

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020123\
 Data File : VY012448.D
 Acq On : 01 Feb 2023 17:36
 Operator : KP/MD
 Sample : 01390-04
 Misc : 5.03g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 STOCKPILE-2

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y011623S.M

Title : SW846 8260

Signal : TIC: VY012448.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.327	81	83	87	rVB2	282	357	1.63%	0.187%
2	2.375	89	91	93	rBV3	389	424	1.93%	0.222%
3	2.497	109	111	114	rVB2	333	377	1.72%	0.198%
4	2.534	114	117	118	rBV	299	250	1.14%	0.131%
5	2.607	127	129	132	rVB2	347	405	1.84%	0.212%
6	2.851	166	169	173	rBV3	201	330	1.50%	0.173%
7	3.808	324	326	330	rVB2	216	252	1.15%	0.132%
8	3.942	340	348	355	rBV	2092	5689	25.91%	2.983%
9	4.095	369	373	375	rBV3	418	678	3.09%	0.355%
10	4.113	375	376	380	rVB2	393	409	1.86%	0.214%
11	4.314	406	409	413	rVB2	234	372	1.69%	0.195%
12	4.710	472	474	475	rVV2	378	352	1.60%	0.185%
13	4.723	475	476	479	rVB2	284	266	1.21%	0.139%
14	5.125	536	542	544	rBV	165	346	1.58%	0.181%
15	5.344	575	578	580	rBV2	243	290	1.32%	0.152%
16	5.399	585	587	590	rBV	217	251	1.14%	0.132%
17	5.533	605	609	613	rVB2	137	244	1.11%	0.128%
18	5.582	613	617	620	rVB2	338	496	2.26%	0.260%
19	5.747	642	644	648	rVV	221	339	1.54%	0.178%
