

**Integrating Medicinal Chemistry, Organic/Combinatorial Chemistry
and Computational Chemistry for the Discovery of Selective Estrogen
Receptor Modulators with FORECASTER, a Novel Platform for Drug
Discovery**

Supporting Information

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REACT

The chemical transformations to be carried out are defined in an editable text file (Figure S1). A set of defined reactions is given in Figure S1 but additional reactions can be added. It is also possible to use a generic functional group (e.g., X in reactant 1 and Y in reactant 2).

#rule	funct_group	cp	keep_atom	rm_atom	new_atom
#----	-----	--	-----	-----	-----
#1: peptide bond formation					
Rule1	carboxyl	c	o	oh	-
Rule1	carboxylate	c	o	o	-
Rule1	ester	c	o	os	-
Rule2	amine_1	n3	hn, c3	hn	-
Rule2	ammonium_1	n4	hn, c3	hn, hn	-
Rule2	amine_2	n3	hn, c3, c3	hn	-
Rule2	ammonium_2	n4	hn, c3, c3	hn, hn	-
#2: sulfonamide formation					
#Rule1	sulfonyl_cl	s6	o, o	cl	-
#Rule1	sulfonyl_br	s6	o, o	br	-
#Rule2	amine_1	n3	hn	hn	-
#Rule2	ammonium_1	n4	hn	hn, hn	-
#Rule2	amine_2	n3	hn	hn	-
#Rule2	ammonium_2	n4	hn	hn, hn	-
#3: reductive amination					
#Rule1	aldehyde	c	hc	o	H
#Rule1	ketone	c	c3, c3	o	H
#Rule2	amine_1	n3	c3	hn	-
#Rule2	ammonium_1	n4	c3	hn, hn	-
#Rule2	amine_2	n3	c3, c3	hn	-
#Rule2	ammonium_2	n4	c3, c3	hn, hn	-
#4: Suzuki coupling					
#Rule1	aryl_chloride	ca	-	cl	-
#Rule1	aryl_bromide	ca	-	br	-
#Rule1	aryl_iodide	ca	i	-	-
#Rule1	vinyl_chloride	c2	-	cl	-
#Rule1	vinyl_bromide	c2	-	br	-
#Rule1	vinyl_iodide	c2	-	i	-
#Rule2	boron_acid_ar	ca	-	b	-
#Rule2	boron_acid_al	c3	-	b	-
#Rule2	boron_acid_vi	c2	-	b	-
#Rule2	boron_ester_ar	ca	-	b	-
#Rule2	boron_ester_al	c3	-	b	-
#Rule2	boron_ester_vi	c2	-	b	-

#5: Dummy atoms

Raloxifene
Forecaster10031114513D

62	66	0	0	0	0	0	0	0999	V2000					
-6.9691	-1.3556					0.0259	C	0	0	0	0	0	0	0
-7.0342	-2.6926					0.0795	C	0	0	0	0	0	0	0
-5.7955	-3.4850					0.1306	C	0	0	0	0	0	0	0
-4.6469	-2.8221					0.1112	C	0	0	0	0	0	0	0
-4.5505	-1.4118					0.0374	C	0	0	0	0	0	0	0
-5.6556	-0.6685					0.0022	C	0	0	0	0	0	0	0
-8.2708	-3.3317					0.0866	O	0	0	0	0	0	0	0
-3.1316	-3.4303					0.1542	S	0	0	0	0	0	0	0
-2.2258	-1.9954					-0.0013	C	0	0	0	0	0	0	0
-3.0879	-0.9056					-0.0140	C	0	0	0	0	0	0	0
-0.7328	-2.1408					-0.1396	C	0	0	0	0	0	0	0
-0.1588	-3.1868					0.4559	C	0	0	0	0	0	0	0
1.2930	-3.3777					0.3922	C	0	0	0	0	0	0	0
2.0499	-2.5241					-0.2926	C	0	0	0	0	0	0	0
1.4266	-1.4263					-1.0192	C	0	0	0	0	0	0	0
0.1074	-1.2538					-0.9591	C	0	0	0	0	0	0	0
3.4315	-2.6829					-0.3212	O	0	0	0	0	0	0	0
-2.8444	0.6485					-0.0950	C	0	0	0	0	0	0	0
-1.5749	1.4284					0.1274	C	0	0	0	0	0	0	0
-3.8150	1.3426					-0.4193	O	0	0	0	0	0	0	0
-0.5265	0.9749					0.8121	C	0	0	0	0	0	0	0
0.7464	1.7172					0.8090	C	0	0	0	0	0	0	0
0.8357	2.8773					0.1608	C	0	0	0	0	0	0	0
-0.3569	3.4443					-0.4615	C	0	0	0	0	0	0	0
-1.4961	2.7576					-0.4777	C	0	0	0	0	0	0	0
2.0672	3.5434					-0.0034	O	0	0	0	0	0	0	0
3.1992	2.8006					0.5015	C	0	0	0	0	0	0	0
4.4805	3.5560					0.0527	C	0	0	0	0	0	0	0
5.7307	2.8439					0.4119	N	0	0	0	0	0	0	0
5.8068	1.5412					-0.3047	C	0	0	0	0	0	0	0
7.1227	0.8088					0.0619	C	0	0	0	0	0	0	0
8.3209	1.6892					-0.3364	C	0	0	0	0	0	0	0
8.2111	3.0313					0.4012	C	0	0	0	0	0	0	0
6.8755	3.7033					0.0208	C	0	0	0	0	0	0	0
-7.8876	-0.7693					-0.0005	H	0	0	0	0	0	0	0
-5.8208	-4.5735					0.1823	H	0	0	0	0	0	0	0
-5.5955	0.4189					-0.0429	H	0	0	0	0	0	0	0
-8.8224	-3.0185					0.9234	H	0	0	0	0	0	0	0
-0.7749	-3.9064					0.9950	H	0	0	0	0	0	0	0
1.7537	-4.2208					0.9070	H	0	0	0	0	0	0	0

	5.7806	1.7190	-1.3798	H	0	0	0	0	0
	7.1488	0.6221	1.1355	H	0	0	0	0	0
	7.1733	-0.1392	-0.4736	H	0	0	0	0	0
	9.2500	1.1922	-0.0574	H	0	0	0	0	0
	8.3087	1.8602	-1.4128	H	0	0	0	0	0
	8.2411	2.8607	1.4773	H	0	0	0	0	0
	9.0406	3.6765	0.1118	H	0	0	0	0	0
	6.7969	4.6611	0.5351	H	0	0	0	0	0
	6.8501	3.8658	-1.0567	H	0	0	0	0	0
	5.7551	2.6736	1.4680	H	0	0	0	0	0
2	1	1	0	0	0				
35	1	1	0	0	0				
6	1	2	0	0	0				
3	2	2	0	0	0				
7	2	1	0	0	0				
4	3	1	0	0	0				
36	3	1	0	0	0				
5	4	2	0	0	0				
8	4	1	0	0	0				
6	5	1	0	0	0				
10	5	1	0	0	0				
37	6	1	0	0	0				
38	7	1	0	0	0				
9	8	1	0	0	0				
10	9	2	0	0	0				
11	9	1	0	0	0				
18	10	1	0	0	0				
12	11	1	0	0	0				
16	11	2	0	0	0				
13	12	2	0	0	0				
39	12	1	0	0	0				
14	13	1	0	0	0				
40	13	1	0	0	0				
15	14	2	0	0	0				
17	14	1	0	0	0				
16	15	1	0	0	0				
41	15	1	0	0	0				
42	16	1	0	0	0				
43	17	1	0	0	0				
19	18	1	0	0	0				
20	18	2	0	0	0				
21	19	1	0	0	0				
25	19	2	0	0	0				
22	21	2	0	0	0				
44	21	1	0	0	0				
23	22	1	0	0	0				
45	22	1	0	0	0				
24	23	2	0	0	0				
26	23	1	0	0	0				
25	24	1	0	0	0				
46	24	1	0	0	0				
47	25	1	0	0	0				
27	26	1	0	0	0				

29	28	1	0	0	0
50	28	1	0	0	0
51	28	1	0	0	0
30	29	1	0	0	0
62	29	1	0	0	0
34	29	1	0	0	0
31	30	1	0	0	0
52	30	1	0	0	0
53	30	1	0	0	0
32	31	1	0	0	0
54	31	1	0	0	0
55	31	1	0	0	0
33	32	1	0	0	0
56	32	1	0	0	0
57	32	1	0	0	0
34	33	1	0	0	0
58	33	1	0	0	0
59	33	1	0	0	0
60	34	1	0	0	0
61	34	1	0	0	0

M END

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Arzoxifene

Forecaster10031114513D

64	68	0	0	0	0	0	0	0	0	0999	V2000					
-6.9927	-1.2114	0.0546	C	0	0	0	0	0	0							
-7.0953	-2.5443	-0.0553	C	0	0	0	0	0	0							
-5.8803	-3.3691	-0.1394	C	0	0	0	0	0	0							
-4.7160	-2.7390	-0.0943	C	0	0	0	0	0	0							
-4.5806	-1.3374	0.0334	C	0	0	0	0	0	0							
-5.6578	-0.5577	0.1027	C	0	0	0	0	0	0							
-8.3485	-3.1497	-0.0913	O	0	0	0	0	0	0							
-3.2188	-3.3812	-0.1686	S	0	0	0	0	0	0							
-2.2819	-1.9721	0.0181	C	0	0	0	0	0	0							
-3.1265	-0.8642	0.0783	C	0	0	0	0	0	0							
-0.7940	-2.1570	0.1280	C	0	0	0	0	0	0							
-0.2659	-3.2088	-0.4996	C	0	0	0	0	0	0							
1.1816	-3.4115	-0.5197	C	0	0	0	0	0	0							
1.9862	-2.5585	0.1070	C	0	0	0	0	0	0							
1.4111	-1.4655	0.8879	C	0	0	0	0	0	0							
0.0930	-1.2944	0.9151	C	0	0	0	0	0	0							
3.3719	-2.7112	-0.0011	O	0	0	0	0	0	0							
-2.9192	0.6215	0.1895	O	0	0	0	0	0	0							
-1.7099	1.3972	-0.0508	C	0	0	0	0	0	0							
-0.6505	0.9523	-0.7197	C	0	0	0	0	0	0							
0.6079	1.7160	-0.7552	C	0	0	0	0	0	0							
0.6787	2.9023	-0.1600	C	0	0	0	0	0	0							
-0.5326	3.4733	0.4357	C	0	0	0	0	0	0							
-1.6604	2.7626	0.4857	C	0	0	0	0	0	0							
1.9087	3.5942	-0.0258	O	0	0	0	0	0	0							
3.0613	2.8420	-0.4963	C	0	0	0	0	0	0							
4.3414	3.6416	-0.0966	C	0	0	0	0	0	0							

8.2428	1.8815	0.3495	C	0	0	0	0	0
8.0921	3.1762	-0.4616	C	0	0	0	0	0
6.7442	3.8413	-0.1025	C	0	0	0	0	0
4.0535	-1.6623	0.6910	C	0	0	0	0	0
-7.8951	-0.6024	0.1091	H	0	0	0	0	0
-5.9357	-4.4535	-0.2348	H	0	0	0	0	0
-5.5642	0.5246	0.1918	H	0	0	0	0	0
-8.8696	-2.9296	0.7933	H	0	0	0	0	0
-0.9189	-3.9228	-1.0015	H	0	0	0	0	0
1.6029	-4.2652	-1.0505	H	0	0	0	0	0
2.0611	-0.7922	1.4467	H	0	0	0	0	0
-0.3340	-0.5026	1.5305	H	0	0	0	0	0
-0.7148	0.0035	-1.2523	H	0	0	0	0	0
1.4794	1.3094	-1.2684	H	0	0	0	0	0
-0.5118	4.4851	0.8405	H	0	0	0	0	0
-2.5545	3.2004	0.9296	H	0	0	0	0	0
3.0777	1.8569	-0.0300	H	0	0	0	0	0
3.0156	2.7310	-1.5797	H	0	0	0	0	0
4.3294	4.5964	-0.6222	H	0	0	0	0	0
4.3159	3.8179	0.9787	H	0	0	0	0	0
5.7185	1.9276	1.4244	H	0	0	0	0	0
4.8923	1.0301	0.1278	H	0	0	0	0	0
7.1359	0.0432	0.6074	H	0	0	0	0	0
7.0755	0.7102	-1.0421	H	0	0	0	0	0
8.2422	2.1130	1.4146	H	0	0	0	0	0
9.1784	1.3889	0.0848	H	0	0	0	0	0
8.9100	3.8553	-0.2209	H	0	0	0	0	0
8.1129	2.9446	-1.5265	H	0	0	0	0	0
6.7282	4.0650	0.9642	H	0	0	0	0	0
6.6387	4.7660	-0.6698	H	0	0	0	0	0
5.1301	-1.8016	0.5933	H	0	0	0	0	0
3.7791	-1.6840	1.7457	H	0	0	0	0	0
3.7717	-0.7005	0.2624	H	0	0	0	0	0
5.6294	2.7038	-1.4727	H	0	0	0	0	0

2	1	1	0	0	0
6	1	2	0	0	0
35	1	1	0	0	0
3	2	2	0	0	0
7	2	1	0	0	0
4	3	1	0	0	0
36	3	1	0	0	0
5	4	2	0	0	0
8	4	1	0	0	0
6	5	1	0	0	0
10	5	1	0	0	0
37	6	1	0	0	0
38	7	1	0	0	0
9	8	1	0	0	0
10	9	2	0	0	0
11	9	1	0	0	0
18	10	1	0	0	0
12	11	1	0	0	0
16	11	2	0	0	0

40	13	1	0	0	0
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17	14	1	0	0	0
16	15	1	0	0	0
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42	16	1	0	0	0
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19	18	1	0	0	0
20	19	1	0	0	0
24	19	2	0	0	0
21	20	2	0	0	0
43	20	1	0	0	0
22	21	1	0	0	0
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47	26	1	0	0	0
48	26	1	0	0	0
28	27	1	0	0	0
49	27	1	0	0	0
50	27	1	0	0	0
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33	28	1	0	0	0
64	28	1	0	0	0
30	29	1	0	0	0
51	29	1	0	0	0
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54	30	1	0	0	0
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55	31	1	0	0	0
56	31	1	0	0	0
33	32	1	0	0	0
57	32	1	0	0	0
58	32	1	0	0	0
59	33	1	0	0	0
60	33	1	0	0	0
61	34	1	0	0	0
62	34	1	0	0	0
63	34	1	0	0	0

M END

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lasofoxidene

Forecaster10031114513D

63 67 0 0 0 0 0 0 0 0999 V2000

-4 3953 -3 4546 -0 8620 C 0 0 0 0 0

-2.0474	-3.0359	-0.3739	C	0	0	0	0	0
-3.1456	-2.7260	-1.0728	C	0	0	0	0	0
-0.9031	-4.5809	1.4137	C	0	0	0	0	0
0.3214	-3.6370	1.3074	C	0	0	0	0	0
0.4872	-3.2014	-0.1460	C	0	0	0	0	0
-0.7430	-2.2858	-0.6133	C	0	0	0	0	0
-5.6337	-5.1479	0.2146	O	0	0	0	0	0
-0.8498	-0.8217	0.0050	C	0	0	0	0	0
1.8880	-2.5733	-0.3308	C	0	0	0	0	0
0.0863	-0.3235	0.8159	C	0	0	0	0	0
0.1523	1.1013	1.1016	C	0	0	0	0	0
-0.7352	1.9404	0.5614	C	0	0	0	0	0
-1.8321	1.3998	-0.2273	C	0	0	0	0	0
-1.8775	0.1008	-0.5079	C	0	0	0	0	0
2.8803	-3.0004	0.4518	C	0	0	0	0	0
4.2092	-2.3954	0.3687	C	0	0	0	0	0
4.4331	-1.3921	-0.4767	C	0	0	0	0	0
3.3560	-0.9147	-1.3483	C	0	0	0	0	0
2.1508	-1.4819	-1.2950	C	0	0	0	0	0
-0.6116	3.3578	0.6571	O	0	0	0	0	0
0.6661	3.8366	1.1720	C	0	0	0	0	0
1.7552	3.6546	0.0372	C	0	0	0	0	0
3.0445	4.2716	0.3714	N	0	0	0	0	0
4.0455	4.0083	-0.6597	C	0	0	0	0	0
5.1891	4.9131	-0.1813	C	0	0	0	0	0
4.4374	6.1737	0.3248	C	0	0	0	0	0
2.9515	5.7310	0.3123	C	0	0	0	0	0
-5.2865	-3.1817	-1.4271	H	0	0	0	0	0
-3.2949	-5.6350	1.4910	H	0	0	0	0	0
-3.1080	-1.9215	-1.8073	H	0	0	0	0	0
-1.1955	-4.6403	2.4621	H	0	0	0	0	0
-0.6017	-5.5681	1.0635	H	0	0	0	0	0
0.1629	-2.7606	1.9358	H	0	0	0	0	0
1.2179	-4.1629	1.6358	H	0	0	0	0	0
0.4606	-4.1054	-0.7545	H	0	0	0	0	0
-0.6477	-2.1625	-1.6921	H	0	0	0	0	0
-6.3802	-4.4849	0.5398	H	0	0	0	0	0
0.8134	-0.9956	1.2716	H	0	0	0	0	0
0.9306	1.4863	1.7604	H	0	0	0	0	0
-2.6189	2.0617	-0.5892	H	0	0	0	0	0
-2.6869	-0.2871	-1.1264	H	0	0	0	0	0
2.6988	-3.8085	1.1604	H	0	0	0	0	0
5.0169	-2.7664	0.9996	H	0	0	0	0	0
5.4173	-0.9257	-0.5208	H	0	0	0	0	0
3.5407	-0.0941	-2.0416	H	0	0	0	0	0
1.3586	-1.1416	-1.9619	H	0	0	0	0	0
0.5846	4.8901	1.4397	H	0	0	0	0	0
0.9495	3.2585	2.0516	H	0	0	0	0	0
1.9127	2.5882	-0.1243	H	0	0	0	0	0
1.3802	4.1099	-0.8794	H	0	0	0	0	0
4.3419	2.9595	-0.6734	H	0	0	0	0	0
3.6900	4.2989	-1.6483	H	0	0	0	0	0
5.7525	4.4418	0.6240	H	0	0	0	0	0

	2.4178	6.1251	1.1771 H	0	0	0	0	0
	2.4535	6.0554	-0.6014 H	0	0	0	0	0
	3.3879	3.9474	1.3315 H	0	0	0	0	0
2	1	1	0	0	0			
6	1	2	0	0	0			
32	1	1	0	0	0			
3	2	2	0	0	0			
11	2	1	0	0	0			
4	3	1	0	0	0			
33	3	1	0	0	0			
5	4	2	0	0	0			
7	4	1	0	0	0			
6	5	1	0	0	0			
10	5	1	0	0	0			
34	6	1	0	0	0			
8	7	1	0	0	0			
35	7	1	0	0	0			
36	7	1	0	0	0			
9	8	1	0	0	0			
37	8	1	0	0	0			
38	8	1	0	0	0			
10	9	1	0	0	0			
13	9	1	0	0	0			
39	9	1	0	0	0			
12	10	1	0	0	0			
40	10	1	0	0	0			
41	11	1	0	0	0			
14	12	1	0	0	0			
18	12	2	0	0	0			
19	13	1	0	0	0			
23	13	2	0	0	0			
15	14	2	0	0	0			
42	14	1	0	0	0			
16	15	1	0	0	0			
43	15	1	0	0	0			
17	16	2	0	0	0			
24	16	1	0	0	0			
18	17	1	0	0	0			
44	17	1	0	0	0			
45	18	1	0	0	0			
20	19	2	0	0	0			
46	19	1	0	0	0			
21	20	1	0	0	0			
47	20	1	0	0	0			
22	21	2	0	0	0			
48	21	1	0	0	0			
23	22	1	0	0	0			
49	22	1	0	0	0			
50	23	1	0	0	0			
25	24	1	0	0	0			
26	25	1	0	0	0			
51	25	1	0	0	0			
52	25	1	0	0	0			

28	27	1	0	0	0
31	27	1	0	0	0
63	27	1	0	0	0
29	28	1	0	0	0
55	28	1	0	0	0
56	28	1	0	0	0
30	29	1	0	0	0
57	29	1	0	0	0
58	29	1	0	0	0
31	30	1	0	0	0
59	30	1	0	0	0
60	30	1	0	0	0
61	31	1	0	0	0
62	31	1	0	0	0

M END

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basedoxifene

Forecaster10031114513D

67	71	0	0	0	0	0	0	0	0	0999	V2000			
-7.2569	-1.2574	-0.0420	C	0	0	0	0	0						
-7.2408	-2.5964	-0.1190	C	0	0	0	0	0						
-5.9518	-3.3196	-0.1487	C	0	0	0	0	0						
-4.8421	-2.5915	-0.0926	C	0	0	0	0	0						
-4.8572	-1.2045	0.0014	C	0	0	0	0	0						
-5.9832	-0.5022	0.0226	C	0	0	0	0	0						
-8.4378	-3.3064	-0.1644	O	0	0	0	0	0						
-3.4760	-3.0619	-0.0787	C	0	0	0	0	0						
-2.6871	-1.9807	0.0612	C	0	0	0	0	0						
-3.5540	-0.7396	0.0708	N	0	0	0	0	0						
-3.3009	0.7571	0.0910	C	0	0	0	0	0						
-1.9361	1.4325	-0.1255	C	0	0	0	0	0						
-0.9726	0.9671	-0.9268	C	0	0	0	0	0						
0.3779	1.6106	-0.9111	C	0	0	0	0	0						
0.5885	2.6873	-0.1479	C	0	0	0	0	0						
-0.5166	3.2587	0.6024	C	0	0	0	0	0						
-1.7003	2.6600	0.6239	C	0	0	0	0	0						
1.8611	3.2731	0.0336	O	0	0	0	0	0						
2.9780	2.5598	-0.5345	C	0	0	0	0	0						
4.2392	3.3720	-0.1099	C	0	0	0	0	0						
5.5332	2.6752	-0.3237	N	0	0	0	0	0						
-1.2073	-2.1918	0.2014	C	0	0	0	0	0						
-0.6912	-3.3010	-0.3267	C	0	0	0	0	0						
0.7507	-3.5483	-0.2819	C	0	0	0	0	0						
1.5573	-2.6730	0.3124	C	0	0	0	0	0						
0.9965	-1.4920	0.9549	C	0	0	0	0	0						
-0.3158	-1.2705	0.9105	C	0	0	0	0	0						
2.9310	-2.8862	0.3241	O	0	0	0	0	0						
5.6072	1.4827	0.5505	C	0	0	0	0	0						
6.6028	0.4267	-0.0222	C	0	0	0	0	0						
8.1082	0.7853	0.0086	C	0	0	0	0	0						
8.4736	2.1255	-0.6557	C	0	0	0	0	0						
7.9961	3.2438	0.2559	C	0	0	0	0	0						

-5.9717	0.5860	0.0850	H	0	0	0	0	0
-8.9952	-3.1096	0.7035	H	0	0	0	0	0
-3.1465	-4.0973	-0.1652	H	0	0	0	0	0
-3.9528	1.1705	-0.6786	H	0	0	0	0	0
-3.6370	1.0935	1.0718	H	0	0	0	0	0
-1.1699	0.1233	-1.5880	H	0	0	0	0	0
1.1859	1.2034	-1.5190	H	0	0	0	0	0
-0.3718	4.1882	1.1529	H	0	0	0	0	0
-2.5096	3.0932	1.2116	H	0	0	0	0	0
3.0253	1.5455	-0.1382	H	0	0	0	0	0
2.8952	2.5225	-1.6207	H	0	0	0	0	0
4.2546	4.2981	-0.6845	H	0	0	0	0	0
4.1510	3.6037	0.9515	H	0	0	0	0	0
-1.3495	-4.0316	-0.7968	H	0	0	0	0	0
1.1636	-4.4494	-0.7354	H	0	0	0	0	0
1.6508	-0.7900	1.4718	H	0	0	0	0	0
-0.7314	-0.3938	1.4073	H	0	0	0	0	0
3.1408	-3.7929	0.8104	H	0	0	0	0	0
5.9436	1.7882	1.5413	H	0	0	0	0	0
4.6166	1.0341	0.6249	H	0	0	0	0	0
6.4726	-0.4914	0.5508	H	0	0	0	0	0
6.3294	0.2484	-1.0622	H	0	0	0	0	0
8.4239	0.8280	1.0510	H	0	0	0	0	0
8.6544	-0.0060	-0.5048	H	0	0	0	0	0
9.5536	2.1910	-0.7877	H	0	0	0	0	0
7.9831	2.2037	-1.6259	H	0	0	0	0	0
8.0618	2.8941	1.2862	H	0	0	0	0	0
8.6573	4.0995	0.1193	H	0	0	0	0	0
6.2141	4.2274	0.8937	H	0	0	0	0	0
6.5810	4.4048	-0.8393	H	0	0	0	0	0
5.6234	2.3813	-1.3486	H	0	0	0	0	0

2	1	1	0	0	0
6	1	2	0	0	0
35	1	1	0	0	0
3	2	2	0	0	0
7	2	1	0	0	0
4	3	1	0	0	0
36	3	1	0	0	0
5	4	2	0	0	0
8	4	1	0	0	0
6	5	1	0	0	0
10	5	1	0	0	0
37	6	1	0	0	0
38	7	1	0	0	0
9	8	2	0	0	0
39	8	1	0	0	0
10	9	1	0	0	0
22	9	1	0	0	0
11	10	1	0	0	0
12	11	1	0	0	0
40	11	1	0	0	0
41	11	1	0	0	0
13	12	1	0	0	0

15	14	1	0	0	0
43	14	1	0	0	0
16	15	2	0	0	0
18	15	1	0	0	0
17	16	1	0	0	0
44	16	1	0	0	0
45	17	1	0	0	0
19	18	1	0	0	0
20	19	1	0	0	0
46	19	1	0	0	0
47	19	1	0	0	0
21	20	1	0	0	0
48	20	1	0	0	0
49	20	1	0	0	0
29	21	1	0	0	0
34	21	1	0	0	0
67	21	1	0	0	0
23	22	1	0	0	0
27	22	2	0	0	0
24	23	2	0	0	0
50	23	1	0	0	0
25	24	1	0	0	0
51	24	1	0	0	0
26	25	2	0	0	0
28	25	1	0	0	0
27	26	1	0	0	0
52	26	1	0	0	0
53	27	1	0	0	0
54	28	1	0	0	0
30	29	1	0	0	0
55	29	1	0	0	0
56	29	1	0	0	0
31	30	1	0	0	0
57	30	1	0	0	0
58	30	1	0	0	0
32	31	1	0	0	0
59	31	1	0	0	0
60	31	1	0	0	0
33	32	1	0	0	0
61	32	1	0	0	0
62	32	1	0	0	0
34	33	1	0	0	0
63	33	1	0	0	0
64	33	1	0	0	0
65	34	1	0	0	0
66	34	1	0	0	0

M END

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Pipendoxifene

Forecaster10031114513D

64	68	0	0	0	0	0	0	0	0	0999	V2000
-6	9758	-1	2337	-0	0464	C	0	0	0	0	0

-4.5770	-1.1667	-0.0067	C	0	0	0	0	0
-5.7071	-0.4712	0.0143	C	0	0	0	0	0
-8.1446	-3.2895	-0.1609	O	0	0	0	0	0
-3.1837	-3.0149	-0.0829	C	0	0	0	0	0
-2.4012	-1.9282	0.0517	C	0	0	0	0	0
-3.2782	-0.6929	0.0602	N	0	0	0	0	0
-3.0391	0.8042	0.0864	C	0	0	0	0	0
-1.6779	1.4833	-0.1032	C	0	0	0	0	0
-0.7262	1.0622	-0.9432	C	0	0	0	0	0
0.6236	1.7079	-0.9101	C	0	0	0	0	0
0.8436	2.7392	-0.0878	C	0	0	0	0	0
-0.2490	3.2625	0.7119	C	0	0	0	0	0
-1.4321	2.6636	0.7135	C	0	0	0	0	0
2.1160	3.3182	0.1054	O	0	0	0	0	0
3.2150	2.6527	-0.5415	C	0	0	0	0	0
4.4924	3.4111	-0.0729	C	0	0	0	0	0
5.7615	2.7472	-0.4504	N	0	0	0	0	0
-0.9183	-2.1314	0.1885	C	0	0	0	0	0
-0.4019	-3.2518	-0.3158	C	0	0	0	0	0
1.0410	-3.4962	-0.2708	C	0	0	0	0	0
1.8483	-2.6059	0.2997	C	0	0	0	0	0
1.2877	-1.4109	0.9143	C	0	0	0	0	0
-0.0251	-1.1931	0.8693	C	0	0	0	0	0
3.2224	-2.8168	0.3131	O	0	0	0	0	0
5.8787	1.4457	0.2636	C	0	0	0	0	0
7.2236	0.7607	-0.0872	C	0	0	0	0	0
8.3855	1.6819	0.3261	C	0	0	0	0	0
8.2372	3.0189	-0.4138	C	0	0	0	0	0
6.8752	3.6430	-0.0461	C	0	0	0	0	0
-7.9295	-0.7061	-0.0318	H	0	0	0	0	0
-5.6135	-4.3757	-0.2106	H	0	0	0	0	0
-5.7020	0.6172	0.0738	H	0	0	0	0	0
-8.7019	-3.0932	0.7071	H	0	0	0	0	0
-2.8478	-4.0485	-0.1661	H	0	0	0	0	0
-3.6788	1.2137	-0.6954	H	0	0	0	0	0
-3.3963	1.1378	1.0607	H	0	0	0	0	0
-0.9320	0.2551	-1.6463	H	0	0	0	0	0
1.4231	1.3395	-1.5529	H	0	0	0	0	0
-0.0955	4.1562	1.3168	H	0	0	0	0	0
-2.2335	3.0612	1.3362	H	0	0	0	0	0
3.2596	1.6069	-0.2374	H	0	0	0	0	0
3.1122	2.7125	-1.6250	H	0	0	0	0	0
4.4816	4.4066	-0.5167	H	0	0	0	0	0
4.4607	3.4966	1.0133	H	0	0	0	0	0
-1.0607	-3.9940	-0.7665	H	0	0	0	0	0
1.4535	-4.4071	-0.7045	H	0	0	0	0	0
1.9425	-0.6949	1.4110	H	0	0	0	0	0
-0.4398	-0.3047	1.3456	H	0	0	0	0	0
3.4348	-3.7110	0.8208	H	0	0	0	0	0
5.8334	1.6198	1.3386	H	0	0	0	0	0
5.0557	0.7963	-0.0348	H	0	0	0	0	0
7.3009	-0.1855	0.4483	H	0	0	0	0	0
7.2692	0.5762	-1.1605	H	0	0	0	0	0

