

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
 Data File : VX006092.D
 Acq On : 19 Nov 2018 15:41
 Operator : JC/MD
 Sample : J5951-04
 Misc : 5.02g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FDSB-04(26.5-28.5)

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.721	65	93	94	rBV6	11499	72528	13.11%	1.717%
2	5.507	701	714	726	rBV2	74313	205867	37.20%	4.873%
3	5.659	728	739	754	rVB2	131932	375721	67.90%	8.894%
4	6.067	795	806	824	rBV2	78533	210406	38.02%	4.981%
5	6.854	926	935	960	rBV2	188745	459033	82.96%	10.866%
6	8.713	1233	1240	1254	rBV	350732	553336	100.00%	13.098%
7	10.115	1464	1470	1484	rBV	361376	489702	88.50%	11.592%
8	11.140	1632	1638	1648	rBV	305653	395825	71.53%	9.370%
9	12.079	1787	1792	1798	rBV	430524	525883	95.04%	12.449%
10	12.371	1835	1840	1846	rBV5	3154	6988	1.26%	0.165%
11	12.524	1861	1865	1870	rVB6	3236	5898	1.07%	0.140%
12	12.609	1870	1879	1880	rBV5	3181	6790	1.23%	0.161%
13	12.639	1880	1884	1887	rVV	4776	6395	1.16%	0.151%
14	12.737	1896	1900	1905	rBV2	8897	12806	2.31%	0.303%
15	12.877	1919	1923	1928	rVB7	5624	8106	1.46%	0.192%
