

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY033125\
 Data File : VY021721.D
 Acq On : 31 Mar 2025 15:48
 Operator : SY/MD
 Sample : Q1675-07
 Misc : 2.16g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 T1

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\82Y032725S.M

Title : SW846 8260

Signal : TIC: VY021721.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.812	10	15	24	rVB	78807	106242	7.08%	0.953%
2	4.610	464	474	482	rBV2	22620	65654	4.37%	0.589%
3	4.702	482	489	501	rVB3	8039	29102	1.94%	0.261%
4	7.634	959	970	976	rBV	215613	515756	34.36%	4.628%
5	7.707	976	982	994	rVB	317257	722461	48.14%	6.483%
6	8.061	1029	1040	1051	rBV	172577	396757	26.44%	3.560%
7	8.244	1063	1070	1078	rVB	10773	24286	1.62%	0.218%
8	8.616	1120	1131	1142	rBV	545768	1081512	72.06%	9.705%
9	10.103	1368	1375	1383	rBV	872155	1500874	100.00%	13.468%
10	11.414	1581	1590	1602	rBV	834894	1343307	89.50%	12.054%
11	12.408	1744	1753	1763	rBV	648689	1074607	71.60%	9.643%
12	12.761	1802	1811	1816	rBV5	18655	48013	3.20%	0.431%
13	12.993	1841	1849	1854	rBV	75723	115874	7.72%	1.040%
14	13.096	1862	1866	1874	rVB	21983	36644	2.44%	0.329%
15	13.206	1875	1884	1891	rBV	144658	261082	17.40%	2.343%
16	13.346	1898	1907	1912	rVV	758191	1215656	81.00%	10.909%
17	13.407	1912	1917	1926	rVB2	177566	398137	26.53%	3.573%
18	13.566	1933	1943	1948	rBV3	79125	160130	10.67%	1.437%
19	13.749	1968	1973	1978	rVB4	26983	50710	3.38%	0.455%
20	13.883	1990	1995	1999	rBV	84687	161350	10.75%	1.448%
21	13.999	2010	2014	2017	rVB3	20487	25195	1.68%	0.226%
22	14.072	2020	2026	2031	rVV5	41409	94318	6.28%	0.846%
23	14.182	2039	2044	2045	rBV4	25611	44745	2.98%	0.402%
24	14.304	2059	2064	2073	rBV3	117872	303172	20.20%	2.720%
25	14.383	2073	2077	2082	rVV5	45450	78800	5.25%	0.707%
26	14.468	2088	2091	2099	rVB7	48918	121640	8.10%	1.092%
27	14.761	2137	2139	2148	rVB6	78095	188249	12.54%	1.689%
28	14.852	2151	2154	2158	rVB2	61450	91362	6.09%	0.820%
29	14.919	2159	2165	2166	rBV4	67409	126820	8.45%	1.138%
30	15.133	2197	2200	2205	rVB2	94670	130424	8.69%	1.170%
31	15.511	2258	2262	2268	rVB2	142544	264099	17.60%	2.370%
32	16.638	2443	2447	2453	rVB3	187982	367077	24.46%	3.294%

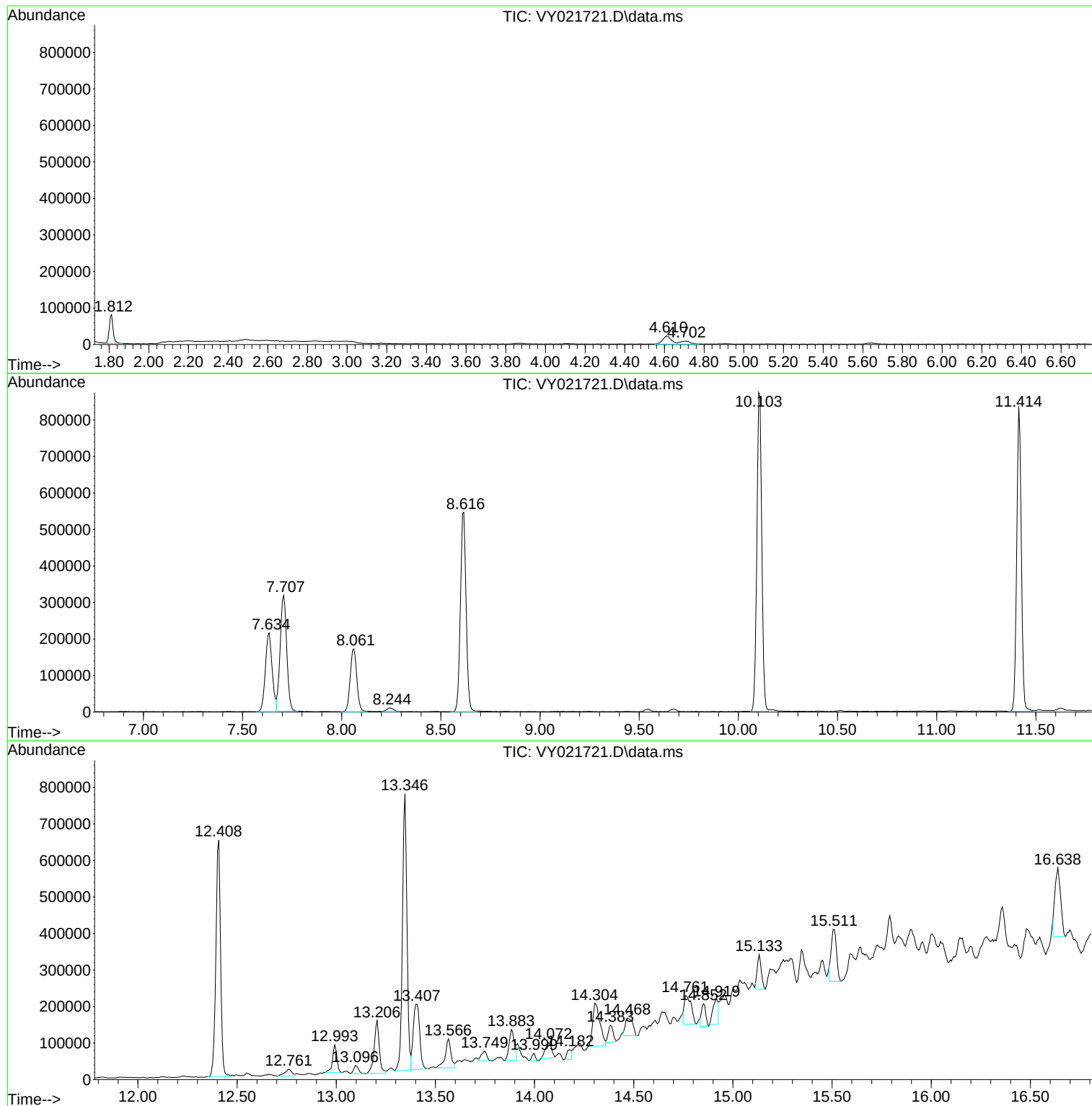
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
T1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y032725S.M
Quant Title : SW846 8260