		8.2836		2.8491		-1.4895	H	0	0	0	0	0
		6.8336		3.8016		1.0315	H	0	0	0	0	0
		6.7696		4.5990		-0.5589	H	0	0	0	0	0
		5.7884		2.5866		-1.5079	H	0	0	0	0	0
2	1	1	0	0	0							
6	1	2	0	0	0							
34	1	1	0	0	0							
3	2	2	0	0	0							
7	2	1	0	0	0							
4	3	1	0	0	0							
35	3	1	0	0	0							
5	4	2	0	0	0							
8	4	1	0	0	0							
6	5	1	0	0	0							
10	5	1	0	0	0							
36	6	1	0	0	0							
37	7	1	0	0	0							
9	8	2	0	0	0							
38	8	1	0	0	0							
10	9	1	0	0	0							
22	9	1	0	0	0							
11	10	1	0	0	0							
12	11	1	0	0	0							
39	11	1	0	0	0							
40	11	1	0	0	0							
13	12	1	0	0	0							
17	12	2	0	0	0							
14	13	2	0	0	0							
41	13	1	0	0	0							
15	14	1	0	0	0							
42	14	1	0	0	0							
16	15	2	0	0	0							
18	15	1	0	0	0							
17	16	1	0	0	0							
43	16	1	0	0	0							
44	17	1	0	0	0							
19	18	1	0	0	0							
20	19	1	0	0	0							
45	19	1	0	0	0							
46	19	1	0	0	0							
21	20	1	0	0	0							
47	20	1	0	0	0							
48	20	1	0	0	0							
29	21	1	0	0	0							
33	21	1	0	0	0							
64	21	1	0	0	0							
23	22	1	0	0	0							
27	22	2	0	0	0							
24	23	2	0	0	0							
49	23	1	0	0	0							
25	24	1	0	0	0							
50	24	1	0	0	0							
26	25	2	0	0	0							

52	27	1	0	0	0
53	28	1	0	0	0
30	29	1	0	0	0
54	29	1	0	0	0
55	29	1	0	0	0
31	30	1	0	0	0
56	30	1	0	0	0
57	30	1	0	0	0
32	31	1	0	0	0
58	31	1	0	0	0
59	31	1	0	0	0
33	32	1	0	0	0
60	32	1	0	0	0
61	32	1	0	0	0
62	33	1	0	0	0
63	33	1	0	0	0

M END

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Forecaster10031114513D

66	70	0	0	0	0	0	0	0	0	0999	V2000					
-7.2166		0.7634		0.1802	C	0	0	0	0	0						
-7.3288		-0.5618		0.1712	C	0	0	0	0	0						
-6.1292		-1.3853		0.1479	C	0	0	0	0	0						
-4.9178		-0.8189		0.1122	C	0	0	0	0	0						
-4.7918		0.6131		0.1064	C	0	0	0	0	0						
-5.8814		1.3793		0.1513	C	0	0	0	0	0						
-8.5857		-1.1639		0.1843	O	0	0	0	0	0						
-3.7455		-1.6761		0.1045	C	0	0	0	0	0						
-2.4944		-1.1404		-0.0772	C	0	0	0	0	0						
-2.4232		0.4512		-0.3368	C	0	0	0	0	0						
-3.5676		1.1779		0.0576	O	0	0	0	0	0						
-4.0567		-3.1595		0.2408	C	0	0	0	0	0						
-1.1844		-2.0430		-0.1441	C	0	0	0	0	0						
-1.0425		-3.1716		0.5625	C	0	0	0	0	0						
0.1897		-3.9537		0.5331	C	0	0	0	0	0						
1.2170		-3.5502		-0.2047	C	0	0	0	0	0						
1.0992		-2.3404		-1.0047	C	0	0	0	0	0						
-0.0299		-1.6335		-0.9867	C	0	0	0	0	0						
2.3978		-4.2839		-0.2131	O	0	0	0	0	0						
-1.1355		1.2909		-0.0006	C	0	0	0	0	0						
-0.1078		0.8309		0.7208	C	0	0	0	0	0						
1.1618		1.5821		0.7901	C	0	0	0	0	0						
1.2729		2.7567		0.1702	C	0	0	0	0	0						
0.1067		3.3211		-0.5087	C	0	0	0	0	0						
-1.0247		2.6238		-0.6010	C	0	0	0	0	0						
2.5087		3.4405		0.0732	O	0	0	0	0	0						
3.6385		2.7008		0.5976	C	0	0	0	0	0						
4.9243		3.4696		0.1651	C	0	0	0	0	0						
6.1855		2.7512		0.4887	N	0	0	0	0	0						
6.2547		1.4705		-0.2681	C	0	0	0	0	0						
7.5823		0.7332		0.0465	C	0	0	0	0	0						

-8.1087	1.3891	0.2088	H	0	0	0	0	0
-6.2184	-2.4716	0.1596	H	0	0	0	0	0
-5.7827	2.4647	0.1666	H	0	0	0	0	0
-9.1033	-0.8759	1.0513	H	0	0	0	0	0
-2.4678	0.5143	-1.4241	H	0	0	0	0	0
-3.1275	-3.7290	0.2261	H	0	0	0	0	0
-4.6895	-3.4762	-0.5883	H	0	0	0	0	0
-4.5763	-3.3372	1.1824	H	0	0	0	0	0
-1.8727	-3.5169	1.1786	H	0	0	0	0	0
0.2665	-4.8704	1.1178	H	0	0	0	0	0
1.9367	-2.0118	-1.6201	H	0	0	0	0	0
-0.1089	-0.7372	-1.6019	H	0	0	0	0	0
2.7882	-4.3308	0.7605	H	0	0	0	0	0
-0.2083	-0.1089	1.2637	H	0	0	0	0	0
2.0064	1.1767	1.3472	H	0	0	0	0	0
0.1638	4.3195	-0.9423	H	0	0	0	0	0
-1.8780	3.0493	-1.1291	H	0	0	0	0	0
3.5806	2.6496	1.6849	H	0	0	0	0	0
3.6492	1.6916	0.1859	H	0	0	0	0	0
4.8849	3.6277	-0.9127	H	0	0	0	0	0
4.9367	4.4334	0.6740	H	0	0	0	0	0
5.4149	0.8374	0.0183	H	0	0	0	0	0
6.2042	1.6806	-1.3365	H	0	0	0	0	0
7.6343	0.5159	1.1134	H	0	0	0	0	0
7.6237	-0.1989	-0.5171	H	0	0	0	0	0
9.7050	1.1284	-0.1126	H	0	0	0	0	0
8.7289	1.8327	-1.4244	H	0	0	0	0	0
8.7264	2.7447	1.4958	H	0	0	0	0	0
9.4897	3.6056	0.1372	H	0	0	0	0	0
7.2528	4.5669	0.6446	H	0	0	0	0	0
7.2713	3.8221	-0.9723	H	0	0	0	0	0
6.2277	2.5520	1.5392	H	0	0	0	0	0

2	1	1	0	0	0
6	1	2	0	0	0
35	1	1	0	0	0
3	2	2	0	0	0
7	2	1	0	0	0
4	3	1	0	0	0
36	3	1	0	0	0
5	4	2	0	0	0
8	4	1	0	0	0
6	5	1	0	0	0
11	5	1	0	0	0
37	6	1	0	0	0
38	7	1	0	0	0
9	8	2	0	0	0
12	8	1	0	0	0
10	9	1	0	0	0
13	9	1	0	0	0
11	10	1	0	0	0
20	10	1	0	0	0
39	10	1	0	0	0
40	12	1	0	0	0

18	13	2	0	0	0
15	14	2	0	0	0
43	14	1	0	0	0
16	15	1	0	0	0
44	15	1	0	0	0
17	16	2	0	0	0
19	16	1	0	0	0
18	17	1	0	0	0
45	17	1	0	0	0
46	18	1	0	0	0
47	19	1	0	0	0
21	20	1	0	0	0
25	20	2	0	0	0
22	21	2	0	0	0
48	21	1	0	0	0
23	22	1	0	0	0
49	22	1	0	0	0
24	23	2	0	0	0
26	23	1	0	0	0
25	24	1	0	0	0
50	24	1	0	0	0
51	25	1	0	0	0
27	26	1	0	0	0
28	27	1	0	0	0
52	27	1	0	0	0
53	27	1	0	0	0
29	28	1	0	0	0
54	28	1	0	0	0
55	28	1	0	0	0
30	29	1	0	0	0
34	29	1	0	0	0
66	29	1	0	0	0
31	30	1	0	0	0
56	30	1	0	0	0
57	30	1	0	0	0
32	31	1	0	0	0
58	31	1	0	0	0
59	31	1	0	0	0
33	32	1	0	0	0
60	32	1	0	0	0
61	32	1	0	0	0
34	33	1	0	0	0
62	33	1	0	0	0
63	33	1	0	0	0
64	34	1	0	0	0
65	34	1	0	0	0

M END

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clomiphene

Forecaster10031114513D

59 61 0 0 0 0 0 0 0 0999 V2000

-4 2903 -3 3308 0 1495 C 0 0 0 0 0

-1.8421	-3.2695	0.0496	C	0	0	0	0	0
-3.0018	-2.6242	0.1807	C	0	0	0	0	0
-0.4585	-2.4857	0.0804	C	0	0	0	0	0
0.7515	-3.1687	0.1021	C	0	0	0	0	0
-0.5325	-0.9142	0.1114	C	0	0	0	0	0
0.3264	-0.2241	0.8681	C	0	0	0	0	0
0.3810	1.2197	0.8403	C	0	0	0	0	0
-0.4545	1.9172	0.0757	C	0	0	0	0	0
-1.4919	1.2020	-0.6719	C	0	0	0	0	0
-1.5293	-0.1311	-0.6629	C	0	0	0	0	0
-0.3443	3.3337	-0.0738	O	0	0	0	0	0
0.8389	3.9446	0.5407	C	0	0	0	0	0
2.1378	3.6078	-0.2997	C	0	0	0	0	0
3.3189	4.3437	0.1913	N	0	0	0	0	0
3.1289	5.7750	-0.0991	C	0	0	0	0	0
4.3581	6.5793	0.3718	C	0	0	0	0	0
4.5353	3.8643	-0.5025	C	0	0	0	0	0
4.8100	2.3950	-0.1366	C	0	0	0	0	0
0.8289	-4.9009	0.2258	C1	0	0	0	0	0
2.1927	-2.6133	-0.0133	C	0	0	0	0	0
3.1780	-3.4088	0.3925	C	0	0	0	0	0
4.5820	-2.9943	0.2823	C	0	0	0	0	0
4.8953	-1.8228	-0.2643	C	0	0	0	0	0
3.8417	-0.9589	-0.7672	C	0	0	0	0	0
2.5686	-1.3263	-0.6580	C	0	0	0	0	0
-5.5415	-5.3236	-0.0379	O	0	0	0	0	0
-5.2199	-2.7716	0.2554	H	0	0	0	0	0
-3.1054	-6.4670	-0.2737	H	0	0	0	0	0
-0.9995	-5.3090	-0.2312	H	0	0	0	0	0
-2.9939	-1.5425	0.3147	H	0	0	0	0	0
1.0058	-0.7664	1.5257	H	0	0	0	0	0
1.1152	1.7430	1.4528	H	0	0	0	0	0
-2.2364	1.7619	-1.2379	H	0	0	0	0	0
-2.3004	-0.6521	-1.2304	H	0	0	0	0	0
0.7060	5.0258	0.5771	H	0	0	0	0	0
0.9568	3.5582	1.5531	H	0	0	0	0	0
2.3352	2.5381	-0.2291	H	0	0	0	0	0
1.9629	3.8776	-1.3412	H	0	0	0	0	0
2.9992	5.9107	-1.1728	H	0	0	0	0	0
2.2418	6.1339	0.4228	H	0	0	0	0	0
4.2072	7.6362	0.1523	H	0	0	0	0	0
5.2470	6.2238	-0.1494	H	0	0	0	0	0
4.4899	6.4470	1.4457	H	0	0	0	0	0
4.3914	3.9463	-1.5798	H	0	0	0	0	0
5.3861	4.4755	-0.2015	H	0	0	0	0	0
5.7071	2.0531	-0.6527	H	0	0	0	0	0
3.9617	1.7803	-0.4377	H	0	0	0	0	0
4.9561	2.3094	0.9402	H	0	0	0	0	0
2.9391	-4.3852	0.8141	H	0	0	0	0	0
5.3715	-3.6497	0.6501	H	0	0	0	0	0
5.9379	-1.5126	-0.3344	H	0	0	0	0	0
4.0952	-0.0076	-1.2350	H	0	0	0	0	0
1.7872	-0.6736	-1.0473	H	0	0	0	0	0

6	1	2	0	0	0
31	1	1	0	0	0
3	2	2	0	0	0
30	2	1	0	0	0
4	3	1	0	0	0
32	3	1	0	0	0
5	4	2	0	0	0
33	4	1	0	0	0
6	5	1	0	0	0
7	5	1	0	0	0
34	6	1	0	0	0
8	7	2	0	0	0
9	7	1	0	0	0
23	8	1	0	0	0
24	8	1	0	0	0
10	9	1	0	0	0
14	9	2	0	0	0
11	10	2	0	0	0
35	10	1	0	0	0
12	11	1	0	0	0
36	11	1	0	0	0
13	12	2	0	0	0
15	12	1	0	0	0
14	13	1	0	0	0
37	13	1	0	0	0
38	14	1	0	0	0
16	15	1	0	0	0
17	16	1	0	0	0
39	16	1	0	0	0
40	16	1	0	0	0
18	17	1	0	0	0
41	17	1	0	0	0
42	17	1	0	0	0
19	18	1	0	0	0
21	18	1	0	0	0
59	18	1	0	0	0
20	19	1	0	0	0
43	19	1	0	0	0
44	19	1	0	0	0
45	20	1	0	0	0
46	20	1	0	0	0
47	20	1	0	0	0
22	21	1	0	0	0
48	21	1	0	0	0
49	21	1	0	0	0
50	22	1	0	0	0
51	22	1	0	0	0
52	22	1	0	0	0
25	24	1	0	0	0
29	24	2	0	0	0
26	25	2	0	0	0
53	25	1	0	0	0
27	26	1	0	0	0

Forecaster10031114513D

59 61 0 0 0 0 0 0 0 0999 v2000

-4.1804	-2.3547	0.2103	C	0	0	0	0	0
-4.2992	-3.6609	0.0035	C	0	0	0	0	0
-3.1094	-4.4633	-0.1853	C	0	0	0	0	0
-1.9072	-3.8926	-0.1548	C	0	0	0	0	0
-1.7218	-2.4201	0.0767	C	0	0	0	0	0
-2.8532	-1.7240	0.2468	C	0	0	0	0	0
-0.2892	-1.6402	0.1034	C	0	0	0	0	0
0.9597	-2.2916	0.1808	C	0	0	0	0	0
-0.3789	-0.0613	0.0935	C	0	0	0	0	0
0.4436	0.6584	0.8612	C	0	0	0	0	0
0.4560	2.1038	0.8279	C	0	0	0	0	0
-0.3927	2.7766	0.0526	C	0	0	0	0	0
-1.3880	2.0310	-0.7173	C	0	0	0	0	0
-1.3817	0.6964	-0.7111	C	0	0	0	0	0
-0.3300	4.1986	-0.0743	O	0	0	0	0	0
0.8383	4.7958	0.5622	C	0	0	0	0	0
2.0955	4.5666	-0.3638	C	0	0	0	0	0
3.3237	5.1201	0.2195	N	0	0	0	0	0
3.2240	6.5849	0.2830	C	0	0	0	0	0
4.4655	4.7467	-0.6307	C	0	0	0	0	0
1.0355	-3.8228	0.4197	C	0	0	0	0	0
2.3861	-1.5872	0.0482	C	0	0	0	0	0
3.4492	-2.0961	0.6853	C	0	0	0	0	0
4.7797	-1.4821	0.5635	C	0	0	0	0	0
4.9617	-0.4065	-0.1979	C	0	0	0	0	0
3.8392	0.1571	-0.9305	C	0	0	0	0	0
2.6326	-0.3962	-0.8298	C	0	0	0	0	0
-5.5576	-4.2556	-0.0327	O	0	0	0	0	0
1.9725	-4.6236	-0.5350	C	0	0	0	0	0
1.9234	-6.3327	-0.0772	C1	0	0	0	0	0
-5.0731	-1.7460	0.3540	H	0	0	0	0	0
-3.1980	-5.5367	-0.3527	H	0	0	0	0	0
-1.0256	-4.5162	-0.3031	H	0	0	0	0	0
-2.7874	-0.6497	0.4187	H	0	0	0	0	0
1.1268	0.1399	1.5338	H	0	0	0	0	0
1.1692	2.6500	1.4453	H	0	0	0	0	0
-2.1380	2.5675	-1.2985	H	0	0	0	0	0
-2.1189	0.1525	-1.3017	H	0	0	0	0	0
0.6744	5.8647	0.6990	H	0	0	0	0	0
1.0071	4.3266	1.5314	H	0	0	0	0	0
2.2302	3.4954	-0.5134	H	0	0	0	0	0
1.9157	5.0484	-1.3248	H	0	0	0	0	0
4.1369	6.9933	0.7163	H	0	0	0	0	0

4.3199	5.1496	-1.6330	H	0	0	0	0	0
4.5400	3.6605	-0.6834	H	0	0	0	0	0
1.3849	-3.9831	1.4397	H	0	0	0	0	0
0.0286	-4.2261	0.3124	H	0	0	0	0	0
3.3253	-2.9832	1.3064	H	0	0	0	0	0
5.6244	-1.9120	1.1018	H	0	0	0	0	0
5.9485	0.0505	-0.2723	H	0	0	0	0	0
3.9858	1.0330	-1.5624	H	0	0	0	0	0
1.8043	0.0261	-1.3987	H	0	0	0	0	0
-6.0442	-4.1025	0.8851	H	0	0	0	0	0
1.6313	-4.5098	-1.5640	H	0	0	0	0	0
2.9925	-4.2495	-0.4464	H	0	0	0	0	0
3.4640	4.7258	1.2043	H	0	0	0	0	0

2	1	1	0	0	0
6	1	2	0	0	0
31	1	1	0	0	0
3	2	2	0	0	0
28	2	1	0	0	0
4	3	1	0	0	0
32	3	1	0	0	0
5	4	2	0	0	0
33	4	1	0	0	0
6	5	1	0	0	0
7	5	1	0	0	0
34	6	1	0	0	0
8	7	2	0	0	0
9	7	1	0	0	0
21	8	1	0	0	0
22	8	1	0	0	0
10	9	1	0	0	0
14	9	2	0	0	0
11	10	2	0	0	0
35	10	1	0	0	0
12	11	1	0	0	0
36	11	1	0	0	0
13	12	2	0	0	0
15	12	1	0	0	0
14	13	1	0	0	0
37	13	1	0	0	0
38	14	1	0	0	0
16	15	1	0	0	0
17	16	1	0	0	0
39	16	1	0	0	0
40	16	1	0	0	0
18	17	1	0	0	0
41	17	1	0	0	0
42	17	1	0	0	0
19	18	1	0	0	0
20	18	1	0	0	0
59	18	1	0	0	0
43	19	1	0	0	0
44	19	1	0	0	0
45	19	1	0	0	0

29	21	1	0	0	0
49	21	1	0	0	0
50	21	1	0	0	0
23	22	1	0	0	0
27	22	2	0	0	0
24	23	2	0	0	0
51	23	1	0	0	0
25	24	1	0	0	0
52	24	1	0	0	0
26	25	2	0	0	0
53	25	1	0	0	0
27	26	1	0	0	0
54	26	1	0	0	0
55	27	1	0	0	0
56	28	1	0	0	0
30	29	1	0	0	0
57	29	1	0	0	0
58	29	1	0	0	0

M END

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benzothiophene_1

Forecaster10031114513D

61	65	0	0	0	0	0	0	0	0	0999	V2000						
-7.4901	-1.1614	-0.0573	C	0	0	0	0	0	0								
-7.6071	-2.4946	-0.1168	C	0	0	0	0	0	0								
-6.3993	-3.3351	-0.1551	C	0	0	0	0	0	0								
-5.2257	-2.7174	-0.1218	C	0	0	0	0	0	0								
-5.0761	-1.3114	-0.0445	C	0	0	0	0	0	0								
-6.1513	-0.5261	-0.0166	C	0	0	0	0	0	0								
-3.7337	-3.3837	-0.1535	S	0	0	0	0	0	0								
-2.7761	-1.9827	0.0056	C	0	0	0	0	0	0								
-3.5956	-0.8627	0.0139	C	0	0	0	0	0	0								
-3.2903	0.6798	0.0926	C	0	0	0	0	0	0								
-1.2910	-2.1765	0.1478	C	0	0	0	0	0	0								
-0.7451	-3.2310	-0.4579	C	0	0	0	0	0	0								
0.7009	-3.4610	-0.3938	C	0	0	0	0	0	0								
1.4789	-2.6349	0.3012	C	0	0	0	0	0	0								
0.8842	-1.5293	1.0397	C	0	0	0	0	0	0								
-0.4297	-1.3208	0.9795	C	0	0	0	0	0	0								
2.8558	-2.8298	0.3287	O	0	0	0	0	0	0								
-4.2317	1.4121	0.4173	O	0	0	0	0	0	0								
-1.9877	1.4074	-0.1302	C	0	0	0	0	0	0								
-0.9582	0.9165	-0.8198	C	0	0	0	0	0	0								
0.3462	1.6098	-0.8147	C	0	0	0	0	0	0								
0.4796	2.7611	-0.1578	C	0	0	0	0	0	0								
-0.6901	3.3674	0.4699	C	0	0	0	0	0	0								
-1.8553	2.7268	0.4828	C	0	0	0	0	0	0								
1.7323	3.3871	0.0110	O	0	0	0	0	0	0								
2.8529	2.6287	-0.4971	C	0	0	0	0	0	0								
4.1370	3.3867	-0.0545	C	0	0	0	0	0	0								
5.3956	2.6893	-0.4152	N	0	0	0	0	0	0								
5.4968	1.3921	0.3080	C	0	0	0	0	0	0								

6.5266	3.5707	-0.0310	C	0	0	0	0	0
-8.3852	-0.5397	-0.0387	H	0	0	0	0	0
-8.5945	-2.9559	-0.1368	H	0	0	0	0	0
-6.4665	-4.4217	-0.2087	H	0	0	0	0	0
-6.0494	0.5579	0.0349	H	0	0	0	0	0
-1.3795	-3.9281	-1.0054	H	0	0	0	0	0
1.1401	-4.3107	-0.9166	H	0	0	0	0	0
1.5138	-0.8734	1.6409	H	0	0	0	0	0
-0.8725	-0.5066	1.5531	H	0	0	0	0	0
3.0679	-3.7754	0.7328	H	0	0	0	0	0
-1.0796	-0.0034	-1.3918	H	0	0	0	0	0
1.1959	1.1812	-1.3461	H	0	0	0	0	0
-0.6081	4.3516	0.9311	H	0	0	0	0	0
-2.7207	3.1910	0.9557	H	0	0	0	0	0
2.8469	1.6223	-0.0786	H	0	0	0	0	0
2.8060	2.5708	-1.5846	H	0	0	0	0	0
4.1387	4.3674	-0.5302	H	0	0	0	0	0
4.1090	3.5076	1.0284	H	0	0	0	0	0
5.4687	1.5749	1.3822	H	0	0	0	0	0
4.6586	0.7552	0.0253	H	0	0	0	0	0
6.8958	-0.2616	0.4832	H	0	0	0	0	0
6.8543	0.4907	-1.1298	H	0	0	0	0	0
7.9961	1.7637	1.4097	H	0	0	0	0	0
8.9471	1.1056	0.0562	H	0	0	0	0	0
8.6914	3.5846	-0.1263	H	0	0	0	0	0
7.9048	2.7463	-1.4857	H	0	0	0	0	0
6.5005	3.7379	1.0458	H	0	0	0	0	0
6.4295	4.5244	-0.5498	H	0	0	0	0	0
5.4193	2.5146	-1.4706	H	0	0	0	0	0
2	1	1	0	0	0			
6	1	2	0	0	0			
34	1	1	0	0	0			
3	2	2	0	0	0			
35	2	1	0	0	0			
4	3	1	0	0	0			
36	3	1	0	0	0			
5	4	2	0	0	0			
7	4	1	0	0	0			
6	5	1	0	0	0			
9	5	1	0	0	0			
37	6	1	0	0	0			
8	7	1	0	0	0			
9	8	2	0	0	0			
11	8	1	0	0	0			
10	9	1	0	0	0			
18	10	2	0	0	0			
19	10	1	0	0	0			
12	11	1	0	0	0			
16	11	2	0	0	0			
13	12	2	0	0	0			
38	12	1	0	0	0			
14	13	1	0	0	0			
39	13	1	0	0	0			

40	15	1	0	0	0
41	16	1	0	0	0
42	17	1	0	0	0
20	19	1	0	0	0
24	19	2	0	0	0
21	20	2	0	0	0
43	20	1	0	0	0
22	21	1	0	0	0
44	21	1	0	0	0
23	22	2	0	0	0
25	22	1	0	0	0
24	23	1	0	0	0
45	23	1	0	0	0
46	24	1	0	0	0
26	25	1	0	0	0
27	26	1	0	0	0
47	26	1	0	0	0
48	26	1	0	0	0
28	27	1	0	0	0
49	27	1	0	0	0
50	27	1	0	0	0
29	28	1	0	0	0
33	28	1	0	0	0
61	28	1	0	0	0
30	29	1	0	0	0
51	29	1	0	0	0
52	29	1	0	0	0
31	30	1	0	0	0
53	30	1	0	0	0
54	30	1	0	0	0
32	31	1	0	0	0
55	31	1	0	0	0
56	31	1	0	0	0
33	32	1	0	0	0
57	32	1	0	0	0
58	32	1	0	0	0
59	33	1	0	0	0
60	33	1	0	0	0

M END

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benzothiophene_2

Forecaster10031114513D

65	69	0	0	0	0	0	0	0	0	0999	V2000					
-6.9300	-0.7279	-0.0282	C	0	0	0	0	0	0							
-7.0373	-2.0632	-0.0619	C	0	0	0	0	0	0							
-5.8137	-2.8910	-0.1084	C	0	0	0	0	0	0							
-4.6473	-2.2590	-0.1012	C	0	0	0	0	0	0							
-4.5119	-0.8507	-0.0419	C	0	0	0	0	0	0							
-5.5961	-0.0769	-0.0151	C	0	0	0	0	0	0							
-3.1483	-2.9094	-0.1425	S	0	0	0	0	0	0							
-2.2046	-1.4985	0.0039	C	0	0	0	0	0	0							
-3.0346	-0.3856	0.0077	C	0	0	0	0	0	0							

1.2922	-2.9257	-0.3967	C	0	0	0	0	0
2.0559	-2.0956	0.3095	C	0	0	0	0	0
1.4431	-1.0052	1.0562	C	0	0	0	0	0
0.1270	-0.8138	0.9918	C	0	0	0	0	0
3.4350	-2.2717	0.3408	O	0	0	0	0	0
-3.6842	1.8866	0.4053	O	0	0	0	0	0
-1.4352	1.8939	-0.1398	C	0	0	0	0	0
-0.4033	1.4071	-0.8307	C	0	0	0	0	0
0.9012	2.1031	-0.8227	C	0	0	0	0	0
1.0331	3.2518	-0.1610	C	0	0	0	0	0
-0.1391	3.8536	0.4688	C	0	0	0	0	0
-1.3040	3.2115	0.4783	C	0	0	0	0	0
2.2859	3.8812	0.0108	O	0	0	0	0	0
3.4129	3.1306	-0.4995	C	0	0	0	0	0
4.6927	3.8994	-0.0570	C	0	0	0	0	0
5.9602	3.2153	-0.4177	N	0	0	0	0	0
6.0772	1.9199	0.3064	C	0	0	0	0	0
7.4162	1.2261	-0.0575	C	0	0	0	0	0
8.5882	2.1449	0.3338	C	0	0	0	0	0
8.4366	3.4776	-0.4123	C	0	0	0	0	0
7.0815	4.1103	-0.0340	C	0	0	0	0	0
-8.3109	-2.6581	-0.0468	O	0	0	0	0	0
-8.2150	-4.0902	-0.0669	C	0	0	0	0	0
-7.8306	-0.1141	-0.0102	H	0	0	0	0	0
-5.8676	-3.9790	-0.1471	H	0	0	0	0	0
-5.5057	1.0089	0.0157	H	0	0	0	0	0
-0.7790	-3.4169	-1.0210	H	0	0	0	0	0
1.7455	-3.7640	-0.9257	H	0	0	0	0	0
2.0611	-0.3469	1.6668	H	0	0	0	0	0
-0.3295	-0.0110	1.5708	H	0	0	0	0	0
3.6586	-3.2182	0.7367	H	0	0	0	0	0
-0.5227	0.4889	-1.4058	H	0	0	0	0	0
1.7515	1.6781	-1.3560	H	0	0	0	0	0
-0.0588	4.8359	0.9344	H	0	0	0	0	0
-2.1702	3.6732	0.9523	H	0	0	0	0	0
3.4151	2.1239	-0.0815	H	0	0	0	0	0
3.3655	3.0729	-1.5869	H	0	0	0	0	0
4.6851	4.8804	-0.5320	H	0	0	0	0	0
4.6637	4.0193	1.0260	H	0	0	0	0	0
6.0462	2.1031	1.3804	H	0	0	0	0	0
5.2471	1.2725	0.0236	H	0	0	0	0	0
7.4965	0.2833	0.4836	H	0	0	0	0	0
7.4468	1.0338	-1.1300	H	0	0	0	0	0
8.5721	2.3224	1.4091	H	0	0	0	0	0
9.5316	1.6745	0.0568	H	0	0	0	0	0
9.2462	4.1499	-0.1284	H	0	0	0	0	0
8.4704	3.3009	-1.4873	H	0	0	0	0	0
7.0531	4.2782	1.0426	H	0	0	0	0	0
6.9735	5.0623	-0.5537	H	0	0	0	0	0
-9.2157	-4.5221	-0.0546	H	0	0	0	0	0
-7.6623	-4.4302	0.8090	H	0	0	0	0	0
-7.6941	-4.4073	-0.9704	H	0	0	0	0	0
5.9858	3.0402	-1.4730	H	0	0	0	0	0

3	2	2	0	0	0
34	2	1	0	0	0
4	3	1	0	0	0
37	3	1	0	0	0
5	4	2	0	0	0
7	4	1	0	0	0
6	5	1	0	0	0
9	5	1	0	0	0
38	6	1	0	0	0
8	7	1	0	0	0
9	8	2	0	0	0
11	8	1	0	0	0
10	9	1	0	0	0
18	10	2	0	0	0
19	10	1	0	0	0
12	11	1	0	0	0
16	11	2	0	0	0
13	12	2	0	0	0
39	12	1	0	0	0
14	13	1	0	0	0
40	13	1	0	0	0
15	14	2	0	0	0
17	14	1	0	0	0
16	15	1	0	0	0
41	15	1	0	0	0
42	16	1	0	0	0
43	17	1	0	0	0
20	19	1	0	0	0
24	19	2	0	0	0
21	20	2	0	0	0
44	20	1	0	0	0
22	21	1	0	0	0
45	21	1	0	0	0
23	22	2	0	0	0
25	22	1	0	0	0
24	23	1	0	0	0
46	23	1	0	0	0
47	24	1	0	0	0
26	25	1	0	0	0
27	26	1	0	0	0
48	26	1	0	0	0
49	26	1	0	0	0
28	27	1	0	0	0
50	27	1	0	0	0
51	27	1	0	0	0
29	28	1	0	0	0
33	28	1	0	0	0
65	28	1	0	0	0
30	29	1	0	0	0
52	29	1	0	0	0
53	29	1	0	0	0
31	30	1	0	0	0
54	30	1	0	0	0

