

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD070721\
 Data File : VD069609.D
 Acq On : 07 Jul 2021 15:36
 Operator : VA/SY
 Sample : M2936-01
 Misc : 5.08G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 TR-05-070221

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_D\Method\82D062121S.M
 Title : SW846 8260

Signal : TIC: VD069609.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.156	379	380	386	rVB2	6478	10948	1.22%	0.161%
2	4.962	509	517	528	rVB4	16406	46931	5.23%	0.692%
3	7.191	886	896	905	rBV2	32290	92533	10.31%	1.364%
4	7.697	976	982	986	rBV4	6532	13212	1.47%	0.195%
5	7.914	1007	1019	1024	rBV2	143930	339634	37.83%	5.005%
6	7.973	1024	1029	1038	rVB	184041	421178	46.91%	6.207%
7	8.332	1074	1090	1099	rBV	139524	318325	35.45%	4.691%
8	8.861	1171	1180	1189	rBV	305272	629553	70.12%	9.278%
9	10.338	1423	1431	1440	rBV	497519	897848	100.00%	13.232%
10	11.085	1552	1558	1561	rVB5	13047	19134	2.13%	0.282%
11	11.638	1643	1652	1661	rBV	497376	872646	97.19%	12.861%
12	12.261	1755	1758	1764	rVB6	8770	14290	1.59%	0.211%
13	12.626	1813	1820	1830	rVB	350099	587294	65.41%	8.655%
14	12.943	1869	1874	1875	rBV4	9333	11136	1.24%	0.164%
15	13.173	1909	1913	1919	rVB5	15295	25679	2.86%	0.378%
16	13.249	1924	1926	1931	rVB5	7459	9669	1.08%	0.142%
17	13.308	1931	1936	1939	rBV3	7968	11894	1.32%	0.175%
18	13.567	1974	1980	1989	rVB	464317	744365	82.91%	10.970%
19	13.890	2029	2035	2039	rBV6	13099	26646	2.97%	0.393%
20	14.208	2086	2089	2094	rVB7	9779	16480	1.84%	0.243%
21	14.273	2094	2100	2105	rBV8	23647	46986	5.23%	0.692%
22	14.432	2117	2127	2134	rVB3	42475	112641	12.55%	1.660%
23	14.532	2138	2144	2151	rBV	60322	130726	14.56%	1.927%
24	14.596	2151	2155	2161	rVB6	22044	42097	4.69%	0.620%
25	14.679	2166	2169	2172	rBV4	11873	17075	1.90%	0.252%
26	14.743	2177	2180	2185	rBV7	13083	17781	1.98%	0.262%
27	14.820	2187	2193	2195	rBV5	26576	52925	5.89%	0.780%
28	14.861	2195	2200	2207	rVB4	67721	130807	14.57%	1.928%
29	14.932	2207	2212	2218	rBV10	14534	40222	4.48%	0.593%
30	15.085	2233	2238	2242	rVB7	23576	36030	4.01%	0.531%
31	15.149	2245	2249	2251	rBV5	25615	43772	4.88%	0.645%
32	15.267	2267	2269	2277	rVB9	37507	86441	9.63%	1.274%
33	15.355	2278	2284	2291	rBV2	147871	269645	30.03%	3.974%
34	15.420	2291	2295	2300	rBV8	34045	73152	8.15%	1.078%
35	15.761	2351	2353	2359	rVB6	64910	101783	11.34%	1.500%
36	16.332	2445	2450	2458	rVB4	115750	224908	25.05%	3.315%

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ClientSampleId :
TR-05-070221

