

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012524\
 Data File : VX039954.D
 Acq On : 25 Jan 2024 15:18
 Operator : JC/MD
 Sample : P1218-05
 Misc : 1.12g/10mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 134

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_X\Method\82X011024W.M
 Title : SW846 8260

Signal : TIC: VX039954.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	69	84	85	rBV4	8803	31065	6.01%	0.837%
2	2.940	292	304	312	rBV4	1905	5262	1.02%	0.142%
3	5.391	694	706	719	rBV2	49217	152148	29.46%	4.098%
4	5.544	721	731	750	rVB	94189	273807	53.01%	7.374%
5	5.958	789	799	816	rBV	64243	186321	36.08%	5.018%
6	6.757	921	930	948	rBV	151741	377859	73.16%	10.177%
7	7.214	999	1005	1016	rBV5	1941	6040	1.17%	0.163%
8	8.647	1234	1240	1250	rBV	321034	516475	100.00%	13.910%
9	10.055	1465	1471	1485	rBV	340270	471910	91.37%	12.710%
10	11.085	1634	1640	1651	rBV	263969	364632	70.60%	9.820%
11	11.476	1699	1704	1710	rVB7	3697	6469	1.25%	0.174%
12	12.024	1788	1794	1800	rBV	384029	490253	94.92%	13.204%
13	12.103	1804	1807	1811	rVB3	4708	5423	1.05%	0.146%
