Rapid Qualitative GC-TOFMS Analysis of a Petroleum Refinery Reformate Standard

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Key Words: GC-TOFMS, Petrochemical, Deconvolution

1. Introduction

Analyses of petroleum products are complicated by the relatively large number of volatile components contained in these mixtures. As a result, GC or GCMS analyses of these mixtures typically take two hours or more. 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 analysis times. 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 analyses were evaluated using a Petroleum Refinery Reformate Standard (Supelco, Inc.). The mixture contained 284 analytes commonly found in petroleum products. 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 indicating the analyte name, its Retention Time (RT), and the accuracy of its library search result versus the NIST spectral database summarized in Table 2.

Table 1. Pegasus II GC-TOFMS Conditions for a 14 Minute Analysis of a Petroleum Refinery Reformate Standard (Supelco Catalog Number 4-7489).

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.*

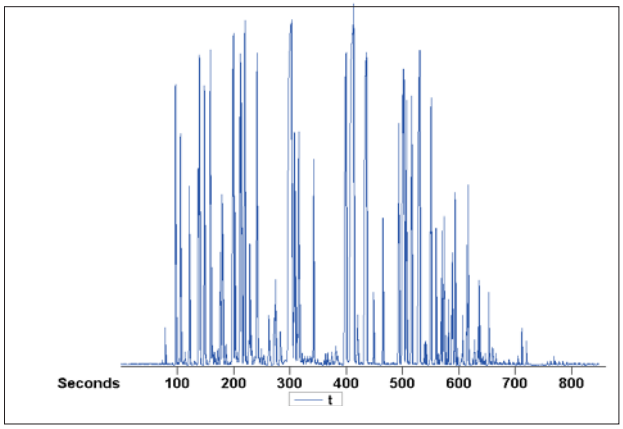

Figure 1. Petroleum Refinery Reformate Standard Total Ion Chromatogram (TIC)—284 Analytes in 14 Minutes.

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 located on the following page. In Figure 2, the positions of all components in a coelution containing three C11 benzene isomers are accurately located by the Peak Find algorithm. The mass spectra for all three 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 C11 benzene isomer coelution (Figure 3), the signal at 91u, 117u, and 148u is appropriately proportioned between the three analytes by the Deconvolution algorithm.

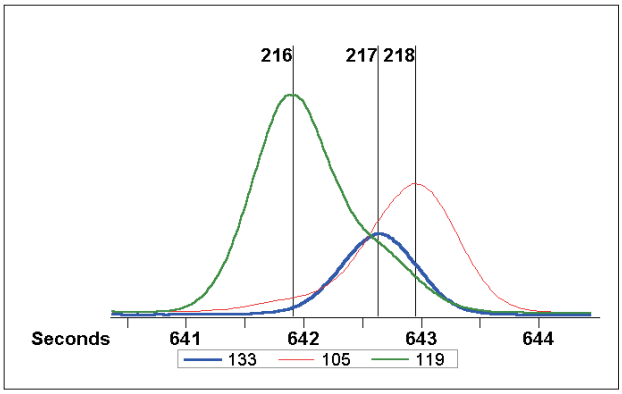

Figure 2. Extracted Ion Profile Chromatogram Showing the Coelution of C11 Benzene Isomers.

