

9.7007	-6.5158	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
18.5257	-9.4991	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
14.7924	-2.4533	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
6.4965	-10.6032	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
10.3340	-6.1533	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
14.1132	-5.4116	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
10.8674	-1.9700	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
10.9466	-9.9366	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
18.5257	-10.2241	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
7.6674	-12.5116	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
5.5218	-9.6021	0.0000	N	0	0	0	0	0	0	0	0	0	0	0	0
12.2424	-1.8075	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
13.7090	-1.8199	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
7.6632	-13.9700	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
12.8382	-9.1366	0.0000	C1	0	0	0	0	0	0	0	0	0	0	0	0
18.5299	-7.7324	0.0000	N	0	0	0	0	0	0	0	0	0	0	0	0
8.9340	-14.7032	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
15.3757	-6.1408	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
9.7007	-4.3366	0.0000	C1	0	0	0	0	0	0	0	0	0	0	0	0
7.7965	-6.1533	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
14.7924	-3.7116	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
12.8299	-10.5825	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
3.2342	-9.4422	0.0000	N	0	0	0	0	0	0	0	0	0	0	0	0
10.3090	-11.0241	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
10.2007	-13.9825	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
17.8840	-11.3158	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
6.4090	-11.7825	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
14.7424	-5.0491	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
14.1132	-6.1366	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
14.7382	-6.4991	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
15.3757	-5.4116	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
4.2037	-9.6141	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
10.2007	-14.7075	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
10.2340	-3.0616	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
4.7727	-10.1345	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
3.5909	-10.0106	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
19.1632	-8.0949	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
3.1822	-8.6000	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
2.4981	-9.7321	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
5.1798	-3.0783	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
9.6049	-2.7033	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
5.8174	-2.7116	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
6.4465	-3.0700	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
8.9715	-3.0699	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
7.0799	-2.7075	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
7.7090	-3.0700	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
8.3424	-2.7075	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
11.7132	-2.5491	0.0000	H	0	0	0	0	0	0	0	0	0	0	0	0
5.8174	-2.0305	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0

2	9	1	0	0	0	0
3	5	1	0	0	0	0
1	4	1	6	0	0	0
5	36	1	1	0	0	0
6	10	1	0	0	0	0
7	8	1	0	0	0	0
8	1	1	0	0	0	0
9	5	1	0	0	0	0
10	15	1	0	0	0	0
10	11	1	1	0	0	0
28	12	1	1	0	0	0
13	32	1	0	0	0	0
14	45	1	1	0	0	0
15	12	1	0	0	0	0
16	18	2	0	0	0	0
17	4	1	0	0	0	0
18	25	1	0	0	0	0
19	13	1	0	0	0	0
20	14	1	0	0	0	0
21	23	1	0	0	0	0
22	16	1	0	0	0	0
23	3	1	0	0	0	0
24	30	1	0	0	0	0
25	7	1	0	0	0	0
26	29	1	0	0	0	0
27	20	1	0	0	0	0
28	19	1	0	0	0	0
42	29	1	1	0	0	0
30	39	1	0	0	0	0
31	11	1	0	0	0	0

32 17 1 6 0 0 0
33 60 1 0 0 0 0
34 14 1 0 0 0 0
35 16 1 0 0 0 0
36 24 1 0 0 0 0
37 28 1 0 0 0 0
38 27 1 0 0 0 0
39 59 1 0 0 0 0
40 6 2 0 0 0 0
41 34 1 0 0 0 0
42 31 1 0 0 0 0
43 1 1 0 0 0 0
44 47 2 0 0 0 0
45 35 1 0 0 0 0
46 55 1 0 0 0 0
47 32 1 0 0 0 0
2 48 1 1 0 0 0
49 33 1 0 0 0 0
50 46 1 0 0 0 0
51 3 1 0 0 0 0
52 43 1 0 0 0 0
25 53 1 1 0 0 0
54 40 1 0 0 0 0
55 64 2 0 0 0 0
56 57 1 0 0 0 0
57 26 1 0 0 0 0
58 37 1 0 0 0 0
59 84 1 0 0 0 0
60 37 2 0 0 0 0
61 55 1 0 0 0 0
62 76 1 0 0 0 0
63 50 1 0 0 0 0
64 6 1 0 0 0 0
65 66 1 0 0 0 0
66 52 2 0 0 0 0
67 22 2 0 0 0 0
68 51 1 0 0 0 0
69 18 1 0 0 0 0
70 8 2 0 0 0 0
71 15 2 0 0 0 0
72 17 2 0 0 0 0
73 19 2 0 0 0 0
74 50 2 0 0 0 0
75 26 2 0 0 0 0
76 69 2 0 0 0 0
77 31 2 0 0 0 0
78 42 1 0 0 0 0
79 47 1 0 0 0 0
80 52 1 0 0 0 0
81 56 1 0 0 0 0
82 48 2 0 0 0 0
83 53 2 0 0 0 0
84 80 2 0 0 0 0
85 49 1 0 0 0 0
86 68 2 0 0 0 0
87 79 2 0 0 0 0
88 74 1 0 0 0 0
20 89 1 6 0 0 0
90 53 1 0 0 0 0
23 91 1 1 0 0 0
21 92 1 6 0 0 0
27 93 1 6 0 0 0
94 40 1 0 0 0 0
57 95 1 6 0 0 0
38 96 1 1 0 0 0
97 78 1 0 0 0 0
98 65 1 0 0 0 0
43 99 1 6 0 0 0
100 48 1 0 0 0 0
101 54 1 0 0 0 0
102115 1 0 0 0 0
103 67 1 0 0 0 0
41104 1 6 0 0 0
105 74 1 0 0 0 0
106 76 1 0 0 0 0
107 85 1 0 0 0 0
108 85 2 0 0 0 0
109108 1 0 0 0 0
110107 2 0 0 0 0

Chemical Structure, MOLFILE

111114	1	0	0	0	0
112104	1	0	0	0	0
113 68	1	0	0	0	0
114 90	1	0	0	0	0
115111	1	0	0	0	0
116 95	1	0	0	0	0
117102	1	0	0	0	0
118102	1	0	0	0	0
119121	1	0	0	0	0
120113	1	0	0	0	0
121122	1	0	0	0	0
122124	1	0	0	0	0
123120	1	0	0	0	0
124125	1	0	0	0	0
125126	1	0	0	0	0
126123	1	0	0	0	0
3127	1	1	0	0	0
65 59	2	0	0	0	0
22 44	1	0	0	0	0
87 67	1	0	0	0	0
35 62	2	0	0	0	0
58 30	2	0	0	0	0
24 33	2	0	0	0	0
41 38	1	0	0	0	0
61 54	2	0	0	0	0
110 97	1	0	0	0	0
97109	2	0	0	0	0
2 21	1	0	0	0	0
63 56	2	0	0	0	0
81 88	2	0	0	0	0
121129	1	0	0	0	0
138145	1	0	0	0	0
139141	1	0	0	0	0
137140	1	6	0	0	0
141172	1	1	0	0	0
142146	1	0	0	0	0
143144	1	0	0	0	0
144137	1	0	0	0	0
145141	1	0	0	0	0
146151	1	0	0	0	0
146147	1	1	0	0	0
164148	1	1	0	0	0
149168	1	0	0	0	0
150181	1	1	0	0	0
151148	1	0	0	0	0
152154	2	0	0	0	0
153140	1	0	0	0	0
154161	1	0	0	0	0
155149	1	0	0	0	0
156150	1	0	0	0	0
157159	1	0	0	0	0
158152	1	0	0	0	0
159139	1	0	0	0	0
160166	1	0	0	0	0
161143	1	0	0	0	0
162165	1	0	0	0	0
163156	1	0	0	0	0
164155	1	0	0	0	0
178165	1	1	0	0	0
166175	1	0	0	0	0
167147	1	0	0	0	0
168153	1	6	0	0	0
169196	1	0	0	0	0
170150	1	0	0	0	0
171152	1	0	0	0	0
172160	1	0	0	0	0
173164	1	0	0	0	0
174163	1	0	0	0	0
175195	1	0	0	0	0
176142	2	0	0	0	0
177170	1	0	0	0	0
178167	1	0	0	0	0
179137	1	0	0	0	0
180183	2	0	0	0	0
181171	1	0	0	0	0
182191	1	0	0	0	0
183168	1	0	0	0	0
138184	1	1	0	0	0
185169	1	0	0	0	0

186182	1	0	0	0	0
187139	1	0	0	0	0
188179	1	0	0	0	0
161189	1	1	0	0	0
190176	1	0	0	0	0
191200	2	0	0	0	0
192193	1	0	0	0	0
193162	1	0	0	0	0
194173	1	0	0	0	0
195220	1	0	0	0	0
196173	2	0	0	0	0
197191	1	0	0	0	0
198212	1	0	0	0	0
199186	1	0	0	0	0
200142	1	0	0	0	0
201202	1	0	0	0	0
202188	2	0	0	0	0
203158	2	0	0	0	0
204187	1	0	0	0	0
205154	1	0	0	0	0
206144	2	0	0	0	0
207151	2	0	0	0	0
208153	2	0	0	0	0
209155	2	0	0	0	0
210186	2	0	0	0	0
211162	2	0	0	0	0
212205	2	0	0	0	0
213167	2	0	0	0	0
214178	1	0	0	0	0
215183	1	0	0	0	0
216188	1	0	0	0	0
217192	1	0	0	0	0
218184	2	0	0	0	0
219189	2	0	0	0	0
220216	2	0	0	0	0
221185	1	0	0	0	0
222204	2	0	0	0	0
223215	2	0	0	0	0
224210	1	0	0	0	0
156225	1	6	0	0	0
226189	1	0	0	0	0
159227	1	1	0	0	0
157228	1	6	0	0	0
163229	1	6	0	0	0
230176	1	0	0	0	0
193231	1	6	0	0	0
174232	1	1	0	0	0
233214	1	0	0	0	0
234201	1	0	0	0	0
179235	1	6	0	0	0
236184	1	0	0	0	0
237190	1	0	0	0	0
238251	1	0	0	0	0
239203	1	0	0	0	0
177240	1	6	0	0	0
241210	1	0	0	0	0
242212	1	0	0	0	0
243221	1	0	0	0	0
244221	2	0	0	0	0
245244	1	0	0	0	0
246243	2	0	0	0	0
247250	1	0	0	0	0
248240	1	0	0	0	0
249204	1	0	0	0	0
250226	1	0	0	0	0
251247	1	0	0	0	0
252231	1	0	0	0	0
253238	1	0	0	0	0
254238	1	0	0	0	0
255257	1	0	0	0	0
256249	1	0	0	0	0
257258	1	0	0	0	0
258260	1	0	0	0	0
259256	1	0	0	0	0
260261	1	0	0	0	0
261262	1	0	0	0	0
262259	1	0	0	0	0
139263	1	1	0	0	0
201195	2	0	0	0	0

158180	1	0	0	0	0
223203	1	0	0	0	0
171198	2	0	0	0	0
194166	2	0	0	0	0
160169	2	0	0	0	0
177174	1	0	0	0	0
197190	2	0	0	0	0
246233	1	0	0	0	0
233245	2	0	0	0	0
138157	1	0	0	0	0
199192	2	0	0	0	0
217224	2	0	0	0	0
257264	1	0	0	0	0
266273	1	0	0	0	0
267269	1	0	0	0	0
265268	1	6	0	0	0
269300	1	1	0	0	0
270274	1	0	0	0	0
271272	1	0	0	0	0
272265	1	0	0	0	0
273269	1	0	0	0	0
274279	1	0	0	0	0
274275	1	1	0	0	0
292276	1	1	0	0	0
277296	1	0	0	0	0
278309	1	1	0	0	0
279276	1	0	0	0	0
280282	2	0	0	0	0
281268	1	0	0	0	0
282289	1	0	0	0	0
283277	1	0	0	0	0
284278	1	0	0	0	0
285287	1	0	0	0	0
286280	1	0	0	0	0
287267	1	0	0	0	0
288294	1	0	0	0	0
289271	1	0	0	0	0
290293	1	0	0	0	0
291284	1	0	0	0	0
292283	1	0	0	0	0
306293	1	1	0	0	0
294303	1	0	0	0	0
295275	1	0	0	0	0
296281	1	6	0	0	0
297324	1	0	0	0	0
298278	1	0	0	0	0
299280	1	0	0	0	0
300288	1	0	0	0	0
301292	1	0	0	0	0
302291	1	0	0	0	0
303323	1	0	0	0	0
304270	2	0	0	0	0
305298	1	0	0	0	0
306295	1	0	0	0	0
307265	1	0	0	0	0
308311	2	0	0	0	0
309299	1	0	0	0	0
310319	1	0	0	0	0
311296	1	0	0	0	0
266312	1	1	0	0	0
313297	1	0	0	0	0
314310	1	0	0	0	0
315267	1	0	0	0	0
316307	1	0	0	0	0
289317	1	1	0	0	0
318304	1	0	0	0	0
319328	2	0	0	0	0
320321	1	0	0	0	0
321290	1	0	0	0	0
322301	1	0	0	0	0
323348	1	0	0	0	0
324301	2	0	0	0	0
325319	1	0	0	0	0
326340	1	0	0	0	0
327314	1	0	0	0	0
328270	1	0	0	0	0
329330	1	0	0	0	0
330316	2	0	0	0	0
331286	2	0	0	0	0

332315	1	0	0	0	0
333282	1	0	0	0	0
334272	2	0	0	0	0
335279	2	0	0	0	0
336281	2	0	0	0	0
337283	2	0	0	0	0
338314	2	0	0	0	0
339290	2	0	0	0	0
340333	2	0	0	0	0
341295	2	0	0	0	0
342306	1	0	0	0	0
343311	1	0	0	0	0
344316	1	0	0	0	0
345320	1	0	0	0	0
346312	2	0	0	0	0
347317	2	0	0	0	0
348344	2	0	0	0	0
349313	1	0	0	0	0
350332	2	0	0	0	0
351343	2	0	0	0	0
352338	1	0	0	0	0
284353	1	6	0	0	0
354317	1	0	0	0	0
287355	1	1	0	0	0
285356	1	6	0	0	0
291357	1	6	0	0	0
358304	1	0	0	0	0
321359	1	6	0	0	0
302360	1	1	0	0	0
361342	1	0	0	0	0
362329	1	0	0	0	0
307363	1	6	0	0	0
364312	1	0	0	0	0
365318	1	0	0	0	0
366379	1	0	0	0	0
367331	1	0	0	0	0
305368	1	6	0	0	0
369338	1	0	0	0	0
370340	1	0	0	0	0
371349	1	0	0	0	0
372349	2	0	0	0	0
373372	1	0	0	0	0
374371	2	0	0	0	0
375378	1	0	0	0	0
376368	1	0	0	0	0
377332	1	0	0	0	0
378354	1	0	0	0	0
379375	1	0	0	0	0
380359	1	0	0	0	0
381366	1	0	0	0	0
382366	1	0	0	0	0
383385	1	0	0	0	0
384377	1	0	0	0	0
385386	1	0	0	0	0
386388	1	0	0	0	0
387384	1	0	0	0	0
388389	1	0	0	0	0
389390	1	0	0	0	0
390387	1	0	0	0	0
267391	1	1	0	0	0
329323	2	0	0	0	0
286308	1	0	0	0	0
351331	1	0	0	0	0
299326	2	0	0	0	0
322294	2	0	0	0	0
288297	2	0	0	0	0
305302	1	0	0	0	0
325318	2	0	0	0	0
374361	1	0	0	0	0
361373	2	0	0	0	0
266285	1	0	0	0	0
327320	2	0	0	0	0
345352	2	0	0	0	0
385392	1	0	0	0	0
394401	1	0	0	0	0
395397	1	0	0	0	0
393396	1	6	0	0	0
397428	1	1	0	0	0
398402	1	0	0	0	0

