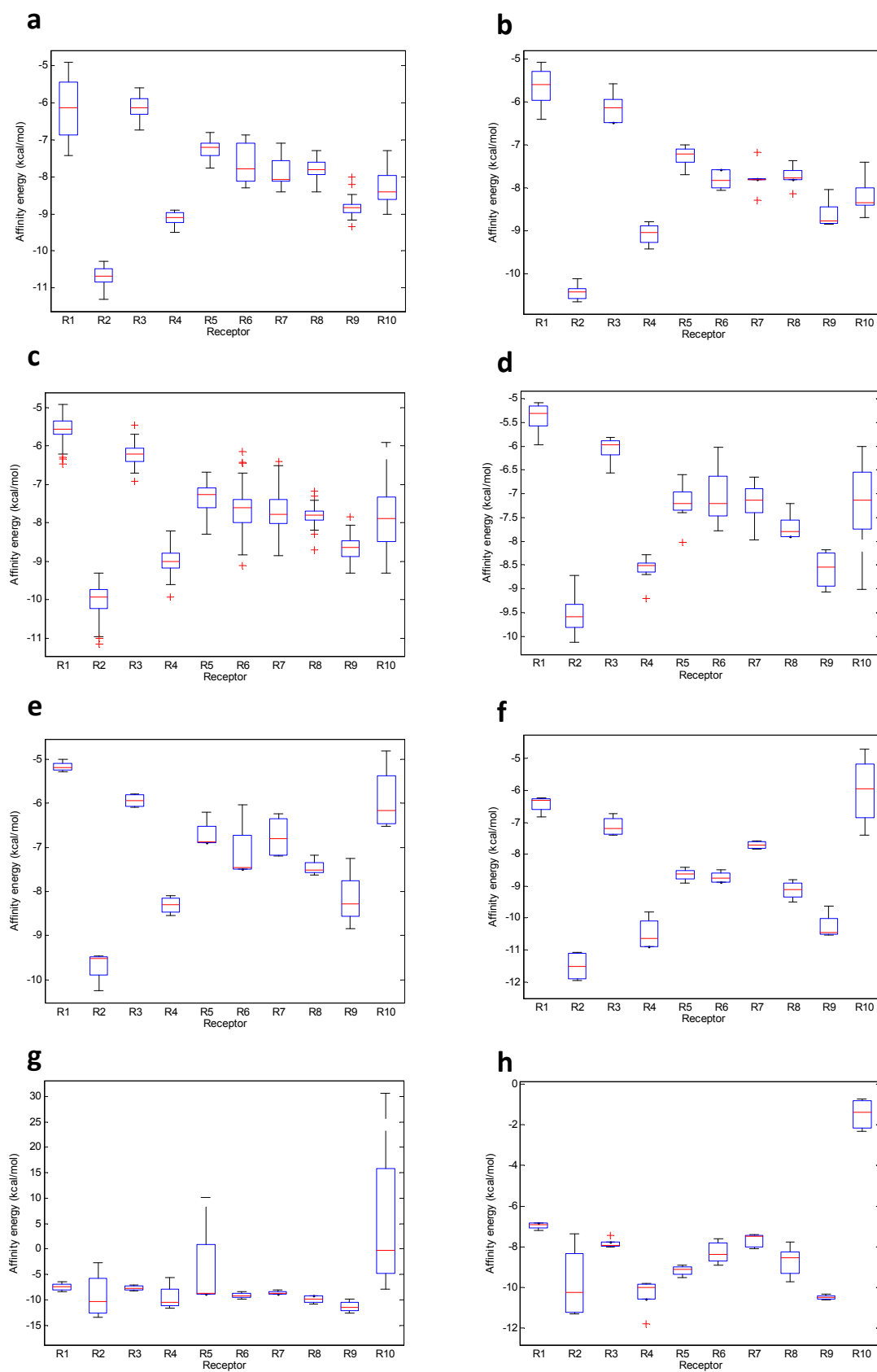
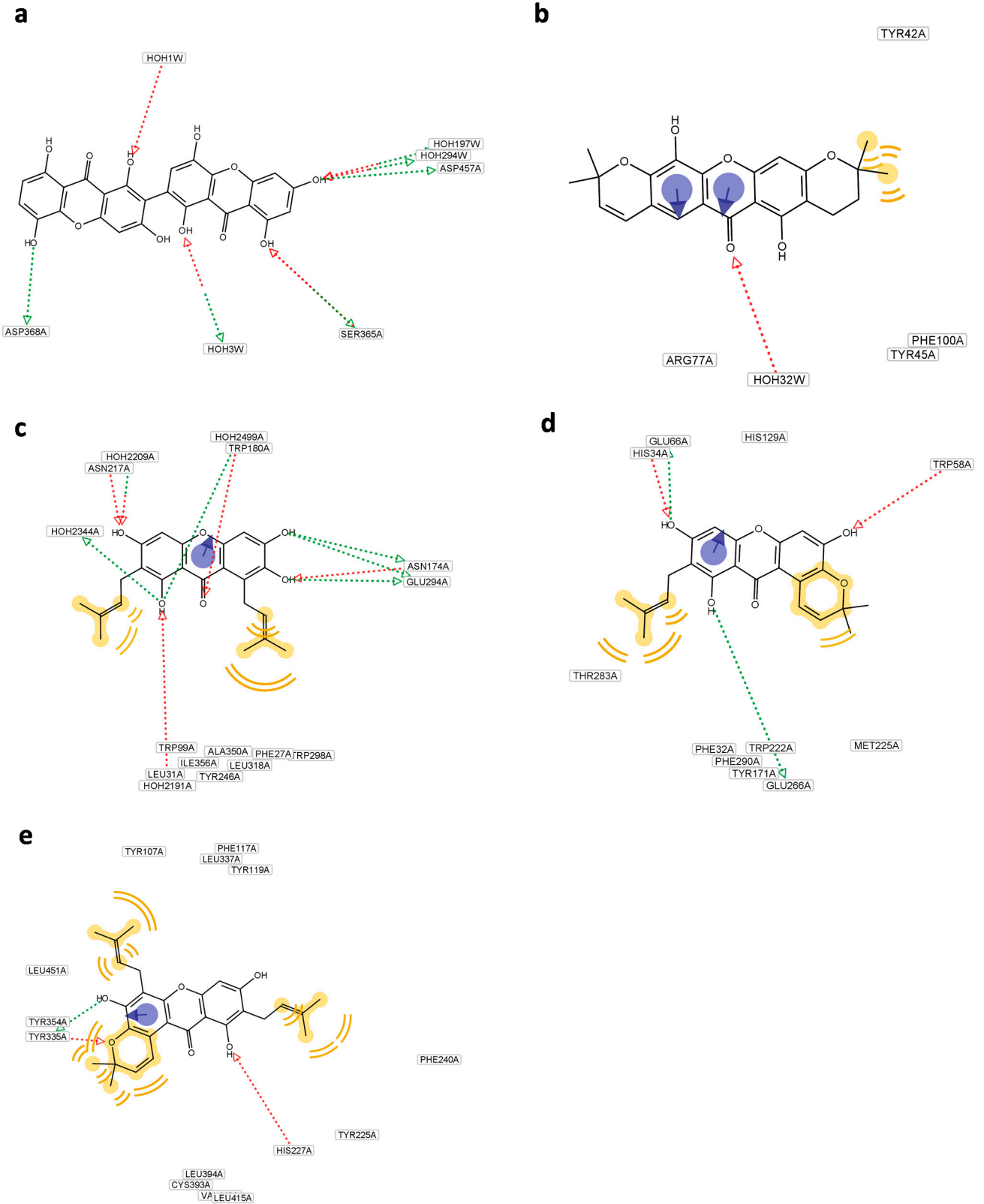


