

SUPPLEMENTARY DATA

Metabolomic Profiling LC-MS Based Bioactive Compound of *Sonneratia alba*, Antioxidant Activities and Its In-silico molecular docking Studies

**Indra Lasmana Tarigan^{1,3}, Madyawati Latief^{1,3*}, Jamaluddin Al Anshori², Fitria Melani¹,
Silvi Ayudiah Putri¹, Naimul Husna¹, Tri Warni¹, Ilham Ifandi Ramadhan¹,
Yusnaidar¹, Sutrisno¹**

¹Department of Chemistry, Faculty of Science and Technology, Universitas Jambi, Indonesia

²Department of Chemistry, Faculty of Mathematic and Natural Sciences, Universitas
Padjajaran, Indonesia

³Natural Product and Biomaterial Chemistry Laboratory, Faculty of Science and Technology,
Universitas Jambi, Indonesia

*Corresponding author email: madyawatilatief@unja.ac.id

Table 1. The physicochemical properties of candidate bioactive compounds (from five different fractions)

No	Bioactive Compounds	Formula	Molar Mass <500	Hydrogen Donor <5	Hydrogen Acceptor <10	Log P <5	Drug-likeness
1	4 <i>H</i> -cyclopenta[def]phenanthrene-4-one	C ₁₅ H ₈ O	204.228	0	1	3.382	Yes
2	Meperidine	C ₁₅ H ₂₁ NO ₂	247.338	0	3	2.213	Yes
3	Scolymoside	C ₂₇ H ₃₀ O ₁₅	594.522	9	15	-1.392	No
4	2'-Hydroxygenistein-7-O-glucoside	C ₂₁ H ₂₀ O ₁₁	488.38	7	11	-0.244	No
5	Kaempferol 3-gluco-xyloside	C ₂₆ H ₂₈ O ₁₅	580.495	9	15	-1.781	No
6	Kaempferol-3-Rhamnoside	C ₂₁ H ₂₀ O ₁₀	432.381	6	10	0.783	Yes
7	2,4-Diamino-6-morpholino-s-triazine	C ₇ H ₁₂ N ₆ O	196.214	2	7	-1.127	Yes
8	3-(4,6-dimorpholino-1,3,5-triazin-2-yl)-1,2,3,4,5,6-hexahydro-8 <i>H</i> -1,5-methanopyridol[1,2- <i>a</i>] [1,5] diazocin-8-one	C ₂₂ H ₂₉ N ₇ O ₃	375.871	1	3	4.3172	No
9	4-[4-(Benzyloxy)-2-methylbenzoyl]-5-(4-ethoxyphenyl)-3-hydroxy-1-[3-(4-morpholinyl)propyl]-1,5-dihydro-2 <i>H</i> -pyrrol-2-one	C ₃₄ H ₃₈ N ₂ O ₆	570.686	1	7	5.273	No
10	N-[3-(4-{[(5-Isopropyl-1,2-oxazol-3-yl)carbamoyl]amino}-3-methylphenyl)-1 <i>H</i> -pyrazol-5-yl]-4-[(4-methyl-1-piperazinyl)methyl]benzamide	C ₃₀ H ₃₆ N ₈ O ₃	556.671	4	7	5.140	No
11	Linetastine	C ₃₅ H ₄₀ N ₂ O ₆	584.713	1	7	6.186	No
12	L-Histidyl-1-(2-hydroxy-5-nitrobenzyl)-L-tryptophyl-L-lysine	C ₃₀ H ₃₆ N ₈ O ₇	620.667	7	10	1.322	No
13	5-Isothiocyanatoindane	C ₂₄ H ₄₂ N ₈ O ₈	570.648	8	9	-3.934	No
14	N-[3-(4-{[(5-Tert-Butyl-1,2-Oxazol-3-Yl)carbamoyl]amino}-3-Methylphenyl)-1 <i>H</i> -Pyrazol-5-Yl]-4-[(4-Methylpiperazin-1-Yl)methyl]benzamide	C ₃₁ H ₃₈ N ₈ O ₃	570.698	4	7	5.314	No
15	1-{6-(3,4-Dihydro-2(1 <i>H</i>)-isoquinolinyl)-2-[4-(2-methyl-2-propanyl)phenyl]-4-pyrimidinyl}-3-(1-methyl-1 <i>H</i> -indol-3-yl)-2-piperazinone	C ₃₆ H ₃₈ N ₆ O	570.741	1	6	6.173	No
16	2-[(2-Methoxy-4-{[4-(4-methyl-1-piperazinyl)-1-piperidinyl]carbonyl}phenyl)amino]-5,11-dimethyl-5,11-dihydro-6 <i>H</i> -pyrimido[4,5- <i>b</i>][1,4]benzodiazepin-6-on	C ₃₁ H ₃₈ N ₈ O ₃	570.698	1	9	3.438	Yes
17	N-[2-Amino-6-(butylamino)-3-hydroxy-5-methyl-6-oxohexyl]-N-isopropyl-4-methoxy-3-(3-methoxypropoxy)benzamide	C ₂₆ H ₄₅ N ₃ O ₆	495.661	3	7	2.591	Yes
18	4-[(4-{3-Ethyl-7-(4-morpholinyl)-3 <i>H</i> -[1,2,3]triazolo[4,5- <i>d</i>]pyrimidin-5-yl}phenyl)carbamoyl]amino]-N-[2-(2-pyridinyl)ethyl]benzamide	C ₃₁ H ₃₂ N ₁₀ O ₃	592.664	3	10	3.756	Yes

