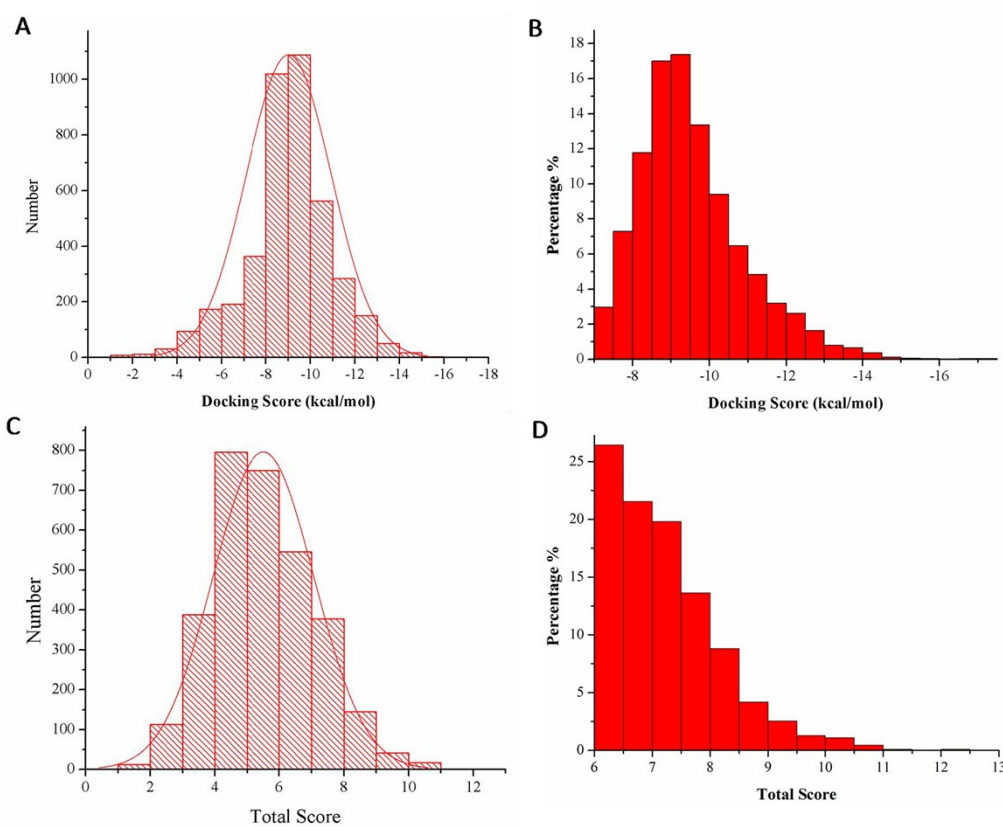


1 Supplementary Material



2
3 Fig.S1 The distribution of scores according to the docking software. A. Results by Glide-XP;
4 B.Docking Score < -7 kcal/mol by Glide-XP; C. Results by Sybyl-Surflex;D. Total Score > 4 by
5 Sybyl-Surflex