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Table 2: Petroleum Refinery Reformate Standard 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	Formula
1	Isobutane	73.51	899	900	C4H10
2	Butane	78.83	961	964	C4H10
3	Propane, 2,2-dimethyl-	81.47	875	875	C5H12
4	2-Butene, (Z)-	83.51	687	898	C4H8
5	1-Butene, 3-methyl-	91.49	892	892	C5H10
6	iso-Pentane	96.93	876	900	C5H12
7	1-Pentene	101.47	852	872	C5H10
8	1-Butene, 2-methyl-	103.81	868	917	C5H10
9	Pentane	105.71	946	949	C5H12
10	2-Pentene, (Z)-	108.29	885	905	C5H10
11	2-Pentene, (E)-	111.57	860	863	C5H10
12	2-Butene, 2-methyl-	113.67	877	933	C5H10
13	Butane, 2,2-dimethyl-	121.53	915	915	C6H14
14	Cyclopentene	130.59	912	918	C5H8
15	1-Pentene, 4-methyl-	131.63	817	818	C6H12
16	1-Pentene, 3-methyl-	132.71	895	896	C6H12
17	Cyclopentane	136.99	874	875	C5H10
18	Butane, 2,3-dimethyl-	137.31	878	882	C6H14
19	Pentane, 2-methyl-	139.37	877	882	C6H14
20	Pentane, 3-methyl-	148.13	926	928	C6H14
21	1-Pentene, 2-methyl-	150.45	915	916	C6H12
22	Pentane, 2,4-dimethyl-	157.89	795	797	C7H16
23	Hexane	159.05	944	951	C6H14
24	2-Hexene, (E)-	161.33	911	934	C6H12
25	2-Pentene, 4-methyl-	162.85	853	859	C6H12
26	2-Pentene, 3-methyl-, (Z)-	165.69	917	917	C6H12
27	Cyclopentene, 3-methyl-	166.03	828	916	C6H10
28	2-Hexene, (Z)-	168.07	856	856	C6H12
29	Cyclopentene, 4-methyl-	168.25	756	770	C6H10
30	1-Butene, 2,3-dimethyl-	172.41	909	909	C6H12
31	Pentane, 2,2-dimethyl-	176.51	896	897	C7H16
32	Cyclopentane, methyl-	179.53	873	874	C6H12
33	Pentane, 2,4-dimethyl-	180.81	873	877	C7H16
34	1,3-Cyclopentadiene, 1-methyl-	184.19	704	910	C6H8
35	Butane, 2,2,3-trimethyl-	186.31	880	881	C7H16
36	1-Pentene, 3,4-dimethyl-	190.81	657	810	C7H14
37	1-Pentene, 2,4-dimethyl-	193.77	793	866	C7H14
38	Cyclopentane, methylene-	197.31	831	853	C6H10
39	Benzene	199.85	927	944	C6H6
40	Pentane, 3,3-dimethyl-	202.53	834	839	C7H16
41	2-Pentene, 3-ethyl-	204.21	869	869	C7H14
42	Cyclohexane	206.79	918	920	C6H12
43	Pentane, 2,2,3-trimethyl-	208.35	658	679	C8H18
44	Hexane, 2-methyl-	212.13	872	874	C7H16
45	Pentane, 2,3-dimethyl-	214.47	938	938	C7H16
46	Cyclopentane, 1,1-dimethyl-	217.93	897	900	C7H14
47	Hexane, 3-methyl-	220.35	872	876	C7H16
48	5-Methyl-2-hexene,c&t	222.25	885	889	C7H14
49	Cyclopentane, 1,3-dimethyl-	226.73	914	921	C7H14
50	Pentane, 3-ethyl-	228.63	727	755	C7H16
51	Cyclopentane, 1,3-dimethyl-	229.41	913	927	C7H14
52	Cyclopentane, 1,2-dimethyl-, trans-	231.77	893	893	C7H14
53	3-Methyl-3-hexene,c&t	235.65	935	954	C7H14
54	3-Heptene	238.27	918	951	C7H14