20	5.796	651	652	656	rBV2	213	242	1.10%	0.127%
21	6.119	703	705	710	rBV2	248	354	1.61%	0.186%
22	6.716	797	803	805	rVB	244	429	1.95%	0.225%
23	6.923	835	837	838	rVV	283	234	1.07%	0.123%
24	6.966	838	844	853	rVV4	1290	3700	16.85%	1.940%
25	7.045	855	857	862	rVB2	203	273	1.24%	0.143%
26	7.204	882	883	891	rVB	193	354	1.61%	0.186%
27	7.509	930	933	937	rBV2	310	513	2.34%	0.269%
28	7.582	943	945	952	rVB3	193	301	1.37%	0.158%
29	7.716	960	967	969	rBV4	1441	2754	12.54%	1.444%
30	7.789	972	979	987	rVV3	5705	14169	64.54%	7.429%
31	7.874	989	993	995	rVV2	458	668	3.04%	0.350%
32	7.893	995	996	1000	rVV2	272	269	1.23%	0.141%
33	8.002	1007	1014	1022	rVB4	2947	6656	30.32%	3.490%
34	8.088	1022	1028	1030	rBV2	256	341	1.55%	0.179%
35	8.143	1030	1037	1049	rVB2	3985	8913	40.60%	4.673%
36	8.228	1049	1051	1053	rBV	282	255	1.16%	0.134%

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37	8.258	1053	1056	1064	rVB4	392	869	3.96%	0.456%
38	8.551	1098	1104	1109	rBV4	4656	8196	37.33%	4.297%
39	8.691	1120	1127	1136	rBV2	8405	16078	73.24%	8.430%
40	9.130	1193	1199	1201	rBV2	213	267	1.22%	0.140%
41	9.197	1201	1210	1212	rBV4	506	975	4.44%	0.511%
42	10.185	1363	1372	1377	rBV	12547	21953	100.00%	11.511%
43	10.246	1377	1382	1392	rVB	4309	7783	35.45%	4.081%
44	10.368	1398	1402	1406	rBV3	476	562	2.56%	0.295%