6

7

8

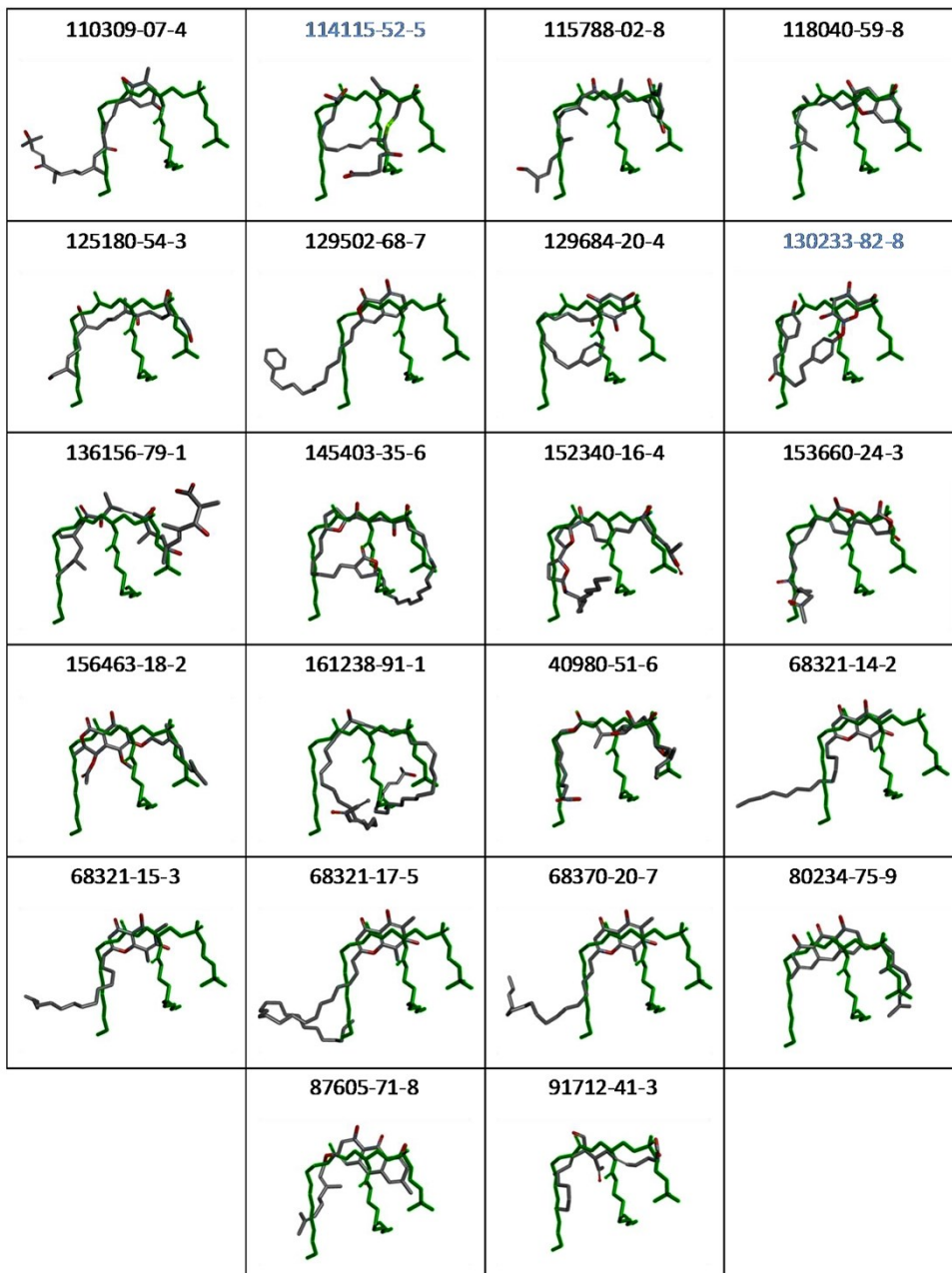
9

10

11

12

13

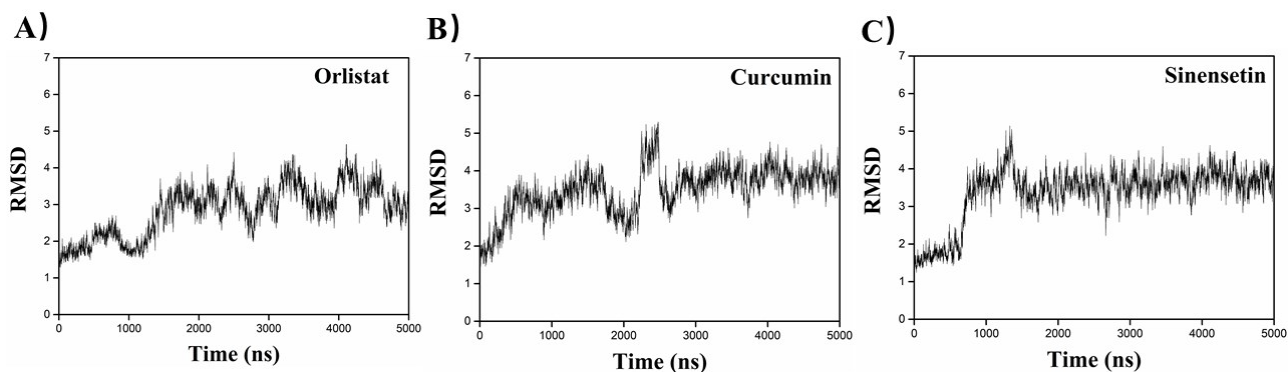


14

15 Fig S2 The position comparison of top hits to the original ligand PLC. (The green one represents

16 the PLC, the forest green ones are those top hits).

