Rapid Qualitative GC-TOFMS Analysis of Unleaded Gasoline

LECO Corporation; Saint Joseph, Michigan USA

Key Words: GC-TOFMS, Petrochemical, Deconvolution

1. Introduction

Analyses of petroleum fuels are complicated by the relatively large number of volatile and semivolatile components contained in these mixtures. As a result, GC or GCMS analyses of these mixtures typically take well over two hours. Previous analytical conditions have focused on complete chromatographic resolution of as many individual analytes as possible. While all mass spectrometers offer multi-channel detection capabilities that may be used to identify coeluting analytes, slow spectral acquisition rates and under-developed software algorithms have minimized the impact of MS detectors on faster GC separation times.

The LECO Pegasus II GC-TOFMS offers several unique advantages for reducing the time of fuel analyses. The Pegasus II provides acquisition rates of up to 500 full range mass spectra/second to allow accurate definition of the narrowest GC peaks. Fast GC techniques may now be effectively used to reduce separation times without sacrificing data quality. The unique degree of spectral continuity across a chromatographic peak provided by the Pegasus II has allowed the development of several revolutionary software algorithms. The Peak Find algorithm effectively locates the position of all peaks in the chromatogram including multiple components in complex coelutions. The Deconvolution algorithm effectively resolves the mixed mass spectra of the coelution into accurate individual mass spectra for each analyte, including the accurate distribution of signal from masses shared by several components in the coelution.

2. Experimental Conditions

The potential benefit of these unique features of the Pegasus II in petroleum fuel analyses were evaluated using an unleaded gasoline sample obtained from a local distributor. The analytical conditions used for the 14 minute analysis of this complex mixture are summarized in Table 1. The resulting total ion chromatogram from the separation is shown in Figure 1 with the peak table (Table 2) indicating the analyte name, its Retention Time (RT), and the accuracy of its library search result versus the NIST spectral database.

Table 1. Pegasus II GC-TOFMS Conditions for a 14 minute Analysis of an Unleaded Gasoline Sample.

Detector:	LECO Corporation Pegasus II Time-of-Flight Mass Spectrometer
Transfer Line:	275°C
Source:	210°C
Acquisition Rate:	50 spectra/sec
GC:	Hewlett Packard® 6890*
Column:	DB-1 20 m x 0.1 mm ID, 0.4 µm phase film
Oven:	40°C for 0.4 min., then to 110°C at 10°C/min., then to 260°C at 20°C/min., hold for 1 min.
Injector:	225°C
Carrier Gas:	Helium, 0.6 ml/min. constant flow
Sample:	No preparation required. 0.2 µL split (1000:1) injection

**HP6890 GC is equipped with fast oven temperature ramp capabilities and a high pressure EPC module.*

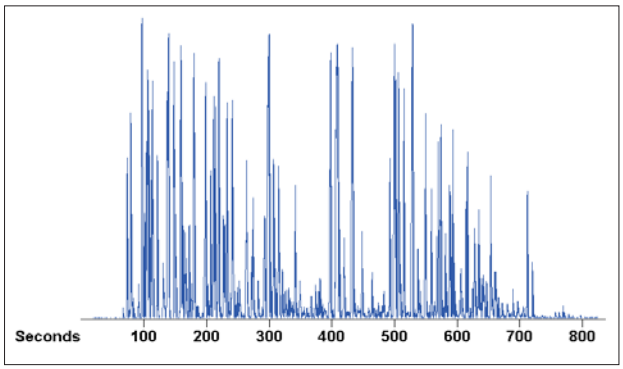

Figure 1: Unleaded Gasoline Total Ion Chromatogram (TIC)—573 Analytes in 14 Minutes.

3. Results

The effectiveness of the Peak Find and Deconvolution algorithms to accurately locate and identify analytes in complex coelutions resulting from the rapid separation conditions used in this analysis can be evaluated in Figures 2 and 3. In Figure 2, the positions of all components in a coelution containing five C7 hydrocarbons are accurately located by the Peak Find algorithm. The mass spectra for all five analytes are accurately resolved from one another by the Deconvolution algorithm. Library search results for these mass spectra versus the NIST spectral database are presented in Figure 3. The Deconvolution algorithm not only separates out ions unique to the spectra of each analyte but also successfully assigns the appropriate amount of signal to each analyte spectrum for masses that are shared between multiple analytes in the coelution. In the C7 hydrocarbon coelution (Figure 3), the signal at 55u, 81u, 96u, and 98u is appropriately proportioned between the five analytes by the Deconvolution algorithm.

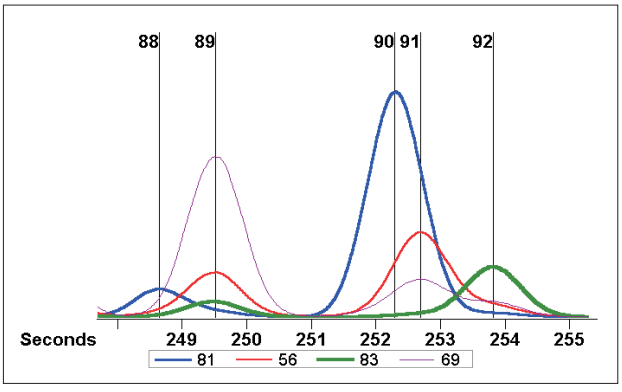

Figure 2. Extracted Ion Profile Chromatogram Showing the Coelution of C7 Hydrocarbons. The markers indicate peak positions as determined by the Pegasus II GC-TOFMS Peak Find algorithm.

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Table 2. Unleaded Gasoline Peak Table With the Similarity and Reverse Similarity Numbers Resulting From Comparison of the Acquired Spectra to the NIST Mass Spectral Database.

