

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112024\
 Data File : VY020353.D
 Acq On : 20 Nov 2024 12:44
 Operator : SY/MD
 Sample : P4929-01
 Misc : 3.16g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 ARS520

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_Y\methods\82Y111924S.M
 Title : SW846 8260

Signal : TIC: VY020353.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.141	544	561	582	rBV2	271780	986834	19.45%	6.052%
2	5.647	627	644	669	rBV	1607041	5073123	100.00%	31.114%
3	6.695	802	816	834	rBV	409178	1260337	24.84%	7.730%
4	7.634	959	970	976	rBV	111968	264536	5.21%	1.622%
5	7.707	976	982	993	rVB	180124	400428	7.89%	2.456%
6	8.061	1029	1040	1051	rBV	103714	232913	4.59%	1.428%
7	8.616	1122	1131	1140	rBV	299817	585688	11.54%	3.592%
8	10.103	1368	1375	1383	rBV	441786	747003	14.72%	4.581%
9	11.414	1579	1590	1601	rBV	382581	618513	12.19%	3.793%
10	12.261	1718	1729	1735	rBV	47341	82240	1.62%	0.504%
11	12.408	1744	1753	1759	rBV	243106	397237	7.83%	2.436%
12	12.731	1802	1806	1811	rVV2	72810	111158	2.19%	0.682%
13	12.816	1815	1820	1825	rVB	31232	51946	1.02%	0.319%
14	13.042	1852	1857	1863	rBV	63621	113099	2.23%	0.694%
15	13.103	1863	1867	1873	rVB	32931	58524	1.15%	0.359%
16	13.347	1900	1907	1916	rVV3	249584	480319	9.47%	2.946%
17	13.542	1933	1939	1942	rBV5	25802	51486	1.01%	0.316%
18	13.676	1954	1961	1969	rBV2	170185	314191	6.19%	1.927%
19	13.889	1992	1996	2001	rVB3	42629	67428	1.33%	0.414%
20	13.999	2009	2014	2018	rBV3	51087	91275	1.80%	0.560%
21	14.048	2018	2022	2030	rBV7	52828	123400	2.43%	0.757%
22	14.133	2030	2036	2038	rBV5	42127	93825	1.85%	0.575%
23	14.176	2038	2043	2044	rBV5	77696	116945	2.31%	0.717%
24	14.200	2044	2047	2051	rVB2	80329	133236	2.63%	0.817%
25	14.310	2060	2065	2068	rBV2	143147	238802	4.71%	1.465%
26	14.340	2068	2070	2073	rVV3	77503	99847	1.97%	0.612%
27	14.389	2073	2078	2084	rVB6	80661	183024	3.61%	1.122%
28	14.505	2093	2097	2098	rBV3	74858	90991	1.79%	0.558%
29	14.529	2098	2101	2106	rVB	264814	368122	7.26%	2.258%
30	14.602	2107	2113	2117	rBV4	115778	288648	5.69%	1.770%
31	14.651	2117	2121	2127	rVB3	140999	233123	4.60%	1.430%
32	14.761	2136	2139	2141	rBV4	59041	86201	1.70%	0.529%
33	14.791	2141	2144	2148	rVB	129997	185067	3.65%	1.135%
34	14.858	2151	2155	2159	rVB3	151653	223785	4.41%	1.372%
35	14.919	2160	2165	2167	rBV	113350	198004	3.90%	1.214%
36	15.011	2176	2180	2183	rBV4	69534	104621	2.06%	0.642%

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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

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37	15.054	2184	2187	2192	rVB5	101724	158100	3.12%	0.970%
38	15.188	2205	2209	2216	rBV4	119285	269192	5.31%	1.651%
39	15.346	2231	2235	2239	rBV	157554	213648	4.21%	1.310%
40	16.364	2398	2402	2416	rVB5	235577	620459	12.23%	3.805%
41	16.645	2444	2448	2454	rVB2	147497	287823	5.67%	1.765%

