

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051523\
 Data File : VY013735.D
 Acq On : 15 May 2023 14:29
 Operator : KP/MD
 Sample : VIBLK
 Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 VIBLK

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: VY013735.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	20	rVB	60527	82458	6.89%	0.999%
2	2.223	60	66	70	rBV3	7277	12166	1.02%	0.147%
3	4.716	463	475	489	rVB2	28506	92318	7.71%	1.118%
4	5.747	634	644	653	rBV5	6468	20378	1.70%	0.247%
5	6.972	833	845	847	rBV2	12510	26748	2.23%	0.324%
6	7.716	956	967	973	rBV	170003	403540	33.72%	4.889%
7	7.789	973	979	994	rVB	263618	608195	50.82%	7.368%
8	8.143	1023	1037	1048	rBV	164944	374178	31.27%	4.533%
9	8.691	1117	1127	1136	rBV	435597	856458	71.56%	10.375%
10	10.179	1364	1371	1378	rBV	718573	1196788	100.00%	14.498%
11	10.575	1430	1436	1444	rVB	64509	121382	10.14%	1.470%
12	10.941	1488	1496	1503	rBV	38873	70706	5.91%	0.857%
13	11.319	1553	1558	1565	rVB2	24882	42771	3.57%	0.518%
14	11.489	1577	1586	1596	rBV	675737	1088095	90.92%	13.181%
15	12.483	1742	1749	1756	rBV2	577732	980391	81.92%	11.877%
16	12.812	1796	1803	1810	rVB4	9375	19468	1.63%	0.236%
17	13.184	1857	1864	1868	rBV2	12471	23564	1.97%	0.285%
18	13.422	1896	1903	1911	rVB	649531	993783	83.04%	12.039%
19	13.745	1951	1956	1961	rBV7	14222	26917	2.25%	0.326%
20	13.959	1986	1991	1996	rBV2	23737	38029	3.18%	0.461%
21	14.068	2005	2009	2015	rBV9	6951	12254	1.02%	0.148%
22	14.251	2036	2039	2046	rVB8	20242	36360	3.04%	0.440%
23	14.416	2062	2066	2070	rVV5	20626	31637	2.64%	0.383%
24	14.617	2095	2099	2102	rBV5	13041	19546	1.63%	0.237%
25	14.678	2105	2109	2113	rVV6	16380	30169	2.52%	0.365%
26	14.727	2113	2117	2124	rVV2	102530	166985	13.95%	2.023%
27	14.794	2124	2128	2133	rVB7	12609	22917	1.91%	0.278%
28	14.843	2133	2136	2138	rBV4	15129	19458	1.63%	0.236%
29	15.007	2159	2163	2166	rBV4	15402	23913	2.00%	0.290%
30	15.208	2191	2196	2202	rBV	166368	263968	22.06%	3.198%
31	15.275	2203	2207	2210	rVV6	20469	39673	3.31%	0.481%
32	15.318	2211	2214	2220	rVV5	20911	51599	4.31%	0.625%
33	15.452	2231	2236	2240	rBV7	20831	48429	4.05%	0.587%
34	15.605	2256	2261	2265	rVB4	61775	99421	8.31%	1.204%
35	16.153	2346	2351	2355	rBV	76040	128661	10.75%	1.559%
36	16.476	2398	2404	2409	rBV5	56957	131788	11.01%	1.596%