Forecaster10031114513D

65 69 0 0 0 0 0 0 0 0999 v2000

-7.10658	-1.1396	-0.0505	C	0	0	0	0	0
-7.1663	-2.4758	-0.0913	C	0	0	0	0	0
-5.9514	-3.3026	-0.1314	C	0	0	0	0	0
-4.7790	-2.6713	-0.1149	C	0	0	0	0	0
-4.6550	-1.2566	-0.0527	C	0	0	0	0	0
-5.7303	-0.4914	-0.0291	C	0	0	0	0	0
-3.2821	-3.3227	-0.1430	S	0	0	0	0	0
-2.3462	-1.9008	0.0151	C	0	0	0	0	0
-3.1663	-0.8057	0.0010	C	0	0	0	0	0
-2.8881	0.7541	0.0804	C	0	0	0	0	0
-0.8540	-2.0809	0.1742	C	0	0	0	0	0
-0.2759	-3.1229	-0.4049	C	0	0	0	0	0
1.1773	-3.3200	-0.3110	C	0	0	0	0	0
1.9253	-2.4689	0.3950	C	0	0	0	0	0
1.2852	-1.3766	1.1105	C	0	0	0	0	0
-0.0317	-1.1967	1.0192	C	0	0	0	0	0
3.3243	-2.6068	0.4591	O	0	0	0	0	0
-3.8256	1.4723	0.3986	O	0	0	0	0	0
-1.5763	1.4810	-0.1473	C	0	0	0	0	0
-0.5507	1.0027	-0.8371	C	0	0	0	0	0
0.7541	1.7000	-0.8306	C	0	0	0	0	0
0.8832	2.8486	-0.1654	C	0	0	0	0	0
-0.2880	3.4457	0.4669	C	0	0	0	0	0
-1.4532	2.8015	0.4769	C	0	0	0	0	0
2.1348	3.4789	0.0067	O	0	0	0	0	0
3.2598	2.7290	-0.5062	C	0	0	0	0	0
4.5421	3.4890	-0.0583	C	0	0	0	0	0
5.8040	2.7959	-0.4194	N	0	0	0	0	0
5.9066	1.4962	0.2993	C	0	0	0	0	0
7.2389	0.7905	-0.0648	C	0	0	0	0	0
8.4190	1.6960	0.3329	C	0	0	0	0	0
8.2824	3.0336	-0.4077	C	0	0	0	0	0
6.9329	3.6783	-0.0294	C	0	0	0	0	0
-8.4209	-3.0804	-0.0937	O	0	0	0	0	0
3.7822	-3.7219	-0.3197	C	0	0	0	0	0
-7.9673	-0.5272	-0.0330	H	0	0	0	0	0
-6.0081	-4.3903	-0.1730	H	0	0	0	0	0

1.8845	-0.7032	1.7232	H	0	0	0	0	0
-0.5056	-0.3876	1.5749	H	0	0	0	0	0
-0.6697	0.0863	-1.4151	H	0	0	0	0	0
1.6044	1.2777	-1.3660	H	0	0	0	0	0
-0.2086	4.4269	0.9348	H	0	0	0	0	0
-2.3209	3.2589	0.9522	H	0	0	0	0	0
3.2579	1.7197	-0.0946	H	0	0	0	0	0
3.2134	2.6784	-1.5940	H	0	0	0	0	0
4.5421	4.4714	-0.5304	H	0	0	0	0	0
4.5118	3.6059	1.0250	H	0	0	0	0	0
5.8754	1.6751	1.3741	H	0	0	0	0	0
5.0706	0.8584	0.0121	H	0	0	0	0	0
7.3086	-0.1553	0.4725	H	0	0	0	0	0
7.2698	0.6025	-1.1380	H	0	0	0	0	0
8.4023	1.8690	1.4090	H	0	0	0	0	0
9.3583	1.2174	0.0558	H	0	0	0	0	0
9.0982	3.6965	-0.1192	H	0	0	0	0	0
8.3167	2.8613	-1.4834	H	0	0	0	0	0
6.9038	3.8419	1.0479	H	0	0	0	0	0
6.8354	4.6335	-0.5453	H	0	0	0	0	0
-8.9400	-2.8140	0.7793	H	0	0	0	0	0
4.8671	-3.7964	-0.2457	H	0	0	0	0	0
3.4987	-3.5784	-1.3624	H	0	0	0	0	0
3.3291	-4.6391	0.0567	H	0	0	0	0	0
5.8302	2.6251	-1.4754	H	0	0	0	0	0
2	1	1	0	0	0			
6	1	2	0	0	0			
36	1	1	0	0	0			
3	2	2	0	0	0			
34	2	1	0	0	0			
4	3	1	0	0	0			
37	3	1	0	0	0			
5	4	2	0	0	0			
7	4	1	0	0	0			
6	5	1	0	0	0			
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38	6	1	0	0	0			
8	7	1	0	0	0			
9	8	2	0	0	0			
11	8	1	0	0	0			
10	9	1	0	0	0			
18	10	2	0	0	0			
19	10	1	0	0	0			
12	11	1	0	0	0			
16	11	2	0	0	0			
13	12	2	0	0	0			
39	12	1	0	0	0			
14	13	1	0	0	0			
40	13	1	0	0	0			
15	14	2	0	0	0			
17	14	1	0	0	0			
16	15	1	0	0	0			
41	15	1	0	0	0			

24	19	2	0	0	0
21	20	2	0	0	0
43	20	1	0	0	0
22	21	1	0	0	0
44	21	1	0	0	0
23	22	2	0	0	0
25	22	1	0	0	0
24	23	1	0	0	0
45	23	1	0	0	0
46	24	1	0	0	0
26	25	1	0	0	0
27	26	1	0	0	0
47	26	1	0	0	0
48	26	1	0	0	0
28	27	1	0	0	0
49	27	1	0	0	0
50	27	1	0	0	0
29	28	1	0	0	0
33	28	1	0	0	0
65	28	1	0	0	0
30	29	1	0	0	0
51	29	1	0	0	0
52	29	1	0	0	0
31	30	1	0	0	0
53	30	1	0	0	0
54	30	1	0	0	0
32	31	1	0	0	0
55	31	1	0	0	0
56	31	1	0	0	0
33	32	1	0	0	0
57	32	1	0	0	0
58	32	1	0	0	0
59	33	1	0	0	0
60	33	1	0	0	0
61	34	1	0	0	0
62	35	1	0	0	0
63	35	1	0	0	0
64	35	1	0	0	0

M END

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benzothiophene_4

Forecaster10031114513D

64	68	0	0	0	0	0	0	0	0	0999	V2000					
-6.9971	-0.7392	0.0705	C	0	0	0	0	0	0							
-7.1568	-2.0688	0.0545	C	0	0	0	0	0	0							
-5.9796	-2.9408	0.0373	C	0	0	0	0	0	0							
-4.7887	-2.3594	0.0320	C	0	0	0	0	0	0							
-4.5834	-0.9684	0.0358	C	0	0	0	0	0	0							
-5.6346	-0.1467	0.0595	C	0	0	0	0	0	0							
-3.3428	-3.0749	0.0074	S	0	0	0	0	0	0							
-2.2842	-1.7211	-0.0566	C	0	0	0	0	0	0							
-3.0759	-0.5658	-0.0108	C	0	0	0	0	0	0							

1.3359	-3.2494	-0.0201	C	0	0	0	0	0
2.0533	-2.3215	-0.6373	C	0	0	0	0	0
1.3959	-1.1435	-1.1438	C	0	0	0	0	0
0.0857	-0.9843	-0.9716	C	0	0	0	0	0
-3.6897	1.7296	-0.3494	O	0	0	0	0	0
-1.4522	1.7140	0.1688	C	0	0	0	0	0
-0.4129	1.2332	0.8516	C	0	0	0	0	0
0.8831	1.9487	0.8341	C	0	0	0	0	0
0.9983	3.1012	0.1733	C	0	0	0	0	0
-0.1811	3.6910	-0.4495	C	0	0	0	0	0
-1.3375	3.0358	-0.4503	C	0	0	0	0	0
2.2426	3.7443	-0.0026	O	0	0	0	0	0
3.3738	3.0017	0.5059	C	0	0	0	0	0
4.6507	3.7690	0.0571	C	0	0	0	0	0
5.9162	3.0828	0.4193	N	0	0	0	0	0
6.0258	1.7825	-0.2970	C	0	0	0	0	0
7.3616	1.0843	0.0691	C	0	0	0	0	0
8.5371	1.9950	-0.3298	C	0	0	0	0	0
8.3930	3.3331	0.4085	C	0	0	0	0	0
7.0404	3.9702	0.0285	C	0	0	0	0	0
-8.4334	-2.6241	0.0530	O	0	0	0	0	0
-0.7994	-4.2000	0.9198	C	0	0	0	0	0
-7.8712	-0.0884	0.0917	H	0	0	0	0	0
-6.0795	-4.0262	0.0292	H	0	0	0	0	0
-5.4968	0.9345	0.0705	H	0	0	0	0	0
1.8275	-4.1525	0.3417	H	0	0	0	0	0
3.1289	-2.4481	-0.7604	H	0	0	0	0	0
1.9724	-0.3817	-1.6687	H	0	0	0	0	0
-0.3934	-0.0974	-1.3864	H	0	0	0	0	0
-0.5176	0.3114	1.4239	H	0	0	0	0	0
1.7424	1.5338	1.3609	H	0	0	0	0	0
-0.1140	4.6736	-0.9165	H	0	0	0	0	0
-2.2119	3.4884	-0.9180	H	0	0	0	0	0
3.3302	2.9492	1.5938	H	0	0	0	0	0
3.3772	1.9930	0.0928	H	0	0	0	0	0
4.6198	3.8847	-1.0263	H	0	0	0	0	0
4.6451	4.7519	0.5283	H	0	0	0	0	0
5.1929	1.1410	-0.0091	H	0	0	0	0	0
5.9942	1.9593	-1.3721	H	0	0	0	0	0
7.3930	0.8985	1.1427	H	0	0	0	0	0
7.4364	0.1378	-0.4663	H	0	0	0	0	0
9.4788	1.5218	-0.0515	H	0	0	0	0	0
8.5200	2.1660	-1.4062	H	0	0	0	0	0
8.4276	3.1627	1.4845	H	0	0	0	0	0
9.2054	3.9998	0.1193	H	0	0	0	0	0
6.9377	4.9258	0.5428	H	0	0	0	0	0
7.0110	4.1319	-1.0490	H	0	0	0	0	0
-8.9485	-2.3209	0.9163	H	0	0	0	0	0
-0.0776	-4.9830	1.1521	H	0	0	0	0	0
-1.5923	-4.6112	0.2950	H	0	0	0	0	0
-1.2288	-3.8162	1.8453	H	0	0	0	0	0
5.9430	2.9139	1.4755	H	0	0	0	0	0

33	2	1	0	0	0
4	3	1	0	0	0
36	3	1	0	0	0
5	4	2	0	0	0
7	4	1	0	0	0
6	5	1	0	0	0
9	5	1	0	0	0
37	6	1	0	0	0
8	7	1	0	0	0
9	8	2	0	0	0
11	8	1	0	0	0
10	9	1	0	0	0
17	10	2	0	0	0
18	10	1	0	0	0
12	11	1	0	0	0
16	11	2	0	0	0
13	12	2	0	0	0
34	12	1	0	0	0
14	13	1	0	0	0
38	13	1	0	0	0
15	14	2	0	0	0
39	14	1	0	0	0
16	15	1	0	0	0
40	15	1	0	0	0
41	16	1	0	0	0
19	18	1	0	0	0
23	18	2	0	0	0
20	19	2	0	0	0
42	19	1	0	0	0
21	20	1	0	0	0
43	20	1	0	0	0
22	21	2	0	0	0
24	21	1	0	0	0
23	22	1	0	0	0
44	22	1	0	0	0
45	23	1	0	0	0
25	24	1	0	0	0
26	25	1	0	0	0
46	25	1	0	0	0
47	25	1	0	0	0
27	26	1	0	0	0
48	26	1	0	0	0
49	26	1	0	0	0
28	27	1	0	0	0
32	27	1	0	0	0
64	27	1	0	0	0
29	28	1	0	0	0
50	28	1	0	0	0
51	28	1	0	0	0
30	29	1	0	0	0
52	29	1	0	0	0
53	29	1	0	0	0
31	30	1	0	0	0

Forecaster10031114513D

	54	57	0	0	0	0	0	0	0999	V2000					
-6.9817				-1.3428				-0.0082	C	0	0	0	0	0	0
-7.1389				-2.6740				-0.0189	C	0	0	0	0	0	0
-5.9625				-3.5493				-0.0305	C	0	0	0	0	0	0
-4.7719				-2.9694				-0.0290	C	0	0	0	0	0	0
-4.5720				-1.5631				-0.0154	C	0	0	0	0	0	0
-5.6223				-0.7434				-0.0057	C	0	0	0	0	0	0
-3.3114				-3.6910				-0.0374	S	0	0	0	0	0	0
-2.3107				-2.3211				-0.0157	C	0	0	0	0	0	0
-3.0714				-1.1686				-0.0079	C	0	0	0	0	0	0
-2.6811				0.3714				0.0282	C	0	0	0	0	0	0
-0.8322				-2.5185				0.0110	C	0	0	0	0	0	0
-3.6276				1.1638				0.1122	O	0	0	0	0	0	0
-1.3145				1.0611				0.0006	C	0	0	0	0	0	0
-0.1541				0.4410				-0.1785	C	0	0	0	0	0	0
1.1153				1.1606				-0.1714	C	0	0	0	0	0	0
1.1338				2.4752				0.0196	C	0	0	0	0	0	0
-0.1332				3.1890				0.2026	C	0	0	0	0	0	0
-1.2890				2.5224				0.1881	C	0	0	0	0	0	0
2.3488				3.1854				0.0574	O	0	0	0	0	0	0
3.4988				2.3362				-0.1647	C	0	0	0	0	0	0
4.7711				3.1920				0.0350	C	0	0	0	0	0	0
6.0096				2.4600				-0.3164	N	0	0	0	0	0	0
6.1608				1.2349				0.5077	C	0	0	0	0	0	0
7.4607				0.4927				0.1077	C	0	0	0	0	0	0
8.6640				1.4232				0.3419	C	0	0	0	0	0	0
8.4767				2.6923				-0.5012	C	0	0	0	0	0	0
7.1559				3.3742				-0.0945	C	0	0	0	0	0	0
-8.4145				-3.2293				-0.0182	O	0	0	0	0	0	0
-7.8582				-0.6949				-0.0013	H	0	0	0	0	0	0
-6.0640				-4.6345				-0.0400	H	0	0	0	0	0	0
-5.4878				0.3382				0.0038	H	0	0	0	0	0	0
-0.3357				-1.5482				0.0225	H	0	0	0	0	0	0
-0.5232				-3.0737				-0.8747	H	0	0	0	0	0	0
-0.5559				-3.0780				0.9048	H	0	0	0	0	0	0
-0.1496				-0.6376				-0.3355	H	0	0	0	0	0	0
2.0491				0.6191				-0.3229	H	0	0	0	0	0	0
-0.1313				4.2688				0.3512	H	0	0	0	0	0	0
-2.2254				3.0653				0.3165	H	0	0	0	0	0	0
3.4924				1.5114				0.5479	H	0	0	0	0	0	0

6.2110	1.5110	1.5610	H	0	0	0	0	0
5.3049	0.5802	0.3435	H	0	0	0	0	0
7.5700	-0.4053	0.7158	H	0	0	0	0	0
7.4133	0.2155	-0.9454	H	0	0	0	0	0
8.7216	1.6894	1.3973	H	0	0	0	0	0
9.5822	0.9172	0.0437	H	0	0	0	0	0
9.3090	3.3738	-0.3254	H	0	0	0	0	0
8.4406	2.4270	-1.5578	H	0	0	0	0	0
7.2012	3.6428	0.9609	H	0	0	0	0	0
7.0178	4.2743	-0.6935	H	0	0	0	0	0
-8.9297	-2.9228	0.8439	H	0	0	0	0	0
5.9741	2.1857	-1.3500	H	0	0	0	0	0
2	1	1	0	0	0			
6	1	2	0	0	0			
29	1	1	0	0	0			
3	2	2	0	0	0			
28	2	1	0	0	0			
4	3	1	0	0	0			
30	3	1	0	0	0			
5	4	2	0	0	0			
7	4	1	0	0	0			
6	5	1	0	0	0			
9	5	1	0	0	0			
31	6	1	0	0	0			
8	7	1	0	0	0			
9	8	2	0	0	0			
11	8	1	0	0	0			
10	9	1	0	0	0			
12	10	2	0	0	0			
13	10	1	0	0	0			
32	11	1	0	0	0			
33	11	1	0	0	0			
34	11	1	0	0	0			
14	13	1	0	0	0			
18	13	2	0	0	0			
15	14	2	0	0	0			
35	14	1	0	0	0			
16	15	1	0	0	0			
36	15	1	0	0	0			
17	16	2	0	0	0			
19	16	1	0	0	0			
18	17	1	0	0	0			
37	17	1	0	0	0			
38	18	1	0	0	0			
20	19	1	0	0	0			
21	20	1	0	0	0			
39	20	1	0	0	0			
40	20	1	0	0	0			
22	21	1	0	0	0			
41	21	1	0	0	0			
42	21	1	0	0	0			
23	22	1	0	0	0			
27	22	1	0	0	0			

Forecaster10031114513D

[illegible]

-0.3029	-0.1472	0.8286	H	0	0	0	0	0
1.8815	1.0938	0.7458	H	0	0	0	0	0
-0.2881	4.6733	-0.2606	H	0	0	0	0	0
-2.3746	3.4420	-0.2675	H	0	0	0	0	0
3.2942	2.1246	1.1208	H	0	0	0	0	0
3.3279	1.9747	-0.6529	H	0	0	0	0	0
4.5330	4.2938	-0.6091	H	0	0	0	0	0
4.8088	3.9555	1.1168	H	0	0	0	0	0
6.1664	1.8912	1.7128	H	0	0	0	0	0
5.1508	0.8956	0.6420	H	0	0	0	0	0
7.4156	-0.1266	0.9171	H	0	0	0	0	0
7.1531	0.3786	-0.7697	H	0	0	0	0	0
8.6602	1.9823	1.3593	H	0	0	0	0	0
9.4056	1.0853	0.0142	H	0	0	0	0	0
9.1636	3.5148	-0.5219	H	0	0	0	0	0
8.1943	2.5011	-1.6183	H	0	0	0	0	0
7.1575	3.9483	0.8690	H	0	0	0	0	0
6.8700	4.4421	-0.8171	H	0	0	0	0	0
-8.8885	-2.8468	0.7195	H	0	0	0	0	0
-0.7695	-3.8317	1.4106	H	0	0	0	0	0
-0.6784	-4.2217	-0.3240	H	0	0	0	0	0
1.5609	-2.9434	1.3329	H	0	0	0	0	0
1.5089	-4.6428	0.8051	H	0	0	0	0	0
2.9408	-3.2602	-0.7002	H	0	0	0	0	0
1.5325	-3.9214	-1.5656	H	0	0	0	0	0
1.7630	-1.0998	-0.4122	H	0	0	0	0	0
1.8597	-1.5335	-2.1361	H	0	0	0	0	0
-0.4314	-0.7321	-1.5603	H	0	0	0	0	0
-0.4690	-2.4496	-2.0273	H	0	0	0	0	0
5.7405	2.3370	-1.2164	H	0	0	0	0	0

2	1	1	0	0	0
6	1	2	0	0	0
34	1	1	0	0	0
3	2	2	0	0	0
28	2	1	0	0	0
4	3	1	0	0	0
35	3	1	0	0	0
5	4	2	0	0	0
7	4	1	0	0	0
6	5	1	0	0	0
9	5	1	0	0	0
36	6	1	0	0	0
8	7	1	0	0	0
9	8	2	0	0	0
11	8	1	0	0	0
10	9	1	0	0	0
12	10	2	0	0	0
13	10	1	0	0	0
29	11	1	0	0	0
33	11	1	0	0	0
37	11	1	0	0	0
14	13	1	0	0	0
18	13	2	0	0	0

39	15	1	0	0	0
17	16	2	0	0	0
19	16	1	0	0	0
18	17	1	0	0	0
40	17	1	0	0	0
41	18	1	0	0	0
20	19	1	0	0	0
21	20	1	0	0	0
42	20	1	0	0	0
43	20	1	0	0	0
22	21	1	0	0	0
44	21	1	0	0	0
45	21	1	0	0	0
23	22	1	0	0	0
27	22	1	0	0	0
67	22	1	0	0	0
24	23	1	0	0	0
46	23	1	0	0	0
47	23	1	0	0	0
25	24	1	0	0	0
48	24	1	0	0	0
49	24	1	0	0	0
26	25	1	0	0	0
50	25	1	0	0	0
51	25	1	0	0	0
27	26	1	0	0	0
52	26	1	0	0	0
53	26	1	0	0	0
54	27	1	0	0	0
55	27	1	0	0	0
56	28	1	0	0	0
30	29	1	0	0	0
57	29	1	0	0	0
58	29	1	0	0	0
31	30	1	0	0	0
59	30	1	0	0	0
60	30	1	0	0	0
32	31	1	0	0	0
61	31	1	0	0	0
62	31	1	0	0	0
33	32	1	0	0	0
63	32	1	0	0	0
64	32	1	0	0	0
65	33	1	0	0	0
66	33	1	0	0	0

M END

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flavanone_1

Forecaster10031114513D

62	65	0	0	0	0	0	0	0	0	0999	V2000
-7.2981		0.9001		-0.0423	C	0	0	0	0	0	
-7.1298		-0.4096		0.1215	C	0	0	0	0	0	

-6.1371	1.7667	-0.1664	C	0	0	0	0	0
-8.2403	-1.2361	0.2528	O	0	0	0	0	0
-3.4302	-0.6959	-0.0515	O	0	0	0	0	0
-2.3103	0.0892	-0.5065	C	0	0	0	0	0
-2.3926	1.5520	0.2207	C	0	0	0	0	0
-3.7788	2.1101	-0.1716	C	0	0	0	0	0
-3.9688	3.2972	-0.4382	O	0	0	0	0	0
-1.2698	2.6918	-0.0847	C	0	0	0	0	0
-1.0280	-0.7433	-0.2660	C	0	0	0	0	0
-1.5623	3.9960	0.7000	C	0	0	0	0	0
0.1534	2.3270	0.3638	C	0	0	0	0	0
-1.0141	-1.7270	0.6354	C	0	0	0	0	0
0.2320	-2.4937	0.8770	C	0	0	0	0	0
1.3495	-2.1968	0.2076	C	0	0	0	0	0
1.3164	-1.1548	-0.8166	C	0	0	0	0	0
0.1889	-0.4897	-1.0597	C	0	0	0	0	0
2.5572	-2.8665	0.5164	O	0	0	0	0	0
3.6862	-2.2950	-0.1932	C	0	0	0	0	0
4.9859	-3.0363	0.2243	C	0	0	0	0	0
6.2035	-2.3400	-0.2711	N	0	0	0	0	0
7.3892	-3.1697	0.0575	C	0	0	0	0	0
8.6839	-2.4852	-0.4361	C	0	0	0	0	0
8.8245	-1.1235	0.2613	C	0	0	0	0	0
7.5896	-0.2713	-0.0767	C	0	0	0	0	0
6.3152	-1.0121	0.3968	C	0	0	0	0	0
-8.3024	1.3217	-0.0833	H	0	0	0	0	0
-5.6251	-2.0560	0.2497	H	0	0	0	0	0
-6.2690	2.8410	-0.2954	H	0	0	0	0	0
-8.7983	-0.9426	1.0925	H	0	0	0	0	0
-2.4182	0.2399	-1.5806	H	0	0	0	0	0
-2.4014	1.3819	1.2973	H	0	0	0	0	0
-1.2634	2.9106	-1.1525	H	0	0	0	0	0
-0.7949	4.7363	0.4742	H	0	0	0	0	0
-1.5598	3.7855	1.7695	H	0	0	0	0	0
-2.5382	4.3847	0.4089	H	0	0	0	0	0
0.8324	3.1441	0.1201	H	0	0	0	0	0
0.4761	1.4216	-0.1503	H	0	0	0	0	0
0.1631	2.1561	1.4403	H	0	0	0	0	0
-1.9187	-1.9670	1.1942	H	0	0	0	0	0
0.2363	-3.3046	1.6053	H	0	0	0	0	0
2.2177	-0.9214	-1.3833	H	0	0	0	0	0
0.1649	0.2531	-1.8570	H	0	0	0	0	0
3.5340	-2.4045	-1.2670	H	0	0	0	0	0
3.7747	-1.2375	0.0558	H	0	0	0	0	0
5.0279	-3.0887	1.3122	H	0	0	0	0	0
4.9643	-4.0451	-0.1880	H	0	0	0	0	0
7.4443	-3.3041	1.1378	H	0	0	0	0	0
7.2913	-4.1419	-0.4255	H	0	0	0	0	0
9.5433	-3.1105	-0.1940	H	0	0	0	0	0
8.6321	-2.3398	-1.5151	H	0	0	0	0	0
8.8872	-1.2679	1.3399	H	0	0	0	0	0
9.7252	-0.6213	-0.0916	H	0	0	0	0	0
7.6612	0.6912	0.4299	H	0	0	0	0	0

	6.1379	-2.2071	-1.3308 H	0	0	0	0	0
2	1	1	0	0	0			
6	1	2	0	0	0			
31	1	1	0	0	0			
3	2	2	0	0	0			
7	2	1	0	0	0			
4	3	1	0	0	0			
32	3	1	0	0	0			
5	4	2	0	0	0			
8	4	1	0	0	0			
6	5	1	0	0	0			
11	5	1	0	0	0			
33	6	1	0	0	0			
34	7	1	0	0	0			
9	8	1	0	0	0			
10	9	1	0	0	0			
14	9	1	0	0	0			
35	9	1	0	0	0			
11	10	1	0	0	0			
13	10	1	0	0	0			
36	10	1	0	0	0			
12	11	2	0	0	0			
15	13	1	0	0	0			
16	13	1	0	0	0			
37	13	1	0	0	0			
17	14	1	0	0	0			
21	14	2	0	0	0			
38	15	1	0	0	0			
39	15	1	0	0	0			
40	15	1	0	0	0			
41	16	1	0	0	0			
42	16	1	0	0	0			
43	16	1	0	0	0			
18	17	2	0	0	0			
44	17	1	0	0	0			
19	18	1	0	0	0			
45	18	1	0	0	0			
20	19	2	0	0	0			
22	19	1	0	0	0			
21	20	1	0	0	0			
46	20	1	0	0	0			
47	21	1	0	0	0			
23	22	1	0	0	0			
24	23	1	0	0	0			
48	23	1	0	0	0			
49	23	1	0	0	0			
25	24	1	0	0	0			
50	24	1	0	0	0			
51	24	1	0	0	0			
26	25	1	0	0	0			
30	25	1	0	0	0			
62	25	1	0	0	0			
27	26	1	0	0	0			

54 27 1 0 0 0
55 27 1 0 0 0
29 28 1 0 0 0
56 28 1 0 0 0
57 28 1 0 0 0
30 29 1 0 0 0
58 29 1 0 0 0
59 29 1 0 0 0
60 30 1 0 0 0
61 30 1 0 0 0

M END

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flavanone_2

Forecaster10031114513D

63 67 0 0 0 0 0 0 0 0999 V2000
-7.1339 0.6954 0.0737 C 0 0 0 0 0
-6.9341 -0.4579 0.7109 C 0 0 0 0 0
-5.5629 -0.9751 0.8860 C 0 0 0 0 0
-4.5341 -0.2965 0.3894 C 0 0 0 0 0
-4.7548 0.9704 -0.3244 C 0 0 0 0 0
-5.9987 1.4516 -0.4613 C 0 0 0 0 0
-8.0228 -1.1835 1.1894 O 0 0 0 0 0
-3.2489 -0.7792 0.4911 O 0 0 0 0 0
-2.4105 -0.4782 -0.5779 C 0 0 0 0 0
-2.2248 1.0838 -0.7893 C 0 0 0 0 0
-3.6071 1.7153 -0.8756 C 0 0 0 0 0
-3.7717 2.8166 -1.3985 O 0 0 0 0 0
-1.3587 1.9147 0.2182 C 0 0 0 0 0
-1.1123 -1.2702 -0.4922 C 0 0 0 0 0
-0.5395 1.3426 1.1081 C 0 0 0 0 0
0.3795 2.1515 1.9140 C 0 0 0 0 0
0.4238 3.4710 1.7518 C 0 0 0 0 0
-0.4683 4.1118 0.7891 C 0 0 0 0 0
-1.3115 3.3763 0.0660 C 0 0 0 0 0
-1.0591 -2.3257 0.3168 C 0 0 0 0 0
0.2078 -3.0220 0.5351 C 0 0 0 0 0
1.3245 -2.5866 -0.0471 C 0 0 0 0 0
1.2678 -1.4403 -0.9671 C 0 0 0 0 0
0.1070 -0.8254 -1.1932 C 0 0 0 0 0
2.5414 -3.2189 0.2617 O 0 0 0 0 0
3.6782 -2.5687 -0.3378 C 0 0 0 0 0
4.9506 -3.3290 0.1134 C 0 0 0 0 0
6.1927 -2.6547 -0.3261 N 0 0 0 0 0
7.3426 -3.5115 0.0501 C 0 0 0 0 0
8.6680 -2.8633 -0.4011 C 0 0 0 0 0
8.8150 -1.4999 0.2904 C 0 0 0 0 0
7.6120 -0.6213 -0.0940 C 0 0 0 0 0
6.3062 -1.3292 0.3410 C 0 0 0 0 0
-8.1470 1.0781 -0.0501 H 0 0 0 0 0
-5.3949 -1.9100 1.4206 H 0 0 0 0 0
-6.1648 2.4019 -0.9687 H 0 0 0 0 0
-8.5566 -0.6000 1.8802 H 0 0 0 0 0

1.0275	1.6712	2.6472	H	0	0	0	0	0
1.1225	4.0712	2.3346	H	0	0	0	0	0
-0.4441	5.1941	0.6620	H	0	0	0	0	0
-1.9751	3.8645	-0.6478	H	0	0	0	0	0
-1.9629	-2.6721	0.8182	H	0	0	0	0	0
0.2390	-3.9020	1.1775	H	0	0	0	0	0
2.1743	-1.0940	-1.4635	H	0	0	0	0	0
0.0587	0.0062	-1.8962	H	0	0	0	0	0
3.5931	-2.6002	-1.4240	H	0	0	0	0	0
3.7292	-1.5314	-0.0068	H	0	0	0	0	0
4.9530	-3.3936	1.2015	H	0	0	0	0	0
4.9279	-4.3329	-0.3106	H	0	0	0	0	0
7.3559	-3.6393	1.1325	H	0	0	0	0	0
7.2373	-4.4844	-0.4299	H	0	0	0	0	0
9.5030	-3.5064	-0.1232	H	0	0	0	0	0
8.6587	-2.7260	-1.4824	H	0	0	0	0	0
8.8384	-1.6374	1.3714	H	0	0	0	0	0
9.7383	-1.0208	-0.0355	H	0	0	0	0	0
7.6891	0.3427	0.4089	H	0	0	0	0	0
7.6020	-0.4689	-1.1732	H	0	0	0	0	0
6.3161	-1.4700	1.4218	H	0	0	0	0	0
5.4522	-0.7118	0.0623	H	0	0	0	0	0
6.1743	-2.5229	-1.3878	H	0	0	0	0	0