399400	1	0	0	0	0
400393	1	0	0	0	0
401397	1	0	0	0	0
402407	1	0	0	0	0
402403	1	1	0	0	0
420404	1	1	0	0	0
405424	1	0	0	0	0
406437	1	1	0	0	0
407404	1	0	0	0	0
408410	2	0	0	0	0
409396	1	0	0	0	0
410417	1	0	0	0	0
411405	1	0	0	0	0
412406	1	0	0	0	0
413415	1	0	0	0	0
414408	1	0	0	0	0
415395	1	0	0	0	0
416422	1	0	0	0	0
417399	1	0	0	0	0
418421	1	0	0	0	0
419412	1	0	0	0	0
420411	1	0	0	0	0
434421	1	1	0	0	0
422431	1	0	0	0	0
423403	1	0	0	0	0
424409	1	6	0	0	0
425452	1	0	0	0	0
426406	1	0	0	0	0
427408	1	0	0	0	0
428416	1	0	0	0	0
429420	1	0	0	0	0
430419	1	0	0	0	0
431451	1	0	0	0	0
432398	2	0	0	0	0
433426	1	0	0	0	0
434423	1	0	0	0	0
435393	1	0	0	0	0
436439	2	0	0	0	0
437427	1	0	0	0	0
438447	1	0	0	0	0
439424	1	0	0	0	0
394440	1	1	0	0	0
441425	1	0	0	0	0
442438	1	0	0	0	0
443395	1	0	0	0	0
444435	1	0	0	0	0
417445	1	1	0	0	0
446432	1	0	0	0	0
447456	2	0	0	0	0
448449	1	0	0	0	0
449418	1	0	0	0	0
450429	1	0	0	0	0
451476	1	0	0	0	0
452429	2	0	0	0	0
453447	1	0	0	0	0
454468	1	0	0	0	0
455442	1	0	0	0	0
456398	1	0	0	0	0
457458	1	0	0	0	0
458444	2	0	0	0	0
459414	2	0	0	0	0
460443	1	0	0	0	0
461410	1	0	0	0	0
462400	2	0	0	0	0
463407	2	0	0	0	0
464409	2	0	0	0	0
465411	2	0	0	0	0
466442	2	0	0	0	0
467418	2	0	0	0	0
468461	2	0	0	0	0
469423	2	0	0	0	0
470434	1	0	0	0	0
471439	1	0	0	0	0
472444	1	0	0	0	0
473448	1	0	0	0	0
474440	2	0	0	0	0
475445	2	0	0	0	0
476472	2	0	0	0	0
477441	1	0	0	0	0

478460	2	0	0	0	0
479471	2	0	0	0	0
480466	1	0	0	0	0
412481	1	6	0	0	0
482445	1	0	0	0	0
415483	1	1	0	0	0
413484	1	6	0	0	0
419485	1	6	0	0	0
486432	1	0	0	0	0
449487	1	6	0	0	0
430488	1	1	0	0	0
489470	1	0	0	0	0
490457	1	0	0	0	0
435491	1	6	0	0	0
492440	1	0	0	0	0
493446	1	0	0	0	0
494507	1	0	0	0	0
495459	1	0	0	0	0
433496	1	6	0	0	0
497466	1	0	0	0	0
498468	1	0	0	0	0
499477	1	0	0	0	0
500477	2	0	0	0	0
501500	1	0	0	0	0
502499	2	0	0	0	0
503506	1	0	0	0	0
504496	1	0	0	0	0
505460	1	0	0	0	0
506482	1	0	0	0	0
507503	1	0	0	0	0
508487	1	0	0	0	0
509494	1	0	0	0	0
510494	1	0	0	0	0
511513	1	0	0	0	0
512505	1	0	0	0	0
513514	1	0	0	0	0
514516	1	0	0	0	0
515512	1	0	0	0	0
516517	1	0	0	0	0
517518	1	0	0	0	0
518515	1	0	0	0	0
395519	1	1	0	0	0
457451	2	0	0	0	0
414436	1	0	0	0	0
479459	1	0	0	0	0
427454	2	0	0	0	0
450422	2	0	0	0	0
416425	2	0	0	0	0
433430	1	0	0	0	0
453446	2	0	0	0	0
502489	1	0	0	0	0
489501	2	0	0	0	0
394413	1	0	0	0	0
455448	2	0	0	0	0
473480	2	0	0	0	0
513520	1	0	0	0	0
522529	1	0	0	0	0
523525	1	0	0	0	0
521524	1	6	0	0	0
525556	1	1	0	0	0
526530	1	0	0	0	0
527528	1	0	0	0	0
528521	1	0	0	0	0
529525	1	0	0	0	0
530535	1	0	0	0	0
530531	1	1	0	0	0
548532	1	1	0	0	0
533552	1	0	0	0	0
534565	1	1	0	0	0
535532	1	0	0	0	0
536538	2	0	0	0	0
537524	1	0	0	0	0
538545	1	0	0	0	0
539533	1	0	0	0	0
540534	1	0	0	0	0
541543	1	0	0	0	0
542536	1	0	0	0	0
543523	1	0	0	0	0
544550	1	0	0	0	0

545527	1	0	0	0	0
546549	1	0	0	0	0
547540	1	0	0	0	0
548539	1	0	0	0	0
562549	1	1	0	0	0
550559	1	0	0	0	0
551531	1	0	0	0	0
552537	1	6	0	0	0
553580	1	0	0	0	0
554534	1	0	0	0	0
555536	1	0	0	0	0
556544	1	0	0	0	0
557548	1	0	0	0	0
558547	1	0	0	0	0
559579	1	0	0	0	0
560526	2	0	0	0	0
561554	1	0	0	0	0
562551	1	0	0	0	0
563521	1	0	0	0	0
564567	2	0	0	0	0
565555	1	0	0	0	0
566575	1	0	0	0	0
567552	1	0	0	0	0
522568	1	1	0	0	0
569553	1	0	0	0	0
570566	1	0	0	0	0
571523	1	0	0	0	0
572563	1	0	0	0	0
545573	1	1	0	0	0
574560	1	0	0	0	0
575584	2	0	0	0	0
576577	1	0	0	0	0
577546	1	0	0	0	0
578557	1	0	0	0	0
579604	1	0	0	0	0
580557	2	0	0	0	0
581575	1	0	0	0	0
582596	1	0	0	0	0
583570	1	0	0	0	0
584526	1	0	0	0	0
585586	1	0	0	0	0
586572	2	0	0	0	0
587542	2	0	0	0	0
588571	1	0	0	0	0
589538	1	0	0	0	0
590528	2	0	0	0	0
591535	2	0	0	0	0
592537	2	0	0	0	0
593539	2	0	0	0	0
594570	2	0	0	0	0
595546	2	0	0	0	0
596589	2	0	0	0	0
597551	2	0	0	0	0
598562	1	0	0	0	0
599567	1	0	0	0	0
600572	1	0	0	0	0
601576	1	0	0	0	0
602568	2	0	0	0	0
603573	2	0	0	0	0
604600	2	0	0	0	0
605569	1	0	0	0	0
606588	2	0	0	0	0
607599	2	0	0	0	0
608594	1	0	0	0	0
540609	1	6	0	0	0
610573	1	0	0	0	0
543611	1	1	0	0	0
541612	1	6	0	0	0
547613	1	6	0	0	0
614560	1	0	0	0	0
577615	1	6	0	0	0
558616	1	1	0	0	0
617598	1	0	0	0	0
618585	1	0	0	0	0
563619	1	6	0	0	0
620568	1	0	0	0	0
621574	1	0	0	0	0
622635	1	0	0	0	0
623587	1	0	0	0	0

M	SAL	1	8	336	337	338	339	340	341	342	343
M	SAL	1	8	344	345	346	347	348	349	350	351
M	SAL	1	8	352	353	354	355	356	357	358	359
M	SAL	1	8	360	361	362	363	364	365	366	367
M	SAL	1	8	368	369	370	371	372	373	374	375
M	SAL	1	8	376	377	378	379	380	381	382	383
M	SAL	1	8	384	385	386	387	388	389	390	391
M	SAL	1	8	392	393	394	395	396	397	398	399
M	SAL	1	8	400	401	402	403	404	405	406	407
M	SAL	1	8	408	409	410	411	412	413	414	415
M	SAL	1	8	416	417	418	419	420	421	422	423
M	SAL	1	8	424	425	426	427	428	429	430	431
M	SAL	1	8	432	433	434	435	436	437	438	439
M	SAL	1	8	440	441	442	443	444	445	446	447
M	SAL	1	8	448	449	450	451	452	453	454	455
M	SAL	1	8	456	457	458	459	460	461	462	463
M	SAL	1	8	464	465	466	467	468	469	470	471
M	SAL	1	8	472	473	474	475	476	477	478	479
M	SAL	1	8	480	481	482	483	484	485	486	487
M	SAL	1	8	488	489	490	491	492	493	494	495
M	SAL	1	8	496	497	498	499	500	501	502	503
M	SAL	1	8	504	505	506	507	508	509	510	511
M	SAL	1	8	512	513	514	515	516	517	518	519
M	SAL	1	8	520	521	522	523	524	525	526	527
M	SAL	1	8	528	529	530	531	532	533	534	535
M	SAL	1	8	536	537	538	539	540	541	542	543
M	SAL	1	8	544	545	546	547	548	549	550	551
M	SAL	1	8	552	553	554	555	556	557	558	559
M	SAL	1	8	560	561	562	563	564	565	566	567
M	SAL	1	8	568	569	570	571	572	573	574	575
M	SAL	1	8	576	577	578	579	580	581	582	583
M	SAL	1	8	584	585	586	587	588	589	590	591
M	SAL	1	8	592	593	594	595	596	597	598	599
M	SAL	1	8	600	601	602	603	604	605	606	607
M	SAL	1	8	608	609	610	611	612	613	614	615
M	SAL	1	8	616	617	618	619	620	621	622	623
M	SAL	1	8	624	625	626	627	628	629	630	631
M	SAL	1	8	632	633	634	635	636	637	638	639
M	SAL	1	8	640	641	642	643	644	645	646	647
M	SAL	1	1	648							
M	SPA	1	8	1	2	3	4	5	6	7	8
M	SPA	1	8	9	10	11	12	13	14	15	16
M	SPA	1	8	17	18	19	20	21	22	23	24
M	SPA	1	8	25	26	27	28	29	30	31	32
M	SPA	1	8	33	34	35	36	37	38	39	40
M	SPA	1	8	41	42	43	44	45	46	47	48
M	SPA	1	8	49	50	51	52	53	54	55	56
M	SPA	1	8	57	58	59	60	61	62	63	64
M	SPA	1	8	65	66	67	68	69	70	71	72
M	SPA	1	8	73	74	75	76	77	78	79	80
M	SPA	1	8	81	82	83	84	85	86	87	88
M	SPA	1	8	89	90	91	92	93	94	95	96
M	SPA	1	8	97	98	99	100	101	102	103	104
M	SPA	1	8	105	106	107	108	109	110	111	112
M	SPA	1	8	113	114	115	116	117	118	119	120
M	SPA	1	8	121	122	123	124	125	126	127	129
M	SMT	1	5								
M	SDI	1	4	1.1462		-15.4767		1.1462		-1.0383	
M	SDI	1	4	20.5130		-1.0383		20.5130		-15.4767	
M	SAL	2	8	128	130	131	132	133	134	135	136
M	SPA	2	1	128							
M	SMT	2	8								
M	SDI	2	4	21.8186		-8.7142		21.8186		-7.1758	
M	SDI	2	4	23.8093		-7.1758		23.8093		-8.7142	
M	END										

Chemical Structures, InChI

InChI=1S/5C87H98Cl2N10O28.8ClH/c5*1-37(2)12-9-7-6-8-10-13-60(105)93-69-72(108)74(110)77(85(119)120)127-86(69)126-76-57-30-42-31-58(76)123-54-23-18-41(28-49(54)88)70(106)68-84(118)97-66(79(113)91-24-11-25-99(4)5)47-32-43(101)33-56(124-87-75(111)73(109)71(107)59(36-100)125-87)61(47)46-27-39(16-21-51(46)10)2)64(81(115)98-68)94-82(116)65(42)95-83(117)67-48-34-45(35-53(104)62(48)89)122-55-29-40(17-22-52(55)103)63(90-3)80(114)92-50(78(112)96-67)26-38-14-19-44(121-57)20-15-38;;;;;;/h5*14-23,27-35,37,50,59,63-75,77,86-87,90,100-104,106-111H,6-13,24-26,36H2,1-5H3,(H,91,113)(H,92,114)(H,93,105)(H,94,116)(H,95,117)(H,96,112)(H,97,118)(H,98,115)(H,119,120);8*1H/t5*50-,59-,63-,64-,65-,66+,67+,68+,69-,70-,71-,72-,73+,74+,75+,77+,86-,87+;;;;;;/m11111...../s1

Chemical Structure, InChI Key

WPNCURJEDGILLS-BBMAAFOLSA-N

Chemical Structure, MOLFILE

50	46	1	0	0	0	0
51	3	1	0	0	0	0
52	43	1	0	0	0	0
25	53	1	1	0	0	0
54	40	1	0	0	0	0
55	64	2	0	0	0	0
56	57	1	0	0	0	0
57	26	1	0	0	0	0
58	37	1	0	0	0	0
59	84	1	0	0	0	0
60	37	2	0	0	0	0
61	55	1	0	0	0	0
62	76	1	0	0	0	0
63	50	1	0	0	0	0
64	6	1	0	0	0	0
65	66	1	0	0	0	0
66	52	2	0	0	0	0
67	22	2	0	0	0	0
68	51	1	0	0	0	0
69	18	1	0	0	0	0
70	8	2	0	0	0	0
71	15	2	0	0	0	0
72	17	2	0	0	0	0
73	19	2	0	0	0	0
74	50	2	0	0	0	0
75	26	2	0	0	0	0
76	69	2	0	0	0	0
77	31	2	0	0	0	0
78	42	1	0	0	0	0
79	47	1	0	0	0	0
80	52	1	0	0	0	0
81	56	1	0	0	0	0
82	48	2	0	0	0	0
83	53	2	0	0	0	0
84	80	2	0	0	0	0
85	49	1	0	0	0	0
86	68	2	0	0	0	0
87	79	2	0	0	0	0
88	74	1	0	0	0	0
20	89	1	6	0	0	0
90	53	1	0	0	0	0
23	91	1	1	0	0	0
21	92	1	6	0	0	0
27	93	1	6	0	0	0
94	40	1	0	0	0	0
57	95	1	6	0	0	0
38	96	1	1	0	0	0
97	78	1	0	0	0	0
98	65	1	0	0	0	0
43	99	1	6	0	0	0
100	48	1	0	0	0	0
101	54	1	0	0	0	0
102	115	1	0	0	0	0
103	67	1	0	0	0	0
41	104	1	6	0	0	0
105	74	1	0	0	0	0
106	76	1	0	0	0	0
107	85	1	0	0	0	0
108	85	2	0	0	0	0
109	108	1	0	0	0	0
110	107	2	0	0	0	0
111	114	1	0	0	0	0
112	104	1	0	0	0	0
113	68	1	0	0	0	0
114	90	1	0	0	0	0
115	111	1	0	0	0	0
116	95	1	0	0	0	0
117	102	1	0	0	0	0
118	102	1	0	0	0	0
119	121	1	0	0	0	0
120	113	1	0	0	0	0
121	122	1	0	0	0	0
122	124	1	0	0	0	0
123	120	1	0	0	0	0
124	125	1	0	0	0	0
125	126	1	0	0	0	0
126	123	1	0	0	0	0
127	119	1	0	0	0	0
31	28	1	1	0	0	0

65 59	2	0	0	0	0
22 44	1	0	0	0	0
87 67	1	0	0	0	0
35 62	2	0	0	0	0
58 30	2	0	0	0	0
24 33	2	0	0	0	0
41 38	1	0	0	0	0
61 54	2	0	0	0	0
110 97	1	0	0	0	0
97109	2	0	0	0	0
2 21	1	0	0	0	0
63 56	2	0	0	0	0
81 88	2	0	0	0	0
138145	1	0	0	0	0
139141	1	0	0	0	0
137140	1	6	0	0	0
141172	1	1	0	0	0
142146	1	0	0	0	0
143144	1	0	0	0	0
144137	1	0	0	0	0
145141	1	0	0	0	0
146151	1	0	0	0	0
146147	1	1	0	0	0
164148	1	1	0	0	0
149168	1	0	0	0	0
150181	1	1	0	0	0
151148	1	0	0	0	0
152154	2	0	0	0	0
153140	1	0	0	0	0
154161	1	0	0	0	0
155149	1	0	0	0	0
156150	1	0	0	0	0
157159	1	0	0	0	0
158152	1	0	0	0	0
159139	1	0	0	0	0
160166	1	0	0	0	0
161143	1	0	0	0	0
162165	1	0	0	0	0
163156	1	0	0	0	0
164155	1	0	0	0	0
178165	1	1	0	0	0
166175	1	0	0	0	0
167147	1	0	0	0	0
168153	1	6	0	0	0
169196	1	0	0	0	0
170150	1	0	0	0	0
171152	1	0	0	0	0
172160	1	0	0	0	0
173164	1	0	0	0	0
174163	1	0	0	0	0
175195	1	0	0	0	0
176142	2	0	0	0	0
177170	1	0	0	0	0
178167	1	0	0	0	0
179137	1	0	0	0	0
180183	2	0	0	0	0
181171	1	0	0	0	0
182191	1	0	0	0	0
183168	1	0	0	0	0
138184	1	1	0	0	0
185169	1	0	0	0	0
186182	1	0	0	0	0
187139	1	0	0	0	0
188179	1	0	0	0	0
161189	1	1	0	0	0
190176	1	0	0	0	0
191200	2	0	0	0	0
192193	1	0	0	0	0
193162	1	0	0	0	0
194173	1	0	0	0	0
195220	1	0	0	0	0
196173	2	0	0	0	0
197191	1	0	0	0	0
198212	1	0	0	0	0
199186	1	0	0	0	0
200142	1	0	0	0	0
201202	1	0	0	0	0
202188	2	0	0	0	0
203158	2	0	0	0	0

