.nih.gov/compound/173183#section=3D-Conformer	CC(C)C(C)CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C
24	24-	400.7	*Schizochytrium*	https://pubchem.ncbi.nlm.nih.gov/compound/	C[C@H](CCC(C)C(C)C)[C@H]1CC[C@@H]2[C@

	Methylcholesterol		*aggregatum*	12358784#section=3D-Conformer	@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C
25	24-Methylcholestan-3beta-ol	402.7	*Micromonas aff.pusilla*	https://pubchem.ncbi.nlm.nih.gov/compound/89871363#section=3D-Conformer	CC(C)C(C)CCC(C)C1CCC2C1(CCC3C2CCC4C3(CCC(C4)O)C)C
26	7-Dehydroporiferasterol	410.7	*Dunaliella salina*	https://pubchem.ncbi.nlm.nih.gov/compound/20843308#section=3D-Conformer	CCC(C=CC(C)C1CCC2C1(CCC3C2=CC=C4C3(CCC(C4)O)C)C)C(C)C
27	Stigmasterol	412.69	*Bigelowiella natans*	https://pubchem.ncbi.nlm.nih.gov/compound/5280794#section=3D-Conformer	CCC(C=CC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)C(C)C
28	Isofucosterol atau 28-isofucosterol	412.7	*Chattonella antique*	https://pubchem.ncbi.nlm.nih.gov/compound/5281326#section=3D-Conformer	C/C=C(/CC[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C)\C(C)C
29	24-Ethylcholest-5-en-3β-ol	414.7	*Attheya ussurensis*	https://pubchem.ncbi.nlm.nih.gov/compound/12303641#section=3D-Conformer	CCC(CC[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CCC(C4)O)C)C)C(C)C
30	24-Ethylcholesterol	414.7	*Cyanophora paradoxa*	https://pubchem.ncbi.nlm.nih.gov/compound/9823110#section=3D-Conformer	CCC(CC[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C)C(C)C
31	Clionasterol	414.7	*Nostoc commune var. sphaeroides Kützing*	https://pubchem.ncbi.nlm.nih.gov/compound/457801#section=3D-Conformer	CC[C@@H](CC[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C)C(C)C
32	Beta-Sitosterol	414.7	*Porphyridium cruentum*	https://pubchem.ncbi.nlm.nih.gov/compound/222284#section=3D-Conformer	CC[C@H](CC[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C)C(C)C
33	Sitosterol	414.71	*Chrysoderma* sp.	https://pubchem.ncbi.nlm.nih.gov/compound/222284#section=3D-Conformer	CCC(CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)C(C)C
34	24E-propylidenecholesterol	426.7	*Nematochrysopsis* sp.	https://pubchem.ncbi.nlm.nih.gov/compound/21603767#section=3D-Conformer	CC/C=C(\CC[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C)/C(C)C
35	Ergosterol peroxide	428.65	*Chlorella vulgaris*	https://pubchem.ncbi.nlm.nih.gov/compound/5351516#section=3D-Conformer	CC(C)C(C)C=CC(C)C1CCC2C1(CCC3C24C=CC5(C3(CCC(C5)O)C)OO4)C
36	Dinosterol	428.7	*Crypthecodinium cohnii*	https://pubchem.ncbi.nlm.nih.gov/compound/6441076#section=3D-Conformer	C[C@H]1[C@@H]2CC[C@H]3[C@@H]4CC[C@@H]([C@]4(CC[C@@H]3[C@]2(CC[C@@H]1O)C)C)[C@H](C)/C=C(\C)/[C@H](C)C(C)C
37	Saringosterol	428.7	*Micromonas aff.pusilla*	https://pubchem.ncbi.nlm.nih.gov/compound/14161394#section=3D-Conformer	C[C@H](CCC(C=C)(C(C)C)O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C
38	7-Dehydroporiferaste	442.7	*Chlorella vulgaris*	https://pubchem.ncbi.nlm.nih.gov/compound/15454715#section=3D-Conformer	CCC(C=CC(C)C1CCC2C1(CCC3C24C=CC5(C3(CCC(C5)O)C)OO4)C)C(C)C