Peak	Name	RT (sec)	Similarity	Reverse
1	Propane	67.03	964	964
2	Isobutane	73.55	879	879
3	1-Propene, 2-methyl-	77.15	931	941
4	1-Butyne	77.73	693	916
5	Butane	79.05	937	941
6	Acetic acid, 2-propenyl ester	79.83	761	765
7	1-Butene	80.59	917	929
8	Propane, 2,2-dimethyl-	81.53	904	904
9	2-Butene	83.53	919	930
10	Ethanol	86.67	920	920
11	Cyclopropane, 1,1-dimethyl-	91.53	942	961
12	Butane, 2-methyl-	97.19	874	899
13	1-Pentene	101.57	949	952
14	Cyclopropane, 1,2-dimethyl-, cis-	103.95	913	913
15	Pentane	106.03	940	941
16	1,3-Pentadiene, (Z)-	107.69	910	932
17	Cyclopropane, 1,2-dimethyl-, trans-	108.47	925	925
18	2-Pentene, (Z)-	111.71	908	908
19	2-Butene, 2-methyl-	113.79	878	944
20	1,2-Pentadiene	114.81	910	957
21	1,3-Butadiene, 2-methyl-	120.21	944	946
22	3-Penten-1-yne	120.53	893	904
23	Butane, 2,2-dimethyl-	121.63	937	937
24	1,3-Pentadiene, (Z)-	130.69	929	944
25	1-Pentene, 4-methyl-	131.73	891	891
26	Cyclopropane, 1-ethyl-1-methyl-	132.83	912	913
27	Propane, 2-methoxy-2-methyl-	135.83	797	813
28	Cyclobutane, methyl-	137.05	858	876
29	Butane, 2,3-dimethyl-	137.89	863	878
30	Pentane, 2-methyl-	139.79	886	890
31	2-Butanone	142.37	629	866
32	Pentane, 3-methyl-	148.39	925	927
33	1-Pentene, 2-methyl-	150.59	913	916
34	1-Hexene	151.11	909	911
35	trans-1,4-Hexadiene	154.89	774	868
36	Cyclopropane, (1-methylethyl)-	157.87	791	795
37	Hexane	159.27	933	938
38	3-Hexene, (Z)-	159.81	862	863
39	2-Hexene	161.47	913	920
40	2-Pentene, 4-methyl-	163.05	940	949
41	2-Pentene, 3-methyl-, (Z)-	165.85	917	917
42	Cyclopentene, 3-methyl-	166.25	928	949
43	2-Hexene	168.23	881	909
44	2-Pentene, 3-methyl-, (Z)-	172.57	922	922
45	2-Pentene, 4-methyl-	172.97	822	848
46	Butane, 2,2,3-trimethyl-	176.63	867	869
47	Cyclopentane, methyl-	179.93	875	875
48	Pentane, 2,4-dimethyl-	181.01	836	841
49	Cyclopropane, (1-methylethylidene)-	181.73	852	857
50	1,3-Cyclopentadiene, 5-methyl-	184.29	822	855
51	Butane, 2,2,3-trimethyl-	186.37	900	900
52	1,3-Cyclopentadiene, 5-methyl-	187.07	909	910
53	2,4-Hexadiene, (E,E)-	189.73	924	934
54	1-Pentene, 3,4-dimethyl-	190.75	816	855
55	2-Pentyne, 4,4-dimethyl-	192.29	842	857
56	1-Pentene, 2,4-dimethyl-	193.61	886	915
57	Cyclopentene, 3-methyl-	196.79	894	907
58	1-Hexene, 3-methyl-	197.93	745	747
59	Benzene	198.25	857	900
60	Cyclopropane, 1,1,2,2-tetramethyl-	199.37	854	863
61	Thiophene	201.73	800	813
62	Pentane, 3,3-dimethyl-	202.27	894	895
63	2-Pentene, 3-ethyl-	204.23	921	921
64	Cyclobutene, 3,3-dimethyl-	205.83	744	761
65	Cyclohexane	206.91	934	936
66	1,3-Cyclopentadiene, 1-methyl-	207.87	750	903
67	Azetidine	208.35	865	945
68	3,5-Dimethylcyclopentene	209.33	780	800
69	1-Pentene, 3-ethyl-	210.25	879	879
70	Hexane, 2-methyl-	211.89	904	904
71	Pentane, 2,3-dimethyl-	214.35	930	931
72	Hexane, 3-methoxy-	215.27	801	801
73	Cyclopentane, 1,1-dimethyl-	217.81	896	901
74	Hexane, 3-methyl-	219.79	884	886
75	1,4-Hexadiene, (Z)-	220.35	753	820
76	2-Hexene, 5-methyl-, (Z)-	222.19	890	908
77	Cyclopentane, 1,3-dimethyl-	226.85	936	949
78	Pentane, 3-ethyl-	228.77	897	897
79	Cyclopentane, 1,3-dimethyl-	229.51	933	945
80	Cyclopentane, 1,2-dimethyl-, cis-	231.87	918	928
81	Butane, 2,2,3,3-tetramethyl-	233.05	922	936
82	3-Hexene, 3-methyl-, (Z)-	235.69	933	953
83	Cyclopentene, 1,2,3-trimethyl-	236.63	748	814
84	3-Heptene	238.33	945	949
85	Heptane	241.27	899	947
86	3-Hexene, 3-methyl-, (Z)-	242.63	824	876
87	2-Heptene	244.59	915	917
88	3-Methyl-3-hexene,c&t	246.89	918	937
89	1,4-Hexadiene, 2-methyl-	248.65	896	911
90	1-Pentene, 2,3-dimethyl-	249.51	914	934
91	3,5-Dimethylcyclopentene	252.29	916	944
92	2-Heptene	252.69	918	920
93	2-Pentene, 3,4-dimethyl-, (Z)-	253.81	917	924
94	3,4-Heptadiene	256.83	872	880
95	6-Methyl-2-heptyne	257.35	650	730
96	Cyclopentene, 3-ethyl-	259.45	879	880
97	1,4-Heptadiene	260.01	597	598
98	Cyclopentane, 1, 3-dimethyl-	262.55	869	882
99	Cyclohexane, methyl-	264.09	899	899
100	Cyclopentane, 1,1,3-trimethyl-	265.67	878	879
101	Cyclopentene, 1,2,3-trimethyl-	266.85	888	891
102	5,5-Dimethyl-1,3-hexadiene	269.49	888	892
103	Hexane, 2,5-dimethyl-	272.11	940	951
104	Cyclopentane, ethyl-	274.19	855	857
105	Hexane, 2,4-dimethyl-	274.57	917	919
106	5-Methyl-1,5-hexadien-3-ol	275.05	729	741
107	Cyclohexane, methylene-	277.73	717	802