2	1	1	0	0	0
6	1	2	0	0	0
34	1	1	0	0	0
3	2	2	0	0	0
7	2	1	0	0	0
4	3	1	0	0	0
35	3	1	0	0	0
5	4	2	0	0	0
8	4	1	0	0	0
6	5	1	0	0	0
11	5	1	0	0	0
36	6	1	0	0	0
37	7	1	0	0	0
9	8	1	0	0	0
10	9	1	0	0	0
14	9	1	0	0	0
38	9	1	0	0	0
11	10	1	0	0	0
13	10	1	0	0	0
39	10	1	0	0	0
12	11	2	0	0	0
15	13	1	0	0	0
19	13	2	0	0	0
20	14	1	0	0	0
24	14	2	0	0	0
16	15	2	0	0	0
40	15	1	0	0	0
17	16	1	0	0	0
41	16	1	0	0	0
18	17	2	0	0	0

44	19	1	0	0	0
21	20	2	0	0	0
45	20	1	0	0	0
22	21	1	0	0	0
46	21	1	0	0	0
23	22	2	0	0	0
25	22	1	0	0	0
24	23	1	0	0	0
47	23	1	0	0	0
48	24	1	0	0	0
26	25	1	0	0	0
27	26	1	0	0	0
49	26	1	0	0	0
50	26	1	0	0	0
28	27	1	0	0	0
51	27	1	0	0	0
52	27	1	0	0	0
29	28	1	0	0	0
33	28	1	0	0	0
63	28	1	0	0	0
30	29	1	0	0	0
53	29	1	0	0	0
54	29	1	0	0	0
31	30	1	0	0	0
55	30	1	0	0	0
56	30	1	0	0	0
32	31	1	0	0	0
57	31	1	0	0	0
58	31	1	0	0	0
33	32	1	0	0	0
59	32	1	0	0	0
60	32	1	0	0	0
61	33	1	0	0	0
62	33	1	0	0	0

M END

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flavanone_3

Forecaster10031114513D

65	69	0	0	0	0	0	0	0	0	0999	V2000					
-7.0467		0.4499		1.0237	C	0	0	0	0	0						
-7.1195		-0.5880		0.2007	C	0	0	0	0	0						
-5.9140		-1.1291		-0.4333	C	0	0	0	0	0						
-4.7068		-0.5522		-0.1895	C	0	0	0	0	0						
-4.6538		0.6037		0.7283	C	0	0	0	0	0						
-5.7415		1.0750		1.2982	C	0	0	0	0	0						
-8.3598		-1.1700		-0.0740	O	0	0	0	0	0						
-3.5828		-1.0636		-0.8088	O	0	0	0	0	0						
-2.3503		-0.3491		-0.7841	C	0	0	0	0	0						
-2.6079		1.1640		-0.3784	C	0	0	0	0	0						
-3.3274		1.2976		0.9495	C	0	0	0	0	0						
-1.3630		2.0371		-0.4067	C	0	0	0	0	0						
-1.2335		-1.2060		-0.0556	C	0	0	0	0	0						

-0.0830	3.7899	0.6726	C	0	0	0	0	0
-1.1936	3.0598	0.6285	C	0	0	0	0	0
-1.1797	-2.5029	-0.3420	C	0	0	0	0	0
0.0405	-3.2893	-0.0501	C	0	0	0	0	0
1.1305	-2.6891	0.4376	C	0	0	0	0	0
1.0639	-1.2817	0.8134	C	0	0	0	0	0
-0.0555	-0.5885	0.6058	C	0	0	0	0	0
2.3499	-3.4135	0.4869	O	0	0	0	0	0
3.5023	-2.5916	0.8307	C	0	0	0	0	0
4.7831	-3.3865	0.4074	C	0	0	0	0	0
6.0593	-2.6367	0.6064	N	0	0	0	0	0
7.1826	-3.5279	0.2053	C	0	0	0	0	0
8.5427	-2.8260	0.4192	C	0	0	0	0	0
8.5880	-1.5510	-0.4349	C	0	0	0	0	0
7.4173	-0.6413	-0.0207	C	0	0	0	0	0
6.0792	-1.4020	-0.2253	C	0	0	0	0	0
2.1469	4.3111	-0.2440	O	0	0	0	0	0
-7.9494	0.8387	1.4950	H	0	0	0	0	0
-5.9847	-1.9904	-1.0975	H	0	0	0	0	0
-5.6770	1.9281	1.9736	H	0	0	0	0	0
-8.7876	-1.5210	0.8184	H	0	0	0	0	0
-2.0327	-0.3071	-1.8259	H	0	0	0	0	0
-3.2821	1.5707	-1.1322	H	0	0	0	0	0
-2.7641	0.8089	1.7445	H	0	0	0	0	0
-3.4784	2.3470	1.2027	H	0	0	0	0	0
-0.5490	1.1296	-2.1215	H	0	0	0	0	0
1.5939	2.5140	-2.0189	H	0	0	0	0	0
0.0392	4.5509	1.4433	H	0	0	0	0	0
-1.9805	3.2228	1.3650	H	0	0	0	0	0
-2.0416	-2.9919	-0.7959	H	0	0	0	0	0
0.0498	-4.3636	-0.2340	H	0	0	0	0	0
1.9296	-0.7965	1.2641	H	0	0	0	0	0
-0.1075	0.4516	0.9276	H	0	0	0	0	0
3.4575	-1.6436	0.2947	H	0	0	0	0	0
3.5185	-2.4023	1.9040	H	0	0	0	0	0
4.8284	-4.3019	0.9975	H	0	0	0	0	0
4.6956	-3.6388	-0.6494	H	0	0	0	0	0
7.1506	-4.4361	0.8072	H	0	0	0	0	0
7.0754	-3.7858	-0.8483	H	0	0	0	0	0
8.6575	-2.5650	1.4713	H	0	0	0	0	0
9.3498	-3.4948	0.1201	H	0	0	0	0	0
9.5323	-1.0321	-0.2702	H	0	0	0	0	0
8.4952	-1.8118	-1.4892	H	0	0	0	0	0
7.5232	-0.3669	1.0289	H	0	0	0	0	0
7.4215	0.2595	-0.6345	H	0	0	0	0	0
5.2501	-0.7575	0.0668	H	0	0	0	0	0
5.9762	-1.6736	-1.2759	H	0	0	0	0	0
2.9631	3.6627	-0.1178	H	0	0	0	0	0
6.1624	-2.3741	1.6385	H	0	0	0	0	0

2 1 1 0 0 0

6 1 2 0 0 0

34 1 1 0 0 0

3 2 2 0 0 0

5	4	2	0	0	0
8	4	1	0	0	0
6	5	1	0	0	0
11	5	1	0	0	0
36	6	1	0	0	0
37	7	1	0	0	0
9	8	1	0	0	0
10	9	1	0	0	0
13	9	1	0	0	0
38	9	1	0	0	0
11	10	1	0	0	0
12	10	1	0	0	0
39	10	1	0	0	0
40	11	1	0	0	0
41	11	1	0	0	0
14	12	1	0	0	0
18	12	2	0	0	0
19	13	1	0	0	0
23	13	2	0	0	0
15	14	2	0	0	0
42	14	1	0	0	0
16	15	1	0	0	0
43	15	1	0	0	0
17	16	2	0	0	0
33	16	1	0	0	0
18	17	1	0	0	0
44	17	1	0	0	0
45	18	1	0	0	0
20	19	2	0	0	0
46	19	1	0	0	0
21	20	1	0	0	0
47	20	1	0	0	0
22	21	2	0	0	0
24	21	1	0	0	0
23	22	1	0	0	0
48	22	1	0	0	0
49	23	1	0	0	0
25	24	1	0	0	0
26	25	1	0	0	0
50	25	1	0	0	0
51	25	1	0	0	0
27	26	1	0	0	0
52	26	1	0	0	0
53	26	1	0	0	0
28	27	1	0	0	0
32	27	1	0	0	0
65	27	1	0	0	0
29	28	1	0	0	0
54	28	1	0	0	0
55	28	1	0	0	0
30	29	1	0	0	0
56	29	1	0	0	0
57	29	1	0	0	0

32 31 1 0 0 0
60 31 1 0 0 0
61 31 1 0 0 0
62 32 1 0 0 0
63 32 1 0 0 0
64 33 1 0 0 0

M END

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benzoxathiin_1

Forecaster10031114513D

63 67 0 0 0 0 0 0 0 0999 V2000
-7.2760 0.5537 -0.3468 C 0 0 0 0 0
-6.9261 -0.4774 -1.1176 C 0 0 0 0 0
-5.5119 -0.8871 -1.2161 C 0 0 0 0 0
-4.5778 -0.2284 -0.5271 C 0 0 0 0 0
-4.9749 0.9204 0.3069 C 0 0 0 0 0
-6.2495 1.2950 0.3921 C 0 0 0 0 0
-8.6150 0.9282 -0.2446 O 0 0 0 0 0
-3.2366 -0.6431 -0.5677 O 0 0 0 0 0
-2.4297 -0.4727 0.5949 C 0 0 0 0 0
-2.1793 1.0478 0.9865 C 0 0 0 0 0
-3.7495 1.7649 1.1309 S 0 0 0 0 0
-1.2762 1.9586 0.0970 C 0 0 0 0 0
-1.1539 -1.3311 0.4925 C 0 0 0 0 0
-0.5326 1.4875 -0.9097 C 0 0 0 0 0
0.4666 2.3421 -1.5643 C 0 0 0 0 0
0.6436 3.5951 -1.1506 C 0 0 0 0 0
-0.1945 4.1309 -0.0808 C 0 0 0 0 0
-1.1039 3.3560 0.5084 C 0 0 0 0 0
-1.1916 -2.4992 -0.1478 C 0 0 0 0 0
0.0493 -3.2721 -0.3480 C 0 0 0 0 0
1.2194 -2.7847 0.0706 C 0 0 0 0 0
1.2549 -1.5200 0.8009 C 0 0 0 0 0
0.1309 -0.8494 1.0284 C 0 0 0 0 0
1.6299 4.3915 -1.7290 O 0 0 0 0 0
2.4109 -3.4797 -0.2101 O 0 0 0 0 0
3.5732 -2.6857 0.1264 C 0 0 0 0 0
4.8542 -3.5411 -0.0144 C 0 0 0 0 0
6.0558 -2.7013 -0.2749 N 0 0 0 0 0
7.2535 -3.5785 -0.2614 C 0 0 0 0 0
8.5173 -2.7724 -0.6287 C 0 0 0 0 0
8.6938 -1.6229 0.3741 C 0 0 0 0 0
7.4344 -0.7400 0.3411 C 0 0 0 0 0
6.2020 -1.6054 0.7109 C 0 0 0 0 0
-7.6883 -1.0197 -1.6772 H 0 0 0 0 0
-5.2304 -1.7271 -1.8511 H 0 0 0 0 0
-6.5288 2.1494 1.0087 H 0 0 0 0 0
-8.9797 1.1882 -1.1943 H 0 0 0 0 0
-3.0051 -0.8976 1.4174 H 0 0 0 0 0
-1.7404 1.0477 1.9842 H 0 0 0 0 0
-0.6692 0.4602 -1.2474 H 0 0 0 0 0
1.0630 1.9506 -2.3884 H 0 0 0 0 0

0.0104	-4.2443	-0.8393	H	0	0	0	0	0
2.2056	-1.1258	1.1599	H	0	0	0	0	0
0.1597	0.0670	1.6179	H	0	0	0	0	0
2.5694	3.9447	-1.5866	H	0	0	0	0	0
3.6339	-1.8307	-0.5470	H	0	0	0	0	0
3.4850	-2.3338	1.1542	H	0	0	0	0	0
5.0081	-4.0998	0.9088	H	0	0	0	0	0
4.7240	-4.2368	-0.8433	H	0	0	0	0	0
7.3759	-4.0031	0.7350	H	0	0	0	0	0
7.1177	-4.3821	-0.9852	H	0	0	0	0	0
9.3893	-3.4253	-0.5915	H	0	0	0	0	0
8.4102	-2.3653	-1.6342	H	0	0	0	0	0
8.8306	-2.0288	1.3764	H	0	0	0	0	0
9.5654	-1.0284	0.1003	H	0	0	0	0	0
7.5390	0.0728	1.0598	H	0	0	0	0	0
7.3039	-0.3268	-0.6591	H	0	0	0	0	0
6.3401	-2.0279	1.7062	H	0	0	0	0	0
5.3059	-0.9850	0.7001	H	0	0	0	0	0
5.9628	-2.2699	-1.2497	H	0	0	0	0	0

1	2	1	0	0	0
6	1	2	0	0	0
7	1	1	0	0	0
3	2	2	0	0	0
34	2	1	0	0	0
4	3	1	0	0	0
35	3	1	0	0	0
5	4	2	0	0	0
8	4	1	0	0	0
6	5	1	0	0	0
11	5	1	0	0	0
36	6	1	0	0	0
37	7	1	0	0	0
9	8	1	0	0	0
10	9	1	0	0	0
13	9	1	0	0	0
38	9	1	0	0	0
11	10	1	0	0	0
12	10	1	0	0	0
39	10	1	0	0	0
14	12	1	0	0	0
18	12	2	0	0	0
19	13	1	0	0	0
23	13	2	0	0	0
15	14	2	0	0	0
40	14	1	0	0	0
16	15	1	0	0	0
41	15	1	0	0	0
17	16	2	0	0	0
24	16	1	0	0	0
18	17	1	0	0	0
42	17	1	0	0	0
43	18	1	0	0	0
20	19	2	0	0	0

22	21	2	0	0	0
25	21	1	0	0	0
23	22	1	0	0	0
46	22	1	0	0	0
47	23	1	0	0	0
48	24	1	0	0	0
26	25	1	0	0	0
27	26	1	0	0	0
49	26	1	0	0	0
50	26	1	0	0	0
28	27	1	0	0	0
51	27	1	0	0	0
52	27	1	0	0	0
29	28	1	0	0	0
33	28	1	0	0	0
63	28	1	0	0	0
30	29	1	0	0	0
53	29	1	0	0	0
54	29	1	0	0	0
31	30	1	0	0	0
55	30	1	0	0	0
56	30	1	0	0	0
32	31	1	0	0	0
57	31	1	0	0	0
58	31	1	0	0	0
33	32	1	0	0	0
59	32	1	0	0	0
60	32	1	0	0	0
61	33	1	0	0	0
62	33	1	0	0	0

M END

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benzoxathiin_2

Forecaster10031114513D

63	67	0	0	0	0	0	0	0	0	0999	V2000					
-7.2855				0.5833				0.3270	C		0	0	0	0	0	0
-6.9457				-0.4397				1.1127	C		0	0	0	0	0	0
-5.5360				-0.8580				1.2193	C		0	0	0	0	0	0
-4.5972				-0.2169				0.5243	C		0	0	0	0	0	0
-4.9787				0.9246				-0.3280	C		0	0	0	0	0	0
-6.2519				1.3082				-0.4208	C		0	0	0	0	0	0
-8.6218				0.9649				0.2172	O		0	0	0	0	0	0
-3.2632				-0.6421				0.5730	O		0	0	0	0	0	0
-2.4591				-0.5067				-0.5917	C		0	0	0	0	0	0
-2.1802				1.0043				-1.0039	C		0	0	0	0	0	0
-3.7397				1.7464				-1.1620	S		0	0	0	0	0	0
-1.2448				1.9047				-0.1226	C		0	0	0	0	0	0
-1.1938				-1.3538				-0.4735	C		0	0	0	0	0	0
-0.3245				1.3911				0.6999	C		0	0	0	0	0	0
0.6775				2.2364				1.3433	C		0	0	0	0	0	0
0.6943				3.5424				1.0995	C		0	0	0	0	0	0
-0.3242				4.1303				0.2253	C		0	0	0	0	0	0

1.2194	-2.6988	0.0193	C	0	0	0	0	0
1.1580	-1.6652	-1.0209	C	0	0	0	0	0
0.0081	-1.0435	-1.2729	C	0	0	0	0	0
1.6818	4.3441	1.6676	O	0	0	0	0	0
2.4347	-3.3194	0.3567	O	0	0	0	0	0
3.5595	-2.7346	-0.3305	C	0	0	0	0	0
4.8453	-3.4541	0.1475	C	0	0	0	0	0
6.0735	-2.7701	-0.3201	N	0	0	0	0	0
7.2415	-3.5955	0.0694	C	0	0	0	0	0
8.5535	-2.9289	-0.3961	C	0	0	0	0	0
8.6756	-1.5517	0.2731	C	0	0	0	0	0
7.4564	-0.7030	-0.1256	C	0	0	0	0	0
6.1643	-1.4284	0.3212	C	0	0	0	0	0
-7.7132	-0.9684	1.6780	H	0	0	0	0	0
-5.2619	-1.6913	1.8663	H	0	0	0	0	0
-6.5239	2.1563	-1.0492	H	0	0	0	0	0
-9.1862	0.1616	-0.1551	H	0	0	0	0	0
-3.0365	-0.9400	-1.4084	H	0	0	0	0	0
-1.7423	0.9807	-2.0018	H	0	0	0	0	0
-0.3220	0.3186	0.8944	H	0	0	0	0	0
1.4093	1.7973	2.0214	H	0	0	0	0	0
-0.3306	5.2054	0.0461	H	0	0	0	0	0
-1.9997	3.8008	-0.9990	H	0	0	0	0	0
-2.0336	-2.5729	1.0161	H	0	0	0	0	0
0.1446	-3.8430	1.4149	H	0	0	0	0	0
2.0532	-1.4068	-1.5866	H	0	0	0	0	0
-0.0462	-0.3035	-2.0714	H	0	0	0	0	0
1.6242	4.2824	2.7142	H	0	0	0	0	0
3.4425	-2.8641	-1.4064	H	0	0	0	0	0
3.6228	-1.6718	-0.0967	H	0	0	0	0	0
4.8499	-3.4783	1.2372	H	0	0	0	0	0
4.8419	-4.4732	-0.2391	H	0	0	0	0	0
7.2590	-3.7030	1.1539	H	0	0	0	0	0
7.1555	-4.5791	-0.3924	H	0	0	0	0	0
9.4015	-3.5511	-0.1102	H	0	0	0	0	0
8.5388	-2.8093	-1.4794	H	0	0	0	0	0
8.7016	-1.6708	1.3563	H	0	0	0	0	0
9.5897	-1.0609	-0.0610	H	0	0	0	0	0
7.5149	0.2705	0.3613	H	0	0	0	0	0
7.4437	-0.5687	-1.2072	H	0	0	0	0	0
6.1762	-1.5484	1.4045	H	0	0	0	0	0
5.2992	-0.8323	0.0307	H	0	0	0	0	0
6.0451	-2.6618	-1.3842	H	0	0	0	0	0

1	2	1	0	0	0
6	1	2	0	0	0
7	1	1	0	0	0
3	2	2	0	0	0
34	2	1	0	0	0
4	3	1	0	0	0
35	3	1	0	0	0
5	4	2	0	0	0
8	4	1	0	0	0
6	5	1	0	0	0

9	8	1	0	0	0
10	9	1	0	0	0
13	9	1	0	0	0
38	9	1	0	0	0
11	10	1	0	0	0
12	10	1	0	0	0
39	10	1	0	0	0
14	12	1	0	0	0
18	12	2	0	0	0
19	13	1	0	0	0
23	13	2	0	0	0
15	14	2	0	0	0
40	14	1	0	0	0
16	15	1	0	0	0
41	15	1	0	0	0
17	16	2	0	0	0
24	16	1	0	0	0
18	17	1	0	0	0
42	17	1	0	0	0
43	18	1	0	0	0
20	19	2	0	0	0
44	19	1	0	0	0
21	20	1	0	0	0
45	20	1	0	0	0
22	21	2	0	0	0
25	21	1	0	0	0
23	22	1	0	0	0
46	22	1	0	0	0
47	23	1	0	0	0
48	24	1	0	0	0
26	25	1	0	0	0
27	26	1	0	0	0
49	26	1	0	0	0
50	26	1	0	0	0
28	27	1	0	0	0
51	27	1	0	0	0
52	27	1	0	0	0
29	28	1	0	0	0
33	28	1	0	0	0
63	28	1	0	0	0
30	29	1	0	0	0
53	29	1	0	0	0
54	29	1	0	0	0
31	30	1	0	0	0
55	30	1	0	0	0
56	30	1	0	0	0
32	31	1	0	0	0
57	31	1	0	0	0
58	31	1	0	0	0
33	32	1	0	0	0
59	32	1	0	0	0
60	32	1	0	0	0
61	33	1	0	0	0

benzoxathiin_3

Forecaster10031114513D

63	67	0	0	0	0	0	0	0	0	0999	V2000					
-7.4836		0.5206		-0.0387	C	0	0	0	0	0						
-7.2964		-0.7933		-0.1651	C	0	0	0	0	0						
-5.9306		-1.3469		-0.1874	C	0	0	0	0	0						
-4.8806		-0.5368		-0.0770	C	0	0	0	0	0						
-5.1017		0.8965		0.0905	C	0	0	0	0	0						
-6.3323		1.4082		0.1061	C	0	0	0	0	0						
-8.7739		1.0453		-0.0230	O	0	0	0	0	0						
-3.5755		-1.0637		-0.1403	O	0	0	0	0	0						
-2.3928		-0.2729		-0.4253	C	0	0	0	0	0						
-2.3073		0.9630		0.5781	C	0	0	0	0	0						
-3.7615		1.8578		0.3343	S	0	0	0	0	0						
-1.1221		1.8781		0.3296	C	0	0	0	0	0						
-1.1438		-1.1513		-0.2856	C	0	0	0	0	0						
0.0217		1.7047		0.9957	C	0	0	0	0	0						
1.1623		2.5840		0.7431	C	0	0	0	0	0						
1.0538		3.5783		-0.1353	C	0	0	0	0	0						
-0.2109		3.7941		-0.8444	C	0	0	0	0	0						
-1.2452		2.9828		-0.6261	C	0	0	0	0	0						
-1.1520		-2.1954		0.5439	C	0	0	0	0	0						
0.0788		-2.9809		0.7559	C	0	0	0	0	0						
1.2125		-2.6377		0.1409	C	0	0	0	0	0						
1.2117		-1.5129		-0.8007	C	0	0	0	0	0						
0.0935		-0.8234		-1.0188	C	0	0	0	0	0						
2.1415		4.4108		-0.3799	O	0	0	0	0	0						
2.4047		-3.3381		0.4298	O	0	0	0	0	0						
3.5491		-2.7357		-0.2175	C	0	0	0	0	0						
4.8350		-3.4995		0.1960	C	0	0	0	0	0						
6.0567		-2.7997		-0.2758	N	0	0	0	0	0						
7.2401		-3.6312		0.0543	C	0	0	0	0	0						
8.5355		-2.9408		-0.4286	C	0	0	0	0	0						
8.6690		-1.5819		0.2760	C	0	0	0	0	0						
7.4335		-0.7310		-0.0616	C	0	0	0	0	0						
6.1604		-1.4779		0.4027	C	0	0	0	0	0						
-8.1549		-1.4593		-0.2521	H	0	0	0	0	0						
-5.7804		-2.4212		-0.2945	H	0	0	0	0	0						
-6.4787		2.4816		0.2261	H	0	0	0	0	0						
-9.2601		0.8071		-0.9227	H	0	0	0	0	0						
-2.4524		0.1015		-1.4472	H	0	0	0	0	0						
-2.2742		0.5963		1.6040	H	0	0	0	0	0						
0.1057		0.9044		1.7309	H	0	0	0	0	0						
2.1010		2.4254		1.2738	H	0	0	0	0	0						
-0.3053		4.6188		-1.5508	H	0	0	0	0	0						
-2.1832		3.1407		-1.1584	H	0	0	0	0	0						
-2.0690		-2.4688		1.0659	H	0	0	0	0	0						
0.0621		-3.8463		1.4184	H	0	0	0	0	0						
2.1288		-1.2408		-1.3232	H	0	0	0	0	0						
0.0925		-0.0104		-1.7448	H	0	0	0	0	0						
2.4242		4.8890		0.5111	H	0	0	0	0	0						
3.4256		-2.7902		-1.2991	H	0	0	0	0	0						

7.2897	-3.7725	1.1340	H	0	0	0	0	0
7.1458	-4.6004	-0.4355	H	0	0	0	0	0
9.3952	-3.5650	-0.1848	H	0	0	0	0	0
8.4893	-2.7904	-1.5072	H	0	0	0	0	0
8.7282	-1.7316	1.3540	H	0	0	0	0	0
9.5696	-1.0753	-0.0710	H	0	0	0	0	0
7.5006	0.2287	0.4509	H	0	0	0	0	0
7.3874	-0.5662	-1.1381	H	0	0	0	0	0
6.2070	-1.6306	1.4809	H	0	0	0	0	0
5.2834	-0.8789	0.1576	H	0	0	0	0	0
6.0023	-2.6566	-1.3348	H	0	0	0	0	0
1	2	1	0	0	0			
6	1	2	0	0	0			
7	1	1	0	0	0			
3	2	2	0	0	0			
34	2	1	0	0	0			
4	3	1	0	0	0			
35	3	1	0	0	0			
5	4	2	0	0	0			
8	4	1	0	0	0			
6	5	1	0	0	0			
11	5	1	0	0	0			
36	6	1	0	0	0			
37	7	1	0	0	0			
9	8	1	0	0	0			
10	9	1	0	0	0			
13	9	1	0	0	0			
38	9	1	0	0	0			
11	10	1	0	0	0			
12	10	1	0	0	0			
39	10	1	0	0	0			
14	12	1	0	0	0			
18	12	2	0	0	0			
19	13	1	0	0	0			
23	13	2	0	0	0			
15	14	2	0	0	0			
40	14	1	0	0	0			
16	15	1	0	0	0			
41	15	1	0	0	0			
17	16	2	0	0	0			
24	16	1	0	0	0			
18	17	1	0	0	0			
42	17	1	0	0	0			
43	18	1	0	0	0			
20	19	2	0	0	0			
44	19	1	0	0	0			
21	20	1	0	0	0			
45	20	1	0	0	0			
22	21	2	0	0	0			
25	21	1	0	0	0			
23	22	1	0	0	0			
46	22	1	0	0	0			
47	23	1	0	0	0			

49	26	1	0	0	0
50	26	1	0	0	0
28	27	1	0	0	0
51	27	1	0	0	0
52	27	1	0	0	0
29	28	1	0	0	0
33	28	1	0	0	0
63	28	1	0	0	0
30	29	1	0	0	0
53	29	1	0	0	0
54	29	1	0	0	0
31	30	1	0	0	0
55	30	1	0	0	0
56	30	1	0	0	0
32	31	1	0	0	0
57	31	1	0	0	0
58	31	1	0	0	0
33	32	1	0	0	0
59	32	1	0	0	0
60	32	1	0	0	0
61	33	1	0	0	0
62	33	1	0	0	0

M END

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benzoxathiin_4

Forecaster10031114513D

61	65	0	0	0	0	0	0	0	0	0999	V2000					
-7.5069			0.5243							-0.0076	C	0	0	0	0	0
-7.3114			-0.7932							0.0170	C	0	0	0	0	0
-5.9396			-1.3343							0.0106	C	0	0	0	0	0
-4.8913			-0.5068							-0.0198	C	0	0	0	0	0
-5.1248			0.9125							-0.0523	C	0	0	0	0	0
-6.3556			1.4223							-0.0455	C	0	0	0	0	0
-8.8002			1.0442							0.0035	O	0	0	0	0	0
-3.5815			-1.0362							-0.0221	O	0	0	0	0	0
-2.3351			-0.3151							-0.0418	C	0	0	0	0	0
-2.3131			1.0637							-0.0332	C	0	0	0	0	0
-3.7922			1.8799							-0.0901	S	0	0	0	0	0
-1.1040			2.0046							0.0726	C	0	0	0	0	0
-1.0846			-1.2392							-0.0926	C	0	0	0	0	0
0.0195			1.6771							0.7203	C	0	0	0	0	0
1.1561			2.5697							0.7875	C	0	0	0	0	0
1.0832			3.7648							0.2217	C	0	0	0	0	0
-0.1620			4.1849							-0.4300	C	0	0	0	0	0
-1.2041			3.3531							-0.4886	C	0	0	0	0	0
-1.1443			-2.4741							0.4038	C	0	0	0	0	0
0.0898			-3.3142							0.4560	C	0	0	0	0	0
1.2519			-2.8440							-0.0127	C	0	0	0	0	0
1.2846			-1.5554							-0.6519	C	0	0	0	0	0
0.1885			-0.8162							-0.7082	C	0	0	0	0	0
2.1841			4.6111							0.2554	O	0	0	0	0	0
2.4491			-3.5754							0.1500	O	0	0	0	0	0

7.3149	-3.6288	-0.0214	C	0	0	0	0	0
8.6132	-2.9057	-0.4417	C	0	0	0	0	0
8.7117	-1.5742	0.3169	C	0	0	0	0	0
7.4721	-0.7261	-0.0177	C	0	0	0	0	0
6.1947	-1.5065	0.3888	C	0	0	0	0	0
-8.1648	-1.4708	0.0418	H	0	0	0	0	0
-5.7805	-2.4124	0.0307	H	0	0	0	0	0
-6.5024	2.5021	-0.0681	H	0	0	0	0	0
-9.3245	0.6977	-0.8377	H	0	0	0	0	0
0.0807	0.7068	1.2132	H	0	0	0	0	0
2.0667	2.2605	1.3006	H	0	0	0	0	0
-0.2365	5.1802	-0.8681	H	0	0	0	0	0
-2.1333	3.6790	-0.9561	H	0	0	0	0	0
-2.0911	-2.8704	0.7708	H	0	0	0	0	0
0.0435	-4.3177	0.8790	H	0	0	0	0	0
2.2126	-1.1879	-1.0899	H	0	0	0	0	0
0.2272	0.1408	-1.2286	H	0	0	0	0	0
2.4386	4.8155	1.2534	H	0	0	0	0	0
3.5393	-2.7053	-1.4087	H	0	0	0	0	0
3.5983	-1.8277	0.1392	H	0	0	0	0	0
4.9253	-3.7167	1.1267	H	0	0	0	0	0
4.9165	-4.5255	-0.4592	H	0	0	0	0	0
7.3396	-3.8137	1.0525	H	0	0	0	0	0
7.2457	-4.5781	-0.5526	H	0	0	0	0	0
9.4737	-3.5291	-0.1987	H	0	0	0	0	0
8.5939	-2.7143	-1.5146	H	0	0	0	0	0
8.7477	-1.7646	1.3895	H	0	0	0	0	0
9.6132	-1.0433	0.0112	H	0	0	0	0	0
7.5149	0.2143	0.5318	H	0	0	0	0	0
7.4488	-0.5213	-1.0880	H	0	0	0	0	0
6.2183	-1.7022	1.4608	H	0	0	0	0	0
5.3157	-0.9089	0.1473	H	0	0	0	0	0
6.1029	-2.6109	-1.3991	H	0	0	0	0	0

1	2	1	0	0	0
6	1	2	0	0	0
7	1	1	0	0	0
3	2	2	0	0	0
34	2	1	0	0	0
4	3	1	0	0	0
35	3	1	0	0	0
5	4	2	0	0	0
8	4	1	0	0	0
6	5	1	0	0	0
11	5	1	0	0	0
36	6	1	0	0	0
37	7	1	0	0	0
9	8	1	0	0	0
10	9	2	0	0	0
13	9	1	0	0	0
11	10	1	0	0	0
12	10	1	0	0	0
14	12	1	0	0	0
18	12	2	0	0	0