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VIBLK

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

37	16.763	2447	2451	2455	rVB4	26893	49698	4.15%	0.602%
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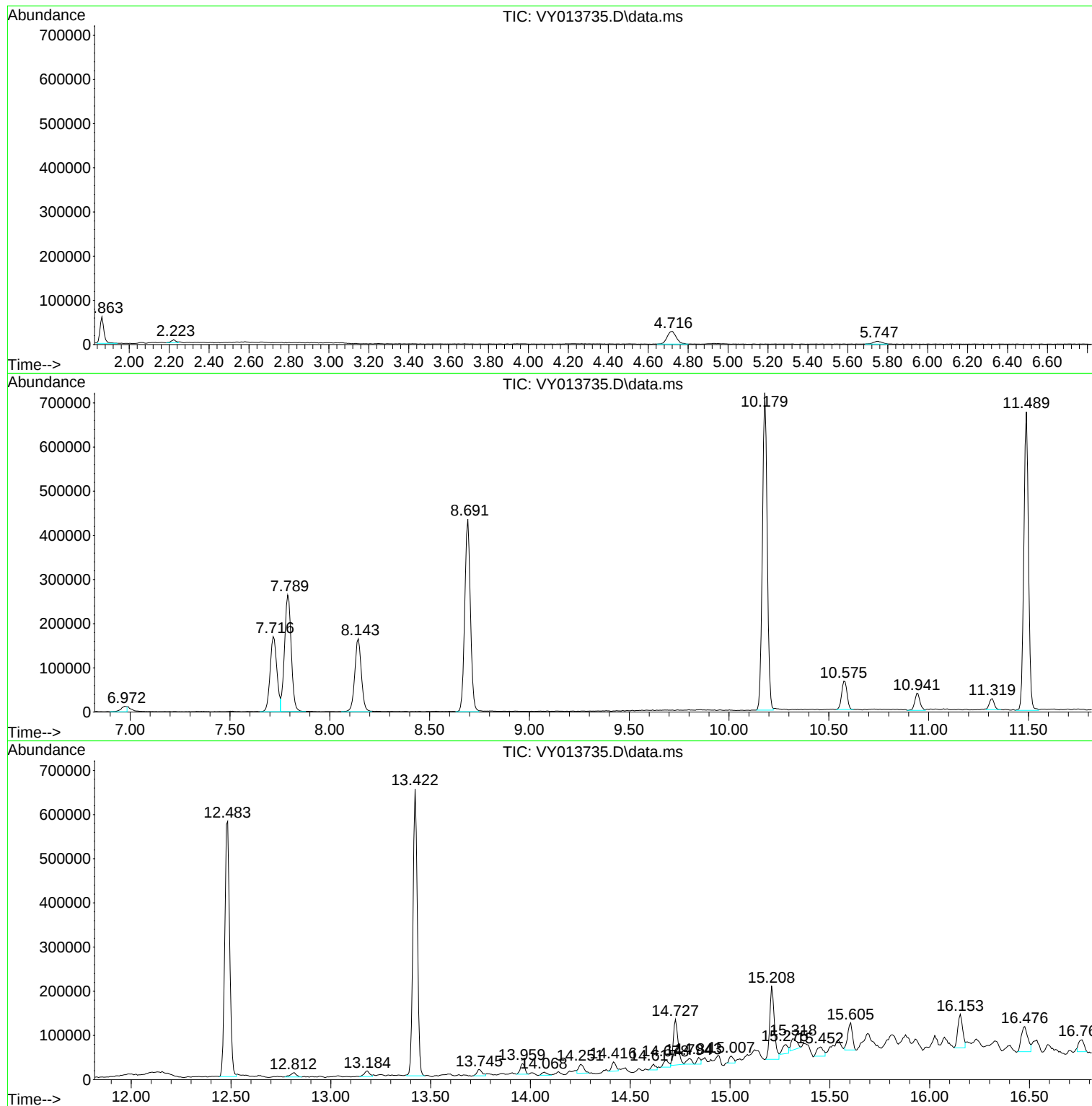
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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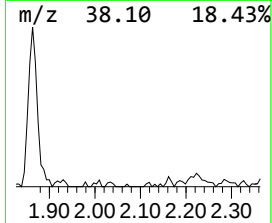