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	16.684	2504	2510	2524	rVB4	61676	248887	27.72%	3.668%
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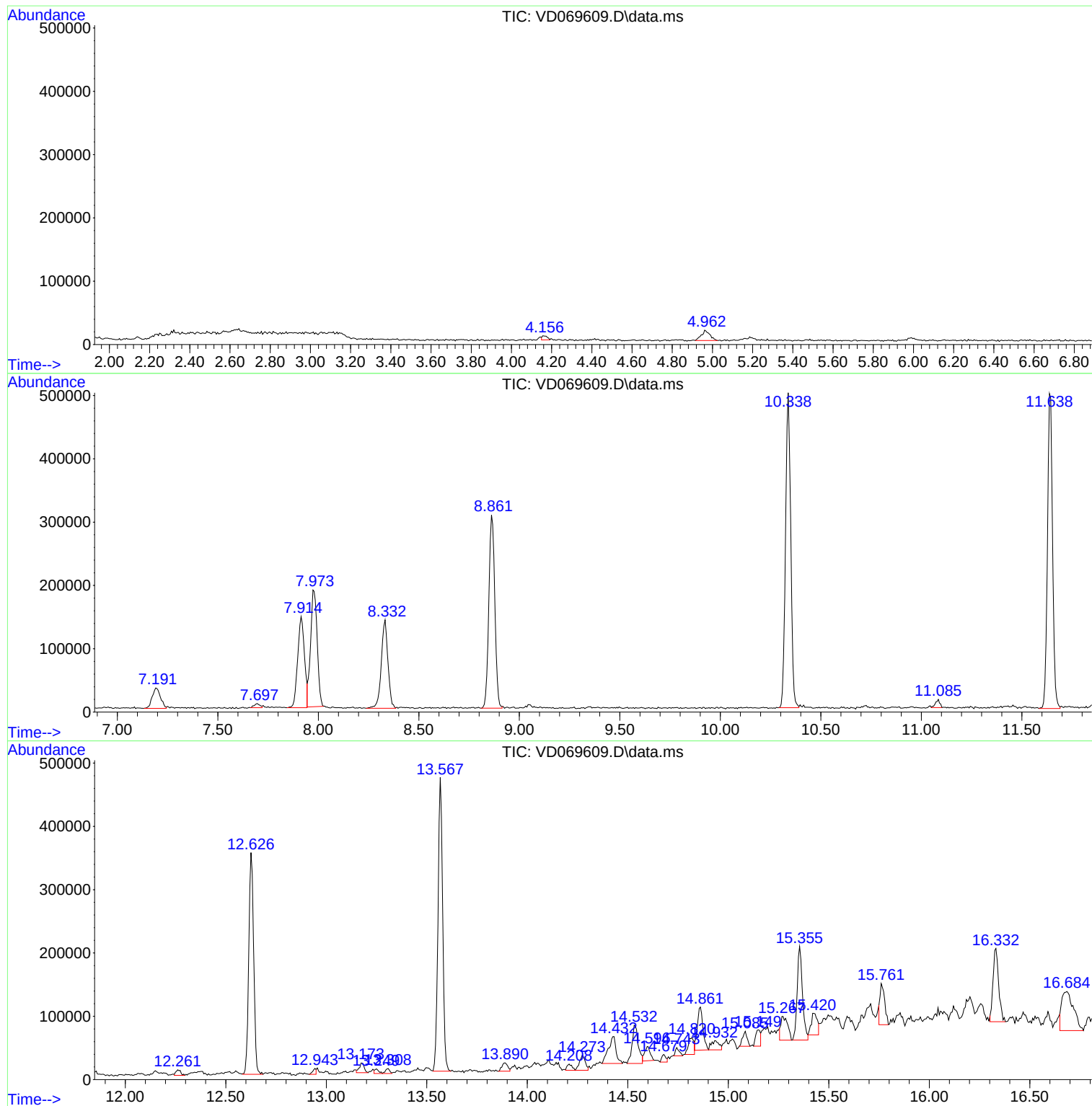
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Quant Title : SW846 8260