45	10.953	1494	1498	1502	rBV4	663	1013	4.61%	0.531%
46	11.221	1539	1542	1545	rVB2	253	264	1.20%	0.138%
47	11.282	1547	1552	1553	rBV3	231	271	1.23%	0.142%
48	11.368	1561	1566	1567	rVV2	214	335	1.53%	0.176%
49	11.490	1580	1586	1595	rVB	11709	19949	90.87%	10.460%
50	11.599	1598	1604	1610	rBV4	1040	1976	9.00%	1.036%
51	11.703	1614	1621	1629	rVB4	4822	10166	46.31%	5.330%
52	11.788	1632	1635	1636	rBV2	256	245	1.12%	0.128%
53	12.032	1670	1675	1683	rVB	1561	2771	12.62%	1.453%
54	12.252	1710	1711	1714	rVB2	360	338	1.54%	0.177%
55	12.483	1744	1749	1759	rVB3	7423	12970	59.08%	6.801%
56	12.569	1759	1763	1765	rVV	264	329	1.50%	0.173%
57	12.678	1776	1781	1783	rBV3	407	601	2.74%	0.315%
58	12.739	1788	1791	1793	rVV2	908	1091	4.97%	0.572%
59	12.776	1795	1797	1798	rVV2	406	355	1.62%	0.186%
60	12.806	1798	1802	1807	rVB3	1674	2468	11.24%	1.294%
61	12.922	1819	1821	1825	rVB2	196	247	1.13%	0.130%
62	12.983	1825	1831	1833	rBV3	376	592	2.70%	0.310%
63	13.123	1849	1854	1859	rBV	1082	1594	7.26%	0.836%
64	13.428	1899	1904	1912	rVB2	5941	9826	44.76%	5.152%
65	13.526	1916	1920	1925	rBV2	428	634	2.89%	0.332%
66	13.629	1935	1937	1940	rVB3	322	394	1.79%	0.207%
67	13.983	1992	1995	1998	rVB3	385	438	2.00%	0.230%
68	14.105	2011	2015	2018	rBV2	200	239	1.09%	0.125%
69	14.349	2050	2055	2058	rBV2	443	695	3.17%	0.364%