38	14	1	0	0	0
16	15	1	0	0	0
39	15	1	0	0	0
17	16	2	0	0	0
24	16	1	0	0	0
18	17	1	0	0	0
40	17	1	0	0	0
41	18	1	0	0	0
20	19	2	0	0	0
42	19	1	0	0	0
21	20	1	0	0	0
43	20	1	0	0	0
22	21	2	0	0	0
25	21	1	0	0	0
23	22	1	0	0	0
44	22	1	0	0	0
45	23	1	0	0	0
46	24	1	0	0	0
26	25	1	0	0	0
27	26	1	0	0	0
47	26	1	0	0	0
48	26	1	0	0	0
28	27	1	0	0	0
49	27	1	0	0	0
50	27	1	0	0	0
29	28	1	0	0	0
33	28	1	0	0	0
61	28	1	0	0	0
30	29	1	0	0	0
51	29	1	0	0	0
52	29	1	0	0	0
31	30	1	0	0	0
53	30	1	0	0	0
54	30	1	0	0	0
32	31	1	0	0	0
55	31	1	0	0	0
56	31	1	0	0	0
33	32	1	0	0	0
57	32	1	0	0	0
58	32	1	0	0	0
59	33	1	0	0	0
60	33	1	0	0	0

M END

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benzopyran_1

Forecaster10031114513D

66	70	0	0	0	0	0	0	0	0	0999	V2000					
-5.4439	-2.5108	-0.1063	C	0	0	0	0	0	0							
-5.5839	-3.8331	-0.1050	C	0	0	0	0	0	0							
-4.4197	-4.6816	-0.0575	C	0	0	0	0	0	0							
-3.2049	-4.1447	0.0074	C	0	0	0	0	0	0							
-3.0312	-2.6846	0.0417	C	0	0	0	0	0	0							

-2.9877	0.7365	-0.1009	C	0	0	0	0	0
-1.9054	0.5755	-0.8682	C	0	0	0	0	0
-0.7802	1.5434	-0.7977	C	0	0	0	0	0
-0.8664	2.6067	0.0009	C	0	0	0	0	0
-2.0972	2.8349	0.7505	C	0	0	0	0	0
-3.0917	1.9516	0.7087	C	0	0	0	0	0
-2.1261	-4.9799	0.0212	O	0	0	0	0	0
-0.7860	-4.5332	-0.0063	C	0	0	0	0	0
-0.6338	-3.0362	0.1280	C	0	0	0	0	0
-1.6795	-2.2202	0.1542	C	0	0	0	0	0
0.7035	-2.4423	0.1711	C	0	0	0	0	0
1.7899	-3.1767	-0.0477	C	0	0	0	0	0
3.1120	-2.5334	-0.0615	C	0	0	0	0	0
3.2172	-1.2212	0.1476	C	0	0	0	0	0
2.0270	-0.4311	0.4059	C	0	0	0	0	0
0.8339	-1.0153	0.4154	C	0	0	0	0	0
0.2137	3.5041	0.2002	O	0	0	0	0	0
1.4641	3.1366	-0.4347	C	0	0	0	0	0
2.5008	4.2245	-0.0129	C	0	0	0	0	0
3.9040	3.9392	-0.4199	N	0	0	0	0	0
4.4231	2.7555	0.3189	C	0	0	0	0	0
5.9029	2.4855	-0.0662	C	0	0	0	0	0
6.7532	3.7201	0.2813	C	0	0	0	0	0
6.1939	4.9268	-0.4837	C	0	0	0	0	0
4.7189	5.1338	-0.0792	C	0	0	0	0	0
4.4609	-0.6059	0.1179	O	0	0	0	0	0
-6.3337	-1.8835	-0.1600	H	0	0	0	0	0
-4.5353	-5.7653	-0.0748	H	0	0	0	0	0
-7.4135	-4.0862	0.6721	H	0	0	0	0	0
-4.8171	-0.0085	-0.8743	H	0	0	0	0	0
-4.6988	-0.0160	0.9020	H	0	0	0	0	0
-1.8476	-0.2723	-1.5509	H	0	0	0	0	0
0.1150	1.3838	-1.3987	H	0	0	0	0	0
-2.2032	3.7383	1.3510	H	0	0	0	0	0
-3.9976	2.1358	1.2862	H	0	0	0	0	0
-0.2500	-5.0071	0.8161	H	0	0	0	0	0
-0.3424	-4.8389	-0.9539	H	0	0	0	0	0
-1.5034	-1.1504	0.2661	H	0	0	0	0	0
1.7010	-4.2500	-0.2160	H	0	0	0	0	0
4.0062	-3.1297	-0.2428	H	0	0	0	0	0
2.1121	0.6396	0.5917	H	0	0	0	0	0
-0.0571	-0.4179	0.6085	H	0	0	0	0	0
1.7873	2.1535	-0.0923	H	0	0	0	0	0
1.3485	3.1246	-1.5185	H	0	0	0	0	0
2.2024	5.1706	-0.4645	H	0	0	0	0	0
2.4744	4.3153	1.0730	H	0	0	0	0	0
4.3594	2.9445	1.3905	H	0	0	0	0	0
3.8212	1.8824	0.0670	H	0	0	0	0	0
6.2714	1.6223	0.4880	H	0	0	0	0	0
5.9700	2.2869	-1.1358	H	0	0	0	0	0
6.7047	3.9099	1.3535	H	0	0	0	0	0
7.7889	3.5473	-0.0111	H	0	0	0	0	0
6.7703	5.8176	-0.2340	H	0	0	0	0	0

		5.0783		-1.0277		0.8551	H	0	0	0	0	0
		3.9473		3.7579		-1.4735	H	0	0	0	0	0
2	1	1	0	0	0							
6	1	2	0	0	0							
35	1	1	0	0	0							
3	2	2	0	0	0							
7	2	1	0	0	0							
4	3	1	0	0	0							
36	3	1	0	0	0							
5	4	2	0	0	0							
15	4	1	0	0	0							
6	5	1	0	0	0							
18	5	1	0	0	0							
8	6	1	0	0	0							
37	7	1	0	0	0							
9	8	1	0	0	0							
38	8	1	0	0	0							
39	8	1	0	0	0							
10	9	1	0	0	0							
14	9	2	0	0	0							
11	10	2	0	0	0							
40	10	1	0	0	0							
12	11	1	0	0	0							
41	11	1	0	0	0							
13	12	2	0	0	0							
25	12	1	0	0	0							
14	13	1	0	0	0							
42	13	1	0	0	0							
43	14	1	0	0	0							
16	15	1	0	0	0							
17	16	1	0	0	0							
44	16	1	0	0	0							
45	16	1	0	0	0							
18	17	2	0	0	0							
19	17	1	0	0	0							
46	18	1	0	0	0							
20	19	1	0	0	0							
24	19	2	0	0	0							
21	20	2	0	0	0							
47	20	1	0	0	0							
22	21	1	0	0	0							
48	21	1	0	0	0							
23	22	2	0	0	0							
34	22	1	0	0	0							
24	23	1	0	0	0							
49	23	1	0	0	0							
50	24	1	0	0	0							
26	25	1	0	0	0							
27	26	1	0	0	0							
51	26	1	0	0	0							
52	26	1	0	0	0							
28	27	1	0	0	0							
53	27	1	0	0	0							

66	28	1	0	0	0
30	29	1	0	0	0
55	29	1	0	0	0
56	29	1	0	0	0
31	30	1	0	0	0
57	30	1	0	0	0
58	30	1	0	0	0
32	31	1	0	0	0
59	31	1	0	0	0
60	31	1	0	0	0
33	32	1	0	0	0
61	32	1	0	0	0
62	32	1	0	0	0
63	33	1	0	0	0
64	33	1	0	0	0
65	34	1	0	0	0

M END

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benzopyran_2

Forecaster10031114513D

65	69	0	0	0	0	0	0	0	0	0999	V2000					
-5.3911	-2.4943	-0.1073	C	0	0	0	0	0	0							
-5.5374	-3.8155	-0.1052	C	0	0	0	0	0	0							
-4.3774	-4.6686	-0.0617	C	0	0	0	0	0	0							
-3.1600	-4.1375	-0.0021	C	0	0	0	0	0	0							
-2.9772	-2.6783	0.0307	C	0	0	0	0	0	0							
-4.0591	-1.8573	-0.0431	C	0	0	0	0	0	0							
-6.8101	-4.3770	-0.1538	O	0	0	0	0	0	0							
-4.1245	-0.2563	-0.0296	C	0	0	0	0	0	0							
-2.9275	0.7416	-0.1002	C	0	0	0	0	0	0							
-1.8416	0.5742	-0.8602	C	0	0	0	0	0	0							
-0.7153	1.5357	-0.7872	C	0	0	0	0	0	0							
-0.8025	2.6023	0.0063	C	0	0	0	0	0	0							
-2.0355	2.8386	0.7496	C	0	0	0	0	0	0							
-3.0327	1.9589	0.7056	C	0	0	0	0	0	0							
-2.0873	-4.9785	0.0100	O	0	0	0	0	0	0							
-0.7453	-4.5416	-0.0154	C	0	0	0	0	0	0							
-0.5789	-3.0459	0.1146	C	0	0	0	0	0	0							
-1.6189	-2.2210	0.1402	C	0	0	0	0	0	0							
0.7704	-2.4728	0.1715	C	0	0	0	0	0	0							
1.8432	-3.2375	-0.0102	C	0	0	0	0	0	0							
3.1827	-2.6350	0.0131	C	0	0	0	0	0	0							
3.3233	-1.3261	0.2181	C	0	0	0	0	0	0							
2.1450	-0.4949	0.4273	C	0	0	0	0	0	0							
0.9335	-1.0435	0.4034	C	0	0	0	0	0	0							
0.2782	3.4941	0.2038	O	0	0	0	0	0	0							
1.5234	3.1166	-0.4316	C	0	0	0	0	0	0							
2.5676	4.1899	-0.0008	C	0	0	0	0	0	0							
3.9646	3.9008	-0.4190	N	0	0	0	0	0	0							
4.4750	2.6925	0.2874	C	0	0	0	0	0	0							
5.9512	2.4217	-0.1081	C	0	0	0	0	0	0							
6.8113	3.6420	0.2698	C	0	0	0	0	0	0							

-4.4980	-5.7518	-0.0777	H	0	0	0	0	0
-7.3649	-4.0603	0.6795	H	0	0	0	0	0
-4.7549	0.0041	-0.8798	H	0	0	0	0	0
-4.6415	-0.0063	0.8968	H	0	0	0	0	0
-1.7831	-0.2762	-1.5395	H	0	0	0	0	0
0.1830	1.3701	-1.3820	H	0	0	0	0	0
-2.1407	3.7445	1.3466	H	0	0	0	0	0
-3.9410	2.1475	1.2779	H	0	0	0	0	0
-0.2153	-5.0174	0.8097	H	0	0	0	0	0
-0.3020	-4.8539	-0.9610	H	0	0	0	0	0
-1.4350	-1.1521	0.2488	H	0	0	0	0	0
1.7288	-4.3087	-0.1760	H	0	0	0	0	0
4.0630	-3.2598	-0.1376	H	0	0	0	0	0
4.3170	-0.8783	0.2293	H	0	0	0	0	0
2.2562	0.5751	0.6032	H	0	0	0	0	0
0.0545	-0.4180	0.5587	H	0	0	0	0	0
1.8357	2.1280	-0.0951	H	0	0	0	0	0
1.4094	3.1128	-1.5156	H	0	0	0	0	0
2.2732	5.1442	-0.4375	H	0	0	0	0	0
2.5476	4.2656	1.0864	H	0	0	0	0	0
4.4148	2.8530	1.3638	H	0	0	0	0	0
3.8655	1.8314	0.0133	H	0	0	0	0	0
6.3147	1.5418	0.4227	H	0	0	0	0	0
6.0146	2.2504	-1.1827	H	0	0	0	0	0
6.7654	3.8045	1.3466	H	0	0	0	0	0
7.8454	3.4691	-0.0284	H	0	0	0	0	0
6.8444	5.7522	-0.1912	H	0	0	0	0	0
6.3203	4.7149	-1.5397	H	0	0	0	0	0
4.7380	5.2286	1.0281	H	0	0	0	0	0
4.3971	5.9620	-0.5579	H	0	0	0	0	0
4.0029	3.7466	-1.4771	H	0	0	0	0	0
2	1	1	0	0	0			
6	1	2	0	0	0			
34	1	1	0	0	0			
3	2	2	0	0	0			
7	2	1	0	0	0			
4	3	1	0	0	0			
35	3	1	0	0	0			
5	4	2	0	0	0			
15	4	1	0	0	0			
6	5	1	0	0	0			
18	5	1	0	0	0			
8	6	1	0	0	0			
36	7	1	0	0	0			
9	8	1	0	0	0			
37	8	1	0	0	0			
38	8	1	0	0	0			
10	9	1	0	0	0			
14	9	2	0	0	0			
11	10	2	0	0	0			
39	10	1	0	0	0			
12	11	1	0	0	0			
40	11	1	0	0	0			

-4.3577	-7.2882	0.0696	O	0	0	0	0	0
-0.0475	-3.5623	-0.0541	N	0	0	0	0	0
1.2046	-4.0764	-0.0585	N	0	0	0	0	0
2.0671	-3.1460	0.0853	C	0	0	0	0	0
1.3660	-1.8212	0.1886	C	0	0	0	0	0
0.0421	-2.0627	0.0683	C	0	0	0	0	0
2.0910	-0.4634	0.3543	C	0	0	0	0	0
2.0255	0.4037	-0.9292	C	0	0	0	0	0
3.5586	-3.4460	0.0799	C	0	0	0	0	0
3.9511	-4.7167	-0.0124	C	0	0	0	0	0
5.3839	-5.0601	-0.0436	C	0	0	0	0	0
6.3048	-4.0990	0.0106	C	0	0	0	0	0
5.8912	-2.7049	0.1067	C	0	0	0	0	0
4.5969	-2.3938	0.1426	C	0	0	0	0	0
7.6596	-4.4222	-0.0227	O	0	0	0	0	0
-1.1344	-0.9866	0.0457	C	0	0	0	0	0
-0.9864	0.2701	0.4956	C	0	0	0	0	0
-2.0931	1.2516	0.4220	C	0	0	0	0	0
-3.2617	0.8869	-0.1033	C	0	0	0	0	0
-3.4272	-0.4497	-0.5913	C	0	0	0	0	0
-2.4297	-1.3161	-0.5271	C	0	0	0	0	0
-4.3462	1.7519	-0.2210	O	0	0	0	0	0
-4.1091	3.0723	0.2472	C	0	0	0	0	0
-5.4200	3.8329	-0.0208	C	0	0	0	0	0
-5.3409	5.2410	0.3669	N	0	0	0	0	0
-4.2879	5.9198	-0.4260	C	0	0	0	0	0
-4.2183	7.4113	-0.0361	C	0	0	0	0	0
-5.5818	8.0650	-0.3181	C	0	0	0	0	0
-6.6584	7.3345	0.4974	C	0	0	0	0	0
-6.6624	5.8500	0.0961	C	0	0	0	0	0
-4.5636	-4.7436	0.4365	H	0	0	0	0	0
-1.7238	-7.8822	-0.3431	H	0	0	0	0	0
0.0889	-6.2808	-0.4019	H	0	0	0	0	0
-2.6598	-3.0803	0.4099	H	0	0	0	0	0
-4.8283	-7.2605	1.0079	H	0	0	0	0	0
1.6228	0.0855	1.1714	H	0	0	0	0	0
3.1370	-0.6527	0.5954	H	0	0	0	0	0
2.5488	1.3447	-0.7597	H	0	0	0	0	0
0.9840	0.6074	-1.1779	H	0	0	0	0	0
2.4977	-0.1305	-1.7537	H	0	0	0	0	0
3.2049	-5.5095	-0.0653	H	0	0	0	0	0
5.6911	-6.1037	-0.1112	H	0	0	0	0	0
6.6421	-1.9160	0.1492	H	0	0	0	0	0
4.2979	-1.3484	0.2193	H	0	0	0	0	0
7.8929	-5.0395	0.7941	H	0	0	0	0	0
-0.0314	0.5742	0.9241	H	0	0	0	0	0
-1.9523	2.2660	0.7953	H	0	0	0	0	0
-4.3823	-0.7551	-1.0187	H	0	0	0	0	0
-2.5854	-2.3206	-0.9206	H	0	0	0	0	0
-3.8817	3.0653	1.3132	H	0	0	0	0	0
-3.2832	3.5292	-0.2980	H	0	0	0	0	0
-5.6454	3.7760	-1.0857	H	0	0	0	0	0
-6.2210	3.3589	0.5465	H	0	0	0	0	0

-3.4463	7.9074	-0.6244	H	0	0	0	0	0
-5.5517	9.1151	-0.0274	H	0	0	0	0	0
-5.8121	7.9881	-1.3807	H	0	0	0	0	0
-6.4370	7.4257	1.5608	H	0	0	0	0	0
-7.6348	7.7725	0.2901	H	0	0	0	0	0
-7.4250	5.3244	0.6708	H	0	0	0	0	0
-6.8858	5.7658	-0.9674	H	0	0	0	0	0
-5.1142	5.3171	1.4098	H	0	0	0	0	0
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37	1	1	0	0	0			
3	2	2	0	0	0			
7	2	1	0	0	0			
4	3	1	0	0	0			
38	3	1	0	0	0			
5	4	2	0	0	0			
39	4	1	0	0	0			
6	5	1	0	0	0			
8	5	1	0	0	0			
40	6	1	0	0	0			
41	7	1	0	0	0			
9	8	1	0	0	0			
12	8	1	0	0	0			
10	9	2	0	0	0			
11	10	1	0	0	0			
15	10	1	0	0	0			
12	11	2	0	0	0			
13	11	1	0	0	0			
22	12	1	0	0	0			
14	13	1	0	0	0			
42	13	1	0	0	0			
43	13	1	0	0	0			
44	14	1	0	0	0			
45	14	1	0	0	0			
46	14	1	0	0	0			
16	15	1	0	0	0			
20	15	2	0	0	0			
17	16	2	0	0	0			
47	16	1	0	0	0			
18	17	1	0	0	0			
48	17	1	0	0	0			
19	18	2	0	0	0			
21	18	1	0	0	0			
20	19	1	0	0	0			
49	19	1	0	0	0			
50	20	1	0	0	0			
51	21	1	0	0	0			
23	22	1	0	0	0			
27	22	2	0	0	0			
24	23	2	0	0	0			
52	23	1	0	0	0			
25	24	1	0	0	0			
53	24	1	0	0	0			

54 26 1 0 0 0
55 27 1 0 0 0
29 28 1 0 0 0
30 29 1 0 0 0
56 29 1 0 0 0
57 29 1 0 0 0
31 30 1 0 0 0
58 30 1 0 0 0
59 30 1 0 0 0
32 31 1 0 0 0
36 31 1 0 0 0
70 31 1 0 0 0
33 32 1 0 0 0
60 32 1 0 0 0
61 32 1 0 0 0
34 33 1 0 0 0
62 33 1 0 0 0
63 33 1 0 0 0
35 34 1 0 0 0
64 34 1 0 0 0
65 34 1 0 0 0
36 35 1 0 0 0
66 35 1 0 0 0
67 35 1 0 0 0
68 36 1 0 0 0
69 36 1 0 0 0

M END

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pyrrazole_2

Forecaster10031114513D

67 71 0 0 0 0 0 0 0 0999 V2000
-3.5389 -5.0882 -0.1727 C 0 0 0 0 0
-3.2987 -6.3835 -0.0396 C 0 0 0 0 0
-1.9154 -6.8479 0.1072 C 0 0 0 0 0
-0.9066 -5.9694 0.1217 C 0 0 0 0 0
-1.1697 -4.5229 -0.0070 C 0 0 0 0 0
-2.4326 -4.1466 -0.1609 C 0 0 0 0 0
-4.3583 -7.2871 -0.0411 O 0 0 0 0 0
-0.0175 -3.5881 0.0245 N 0 0 0 0 0
1.2399 -4.1064 0.0273 N 0 0 0 0 0
2.1052 -3.1724 -0.0223 C 0 0 0 0 0
1.4148 -1.8453 -0.0548 C 0 0 0 0 0
0.0834 -2.0772 -0.0112 C 0 0 0 0 0
2.1210 -0.4937 -0.0846 C 0 0 0 0 0
3.6024 -3.4569 -0.0221 C 0 0 0 0 0
4.0123 -4.7271 0.0099 C 0 0 0 0 0
5.4521 -5.0470 0.0174 C 0 0 0 0 0
6.3585 -4.0706 -0.0048 C 0 0 0 0 0
5.9254 -2.6825 -0.0386 C 0 0 0 0 0
4.6277 -2.3916 -0.0478 C 0 0 0 0 0
7.7179 -4.3723 0.0037 O 0 0 0 0 0
-1.0654 -0.9583 0.0195 C 0 0 0 0 0

-3.4120	-0.4252	0.3940	C	0	0	0	0	0
-2.4270	-1.3047	0.3571	C	0	0	0	0	0
-4.2584	1.8058	0.1538	O	0	0	0	0	0
-3.9805	3.1566	-0.1636	C	0	0	0	0	0
-5.3252	3.8775	0.0246	C	0	0	0	0	0
-5.2601	5.2886	-0.3391	N	0	0	0	0	0
-4.2524	5.9834	0.4919	C	0	0	0	0	0
-4.1982	7.4740	0.0996	C	0	0	0	0	0
-5.5834	8.1009	0.3330	C	0	0	0	0	0
-6.6180	7.3492	-0.5167	C	0	0	0	0	0
-6.6045	5.8655	-0.1169	C	0	0	0	0	0
-4.5616	-4.7301	-0.2905	H	0	0	0	0	0
-1.7083	-7.9136	0.2049	H	0	0	0	0	0
0.1182	-6.3249	0.2295	H	0	0	0	0	0
-2.6494	-3.0855	-0.2838	H	0	0	0	0	0
-5.0093	-7.0652	0.7523	H	0	0	0	0	0
1.3788	0.3042	-0.1049	H	0	0	0	0	0
2.7469	-0.4298	-0.9747	H	0	0	0	0	0
2.7427	-0.3883	0.8045	H	0	0	0	0	0
3.2784	-5.5327	0.0306	H	0	0	0	0	0
5.7763	-6.0874	0.0412	H	0	0	0	0	0
6.6640	-1.8811	-0.0564	H	0	0	0	0	0
4.3139	-1.3481	-0.0748	H	0	0	0	0	0
7.9519	-4.9109	0.8741	H	0	0	0	0	0
0.1719	0.6662	-0.4781	H	0	0	0	0	0
-1.7285	2.3895	-0.4228	H	0	0	0	0	0
-4.4194	-0.7528	0.6508	H	0	0	0	0	0
-2.6529	-2.3445	0.5933	H	0	0	0	0	0
-3.2269	3.5639	0.5104	H	0	0	0	0	0
-3.6350	3.2476	-1.1934	H	0	0	0	0	0
-6.0732	3.3900	-0.6007	H	0	0	0	0	0
-5.6194	3.8000	1.0713	H	0	0	0	0	0
-4.5257	5.8947	1.5433	H	0	0	0	0	0
-3.2743	5.5301	0.3307	H	0	0	0	0	0
-3.4566	7.9868	0.7122	H	0	0	0	0	0
-3.9276	7.5659	-0.9523	H	0	0	0	0	0
-5.8482	8.0211	1.3873	H	0	0	0	0	0
-5.5637	9.1510	0.0413	H	0	0	0	0	0
-7.6093	7.7668	-0.3406	H	0	0	0	0	0
-6.3647	7.4462	-1.5724	H	0	0	0	0	0
-6.8654	5.7745	0.9375	H	0	0	0	0	0
-7.3329	5.3236	-0.7201	H	0	0	0	0	0
-4.9972	5.3804	-1.3722	H	0	0	0	0	0
2	1	1	0	0	0			
6	1	2	0	0	0			
36	1	1	0	0	0			
3	2	2	0	0	0			
7	2	1	0	0	0			
4	3	1	0	0	0			
37	3	1	0	0	0			
5	4	2	0	0	0			
38	4	1	0	0	0			
6	5	1	0	0	0			

9	8	1	0	0	0
12	8	1	0	0	0
10	9	2	0	0	0
11	10	1	0	0	0
14	10	1	0	0	0
12	11	2	0	0	0
13	11	1	0	0	0
21	12	1	0	0	0
41	13	1	0	0	0
42	13	1	0	0	0
43	13	1	0	0	0
15	14	1	0	0	0
19	14	2	0	0	0
16	15	2	0	0	0
44	15	1	0	0	0
17	16	1	0	0	0
45	16	1	0	0	0
18	17	2	0	0	0
20	17	1	0	0	0
19	18	1	0	0	0
46	18	1	0	0	0
47	19	1	0	0	0
48	20	1	0	0	0
22	21	1	0	0	0
26	21	2	0	0	0
23	22	2	0	0	0
49	22	1	0	0	0
24	23	1	0	0	0
50	23	1	0	0	0
25	24	2	0	0	0
27	24	1	0	0	0
26	25	1	0	0	0
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28	27	1	0	0	0
29	28	1	0	0	0
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54	28	1	0	0	0
30	29	1	0	0	0
55	29	1	0	0	0
56	29	1	0	0	0
31	30	1	0	0	0
35	30	1	0	0	0
67	30	1	0	0	0
32	31	1	0	0	0
57	31	1	0	0	0
58	31	1	0	0	0
33	32	1	0	0	0
59	32	1	0	0	0
60	32	1	0	0	0
34	33	1	0	0	0
61	33	1	0	0	0
62	33	1	0	0	0