17



18

19 Fig S3 RMSD of orlistat (A), curcumin (B) and sinensetin (C).

20

21

22

23 Table S1 Docking results of 40 molecules selected by virtual screening from CNPD.

	Glide-XP		Sybyl-Surflex				
	Docking-score (kcal/mol)	Total-score	G-score	PMF-score	D-score	Chem-score	C-score
136156-79-1	-13.1353	7.8770	-352.289	-97.5616	-172.273	-34.5039	4
130233-82-8	-11.6786	7.3024	-229.345	-115.3030	-141.019	-36.4753	4
91851-48-8	-11.0952	6.8822	-375.566	-92.1285	-180.220	-38.8126	3
99529-30-3	-11.0243	6.4263	-281.599	-66.6293	-150.021	-40.3004	3
68321-14-2	-10.6166	8.3346	-263.338	-89.6224	-134.716	-39.2833	2
40980-51-6	-10.5838	10.9569	-324.877	-125.8860	-175.455	-41.7011	4
68321-17-5	-10.4488	7.9592	-258.301	-94.9902	-174.307	-47.5516	4
87605-71-8	-10.3861	7.6826	-294.26	-106.1570	-162.538	-48.9586	4
68321-15-3	-10.3426	7.8066	-261.491	-108.1260	-157.726	-42.6039	4

68370-20-7	-10.088	7.6779	-250.167	-69.5592	-127.215	-37.0894	2
153660-24-3	-10.0801	7.7583	-263.205	-94.3052	-147.642	-27.9235	3
144599-01-9	-9.97607	8.0259	-252.68	-97.1004	-143.558	-37.3679	4
129502-68-7	-9.86629	7.6338	-248.199	-84.5675	-145.388	-43.5301	3
115788-02-8	-9.85014	9.9850	-327.577	-112.3980	-158.267	-50.4833	4
122617-02-1	-9.7982	8.6888	-281.752	-105.3610	-141.843	-40.2707	4
21389-98-0	-9.71857	8.5166	-267.037	-75.0768	-141.238	-41.2080	3
91712-41-3	-9.69655	8.1441	-269.506	-83.9743	-151.392	-44.1375	3
111074-75-0	-9.63016	8.2638	-291.372	-58.5816	-150.666	-42.7266	3
152340-16-4	-9.62566	12.4597	-291.712	-98.7407	-173.500	-47.1479	4
103538-03-0	-9.59084	7.3111	-237.756	-93.0506	-148.356	-32.4160	3
118040-59-8	-9.43361	7.4682	-258.058	-71.5662	-133.933	-38.3473	2
129684-20-4	-9.31833	8.5910	-292.013	-102.6060	-147.334	-42.7671	4
155661-16-8	-9.1964	7.6442	-211.135	-95.6962	-121.448	-34.1965	3
153660-25-4	-9.19495	10.1305	-336.042	-105.7020	-153.923	-41.3133	4
110309-07-4	-9.10702	9.7738	-284.456	-89.4377	-153.744	-42.3642	3
93822-73-2	-9.06388	8.8099	-352.509	-90.0620	-174.520	-42.8167	3
80234-75-9	-8.97052	7.1198	-233.508	-127.3570	-147.422	-46.3742	4
95690-76-9	-8.94501	6.2271	-243.54	-76.9609	-122.814	-40.9401	2
145403-35-6	-8.87812	10.7901	-328.827	-93.0048	-197.621	-50.2736	3
119980-00-6	-8.75798	8.3194	-299.599	-94.3961	-159.690	-50.6864	4
89362-84-5	-8.71471	7.7997	-272.15	-82.1696	-142.925	-44.1357	3

114115-52-5	-8.66435	6.9931	-263.174	-101.5610	-140.254	-18.6350	3
161238-91-1	-8.64876	11.1503	-409.482	-89.7103	-215.049	-60.9947	3
125180-54-3	-8.57326	9.0519	-262.375	-82.5333	-156.117	-42.8845	3
133084-69-2	-8.56674	8.9465	-221.569	-85.8384	-136.595	-44.0783	3
156463-18-2	-8.55069	6.5795	-277.979	-116.1590	-162.336	-34.7843	4
88674-93-5	-8.5121	8.7151	-263.932	-86.6165	-133.346	-40.7347	2
137592-04-2	-8.21459	7.9155	-258.756	-96.8473	-162.676	-45.7731	4
121254-96-4	-8.08763	10.5372	-337.841	-87.3209	-196.112	-54.4733	3
62758-06-9	-8.04284	8.2020	-327.506	-108.7150	-173.048	-41.6204	4