55	Heptane	241.77	939	942	C7H16
56	3-Methyl-3-hexene,c&t	242.79	912	941	C7H14
57	2-Heptene	244.63	825	832	C7H14
58	3-Methyl-3-hexene,c&t	246.93	909	926	C7H14
59	1-Pentene, 2,3-dimethyl-	249.53	907	928	C7H14
60	2,3-Dimethyl-1,4-pentadiene	252.31	854	871	C7H12
61	2-Heptene	252.75	909	911	C7H14
62	2-Pentene, 3,4-dimethyl-, (Z)-	253.85	909	914	C7H14
63	2-Hexene, 5,5-dimethyl-, (Z)-	257.35	711	825	C8H16
64	Hexane, 2,2-dimethyl-	262.51	847	848	C8H18
65	Cyclohexane, methyl-	263.79	878	878	C7H14
66	Cyclopentane, 1,1,3-trimethyl-	265.71	864	876	C8H16
67	Hexane, 2,5-dimethyl-	272.15	933	944	C8H18
68	Hexane, 2,4-dimethyl-	274.63	890	897	C8H18
69	3,4-Dimethyl-2-hexene (c,t)	278.97	684	765	C8H16
70	Hexane, 3,3-dimethyl-	283.03	888	890	C8H18
71	3-Ethyl-4-methyl-2-pentene	285.39	727	832	C8H16
72	Cyclopentane, 1,2,3-trimethyl-, (1à,2à,3á)-	290.29	852	852	C8H16
73	1,2-Hexadiene, 5-methyl-	292.85	670	735	C7H12
74	1-Heptene, 3-methoxy-	293.81	465	622	C8H16O
75	Toluene	303.55	848	854	C7H8
76	Hexane, 2,3-dimethyl-	303.99	886	887	C8H18
77	Cyclopentane, 1,2,4-trimethyl-, (1à,2á,4à)-	304.49	692	707	C8H16
78	Pentane, 3-ethyl-2-methyl-	305.35	893	894	C8H18
79	Heptane, 2-methyl-	307.95	876	882	C8H18
80	Heptane, 4-methyl-	309.53	886	887	C8H18
81	Butane, 2,2,3-trimethyl-	312.41	873	877	C7H16
82	Heptane, 3-methyl-	315.89	879	891	C8H18
83	Hexane, 3-ethyl-	317.11	887	888	C8H18
84	Cyclopropane, 1,1-dimethyl-	317.67	750	829	C5H10
85	Cyclopentane, 1,1,3,4-tetramethyl-, trans-	319.95	773	805	C9H18
86	1,3-Dimethyl-cyclohexane,c&t	321.57	861	907	C8H16
87	Cyclopentane, 1,2,3-trimethyl-, (1à,2à,3à)-	321.83	895	906	C8H16
88	1,3-Dimethyl-cyclohexane,c&t	323.33	865	917	C8H16
89	Oxetane, 3,3-dimethyl-	325.27	792	826	C5H10O
90	3-Heptene, 4-methyl-	325.87	794	801	C8H16
91	Heptane, 2,2-dimethyl-	326.33	863	863	C9H20
92	5-Methyl-3-heptene	327.05	844	847	C8H16
93	Heptane, 3-methylene-	327.67	816	818	C8H16
94	2,4-Dimethyl hexene-1	328.03	724	739	C8H16
95	Cyclohexane, 1,1-dimethyl-	329.79	808	857	C8H16
96	Cyclopentane, 1-ethyl-3-methyl-, trans-	330.97	864	865	C8H16
97	3-Heptene, 4-methyl-	332.41	816	818	C8H16
98	Cyclopentane, 1-ethyl-3-methyl-	333.33	841	842	C8H16
99	2-Octene	335.07	870	877	C8H16
100	5,5-Dimethyl-1,3-hexadiene	336.45	704	779	C8H14
101	3-Heptene, 3-methyl-	338.05	896	928	C8H16
102	2,3-Dimethyl-1-hexene	339.55	763	769	C8H16
103	1-Pentanol, 2-ethyl-	341.95	785	814	C7H16O
104	Hexane, 2,4-dimethyl-	342.35	917	918	C8H18
105	3-Heptene, 3-methyl-	344.45	858	889	C8H16
106	1à,2á,3à,4á-Tetra-methylcyclopentane	346.39	667	786	C9H18