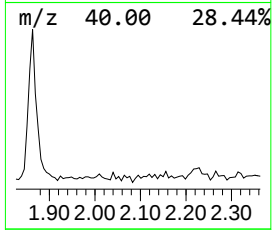
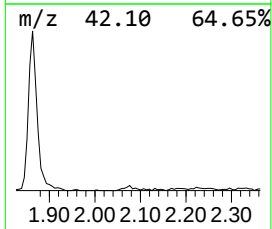
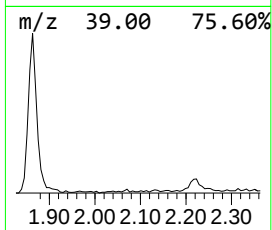
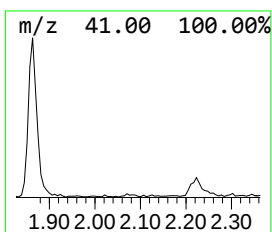
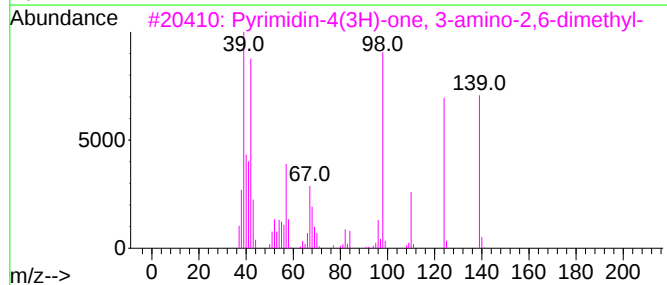
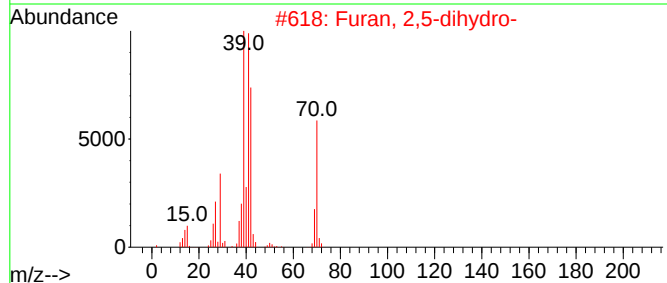
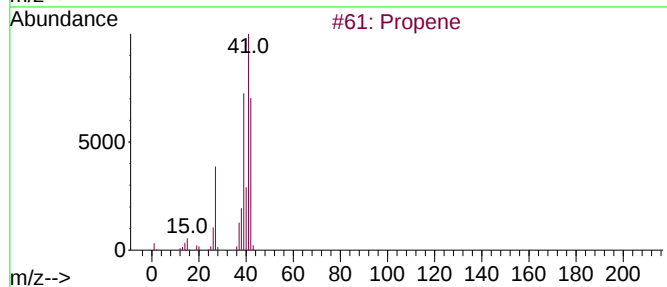
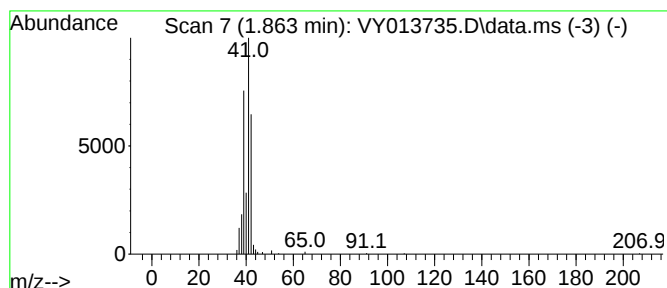
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
Quant Title : SW846 8260