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



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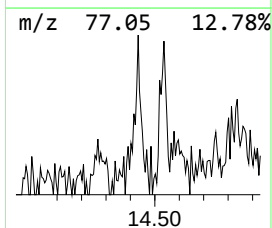
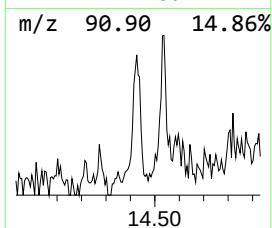
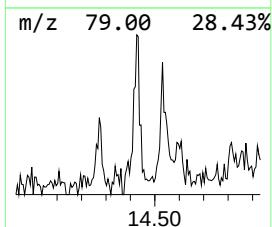
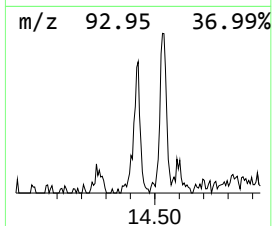
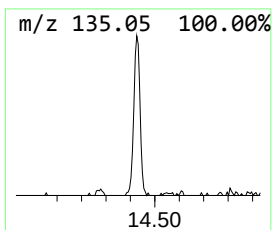
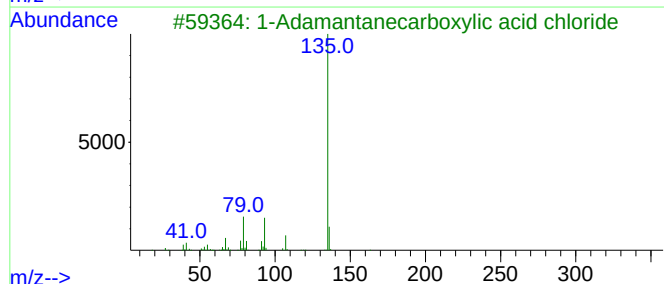
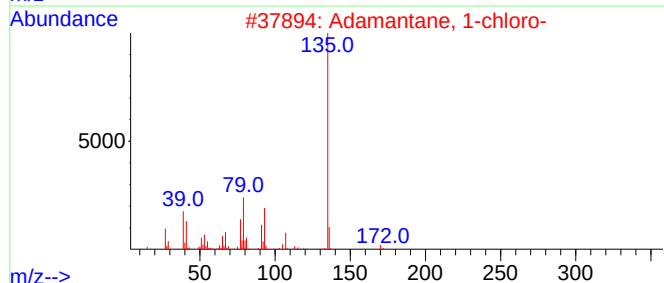
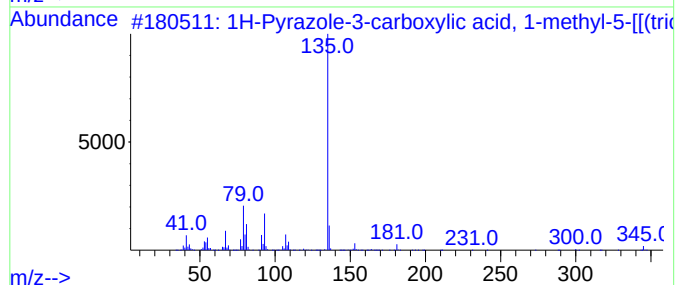
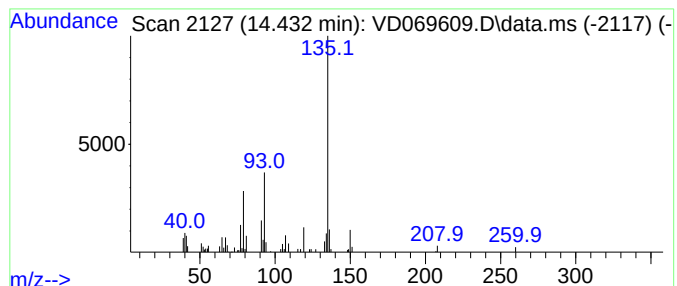
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D062121S.M
Quant Title : SW846 8260

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

Peak Number 3 1H-Pyrazole-3-carboxylic ac... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.432	7.57 ug/l	112641	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Pyrazole-3-carboxylic acid, 1...	345	C19H27N3O3	1000351-30-4	59
2			Adamantane, 1-chloro-	170	C10H15Cl	000935-56-8	59
3			1-Adamantanecarboxylic acid chlo...	198	C11H15ClO	002094-72-6	59
4			N-[2-(Trifluoromethyl)phenyl]-1-...	323	C18H20F3NO	314055-04-4	59
5			4-(1-Adamantanecarboxamido)-2-et...	476	C30H40N2O3	143413-39-2	59