Peak	Name	RT (sec)	Similarity	Reverse	Formula
107	3-Octene, (E)-	349.13	842	857	C8H16
108	4-Methyl-1,3-heptadiene (c,t)	350.39	878	888	C8H14
109	Hexane, 2,4,4-trimethyl-	352.67	837	838	C9H20
110	2-Octene	354.01	861	865	C8H16
111	Cyclopentane, (1-methylethyl)-	356.01	808	808	C8H16
112	Hexane, 2,3,5-trimethyl-	360.55	863	877	C9H20
113	Butane, 2-cyclopropyl-	362.39	731	765	C7H14
114	Heptane, 2,2-dimethyl-	363.21	913	913	C9H20
115	Cyclopentane, 1-ethyl-3-methyl-, trans-	366.43	855	855	C8H16
116	Heptane, 2,4-dimethyl-	367.37	910	911	C9H20
117	Pentane, 3-ethyl-2,2-dimethyl-	369.71	811	856	C9H20
118	Heptane, 4,4-dimethyl-	371.07	870	871	C9H20
119	Octane, 3,5-dimethyl-	374.11	858	883	C10H22
120	Cyclopentane, propyl-	376.55	779	843	C8H16
121	Cyclopentane, 1-methyl-2-(2-propenyl)-, trans-	379.17	830	861	C9H16
122	Heptane, 2,5-dimethyl-	381.53	915	915	C9H20
123	1-Hexene, 3,5,5-trimethyl-	385.09	830	852	C9H18
124	1à,2á,3à,4á-Tetramethylcyclopentane	389.41	752	760	C9H18
125	Cyclohexane, 1-ethyl-1-methyl-	391.25	796	813	C9H18
126	Ethylbenzene	399.93	875	876	C8H10
127	Hexane, 2,3-dimethyl-	401.15	516	686	C8H18
128	1-Hexene, 2,5,5-trimethyl-	402.55	698	749	C9H18
129	m-Xylene	407.37	838	854	C8H10
130	p-Xylene	410.79	898	945	C8H10
131	3,4-Dimethylheptane (manual)	412.41	590	632	C4H7N3O
132	4-Methyloctane (manual)	413.25	590	632	C4H7N3O
133	p-Xylene	413.45	847	863	C8H10
134	1-Hexene, 3,3,5-trimethyl-	414.93	574	775	C9H18
135	Heptane, 3-ethyl-	418.87	796	844	C9H20
136	Octane, 3-methyl-	420.41	901	901	C9H20
137	o-Xylene	435.99	670	671	C8H10
138	1-Ethyl-3-methylcyclohexane (c,t)	442.19	757	795	C9H18
139	1-Heptene, 3-methyl-	442.91	785	802	C8H16
140	2-Methyl-2-octene	445.11	798	817	C9H18
141	Cyclopentane, 1,3-dimethyl-2-(1-methylethenyl)-, (1à,2à,3á)-	446.05	731	757	C10H18
142	Nonane	448.59	897	897	C9H20
143	2-Furanol, tetrahydro-2-methyl-	450.39	785	804	C5H10O2
144	2-Nonene, (E)-	450.79	799	799	C9H18
145	Butane, 2-cyclopropyl-	452.99	772	874	C7H14
146	Cyclohexane, 1-ethyl-2-methyl-, cis-	459.33	854	854	C9H18
147	Isooctane, (ethenyloxy)-	463.35	763	786	C10H20O
148	Isopropylbenzene	465.13	893	894	C9H12
149	2-Octenal, (E)-	467.17	536	749	C8H14O
150	Heptane, 3-methyl-	467.85	844	865	C8H18
151	Hexane, 3-ethyl-4-methyl-	474.43	880	881	C9H20
152	Pentane, 2,2,3,3-tetramethyl-	475.87	785	785	C9H20
153	Octane, 2,7-dimethyl-	478.39	791	793	C10H22
154	Cyclohexane, propyl-	480.77	783	792	C9H18
155	Benzene, 2-propenyl-	482.25	722	724	C9H10
156	Nonane, 3-methyl-	483.45	863	863	C10H22