14	12.323	1838	1843	1848	rVB7	2327	5169	1.00%	0.139%
15	12.420	1855	1859	1864	rVV	47669	56894	11.02%	1.532%
16	12.469	1864	1867	1873	rVB6	3959	8335	1.61%	0.224%
17	12.549	1873	1880	1882	rBV5	5533	10525	2.04%	0.283%
18	12.585	1882	1886	1890	rVV5	8383	14833	2.87%	0.399%
19	12.683	1898	1902	1906	rBV2	12216	14951	2.89%	0.403%
20	12.762	1913	1915	1920	rBV5	4570	7810	1.51%	0.210%
21	12.817	1921	1924	1929	rVB4	9539	12795	2.48%	0.345%
22	12.896	1929	1937	1942	rBV4	20130	51801	10.03%	1.395%
23	12.945	1942	1945	1947	rVV2	10569	13272	2.57%	0.357%
24	12.975	1947	1950	1954	rVV4	19497	26559	5.14%	0.715%
25	13.042	1957	1961	1964	rVV2	16712	20831	4.03%	0.561%
26	13.085	1966	1968	1974	rVB7	4768	8281	1.60%	0.223%
27	13.158	1974	1980	1984	rBV8	6088	13071	2.53%	0.352%
28	13.207	1985	1988	1991	rVV3	7539	10335	2.00%	0.278%
29	13.268	1993	1998	2001	rVV	78235	105299	20.39%	2.836%
30	13.292	2001	2002	2007	rVV3	26413	30971	6.00%	0.834%
31	13.341	2007	2010	2013	rVV5	7904	9822	1.90%	0.265%
32	13.384	2013	2017	2020	rVV2	21791	29872	5.78%	0.805%
33	13.420	2020	2023	2032	rVB8	18461	43418	8.41%	1.169%