19	Ethyl N-[(2-{[(4-carbamoylphenyl)amino]methyl}-1-methyl-1H-benzimidazol-5-yl)carbonyl]-N-2-pyridinyl-β-alaninate	C ₂₇ H ₂₈ N ₆ O ₄	500.559	2	8	3.279	Yes
20	N-[3-(4-{[(5-Isopropyl-1,2-oxazol-3-yl)carbamoyl]amino}-3-methylphenyl)-1H-pyrazol-5-yl]-4-[(4-methyl-1-piperazinyl)methyl]benzamide	C ₃₀ H ₃₆ N ₈ O ₃	556.671	4	7	5.140	No
21	6-[2-(2-Ethyl-4-methyl-1H-imidazol-1-yl)ethyl]-1,3,5-triazin-2,4-diamin	C ₁₁ H ₁₇ N ₇	247.306	2	7	0.346	Yes
22	Biurea, 1,6-dimethyl-1,6-dinitroso-	C ₄ H ₈ N ₆ O ₄	204.146	2	6	-0.453	Yes
23	1,8-Dihydroxy-6-methoxy-9-oxo-9H-xanthen-2-yl 2-O-(6-deoxy-α-L-mannopyranosyl)-β-D-xylopyranoside	C ₂₅ H ₂₈ O ₁₄	552.485	7	14	-1.329	No
24	Carlinside	C ₂₆ H ₂₈ O ₁₅	580.495	11	15	-2.048	No
25	7-(4-Aminobenzyl)-7H-pyrrolo[3,2-f]quinazoline-1,3-diamine	C ₁₇ H ₁₆ N ₆	304.357	3	6	3.204	Yes
26	2,4-Diamino-6-morpholino-s-triazine	C ₇ H ₁₂ N ₆ O	196.214	2	7	-1.127	Yes
27	11-[4,6-Di(4-morpholinyl)-1,3,5-triazin-2-yl]-7,11-diazatricyclo[7.3.1.0~2,7~]trideca-2,4-dien-6-one	C ₂₂ H ₂₉ N ₇ O ₃	439.52	0	10	0.330	Yes
28	4-[(4-Methylpiperazin-1-Yl)methyl]-N-{3-[3-Methyl-4-({[5-(Propan-2-Yl)-1,2-Oxazol-3-Yl]carbamoyl}amino)phenyl]-1h-Pyrazol-5-Yl}benzamide	C ₃₀ H ₃₆ N ₈ O ₃	556.671	4	7	5.140	No
29	2-Methyl-2-propanyl {(2S,3S)-1-[(3S)-7-[2-(hydroxyamino)-2-oxoethoxy]-3-[(4-methoxyphenyl)carbamoyl]-3,4-dihydro-2(1H)-isoquinolinyl]-3-methyl-1-oxo-2-pentanyl} carbamate	C ₃₀ H ₄₀ N ₄ O ₈	584.67	4	8	3.410	Yes
30	N-Methyl-D-phenylalanyl-N-[5-carbamimidamido-1-(1-methyl-1H-benzimidazol-2-yl)-1-oxo-2-pentanyl]-L-prolinamide	C ₂₉ H ₃₈ N ₈ O ₃	546.676	5	7	1.325	Yes
31	5-[4-(Benzyloxy)phenyl]-4-(4-butoxybenzoyl)-1-[3-(diethylamino)propyl]-3-hydroxy-1,5-dihydro-2H-pyrrol-2-one	C ₃₅ H ₄₂ N ₂ O ₅	570.73	1	6	6.754	No
32	2-{(2R,3R,6S)-2-{[(1R,2S,3S,4R,6S)-4,6-Diamino-3-{[3-deoxy-4-C-methyl-3-(methylamino)-L-arabinopyranosyl]oxy}-2-hydroxycyclohexyl]oxy}-6-[(1R)-1-(methylamino)ethyl]tetrahydro-2H-pyran-3-yl} guanidine	C ₂₂ H ₄₅ N ₇ O ₇	519.644	9	12	-4.012	No
33	N-Cyclopentyl-N-[2-(dimethylamino)ethyl]-2-(5-{[isopropyl(methyl)amino]methyl}-1-tetrazolidinyl)acetamid	C ₁₇ H ₃₇ N ₇ O	355.531	3	7	-0.185	Yes
34	Salicyloylaminotriazole	C ₉ H ₈ N ₄ O ₂	204.189	3	4	0.762	Yes
35	Kaempferol-3-O-rutinoside	C ₂₇ H ₃₀ O ₁₅	594.522	9	15	-1.392	No
36	Quercitrin	C ₂₁ H ₂₀ O ₁₁	448.380	7	11	0.488	No
37	Quercetin 3-[rhamnosyl-(1->2)-alpha-L-arabinopyranoside]	C ₂₆ H ₂₈ O ₁₅	580.495	9	15	-1.048	No