16	12.944	1928	1934	1941	rBV4	15340	35703	6.45%	0.845%
17	13.158	1962	1969	1973	rBV8	3726	10085	1.82%	0.239%
18	13.267	1983	1987	1991	rBV2	7188	10414	1.88%	0.247%
19	13.347	1995	2000	2006	rVB4	21817	39403	7.12%	0.933%
20	13.401	2006	2009	2011	rBV2	7454	9340	1.69%	0.221%
21	13.438	2011	2015	2019	rBV	43549	54438	9.84%	1.289%
22	13.566	2030	2036	2039	rBV7	5180	11548	2.09%	0.273%
23	13.639	2045	2048	2050	rBV2	7112	8458	1.53%	0.200%
24	13.731	2059	2063	2065	rBV5	5296	8251	1.49%	0.195%
25	13.761	2065	2068	2070	rBV2	7123	7111	1.29%	0.168%
26	13.859	2080	2084	2087	rBV3	13092	17624	3.19%	0.417%
27	13.901	2087	2091	2097	rVB	57642	71990	13.01%	1.704%
28	13.962	2097	2101	2103	rBV4	11822	18169	3.28%	0.430%
29	14.048	2109	2115	2117	rBV6	7417	14862	2.69%	0.352%
30	14.127	2125	2128	2131	rBV3	12704	17247	3.12%	0.408%
31	14.164	2131	2134	2136	rVV2	13161	18331	3.31%	0.434%
32	14.194	2136	2139	2141	rVV3	14826	17532	3.17%	0.415%
33	14.243	2145	2147	2149	rVV	15689	18209	3.29%	0.431%
34	14.279	2149	2153	2159	rVB4	17802	37054	6.70%	0.877%

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 FDSB-04(26.5-28.5)