	rol peroxide				
39	24-Oxocholesterol acetate	442.7	*Isochrysis galbana*	https://pubchem.ncbi.nlm.nih.gov/compound/10972273#section=3D-Conformer	CC(C)C(=O)CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)OC(=O)C)C)C
40	Botryococcene	466.8	*Botryococcus braunii*	https://pubchem.ncbi.nlm.nih.gov/compound/10885141#section=2D-Structure	CC(CCC(C)C(=C)CCC(C)C(=C)C)C=CC(C)(CCC(C)C(=C)CCC(C)C(=C)C)C=C
41	Terpenoid-EA-I	528.6	*Chlorella vulgaris*	https://pubchem.ncbi.nlm.nih.gov/compound/5281400#section=3D-Conformer	CCCCCC=CC=CC12OC3C4C5C(O5)(C(C6(C(C4(O1)C(CC3(O2)C(=C)C)C)C=C(C6=O)C)O)O)CO
42	B-carotene	536.87	*Dunaliella salina*	https://pubchem.ncbi.nlm.nih.gov/compound/5280489#section=3D-Conformer	CC1=C(C(CCC1)(C)C)C=CC(=CC=CC(=CC=CC=C(C)C=CC=C(C)C=CC2=C(CCCC2(C)C)C)C)C
43	Carotenoids, Astaxanthin	536.9	*Dunaliella salina*	https://pubchem.ncbi.nlm.nih.gov/compound/6419725#section=3D-Conformer	CC1=C(C(CCC1)(C)C)C=CC(=CC=CC(=CC=CC=C(C)C=CC=C(C)C=CC2C(=CCCC2(C)C)C)C)C
44	Scytovirin N	544.6	*Scytonema varium*	https://pubchem.ncbi.nlm.nih.gov/compound/135473381#section=3D-Conformer	C1=CC=C2C(=C1)C3=C(C(=O)C(=CC4=CC=C(C=C4)O)C3=N2)C5=C6C7=CC=CC=C7N=C6C(=CC8=CC=C(C=C8)O)C5=O
45	Triterpenoid	552.8	*Phaeodactylum tricornutum*	https://pubchem.ncbi.nlm.nih.gov/compound/451674#section=3D-Conformer	CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)COS(=O)(=O)O)O)C)C)C2C1)C)C(=O)O)C
46	Canthaxanthin	564.84	*Chlorella vulgaris*	https://pubchem.ncbi.nlm.nih.gov/compound/5281227#section=3D-Conformer	CC1=C(C(CCC1=O)(C)C)C=CC(=CC=CC(=CC=CC=C(C)C=CC=C(C)C=CC2=C(C(=O)CCC2(C)C)C)C)C
47	Zeaxanthin	568.87	*Haematococcus pluvialis*	https://pubchem.ncbi.nlm.nih.gov/compound/5280899#section=3D-Conformer	CC1=C(C(CC(C1)O)(C)C)C=CC(=CC=CC(=CC=CC=C(C)C=CC=C(C)C=CC2=C(CC(CC2(C)C)O)C)C)C
48	Lutein	568.9	*Chlorella protothecoides*	https://pubchem.ncbi.nlm.nih.gov/compound/5281243#section=3D-Conformer	CC1=C(C(CC(C1)O)(C)C)C=CC(=CC=CC(=CC=CC=C(C)C=CC=C(C)C=CC2C(=CC(CC2(C)C)O)C)C)C
49	Phycocyanobilin	586.68	*Spirulina sp.*	https://pubchem.ncbi.nlm.nih.gov/compound/365902#section=3D-Conformer	CCC1=C(C(=NC1=O)C=C2C(=C(C(=CC3=C(C(=C(N3)C=C4C(=CC)C(C(=O)N4)C)C)CCC(=O)O)N2)CCC(=O)O)C)C
50	Astaxanthin, ketocarotenoids	596.8	*Haematococcus pluvialis*	https://pubchem.ncbi.nlm.nih.gov/compound/5281224#section=3D-Conformer	CC1=C(C(CC(C1=O)O)(C)C)C=CC(=CC=CC(=CC=CC=C(C)C=CC=C(C)C=CC2=C(C(=O)C(CC2(C)C)O)C)C)C
51	Violaxanthin	600.87	*Chlorella ellipsoidea*	https://pubchem.ncbi.nlm.nih.gov/compound/448438#section=3D-Conformer	CC(=CC=CC=C(C)C=CC=C(C)C=CC12C(CC(CC1(O2)C)O)(C)C)C=CC=C(C)C=CC34C(CC(CC3(O4)C)O)(C)C
52	Cryptophycin	655.18	*Nostoc sp.*	https://pubchem.ncbi.nlm.nih.gov/compound/6438401#section=3D-Conformer	CC1CNC(=O)C(NC(=O)C=CCC(OC(=O)C(OC1=O)CC(C)C)C(C)C2C(O2)C3=CC=CC=C3)CC4=CC(=C(C=C4)OC)Cl
53	Fucoxanthin	658.91	*Chaetoceros sp*	https://pubchem.ncbi.nlm.nih.gov/compound/5281239#section=3D-Conformer	CC(=CC=CC=C(C)C=CC=C(C)C(=O)CC12C(CC(CC1(O2)C)O)(C)C)C=CC=C(C)C=C=C3C(CC(CC3(C)O)OC(=O)C)(C)C
54	Phycocyanin	719.8	*Spirulina sp.*	https://pubchem.ncbi.nlm.nih.gov/compound/365902#section=3D-Conformer	CCC1=C(C)C(\C=C2\N\C(=C/C3=C(CCC(O)=O)C(C)=C(N3)\C=C3/NC(=O)[C@H](C)C3CSCC(NC)C(