38	Apigenin-7-O-glucoside	C ₂₁ H ₂₀ O ₁₀	432.381	6	10	0.049	Yes
39	Isobutyl furfurylacetate	C ₁₁ H ₁₆ O ₃	196.246	0	3	2.411	Yes
40	(S)-2-(3-(1-((4-Isopropylbenzyloxy)carbonyl)piperidin-3-yl)phenoxy)-2-methylpropanoic acid	C ₂₆ H ₃₃ NO ₅	439.552	1	4	5.568	Yes
41	Dipiperamide A	C ₃₄ H ₃₈ N ₂ O ₆	570.686	0	6	5.394	No
42	Omadacycline	C ₂₉ H ₄₀ N ₄ O ₇	556.660	6	10	1.165	No
43	2-[[1-[(1-Carboxy-2-phenylethyl)amino]-4-methyl-1-oxopentan-2-yl]amino]-4-[2-(phenylmethoxycarbonylamino)propanoylamino]butanoic acid	C ₃₀ H ₄₀ N ₄ O ₈	584.670	6	7	2.077	No
44	2-ketobenzothiazole 54	C ₂₉ H ₃₈ N ₈ O ₃	546.676	4	7	1.116	Yes
45	N-{2-(2-Methyl-2-propanyl)-6-[4-(4-phenoxyphenyl)-1-piperazinyl]-4-pyrimidinyl}-N'-phenyl-1,4-benzenediamine	C ₃₆ H ₃₈ N ₆ O	570.741	2	7	8.380	No
46	Pyrazolo[3,4-d]pyrimidine 6	C ₃₁ H ₃₈ N ₈ O ₃	570.698	2	8	3.340	Yes
47	(3-Aminopropyl)carbamodithioic acid	C ₄ H ₁₀ N ₂ S ₂	150.272	3	2	0.139	Yes
48	3-O-Ethylascorbic acid	C ₈ H ₁₂ O ₆	204.178	3	6	-0.928	Yes
49	Nictoflorin	C ₂₇ H ₃₀ O ₁₅	594.522	9	15	-1.329	No
50	3,5-Dicaffeoyl-4-succinoylquinic acid	C ₂₉ H ₂₈ O ₁₅	616.528	7	13	1.445	No
51	Genistin	C ₂₁ H ₂₀ O ₁₀	432.381	6	10	0.049	Yes
52	Ibuprofen	C ₁₃ H ₁₈ O ₂	206.285	1	1	3.073	Yes
53	p-Hexyloxybenzoic Acid	C ₁₃ H ₁₈ O ₃	222.284	1	2	3.343	Yes
54	Salicylihalamide A	C ₂₆ H ₃₃ NO ₅	439.552	3	5	4.349	Yes
55	3,3-Bis-(4-ethyl-phenyl)-2-(4-methoxy-6-methyl-pyrimidin-2-yloxy)-3-[2-(4-methoxy-phenyl)-ethoxy]-propionic acid	C ₃₄ H ₃₈ N ₂ O ₆	570.686	1	7	5.962	No
56	Methyloctadecylamine	C ₁₉ H ₄₁ N	283.544	1	1	6.467	Yes
57	2-Aminobenzothiazole	C ₇ H ₆ N ₂ S	150.206	1	3	1.878	Yes
58	Homocycloleucine	C ₇ H ₁₃ NO ₂	143.186	2	2	0.732	Yes
59	Pantothenic acid	C ₉ H ₁₇ NO ₅	219.237	4	4	-1.043	Yes
60	Carlinoside	C ₂₆ H ₂₈ O ₁₅	580.495	11	15	-2.048	No
61	2-Hydroxyibuprofen	C ₁₃ H ₁₈ O ₃	222.284	2	4	2.188	Yes
62	1-(1-(2-ethoxyethyl)-3-methyl-7-((4-methylpyridin-2-yl)amino)-1H-pyrazolo[4,3-d]pyrimidin-5-yl)piperidine-4-carboxylic acid	C ₂₂ H ₂₉ N ₇ O ₃	439.520	2	9	2.919	Yes
63	Gibberellin A7	C ₁₉ H ₂₂ O ₅	330.380	2	4	1.912	Yes
64	N-(3-((2-(4-amino-1,2,5-oxadiazol-3-yl)-1-ethyl-1H-imidazo[4,5-c]pyridin-6-yl)oxy)phenyl)-4-(2-(diisopropylamino)ethoxy)benzamide	C ₃₁ H ₃₆ N ₈ O ₄	584.681	2	11	5.625	No