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

Peak Number 1 Propene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.863	6.78 ug/l	82458	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	83
3			Pyrimidin-4(3H)-one, 3-amino-2,6...	139	C6H9N3O	093098-74-9	78
4			Aluminum, tripropyl-	156	C9H21Al	000102-67-0	74
5			N-Methyl-7-azabicyclo(2,2,1)hept...	109	C7H11N	055590-26-6	64



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ClientSampleId :
VIBLK

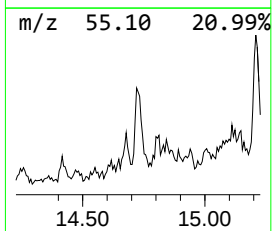
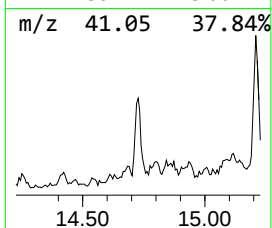
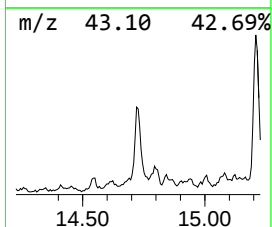
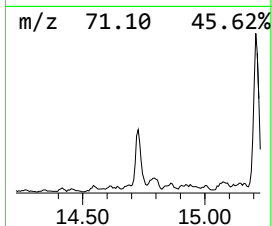
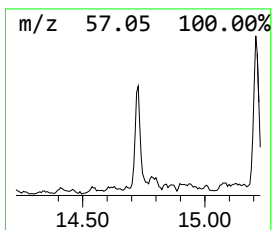
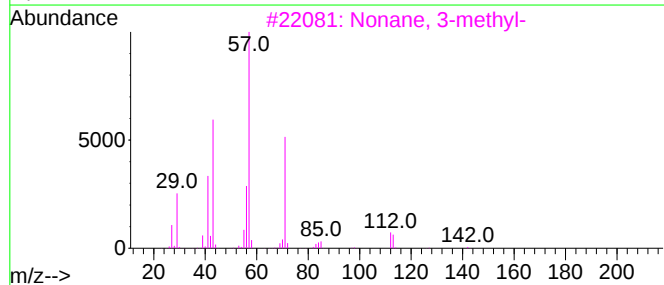
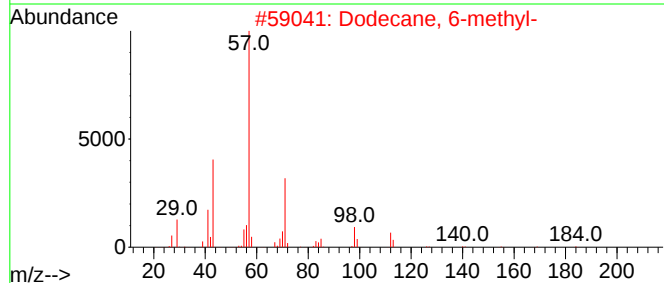
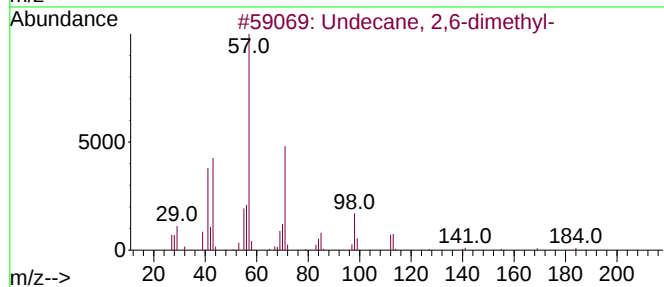
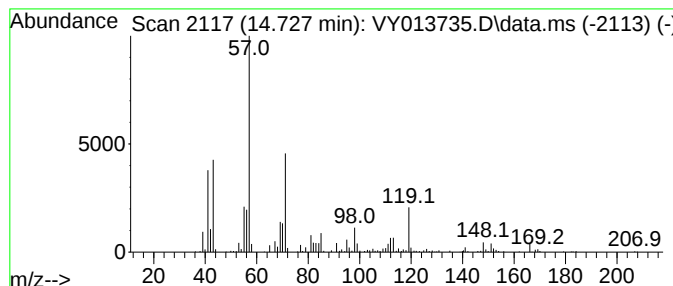
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.727	8.40 ug/l	166985	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	64
2			Dodecane, 6-methyl-	184	C13H28	006044-71-9	64
3			Nonane, 3-methyl-	142	C10H22	005911-04-6	52
4			Dodecane, 2,5-dimethyl-	198	C14H30	056292-65-0	50
5			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	47