	C)=O)C(CCC(O)O)=C2C)=NC1=O

Table S2. Molecular docking parameter optimization.

No.	Receptor Preparation	Grid Box (0.375Å)	Binding Energy (kcal/mol)	Inhibition Constant (µM)
1.	Protein Modelling	20 x 20 x 20	-8,95	0,28
2.	Protein Modelling	22 x 30 x 20	- 8,84	0,33
3.	3 Step of Minimization	20 x 20 x 20	-7,66	2,41
4.	3 Step of Minimization	22 x 30 x 20	- 7,35	4,09
5.	6 Step of Minimization	20 x 20 x 20	-7,54	2,97
6.	6 Step of Minimization	22 x 30 x 20	- 7,26	4,77

Table S3. Alanine scanning analysis of B-Raf V600E structure.

No	Residue	Delta G (kcal/mol)	Effect to B-Raf Receptor
1	ASP1	0.379477	**Destabilize**
2	TRP2	-0.871411	Stabilize
3	GLU3	-0.378829	Stabilize
4	ILE4	-2.29437	Stabilize
5	PRO5	0.974839	**Destabilize**
6	ASP6	-2.03095	Stabilize
7	GLY7	3.63669	**Destabilize**
8	GLN8	-5.07004	Stabilize
9	ILE9	-2.86979	Stabilize
10	THR10	-0.799588	Stabilize
11	VAL11	0.590647	**Destabilize**
12	GLY12	2.15317	**Destabilize**
13	GLN13	-0.999605	Stabilize
14	ARG14	-1.25348	Stabilize
15	ILE15	-1.69835	Stabilize
16	GLY16	2.56932	**Destabilize**
17	SER17	-0.454405	Stabilize
18	GLY18	1.91792	**Destabilize**

19	SER19	-3.31033	Stabilize
20	PHE20	-4.10426	Stabilize
21	GLY21	4.13288	**Destabilize**
22	THR22	-3.13501	Stabilize
23	VAL23	-0.874686	Stabilize
24	TYR24	1.25367	**Destabilize**
25	LYS25	0.171456	**Destabilize**
26	GLY26	1.70135	**Destabilize**
27	LYS27	-0.27369	Stabilize
28	TRP28	-2.92023	Stabilize
29	H2S29	-0.284182	Stabilize
30	GLY30	3.32285	**Destabilize**
31	ASP31	-2.0747	Stabilize
32	VAL32	-1.08149	Stabilize
33	ALA33	0	Stabilize
34	VAL34	1.86774	**Destabilize**
35	LYS35	0.230005	**Destabilize**
36	MET36	1.43575	**Destabilize**
37	LEU37	1.78137	**Destabilize**
38	ASN38	-0.475943	Stabilize
39	VAL39	0.0378436	**Destabilize**
40	THR40	-0.276346	Stabilize
41	ALA41	0	Stabilize
42	PRO42	0.616177	**Destabilize**
43	THR43	-0.970886	Stabilize
44	PRO44	0.925341	**Destabilize**
45	GLN45	0.134429	**Destabilize**
46	GLN46	-0.807148	Stabilize
47	LEU47	0.64482	**Destabilize**
48	GLN48	-4.71631	Stabilize
49	ALA49	0	Stabilize
50	PHE50	3.72512	**Destabilize**
51	LYS51	-0.0523744	Stabilize
52	ASN52	-2.65961	Stabilize
53	GLU53	-2.403	Stabilize