204187	1	0	0	0	0
205154	1	0	0	0	0
206144	2	0	0	0	0
207151	2	0	0	0	0
208153	2	0	0	0	0
209155	2	0	0	0	0
210186	2	0	0	0	0
211162	2	0	0	0	0
212205	2	0	0	0	0
213167	2	0	0	0	0
214178	1	0	0	0	0
215183	1	0	0	0	0
216188	1	0	0	0	0
217192	1	0	0	0	0
218184	2	0	0	0	0
219189	2	0	0	0	0
220216	2	0	0	0	0
221185	1	0	0	0	0
222204	2	0	0	0	0
223215	2	0	0	0	0
224210	1	0	0	0	0
156225	1	6	0	0	0
226189	1	0	0	0	0
159227	1	1	0	0	0
157228	1	6	0	0	0
163229	1	6	0	0	0
230176	1	0	0	0	0
193231	1	6	0	0	0
174232	1	1	0	0	0
233214	1	0	0	0	0
234201	1	0	0	0	0
179235	1	6	0	0	0
236184	1	0	0	0	0
237190	1	0	0	0	0
238251	1	0	0	0	0
239203	1	0	0	0	0
177240	1	6	0	0	0
241210	1	0	0	0	0
242212	1	0	0	0	0
243221	1	0	0	0	0
244221	2	0	0	0	0
245244	1	0	0	0	0
246243	2	0	0	0	0
247250	1	0	0	0	0
248240	1	0	0	0	0
249204	1	0	0	0	0
250226	1	0	0	0	0
251247	1	0	0	0	0
252231	1	0	0	0	0
253238	1	0	0	0	0
254238	1	0	0	0	0
255257	1	0	0	0	0
256249	1	0	0	0	0
257258	1	0	0	0	0
258260	1	0	0	0	0
259256	1	0	0	0	0
260261	1	0	0	0	0
261262	1	0	0	0	0
262259	1	0	0	0	0
263255	1	0	0	0	0
139264	1	1	0	0	0
201195	2	0	0	0	0
158180	1	0	0	0	0
223203	1	0	0	0	0
171198	2	0	0	0	0
194166	2	0	0	0	0
160169	2	0	0	0	0
177174	1	0	0	0	0
197190	2	0	0	0	0
246233	1	0	0	0	0
233245	2	0	0	0	0
138157	1	0	0	0	0
199192	2	0	0	0	0
217224	2	0	0	0	0
266273	1	0	0	0	0
267269	1	0	0	0	0
265268	1	6	0	0	0
269300	1	1	0	0	0
270274	1	0	0	0	0

271272	1	0	0	0	0
272265	1	0	0	0	0
273269	1	0	0	0	0
274279	1	0	0	0	0
274275	1	1	0	0	0
292276	1	1	0	0	0
277296	1	0	0	0	0
278309	1	1	0	0	0
279276	1	0	0	0	0
280282	2	0	0	0	0
281268	1	0	0	0	0
282289	1	0	0	0	0
283277	1	0	0	0	0
284278	1	0	0	0	0
285287	1	0	0	0	0
286280	1	0	0	0	0
287267	1	0	0	0	0
288294	1	0	0	0	0
289271	1	0	0	0	0
290293	1	0	0	0	0
291284	1	0	0	0	0
292283	1	0	0	0	0
306293	1	1	0	0	0
294303	1	0	0	0	0
295275	1	0	0	0	0
296281	1	6	0	0	0
297324	1	0	0	0	0
298278	1	0	0	0	0
299280	1	0	0	0	0
300288	1	0	0	0	0
301292	1	0	0	0	0
302291	1	0	0	0	0
303323	1	0	0	0	0
304270	2	0	0	0	0
305298	1	0	0	0	0
306295	1	0	0	0	0
307265	1	0	0	0	0
308311	2	0	0	0	0
309299	1	0	0	0	0
310319	1	0	0	0	0
311296	1	0	0	0	0
266312	1	1	0	0	0
313297	1	0	0	0	0
314310	1	0	0	0	0
315267	1	0	0	0	0
316307	1	0	0	0	0
289317	1	1	0	0	0
318304	1	0	0	0	0
319328	2	0	0	0	0
320321	1	0	0	0	0
321290	1	0	0	0	0
322301	1	0	0	0	0
323348	1	0	0	0	0
324301	2	0	0	0	0
325319	1	0	0	0	0
326340	1	0	0	0	0
327314	1	0	0	0	0
328270	1	0	0	0	0
329330	1	0	0	0	0
330316	2	0	0	0	0
331286	2	0	0	0	0
332315	1	0	0	0	0
333282	1	0	0	0	0
334272	2	0	0	0	0
335279	2	0	0	0	0
336281	2	0	0	0	0
337283	2	0	0	0	0
338314	2	0	0	0	0
339290	2	0	0	0	0
340333	2	0	0	0	0
341295	2	0	0	0	0
342306	1	0	0	0	0
343311	1	0	0	0	0
344316	1	0	0	0	0
345320	1	0	0	0	0
346312	2	0	0	0	0
347317	2	0	0	0	0
348344	2	0	0	0	0
349313	1	0	0	0	0

350332	2	0	0	0	0
351343	2	0	0	0	0
352338	1	0	0	0	0
284353	1	6	0	0	0
354317	1	0	0	0	0
287355	1	1	0	0	0
285356	1	6	0	0	0
291357	1	6	0	0	0
358304	1	0	0	0	0
321359	1	6	0	0	0
302360	1	1	0	0	0
361342	1	0	0	0	0
362329	1	0	0	0	0
307363	1	6	0	0	0
364312	1	0	0	0	0
365318	1	0	0	0	0
366379	1	0	0	0	0
367331	1	0	0	0	0
305368	1	6	0	0	0
369338	1	0	0	0	0
370340	1	0	0	0	0
371349	1	0	0	0	0
372349	2	0	0	0	0
373372	1	0	0	0	0
374371	2	0	0	0	0
375378	1	0	0	0	0
376368	1	0	0	0	0
377332	1	0	0	0	0
378354	1	0	0	0	0
379375	1	0	0	0	0
380359	1	0	0	0	0
381366	1	0	0	0	0
382366	1	0	0	0	0
383385	1	0	0	0	0
384377	1	0	0	0	0
385386	1	0	0	0	0
386388	1	0	0	0	0
387384	1	0	0	0	0
388389	1	0	0	0	0
389390	1	0	0	0	0
390387	1	0	0	0	0
391383	1	0	0	0	0
267392	1	1	0	0	0
329323	2	0	0	0	0
286308	1	0	0	0	0
351331	1	0	0	0	0
299326	2	0	0	0	0
322294	2	0	0	0	0
288297	2	0	0	0	0
305302	1	0	0	0	0
325318	2	0	0	0	0
374361	1	0	0	0	0
361373	2	0	0	0	0
266285	1	0	0	0	0
327320	2	0	0	0	0
345352	2	0	0	0	0
394401	1	0	0	0	0
395397	1	0	0	0	0
393396	1	6	0	0	0
397428	1	1	0	0	0
398402	1	0	0	0	0
399400	1	0	0	0	0
400393	1	0	0	0	0
401397	1	0	0	0	0
402407	1	0	0	0	0
402403	1	1	0	0	0
420404	1	1	0	0	0
405424	1	0	0	0	0
406437	1	1	0	0	0
407404	1	0	0	0	0
408410	2	0	0	0	0
409396	1	0	0	0	0
410417	1	0	0	0	0
411405	1	0	0	0	0
412406	1	0	0	0	0
413415	1	0	0	0	0
414408	1	0	0	0	0
415395	1	0	0	0	0
416422	1	0	0	0	0

417399	1	0	0	0	0
418421	1	0	0	0	0
419412	1	0	0	0	0
420411	1	0	0	0	0
434421	1	1	0	0	0
422431	1	0	0	0	0
423403	1	0	0	0	0
424409	1	6	0	0	0
425452	1	0	0	0	0
426406	1	0	0	0	0
427408	1	0	0	0	0
428416	1	0	0	0	0
429420	1	0	0	0	0
430419	1	0	0	0	0
431451	1	0	0	0	0
432398	2	0	0	0	0
433426	1	0	0	0	0
434423	1	0	0	0	0
435393	1	0	0	0	0
436439	2	0	0	0	0
437427	1	0	0	0	0
438447	1	0	0	0	0
439424	1	0	0	0	0
394440	1	1	0	0	0
441425	1	0	0	0	0
442438	1	0	0	0	0
443395	1	0	0	0	0
444435	1	0	0	0	0
417445	1	1	0	0	0
446432	1	0	0	0	0
447456	2	0	0	0	0
448449	1	0	0	0	0
449418	1	0	0	0	0
450429	1	0	0	0	0
451476	1	0	0	0	0
452429	2	0	0	0	0
453447	1	0	0	0	0
454468	1	0	0	0	0
455442	1	0	0	0	0
456398	1	0	0	0	0
457458	1	0	0	0	0
458444	2	0	0	0	0
459414	2	0	0	0	0
460443	1	0	0	0	0
461410	1	0	0	0	0
462400	2	0	0	0	0
463407	2	0	0	0	0
464409	2	0	0	0	0
465411	2	0	0	0	0
466442	2	0	0	0	0
467418	2	0	0	0	0
468461	2	0	0	0	0
469423	2	0	0	0	0
470434	1	0	0	0	0
471439	1	0	0	0	0
472444	1	0	0	0	0
473448	1	0	0	0	0
474440	2	0	0	0	0
475445	2	0	0	0	0
476472	2	0	0	0	0
477441	1	0	0	0	0
478460	2	0	0	0	0
479471	2	0	0	0	0
480466	1	0	0	0	0
412481	1	6	0	0	0
482445	1	0	0	0	0
415483	1	1	0	0	0
413484	1	6	0	0	0
419485	1	6	0	0	0
486432	1	0	0	0	0
449487	1	6	0	0	0
430488	1	1	0	0	0
489470	1	0	0	0	0
490457	1	0	0	0	0
435491	1	6	0	0	0
492440	1	0	0	0	0
493446	1	0	0	0	0
494507	1	0	0	0	0
495459	1	0	0	0	0

433496	1	6	0	0	0
497466	1	0	0	0	0
498468	1	0	0	0	0
499477	1	0	0	0	0
500477	2	0	0	0	0
501500	1	0	0	0	0
502499	2	0	0	0	0
503506	1	0	0	0	0
504496	1	0	0	0	0
505460	1	0	0	0	0
506482	1	0	0	0	0
507503	1	0	0	0	0
508487	1	0	0	0	0
509494	1	0	0	0	0
510494	1	0	0	0	0
511513	1	0	0	0	0
512505	1	0	0	0	0
513514	1	0	0	0	0
514516	1	0	0	0	0
515512	1	0	0	0	0
516517	1	0	0	0	0
517518	1	0	0	0	0
518515	1	0	0	0	0
519511	1	0	0	0	0
395520	1	1	0	0	0
457451	2	0	0	0	0
414436	1	0	0	0	0
479459	1	0	0	0	0
427454	2	0	0	0	0
450422	2	0	0	0	0
416425	2	0	0	0	0
433430	1	0	0	0	0
453446	2	0	0	0	0
502489	1	0	0	0	0
489501	2	0	0	0	0
394413	1	0	0	0	0
455448	2	0	0	0	0
473480	2	0	0	0	0
522529	1	0	0	0	0
523525	1	0	0	0	0
521524	1	6	0	0	0
525556	1	1	0	0	0
526530	1	0	0	0	0
527528	1	0	0	0	0
528521	1	0	0	0	0
529525	1	0	0	0	0
530535	1	0	0	0	0
530531	1	1	0	0	0
548532	1	1	0	0	0
533552	1	0	0	0	0
534565	1	1	0	0	0
535532	1	0	0	0	0
536538	2	0	0	0	0
537524	1	0	0	0	0
538545	1	0	0	0	0
539533	1	0	0	0	0
540534	1	0	0	0	0
541543	1	0	0	0	0
542536	1	0	0	0	0
543523	1	0	0	0	0
544550	1	0	0	0	0
545527	1	0	0	0	0
546549	1	0	0	0	0
547540	1	0	0	0	0
548539	1	0	0	0	0
562549	1	1	0	0	0
550559	1	0	0	0	0
551531	1	0	0	0	0
552537	1	6	0	0	0
553580	1	0	0	0	0
554534	1	0	0	0	0
555536	1	0	0	0	0
556544	1	0	0	0	0
557548	1	0	0	0	0
558547	1	0	0	0	0
559579	1	0	0	0	0
560526	2	0	0	0	0
561554	1	0	0	0	0
562551	1	0	0	0	0

563521	1	0	0	0	0
564567	2	0	0	0	0
565555	1	0	0	0	0
566575	1	0	0	0	0
567552	1	0	0	0	0
522568	1	1	0	0	0
569553	1	0	0	0	0
570566	1	0	0	0	0
571523	1	0	0	0	0
572563	1	0	0	0	0
545573	1	1	0	0	0
574560	1	0	0	0	0
575584	2	0	0	0	0
576577	1	0	0	0	0
577546	1	0	0	0	0
578557	1	0	0	0	0
579604	1	0	0	0	0
580557	2	0	0	0	0
581575	1	0	0	0	0
582596	1	0	0	0	0
583570	1	0	0	0	0
584526	1	0	0	0	0
585586	1	0	0	0	0
586572	2	0	0	0	0
587542	2	0	0	0	0
588571	1	0	0	0	0
589538	1	0	0	0	0
590528	2	0	0	0	0
591535	2	0	0	0	0
592537	2	0	0	0	0
593539	2	0	0	0	0
594570	2	0	0	0	0
595546	2	0	0	0	0
596589	2	0	0	0	0
597551	2	0	0	0	0
598562	1	0	0	0	0
599567	1	0	0	0	0
600572	1	0	0	0	0
601576	1	0	0	0	0
602568	2	0	0	0	0
603573	2	0	0	0	0
604600	2	0	0	0	0
605569	1	0	0	0	0
606588	2	0	0	0	0
607599	2	0	0	0	0
608594	1	0	0	0	0
540609	1	6	0	0	0
610573	1	0	0	0	0
543611	1	1	0	0	0
541612	1	6	0	0	0
547613	1	6	0	0	0
614560	1	0	0	0	0
577615	1	6	0	0	0
558616	1	1	0	0	0
617598	1	0	0	0	0
618585	1	0	0	0	0
563619	1	6	0	0	0
620568	1	0	0	0	0
621574	1	0	0	0	0
622635	1	0	0	0	0
623587	1	0	0	0	0
561624	1	6	0	0	0
625594	1	0	0	0	0
626596	1	0	0	0	0
627605	1	0	0	0	0
628605	2	0	0	0	0
629628	1	0	0	0	0
630627	2	0	0	0	0
631634	1	0	0	0	0
632624	1	0	0	0	0
633588	1	0	0	0	0
634610	1	0	0	0	0
635631	1	0	0	0	0
636615	1	0	0	0	0
637622	1	0	0	0	0
638622	1	0	0	0	0
639641	1	0	0	0	0
640633	1	0	0	0	0
641642	1	0	0	0	0