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Instrument :
MSVOA_D
ClientSampleId :
TR-05-070221

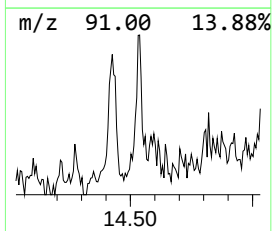
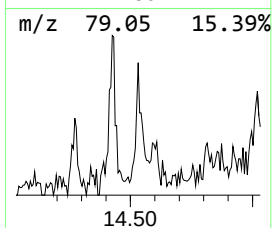
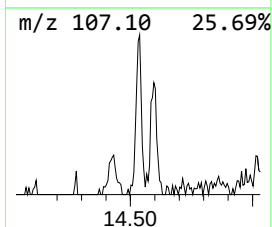
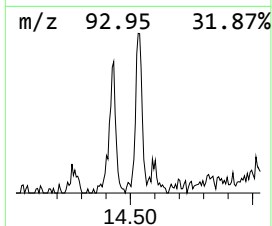
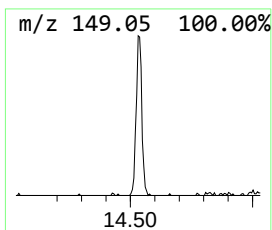
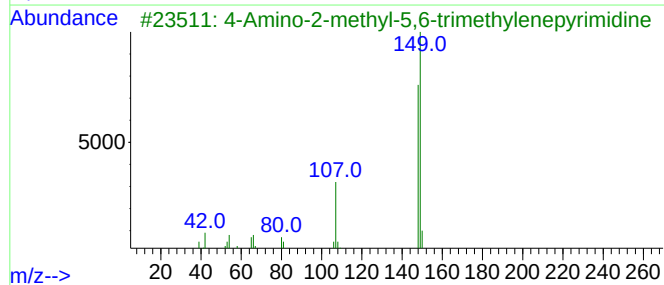
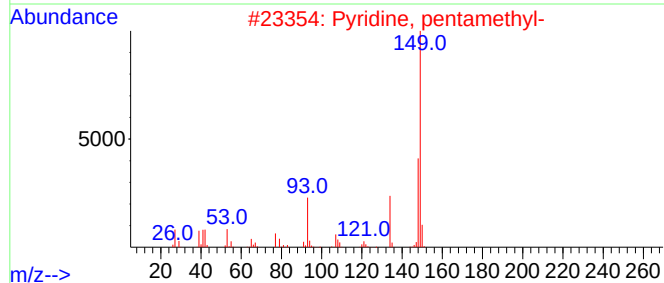
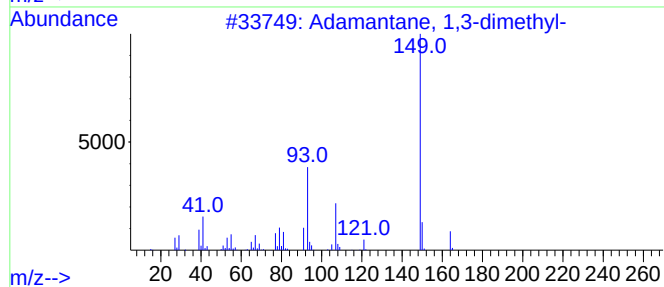
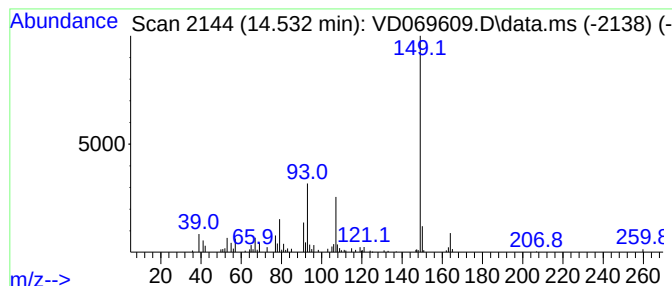
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D062121S.M
Quant Title : SW846 8260