24 Table S2 Similarity results of 40 molecules selected by virtual screening from CNPD.

	TOPDIST	QREGID	Sim_PLC	Sim_Cetilistat	Sim-Orlistat
Orlistat	157	l1pa_ligand	6.1750	5.1580	8.2291
136156-79-1	183	l1pa_ligand	4.4999	-	4.0026
130233-82-8	175	orlistat	5.0084	4.6788	4.7906
91851-48-8	184	l1pa_ligand	4.8293	4.4441	4.7431
99529-30-3	182	l1pa_ligand	5.1299	4.4008	5.0874
68321-14-2	142	cetilistat	5.4010	6.5849	5.9613
40980-51-6	183	l1pa_ligand	4.944	4.3787	4.5298
68321-17-5	151	cetilistat	5.3502	6.3348	5.8630
87605-71-8	174	orlistat	5.5462	5.7555	5.4287
68321-15-3	133	cetilistat	5.6410	7.2256	5.8189
68370-20-7	129	cetilistat	5.4593	7.0622	5.6146

153660-24-3	181	l1pa_ligand	4.9921	4.8834	4.6379
144599-01-9	173	l1pa_ligand	5.5377	5.0503	5.7080
129502-68-7	139	cetilistat	4.8974	6.9266	5.5548
115788-02-8	176	l1pa_ligand	5.0019	4.8074	4.7878
122617-02-1	170	cetilistat	5.1092	4.8017	4.9962
21389-98-0	166	cetilistat	5.0362	4.9506	4.7677
91712-41-3	150	l1pa_ligand	5.1691	4.9117	5.4074
111074-75-0	172	cetilistat	4.8886	5.7676	5.8609
89362-84-5	169	orlistat	4.8795	4.9695	5.0952
152340-16-4	179	orlistat	4.9366	4.0829	5.0616
103538-03-0	167	l1pa_ligand	5.4430	5.2391	5.2507
118040-59-8	165	orlistat	5.2731	5.5041	5.5902
129684-20-4	170	cetilistat	5.4842	5.9984	5.5932
155661-16-8	184	cetilistat	5.2363	5.3386	5.3058
153660-25-4	175	cetilistat	5.0460	4.8918	5.1683
110309-07-4	176	cetilistat	5.0842	4.2104	4.7552
93822-73-2	173	cetilistat	5.5218	5.0854	5.3417
80234-75-9	182	orlistat	5.3095	5.9898	5.5499
95690-76-9	144	cetilistat	5.2562	7.1645	6.2504
145403-35-6	183	cetilistat	5.3819	4.0338	5.3380
119980-00-6	179	cetilistat	4.4654	5.3079	4.8156
89362-84-5	169	orlistat	4.8795	4.9695	5.0952

114115-52-5	176	1lpa_ligand	5.0513	-	4.2279
161238-91-1	182	cetilistat	4.6886	4.3915	5.3642
125180-54-3	179	1lpa_ligand	4.7550	4.0991	4.2911
133084-69-2	166	cetilistat	4.9117	6.4215	5.7741
156463-18-2	181	orlistat	5.3683	5.0862	5.4158
88674-93-5	178	1lpa_ligand	4.5677	5.0516	5.0802
137592-04-2	168	cetilistat	6.1549	5.5828	5.8507
121254-96-4	184	cetilistat	5.2539	4.2244	4.4345
62758-06-9	156	orlistat	5.0514	-	5.5259

25

26

27

28

29

30

31

32

33

34

35

36

37

38
39
40
41
42
43
44
45
46

47 Table S3 Interaction analyses between selected molecules from CNPD with pancreatic lipase by
48 Glide.

Glide	Ser152	Phe77	Leu153	Other Hydrogen bonding	Hydrophobic interaction
136156-79-1	Y	Y	N	Arg256 Arg111Lys80Asp79	Ile78 Phe215 Phe77
130233-82-8	Y	N	N	Arg256 Asp79	Phe215Phe77 Tyr114
91851-48-8	N	N	N	Arg256	Ala259 Phe77 Phe215 Ile78 Tyr114 Pro180
99529-30-3	N	N	N	Arg256 Asp79 Glu179	Phe215 Ile209 Phe77 Pro180 Ala260 Ile78 Tyr114
68321-14-2	Y	Y	Y	-	Tyr114 Pro180 Phe77 His263 Cys181 Phe215 Thr115
40980-51-6	Y	Y	N	Arg256 Asp79 Tyr114	Phe77 Phe215 Tyr114