34	13.500	2032	2036	2040	rBV5	7664	11885	2.30%	0.320%
35	13.591	2046	2051	2055	rBV7	8150	14927	2.89%	0.402%
36	13.682	2060	2066	2067	rBV6	7413	13099	2.54%	0.353%

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37	13.798	2082	2085	2088	rBV4	6207	7086	1.37%	0.191%
38	13.841	2088	2092	2100	rVB6	12124	26563	5.14%	0.715%
39	13.920	2100	2105	2111	rBV8	9072	19372	3.75%	0.522%
40	14.036	2121	2124	2127	rVB	20594	21278	4.12%	0.573%
41	14.073	2127	2130	2134	rBV2	8003	10102	1.96%	0.272%
42	14.225	2149	2155	2162	rVB3	19695	37960	7.35%	1.022%
43	14.371	2174	2179	2182	rBV4	6608	9358	1.81%	0.252%
44	14.408	2182	2185	2189	rVV6	5209	9145	1.77%	0.246%
45	14.445	2189	2191	2193	rVV3	7626	8305	1.61%	0.224%
46	14.481	2193	2197	2206	rVB6	13420	28137	5.45%	0.758%
47	14.554	2206	2209	2215	rBV7	3024	6531	1.26%	0.176%
48	14.615	2215	2219	2222	rBV3	13538	20520	3.97%	0.553%
49	14.670	2225	2228	2233	rVB5	7373	11223	2.17%	0.302%
50	14.731	2233	2238	2239	rBV5	5456	7761	1.50%	0.209%
51	14.755	2239	2242	2245	rVB3	7015	7707	1.49%	0.208%
52	14.847	2254	2257	2263	rVB7	4658	6385	1.24%	0.172%