Forecaster10031114513D

```
73 77  0  0  0  0  0  0  0  0  0999 v2000
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-3.5460	-5.1351	0.0746	C	0	0	0	0	0
-3.2633	-6.4254	0.0452	C	0	0	0	0	0
-1.8575	-6.8484	-0.0114	C	0	0	0	0	0
-0.8743	-5.9370	-0.0365	C	0	0	0	0	0
-1.1843	-4.4888	-0.0086	C	0	0	0	0	0
-2.4687	-4.1644	0.0495	C	0	0	0	0	0
-4.2978	-7.3600	0.0685	O	0	0	0	0	0
-0.0406	-3.4965	-0.0285	N	0	0	0	0	0
1.1940	-4.0059	-0.0190	N	0	0	0	0	0
2.0851	-3.0990	0.0026	C	0	0	0	0	0
1.4043	-1.6836	0.0656	C	0	0	0	0	0
0.0450	-1.9459	-0.0324	C	0	0	0	0	0
2.2442	-0.2355	0.2336	C	0	0	0	0	0
1.6040	0.9506	0.9608	C	0	0	0	0	0
3.5724	-3.5398	-0.0879	C	0	0	0	0	0
3.8807	-4.8028	0.2138	C	0	0	0	0	0
5.2885	-5.2628	0.1836	C	0	0	0	0	0
6.2639	-4.4246	-0.1666	C	0	0	0	0	0
5.9373	-3.0695	-0.5524	C	0	0	0	0	0
4.6733	-2.6581	-0.5255	C	0	0	0	0	0
7.5930	-4.8435	-0.1680	O	0	0	0	0	0
-1.2155	-0.8923	-0.1069	C	0	0	0	0	0
-1.0703	0.4262	-0.2173	C	0	0	0	0	0
-2.2024	1.3616	-0.2231	C	0	0	0	0	0
-3.4400	0.8897	-0.1656	C	0	0	0	0	0
-3.6361	-0.5156	-0.1214	C	0	0	0	0	0
-2.5928	-1.3299	-0.0857	C	0	0	0	0	0
-4.5539	1.7133	-0.1224	O	0	0	0	0	0
-4.2287	3.0938	-0.0406	C	0	0	0	0	0
-5.5632	3.8437	-0.0873	C	0	0	0	0	0
-5.4144	5.2534	0.2738	N	0	0	0	0	0
-4.4233	5.9238	-0.5955	C	0	0	0	0	0
-4.2882	7.4027	-0.1729	C	0	0	0	0	0
-5.6569	8.0885	-0.3230	C	0	0	0	0	0
-6.6767	7.3607	0.5642	C	0	0	0	0	0
-6.7438	5.8859	0.1394	C	0	0	0	0	0
3.5483	-0.3168	1.0252	C	0	0	0	0	0
-4.5830	-4.8020	0.1175	H	0	0	0	0	0
-1.6121	-7.9102	-0.0331	H	0	0	0	0	0
0.1643	-6.2653	-0.0779	H	0	0	0	0	0
-2.7301	-3.1066	0.0802	H	0	0	0	0	0
-4.8583	-7.2405	0.9483	H	0	0	0	0	0
2.4997	0.1045	-0.7700	H	0	0	0	0	0
2.2978	1.7912	0.9668	H	0	0	0	0	0
1.3707	0.6655	1.9867	H	0	0	0	0	0

6.7268	-2.3861	-0.8650	H	0	0	0	0	0
4.4426	-1.6390	-0.8359	H	0	0	0	0	0
7.8650	-5.1496	0.7989	H	0	0	0	0	0
-0.0624	0.8312	-0.3078	H	0	0	0	0	0
-2.0264	2.4361	-0.2743	H	0	0	0	0	0
-4.6465	-0.9246	-0.1168	H	0	0	0	0	0
-2.7854	-2.4017	-0.0371	H	0	0	0	0	0
-3.7076	3.3056	0.8930	H	0	0	0	0	0
-3.6005	3.3856	-0.8822	H	0	0	0	0	0
-5.9667	3.7804	-1.0979	H	0	0	0	0	0
-6.2554	3.3732	0.6110	H	0	0	0	0	0
-3.4579	5.4276	-0.4961	H	0	0	0	0	0
-4.7545	5.8708	-1.6326	H	0	0	0	0	0
-3.9627	7.4584	0.8659	H	0	0	0	0	0
-3.5574	7.9004	-0.8104	H	0	0	0	0	0
-5.5800	9.1306	-0.0129	H	0	0	0	0	0
-5.9777	8.0413	-1.3637	H	0	0	0	0	0
-6.3671	7.4271	1.6072	H	0	0	0	0	0
-7.6580	7.8203	0.4460	H	0	0	0	0	0
-7.4577	5.3609	0.7741	H	0	0	0	0	0
-7.0675	5.8253	-0.8997	H	0	0	0	0	0
4.0074	0.6706	1.0724	H	0	0	0	0	0
4.2299	-1.0107	0.5332	H	0	0	0	0	0
3.3393	-0.6684	2.0356	H	0	0	0	0	0
-5.0932	5.3234	1.2920	H	0	0	0	0	0
2	1	1	0	0	0			
6	1	2	0	0	0			
38	1	1	0	0	0			
3	2	2	0	0	0			
7	2	1	0	0	0			
4	3	1	0	0	0			
39	3	1	0	0	0			
5	4	2	0	0	0			
40	4	1	0	0	0			
6	5	1	0	0	0			
8	5	1	0	0	0			
41	6	1	0	0	0			
42	7	1	0	0	0			
9	8	1	0	0	0			
12	8	1	0	0	0			
10	9	2	0	0	0			
11	10	1	0	0	0			
15	10	1	0	0	0			
12	11	2	0	0	0			
13	11	1	0	0	0			
22	12	1	0	0	0			
14	13	1	0	0	0			
37	13	1	0	0	0			
43	13	1	0	0	0			
44	14	1	0	0	0			
45	14	1	0	0	0			
46	14	1	0	0	0			
16	15	1	0	0	0			

18	17	1	0	0	0
48	17	1	0	0	0
19	18	2	0	0	0
21	18	1	0	0	0
20	19	1	0	0	0
49	19	1	0	0	0
50	20	1	0	0	0
51	21	1	0	0	0
23	22	1	0	0	0
27	22	2	0	0	0
24	23	2	0	0	0
52	23	1	0	0	0
25	24	1	0	0	0
53	24	1	0	0	0
26	25	2	0	0	0
28	25	1	0	0	0
27	26	1	0	0	0
54	26	1	0	0	0
55	27	1	0	0	0
29	28	1	0	0	0
30	29	1	0	0	0
56	29	1	0	0	0
57	29	1	0	0	0
31	30	1	0	0	0
58	30	1	0	0	0
59	30	1	0	0	0
32	31	1	0	0	0
36	31	1	0	0	0
73	31	1	0	0	0
33	32	1	0	0	0
60	32	1	0	0	0
61	32	1	0	0	0
34	33	1	0	0	0
62	33	1	0	0	0
63	33	1	0	0	0
35	34	1	0	0	0
64	34	1	0	0	0
65	34	1	0	0	0
36	35	1	0	0	0
66	35	1	0	0	0
67	35	1	0	0	0
68	36	1	0	0	0
69	36	1	0	0	0
70	37	1	0	0	0
71	37	1	0	0	0
72	37	1	0	0	0

M END

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pyrrazole_4

Forecaster10031114513D

70 74 0 0 0 0 0 0 0 0999 V2000

-6.6366 -3.1461 -0.0994 C 0 0 0 0 0

-4.2044	-3.4406	0.0617	C	0	0	0	0	0
-5.2520	-2.6071	-0.0825	C	0	0	0	0	0
-8.1541	-4.9669	-0.0045	O	0	0	0	0	0
-2.7667	-2.8396	0.0497	C	0	0	0	0	0
-1.4257	-3.5864	0.1704	C	0	0	0	0	0
-0.4418	-2.6176	0.0688	C	0	0	0	0	0
-2.5599	-1.5952	-0.0780	N	0	0	0	0	0
1.1712	-2.9132	0.0517	C	0	0	0	0	0
1.6960	-4.1165	0.2563	C	0	0	0	0	0
3.1486	-4.3689	0.2204	C	0	0	0	0	0
3.9922	-3.3726	-0.0303	C	0	0	0	0	0
3.4715	-2.0615	-0.2800	C	0	0	0	0	0
2.1583	-1.8518	-0.2517	C	0	0	0	0	0
5.3648	-3.5964	-0.0570	O	0	0	0	0	0
-1.2184	-1.3147	-0.0419	N	0	0	0	0	0
-1.1888	-5.1197	0.3732	C	0	0	0	0	0
-1.7164	-6.0579	-0.7438	C	0	0	0	0	0
-0.7222	0.1120	0.0004	C	0	0	0	0	0
0.5101	0.4081	0.3541	C	0	0	0	0	0
1.0616	1.7403	0.3389	C	0	0	0	0	0
0.3103	2.7670	-0.0183	C	0	0	0	0	0
-1.1205	2.5146	-0.3545	C	0	0	0	0	0
-1.6142	1.2587	-0.3455	C	0	0	0	0	0
0.9004	4.0671	-0.1063	O	0	0	0	0	0
2.3380	4.0210	0.2243	C	0	0	0	0	0
3.0236	5.3949	-0.0582	C	0	0	0	0	0
4.4787	5.3992	0.3131	N	0	0	0	0	0
5.2377	4.3866	-0.4725	C	0	0	0	0	0
6.7366	4.4050	-0.0628	C	0	0	0	0	0
7.3207	5.8031	-0.3332	C	0	0	0	0	0
6.5169	6.8329	0.4737	C	0	0	0	0	0
5.0298	6.7563	0.0539	C	0	0	0	0	0
-7.4801	-2.4647	-0.2106	H	0	0	0	0	0
-5.9023	-6.4259	0.2829	H	0	0	0	0	0
-3.6647	-5.5632	0.3461	H	0	0	0	0	0
-5.0841	-1.5352	-0.1870	H	0	0	0	0	0
-8.7098	-4.5518	0.7838	H	0	0	0	0	0
1.0254	-4.9515	0.4590	H	0	0	0	0	0
3.5310	-5.3738	0.3997	H	0	0	0	0	0
4.1510	-1.2363	-0.4930	H	0	0	0	0	0
1.7901	-0.8478	-0.4625	H	0	0	0	0	0
5.6793	-3.9576	0.8774	H	0	0	0	0	0
-0.1140	-5.2796	0.4589	H	0	0	0	0	0
-1.6751	-5.4089	1.3048	H	0	0	0	0	0
-1.4911	-7.0928	-0.4863	H	0	0	0	0	0
-1.2343	-5.8059	-1.6884	H	0	0	0	0	0
-2.7950	-5.9352	-0.8427	H	0	0	0	0	0
1.1563	-0.4070	0.6799	H	0	0	0	0	0
2.1016	1.9010	0.6230	H	0	0	0	0	0
-1.7721	3.3504	-0.6093	H	0	0	0	0	0
-2.6615	1.0817	-0.5901	H	0	0	0	0	0
2.4527	3.7764	1.2803	H	0	0	0	0	0
2.8181	3.2524	-0.3814	H	0	0	0	0	0

	5.1518	4.6163	-1.5345	H	0	0	0	0	0
	6.8268	4.1718	0.9981	H	0	0	0	0	0
	7.2825	3.6634	-0.6461	H	0	0	0	0	0
	8.3660	5.8303	-0.0255	H	0	0	0	0	0
	7.2483	6.0321	-1.3964	H	0	0	0	0	0
	6.6074	6.6139	1.5376	H	0	0	0	0	0
	6.9012	7.8332	0.2742	H	0	0	0	0	0
	4.4590	7.4889	0.6245	H	0	0	0	0	0
	4.9467	6.9787	-1.0099	H	0	0	0	0	0
	4.5742	5.1764	1.3553	H	0	0	0	0	0
2	1	1	0	0	0				
6	1	2	0	0	0				
37	1	1	0	0	0				
3	2	2	0	0	0				
7	2	1	0	0	0				
4	3	1	0	0	0				
38	3	1	0	0	0				
5	4	2	0	0	0				
39	4	1	0	0	0				
6	5	1	0	0	0				
8	5	1	0	0	0				
40	6	1	0	0	0				
41	7	1	0	0	0				
9	8	1	0	0	0				
11	8	2	0	0	0				
10	9	2	0	0	0				
20	9	1	0	0	0				
12	10	1	0	0	0				
19	10	1	0	0	0				
19	11	1	0	0	0				
13	12	1	0	0	0				
17	12	2	0	0	0				
14	13	2	0	0	0				
42	13	1	0	0	0				
15	14	1	0	0	0				
43	14	1	0	0	0				
16	15	2	0	0	0				
18	15	1	0	0	0				
17	16	1	0	0	0				
44	16	1	0	0	0				
45	17	1	0	0	0				
46	18	1	0	0	0				
22	19	1	0	0	0				
21	20	1	0	0	0				
47	20	1	0	0	0				
48	20	1	0	0	0				
49	21	1	0	0	0				
50	21	1	0	0	0				
51	21	1	0	0	0				
23	22	1	0	0	0				
27	22	2	0	0	0				
24	23	2	0	0	0				
52	23	1	0	0	0				

28	25	1	0	0	0
27	26	1	0	0	0
54	26	1	0	0	0
55	27	1	0	0	0
29	28	1	0	0	0
30	29	1	0	0	0
56	29	1	0	0	0
57	29	1	0	0	0
31	30	1	0	0	0
58	30	1	0	0	0
59	30	1	0	0	0
32	31	1	0	0	0
36	31	1	0	0	0
70	31	1	0	0	0
33	32	1	0	0	0
60	32	1	0	0	0
61	32	1	0	0	0
34	33	1	0	0	0
62	33	1	0	0	0
63	33	1	0	0	0
35	34	1	0	0	0
64	34	1	0	0	0
65	34	1	0	0	0
36	35	1	0	0	0
66	35	1	0	0	0
67	35	1	0	0	0
68	36	1	0	0	0
69	36	1	0	0	0

M END

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phenantrene_1

Forecaster10031114513D

65	70	0	0	0	0	0	0	0	0	0999	V2000					
-2.7613	-4.9355	0.3045	C	0	0	0	0	0	0							
-2.5920	-6.2392	0.1424	C	0	0	0	0	0	0							
-1.2487	-6.7685	-0.0204	C	0	0	0	0	0	0							
-0.1993	-5.9455	-0.0458	C	0	0	0	0	0	0							
-0.3703	-4.4961	0.0784	C	0	0	0	0	0	0							
-1.6055	-4.0509	0.2801	C	0	0	0	0	0	0							
-3.6903	-7.0913	0.1458	O	0	0	0	0	0	0							
1.1125	-6.4954	-0.1568	C	0	0	0	0	0	0							
2.1705	-5.6979	-0.1461	C	0	0	0	0	0	0							
2.0693	-4.2293	-0.0637	C	0	0	0	0	0	0							
0.8934	-3.5826	0.0102	C	0	0	0	0	0	0							
3.3166	-3.5185	-0.0572	C	0	0	0	0	0	0							
3.3731	-2.2044	0.0203	C	0	0	0	0	0	0							
2.1681	-1.3937	0.0712	C	0	0	0	0	0	0							
0.9305	-1.9774	0.0590	C	0	0	0	0	0	0							
4.6859	-1.5625	0.0120	C	0	0	0	0	0	0							
4.7956	-0.2376	0.0198	C	0	0	0	0	0	0							
3.6067	0.6096	0.0327	C	0	0	0	0	0	0							
2.3856	0.0755	0.0565	C	0	0	0	0	0	0							

-2.6720	0.5654	-0.1155	C	0	0	0	0	0
-2.5710	-0.6294	-0.9174	C	0	0	0	0	0
-1.4787	-1.3816	-0.8671	C	0	0	0	0	0
-3.8459	1.3575	-0.2506	O	0	0	0	0	0
-3.8072	2.6226	0.4311	C	0	0	0	0	0
-2.9284	3.5896	-0.4183	C	0	0	0	0	0
-2.8980	4.9247	0.1454	N	0	0	0	0	0
-1.9134	5.7144	-0.6197	C	0	0	0	0	0
-1.8392	7.1433	-0.0611	C	0	0	0	0	0
-3.2246	7.7923	-0.1936	C	0	0	0	0	0
-4.2448	6.9497	0.5902	C	0	0	0	0	0
-4.2490	5.5179	0.0265	C	0	0	0	0	0
3.7500	1.9934	0.0175	O	0	0	0	0	0
-3.7607	-4.5273	0.4553	H	0	0	0	0	0
-1.0978	-7.8432	-0.1223	H	0	0	0	0	0
-1.7594	-2.9827	0.4331	H	0	0	0	0	0
-4.1906	-7.0146	1.0658	H	0	0	0	0	0
1.2445	-7.5733	-0.2506	H	0	0	0	0	0
3.1616	-6.1484	-0.2007	H	0	0	0	0	0
4.2465	-4.0839	-0.1183	H	0	0	0	0	0
5.5859	-2.1773	-0.0007	H	0	0	0	0	0
5.7843	0.2213	0.0165	H	0	0	0	0	0
1.5198	0.7376	0.0655	H	0	0	0	0	0
0.3447	0.3260	1.4381	H	0	0	0	0	0
-1.7242	1.7858	1.3102	H	0	0	0	0	0
-3.3967	-0.9162	-1.5686	H	0	0	0	0	0
-1.4123	-2.2609	-1.5078	H	0	0	0	0	0
-4.8160	3.0243	0.5262	H	0	0	0	0	0
-3.3705	2.4974	1.4219	H	0	0	0	0	0
-1.9112	3.1998	-0.4568	H	0	0	0	0	0
-3.3364	3.6421	-1.4277	H	0	0	0	0	0
-0.9332	5.2443	-0.5400	H	0	0	0	0	0
-2.2152	5.7512	-1.6664	H	0	0	0	0	0
-1.5468	7.1126	0.9885	H	0	0	0	0	0
-1.1075	7.7209	-0.6259	H	0	0	0	0	0
-3.1956	8.8033	0.2128	H	0	0	0	0	0
-3.5118	7.8307	-1.2444	H	0	0	0	0	0
-3.9672	6.9268	1.6440	H	0	0	0	0	0
-5.2377	7.3869	0.4849	H	0	0	0	0	0
-4.9604	4.9113	0.5869	H	0	0	0	0	0
-4.5408	5.5440	-1.0234	H	0	0	0	0	0
4.2932	2.2988	0.8626	H	0	0	0	0	0
-2.6088	4.8796	1.1746	H	0	0	0	0	0
2	1	1	0	0	0			
6	1	2	0	0	0			
36	1	1	0	0	0			
3	2	2	0	0	0			
7	2	1	0	0	0			
4	3	1	0	0	0			
37	3	1	0	0	0			
5	4	2	0	0	0			
8	4	1	0	0	0			
6	5	1	0	0	0			

9	8	2	0	0	0
40	8	1	0	0	0
10	9	1	0	0	0
41	9	1	0	0	0
11	10	1	0	0	0
12	10	2	0	0	0
15	11	2	0	0	0
13	12	1	0	0	0
42	12	1	0	0	0
14	13	2	0	0	0
16	13	1	0	0	0
15	14	1	0	0	0
19	14	1	0	0	0
20	15	1	0	0	0
17	16	2	0	0	0
43	16	1	0	0	0
18	17	1	0	0	0
44	17	1	0	0	0
19	18	2	0	0	0
35	18	1	0	0	0
45	19	1	0	0	0
21	20	1	0	0	0
25	20	2	0	0	0
22	21	2	0	0	0
46	21	1	0	0	0
23	22	1	0	0	0
47	22	1	0	0	0
24	23	2	0	0	0
26	23	1	0	0	0
25	24	1	0	0	0
48	24	1	0	0	0
49	25	1	0	0	0
27	26	1	0	0	0
28	27	1	0	0	0
50	27	1	0	0	0
51	27	1	0	0	0
29	28	1	0	0	0
52	28	1	0	0	0
53	28	1	0	0	0
30	29	1	0	0	0
34	29	1	0	0	0
65	29	1	0	0	0
31	30	1	0	0	0
54	30	1	0	0	0
55	30	1	0	0	0
32	31	1	0	0	0
56	31	1	0	0	0
57	31	1	0	0	0
33	32	1	0	0	0
58	32	1	0	0	0
59	32	1	0	0	0
34	33	1	0	0	0
60	33	1	0	0	0

64 35 1 0 0 0

M END

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phenantrene_2

Forecaster10031114513D

62	67	0	0	0	0	0	0	0	0	0999	V2000					
-3.3332	-5.0525	0.1200	C	0	0	0	0	0	0							
-3.0622	-6.3588	0.0323	C	0	0	0	0	0	0							
-1.6682	-6.8115	-0.0526	C	0	0	0	0	0	0							
-0.7216	-5.8827	-0.0549	C	0	0	0	0	0	0							
-0.9819	-4.4725	0.0192	C	0	0	0	0	0	0							
-2.2406	-4.0590	0.1205	C	0	0	0	0	0	0							
-4.0987	-7.2857	0.0281	O	0	0	0	0	0	0							
1.4001	-4.4911	-0.0619	C	0	0	0	0	0	0							
0.3617	-3.6403	-0.0088	C	0	0	0	0	0	0							
2.7561	-4.0768	-0.0579	C	0	0	0	0	0	0							
3.0425	-2.7866	0.0073	C	0	0	0	0	0	0							
1.9795	-1.7527	0.0639	C	0	0	0	0	0	0							
0.6486	-2.0969	0.0560	C	0	0	0	0	0	0							
4.4467	-2.3856	-0.0008	C	0	0	0	0	0	0							
4.7909	-1.1011	0.0183	C	0	0	0	0	0	0							
3.7756	-0.0524	0.0468	C	0	0	0	0	0	0							
2.4793	-0.3526	0.0689	C	0	0	0	0	0	0							
-0.4940	-0.9907	0.0756	C	0	0	0	0	0	0							
-0.3099	0.2078	0.6404	C	0	0	0	0	0	0							
-1.3245	1.2387	0.6139	C	0	0	0	0	0	0							
-2.4899	1.0313	0.0046	C	0	0	0	0	0	0							
-2.7347	-0.2687	-0.5933	C	0	0	0	0	0	0							
-1.7944	-1.2117	-0.5604	C	0	0	0	0	0	0							
-3.4997	2.0401	-0.0929	O	0	0	0	0	0	0							
-3.1325	3.3404	0.4517	C	0	0	0	0	0	0							
-2.1212	4.0854	-0.4857	C	0	0	0	0	0	0							
-1.7741	5.3896	0.0736	N	0	0	0	0	0	0							
-0.6531	5.9614	-0.7000	C	0	0	0	0	0	0							
-0.2529	7.3257	-0.1078	C	0	0	0	0	0	0							
-1.4614	8.2702	-0.1921	C	0	0	0	0	0	0							
-2.6291	7.6533	0.5956	C	0	0	0	0	0	0							
-2.9620	6.2707	0.0036	C	0	0	0	0	0	0							
4.1675	1.2829	0.0490	O	0	0	0	0	0	0							
0.9074	-6.1089	-0.1184	S	0	0	0	0	0	0							
-4.3682	-4.7184	0.1917	H	0	0	0	0	0	0							
-1.4205	-7.8713	-0.1115	H	0	0	0	0	0	0							
-2.4648	-2.9955	0.2033	H	0	0	0	0	0	0							
-4.6486	-7.2006	0.9185	H	0	0	0	0	0	0							
3.5563	-4.8153	-0.1081	H	0	0	0	0	0	0							
5.2236	-3.1498	-0.0228	H	0	0	0	0	0	0							
5.8460	-0.8274	0.0126	H	0	0	0	0	0	0							
1.7545	0.4612	0.0916	H	0	0	0	0	0	0							
0.6376	0.4149	1.1379	H	0	0	0	0	0	0							
-1.1326	2.1961	1.0983	H	0	0	0	0	0	0							
-3.6925	-0.4742	-1.0714	H	0	0	0	0	0	0							
-1.9993	-2.1780	-1.0213	H	0	0	0	0	0	0							

-2.5764	4.2249	-1.4662	H	0	0	0	0	0
0.1996	5.2838	-0.6560	H	0	0	0	0	0
-0.9598	6.0934	-1.7376	H	0	0	0	0	0
0.0436	7.2010	0.9337	H	0	0	0	0	0
0.5790	7.7425	-0.6755	H	0	0	0	0	0
-1.2007	9.2375	0.2373	H	0	0	0	0	0
-1.7517	8.4012	-1.2345	H	0	0	0	0	0
-2.3454	7.5433	1.6423	H	0	0	0	0	0
-3.5021	8.3017	0.5215	H	0	0	0	0	0
-3.7776	5.8223	0.5709	H	0	0	0	0	0
-3.2638	6.3872	-1.0373	H	0	0	0	0	0
4.7583	1.4734	0.8959	H	0	0	0	0	0
-1.4781	5.2716	1.0950	H	0	0	0	0	0
2	1	1	0	0	0			
6	1	2	0	0	0			
35	1	1	0	0	0			
3	2	2	0	0	0			
7	2	1	0	0	0			
4	3	1	0	0	0			
36	3	1	0	0	0			
5	4	1	0	0	0			
34	4	2	0	0	0			
6	5	1	0	0	0			
9	5	2	0	0	0			
37	6	1	0	0	0			
38	7	1	0	0	0			
8	9	1	0	0	0			
10	8	1	0	0	0			
34	8	2	0	0	0			
13	9	1	0	0	0			
11	10	2	0	0	0			
39	10	1	0	0	0			
12	11	1	0	0	0			
14	11	1	0	0	0			
13	12	2	0	0	0			
17	12	1	0	0	0			
18	13	1	0	0	0			
15	14	2	0	0	0			
40	14	1	0	0	0			
16	15	1	0	0	0			
41	15	1	0	0	0			
17	16	2	0	0	0			
33	16	1	0	0	0			
42	17	1	0	0	0			
19	18	1	0	0	0			
23	18	2	0	0	0			
20	19	2	0	0	0			
43	19	1	0	0	0			
21	20	1	0	0	0			
44	20	1	0	0	0			
22	21	2	0	0	0			
24	21	1	0	0	0			
23	22	1	0	0	0			

26	25	1	0	0	0
47	25	1	0	0	0
48	25	1	0	0	0
27	26	1	0	0	0
49	26	1	0	0	0
50	26	1	0	0	0
28	27	1	0	0	0
32	27	1	0	0	0
62	27	1	0	0	0
29	28	1	0	0	0
51	28	1	0	0	0
52	28	1	0	0	0
30	29	1	0	0	0
53	29	1	0	0	0
54	29	1	0	0	0
31	30	1	0	0	0
55	30	1	0	0	0
56	30	1	0	0	0
32	31	1	0	0	0
57	31	1	0	0	0
58	31	1	0	0	0
59	32	1	0	0	0
60	32	1	0	0	0
61	33	1	0	0	0

M END

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indole_1

Forecaster10031114513D

85	89	0	0	0	0	0	0	0	0999	V2000					
-2.0706	-2.6123	0.0363	C	0	0	0	0	0							
-1.9805	-3.9501	0.0157	C	0	0	0	0	0							
-0.6617	-4.6009	-0.0210	C	0	0	0	0	0							
0.4157	-3.8238	-0.0175	C	0	0	0	0	0							
0.3591	-2.4378	0.0300	C	0	0	0	0	0							
-0.8013	-1.7809	0.0478	C	0	0	0	0	0							
1.7233	-4.2268	-0.0476	N	0	0	0	0	0							
2.5510	-3.0562	0.0427	C	0	0	0	0	0							
1.7582	-1.9320	0.0716	C	0	0	0	0	0							
4.0534	-3.3004	0.1157	C	0	0	0	0	0							
4.4721	-4.5325	-0.1689	C	0	0	0	0	0							
5.8974	-4.8769	-0.1281	C	0	0	0	0	0							
6.7947	-3.9576	0.2120	C	0	0	0	0	0							
6.3490	-2.6208	0.5547	C	0	0	0	0	0							
5.0530	-2.3151	0.5136	C	0	0	0	0	0							
2.0848	-0.3769	0.1754	C	0	0	0	0	0							
3.4462	0.1072	-0.3250	C	0	0	0	0	0							
4.0880	1.0933	0.3311	N	0	0	0	0	0							
4.0036	-0.4750	-1.2623	O	0	0	0	0	0							
5.4719	1.4470	0.0044	C	0	0	0	0	0							
6.3576	0.8786	1.1332	C	0	0	0	0	0							
5.7503	2.9688	-0.0125	C	0	0	0	0	0							
7.2858	3.1312	-0.2475	C	0	0	0	0	0							

8.6728	7.1961	0.0433	C	0	0	0	0	0
7.2340	6.9118	0.0860	C	0	0	0	0	0
6.7969	5.6558	-0.0051	C	0	0	0	0	0
-3.3479	-1.9841	0.0581	O	0	0	0	0	0
-4.4612	-2.9388	0.1453	C	0	0	0	0	0
-5.8029	-2.1576	0.0077	C	0	0	0	0	0
-7.0667	-2.9722	0.4577	C	0	0	0	0	0
-7.3164	-4.2842	-0.3340	C	0	0	0	0	0
-8.5919	-4.8994	0.1553	N	0	0	0	0	0
-9.7329	-3.9858	-0.1365	C	0	0	0	0	0
-11.0547	-4.5782	0.4081	C	0	0	0	0	0
-11.3059	-5.9422	-0.2526	C	0	0	0	0	0
-10.1134	-6.8636	0.0542	C	0	0	0	0	0
-8.8152	-6.2150	-0.4922	C	0	0	0	0	0
9.1272	8.5078	0.1387	O	0	0	0	0	0
-2.8862	-4.5565	0.0262	H	0	0	0	0	0
-0.5714	-5.6868	-0.0502	H	0	0	0	0	0
-0.8365	-0.6917	0.0697	H	0	0	0	0	0
2.0685	-5.2366	-0.1248	H	0	0	0	0	0
3.7434	-5.2976	-0.4366	H	0	0	0	0	0
6.2208	-5.8877	-0.3769	H	0	0	0	0	0
7.8558	-4.2060	0.2332	H	0	0	0	0	0
7.0767	-1.8637	0.8468	H	0	0	0	0	0
4.7330	-1.3085	0.7827	H	0	0	0	0	0
1.3227	0.1528	-0.3963	H	0	0	0	0	0
2.0091	-0.0997	1.2268	H	0	0	0	0	0
3.5779	1.6280	1.1049	H	0	0	0	0	0
5.7548	1.0049	-0.9509	H	0	0	0	0	0
7.4017	1.1184	0.9322	H	0	0	0	0	0
6.2366	-0.2037	1.1806	H	0	0	0	0	0
6.0610	1.3190	2.0852	H	0	0	0	0	0
5.1928	3.4454	-0.8188	H	0	0	0	0	0
5.4652	3.4151	0.9402	H	0	0	0	0	0
7.8147	2.5426	0.5021	H	0	0	0	0	0
7.5254	2.7541	-1.2417	H	0	0	0	0	0
9.7754	4.0014	-0.2963	H	0	0	0	0	0
10.6134	6.4066	-0.1175	H	0	0	0	0	0
6.5210	7.7294	0.1924	H	0	0	0	0	0
5.7279	5.4459	0.0298	H	0	0	0	0	0
-4.3796	-3.6712	-0.6578	H	0	0	0	0	0
-4.4315	-3.4494	1.1078	H	0	0	0	0	0
-5.7396	-1.2580	0.6199	H	0	0	0	0	0
-5.9304	-1.8778	-1.0380	H	0	0	0	0	0
-6.9460	-3.2299	1.5099	H	0	0	0	0	0
-7.9414	-2.3330	0.3377	H	0	0	0	0	0
-7.4002	-4.0613	-1.3977	H	0	0	0	0	0
-6.4891	-4.9749	-0.1711	H	0	0	0	0	0
-9.5502	-3.0213	0.3373	H	0	0	0	0	0
-9.8177	-3.8512	-1.2148	H	0	0	0	0	0
-10.9799	-4.7045	1.4882	H	0	0	0	0	0
-11.8791	-3.9037	0.1768	H	0	0	0	0	0
-12.2206	-6.3805	0.1467	H	0	0	0	0	0
-11.4037	-5.8153	-1.3308	H	0	0	0	0	0

-8.9076	-6.0756	-1.5693 H	0	0	0	0	0
9.7492	8.6030	0.9793 H	0	0	0	0	0
-8.5241	-5.0415	1.2137 H	0	0	0	0	0
1	2	1	0	0	0		
6	1	2	0	0	0		
30	1	1	0	0	0		
3	2	2	0	0	0		
42	2	1	0	0	0		
4	3	1	0	0	0		
43	3	1	0	0	0		
5	4	2	0	0	0		
7	4	1	0	0	0		
6	5	1	0	0	0		
9	5	1	0	0	0		
44	6	1	0	0	0		
8	7	1	0	0	0		
45	7	1	0	0	0		
9	8	2	0	0	0		
10	8	1	0	0	0		
16	9	1	0	0	0		
11	10	1	0	0	0		
15	10	2	0	0	0		
12	11	2	0	0	0		
46	11	1	0	0	0		
13	12	1	0	0	0		
47	12	1	0	0	0		
14	13	2	0	0	0		
48	13	1	0	0	0		
15	14	1	0	0	0		
49	14	1	0	0	0		
50	15	1	0	0	0		
17	16	1	0	0	0		
51	16	1	0	0	0		
52	16	1	0	0	0		
18	17	1	0	0	0		
19	17	2	0	0	0		
20	18	1	0	0	0		
53	18	1	0	0	0		
21	20	1	0	0	0		
22	20	1	0	0	0		
54	20	1	0	0	0		
55	21	1	0	0	0		
56	21	1	0	0	0		
57	21	1	0	0	0		
23	22	1	0	0	0		
58	22	1	0	0	0		
59	22	1	0	0	0		
24	23	1	0	0	0		
60	23	1	0	0	0		
61	23	1	0	0	0		
25	24	1	0	0	0		
29	24	2	0	0	0		
26	25	2	0	0	0		

28	27	2	0	0	0
41	27	1	0	0	0
29	28	1	0	0	0
64	28	1	0	0	0
65	29	1	0	0	0
31	30	1	0	0	0
32	31	1	0	0	0
66	31	1	0	0	0
67	31	1	0	0	0
33	32	1	0	0	0
68	32	1	0	0	0
69	32	1	0	0	0
34	33	1	0	0	0
70	33	1	0	0	0
71	33	1	0	0	0
35	34	1	0	0	0
72	34	1	0	0	0
73	34	1	0	0	0
36	35	1	0	0	0
40	35	1	0	0	0
85	35	1	0	0	0
37	36	1	0	0	0