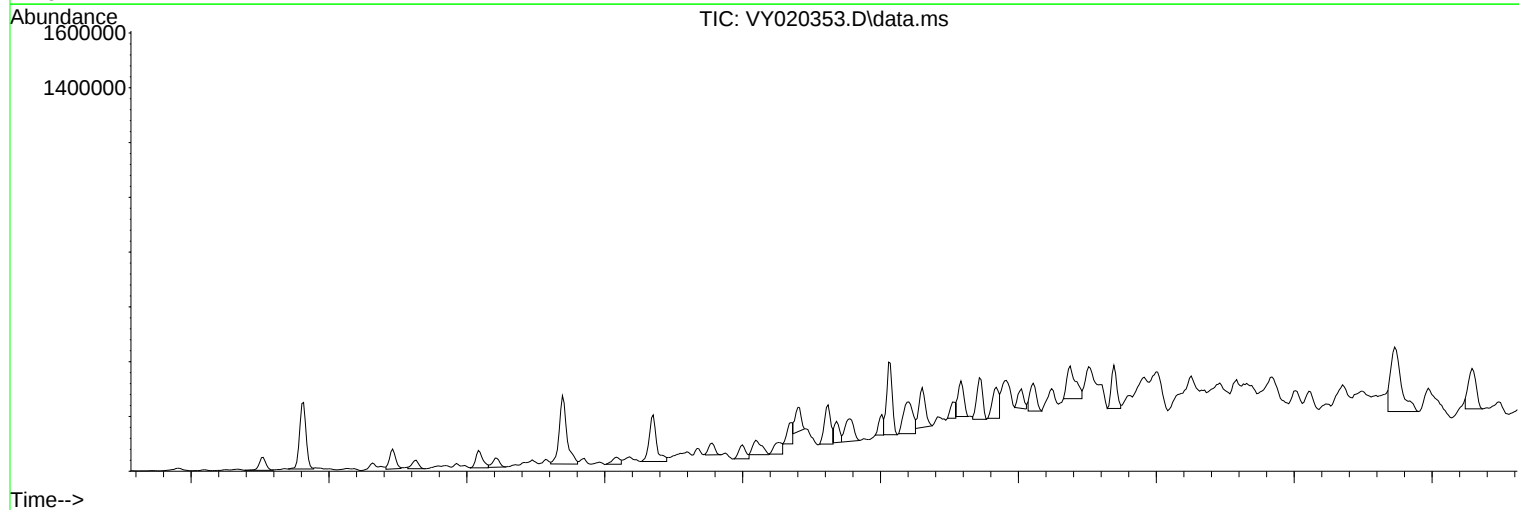
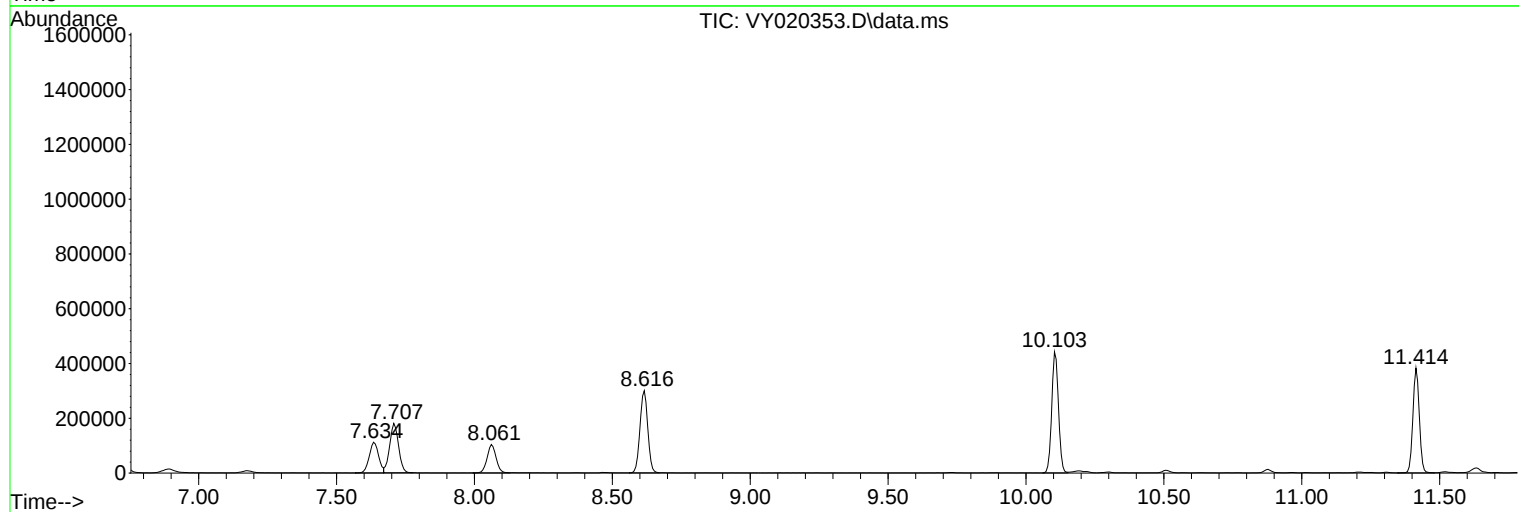
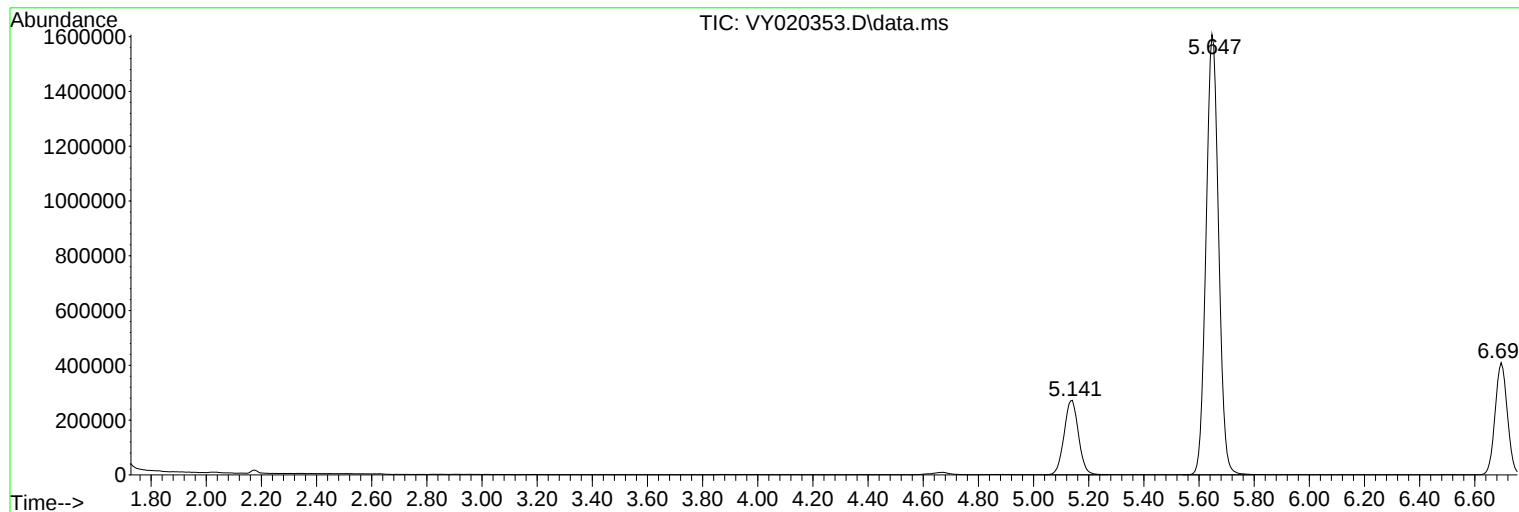
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Quant Title : SW846 8260

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



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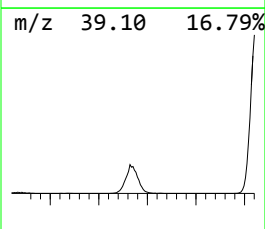
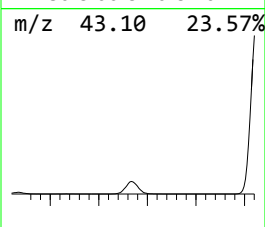
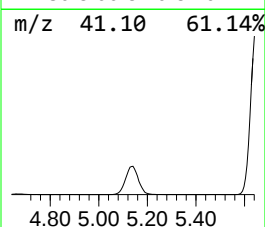
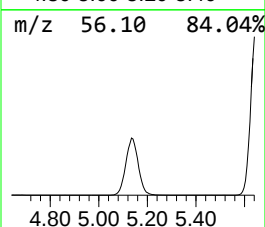
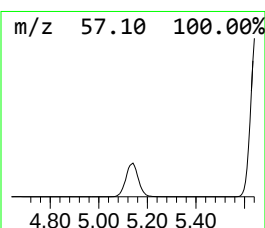
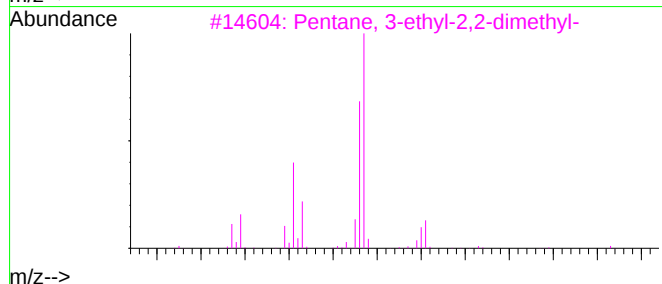
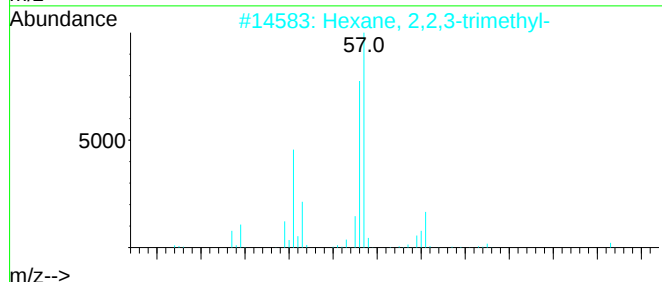
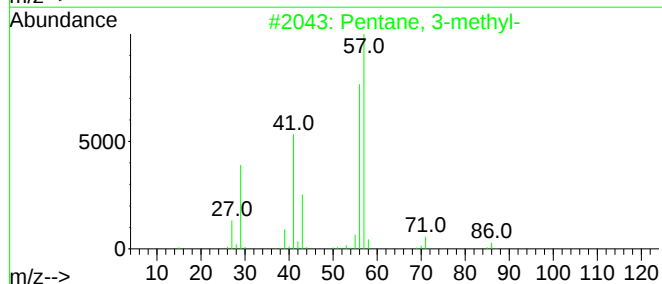
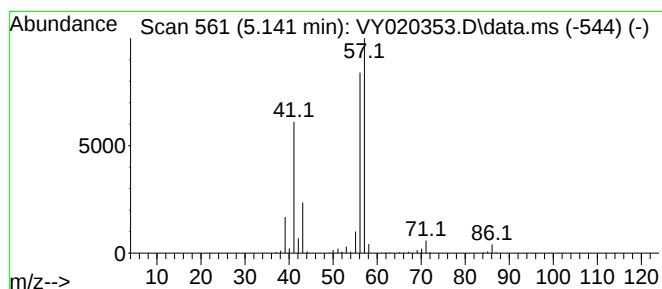
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.141	123.22 ug/l	986834	Pentafluorobenzene	7.707

