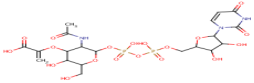
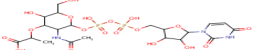
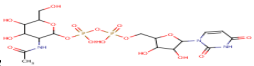
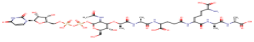
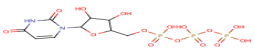
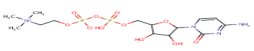


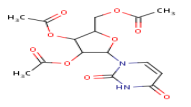
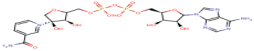
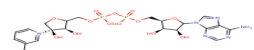
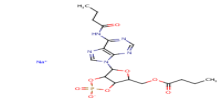
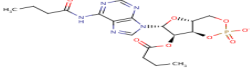
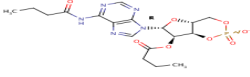
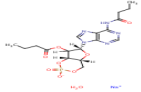
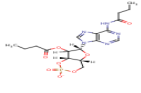
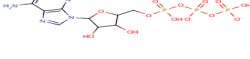
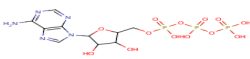
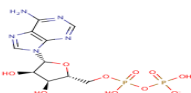
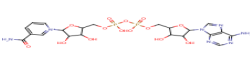
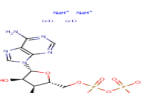
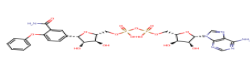

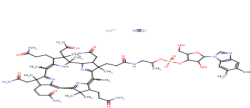
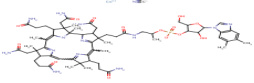
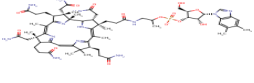
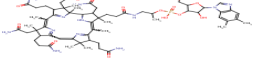
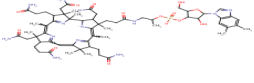
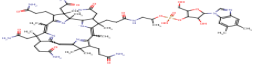
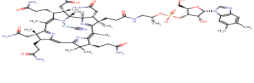
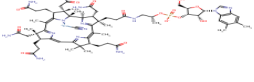
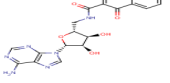
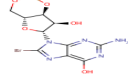
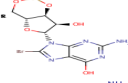
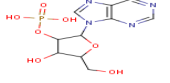
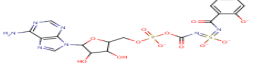
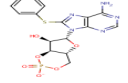
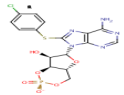
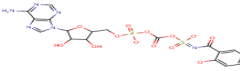
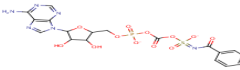


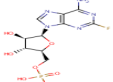
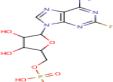
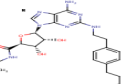
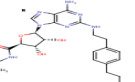
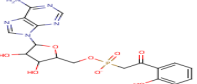
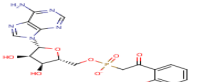
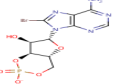
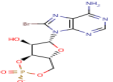


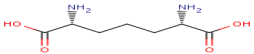
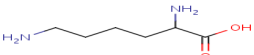
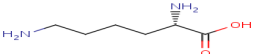
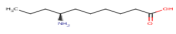

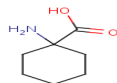

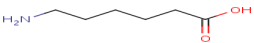
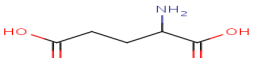
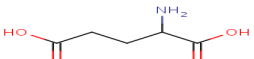
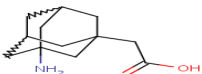
Molecule	Structure	CDD Number	Similarity Score (%)	Alamar Blue: Percent	TB Prathiparti MIC B: MIC	TB Prathiparti MIC A: MIC	MTb (H37Rv) Inhibitory	MTb (H37Rv) Inhibitory	MTb (H37Rv) Inhibitory Dose
<b>ESSENTIAL MOLECULE: UDP-GlcNAc-enol pyruvate</b>									
UDP-GlcNAc-enol pyruvate			100						
UDP-N-acetyl-muramate			98						
UDP-N-acetyl-D-glucosamine			95						
UDP-N-acetylmuramoyl-L-alanine			89						
JHU- 12039		CDD-42391	73						
JHU- 2276		CDD-128568	70						
TBL-7912			67						
TBL-7912		CDD-343091	67						
ST013879		CDD-45534	64						
Nadide		CDD-1644	61						
Nadide		CDD-1644	61	-3					

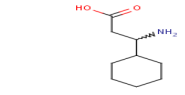
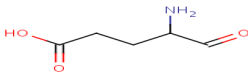
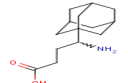


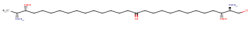
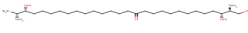
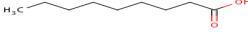
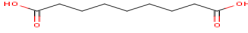
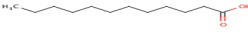
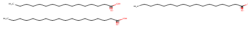
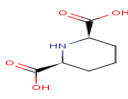
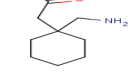
JHU- 1441		CDD-128664	60	
SMR000058940			60	
SMR000058940		CDD-303017	60	
Bucladesine sodium salt		CDD-1701	60	
Bucladesine sodium salt		CDD-1701	60	-1
ST075421		CDD-45861	60	
JHU- 178		CDD-42157	60	
ST057097		CDD-45679	60	
JHU- 6717		CDD-47258	60	
ST057081		CDD-44446	59	
TBL-8595		CDD-343074	59	
TBL-8595		CDD-343074	59	
JHU- 2633		CDD-45948	58	



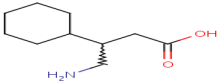

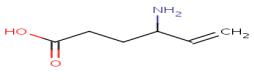
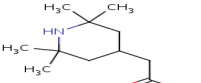
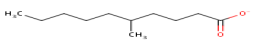

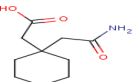

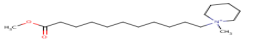
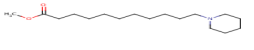
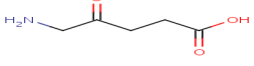
JHU- 5184		CDD-45951	58	
Hydroxocobalamin		CDD-891	58	
JHU- 2457		CDD-46421	58	
JHU- 4913		CDD-47349	58	
JHU- 10786		CDD-45950	58	
Cyanocobalamin		CDD-1384	58	
Cyanocobalamin		CDD-1384	58	33
TBL-2459		CDD-341600	58	
SMR000326870			58	
SMR000326870		CDD-298228	58	
ST013860		CDD-45528	57	
351369		CDD-51464	57	0.131533
SMR000326853			57	

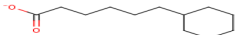

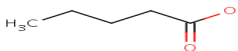
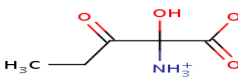
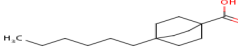
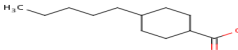
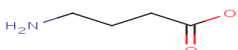
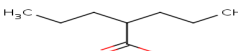
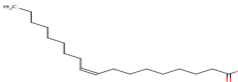
SMR000326853		CDD-215826	57	
351366		CDD-51487	56	0.154921
351368		CDD-53049	56	7.86158
SMR000450983			56	
SMR000450983		CDD-308570	56	
Fludarabine phosphate		CDD-864	56	
JHU- 12275		CDD-47321	56	
SMR000058796		CDD-327201	55	
SMR000058796		CDD-327201	55	
213648		CDD-50448	55	100
TBL-1747		CDD-341006	55	
SMR000326869			55	
SMR000326869		CDD-215785	55	

**ESSENTIAL MOLECULE: MESO-DIAMINOPIMELATE**

meso-diaminopimelate		CDD-47339	100	
JHU-5918		CDD-47339	98	
692_FDAMDD_v3b		CDD-47990	98	
SMR000102743		CDD-258204	90	-7.02
SMR000387093		CDD-170625	81	-15.48
SN-5889		CDD-5133	81	
SMR000102742		CDD-161620	80	-9.8
6-aminohexanoic acid		CDD-7	77	
L-glutamate		CDD-41783	69	
SMR000033946		CDD-41783	69	0
SMR000278375		CDD-222679	68	3.53, 4.04

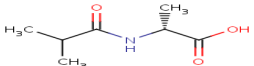
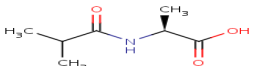
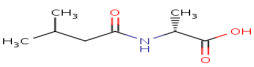
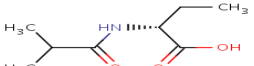
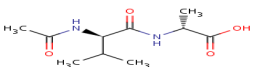
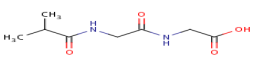
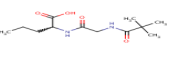
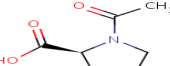
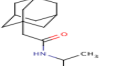
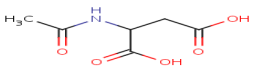
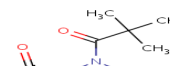
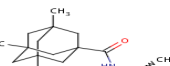
SMR000338326		CDD-171480	67	1.31		
Glutamate-1-semialdehyde			66			
SMR000299536		CDD-221626	65	0.31		
Tranexamic acid		CDD-689	65			
Tranexamic acid		CDD-689	65	-33		
TBL-734		CDD-340419	65			
TBL-734		CDD-340419	65		Inhibition of I Invitro	12538025
SMR000112203		CDD-46795	62	7.39		
SMR000059164		CDD-61	62	-11.58		
TBL-1707		CDD-2534	62		Antimycobac Invitro	16180806
TBL-1710		CDD-340981	62		Antimycobac Invitro	16180806
TBL-2523		CDD-341652	62		Inhibition of I Invitro	18054225
Gabapentin		CDD-297	62	10		

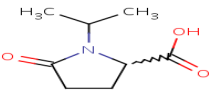
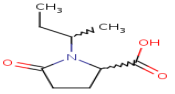
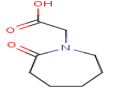


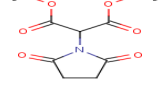
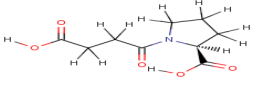
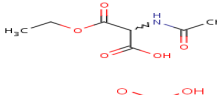
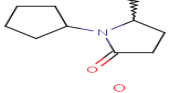
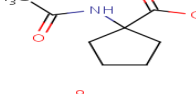
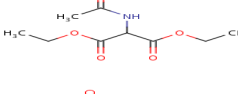
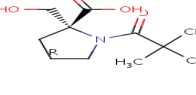
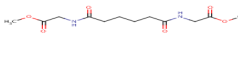
SMR000058664		CDD-160221	59		-0.52
SMR000326773		CDD-254061	59		-11.86
SMR000131763		CDD-161284	58		1.27
SMR000386957		CDD-42709	58		9.95
Vigabatrin		CDD-1052	58	0	
SMR000315130		CDD-60021	57		2.4
17609		CDD-53758	57	16.8387	
SMR000127417		CDD-255913	57		6.65
SMR000036610		CDD-154969	55		-7.64
SMR000416006		CDD-192760	55		-0.4
SMR000175091		CDD-271453	55		6.47
SMR000175090		CDD-304261	55		3.77
5-amino-levulinate		CDD-15328	55		