74	36	1	0	0	0
75	36	1	0	0	0
38	37	1	0	0	0
76	37	1	0	0	0
77	37	1	0	0	0
39	38	1	0	0	0
78	38	1	0	0	0
79	38	1	0	0	0
40	39	1	0	0	0
80	39	1	0	0	0
81	39	1	0	0	0
82	40	1	0	0	0
83	40	1	0	0	0
84	41	1	0	0	0

M END

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indole_2

Forecaster10031114513D

88	92	0	0	0	0	0	0	0	0999	V2000					
	-0.1636		-3.4886		-0.0250	C	0	0	0	0	0				
	-0.3668		-4.8126		-0.0559	C	0	0	0	0	0				
	0.7977		-5.7302		-0.0498	C	0	0	0	0	0				
	2.0067		-5.1877		-0.0205	C	0	0	0	0	0				
	2.2284		-3.8160		0.0006	C	0	0	0	0	0				
	1.2100		-2.9545		-0.0004	C	0	0	0	0	0				
	3.2281		-5.8394		-0.0147	N	0	0	0	0	0				
	4.2553		-4.8367		-0.0059	C	0	0	0	0	0				
	3.6955		-3.5825		0.0061	C	0	0	0	0	0				
	5.7135		-5.2365		-0.0164	C	0	0	0	0	0				
	5.9830		-6.5477		-0.0303	C	0	0	0	0	0				

6.8477	-4.2902	-0.0082	C	0	0	0	0	0
4.4944	-2.2276	-0.0113	C	0	0	0	0	0
3.7903	-0.8878	0.1780	C	0	0	0	0	0
4.4441	0.2383	-0.1280	N	0	0	0	0	0
2.6433	-0.8105	0.6160	O	0	0	0	0	0
3.7766	1.5056	0.0219	C	0	0	0	0	0
2.7925	1.6778	-1.1589	C	0	0	0	0	0
4.7666	2.6932	0.0071	C	0	0	0	0	0
3.9177	3.9798	0.1410	C	0	0	0	0	0
4.7351	5.2405	0.0774	C	0	0	0	0	0
4.1057	6.4140	0.1091	C	0	0	0	0	0
4.8636	7.6604	0.0415	C	0	0	0	0	0
6.1906	7.6262	-0.0522	C	0	0	0	0	0
6.8912	6.3353	-0.0875	C	0	0	0	0	0
6.1983	5.1971	-0.0267	C	0	0	0	0	0
-1.2289	-2.5752	-0.0317	O	0	0	0	0	0
-2.5238	-3.1890	-0.1349	C	0	0	0	0	0
-3.5446	-2.0344	-0.1782	C	0	0	0	0	0
-5.6062	-3.4853	0.4126	C	0	0	0	0	0
-7.0824	-3.8945	-0.0039	C	0	0	0	0	0
-8.1910	-2.9085	0.3480	N	0	0	0	0	0
-8.0791	-1.5825	-0.3305	C	0	0	0	0	0
-9.2096	-0.6393	0.1203	C	0	0	0	0	0
-10.5527	-1.2649	-0.2676	C	0	0	0	0	0
-10.6694	-2.6336	0.4175	C	0	0	0	0	0
-9.4887	-3.5315	-0.0207	C	0	0	0	0	0
-4.9530	-2.5025	-0.5959	C	0	0	0	0	0
6.9105	8.8147	-0.1166	O	0	0	0	0	0
-1.3805	-5.2120	-0.0853	H	0	0	0	0	0
0.6644	-6.8119	-0.0687	H	0	0	0	0	0
1.3896	-1.8795	0.0166	H	0	0	0	0	0
3.3791	-6.8987	-0.0165	H	0	0	0	0	0
5.1640	-7.2670	-0.0364	H	0	0	0	0	0
7.5730	-8.0962	-0.0493	H	0	0	0	0	0
9.4073	-6.5189	-0.0342	H	0	0	0	0	0
8.9287	-4.0130	-0.0078	H	0	0	0	0	0
6.6517	-3.2180	0.0029	H	0	0	0	0	0
5.2390	-2.2989	0.7816	H	0	0	0	0	0
4.9958	-2.1781	-0.9779	H	0	0	0	0	0
5.4535	0.1979	-0.4808	H	0	0	0	0	0
3.2201	1.5116	0.9591	H	0	0	0	0	0
2.2753	2.6326	-1.0652	H	0	0	0	0	0
2.0635	0.8675	-1.1461	H	0	0	0	0	0
3.3442	1.6548	-2.0987	H	0	0	0	0	0
5.4619	2.6132	0.8427	H	0	0	0	0	0
5.3236	2.7064	-0.9297	H	0	0	0	0	0
3.1886	3.9990	-0.6690	H	0	0	0	0	0
3.3973	3.9528	1.0984	H	0	0	0	0	0
3.0188	6.4441	0.1859	H	0	0	0	0	0
4.3430	8.6177	0.0678	H	0	0	0	0	0
7.9782	6.3076	-0.1634	H	0	0	0	0	0
6.7168	4.2387	-0.0542	H	0	0	0	0	0
-2.5881	-3.7844	-1.0456	H	0	0	0	0	0

-5.6392	-3.0092	1.3926	H	0	0	0	0	0
-4.9961	-4.3869	0.4665	H	0	0	0	0	0
-7.0942	-4.0326	-1.0850	H	0	0	0	0	0
-7.3137	-4.8402	0.4863	H	0	0	0	0	0
-7.1181	-1.1332	-0.0800	H	0	0	0	0	0
-8.1432	-1.7268	-1.4090	H	0	0	0	0	0
-9.1660	-0.5046	1.2011	H	0	0	0	0	0
-9.0992	0.3271	-0.3716	H	0	0	0	0	0
-11.3672	-0.6192	0.0605	H	0	0	0	0	0
-10.6009	-1.3902	-1.3493	H	0	0	0	0	0
-10.6436	-2.5018	1.4992	H	0	0	0	0	0
-11.6097	-3.1044	0.1307	H	0	0	0	0	0
-9.5735	-4.5000	0.4722	H	0	0	0	0	0
-9.5255	-3.6688	-1.1014	H	0	0	0	0	0
-4.8778	-3.0005	-1.5626	H	0	0	0	0	0
-5.5943	-1.6259	-0.6871	H	0	0	0	0	0
6.6093	9.3616	-0.9608	H	0	0	0	0	0
-8.1799	-2.7497	1.4061	H	0	0	0	0	0

1	2	1	0	0	0
6	1	2	0	0	0
30	1	1	0	0	0
3	2	2	0	0	0
43	2	1	0	0	0
4	3	1	0	0	0
44	3	1	0	0	0
5	4	2	0	0	0
7	4	1	0	0	0
6	5	1	0	0	0
9	5	1	0	0	0
45	6	1	0	0	0
8	7	1	0	0	0
46	7	1	0	0	0
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53	16	1	0	0	0
18	17	1	0	0	0
19	17	2	0	0	0
20	18	1	0	0	0
54	18	1	0	0	0

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57	21	1	0	0	0
58	21	1	0	0	0
23	22	1	0	0	0
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60	22	1	0	0	0
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63	25	1	0	0	0
27	26	1	0	0	0
64	26	1	0	0	0
28	27	2	0	0	0
42	27	1	0	0	0
29	28	1	0	0	0
65	28	1	0	0	0
66	29	1	0	0	0
31	30	1	0	0	0
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73	34	1	0	0	0
74	34	1	0	0	0
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40	35	1	0	0	0
88	35	1	0	0	0
37	36	1	0	0	0
75	36	1	0	0	0
76	36	1	0	0	0
38	37	1	0	0	0
77	37	1	0	0	0
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80	38	1	0	0	0
40	39	1	0	0	0
81	39	1	0	0	0
82	39	1	0	0	0
83	40	1	0	0	0
84	40	1	0	0	0
85	41	1	0	0	0
86	41	1	0	0	0

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indole_3
Forecaster10031114513D
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Forecaster10031114513D

79	83	0	0	0	0	0	0	0999	V2000					
-2.7253			-3.1137				0.1643	C	0	0	0	0	0	0
-2.7428			-4.4442				-0.0345	C	0	0	0	0	0	0
-1.4624			-5.1704				-0.1796	C	0	0	0	0	0	0
-0.3372			-4.4724				-0.1006	C	0	0	0	0	0	0
-0.3046			-3.1049				0.1039	C	0	0	0	0	0	0
-1.4162			-2.3823				0.2375	C	0	0	0	0	0	0
0.9523			-4.9461				-0.1844	N	0	0	0	0	0	0
1.8400			-3.8321				0.0192	C	0	0	0	0	0	0
1.0989			-2.6788				0.1632	C	0	0	0	0	0	0
3.3325			-4.1225				0.0715	C	0	0	0	0	0	0
3.7249			-5.3410				-0.3065	C	0	0	0	0	0	0
5.1429			-5.7187				-0.2771	C	0	0	0	0	0	0
6.0571			-4.8510				0.1456	C	0	0	0	0	0	0
5.6396			-3.5340				0.5894	C	0	0	0	0	0	0
4.3527			-3.1956				0.5584	C	0	0	0	0	0	0
1.4966			-1.1716				0.4002	C	0	0	0	0	0	0
2.8180			-0.6895				-0.1883	C	0	0	0	0	0	0
3.5024			0.2817				0.4361	N	0	0	0	0	0	0
3.3092			-1.2617				-1.1693	O	0	0	0	0	0	0
4.8541			0.6382				0.0254	C	0	0	0	0	0	0
5.8126			0.0112				1.0583	C	0	0	0	0	0	0
5.1284			2.1586				0.0588	C	0	0	0	0	0	0
6.6408			2.3459				-0.2642	C	0	0	0	0	0	0
7.0894			3.7777				-0.1578	C	0	0	0	0	0	0
8.3914			4.0582				-0.2212	C	0	0	0	0	0	0
8.8532			5.4427				-0.1123	C	0	0	0	0	0	0
7.9698			6.4257				0.0482	C	0	0	0	0	0	0
6.5368			6.1189				0.1189	C	0	0	0	0	0	0
6.1175			4.8573				0.0234	C	0	0	0	0	0	0
-3.9523			-5.1849				-0.0997	O	0	0	0	0	0	0
-5.1458			-4.3987				0.1126	C	0	0	0	0	0	0
-6.3743			-5.3404				-0.0648	C	0	0	0	0	0	0
-7.6546			-4.6789				0.2911	N	0	0	0	0	0	0
-7.8725			-3.4706				-0.5383	C	0	0	0	0	0	0
-9.1989			-2.7854				-0.1281	C	0	0	0	0	0	0
-10.3624			-3.7682				-0.3455	C	0	0	0	0	0	0
-10.1111			-5.0245				0.5014	C	0	0	0	0	0	0
-8.7617			-5.6501				0.0863	C	0	0	0	0	0	0
8.4062			7.7428				0.1489	O	0	0	0	0	0	0
-3.6618			-2.5666				0.2723	H	0	0	0	0	0	0
-1.4440			-6.2474				-0.3465	H	0	0	0			

6.8419	0.2516	0.7923	H	0	0	0	0	0
5.6829	-1.0711	1.0650	H	0	0	0	0	0
5.5913	0.4093	2.0486	H	0	0	0	0	0
4.5188	2.6670	-0.6882	H	0	0	0	0	0
4.9026	2.5596	1.0469	H	0	0	0	0	0
7.2226	1.7464	0.4359	H	0	0	0	0	0
6.8247	1.9986	-1.2809	H	0	0	0	0	0
9.1144	3.2535	-0.3546	H	0	0	0	0	0
9.9184	5.6686	-0.1625	H	0	0	0	0	0
5.8138	6.9241	0.2497	H	0	0	0	0	0
5.0530	4.6299	0.0801	H	0	0	0	0	0
-5.1407	-3.9818	1.1197	H	0	0	0	0	0
-5.1909	-3.5893	-0.6160	H	0	0	0	0	0
-6.4231	-5.6584	-1.1062	H	0	0	0	0	0
-6.2416	-6.2121	0.5760	H	0	0	0	0	0
-7.0456	-2.7761	-0.3900	H	0	0	0	0	0
-7.9231	-3.7571	-1.5887	H	0	0	0	0	0
-9.1528	-2.5016	0.9233	H	0	0	0	0	0
-9.3539	-1.8959	-0.7387	H	0	0	0	0	0
-11.2987	-3.3013	-0.0398	H	0	0	0	0	0
-10.4192	-4.0417	-1.3991	H	0	0	0	0	0
-10.0785	-4.7531	1.5566	H	0	0	0	0	0
-10.9134	-5.7434	0.3352	H	0	0	0	0	0
-8.5767	-6.5380	0.6908	H	0	0	0	0	0
-8.8042	-5.9291	-0.9665	H	0	0	0	0	0
9.0448	7.8381	0.9769	H	0	0	0	0	0
-7.6259	-4.3943	1.3222	H	0	0	0	0	0
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6	1	2	0	0	0			
40	1	1	0	0	0			
3	2	2	0	0	0			
30	2	1	0	0	0			
4	3	1	0	0	0			
41	3	1	0	0	0			
5	4	2	0	0	0			
7	4	1	0	0	0			
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9	5	1	0	0	0			
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9	8	2	0	0	0			
10	8	1	0	0	0			
16	9	1	0	0	0			
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15	10	2	0	0	0			
12	11	2	0	0	0			
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13	12	1	0	0	0			
45	12	1	0	0	0			
14	13	2	0	0	0			
46	13	1	0	0	0			
15	14	1	0	0	0			

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50	16	1	0	0	0
18	17	1	0	0	0
19	17	2	0	0	0
20	18	1	0	0	0
51	18	1	0	0	0
21	20	1	0	0	0
22	20	1	0	0	0
52	20	1	0	0	0
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60	25	1	0	0	0
27	26	1	0	0	0
61	26	1	0	0	0
28	27	2	0	0	0
39	27	1	0	0	0
29	28	1	0	0	0
62	28	1	0	0	0
63	29	1	0	0	0
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32	31	1	0	0	0
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72	36	1	0	0	0
73	36	1	0	0	0
38	37	1	0	0	0
74	37	1	0	0	0
75	37	1	0	0	0
76	38	1	0	0	0
77	38	1	0	0	0

indole_4

Forecaster10031114513D

79	83	0	0	0	0	0	0	0	0	0999	V2000					
-2.4187	-2.6374	0.1208	C	0	0	0	0	0	0							
-2.3986	-3.9736	-0.0437	C	0	0	0	0	0	0							
-1.0954	-4.6640	-0.1565	C	0	0	0	0	0	0							
0.0104	-3.9321	-0.0860	C	0	0	0	0	0	0							
0.0063	-2.5583	0.0880	C	0	0	0	0	0	0							
-1.1270	-1.8653	0.1937	C	0	0	0	0	0	0							
1.3107	-4.3735	-0.1541	N	0	0	0	0	0	0							
2.1724	-3.2352	0.0281	C	0	0	0	0	0	0							
1.4072	-2.0954	0.1477	C	0	0	0	0	0	0							
3.6695	-3.4985	0.0852	C	0	0	0	0	0	0							
4.0818	-4.7139	-0.2793	C	0	0	0	0	0	0							
5.5054	-5.0681	-0.2487	C	0	0	0	0	0	0							
6.4056	-4.1804	0.1621	C	0	0	0	0	0	0							
5.9665	-2.8660	0.5917	C	0	0	0	0	0	0							
4.6739	-2.5494	0.5596	C	0	0	0	0	0	0							
1.7770	-0.5685	0.3573	C	0	0	0	0	0	0							
3.1087	-0.0725	-0.2120	C	0	0	0	0	0	0							
3.7773	0.9108	0.4172	N	0	0	0	0	0	0							
3.6212	-0.6451	-1.1815	O	0	0	0	0	0	0							
5.1386	1.2748	0.0239	C	0	0	0	0	0	0							
6.0840	0.6627	1.0779	C	0	0	0	0	0	0							
5.4142	2.7984	0.0466	C	0	0	0	0	0	0							
6.9348	2.9784	-0.2580	C	0	0	0	0	0	0							
7.3980	4.4086	-0.1549	C	0	0	0	0	0	0							
8.7034	4.6755	-0.2151	C	0	0	0	0	0	0							
9.1806	6.0557	-0.1089	C	0	0	0	0	0	0							
8.3075	7.0487	0.0466	C	0	0	0	0	0	0							
6.8709	6.7571	0.1139	C	0	0	0	0	0	0							
6.4378	5.4997	0.0205	C	0	0	0	0	0	0							
-3.5934	-4.7528	-0.1153	O	0	0	0	0	0	0							
-4.8103	-3.9834	0.0277	C	0	0	0	0	0	0							
-6.0411	-4.9237	-0.1876	C	0	0	0	0	0	0							
-7.3696	-4.1389	0.0003	C	0	0	0	0	0	0							
-8.5503	-4.9934	-0.3090	N	0	0	0	0	0	0							
-9.8087	-4.2863	-0.0644	C	0	0	0	0	0	0							
-10.8594	-5.4109	-0.2293	C	0	0	0	0	0	0							
-10.0652	-6.6936	0.1457	C	0	0	0	0	0	0							
-8.6918	-6.1389	0.5872	C	0	0	0	0	0	0							
8.7580	8.3617	0.1451	O	0	0	0	0	0	0							
-3.3711	-2.1134	0.2014	H	0	0	0	0	0	0							
-1.0441	-5.7441	-0.2938	H	0	0	0	0	0	0							
-1.1198	-0.7836	0.3275	H	0	0	0	0	0	0							
1.6259	-5.3834	-0.3141	H	0	0	0	0	0	0							
3.3508	-5.4542	-0.6044	H	0	0	0	0	0	0							
5.8255	-6.0613	-0.5635	H	0	0	0	0	0	0							
7.4647	-4.4378	0.1761	H	0	0	0	0	0	0							
6.6966	-2.1362	0.9415	H	0	0	0	0	0	0							
4.3582	-1.5613	0.8943	H	0	0	0	0	0	0							
0.9860	0.0237	-0.1029	H	0	0	0	0	0	0							

7.1160	0.9078	0.8271	H	0	0	0	0	0
5.9613	-0.4203	1.0914	H	0	0	0	0	0
5.8437	1.0675	2.0610	H	0	0	0	0	0
4.8160	3.3005	-0.7137	H	0	0	0	0	0
5.1755	3.2095	1.0275	H	0	0	0	0	0
7.5033	2.3786	0.4528	H	0	0	0	0	0
7.1291	2.6241	-1.2703	H	0	0	0	0	0
9.4181	3.8626	-0.3439	H	0	0	0	0	0
10.2483	6.2697	-0.1570	H	0	0	0	0	0
6.1563	7.5704	0.2405	H	0	0	0	0	0
5.3706	5.2844	0.0746	H	0	0	0	0	0
-4.8526	-3.5507	1.0272	H	0	0	0	0	0
-4.8266	-3.1858	-0.7150	H	0	0	0	0	0
-6.0067	-5.3328	-1.1973	H	0	0	0	0	0
-6.0007	-5.7376	0.5363	H	0	0	0	0	0
-7.4382	-3.7990	1.0337	H	0	0	0	0	0
-7.3704	-3.2771	-0.6670	H	0	0	0	0	0
-9.8357	-3.8660	0.9409	H	0	0	0	0	0
-9.9632	-3.4923	-0.7950	H	0	0	0	0	0
-11.7019	-5.2611	0.4459	H	0	0	0	0	0
-11.2208	-5.4609	-1.2564	H	0	0	0	0	0
-10.5508	-7.2300	0.9609	H	0	0	0	0	0
-9.9617	-7.3551	-0.7144	H	0	0	0	0	0
-8.7027	-5.8298	1.6324	H	0	0	0	0	0
-7.8972	-6.8686	0.4318	H	0	0	0	0	0
9.3953	8.4523	0.9747	H	0	0	0	0	0
-8.5072	-5.3254	-1.3253	H	0	0	0	0	0
2	1	1	0	0	0			
6	1	2	0	0	0			
40	1	1	0	0	0			
3	2	2	0	0	0			
30	2	1	0	0	0			
4	3	1	0	0	0			
41	3	1	0	0	0			
5	4	2	0	0	0			
7	4	1	0	0	0			
6	5	1	0	0	0			
9	5	1	0	0	0			
42	6	1	0	0	0			
8	7	1	0	0	0			
43	7	1	0	0	0			
9	8	2	0	0	0			
10	8	1	0	0	0			
16	9	1	0	0	0			
11	10	1	0	0	0			
15	10	2	0	0	0			
12	11	2	0	0	0			
44	11	1	0	0	0			
13	12	1	0	0	0			
45	12	1	0	0	0			
14	13	2	0	0	0			
46	13	1	0	0	0			
15	14	1	0	0	0			

49	16	1	0	0	0
50	16	1	0	0	0
18	17	1	0	0	0
19	17	2	0	0	0
20	18	1	0	0	0
51	18	1	0	0	0
21	20	1	0	0	0
22	20	1	0	0	0
52	20	1	0	0	0
53	21	1	0	0	0
54	21	1	0	0	0
55	21	1	0	0	0
23	22	1	0	0	0
56	22	1	0	0	0
57	22	1	0	0	0
24	23	1	0	0	0
58	23	1	0	0	0
59	23	1	0	0	0
25	24	1	0	0	0
29	24	2	0	0	0
26	25	2	0	0	0
60	25	1	0	0	0
27	26	1	0	0	0
61	26	1	0	0	0
28	27	2	0	0	0
39	27	1	0	0	0
29	28	1	0	0	0
62	28	1	0	0	0
63	29	1	0	0	0
31	30	1	0	0	0
32	31	1	0	0	0
64	31	1	0	0	0
65	31	1	0	0	0
33	32	1	0	0	0
66	32	1	0	0	0
67	32	1	0	0	0
34	33	1	0	0	0
68	33	1	0	0	0
69	33	1	0	0	0
35	34	1	0	0	0
38	34	1	0	0	0
79	34	1	0	0	0
36	35	1	0	0	0
70	35	1	0	0	0
71	35	1	0	0	0
37	36	1	0	0	0
72	36	1	0	0	0
73	36	1	0	0	0
38	37	1	0	0	0
74	37	1	0	0	0
75	37	1	0	0	0
76	38	1	0	0	0
77	38	1	0	0	0

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Forecaster10031114513D

62	66	0	0	0	0	0	0	0	0	0999	V2000					
-4.9416	-4.6120	0.0344	C	0	0	0	0	0	0							
-4.8980	-5.9414	0.0321	C	0	0	0	0	0	0							
-3.6089	-6.6228	0.0493	C	0	0	0	0	0	0							
-2.4821	-5.9135	0.0632	C	0	0	0	0	0	0							
-2.5117	-4.4425	0.0564	C	0	0	0	0	0	0							
-3.6984	-3.8337	0.0471	C	0	0	0	0	0	0							
-6.0774	-6.6801	0.0143	O	0	0	0	0	0	0							
-1.1685	-3.7316	0.0537	C	0	0	0	0	0	0							
0.2187	-4.6895	0.1455	S	0	0	0	0	0	0							
1.3743	-3.5381	0.0725	C	0	0	0	0	0	0							
0.8068	-2.3407	-0.0167	C	0	0	0	0	0	0							
-0.7991	-2.4132	-0.0107	C	0	0	0	0	0	0							
2.8168	-3.7396	0.0711	C	0	0	0	0	0	0							
3.6045	-2.6702	-0.0367	C	0	0	0	0	0	0							
3.0079	-1.3332	-0.1618	C	0	0	0	0	0	0							
1.6845	-1.1862	-0.1571	C	0	0	0	0	0	0							
4.9873	-2.8105	-0.0380	O	0	0	0	0	0	0							
-1.7931	-1.1684	-0.1339	C	0	0	0	0	0	0							
-2.9623	-1.3816	-0.4666	O	0	0	0	0	0	0							
-1.4640	0.2988	0.0169	C	0	0	0	0	0	0							
-0.3633	0.7417	0.6146	C	0	0	0	0	0	0							
-0.0309	2.1516	0.6548	C	0	0	0	0	0	0							
-0.8362	3.0475	0.0922	C	0	0	0	0	0	0							
-2.1017	2.5876	-0.4980	C	0	0	0	0	0	0							
-2.3996	1.2879	-0.5268	C	0	0	0	0	0	0							
-0.5101	4.4356	0.0365	O	0	0	0	0	0	0							
0.7985	4.8233	0.5758	C	0	0	0	0	0	0							
1.9995	4.4451	-0.3710	C	0	0	0	0	0	0							
3.2500	5.0425	0.1457	N	0	0	0	0	0	0							
4.4055	4.5735	-0.6582	C	0	0	0	0	0	0							
5.7137	5.2025	-0.1213	C	0	0	0	0	0	0							
5.6105	6.7332	-0.2271	C	0	0	0	0	0	0							
4.4007	7.2019	0.5952	C	0	0	0	0	0	0							
3.1288	6.5193	0.0544	C	0	0	0	0	0	0							
-5.9036	-4.0996	0.0268	H	0	0	0	0	0	0							
-3.5677	-7.7120	0.0508	H	0	0	0	0	0	0							
-1.5228	-6.4307	0.0799	H	0	0	0	0	0	0							
-3.7449	-2.7447	0.0490	H	0	0	0	0	0	0							
-6.6488	-6.4486	0.8643	H	0	0	0	0	0	0							
3.2413	-4.7399	0.1561	H	0	0	0	0	0	0							
3.6510	-0.4585	-0.2588	H	0	0	0	0	0	0							
1.2528	-0.1906	-0.2595	H	0	0	0	0	0	0							
5.2952	-3.2566	0.8613	H	0	0	0	0	0	0							
0.3081	0.0250	1.0877	H	0	0	0	0	0	0							
0.8839	2.4792	1.1487	H	0	0	0	0	0	0							
-2.8006	3.3130	-0.9145	H	0	0	0	0	0	0							
-3.3452	0.9588	-0.9576	H	0	0	0	0	0	0							
0.8041	5.9027	0.7272	H	0	0	0	0	0	0							
0.9409	4.3209	1.5326	H	0	0	0	0	0	0							

	4.2643	4.8670	-1.6984	H	0	0	0	0	0
	5.8561	4.9167	0.9209	H	0	0	0	0	0
	6.5585	4.8511	-0.7137	H	0	0	0	0	0
	6.5194	7.1901	0.1643	H	0	0	0	0	0
	5.4788	7.0208	-1.2702	H	0	0	0	0	0
	4.5435	6.9311	1.6413	H	0	0	0	0	0
	4.2986	8.2838	0.5100	H	0	0	0	0	0
	2.2702	6.8452	0.6414	H	0	0	0	0	0
	2.9856	6.8032	-0.9882	H	0	0	0	0	0
	3.3865	4.7575	1.1680	H	0	0	0	0	0
2	1	1	0	0	0				
6	1	2	0	0	0				
35	1	1	0	0	0				
3	2	2	0	0	0				
7	2	1	0	0	0				
4	3	1	0	0	0				
36	3	1	0	0	0				
5	4	2	0	0	0				
37	4	1	0	0	0				
6	5	1	0	0	0				
8	5	1	0	0	0				
38	6	1	0	0	0				
39	7	1	0	0	0				
9	8	1	0	0	0				
12	8	2	0	0	0				
10	9	1	0	0	0				
11	10	1	0	0	0				
13	10	2	0	0	0				
12	11	1	0	0	0				
16	11	2	0	0	0				
18	12	1	0	0	0				
14	13	1	0	0	0				
40	13	1	0	0	0				
15	14	2	0	0	0				
17	14	1	0	0	0				
16	15	1	0	0	0				
41	15	1	0	0	0				
42	16	1	0	0	0				
43	17	1	0	0	0				
19	18	2	0	0	0				
20	18	1	0	0	0				
21	20	1	0	0	0				
25	20	2	0	0	0				
22	21	2	0	0	0				
44	21	1	0	0	0				
23	22	1	0	0	0				
45	22	1	0	0	0				
24	23	2	0	0	0				
26	23	1	0	0	0				
25	24	1	0	0	0				
46	24	1	0	0	0				
47	25	1	0	0	0				
27	26	1	0	0	0				

29	28	1	0	0	0
50	28	1	0	0	0
51	28	1	0	0	0
30	29	1	0	0	0
34	29	1	0	0	0
62	29	1	0	0	0
31	30	1	0	0	0
52	30	1	0	0	0
53	30	1	0	0	0
32	31	1	0	0	0
54	31	1	0	0	0
55	31	1	0	0	0
33	32	1	0	0	0
56	32	1	0	0	0
57	32	1	0	0	0
34	33	1	0	0	0
58	33	1	0	0	0
59	33	1	0	0	0
60	34	1	0	0	0
61	34	1	0	0	0

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Forecaster10031114513D

66	70	0	0	0	0	0	0	0	0	0999	V2000					
	2.5438		5.3869		-1.2165	C	0	0	0	0	0					
	2.6324		4.2222		-0.5173	C	0	0	0	0	0					
	3.8341		4.0031		0.3051	C	0	0	0	0	0					
	4.7924		4.8907		0.3955	C	0	0	0	0	0					
	4.6844		6.1630		-0.3405	C	0	0	0	0	0					
	3.6159		6.3845		-1.1099	C	0	0	0	0	0					
	5.6862		7.1226		-0.2346	O	0	0	0	0	0					
	1.5894		3.2964		-0.5705	O	0	0	0	0	0					
	1.3277		2.5110		0.5978	C	0	0	0	0	0					
	2.5120		1.5177		0.9818	C	0	0	0	0	0					
	3.9280		2.5015		1.1280	S	0	0	0	0	0					
	2.8393		0.2643		0.0980	C	0	0	0	0	0					
	-0.0684		1.8537		0.5053	C	0	0	0	0	0					
	1.9584		-0.2695		-0.7541	C	0	0	0	0	0					
	2.2102		-1.5633		-1.3913	C	0	0	0	0	0					
	3.3260		-2.2315		-1.1153	C	0	0	0	0	0					
	4.3193		-1.6433		-0.2156	C	0	0	0	0	0					
	4.0892		-0.4611		0.3577	C	0	0	0	0	0					
	3.5431		-3.4894		-1.6742	O	0	0	0	0	0					
	-1.0312		2.4330		-0.2037	C	0	0	0	0	0					
	-2.3249		1.7446		-0.3981	C	0	0	0	0	0					
	-2.5164		0.5197		0.1014	C	0	0	0	0	0					
	-1.4735		-0.0969		0.9164	C	0	0	0	0	0					
	-0.3287		0.5450		1.1365	C	0	0	0	0	0					
	-3.7081		-0.1794		-0.1948	O	0	0	0	0	0					
	-3.6413		-1.5684		0.2289	C	0	0	0	0	0					
	-4.9867		-2.2701		-0.1040	C	0	0	0	0	0					

-4.5606	-5.9681	0.0015	C	0	0	0	0	0
-4.0571	-4.5805	0.4637	C	0	0	0	0	0
-6.9698	-6.7824	-0.3441	C	0	0	0	0	0
-4.1221	-7.1251	0.9184	C	0	0	0	0	0
1.6800	5.5782	-1.8532	H	0	0	0	0	0
5.6675	4.6892	1.0133	H	0	0	0	0	0
3.5384	7.3185	-1.6664	H	0	0	0	0	0
5.7816	7.4205	0.7677	H	0	0	0	0	0
1.2630	3.2224	1.4211	H	0	0	0	0	0
2.2905	1.1430	1.9811	H	0	0	0	0	0
1.0369	0.2677	-0.9783	H	0	0	0	0	0
1.4843	-1.9780	-2.0907	H	0	0	0	0	0
5.2502	-2.1731	-0.0134	H	0	0	0	0	0
4.8356	-0.0298	1.0248	H	0	0	0	0	0
2.7771	-4.1426	-1.3755	H	0	0	0	0	0
-0.8670	3.4171	-0.6426	H	0	0	0	0	0
-3.1250	2.2374	-0.9504	H	0	0	0	0	0
-1.6331	-1.0859	1.3458	H	0	0	0	0	0
0.4232	0.1005	1.7885	H	0	0	0	0	0
-2.8288	-2.0707	-0.2961	H	0	0	0	0	0
-3.4631	-1.6134	1.3033	H	0	0	0	0	0
-5.6329	-2.2233	0.7726	H	0	0	0	0	0