642644	1	0	0	0	0					
643640	1	0	0	0	0					
644645	1	0	0	0	0					
645646	1	0	0	0	0					
646643	1	0	0	0	0					
647639	1	0	0	0	0					
523648	1	1	0	0	0					
585579	2	0	0	0	0					
542564	1	0	0	0	0					
607587	1	0	0	0	0					
555582	2	0	0	0	0					
578550	2	0	0	0	0					
544553	2	0	0	0	0					
561558	1	0	0	0	0					
581574	2	0	0	0	0					
630617	1	0	0	0	0					
617629	2	0	0	0	0					
522541	1	0	0	0	0					
583576	2	0	0	0	0					
601608	2	0	0	0	0					
M STY	2	1	MUL	2	MUL					
M SLB	2	1	1	2	2					
M SAL	1	8	16	17	18	19	20	21	22	23
M SAL	1	8	24	25	26	27	28	29	30	31
M SAL	1	8	32	33	34	35	36	37	38	39
M SAL	1	8	40	41	42	43	44	45	46	47
M SAL	1	8	48	49	50	51	52	53	54	55
M SAL	1	8	56	57	58	59	60	61	62	63
M SAL	1	8	64	65	66	67	68	69	70	71
M SAL	1	8	72	73	74	75	76	77	78	79
M SAL	1	8	80	81	82	83	84	85	86	87
M SAL	1	8	88	89	90	91	92	93	94	95
M SAL	1	8	96	97	98	99	100	101	102	103
M SAL	1	8	104	105	106	107	108	109	110	111
M SAL	1	8	112	113	114	115	116	117	118	119
M SAL	1	8	120	121	122	123	124	125	126	127
M SAL	1	8	128	137	138	139	140	141	142	143
M SAL	1	8	144	145	146	147	148	149	150	151
M SAL	1	8	152	153	154	155	156	157	158	159
M SAL	1	8	160	161	162	163	164	165	166	167
M SAL	1	8	168	169	170	171	172	173	174	175
M SAL	1	8	176	177	178	179	180	181	182	183
M SAL	1	8	184	185	186	187	188	189	190	191
M SAL	1	8	192	193	194	195	196	197	198	199
M SAL	1	8	200	201	202	203	204	205	206	207
M SAL	1	8	208	209	210	211	212	213	214	215
M SAL	1	8	216	217	218	219	220	221	222	223
M SAL	1	8	224	225	226	227	228	229	230	231
M SAL	1	8	232	233	234	235	236	237	238	239
M SAL	1	8	240	241	242	243	244	245	246	247
M SAL	1	8	248	249	250	251	252	253	254	255
M SAL	1	8	256	257	258	259	260	261	262	263
M SAL	1	8	264	265	266	267	268	269	270	271
M SAL	1	8	272	273	274	275	276	277	278	279
M SAL	1	8	280	281	282	283	284	285	286	287
M SAL	1	8	288	289	290	291	292	293	294	295
M SAL	1	8	296	297	298	299	300	301	302	303
M SAL	1	8	304	305	306	307	308	309	310	311
M SAL	1	8	312	313	314	315	316	317	318	319
M SAL	1	8	320	321	322	323	324	325	326	327
M SAL	1	8	328	329	330	331	332	333	334	335
M SAL	1	8	336	337	338	339	340	341	342	343
M SAL	1	8	344	345	346	347	348	349	350	351
M SAL	1	8	352	353	354	355	356	357	358	359
M SAL	1	8	360	361	362	363	364	365	366	367
M SAL	1	8	368	369	370	371	372	373	374	375
M SAL	1	8	376	377	378	379	380	381	382	383
M SAL	1	8	384	385	386	387	388	389	390	391
M SAL	1	8	392	393	394	395	396	397	398	399
M SAL	1	8	400	401	402	403	404	405	406	407
M SAL	1	8	408	409	410	411	412	413	414	415
M SAL	1	8	416	417	418	419	420	421	422	423
M SAL	1	8	424	425	426	427	428	429	430	431
M SAL	1	8	432	433	434	435	436	437	438	439
M SAL	1	8	440	441	442	443	444	445	446	447
M SAL	1	8	448	449	450	451	452	453	454	455
M SAL	1	8	456	457	458	459	460	461	462	463
M SAL	1	8	464	465	466	467	468	469	470	471
M SAL	1	8	472	473	474	475	476	477	478	479

M	SAL	1	8	480	481	482	483	484	485	486	487
M	SAL	1	8	488	489	490	491	492	493	494	495
M	SAL	1	8	496	497	498	499	500	501	502	503
M	SAL	1	8	504	505	506	507	508	509	510	511
M	SAL	1	8	512	513	514	515	516	517	518	519
M	SAL	1	8	520	521	522	523	524	525	526	527
M	SAL	1	8	528	529	530	531	532	533	534	535
M	SAL	1	8	536	537	538	539	540	541	542	543
M	SAL	1	8	544	545	546	547	548	549	550	551
M	SAL	1	8	552	553	554	555	556	557	558	559
M	SAL	1	8	560	561	562	563	564	565	566	567
M	SAL	1	8	568	569	570	571	572	573	574	575
M	SAL	1	8	576	577	578	579	580	581	582	583
M	SAL	1	8	584	585	586	587	588	589	590	591
M	SAL	1	8	592	593	594	595	596	597	598	599
M	SAL	1	8	600	601	602	603	604	605	606	607
M	SAL	1	8	608	609	610	611	612	613	614	615
M	SAL	1	8	616	617	618	619	620	621	622	623
M	SAL	1	8	624	625	626	627	628	629	630	631
M	SAL	1	8	632	633	634	635	636	637	638	639
M	SAL	1	8	640	641	642	643	644	645	646	647
M	SAL	1	1	648							
M	SPA	1	8	1	2	3	4	5	6	7	8
M	SPA	1	8	9	10	11	12	13	14	15	16
M	SPA	1	8	17	18	19	20	21	22	23	24
M	SPA	1	8	25	26	27	28	29	30	31	32
M	SPA	1	8	33	34	35	36	37	38	39	40
M	SPA	1	8	41	42	43	44	45	46	47	48
M	SPA	1	8	49	50	51	52	53	54	55	56
M	SPA	1	8	57	58	59	60	61	62	63	64
M	SPA	1	8	65	66	67	68	69	70	71	72
M	SPA	1	8	73	74	75	76	77	78	79	80
M	SPA	1	8	81	82	83	84	85	86	87	88
M	SPA	1	8	89	90	91	92	93	94	95	96
M	SPA	1	8	97	98	99	100	101	102	103	104
M	SPA	1	8	105	106	107	108	109	110	111	112
M	SPA	1	8	113	114	115	116	117	118	119	120
M	SPA	1	8	121	122	123	124	125	126	127	128
M	SMT	1	5								
M	SDI	1	4	1.1462	-15.4767			1.1462	-1.0383		
M	SDI	1	4	20.5130	-1.0383			20.5130	-15.4767		
M	SAL	2	8	129	130	131	132	133	134	135	136
M	SPA	2	1	129							
M	SMT	2	8								
M	SDI	2	4	21.8186	-8.7142			21.8186	-7.1758		
M	SDI	2	4	23.8093	-7.1758			23.8093	-8.7142		
M	END										

Chemical Structures, InChI

InChI=1S/5C87H98Cl2N10O28.8ClH/c5*1-5-6-7-8-9-10-11-12-14-60(105)93-69-72(108)74(110)77(85(119)120)127-86(69)126-76-57-31-42-32-58(76)123-54-24-19-41(29-49(54)88)70(106)68-84(118)97-66(79(113)91-25-13-26-99(3)4)47-33-43(101)34-56(124-87-75(111)73(109)71(107)59(37-100)125-87)61(47)46-28-39(17-22-51(46)102)64(81(115)98-68)94-82(116)65(42)95-83(117)67-48-35-45(36-53(104)62(48)89)122-55-30-40(18-23-52(55)103)63(90-2)80(114)92-50(78(112)96-67)27-38-15-20-44(121-57)21-16-38;;;;;;;;;h5*15-24,28-36,50,59,63-75,77,86-87,90,100-104,106-111H,5-14,25-27,37H2,1-4HB,(H,91,113)(H,92,114)(H,93,105)(H,94,116)(H,95,117)(H,96,112)(H,97,118)(H,98,115)(H,119,120);8*1H/t5*50-,59-,63-,64-,65-,66+,67+,68+,69-,70-,71-,72-,73+,74+,75+,77+,86-,87+;;;;;;;;;m11111...../s1

Chemical Structure, InChI Key

MQVCEBIOFIUZDQ-BBMAAFOLSA-N

Moiety (mixture component)

Name	Quantity
	Undefined not 0

Moiety Characteristics

	-FDASRS-06211411022D
653705	0 0 1 0 0 0 0 0999 V2000
	8.1982 -7.9416 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0
	13.4606 -3.2625 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0

Chemical Structure, MOLFILE

62	76	1	0	0	0	0
63	50	1	0	0	0	0
64	6	1	0	0	0	0
65	66	1	0	0	0	0
66	52	2	0	0	0	0
67	22	2	0	0	0	0
68	51	1	0	0	0	0
69	18	1	0	0	0	0
70	8	2	0	0	0	0
71	15	2	0	0	0	0
72	17	2	0	0	0	0
73	19	2	0	0	0	0
74	50	2	0	0	0	0
75	26	2	0	0	0	0
76	69	2	0	0	0	0
77	31	2	0	0	0	0
78	42	1	0	0	0	0
79	47	1	0	0	0	0
80	52	1	0	0	0	0
81	56	1	0	0	0	0
82	48	2	0	0	0	0
83	53	2	0	0	0	0
84	80	2	0	0	0	0
85	49	1	0	0	0	0
86	68	2	0	0	0	0
87	79	2	0	0	0	0
88	74	1	0	0	0	0
20	89	1	6	0	0	0
90	53	1	0	0	0	0
23	91	1	1	0	0	0
21	92	1	6	0	0	0
27	93	1	6	0	0	0
94	40	1	0	0	0	0
57	95	1	6	0	0	0
38	96	1	1	0	0	0
97	78	1	0	0	0	0
98	65	1	0	0	0	0
43	99	1	6	0	0	0
100	48	1	0	0	0	0
101	54	1	0	0	0	0
102	115	1	0	0	0	0
103	67	1	0	0	0	0
41	104	1	6	0	0	0
105	74	1	0	0	0	0
106	76	1	0	0	0	0
107	85	1	0	0	0	0
108	85	2	0	0	0	0
109	108	1	0	0	0	0
110	107	2	0	0	0	0
111	114	1	0	0	0	0
112	104	1	0	0	0	0
113	68	1	0	0	0	0
114	90	1	0	0	0	0
115	111	1	0	0	0	0
116	95	1	0	0	0	0
117	102	1	0	0	0	0
118	102	1	0	0	0	0
119	121	1	0	0	0	0
120	113	1	0	0	0	0
121	122	1	0	0	0	0
122	124	1	0	0	0	0
123	120	1	0	0	0	0
124	125	1	0	0	0	0
125	126	1	0	0	0	0
126	123	1	0	0	0	0
127	119	1	0	0	0	0
3	128	1	1	0	0	0
65	59	2	0	0	0	0
22	44	1	0	0	0	0
87	67	1	0	0	0	0
35	62	2	0	0	0	0
58	30	2	0	0	0	0
24	33	2	0	0	0	0
41	38	1	0	0	0	0
61	54	2	0	0	0	0
110	97	1	0	0	0	0
97	109	2	0	0	0	0
2	21	1	0	0	0	0
63	56	2	0	0	0	0

81 88	2	0	0	0	0
127129	1	0	0	0	0
139146	1	0	0	0	0
140142	1	0	0	0	0
138141	1	6	0	0	0
142173	1	1	0	0	0
143147	1	0	0	0	0
144145	1	0	0	0	0
145138	1	0	0	0	0
146142	1	0	0	0	0
147152	1	0	0	0	0
147148	1	1	0	0	0
165149	1	1	0	0	0
150169	1	0	0	0	0
151182	1	1	0	0	0
152149	1	0	0	0	0
153155	2	0	0	0	0
154141	1	0	0	0	0
155162	1	0	0	0	0
156150	1	0	0	0	0
157151	1	0	0	0	0
158160	1	0	0	0	0
159153	1	0	0	0	0
160140	1	0	0	0	0
161167	1	0	0	0	0
162144	1	0	0	0	0
163166	1	0	0	0	0
164157	1	0	0	0	0
165156	1	0	0	0	0
179166	1	1	0	0	0
167176	1	0	0	0	0
168148	1	0	0	0	0
169154	1	6	0	0	0
170197	1	0	0	0	0
171151	1	0	0	0	0
172153	1	0	0	0	0
173161	1	0	0	0	0
174165	1	0	0	0	0
175164	1	0	0	0	0
176196	1	0	0	0	0
177143	2	0	0	0	0
178171	1	0	0	0	0
179168	1	0	0	0	0
180138	1	0	0	0	0
181184	2	0	0	0	0
182172	1	0	0	0	0
183192	1	0	0	0	0
184169	1	0	0	0	0
139185	1	1	0	0	0
186170	1	0	0	0	0
187183	1	0	0	0	0
188140	1	0	0	0	0
189180	1	0	0	0	0
162190	1	1	0	0	0
191177	1	0	0	0	0
192201	2	0	0	0	0
193194	1	0	0	0	0
194163	1	0	0	0	0
195174	1	0	0	0	0
196221	1	0	0	0	0
197174	2	0	0	0	0
198192	1	0	0	0	0
199213	1	0	0	0	0
200187	1	0	0	0	0
201143	1	0	0	0	0
202203	1	0	0	0	0
203189	2	0	0	0	0
204159	2	0	0	0	0
205188	1	0	0	0	0
206155	1	0	0	0	0
207145	2	0	0	0	0
208152	2	0	0	0	0
209154	2	0	0	0	0
210156	2	0	0	0	0
211187	2	0	0	0	0
212163	2	0	0	0	0
213206	2	0	0	0	0
214168	2	0	0	0	0
215179	1	0	0	0	0

216184	1	0	0	0	0
217189	1	0	0	0	0
218193	1	0	0	0	0
219185	2	0	0	0	0
220190	2	0	0	0	0
221217	2	0	0	0	0
222186	1	0	0	0	0
223205	2	0	0	0	0
224216	2	0	0	0	0
225211	1	0	0	0	0
157226	1	6	0	0	0
227190	1	0	0	0	0
160228	1	1	0	0	0
158229	1	6	0	0	0
164230	1	6	0	0	0
231177	1	0	0	0	0
194232	1	6	0	0	0
175233	1	1	0	0	0
234215	1	0	0	0	0
235202	1	0	0	0	0
180236	1	6	0	0	0
237185	1	0	0	0	0
238191	1	0	0	0	0
239252	1	0	0	0	0
240204	1	0	0	0	0
178241	1	6	0	0	0
242211	1	0	0	0	0
243213	1	0	0	0	0
244222	1	0	0	0	0
245222	2	0	0	0	0
246245	1	0	0	0	0
247244	2	0	0	0	0
248251	1	0	0	0	0
249241	1	0	0	0	0
250205	1	0	0	0	0
251227	1	0	0	0	0
252248	1	0	0	0	0
253232	1	0	0	0	0
254239	1	0	0	0	0
255239	1	0	0	0	0
256258	1	0	0	0	0
257250	1	0	0	0	0
258259	1	0	0	0	0
259261	1	0	0	0	0
260257	1	0	0	0	0
261262	1	0	0	0	0
262263	1	0	0	0	0
263260	1	0	0	0	0
264256	1	0	0	0	0
140265	1	1	0	0	0
202196	2	0	0	0	0
159181	1	0	0	0	0
224204	1	0	0	0	0
172199	2	0	0	0	0
195167	2	0	0	0	0
161170	2	0	0	0	0
178175	1	0	0	0	0
198191	2	0	0	0	0
247234	1	0	0	0	0
234246	2	0	0	0	0
139158	1	0	0	0	0
200193	2	0	0	0	0
218225	2	0	0	0	0
264266	1	0	0	0	0
268275	1	0	0	0	0
269271	1	0	0	0	0
267270	1	6	0	0	0
271302	1	1	0	0	0
272276	1	0	0	0	0
273274	1	0	0	0	0
274267	1	0	0	0	0
275271	1	0	0	0	0
276281	1	0	0	0	0
276277	1	1	0	0	0
294278	1	1	0	0	0
279298	1	0	0	0	0
280311	1	1	0	0	0
281278	1	0	0	0	0
282284	2	0	0	0	0

283270	1	0	0	0	0
284291	1	0	0	0	0
285279	1	0	0	0	0
286280	1	0	0	0	0
287289	1	0	0	0	0
288282	1	0	0	0	0
289269	1	0	0	0	0
290296	1	0	0	0	0
291273	1	0	0	0	0
292295	1	0	0	0	0
293286	1	0	0	0	0
294285	1	0	0	0	0
308295	1	1	0	0	0
296305	1	0	0	0	0
297277	1	0	0	0	0
298283	1	6	0	0	0
299326	1	0	0	0	0
300280	1	0	0	0	0
301282	1	0	0	0	0
302290	1	0	0	0	0
303294	1	0	0	0	0
304293	1	0	0	0	0
305325	1	0	0	0	0
306272	2	0	0	0	0
307300	1	0	0	0	0
308297	1	0	0	0	0
309267	1	0	0	0	0
310313	2	0	0	0	0
311301	1	0	0	0	0
312321	1	0	0	0	0
313298	1	0	0	0	0
268314	1	1	0	0	0
315299	1	0	0	0	0
316312	1	0	0	0	0
317269	1	0	0	0	0
318309	1	0	0	0	0
291319	1	1	0	0	0
320306	1	0	0	0	0
321330	2	0	0	0	0
322323	1	0	0	0	0
323292	1	0	0	0	0
324303	1	0	0	0	0
325350	1	0	0	0	0
326303	2	0	0	0	0
327321	1	0	0	0	0
328342	1	0	0	0	0
329316	1	0	0	0	0
330272	1	0	0	0	0
331332	1	0	0	0	0
332318	2	0	0	0	0
333288	2	0	0	0	0
334317	1	0	0	0	0
335284	1	0	0	0	0
336274	2	0	0	0	0
337281	2	0	0	0	0
338283	2	0	0	0	0
339285	2	0	0	0	0
340316	2	0	0	0	0
341292	2	0	0	0	0
342335	2	0	0	0	0
343297	2	0	0	0	0
344308	1	0	0	0	0
345313	1	0	0	0	0
346318	1	0	0	0	0
347322	1	0	0	0	0
348314	2	0	0	0	0
349319	2	0	0	0	0
350346	2	0	0	0	0
351315	1	0	0	0	0
352334	2	0	0	0	0
353345	2	0	0	0	0
354340	1	0	0	0	0
286355	1	6	0	0	0
356319	1	0	0	0	0
289357	1	1	0	0	0
287358	1	6	0	0	0
293359	1	6	0	0	0
360306	1	0	0	0	0
323361	1	6	0	0	0