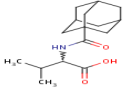
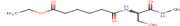
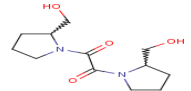
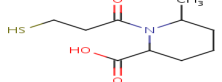
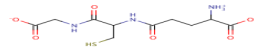
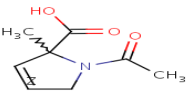
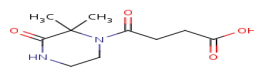
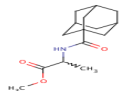
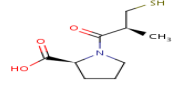
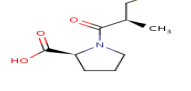
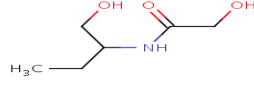
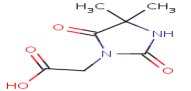
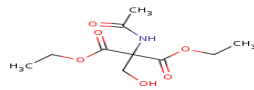
17610		CDD-54322	54	31.4245		
TBL-1709		CDD-340980	54		Antimycobac Invitro	16180806
TBL-2524		CDD-341653	53		Inhibition of I Invitro	18054225
SMR000424877		CDD-285242	53		-3.95	
SMR000471834		CDD-309946	52		-4.9	
92585		CDD-53528	52	13.5934		
17612		CDD-53378	52	11.6665		
SMR000113247		CDD-322745	52		-5.43	
SMR000019012		CDD-338808	52		-15.89	
SMR000058285		CDD-14017	51		-5.23	
SMR000499581		CDD-717	51	14.81		
17614		CDD-54032	51	22.2056		

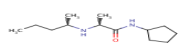
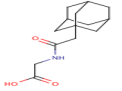
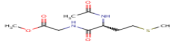
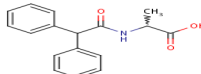
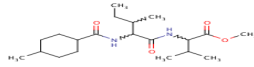
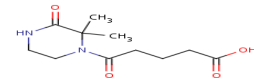
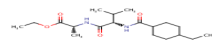
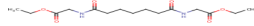
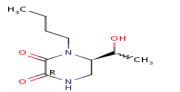
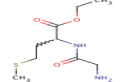
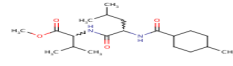
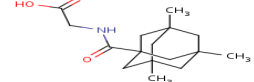


## ESSENTIAL MOLECULE: D-alanine-D-alanine

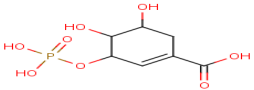
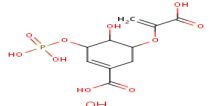
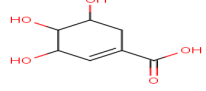
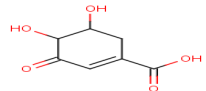
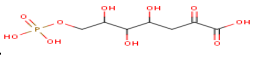
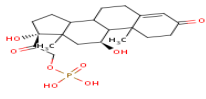
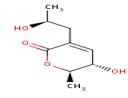
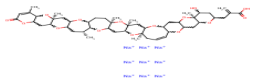
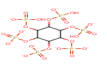
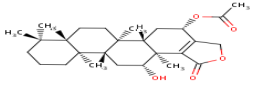
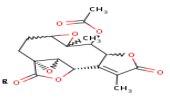
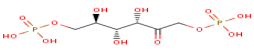
CDD-62785		CDD-62785	82	
CDD-74989		CDD-74989	82	
CDD-63657		CDD-63657	75	
CDD-62786		CDD-62786	74	
CDD-63766		CDD-63766	71	
CDD-57283		CDD-57283	66	
SMR000039488		CDD-234078	65	0.62
SMR000365399		CDD-61098	63	0.28
7561067		CDD-145987	62	2.56
Aspartic acid, N-acetyl (R,S)		CDD-1369	61	1
SMR000135311		CDD-258631	60	0.34
SMR000298068		CDD-240528	60	-6.98

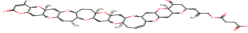
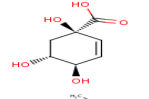
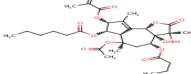
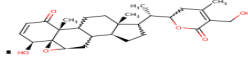
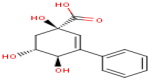
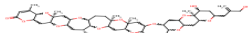
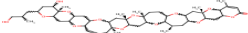
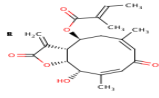
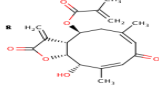
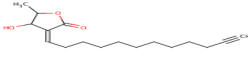
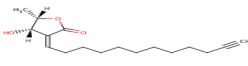
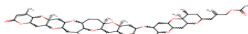
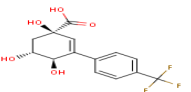
SMR000132432		CDD-168599	59	2.15
SMR000132615		CDD-326812	58	1.77
SMR000368756		CDD-59139	57	-6.48
SMR000324857		CDD-158233	57	-6.28
SMR000275346		CDD-253586	57	4.02
7823679		CDD-131606	57	-1.12
SMR000326657		CDD-327150	57	-8.05
SMR000145624		CDD-161166	56	-1.99
SMR000033650		CDD-165697	56	-0.61
SMR000393684		CDD-197851	56	-3.18
18685		CDD-54256	56	28.7725
SMR000231097		CDD-150148	55	-0.65
SMR000023915		CDD-204064	55	-8.53

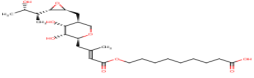
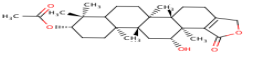
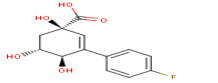
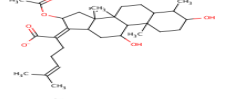
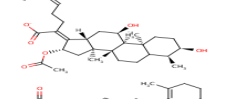
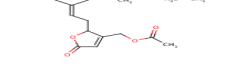
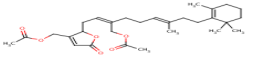
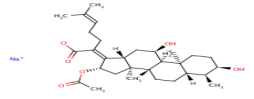
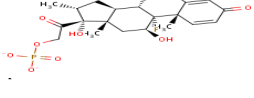
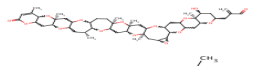
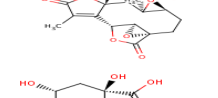
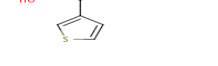
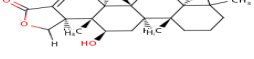
SMR000064358		CDD-159991	54		-7.6
SMR000038218		CDD-335296	54		-3.17
SMR000281812		CDD-265293	54		-7.97
5219863		CDD-130340	54		-11.35
1653		CDD-51090	53	0.00816	
SMR000389080		CDD-169480	53		-3.82
SMR000124115		CDD-58256	53		5.98
SMR000062190		CDD-159948	53		-3.59
Captopril		CDD-1069	53	10	
SMR000059061		CDD-1069	53		-12.15
TBL-6682		CDD-344159	53		Antimycobac Invitro
SMR000151266		CDD-57914	53		1.52
SMR000059905		CDD-287960	53		4.72

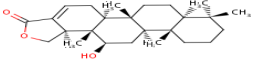
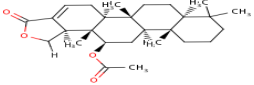
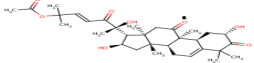
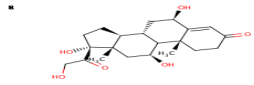
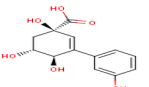
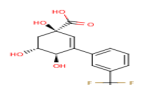
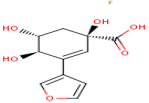
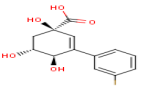
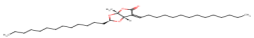
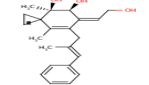
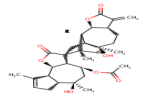
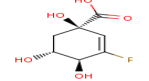
SMR000253920		CDD-316141	52	-6.8
7668592		CDD-129640	52	0.53
SMR000285755		CDD-163261	52	-12.36, -8.9
SMR000065739		CDD-339642	52	-12.06
SMR000025113		CDD-225760	51	6.19
SMR000275429		CDD-58257	51	8.98
SMR000022542		CDD-184338	51	1.14
SMR000038578		CDD-261447	51	-10.28
SMR000462344		CDD-266148	51	-2.35
SMR000010934		CDD-302106	50	-2
SMR000130285		CDD-231616	50	-2.41
7890140		CDD-131621	50	-1.5

**ESSENTIAL MOLECULE: Shikimate-3-phosphate**

Shikimate-3-phosphate			100	
5-enolpyruvyl-shikimate-3-phosphate			80	
Shikimate			67	
3-dehydro-shikimate			57	
3-deoxy-d-arabino-heptulose			54	
CDD-14819		CDD-14819	51	
SMR000440586		CDD-163046	51	8.8
SMR000265086		CDD-291571	50	-8.06
CDD-46044		CDD-46044	50	
TBL-3891		CDD-342011	49	
SMR000156259		CDD-186881	49	-3.61
CDD-870		CDD-870	48	

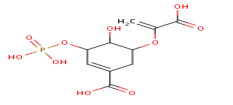
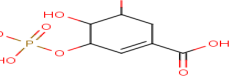
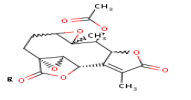

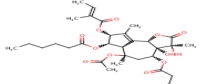
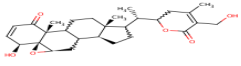

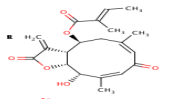
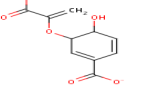
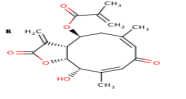
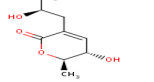
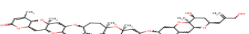
SMR000453594		CDD-168394	48	-9.09
TBL-1582		CDD-340890	48	
SMR000440625		CDD-168409	47	48.57
SMR000440592		CDD-169155	47	1.25
TBL-1585		CDD-340893	47	
SMR000265087		CDD-169952	47	6.08
SMR000265081		CDD-170928	47	7.64
SMR000445667		CDD-270524	47	-10.55
SMR000445666		CDD-337904	47	-4.72
342055		CDD-53251	47	10.16
TBL-1708		CDD-340979	47	
SMR000453593		CDD-327066	46	-1.93
TBL-1587		CDD-340895	46	

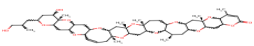
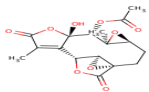
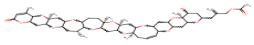
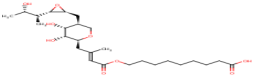
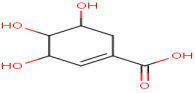
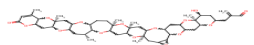
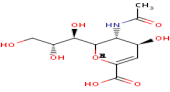
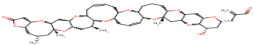
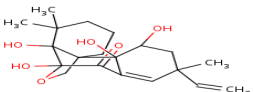
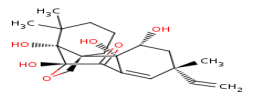
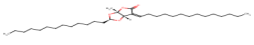
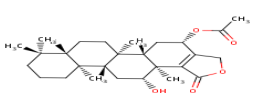

SMR000471888		CDD-164785	46		-9.93
TBL-3894		CDD-342566	46		
TBL-1586		CDD-340894	46		
132		CDD-52622	46	3.87814	
SMR000059232		CDD-152203	46		25.01
TBL-1244		CDD-340732	45		
TBL-1245		CDD-340733	45		
Fusidic acid sodium salt		CDD-1346	45	72	
SMR000058813		CDD-160129	45		11.43
SMR000265080		CDD-163028	45		15.04
SMR000156260		CDD-339894	45		-10.64
TBL-1594		CDD-340902	45		
TBL-1248		CDD-340736	45		

