

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY050423\
 Data File : VY013606.D
 Acq On : 04 May 2023 17:36
 Operator : KP/MD
 Sample : 02588-05
 Misc : 4.63g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 ZONE-C-3-6-05012023

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\82Y042423S.M
 Title : SW846 8260

Signal : TIC: VY013606.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.863	3	7	16	rVB4	7769	17495	1.53%	0.236%
2	3.960	340	351	360	rBV2	14634	51219	4.49%	0.692%
3	4.710	464	474	483	rBV3	10374	31387	2.75%	0.424%
4	5.753	633	645	657	rVB4	10088	32217	2.82%	0.435%
5	6.990	841	848	857	rBV3	5993	17045	1.49%	0.230%
6	7.716	957	967	973	rBV	176064	424214	37.19%	5.728%
7	7.789	973	979	991	rVB	269377	617404	54.12%	8.336%
8	8.136	1027	1036	1053	rBV	188094	422137	37.01%	5.700%
9	8.685	1117	1126	1142	rBV	421887	845043	74.08%	11.410%
10	10.179	1363	1371	1379	rBV	675388	1140707	100.00%	15.402%
11	11.489	1578	1586	1595	rBV	625805	1030395	90.33%	13.913%
12	12.008	1662	1671	1675	rBV9	4305	12067	1.06%	0.163%
13	12.227	1705	1707	1713	rVB5	8251	13349	1.17%	0.180%
14	12.483	1741	1749	1758	rBV	481358	818232	71.73%	11.048%
15	12.629	1767	1773	1782	rVB7	9806	29279	2.57%	0.395%
16	12.812	1795	1803	1804	rBV5	11049	20994	1.84%	0.283%
17	13.038	1836	1840	1841	rVV2	17601	20682	1.81%	0.279%
18	13.068	1841	1845	1853	rVB	33795	55944	4.90%	0.755%
19	13.172	1858	1862	1868	rBV	15729	24251	2.13%	0.327%
20	13.282	1872	1880	1885	rBV	78450	137744	12.08%	1.860%
21	13.422	1895	1903	1908	rBV	588803	935514	82.01%	12.631%
22	13.477	1908	1912	1922	rVB	93147	196414	17.22%	2.652%
23	13.641	1931	1939	1944	rBV4	30115	62067	5.44%	0.838%
24	13.958	1986	1991	1994	rVV3	27716	48258	4.23%	0.652%
25	13.989	1994	1996	2006	rVB3	26993	56740	4.97%	0.766%
26	14.141	2013	2021	2022	rBV4	19659	34682	3.04%	0.468%
27	14.257	2036	2040	2045	rBV7	10126	22693	1.99%	0.306%
28	14.385	2055	2061	2071	rVB2	60990	147478	12.93%	1.991%
29	14.519	2079	2083	2085	rBV4	6932	11638	1.02%	0.157%
30	14.635	2096	2102	2105	rBV8	5194	11692	1.02%	0.158%
31	14.678	2105	2109	2113	rVV7	7437	15925	1.40%	0.215%
32	14.727	2115	2117	2123	rVB6	10892	17732	1.55%	0.239%
33	15.214	2194	2197	2204	rVB7	10421	18789	1.65%	0.254%
34	15.318	2209	2214	2220	rVV2	20654	40772	3.57%	0.551%
35	15.379	2222	2224	2230	rVB6	7806	12285	1.08%	0.166%
36	15.605	2257	2261	2265	rVB5	6924	11736	1.03%	0.158%

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ClientSampleId :
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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\82Y042423S.M
Title : SW846 8260