304362	1	1	0	0	0
363344	1	0	0	0	0
364331	1	0	0	0	0
309365	1	6	0	0	0
366314	1	0	0	0	0
367320	1	0	0	0	0
368381	1	0	0	0	0
369333	1	0	0	0	0
307370	1	6	0	0	0
371340	1	0	0	0	0
372342	1	0	0	0	0
373351	1	0	0	0	0
374351	2	0	0	0	0
375374	1	0	0	0	0
376373	2	0	0	0	0
377380	1	0	0	0	0
378370	1	0	0	0	0
379334	1	0	0	0	0
380356	1	0	0	0	0
381377	1	0	0	0	0
382361	1	0	0	0	0
383368	1	0	0	0	0
384368	1	0	0	0	0
385387	1	0	0	0	0
386379	1	0	0	0	0
387388	1	0	0	0	0
388390	1	0	0	0	0
389386	1	0	0	0	0
390391	1	0	0	0	0
391392	1	0	0	0	0
392389	1	0	0	0	0
393385	1	0	0	0	0
269394	1	1	0	0	0
331325	2	0	0	0	0
288310	1	0	0	0	0
353333	1	0	0	0	0
301328	2	0	0	0	0
324296	2	0	0	0	0
290299	2	0	0	0	0
307304	1	0	0	0	0
327320	2	0	0	0	0
376363	1	0	0	0	0
363375	2	0	0	0	0
268287	1	0	0	0	0
329322	2	0	0	0	0
347354	2	0	0	0	0
393395	1	0	0	0	0
397404	1	0	0	0	0
398400	1	0	0	0	0
396399	1	6	0	0	0
400431	1	1	0	0	0
401405	1	0	0	0	0
402403	1	0	0	0	0
403396	1	0	0	0	0
404400	1	0	0	0	0
405410	1	0	0	0	0
405406	1	1	0	0	0
423407	1	1	0	0	0
408427	1	0	0	0	0
409440	1	1	0	0	0
410407	1	0	0	0	0
411413	2	0	0	0	0
412399	1	0	0	0	0
413420	1	0	0	0	0
414408	1	0	0	0	0
415409	1	0	0	0	0
416418	1	0	0	0	0
417411	1	0	0	0	0
418398	1	0	0	0	0
419425	1	0	0	0	0
420402	1	0	0	0	0
421424	1	0	0	0	0
422415	1	0	0	0	0
423414	1	0	0	0	0
437424	1	1	0	0	0
425434	1	0	0	0	0
426406	1	0	0	0	0
427412	1	6	0	0	0
428455	1	0	0	0	0

429409	1	0	0	0	0
430411	1	0	0	0	0
431419	1	0	0	0	0
432423	1	0	0	0	0
433422	1	0	0	0	0
434454	1	0	0	0	0
435401	2	0	0	0	0
436429	1	0	0	0	0
437426	1	0	0	0	0
438396	1	0	0	0	0
439442	2	0	0	0	0
440430	1	0	0	0	0
441450	1	0	0	0	0
442427	1	0	0	0	0
397443	1	1	0	0	0
444428	1	0	0	0	0
445441	1	0	0	0	0
446398	1	0	0	0	0
447438	1	0	0	0	0
420448	1	1	0	0	0
449435	1	0	0	0	0
450459	2	0	0	0	0
451452	1	0	0	0	0
452421	1	0	0	0	0
453432	1	0	0	0	0
454479	1	0	0	0	0
455432	2	0	0	0	0
456450	1	0	0	0	0
457471	1	0	0	0	0
458445	1	0	0	0	0
459401	1	0	0	0	0
460461	1	0	0	0	0
461447	2	0	0	0	0
462417	2	0	0	0	0
463446	1	0	0	0	0
464413	1	0	0	0	0
465403	2	0	0	0	0
466410	2	0	0	0	0
467412	2	0	0	0	0
468414	2	0	0	0	0
469445	2	0	0	0	0
470421	2	0	0	0	0
471464	2	0	0	0	0
472426	2	0	0	0	0
473437	1	0	0	0	0
474442	1	0	0	0	0
475447	1	0	0	0	0
476451	1	0	0	0	0
477443	2	0	0	0	0
478448	2	0	0	0	0
479475	2	0	0	0	0
480444	1	0	0	0	0
481463	2	0	0	0	0
482474	2	0	0	0	0
483469	1	0	0	0	0
415484	1	6	0	0	0
485448	1	0	0	0	0
418486	1	1	0	0	0
416487	1	6	0	0	0
422488	1	6	0	0	0
489435	1	0	0	0	0
452490	1	6	0	0	0
433491	1	1	0	0	0
492473	1	0	0	0	0
493460	1	0	0	0	0
438494	1	6	0	0	0
495443	1	0	0	0	0
496449	1	0	0	0	0
497510	1	0	0	0	0
498462	1	0	0	0	0
436499	1	6	0	0	0
500469	1	0	0	0	0
501471	1	0	0	0	0
502480	1	0	0	0	0
503480	2	0	0	0	0
504503	1	0	0	0	0
505502	2	0	0	0	0
506509	1	0	0	0	0
507499	1	0	0	0	0

508463	1	0	0	0	0
509485	1	0	0	0	0
510506	1	0	0	0	0
511490	1	0	0	0	0
512497	1	0	0	0	0
513497	1	0	0	0	0
514516	1	0	0	0	0
515508	1	0	0	0	0
516517	1	0	0	0	0
517519	1	0	0	0	0
518515	1	0	0	0	0
519520	1	0	0	0	0
520521	1	0	0	0	0
521518	1	0	0	0	0
522514	1	0	0	0	0
398523	1	1	0	0	0
460454	2	0	0	0	0
417439	1	0	0	0	0
482462	1	0	0	0	0
430457	2	0	0	0	0
453425	2	0	0	0	0
419428	2	0	0	0	0
436433	1	0	0	0	0
456449	2	0	0	0	0
505492	1	0	0	0	0
492504	2	0	0	0	0
397416	1	0	0	0	0
458451	2	0	0	0	0
476483	2	0	0	0	0
522524	1	0	0	0	0
526533	1	0	0	0	0
527529	1	0	0	0	0
525528	1	6	0	0	0
529560	1	1	0	0	0
530534	1	0	0	0	0
531532	1	0	0	0	0
532525	1	0	0	0	0
533529	1	0	0	0	0
534539	1	0	0	0	0
534535	1	1	0	0	0
552536	1	1	0	0	0
537556	1	0	0	0	0
538569	1	1	0	0	0
539536	1	0	0	0	0
540542	2	0	0	0	0
541528	1	0	0	0	0
542549	1	0	0	0	0
543537	1	0	0	0	0
544538	1	0	0	0	0
545547	1	0	0	0	0
546540	1	0	0	0	0
547527	1	0	0	0	0
548554	1	0	0	0	0
549531	1	0	0	0	0
550553	1	0	0	0	0
551544	1	0	0	0	0
552543	1	0	0	0	0
566553	1	1	0	0	0
554563	1	0	0	0	0
555535	1	0	0	0	0
556541	1	6	0	0	0
557584	1	0	0	0	0
558538	1	0	0	0	0
559540	1	0	0	0	0
560548	1	0	0	0	0
561552	1	0	0	0	0
562551	1	0	0	0	0
563583	1	0	0	0	0
564530	2	0	0	0	0
565558	1	0	0	0	0
566555	1	0	0	0	0
567525	1	0	0	0	0
568571	2	0	0	0	0
569559	1	0	0	0	0
570579	1	0	0	0	0
571556	1	0	0	0	0
526572	1	1	0	0	0
573557	1	0	0	0	0
574570	1	0	0	0	0

575527	1	0	0	0	0
576567	1	0	0	0	0
549577	1	1	0	0	0
578564	1	0	0	0	0
579588	2	0	0	0	0
580581	1	0	0	0	0
581550	1	0	0	0	0
582561	1	0	0	0	0
583608	1	0	0	0	0
584561	2	0	0	0	0
585579	1	0	0	0	0
586600	1	0	0	0	0
587574	1	0	0	0	0
588530	1	0	0	0	0
589590	1	0	0	0	0
590576	2	0	0	0	0
591546	2	0	0	0	0
592575	1	0	0	0	0
593542	1	0	0	0	0
594532	2	0	0	0	0
595539	2	0	0	0	0
596541	2	0	0	0	0
597543	2	0	0	0	0
598574	2	0	0	0	0
599550	2	0	0	0	0
600593	2	0	0	0	0
601555	2	0	0	0	0
602566	1	0	0	0	0
603571	1	0	0	0	0
604576	1	0	0	0	0
605580	1	0	0	0	0
606572	2	0	0	0	0
607577	2	0	0	0	0
608604	2	0	0	0	0
609573	1	0	0	0	0
610592	2	0	0	0	0
611603	2	0	0	0	0
612598	1	0	0	0	0
544613	1	6	0	0	0
614577	1	0	0	0	0
547615	1	1	0	0	0
545616	1	6	0	0	0
551617	1	6	0	0	0
618564	1	0	0	0	0
581619	1	6	0	0	0
562620	1	1	0	0	0
621602	1	0	0	0	0
622589	1	0	0	0	0
567623	1	6	0	0	0
624572	1	0	0	0	0
625578	1	0	0	0	0
626639	1	0	0	0	0
627591	1	0	0	0	0
565628	1	6	0	0	0
629598	1	0	0	0	0
630600	1	0	0	0	0
631609	1	0	0	0	0
632609	2	0	0	0	0
633632	1	0	0	0	0
634631	2	0	0	0	0
635638	1	0	0	0	0
636628	1	0	0	0	0
637592	1	0	0	0	0
638614	1	0	0	0	0
639635	1	0	0	0	0
640619	1	0	0	0	0
641626	1	0	0	0	0
642626	1	0	0	0	0
643645	1	0	0	0	0
644637	1	0	0	0	0
645646	1	0	0	0	0
646648	1	0	0	0	0
647644	1	0	0	0	0
648649	1	0	0	0	0
649650	1	0	0	0	0
650647	1	0	0	0	0
651643	1	0	0	0	0
527652	1	1	0	0	0
589583	2	0	0	0	0


```

M SAL 1 8 536 537 538 539 540 541 542 543
M SAL 1 8 544 545 546 547 548 549 550 551
M SAL 1 8 552 553 554 555 556 557 558 559
M SAL 1 8 560 561 562 563 564 565 566 567
M SAL 1 8 568 569 570 571 572 573 574 575
M SAL 1 8 576 577 578 579 580 581 582 583
M SAL 1 8 584 585 586 587 588 589 590 591
M SAL 1 8 592 593 594 595 596 597 598 599
M SAL 1 8 600 601 602 603 604 605 606 607
M SAL 1 8 608 609 610 611 612 613 614 615
M SAL 1 8 616 617 618 619 620 621 622 623
M SAL 1 8 624 625 626 627 628 629 630 631
M SAL 1 8 632 633 634 635 636 637 638 639
M SAL 1 8 640 641 642 643 644 645 646 647
M SAL 1 6 648 649 650 651 652 653
M SPA 1 8 1 2 3 4 5 6 7 8
M SPA 1 8 9 10 11 12 13 14 15 16
M SPA 1 8 17 18 19 20 21 22 23 24
M SPA 1 8 25 26 27 28 29 30 31 32
M SPA 1 8 33 34 35 36 37 38 39 40
M SPA 1 8 41 42 43 44 45 46 47 48
M SPA 1 8 49 50 51 52 53 54 55 56
M SPA 1 8 57 58 59 60 61 62 63 64
M SPA 1 8 65 66 67 68 69 70 71 72
M SPA 1 8 73 74 75 76 77 78 79 80
M SPA 1 8 81 82 83 84 85 86 87 88
M SPA 1 8 89 90 91 92 93 94 95 96
M SPA 1 8 97 98 99 100 101 102 103 104
M SPA 1 8 105 106 107 108 109 110 111 112
M SPA 1 8 113 114 115 116 117 118 119 120
M SPA 1 8 121 122 123 124 125 126 127 128
M SPA 1 1 129
M SMT 1 5
M SDI 1 4 0.9103 -15.6567 0.9103 -1.2183
M SDI 1 4 20.2772 -1.2183 20.2772 -15.6567
M SAL 2 8 130 131 132 133 134 135 136 137
M SPA 2 1 130
M SMT 2 8
M SDI 2 4 22.0203 -7.9567 22.0203 -6.4183
M SDI 2 4 24.0110 -6.4183 24.0110 -7.9567
M END

```

Chemical Structures, InChI

InChI=1S/5C88H100Cl2N10O28.8ClH/c5*1-5-6-7-8-9-10-11-12-13-15-61(106)94-70-73(109)75(111)78(86(120)121)128-87(70)127-77-58-32-43-33-59(77)124-55-25-20-42(30-50(55)89)71(107)69-85(119)98-67(80(114)92-26-14-27-100(3)4)48-34-44(102)35-57(125-88-76(112)74(110)72(108)60(38-101)126-88)62(48)47-29-40(18-23-52(47)103)65(82(116)99-69)95-83(117)66(43)96-84(118)68-49-36-46(37-54(105)63(49)90)123-56-31-41(19-24-53(56)104)64(91-2)81(115)93-51(79(113)97-68)28-39-16-21-45(122-58)22-17-39;;;;;;;;;;/h5*16-25,29-37,51,60,64-76,78,87-88,91,101-105,107-112H,5-15,26-28,38H2,1-4H3,(H,92,114)(H,93,115)(H,94,106)(H,95,117)(H,96,118)(H,97,113)(H,98,119)(H,99,116)(H,120,121);8*1H/t5*51-,60-,64-,65-,66-,67+,68+,69+,70-,71-,72-,73-,74+,75+,76+,78+,87-,88+;;;;;;;;;;/m11111...../s1

Chemical Structure, InChI Key

RCJAZPZRAROQAD-XERKAGHASA-N

Moiety (mixture component)

