

Supplementary Material

Table S1. Fragment ions of chemical constituents tentatively identified in *Rosmarinus officinalis* by HPLC-QTOF-MS/MS

No. Fig. 2	Fragment ions			Identification criteria	References
	Fragment type	Fragment formula	m/z		
1	[M-H] ⁻	[C ₂₂ H ₂₁ O ₁₂] ⁻	477.10570		
	[M-H-CH ₃] ⁻	[C ₂₁ H ₁₈ O ₁₂] ⁻	462.06633		
	[M-H-C ₆ H ₁₁ O ₅] ⁻	[C ₁₆ H ₁₁ O ₇] ⁻	315.04814		
2	[M-H] ⁻	[C ₁₈ H ₁₅ O ₈] ⁻	359.07991	a, b	[1]
	[M-H-C ₉ H ₆ O ₃] ⁻	[C ₉ H ₉ O ₅] ⁻	197.04519		
	[M-H-C ₉ H ₈ O ₄] ⁻	[C ₉ H ₇ O ₄] ⁻	179.03460		
	[M-H-C ₉ H ₈ O ₄ -H ₂ O] ⁻	[C ₉ H ₅ O ₃] ⁻	161.02342		
	[M-H-C ₉ H ₈ O ₄ -H ₂ O-CH ₂ O] ⁻	[C ₈ H ₇ O ₂] ⁻	135.04261		
3	[M-H] ⁻	[C ₃₁ H ₂₇ O ₁₄] ⁻	623.10900	a, b	[2]
	[M-H-C ₁₅ H ₁₆ O ₇] ⁻	[C ₁₆ H ₁₁ O ₇] ⁻	315.04949		
	[M-H-C ₁₅ H ₁₆ O ₇ -CH ₃] ⁻	[C ₁₅ H ₈ O ₇] ⁻	300.03166		
4	[M-H] ⁻	[C ₁₇ H ₁₃ O ₆] ⁻	313.07089	a, b	[1]
	[M-H-CH ₃] ⁻	[C ₁₆ H ₁₀ O ₆] ⁻	298.04655		
	[M-H-CH ₃ -CH ₃] ⁻	[C ₁₅ H ₇ O ₆] ⁻	283.01956		
5	[M+CH ₃ COO] ⁻	[C ₃₉ H ₅₁ O ₁₀] ⁻	691.34456		
	[M+CH ₃ COO-C ₁₇ H ₁₉ O] ⁻	[C ₂₀ H ₂₅ O ₅] ⁻	345.17075		
	[M+CH ₃ COO-C ₁₇ H ₁₉ O-CO ₂ -H ₂ O] ⁻	[C ₁₉ H ₂₃ O ₂] ⁻	283.17058		
6	[M-H] ⁻	[C ₂₀ H ₂₅ O ₅] ⁻	345.17019	a, b	[3]
	[M-H-CO ₂ -H ₂ O] ⁻	[C ₁₉ H ₂₃ O ₂] ⁻	283.16949		
7	[M-H] ⁻	[C ₂₀ H ₂₃ O ₅] ⁻	343.15454	a, b	[4]
	[M-H-CO ₂] ⁻	[C ₁₉ H ₂₃ O ₃] ⁻	283.16949		
8	[M-H] ⁻	[C ₂₄ H ₂₇ O ₉] ⁻	457.1481		
	[M-H-C ₄ H ₄ O ₅] ⁻	[C ₂₀ H ₂₃ O ₅] ⁻	343.15461		
	[M-H-C ₄ H ₄ O ₅ -CO ₂] ⁻	[C ₁₉ H ₂₃ O ₃] ⁻	299.16542		

9	[M-H] ⁻ [M-H-CO ₂] ⁻	[C ₂₀ H ₂₅ O ₄] ⁻ [C ₁₉ H ₂₅ O ₂] ⁻	329.17600 285.18618	a, b	[1]
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^a Collision energy used to these fragments was 20 or 40 eV. ^a Tentative identification based on m/z negative mode, reported in the literature for *Rosmarinus officinalis* or other species of the *Lamiaceae* family. ^b Tentative identification based on the fragmentation pattern study (ESI-QTOF) and data reported in scientific articles.

Figure S1. Compound fragment spectrum results (MS/MS)

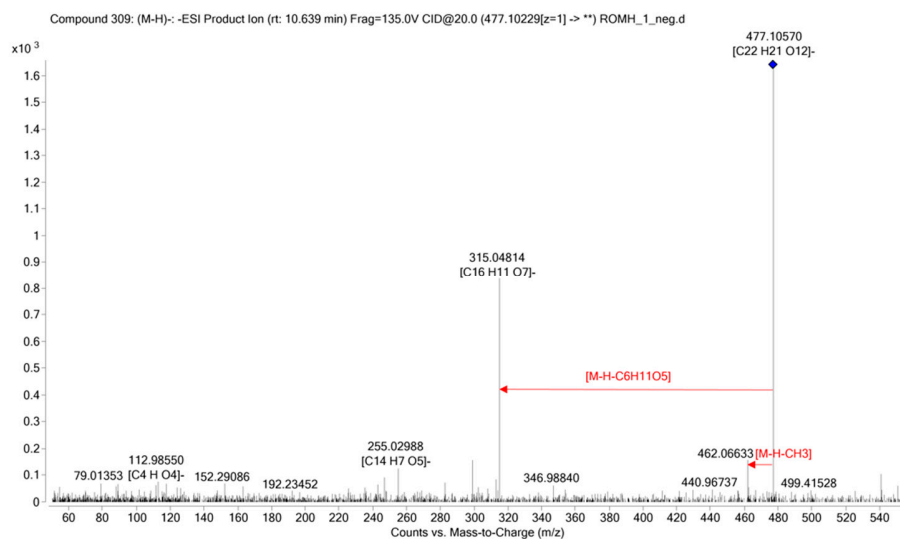
Compound 1

Retention time: 10.639

m/z [M-H]: 477.1028

Formula: C₂₂H₂₂O₁₂

Tentative annotation: Flavonoid-glycosylated type



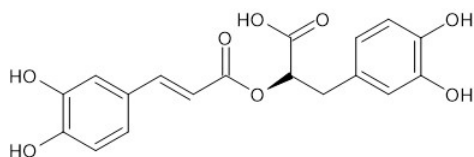
Compound 2

Retention time: 11.256

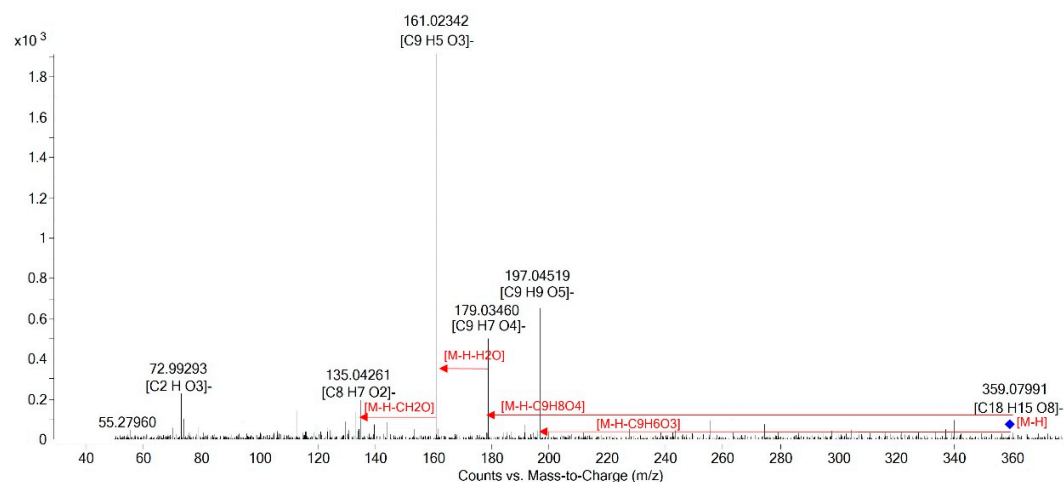
m/z [M-H]: 359.0772

Formula: C₁₈H₁₆O₈

Tentative annotation: Rosmarinic acid



Compound 326: (M-H)⁻ -ESI Product Ion (rt: 11.256 min) Frag=135.0V CID@20.0 (359.07651[z=1] -> **) ROMH_1_neg.d