68321-17-5	Y	Y	Y	-	Phe77 His263 Phe215 Tyr114
87605-71-8	Y	N	N	His263 Arg256 Asp79	Phe77 His263 Tyr114
68321-15-3	Y	Y	Y	-	Phe77 His263 Phe215 Tyr114
68370-20-7	Y	Y	Y	-	Tyr114 Phe215 Phe77 Pro180 Cys181 His263
153660-24-3	N	Y	N	Tyr114 Arg256 Asp79	Tyr114 Phe215 Phe77
144599-01-9	N	N	N	Arg256 Asp79	Ala260 Phe215 His263
129502-68-7	Y	Y	N	-	His263 Tyr114 Phe215
115788-02-8	Y	N	N	His263 Arg256 Asp79	Phe215 Tyr114
122617-02-1	N	N	N	His263 Asp79 Arg256 Phe215	Phe215 Leu264 Ile209 Tyr114 Pro118
21389-98-0	N	N	N	Phe215 Asp79	His263 Phe77 Pro180
91712-41-3	Y	Y	N	Phe215 Arg256	Phe77 Phe215 Tyr114
111074-75-0	N	N	N	Asp79 Arg256	His263 Phe77 Ile209
152340-16-4	Y	N	N	His263 Asp79 Arg256	Tyr114 Phe215 His263
103538-03-0	N	N	N	Arg256 Asp79	Pro180 His263 Tyr114
118040-59-8	N	Y	N	Asp79 Arg256	Pro80 Phe77 Phe215 Tyr114 His263
129684-20-4	N	Y	N	Asp79 Arg256	Pro180 Tyr114 Phe77
155661-16-8	N	N	N	Asp79 Arg256	Thr114 Phe215 Ser152
153660-25-4	N	N	N	Asp79 Arg256 Tyr114	Tyr114 Phe215 Phe77
110309-07-4	Y	Y	N	Cys181 Gln183	Tyr114 His263 Ile209
93822-73-2	N	N	N	Asp79 Arg256	Phe215 His263
80234-75-9	Y	N	Y	-	Phe215 Thr255 Ala259

				Phe215 Tyr114 Arg256	Ala259 His263 Ala260 Phe215 Phe77
95690-76-9	N	N	N	Asp79	Tyr114
145403-35-6	N	Y	N	Arg256	Phe215 Tyr114 His253
119980-00-6	N	N	N	Arg256 Asp79	Phe77 Tyr114 Ala260
89362-84-5	N	N	N	Arg256 Asp79	Phe215 Tyr114 Ala259
114115-52-5	Y	N	N	His163 Arg256	Ile78 Phe215
161238-91-1	N	Y	N	Phe258	Phe77 Ala259
125180-54-3	Y	N	N	Asp79 Arg256	His263 Phe215 Tyr114
133084-69-2	N	N	N	Asp79	Phe77 His263 Tyr114
156463-18-2	Y	Y	Y	-	Ile78
88674-93-5	N	N	N	Asp79 Arg256 Tyr114	His263 Phe215 Phe77 Tyr114
137592-04-2	N	N	N	Arg256	Phe215 Phe258 Thr255
121254-96-4	N	N	N	Asp205	Phe77 His263 Tyr114
62758-06-9	N	N	N	Arg256	Tyr114 Phe77 Phe215

49 The blue ones are inappropriate and should be deleted.

50

51

52

53

54

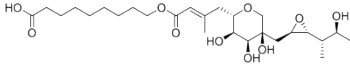
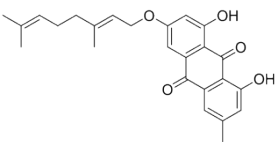
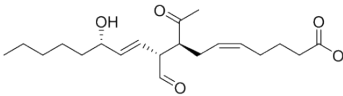
55