Name	Quantity
	Undefined not 0

Moiety Characteristics

```

-FDASRS-06211411022D
653705 0 0 1 0 0 0 0 0999 V2000
8.3545 -7.6916 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0
13.6169 -3.0125 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0
12.1545 -2.9999 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0
8.9794 -8.0541 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.5128 -3.6332 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0
14.0294 -9.0749 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.2253 -9.0958 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.7877 -8.4999 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```


Chemical Structure, MOLFILE

68 51 1 0 0 0 0
69 18 1 0 0 0 0
70 8 2 0 0 0 0
71 15 2 0 0 0 0
72 17 2 0 0 0 0
73 19 2 0 0 0 0
74 50 2 0 0 0 0
75 26 2 0 0 0 0
76 69 2 0 0 0 0
77 31 2 0 0 0 0
78 42 1 0 0 0 0
79 47 1 0 0 0 0
80 52 1 0 0 0 0
81 56 1 0 0 0 0
82 48 2 0 0 0 0
83 53 2 0 0 0 0
84 80 2 0 0 0 0
85 49 1 0 0 0 0
86 68 2 0 0 0 0
87 79 2 0 0 0 0
88 74 1 0 0 0 0
20 89 1 6 0 0 0
90 53 1 0 0 0 0
23 91 1 1 0 0 0
21 92 1 6 0 0 0
27 93 1 6 0 0 0
94 40 1 0 0 0 0
57 95 1 6 0 0 0
38 96 1 1 0 0 0
97 78 1 0 0 0 0
98 65 1 0 0 0 0
43 99 1 6 0 0 0
100 48 1 0 0 0 0
101 54 1 0 0 0 0
102115 1 0 0 0 0
103 67 1 0 0 0 0
41104 1 6 0 0 0
105 74 1 0 0 0 0
106 76 1 0 0 0 0
107 85 1 0 0 0 0
108 85 2 0 0 0 0
109108 1 0 0 0 0
110107 2 0 0 0 0
111114 1 0 0 0 0
112104 1 0 0 0 0
113 68 1 0 0 0 0
114 90 1 0 0 0 0
115111 1 0 0 0 0
116 95 1 0 0 0 0
117102 1 0 0 0 0
118102 1 0 0 0 0
119121 1 0 0 0 0
120113 1 0 0 0 0
121122 1 0 0 0 0
122124 1 0 0 0 0
123120 1 0 0 0 0
124125 1 0 0 0 0
125126 1 0 0 0 0
126123 1 0 0 0 0
127119 1 0 0 0 0
128119 1 0 0 0 0
3129 1 1 0 0 0
65 59 2 0 0 0 0
22 44 1 0 0 0 0
87 67 1 0 0 0 0
35 62 2 0 0 0 0
58 30 2 0 0 0 0
24 33 2 0 0 0 0
41 38 1 0 0 0 0
61 54 2 0 0 0 0
110 97 1 0 0 0 0
97109 2 0 0 0 0
2 21 1 0 0 0 0
63 56 2 0 0 0 0
81 88 2 0 0 0 0
139146 1 0 0 0 0
140142 1 0 0 0 0
138141 1 6 0 0 0
142173 1 1 0 0 0

143147	1	0	0	0	0
144145	1	0	0	0	0
145138	1	0	0	0	0
146142	1	0	0	0	0
147152	1	0	0	0	0
147148	1	1	0	0	0
165149	1	1	0	0	0
150169	1	0	0	0	0
151182	1	1	0	0	0
152149	1	0	0	0	0
153155	2	0	0	0	0
154141	1	0	0	0	0
155162	1	0	0	0	0
156150	1	0	0	0	0
157151	1	0	0	0	0
158160	1	0	0	0	0
159153	1	0	0	0	0
160140	1	0	0	0	0
161167	1	0	0	0	0
162144	1	0	0	0	0
163166	1	0	0	0	0
164157	1	0	0	0	0
165156	1	0	0	0	0
179166	1	1	0	0	0
167176	1	0	0	0	0
168148	1	0	0	0	0
169154	1	6	0	0	0
170197	1	0	0	0	0
171151	1	0	0	0	0
172153	1	0	0	0	0
173161	1	0	0	0	0
174165	1	0	0	0	0
175164	1	0	0	0	0
176196	1	0	0	0	0
177143	2	0	0	0	0
178171	1	0	0	0	0
179168	1	0	0	0	0
180138	1	0	0	0	0
181184	2	0	0	0	0
182172	1	0	0	0	0
183192	1	0	0	0	0
184169	1	0	0	0	0
139185	1	1	0	0	0
186170	1	0	0	0	0
187183	1	0	0	0	0
188140	1	0	0	0	0
189180	1	0	0	0	0
162190	1	1	0	0	0
191177	1	0	0	0	0
192201	2	0	0	0	0
193194	1	0	0	0	0
194163	1	0	0	0	0
195174	1	0	0	0	0
196221	1	0	0	0	0
197174	2	0	0	0	0
198192	1	0	0	0	0
199213	1	0	0	0	0
200187	1	0	0	0	0
201143	1	0	0	0	0
202203	1	0	0	0	0
203189	2	0	0	0	0
204159	2	0	0	0	0
205188	1	0	0	0	0
206155	1	0	0	0	0
207145	2	0	0	0	0
208152	2	0	0	0	0
209154	2	0	0	0	0
210156	2	0	0	0	0
211187	2	0	0	0	0
212163	2	0	0	0	0
213206	2	0	0	0	0
214168	2	0	0	0	0
215179	1	0	0	0	0
216184	1	0	0	0	0
217189	1	0	0	0	0
218193	1	0	0	0	0
219185	2	0	0	0	0
220190	2	0	0	0	0
221217	2	0	0	0	0

222186	1	0	0	0	0
223205	2	0	0	0	0
224216	2	0	0	0	0
225211	1	0	0	0	0
157226	1	6	0	0	0
227190	1	0	0	0	0
160228	1	1	0	0	0
158229	1	6	0	0	0
164230	1	6	0	0	0
231177	1	0	0	0	0
194232	1	6	0	0	0
175233	1	1	0	0	0
234215	1	0	0	0	0
235202	1	0	0	0	0
180236	1	6	0	0	0
237185	1	0	0	0	0
238191	1	0	0	0	0
239252	1	0	0	0	0
240204	1	0	0	0	0
178241	1	6	0	0	0
242211	1	0	0	0	0
243213	1	0	0	0	0
244222	1	0	0	0	0
245222	2	0	0	0	0
246245	1	0	0	0	0
247244	2	0	0	0	0
248251	1	0	0	0	0
249241	1	0	0	0	0
250205	1	0	0	0	0
251227	1	0	0	0	0
252248	1	0	0	0	0
253232	1	0	0	0	0
254239	1	0	0	0	0
255239	1	0	0	0	0
256258	1	0	0	0	0
257250	1	0	0	0	0
258259	1	0	0	0	0
259261	1	0	0	0	0
260257	1	0	0	0	0
261262	1	0	0	0	0
262263	1	0	0	0	0
263260	1	0	0	0	0
264256	1	0	0	0	0
265256	1	0	0	0	0
140266	1	1	0	0	0
202196	2	0	0	0	0
159181	1	0	0	0	0
224204	1	0	0	0	0
172199	2	0	0	0	0
195167	2	0	0	0	0
161170	2	0	0	0	0
178175	1	0	0	0	0
198191	2	0	0	0	0
247234	1	0	0	0	0
234246	2	0	0	0	0
139158	1	0	0	0	0
200193	2	0	0	0	0
218225	2	0	0	0	0
268275	1	0	0	0	0
269271	1	0	0	0	0
267270	1	6	0	0	0
271302	1	1	0	0	0
272276	1	0	0	0	0
273274	1	0	0	0	0
274267	1	0	0	0	0
275271	1	0	0	0	0
276281	1	0	0	0	0
276277	1	1	0	0	0
294278	1	1	0	0	0
279298	1	0	0	0	0
280311	1	1	0	0	0
281278	1	0	0	0	0
282284	2	0	0	0	0
283270	1	0	0	0	0
284291	1	0	0	0	0
285279	1	0	0	0	0
286280	1	0	0	0	0
287289	1	0	0	0	0
288282	1	0	0	0	0

289269	1	0	0	0	0
290296	1	0	0	0	0
291273	1	0	0	0	0
292295	1	0	0	0	0
293286	1	0	0	0	0
294285	1	0	0	0	0
308295	1	1	0	0	0
296305	1	0	0	0	0
297277	1	0	0	0	0
298283	1	6	0	0	0
299326	1	0	0	0	0
300280	1	0	0	0	0
301282	1	0	0	0	0
302290	1	0	0	0	0
303294	1	0	0	0	0
304293	1	0	0	0	0
305325	1	0	0	0	0
306272	2	0	0	0	0
307300	1	0	0	0	0
308297	1	0	0	0	0
309267	1	0	0	0	0
310313	2	0	0	0	0
311301	1	0	0	0	0
312321	1	0	0	0	0
313298	1	0	0	0	0
268314	1	1	0	0	0
315299	1	0	0	0	0
316312	1	0	0	0	0
317269	1	0	0	0	0
318309	1	0	0	0	0
291319	1	1	0	0	0
320306	1	0	0	0	0
321330	2	0	0	0	0
322323	1	0	0	0	0
323292	1	0	0	0	0
324303	1	0	0	0	0
325350	1	0	0	0	0
326303	2	0	0	0	0
327321	1	0	0	0	0
328342	1	0	0	0	0
329316	1	0	0	0	0
330272	1	0	0	0	0
331332	1	0	0	0	0
332318	2	0	0	0	0
333288	2	0	0	0	0
334317	1	0	0	0	0
335284	1	0	0	0	0
336274	2	0	0	0	0
337281	2	0	0	0	0
338283	2	0	0	0	0
339285	2	0	0	0	0
340316	2	0	0	0	0
341292	2	0	0	0	0
342335	2	0	0	0	0
343297	2	0	0	0	0
344308	1	0	0	0	0
345313	1	0	0	0	0
346318	1	0	0	0	0
347322	1	0	0	0	0
348314	2	0	0	0	0
349319	2	0	0	0	0
350346	2	0	0	0	0
351315	1	0	0	0	0
352334	2	0	0	0	0
353345	2	0	0	0	0
354340	1	0	0	0	0
286355	1	6	0	0	0
356319	1	0	0	0	0
289357	1	1	0	0	0
287358	1	6	0	0	0
293359	1	6	0	0	0
360306	1	0	0	0	0
323361	1	6	0	0	0
304362	1	1	0	0	0
363344	1	0	0	0	0
364331	1	0	0	0	0
309365	1	6	0	0	0
366314	1	0	0	0	0
367320	1	0	0	0	0

368381	1	0	0	0	0
369333	1	0	0	0	0
307370	1	6	0	0	0
371340	1	0	0	0	0
372342	1	0	0	0	0
373351	1	0	0	0	0
374351	2	0	0	0	0
375374	1	0	0	0	0
376373	2	0	0	0	0
377380	1	0	0	0	0
378370	1	0	0	0	0
379334	1	0	0	0	0
380356	1	0	0	0	0
381377	1	0	0	0	0
382361	1	0	0	0	0
383368	1	0	0	0	0
384368	1	0	0	0	0
385387	1	0	0	0	0
386379	1	0	0	0	0
387388	1	0	0	0	0
388390	1	0	0	0	0
389386	1	0	0	0	0
390391	1	0	0	0	0
391392	1	0	0	0	0
392389	1	0	0	0	0
393385	1	0	0	0	0
394385	1	0	0	0	0
269395	1	1	0	0	0
331325	2	0	0	0	0
288310	1	0	0	0	0
353333	1	0	0	0	0
301328	2	0	0	0	0
324296	2	0	0	0	0
290299	2	0	0	0	0
307304	1	0	0	0	0
327320	2	0	0	0	0
376363	1	0	0	0	0
363375	2	0	0	0	0
268287	1	0	0	0	0
329322	2	0	0	0	0
347354	2	0	0	0	0
397404	1	0	0	0	0
398400	1	0	0	0	0
396399	1	6	0	0	0
400431	1	1	0	0	0
401405	1	0	0	0	0
402403	1	0	0	0	0
403396	1	0	0	0	0
404400	1	0	0	0	0
405410	1	0	0	0	0
405406	1	1	0	0	0
423407	1	1	0	0	0
408427	1	0	0	0	0
409440	1	1	0	0	0
410407	1	0	0	0	0
411413	2	0	0	0	0
412399	1	0	0	0	0
413420	1	0	0	0	0
414408	1	0	0	0	0
415409	1	0	0	0	0
416418	1	0	0	0	0
417411	1	0	0	0	0
418398	1	0	0	0	0
419425	1	0	0	0	0
420402	1	0	0	0	0
421424	1	0	0	0	0
422415	1	0	0	0	0
423414	1	0	0	0	0
437424	1	1	0	0	0
425434	1	0	0	0	0
426406	1	0	0	0	0
427412	1	6	0	0	0
428455	1	0	0	0	0
429409	1	0	0	0	0
430411	1	0	0	0	0
431419	1	0	0	0	0
432423	1	0	0	0	0
433422	1	0	0	0	0
434454	1	0	0	0	0

435401	2	0	0	0	0
436429	1	0	0	0	0
437426	1	0	0	0	0
438396	1	0	0	0	0
439442	2	0	0	0	0
440430	1	0	0	0	0
441450	1	0	0	0	0
442427	1	0	0	0	0
397443	1	1	0	0	0
444428	1	0	0	0	0
445441	1	0	0	0	0
446398	1	0	0	0	0
447438	1	0	0	0	0
420448	1	1	0	0	0
449435	1	0	0	0	0
450459	2	0	0	0	0
451452	1	0	0	0	0
452421	1	0	0	0	0
453432	1	0	0	0	0
454479	1	0	0	0	0
455432	2	0	0	0	0
456450	1	0	0	0	0
457471	1	0	0	0	0
458445	1	0	0	0	0
459401	1	0	0	0	0
460461	1	0	0	0	0
461447	2	0	0	0	0
462417	2	0	0	0	0
463446	1	0	0	0	0
464413	1	0	0	0	0
465403	2	0	0	0	0
466410	2	0	0	0	0
467412	2	0	0	0	0
468414	2	0	0	0	0
469445	2	0	0	0	0
470421	2	0	0	0	0
471464	2	0	0	0	0
472426	2	0	0	0	0
473437	1	0	0	0	0
474442	1	0	0	0	0
475447	1	0	0	0	0
476451	1	0	0	0	0
477443	2	0	0	0	0
478448	2	0	0	0	0
479475	2	0	0	0	0
480444	1	0	0	0	0
481463	2	0	0	0	0
482474	2	0	0	0	0
483469	1	0	0	0	0
415484	1	6	0	0	0
485448	1	0	0	0	0
418486	1	1	0	0	0
416487	1	6	0	0	0
422488	1	6	0	0	0
489435	1	0	0	0	0
452490	1	6	0	0	0
433491	1	1	0	0	0
492473	1	0	0	0	0
493460	1	0	0	0	0
438494	1	6	0	0	0
495443	1	0	0	0	0
496449	1	0	0	0	0
497510	1	0	0	0	0
498462	1	0	0	0	0
436499	1	6	0	0	0
500469	1	0	0	0	0
501471	1	0	0	0	0
502480	1	0	0	0	0
503480	2	0	0	0	0
504503	1	0	0	0	0
505502	2	0	0	0	0
506509	1	0	0	0	0
507499	1	0	0	0	0
508463	1	0	0	0	0
509485	1	0	0	0	0
510506	1	0	0	0	0
511490	1	0	0	0	0
512497	1	0	0	0	0
513497	1	0	0	0	0

514516	1	0	0	0	0
515508	1	0	0	0	0
516517	1	0	0	0	0
517519	1	0	0	0	0
518515	1	0	0	0	0
519520	1	0	0	0	0
520521	1	0	0	0	0
521518	1	0	0	0	0
522514	1	0	0	0	0
523514	1	0	0	0	0
398524	1	1	0	0	0
460454	2	0	0	0	0
417439	1	0	0	0	0
482462	1	0	0	0	0
430457	2	0	0	0	0
453425	2	0	0	0	0
419428	2	0	0	0	0
436433	1	0	0	0	0
456449	2	0	0	0	0
505492	1	0	0	0	0
492504	2	0	0	0	0
397416	1	0	0	0	0
458451	2	0	0	0	0
476483	2	0	0	0	0
526533	1	0	0	0	0
527529	1	0	0	0	0
525528	1	6	0	0	0
529560	1	1	0	0	0
530534	1	0	0	0	0
531532	1	0	0	0	0
532525	1	0	0	0	0
533529	1	0	0	0	0
534539	1	0	0	0	0
534535	1	1	0	0	0
552536	1	1	0	0	0
537556	1	0	0	0	0
538569	1	1	0	0	0
539536	1	0	0	0	0
540542	2	0	0	0	0
541528	1	0	0	0	0
542549	1	0	0	0	0
543537	1	0	0	0	0
544538	1	0	0	0	0
545547	1	0	0	0	0
546540	1	0	0	0	0
547527	1	0	0	0	0
548554	1	0	0	0	0
549531	1	0	0	0	0
550553	1	0	0	0	0
551544	1	0	0	0	0
552543	1	0	0	0	0
566553	1	1	0	0	0
554563	1	0	0	0	0
555535	1	0	0	0	0
556541	1	6	0	0	0
557584	1	0	0	0	0
558538	1	0	0	0	0
559540	1	0	0	0	0
560548	1	0	0	0	0
561552	1	0	0	0	0
562551	1	0	0	0	0
563583	1	0	0	0	0
564530	2	0	0	0	0
565558	1	0	0	0	0
566555	1	0	0	0	0
567525	1	0	0	0	0
568571	2	0	0	0	0
569559	1	0	0	0	0
570579	1	0	0	0	0
571556	1	0	0	0	0
526572	1	1	0	0	0
573557	1	0	0	0	0
574570	1	0	0	0	0
575527	1	0	0	0	0
576567	1	0	0	0	0
549577	1	1	0	0	0
578564	1	0	0	0	0
579588	2	0	0	0	0
580581	1	0	0	0	0

581550	1	0	0	0	0
582561	1	0	0	0	0
583608	1	0	0	0	0
584561	2	0	0	0	0
585579	1	0	0	0	0
586600	1	0	0	0	0
587574	1	0	0	0	0
588530	1	0	0	0	0
589590	1	0	0	0	0
590576	2	0	0	0	0
591546	2	0	0	0	0