# Supplementary Materials



**Figure S1.** Boxplot of affinity energy values datasets for R1-R10. (a) DX; (b) TrX; (c) TeX; (d) PeX; (e) HX; (f) PePX; (g) Dim; (h) XD.



**Figure S2.** Residual interaction maps for some xanthones. (a) 266—R1; (b) 214—R3; (c) 166—R5; (d) 225—R6; (e) 256—R9.

**Table S1.** Systematic name of the tested xanthenes.

<b>ID</b>	<b>Name</b>	<b>ID</b>	<b>Name</b>
1	9 <i>H</i> -xanthen-9-one	29	3,5-dimethoxy-9 <i>H</i> -xanthen-9-one
2	1-hydroxy-9 <i>H</i> -xanthen-9-one	30	1,3-dimethoxy-9 <i>H</i> -xanthen-9-one
3	2-hydroxy-9 <i>H</i> -xanthen-9-one	31	2,7-dimethoxy-9 <i>H</i> -xanthen-9-one
4	3-hydroxy-9 <i>H</i> -xanthen-9-one	32	2-hydroxy-1,8-dimethoxy-9 <i>H</i> -xanthen-9-one
5	4-hydroxy-9 <i>H</i> -xanthen-9-one	33	1,2,7-trimethoxy-9 <i>H</i> -xanthen-9-one
6	4-hydroxy-9 <i>H</i> -xanthen-9-one	34	1,5-dihydroxy-3-methoxy-9 <i>H</i> -xanthen-9-one
7	1-methoxy-9 <i>H</i> -xanthen-9-one	35	1,6-dihydroxy-5-methoxy-9 <i>H</i> -xanthen-9-one
8	2-methoxy-9 <i>H</i> -xanthen-9-one	36	1-hydroxy-5,6-dimethoxy-9 <i>H</i> -xanthen-9-one
9	3-methoxy-9 <i>H</i> -xanthen-9-one	37	1,5-dihydroxy-6-methoxy-9 <i>H</i> -xanthen-9-one
10	4-methoxy-9 <i>H</i> -xanthen-9-one	38	1-hydroxy-2,3,5-trimethoxy-9 <i>H</i> -xanthen-9-one
11	1,2-dihydroxy-9 <i>H</i> -xanthen-9-one	39	1-hydroxy-2,3,7-trimethoxy-9 <i>H</i> -xanthen-9-one
12	2,3-dihydroxy-9 <i>H</i> -xanthen-9-one	40	1-hydroxy-3,4,5-trimethoxy-9 <i>H</i> -xanthen-9-one
13	3,4-dihydroxy-9 <i>H</i> -xanthen-9-one	41	1-hydroxy-3,4,7-trimethoxy-9 <i>H</i> -xanthen-9-one
14	3,5-dihydroxy-9 <i>H</i> -xanthen-9-one	42	1-hydroxy-3,5,6-trimethoxy-9 <i>H</i> -xanthen-9-one
15	3,6-dihydroxy-9 <i>H</i> -xanthen-9-one	43	1-hydroxy-3,5,8-trimethoxy-9 <i>H</i> -xanthen-9-one
16	1,7-dihydroxy-9 <i>H</i> -xanthen-9-one	44	1-hydroxy-3,6,7-trimethoxy-9 <i>H</i> -xanthen-9-one
17	1,5-dihydroxy-9 <i>H</i> -xanthen-9-one	45	1-hydroxy-3,6,8-trimethoxy-9 <i>H</i> -xanthen-9-one
18	3-hydroxy-4-methoxy-9 <i>H</i> -xanthen-9-one	46	8-hydroxy-1,2,6-trimethoxy-9 <i>H</i> -xanthen-9-one
19	4-hydroxy-3-methoxy-9 <i>H</i> -xanthen-9-one	47	2-hydroxy-1,3,7-trimethoxy-9 <i>H</i> -xanthen-9-one
20	3-hydroxy-5-methoxy-9 <i>H</i> -xanthen-9-one	48	7-hydroxy-2,3,4-trimethoxy-9 <i>H</i> -xanthen-9-one
21	2-hydroxy-1-methoxy-9 <i>H</i> -xanthen-9-one	49	3-hydroxy-1,2,4-trimethoxy-9 <i>H</i> -xanthen-9-one
22	3-hydroxy-2-methoxy-9 <i>H</i> -xanthen-9-one	50	3-hydroxy-1,2,7-trimethoxy-9 <i>H</i> -xanthen-9-one
23	1-hydroxy-5-methoxy-9 <i>H</i> -xanthen-9-one	51	3-hydroxy-1,5,6-trimethoxy-9 <i>H</i> -xanthen-9-one
24	5-hydroxy-1-methoxy-9 <i>H</i> -xanthen-9-one	52	6-hydroxy-1,2,8-trimethoxy-9 <i>H</i> -xanthen-9-one
25	1-hydroxy-7-methoxy-9 <i>H</i> -xanthen-9-one	53	4-hydroxy-2,3,6-trimethoxy-9 <i>H</i> -xanthen-9-one
26	1,2-dimethoxy-9 <i>H</i> -xanthen-9-one	54	5-hydroxy-1,2,3-trimethoxy-9 <i>H</i> -xanthen-9-one
27	2,3-dimethoxy-9 <i>H</i> -xanthen-9-one	55	6-hydroxy-1,3,5-trimethoxy-9 <i>H</i> -xanthen-9-one
28	3,4-dimethoxy-9 <i>H</i> -xanthen-9-one	56	7-hydroxy-1,2,3-trimethoxy-9 <i>H</i> -xanthen-9-one