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



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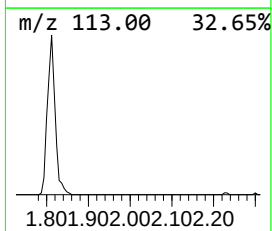
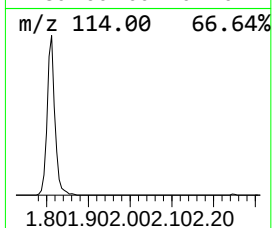
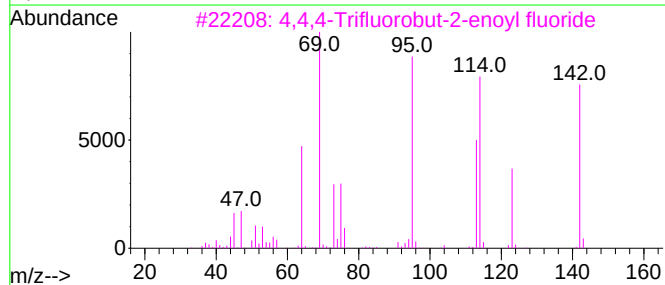
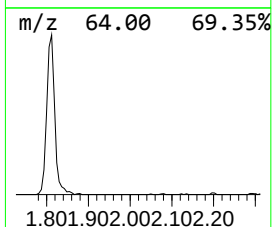
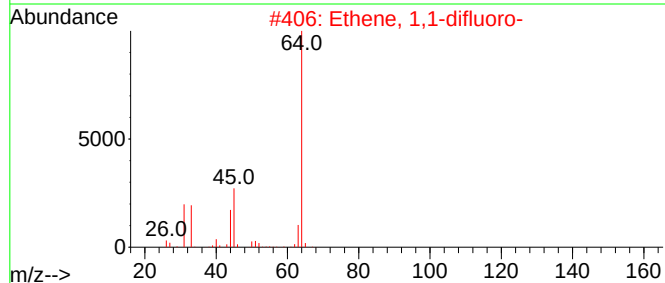
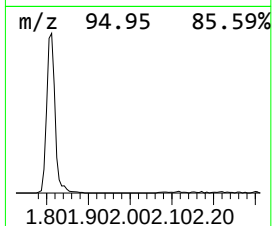
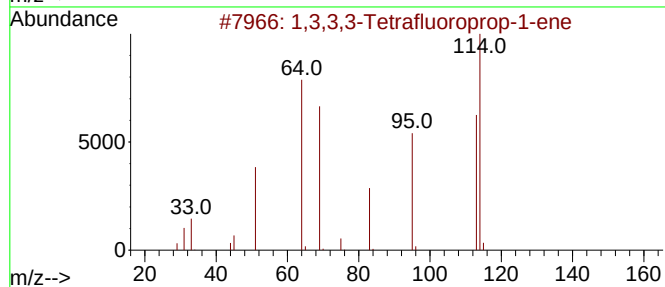
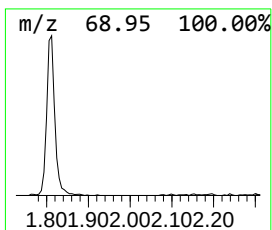
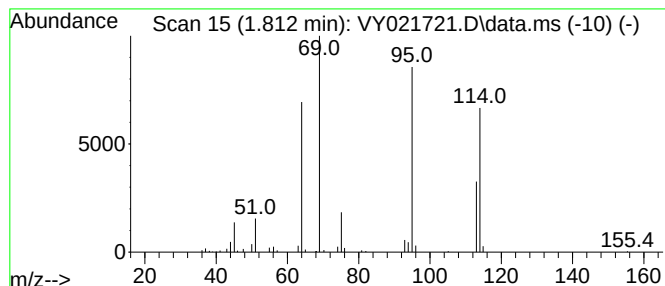
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y032725S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown1.812 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.812	7.35 ug/l	106242	Pentafluorobenzene	7.707

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,3,3-Tetrafluoroprop-1-ene	114	C3H2F4	1000389-53-0	25
2			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	12
3			4,4,4-Trifluorobut-2-enoyl fluoride	142	C4H2F4O	1000394-29-0	10
4			Ethyl diazoacetate	114	C4H6N2O2	000623-73-4	9
5			2-Pentenoic acid, 2-methyl-	114	C6H10O2	003142-72-1	9