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

Peak Number 4 Adamantane, 1,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.532	8.78 ug/l	130726	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	87
2			Pyridine, pentamethyl-	149	C10H15N	003748-83-2	64
3			4-Amino-2-methyl-5,6-trimethylen...	149	C8H11N3	076881-49-7	58
4			Phthalic acid, 2-chloropropyl oc...	494	C29H47ClO4	1000356-83-9	43
5			1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	43



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ALS Vial : 10 Sample Multiplier: 1

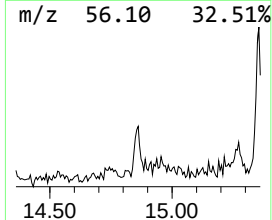
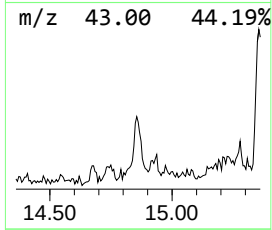
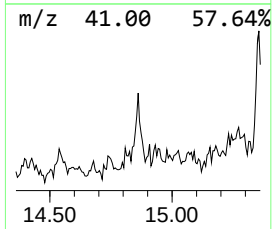
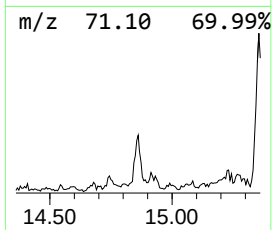
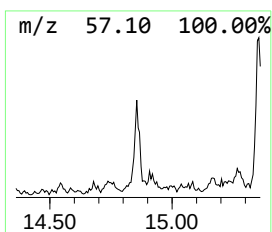
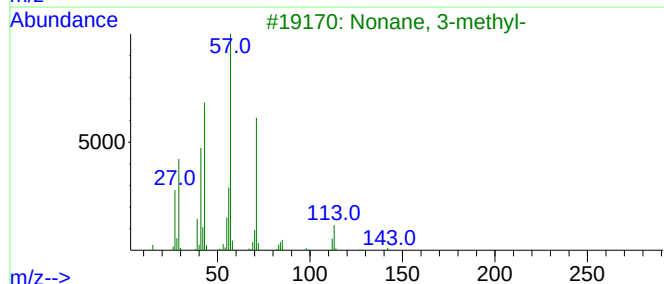
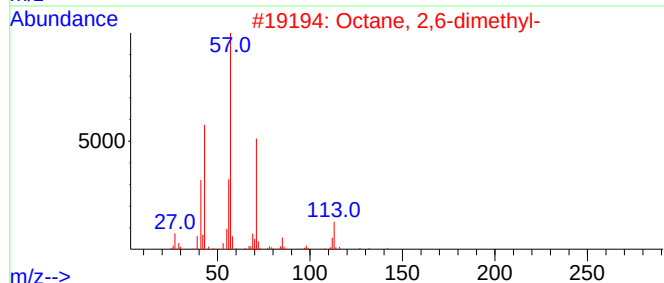
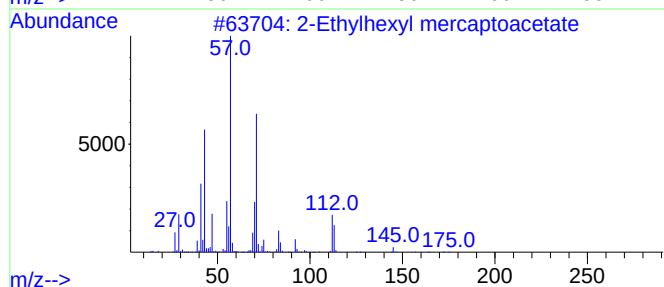
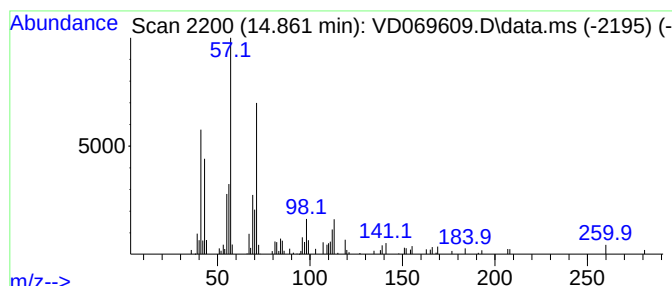
Instrument :
MSVOA_D
ClientSampleId :
TR-05-070221