Table S1. *Cont.*

ID	Name	ID	Name
57	2-hydroxy-1,6,8-trimethoxy-9 <i>H</i> -xanthen-9-one	85	2,8-dihydroxy-1,6-dimethoxy-9 <i>H</i> -xanthen-9-one
58	8-hydroxy-1,3,5-trimethoxy-9 <i>H</i> -xanthen-9-one	86	1,8-dihydroxy-2,7-dimethoxy-9 <i>H</i> -xanthen-9-one
59	1,3,5-trihydroxy-2-methoxy-9 <i>H</i> -xanthen-9-one	87	1,8-dihydroxy-3,5-dimethoxy-9 <i>H</i> -xanthen-9-one
60	1,2-dihydroxy-5,6-dimethoxy-9 <i>H</i> -xanthen-9-one	88	1,8-dihydroxy-3,6-dimethoxy-9 <i>H</i> -xanthen-9-one
61	1,3-dihydroxy-2,5-dimethoxy-9 <i>H</i> -xanthen-9-one	89	1,8-dihydroxy-2,6-dimethoxy-9 <i>H</i> -xanthen-9-one
62	1,3-dihydroxy-2,7-dimethoxy-9 <i>H</i> -xanthen-9-one	90	2,4-dihydroxy-3,6-dimethoxy-9 <i>H</i> -xanthen-9-one
63	1,3-dihydroxy-2,8-dimethoxy-9 <i>H</i> -xanthen-9-one	91	2,5-dihydroxy-1,6-dimethoxy-9 <i>H</i> -xanthen-9-one
64	1,3-dihydroxy-4,5-dimethoxy-9 <i>H</i> -xanthen-9-one	92	2,6-dihydroxy-1,5-dimethoxy-9 <i>H</i> -xanthen-9-one
65	1,3-dihydroxy-4,7-dimethoxy-9 <i>H</i> -xanthen-9-one	93	2,7-dihydroxy-1,8-dimethoxy-9 <i>H</i> -xanthen-9-one
66	1,3-dihydroxy-5,6-dimethoxy-9 <i>H</i> -xanthen-9-one	94	3,8-dihydroxy-1,2-dimethoxy-9 <i>H</i> -xanthen-9-one
67	1,3-dihydroxy-5,8-dimethoxy-9 <i>H</i> -xanthen-9-one	95	2,6-dihydroxy-1,8-dimethoxy-9 <i>H</i> -xanthen-9-one
68	1,3-dihydroxy-6,7-dimethoxy-9 <i>H</i> -xanthen-9-one	96	3,6-dihydroxy-1,5-dimethoxy-9 <i>H</i> -xanthen-9-one
69	6,8-dihydroxy-1,2-dimethoxy-9 <i>H</i> -xanthen-9-one	97	1,6-dihydroxy-2,8-dimethoxy-9 <i>H</i> -xanthen-9-one
70	1,4-dihydroxy-3,5-dimethoxy-9 <i>H</i> -xanthen-9-one	98	4,6-dihydroxy-1,3-dimethoxy-9 <i>H</i> -xanthen-9-one
71	1,5-dihydroxy-2,3-dimethoxy-9 <i>H</i> -xanthen-9-one	99	5,6-dihydroxy-1,3-dimethoxy-9 <i>H</i> -xanthen-9-one
72	1,5-dihydroxy-3,4-dimethoxy-9 <i>H</i> -xanthen-9-one	100	1,2,3-trihydroxy-5-methoxy-9 <i>H</i> -xanthen-9-one
73	1,5-dihydroxy-3,7-dimethoxy-9 <i>H</i> -xanthen-9-one	101	1,2,8-trihydroxy-3-methoxy-9 <i>H</i> -xanthen-9-one
74	1,5-dihydroxy-3,8-dimethoxy-9 <i>H</i> -xanthen-9-one	102	1,3,5-trihydroxy-2-methoxy-9 <i>H</i> -xanthen-9-one
75	1,5-dihydroxy-6,7-dimethoxy-9 <i>H</i> -xanthen-9-one	103	1,3,5-trihydroxy-6-methoxy-9 <i>H</i> -xanthen-9-one
76	1,6-dihydroxy-3,5-dimethoxy-9 <i>H</i> -xanthen-9-one	104	1,3,6-trihydroxy-5-methoxy-9 <i>H</i> -xanthen-9-one
77	1,6-dihydroxy-3,7-dimethoxy-9 <i>H</i> -xanthen-9-one	105	1,3,6-trihydroxy-7-methoxy-9 <i>H</i> -xanthen-9-one
78	1,6-dihydroxy-5,7-dimethoxy-9 <i>H</i> -xanthen-9-one	106	1,3,7-trihydroxy-6-methoxy-9 <i>H</i> -xanthen-9-one
79	3,8-dihydroxy-1,2-dimethoxy-9 <i>H</i> -xanthen-9-one	107	2,6,8-trihydroxy-1-methoxy-9 <i>H</i> -xanthen-9-one
80	4,10-dihydroxy-11 <i>H</i> -[1,3]dioxolo[4,5- <i>a</i> ]xanthen-11-one	108	1,3,8-trihydroxy-5-methoxy-9 <i>H</i> -xanthen-9-one
81	1,7-dihydroxy-2,3-dimethoxy-9 <i>H</i> -xanthen-9-one	109	1,6,8-trihydroxy-2-methoxy-9 <i>H</i> -xanthen-9-one
82	1,7-dihydroxy-3,4-dimethoxy-9 <i>H</i> -xanthen-9-one	110	1,4,7-trihydroxy-3-methoxy-9 <i>H</i> -xanthen-9-one
83	1,7-dihydroxy-3,5-dimethoxy-9 <i>H</i> -xanthen-9-one	111	2,5,8-trihydroxy-1-methoxy-9 <i>H</i> -xanthen-9-one
84	1,7-dihydroxy-3,6-dimethoxy-9 <i>H</i> -xanthen-9-one	112	1,4,8-trihydroxy-3-methoxy-9 <i>H</i> -xanthen-9-one