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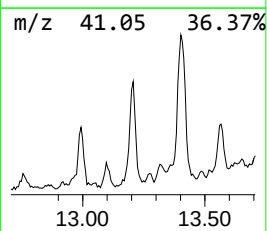
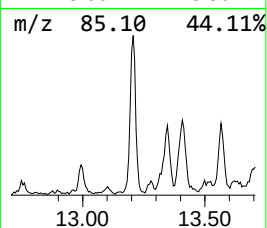
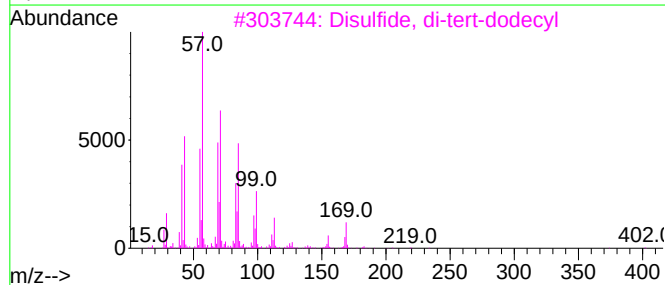
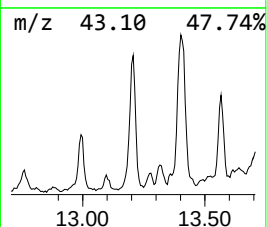
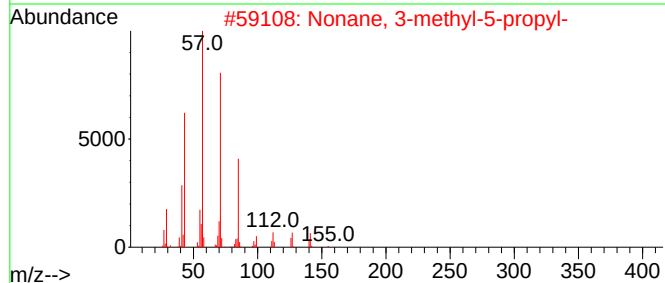
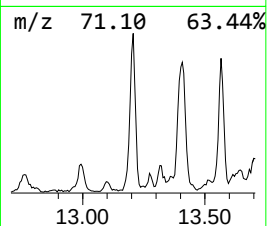
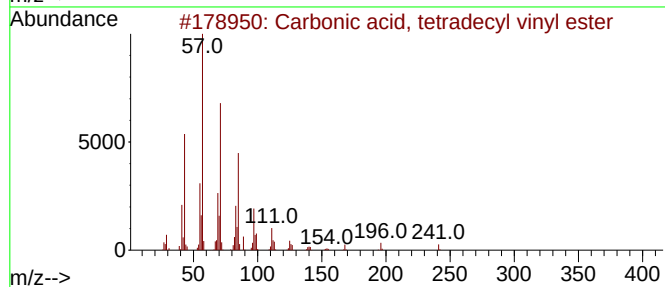
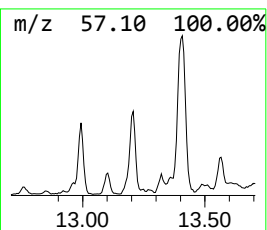
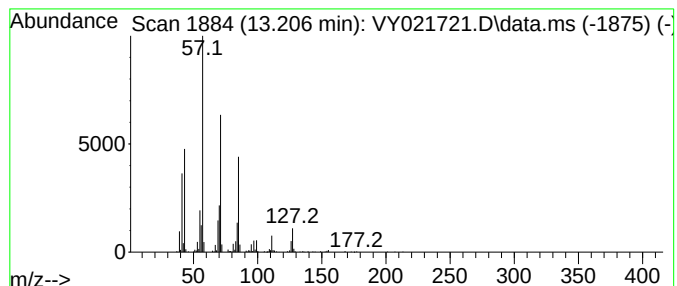
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y032725S.M
Quant Title : SW846 8260

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

Peak Number 2 Carbonic acid, tetradecyl v... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.206	10.74 ug/l	261082	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	72
2			Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	72
3			Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	72
4			Heptadecane	240	C17H36	000629-78-7	59
5			2-Bromotetradecane	276	C14H29Br	074036-95-6	59



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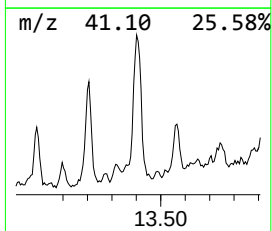
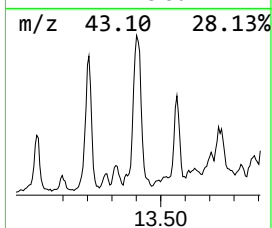
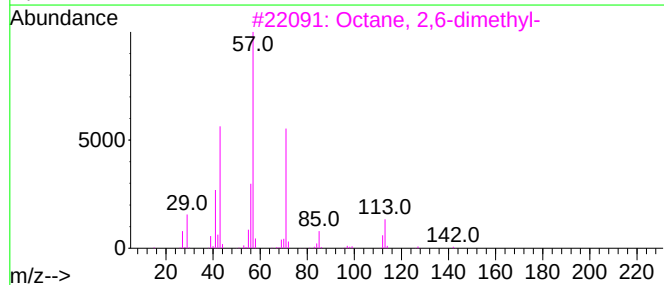
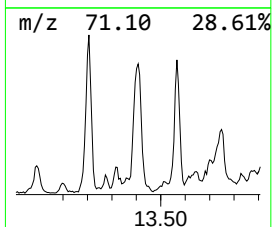
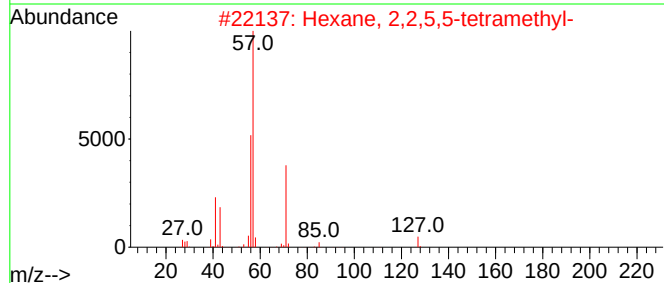
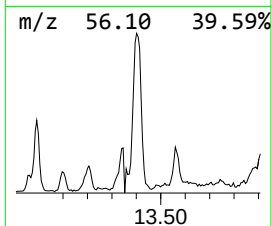
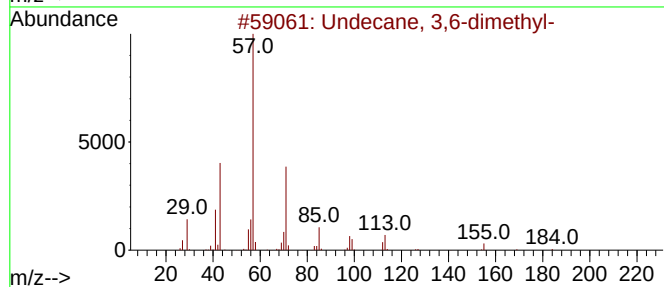
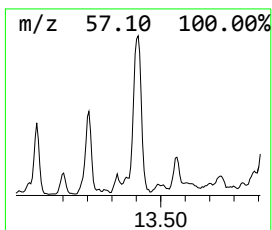
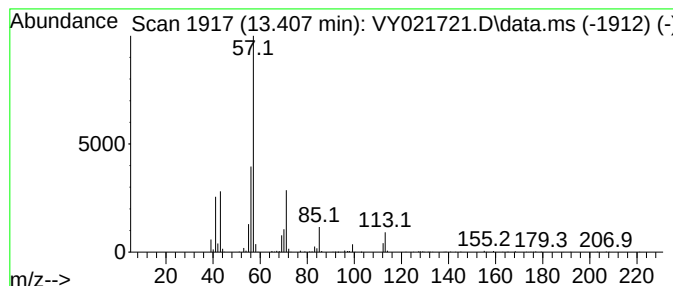
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y032725S.M
Quant Title : SW846 8260