592575	1	0	0	0	0
593542	1	0	0	0	0
594532	2	0	0	0	0
595539	2	0	0	0	0
596541	2	0	0	0	0
597543	2	0	0	0	0
598574	2	0	0	0	0
599550	2	0	0	0	0
600593	2	0	0	0	0
601555	2	0	0	0	0
602566	1	0	0	0	0
603571	1	0	0	0	0
604576	1	0	0	0	0
605580	1	0	0	0	0
606572	2	0	0	0	0
607577	2	0	0	0	0
608604	2	0	0	0	0
609573	1	0	0	0	0
610592	2	0	0	0	0
611603	2	0	0	0	0
612598	1	0	0	0	0
544613	1	6	0	0	0
614577	1	0	0	0	0
547615	1	1	0	0	0
545616	1	6	0	0	0
551617	1	6	0	0	0
618564	1	0	0	0	0
581619	1	6	0	0	0
562620	1	1	0	0	0
621602	1	0	0	0	0
622589	1	0	0	0	0
567623	1	6	0	0	0
624572	1	0	0	0	0
625578	1	0	0	0	0
626639	1	0	0	0	0
627591	1	0	0	0	0
565628	1	6	0	0	0
629598	1	0	0	0	0
630600	1	0	0	0	0
631609	1	0	0	0	0
632609	2	0	0	0	0
633632	1	0	0	0	0
634631	2	0	0	0	0
635638	1	0	0	0	0
636628	1	0	0	0	0
637592	1	0	0	0	0
638614	1	0	0	0	0
639635	1	0	0	0	0
640619	1	0	0	0	0
641626	1	0	0	0	0
642626	1	0	0	0	0
643645	1	0	0	0	0
644637	1	0	0	0	0
645646	1	0	0	0	0
646648	1	0	0	0	0
647644	1	0	0	0	0
648649	1	0	0	0	0
649650	1	0	0	0	0
650647	1	0	0	0	0
651643	1	0	0	0	0
652643	1	0	0	0	0
527653	1	1	0	0	0
589583	2	0	0	0	0
546568	1	0	0	0	0
611591	1	0	0	0	0
559586	2	0	0	0	0
582554	2	0	0	0	0
548557	2	0	0	0	0

565562	1	0	0	0	0					
585578	2	0	0	0	0					
634621	1	0	0	0	0					
621633	2	0	0	0	0					
526545	1	0	0	0	0					
587580	2	0	0	0	0					
605612	2	0	0	0	0					
M STY	2	1	MUL	2	MUL					
M SLB	2	1	1	2	2					
M SAL	1	8	16	17	18	19	20	21	22	23
M SAL	1	8	24	25	26	27	28	29	30	31
M SAL	1	8	32	33	34	35	36	37	38	39
M SAL	1	8	40	41	42	43	44	45	46	47
M SAL	1	8	48	49	50	51	52	53	54	55
M SAL	1	8	56	57	58	59	60	61	62	63
M SAL	1	8	64	65	66	67	68	69	70	71
M SAL	1	8	72	73	74	75	76	77	78	79
M SAL	1	8	80	81	82	83	84	85	86	87
M SAL	1	8	88	89	90	91	92	93	94	95
M SAL	1	8	96	97	98	99	100	101	102	103
M SAL	1	8	104	105	106	107	108	109	110	111
M SAL	1	8	112	113	114	115	116	117	118	119
M SAL	1	8	120	121	122	123	124	125	126	127
M SAL	1	8	128	129	138	139	140	141	142	143
M SAL	1	8	144	145	146	147	148	149	150	151
M SAL	1	8	152	153	154	155	156	157	158	159
M SAL	1	8	160	161	162	163	164	165	166	167
M SAL	1	8	168	169	170	171	172	173	174	175
M SAL	1	8	176	177	178	179	180	181	182	183
M SAL	1	8	184	185	186	187	188	189	190	191
M SAL	1	8	192	193	194	195	196	197	198	199
M SAL	1	8	200	201	202	203	204	205	206	207
M SAL	1	8	208	209	210	211	212	213	214	215
M SAL	1	8	216	217	218	219	220	221	222	223
M SAL	1	8	224	225	226	227	228	229	230	231
M SAL	1	8	232	233	234	235	236	237	238	239
M SAL	1	8	240	241	242	243	244	245	246	247
M SAL	1	8	248	249	250	251	252	253	254	255
M SAL	1	8	256	257	258	259	260	261	262	263
M SAL	1	8	264	265	266	267	268	269	270	271
M SAL	1	8	272	273	274	275	276	277	278	279
M SAL	1	8	280	281	282	283	284	285	286	287
M SAL	1	8	288	289	290	291	292	293	294	295
M SAL	1	8	296	297	298	299	300	301	302	303
M SAL	1	8	304	305	306	307	308	309	310	311
M SAL	1	8	312	313	314	315	316	317	318	319
M SAL	1	8	320	321	322	323	324	325	326	327
M SAL	1	8	328	329	330	331	332	333	334	335
M SAL	1	8	336	337	338	339	340	341	342	343
M SAL	1	8	344	345	346	347	348	349	350	351
M SAL	1	8	352	353	354	355	356	357	358	359
M SAL	1	8	360	361	362	363	364	365	366	367
M SAL	1	8	368	369	370	371	372	373	374	375
M SAL	1	8	376	377	378	379	380	381	382	383
M SAL	1	8	384	385	386	387	388	389	390	391
M SAL	1	8	392	393	394	395	396	397	398	399
M SAL	1	8	400	401	402	403	404	405	406	407
M SAL	1	8	408	409	410	411	412	413	414	415
M SAL	1	8	416	417	418	419	420	421	422	423
M SAL	1	8	424	425	426	427	428	429	430	431
M SAL	1	8	432	433	434	435	436	437	438	439
M SAL	1	8	440	441	442	443	444	445	446	447
M SAL	1	8	448	449	450	451	452	453	454	455
M SAL	1	8	456	457	458	459	460	461	462	463
M SAL	1	8	464	465	466	467	468	469	470	471
M SAL	1	8	472	473	474	475	476	477	478	479
M SAL	1	8	480	481	482	483	484	485	486	487
M SAL	1	8	488	489	490	491	492	493	494	495
M SAL	1	8	496	497	498	499	500	501	502	503
M SAL	1	8	504	505	506	507	508	509	510	511
M SAL	1	8	512	513	514	515	516	517	518	519
M SAL	1	8	520	521	522	523	524	525	526	527
M SAL	1	8	528	529	530	531	532	533	534	535
M SAL	1	8	536	537	538	539	540	541	542	543
M SAL	1	8	544	545	546	547	548	549	550	551
M SAL	1	8	552	553	554	555	556	557	558	559
M SAL	1	8	560	561	562	563	564	565	566	567
M SAL	1	8	568	569	570	571	572	573	574	575
M SAL	1	8	576	577	578	579	580	581	582	583

Chemical Structure, MOLFILE

69	18	1	0	0	0	0
70	8	2	0	0	0	0
71	15	2	0	0	0	0
72	17	2	0	0	0	0
73	19	2	0	0	0	0
74	50	2	0	0	0	0
75	26	2	0	0	0	0
76	69	2	0	0	0	0
77	31	2	0	0	0	0
78	42	1	0	0	0	0
79	47	1	0	0	0	0
80	52	1	0	0	0	0
81	56	1	0	0	0	0
82	48	2	0	0	0	0
83	53	2	0	0	0	0
84	80	2	0	0	0	0
85	49	1	0	0	0	0
86	68	2	0	0	0	0
87	79	2	0	0	0	0
88	74	1	0	0	0	0
20	89	1	6	0	0	0
90	53	1	0	0	0	0
23	91	1	1	0	0	0
21	92	1	6	0	0	0
27	93	1	6	0	0	0
94	40	1	0	0	0	0
57	95	1	6	0	0	0
38	96	1	1	0	0	0
97	78	1	0	0	0	0
98	65	1	0	0	0	0
43	99	1	6	0	0	0
100	48	1	0	0	0	0
101	54	1	0	0	0	0
102	115	1	0	0	0	0
103	67	1	0	0	0	0
41	104	1	6	0	0	0
105	74	1	0	0	0	0
106	76	1	0	0	0	0
107	85	1	0	0	0	0
108	85	2	0	0	0	0
109	108	1	0	0	0	0
110	107	2	0	0	0	0
111	114	1	0	0	0	0
112	104	1	0	0	0	0
113	68	1	0	0	0	0
114	90	1	0	0	0	0
115	111	1	0	0	0	0
116	95	1	0	0	0	0
117	102	1	0	0	0	0
118	102	1	0	0	0	0
119	121	1	0	0	0	0
120	113	1	0	0	0	0
121	122	1	0	0	0	0
122	124	1	0	0	0	0
123	120	1	0	0	0	0
124	125	1	0	0	0	0
125	126	1	0	0	0	0
126	123	1	0	0	0	0
127	119	1	0	0	0	0
128	119	1	0	0	0	0
3	129	1	1	0	0	0
65	59	2	0	0	0	0
22	44	1	0	0	0	0
87	67	1	0	0	0	0
35	62	2	0	0	0	0
58	30	2	0	0	0	0
24	33	2	0	0	0	0
41	38	1	0	0	0	0
61	54	2	0	0	0	0
110	97	1	0	0	0	0
97	109	2	0	0	0	0
2	21	1	0	0	0	0
63	56	2	0	0	0	0
81	88	2	0	0	0	0
95	130	1	0	0	0	0
140	147	1	0	0	0	0
141	143	1	0	0	0	0
139	142	1	6	0	0	0
143	174	1	1	0	0	0

144148	1	0	0	0	0
145146	1	0	0	0	0
146139	1	0	0	0	0
147143	1	0	0	0	0
148153	1	0	0	0	0
148149	1	1	0	0	0
166150	1	1	0	0	0
151170	1	0	0	0	0
152183	1	1	0	0	0
153150	1	0	0	0	0
154156	2	0	0	0	0
155142	1	0	0	0	0
156163	1	0	0	0	0
157151	1	0	0	0	0
158152	1	0	0	0	0
159161	1	0	0	0	0
160154	1	0	0	0	0
161141	1	0	0	0	0
162168	1	0	0	0	0
163145	1	0	0	0	0
164167	1	0	0	0	0
165158	1	0	0	0	0
166157	1	0	0	0	0
180167	1	1	0	0	0
168177	1	0	0	0	0
169149	1	0	0	0	0
170155	1	6	0	0	0
171198	1	0	0	0	0
172152	1	0	0	0	0
173154	1	0	0	0	0
174162	1	0	0	0	0
175166	1	0	0	0	0
176165	1	0	0	0	0
177197	1	0	0	0	0
178144	2	0	0	0	0
179172	1	0	0	0	0
180169	1	0	0	0	0
181139	1	0	0	0	0
182185	2	0	0	0	0
183173	1	0	0	0	0
184193	1	0	0	0	0
185170	1	0	0	0	0
140186	1	1	0	0	0
187171	1	0	0	0	0
188184	1	0	0	0	0
189141	1	0	0	0	0
190181	1	0	0	0	0
163191	1	1	0	0	0
192178	1	0	0	0	0
193202	2	0	0	0	0
194195	1	0	0	0	0
195164	1	0	0	0	0
196175	1	0	0	0	0
197222	1	0	0	0	0
198175	2	0	0	0	0
199193	1	0	0	0	0
200214	1	0	0	0	0
201188	1	0	0	0	0
202144	1	0	0	0	0
203204	1	0	0	0	0
204190	2	0	0	0	0
205160	2	0	0	0	0
206189	1	0	0	0	0
207156	1	0	0	0	0
208146	2	0	0	0	0
209153	2	0	0	0	0
210155	2	0	0	0	0
211157	2	0	0	0	0
212188	2	0	0	0	0
213164	2	0	0	0	0
214207	2	0	0	0	0
215169	2	0	0	0	0
216180	1	0	0	0	0
217185	1	0	0	0	0
218190	1	0	0	0	0
219194	1	0	0	0	0
220186	2	0	0	0	0
221191	2	0	0	0	0
222218	2	0	0	0	0

223187	1	0	0	0	0
224206	2	0	0	0	0
225217	2	0	0	0	0
226212	1	0	0	0	0
158227	1	6	0	0	0
228191	1	0	0	0	0
161229	1	1	0	0	0
159230	1	6	0	0	0
165231	1	6	0	0	0
232178	1	0	0	0	0
195233	1	6	0	0	0
176234	1	1	0	0	0
235216	1	0	0	0	0
236203	1	0	0	0	0
181237	1	6	0	0	0
238186	1	0	0	0	0
239192	1	0	0	0	0
240253	1	0	0	0	0
241205	1	0	0	0	0
179242	1	6	0	0	0
243212	1	0	0	0	0
244214	1	0	0	0	0
245223	1	0	0	0	0
246223	2	0	0	0	0
247246	1	0	0	0	0
248245	2	0	0	0	0
249252	1	0	0	0	0
250242	1	0	0	0	0
251206	1	0	0	0	0
252228	1	0	0	0	0
253249	1	0	0	0	0
254233	1	0	0	0	0
255240	1	0	0	0	0
256240	1	0	0	0	0
257259	1	0	0	0	0
258251	1	0	0	0	0
259260	1	0	0	0	0
260262	1	0	0	0	0
261258	1	0	0	0	0
262263	1	0	0	0	0
263264	1	0	0	0	0
264261	1	0	0	0	0
265257	1	0	0	0	0
266257	1	0	0	0	0
141267	1	1	0	0	0
203197	2	0	0	0	0
160182	1	0	0	0	0
225205	1	0	0	0	0
173200	2	0	0	0	0
196168	2	0	0	0	0
162171	2	0	0	0	0
179176	1	0	0	0	0
199192	2	0	0	0	0
248235	1	0	0	0	0
235247	2	0	0	0	0
140159	1	0	0	0	0
201194	2	0	0	0	0
219226	2	0	0	0	0
233268	1	0	0	0	0
270277	1	0	0	0	0
271273	1	0	0	0	0
269272	1	6	0	0	0
273304	1	1	0	0	0
274278	1	0	0	0	0
275276	1	0	0	0	0
276269	1	0	0	0	0
277273	1	0	0	0	0
278283	1	0	0	0	0
278279	1	1	0	0	0
296280	1	1	0	0	0
281300	1	0	0	0	0
282313	1	1	0	0	0
283280	1	0	0	0	0
284286	2	0	0	0	0
285272	1	0	0	0	0
286293	1	0	0	0	0
287281	1	0	0	0	0
288282	1	0	0	0	0
289291	1	0	0	0	0

290284	1	0	0	0	0
291271	1	0	0	0	0
292298	1	0	0	0	0
293275	1	0	0	0	0
294297	1	0	0	0	0
295288	1	0	0	0	0
296287	1	0	0	0	0
310297	1	1	0	0	0
298307	1	0	0	0	0
299279	1	0	0	0	0
300285	1	6	0	0	0
301328	1	0	0	0	0
302282	1	0	0	0	0
303284	1	0	0	0	0
304292	1	0	0	0	0
305296	1	0	0	0	0
306295	1	0	0	0	0
307327	1	0	0	0	0
308274	2	0	0	0	0
309302	1	0	0	0	0
310299	1	0	0	0	0
311269	1	0	0	0	0
312315	2	0	0	0	0
313303	1	0	0	0	0
314323	1	0	0	0	0
315300	1	0	0	0	0
270316	1	1	0	0	0
317301	1	0	0	0	0
318314	1	0	0	0	0
319271	1	0	0	0	0
320311	1	0	0	0	0
293321	1	1	0	0	0
322308	1	0	0	0	0
323332	2	0	0	0	0
324325	1	0	0	0	0
325294	1	0	0	0	0
326305	1	0	0	0	0
327352	1	0	0	0	0
328305	2	0	0	0	0
329323	1	0	0	0	0
330344	1	0	0	0	0
331318	1	0	0	0	0
332274	1	0	0	0	0
333334	1	0	0	0	0
334320	2	0	0	0	0
335290	2	0	0	0	0
336319	1	0	0	0	0
337286	1	0	0	0	0
338276	2	0	0	0	0
339283	2	0	0	0	0
340285	2	0	0	0	0
341287	2	0	0	0	0
342318	2	0	0	0	0
343294	2	0	0	0	0
344337	2	0	0	0	0
345299	2	0	0	0	0
346310	1	0	0	0	0
347315	1	0	0	0	0
348320	1	0	0	0	0
349324	1	0	0	0	0
350316	2	0	0	0	0
351321	2	0	0	0	0
352348	2	0	0	0	0
353317	1	0	0	0	0
354336	2	0	0	0	0
355347	2	0	0	0	0
356342	1	0	0	0	0
288357	1	6	0	0	0
358321	1	0	0	0	0
291359	1	1	0	0	0
289360	1	6	0	0	0
295361	1	6	0	0	0
362308	1	0	0	0	0
325363	1	6	0	0	0
306364	1	1	0	0	0
365346	1	0	0	0	0
366333	1	0	0	0	0
311367	1	6	0	0	0
368316	1	0	0	0	0

369322	1	0	0	0	0
370383	1	0	0	0	0
371335	1	0	0	0	0
309372	1	6	0	0	0
373342	1	0	0	0	0
374344	1	0	0	0	0
375353	1	0	0	0	0
376353	2	0	0	0	0
377376	1	0	0	0	0
378375	2	0	0	0	0
379382	1	0	0	0	0
380372	1	0	0	0	0
381336	1	0	0	0	0
382358	1	0	0	0	0
383379	1	0	0	0	0
384363	1	0	0	0	0
385370	1	0	0	0	0
386370	1	0	0	0	0
387389	1	0	0	0	0
388381	1	0	0	0	0
389390	1	0	0	0	0
390392	1	0	0	0	0
391388	1	0	0	0	0
392393	1	0	0	0	0
393394	1	0	0	0	0
394391	1	0	0	0	0
395387	1	0	0	0	0
396387	1	0	0	0	0
271397	1	1	0	0	0
333327	2	0	0	0	0
290312	1	0	0	0	0
355335	1	0	0	0	0
303330	2	0	0	0	0
326298	2	0	0	0	0
292301	2	0	0	0	0
309306	1	0	0	0	0
329322	2	0	0	0	0
378365	1	0	0	0	0
365377	2	0	0	0	0