70	14.446	2068	2071	2072	rBV2	273	244	1.11%	0.128%
71	14.556	2086	2089	2091	rVB3	274	250	1.14%	0.131%
72	14.581	2091	2093	2096	rVB3	400	327	1.49%	0.171%
73	14.611	2096	2098	2100	rBV2	327	402	1.83%	0.211%
74	14.678	2108	2109	2113	rVB2	229	248	1.13%	0.130%
75	14.721	2113	2116	2118	rVB	457	322	1.47%	0.169%
76	14.739	2118	2119	2121	rBV	418	303	1.38%	0.159%

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77	14.843	2132	2136	2138	rBV4	276	448	2.04%	0.235%
78	14.879	2141	2142	2147	rVB2	385	336	1.53%	0.176%
79	14.946	2151	2153	2155	rVV2	232	252	1.15%	0.132%
80	15.111	2177	2180	2181	rVV2	292	272	1.24%	0.143%
81	15.172	2188	2190	2193	rBV3	239	284	1.29%	0.149%
82	15.227	2197	2199	2201	rBV2	373	274	1.25%	0.144%
83	15.318	2211	2214	2217	rVV2	376	396	1.80%	0.208%
84	15.525	2246	2248	2251	rVB2	307	303	1.38%	0.159%
85	15.623	2259	2264	2267	rVB2	459	853	3.89%	0.447%
86	15.653	2267	2269	2270	rBV	321	241	1.10%	0.126%
87	15.800	2290	2293	2296	rBV3	333	446	2.03%	0.234%
88	15.879	2304	2306	2309	rVB2	268	259	1.18%	0.136%
89	16.099	2341	2342	2346	rVV2	513	455	2.07%	0.239%
90	16.135	2346	2348	2354	rVV4	456	619	2.82%	0.325%
91	16.196	2356	2358	2361	rVV3	330	243	1.11%	0.127%
92	16.263	2366	2369	2371	rVB2	447	482	2.20%	0.253%
93	16.300	2373	2375	2377	rVV3	360	433	1.97%	0.227%