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

Peak Number 3 Undecane, 3,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.407	16.38 ug/l	398137	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	53
2			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	50
3			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	50
4			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	47
5			Heptane, 3-(bromomethyl)-	192	C8H17Br	018908-66-2	46



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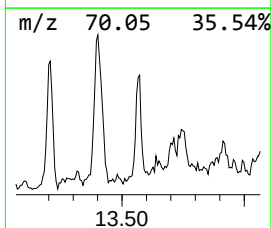
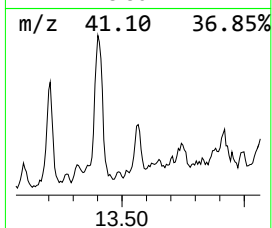
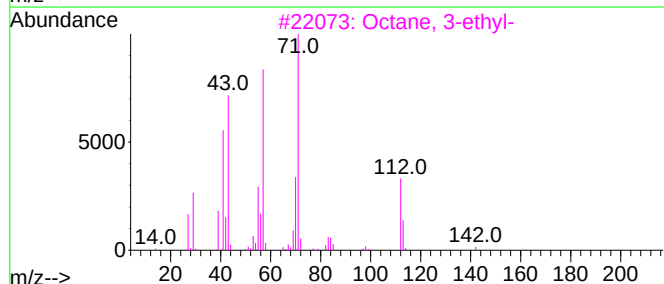
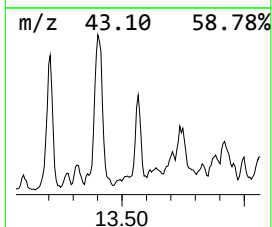
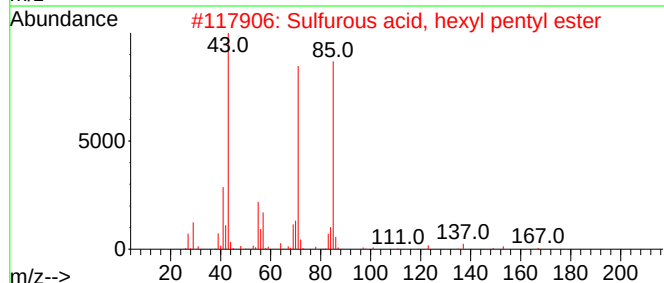
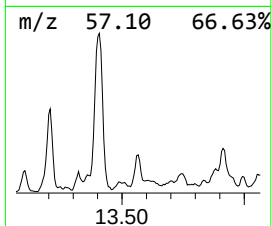
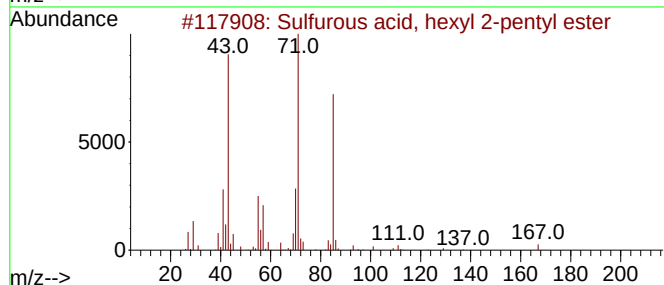
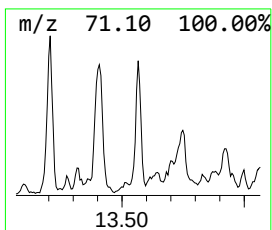
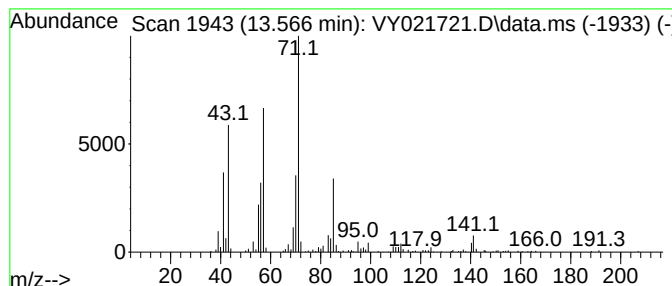
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Sulfurous acid, hexyl 2-pen... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.566	6.59 ug/l	160130	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	59
2			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	58
3			Octane, 3-ethyl-	142	C10H22	005881-17-4	58
4			Sulfurous acid, 2-pentyl tetradec...	348	C19H40O3S	1000309-16-3	53
5			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	53