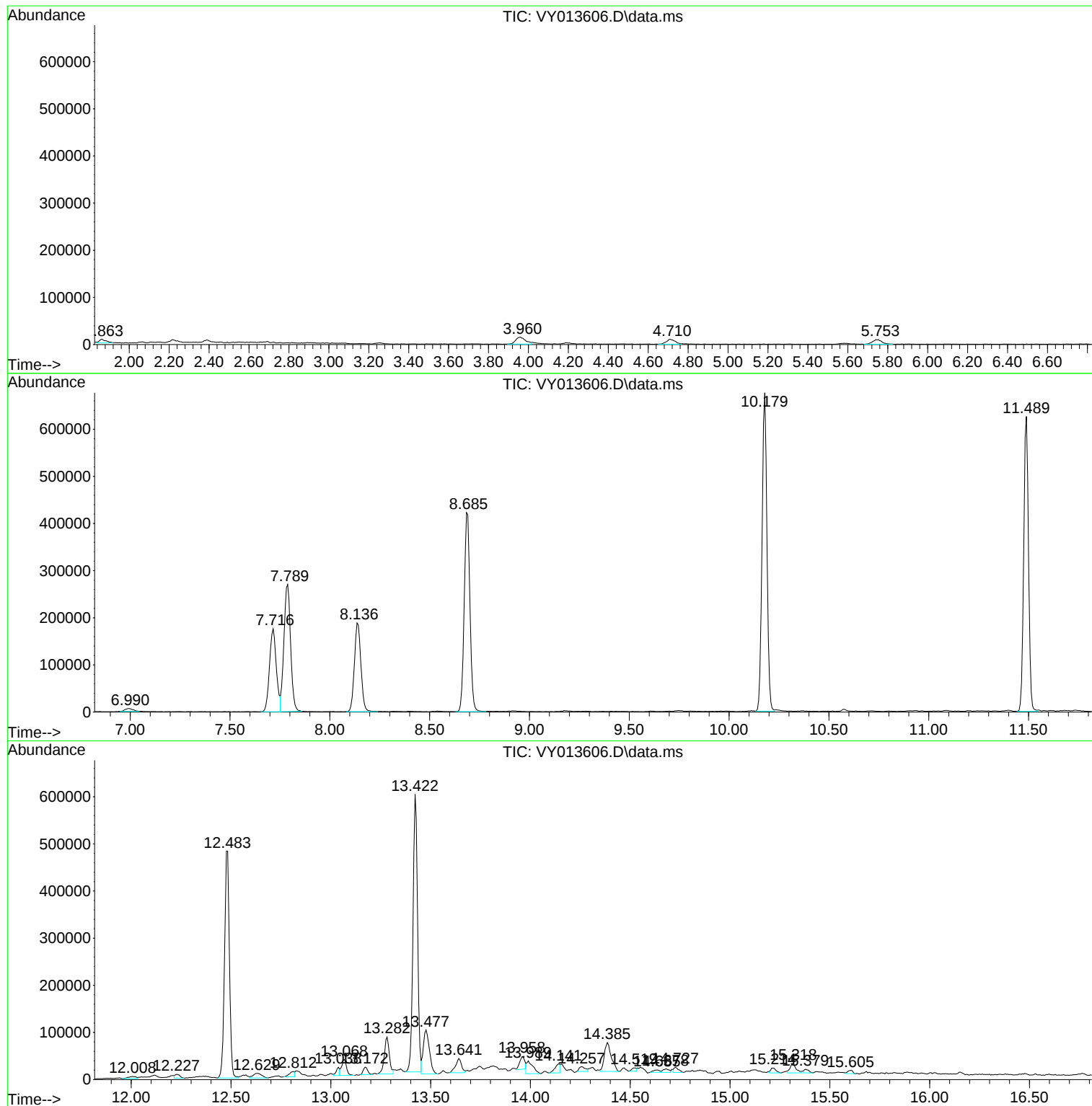
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Quant Title : SW846 8260