53	14.908	2263	2267	2277	rVB10	3381	10914	2.11%	0.294%
54	15.188	2307	2313	2325	rBV3	18665	34742	6.73%	0.936%
55	15.487	2356	2362	2367	rBV5	3959	7469	1.45%	0.201%

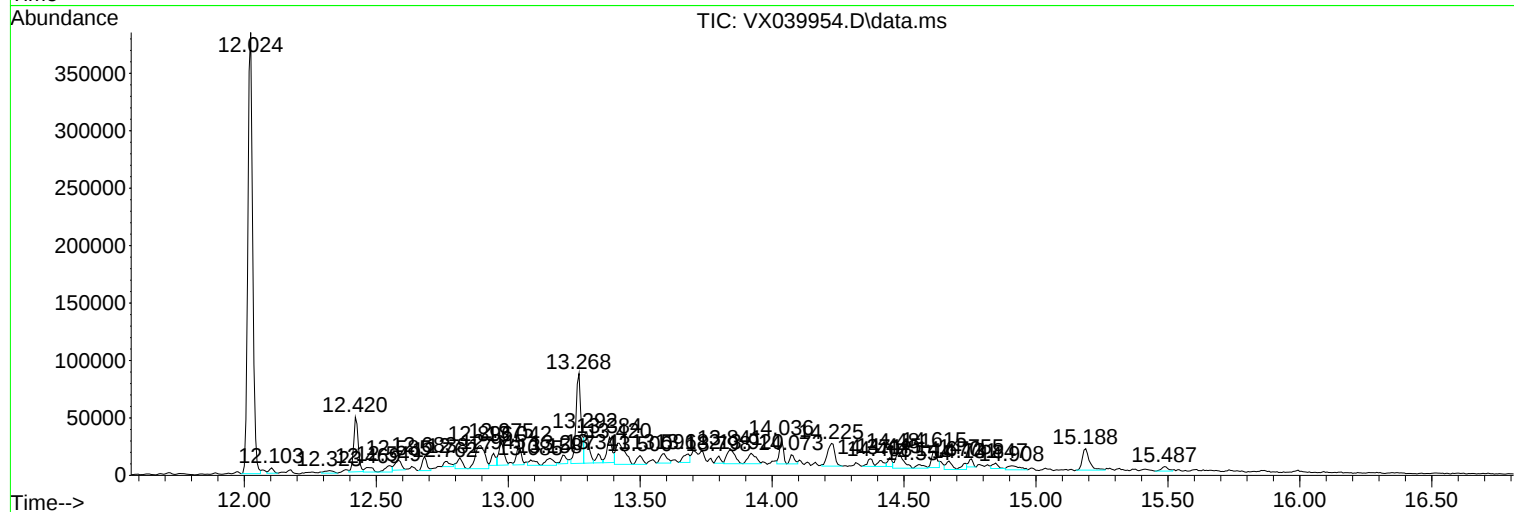
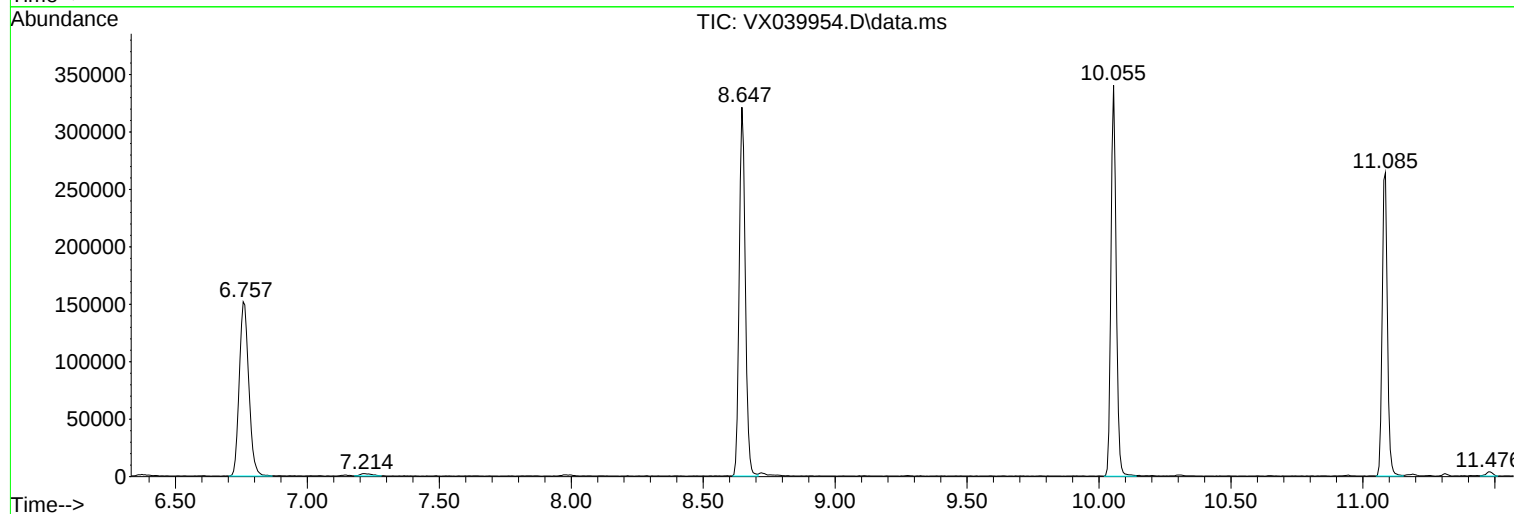
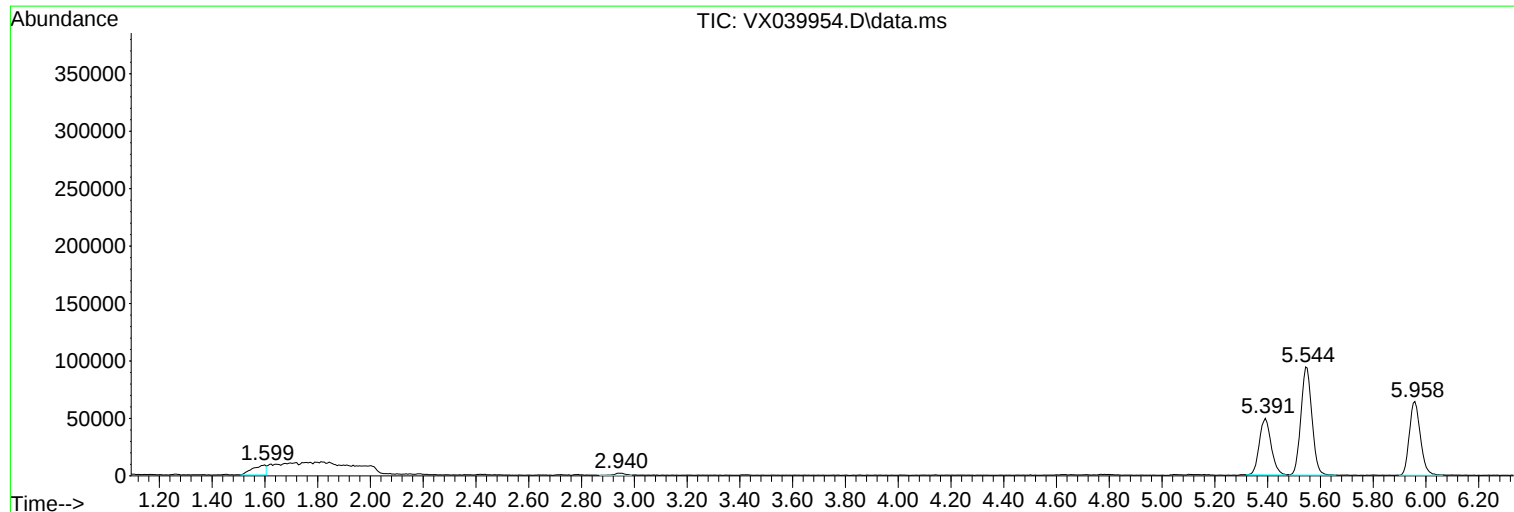
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
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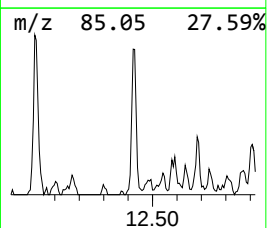
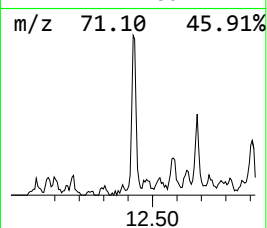
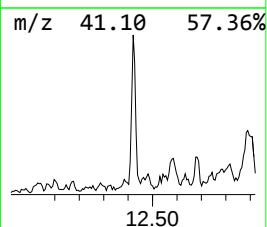
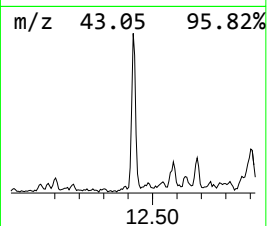
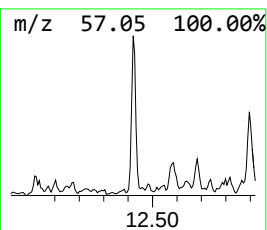
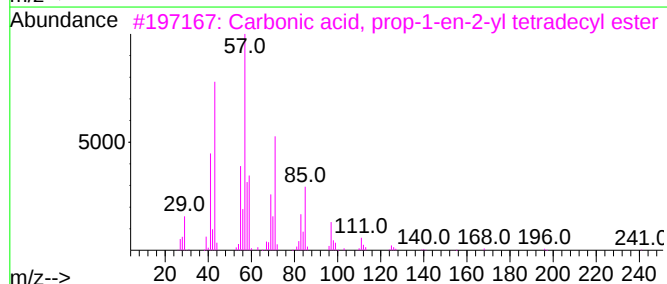
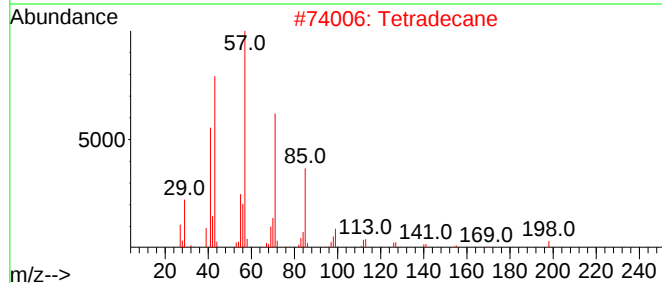
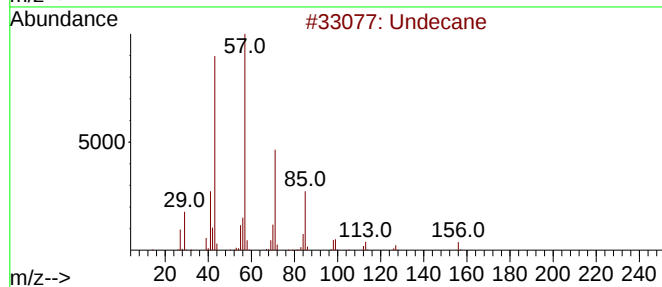
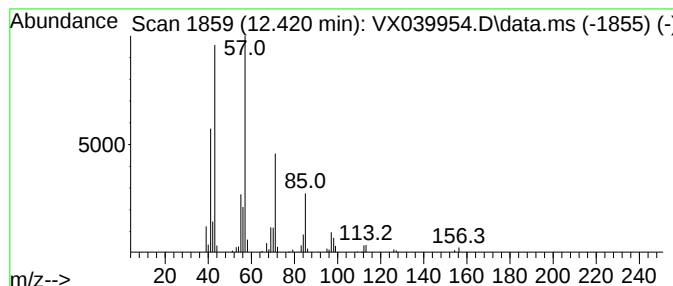
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Undecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	5.80 ug/l	56894	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	87
2	Tetradecane			198	C14H30	000629-59-4	80
3	Carbonic acid, prop-1-en-2-yl te...			298	C18H34O3	1000382-90-9	80