Peak	Name	RT (sec)	Similarity	Reverse
108	Cyclopentane, 1,2,4-trimethyl-, (1à,2á,4à)-	282.25	886	888
109	Hexane, 3,3-dimethyl-	282.77	824	825
110	1,3,6-Heptatriene	283.43	864	879
111	5-Methyl-3-heptene	285.33	799	856
112	1-Butene, 2,3-dimethyl-	285.63	800	800
113	1,4-Hexadiene, 2,3-dimethyl-	288.19	831	845
114	Cyclopentane, 1,2,3-trimethyl-, (1à,2à,3á)-	289.73	903	905
115	Cyclopentene, 4,4-dimethyl-	292.31	833	866
116	Pentane, 2,3,4-trimethyl-	292.77	904	916
117	Cyclopentene, 3-ethyl-	293.85	734	742
118	5-Methyl-3-heptene	296.79	692	729
119	2-Heptene, 4-methyl-, (E)-	298.85	875	930
120	Toluene	299.97	851	856
121	Pentane, 2,3,3-trimethyl-	300.25	858	869
122	Thiophene, 2-methyl-	300.81	827	848
123	Pentane, 2,3,4-trimethyl-	302.01	919	928
124	4-Methyl-1,4-heptadiene	302.57	783	812
125	1-Pentene, 3-ethyl-4-methyl-	303.47	818	832
126	Pentane, 3-ethyl-2-methyl-	303.89	894	897
127	3,5-Dimethylcyclopentene	305.03	507	730
128	Cyclohexane, 1,1-dimethyl-	306.61	688	707
129	Heptane, 2-methyl-	306.95	895	899
130	Cyclohexane, methylene-	308.17	878	915
131	Heptane, 4-methyl-	308.57	890	891
132	2-Hexene, 2,3-dimethyl-	309.85	710	765
133	Hexane, 3,4-dimethyl-	311.61	820	852
134	3-Methyl-3-hexen-2-ol	313.23	631	729
135	1-Pentene, 3-ethyl-3-methyl-	313.99	609	651
136	Heptane, 3-methyl-	315.09	892	909
137	2-Butene, (Z)-	315.53	761	849
138	Hexane, 3-ethyl-	316.39	886	887
139	2-Pentene	316.99	829	869
140	Pentane, 3-methyl-	318.39	546	817
141	1,1,3,4-Tetramethylcyclohexane	319.37	759	770
142	1,3-Dimethylcyclohexane,c&t	320.99	869	899
143	Cyclopentane, 1,2,3-trimethyl-, (1à,2à,3à)-	321.29	880	885
144	Cyclohexane, 1,4-dimethyl-	322.81	899	907
145	3-Heptene, 2-methyl-, (E)-	325.75	783	846
146	Heptane, 2,2-dimethyl-	326.19	897	897
147	3-Ethyl-3-hexene	326.95	758	856
148	Heptane, 3-methylene-	327.53	824	827
149	1-Octene	329.23	882	886
150	Cyclohexane, 1,1-dimethyl-	329.45	778	820
151	Cyclopentane, 1-ethyl-3-methyl-, trans-	330.87	894	906
152	3-Hexene, 2,5-dimethyl-, (E)-	332.31	799	799
153	Cyclopentane, 1-ethyl-3-methyl-, trans-	333.17	892	893
154	Cyclopentane, 1-ethyl-2-methyl-, cis-	334.83	864	879
155	Cyclopentene, 1,2,3-trimethyl-	336.31	911	926
156	3-Octene, (E)-	337.93	886	895
157	Heptane, 3-methylene-	339.43	859	860
158	4-Methyl-1,4-heptadiene	340.97	809	827
159	Hexane, 2,4-dimethyl-	341.83	877	900
160	1,4-Heptadiene, 3-methyl-	344.31	759	838
161	2-Octene	344.59	898	900

Peak	Name	RT (sec)	Similarity	Reverse
162	1à,2á,3à,4á-Tetramethylcyclopentane	346.11	837	856
163	Cyclohexane, 1,4-dimethyl-	348.91	869	883
164	4-Methyl-1,3-heptadiene (c,t)	350.27	918	933
165	Heptane, 3,3-dimethyl-	352.57	861	905
166	2-Octene	353.89	881	884
167	2-Ethyl-3-methylcyclopentene	354.75	863	876
168	Cyclopentane, (1-methylethyl)-	355.79	825	830
169	3-Heptene, 2,6-dimethyl-	356.33	733	831
170	1,4-Hexadiene, 3-ethyl-	359.69	837	866
171	Hexane, 2,3,5-trimethyl-	360.45	796	827
172	Butane, 2-cyclopropyl-	362.13	828	888
173	Pentane, 3-methyl-	363.07	853	893
174	Ethanone, 1-(1,3-dimethyl-3-cyclohexen-1-yl)-	364.69	707	708
175	1,3-Dimethyl-1-cyclohexene	365.53	913	940
176	Cyclopentane, 1-ethyl-2-methyl-, cis-	366.29	874	886
177	Hexane, 2,4-dimethyl-	367.25	823	867
178	1,4-Dimethyl-1-cyclohexene	369.79	908	932
179	4-Methyl-1,6-heptadien-4-ol	370.91	743	843
180	Cyclopentane, 1,1,3,3-tetramethyl-	372.65	787	788
181	Heptane, 2,6-dimethyl-	373.89	887	898
182	Cyclohexane, 1,2-dimethyl-	374.39	782	800
183	Cyclopentane, propyl-	376.49	844	847
184	2-Pyrazoline, 1-isopropyl-5-methyl-	378.15	820	856
185	Cyclohexane, ethyl-	379.11	884	895
186	2-Ethyl-3-methylcyclopentene	379.49	839	898
187	Heptane, 2,5-dimethyl-	381.33	902	904
188	1,2-Dimethyl-1,4-cyclohexadiene	383.71	666	898
189	Cyclohexane, 1,1,3-trimethyl-	384.93	812	813
190	Cyclooctane, butyl-	385.75	716	752
191	3,3,5,5-Tetramethylcyclopentene	386.59	796	800
192	1,1,4-Trimethylcyclohexane	387.95	791	826
193	cis-4-Nonene	389.19	794	831
194	Cyclohexane, 1-ethyl-2-methyl-, cis-	391.05	831	833
195	1,4-Octadiene,c&t	393.69	758	786
196	Ethylbenzene	398.11	865	868
197	Thiophene, 3-ethyl-	399.09	695	712
198	Cyclohexane, 1,2,3-trimethyl-, (1à,2á,3à)-	401.59	866	880
199	p-Xylene	406.33	796	844
200	p-Xylene	409.93	913	936
201	Benzene, 1,3-dimethyl-	410.51	802	811
202	Octane, 4-methyl-	411.41	898	910
203	Thiophene, 2-ethyl-	411.85	597	597
204	Octane, 2-methyl-	412.23	904	919
205	Thiophene, 2,4-dimethyl-	412.75	739	742
206	1-Nonyne, 7-methyl-	414.25	781	804
207	5-Methyl-1-heptanol	415.81	757	793
208	Cyclopentene, 4-methyl-	417.17	845	878
209	Octane, 3-methyl-	419.83	885	886
210	Cyclopentane, 1-methyl-3-(1-methylethyl)-	422.07	788	797
211	1,3-Hexadiene, 3-ethyl-2-methyl-	423.13	763	776