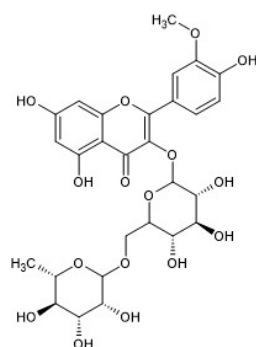
Compound 3

Retention time: 11.35

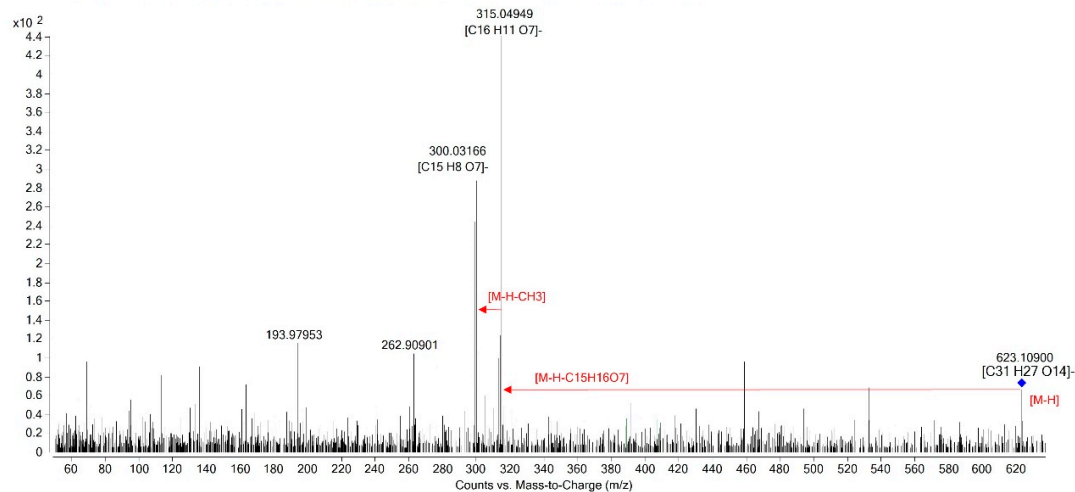
m/z [M-H]⁻: 623.1396

Formula: C₃₁H₂₈O₁₄

Tentative annotation: Isorhamnetin-rutinoside



Compound 331: (M-H)⁻ -ESI Product Ion (rt: 11.355 min) Frag=135.0V CID@40.0 (623.13940[z=1] -> **) ROMH_1_neg.d



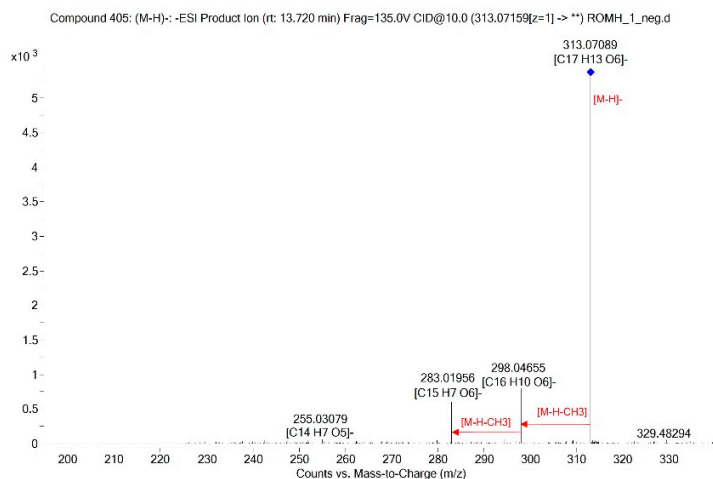
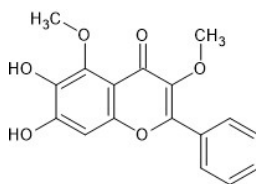
Compound 4

Retention time: 13.726

m/z [M-H]: 313.0709

Formula: C₁₇H₁₄O₆

Tentative annotation: Dihydroxy-dimethoxyflavone



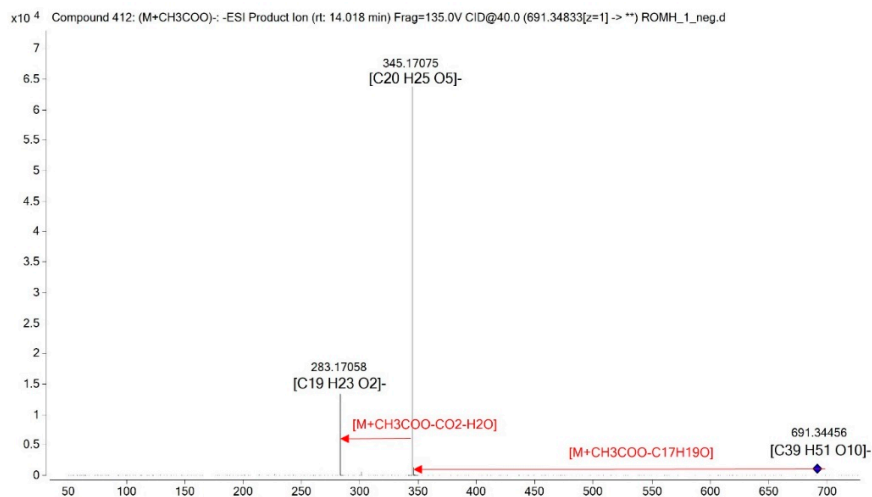
Compound 5

Retention time: 14.012

m/z [M+CH₃COO]⁻: 632.33497

Formula: C₃₈H₄₈O₈

Tentative annotation: Diterpene



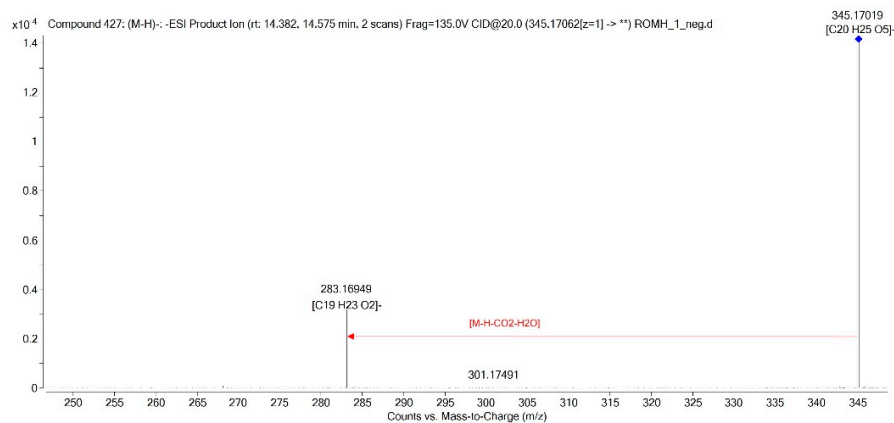
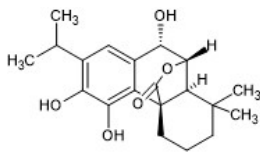
Compound 6