65	4-(1-(adamantan-1-ylmethyl)-3,3-bis((1-methyl-1H-imidazol-5-yl)methyl)-2-oxoindolin-6-yl)benzonitrile	C ₃₆ H ₃₈ N ₆ O	570.741	0	7	5.978	No
66	Adamantanecarboxylic acid	C ₁₁ H ₁₆ O ₂	180.247	1	1	2.287	Yes
67	Hydroxyethylene dipeptide isostere 8	C ₃₅ H ₄₂ N ₂ O ₅	570.73	4	5	5.367	No
68	1-hexadecanal	C ₁₆ H ₃₂ O	240.431	0	1	5.666	Yes
69	4-(((5S,8S,11S,14S,17S,18S)-8-(aminomethyl)-11-isobutyl-5-isopropyl-18-methyl-4,7,13,16-tetraoxo-14-propyl-3,6,9,12,15-pentaazaicosan-17-yl)carbamoyl)pyridine 1-oxide	C ₃₃ H ₅₈ N ₈ O ₆	662.877	7	8	0.474	No

Supplementary Table 2. ADMET Profile

Bioactive Compounds	Absorption				Distribution		Excretion	Toxicity	
	Caco-2 (log Papp in 10 ⁻⁶ cm/s)	Intestinal Absorption (% absorbed)	Skin Permeability (log Kp)	VD _{ess} (log L/kg)	BBB Permeability (log BBB)	CNS Permeability (log PS)	Total Clearance (log mL/min/kg)	Oral Rat Acute Toxicity (LD ₅₀ = mol/kg)	Oral Rat Chronic Toxicity (LOAEL = log mg/kg bw/day)
C ₁₅ H ₈ O	0.986	98.817	-2.611	0.362	0.559	-1.327	0.344	2.423	1.096
C ₁₅ H ₂₁ NO ₂	1.671	95.134	-2.575	0.666	0.310	-2.119	0.911	2.737	1.559
C ₂₁ H ₂₀ O ₁₀	0.123	60.006	-2.735	1.15	-1.265	-3.994	0.431	2.61	2.799
C ₇ H ₁₂ N ₆ O	0.087	71.5	-2.767	0.184	-0.024	-3.578	0.054	2.255	1.726
C ₃₁ H ₃₈ N ₈ O ₃	0.864	92.431	-2.735	1.969	-1.025	-2.58	0.422	2.943	2.268
C ₂₆ H ₄₅ N ₃ O ₆	0.736	49.104	-2.735	0.015	-1.633	-3.676	0.919	3.678	2.963
C ₃₁ H ₃₂ N ₁₀ O ₃	1.115	87.972	-2.735	-0.112	-1.966	-3.899	0.444	2.527	1.794
C ₂₇ H ₂₈ N ₆ O ₄	1.117	79.981	-2.735	0.361	-0.706	-3.704	1.006	2.3	0.978
C ₁₁ H ₁₇ N ₇	0.069	74.874	-2.735	-0.06	-0.266	-3.492	0.939	2.446	1.8
C ₄ H ₈ N ₆ O ₄	-0.29	64.636	-3.753	-0.877	-1.096	-3.611	1.083	2.737	2.014
C ₁₇ H ₁₆ N ₆	1.246	97.921	-2.735	0.565	-0.637	-2.257	0.744	2.717	1.183
C ₇ H ₁₂ N ₆ O	0.087	71.5	-2.767	0.184	-0.024	-3.578	0.054	2.255	1.726
C ₂₂ H ₂₉ N ₇ O ₃	1.086	99.348	-2.923	-0.502	-1.158	-3.08	0.3	2.618	1.195
C ₃₀ H ₄₀ N ₄ O ₈	0.515	62.483	-2.735	-0.599	-1.55	-3.492	0.487	3.031	2.849
C ₂₉ H ₃₈ N ₈ O ₃	-0.447	52.13	-2.735	0.091	-1.035	-3.815	0.72	2.483	3.539
C ₁₇ H ₃₇ N ₇ O	0.808	64.162	-2.859	-0.059	0.023	-4.43	0.884	2.403	1.72
C ₉ H ₈ N ₄ O ₂	0g.302	88.842	-2.735	0.384	-1.467	-5.254	0.054	2.622	3.596