Delivering the Right Results

Peak	Name	RT (sec)	Similarity	Reverse
212	Thiophene, 2,3-dimethyl-	423.75	862	862
213	Bicyclo[4.2.0]octa-1,3,5-triene	425.19	684	751
214	1,6-Heptadiene, 3,3-dimethyl-	426.59	758	818
215	Cyclohexane, 1,2,4-trimethyl-	427.35	849	849
216	Heptane, 2,2,4-trimethyl-	429.33	908	925
217	Benzene, 1,2-dimethyl-	431.75	899	903
218	3-Heptene, 4-ethyl-	433.67	735	761
219	2-Undecanethiol, 2-methyl-	435.95	779	784
220	Cycloheptanone, 4-methyl-, (R)-	437.43	781	818
221	cis-1-Ethyl-3-methyl-cyclohexane	438.69	896	912
222	2-Thiophenecarboxaldehyde	439.65	788	856
223	cis-4-Nonene	441.03	760	813
224	1-Ethyl-3-methylcyclohexane (c,t)	441.33	775	779
225	4-Nonene	442.45	877	881
226	Cyclopentanone, 2-methyl-4-(2-methylpropyl)-	444.13	773	790
227	trans-2-Methyl-3-octene	445.11	738	781
228	Nonane	448.31	900	900
229	1,3-Hexadiene, 3-ethyl-2-methyl-	448.97	806	814
230	Heptane, 2,5,5-trimethyl-	450.07	877	878
231	cis-2-Nonene	450.43	884	893
232	cis-4-Nonene	452.61	797	831
233	4-Methyl-1,4-heptadiene	453.79	732	812
234	3-Nonyne	455.47	800	801
235	Cyclohexane, 1,2,3-trimethyl-, (1à,2à,3á)-	456.37	844	907
236	Furan, 4-methyl-2-propyl-	457.93	771	826
237	Cyclohexane, 1-ethyl-4-methyl-, cis-	458.79	918	922
238	3-Heptene, 2,6-dimethyl-	459.63	781	839
239	Cyclohexane, 1-ethyl-4-methyl-, cis-	461.59	851	857
240	Undecane, 5-methyl-	463.03	844	869
241	Benzene, (1-methylethyl)-	464.27	885	886
242	1,5-Octadiene, 7-methyl-3-(1-methylethyl)-	466.69	618	676
243	Nonane, 4-methyl-	466.89	815	853
244	Heptane, 3-methyl-	467.81	861	884
245	Heptane, 2,3,5-trimethyl-	469.19	754	845
246	1,1'-Bicycloheptyl	470.09	696	702
247	Cyclohexane, 1-propenyl-	471.35	806	808
248	3-Hexene, 3-ethyl-2,5-dimethyl-	472.93	705	713
249	Nonane, 4-methyl-	474.39	816	866
250	Heptane, 3,5-dimethyl-	475.73	830	839
251	Pentalene, octahydro-2-methyl-	477.27	738	741
252	Octane, 2,7-dimethyl-	478.31	859	867
253	Diisoamylene	480.07	781	782
254	Cyclohexane, (1-methylethyl)-	480.65	889	908
255	Oxirane, (3,3-dimethylbutyl)-	481.39	779	838
256	Cyclopentane, butyl-	482.71	829	832
257	Nonane, 3-methyl-	483.33	893	895
258	Octane, 3,6-dimethyl-	489.01	894	897
259	Cyclohexane, 1-methyl-2-propyl-	489.89	713	790
260	3,4-Diethyl-3-hexene	490.67	673	725

Peak	Name	RT (sec)	Similarity	Reverse
261	Heptane, 3-ethyl-2-methyl-	491.27	757	852
262	Benzene, propyl-	492.71	855	856
263	Heptane, 3-ethyl-	494.03	651	740
264	Benzene, 1-ethyl-2-methyl-	496.91	855	881
265	(6Z)-Nonen-1-ol	497.15	746	752
266	1,2,4-Trimethylbenzene	498.03	898	913
267	Benzene, 1,2,3-trimethyl-	500.03	875	877
268	Benzene, 1-ethyl-4-methyl-	501.85	864	864
269	Octane, 4-ethyl-	502.47	742	874
270	Cyclooctane, ethyl-	504.07	722	748
271	Benzene, 1,2,3-trimethyl-	506.39	906	908
272	Nonane, 4-methyl-	507.37	900	908
273	Nonane, 2-methyl-	509.41	855	858
274	2,2,6,6-Tetramethylheptane	510.31	837	854
275	Cyclohexane, 1-ethyl-2,3-dimethyl-	511.09	694	708
276	Octane, 3-ethyl-	512.63	831	857
277	Benzene, 1,2,3-trimethyl-	515.21	863	884
278	1-Pentanol, 4-methyl-2-propyl-	516.03	764	798
279	1-Methyl-4-(1-methylethyl)-cyclohexane	516.69	736	784
280	Cyclohexane, 1-methyl-4-(1-methylethylidene)-	518.81	789	799
281	Heptane, 2,2,4-trimethyl-	521.51	735	792
282	Octane, 2-methyl-	522.41	683	767
283	1-Methyl-4-(1-methylethyl)-cyclohexane	523.05	757	836
284	2-Nonene, 3-methyl-, (E)-	524.99	576	757
285	1-Octanol, 2,7-dimethyl-	525.75	684	765
286	Benzene, 1,2,3-trimethyl-	528.91	903	905
287	Cyclohexane, 1-ethyl-2-methyl-	529.23	584	769
288	cis-4-Decene	530.11	718	776
289	Cyclobutane, 1,2-diethyl-, cis-	530.49	758	827
290	1,1'-Bicyclohexyl, 2-methyl-, trans-	532.79	756	758
291	6-Octen-1-ol, 7-methyl-3-methylene-	533.07	724	784
292	3-Ethyl-3-methylheptane	535.55	717	823
293	Octane, 3,5-dimethyl-	537.29	880	915
294	trans-3-Decene	538.83	841	889
295	Benzene, (2-methylpropyl)-	539.09	843	861
296	Thiophene, 2,3,4-trimethyl-	539.73	767	775
297	Benzene, (1-methylpropyl)-	541.27	842	896
298	Benzeneacetaldehyde, à-methyl-	541.69	705	789
299	Cyclohexane, 1-methyl-4-(1-methylbutyl)-	542.01	621	648
300	Benzeneacetaldehyde, à-methyl-	542.19	700	770
301	Tridecane, 6-methyl-	542.99	747	794
302	Cyclopentane, 1-methyl-3-(2-methylpropyl)-	544.85	796	806
303	2-Decene, (E)-	545.79	865	899
304	Benzene, 1-methyl-2-(1-methylethyl)-	547.95	851	855
305	Benzene, 1-ethyl-4-methyl-	549.15	773	786
306	Benzene, 1,2,3-trimethyl-	549.63	898	903
307	1,2,4-Trimethylbenzene	550.05	834	854
308	Benzene, 1-methyl-2-(1-methylethyl)-	550.67	811	817
309	Octane, 2,3,7-trimethyl-	551.23	653	822
310	Octane, 2,4,6-trimethyl-	552.09	720	779
311	Decane, 3,4-dimethyl-	553.03	778	809
312	Decane, 4-methyl-	555.35	846	868
313	Phenol, 2-methyl-	556.67	715	849