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D062121S.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Ethylhexyl mercaptoacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.861	8.79 ug/l	130807	1,4-Dichlorobenzene-d4	13.567	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	59
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	59
3	Nonane, 3-methyl-	142	C10H22	005911-04-6	59
4	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	59
5	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	58



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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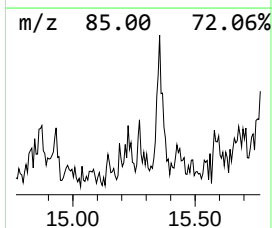
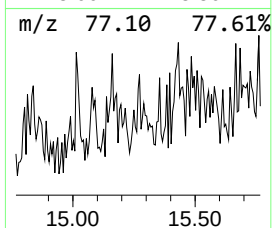
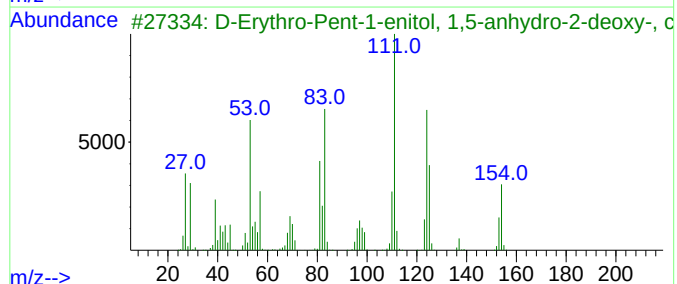
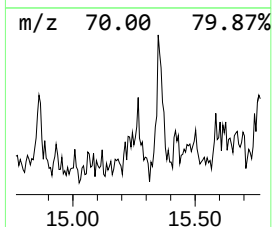
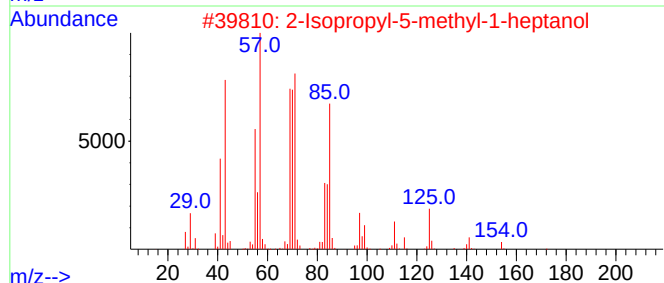
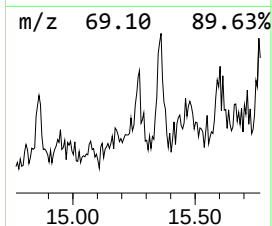
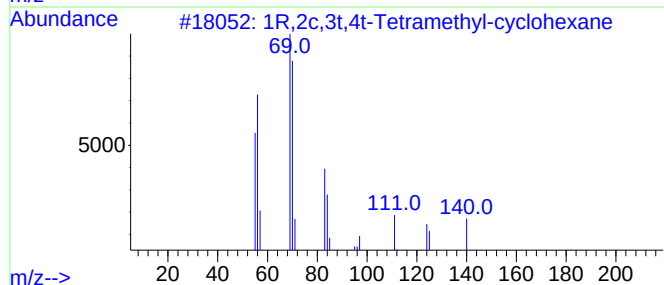
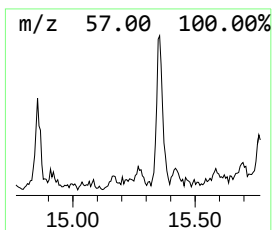
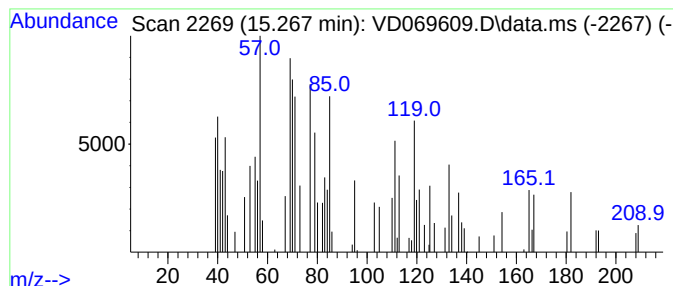
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Quant Title : SW846 8260