Retention time: 14.478

m/z [M-H]⁻: 345.1707

Formula: C₂₀H₂₆O₅

Tentative annotation: Rosmanol



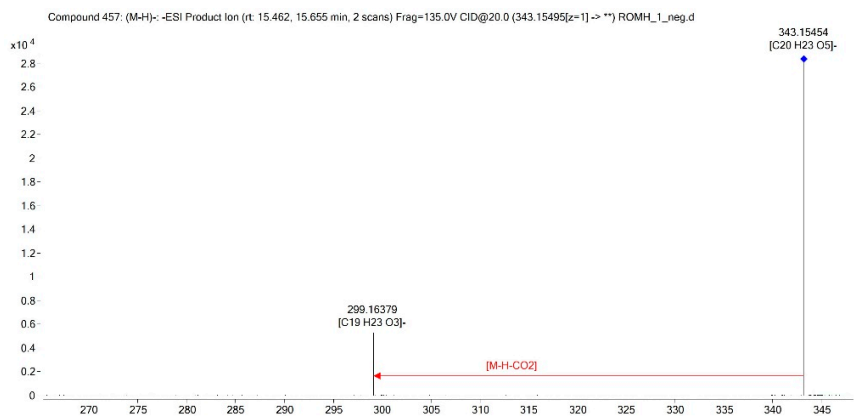
Compound 7

Retention time: 15.558

m/z [M-H]⁻: 343.1551

Formula: C₂₀H₂₄O₅

Tentative annotation: Rosmadial



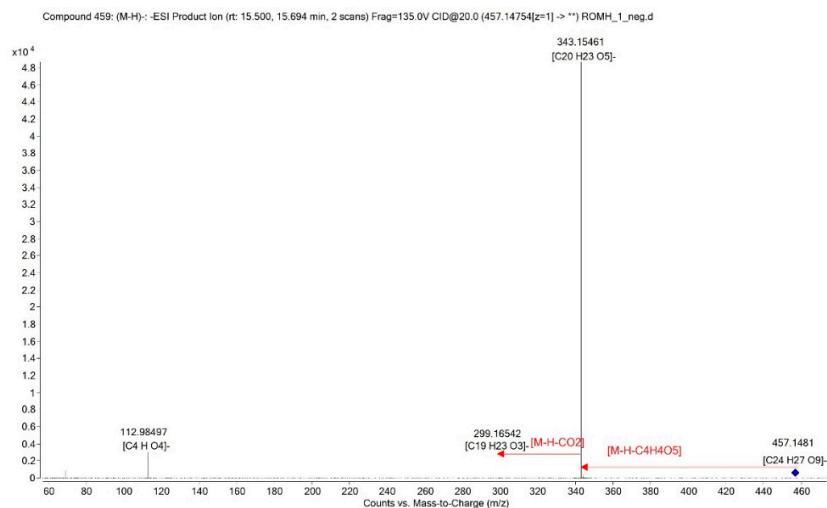
Compound 8

Retention time: 15.597

m/z [M-H]⁻: 457.1481

Formula: C₂₄H₂₆O₉

Tentative annotation: Diterpene type



Compound 9

Retention time: 16.077

m/z [M-H]⁻: 329.1764

Formula: C₂₀H₂₆O₄

Tentative annotation: Carnosol

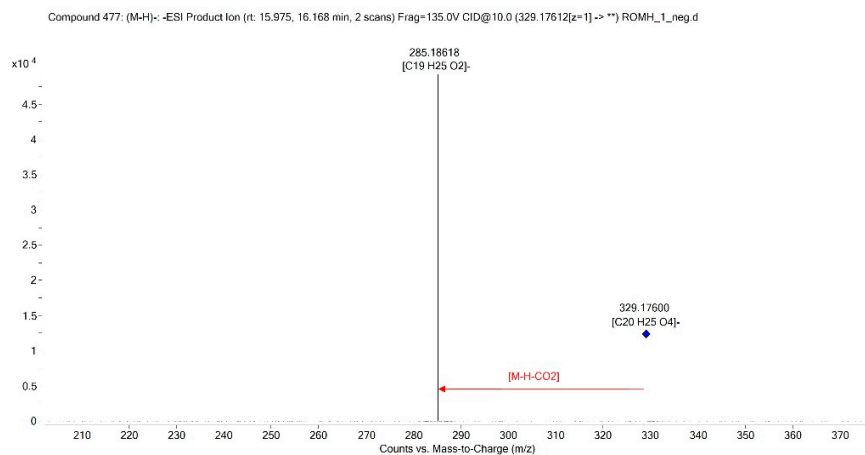
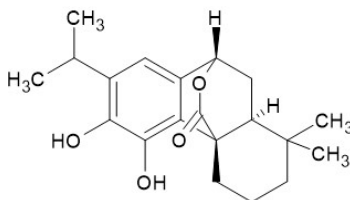


Table S2. Docking score for 708 human proteins with carnosol.

	Carnosol				
	Binding Affinity (kcal/mol)				
	Protein	Run 1	Run 2	Run 3	<i>Average</i>
1	3O0I	-10.9	-10.9	-10.9	-10.9
2	3NMQ	-10.4	-10.4	-10.4	-10.4
3	1RY8	-10.4	-10.4	-10.4	-10.4
4	2WKM	-10.3	-10.3	-10.3	-10.3
5	1N83	-10.0	-10.0	-10.0	-10.0
6	1HFQ	-10.0	-10.0	-10.0	-10.0
7	3WHW	-9.9	-9.9	-9.9	-9.9
8	3L0L	-9.9	-9.9	-9.9	-9.9
9	2XVT	-9.9	-9.9	-9.9	-9.9
10	1TQN	-9.8	-9.8	-9.8	-9.8
11	1DGB	-9.8	-9.8	-9.8	-9.8
12	4XII	-9.8	-9.8	-9.8	-9.8
13	1P8D	-9.7	-9.7	-9.7	-9.7
14	4DRJ	-9.7	-9.7	-9.7	-9.7
15	4AOJ	-9.6	-9.6	-9.6	-9.6
16	1UHL	-9.6	-9.6	-9.6	-9.6
17	1ZXM	-9.6	-9.6	-9.6	-9.6
18	4FA2	-9.5	-9.5	-9.5	-9.5
19	4J52	-9.5	-9.5	-9.5	-9.5
20	3X36	-9.2	-9.2	-9.2	-9.2
21	1UY7	-10.9	-10.9	-10.9	-10.9
22	1UY8	-10.9	-10.9	-10.8	-10.9
23	1UY9	-10.8	-10.8	-10.8	-10.8
24	2FWY	-10.7	-10.7	-10.7	-10.7
25	2H55	-10.7	-10.7	-10.7	-10.7
26	1UYC	-10.6	-10.6	-10.6	-10.6
27	1UYG	-10.6	-10.6	-10.6	-10.6
28	5FNC	-10.6	-10.6	-10.6	-10.6
29	1UYF	-10.4	-10.4	-10.4	-10.4
30	3FT8	-10.4	-10.4	-10.4	-10.4
31	1UY6	-10.4	-10.3	-10.3	-10.3
32	1UYD	-10.3	-10.3	-10.3	-10.3
33	1UYE	-10.3	-10.3	-10.3	-10.3
34	1UYH	-10.3	-10.3	-10.3	-10.3
35	1UYK	-10.3	-10.3	-10.3	-10.3

36	2FWZ	-10.3	-10.3	-10.3	-10.3
37	1UYM	-10.2	-10.2	-10.2	-10.2
38	4B0O	-9.7	-9.7	-9.7	-9.7
39	5GT4	-9.6	-9.6	-9.6	-9.6
40	3IAI	-9.9	-9.6	-8.6	-9.4
41	4BDS	-9.3	-9.4	-9.4	-9.4
42	3LDQ	-9.3	-9.4	-9.4	-9.4
43	1G1U	-9.3	-9.6	-9.3	-9.4
44	1H9U	-9.4	-9.4	-9.4	-9.4
45	2W5B	-9.4	-9.4	-9.4	-9.4
46	3PP1	-9.9	-8.6	-9.8	-9.4
47	4MJH	-9.1	-9.4	-9.3	-9.3
48	3O96	-8.6	-9.2	-10	-9.3
49	3UT3	-9.1	-9.5	-9.2	-9.3
50	2VQQ	-9.1	-9.1	-9.6	-9.3
51	1M13	-9.3	-9.3	-9.3	-9.3
52	1P0I	-9.3	-9.3	-9.3	-9.3
53	4TPK	-9.2	-9.3	-9.3	-9.3
54	5GPG	-9.3	-9.3	-9.3	-9.3
55	4C9X	-9.3	-9.3	-9.3	-9.3
56	1KV2	-9.3	-9.3	-9.3	-9.3
57	1W22	-9.2	-9.2	-9.2	-9.2
58	2OC2	-9.2	-9.2	-9.2	-9.2
59	4NRE	-9.2	-9.2	-9.2	-9.2
60	4R6A	-9.2	-9.2	-9.2	-9.2
61	1Z6T	-8.9	-9.3	-9.3	-9.2
62	3VI8	-9.4	-8.9	-9.3	-9.2
63	3MVH	-9.2	-9.2	-9.2	-9.2
64	2X0W	-9.1	-9.1	-9.1	-9.1
65	3SOS	-9.1	-9.1	-9.1	-9.1
66	3EAH	-9.1	-9.1	-9.1	-9.1
67	2V0M	-9.6	-8.4	-9.4	-9.1
68	4D6Z	-9.2	-9	-9.2	-9.1
69	3UA1	-9.3	-9.1	-9	-9.1
70	3W3N	-9.1	-9.1	-9.1	-9.1
71	4QC0	-9.1	-9.1	-9.1	-9.1
72	3S95	-9.1	-9.1	-9.1	-9.1
73	3C4C	-9.1	-9.1	-9.1	-9.1
74	1DB1	-9.1	-9.1	-9.1	-9.1
75	1PQ6	-9.1	-8.2	-9.9	-9.1
76	5IXS	-8.5	-8.6	-10.1	-9.1