94	16.330	2379	2380	2382	rBV	417	370	1.69%	0.194%
95	16.428	2394	2396	2398	rVB3	342	253	1.15%	0.133%
96	16.446	2398	2399	2403	rBV3	540	505	2.30%	0.265%
97	16.513	2408	2410	2413	rBV3	659	647	2.95%	0.339%
98	16.647	2430	2432	2433	rVB	531	366	1.67%	0.192%
99	16.666	2433	2435	2436	rBV	532	418	1.90%	0.219%
100	16.720	2443	2444	2447	rBV3	316	432	1.97%	0.227%

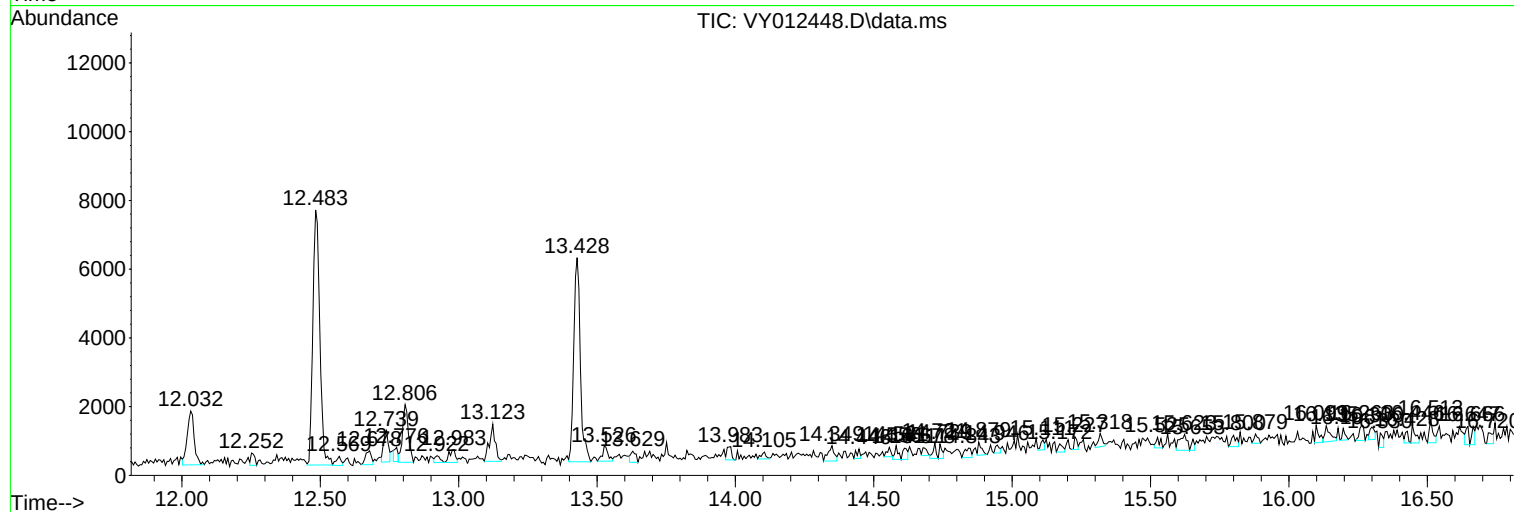
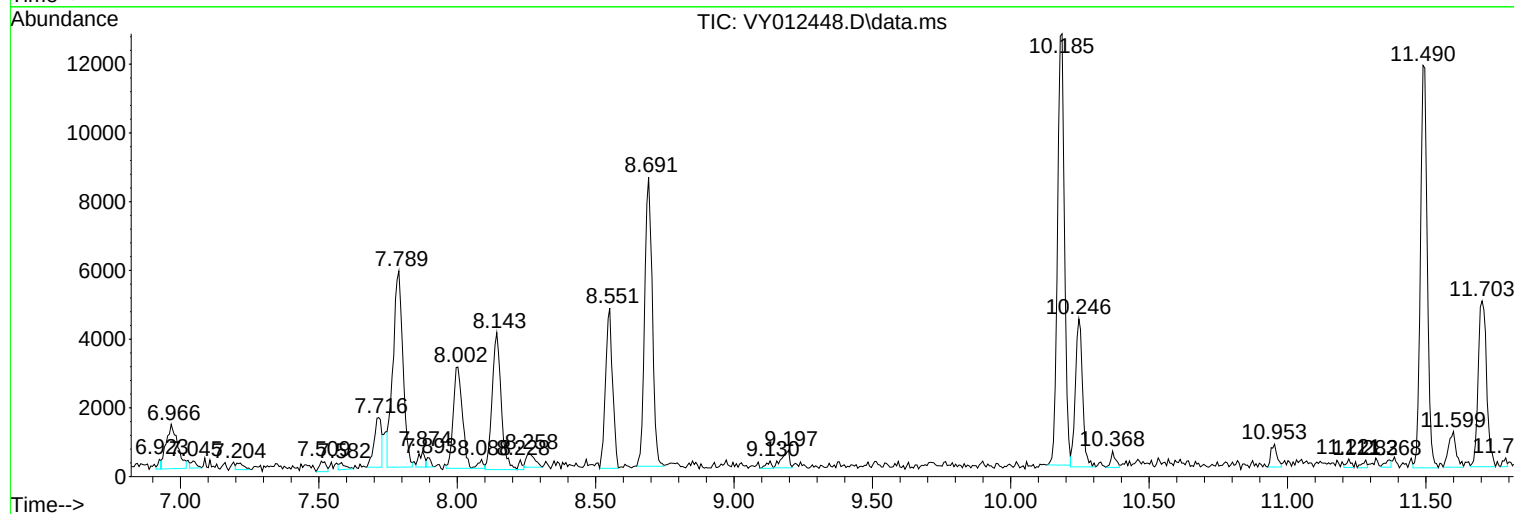
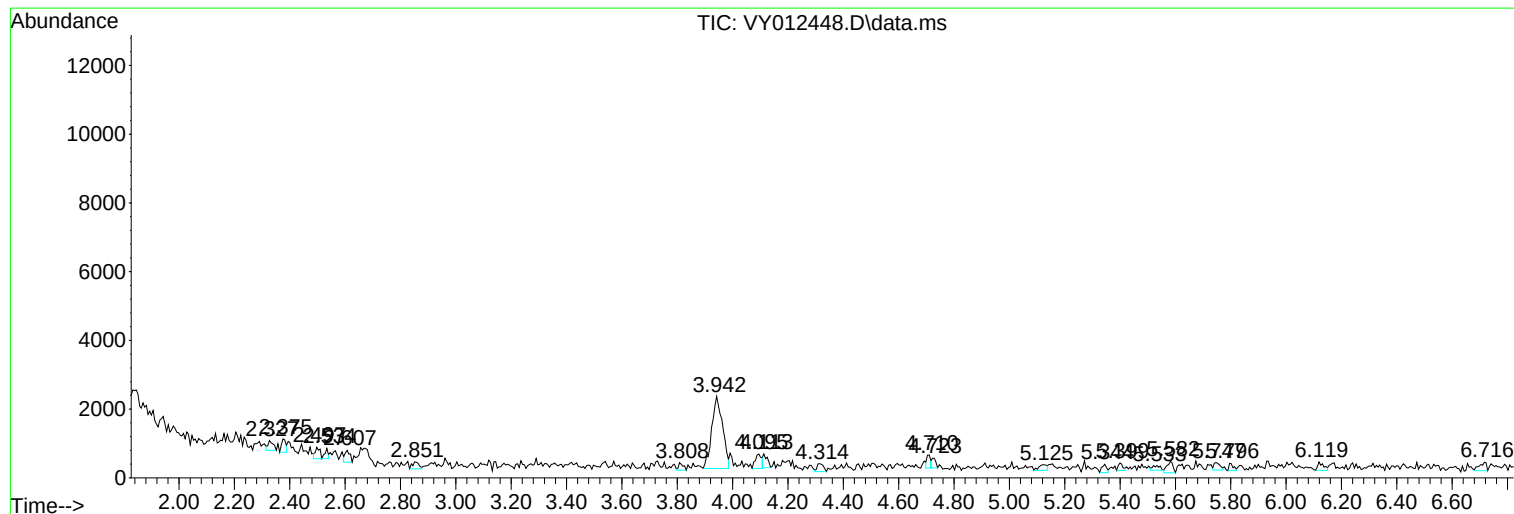
Sum of corrected areas: 190719

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y011623S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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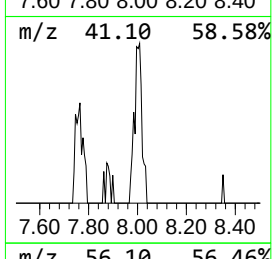
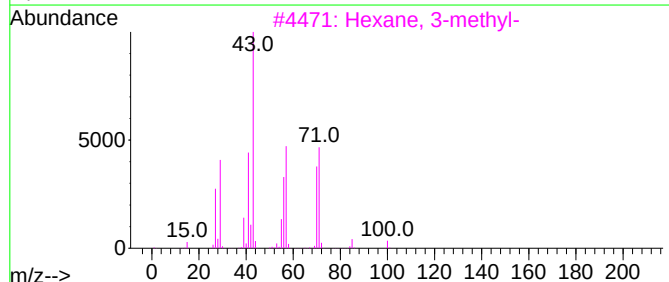
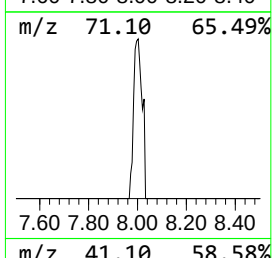
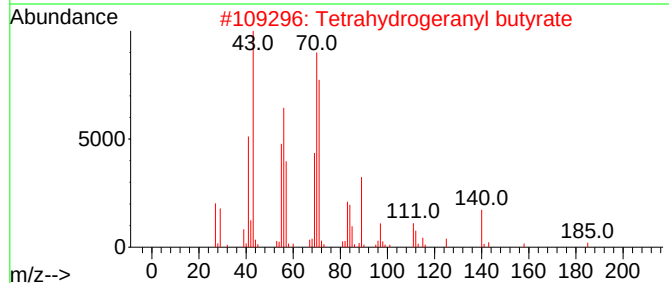
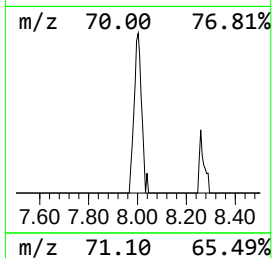
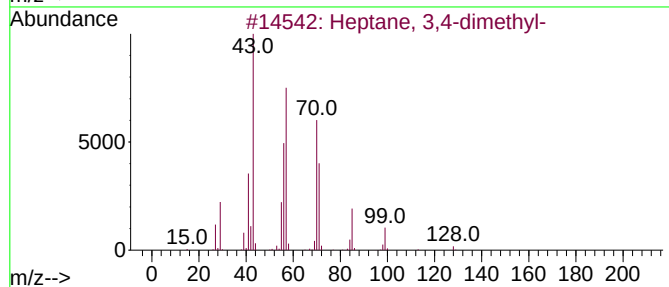
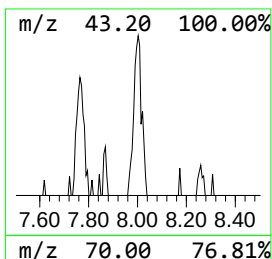
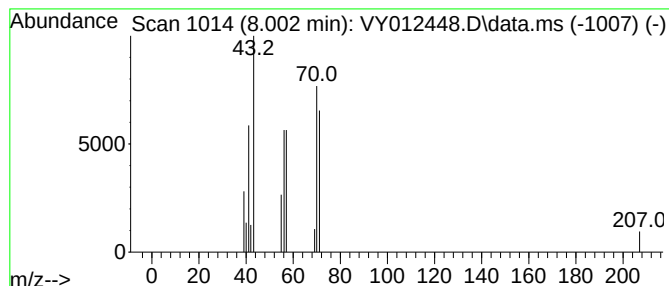
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y011623S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Heptane, 3,4-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.002	23.49 ug/l	6656	Pentafluorobenzene	7.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	64