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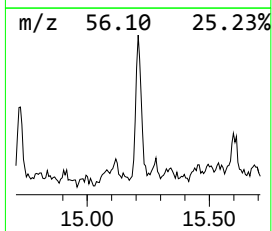
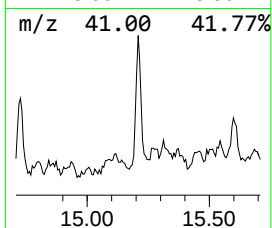
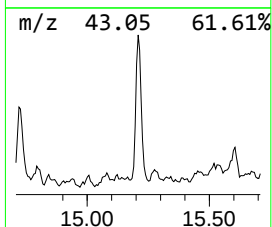
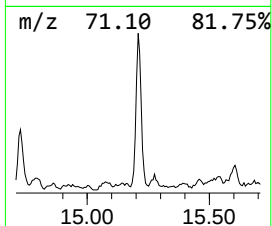
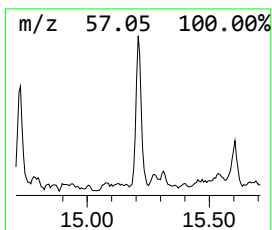
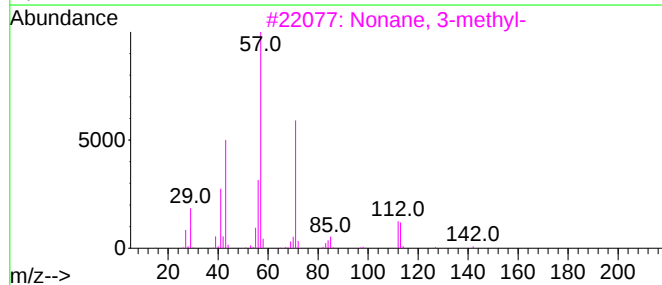
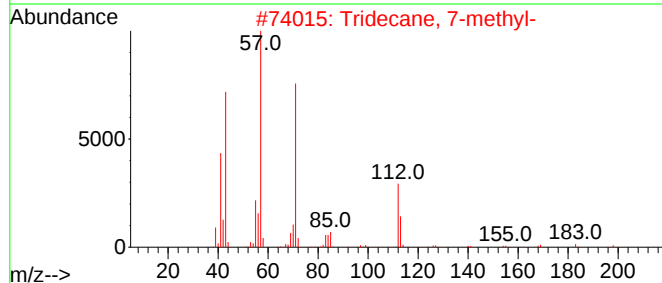
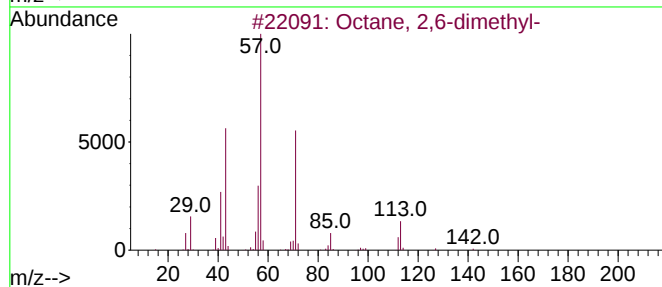
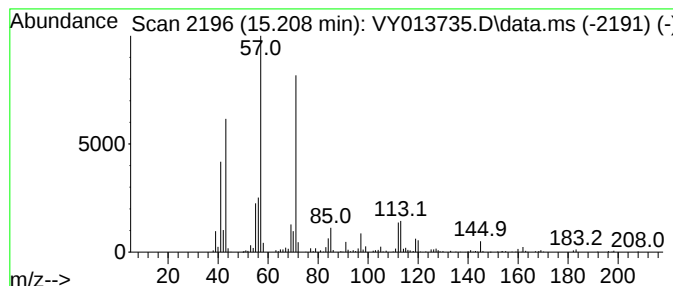
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octane, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.208	13.28 ug/l	263968	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	78
2			Tridecane, 7-methyl-	198	C14H30	026730-14-3	76
3			Nonane, 3-methyl-	142	C10H22	005911-04-6	64
4			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	64
5			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	59