Peak	Name	RT (sec)	Similarity	Reverse	Formula
157	Heptane, 3,3,5-trimethyl-	486.01	832	832	C10H22
158	Octane, 3,6-dimethyl-	489.45	838	845	C10H22
159	Benzene, propyl-	493.65	871	872	C9H12
160	Benzene, 1-ethyl-3-methyl-	501.47	867	868	C9H12
161	Benzene, 1-ethyl-4-methyl-	503.15	868	868	C9H12
162	Benzene, 1,3,5-trimethyl-	506.49	885	897	C9H12
163	Benzene, 1,2,3-trimethyl-	507.37	924	925	C9H12
164	Nonane, 2-methyl-	509.97	869	869	C10H22
165	Octane, 3-ethyl-	513.13	860	870	C10H22
166	Benzene, 1-ethyl-2-methyl-	515.37	836	846	C9H12
167	1,2,4-Trimethylbenzene	516.35	881	894	C9H12
168	Benzene, 1-propenyl-, (E)-	522.27	825	843	C9H10
169	Benzene, 1,2,3-trimethyl-	529.77	905	906	C9H12
170	Benzene, 1,2,3-trimethyl-	530.93	901	903	C9H12
171	Decane	537.65	870	878	C10H22
172	Isobutylbenzene	539.45	858	862	C10H14
173	sec-Butylbenzene	541.61	889	905	C10H14
174	Benzene, 1-methyl-4-(1-methylethyl)-	548.95	830	830	C10H14
175	Benzene, 1,2,3-trimethyl-	550.77	918	920	C9H12
176	Benzene, 1,2-diethyl-	551.11	826	838	C10H14
177	Indane	559.35	877	889	C9H10
178	Benzene, 1-methyl-2-(1-methylethyl)-	560.57	850	866	C10H14
179	Indene	563.31	850	859	C9H8
180	Benzene, 1,3-diethyl-	567.59	868	871	C10H14
181	Benzene, 1-methyl-3-propyl-	569.83	888	888	C10H14
182	Benzene, 1-methyl-4-propyl-	572.79	869	869	C10H14
183	Benzene, butyl-	573.55	826	835	C10H14
184	Benzene, 4-ethyl-1,2-dimethyl-	574.07	885	885	C10H14
185	Benzene, 1,4-diethyl-	576.99	836	840	C10H14
186	Benzene, 1-methyl-2-propyl-	581.21	850	854	C10H14
187	Benzene, 2-ethyl-1,4-dimethyl-	587.55	882	882	C10H14
188	Benzene, 1-ethyl-2,4-dimethyl-	589.07	866	866	C10H14
189	Benzene, 1-butenyl-, (E)-	591.21	909	924	C10H12
190	Benzene, 4-ethyl-1,2-dimethyl-	593.19	884	884	C10H14
191	2,3-Dihydro-1-methylindene	594.73	891	927	C10H12
192	Benzene, 1-methyl-2-(1-methylethyl)-	597.51	889	889	C10H14
193	Benzene, 1-methyl-4-(2-methylpropyl)-	603.79	842	850	C11H16
194	Benzene, 1-ethyl-4-(1-methylethyl)-	604.01	775	838	C11H16
195	Benzene, (1,1-dimethylpropyl)-	605.07	846	848	C11H16
196	Undecane	605.67	805	838	C11H24
197	Benzene, 1-methyl-2-(1-methylethyl)-	606.55	881	881	C10H14
198	Benzene, (1-methylbutyl)-	608.13	878	896	C11H16
199	Benzene, (1,1-dimethylpropyl)-	609.45	760	760	C11H16
200	Benzene, 2,4-dimethyl-1-(1-methylethyl)-	610.53	859	877	C11H16
201	Benzene, 1,2,4,5-tetramethyl-	614.15	898	898	C10H14