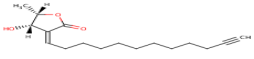
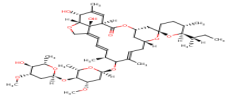
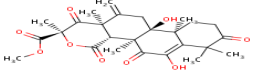
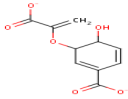
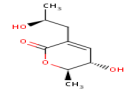
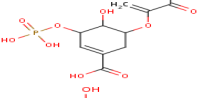
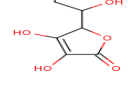
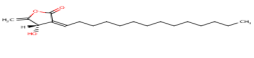
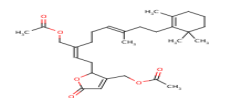
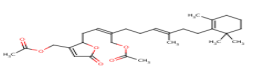
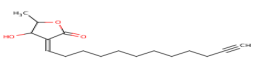
TBL-3893		CDD-342392	45	
TBL-1247		CDD-340735	44	
SMR000232280		CDD-169346	44	-1.64
SMR000058916		CDD-168620	44	-2.26
TBL-1590		CDD-340898	44	
TBL-1589		CDD-340897	44	
TBL-1596		CDD-340904	44	
TBL-1588		CDD-340896	44	
TBL-1706		CDD-340978	43	
SMR000545216		CDD-200281	43	1.22
SMR000226339		CDD-161966	43	1.15
TBL-1583		CDD-340891	43	

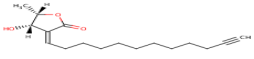
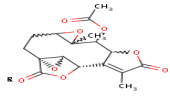
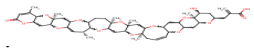
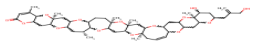
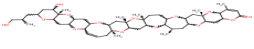
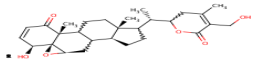
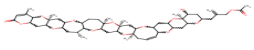
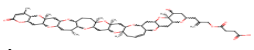
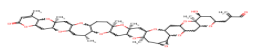
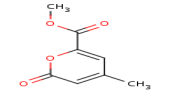
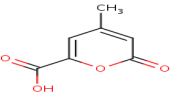
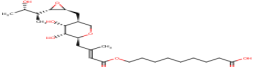
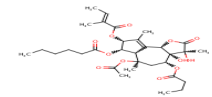


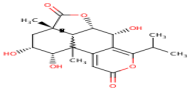
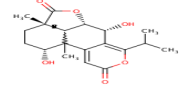
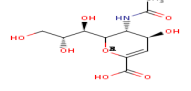
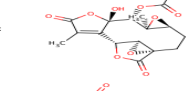
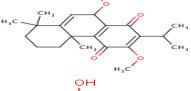
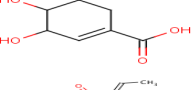
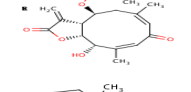
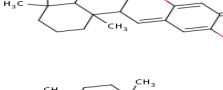
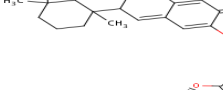
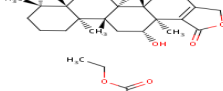
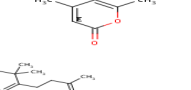
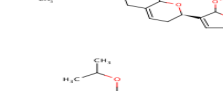
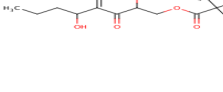
**ESSENTIAL MOLECULE: 5-enolpyruvyl-shikimate-3-phosphate**

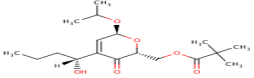
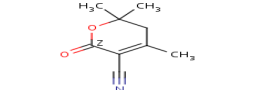
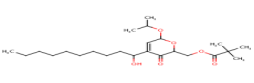
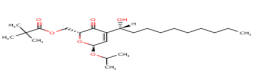
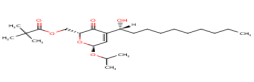
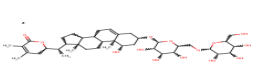
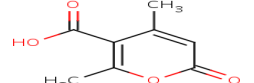
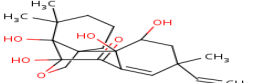
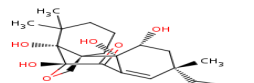
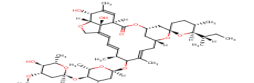
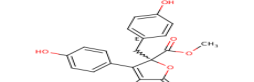
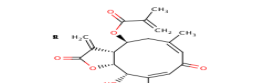
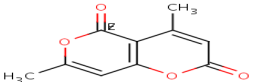
5-enolpyruvyl-shikimate-3-pl			100	
Shikimate-3-phosphate			80	
SMR000156259	 CDD-186881		58	-3.61
SMR000265086	 CDD-291571		58	-8.06
SMR000440625	 CDD-168409		56	48.57
SMR000440592	 CDD-169155		56	1.25
SMR000453594	 CDD-168394		56	-9.09
SMR000445667	 CDD-270524		55	-10.55
Chorismate			55	
SMR000445666	 CDD-337904		55	-4.72
SMR000440586	 CDD-163046		55	8.8
SMR000265087	 CDD-169952		55	6.08

SMR000265081		CDD-170928	55	7.64	
SMR000156260		CDD-339894	54	-10.64	
SMR000453593		CDD-327066	54	-1.93	
SMR000471888		CDD-164785	54	-9.93	
Shikimate			54		
SMR000265080		CDD-163028	53	15.04	
SMR000471880		CDD-216139	53	-10.88	
SMR000265084		CDD-168393	52	83.59	
166619		CDD-53115	52	8.50625	
TBL-745		CDD-340430	52		Antimycobac Invitro, Invit 12657257, 12657258
TBL-1706		CDD-340978	51		Antimycobac Invitro 16180806
TBL-3891		CDD-342011	51		Antimycobac Invitro 16378375
342055		CDD-53251	50	10.16	

TBL-1708		CDD-340979	50		Antimycobac Invitro	16180806
Ivermectin		CDD-1173	50	95		
SMR000440631		CDD-170291	50			-10.11
<b>ESSENTIAL MOLECULE: Chorismate</b>						
Chorismate			100			
SMR000440586		CDD-163046	58			
5-enolpyruvyl-shikimate-3-phosphate			55			
Ascorbic acid		CDD-1295	52	-6		
TBL-1704		CDD-340976	51			
TBL-1244		CDD-340732	50			
TBL-1245		CDD-340733	50			
342055		CDD-53251	50			10.16

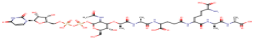
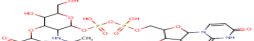


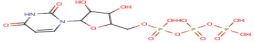



TBL-1708		CDD-340979	50
SMR000156259		CDD-186881	50
SMR000265086		CDD-291571	49
SMR000265087		CDD-169952	49
SMR000265081		CDD-170928	49
SMR000440592		CDD-169155	48
SMR000453593		CDD-327066	48
SMR000453594		CDD-168394	48
SMR000265080		CDD-163028	48
SMR000460905		CDD-263155	48
SMR000456927		CDD-257348	47
SMR000471888		CDD-164785	47
SMR000440625		CDD-168409	47

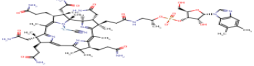
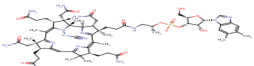
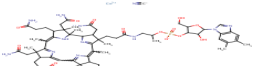
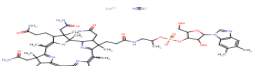
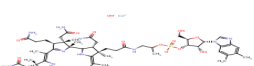
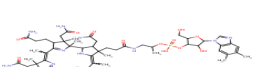
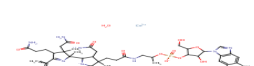
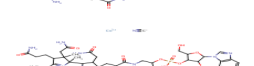
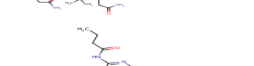
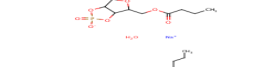
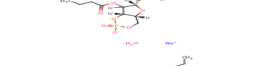
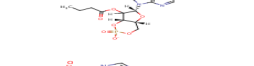
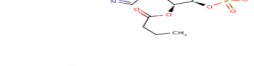
SMR000232308		CDD-168813	46	
SMR000232307		CDD-186948	46	
SMR000471880		CDD-216139	46	
SMR000156260		CDD-339894	45	
167369		CDD-52019	45	0.983213, 2.30279
Shikimate			45	
SMR000445667		CDD-270524	45	
10666		CDD-48179	44	38.058
10666		CDD-48179	44	38.0573
TBL-3891		CDD-342011	44	
SMR000147083		CDD-338334	44	
TBL-1249		CDD-340737	44	
419060		CDD-50320	43	73.008

TBL-6663		CDD-344460	43	
SMR000037070		CDD-207739	43	
17922		CDD-48991	43	14.651
TBL-5660		CDD-344465	43	
TBL-5660		CDD-344465	43	
SMR000440588		CDD-325620	43	
SMR000031519		CDD-44177	43	
166619		CDD-53115	43	8.50625
TBL-745		CDD-340430	43	
Ivermectin		CDD-1173	43	95
SMR000440685		CDD-254770	43	
SMR000445666		CDD-337904	43	
SMR000020726		CDD-165542	43	

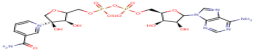
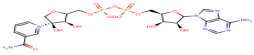
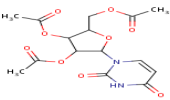
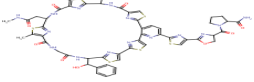
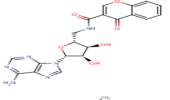
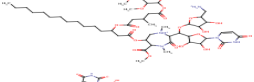


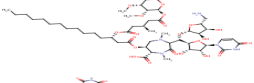

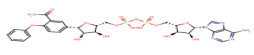
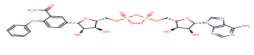
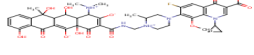
132		CDD-52622	43	3.87814
SMR000059232		CDD-152203	43	
SMR000265084		CDD-168393	43	

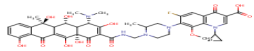
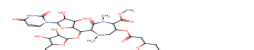
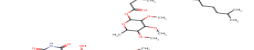
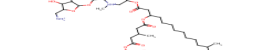
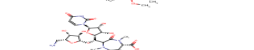
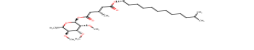
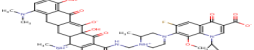

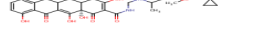
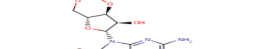
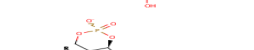
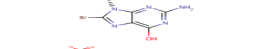

### ESSENTIAL MOLECULE: UDP-N-acetylmuramoyl-L-alanyl-D-glutamyl-meso-2,6-diaminopimelyl-D-alanyl-D-alanine

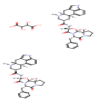

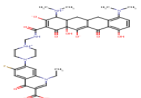
UDP-N-acetylmuramoyl-L-al			100	
UDP-N-acetyl-muramate			91	
UDP-GlcNAc-enol pyruvate			89	
UDP-N-acetyl-D-glucosamine			88	
JHU- 12039		CDD-42391	68	
JHU- 2276		CDD-128568	67	
TBL-7912			64	
TBL-7912		CDD-343091	64	Binding affir Invitro