Peak	Name	RT (sec)	Similarity	Reverse
314	Cyclohexane, 1-ethyl-1-methyl-	557.11	827	867
315	Benzene, 1-propenyl-	558.35	806	829
316	Benzene, 1-ethenyl-2-methyl-	558.87	868	896
317	Benzene, 1-propenyl-	559.27	792	794
318	Decane, 2,2,3-trimethyl-	559.49	693	787
319	Benzene, 1-propynyl-	563.03	864	914
320	1-Undecene, 5-methyl-	564.13	754	759
321	Cyclopentane, pentyl-	565.57	781	808
322	Cyclopentane, 1,1,3-trimethyl-3-(2-methyl-2-propenyl)-	566.29	717	734
323	Benzene, 1,2-diethyl-	567.57	870	903
324	Benzene, 1-methyl-2-propyl-	569.55	823	846
325	Benzene, (1-methylpropyl)-	569.79	868	887
326	Benzene, 1-methyl-3-propyl-	570.37	846	856
327	Decane, 2,5,9-trimethyl-	570.73	646	753
328	Benzene, (1-methylpropyl)-	572.81	897	916
329	Benzene, (2-methylpropyl)-	573.53	820	843
330	Benzene, 4-ethyl-1,2-dimethyl-	574.15	851	851
331	Decane, 2,4-dimethyl-	575.53	699	858
332	Benzene, 1,2-diethyl-	577.01	885	910
333	Nonane, 2,3-dimethyl-	577.47	831	845
334	4-Octene, 2,3,6-trimethyl-	577.95	750	858
335	2-Propyl-1-pentanol	578.45	762	837
336	Decane, 5-methyl-	579.05	857	871
337	Benzene, 1-methyl-2-propyl-	580.55	729	784
338	Benzene, (1-methylpropyl)-	581.15	853	905
339	Hexane, 2,2,5-trimethyl-	581.99	708	787
340	Pentane, 3-ethyl-2,2-dimethyl-	582.89	849	882
341	Decane, 2-methyl-	583.57	864	864
342	2-Decen-1-ol, (Z)-	583.81	822	827
343	Decane, 3-methyl-	585.65	730	796
344	Decane, 2,5,9-trimethyl-	586.49	799	815
345	Benzene, 2-ethyl-1,4-dimethyl-	587.57	881	881
346	2,3-Dimethyldecane	587.89	865	880
347	Benzene, 1-methyl-2-(1-methylethyl)-	589.11	875	876
348	Benzene, 1-butenyl-, (E)-	591.23	902	934
349	Benzene, 4-ethyl-1,2-dimethyl-	593.19	878	878
350	Benzene, 1-butenyl-, (E)-	594.87	889	909
351	1-Octanol, 2,7-dimethyl-	595.57	698	766
352	Benzene, 1-methyl-2-(1-methylethyl)-	597.49	873	880
353	4-Decene, 8-methyl-, (E)-	598.73	799	876
354	Cyclopentane, 1,1'-(1,4-butandiyl)bis-	599.41	749	749
355	Cyclohexane, 1-methyl-2-propyl-	599.63	656	757
356	Bicyclo[2.2.2]oct-5-en-2-one	600.45	772	812
357	3-Undecene, (E)-	601.35	703	778
358	Decane, 3,4-dimethyl-	601.77	639	734
359	1H-Indene, 2,3-dihydro-1,6-dimethyl-	602.57	751	771
360	Benzene, 1-methyl-4-(2-methylpropyl)-	603.93	799	828
361	Benzene, (1,1-dimethylethyl)methyl-	604.05	684	804
362	Benzene, (1,2-dimethylpropyl)-	604.75	715	741
363	Benzene, (1,1-dimethylpropyl)-	605.09	836	837

Peak	Name	RT (sec)	Similarity	Reverse
344	Decane, 2,5,9-trimethyl-	586.49	799	815
345	Benzene, 2-ethyl-1,4-dimethyl-	587.57	881	881
346	2,3-Dimethyldecane	587.89	865	880
347	Benzene, 1-methyl-2-(1-methylethyl)-	589.11	875	876
348	Benzene, 1-butenyl-, (E)-	591.23	902	934
349	Benzene, 4-ethyl-1,2-dimethyl-	593.19	878	878
350	Benzene, 1-butenyl-, (E)-	594.87	889	909
351	1-Octanol, 2,7-dimethyl-	595.57	698	766
352	Benzene, 1-methyl-2-(1-methylethyl)-	597.49	873	880
353	4-Decene, 8-methyl-, (E)-	598.73	799	876
354	Cyclopentane, 1,1'-(1,4-butandiyl)bis-	599.41	749	749
355	Cyclohexane, 1-methyl-2-propyl-	599.63	656	757
356	Bicyclo[2.2.2]oct-5-en-2-one	600.45	772	812
357	3-Undecene, (E)-	601.35	703	778
358	Decane, 3,4-dimethyl-	601.77	639	734
359	1H-Indene, 2,3-dihydro-1,6-dimethyl-	602.57	751	771
360	Benzene, 1-methyl-4-(2-methylpropyl)-	603.93	799	828
361	Benzene, (1,1-dimethylethyl)methyl-	604.05	684	804
362	Benzene, (1,2-dimethylpropyl)-	604.75	715	741
363	Benzene, (1,1-dimethylpropyl)-	605.09	836	837
364	Undecane	605.73	924	925
365	Benzene, 4-ethyl-1,2-dimethyl-	606.53	879	880
366	1H-Indene, 1-ethyl-2,3-dihydro-1-methyl-	607.55	705	762
367	Benzene, (1,2-dimethylpropyl)-	608.13	741	769
368	1-Cyclopentylcyclopentene	608.73	891	915
369	Benzene, methyl(1-methylethyl)-	609.51	653	694
370	Benzene, 2,4-dimethyl-1-(1-methylethyl)-	610.47	786	855
371	Benzene, 1,2,4,5-tetramethyl-	614.07	892	893
372	Benzene, 1-methyl-4-(2-methylpropyl)-	614.61	730	771
373	Benzene, 4-ethyl-1,2-dimethyl-	616.47	890	890
374	Bicyclo[4.1.0]hept-4-en-3-ol, 3,7,7-trimethyl-, [1S-(1à,3à,6à)]-	616.97	661	774
375	2,6-Dimethyldecane	617.53	829	899
376	Benzene, (2-methyl-1-propenyl)-	618.61	831	897
377	Nonane, 3,7-dimethyl-	623.59	850	861
378	Benzene, (1,1-dimethylpropyl)-	624.63	856	858
379	Benzene, 2,4-diethyl-1-methyl-	626.89	906	916
380	Butyl pentyl carbonate	627.31	538	678
381	1H-Indene, 2,3-dihydro-5,6-dimethyl-	627.47	662	708
382	Benzene, 1-methyl-2-(2-propenyl)-	627.91	916	923
383	Benzene, (1,1-dimethylpropyl)-	628.79	848	854
384	Benzene, (1,1-dimethylpropyl)-	630.71	836	853
385	1H-Indene, 2,3-dihydro-1,2-dimethyl-	631.07	707	767
386	Benzene, 1-butynyl-	632.79	824	897