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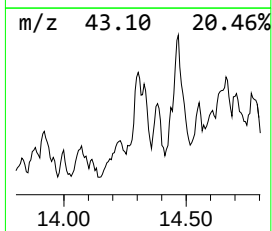
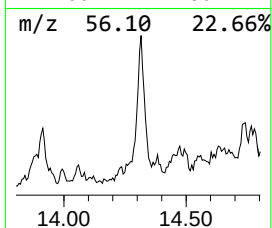
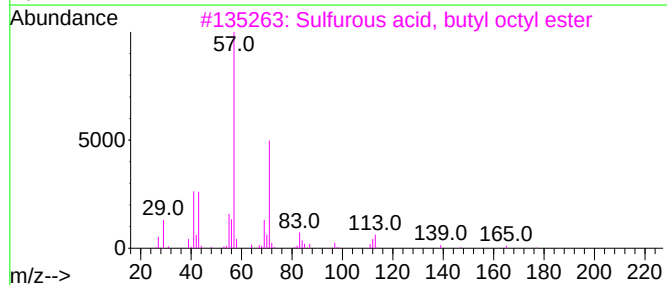
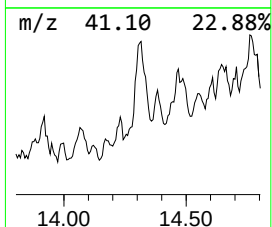
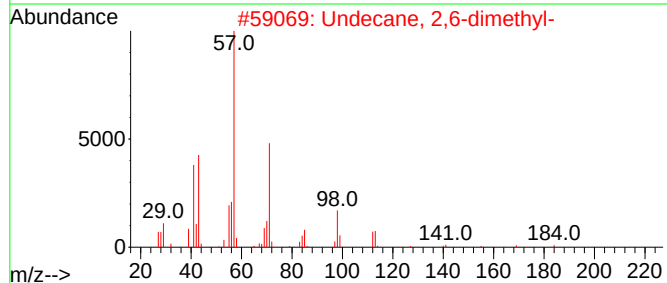
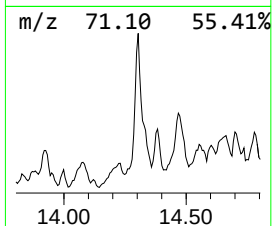
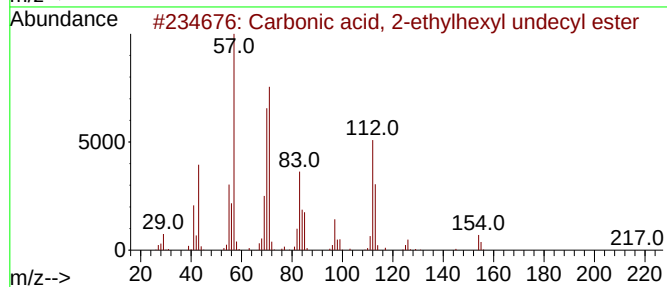
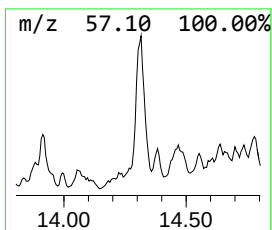
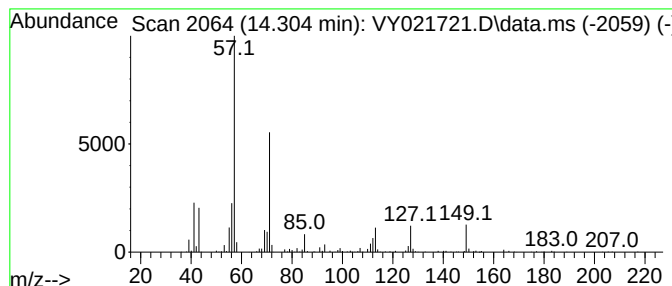
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y032725S.M
Quant Title : SW846 8260

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

Peak Number 6 Carbonic acid, 2-ethylhexyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.304	12.47 ug/l	303172	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, 2-ethylhexyl unde...	328	C20H40O3	1000383-13-8	59
2			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	53
3			Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	53
4			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	53
5			Octyl thioglycolate	204	C10H20O2S	007664-80-4	53