Cyanocobalamin		CDD-1384	63	
Cyanocobalamin		CDD-1384	63	33
JHU- 2633		CDD-45948	63	
JHU- 5184		CDD-45951	63	
Hydroxocobalamin		CDD-891	63	
JHU- 2457		CDD-46421	63	
JHU- 4913		CDD-47349	63	
JHU- 10786		CDD-45950	63	
JHU- 1441		CDD-128664	61	
Bucladesine sodium salt		CDD-1701	60	
Bucladesine sodium salt		CDD-1701	60	-1
SMR000058940			60	
SMR000058940		CDD-303017	60	-9.01

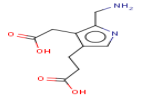
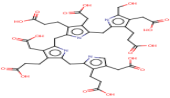


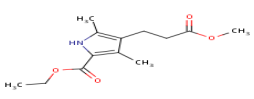
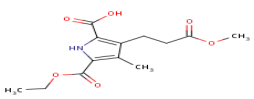
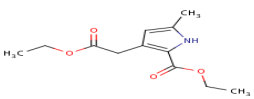
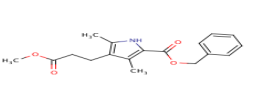


Nadide		CDD-1644	59		
Nadide		CDD-1644	59	-3	
ST013879		CDD-45534	59		
71645		CDD-51970	59		0.774865
TBL-2459		CDD-341600	58		Antimycoba Invitro, Invitro,
337554		CDD-51939	58		0.67926
337555		CDD-51946	58		0.68766
337553		CDD-52135	58		1.34213
TBL-6222		CDD-343099	58		Antimycoba Invitro, Invitro
TBL-6224		CDD-343101	58		Antimycoba Invitro, Invitro
TBL-8595		CDD-343074	58		
TBL-8595		CDD-343074	58		Inhibition of Invitro
195926		CDD-48298	58		0.46

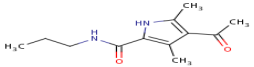
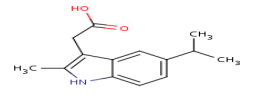
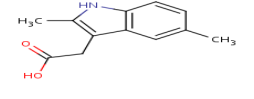
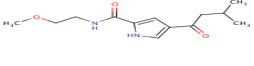
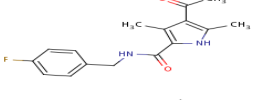
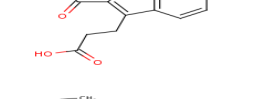
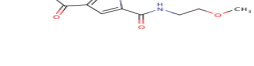
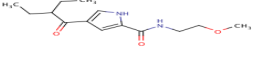
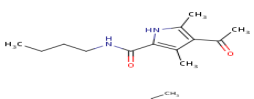
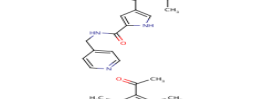
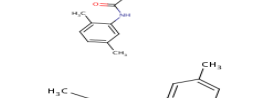
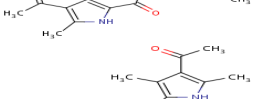
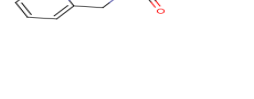
TBL-2165		CDD-341359	58		Antimycoba Invitro
181984		CDD-52136	58	1.34213	
337556		CDD-52150	58	1.37532	
TBL-6223		CDD-343100	58		Antimycoba Invitro, Invitro
228906		CDD-48239	58	0.237	
TBL-2158		CDD-341352	58		Antimycoba Invitro
SMR000326870		CDD-298228	58		
SMR000326870		CDD-298228	58		-6.79
117174		CDD-48351	58	0.985	
TBL-2162		CDD-341356	58		Antimycoba Invitro
SMR000058761		CDD-165952	58		17.86, 15.31
586074		CDD-48242	58	0.24	
TBL-2161		CDD-341355	58		Antimycoba Invitro

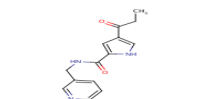
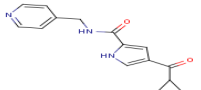
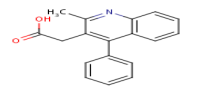
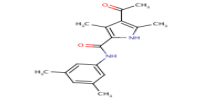
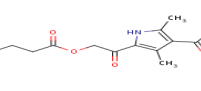
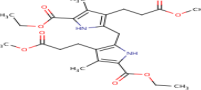
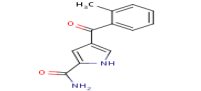
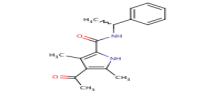
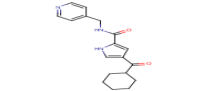
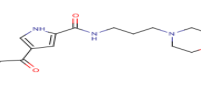
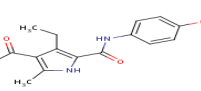
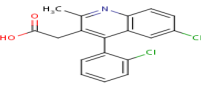
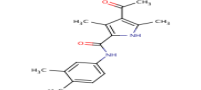
Dihydroergotamine tartrate		CDD-1167	58	17	
JHU- 6717		CDD-47258	58		
S87482		CDD-48352	58		0.989

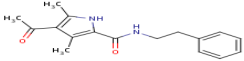
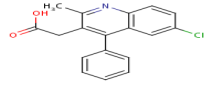
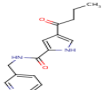
### ESSENTIAL MOLECULE: Porphobilinogen

Porphobilinogen			100		
Hydroxymethylbilane			66		
SMR000117351		CDD-208163	55	-5.91	
SMR000123140		CDD-55430	55	-2.28	
5211865		CDD-138969	54	9.74	
SMR000024024		CDD-149482	54	-3.92	
SMR000459807		CDD-152742	52	5.35	
SMR000037041		CDD-334358	52	5.97	

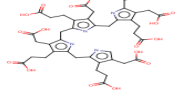
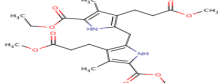
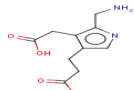
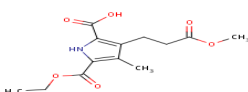
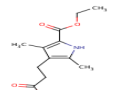
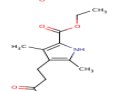
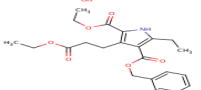
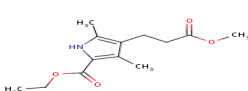
SMR000278254		CDD-216976	51	-0.71
SMR000025645		CDD-231080	51	-3
SMR000036607		CDD-337101	51	0.17
SMR000155142		CDD-183928	51	-3.19
SMR000336071		CDD-282511	51	0.64
SMR000335595		CDD-241050	51	-3.62
5986957		CDD-130567	51	-4.65
SMR000335954		CDD-156346	51	-10.08
SMR000153824		CDD-194562	50	-6.76
SMR000026827		CDD-179263	50	-10.38
SMR000278070		CDD-186584	50	10.91
CDD-117099		CDD-117099	50	
SMR000335875		CDD-240393	50	3.35

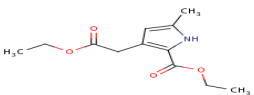
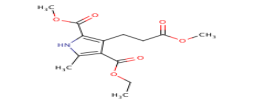
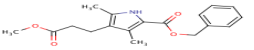
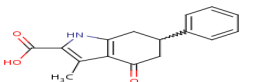
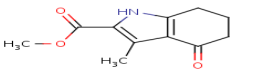
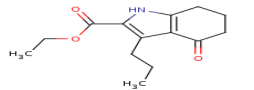
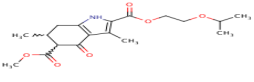
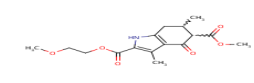
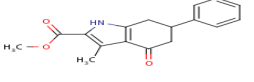
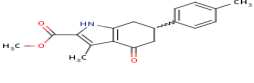
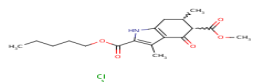
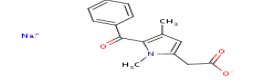
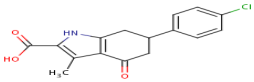
SMR000026822		CDD-179193	50	-14.03
SMR000456742		CDD-256082	50	3.69
7823323		CDD-58764	50	0.5
SMR000335871		CDD-331448	49	-1.86
SMR000375722		CDD-294239	49	5.54
7587340		CDD-129634	49	1.98
CDD-148185		CDD-148185	49	
SMR000335921		CDD-148185	49	2.24
SMR000309262		CDD-149384	49	-1.66
SMR000336065		CDD-281580	49	-6.09
SMR000094066		CDD-230624	49	-1.59
SMR000130725		CDD-150735	49	-4.14
SMR000026815		CDD-179261	49	-4.86

SMR000335872		CDD-158685	49	4.38
SMR000335950		CDD-331972	49	-1.89
SMR000243841		CDD-292749	49	3.93
SMR000153247		CDD-159312	48	-2.14
SMR000352704		CDD-241355	48	-0.41
SMR000107043		CDD-257352	48	-0.81
SMR000179978		CDD-210689	48	4.33
SMR000343464		CDD-281709	48	-0.06
SMR000336142		CDD-305702	48	2.26
SMR000179924		CDD-255030	48	15.83
SMR000027355		CDD-288736	48	-16.3
SMR000242789		CDD-215687	48	0.38
SMR000130680		CDD-207723	48	2.4

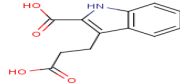
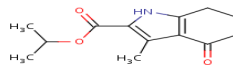
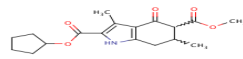
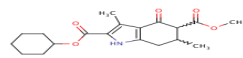
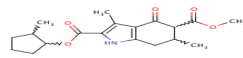
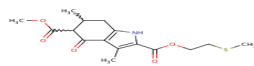
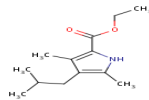
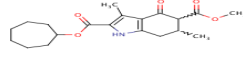
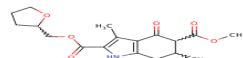
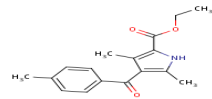
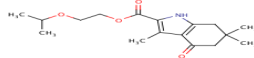
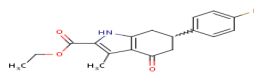
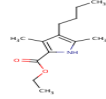
SMR000066691		CDD-225576	48	-0.84
SMR000242790		CDD-272930	48	3.64
SMR000335874		CDD-194417	48	5.43

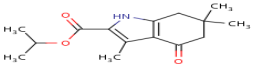
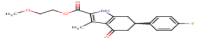
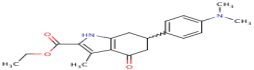
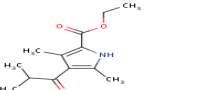
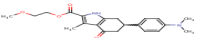
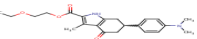
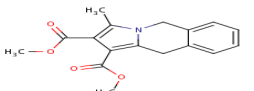
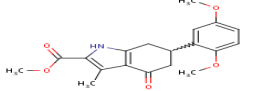
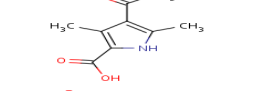
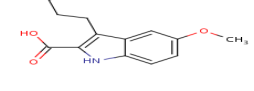
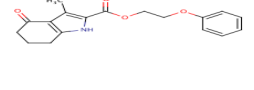
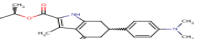
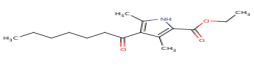
### ESSENTIAL MOLECULE: Hydroxymethylbilane

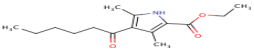
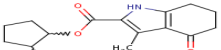
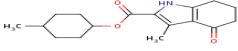
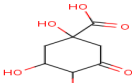