4	Carbonic acid, prop-1-en-2-yl tr...			284	C17H32O3	1000382-90-8	78
5	Tridecane			184	C13H28	000629-50-5	64



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
134

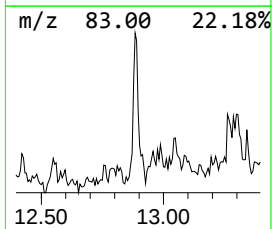
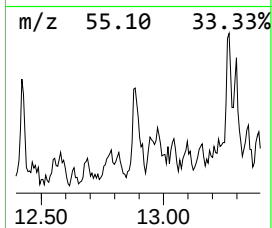
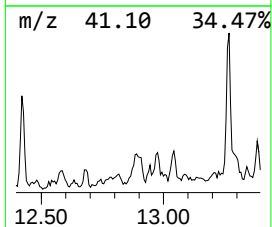
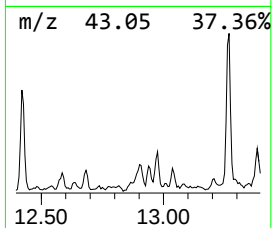
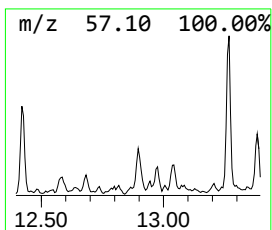
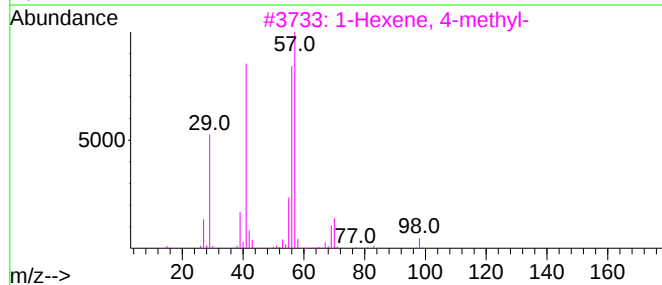
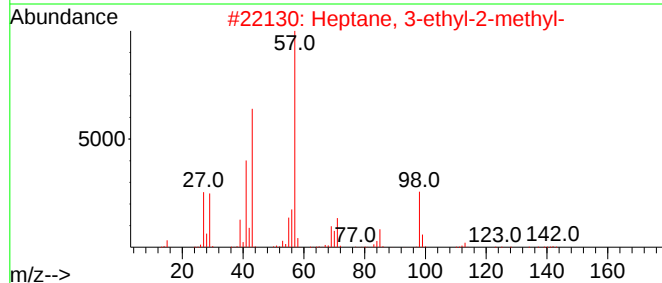
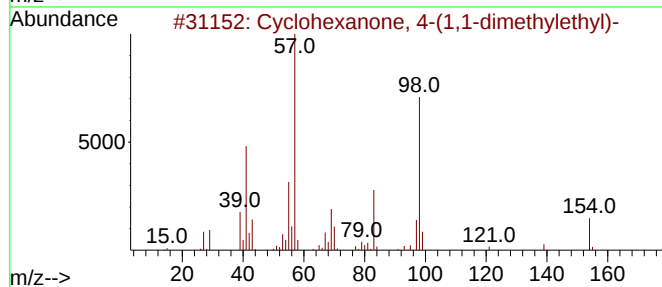
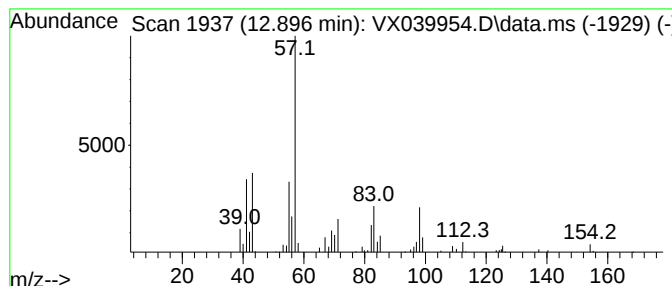
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclohexanone, 4-(1,1-dimet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.896	5.28 ug/l	51801	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 4-(1,1-dimethylet...	154	C10H18O	000098-53-3	50
2			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	38
3			1-Hexene, 4-methyl-	98	C7H14	003769-23-1	35
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	35
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	35



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ALS Vial : 13 Sample Multiplier: 1