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



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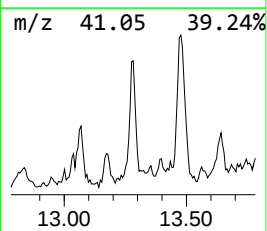
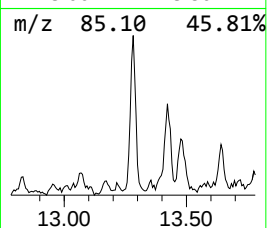
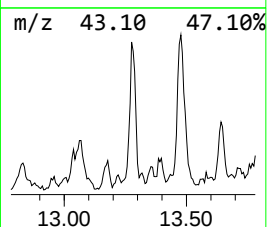
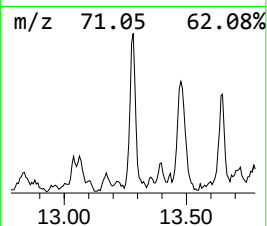
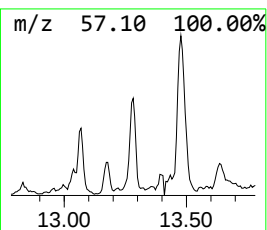
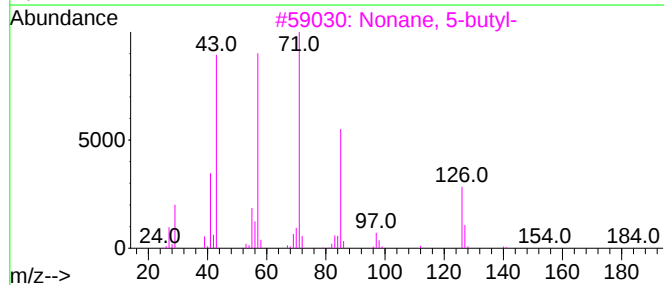
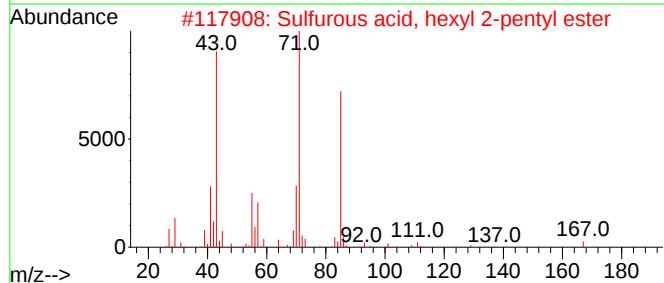
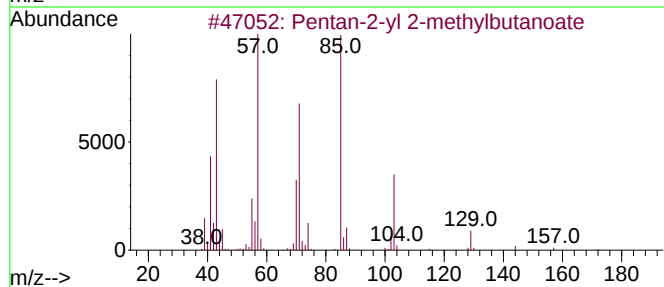
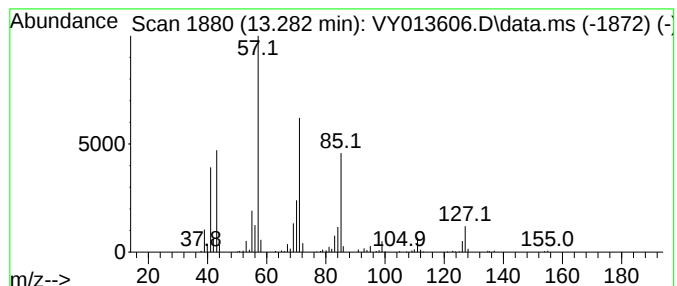
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
Quant Title : SW846 8260

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

Peak Number 1 Pentan-2-yl 2-methylbutanoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	7.36 ug/l	137744	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentan-2-yl 2-methylbutanoate	172	C10H20O2	1000372-71-7	59
2			Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	53
3			Nonane, 5-butyl-	184	C13H28	017312-63-9	53
4			Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	53
5			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	53