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 >
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35	14.474	2183	2185	2188	rBV4	6077	6268	1.13%	0.148%
36	14.541	2193	2196	2199	rVV3	13741	21985	3.97%	0.520%
37	14.572	2199	2201	2205	rVB	15310	18067	3.27%	0.428%
38	14.670	2214	2217	2219	rBV2	49298	55786	10.08%	1.321%
39	14.694	2219	2221	2225	rVV	34600	41358	7.47%	0.979%
40	14.730	2225	2227	2231	rVB4	12993	14406	2.60%	0.341%
41	14.785	2231	2236	2238	rBV4	10405	17346	3.13%	0.411%
42	14.840	2242	2245	2252	rVV2	22330	38963	7.04%	0.922%
43	14.907	2253	2256	2259	rVB2	13062	14718	2.66%	0.348%
44	15.023	2273	2275	2284	rVB9	9720	19739	3.57%	0.467%
45	15.249	2309	2312	2314	rBV2	8346	12281	2.22%	0.291%
46	15.273	2314	2316	2320	rVV2	18992	24076	4.35%	0.570%
47	15.340	2324	2327	2331	rVB	8092	10780	1.95%	0.255%
48	15.444	2340	2344	2348	rBV4	10086	17809	3.22%	0.422%
49	15.493	2348	2352	2356	rVV3	11236	19627	3.55%	0.465%
50	15.547	2357	2361	2368	rVB	20128	35831	6.48%	0.848%
51	15.688	2380	2384	2387	rBV	16813	26935	4.87%	0.638%