Bioactive Compounds	Absorption				Distribution		Excretion	Toxicity	
	Caco-2 (log Papp in 10 ⁻⁶ cm/s)	Intestinal Absorption (% absorbed)	Skin Permeability (log Kp)	VD _{ess} (log L/kg)	BBB Permeability (log BBB)	CNS Permeability (log PS)	Total Clearance (log mL/min/kg)	Oral Rat Acute Toxicity (LD ₅₀ = mol/kg)	Oral Rat Chronic Toxicity (LOAEL = log mg/kg bw/day)
C ₂₁ H ₂₀ O ₁₀	0.330	37.609	-2.735	0.342	-1.391	-3.746	0.547	2.595	4.359
C ₁₁ H ₁₆ O ₃	1.317	97.134	-2.287	-0.05	0.268	-2.479	0.482	2.378	2.085
C ₂₉ H ₃₈ N ₈ O ₃	-0.315	55.327	-2.735	-0.006	-0.741	-3.769	0.566	2.481	3.346
C ₂₆ H ₃₃ NO ₅	0.666	88.283	-2.701	-0.584	-0.005	-1.973	0.49	2.889	0.909
C ₄ H ₁₀ N ₂ S ₂	1.301	85.761	-3.495	0.097	-0.267	-3.161	0.925	2.403	0.508
C ₈ H ₁₂ O ₆	0.015	74.441	-3.207	-0.364	-1.183	-3.959	0.722	1.860	2.741
C ₂₁ H ₂₀ O ₁₀	0.066	37.511	-2.735	0.274	-1.417	-3.687	0.096	2.643	4.406
C ₁₃ H ₁₈ O ₂	1.729	94.064	-2.685	-0.803	0.310	-1.695	0.263	2.303	2.438
C ₁₃ H ₁₈ O ₃	1.373	100	-2.728	-1.607	-0.039	-2.1	0.768	2.159	2.142
C ₂₆ H ₃₃ NO ₅	0.973	75.585	-3.011	0.16	-0.811	-2.194	1.462	2.137	2.019
C ₃₁ H ₃₈ N ₈ O ₃	0.847	86.329	-2.735	1.081	-1.575	-3.331	0.307	2.74	2.179
C ₇ H ₆ N ₂ S	1.655	92.748	-3.026	0.135	0.398	-2.071	0.248	2.503	1.809
C ₇ H ₁₃ NO ₂	0.468	81.472	-2.739	-0.665	-0.351	-3.37	1.153	1.836	2.653
C ₉ H ₁₇ NO ₅	-0.453	30.442	-2.735	-1.15	-0.8	-3.611	0.595	1.28	2.448
C ₁₃ H ₁₈ O ₃	1.213	94.245	-2.654	-1.311	0.21	-2.401	0.319	2.527	1.829
C ₂₂ H ₂₉ N ₇ O ₃	1.125	72.014	-2.735	-0.202	-0.73	-3.303	0.287	2.122	1.537
C ₁₉ H ₂₂ O ₅	1.146	100	-2.735	-0.970	-0.084	-2.458	0.752	2.087	2.379
C ₁₁ H ₁₆ O ₂	1.555	100	-2.731	-0.916	0.406	-1.889	-0.013	1.822	2.161
C ₁₆ H ₃₂ O	1.478	92.332	-2.482	0.487	0.819	-1.564	1.827	1.506	1.155
C ₁₉ H ₄₁ N	1.34	88.016	-2.742	0.934	0.951	-1.69	1.537	2.35	0.882