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
4	Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	50
5	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
ARS520

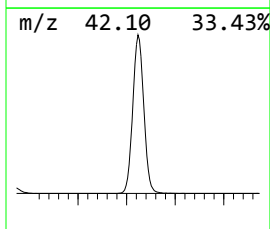
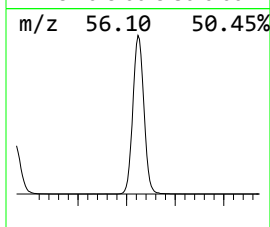
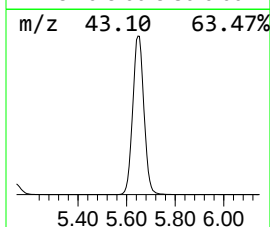
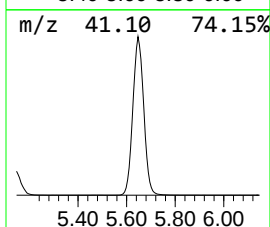
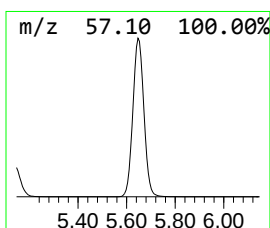
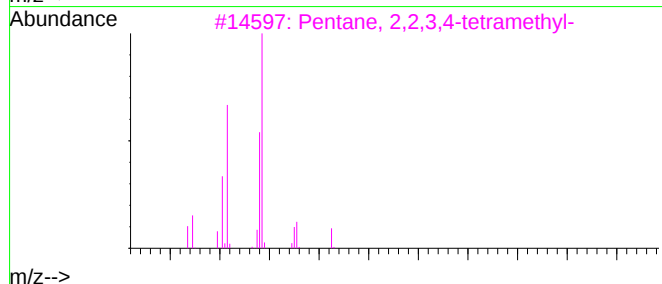
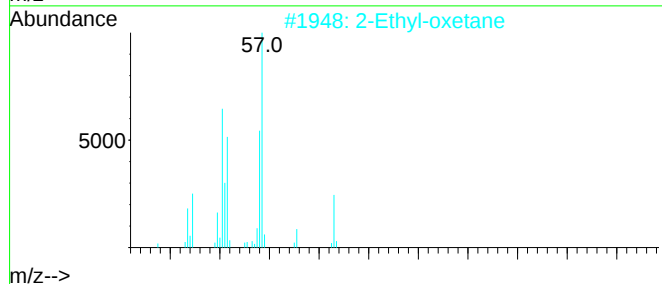
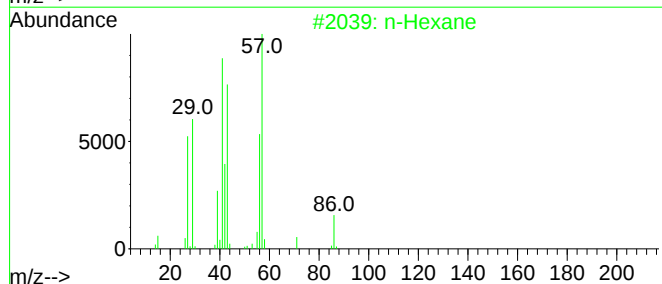
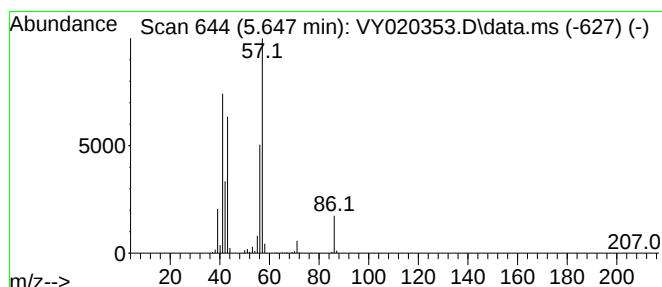
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
Quant Title : SW846 8260

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

Peak Number 2 n-Hexane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.647	633.46 ug/l	5073120	Pentafluorobenzene	7.707

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	91
2	2-Ethyl-oxetane	86	C5H10O	1010386-40-2	78
3	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	40
4	Butanal, 2-methyl-	86	C5H10O	000096-17-3	38
5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	38