Table S1. Cont.

ID	Name	ID	Name
113	1,5,8-trihydroxy-3-methoxy-9 <i>H</i> -xanthen-9-one	141	2,8-dihydroxy-1,5,6-trimethoxy-9 <i>H</i> -xanthen-9-one
114	1,5,6-trihydroxy-3-methoxy-9 <i>H</i> -xanthen-9-one	142	1,3,8-trihydroxy-4,5-dimethoxy-9 <i>H</i> -xanthen-9-one
115	1,5,7-trihydroxy-3-methoxy-9 <i>H</i> -xanthen-9-one	143	3,6,8-trihydroxy-1,2-dimethoxy-9 <i>H</i> -xanthen-9-one
116	1,6,7-trihydroxy-3-methoxy-9 <i>H</i> -xanthen-9-one	144	8-hydroxy-1,2,3,4,6-pentamethoxy-9 <i>H</i> -xanthen-9-one
117	1,6,8-trihydroxy-2-methoxy-9 <i>H</i> -xanthen-9-one	145	1,8-dihydroxy-2,3,4,6-tetramethoxy-9 <i>H</i> -xanthen-9-one
118	1,2,8-trihydroxy-6-methoxy-9 <i>H</i> -xanthen-9-one	146	1,8-dihydroxy-2,3,4,6-tetramethoxy-9 <i>H</i> -xanthen-9-one
119	1,2,8-trihydroxy-3-methoxy-9 <i>H</i> -xanthen-9-one	147	1,2,3,4,6,7-hexamethoxy-9 <i>H</i> -xanthen-9-one
120	2,4,5-trihydroxy-1-methoxy-9 <i>H</i> -xanthen-9-one	148	1,3,5,6-tetrahydroxy-2-(3-methylbut-2-en-1-yl)-9 <i>H</i> -xanthen-9-one
121	3,5,6-trihydroxy-1-methoxy-9 <i>H</i> -xanthen-9-one	149	1,3,5,6-tetrahydroxy-4-(3-methylbut-2-en-1-yl)-9 <i>H</i> -xanthen-9-one
122	1,3,5,6-tetrahydroxy-9 <i>H</i> -xanthen-9-one	150	1,3-dihydroxy-5,6-dimethoxy-2-(3-methylbut-2-en-1-yl)-9 <i>H</i> -xanthen-9-one
123	1,3,5,7-tetrahydroxy-9 <i>H</i> -xanthen-9-one	151	1,3,6-trihydroxy-5-methoxy-2-(3-methylbut-2-en-1-yl)-9 <i>H</i> -xanthen-9-one
124	1,3,5,8-tetrahydroxy-9 <i>H</i> -xanthen-9-one	152	2,3,6,8-tetrahydroxy-1-(3-methylbut-2-en-1-yl)-9 <i>H</i> -xanthen-9-one
125	1,3,6,7-tetrahydroxy-9 <i>H</i> -xanthen-9-one	153	1,5,8-trihydroxy-3-methoxy-2-(3-methylbut-2-en-1-yl)-9 <i>H</i> -xanthen-9-one
126	1,2,6,8-tetrahydroxy-9 <i>H</i> -xanthen-9-one	154	1,3,5,8-tetrahydroxy-2-(3-methylbut-2-en-1-yl)-9 <i>H</i> -xanthen-9-one
127	8,11-dimethoxy-10 <i>H</i> -[1,3]dioxolo[4,5- <i>b</i> ]xanthen-10-one	155	1,3,5,8-tetrahydroxy-4-(3-methylbut-2-en-1-yl)-9 <i>H</i> -xanthen-9-one
128	9,11-dimethoxy-10 <i>H</i> -[1,3]dioxolo[4,5- <i>b</i> ]xanthen-10-one	156	1,4,6-trihydroxy-5-methoxy-7-(3-methylbut-2-en-1-yl)-9 <i>H</i> -xanthen-9-one
129	1,2,3,7-tetramethoxy-9 <i>H</i> -xanthen-9-one	157	3,4,8-trihydroxy-2-methoxy-1-(3-methylbut-2-en-1-yl)-9 <i>H</i> -xanthen-9-one
130	1,2,6,8-tetramethoxy-9 <i>H</i> -xanthen-9-one	158	1,4,5,6-tetrahydroxy-2-(2-methylbut-3-en-2-yl)-9 <i>H</i> -xanthen-9-one
131	1,3,4,5-tetramethoxy-9 <i>H</i> -xanthen-9-one	159	1,5,6-trihydroxy-3-methoxy-2-(2-methylbut-3-en-2-yl)-9 <i>H</i> -xanthen-9-one
132	1,3,4,7-tetramethoxy-9 <i>H</i> -xanthen-9-one	160	1,3,6,7-tetrahydroxy-4-(2-methylbut-3-en-2-yl)-9 <i>H</i> -xanthen-9-one
133	1,3,5,8-tetramethoxy-9 <i>H</i> -xanthen-9-one	161	1,2,5,6-tetrahydroxy-4-(2-methylbut-3-en-2-yl)-9 <i>H</i> -xanthen-9-one
134	1,3,6,7-tetramethoxy-9 <i>H</i> -xanthen-9-one	162	2,5,6-trihydroxy-1-methoxy-4-(2-methylbut-3-en-2-yl)-9 <i>H</i> -xanthen-9-one
135	2,3,4,5-tetramethoxy-9 <i>H</i> -xanthen-9-one	163	1,3,5,6-tetrahydroxy-2-(3-hydroxy-3-methylbutyl)-9 <i>H</i> -xanthen-9-one
136	1-hydroxy-2,3,4,5-tetramethoxy-9 <i>H</i> -xanthen-9-one	164	1,3,6-trihydroxy-7-methoxy-2,5-bis(3-methylbut-2-en-1-yl)-9 <i>H</i> -xanthen-9-one
137	1-hydroxy-2,3,4,7-tetramethoxy-9 <i>H</i> -xanthen-9-one	165	1,3,6-trihydroxy-5-methoxy-2,7-bis(3-methylbut-2-en-1-yl)-9 <i>H</i> -xanthen-9-one
138	8-hydroxy-1,2,5,6-tetramethoxy-9 <i>H</i> -xanthen-9-one	166	1,3,6,7-tetrahydroxy-2,8-bis(3-methylbut-2-en-1-yl)-9 <i>H</i> -xanthen-9-one
139	1-hydroxy-3,5,6,7-tetramethoxy-9 <i>H</i> -xanthen-9-one	167	1,6-dihydroxy-3,7-dimethoxy-2,8-bis(3-methylbut-2-en-1-yl)-9 <i>H</i> -xanthen-9-one
140	8-hydroxy-1,2,4,6-tetramethoxy-9 <i>H</i> -xanthen-9-one	168	1,3,6-trihydroxy-7-methoxy-2,8-bis(3-methylbut-2-en-1-yl)-9 <i>H</i> -xanthen-9-one