Table 3. Binding free energy of 37 potential compounds

Ligands	Binding Free Energy (Kcal/mol)	Inhibitory Constanti (μM)	Hydrogen Bond	Amino Acid Residue
Native Ligan (Adenosin Difosfat)	-7.14	5.84	Asp179, Lys187, Lys213, Ile243, Gly244, His181	Gly158, Tyr188, Phe245, Gly244, Ile243, Gly156, Ser157, Asp179, Gly180, Lys187 , His181, Lys213

Kampferol-3-Rhamnoside	-7.11	6.10	Asp179, Lys187, Gly180, Lys213	Leu185, Tyr186, Gly158, Ser157, His181, Asp179, Gly156, Gly180, Ile155, Leu241, Phe217, Ile122, Pro120, Ile243, Val214, Lys213, Lys187, Tyr188, Thr118,
Meperidin	-7.32	4.30	Ile243, His181	Thr118, Ile243, Lys187, Asp179, Ser157, Gly158, Cys242, Gly156, Ile178, Gly180, Lys213, Val214, Ile155, His181, Lys187
N-[2-Amino-6-(butylamino)-3-hydroxy-5-methyl-6-oxohexyl]-N-isopropyl-4-methoxy-3-(3-methoxypropoxy)benzamide	-4.62	408.65	Lys213, Val214, Gly156, Ile243	Phe245, Gly244, Ser157, Asp179, Pro120, Gly156, Lys213, Ile122, Val214, Ile155, Ile178, Ile243, His181, Gly180, Lys187, Thr118
2-[(2-Methoxy-4-{[4-(4-methyl-1-piperazinyl)-1-piperidinyl]carbonyl}phenyl)amino]-5,11-dimethyl-5,11-dihydro-6H-pyrimido[4,5-b][1,4]benzodiazepin-6-on	-5.82	53.89	Cys242	Asp179, Cys242, Tyr159, Gly161, Gly158, Ile160, Lys213, Ile243, Gly244, Gly156, Gly180, Ile243, Tyr188, Lys187, His181, Val119, Leu241, Ile125, Pro120, Phe217, Ile122, Ile155, Val214
4-[(4-[3-Ethyl-7-(4-morpholinyl)-3H-[1,2,3]triazolo[4,5-d]pyrimidin-5-yl]phenyl}carbamoyl)amino]-N-[2-(2-pyridinyl)ethyl]benzamide	-4.62	408.65	Ser212	Leu229, Ser212, Ile178, Gly180, Val214, Asp179, Ile155, Ile243, Gly156, Thr118, Cys242, Gly244, Tyr188, Tyr159, Ile160, Phe245, Leu299, Pro298, Pro120, Ile122, Lys213, Ala215, Thr228
4H-cyclopenta[def]phenanthrene-4-one	-6.80	10.44	Val214	Ser157, Gly156, Asp179, Gly180, Ile155, Ile178, Val214, Ile122, Pro120, Lys213, Ile243
2,4-Diamino-6-morpholino-s-triazine	-5.67	70.39	Ile243, Val214, Gly156, Asp179	Ile243, Lys213, Val214, Ile155, Ile178, Gly156, Gly180, Ser157, Gly158, Asp179, His181, Lys187
3-(4,6-dimorpholino-1,3,5-triazin-2-yl)-1,2,3,4,5,6-hexahydro-8H-1,5-methanopyridol[1,2-a] [1,5] diazocin-8-one	-4.62	377.04	Lys187	Pro120, Ile122, Lys213, Ile243, Thr118, Val214, Gly180, Gly156, Ser157, Asp179, His181, Gly158, Tyr188, Gly244, Lys187
Ethyl N-[(2-{[(4-carbamoylphenyl)amino]methyl}-1-methyl-1H-benzimidazol-5-yl)carbonyl]-N-2-pyridinyl-β-alaninate	-5.38	133.08	Val214, Lys213, Ile243, Gly180, Asp179	Ile122, Ile155, Gly156, Gly180, Ser157, Asp179, His181, Gly158, Lys187, Gly244, Tyr188, Thr118, Ile243, Pro120, Lys213, Val214
2-Methyl-2-propanyl {(2S,3S)-1-[(3S)-7-[2-(hydroxyamino)-2-oxoethoxy]-3-(4-methoxyphenyl)carbamoyl]-3,4-dihydro-2(1H)-isoquinolinyl]-3-methyl-1-oxo-2-pentanyl} carbamate	-8.27	869.30	Ala11, His10, Asp282, Gln426, Tyr159, Pro298, Thr9	Leu40, Pro427, Phe425, Ala11, His10, Asp282, Gln426, Tyr159, Pro298, Thr9
11-[4,6-Di(4-morpholinyl)-1,3,5-triazin-2-yl]-7,11-diazatricyclo[7.3.1.0~2,7~]trideca-2,4-dien-6-one	-4.69	362.46	Lys187, Gly158, Asp179	Lys213, Ile243, Val214, Thr118, Lys187, Gly244, Gly158, Tyr188, Asp179, His181, Ser157, Gly180