54	VAL54	1.75897	**Destabilize**
55	GLY55	-0.851372	Stabilize
56	VAL56	-1.24991	Stabilize
57	LEU57	2.13139	**Destabilize**
58	ARG58	-1.19456	Stabilize
59	LYS59	-2.35727	Stabilize
60	THR60	0.938762	**Destabilize**
61	ARG61	0.0190215	**Destabilize**
62	H2S62	0.558416	**Destabilize**
63	VAL63	-0.906405	Stabilize
64	ASN64	-2.73269	Stabilize
65	ILE65	3.60096	**Destabilize**
66	LEU66	1.32177	**Destabilize**
67	LEU67	-0.731836	Stabilize
68	PHE68	4.48493	**Destabilize**
69	MET69	-0.918792	Stabilize
70	GLY70	4.28128	**Destabilize**
71	TYR71	1.65054	**Destabilize**
72	SER72	-1.36819	Stabilize
73	THR73	-0.564572	Stabilize
74	LYS74	-3.59163	Stabilize
75	PRO75	0.863057	**Destabilize**
76	GLN76	-1.90124	Stabilize
77	LEU77	2.11426	**Destabilize**
78	ALA78	0	Stabilize
79	ILE79	2.85221	**Destabilize**
80	VAL80	0.325266	**Destabilize**
81	THR81	1.51202	**Destabilize**
82	GLN82	-2.08172	Stabilize
83	TRP83	0.623359	**Destabilize**
84	CYS84	0.300276	**Destabilize**
85	GLU85	-2.48514	Stabilize
86	GLY86	4.44411	**Destabilize**
87	SER87	-0.962607	Stabilize
88	SER88	-1.46833	Stabilize

89	LEU89	3.72662	**Destabilize**
90	TYR90	-1.88159	Stabilize
91	H1S91	-1.53609	Stabilize
92	H2S92	-3.23655	Stabilize
93	LEU93	2.42966	**Destabilize**
94	H2S94	0.537644	**Destabilize**
95	ILE95	-0.357317	Stabilize
96	ILE96	-3.28905	Stabilize
97	GLU97	-2.77292	Stabilize
98	THR98	-0.970765	Stabilize
99	LYS99	-0.578073	Stabilize
100	PHE100	2.78106	**Destabilize**
101	GLU101	0.404485	**Destabilize**
102	MET102	-0.791813	Stabilize
103	ILE103	-2.87494	Stabilize
104	LYS104	0.42932	**Destabilize**
105	LEU105	0.995213	**Destabilize**
106	ILE106	-1.91772	Stabilize
107	ASP107	-2.69408	Stabilize
108	ILE108	2.25843	**Destabilize**
109	ALA109	0	Stabilize
110	ARG110	-3.48373	Stabilize
111	GLN111	-1.1511	Stabilize
112	THR112	-1.68692	Stabilize
113	ALA113	0	Stabilize
114	GLN114	-5.78606	Stabilize
115	GLY115	0.655945	**Destabilize**
116	MET116	2.42141	**Destabilize**
117	ASP117	-2.84272	Stabilize
118	TYR118	0.797264	**Destabilize**
119	LEU119	3.72074	**Destabilize**
120	H2S120	-4.56969	Stabilize
121	ALA121	0	Stabilize
122	LYS122	-1.5352	Stabilize
123	SER123	0.0660321	**Destabilize**