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Misc : 3.16g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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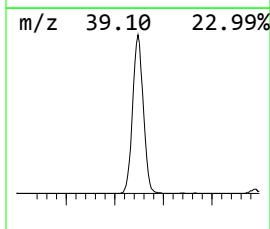
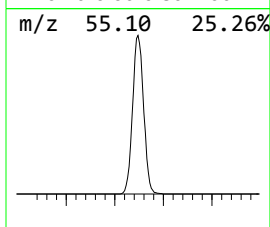
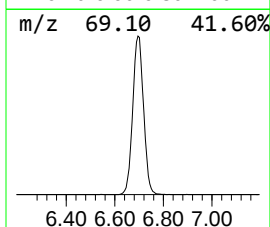
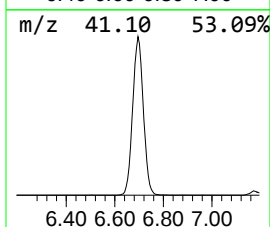
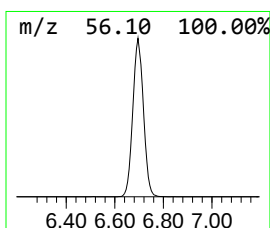
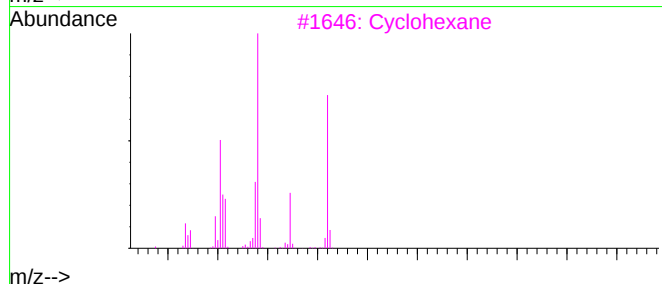
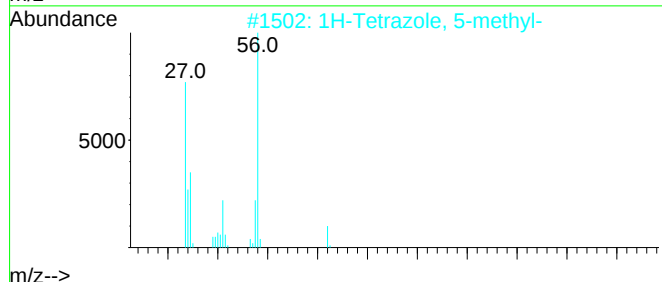
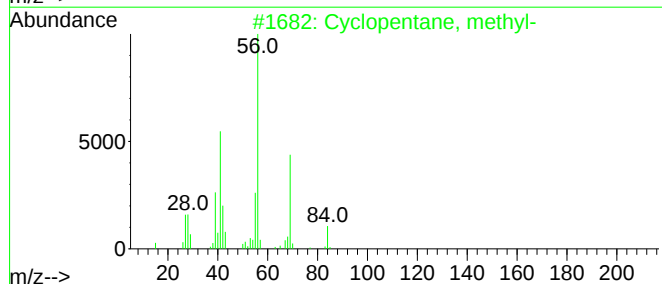
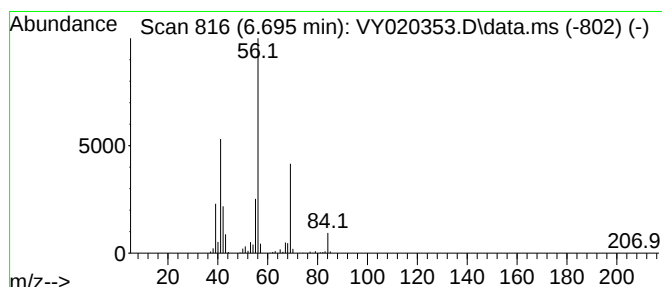
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Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.695	157.37 ug/l	1260340	Pentafluorobenzene	7.707

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3	Cyclohexane	84	C6H12	000110-82-7	78
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50



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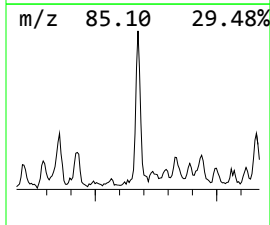
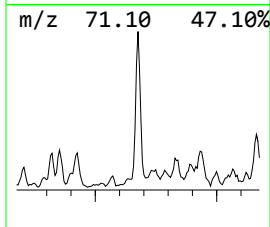
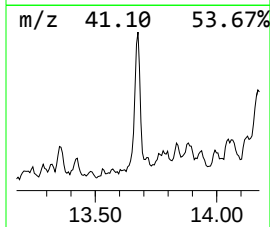
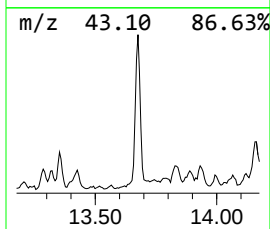
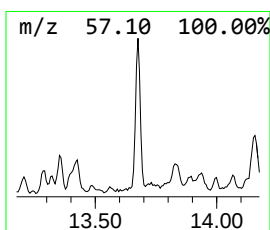
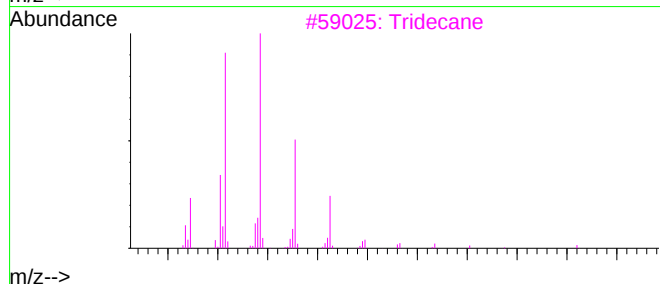
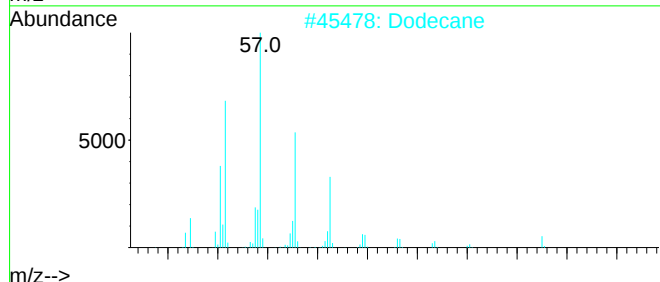
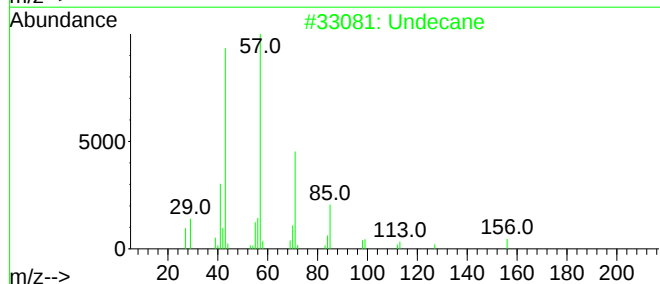
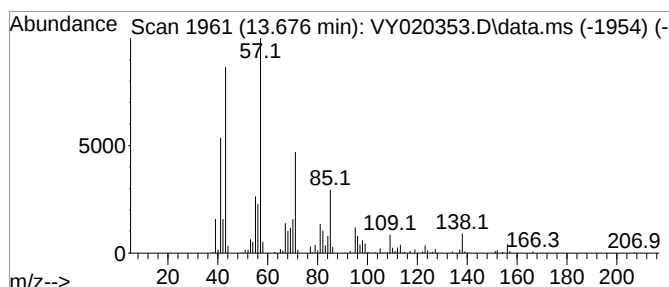
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Peak Number 4 Undecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	32.71 ug/l	314191	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	64
2	Dodecane	170	C12H26	000112-40-3	59
3	Tridecane	184	C13H28	000629-50-5	50
4	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	50
5	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	50