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Peak	Name	RT (sec)	Similarity	Reverse	Formula
202	Benzene, 1,2,3,5-tetramethyl-	616.69	876	877	C10H14
203	Benzene, (2-methyl-1-propenyl)-	618.55	795	882	C10H12
204	Benzene, (1,1-dimethylpropyl)-	624.45	848	849	C11H16
205	Benzene, 2,4-diethyl-1-methyl-	626.71	915	923	C11H16
206	Indan, 1-methyl-	627.71	898	898	C10H12
207	Benzene, 1,3-diethyl-5-methyl-	628.61	850	859	C11H16
208	Benzene, (1-ethylpropyl)-	630.51	783	803	C11H16
209	Benzene, 1-butynyl-	632.61	907	913	C10H10
210	Benzene, 1-methyl-4-(2-methylpropyl)-	633.45	837	838	C11H16
211	Benzene, (2-methyl-1-propenyl)-	634.19	908	924	C10H12
212	Benzene, 1,2,3,4-tetramethyl-	635.93	878	879	C10H14
213	Benzene, (1-methylbutyl)-	637.07	795	817	C11H16
214	Benzene, (1,1-dimethylpropyl)-	639.09	865	869	C11H16
215	Benzene, 2,4-dimethyl-1-(1-methylethyl)-	639.37	868	875	C11H16
216	Benzene, (1,1-dimethylpropyl)-	641.91	843	845	C11H16
217	Benzene, 2,4-dimethyl-1-(1-methylethyl)-	642.63	847	855	C11H16
218	Benzene, 1-methyl-4-(2-methylpropyl)-	642.95	860	861	C11H16
219	Benzene, (1,1-dimethylpropyl)-	646.61	858	862	C11H16
220	Naphthalene	653.21	866	870	C10H8
221	Benzene, 1-ethyl-4-(1-methylethyl)-	654.09	843	876	C11H16
222	1H-Indene, 2,3-dihydro-1,6-dimethyl-	656.53	792	860	C11H14
223	Benzene, (1,1-dimethylpropyl)-	657.57	829	830	C11H16
224	Benzene, 2,4-dimethyl-1-(1-methylethyl)-	659.81	918	936	C11H16
225	Benzene, 2,4-diethyl-1-methyl-	660.83	893	914	C11H16
226	1H-Indene, 2,3-dihydro-4,7-dimethyl-	661.01	704	715	C11H14
227	Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	664.15	628	805	C12H18
228	Benzene, 2,4-dimethyl-1-(1-methylethyl)-	665.67	910	926	C11H16
229	Benzene, (1,1-dimethylbutyl)-	668.73	740	748	C12H18
230	Benzene, 1-ethyl-4-(1-methylethyl)-	671.63	871	886	C11H16
231	Benzene, 1,4-dipropyl-	673.05	796	802	C12H18
232	Benzene, (1,1-dimethylbutyl)-	673.51	742	781	C12H18
233	Naphthalene, 1,2,3,4-tetrahydro-1-methyl-	679.21	763	768	C11H14
234	Benzene, 1-ethyl-4-(1-methylethyl)-	680.17	851	862	C11H16
235	Benzene, (1-ethyl-2-propenyl)-	680.69	792	800	C11H14
236	Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	682.09	601	722	C12H18
237	Benzene, 2,4-dimethyl-1-(1-methylpropyl)-	683.67	753	767	C12H18
238	Benzene, 2,4-dimethyl-1-(1-methylpropyl)-	685.91	768	771	C12H18
239	Benzene, 1-(1-ethylpropyl)-4-methyl-	688.33	758	759	C12H18
240	1H-Indene, 2,3-dihydro-1,2-dimethyl-	688.81	877	877	C11H14
241	Benzene, 1-(1-ethylpropyl)-4-methyl-	689.31	647	647	C12H18
242	Benzene, (1,1-dimethylbutyl)-	691.01	703	718	C12H18
243	1H-Indene, 2,3-dihydro-1,3-dimethyl-	696.25	852	852	C11H14
244	Benzene, 2-ethenyl-1,3,5-trimethyl-	698.01	821	844	C11H14
245	Benzene, 2,4-dimethyl-1-(1-methylethyl)-	704.93	895	911	C11H16
246	1H-Indene, 2,3-dihydro-1,2-dimethyl-	705.81	866	881	C11H14
247	Benzene, 2,4-dimethyl-1-(1-methylpropyl)-	709.25	781	784	C12H18
248	Naphthalene, 2-methyl-	711.61	831	832	C11H10
249	Naphthalene, 1-methyl-	719.75	843	845	C11H10
250	Biphenyl	747.31	861	867	C12H10
251	Diphenylmethane	756.23	794	794	C13H12
252	Naphthalene, 2-ethyl-	757.13	891	907	C12H12
253	Naphthalene, 1-ethyl-	758.29	853	853	C12H12
254	Naphthalene, 2,6-dimethyl-	762.33	936	945	C12H12
255	Naphthalene, 1,7-dimethyl-	762.93	924	932	C12H12
256	1H-Indene, 2,3-dihydro-1,5,7-trimethyl-	767.09	783	813	C12H16
257	Naphthalene, 1,4-dimethyl-	768.87	922	940	C12H12
258	Naphthalene, 1,8-dimethyl-	770.63	903	912	C12H12
259	Naphthalene, 1,3-dimethyl-	777.85	880	880	C12H12
260	Naphthalene, 2,3-dimethyl-	779.07	843	843	C12H12
261	Naphthalene, 1,4-dimethyl-	784.45	890	895	C12H12
262	1,1'-Biphenyl, 4-methyl-	791.95	921	943	C13H12
263	1,1'-Biphenyl, 2-methyl-	796.25	870	870	C13H12
264	Naphthalene, 1,3,6-trimethyl-	799.71	754	796	C13H14
265	1,1'-Biphenyl, 2,3'-dimethyl-	800.51	779	779	C14H14
266	Naphthalene, 2-(1-methylethyl)-	801.15	789	792	C13H14
267	Naphthalene, 1,4,5-trimethyl-	803.83	836	855	C13H14
268	Naphthalene, 1,4,6-trimethyl-	805.79	753	786	C13H14
269	1,1'-Biphenyl, 2-ethyl-	806.17	736	785	C14H14
270	Benzene, 1-methyl-2-(phenylmethyl)-	810.23	711	716	C14H14
271	Naphthalene, 2-(1-methylethyl)-	811.01	858	873	C13H14
272	2,2'-Dimethylbiphenyl	812.19	773	783	C14H14
273	Naphthalene, 1,4,6-trimethyl-	812.59	906	907	C13H14
274	Naphthalene, 1,4,5-trimethyl-	815.05	892	909	C13H14
275	Naphthalene, 1,4,5-trimethyl-	821.33	890	899	C13H14
276	Naphthalene, 1,4,5-trimethyl-	823.23	874	878	C13H14
277	2,2'-Dimethylbiphenyl	830.93	730	736	C14H14
278	4,4'-Dimethylbiphenyl	832.39	858	880	C14H14
279	Naphthalene, 1,4,5-trimethyl-	835.05	874	879	C13H14
280	Benzene, 1,1'-ethylidenebis-	835.55	745	745	C14H14
281	Fluorene	836.09	745	827	C13H10
282	3,3'-Dimethylbiphenyl	837.27	869	879	C14H14
283	Benzene, 1,1'-methylenebis[4-methyl-	838.95	771	825	C15H16
284	Naphthalene, 1,2(or 2,3)-diethyl-	840.49	583	594	C14H16