Table S1. Cont.

ID	Name	ID	Name
169	1,3,5,6-tetrahydroxy-2,4-bis(3-methylbut-2-en-1-yl)-9H-xanthen-9-one	183	1,3,6-trihydroxy-8-(3-hydroxy-3-methylbutyl)-7-methoxy-2-(3-methylbut-2-en-1-yl)-9H-xanthen-9-one
170	1,3,5,6-tetrahydroxy-2,7-bis(3-methylbut-2-en-1-yl)-9H-xanthen-9-one	184	1,3,6-trihydroxy-2-(3-hydroxy-3-methylbutyl)-7-methoxy-8-(3-methylbut-2-en-1-yl)-9H-xanthen-9-one
171	1,3,5,8-tetrahydroxy-2,4-bis(3-methylbut-2-en-1-yl)-9H-xanthen-9-one	185	1,3,6,7-tetrahydroxy-8-(3-hydroxy-3-methylbutyl)-2-(3-methylbut-2-en-1-yl)-9H-xanthen-9-one
172	1,3,5,8-tetrahydroxy-2,4-bis(3-methylbut-2-en-1-yl)-9H-xanthen-9-one	186	1,3,5,6-tetrahydroxy-2-(3-methylbut-2-en-1-yl)-4-(2-methylbut-3-en-2-yl)-9H-xanthen-9-one
173	1,6-dihydroxy-3,7-dimethoxy-2,8-bis(3-methylbut-2-en-1-yl)-9H-xanthen-9-one	187	1,2,5,6-tetrahydroxy-7-(3-methylbut-2-en-1-yl)-4-(2-methylbut-3-en-2-yl)-9H-xanthen-9-one
174	1,3,6-trihydroxy-7-methoxy-2,8-bis(3-methylbut-2-en-1-yl)-9H-xanthen-9-one	188	1,3,5,6-tetrahydroxy-7-(3-methylbut-2-en-1-yl)-4-(2-methylbut-3-en-2-yl)-9H-xanthen-9-one
175	1-hydroxy-3,6,7-trimethoxy-2,8-bis(3-methylbut-2-en-1-yl)-9H-xanthen-9-one	189	1,3,6,7-tetrahydroxy-5-(3-methylbut-2-en-1-yl)-2-(2-methylbut-3-en-2-yl)-9H-xanthen-9-one
176	3,6-diethoxy-1-hydroxy-7-methoxy-2,8-bis(3-methylbut-2-en-1-yl)-9H-xanthen-9-one	190	1,3,5,6-tetrahydroxy-8-(3-methylbut-2-en-1-yl)-2-(2-methylbut-3-en-2-yl)-9H-xanthen-9-one
177	1-hydroxy-7-methoxy-2,8-bis(3-methylbut-2-en-1-yl)-3,6-dipropoxy-9H-xanthen-9-one	191	3,6,8-trihydroxy-2-methoxy-1-(3-methylbut-2-en-1-yl)-5-(2-methylbut-3-en-2-yl)-9H-xanthen-9-one
178	3,6-dibutoxy-1-hydroxy-7-methoxy-2,8-bis(3-methylbut-2-en-1-yl)-9H-xanthen-9-one	192	1,3,6-trihydroxy-5-methoxy-7-(3-methylbut-2-en-1-yl)-2-(2-methylbut-3-en-2-yl)-9H-xanthen-9-one
179	1-hydroxy-3,6-diisopropoxy-7-methoxy-2,8-bis(3-methylbut-2-en-1-yl)-9H-xanthen-9-one	193	1,3,6-trihydroxy-8-(3-hydroxy-3-methylbutyl)-7-methoxy-2-(3-methylbut-2-en-1-yl)-9H-xanthen-9-one
180	3,6-bis(allyloxy)-1-hydroxy-7-methoxy-2,8-bis(3-methylbut-2-en-1-yl)-9H-xanthen-9-one	194	2,3,6,8-tetrahydroxy-1,4,7-tris(3-methylbut-2-en-1-yl)-9H-xanthen-9-one
181	1-hydroxy-7-methoxy-3,6-bis((2-methylallyl)oxy)-2,8-bis(3-methylbut-2-en-1-yl)-9H-xanthen-9-one	195	3,6,8-trihydroxy-2-methoxy-1,4,7-tris(3-methylbut-2-en-1-yl)-9H-xanthen-9-one
182	1-hydroxy-7-methoxy-2,8-bis(3-methylbut-2-en-1-yl)-9-oxo-9H-xanthen-3,6-diyl diacetate	196	3,4,5,8-tetrahydroxy-1,2-bis(3-methylbut-2-en-1-yl)-7-(2-methylbut-3-en-2-yl)-9H-xanthen-9-one