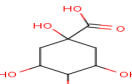
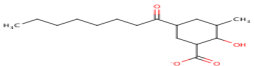
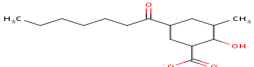
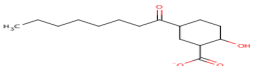
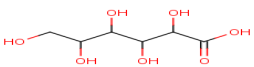
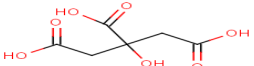
Hydroxymethylbilane			100	
SMR000107043		CDD-257352	73	
Porphobilinogen			66	
SMR000024024		CDD-149482	58	
SMR000117351		CDD-208163	58	
SMR000123140		CDD-55430	58	
SMR000459808		CDD-198465	57	
5211865		CDD-138969	57	

SMR000459807		CDD-152742	57	
5986957		CDD-130567	57	
SMR000037041		CDD-334358	56	
SMR000025512		CDD-210467	55	
SMR000024321		CDD-339602	55	
SMR000093505		CDD-154640	54	
SMR000025514		CDD-209686	54	
SMR000093494		CDD-182122	54	
7906781		CDD-136039	54	
SMR000025506		CDD-166484	54	
SMR000025513		CDD-209635	54	
Zomepirac sodium salt		CDD-1673	53	-35
7906780		CDD-136031	53	

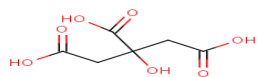


7587340		CDD-129634	53
SMR000081378		CDD-303193	53
SMR000025515		CDD-209746	52
SMR000093486		CDD-212908	52
SMR000093466		CDD-339231	52
SMR000093495		CDD-182140	52
SMR000306976		CDD-148558	52
SMR000093501		CDD-257704	52
SMR000093496		CDD-182155	52
SMR000136914		CDD-152896	52
SMR000093493		CDD-153474	52
SMR000092996		CDD-160023	52
SMR000307292		CDD-296215	52

7906779		CDD-136030	52
SMR000096120		CDD-181455	52
SMR000093499		CDD-166337	51
SMR000136941		CDD-179490	51
SMR000025570		CDD-286570	51
SMR000093490		CDD-338081	51
6954555		CDD-134916	51
SMR000093015		CDD-174968	51
SMR000274100		CDD-293633	51
7744779		CDD-131846	50
SMR000025504		CDD-286801	50
SMR000093500		CDD-270619	50
SMR000102649		CDD-212741	50

SMR000102569		CDD-328715	50	
SMR000093492		CDD-182049	50	
SMR000093504		CDD-270948	50	
<b>ESSENTIAL MOLECULE: 3-dehydroquinate</b>				
3-dehydroquinate			100	
JHU- 1639		CDD-45916	83	
ST069282		CDD-45776	83	
110597		CDD-53000	70	7.05746
110596		CDD-53864	70	18.5625
110595		CDD-54402	70	37.1249
JHU- 12273		CDD-2617	69	
anhydrous citric acid		CDD-48	68	

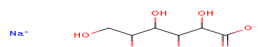
SMR000471840



CDD-48

68

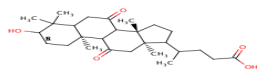
JHU- 9224



CDD-46125

68

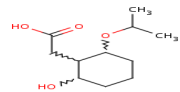
SMR000528036



CDD-150659

66

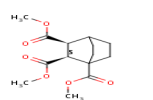
SMR000393714



CDD-197336

64

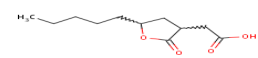
SMR000039502



CDD-147934

62

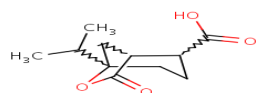
SMR000019361



CDD-229928

60

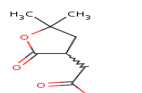
SMR000104203



CDD-257145

60

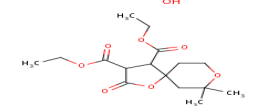
SMR000123336



CDD-166825

59

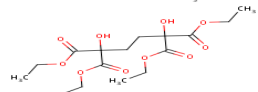
5238109



CDD-130298

59

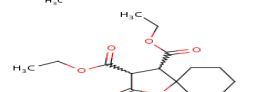
SMR000111707



CDD-229008

59

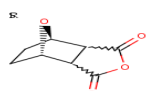
SMR000137265



CDD-161355

58

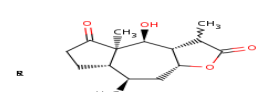
SMR000058587



CDD-270132

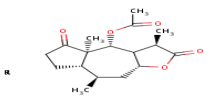
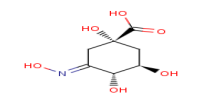
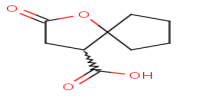
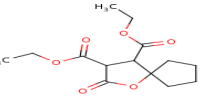
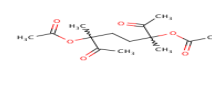
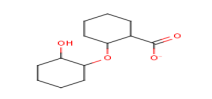
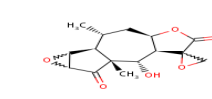
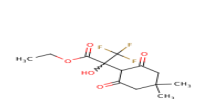
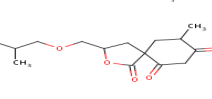
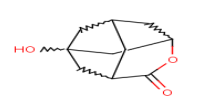
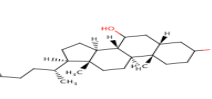
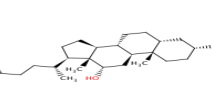
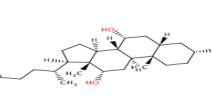
58

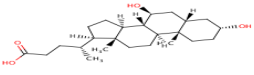
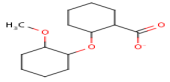
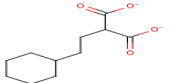
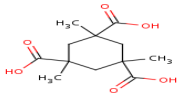
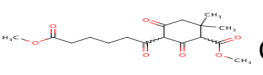
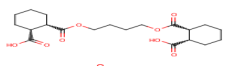
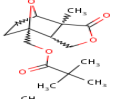
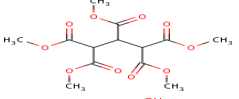
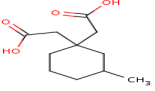
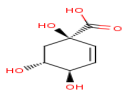
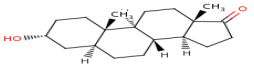
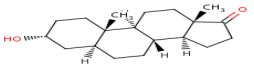
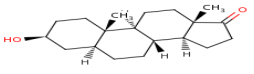
SMR000445654

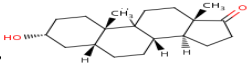
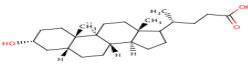
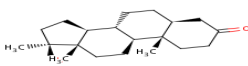


CDD-170204

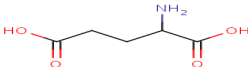
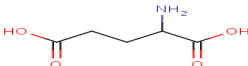
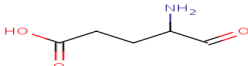
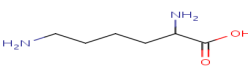
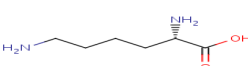
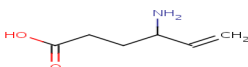
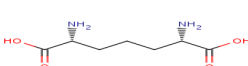
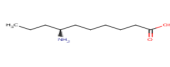
58

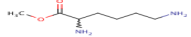
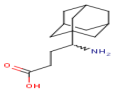
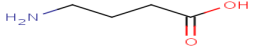
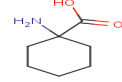
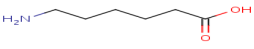

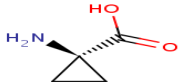
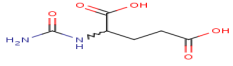
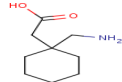
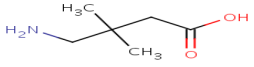
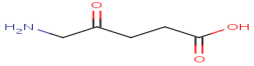
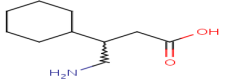

SMR000445680		CDD-270520	57	
TBL-1584		CDD-340892	57	
SMR000123994		CDD-166641	57	
SMR000069228		CDD-258722	57	
SMR000104230		CDD-260656	56	
110164		CDD-52283	56	2.07205
SMR000445659		CDD-254695	56	
SMR000034660		CDD-301107	55	
SMR000009949		CDD-285479	55	
SMR000019471		CDD-289161	55	
Chenodiol		CDD-1265	55	-5
SMR000112166		CDD-147252	55	
SMR000112165		CDD-799	55	

SMR000058403		CDD-714	55	
110165		CDD-52626	55	3.91644
17699		CDD-53608	55	14.7
SMR000074082		CDD-205425	55	
SMR000054222		CDD-264022	55	
SMR000107058		CDD-257426	54	
SMR000225910		CDD-280341	54	
SMR000054383		CDD-156070	54	
SMR000528042		CDD-200173	54	
TBL-1582		CDD-340890	54	
Androsterone		CDD-1366	54	-8
SMR000058571		CDD-1366	54	
Epiandrosterone		CDD-1390	54	-4

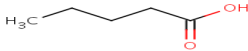
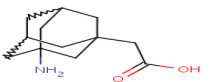
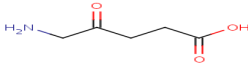
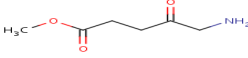
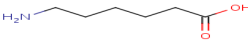
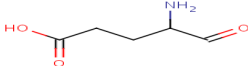
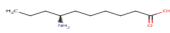
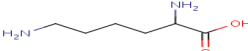
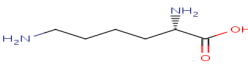
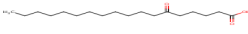
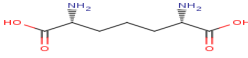
3-alpha-hydroxy-5-beta-andr		CDD-1605	54	-5
Lithocholic acid		CDD-1685	54	18
SMR000238198		CDD-339913	54	

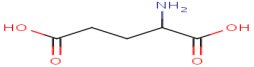
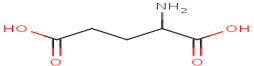
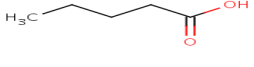
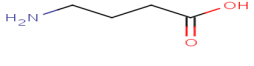
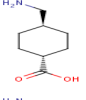

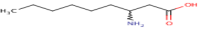
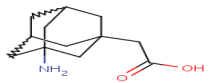


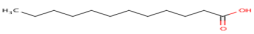
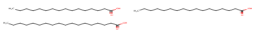
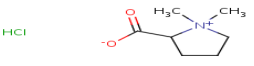
**ESSENTIAL MOLECULE: L-glutamate**

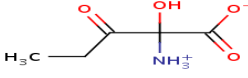
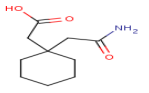
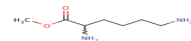
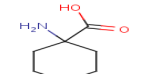
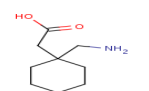
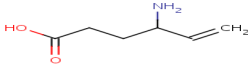
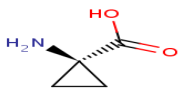
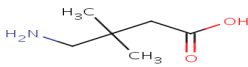
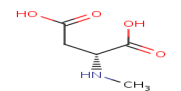
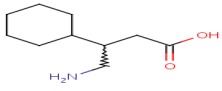
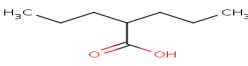
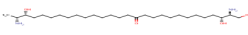
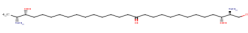
L-glutamate		CDD-41783	100	
SMR000033946		CDD-41783	100	0
Glutamate-1-semialdehyde			93	
JHU-5918		CDD-47339	70	
692_FDAMDD_v3b		CDD-47990	70	
Vigabatrin		CDD-1052	69	0
meso-diaminopimelate			69	
SMR000102743		CDD-258204	64	-7.02