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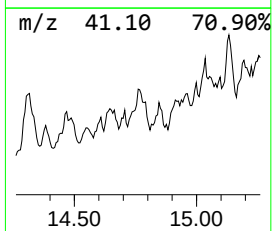
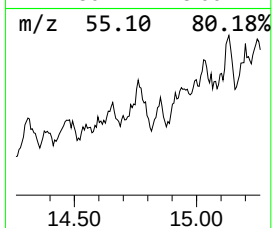
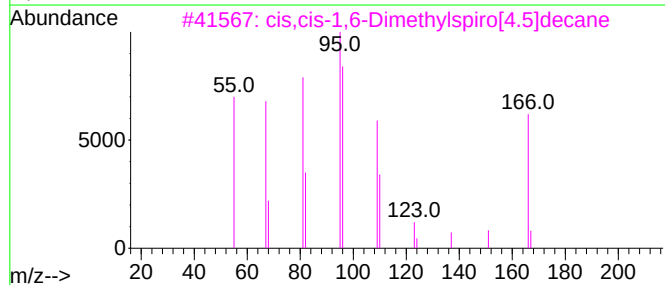
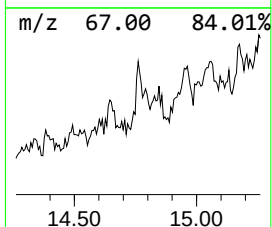
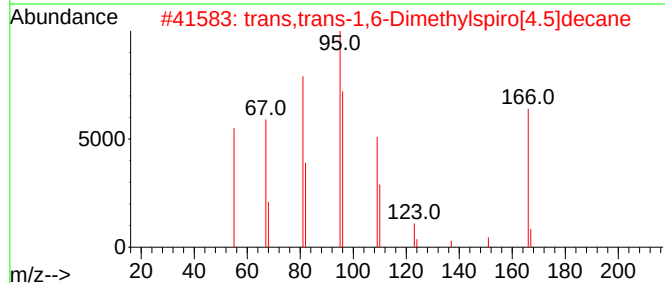
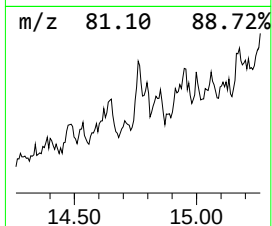
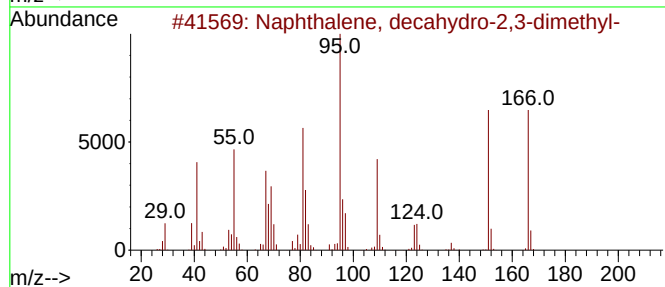
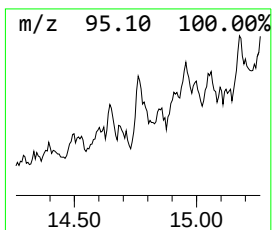
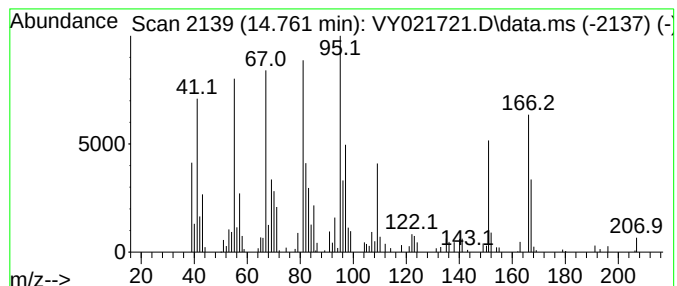
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y032725S.M
Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, decahydro-2,3-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.761	7.74 ug/l	188249	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2,3-dimet...	166	C12H22	001008-80-6	64
2			trans,trans-1,6-Dimethylspiro[4...	166	C12H22	1000111-72-1	62
3			cis,cis-1,6-Dimethylspiro[4.5]de...	166	C12H22	1000111-72-4	49
4			Cyclopropane, 1-(1-methylethyl)-...	152	C11H20	056259-17-7	22
5			4-Decyne	138	C10H18	002384-86-3	18



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY033125\
Data File : VY021721.D
Acq On : 31 Mar 2025 15:48
Operator : SY/MD
Sample : Q1675-07
Misc : 2.16g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
T1

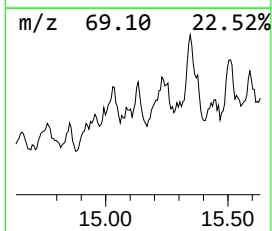
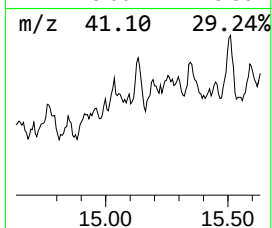
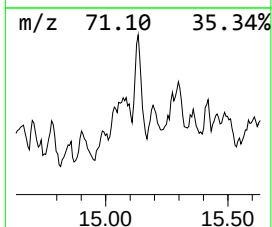
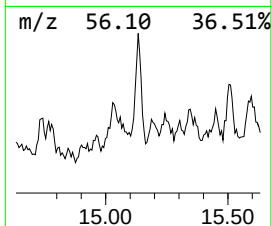
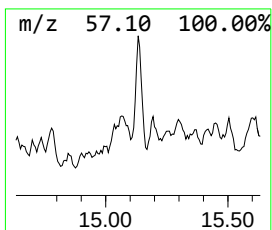
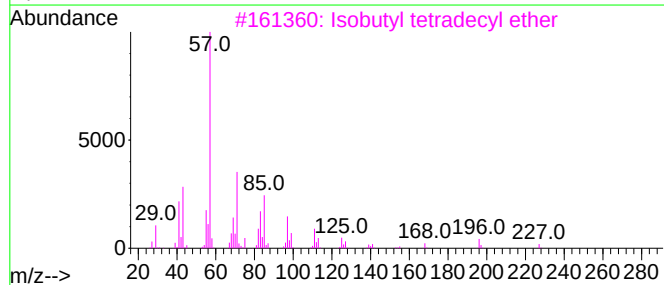
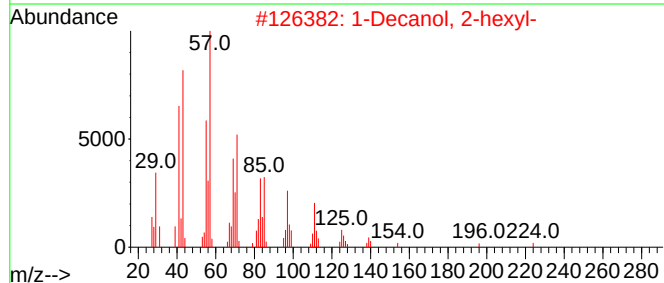
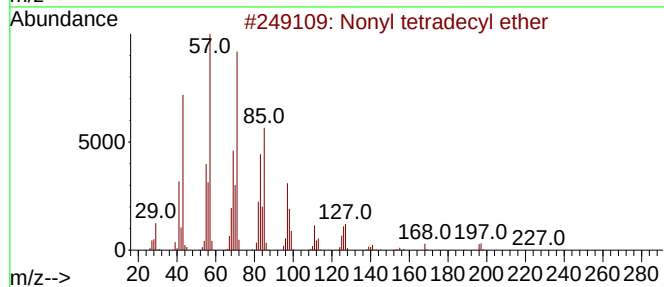
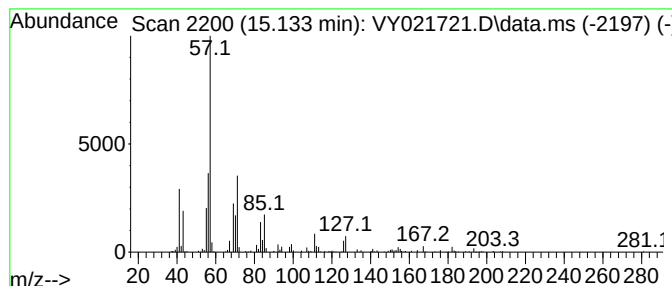
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Quant Title : SW846 8260