Table S1. Cont.

ID	Name	ID	Name
198	1,3,5,6-tetrahydroxy-4,8-bis(3-methylbut-2-en-1-yl)-2-(2-methylbut-3-en-2-yl)-9 <i>H</i> -xanthen-9-one	212	5,13-dihydroxy-3,3,10,10-tetramethyl-2,3,11,12-tetrahydro-1 <i>H</i> -dipyrano[3,2-a:2',3'- <i>i</i> ]xanthen-14(10 <i>H</i> )-one
199	7,12-dihydroxy-9-methoxy-2,2-dimethylpyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one	213	5,13-dihydroxy-3,3,10,10-tetramethyl-3 <i>H</i> -dipyrano[3,2-a:2',3'- <i>i</i> ]xanthen-14(10 <i>H</i> )-one
200	7,9,12-trihydroxy-2,2-dimethylpyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one	214	7,14-dihydroxy-2,2,10,10-tetramethyl-9,10-dihydro-2 <i>H</i> -dipyrano[3,2-b:2',3'- <i>i</i> ]xanthen-6(8 <i>H</i> )-one
201	6,10-dihydroxy-11-methoxy-3,3-dimethylpyrano[2,3- <i>c</i> ]xanthen-7(3 <i>H</i> )-one	215	5,12-dihydroxy-2,2,10,10-tetramethyl-2 <i>H</i> -dipyrano[3,2-b:2',3'- <i>i</i> ]xanthen-6(10 <i>H</i> )-one
202	6,10,11-trihydroxy-3,3-dimethylpyrano[2,3- <i>c</i> ]xanthen-7(3 <i>H</i> )-one	216	6,13-dihydroxy-3,3,11,11-tetramethyl-3 <i>H</i> -dipyrano[3,2-b:3',2'- <i>h</i> ]xanthen-7(11 <i>H</i> )-one
203	6,8,11-trihydroxy-3,3-dimethylpyrano[2,3- <i>c</i> ]xanthen-7(3 <i>H</i> )-one	217	6,13-dihydroxy-3,3,11,11-tetramethyl-2,3-dihydro-1 <i>H</i> -dipyrano[3,2-b:3',2'- <i>h</i> ]xanthen-7(11 <i>H</i> )-one
204	5,8,9-trihydroxy-1,1,2-trimethyl-1 <i>H</i> -furo[2,3- <i>c</i> ]xanthen-6(2 <i>H</i> )-one	218	8,9-dihydroxy-2,3,3,5,6,6-hexamethyl-5,6-dihydro-2 <i>H</i> -difuro[2,3-a:2',3'- <i>c</i> ]xanthen-12(3 <i>H</i> )-one
205	5,9-dihydroxy-10-methoxy-1,1,2-trimethyl-1 <i>H</i> -furo[2,3- <i>c</i> ]xanthen-6(2 <i>H</i> )-one	219	5,12-dihydroxy-2,3,3,10,10-pentamethyl-2,3-dihydrofuro[2,3- <i>h</i> ]pyrano[3,2- <i>b</i> ]xanthen-6(10 <i>H</i> )-one
206	5,9,10-trihydroxy-1,1,2-trimethyl-1 <i>H</i> -furo[2,3- <i>c</i> ]xanthen-6(2 <i>H</i> )-one	220	5,8-dihydroxy-2,2,10,10-tetramethyl-3,4-dihydro-2 <i>H</i> -dipyrano[2,3-a:2',3'- <i>i</i> ]xanthen-14(10 <i>H</i> )-one
207	4,8,9-trihydroxy-2,3,3-trimethyl-2 <i>H</i> -furo[3,2- <i>b</i> ]xanthen-5(3 <i>H</i> )-one	221	1,4,7-trihydroxy-2-(2-hydroxypropan-2-yl)-10,10-dimethyl-1,2-dihydrofuro[3,2- <i>h</i> ]pyrano[3,2- <i>b</i> ]xanthen-6(10 <i>H</i> )-one
208	8,9-dihydroxy-4-methoxy-2,3,3-trimethyl-2 <i>H</i> -furo[3,2- <i>b</i> ]xanthen-5(3 <i>H</i> )-one	222	7,9,12-trihydroxy-2,2-dimethyl-10-(2-methylbut-3-en-2-yl)pyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one
209	9,10-dihydroxy-6-methoxy-3,3-dimethylpyrano[2,3- <i>c</i> ]xanthen-7(3 <i>H</i> )-one	223	7,9,12-trihydroxy-2,2-dimethyl-8-(2-methylbut-3-en-2-yl)pyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one
210	5,9,10-trihydroxy-2,2-dimethylpyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one	224	7,8,12-trihydroxy-2,2-dimethyl-10-(2-methylbut-3-en-2-yl)pyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one
211	5,9,11-trihydroxy-3,3-dimethylpyrano[3,2- <i>a</i> ]xanthen-12(3 <i>H</i> )-one	225	5,9,11-trihydroxy-3,3-dimethyl-10-(3-methylbut-2-en-1-yl)pyrano[3,2- <i>a</i> ]xanthen-12(3 <i>H</i> )-one