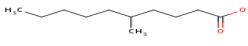
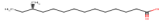

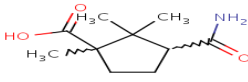

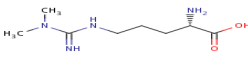

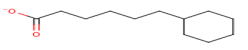
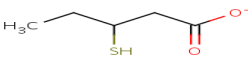
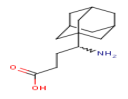

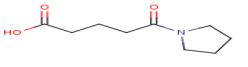
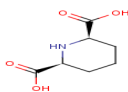
SMR000387093		CDD-170625	63	-15.48
SMR000299536		CDD-221626	61	0.31
SMR000058285		CDD-14017	61	-5.23
SN-5889		CDD-5133	60	
6-aminohexanoic acid		CDD-7	60	
SMR000102742		CDD-161620	58	-9.8
SMR000326773		CDD-254061	57	-11.86
SMR000387065		CDD-255763	55	-8.88
Gabapentin		CDD-297	55	10
SMR000413942		CDD-297226	54	-8.57
5-amino-levulinate		CDD-15328	54	
SMR000131763		CDD-161284	52	1.27
92585		CDD-53528	52	13.5934

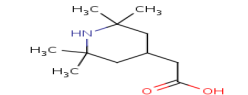
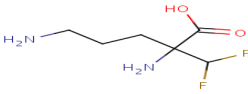
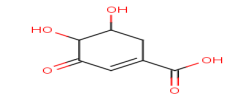
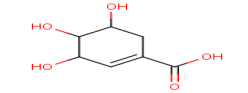
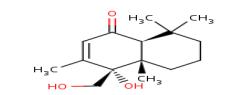
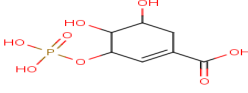
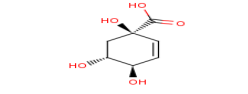
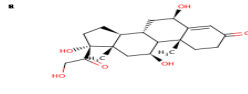
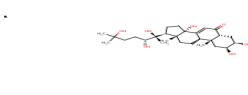
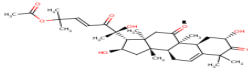


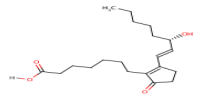
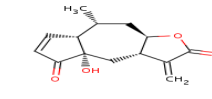
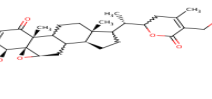
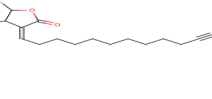
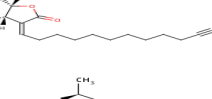
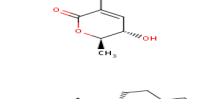
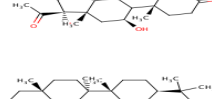
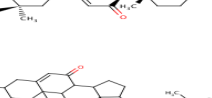
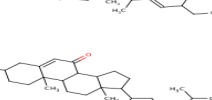
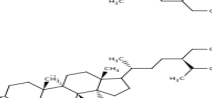
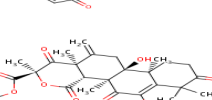
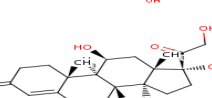

SMR000471834		CDD-309946	51	-4.9
SMR000278375		CDD-222679	50	3.53, 4.04
<b>ESSENTIAL MOLECULE: 5-amino-levulinate</b>				
5-amino-levulinate		CDD-15328	100	
SMR000058997		CDD-47114	85	-6.59
6-aminohexanoic acid		CDD-7	63	
Glutamate-1-semialdehyde			57	
SMR000102743		CDD-258204	56	-7.02
JHU-5918		CDD-47339	56	
692_FDAMDD_v3b		CDD-47990	56	
SMR000386957		CDD-42709	56	9.95
meso-diaminopimelate			55	

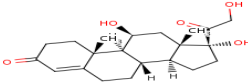
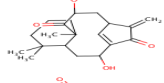
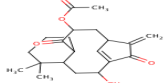
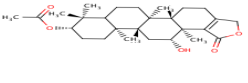
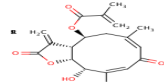
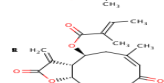
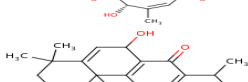
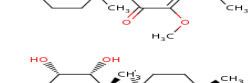
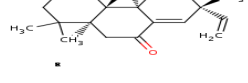
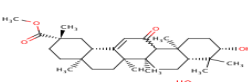
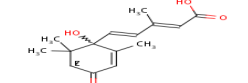
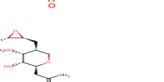
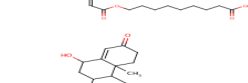
L-glutamate		CDD-41783	54			
SMR000033946		CDD-41783	54		0	
SMR000471834		CDD-309946	54		-4.9	
SMR000058285		CDD-14017	52		-5.23	
Tranexamic acid		CDD-689	51			
Tranexamic acid		CDD-689	51	-33		
SMR000102742		CDD-161620	51		-9.8	
SMR000278375		CDD-222679	49		3.53, 4.04	
SMR000112203		CDD-46795	49		7.39	
SMR000059164		CDD-61	49		-11.58	
TBL-1707		CDD-2534	49			Antimycobac Invitro 16180806
TBL-1710		CDD-340981	49			Antimycobac Invitro 16180806
Stachydrine hydrochloride		CDD-1538	48	6		

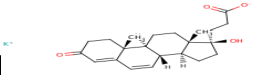
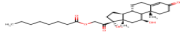
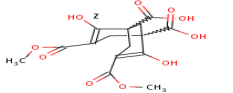
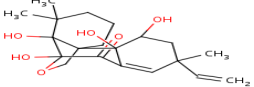
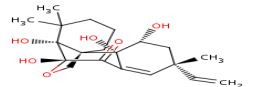
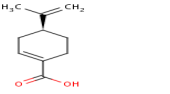
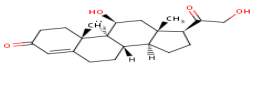
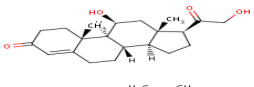
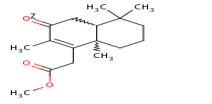
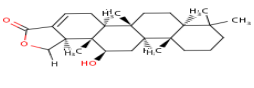
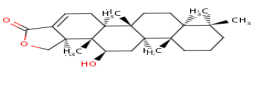
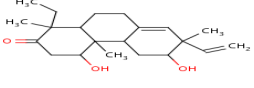
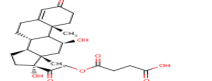
92585		CDD-53528	48	13.5934	
SMR000036610		CDD-154969	48	-7.64	
SMR000387093		CDD-170625	48	-15.48	
SN-5889		CDD-5133	48		
Gabapentin		CDD-297	48	10	
Vigabatrin		CDD-1052	47	0	
SMR000326773		CDD-254061	47	-11.86	
SMR000413942		CDD-297226	47	-8.57	
SMR000326806		CDD-15187	47	-4.11	
SMR000131763		CDD-161284	46	1.27	
SMR000499581		CDD-717	46	14.81	
TBL-734		CDD-340419	45		
TBL-734		CDD-340419	45	Inhibition of I Invitro	12538025

17609		CDD-53758	45	16.8387		
SMR000127417		CDD-255913	45		6.65	
SMR000059031		CDD-14310	45		-9.78	
SMR000368338		CDD-199400	44		-17.3	
SMR000416006		CDD-192760	44		-0.4	
SMR000326864		CDD-255416	44		-8.82	
SMR000338326		CDD-171480	44		1.31	
17610		CDD-54322	43	31.4245		
95069		CDD-54519	43	75.0801		
SMR000299536		CDD-221626	43		0.31	
TBL-1709		CDD-340980	43			Antimycobac Invitro 16180806
SMR000278049		CDD-57028	43		-6.16	
TBL-2523		CDD-341652	42			Inhibition of I Invitro 18054225

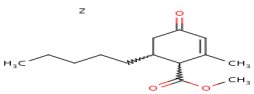
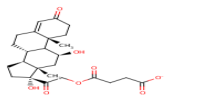
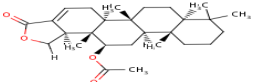
SMR000315130		CDD-60021	42	2.4		
SMR000058442		CDD-847	42	-8.4		
<b>ESSENTIAL MOLECULE: 3-dehydro-shikimate</b>						
3-dehydro-shikimate			100			
Shikimate			76			
SMR000440589		CDD-289581	59	-5.11		
Shikimate-3-phosphate			57			
TBL-1582		CDD-340890	57		Inhibition of I Invitro 16033267	
SMR000058916		CDD-168620	57	-2.26		
SMR000440684		CDD-170440	56	14.46		
SMR000232280		CDD-169346	56	-1.64		

SMR000058636		CDD-289603	56	-6.46		
SMR000445663		CDD-254713	54	-7.5		
SMR000440592		CDD-169155	54	1.25		
342055		CDD-53251	54	10.16		
TBL-1708		CDD-340979	54		Antimycobac Invitro	16180806
SMR000440586		CDD-163046	53	8.8		
SMR000058692		CDD-303018	53	15.5		
SMR000058239		CDD-45644	53	10.23		
398410		CDD-52342	52	2.34365		
398407		CDD-52727	52	4.6186		
TBL-2624		CDD-341738	52		Antimycobac Invitro	18471021
SMR000440631		CDD-170291	52	-10.11		
Hydrocortisone base		CDD-327	52	-26		

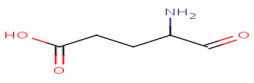
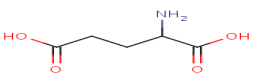
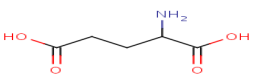
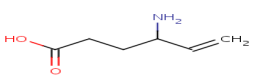
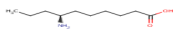
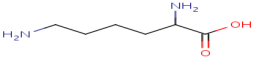
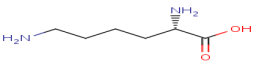
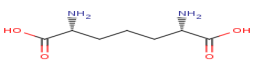
SMR000059022		CDD-327	52		-0.09	
213299		CDD-53747	52	16.6899		
236245		CDD-53789	52	17.3394		
TBL-3894		CDD-342566	52			Antimycobac Invitro 16378375
SMR000445666		CDD-337904	52		-4.72	
SMR000445667		CDD-270524	52		-10.55	
57093		CDD-52554	51	3.48381		
TBL-1735		CDD-340999	51			Antimycobac Invitro 16309313
SMR000445583		CDD-164542	51		-1.26	
SMR000528625		CDD-255676	51		-6.63, -9.71	
SMR000471888		CDD-164785	51		-9.93	
181896		CDD-52734	51	4.66526, 9.79704		
398411		CDD-52783	51	5.15603		

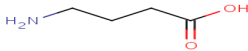
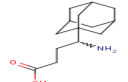
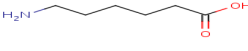