124	ILE124	1.86754	**Destabilize**
125	ILE125	1.63693	**Destabilize**
126	H2S126	0.46964	**Destabilize**
127	ARG127	-1.55096	Stabilize
128	ASP128	-5.74511	Stabilize
129	LEU129	-0.261144	Stabilize
130	LYS130	-2.20477	Stabilize
131	SER131	-2.34588	Stabilize
132	ASN132	-1.31738	Stabilize
133	ASN133	-4.60745	Stabilize
134	ILE134	3.14402	**Destabilize**
135	PHE135	1.3324	**Destabilize**
136	LEU136	2.15839	**Destabilize**
137	H2S137	-1.30322	Stabilize
138	GLU138	0.659159	**Destabilize**
139	ASP139	-1.14894	Stabilize
140	LEU140	0.120572	**Destabilize**
141	THR141	-2.26862	Stabilize
142	VAL142	-2.21714	Stabilize
143	LYS143	-0.0107411	Stabilize
144	ILE144	2.99796	**Destabilize**
145	GLY145	0.335407	**Destabilize**
146	ASP146	-3.52552	Stabilize
147	PHE147	3.60967	**Destabilize**
148	GLY148	4.60952	**Destabilize**
149	LEU149	-0.899227	Stabilize
150	ALA150	0	Stabilize
151	THR151	-0.0913761	Stabilize
152	GLU152	-3.29139	Stabilize
153	LYS153	-1.23008	Stabilize
154	SER154	-1.92521	Stabilize
155	ARG155	-0.316092	Stabilize
156	TRP156	0.55954	**Destabilize**
157	SER157	0.139427	**Destabilize**
158	GLY158	-0.527173	Stabilize

159	SER159	0.00116084	**Destabilize**
160	H1S160	-7.19591	Stabilize
161	GLN161	-2.78866	Stabilize
162	PHE162	0.176435	**Destabilize**
163	GLU163	-1.79887	Stabilize
164	GLN164	-0.641348	Stabilize
165	LEU165	-2.247	Stabilize
166	SER166	-0.355262	Stabilize
167	GLY167	2.96211	**Destabilize**
168	SER168	-3.85706	Stabilize
169	ILE169	-4.763	Stabilize
170	LEU170	-1.67541	Stabilize
171	TRP171	-0.998409	Stabilize
172	MET172	-2.11692	Stabilize
173	ALA173	0	Stabilize
174	PRO174	1.33553	**Destabilize**
175	GLU175	1.28126	**Destabilize**
176	VAL176	-3.34458	Stabilize
177	ILE177	0.923789	**Destabilize**
178	ARG178	-1.7461	Stabilize
179	MET179	-1.46292	Stabilize
180	GLN180	-0.422139	Stabilize
181	ASP181	-0.727591	Stabilize
182	LYS182	-2.16735	Stabilize
183	ASN183	-2.3301	Stabilize
184	PRO184	1.36013	**Destabilize**
185	TYR185	-0.303514	Stabilize
186	SER186	0.204912	**Destabilize**
187	PHE187	-1.26943	Stabilize
188	GLN188	-0.559624	Stabilize
189	SER189	-0.326687	Stabilize
190	ASP190	-2.18411	Stabilize
191	VAL191	0.553976	**Destabilize**
192	TYR192	0.663931	**Destabilize**
193	ALA193	0	Stabilize

194	PHE194	3.73285	**Destabilize**
195	GLY195	1.20208	**Destabilize**
196	ILE196	0.176992	**Destabilize**
197	VAL197	0.497778	**Destabilize**
198	LEU198	3.11958	**Destabilize**
199	TYR199	-0.203002	Stabilize
200	GLU200	1.63251	**Destabilize**
201	LEU201	3.34407	**Destabilize**
202	MET202	1.14207	**Destabilize**
203	THR203	-2.40815	Stabilize
204	GLY204	4.0476	**Destabilize**
205	GLN205	-1.41337	Stabilize
206	LEU206	-0.232927	Stabilize
207	PRO207	1.94438	**Destabilize**
208	TYR208	-3.90846	Stabilize
209	SER209	-0.868319	Stabilize
210	ASN210	-0.829629	Stabilize
211	ILE211	0.127751	**Destabilize**
212	ASN212	-0.736284	Stabilize
213	ASN213	1.12013	**Destabilize**
214	ARG214	-1.32282	Stabilize
215	ASP215	-0.46353	Stabilize
216	GLN216	-0.226606	Stabilize
217	ILE217	-0.33109	Stabilize
218	ILE218	-1.8681	Stabilize
219	PHE219	-2.33141	Stabilize
220	MET220	-1.0014	Stabilize
221	VAL221	-1.80524	Stabilize
222	GLY222	-1.11378	Stabilize
223	ARG223	-2.08557	Stabilize
224	GLY224	3.95668	**Destabilize**
225	TYR225	-2.27168	Stabilize
226	LEU226	-4.54864	Stabilize
227	SER227	-0.759242	Stabilize
228	PRO228	0.641026	**Destabilize**