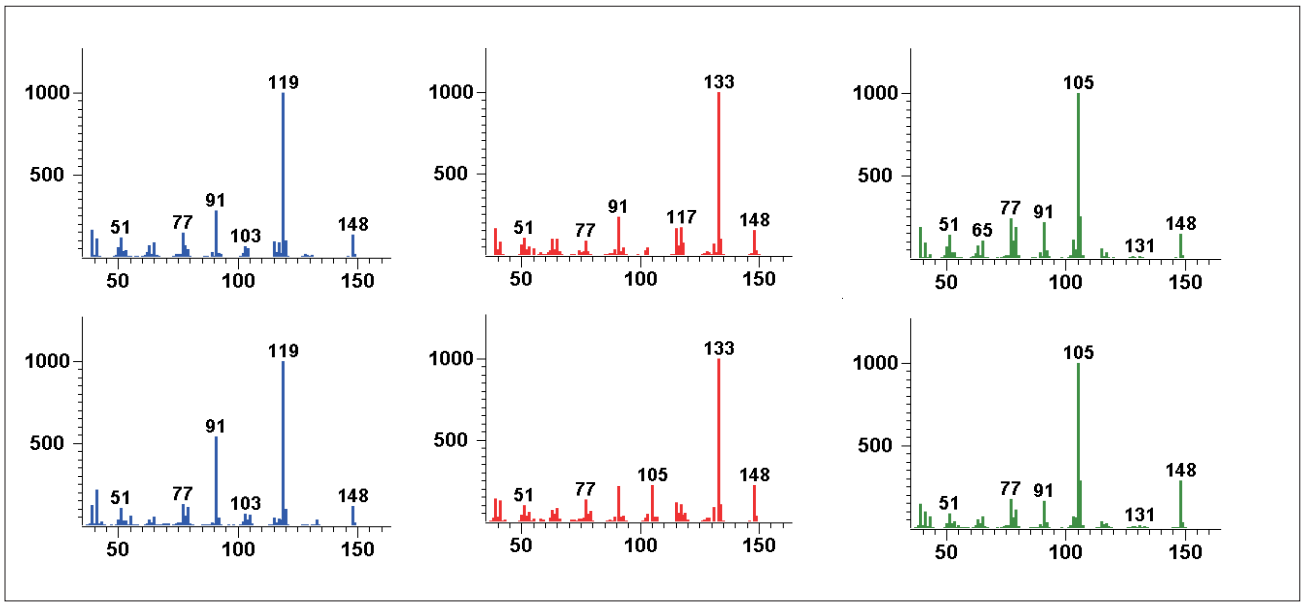

Figure 3. Mass spectra for coeluting C11 Benzene isomers as determined by the Pegasus II GC-TOFMS Deconvolution algorithm.

Top: Pegasus II spectrum. Bottom: NIST Library spectrum. Left: Peak 216; 1,1-dimethylpropyl-benzene; Similarity 843; Reverse Similarity 845. Center: Peak 217; 2,4-dimethyl-1-(1-methylethyl)-benzene; Similarity 847; Reverse Similarity 855. Right: Peak 218; 1-methyl-4-(2-methylpropyl)-benzene; Similarity 860; Reverse Similarity 861.

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 a 284 component Petroleum Refinery Reformate Standard in only 14 minutes using the Pegasus II GC-TOFMS. This represents a 10 fold decrease in data acquistion 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.

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