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

Peak Number 8 Nonyl tetradecyl ether Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	5.36 ug/l	130424	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonyl tetradecyl ether	340	C23H48O	1000406-37-6	72
2			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	64
3			Isobutyl tetradecyl ether	270	C18H38O	1000406-32-7	59
4			Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1010309-37-4	59
5			Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY033125\
Data File : VY021721.D
Acq On : 31 Mar 2025 15:48
Operator : SY/MD
Sample : Q1675-07
Misc : 2.16g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
T1

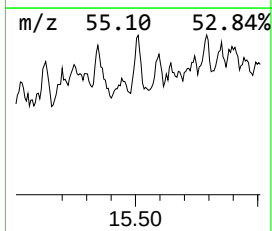
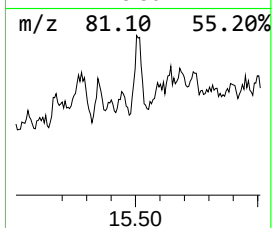
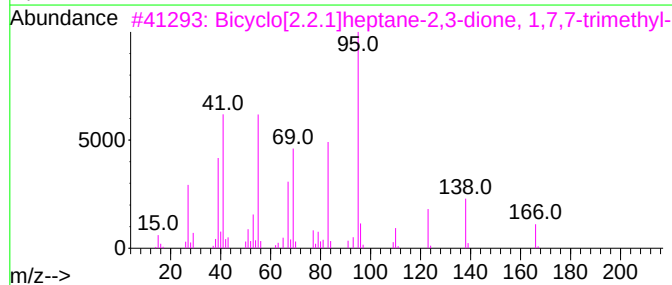
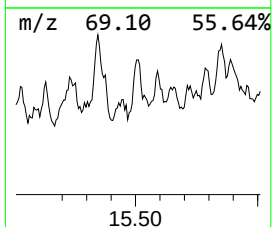
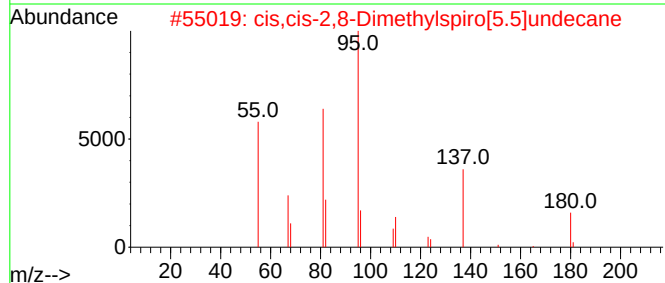
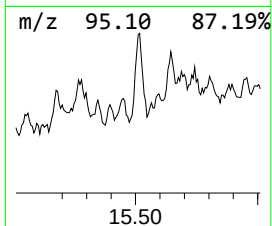
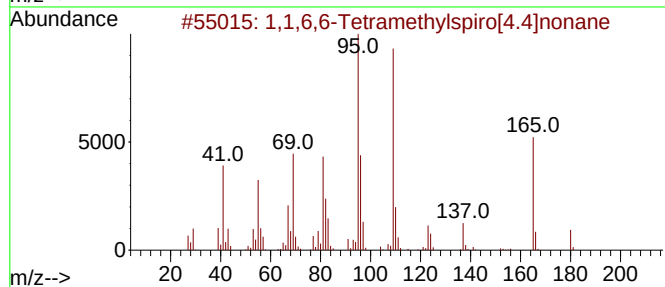
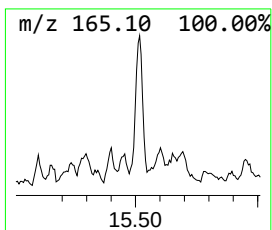
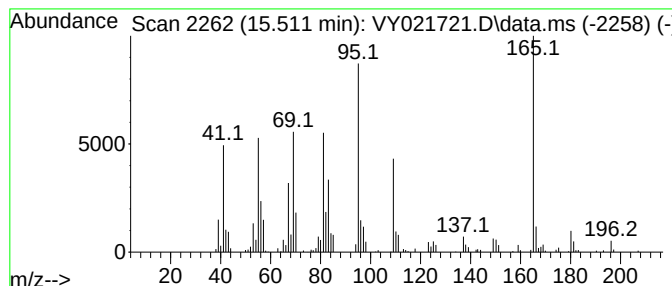
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Quant Title : SW846 8260

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

Peak Number 9 unknown15.511 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.511	10.86 ug/l	264099	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1,6,6-Tetramethylspiro[4.4]nonane	180	C13H24	074054-92-5	45
2			cis,cis-2,8-Dimethylspiro[5.5]un...	180	C13H24	095530-75-9	42
3			Bicyclo[2.2.1]heptane-2,3-dione,...	166	C10H14O2	002767-84-2	42
4			d1-Camphoroquinone	166	C10H14O2	010373-78-1	38
5			1,5-Dihydro-1,5-dimethyl-6H-imid...	165	C6H7N5O	106284-73-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY033125\
Data File : VY021721.D
Acq On : 31 Mar 2025 15:48
Operator : SY/MD
Sample : Q1675-07
Misc : 2.16g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 12 Sample Multiplier: 1