Table S1. Cont.

ID	Name	ID	Name
226	5,9,11-trihydroxy-3,3-dimethyl-10-(2-methylbut-3-en-2-yl)pyrano[3,2- <i>a</i> ]xanthen-12(3 <i>H</i> )-one	240	4,8-dihydroxy-9-methoxy-2,3,3-trimethyl-7-(3-methylbut-2-en-1-yl)-2 <i>H</i> -furo[3,2- <i>b</i> ]xanthen-5(3 <i>H</i> )-one
227	5,9,11-trihydroxy-3,3-dimethyl-8-(3-methylbut-2-en-1-yl)pyrano[3,2- <i>a</i> ]xanthen-12(3 <i>H</i> )-one	241	4,8,9-trihydroxy-2,3,3-trimethyl-7-(3-methylbut-2-en-1-yl)-2 <i>H</i> -furo[3,2- <i>b</i> ]xanthen-5(3 <i>H</i> )-one
228	5,9,11-trihydroxy-3,3-dimethyl-8-(2-methylbut-3-en-2-yl)pyrano[3,2- <i>a</i> ]xanthen-12(3 <i>H</i> )-one	242	4,8,9-trihydroxy-2,3,3-trimethyl-11-(3-methylbut-2-en-1-yl)-2 <i>H</i> -furo[3,2- <i>b</i> ]xanthen-5(3 <i>H</i> )-one
229	7,10,12-trihydroxy-2,2-dimethyl-8-(2-methylbut-3-en-2-yl)-3,4-dihydropyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one	243	4,8,9-trihydroxy-2,3,3-trimethyl-11-(2-methylbut-3-en-2-yl)-2 <i>H</i> -furo[3,2- <i>b</i> ]xanthen-5(3 <i>H</i> )-one
230	5,9,10-trihydroxy-2,2-dimethyl-12-(2-methylbut-3-en-2-yl)pyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one	244	4,7,8-trihydroxy-2,3,3-trimethyl-9-(3-methylbut-2-en-1-yl)-2 <i>H</i> -furo[3,2- <i>b</i> ]xanthen-5(3 <i>H</i> )-one
231	5,9,10-trihydroxy-2,2-dimethyl-12-(3-methylbut-2-en-1-yl)pyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one	245	4,6,9-trihydroxy-2-(2-hydroxypropan-2-yl)-11-(3-methylbut-2-en-1-yl)-2 <i>H</i> -furo[3,2- <i>b</i> ]xanthen-5(3 <i>H</i> )-one
232	5,9,10-trihydroxy-2,2-dimethyl-8-(3-methylbut-2-en-1-yl)pyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one	246	5,7,10-trihydroxy-2-(2-hydroxypropan-2-yl)-4-(3-methylbut-2-en-1-yl)-1 <i>H</i> -furo[2,3- <i>c</i> ]xanthen-6(2 <i>H</i> )-one
233	5,8-dihydroxy-9-methoxy-2,2-dimethyl-10-(3-methylbut-2-en-1-yl)pyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one	247	5,9,10-trihydroxy-1,1,2-trimethyl-4-(2-methylbut-3-en-2-yl)-1 <i>H</i> -furo[2,3- <i>c</i> ]xanthen-6(2 <i>H</i> )-one
234	5,9-dihydroxy-10-methoxy-2,2-dimethyl-12-(2-methylbut-3-en-2-yl)pyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one	248	5,9-dihydroxy-10-methoxy-1,1,2-trimethyl-7-(3-methylbut-2-en-1-yl)-1 <i>H</i> -furo[2,3- <i>c</i> ]xanthen-6(2 <i>H</i> )-one
235	5,9-dihydroxy-7-(3-hydroxy-3-methylbutyl)-8-methoxy-2,2-dimethyl-3,4-dihydropyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one	249	5,9-dihydroxy-10-methoxy-2,2-dimethyl-11-(3-methylbut-2-en-1-yl)-3,4-dihydropyrano[2,3- <i>a</i> ]xanthen-12(2 <i>H</i> )-one
236	5,8,9-trihydroxy-2,2-dimethyl-10-(3-methylbut-2-en-1-yl)pyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one	250	3,5,9-trihydroxy-10-methoxy-2,2-dimethyl-11-(3-methylbut-2-en-1-yl)-3,4-dihydropyrano[2,3- <i>a</i> ]xanthen-12(2 <i>H</i> )-one
237	5,9-dihydroxy-8-methoxy-2,2-dimethyl-7-(3-methylbut-2-en-1-yl)pyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one	251	5,9-dihydroxy-11-(3-hydroxy-3-methylbutyl)-10-methoxy-2,2-dimethyl-3,4-dihydropyrano[2,3- <i>a</i> ]xanthen-12(2 <i>H</i> )-one
238	5,9-dihydroxy-8-methoxy-2,2-dimethyl-7-(3-methylbut-2-en-1-yl)-3,4-dihydropyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one	252	9-hydroxy-8,10-dimethoxy-2,2-dimethyl-11-(2-methylbut-3-en-2-yl)pyrano[3,2- <i>c</i> ]xanthen-7(2 <i>H</i> )-one
239	3,5,9-trihydroxy-8-methoxy-2,2-dimethyl-7-(3-methylbut-2-en-1-yl)-3,4-dihydropyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one	253	5,12-dihydroxy-1,1,2,10,10-pentamethyl-4-(3-methylbut-2-en-1-yl)-1,2-dihydrofuro[3,2- <i>h</i> ]pyrano[3,2- <i>b</i> ]xanthen-6(10 <i>H</i> )-one