Peak	Name	RT (sec)	Similarity	Reverse
387	Benzene, 1-methyl-4-(2-methylpropyl)-	633.61	833	840
388	Benzene, 1-methyl-2-(2-propenyl)-	634.45	913	920
389	Benzene, 1-methyl-2-(1-methylethyl)-	635.95	841	842
390	Benzene, 1,4-diethyl-2-methyl-	636.17	812	829
391	Benzene, (2-methylbutyl)-	636.89	749	754
392	Benzene, (1-methylbutyl)-	637.25	866	879
393	Undecane, 6-methyl-	638.15	864	890
394	Undecane, 5-methyl-	638.89	893	899
395	Benzene, (1,1-dimethylpropyl)-	639.27	839	843
396	Benzene, 2,4-dimethyl-1-(1-methylethyl)-	639.57	869	878
397	Naphthalene, 1,2,3,4-tetrahydro-	641.21	833	856
398	Benzene, (1,1-dimethylpropyl)-	642.13	837	841
399	Benzene, 2,4-dimethyl-1-(1-methylethyl)-	642.87	870	895
400	Benzene, 1-methyl-4-(2-methylpropyl)-	643.21	820	825
401	Undecane, 2-methyl-	643.39	797	869
402	Dodecane, 4-methyl-	644.99	795	830
403	Benzene, (1,1-dimethylpropyl)-	646.83	861	865
404	Undecane, 3-methyl-	647.33	882	888
405	Benzene, (1,1-dimethylpropyl)-	648.19	823	840
406	Heptane, 3-ethyl-5-methyl-	649.11	756	843
407	2-Hexen-4-yne, (Z)-	650.05	668	723
408	1H-Indene, 1,1-dimethyl-	650.33	623	652
409	Heptane, 3,5-dimethyl-	651.17	727	794
410	Bicyclo[2.2.2]octane, 2-chloro-	651.69	639	666
411	Benzene, 1-(1-ethylpropyl)-4-methyl-	652.07	679	695
412	Benzene, 2-ethenyl-1,3,5-trimethyl-	653.07	776	787
413	Naphthalene	653.49	846	852
414	1H-Indene, 1-methylene-	654.31	768	894
415	1H-Indene, 2,3-dihydro-1,2-dimethyl-	655.47	874	875
416	Benzo[c]thiophene	656.05	830	869
417	Benzene, 2-ethenyl-1,3,5-trimethyl-	656.79	853	895
418	Benzene, (1,1-dimethylpropyl)-	657.73	826	829
419	1-Decanol, 2-ethyl-	658.19	731	779
420	Benzene, (1-ethyl-2-propenyl)-	659.03	762	801
421	1H-Indene, 2,3-dihydro-1,3-dimethyl-	659.83	781	797
422	Benzene, 2,4-dimethyl-1-(1-methylethyl)-	660.03	837	850
423	Benzene, 2,4-diethyl-1-methyl-	661.01	862	902
424	1H-Indene, 2,3-dihydro-1,6-dimethyl-	661.37	867	871
425	Undecane	662.35	864	882
426	1,11-Dodecadiene	663.29	639	644
427	Benzene, 1-(1-methylethenyl)-3-(1-methylethyl)-	664.41	693	812
428	Benzene, 2,4-dimethyl-1-(1-methylethyl)-	665.81	905	921
429	Benzene, (1,2,2-trimethylpropyl)-	666.17	695	737
430	Cyclopentane, 1,2-dimethyl-3-(1-methylethyl)-	667.87	685	685
431	Benzene, (1,1-dimethylbutyl)-	668.87	689	743
432	Benzene, 1-methyl-2-(1-ethylpropyl)-	669.71	638	639
433	Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	669.87	656	726
434	Undecane, 2,6-dimethyl-	670.79	845	880
435	Benzene, 2,4-dimethyl-1-(1-methylethyl)-	671.77	796	848
436	Naphthalene, 1,2,3,4-tetrahydro-2-methyl-	671.91	795	805
437	Benzene, 2,4-dimethyl-1-(1-methylpropyl)-	673.19	794	795
438	Undecane, 4,8-dimethyl-	675.01	824	839
439	Benzene, 1-(1,1-dimethylethyl)-4-ethenyl-	675.39	814	864
440	Naphthalene, 1,2,3,4-tetrahydro-1-methyl-	676.43	860	860
441	Benzene, (2-methylpentyl)-	677.71	705	823
442	Benzene, (1,3-dimethylbutyl)-	677.97	684	694
443	Undecane, 2,8-dimethyl-	678.63	720	794
444	Benzene, 1,1'-(1,1,3,3-tetramethyl-1,3-propanediyl)bis-	679.21	737	782
445	Naphthalene, 1,2,3,4-tetrahydro-1-methyl-	679.37	781	785
446	Benzene, 2,4-dimethyl-1-(1-methylethyl)-	680.31	869	887
447	Benzene, 1-methyl-4-(2-propenyl)-	680.87	786	855
448	Benzene, (1,1-dimethylethyl)methyl-	681.23	600	768
449	Benzene, 1,2,4-trimethyl-5-(1-methylethenyl)-	682.25	697	703
450	3,5-Decadiyne, 2,2-dimethyl-	683.85	747	755
451	3-Hexanone, 2,4-dimethyl-	684.53	684	798
452	1H-Indene, 2,3-dihydro-1,1,5-trimethyl-	684.89	774	799
453	3,5-Decadiyne, 2,2-dimethyl-	686.07	746	757
454	Benzene, (1,3-dimethylbutyl)-	686.71	833	843
455	Cyclohexane, hexyl-	687.03	776	855
456	Benzene, 2,4-dimethyl-1-(1-methylpropyl)-	688.49	745	747
457	Benzene, 2-ethenyl-1,3,5-trimethyl-	689.05	893	906
458	Dodecane, 5-methyl-	690.55	770	854
459	Benzene, (1-methyl-3-butenyl)-	690.69	678	728
460	1-Naphthol, 1,2,3,4-tetrahydro-2-methyl-	691.17	777	778
461	Benzene, hexyl-	691.81	784	809
462	Dodecane, 4-methyl-	692.97	748	856
463	Benzene, 1,2-diethyl-3,4-dimethyl-	693.27	699	725
464	Naphthalene, 1,2-dihydro-6-methyl-	694.39	760	786
465	Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	694.87	778	788
466	Tridecane, 3-methyl-	695.13	838	884
467	Benzene, (1,3-dimethylbutyl)-	695.59	725	777
468	Benzene, 2-ethenyl-1,3,5-trimethyl-	696.53	879	905
469	Naphthalene, 1,2,3,4-tetrahydro-6-methyl-	697.11	695	700
470	1H-Indene, 2,3-dihydro-1,2-dimethyl-	698.15	862	862