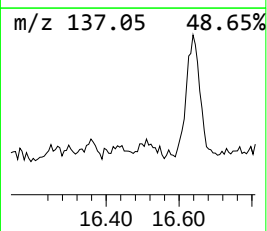
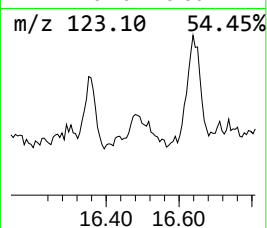
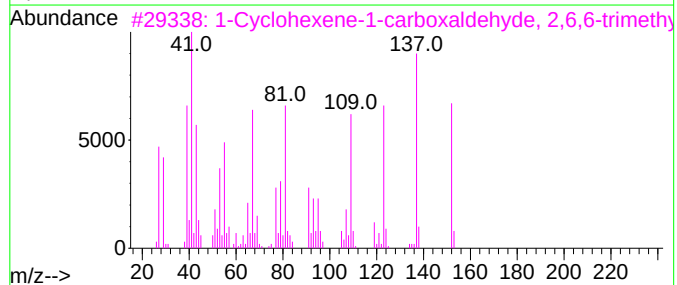
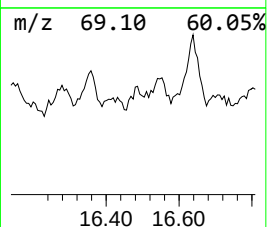
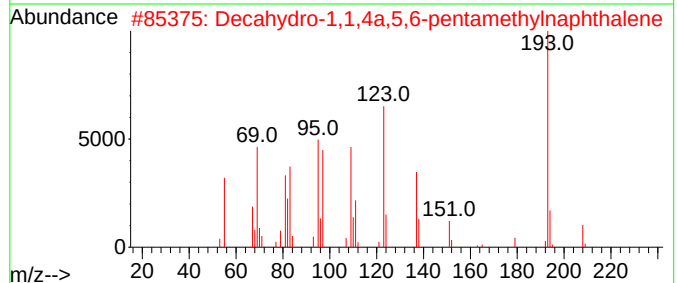
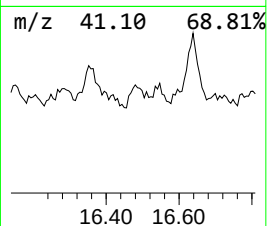
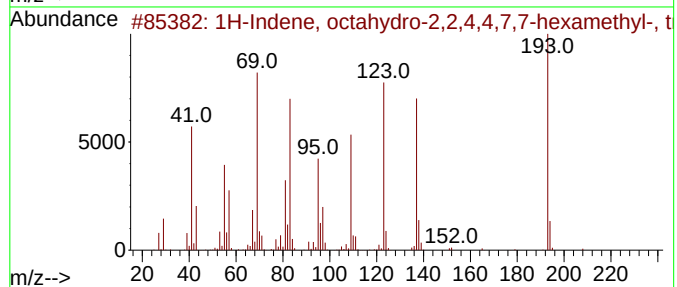
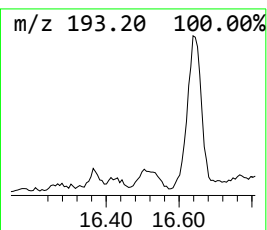
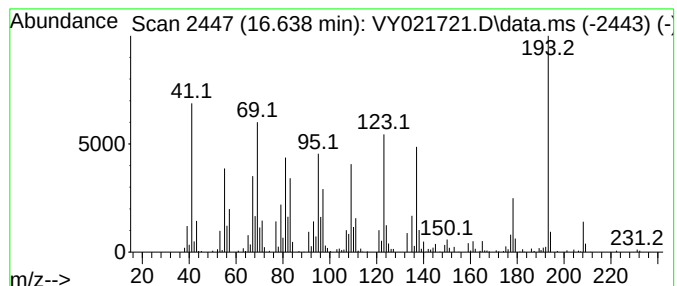
Instrument :
MSVOA_Y
ClientSampleId :
T1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y032725S.M
Quant Title : SW846 8260

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

Peak Number 10 1H-Indene, octahydro-2,2,4,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.639	15.10 ug/l	367077	1,4-Dichlorobenzene-d4	13.346	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	72
2	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	64
3	1-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	000432-25-7	25
4	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	22
5	2,5,5,6,1a-Pentamethyl-cis-1a,4a...	208	C14H24O	1010215-77-9	15



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY033125\
Data File : VY021721.D
Acq On : 31 Mar 2025 15:48
Operator : SY/MD
Sample : Q1675-07
Misc : 2.16g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
T1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y032725S.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.812	1.812	7.3	ug/l	106242	1	7.707	722461	50.0
Carbonic acid, ...	13.206	10.7	ug/l	261082	4	13.346	1215660	50.0
Undecane, 3,6-d...	13.407	16.4	ug/l	398137	4	13.346	1215660	50.0
Sulfurous acid,...	13.566	6.6	ug/l	160130	4	13.346	1215660	50.0
Carbonic acid, ...	14.304	12.5	ug/l	303172	4	13.346	1215660	50.0
Naphthalene, de...	14.761	7.7	ug/l	188249	4	13.346	1215660	50.0
Nonyl tetradecy...	15.133	5.4	ug/l	130424	4	13.346	1215660	50.0
unknown15.511	15.511	10.9	ug/l	264099	4	13.346	1215660	50.0
1H-Indene, octa...	16.639	15.1	ug/l	367077	4	13.346	1215660	50.0