229	ASP229	0.971473	**Destabilize**
230	LEU230	1.06597	**Destabilize**
231	SER231	0.102458	**Destabilize**
232	LYS232	-2.17108	Stabilize
233	VAL233	0.585946	**Destabilize**
234	ARG234	-3.89664	Stabilize
235	SER235	-0.25658	Stabilize
236	ASN236	-0.998275	Stabilize
237	CYS237	-0.940372	Stabilize
238	PRO238	2.34365	**Destabilize**
239	LYS239	-0.923873	Stabilize
240	ALA240	0	Stabilize
241	MET241	-3.6713	Stabilize
242	LYS242	-1.23802	Stabilize
243	ARG243	-1.64316	Stabilize
244	LEU244	1.52471	**Destabilize**
245	MET245	1.06481	**Destabilize**
246	ALA246	0	Stabilize
247	GLU247	-1.28455	Stabilize
248	CYS248	-0.388529	Stabilize
249	LEU249	2.2357	**Destabilize**
250	LYS250	-0.779282	Stabilize
251	LYS251	-0.715215	Stabilize
252	LYS252	-2.939	Stabilize
253	ARG253	-2.60359	Stabilize
254	ASP254	-1.20748	Stabilize
255	GLU255	-0.595169	Stabilize
256	ARG256	0.293405	**Destabilize**
257	PRO257	1.80225	**Destabilize**
258	LEU258	-0.90809	Stabilize
259	PHE259	2.12133	**Destabilize**
260	PRO260	1.28583	**Destabilize**
261	GLN261	-0.47604	Stabilize
262	ILE262	0.539203	**Destabilize**
263	LEU263	-0.236755	Stabilize

264	ALA264	0	Stabilize
265	SER265	-1.45305	Stabilize
266	ILE266	1.89134	**Destabilize**
267	GLU267	-0.52873	Stabilize
268	LEU268	-0.88603	Stabilize
269	LEU269	-0.260953	Stabilize
270	ALA270	0	Stabilize
271	ARG271	-1.8554	Stabilize
272	SER272	-0.670974	Stabilize
273	LYS273	-4.05183	Stabilize
274	SER274	-0.103799	Stabilize
275	ARG275	-1.17095	Stabilize
276	TRP276	-2.41254	Stabilize
277	SER277	0.395745	**Destabilize**
278	GLY278	-0.0513357	Stabilize
279	SER279	-0.225989	Stabilize
280	H2S280	-0.352939	Stabilize
281	GLN281	0.00987052	**Destabilize**
282	PHE282	0.292604	**Destabilize**
283	GLU283	-2.56996	Stabilize
284	GLN284	-0.651101	Stabilize
285	LEU285	-0.374344	Stabilize
286	SER286	-0.137568	Stabilize
287	GLY287	3.87261	**Destabilize**
288	LEU288	-0.644037	Stabilize
289	PRO289	-0.0382287	Stabilize
290	LYS290	-3.04783	Stabilize
291	ILE291	-1.08112	Stabilize
292	H1S292	-1.0526	Stabilize
293	ARG293	-0.019539	Stabilize
294	SER294	-0.983069	Stabilize
295	ALA295	0	Stabilize
296	GLU296	0.111129	**Destabilize**
297	PRO297	-0.127943	Stabilize
298	SER298	-0.37655	Stabilize

299	LEU299	-0.926388	Stabilize
300	ASN300	-2.10508	Stabilize
301	ARG301	-0.294721	Stabilize
302	ALA302	0	Stabilize
303	GLY303	1.33515	**Destabilize**