Table S1. Cont.

ID	Name	ID	Name
254	5,13-dihydroxy-3,3,10,10-tetramethyl-6-(3-methylbut-2-en-1-yl)-3 <i>H</i> -dipyrano[3,2- <i>a</i> :2',3'- <i>i</i> ]xanthen-14(10 <i>H</i> )-one	267	(2 <i>S</i> ,3 <i>R</i> )-4-hydroxy-3-(1-hydroxy-3,6,7-trimethoxy-2,8-bis(3-methylbut-2-en-1-yl)-9-oxo-9 <i>H</i> -xanthen-4-yl)-2-(2-hydroxypropan-2-yl)-7,8-dimethoxy-6-(3-methylbut-2-en-1-yl)-2 <i>H</i> -furo[3,2- <i>b</i> ]xanthen-5(3 <i>H</i> )-one
255	7,9,12-trihydroxy-2,2-dimethyl-8-(3-methylbut-2-en-1-yl)-10-(2-methylbut-3-en-2-yl)pyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one	268	8-hydroxy-3-(3-hydroxy-4-methoxyphenyl)-2-(hydroxymethyl)-5-methoxy-2 <i>H</i> -[1,4]dioxino[2,3- <i>c</i> ]xanthen-7(3 <i>H</i> )-one
256	5,9,11-trihydroxy-3,3-dimethyl-6,10-bis(3-methylbut-2-en-1-yl)pyrano[3,2- <i>a</i> ]xanthen-12(3 <i>H</i> )-one	269	8-hydroxy-3-(5-hydroxy-2,4-dimethoxyphenyl)-2-(hydroxymethyl)-5-methoxy-2 <i>H</i> -[1,4]dioxino[2,3- <i>c</i> ]xanthen-7(3 <i>H</i> )-one
257	5,9,11-trihydroxy-3,3-dimethyl-6,8-bis(3-methylbut-2-en-1-yl)pyrano[3,2- <i>a</i> ]xanthen-12(3 <i>H</i> )-one	270	8-hydroxy-3-(4-hydroxy-3,5-dimethoxyphenyl)-2-(hydroxymethyl)-5-methoxy-2 <i>H</i> -[1,4]dioxino[2,3- <i>c</i> ]xanthen-7(3 <i>H</i> )-one
258	7,10,12-trihydroxy-4-(3-hydroxy-3-methylbutyl)-2,2-dimethyl-8-(2-methylbut-3-en-2-yl)-3,4-dihydropyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one	271	3-(4-hydroxy-3,5-dimethoxyphenyl)-2-(hydroxymethyl)-5,8-dimethoxy-2 <i>H</i> -[1,4]dioxino[2,3- <i>c</i> ]xanthen-7(3 <i>H</i> )-one
259	2,3,5,8-tetrahydroxy-1-(3-hydroxy-3-methylbutyl)-4-(3-methylbut-2-en-1-yl)-7-(2-methylbut-3-en-2-yl)-9 <i>H</i> -xanthen-9-one	272	8,10-dihydroxy-3-(4-hydroxy-3,5-dimethoxyphenyl)-2-(hydroxymethyl)-2 <i>H</i> -[1,4]dioxino[2,3- <i>c</i> ]xanthen-7(3 <i>H</i> )-one
260	1,3,5,6-tetrahydroxy-7-methoxy-2,4-bis(3-methylbut-2-en-1-yl)-9 <i>H</i> -xanthen-9-one		
261	5,9,10-trihydroxy-8-methoxy-2,2-dimethylpyrano[3,2- <i>b</i> ]xanthen-6(2 <i>H</i> )-one		
262	6,9,11-trihydroxy-5-methoxy-3,3-dimethylpyrano[3,2- <i>a</i> ]xanthen-12(3 <i>H</i> )-one		
263	4,8,9-trihydroxy-11-methoxy-2,3,3-trimethyl-2 <i>H</i> -furo[3,2- <i>b</i> ]xanthen-5(3 <i>H</i> )-one		
264	2,2',8,8'-tetrahydroxy-9 <i>H</i> ,9' <i>H</i> -[1,1'-bixanthen]-9,9'-dione		
265	3-((1,8-dihydroxy-3,6-dimethoxy-9-oxo-9 <i>H</i> -xanthen-4-yl)oxy)-1,8-dihydroxy-4,6-dimethoxy-9 <i>H</i> -xanthen-9-one		
266	1,1',3,4',5,6',8,8'-octahydroxy-9 <i>H</i> ,9' <i>H</i> -[2,2'-bixanthen]-9,9'-dione		