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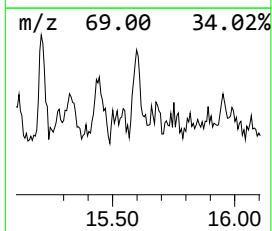
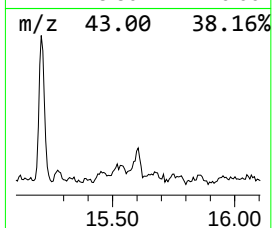
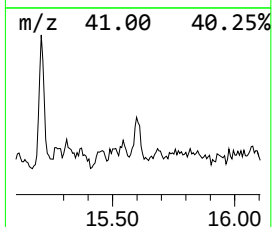
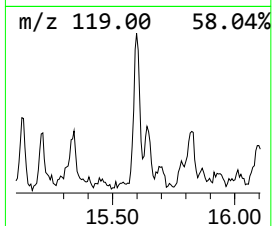
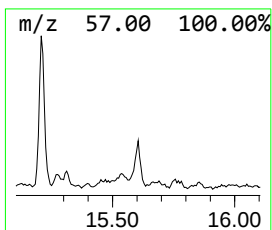
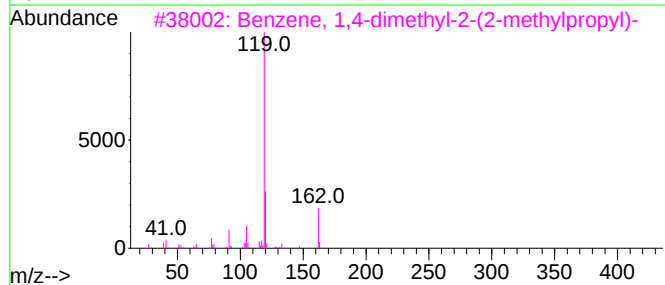
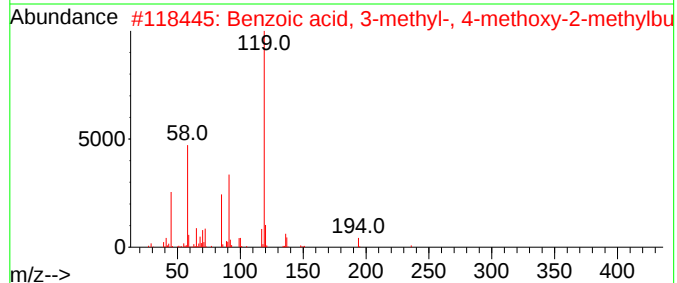
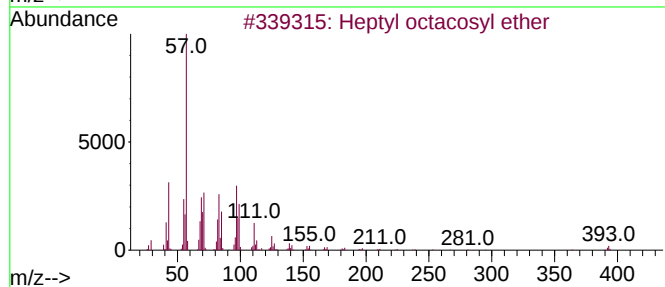
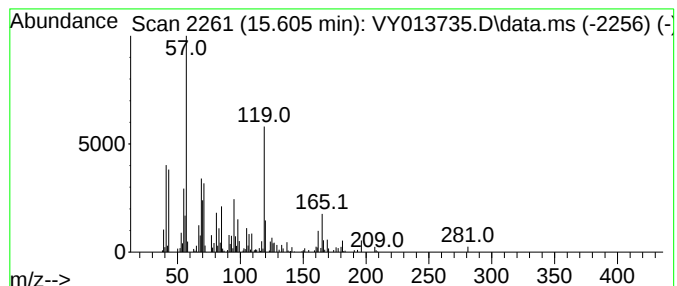
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown15.605 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.605	5.00 ug/l	99421	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptyl octacosyl ether	509	C35H72O	1000406-40-0	27
2			Benzoic acid, 3-methyl-, 4-metho...	236	C14H20O3	1000355-71-0	27
3			Benzene, 1,4-dimethyl-2-(2-methy...	162	C12H18	055669-88-0	25
4			Tetradecane, 2,5-dimethyl-	226	C16H34	056292-69-4	22
5			Ether, 3-hydroxy-2-butyl 1-(p-to...	208	C13H20O2	1000149-41-9	18