2			Tetrahydrogeranyl butyrate	228	C14H28O2	1000428-75-4	56
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	53
4			Propanoic acid, 2-methyl-, 3-met...	158	C9H18O2	002050-01-3	42
5			Heptane, 4-methyl-	114	C8H18	000589-53-7	38



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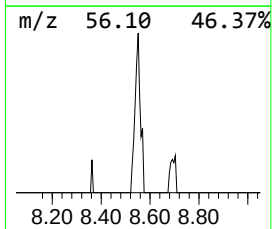
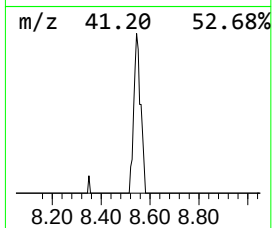
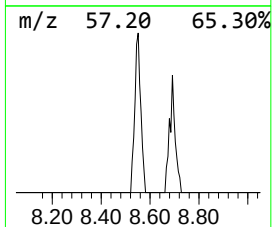
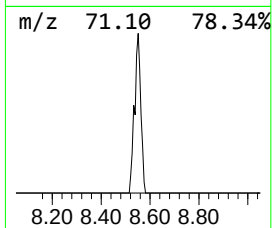
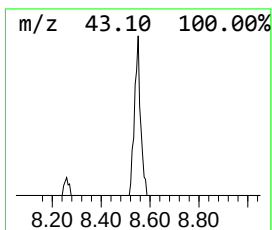
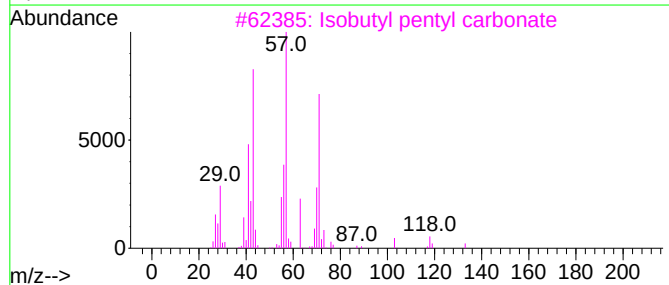
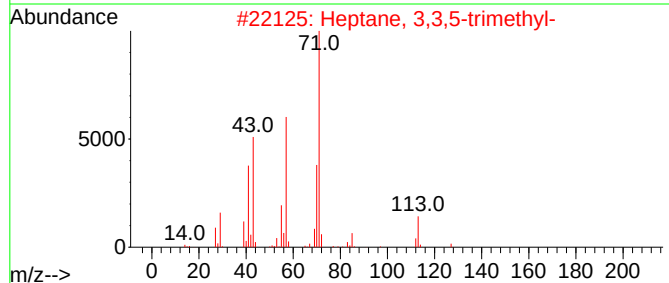
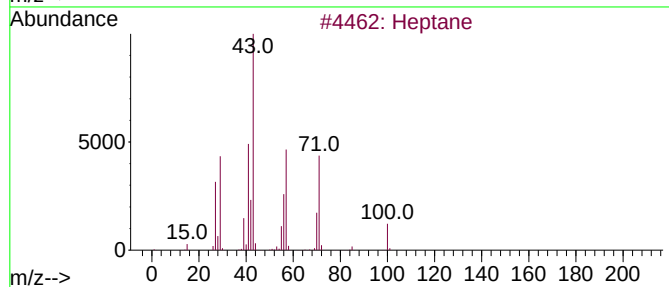
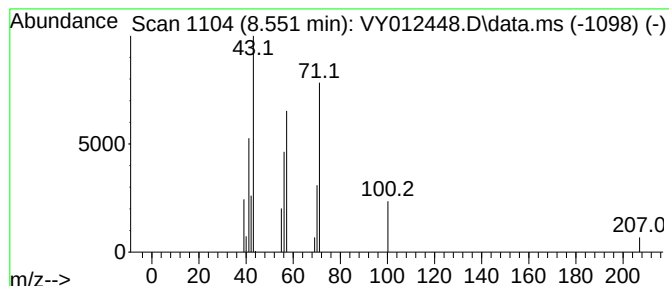
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Peak Number 3 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.551	25.49 ug/l	8196	1,4-Difluorobenzene	8.691

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	90
2			Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	40
3			Isobutyl pentyl carbonate	188	C10H20O3	178442-32-5	39
4			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	39
5			1-Trifluoroacetoxy-2-methylpentane	198	C8H13F3O2	155089-96-6	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Heptane, 3,4-di...	8.002	23.5	ug/l	6656	1	7.795	14169	50.0
Heptane	8.551	25.5	ug/l	8196	2	8.691	16078	50.0