52	15.724	2387	2390	2399	rVB	18238	36421	6.58%	0.862%
53	15.919	2415	2422	2432	rVB9	5407	17648	3.19%	0.418%
54	16.438	2505	2507	2515	rVB7	3385	6852	1.24%	0.162%
55	16.694	2545	2549	2554	rVB6	3321	6494	1.17%	0.154%

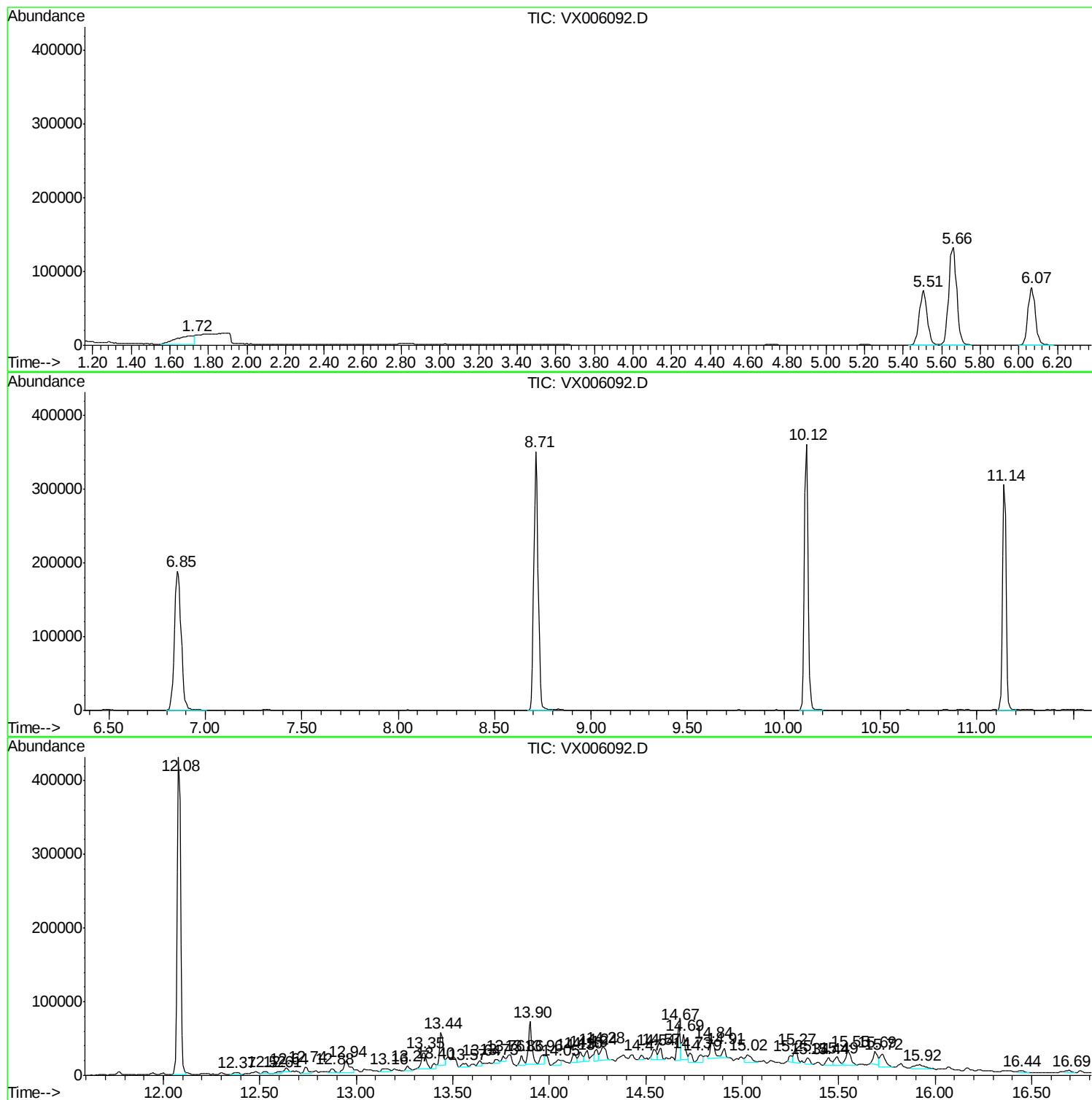
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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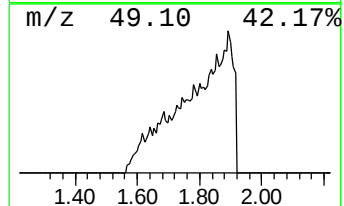
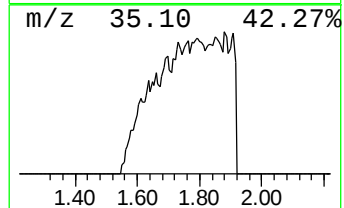
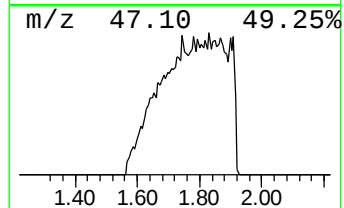
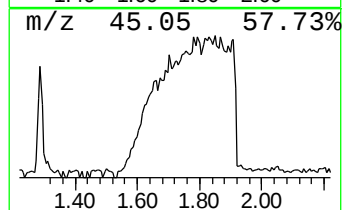
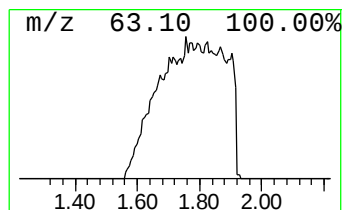
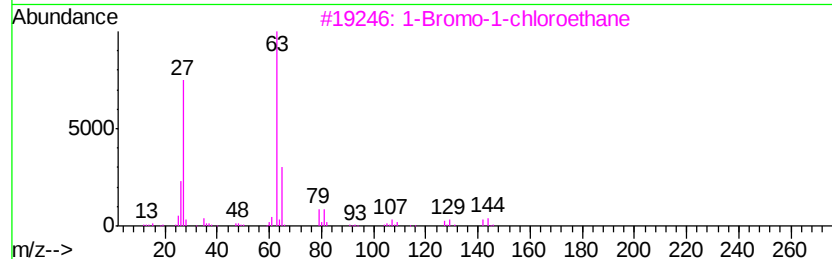
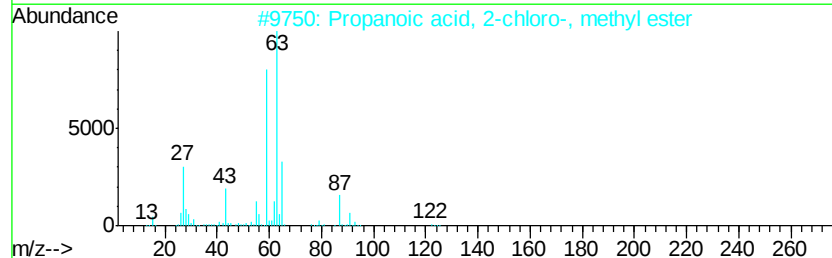
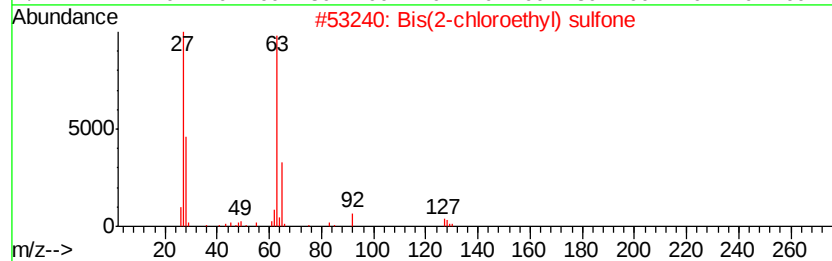
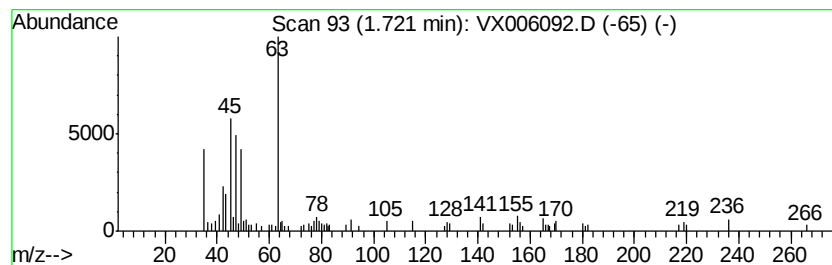
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.72	9.65 ug/l	72528	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bis(2-chloroethyl) sulfone	190	C4H8Cl2O2S	000471-03-4	12
2		Propanoic acid, 2-chloro-, methy...	122	C4H7ClO2	017639-93-9	9
3		1-Bromo-1-chloroethane	142	C2H4BrCl	000593-96-4	9
4		Acetaldehyde, bis(2-chloroethyl)...	186	C6H12Cl2O2	014689-97-5	9