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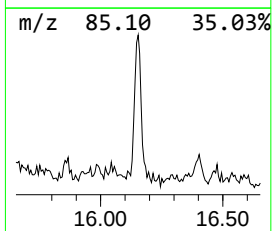
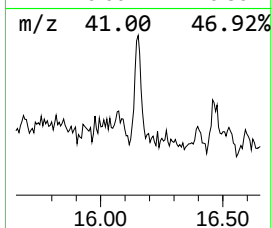
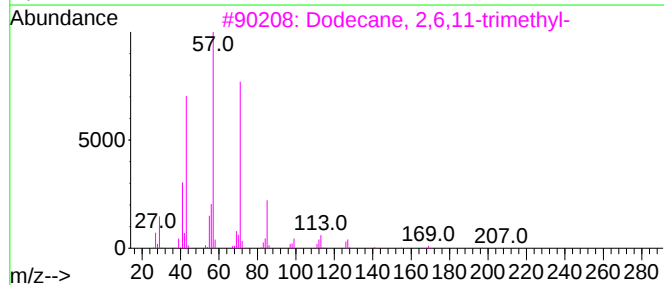
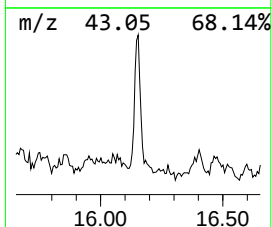
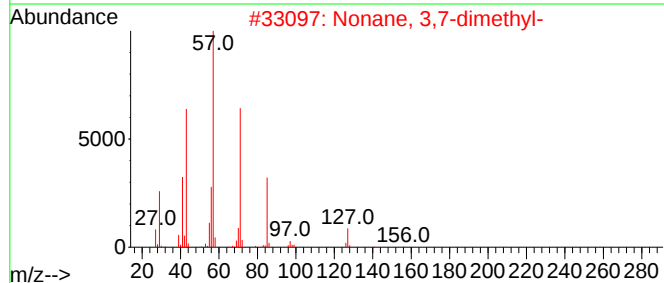
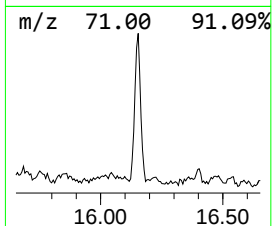
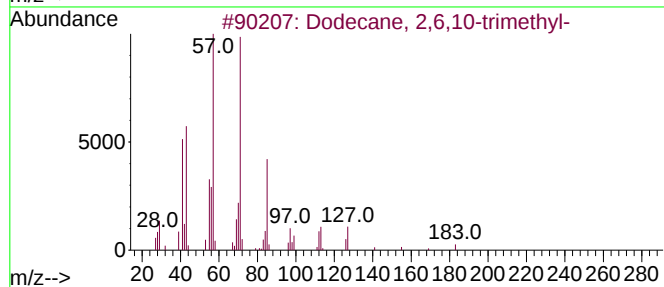
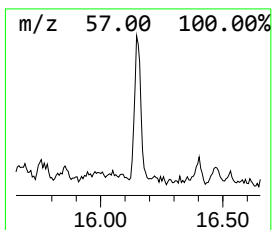
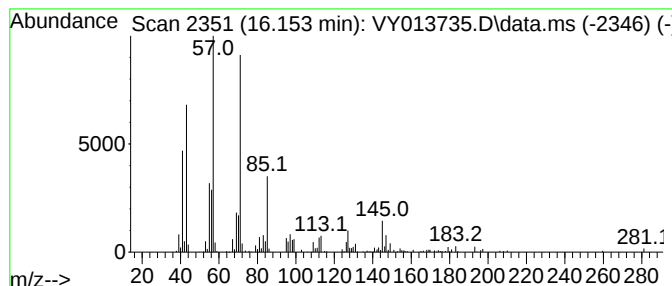
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TIC Integration Parameters: LSCINT.P

Peak Number 7 Dodecane, 2,6,10-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.153	6.47 ug/l	128661	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	83
2			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	72
3			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64
4			Decane, 5-propyl-	184	C13H28	017312-62-8	64
5			Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051523\
Data File : VY013735.D
Acq On : 15 May 2023 14:29
Operator : KP/MD
Sample : VIBLK
Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VIBLK