270289	1	0	0	0	0
331324	2	0	0	0	0
349356	2	0	0	0	0
363398	1	0	0	0	0
400407	1	0	0	0	0
401403	1	0	0	0	0
399402	1	6	0	0	0
403434	1	1	0	0	0
404408	1	0	0	0	0
405406	1	0	0	0	0
406399	1	0	0	0	0
407403	1	0	0	0	0
408413	1	0	0	0	0
408409	1	1	0	0	0
426410	1	1	0	0	0
411430	1	0	0	0	0
412443	1	1	0	0	0
413410	1	0	0	0	0
414416	2	0	0	0	0
415402	1	0	0	0	0
416423	1	0	0	0	0
417411	1	0	0	0	0
418412	1	0	0	0	0
419421	1	0	0	0	0
420414	1	0	0	0	0
421401	1	0	0	0	0
422428	1	0	0	0	0
423405	1	0	0	0	0
424427	1	0	0	0	0
425418	1	0	0	0	0
426417	1	0	0	0	0
440427	1	1	0	0	0
428437	1	0	0	0	0
429409	1	0	0	0	0
430415	1	6	0	0	0
431458	1	0	0	0	0
432412	1	0	0	0	0
433414	1	0	0	0	0
434422	1	0	0	0	0
435426	1	0	0	0	0

436425	1	0	0	0	0
437457	1	0	0	0	0
438404	2	0	0	0	0
439432	1	0	0	0	0
440429	1	0	0	0	0
441399	1	0	0	0	0
442445	2	0	0	0	0
443433	1	0	0	0	0
444453	1	0	0	0	0
445430	1	0	0	0	0
400446	1	1	0	0	0
447431	1	0	0	0	0
448444	1	0	0	0	0
449401	1	0	0	0	0
450441	1	0	0	0	0
423451	1	1	0	0	0
452438	1	0	0	0	0
453462	2	0	0	0	0
454455	1	0	0	0	0
455424	1	0	0	0	0
456435	1	0	0	0	0
457482	1	0	0	0	0
458435	2	0	0	0	0
459453	1	0	0	0	0
460474	1	0	0	0	0
461448	1	0	0	0	0
462404	1	0	0	0	0
463464	1	0	0	0	0
464450	2	0	0	0	0
465420	2	0	0	0	0
466449	1	0	0	0	0
467416	1	0	0	0	0
468406	2	0	0	0	0
469413	2	0	0	0	0
470415	2	0	0	0	0
471417	2	0	0	0	0
472448	2	0	0	0	0
473424	2	0	0	0	0
474467	2	0	0	0	0
475429	2	0	0	0	0
476440	1	0	0	0	0
477445	1	0	0	0	0
478450	1	0	0	0	0
479454	1	0	0	0	0
480446	2	0	0	0	0
481451	2	0	0	0	0
482478	2	0	0	0	0
483447	1	0	0	0	0
484466	2	0	0	0	0
485477	2	0	0	0	0
486472	1	0	0	0	0
418487	1	6	0	0	0
488451	1	0	0	0	0
421489	1	1	0	0	0
419490	1	6	0	0	0
425491	1	6	0	0	0
492438	1	0	0	0	0
455493	1	6	0	0	0
436494	1	1	0	0	0
495476	1	0	0	0	0
496463	1	0	0	0	0
441497	1	6	0	0	0
498446	1	0	0	0	0
499452	1	0	0	0	0
500513	1	0	0	0	0
501465	1	0	0	0	0
439502	1	6	0	0	0
503472	1	0	0	0	0
504474	1	0	0	0	0
505483	1	0	0	0	0
506483	2	0	0	0	0
507506	1	0	0	0	0
508505	2	0	0	0	0
509512	1	0	0	0	0
510502	1	0	0	0	0
511466	1	0	0	0	0
512488	1	0	0	0	0
513509	1	0	0	0	0
514493	1	0	0	0	0

515500	1	0	0	0	0
516500	1	0	0	0	0
517519	1	0	0	0	0
518511	1	0	0	0	0
519520	1	0	0	0	0
520522	1	0	0	0	0
521518	1	0	0	0	0
522523	1	0	0	0	0
523524	1	0	0	0	0
524521	1	0	0	0	0
525517	1	0	0	0	0
526517	1	0	0	0	0
401527	1	1	0	0	0
463457	2	0	0	0	0
420442	1	0	0	0	0
485465	1	0	0	0	0
433460	2	0	0	0	0
456428	2	0	0	0	0
422431	2	0	0	0	0
439436	1	0	0	0	0
459452	2	0	0	0	0
508495	1	0	0	0	0
495507	2	0	0	0	0
400419	1	0	0	0	0
461454	2	0	0	0	0
479486	2	0	0	0	0
493528	1	0	0	0	0
530537	1	0	0	0	0
531533	1	0	0	0	0
529532	1	6	0	0	0
533564	1	1	0	0	0
534538	1	0	0	0	0
535536	1	0	0	0	0
536529	1	0	0	0	0
537533	1	0	0	0	0
538543	1	0	0	0	0
538539	1	1	0	0	0
556540	1	1	0	0	0
541560	1	0	0	0	0
542573	1	1	0	0	0
543540	1	0	0	0	0
544546	2	0	0	0	0
545532	1	0	0	0	0
546553	1	0	0	0	0
547541	1	0	0	0	0
548542	1	0	0	0	0
549551	1	0	0	0	0
550544	1	0	0	0	0
551531	1	0	0	0	0
552558	1	0	0	0	0
553535	1	0	0	0	0
554557	1	0	0	0	0
555548	1	0	0	0	0
556547	1	0	0	0	0
570557	1	1	0	0	0
558567	1	0	0	0	0
559539	1	0	0	0	0
560545	1	6	0	0	0
561588	1	0	0	0	0
562542	1	0	0	0	0
563544	1	0	0	0	0
564552	1	0	0	0	0
565556	1	0	0	0	0
566555	1	0	0	0	0
567587	1	0	0	0	0
568534	2	0	0	0	0
569562	1	0	0	0	0
570559	1	0	0	0	0
571529	1	0	0	0	0
572575	2	0	0	0	0
573563	1	0	0	0	0
574583	1	0	0	0	0
575560	1	0	0	0	0
530576	1	1	0	0	0
577561	1	0	0	0	0
578574	1	0	0	0	0
579531	1	0	0	0	0
580571	1	0	0	0	0
553581	1	1	0	0	0

582568	1	0	0	0	0
583592	2	0	0	0	0
584585	1	0	0	0	0
585554	1	0	0	0	0
586565	1	0	0	0	0
587612	1	0	0	0	0
588565	2	0	0	0	0
589583	1	0	0	0	0
590604	1	0	0	0	0
591578	1	0	0	0	0
592534	1	0	0	0	0
593594	1	0	0	0	0
594580	2	0	0	0	0
595550	2	0	0	0	0
596579	1	0	0	0	0
597546	1	0	0	0	0
598536	2	0	0	0	0
599543	2	0	0	0	0
600545	2	0	0	0	0
601547	2	0	0	0	0
602578	2	0	0	0	0
603554	2	0	0	0	0
604597	2	0	0	0	0
605559	2	0	0	0	0
606570	1	0	0	0	0
607575	1	0	0	0	0
608580	1	0	0	0	0
609584	1	0	0	0	0
610576	2	0	0	0	0
611581	2	0	0	0	0
612608	2	0	0	0	0
613577	1	0	0	0	0
614596	2	0	0	0	0
615607	2	0	0	0	0
616602	1	0	0	0	0
548617	1	6	0	0	0
618581	1	0	0	0	0
551619	1	1	0	0	0
549620	1	6	0	0	0
555621	1	6	0	0	0
622568	1	0	0	0	0
585623	1	6	0	0	0
566624	1	1	0	0	0
625606	1	0	0	0	0
626593	1	0	0	0	0
571627	1	6	0	0	0
628576	1	0	0	0	0
629582	1	0	0	0	0
630643	1	0	0	0	0
631595	1	0	0	0	0
569632	1	6	0	0	0
633602	1	0	0	0	0
634604	1	0	0	0	0
635613	1	0	0	0	0
636613	2	0	0	0	0
637636	1	0	0	0	0
638635	2	0	0	0	0
639642	1	0	0	0	0
640632	1	0	0	0	0
641596	1	0	0	0	0
642618	1	0	0	0	0
643639	1	0	0	0	0
644623	1	0	0	0	0
645630	1	0	0	0	0
646630	1	0	0	0	0
647649	1	0	0	0	0
648641	1	0	0	0	0
649650	1	0	0	0	0
650652	1	0	0	0	0
651648	1	0	0	0	0
652653	1	0	0	0	0
653654	1	0	0	0	0
654651	1	0	0	0	0
655647	1	0	0	0	0
656647	1	0	0	0	0
531657	1	1	0	0	0
593587	2	0	0	0	0
550572	1	0	0	0	0
615595	1	0	0	0	0

563590	2	0	0	0	0					
586558	2	0	0	0	0					
552561	2	0	0	0	0					
569566	1	0	0	0	0					
589582	2	0	0	0	0					
638625	1	0	0	0	0					
625637	2	0	0	0	0					
530549	1	0	0	0	0					
591584	2	0	0	0	0					
609616	2	0	0	0	0					
623658	1	0	0	0	0					
M STY	2	1	MUL	2	MUL					
M SLB	2	1	1	2	2					
M SAL	1	8	16	17	18	19	20	21	22	23
M SAL	1	8	24	25	26	27	28	29	30	31
M SAL	1	8	32	33	34	35	36	37	38	39
M SAL	1	8	40	41	42	43	44	45	46	47
M SAL	1	8	48	49	50	51	52	53	54	55
M SAL	1	8	56	57	58	59	60	61	62	63
M SAL	1	8	64	65	66	67	68	69	70	71
M SAL	1	8	72	73	74	75	76	77	78	79
M SAL	1	8	80	81	82	83	84	85	86	87
M SAL	1	8	88	89	90	91	92	93	94	95
M SAL	1	8	96	97	98	99	100	101	102	103
M SAL	1	8	104	105	106	107	108	109	110	111
M SAL	1	8	112	113	114	115	116	117	118	119
M SAL	1	8	120	121	122	123	124	125	126	127
M SAL	1	8	128	129	130	139	140	141	142	143
M SAL	1	8	144	145	146	147	148	149	150	151
M SAL	1	8	152	153	154	155	156	157	158	159
M SAL	1	8	160	161	162	163	164	165	166	167
M SAL	1	8	168	169	170	171	172	173	174	175
M SAL	1	8	176	177	178	179	180	181	182	183
M SAL	1	8	184	185	186	187	188	189	190	191
M SAL	1	8	192	193	194	195	196	197	198	199
M SAL	1	8	200	201	202	203	204	205	206	207
M SAL	1	8	208	209	210	211	212	213	214	215
M SAL	1	8	216	217	218	219	220	221	222	223
M SAL	1	8	224	225	226	227	228	229	230	231
M SAL	1	8	232	233	234	235	236	237	238	239
M SAL	1	8	240	241	242	243	244	245	246	247
M SAL	1	8	248	249	250	251	252	253	254	255
M SAL	1	8	256	257	258	259	260	261	262	263
M SAL	1	8	264	265	266	267	268	269	270	271
M SAL	1	8	272	273	274	275	276	277	278	279
M SAL	1	8	280	281	282	283	284	285	286	287
M SAL	1	8	288	289	290	291	292	293	294	295
M SAL	1	8	296	297	298	299	300	301	302	303
M SAL	1	8	304	305	306	307	308	309	310	311
M SAL	1	8	312	313	314	315	316	317	318	319
M SAL	1	8	320	321	322	323	324	325	326	327
M SAL	1	8	328	329	330	331	332	333	334	335
M SAL	1	8	336	337	338	339	340	341	342	343
M SAL	1	8	344	345	346	347	348	349	350	351
M SAL	1	8	352	353	354	355	356	357	358	359
M SAL	1	8	360	361	362	363	364	365	366	367
M SAL	1	8	368	369	370	371	372	373	374	375
M SAL	1	8	376	377	378	379	380	381	382	383
M SAL	1	8	384	385	386	387	388	389	390	391
M SAL	1	8	392	393	394	395	396	397	398	399
M SAL	1	8	400	401	402	403	404	405	406	407
M SAL	1	8	408	409	410	411	412	413	414	415
M SAL	1	8	416	417	418	419	420	421	422	423
M SAL	1	8	424	425	426	427	428	429	430	431
M SAL	1	8	432	433	434	435	436	437	438	439
M SAL	1	8	440	441	442	443	444	445	446	447
M SAL	1	8	448	449	450	451	452	453	454	455
M SAL	1	8	456	457	458	459	460	461	462	463
M SAL	1	8	464	465	466	467	468	469	470	471
M SAL	1	8	472	473	474	475	476	477	478	479
M SAL	1	8	480	481	482	483	484	485	486	487
M SAL	1	8	488	489	490	491	492	493	494	495
M SAL	1	8	496	497	498	499	500	501	502	503
M SAL	1	8	504	505	506	507	508	509	510	511
M SAL	1	8	512	513	514	515	516	517	518	519
M SAL	1	8	520	521	522	523	524	525	526	527
M SAL	1	8	528	529	530	531	532	533	534	535
M SAL	1	8	536	537	538	539	540	541	542	543
M SAL	1	8	544	545	546	547	548	549	550	551

M	SAL	1	8	552	553	554	555	556	557	558	559
M	SAL	1	8	560	561	562	563	564	565	566	567
M	SAL	1	8	568	569	570	571	572	573	574	575
M	SAL	1	8	576	577	578	579	580	581	582	583
M	SAL	1	8	584	585	586	587	588	589	590	591
M	SAL	1	8	592	593	594	595	596	597	598	599
M	SAL	1	8	600	601	602	603	604	605	606	607
M	SAL	1	8	608	609	610	611	612	613	614	615
M	SAL	1	8	616	617	618	619	620	621	622	623
M	SAL	1	8	624	625	626	627	628	629	630	631
M	SAL	1	8	632	633	634	635	636	637	638	639
M	SAL	1	8	640	641	642	643	644	645	646	647
M	SAL	1	8	648	649	650	651	652	653	654	655
M	SAL	1	3	656	657	658					
M	SPA	1	8	1	2	3	4	5	6	7	8
M	SPA	1	8	9	10	11	12	13	14	15	16
M	SPA	1	8	17	18	19	20	21	22	23	24
M	SPA	1	8	25	26	27	28	29	30	31	32
M	SPA	1	8	33	34	35	36	37	38	39	40
M	SPA	1	8	41	42	43	44	45	46	47	48
M	SPA	1	8	49	50	51	52	53	54	55	56
M	SPA	1	8	57	58	59	60	61	62	63	64
M	SPA	1	8	65	66	67	68	69	70	71	72
M	SPA	1	8	73	74	75	76	77	78	79	80
M	SPA	1	8	81	82	83	84	85	86	87	88
M	SPA	1	8	89	90	91	92	93	94	95	96
M	SPA	1	8	97	98	99	100	101	102	103	104
M	SPA	1	8	105	106	107	108	109	110	111	112
M	SPA	1	8	113	114	115	116	117	118	119	120
M	SPA	1	8	121	122	123	124	125	126	127	128
M	SPA	1	2	129	130						
M	SMT	1	5								
M	SDI	1	4	1.0978	-15.4692		1.0978	-1.0308			
M	SDI	1	4	20.4647	-1.0308		20.4647	-15.4692			
M	SAL	2	8	131	132	133	134	135	136	137	138
M	SPA	2	1	131							
M	SMT	2	8								
M	SDI	2	4	21.7703	-7.9963		21.7703	-6.4579			
M	SDI	2	4	23.7610	-6.4579		23.7610	-7.9963			
M	END										

Chemical Structures, InChI

InChI=1S/5C89H102Cl2N10O28.8ClH/c5*1-39(2)14-11-9-7-8-10-12-15-62(107)94-70-74(110)76(12)79(87(121)122)129-88(70)128-78-59-32-44-33-60(78)125-56-25-20-43(30-51(56)90)72(108)69-85(119)98-67(81(115)92-26-13-27-100(3)4)49-34-45(103)35-58(126-89-77(113)75(111)73(109)61(38-102)127-89)63(49)48-29-41(18-23-53(48)104)65(82(116)99-69)95-83(117)66(44)96-84(118)68-50-36-47(37-55(106)64(50)91)124-57-31-42(19-24-54(57)105)71(101(5)6)86(120)93-52(80(114)97-68)28-40-16-21-46(123-59)22-17-40;;;;;;;;;h5*16-25,29-37,39,52,61,65-77,79,88-89,102-106,108-113H,7-15,26-28,38H2,1-6H3,(H,92,115)(H,93,120)(H,94,107)(H,95,117)(H,96,118)(H,97,114)(H,98,119)(H,99,116)(H,121,122);8*1H/t5*52-,61-,65-,66-,67+,68+,69+,70-,71-,72-,73-,74-,75+,76+,77+,79+,88-,89+;;;;;;;;;m11111...../s1

Chemical Structure, InChI Key

FATPOJKTNNJYCL-UTJFGVATSA-N

Molecular Bond Types

Product Information

Product Type	INDEXING - SUBSTANCE	Item Code (Source)	33WDQ7T81E
---------------------	----------------------	---------------------------	------------

Labeler - Food and Drug Administration (927645523)