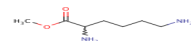
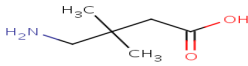
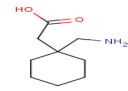
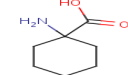
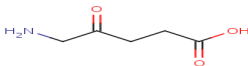
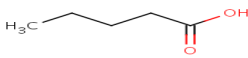
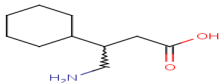
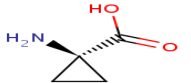
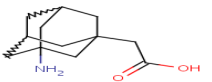
Canrenoic acid potassium salt		CDD-1165	51	-2	
SMR000058694		CDD-160272	51		21.67
SMR000456667		CDD-197541	51		4.01
166619		CDD-53115	51		8.50625
TBL-745		CDD-340430	51		Antimycobac Invitro, Invit 12657257, 1265
SMR000326722		CDD-164631	50		-9.77
Corticosterone		CDD-1383	50	-50	
SMR000058318		CDD-1383	50		-4.43
SMR000111539		CDD-259994	50		-0.99
TBL-1248		CDD-340736	50		Antimycobac Invitro, Invit 15497961, 1549
TBL-3893		CDD-342392	50		Antimycobac Invitro 16378375
209508		CDD-53407	50		12.0307
SMR000058328		CDD-45851	50		-12.2




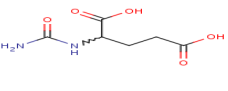
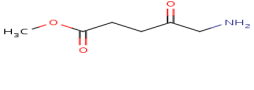
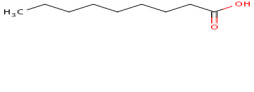
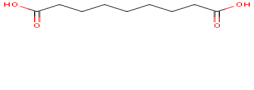
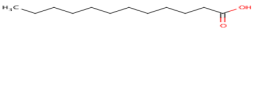
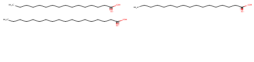


SMR000440162		CDD-239257	50	-5.74
SMR000058768		CDD-301527	50	-7.52
TBL-1247		CDD-340735	50	Antimycobac Invitro, Invit 15497961, 1549

### ESSENTIAL MOLECULE: Glutamate-1-semialdehyde

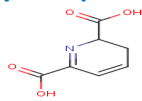
Glutamate-1-semialdehyde			100	
L-glutamate		CDD-41783	93	
SMR000033946		CDD-41783	93	0
Vigabatrin		CDD-1052	74	0
SMR000102743		CDD-258204	68	-7.02
JHU-5918		CDD-47339	67	
692_FDAMDD_v3b		CDD-47990	67	
meso-diaminopimelate			66	

SMR000058285		CDD-14017	66	-5.23
SMR000299536		CDD-221626	65	0.31
6-aminohexanoic acid		CDD-7	64	
SMR000102742		CDD-161620	61	-9.8
SMR000387093		CDD-170625	60	-15.48
SMR000413942		CDD-297226	58	-8.57
Gabapentin		CDD-297	58	10
SN-5889		CDD-5133	57	
5-amino-levulinate		CDD-15328	57	
SMR000471834		CDD-309946	55	-4.9
SMR000131763		CDD-161284	55	1.27
SMR000326773		CDD-254061	54	-11.86
SMR000278375		CDD-222679	53	3.53, 4.04

Tranexamic acid		CDD-689	52				
Tranexamic acid		CDD-689	52	-33			
SMR000338326		CDD-171480	52		1.31		
SMR000387065		CDD-255763	51		-8.88		
SMR000058997		CDD-47114	50		-6.59		
SMR000112203		CDD-46795	50		7.39		
SMR000059164		CDD-61	50		-11.58		
TBL-1707		CDD-2534	50			Antimycobact Invitro	16180806 Mycobacterium
TBL-1710		CDD-340981	50			Antimycobact Invitro	16180806 Mycobacterium

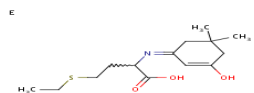
**ESSENTIAL MOLECULE: L-2,3-dihydrodipicolinate**

L-2,3-dihydrodipicolinate



100

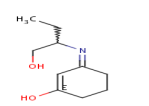
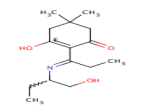
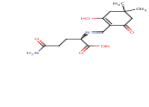
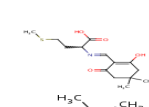
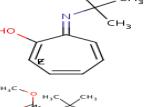
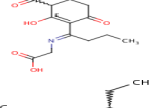
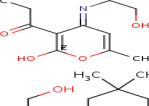
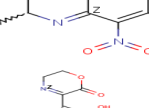
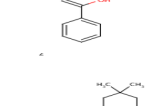
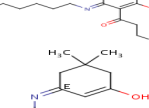
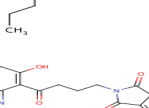
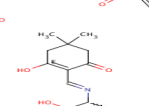
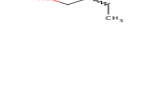
SMR000020451

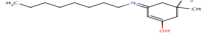
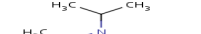
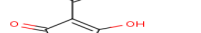
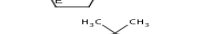
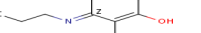

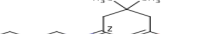



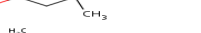
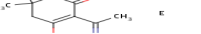



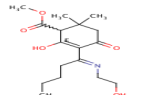
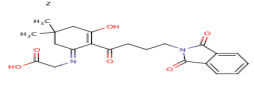
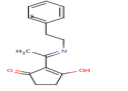
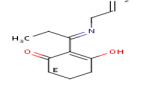
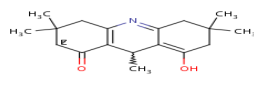
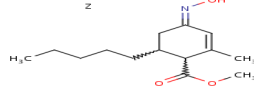
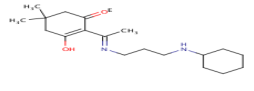
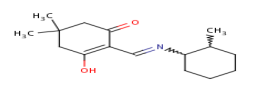
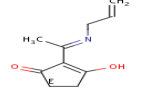
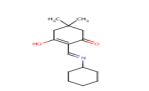
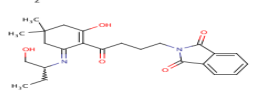
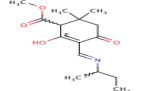
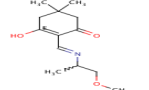
CDD-263791

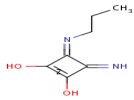
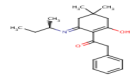
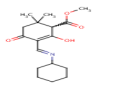

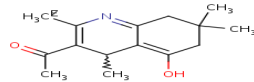
47

1.38

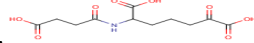
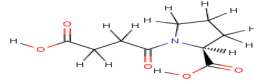
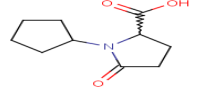
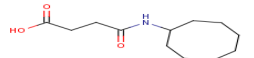
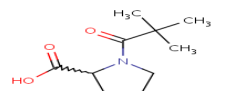
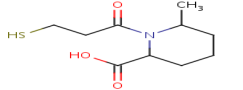
SMR000353541		CDD-215683	45	-3.21, -6.4
SMR000040064		CDD-312894	43	-0.34
SMR000024651		CDD-175568	41	-2.85
SMR000054190		CDD-322314	41	2.31
SMR000039234		CDD-233144	40	2.06
SMR000104276		CDD-298570	40	-6.82
SMR000307573		CDD-241078	39	-0.93
SMR000185101		CDD-189451	38	1.03
SMR000427701		CDD-308769	38	-7.46
SMR000420021		CDD-308909	38	26.21
SMR000230342		CDD-328799	38	-2.03
SMR000313623		CDD-244042	38	2.24
SMR000054242		CDD-181719	38	-10.16

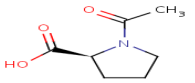
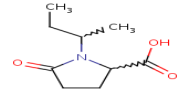
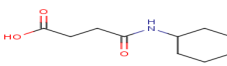
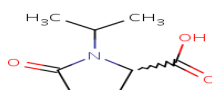
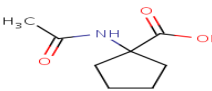
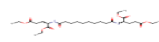
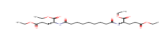
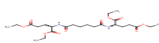
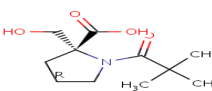
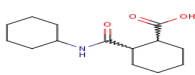
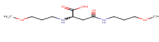
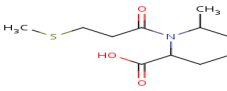

SMR000420031		CDD-275024	38	16.7
SMR000066118		CDD-263668	38	1.35
SMR000281857		CDD-264852	38	-1.82
SMR000420020		CDD-199144	37	3.06
SMR000230885		CDD-247686	37	0
SMR000105014		CDD-167515	37	-1.1
SMR000427702		CDD-196365	37	-11.46
SMR000037970		CDD-299046	37	5.39
SMR000450030		CDD-200701	37	3.96
SMR000054254		CDD-166646	37	-7.71
SMR000104015		CDD-228504	37	-2.62
SMR000105000		CDD-334223	36	4.96
SMR000103577		CDD-213041	36	-5.03

SMR000040276		CDD-234279	36	-0.94
SMR000313622		CDD-241753	36	-8.63
SMR000137201		CDD-192411	36	-0.97
SMR000037713		CDD-210147	36	-17.84
SMR000306744		CDD-190834	36	-3.15
SMR000420277		CDD-201137	36	1.98
SMR000104082		CDD-213106	36	-1.09
SMR000111406		CDD-213420	35	1.38
SMR000037858		CDD-160145	35	-6.58
SMR000054234		CDD-335329	35	-10.74
SMR000307265		CDD-244234	35	2.17
SMR000117846		CDD-244496	35	-0.91
SMR000111392		CDD-159982	35	-2.83


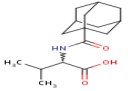
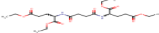
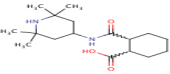
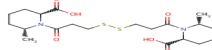
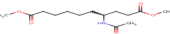
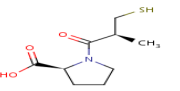
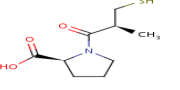
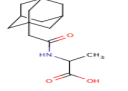
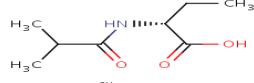
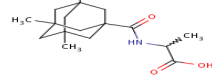
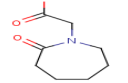
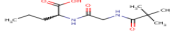
SMR000459869		CDD-310194	35	-0.75
SMR000260499		CDD-192579	35	4.5
SMR000009444		CDD-233876	35	-0.58
SMR000111367		CDD-213555	35	-5.71
SMR000282638		CDD-307029	35	-5.62

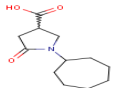
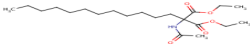
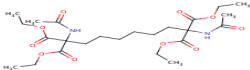
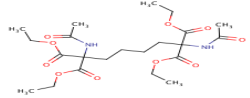
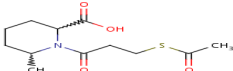
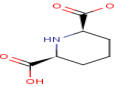
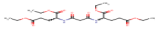
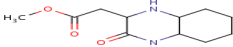
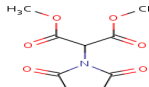
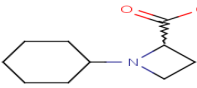
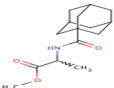
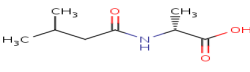
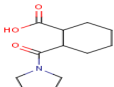
### ESSENTIAL MOLECULE: N-succinyl-2-amino-6-ketopimelate

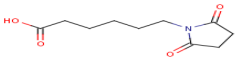
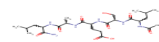
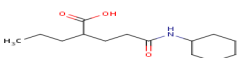
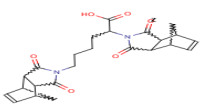
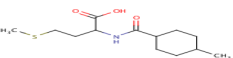
N-succinyl-2-amino-6-ketopi			100	
SMR000326657		CDD-327150	81	-8.05
SMR000033650		CDD-165697	70	-0.61
7260818		CDD-134390	69	-3.7
SMR000135311		CDD-258631	69	0.34
5219863		CDD-130340	69	-11.35