77	3UOK	-9	-9	-9	-9
78	1SR7	-8.3	-9.4	-9.4	-9
79	4FYR	-9	-9	-9	-9
80	1J8F	-9	-9	-9.1	-9
81	3U4S	-8.9	-9	-9	-9
82	5E6H	-9	-9	-9	-9
83	3QKL	-9	-9	-9	-9
84	3NXQ	-9	-9	-9	-9
85	3QM4	-9.4	-9.3	-8.3	-9
86	4EY5	-9	-9	-9	-9
87	5K5E	-9	-9.2	-8.9	-9
88	4R09	-8.6	-9.9	-8.6	-9
89	4C9W	-9	-9	-9	-9
90	1YRP	-8.6	-9.3	-9.2	-9
91	1NMS	-9	-9	-9	-9
92	3EQM	-9	-9	-9	-9
93	3LKJ	-9	-9	-9	-9
94	4JPS	-9.2	-8.8	-8.9	-9
95	3L0J	-8.7	-9.2	-9.2	-9
96	4DOS	-8.9	-9	-9	-9
97	4DQM	-7.5	-8.9	-10.6	-9
98	2RKU	-9	-9	-9	-9
99	2W1C	-9	-9	-9	-9
100	2XRU	-9	-9	-9	-9
101	5CSW	-9	-9	-9	-9
102	4ASD	-8.9	-8.9	-8.9	-8.9
103	3UO5	-8.9	-8.9	-8.9	-8.9
104	4C8B	-8.9	-8.9	-8.8	-8.9
105	4K9W	-8.9	-8.9	-8.9	-8.9
106	2VRL	-8.4	-9.8	-8.4	-8.9
107	4D89	-8.9	-8.9	-8.9	-8.9
108	4EY6	-9	-8.9	-8.9	-8.9
109	3E7G	-8.6	-8.8	-9.4	-8.9
110	3W3K	-8.9	-8.9	-8.9	-8.9
111	2H7C	-8.9	-8.9	-8.9	-8.9
112	2J3N	-9	-8.9	-8.8	-8.9
113	3ZR0	-8.9	-8.9	-8.9	-8.9
114	5KXA	-9.6	-9.5	-7.6	-8.9
115	1G5Y	-9.1	-9.1	-8.6	-8.9
116	1YOK	-8.9	-9	-8.9	-8.9
117	3D24	-8.8	-8.9	-8.9	-8.9

118	3KYT	-8.9	-8.9	-8.9	-8.9
119	4UDC	-9.3	-9.3	-8	-8.9
120	2UW9	-8.9	-8.9	-8.9	-8.9
121	3VHE	-8.8	-8.8	-8.8	-8.8
122	3OCB	-8.8	-8.8	-8.8	-8.8
123	2W8Y	-8.8	-8.8	-8.8	-8.8
124	1AO6	-8.2	-8.9	-9.2	-8.8
125	3L9N	-9.3	-9.3	-7.7	-8.8
126	1OJC	-10	-8.2	-8.2	-8.8
127	2C66	-8.4	-9.5	-8.5	-8.8
128	2V60	-8.1	-8.1	-10.1	-8.8
129	4FVT	-8.8	-8.9	-8.8	-8.8
130	4PZW	-8.8	-8.8	-8.8	-8.8
131	4R08	-8.8	-8.8	-8.7	-8.8
132	5AWB	-8.8	-8.8	-8.8	-8.8
133	1HK1	-8.8	-8.8	-8.9	-8.8
134	1HK2	-8.8	-8.8	-8.8	-8.8
135	1HK5	-7.9	-10.1	-8.5	-8.8
136	4B3E	-9.2	-8.7	-8.6	-8.8
137	3KVW	-8.8	-8.8	-8.8	-8.8
138	4TUH	-8.9	-8.5	-9.1	-8.8
139	4WVT	-8.8	-8.8	-8.8	-8.8
140	1CBS	-9.4	-7.6	-9.4	-8.8
141	1I7I	-8.8	-8.8	-8.8	-8.8
142	1NRL	-8.4	-9.5	-8.4	-8.8
143	1XAP	-9.5	-7.5	-9.4	-8.8
144	2XYW	-9.5	-9.5	-7.4	-8.8
145	3PLZ	-8.8	-8.8	-8.7	-8.8
146	2PVR	-8.8	-8.8	-8.8	-8.8
147	5KDI	-8.7	-8.7	-8.7	-8.7
148	2OK5	-8.6	-8.9	-8.6	-8.7
149	3L54	-8.7	-8.6	-8.7	-8.7
150	1E3K	-8.8	-8.7	-8.7	-8.7
151	3RUK	-8.7	-8.6	-8.7	-8.7
152	4XRY	-8.3	-8.9	-8.9	-8.7
153	4A7A	-8.5	-9.4	-8.1	-8.7
154	4B0Q	-8.7	-8.7	-8.7	-8.7
155	4EY4	-8.7	-8.7	-8.7	-8.7
156	4EY7	-8.7	-8.7	-8.6	-8.7
157	2AZ5	-8.7	-8.7	-8.7	-8.7
158	5HDH	-7.8	-9.1	-9.1	-8.7

159	1HK3	-8.9	-8.4	-8.9	-8.7
160	3Q93	-8.2	-9	-9	-8.7
161	5TQ3	-8.5	-9.2	-8.5	-8.7
162	1X7E	-8.7	-8.7	-8.8	-8.7
163	2YXJ	-8.7	-8.7	-8.7	-8.7
164	4QVX	-8.7	-8.7	-8.7	-8.7
165	1KV6	-9.3	-9.3	-7.6	-8.7
166	2GL8	-9.4	-8.4	-8.4	-8.7
167	2PIN	-8.7	-8.7	-8.7	-8.7
168	3BEJ	-8.9	-8.6	-8.6	-8.7
169	3IPS	-8.6	-8.7	-8.7	-8.7
170	5G3J	-9.1	-7.9	-9.1	-8.7
171	1DHT	-8.7	-8.7	-8.7	-8.7
172	4AG8	-8.6	-8.6	-8.6	-8.6
173	1ZUC	-8.4	-8.9	-8.4	-8.6
174	2OL2	-8.6	-8.6	-8.6	-8.6
175	3IJE	-7.6	-9.1	-9.1	-8.6
176	4LXZ	-9	-7.9	-9	-8.6
177	4L02	-8.6	-8.6	-8.6	-8.6
178	3QU8	-8.2	-9	-8.6	-8.6
179	4W9P	-8.6	-8.6	-8.6	-8.6
180	1NSI	-8.5	-8.4	-8.8	-8.6
181	3KMC	-8.6	-8.6	-8.6	-8.6
182	4R07	-8.8	-8.6	-8.3	-8.6
183	2H79	-8.6	-8.6	-8.6	-8.6
184	2ZZ0	-8.6	-8.5	-8.6	-8.6
185	4NOS	-8.7	-8.6	-8.6	-8.6
186	2W3L	-8.6	-8.6	-8.6	-8.6
187	1K7L	-8.9	-8	-8.9	-8.6
188	3D6D	-8.3	-9.1	-8.3	-8.6
189	2PPL	-7.7	-8.9	-8.9	-8.5
190	3KCG	-8	-8.8	-8.8	-8.5
191	3MAX	-8.5	-8.5	-8.5	-8.5
192	3ZNS	-8	-8.7	-8.7	-8.5
193	4GU0	-8.4	-8.6	-8.5	-8.5
194	2OJI	-8.5	-8.5	-8.5	-8.5
195	3PM0	-8.3	-8.3	-9	-8.5
196	1J1A	-8.5	-8.4	-8.7	-8.5
197	1LYW	-8.5	-8.5	-8.5	-8.5
198	2BYB	-8	-9.4	-8	-8.5
199	2Z5X	-8.5	-8.5	-8.5	-8.5

200	2FV5	-8.5	-8.5	-8.5	-8.5
201	3W3G	-8.4	-8.4	-8.6	-8.5
202	3W3J	-8.5	-8.5	-8.5	-8.5
203	4QBZ	-8.5	-8.5	-8.5	-8.5
204	5ANT	-8.6	-8.2	-8.6	-8.5
205	1GUL	-8.5	-8.5	-8.5	-8.5
206	2JLP	-8.3	-8.6	-8.6	-8.5
207	2VWI	-8.5	-8.5	-8.5	-8.5
208	1EF1	-8.5	-8.5	-8.5	-8.5
209	1MAZ	-8.5	-8.5	-8.5	-8.5
210	2CKE	-8.8	-8.3	-8.4	-8.5
211	2XYJ	-8.5	-8.5	-8.5	-8.5
212	3T03	-8.5	-8.5	-8.6	-8.5
213	4EMA	-8.5	-8.5	-8.5	-8.5
214	4PVU	-8.5	-8.5	-8.5	-8.5
215	4UDD	-8.7	-8.4	-8.4	-8.5
216	4J8M	-8.5	-8.5	-8.5	-8.5
217	1FLT	-8.4	-8.4	-8.5	-8.4
218	4XCT	-8.4	-8.4	-8.4	-8.4
219	5JFR	-8.4	-8.4	-8.4	-8.4
220	2BT0	-8.4	-8.4	-8.4	-8.4
221	2P3T	-8.4	-8.4	-8.4	-8.4
222	3D90	-7.6	-8.8	-8.9	-8.4
223	2D0T	-8.3	-8.4	-8.4	-8.4
224	3G0E	-8.4	-8.4	-8.4	-8.4
225	4ACG	-8.4	-8.4	-8.4	-8.4
226	4OGH	-8.4	-8.4	-8.4	-8.4
227	2C67	-8.1	-9	-8.1	-8.4
228	2WJO	-8.4	-8.4	-8.4	-8.4
229	3HOK	-8.5	-7.6	-9.1	-8.4
230	3ZR1	-8.4	-8.4	-8.3	-8.4
231	3NMM	-8.4	-8.4	-8.4	-8.4
232	1LV2	-8.4	-8.4	-8.4	-8.4
233	1OVL	-8.6	-8.6	-8.1	-8.4
234	3OLL	-8.4	-8.4	-8.4	-8.4
235	4MG5	-8.7	-8.7	-7.9	-8.4
236	4MG7	-7.7	-8.4	-9.2	-8.4
237	4JNK	-7.6	-10.1	-7.6	-8.4
238	4QTD	-8.4	-8.4	-8.4	-8.4
239	5UG8	-8.4	-8.4	-8.4	-8.4
240	2QG2	-8.8	-8.1	-8.1	-8.3