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Quant Title : SW846 8260

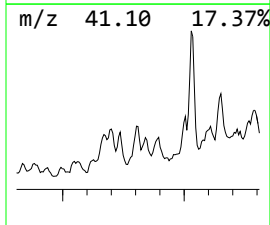
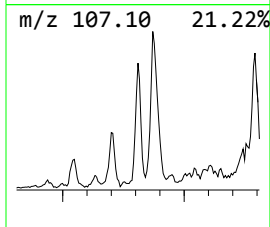
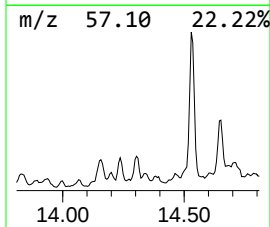
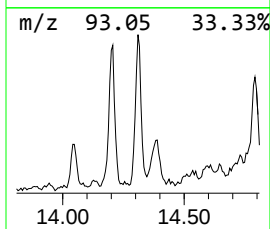
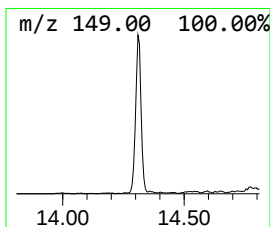
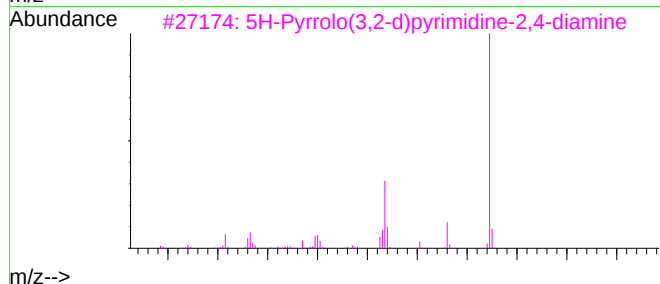
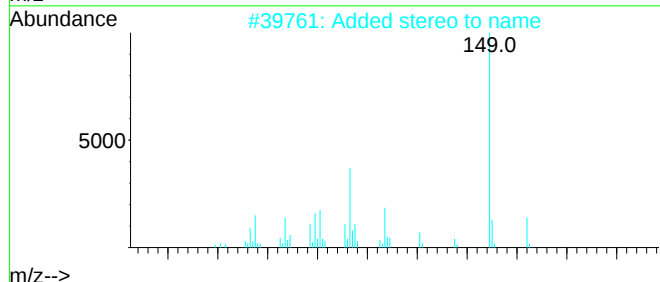
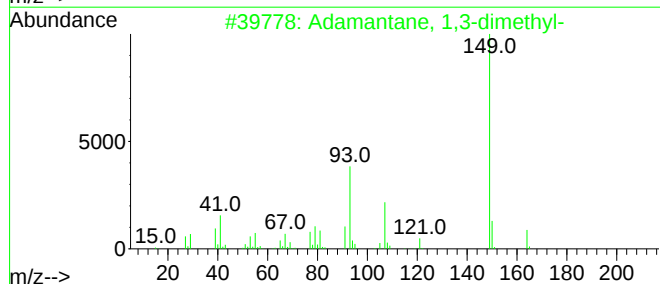
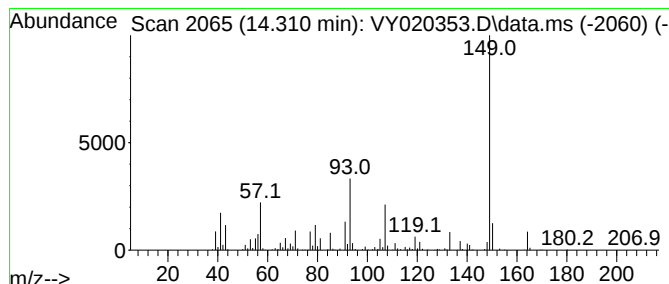
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 Adamantane, 1,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.310	24.86 ug/l	238802	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	91
2	Added stereo to name	164	C12H20	024145-89-9	72
3	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	59
4	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	53
5	Pyridinium, 1-(acetylamino)-2,6-...	164	C9H12N2O	031020-35-6	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112024\
Data File : VY020353.D
Acq On : 20 Nov 2024 12:44
Operator : SY/MD
Sample : P4929-01
Misc : 3.16g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
ARS520

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
Quant Title : SW846 8260

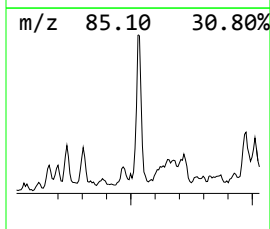
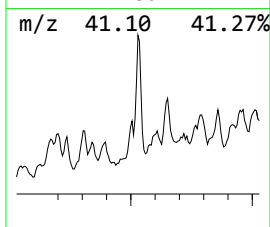
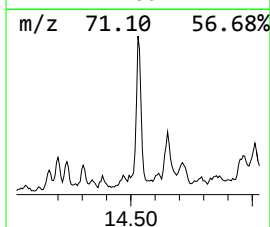
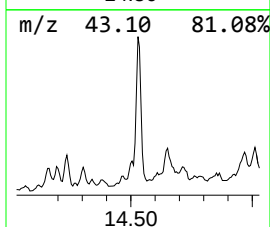
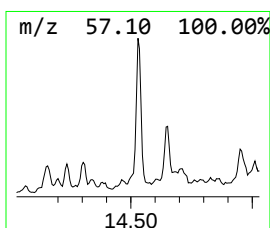
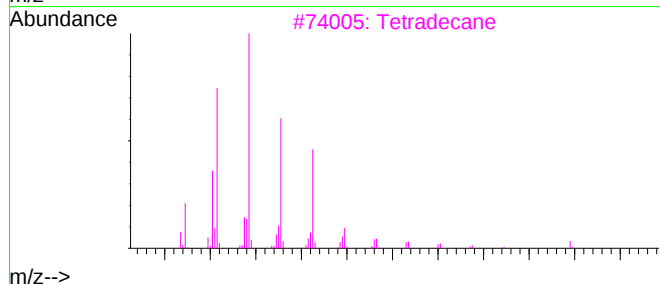
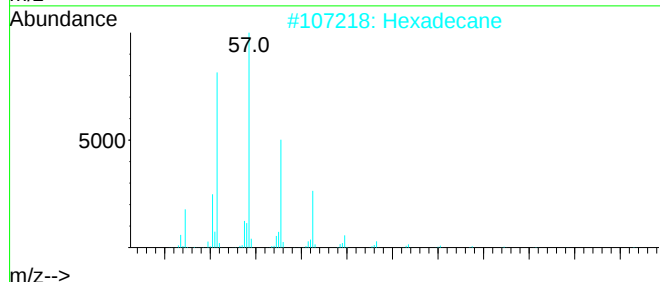
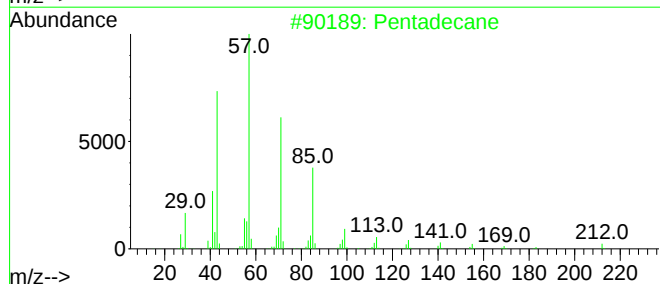
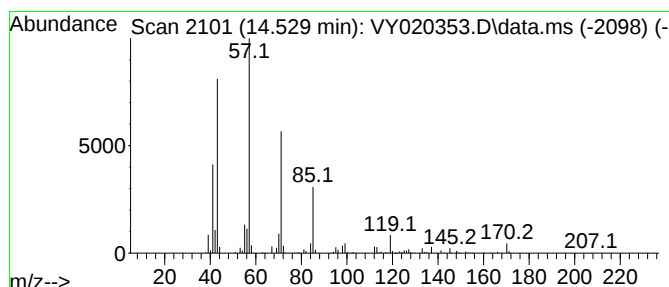
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.529	38.32 ug/l	368122	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	86
2	Hexadecane	226	C16H34	000544-76-3	86
3	Tetradecane	198	C14H30	000629-59-4	80
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
5	Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112024\
Data File : VY020353.D
Acq On : 20 Nov 2024 12:44
Operator : SY/MD
Sample : P4929-01
Misc : 3.16g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
ARS520