SMR000365399		CDD-61098	68	0.28
SMR000132615		CDD-326812	68	1.77
SMR000123689		CDD-56280	68	-1.02
SMR000132432		CDD-168599	67	2.15
SMR000393684		CDD-197851	67	-3.18
SMR000174810		CDD-164142	67	-6.9
SMR000174809		CDD-318181	67	2.58
SMR000174804		CDD-215976	66	-0.28
SMR000231097		CDD-150148	66	-0.65
SMR000069591		CDD-160080	65	-11.92
SMR000230597		CDD-169447	65	-7.92
SMR000145131		CDD-146894	64	-2.49
7830870		CDD-145234	64	4.21

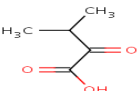
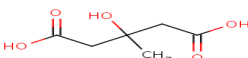

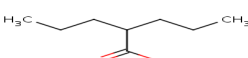
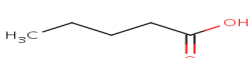
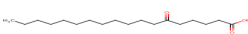


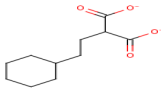
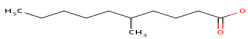
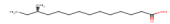
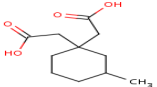
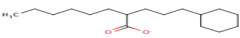
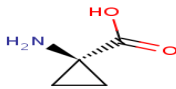
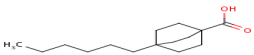
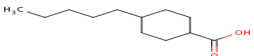
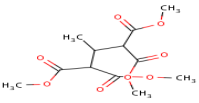
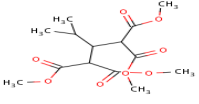
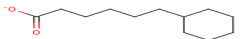
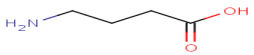
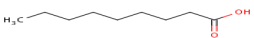
SMR000174803		CDD-282104	64		-3.38
SMR000064358		CDD-159991	63		-7.6
SMR000174802		CDD-247398	63		2.6
SMR000010722		CDD-173740	63		0.33
SMR000135210		CDD-209039	62		-2.17
SMR000102736		CDD-160025	62		-1.41
Captopril		CDD-1069	62	10	
SMR000059061		CDD-1069	62		-12.15
7561067		CDD-145987	61		2.56
CDD-62786		CDD-62786	60		
SMR000298068		CDD-240528	60		-6.98
SMR000368756		CDD-59139	60		-6.48
SMR000039488		CDD-234078	60		0.62


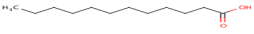
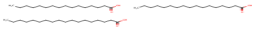
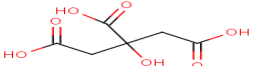
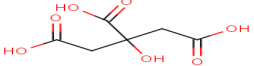
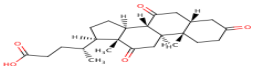
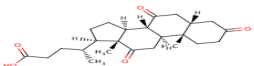
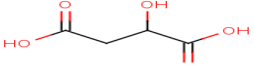
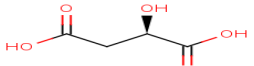
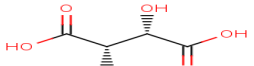
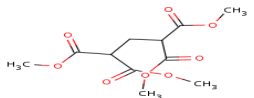
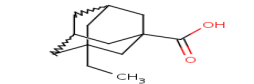
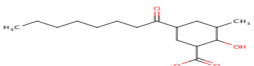
SMR000033651		CDD-207106	60	3.4
SMR000528201		CDD-200110	60	-8.77
SMR000425587		CDD-221604	60	-3.1
SMR000425585		CDD-321276	60	-1.09
SMR000054202		CDD-322035	60	-2.39
TBL-2523		CDD-341652	59	Inhibition of Invitro
SMR000282195		CDD-219073	59	-9.6
7734680		CDD-131947	58	3.09
7823679		CDD-131606	58	-1.12
SMR000012122		CDD-311196	58	0.37
SMR000062190		CDD-159948	58	-3.59
CDD-63657		CDD-63657	58	
SMR000273088		CDD-57025	58	-0.6

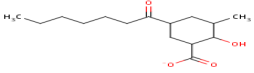
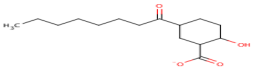
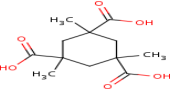
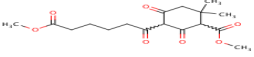
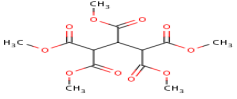
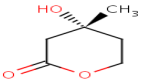
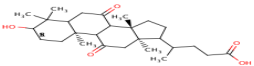
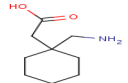


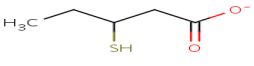

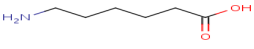
SMR000034328		CDD-117027	58	1.58
SMR000471611		CDD-168517	57	-8.65
7408566		CDD-134674	57	-1.22
SMR000009416		CDD-160151	57	-3.76
7365320		CDD-134616	57	-2.8

**ESSENTIAL MOLECULE: 2-keto-isovalerate**

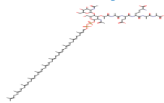
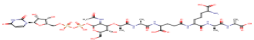
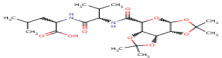
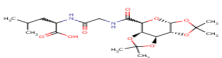
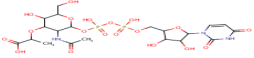
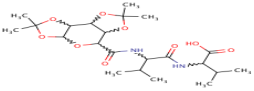
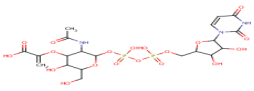
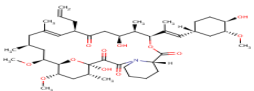
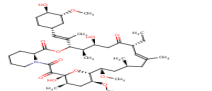
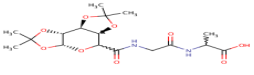
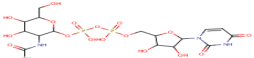
2-keto-isovalerate			100	
SMR000471861		CDD-128597	56	-8.46
SMR000413942		CDD-297226	55	-8.57
SMR000499581		CDD-717	54	14.81
SMR000471834		CDD-309946	52	-4.9
SMR000386957		CDD-42709	50	9.95

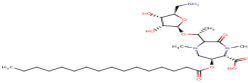
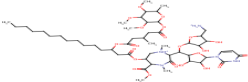
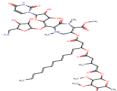
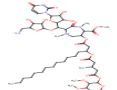
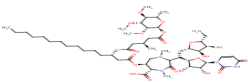
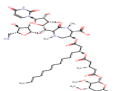
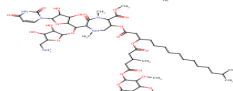
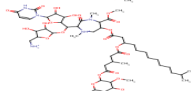
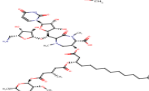
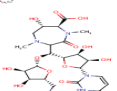
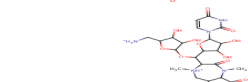
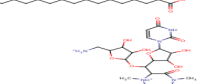
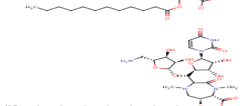
17699		CDD-53608	49	14.7
17609		CDD-53758	49	16.8387
SMR000127417		CDD-255913	49	6.65
SMR000528042		CDD-200173	48	-9.81
17612		CDD-53378	48	11.6665
SMR000326773		CDD-254061	48	-11.86
SMR000113247		CDD-322745	48	-5.43
SMR000019012		CDD-338808	48	-15.89
SMR000137563		CDD-209399	47	-0.15
SMR000054379		CDD-298250	47	-1.21
17610		CDD-54322	46	31.4245
SMR000058285		CDD-14017	46	-5.23
SMR000112203		CDD-46795	46	7.39

SMR000059164		CDD-61	46		-11.58	
TBL-1707		CDD-2534	46			Antimycobac Invitro 16180806
TBL-1710		CDD-340981	46			Antimycobac Invitro 16180806
anhydrous citric acid		CDD-48	45			
SMR000471840		CDD-48	45		-0.98	
Dehydrocholic acid		CDD-1147	44	10		
SMR000058603		CDD-1147	44		-1.56	
SMR000019054		CDD-2665	44		-11.27	
SMR000058580		CDD-212241	44		-0.89	
SMR000499572		CDD-315415	44		9.68	
SMR000141220		CDD-180159	44		-5.64	
SMR000102400		CDD-311365	43		-4.33	
110597		CDD-53000	43		7.05746	

110596		CDD-53864	43	18.5625	
110595		CDD-54402	43	37.1249	
SMR000074082		CDD-205425	43	-1.24	
SMR000054222		CDD-264022	42	-0.89	
SMR000054383		CDD-156070	41	2.58	
Mevalonic-D, L acid lactone		CDD-1651	41	-22	
SMR000528036		CDD-150659	41	-3.78	
Gabapentin		CDD-297	40	10	
Tranexamic acid		CDD-689	40		
Tranexamic acid		CDD-689	40	-33	
95069		CDD-54519	40	75.0801	
TBL-1709		CDD-340980	40		Antimycobac Invitro 16180806
6-aminohexanoic acid		CDD-7	40		

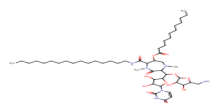
**ESSENTIAL MOLECULE: N-acetylmuramoyl-L-alanyl-D-glutamyl-meso-2,6-diaminopimelyl-D-alanyl-D-alanine-diphosphoundecaprenyl-N-acetylglucosamine**

N-acetylmuramoyl-L-alanyl-L			100	
UDP-N-acetylmuramoyl-L-al			68	
SMR000274374	 CDD-308218		61	2.76
SMR000312992	 CDD-332324		61	4.53
UDP-N-acetyl-muramate			61	
SMR000312993	 CDD-168956		60	-7.3, -2.69
UDP-GlcNAc-enol pyruvate			60	
SMR000466356	 CDD-653		59	-2.63
SMR000127507	 CDD-164290		59	5.69
SMR000312920	 CDD-241500		59	2.71
UDP-N-acetyl-D-glucosamine			58	

TBL-8796		CDD-344703	57		Antimycobact: Invitro	18375127	Mycobacterium
337554		CDD-51939	57	0.67926			
337555		CDD-51946	57	0.68766			
337553		CDD-52135	57	1.34213			
TBL-6222		CDD-343099	57		Antimycobact: Invitro, Invitr	18375127, :	Mycobacterium
TBL-6224		CDD-343101	57		Antimycobact: Invitro, Invitr	18375127, :	Mycobacterium
181984		CDD-52136	56	1.34213			
337556		CDD-52150	56	1.37532			
TBL-6223		CDD-343100	56		Antimycobact: Invitro, Invitr	18375127, :	Mycobacterium
TBL-8792		CDD-343768	56		Antimycobact: Invitro	18375127	Mycobacterium
181972		CDD-52012	56	0.95711			
181971		CDD-52031	56	1.02788			
TBL-8793		CDD-343995	56		Antimycobact: Invitro	18375127	Mycobacterium



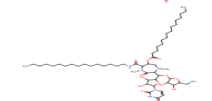
181975



CDD-52500

55 3.18316

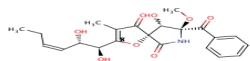
181976



CDD-52885

55 6.01304

SMR000440621



CDD-163045

55 -6.03