241	1DQA	-8.3	-8.3	-8.2	-8.3
242	4ASK	-8.3	-8.4	-8.1	-8.3
243	3C0Z	-8.3	-8.3	-8.4	-8.3
244	1SJ0	-8.2	-8.2	-8.4	-8.3
245	1ZYJ	-8.3	-8.3	-8.3	-8.3
246	4ASX	-8.3	-8.3	-8.3	-8.3
247	4DYM	-8.5	-8.2	-8.2	-8.3
248	4IDT	-8.2	-8.4	-8.3	-8.3
249	4OYA	-8.1	-8.8	-8.1	-8.3
250	3UA5	-8.4	-8	-8.5	-8.3
251	3F6K	-8.7	-7.5	-8.7	-8.3
252	1Q5K	-7.8	-9.2	-8	-8.3
253	1ZXC	-7.9	-9.2	-7.9	-8.3
254	3L0V	-8.3	-8.4	-8.3	-8.3
255	3W3L	-8.3	-8.3	-8.3	-8.3
256	1HK4	-8.1	-8.1	-8.8	-8.3
257	1ICT	-8.3	-8.4	-8.3	-8.3
258	1AWI	-8.3	-8.3	-8.3	-8.3
259	1IG1	-8.3	-8.3	-8.3	-8.3
260	2DUX	-8.3	-8.3	-8.2	-8.3
261	2XIR	-8.3	-8.3	-8.3	-8.3
262	1NAX	-8.3	-8.3	-8.3	-8.3
263	3CDS	-7.5	-8.3	-9.2	-8.3
264	4EM9	-8.4	-8.4	-8.1	-8.3
265	4IS8	-7.9	-8.6	-8.5	-8.3
266	4MG6	-8.5	-8.2	-8.2	-8.3
267	4OAR	-8.3	-8.3	-8.3	-8.3
268	4UDB	-9.1	-8.2	-7.6	-8.3
269	1CG6	-8.3	-8.2	-8.3	-8.3
270	1J1B	-8.3	-9.5	-7.2	-8.3
271	2WGJ	-7.3	-8.7	-9	-8.3
272	3EQH	-8.3	-8.3	-8.3	-8.3
273	3VVH	-8.4	-8.2	-8.4	-8.3
274	3HNG	-8.2	-8.2	-8.2	-8.2
275	4WUA	-8.2	-8.2	-8.2	-8.2
276	1SQN	-8.2	-8.2	-8.1	-8.2
277	3EKO	-8.3	-8	-8.2	-8.2
278	3EKR	-8.4	-7.7	-8.4	-8.2
279	3K97	-8.2	-8.1	-8.2	-8.2
280	1JMJ	-8.2	-8.2	-8.2	-8.2
281	2GS6	-8.2	-8.2	-8.2	-8.2

282	3SOR	-8.5	-7.1	-9	-8.2
283	4NA7	-8.2	-8.2	-8.2	-8.2
284	2Q8E	-8.7	-8	-7.8	-8.2
285	3V6R	-8.3	-8.3	-8.1	-8.2
286	3ZEP	-8.6	-8.2	-7.9	-8.2
287	2XZT	-8.2	-8.2	-8.2	-8.2
288	1BX4	-8.1	-8.1	-8.5	-8.2
289	2V5Z	-8.2	-8.2	-8.2	-8.2
290	2OVX	-8.2	-8.2	-8.2	-8.2
291	2PRG	-8	-8.3	-8.3	-8.2
292	3W3M	-8.7	-8	-8	-8.2
293	4R0A	-8.5	-8.1	-8.1	-8.2
294	2PLL	-8.2	-8.2	-8.2	-8.2
295	4N1U	-8.6	-8	-8	-8.2
296	1GUM	-8.2	-8.2	-8.2	-8.2
297	17GS	-8.2	-8.2	-8.2	-8.2
298	3ZLN	-8.2	-8.2	-8.2	-8.2
299	1A52	-7.4	-9.2	-8	-8.2
300	1KKQ	-8	-8	-8.7	-8.2
301	2QW4	-8.2	-8.2	-8.2	-8.2
302	3B3K	-7.4	-7.4	-9.7	-8.2
303	4MG9	-8.1	-8.2	-8.2	-8.2
304	4MGB	-7.8	-7.9	-8.9	-8.2
305	4PRG	-8.4	-8.2	-8	-8.2
306	4PWL	-8.2	-8.2	-8.2	-8.2
307	5KYJ	-8.2	-8.2	-8.3	-8.2
308	3EQC	-8.2	-8.2	-8.2	-8.2
309	3FGU	-8.2	-8.2	-8.2	-8.2
310	3OWD	-8.2	-8.2	-8.2	-8.2
311	5C91	-8.2	-8.2	-8.2	-8.2
312	3PTA	-8.5	-8	-8.1	-8.2
313	1A28	-7.6	-8.3	-8.3	-8.1
314	3BMY	-8.1	-8.1	-8.1	-8.1
315	3D9I	-7.6	-8.4	-8.4	-8.1
316	4CR5	-8.2	-8.1	-8	-8.1
317	3C10	-7.9	-8.2	-8.2	-8.1
318	4FWF	-8.1	-8.1	-8	-8.1
319	3QX3	-6.6	-8.9	-8.9	-8.1
320	1S3E	-8	-8.1	-8.1	-8.1
321	2PD5	-7.4	-8.4	-8.4	-8.1
322	2VRM	-8.1	-8	-8.3	-8.1

323	3UIU	-8.1	-8.1	-8.1	-8.1
324	4B70	-8.1	-8.1	-8.1	-8.1
325	4I0F	-8	-8.1	-8.1	-8.1
326	4TW8	-8	-8	-8.2	-8.1
327	3G42	-8	-8.1	-8.2	-8.1
328	3LE9	-7.7	-8.3	-8.2	-8.1
329	2XN6	-8.1	-8.1	-8.1	-8.1
330	1JKL	-8	-8.1	-8.1	-8.1
331	1X78	-8	-8.1	-8.1	-8.1
332	2VPF	-8.2	-8.3	-7.9	-8.1
333	1ERR	-8.4	-8.4	-7.6	-8.1
334	1FM9	-7.9	-8.8	-7.6	-8.1
335	1P93	-8.2	-7.9	-8.3	-8.1
336	3LBD	-7.4	-9.4	-7.4	-8.1
337	3VJI	-8.2	-8.1	-8.1	-8.1
338	4HLW	-8	-8	-8.4	-8.1
339	1KE8	-8.1	-8.1	-8.1	-8.1
340	1NFI	-8.1	-8.1	-8.2	-8.1
341	3E8N	-8.4	-7.9	-7.9	-8.1
342	4R3C	-8.2	-8.1	-8.1	-8.1
343	5TWZ	-8	-8.1	-8	-8
344	2BYI	-8.4	-8.4	-7.1	-8
345	2QG0	-8	-8	-8	-8
346	3JXU	-7.9	-8	-8	-8
347	5J20	-7	-7.2	-9.8	-8
348	1TB6	-8.3	-7.4	-8.3	-8
349	2J4I	-8	-8	-8	-8
350	3NXP	-8	-8	-8	-8
351	4BTI	-7.9	-8.1	-7.9	-8
352	4D76	-8.2	-7.7	-8.2	-8
353	5TKS	-8	-8	-8.1	-8
354	3SWR	-7.5	-7.4	-9	-8
355	1D5R	-8	-8.1	-8	-8
356	2HXL	-8.5	-7.7	-7.7	-8
357	3TXO	-7.8	-7.8	-8.3	-8
358	1TNF	-8.2	-7.7	-8.2	-8
359	3QOA	-8.4	-7.1	-8.4	-8
360	1OJA	-7.9	-7.9	-8.2	-8
361	1S3B	-8	-8	-8	-8
362	2C64	-7.9	-8	-8.1	-8
363	2C65	-8.3	-7.9	-7.8	-8