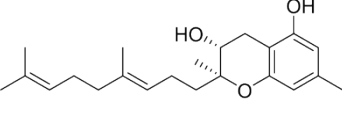
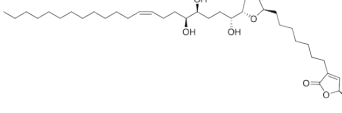
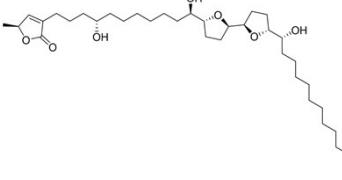
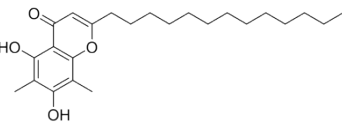
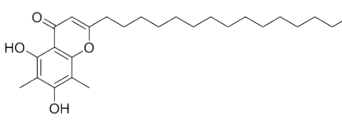
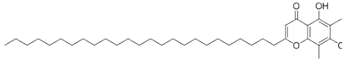
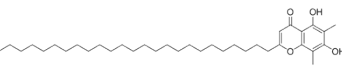
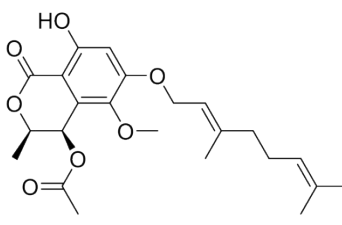
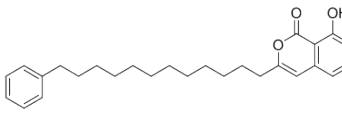
56

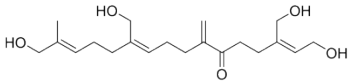
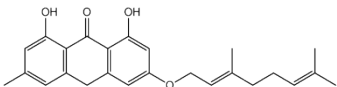
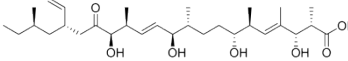
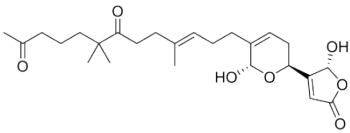
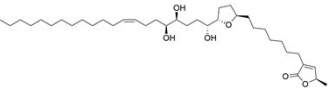
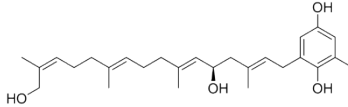
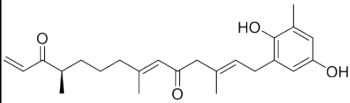
57

58
59
60
61
62
63
64
65
66

67 Table S4 The information of screened molecules from CNPD.

<p>40980-51-6</p> <p>PseudomonicAcidB; <i>Pseudomonas</i>; Commercially available</p> 	<p>87605-71-8</p> <p>3-geranyloxyemodin-6-methyl-1,8-dihydroxyanthrone; <i>Psorospermum febrifugum</i>; Commercially available</p> 	<p>91712-41-3</p> <p>levuglandin E; Chemical synthesis; Commercially available</p> 
<p>118040-59-8</p> <p>Kiwinin; <i>Mushroom</i>; No commercial source</p>	<p>145403-35-6</p> <p>Gigantrionenin; <i>Tomato branch</i>; No commercial source</p>	<p>152340-16-4</p> <p>Bullacin; <i>Tomato branch</i>; No commercial source</p>

		
<p>68321-14-2</p> <p>No common name;</p> <p><i>Sophora flavescens</i>;</p> <p>No commercial source</p> 	<p>68321-15-3</p> <p>No common name;</p> <p><i>Sophora flavescens</i>;</p> <p>No commercial source</p> 	<p>68321-17-5</p> <p>No common name;</p> <p><i>Sophora flavescens</i>;</p> <p>No commercial source</p> 
<p>68370-20-7</p> <p>No common name;</p> <p><i>Sophora flavescens</i>;</p> <p>No commercial source</p> 	<p>156463-18-2</p> <p>No common name;</p> <p>Plants;</p> <p>No commercial source</p> 	<p>129502-68-7</p> <p>8-hydroxy-3-(12-phenyldodecyl)isocoumarin;</p> <p>Plants;</p> <p>No commercial source</p> 

<p>125180-54-3</p> <p>No common name;</p> <p>Plants;</p> <p>No commercial source</p> 	<p>80234-75-9</p> <p>3-geranyloxy-6-methyl-1,8-dihydroxyanthrone;</p> <p>Shrub;</p> <p>No commercial source</p> 	<p>136156-79-1</p> <p>cubensis acid;</p> <p><i>Fungus</i>;</p> <p>No commercial source</p> 
<p>153660-24-3</p> <p>Fasciospongides B;</p> <p><i>Phylum Porifera</i>;</p> <p>No commercial source</p> 	<p>161238-91-1</p> <p>Petroformyne-1;</p> <p><i>Phylum Porifera</i>;</p> <p>No commercial source</p> 	<p>115788-02-8</p> <p>No common name;</p> <p><i>Phaeophyta</i>;</p> <p>No commercial source</p> 
<p>110309-07-4</p> <p>No relevant information found</p> 	<p>129684-20-4</p> <p>No relevant information found</p> 