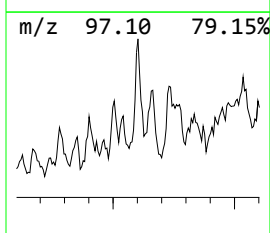
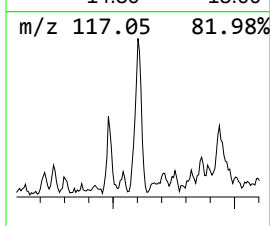
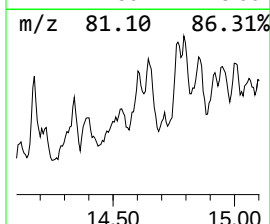
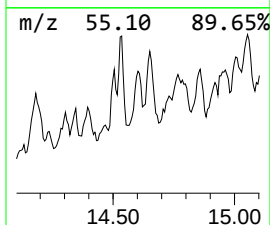
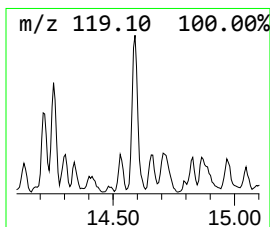
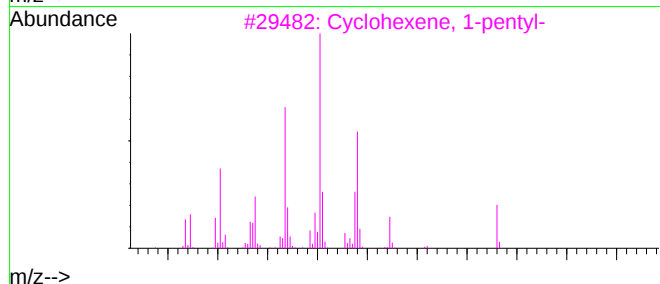
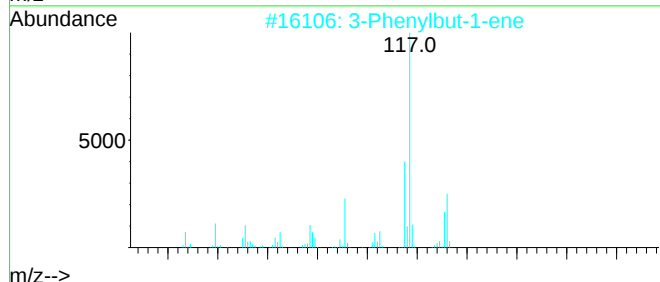
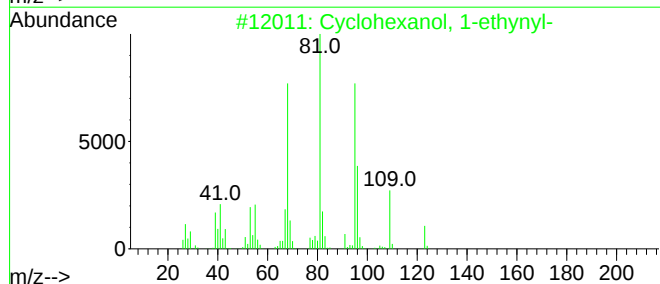
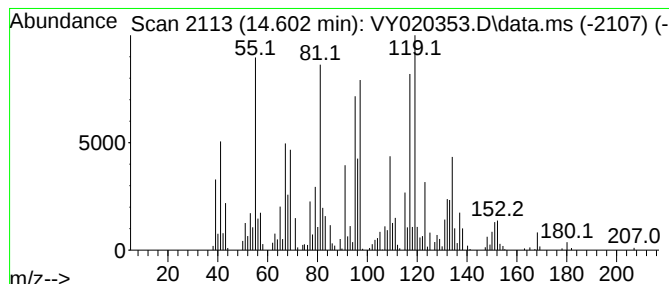
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Quant Title : SW846 8260

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

Peak Number 7 unknown14.602 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.602	30.05 ug/l	288648	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanol, 1-ethynyl-	124	C8H12O	000078-27-3	25
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	25
3			Cyclohexene, 1-pentyl-	152	C11H20	015232-85-6	25
4			Ethanone, 1-(4-methylphenyl)-	134	C9H10O	000122-00-9	25
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112024\
Data File : VY020353.D
Acq On : 20 Nov 2024 12:44
Operator : SY/MD
Sample : P4929-01
Misc : 3.16g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
ARS520