Peak	Name	RT (sec)	Similarity	Reverse
471	Dodecane, 3-methyl-	698.63	757	842
472	Benzene, 1,2-diethyl-4,5-dimethyl-	699.35	597	677
473	Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	699.81	805	822
474	Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	700.29	791	792
475	Octane, 2,3,7-trimethyl-	700.61	745	898
476	1-Butanol, 3,3-dimethyl-	701.59	679	797
477	Benzene, hexamethyl-	702.55	727	753
478	Benzene, 1,4-dipropyl-	702.87	809	813
479	Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	703.53	802	809
480	Benzene, 2,4-dimethyl-1-(1-methylethyl)-	705.17	883	903
481	1H-Indene, 2,3-dihydro-1,2-dimethyl-	705.99	886	887
482	Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	707.25	733	813
483	Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	708.77	724	725
484	Benzene, 2,4-dimethyl-1-(1-methylpropyl)-	709.41	656	656
485	Benzene, 1-(1-methylethenyl)-2-(1-methylethyl)-	710.45	833	885
486	Naphthalene, 1,2,3,4-tetrahydro-6-methyl-	710.83	785	804
487	Benzocycloheptatriene	711.87	849	894
488	1H-Indene, 1-ethylidene-	712.29	847	946
489	Benzaldehyde, 2,4,6-trimethyl-	714.37	666	728
490	1,4-Methanonaphthalen-9-ol, 1,2,3,4-tetrahydro-, stereoisomer	715.45	733	775
491	Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	715.97	865	883
492	Benzene, (1-cyclohexylethyl)-	716.49	600	690
493	Benzo[b]thiophene, 2-methyl-	717.59	762	877
494	Decane, 2,5,9-trimethyl-	718.11	593	855
495	2-Cyclopenten-1-ol, 1-phenyl-	719.39	661	690
496	Benzocycloheptatriene	719.99	879	907
497	1H-Indene, 1-ethylidene-	720.37	652	809
498	Undecane, 3,6-dimethyl-	721.37	672	839
499	Benzene, 1,4-dipropyl-	722.85	573	645
500	1,4-Dimethyl-1,2,3,4-tetrahydronaphthalene	723.43	864	903
501	Disiloxane, pentamethyl-2-propenyl-	725.75	472	622
502	1-Decanol, 2-ethyl-	726.25	689	768
503	Benzene, 1-(1-methylethenyl)-3-(1-methylethyl)-	726.59	720	793
504	Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	727.25	819	819
505	3-Cyclohexen-1-amine, 6-(4-methylphenyl)-2,5-diphenyl-, (1à,2à,5à,6á)-	727.97	791	891
506	Benzene, 1,3,5-trimethyl-	728.33	637	790
507	Undecane, 2,8-dimethyl-	728.69	774	863
508	Naphthalene, 2-ethyl-1,2,3,4-tetrahydro-	729.17	662	713
509	Benzene, [2-methyl-1-(1-methylethyl)propyl]-	729.75	632	687
510	1H-Indene, 2,3-dihydro-1,1,4,7-tetramethyl-	731.13	649	690

Peak	Name	RT (sec)	Similarity	Reverse
511	Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	731.51	791	797
512	3-Cyclohexene-1-ethanol, à-ethenyl-à,3-dimethyl-6-(1-methylethylidene)-	733.27	623	691
513	Benzene, bis(1-methylethyl)-	733.75	700	725
514	Naphthalene, 1,2,3,4-tetrahydro-2,7-dimethyl-	734.15	672	678
515	Benzene, (1,2,2-trimethylpropyl)-	734.77	680	710
516	Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	735.61	729	755
517	1-Octanol, 2-butyl-	736.39	701	809
518	Benzene, octadecyl-	736.75	606	619
519	Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	737.21	668	729
520	Tridecane, 4-methyl-	738.91	698	839
521	Benzene, 4-(2-butenyl)-1,2-dimethyl-, (E)-	739.45	683	706
522	Ethanone, 1-(2,4,6-trimethylphenyl)-	740.01	641	799
523	Benzene, hexyl-	740.41	685	722
524	Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	740.63	735	763
525	Dodecane, 3-methyl-	741.05	822	883
526	Indan, 1,1,6,7-tetramethyl-	741.65	693	726
527	1-Methyl-4-N-hexylbenzene	743.27	628	776
528	1-Iodo-2-methylnonane	744.37	651	822
529	Benzene, 1,1'-(1,1,3,3-tetramethyl-1,3-propanediyl)bis-	745.27	660	722
530	Naphthalene, 2-ethenyl-	747.41	811	888
531	Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	747.83	649	662
532	Dodecane, 2,6,10-trimethyl-	748.09	736	840
533	Benzo[b]thiophene, 2,5-dimethyl-	754.87	711	726
534	Pentadecane	756.23	815	863
535	Naphthalene, 1-ethyl-	757.19	907	910
536	Naphthalene, 1,2,3,4-tetrahydro-1,8-dimethyl-	757.53	820	824
537	Naphthalene, 1-ethyl-	758.35	838	838
538	Octane, 2,4,6-trimethyl-	759.09	705	829
539	1-Decanol, 2-ethyl-	761.49	752	836
540	Naphthalene, 1,4-dimethyl-	762.41	900	927
541	Naphthalene, 2,6-dimethyl-	763.05	921	933
542	Benzene, 1-(1-methylethenyl)-4-(1-methylethyl)-	767.21	801	801
543	Naphthalene, 1,4-dimethyl-	768.97	934	948
544	6-Propyltetraline	770.23	632	717
545	Naphthalene, 2,6-dimethyl-	770.71	916	928
546	Naphthalene, 1,4-dimethyl-	777.93	909	914
547	Naphthalene, 2,6-dimethyl-	779.17	859	883
548	Decane, 2,5,9-trimethyl-	783.41	788	887
549	Naphthalene, 1,4-dimethyl-	784.51	887	897
550	Tridecane, 3-methyl-	786.17	831	849
551	1,1'-Biphenyl, 4-methyl-	791.99	867	874
552	Naphthalene, [[4-(1,1-dimethylethyl)phenoxy]methyl]-	795.47	647	714
553	1,1'-Biphenyl, 4-methyl-	796.27	802	814
554	Decane, 6-ethyl-2-methyl-	797.03	729	828