5		2-[2-(2-Chloro-ethoxy)-ethoxy]-p...	216	C10H13ClO3	1000317-46-1	9



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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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FDSB-04(26.5-28.5)

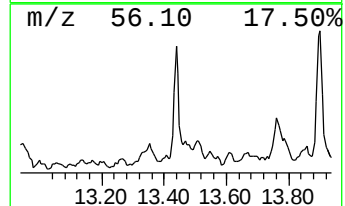
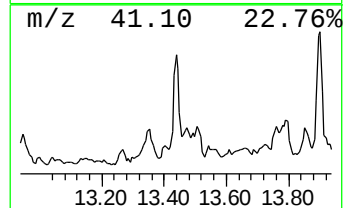
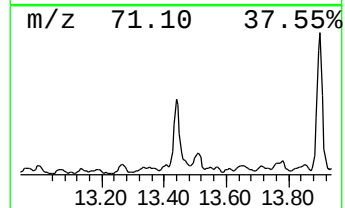
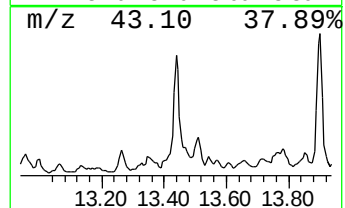
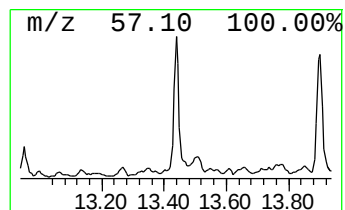
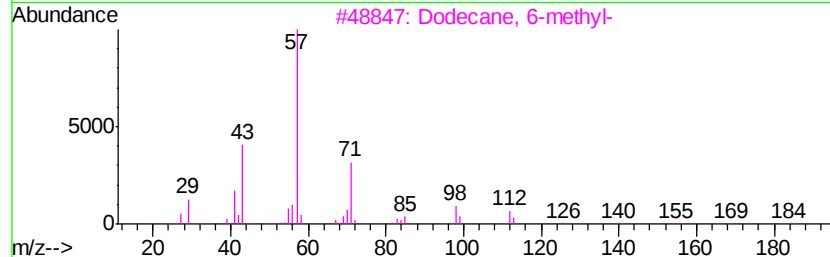
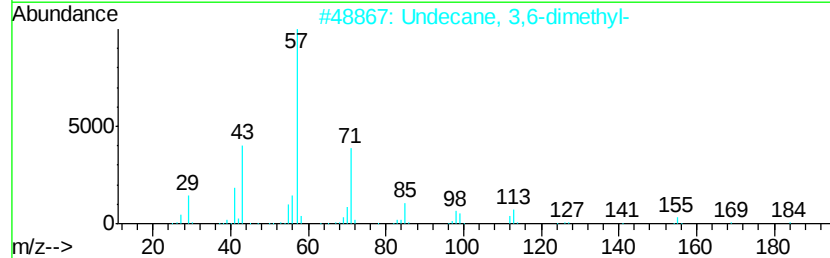
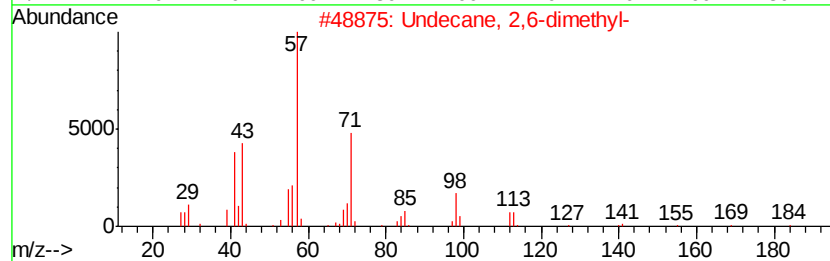
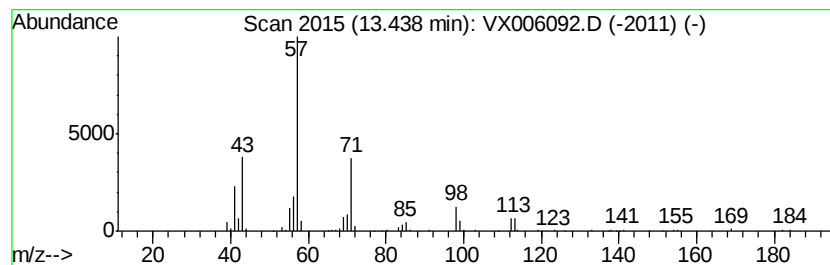
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Undecane, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	5.18 ug/l	54438	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	94
2		Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	91
3		Dodecane, 6-methyl-	184	C13H28	006044-71-9	91
4		Tridecane, 6-methyl-	198	C14H30	013287-21-3	64
5		Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	59



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ALS Vial : 15 Sample Multiplier: 1