364	2OKK	-7.9	-8.2	-7.9	-8
365	2V61	-8	-8	-8	-8
366	2Z5Y	-8	-8	-8	-8
367	3UYT	-7.5	-8.3	-8.3	-8
368	3ZGV	-7.9	-7.7	-8.5	-8
369	3MDY	-8.2	-7.8	-8.1	-8
370	2OW1	-8	-8	-8	-8
371	3WN4	-8	-8	-8	-8
372	5AWD	-7.9	-8.1	-8.1	-8
373	2H77	-8	-8	-8	-8
374	2RIW	-8	-8	-8	-8
375	1DCY	-8	-8	-8	-8
376	2X4Z	-8	-8	-8	-8
377	1L6J	-7.8	-8.3	-7.8	-8
378	1NMQ	-8	-8	-8	-8
379	1QDU	-8.4	-8.4	-7.2	-8
380	3MUP	-8	-8	-8	-8
381	4KMP	-8	-8	-8	-8
382	4MAN	-7.9	-8	-8	-8
383	3GWX	-8.2	-7.7	-8.2	-8
384	3GZ9	-8	-7.9	-8	-8
385	3VJH	-8.1	-7.8	-8	-8
386	4DM6	-8.3	-8.3	-7.5	-8
387	4MG8	-7.8	-7.8	-8.4	-8
388	4MGA	-8	-8	-7.9	-8
389	1OL6	-8.4	-7.2	-8.3	-8
390	2GS2	-8	-8	-7.9	-8
391	3JS2	-7.9	-7.9	-7.9	-7.9
392	4WZV	-7.9	-7.9	-7.9	-7.9
393	5NJK	-7.9	-8	-7.7	-7.9
394	1OSF	-7.9	-7.9	-8	-7.9
395	1UYI	-7.9	-7.9	-7.9	-7.9
396	1DAN	-7.5	-8.1	-8.1	-7.9
397	2BOH	-7.9	-7.9	-7.9	-7.9
398	3BG8	-7.9	-8	-7.9	-7.9
399	3DY7	-7.9	-7.9	-7.9	-7.9
400	3SW2	-7.9	-7.9	-7.9	-7.9
401	4EKG	-8	-7.6	-8	-7.9
402	4LY1	-7.9	-7.9	-7.9	-7.9
403	2H94	-8	-7.6	-8.2	-7.9
404	1OI9	-7.9	-7.9	-7.8	-7.9

405	2BUJ	-8.1	-7.8	-7.7	-7.9
406	1OJ9	-7.9	-7.9	-7.9	-7.9
407	1S2Q	-7.6	-7.6	-8.5	-7.9
408	1S2Y	-7.9	-8	-7.9	-7.9
409	2FDV	-7.9	-7.9	-8	-7.9
410	3INH	-7.9	-7.9	-7.9	-7.9
411	4OM7	-7.9	-8	-7.9	-7.9
412	1Z7J	-7.9	-7.9	-7.9	-7.9
413	5ANW	-7.9	-7.9	-7.9	-7.9
414	4BEX	-7.9	-7.9	-7.9	-7.9
415	2Y1L	-7.9	-7.9	-7.9	-7.9
416	3NPC	-9	-7.4	-7.4	-7.9
417	4IEH	-7.9	-7.9	-7.9	-7.9
418	3CDP	-8.3	-7.6	-7.9	-7.9
419	3HOD	-7.9	-7.9	-7.9	-7.9
420	3OLS	-7.8	-8.1	-7.8	-7.9
421	1GIH	-7.9	-7.9	-8	-7.9
422	3ZXZ	-8.4	-8.3	-7.1	-7.9
423	4ZSA	-7.9	-7.9	-7.9	-7.9
424	2P4I_B	-7.5	-8	-7.9	-7.8
425	4BB4	-7.8	-7.8	-7.8	-7.8
426	2BZ5	-7.8	-7.8	-7.8	-7.8
427	3HHU	-7.9	-7.6	-7.9	-7.8
428	5J6N	-7.8	-7.8	-7.8	-7.8
429	5UCH	-7.8	-7.8	-7.7	-7.8
430	6ASY	-7.4	-8	-8	-7.8
431	2FDA	-7.8	-7.8	-7.8	-7.8
432	2W26	-7.8	-7.8	-7.8	-7.8
433	4JZF	-7.8	-7.8	-7.8	-7.8
434	4NA8	-7.8	-7.8	-7.8	-7.8
435	2QRV	-7.7	-7.7	-7.9	-7.8
436	1U4D	-7.6	-7.6	-8.3	-7.8
437	3P1D	-7.8	-7.8	-7.8	-7.8
438	4WT2	-7.8	-7.8	-7.8	-7.8
439	2YDV	-7.7	-7.8	-7.8	-7.8
440	1DTW	-7.8	-7.8	-7.8	-7.8
441	2BK3	-7.6	-8	-7.9	-7.8
442	3F88	-7.8	-7.8	-7.8	-7.8
443	1FKG	-7.8	-7.8	-7.8	-7.8
444	2ZK1	-8	-7.5	-8	-7.8
445	1ETB	-7.8	-7.8	-7.8	-7.8

446	3GWS	-7.8	-7.8	-7.8	-7.8
447	4LNW	-7.8	-7.8	-7.8	-7.8
448	4LNX	-7.8	-7.8	-7.8	-7.8
449	3TH5	-7.8	-7.8	-7.8	-7.8
450	5UAK	-7.5	-8.2	-7.7	-7.8
451	121P	-7.8	-7.9	-7.6	-7.8
452	1I3O	-7.8	-7.8	-7.8	-7.8
453	3QD6	-7.7	-7.9	-7.9	-7.8
454	1BSX	-7.8	-7.8	-7.8	-7.8
455	1FCX	-7.7	-8.1	-7.7	-7.8
456	1FD0	-7.5	-7.5	-8.4	-7.8
457	1GWX	-7.8	-7.8	-7.8	-7.8
458	2BAW	-7.8	-7.8	-7.8	-7.8
459	2J14	-7.8	-7.7	-7.8	-7.8
460	3BQD	-7.4	-7.4	-8.6	-7.8
461	3U9Q	-8.3	-8	-7	-7.8
462	4MGD	-7.7	-7.8	-7.8	-7.8
463	1ZYS	-7.8	-7.8	-7.8	-7.8
464	3MBL	-7.1	-7.1	-9.3	-7.8
465	3ZME	-8.2	-7.1	-8.2	-7.8
466	4ZZN	-7.8	-7.8	-7.8	-7.8
467	5HG8	-7.8	-7.8	-7.8	-7.8
468	2P4I_A	-7.8	-7.6	-7.8	-7.7
469	1YC3	-7.4	-7.8	-7.8	-7.7
470	1YET	-7.7	-7.7	-7.7	-7.7
471	2BYH	-7.3	-8	-7.9	-7.7
472	1HCG	-7.8	-7.7	-7.6	-7.7
473	2Y7X	-7.7	-7.7	-7.7	-7.7
474	3IIT	-7.7	-7.7	-7.7	-7.7
475	3OS3	-7.7	-7.7	-7.7	-7.7
476	1T64	-7.7	-7.7	-7.7	-7.7
477	2HK5	-7.7	-7.7	-7.7	-7.7
478	3UNJ	-7.7	-7.7	-7.7	-7.7
479	3W33	-7.4	-7.8	-7.8	-7.7
480	4EBV	-7.7	-7.8	-7.5	-7.7
481	4R7H	-7.2	-7.5	-8.3	-7.7
482	2I47	-7.4	-7.4	-8.2	-7.7
483	3F17	-7.6	-7.7	-7.7	-7.7
484	3J0A	-8.1	-7.4	-7.5	-7.7
485	1ETA	-7.8	-7.8	-7.4	-7.7
486	1XZX	-7.7	-7.7	-7.7	-7.7