1-(1-Methylethyl)-3-Quinolin-6-Yl-1h-Pyrazolo[3,4-D]pyrimidin-4-Amine	-7.69	2.31	Ser115, Tyr296	Gly281, Ser283, Gly114, Ser115, Asp282, Lys134, Phe245, Ile160 , Ser41, Thr9, Asn135, Leu299, Pro298, Tyr296
2,4-Diamino-6-morpholino-s-triazine	-5.41	109.07	Tyr188, Tyr159, Ser326, Gly341	Leu299, Tyr188, Tyr159 , Ser326, Gly341
6-[2-(2-Ethyl-4-methyl-1H-imidazol-1-yl)ethyl]-1,3,5-triazin-2,4-diamin	-8.71	411.54	-	Ile44, Ser41, Asn135, His10, Tyr62, Glu32, Ala11, Thr112, Gly12, Thr9, Cys8, Ser38, Ile37, Thr13, Gly7, Phe39, Ser115, Asp282, Gly114, Lys134
Biurea, 1,6-dimethyl-1,6-dinitroso-	-5.45	101.72	Ser38, Phe39, Lys134	Ile37, Ser38, Phe39, Asn36, Lys134, Phe245, Asn135, Ala11, His10, Tyr62, Thr9, Cys8
N-Methyl-D-phenylalanyl-N-[5-carbamimidamido-1-(1-methyl-1H-benzimidazol-2-yl)-1-oxo-2-pentanyl]-L-prolinamide	-7.95	1.49	Ser41, Thr9	Thr113, Asn248, Lys116, Asn135, Gly114, Lys134, Ser115, Asp282, Tyr136, Pro298, Tyr296, Ser41, Leu60, Phe61, Ser63, Asn36, Ile37, Tyr62, Leu40, Ser38, Phe39, Thr9, Cys8, His10, Gly12, Ala11, Gly7, Thr112, Glu32
N-Cyclopentyl-N-[2-(dimethylamino)ethyl]-2-(5-{[isopropyl(methyl)amino]methyl}-1-tetrazolidinyl)acetamid	-9.58	94.83	Asn36, Thr9	Ser41, Asn135, His10, Ala11, Asn34, Glu32, Asn36, Phe39, Cys8, Ile37, Thr12, Ser38, Tyr62, Phe61 , Ser115, Gly114, Asp282, Lys134
Apigenin-7-O-glucoside	-7.57	2.81	Lys213, Ile160, Tyr188	Ile243 , Gly180, Asp179, His181, Lys187, Tyr188, Gly158, Tyr159, Gly161, Ile160, Phe245, Cys242, Gly244, Thr118, Lys213, Pro120, Ile122
Isobutyl furfurylacetate	-5.66	71.09	His181	Lys213 , Gly180, Asp179, Val214, Ile243, Ile155, Ile178, Gly156, Cys242, Gly158, Tyr188, Ser157, Lys187, His181
2-ketobenzothiazole 54	-7.47	3.35	Lys213, Ile243, Gly156, Cys242, Phe245	Leu241, Ile155, Lys213, Val214, Ile122, Ile243 , Pro120, Gly156, Cys242, Gly158, Tyr188, Gly244, Lys187, Ser157, His181, Phe245, Arg246, Thr118, Asp179, Gly180
(S)-2-(3-(1-((4-Isopropylbenzyloxy)carbonyl)piperidin-3-yl)phenoxy)-2-methylpropanoic acid	-8.12	1.12	Lys187	Phe245, Thr118, Pro120, Ile243 , Gly244, Lys213 , Tyr188, Lys187, Gly158, His181, Ser157, Cys242, Asp179, Gly156, Gly180, Ile178, Val214, Ile155
Salicyloylaminotriazole	-7.10	6.27	His181, Lys213, Gly180, Asp179	Tyr188, His181, Lys187, Lys213 , Val214, Ile243, Ile178, Ile155, Gly156, Gly180, Ser157, Asp179, Gly158
(3-Aminopropyl)carbamodithioic acid	-5.02	209.90	Asp179, Ser157, Tyr186, Lys187	Gly156, Gly180, Asp179, Ser157, Gly158, His181, Arg183, Tyr186, Val184, Leu185, Lys187, Tyr188, Cys242, Ile243
3-O-Ethylascorbic acid	-4.43	570.11	Lys213, Cys242, Gly158, Ser157	His181 , Tyr186, Arg183, Leu185, Asp179, Ser157, Gly156, Tyr188, Gly158, Cys242, Gly244, Ile243, Lys213, Lys187, Gly180
Genistin	-6.65	13.33	Ser157, Gly158, Lys213, Ile243, Val214	Lys187, Gly244, Lys213 , Pro120, Thr118, Ile243 , Val214, Ile155, Ile178, Gly180, Ser212, Asp179, Gly156, Cys242, Ser157, Gly158
p-Hexyloxybenzoic Acid	-5.38	113.15	Lys213	Thr118, His181, Ile243 , Gly156, Leu185, Ser157, Tyr186, Asp179, Lys187, Gly158, Tyr188, Lys213
Ibuprofen	-5.68	68.65	Lys187	Ile155, Val214, Lys213 , His181, Lys187, Tyr188, Cys242, Gly158, Ser157, Asp179, Gly156, Ile243 , Gly180