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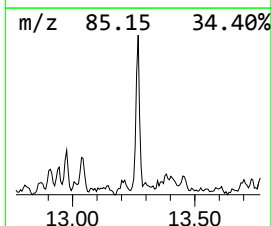
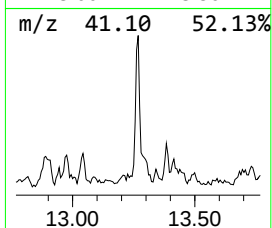
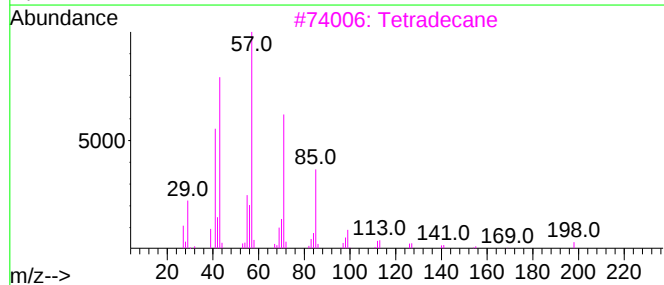
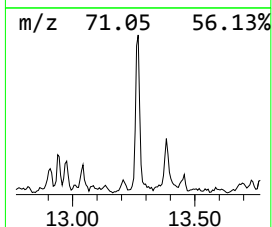
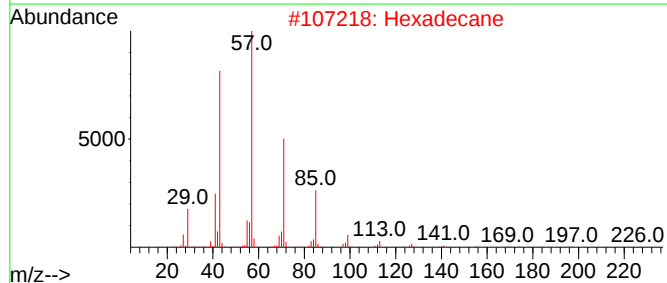
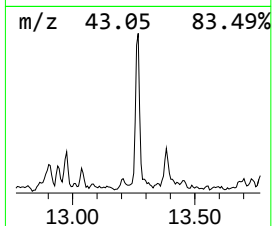
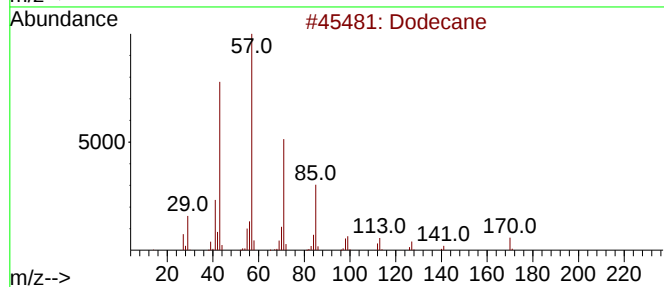
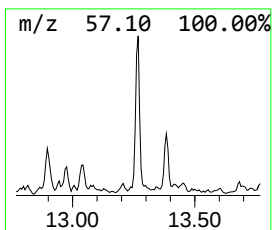
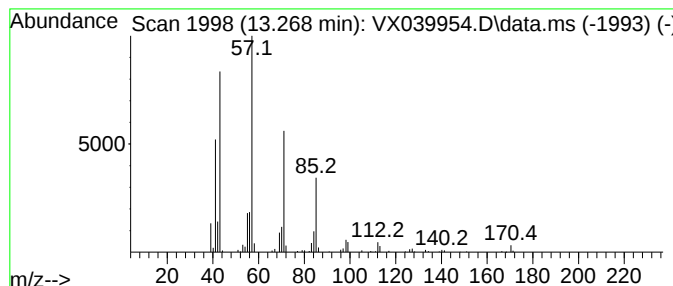
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Dodecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	10.74 ug/l	105299	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	86
2			Hexadecane	226	C16H34	000544-76-3	72
3			Tetradecane	198	C14H30	000629-59-4	72
4			Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	64
5			Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	59



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Undecane	12.421	5.8	ug/l	56894	4	12.024	490253	50.0
Cyclohexanone, ...	12.896	5.3	ug/l	51801	4	12.024	490253	50.0
Dodecane	13.268	10.7	ug/l	105299	4	12.024	490253	50.0