487	1Y0X	-7.7	-7.7	-7.7	-7.7
488	2CEO	-7.6	-8	-7.6	-7.7
489	3KIJ	-7.7	-7.7	-7.7	-7.7
490	2XIK	-7.7	-7.7	-7.7	-7.7
491	3ODW	-7.7	-7.7	-7.6	-7.7
492	1RWW	-7.7	-7.7	-7.7	-7.7
493	3DEH	-7.7	-7.8	-7.7	-7.7
494	5IEZ	-7.7	-7.7	-7.7	-7.7
495	1FBY	-7.8	-7.8	-7.5	-7.7
496	1QKU	-7.8	-7.3	-7.9	-7.7
497	2XYX	-8.5	-7.3	-7.3	-7.7
498	3JZC	-7.7	-7.7	-7.7	-7.7
499	4DM8	-7.4	-8.4	-7.4	-7.7
500	4MGC	-7.8	-7.2	-8	-7.7
501	1MCH	-7.7	-7.7	-7.7	-7.7
502	2ITP	-7.6	-7.6	-7.8	-7.7
503	2XP2	-7.7	-7.6	-7.7	-7.7
504	4EK4	-7.7	-7.7	-7.7	-7.7
505	1M17	-7.6	-7.6	-7.6	-7.6
506	1F9Q	-7.7	-7.5	-7.5	-7.6
507	4A7I	-7.7	-7.7	-7.3	-7.6
508	4AJU	-7.6	-7.6	-7.5	-7.6
509	4DY0	-7.6	-7.6	-7.6	-7.6
510	3F07	-8.6	-7.1	-7.1	-7.6
511	3PP0	-7.6	-7.5	-7.6	-7.6
512	4WH9	-7.5	-7.7	-7.7	-7.6
513	4DVF	-7.6	-7.6	-7.6	-7.6
514	3TKM	-7.6	-7.6	-7.6	-7.6
515	1F86	-7.4	-7.9	-7.4	-7.6
516	2PIW	-8.1	-8.1	-6.7	-7.6
517	2ROX	-7.6	-7.6	-7.6	-7.6
518	1A4R	-7.8	-7.2	-7.8	-7.6
519	1RGP	-7.6	-7.6	-7.6	-7.6
520	4MXO	-7.7	-7.7	-7.5	-7.6
521	4Q9S	-7.6	-7.6	-7.6	-7.6
522	1CP3	-7.6	-7.6	-7.6	-7.6
523	1YWT	-7.6	-7.6	-7.6	-7.6
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525	3GGF	-7.6	-7.6	-7.6	-7.6
526	3VW6	-7.1	-7.9	-7.7	-7.6
527	3ILZ	-7.6	-7.6	-7.5	-7.6

528	4TV1	-7.5	-7.8	-7.5	-7.6
529	1BJ4	-7.6	-7.6	-7.6	-7.6
530	1Z57	-7.3	-8.3	-7.3	-7.6
531	2ITW	-7.6	-7.5	-7.6	-7.6
532	2ITZ	-7.3	-7.2	-8.4	-7.6
533	2QON	-7.1	-7.8	-7.8	-7.6
534	3LQ8	-7.8	-7.6	-7.5	-7.6
535	1GJO	-7.5	-7.5	-7.5	-7.5
536	4U7T	-7.1	-7.5	-7.9	-7.5
537	4MDN	-7.5	-7.4	-7.5	-7.5
538	4Y72	-7.4	-7.5	-7.5	-7.5
539	1K3A	-7.5	-7.5	-7.6	-7.5
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541	5CR1	-7.3	-7.8	-7.3	-7.5
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543	4IZY	-7.6	-7.5	-7.5	-7.5
544	5DCP	-7.8	-7.8	-6.9	-7.5
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549	2V0V	-7.6	-7.5	-7.5	-7.5
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555	4ZSH	-7.5	-7.5	-7.5	-7.5
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558	1A4W	-7.5	-7.5	-7.5	-7.5
559	1C1Y	-7.5	-7.5	-7.4	-7.5
560	1NQL	-7.3	-7.6	-7.6	-7.5
561	2ITN	-7.6	-7.6	-7.4	-7.5
562	2ITU	-7.6	-7.6	-7.3	-7.5
563	3A60	-7.3	-7.3	-7.8	-7.5
564	3LZB	-7.5	-7.5	-7.6	-7.5
565	5VAD	-7.3	-7.7	-7.5	-7.5
566	2P55	-7.4	-7.4	-7.6	-7.5
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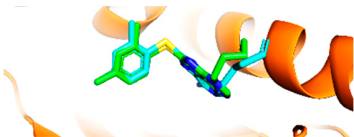
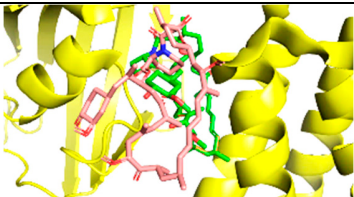
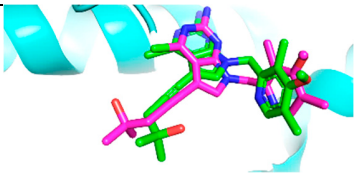

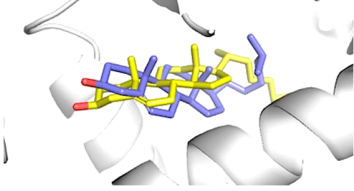
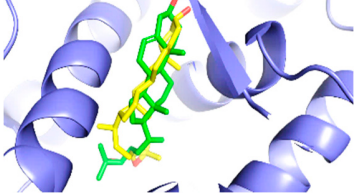
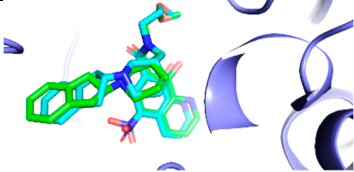
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572	1ZHM	-7.4	-7.6	-7.2	-7.4
573	3IEO	-7.4	-7.4	-7.4	-7.4
574	1Y57	-7.5	-7.2	-7.6	-7.4
575	2XK9	-7.4	-7.4	-7.4	-7.4
576	3ZBF	-7.4	-7.4	-7.4	-7.4
577	4URV	-7.4	-7.4	-7.4	-7.4
578	2HI4	-7.4	-7.4	-7.4	-7.4
579	1B1I	-7.4	-7.4	-7.4	-7.4
580	2QMG	-8.2	-6.8	-7.1	-7.4
581	2QP8	-7.3	-7.7	-7.3	-7.4
582	2WEZ	-7.2	-7.8	-7.1	-7.4
583	4IP9	-7.4	-7.4	-7.4	-7.4
584	2JDF	-7.4	-7.4	-7.4	-7.4
585	1F3M	-7.4	-7.5	-7.4	-7.4
586	1WDZ	-7.4	-7.3	-7.4	-7.4
587	1Y2O	-7.5	-7.5	-7.3	-7.4
588	1G73	-7.5	-7.1	-7.6	-7.4
589	1GFW	-7.3	-7.4	-7.4	-7.4
590	2GCP	-6.7	-7.7	-7.7	-7.4
591	1K74	-7.4	-7.4	-7.4	-7.4
592	3ET3	-7.4	-7.4	-7.4	-7.4
593	4M8E	-7.4	-7.4	-7.4	-7.4
594	4M8H	-7.4	-7.4	-7.3	-7.4
595	1OL5	-7.7	-7.4	-7.1	-7.4
596	4RG2	-7.4	-7.4	-7.4	-7.4
597	4THN	-7.2	-7.1	-7.8	-7.4
598	1YWN	-7.3	-7.3	-7.3	-7.3
599	6BCA	-8.2	-6.4	-7.3	-7.3
600	1C5X	-7.2	-7.7	-7.1	-7.3
601	1PY5	-7.2	-7.3	-7.4	-7.3
602	2O72	-7	-7.8	-7	-7.3
603	3MJ1	-7.3	-7.3	-7.3	-7.3
604	4GQS	-7.7	-7	-7.2	-7.3
605	5HK1	-7.6	-7.3	-7.1	-7.3
606	2XN7	-7.2	-7.6	-7.2	-7.3
607	4N1T	-7.3	-7.3	-7.3	-7.3
608	2J8Z	-7.3	-7.4	-7.3	-7.3
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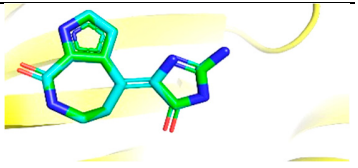
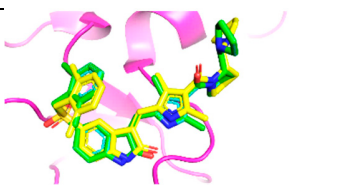
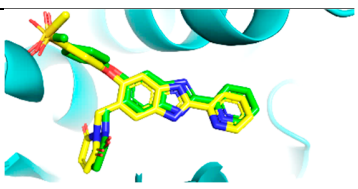
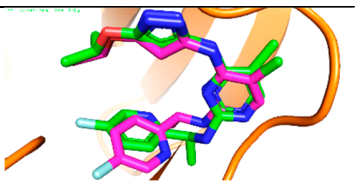
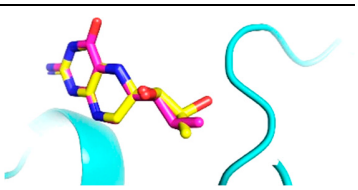
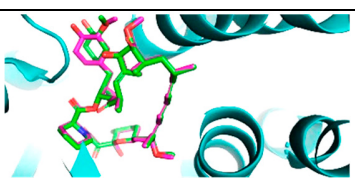
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611	1GS4	-7.1	-7.8	-7.1	-7.3
612	1.00E+99	-7.3	-7.3	-7.3	-7.3
613	2EB3	-7.5	-6.7	-7.6	-7.3
614	2ITX	-7.2	-7.3	-7.3	-7.3
615	5L9B	-7.2	-7.2	-7.2	-7.2
616	4KXQ	-7.2	-7.2	-7.1	-7.2
617	2X2L	-7.2	-7.2	-7.2	-7.2
618	4NJD	-7	-7.6	-7	-7.2
619	5NJX	-7.3	-7.3	-7	-7.2
620	1A9U	-7.2	-7.2	-7.2	-7.2
621	2B7A	-7.2	-7.6	-6.8	-7.2
622	4X30	-7.3	-7.1	-7.1	-7.2
623	4G5J	-7.2	-7.1	-7.2	-7.2
624	1MVC	-7.2	-7.3	-7.2	-7.2
625	5G5W	-7.2	-7.2	-7.2	-7.2
626	1JSV	-7.2	-7.2	-7.2	-7.2
627	1KAO	-7.2	-7.2	-7.2	-7.2
628	1KE5	-7.2	-7.2	-7.2	-7.2
629	1NCF	-7.2	-7.2	-7.2	-7.2
630	2LWI	-7.3	-7.2	-7.2	-7.2
631	3EQB	-7.2	-7.5	-6.8	-7.2
632	3ZZE	-7.2	-7.2	-7.2	-7.2
633	1EK3	-7.1	-7.1	-7.1	-7.1
634	4J1Y	-7.1	-7.1	-7	-7.1
635	3EW8	-7.1	-7.1	-7.1	-7.1
636	1A2B	-7.1	-7.1	-7.1	-7.1
637	3EYG	-7.3	-7	-7	-7.1
638	1SM2	-7.2	-7.2	-7	-7.1
639	3EO2	-7.1	-7.1	-7.1	-7.1
640	1P22	-7.1	-7.2	-7.1	-7.1
641	1R2D	-7.1	-7.1	-7.1	-7.1
642	1RE1	-7.1	-7.1	-7.1	-7.1
643	1MZN	-7.1	-7.1	-7.1	-7.1
644	3CJW	-7.1	-7.1	-7.1	-7.1
645	1GII	-7.2	-7.2	-6.8	-7.1
646	1H00	-6.6	-7.4	-7.4	-7.1
647	2R4B	-7.1	-7.1	-7.1	-7.1
648	1.00E+31	-7	-7	-7	-7
649	1EDM	-7	-7	-7	-7
650	2P55	-6.8	-7.4	-6.8	-7