Salicylihalamide A	-7.67	2.41	Ile243, Lys213	Leu185, Tyr186, Gly158, Tyr188, Ile178, Gly156, Ile155, Val214, Ile122, Ile243 , Pro120, Thr118, Lys187, Gly244, Asp179, Lys213 , His181 , Ser157, Cys242, Gly180
Adamantanecarboxylic acid	-5.43	103.87	Lys213, Lys187	Gly180, Asp179, His181 , Lys213 , Ile243, Gly156, Lys187
2-Aminobenzothiazole	-4.86	273.21	Gly180, Val214	Ser157, Asp179, Ile178, Gly108, Ile155, Val214, Ile122, Lys213 , Gly156, Ile243
1-(1-(2-ethoxyethyl)-3-methyl-7-((4-methylpyridin-2-yl)amino)-1H-pyrazolo[4,3-d]pyrimidin-5-yl)piperidine-4-carboxylic acid	-6.75	11.20	Lys187, Lys213, Gly180, Asp179	Gly244, Lys187, His181, Thr118, Lys213 , Val214 , Leu241 , Ile125 , Phe217 , Ile122 , Ile155, Gly180, Ile178, Asp179, Ile243 , Gly156, Ser157, Cys242, Gly158, Tyr188
Gibberellin A7	-8.14	1.09	Lys213, Gly180	Phe217, Lys213, Lys187, His181, Ser157, Asp179, Gly156, Gly180, Ile243 , Leu241 , Ile122 , Val214 , Ile155
1-hexadecanal	-4.69	361.85	-	His181 , Cys242, Lys187, Gly244, Thr118, Pro120, Ile122, Ile155, Lys213, Ile243, Val214, Gly180, Gly156, Asp179, Ser157, Gly158
2-Hydroxyibuprofen	-6.01	39.41	Lys187, Lys213	Ile243 , Lys213, Lys187, His181, Asp179, Ser157, Tyr188, Tyr186, Gly158, Leu185, Arg183
Homocycloleucine	-4.67	380.26	His181, Lys187, Asp179, Ser157	Gly158, Leu185, Tyr186, Tyr188 , Gly180, Asp179, Gly156, Lys187 , Ser157, His181
N-methyloctadecan-1-amine	-3.87	1.45	Val214	Pro120, Ile122, Val214, Ile160 , Tyr159 , Lys213, Ile243, Phe245, Tyr188, Gly158, Gly244, Cys242, Ser157, Gly156, Gly180, Asp179, Lys187, His181
Pantothenic acid	-3.91	1.36	Lys213, Lys187	His181, Gly244, Ile243, Tyr188, Gly158, Cys242, Lys187, Lys213