Peak	Name	RT (sec)	Similarity	Reverse
555	Naphthalene, 2-(1-methylethyl)-	799.73	776	784
556	Naphthalene, 2-(1-methylethyl)-	801.21	801	833
557	Naphthalene, 2-(1-methylethyl)-	803.89	871	896
558	Naphthalene, 2-(1-methylethyl)-	805.81	767	805
559	5-Methyl-1-phenylhexa-1,3,4-triene	807.71	797	884
560	Naphthalene, 2-(1-methylethyl)-	811.07	794	863
561	Naphthalene, 1,4,6-trimethyl-	812.63	861	894
562	Naphthalene, 1,3,6-trimethyl-	815.09	810	958
563	Naphthalene, 1,4,5-trimethyl-	821.33	884	898
564	Naphthalene, 2,3,6-trimethyl-	823.27	836	850
565	Naphthalene, 1,4,5-trimethyl-	827.73	859	860
566	Naphthalene, 1,4,5-trimethyl-	828.49	871	890
567	Naphthalene, 1,4,6-trimethyl-	829.43	870	873
568	Undecane, 2,9-dimethyl-	835.01	765	856
569	9H-Fluorene-9-carboxylic acid	836.13	835	870
570	Naphthalene, 1,4,6-trimethyl-	838.19	829	836
571	Naphthalene, 2-methyl-1-propyl-	840.47	619	718
572	1,1'-Biphenyl, 4-methyl-	841.39	735	833
573	Naphthalene, 1,3,6-trimethyl-	844.99	668	670

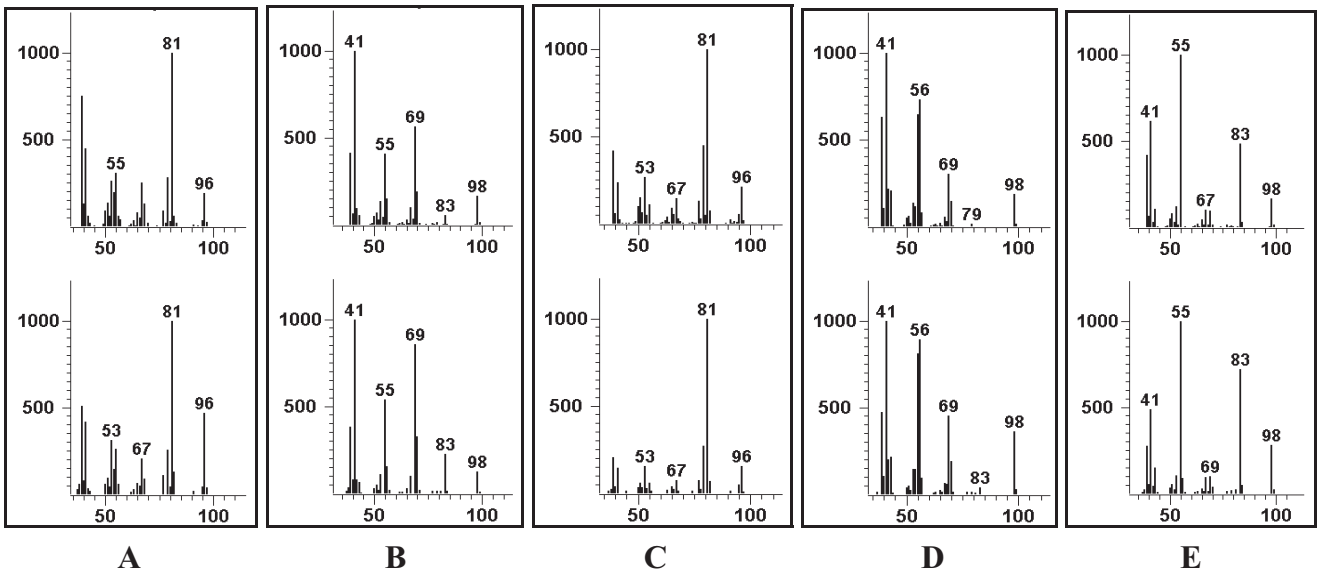

Figure 3. Mass Spectra for Coeluting C7 Hydrocarbons as Determined by the Pegasus II GC-TOFMS Deconvolution algorithm.
Top: Pegasus II spectrum. Bottom: NIST Library spectrum.
A: Peak 88; 2-methyl-1,4-hexadiene; Similarity 896; Reverse Similarity 911. B: Peak 89; 2,3-dimethyl-1-pentene; Similarity 914; Reverse Similarity 934.
C: Peak 90; 3,5-dimethylcyclopentene; Similarity 916; Reverse Similarity 944. D: Peak 91; 2-heptene; Similarity 918; Reverse Similarity 920.
E: Peak 92; 3,4-Dimethyl-2-pentene; Similarity 917; Reverse Similarity 924.

4. Conclusions

The combination of Fast GC techniques (shorter microbore columns and faster temperature program rates), fast mass spectral acquisition rates, and unique Peak Find and spectral Deconvolution algorithms allow accurate analysis of 573 analytes in an unleaded gasoline sample in only 14 minutes using the Pegasus II GC-TOFMS. This represents a 10 fold decrease in data acquisition time. The unique software features also significantly reduce data processing time resulting in an overall decrease of analysis time of well over 1 order of magnitude.

Life Science and Chemical Analysis Solutions

LECO Corporation • 3000 Lakeview Avenue • St. Joseph, MI 49085 • Phone: 800-292-6141 • Fax: 269-982-8977
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