651	3UQP	-7.2	-7.2	-6.7	-7
652	5H1D	-7	-7	-7	-7
653	1TW6	-7.2	-6.7	-7.2	-7
654	1UPK	-7	-7.1	-6.9	-7
655	3U6I	-6.9	-7.1	-7	-7
656	1UOU	-6.9	-6.9	-6.9	-6.9
657	5TQE	-6.9	-6.9	-6.8	-6.9
658	1T69	-7	-6.8	-7	-6.9
659	2KAV	-6.9	-6.9	-6.9	-6.9
660	2PIV	-6.9	-7	-6.9	-6.9
661	2ROY	-6.6	-7.6	-6.6	-6.9
662	3VKX	-6.7	-7.3	-6.7	-6.9
663	3F6Q	-6.9	-6.9	-6.9	-6.9
664	1PAU	-7	-6.9	-6.9	-6.9
665	1SVC	-7.1	-6.7	-6.8	-6.9
666	4KMN	-6.9	-6.9	-6.9	-6.9
667	2JJC	-7.2	-6.8	-6.3	-6.8
668	2QLD	-6.8	-6.7	-6.8	-6.8
669	2UWD	-6.7	-6.7	-6.9	-6.8
670	1T67	-6.8	-6.7	-6.8	-6.8
671	1AIE	-6.8	-6.8	-6.8	-6.8
672	2QU5	-7.1	-6.4	-6.9	-6.8
673	3AYU	-6.8	-6.8	-6.8	-6.8
674	1NME	-6.9	-6.8	-6.8	-6.8
675	1ZUQ	-6.8	-6.8	-6.9	-6.8
676	2EVW	-6.8	-6.8	-6.9	-6.8
677	3MK8	-6.8	-6.8	-6.8	-6.8
678	5C3H	-6.8	-6.8	-6.8	-6.8
679	1UOM	-6.7	-6.6	-7.2	-6.8
680	2YJA	-6.8	-6.8	-6.8	-6.8
681	5NZP	-6.8	-6.8	-6.8	-6.8
682	1JDH	-6.7	-6.7	-6.7	-6.7
683	1CJY	-6.2	-7.2	-6.6	-6.7
684	4KGH	-6.6	-6.5	-6.9	-6.7
685	3UEE	-6.7	-6.7	-6.8	-6.7
686	5FC4	-6.7	-6.7	-6.7	-6.7
687	3K6P	-6.7	-6.7	-6.7	-6.7
688	2CCS	-6.6	-6.6	-6.6	-6.6
689	2CCT	-6.5	-6.8	-6.5	-6.6
690	3BM9	-6.6	-6.5	-6.6	-6.6
691	5J2X	-6.7	-6.5	-6.5	-6.6

692	4LGE	-6.6	-6.6	-6.6	-6.6
693	1UNL	-6.6	-6.7	-6.6	-6.6
694	4AL0	-6.6	-6.6	-6.6	-6.6
695	5EXO	-6.6	-6.6	-6.6	-6.6
696	3UIH	-6.8	-6.4	-6.7	-6.6
697	5NZO	-6.6	-6.6	-6.7	-6.6
698	2CCU	-6.5	-6.5	-6.5	-6.5
699	3BWM	-6.5	-6.5	-6.6	-6.5
700	3OZK	-6.5	-6.4	-6.5	-6.5
701	2BIT	-6.4	-6.5	-6.5	-6.5
702	1GH7	-6.1	-6.9	-6.6	-6.5
703	2BSM	-6.4	-6.4	-6.4	-6.4
704	2VCJ	-6.5	-6.4	-6.4	-6.4
705	4WVS	-6.4	-6.4	-6.5	-6.4
706	1THA	-6.3	-6.3	-6.3	-6.3
707	1DEB	-6.2	-6.2	-6.2	-6.2
708	2FJ5	-5.8	-5.8	-5.8	-5.8

Table S3. RMSD and Superposition between the crystallographic structures of 13 the complexes and the resultant docking pose (Poses obtained is represented in green).

PDB code	Ligand	Reference	Binding Affinity	RMSD (Å)	Overlapping ligand
3O0I	P54	[5]	-9.3	0.984	
4DRJ	RAP	[6]	-8.1	0.322	
3NMQ	7PP	[7]	-10.1	1.579	
1HFQ	MOT	[8]	-9.4	1.159	
1N83	CLR	[9]	-10.9	1.693	
1P8D	CO1	[10]	-8.9	2.578	
4XII	40V	[11]	-10.8	0.765	

1Z57	DBQ	[12]	-9.6	0.000441	
2WKM	SO4	[13]	-11.4	1.619	
3H1V	TK1	[14]	-12.1	0.495	
4AOJ	V4Z	[15]	-8.9	1.421	
4NOS	H2B	[16]	-7.2	0.464	
5GPG	RAP	[17]	-9.5	0.516	

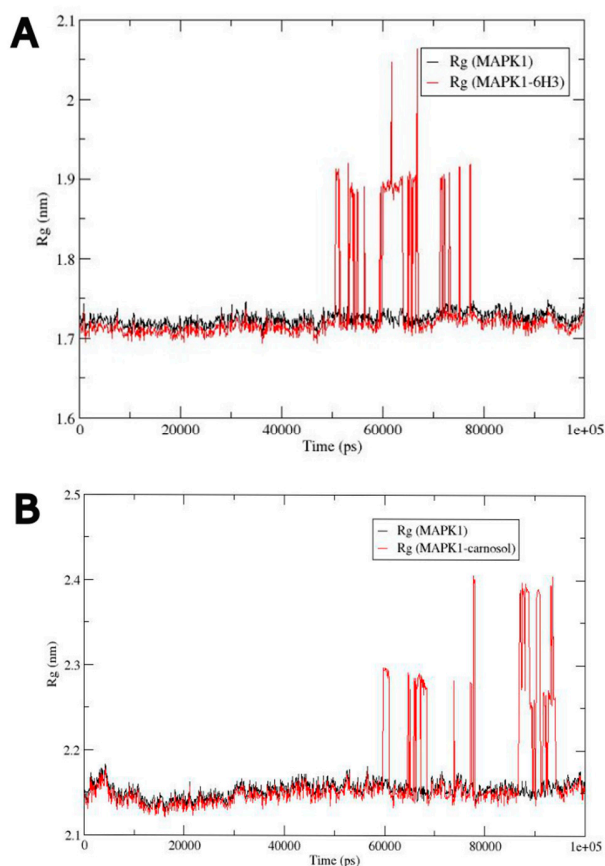


Fig. S2. Radius of gyration for MAPK1 complexes. Radius of gyration for MAPK1-6H3 complex (A) and radius of gyration for MAPK1-carnosol complex (B).

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