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ZONE-C-3-6-05012023

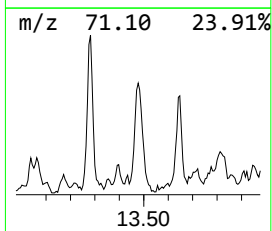
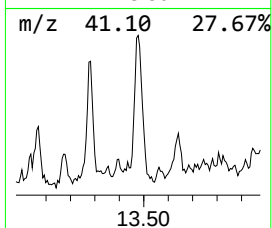
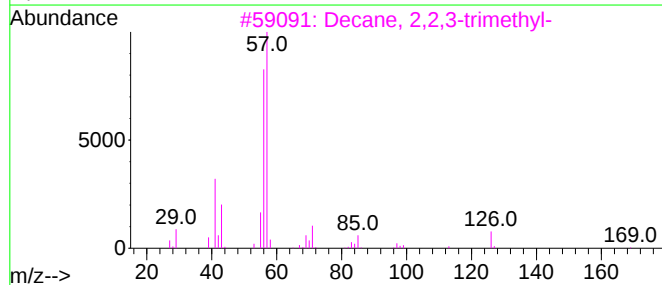
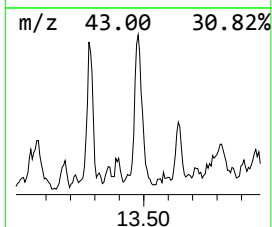
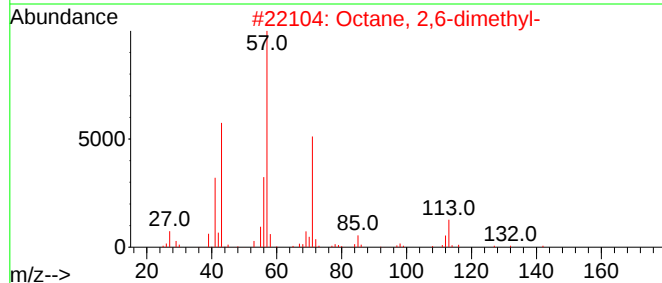
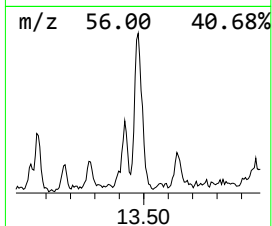
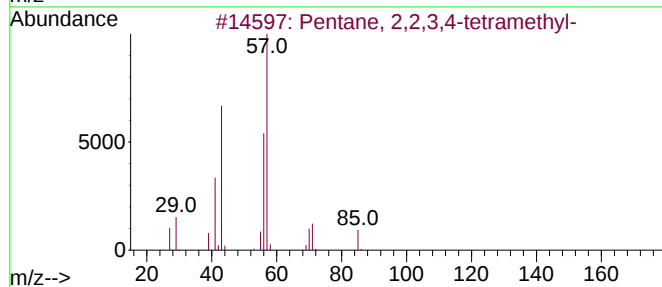
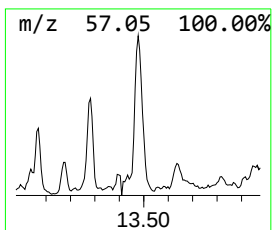
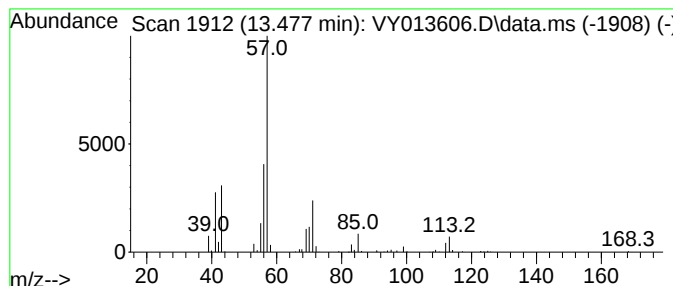
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentane, 2,2,3,4-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.477	10.50 ug/l	196414	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	53
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	50
3			Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	50
4			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	47
5			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	47