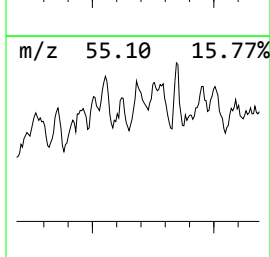
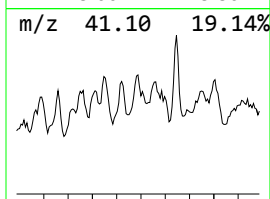
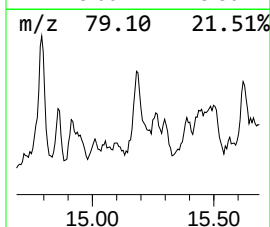
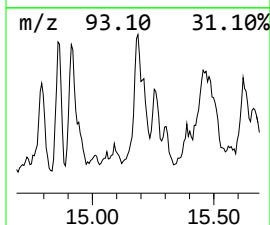
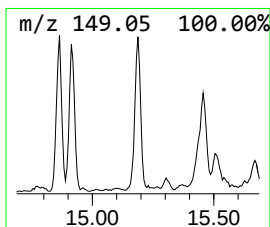
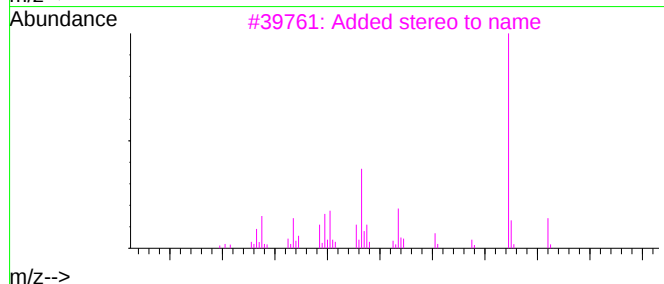
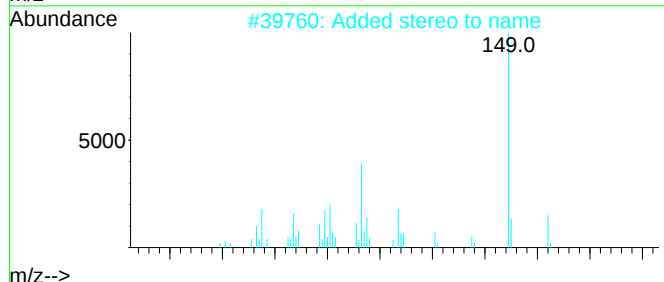
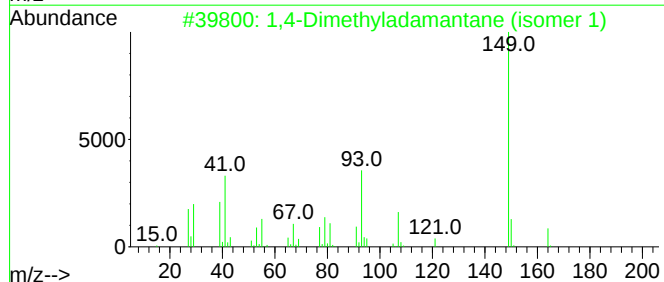
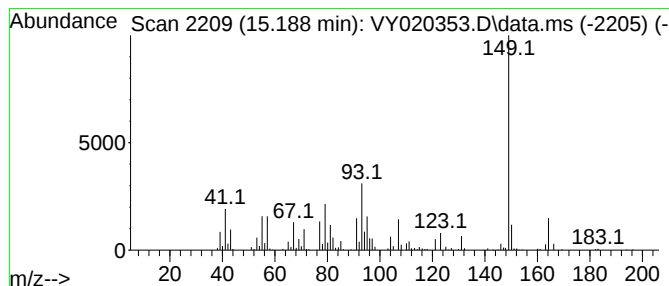
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 1,4-Dimethyladamantane (iso... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.188	28.02 ug/l	269192	1,4-Dichlorobenzene-d4	13.347	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	87
2	Added stereo to name	164	C12H20	024145-88-8	81
3	Added stereo to name	164	C12H20	024145-89-9	74
4	4-(2-Methyl-cyclohex-1-enyl)-but...	164	C11H16O	041437-92-7	72
5	Furan-3-ylethynyltrimethylsilane	164	C9H12OSi	465521-19-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112024\
Data File : VY020353.D
Acq On : 20 Nov 2024 12:44
Operator : SY/MD
Sample : P4929-01
Misc : 3.16g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
ARS520

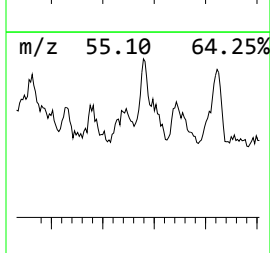
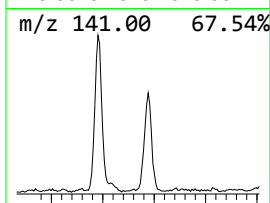
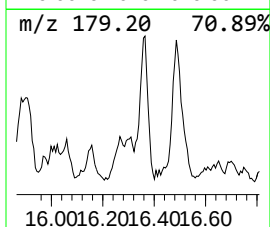
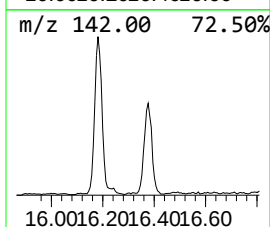
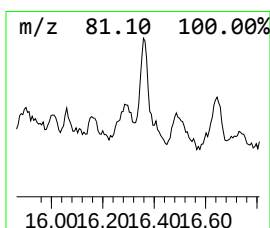
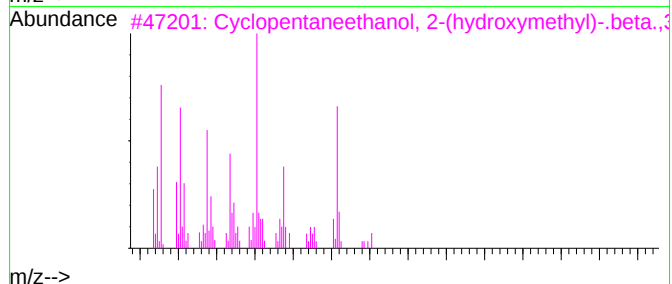
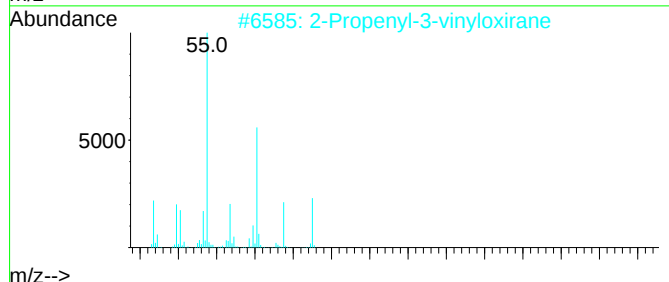
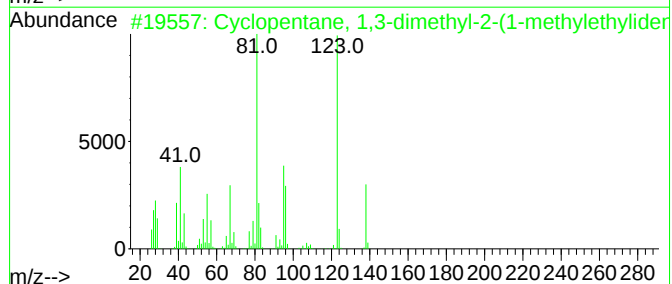
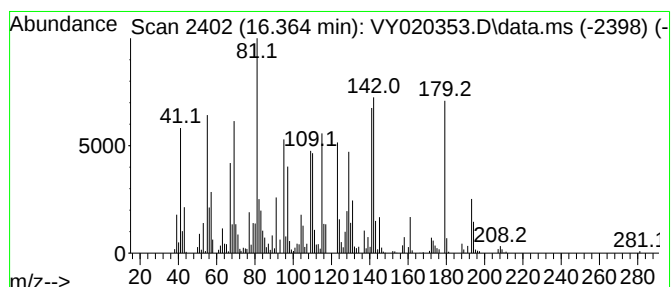
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
Quant Title : SW846 8260