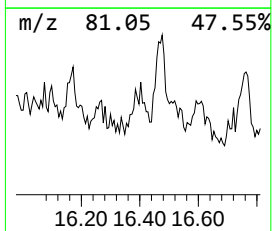
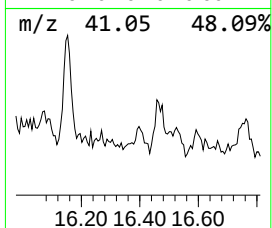
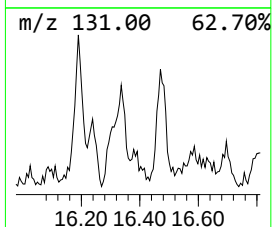
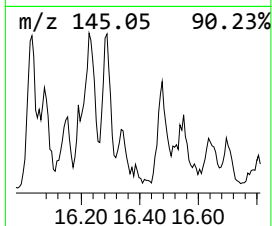
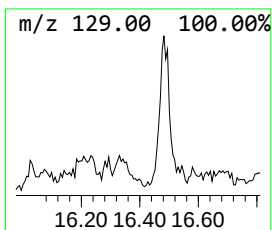
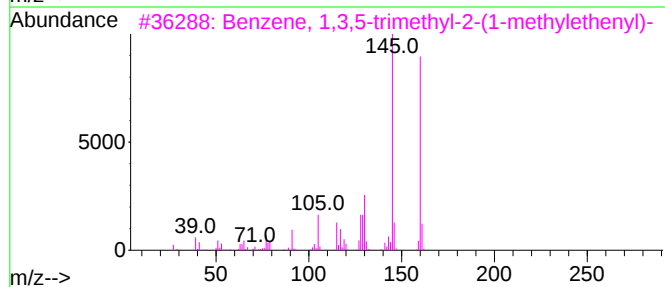
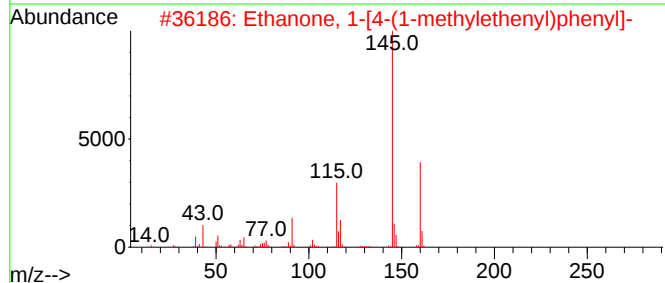
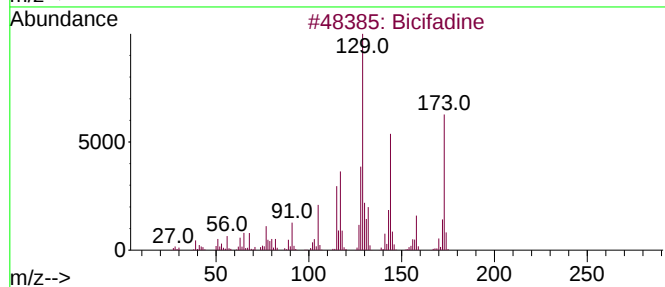
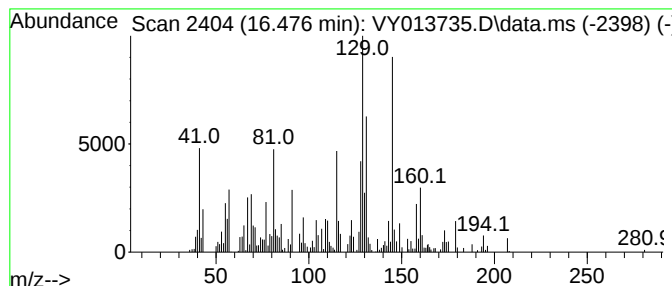
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Quant Title : SW846 8260

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

Peak Number 8 unknown16.476 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.476	6.63 ug/l	131788	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicifadine	173	C12H15N	071195-57-8	46
2			Ethanone, 1-[4-(1-methylethenyl)...]	160	C11H12O	005359-04-6	42
3			Benzene, 1,3,5-trimethyl-2-(1-me...]	160	C12H16	014679-13-1	38
4			5H-Benzocycloheptene, 6,7-dihydro-	144	C11H12	007125-62-4	38
5			Ethanone, 1-(2,3-dihydro-1H-inde...]	160	C11H12O	004228-10-8	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051523\
Data File : VY013735.D
Acq On : 15 May 2023 14:29
Operator : KP/MD
Sample : VIBLK
Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VIBLK

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propene	1.863	6.8	ug/l	82458	1	7.789	608195	50.0
Undecane, 2,6-d...	14.727	8.4	ug/l	166985	4	13.422	993783	50.0
Octane, 2,6-dim...	15.208	13.3	ug/l	263968	4	13.422	993783	50.0
unknown15.605	15.605	5.0	ug/l	99421	4	13.422	993783	50.0
Dodecane, 2,6,1...	16.153	6.5	ug/l	128661	4	13.422	993783	50.0
unknown16.476	16.476	6.6	ug/l	131788	4	13.422	993783	50.0