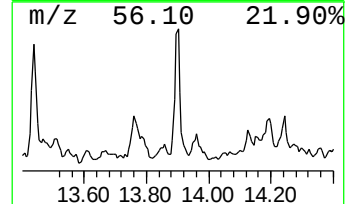
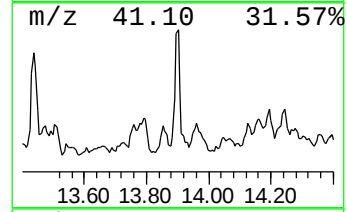
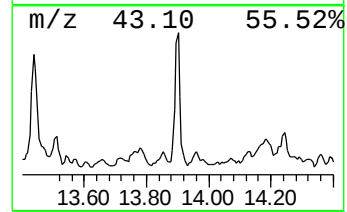
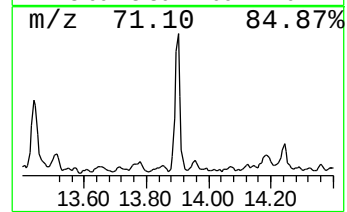
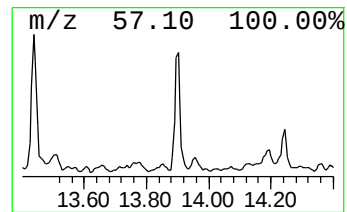
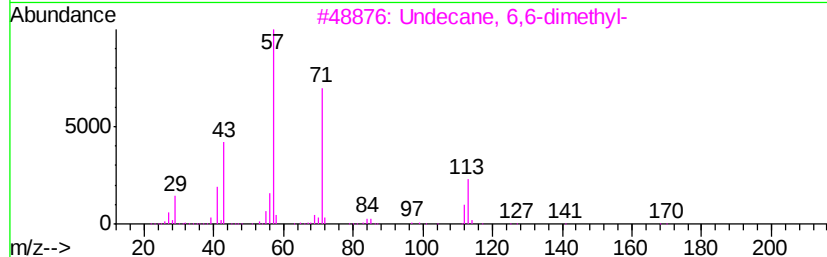
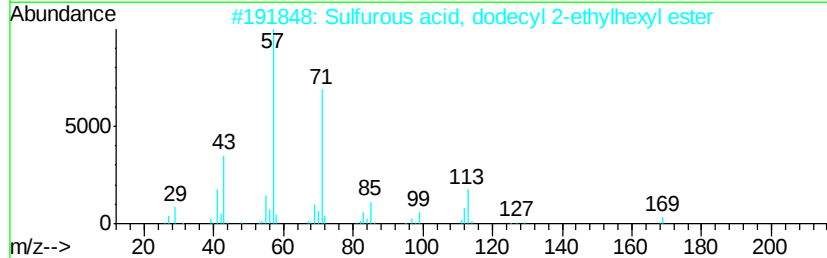
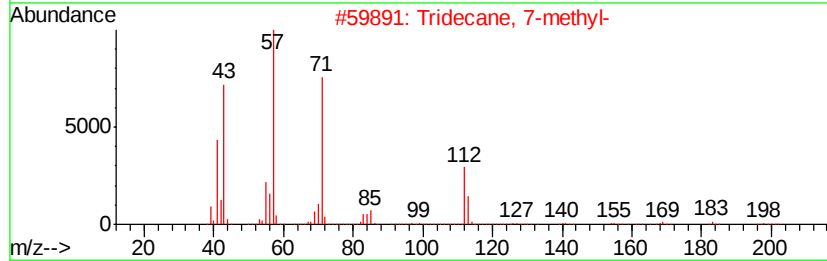
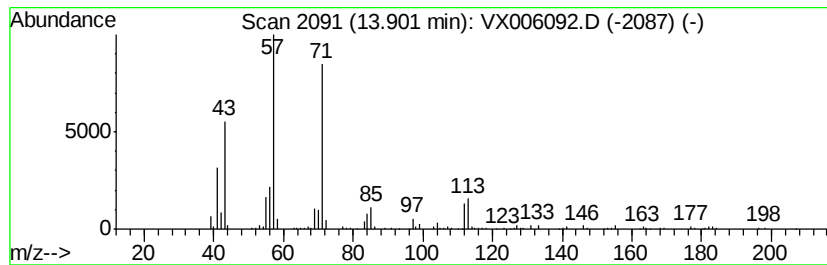
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Peak Number 3 Tridecane, 7-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.90	6.84 ug/l	71990	1,4-Dichlorobenzene-d4		12.08
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 7-methyl-	198	C14H30	026730-14-3	91
2	Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	86
3	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	72
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	64
5	Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	64



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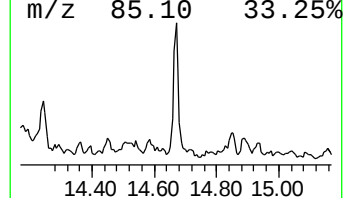
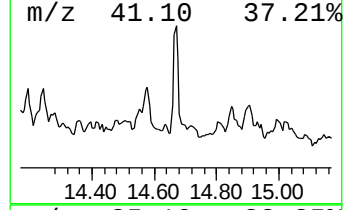
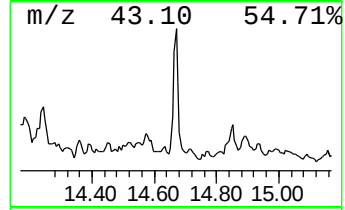