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

Peak Number 9 unknown16.364 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.364	64.59 ug/l	620459	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,3-dimethyl-2-(1-...	138	C10H18	061142-30-1	22
2			2-Propenyl-3-vinyloxirane	110	C7H10O	070597-49-8	22
3			Cyclopentaneethanol, 2-(hydroxym...	172	C10H20O2	000485-42-7	22
4			2-(2-Hydroxycyclooctyl)-furan	194	C12H18O2	115754-90-0	20
5			4-Ethylcyclohexene	110	C8H14	003742-42-5	18



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112024\
Data File : VY020353.D
Acq On : 20 Nov 2024 12:44
Operator : SY/MD
Sample : P4929-01
Misc : 3.16g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
ARS520

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
Quant Title : SW846 8260

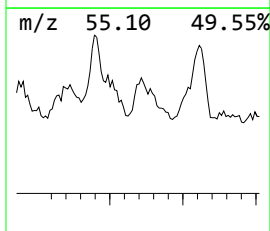
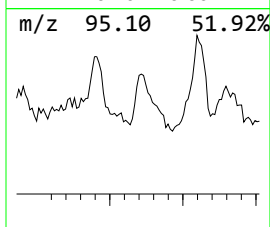
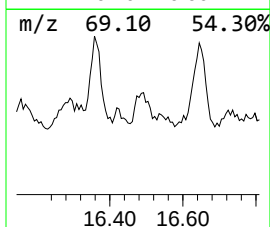
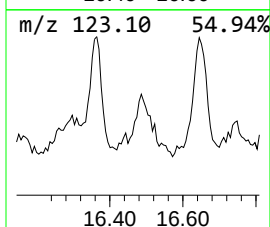
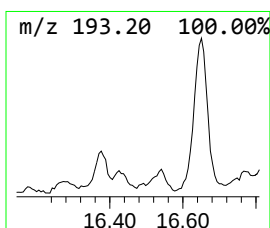
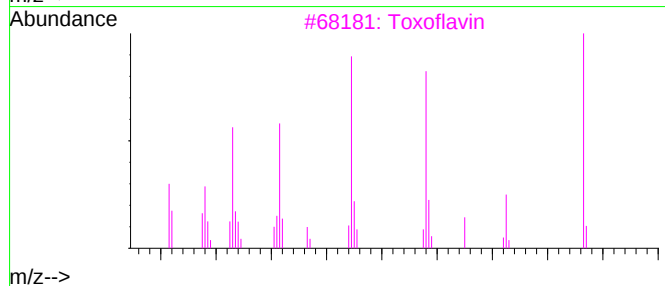
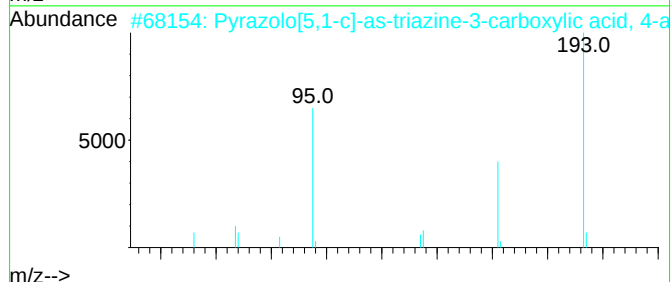
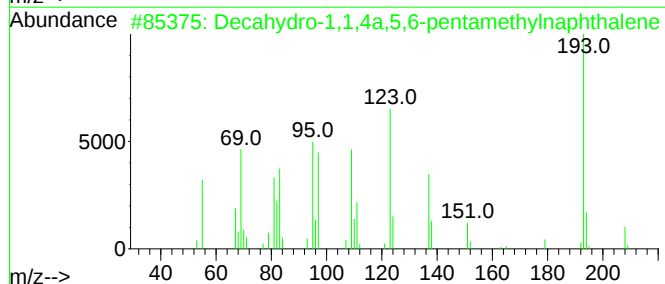
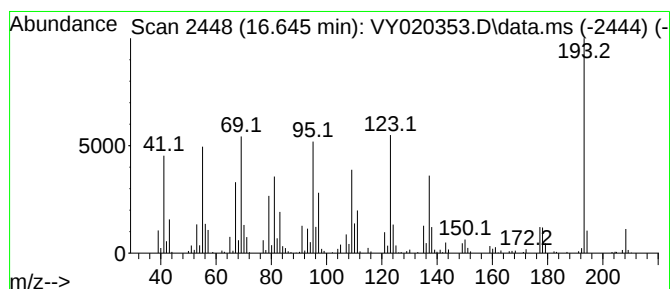
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 10 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.645	29.96 ug/l	287823	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	91
2			Pyrazolo[5,1-c]-as-triazine-3-ca...	193	C6H7N7O	016111-78-7	35
3			Toxoflavin	193	C7H7N5O2	000084-82-2	27
4			Naphthalene, decahydro-1,8a-dime...	208	C15H28	015404-63-4	22
5			Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112024\
Data File : VY020353.D
Acq On : 20 Nov 2024 12:44
Operator : SY/MD
Sample : P4929-01
Misc : 3.16g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
ARS520

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.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
Pentane, 3-methyl-	5.141	123.2	ug/l	986834	1	7.707	400428	50.0
n-Hexane	5.647	633.5	ug/l	5073120	1	7.707	400428	50.0
Cyclopentane, m...	6.695	157.4	ug/l	1260340	1	7.707	400428	50.0
Undecane	13.676	32.7	ug/l	314191	4	13.347	480319	50.0
Adamantane, 1,3...	14.310	24.9	ug/l	238802	4	13.347	480319	50.0
Pentadecane	14.529	38.3	ug/l	368122	4	13.347	480319	50.0
unknown14.602	14.602	30.1	ug/l	288648	4	13.347	480319	50.0
1,4-Dimethylada...	15.188	28.0	ug/l	269192	4	13.347	480319	50.0
unknown16.364	16.364	64.6	ug/l	620459	4	13.347	480319	50.0
Decahydro-1,1,4...	16.645	30.0	ug/l	287823	4	13.347	480319	50.0