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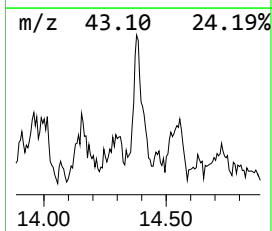
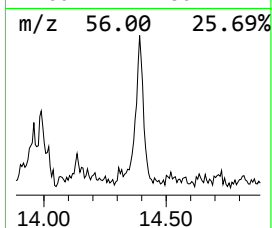
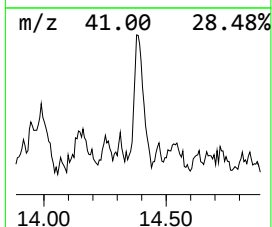
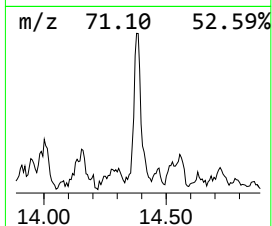
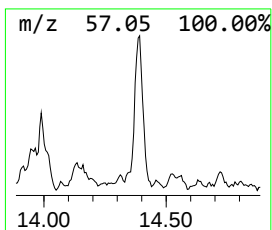
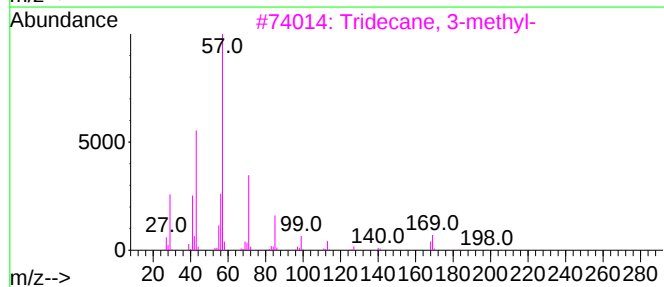
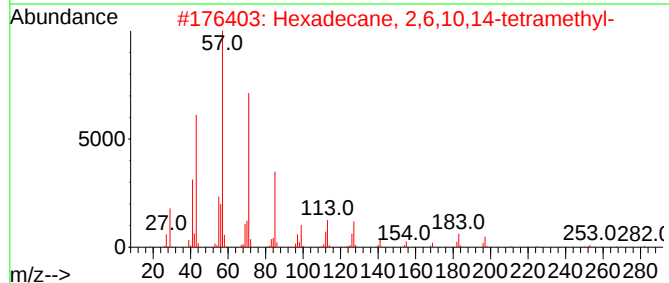
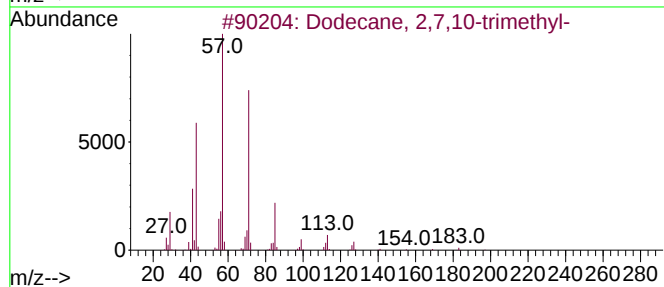
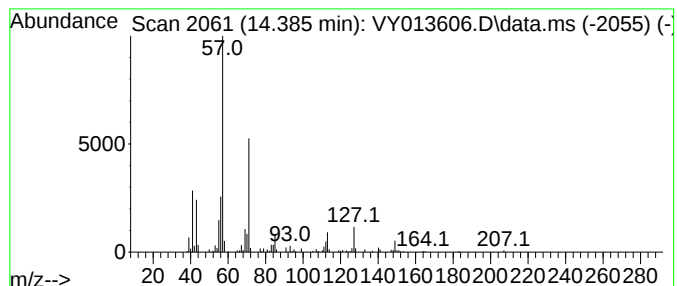
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Quant Title : SW846 8260

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

Peak Number 3 Dodecane, 2,7,10-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.385	7.88 ug/l	147478	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
2			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	59
3			Tridecane, 3-methyl-	198	C14H30	006418-41-3	59
4			Sulfurous acid, 2-ethylhexyl tet...	390	C22H46O3S	1000309-19-7	59
5			Octane, 2-bromo-	192	C8H17Br	000557-35-7	53



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentan-2-yl 2-m...	13.282	7.4	ug/l	137744	4	13.422	935514	50.0
Pentane, 2,2,3,...	13.477	10.5	ug/l	196414	4	13.422	935514	50.0
Dodecane, 2,7,1...	14.385	7.9	ug/l	147478	4	13.422	935514	50.0