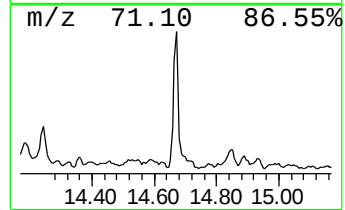
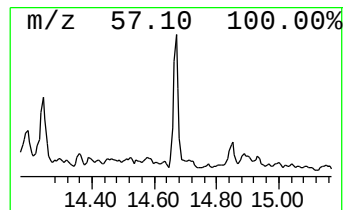
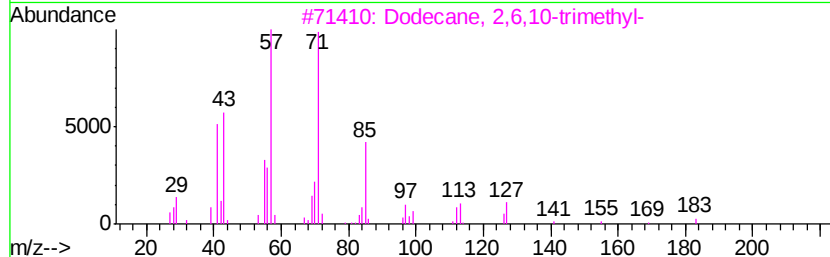
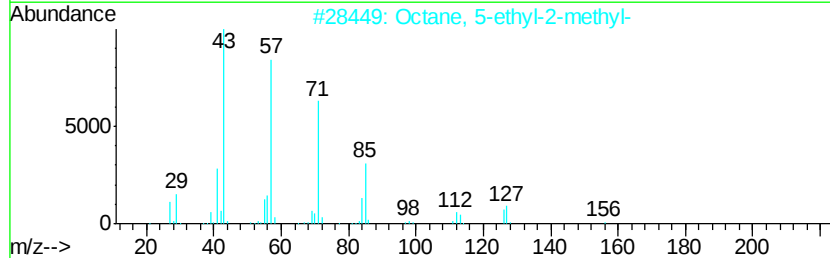
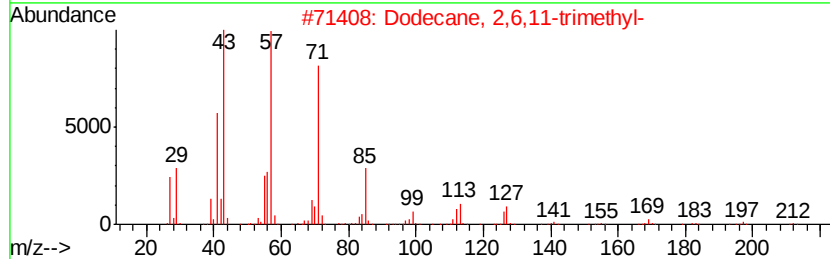
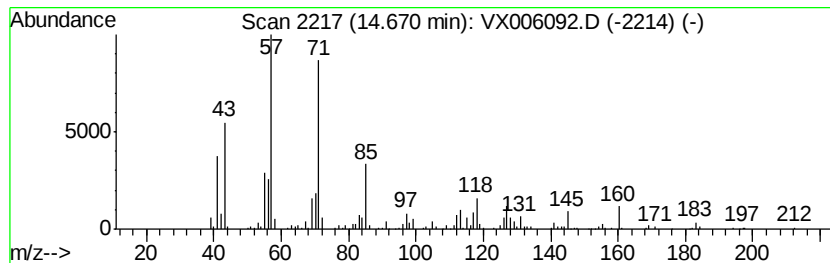
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Peak Number 4 Dodecane, 2,6,11-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	5.30 ug/l	55786	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Dodecane, 2,6,11-trimethyl-	212 C15H32	031295-56-4	83
2	Octane, 5-ethyl-2-methyl-	156 C11H24	062016-18-6	74
3	Dodecane, 2,6,10-trimethyl-	212 C15H32	003891-98-3	74
4	Decane, 2-methyl-	156 C11H24	006975-98-0	72
5	Hexadecane, 2,6,10,14-tetramethyl-	282 C20H42	000638-36-8	72



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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.72	1.72	9.7	ug/l	72528	1	5.66	375721	50.0
Undecane, 2,6-dim...	13.44	5.2	ug/l	54438	4	12.08	525883	50.0
Tridecane, 7-methyl-	13.90	6.8	ug/l	71990	4	12.08	525883	50.0
Dodecane, 2,6,11-...	14.67	5.3	ug/l	55786	4	12.08	525883	50.0