-5.4602	-1.7449	-0.9335	H	0	0	0	0	0
-6.9432	-3.8077	-0.6237	H	0	0	0	0	0
-6.0780	-4.7252	-1.8803	H	0	0	0	0	0
-6.2627	-5.3468	1.1146	H	0	0	0	0	0
-4.2718	-6.1611	-1.0317	H	0	0	0	0	0
-4.3297	-4.3766	1.4992	H	0	0	0	0	0
-2.9779	-4.4828	0.3455	H	0	0	0	0	0
-6.8880	-7.6173	0.3518	H	0	0	0	0	0
-6.6977	-7.1166	-1.3453	H	0	0	0	0	0
-7.9959	-6.4147	-0.3506	H	0	0	0	0	0
-3.0530	-7.2999	0.7977	H	0	0	0	0	0
-4.6699	-8.0288	0.6511	H	0	0	0	0	0
-4.3326	-6.8667	1.9562	H	0	0	0	0	0
-4.2175	-3.6880	-1.3845	H	0	0	0	0	0

2	1	1	0	0	0
6	1	2	0	0	0
35	1	1	0	0	0
3	2	2	0	0	0
8	2	1	0	0	0
4	3	1	0	0	0
11	3	1	0	0	0
5	4	2	0	0	0
36	4	1	0	0	0
6	5	1	0	0	0
7	5	1	0	0	0
37	6	1	0	0	0
38	7	1	0	0	0
9	8	1	0	0	0
10	9	1	0	0	0
13	9	1	0	0	0
39	9	1	0	0	0

14	12	1	0	0	0
18	12	2	0	0	0
20	13	1	0	0	0
24	13	2	0	0	0
15	14	2	0	0	0
41	14	1	0	0	0
16	15	1	0	0	0
42	15	1	0	0	0
17	16	2	0	0	0
19	16	1	0	0	0
18	17	1	0	0	0
43	17	1	0	0	0
44	18	1	0	0	0
45	19	1	0	0	0
21	20	2	0	0	0
46	20	1	0	0	0
22	21	1	0	0	0
47	21	1	0	0	0
23	22	2	0	0	0
25	22	1	0	0	0
24	23	1	0	0	0
48	23	1	0	0	0
49	24	1	0	0	0
26	25	1	0	0	0
27	26	1	0	0	0
50	26	1	0	0	0
51	26	1	0	0	0
28	27	1	0	0	0
52	27	1	0	0	0
53	27	1	0	0	0
29	28	1	0	0	0
32	28	1	0	0	0
66	28	1	0	0	0
30	29	1	0	0	0
54	29	1	0	0	0
55	29	1	0	0	0
31	30	1	0	0	0
33	30	1	0	0	0
56	30	1	0	0	0
32	31	1	0	0	0
34	31	1	0	0	0
57	31	1	0	0	0
58	32	1	0	0	0
59	32	1	0	0	0
60	33	1	0	0	0
61	33	1	0	0	0
62	33	1	0	0	0
63	34	1	0	0	0
64	34	1	0	0	0
65	34	1	0	0	0

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-4.1368	-4.3027	-0.3227	C	0	0	0	0	0
-4.0772	-5.4904	0.2692	C	0	0	0	0	0
-2.7910	-6.0265	0.6773	C	0	0	0	0	0
-1.6675	-5.3421	0.4520	C	0	0	0	0	0
-1.7135	-4.0200	-0.2047	C	0	0	0	0	0
-2.9055	-3.5456	-0.5689	C	0	0	0	0	0
-5.2412	-6.2198	0.4974	O	0	0	0	0	0
-0.3949	-5.9264	0.9020	C	0	0	0	0	0
0.7663	-5.4451	0.0540	C	0	0	0	0	0
0.8704	-4.0110	-0.0974	N	0	0	0	0	0
-0.3895	-3.2159	-0.4914	C	0	0	0	0	0
2.2591	-3.5478	-0.1444	C	0	0	0	0	0
3.1828	-4.3241	0.4284	C	0	0	0	0	0
4.5927	-3.9328	0.4518	C	0	0	0	0	0
4.9756	-2.7892	-0.1084	C	0	0	0	0	0
3.9880	-1.9382	-0.7673	C	0	0	0	0	0
2.7052	-2.2984	-0.7957	C	0	0	0	0	0
-0.4991	-1.6485	-0.1320	C	0	0	0	0	0
0.3985	-1.0215	0.6379	C	0	0	0	0	0
0.4129	0.4544	0.7464	C	0	0	0	0	0
-0.5086	1.1795	0.1128	C	0	0	0	0	0
-1.5562	0.5058	-0.6336	C	0	0	0	0	0
-1.5412	-0.8164	-0.7704	C	0	0	0	0	0
-0.4544	2.5869	0.0584	O	0	0	0	0	0
0.7430	3.1485	0.6289	C	0	0	0	0	0
0.7711	4.6447	0.2085	C	0	0	0	0	0
2.0558	5.3129	0.5199	N	0	0	0	0	0
3.1536	4.6760	-0.2589	C	0	0	0	0	0
4.4986	5.3862	0.0313	C	0	0	0	0	0
4.3824	6.8682	-0.3648	C	0	0	0	0	0
3.2377	7.5023	0.4392	C	0	0	0	0	0
1.9304	6.7412	0.1348	C	0	0	0	0	0
-5.0999	-3.8914	-0.6250	H	0	0	0	0	0
-2.7425	-6.9965	1.1721	H	0	0	0	0	0
-2.9657	-2.5744	-1.0600	H	0	0	0	0	0
-5.8874	-5.6654	1.1119	H	0	0	0	0	0
-0.2198	-5.6387	1.9387	H	0	0	0	0	0
-0.4590	-7.0122	0.8316	H	0	0	0	0	0
1.6883	-5.8027	0.5124	H	0	0	0	0	0
0.6608	-5.8813	-0.9393	H	0	0	0	0	0
-0.3411	-3.2110	-1.5803	H	0	0	0	0	0
2.8810	-5.2659	0.8866	H	0	0	0	0	0
5.3295	-4.5792	0.9287	H	0	0	0	0	0
6.0226	-2.4879	-0.0760	H	0	0	0	0	0
4.3011	-1.0058	-1.2371	H	0	0	0	0	0
1.9780	-1.6654	-1.3042	H	0	0	0	0	0
1.1305	-1.6073	1.1938	H	0	0	0	0	0
1.1779	0.9489	1.3451	H	0	0	0	0	0
-2.3599	1.0879	-1.0845	H	0	0	0	0	0
-2.3154	-1.2985	-1.3673	H	0	0	0	0	0
0.7186	3.0629	1.7153	H	0	0	0	0	0
1.6220	2.6323	0.2430	H	0	0	0	0	0
0.6002	4.7060	-0.8663	H	0	0	0	0	0

	4.7295	5.3097	1.0938	H	0	0	0	0	0
	5.2923	4.9150	-0.5484	H	0	0	0	0	0
	5.3170	7.3824	-0.1407	H	0	0	0	0	0
	4.1700	6.9476	-1.4310	H	0	0	0	0	0
	3.4592	7.4370	1.5045	H	0	0	0	0	0
	3.1265	8.5485	0.1542	H	0	0	0	0	0
	1.1135	7.1934	0.6972	H	0	0	0	0	0
	1.7178	6.8071	-0.9322	H	0	0	0	0	0
	2.2611	5.2356	1.5672	H	0	0	0	0	0
2	1	1	0	0	0				
6	1	2	0	0	0				
33	1	1	0	0	0				
3	2	2	0	0	0				
7	2	1	0	0	0				
4	3	1	0	0	0				
34	3	1	0	0	0				
5	4	2	0	0	0				
8	4	1	0	0	0				
6	5	1	0	0	0				
11	5	1	0	0	0				
35	6	1	0	0	0				
36	7	1	0	0	0				
9	8	1	0	0	0				
37	8	1	0	0	0				
38	8	1	0	0	0				
10	9	1	0	0	0				
39	9	1	0	0	0				
40	9	1	0	0	0				
11	10	1	0	0	0				
12	10	1	0	0	0				
18	11	1	0	0	0				
41	11	1	0	0	0				
13	12	1	0	0	0				
17	12	2	0	0	0				
14	13	2	0	0	0				
42	13	1	0	0	0				
15	14	1	0	0	0				
43	14	1	0	0	0				
16	15	2	0	0	0				
44	15	1	0	0	0				
17	16	1	0	0	0				
45	16	1	0	0	0				
46	17	1	0	0	0				
19	18	1	0	0	0				
23	18	2	0	0	0				
20	19	2	0	0	0				
47	19	1	0	0	0				
21	20	1	0	0	0				
48	20	1	0	0	0				
22	21	2	0	0	0				
24	21	1	0	0	0				
23	22	1	0	0	0				
49	22	1	0	0	0				

51	25	1	0	0	0
52	25	1	0	0	0
27	26	1	0	0	0
53	26	1	0	0	0
54	26	1	0	0	0
28	27	1	0	0	0
32	27	1	0	0	0
65	27	1	0	0	0
29	28	1	0	0	0
55	28	1	0	0	0
56	28	1	0	0	0
30	29	1	0	0	0
57	29	1	0	0	0
58	29	1	0	0	0
31	30	1	0	0	0
59	30	1	0	0	0
60	30	1	0	0	0
32	31	1	0	0	0
61	31	1	0	0	0
62	31	1	0	0	0
63	32	1	0	0	0
64	32	1	0	0	0

M END

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20UZ_lig

Forecaster10031114513D

63	67	0	0	0	0	0	0	0	0	0999	V2000						
2.6448				1.2140						-0.4298	C	0	0	0	0	0	0
3.0057				0.1584						-1.1951	C	0	0	0	0	0	0
4.2897				-0.5073						-0.9854	C	0	0	0	0	0	0
5.1311				-0.0703						-0.0513	C	0	0	0	0	0	0
4.7655				1.0849						0.7652	C	0	0	0	0	0	0
3.6029				1.6861						0.6018	C	0	0	0	0	0	0
6.3530				-0.7043						0.1446	O	0	0	0	0	0	0
3.3017				2.9004						1.4623	C	0	0	0	0	0	0
1.8662				3.4540						1.3356	C	0	0	0	0	0	0
1.4343				3.4314						-0.1277	C	0	0	0	0	0	0
1.3076				1.9119						-0.6559	C	0	0	0	0	0	0
0.1971				4.3366						-0.2876	C	0	0	0	0	0	0
0.1249				1.0139						-0.0409	C	0	0	0	0	0	0
0.0812				5.3856						0.5321	C	0	0	0	0	0	0
-1.0788				6.2698						0.4566	C	0	0	0	0	0	0
-2.0416				6.0278						-0.4287	C	0	0	0	0	0	0
-1.9242				4.8870						-1.3442	C	0	0	0	0	0	0
-0.8570				4.0892						-1.2900	C	0	0	0	0	0	0
-0.9130				1.5475						0.5945	C	0	0	0	0	0	0
-2.0749				0.7526						0.9740	C	0	0	0	0	0	0
-2.1242				-0.5449						0.6880	C	0	0	0	0	0	0
-0.9809				-1.1806						0.0332	C	0	0	0	0	0	0
0.0790				-0.4479						-0.3174	C	0	0	0	0	0	0
-3.2980				-1.2548						0.9807	O	0	0	0	0	0	0
-3.2133				-2.6429						0.6351	C	0	0	0	0	0	0

-5.7035	-6.7189	0.0514	C	0	0	0	0	0
-4.2137	-6.7424	-0.3930	C	0	0	0	0	0
-3.8900	-5.2495	-0.5972	C	0	0	0	0	0
2.3330	-0.1987	-1.9749	H	0	0	0	0	0
4.5601	-1.3674	-1.5980	H	0	0	0	0	0
5.4617	1.4542	1.5182	H	0	0	0	0	0
6.1892	-1.7082	0.4052	H	0	0	0	0	0
3.4664	2.6250	2.5040	H	0	0	0	0	0
3.9951	3.6932	1.1816	H	0	0	0	0	0
1.1867	2.8369	1.9235	H	0	0	0	0	0
1.8392	4.4789	1.7056	H	0	0	0	0	0
2.2382	3.8957	-0.6989	H	0	0	0	0	0
1.1481	1.9588	-1.7331	H	0	0	0	0	0
0.8621	5.5838	1.2662	H	0	0	0	0	0
-1.1555	7.1273	1.1252	H	0	0	0	0	0
-2.9167	6.6761	-0.4741	H	0	0	0	0	0
-2.7123	4.6910	-2.0713	H	0	0	0	0	0
-0.7635	3.2552	-1.9855	H	0	0	0	0	0
-0.8953	2.6096	0.8389	H	0	0	0	0	0
-2.9078	1.2247	1.4951	H	0	0	0	0	0
-0.9942	-2.2517	-0.1684	H	0	0	0	0	0
0.9229	-0.9274	-0.8134	H	0	0	0	0	0
-2.7129	-2.7541	-0.3268	H	0	0	0	0	0
-2.6538	-3.1805	1.4006	H	0	0	0	0	0
-5.2166	-2.8742	1.4167	H	0	0	0	0	0
-5.1245	-2.8268	-0.3605	H	0	0	0	0	0
-6.6366	-5.0481	1.1185	H	0	0	0	0	0
-6.4297	-4.7662	-0.6271	H	0	0	0	0	0
-5.8442	-7.2758	0.9778	H	0	0	0	0	0
-6.3493	-7.1323	-0.7233	H	0	0	0	0	0
-3.5811	-7.1782	0.3803	H	0	0	0	0	0
-4.0905	-7.3005	-1.3212	H	0	0	0	0	0
-2.8224	-5.0503	-0.5039	H	0	0	0	0	0
-4.2449	-4.8865	-1.5618	H	0	0	0	0	0
-4.2703	-5.0588	1.4333	H	0	0	0	0	0

2	1	1	0	0	0
6	1	2	0	0	0
11	1	1	0	0	0
3	2	2	0	0	0
32	2	1	0	0	0
4	3	1	0	0	0
33	3	1	0	0	0
5	4	2	0	0	0
7	4	1	0	0	0
6	5	1	0	0	0
34	5	1	0	0	0
8	6	1	0	0	0
35	7	1	0	0	0
9	8	1	0	0	0
36	8	1	0	0	0
37	8	1	0	0	0
10	9	1	0	0	0
38	9	1	0	0	0

40	10	1	0	0	0
13	11	1	0	0	0
41	11	1	0	0	0
14	12	1	0	0	0
18	12	2	0	0	0
19	13	1	0	0	0
23	13	2	0	0	0
15	14	2	0	0	0
42	14	1	0	0	0
16	15	1	0	0	0
43	15	1	0	0	0
17	16	2	0	0	0
44	16	1	0	0	0
18	17	1	0	0	0
45	17	1	0	0	0
46	18	1	0	0	0
20	19	2	0	0	0
47	19	1	0	0	0
21	20	1	0	0	0
48	20	1	0	0	0
22	21	2	0	0	0
24	21	1	0	0	0
23	22	1	0	0	0
49	22	1	0	0	0
50	23	1	0	0	0
25	24	1	0	0	0
26	25	1	0	0	0
51	25	1	0	0	0
52	25	1	0	0	0
27	26	1	0	0	0
53	26	1	0	0	0
54	26	1	0	0	0
28	27	1	0	0	0
31	27	1	0	0	0
63	27	1	0	0	0
29	28	1	0	0	0
55	28	1	0	0	0
56	28	1	0	0	0
30	29	1	0	0	0
57	29	1	0	0	0
58	29	1	0	0	0
31	30	1	0	0	0
59	30	1	0	0	0
60	30	1	0	0	0
61	31	1	0	0	0
62	31	1	0	0	0

M END

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2IOG_lig

Forecaster10031114513D

79 83 0 0 0 0 0 0 0 0999 V2000

-0.9690 5.5922 0.0377 C 0 0 0 0 0

1.4404	5.4235	0.0342	C	0	0	0	0	0
0.3751	6.2303	0.0397	C	0	0	0	0	0
2.7153	3.4775	0.0383	C	0	0	0	0	0
3.5473	4.5461	0.0335	C	0	0	0	0	0
2.7826	5.7786	0.0272	N	0	0	0	0	0
5.0653	4.6010	0.0363	C	0	0	0	0	0
5.8454	3.5123	0.0315	C	0	0	0	0	0
7.3038	3.6347	0.0311	C	0	0	0	0	0
7.8717	4.8370	0.0352	C	0	0	0	0	0
7.0335	6.0344	0.0401	C	0	0	0	0	0
5.7061	5.9213	0.0404	C	0	0	0	0	0
-2.1389	6.3833	0.0139	O	0	0	0	0	0
-3.3216	5.5512	-0.0817	C	0	0	0	0	0
-4.5989	6.4100	0.0515	C	0	0	0	0	0
-5.8070	5.6137	-0.2811	N	0	0	0	0	0
-7.0059	6.4660	-0.0963	C	0	0	0	0	0
-8.2785	5.6953	-0.5074	C	0	0	0	0	0
-8.4024	4.4300	0.3551	C	0	0	0	0	0
-7.1424	3.5711	0.1571	C	0	0	0	0	0
-5.8994	4.3985	0.5653	C	0	0	0	0	0
3.1295	1.9485	0.0723	C	0	0	0	0	0
2.0584	0.9315	-0.2602	C	0	0	0	0	0
2.0759	-0.2799	0.2921	N	0	0	0	0	0
1.1328	1.2214	-1.0232	O	0	0	0	0	0
0.9594	-1.1418	0.0275	C	0	0	0	0	0
1.2943	-2.6398	0.0935	C	0	0	0	0	0
-0.1018	-0.8404	1.1101	C	0	0	0	0	0
-0.0524	-3.3612	-0.1529	C	0	0	0	0	0
0.0461	-4.8504	-0.0832	C	0	0	0	0	0
-1.0744	-5.5680	-0.1368	C	0	0	0	0	0
-1.0197	-7.0232	-0.0655	C	0	0	0	0	0
0.1552	-7.6369	0.0510	C	0	0	0	0	0
1.3935	-6.8497	0.1087	C	0	0	0	0	0
1.3417	-5.5194	0.0467	C	0	0	0	0	0
0.2067	-9.0239	0.1185	O	0	0	0	0	0
-2.0425	3.7801	0.0481	H	0	0	0	0	0
0.0817	2.3479	0.1009	H	0	0	0	0	0
0.4866	7.3146	0.0454	H	0	0	0	0	0
3.1779	6.7729	0.0188	H	0	0	0	0	0
5.3884	2.5227	0.0278	H	0	0	0	0	0
7.9252	2.7392	0.0274	H	0	0	0	0	0
8.9578	4.9292	0.0349	H	0	0	0	0	0
7.4953	7.0217	0.0435	H	0	0	0	0	0
5.0889	6.8197	0.0437	H	0	0	0	0	0
-3.3279	5.0464	-1.0478	H	0	0	0	0	0
-3.3035	4.8091	0.7165	H	0	0	0	0	0
-4.6807	6.7719	1.0764	H	0	0	0	0	0
-4.5316	7.2583	-0.6296	H	0	0	0	0	0
-7.0834	6.7552	0.9518	H	0	0	0	0	0
-6.9110	7.3590	-0.7141	H	0	0	0	0	0
-9.1530	6.3277	-0.3547	H	0	0	0	0	0
-8.2113	5.4149	-1.5586	H	0	0	0	0	0
-8.4940	4.7096	1.4046	H	0	0	0	0	0

-5.9871	4.6917	1.6115	H	0	0	0	0	0
-5.0021	3.7944	0.4308	H	0	0	0	0	0
3.9420	1.8135	-0.6417	H	0	0	0	0	0
3.4885	1.7289	1.0778	H	0	0	0	0	0
2.8903	-0.5982	0.9089	H	0	0	0	0	0
0.5485	-0.9076	-0.9546	H	0	0	0	0	0
2.0177	-2.9050	-0.6775	H	0	0	0	0	0
1.6948	-2.9001	1.0733	H	0	0	0	0	0
-0.9742	-1.4740	0.9508	H	0	0	0	0	0
-0.3978	0.2068	1.0479	H	0	0	0	0	0
0.3172	-1.0412	2.0962	H	0	0	0	0	0
-0.7652	-3.0273	0.6011	H	0	0	0	0	0
-0.4147	-3.0858	-1.1433	H	0	0	0	0	0
-2.0366	-5.0653	-0.2344	H	0	0	0	0	0
-1.9392	-7.6071	-0.1075	H	0	0	0	0	0
2.3555	-7.3536	0.2023	H	0	0	0	0	0
2.2592	-4.9326	0.0925	H	0	0	0	0	0
-0.3377	-9.3546	0.9533	H	0	0	0	0	0
-5.7512	5.3154	-1.3072	H	0	0	0	0	0

1	2	1	0	0	0
6	1	2	0	0	0
16	1	1	0	0	0
3	2	2	0	0	0
40	2	1	0	0	0
4	3	1	0	0	0
41	3	1	0	0	0
5	4	2	0	0	0
7	4	1	0	0	0
6	5	1	0	0	0
9	5	1	0	0	0
42	6	1	0	0	0
8	7	2	0	0	0
25	7	1	0	0	0
9	8	1	0	0	0
10	8	1	0	0	0
43	9	1	0	0	0
11	10	1	0	0	0
15	10	2	0	0	0
12	11	2	0	0	0
44	11	1	0	0	0
13	12	1	0	0	0
45	12	1	0	0	0
14	13	2	0	0	0
46	13	1	0	0	0
15	14	1	0	0	0
47	14	1	0	0	0
48	15	1	0	0	0
17	16	1	0	0	0
18	17	1	0	0	0
49	17	1	0	0	0
50	17	1	0	0	0
19	18	1	0	0	0
51	18	1	0	0	0

79	19	1	0	0	0
21	20	1	0	0	0
53	20	1	0	0	0
54	20	1	0	0	0
22	21	1	0	0	0
55	21	1	0	0	0
56	21	1	0	0	0
23	22	1	0	0	0
57	22	1	0	0	0
58	22	1	0	0	0
24	23	1	0	0	0
59	23	1	0	0	0
60	23	1	0	0	0
61	24	1	0	0	0
62	24	1	0	0	0
26	25	1	0	0	0
63	25	1	0	0	0
64	25	1	0	0	0
27	26	1	0	0	0
28	26	2	0	0	0
29	27	1	0	0	0
65	27	1	0	0	0
30	29	1	0	0	0
31	29	1	0	0	0
66	29	1	0	0	0
32	30	1	0	0	0
67	30	1	0	0	0
68	30	1	0	0	0
69	31	1	0	0	0
70	31	1	0	0	0
71	31	1	0	0	0
33	32	1	0	0	0
72	32	1	0	0	0
73	32	1	0	0	0
34	33	1	0	0	0
38	33	2	0	0	0
35	34	2	0	0	0
74	34	1	0	0	0
36	35	1	0	0	0
75	35	1	0	0	0
37	36	2	0	0	0
39	36	1	0	0	0
38	37	1	0	0	0
76	37	1	0	0	0
77	38	1	0	0	0
78	39	1	0	0	0

M END

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Forecaster10031114513D

59	61	0	0	0	0	0	0	0	0	0999	V2000
-5	2601	2	8223	-0	5588	C	0	0	0	0	0

-2.8629	2.7932	-0.0304	C	0	0	0	0	0
-3.9010	3.3698	-0.6555	C	0	0	0	0	0
-1.4195	3.4634	-0.1345	C	0	0	0	0	0
-0.1623	2.8139	-0.0498	C	0	0	0	0	0
-1.5025	4.9939	-0.3692	C	0	0	0	0	0
-2.3419	5.7821	0.6881	C	0	0	0	0	0
1.2739	3.6410	-0.0336	C	0	0	0	0	0
-0.0342	1.2029	-0.0470	C	0	0	0	0	0
2.4276	2.9809	-0.2068	C	0	0	0	0	0
3.7399	3.6480	-0.1918	C	0	0	0	0	0
3.8271	4.9590	-0.0055	C	0	0	0	0	0
2.6182	5.7290	0.1850	C	0	0	0	0	0
1.4312	5.1247	0.1768	C	0	0	0	0	0
5.0705	5.5885	0.0082	O	0	0	0	0	0
-0.9195	0.4553	-0.7073	C	0	0	0	0	0
-0.8298	-0.9941	-0.7802	C	0	0	0	0	0
0.1826	-1.6400	-0.2210	C	0	0	0	0	0
1.2148	-0.8763	0.4860	C	0	0	0	0	0
1.1147	0.4550	0.5766	C	0	0	0	0	0
0.2277	-3.0371	-0.3448	O	0	0	0	0	0
1.3949	-3.6230	0.2288	C	0	0	0	0	0
1.3061	-5.1489	-0.0079	C	0	0	0	0	0
2.5523	-5.8166	0.3908	N	0	0	0	0	0
2.4064	-7.2659	0.1860	C	0	0	0	0	0
3.6554	-5.3237	-0.4525	C	0	0	0	0	0
-6.0790	3.3077	-1.0898	H	0	0	0	0	0
-6.5056	1.3288	0.2348	H	0	0	0	0	0
-4.5932	0.2154	1.4968	H	0	0	0	0	0
-2.3626	1.1147	1.3635	H	0	0	0	0	0
-3.7310	4.2674	-1.2501	H	0	0	0	0	0
-0.4880	5.3924	-0.3600	H	0	0	0	0	0
-1.9503	5.1614	-1.3487	H	0	0	0	0	0
-2.3397	6.8428	0.4371	H	0	0	0	0	0
-1.9051	5.6424	1.6770	H	0	0	0	0	0
-3.3670	5.4115	0.6885	H	0	0	0	0	0
2.3926	1.9031	-0.3657	H	0	0	0	0	0
4.6469	3.0606	-0.3348	H	0	0	0	0	0
2.6784	6.8069	0.3357	H	0	0	0	0	0
0.5365	5.7285	0.3286	H	0	0	0	0	0
5.6580	5.1873	0.7805	H	0	0	0	0	0
-1.7464	0.9525	-1.2144	H	0	0	0	0	0
-1.6050	-1.5560	-1.3013	H	0	0	0	0	0
2.0625	-1.3920	0.9372	H	0	0	0	0	0
1.8826	1.0111	1.1143	H	0	0	0	0	0
2.2878	-3.2224	-0.2512	H	0	0	0	0	0
1.4310	-3.4128	1.2977	H	0	0	0	0	0
0.4816	-5.5532	0.5793	H	0	0	0	0	0
1.1248	-5.3354	-1.0664	H	0	0	0	0	0
3.3274	-7.7694	0.4796	H	0	0	0	0	0
2.2030	-7.4660	-0.8660	H	0	0	0	0	0
1.5805	-7.6377	0.7924	H	0	0	0	0	0
4.5836	-5.8155	-0.1616	H	0	0	0	0	0
3.7594	-4.2465	-0.3225	H	0	0	0	0	0

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3	2	2	0	0	0
31	2	1	0	0	0
4	3	1	0	0	0
32	3	1	0	0	0
5	4	2	0	0	0
33	4	1	0	0	0
6	5	1	0	0	0
7	5	1	0	0	0
34	6	1	0	0	0
8	7	2	0	0	0
9	7	1	0	0	0
11	8	1	0	0	0
12	8	1	0	0	0
10	9	1	0	0	0
35	9	1	0	0	0
36	9	1	0	0	0
37	10	1	0	0	0
38	10	1	0	0	0
39	10	1	0	0	0
13	11	1	0	0	0
17	11	2	0	0	0
19	12	1	0	0	0
23	12	2	0	0	0
14	13	2	0	0	0
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41	14	1	0	0	0
16	15	2	0	0	0
18	15	1	0	0	0
17	16	1	0	0	0
42	16	1	0	0	0
43	17	1	0	0	0
44	18	1	0	0	0
20	19	2	0	0	0
45	19	1	0	0	0
21	20	1	0	0	0
46	20	1	0	0	0
22	21	2	0	0	0
24	21	1	0	0	0
23	22	1	0	0	0
47	22	1	0	0	0
48	23	1	0	0	0
25	24	1	0	0	0
26	25	1	0	0	0
49	25	1	0	0	0
50	25	1	0	0	0
27	26	1	0	0	0
51	26	1	0	0	0
52	26	1	0	0	0
28	27	1	0	0	0
29	27	1	0	0	0

55 28 1 0 0 0
56 29 1 0 0 0
57 29 1 0 0 0
58 29 1 0 0 0

M END

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Forecaster10031114513D

65	69	0	0	0	0	0	0	0	0	0999	V2000					
3.4496				3.0014				0.1205	C		0	0	0	0	0	0
3.3558				1.6645				0.0841	C		0	0	0	0	0	0
4.5815				0.8633				-0.0362	C		0	0	0	0	0	0
5.7734				1.4520				-0.1238	C		0	0	0	0	0	0
5.8710				2.9085				-0.1031	C		0	0	0	0	0	0
4.7698				3.6421				0.0185	C		0	0	0	0	0	0
7.1135				3.5279				-0.2123	O		0	0	0	0	0	0
2.2340				3.8617				0.2986	C		0	0	0	0	0	0
1.0037				3.2482				-0.4551	C		0	0	0	0	0	0
0.9023				1.6842				0.0205	C		0	0	0	0	0	0
2.1400				1.0168				0.1561	O		0	0	0	0	0	0
2.6173				5.3069				-0.1721	C		0	0	0	0	0	0
-0.3289				0.7305				0.1241	C		0	0	0	0	0	0
-0.3306				4.1403				-0.2134	C		0	0	0	0	0	0
-0.3841				5.0403				0.7806	C		0	0	0	0	0	0
-1.5717				5.8737				1.0099	C		0	0	0	0	0	0
-2.6455				5.7288				0.2416	C		0	0	0	0	0	0
-2.6236				4.7545				-0.8480	C		0	0	0	0	0	0
-1.5288				4.0233				-1.0803	C		0	0	0	0	0	0
-3.7803				6.5098				0.4689	O		0	0	0	0	0	0
-1.4716				1.0806				-0.4376	C		0	0	0	0	0	0
-2.6076				0.2179				-0.4765	C		0	0	0	0	0	0
-2.5464				-1.0024				0.0237	C		0	0	0	0	0	0
-1.2844				-1.4689				0.6561	C		0	0	0	0	0	0
-0.2260				-0.6388				0.7088	C		0	0	0	0	0	0
-3.7033				-1.7747				-0.1012	O		0	0	0	0	0	0
-3.6336				-3.0999				0.3809	C		0	0	0	0	0	0
-5.0402				-3.6795				0.1080	C		0	0	0	0	0	0
-5.1164				-5.0990				0.4287	N		0	0	0	0	0	0
-6.4314				-5.6359				0.0908	C		0	0	0	0	0	0
-6.2050				-7.1530				0.2454	C		0	0	0	0	0	0
-4.6948				-7.3183				-0.0845	C		0	0	0	0	0	0
-4.2585				-5.8874				-0.4451	C		0	0	0	0	0	0
4.5149				-0.2245				-0.0540	H		0	0	0	0	0	0
6.6755				0.8464				-0.2109	H		0	0	0	0	0	0
4.8455				4.7292				0.0429	H		0	0	0	0	0	0
7.7282				3.2229				0.5825	H		0	0	0	0	0	0
1.9972				3.9012				1.3618	H		0	0	0	0	0	0
1.2252				3.2598				-1.5223	H		0	0	0	0	0	0
0.8616				1.9471				1.0775	H		0	0	0	0	0	0
1.7572				5.9667				-0.0584	H		0	0	0	0	0	0
2.9184				5.2806				-1.2194	H		0	0	0	0	0	0
3.4432				5.6798				0.4337	H		0	0	0	0	0	0

-1.5163	3.3294	-1.9208	H	0	0	0	0	0
-4.1391	6.3325	1.4397	H	0	0	0	0	0
-1.5503	2.0691	-0.8901	H	0	0	0	0	0
-3.5367	0.5705	-0.9244	H	0	0	0	0	0
-1.2168	-2.4737	1.0732	H	0	0	0	0	0
0.7027	-0.9655	1.1767	H	0	0	0	0	0
-2.8720	-3.6662	-0.1552	H	0	0	0	0	0
-3.4117	-3.1113	1.4480	H	0	0	0	0	0
-5.7667	-3.1416	0.7170	H	0	0	0	0	0
-5.2782	-3.5438	-0.9470	H	0	0	0	0	0
-7.1952	-5.2769	0.7806	H	0	0	0	0	0
-6.7137	-5.3794	-0.9303	H	0	0	0	0	0
-6.4214	-7.4793	1.2627	H	0	0	0	0	0
-6.8225	-7.7143	-0.4559	H	0	0	0	0	0
-4.1438	-7.6893	0.7797	H	0	0	0	0	0
-4.5500	-7.9954	-0.9263	H	0	0	0	0	0
-3.2041	-5.7238	-0.2224	H	0	0	0	0	0
-4.4472	-5.6656	-1.4955	H	0	0	0	0	0
-4.8822	-5.2741	1.4580	H	0	0	0	0	0

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8	1	1	0	0	0
3	2	2	0	0	0
11	2	1	0	0	0
4	3	1	0	0	0
34	3	1	0	0	0
5	4	2	0	0	0
35	4	1	0	0	0
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7	5	1	0	0	0
36	6	1	0	0	0
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38	8	1	0	0	0
10	9	1	0	0	0
14	9	1	0	0	0
39	9	1	0	0	0
11	10	1	0	0	0
13	10	1	0	0	0
40	10	1	0	0	0
41	12	1	0	0	0
42	12	1	0	0	0
43	12	1	0	0	0
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19	14	2	0	0	0
16	15	2	0	0	0
44	15	1	0	0	0
17	16	1	0	0	0
45	16	1	0	0	0
18	17	2	0	0	0

47	19	1	0	0	0
48	20	1	0	0	0
22	21	2	0	0	0
49	21	1	0	0	0
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53	27	1	0	0	0
54	27	1	0	0	0
29	28	1	0	0	0
55	28	1	0	0	0
56	28	1	0	0	0
30	29	1	0	0	0
33	29	1	0	0	0
65	29	1	0	0	0
31	30	1	0	0	0
57	30	1	0	0	0
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59	31	1	0	0	0
60	31	1	0	0	0
33	32	1	0	0	0
61	32	1	0	0	0
62	32	1	0	0	0
63	33	1	0	0	0
64	33	1	0	0	0

M END

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