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

Peak Number 6 unknown15.267 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.267	5.81 ug/l	86441	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1R,2c,3t,4t-Tetramethyl-cyclohexane	140	C10H20	1000144-07-3	27		
2	2-Isopropyl-5-methyl-1-heptanol	172	C11H24O	091337-07-4	22		
3	D-Erythro-Pent-1-enitol, 1,5-anh...	154	C7H11BO3	074793-26-3	18		
4	N-Guanyproline	157	C6H11N3O2	1000130-31-0	14		
5	2-Undecene, 2,5-dimethyl-	182	C13H26	049622-16-4	14		



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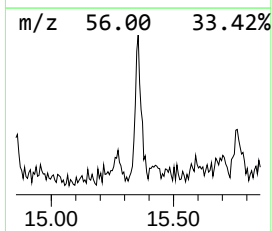
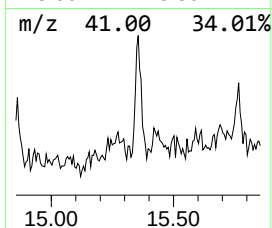
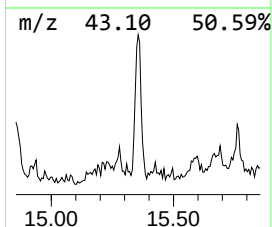
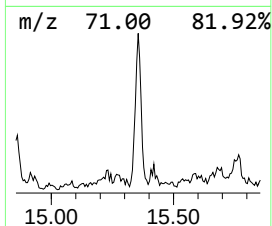
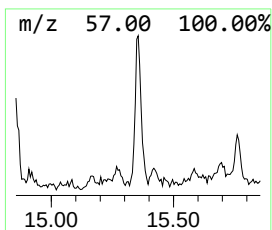
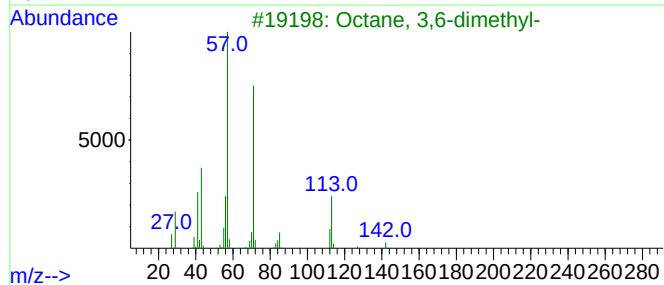
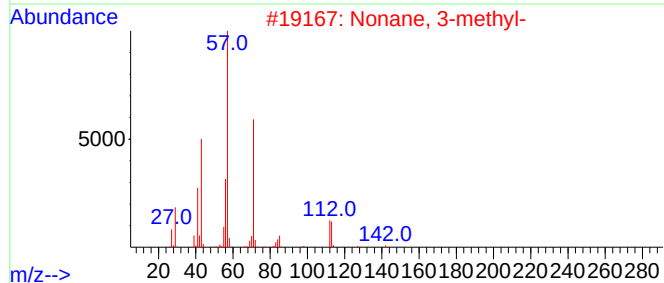
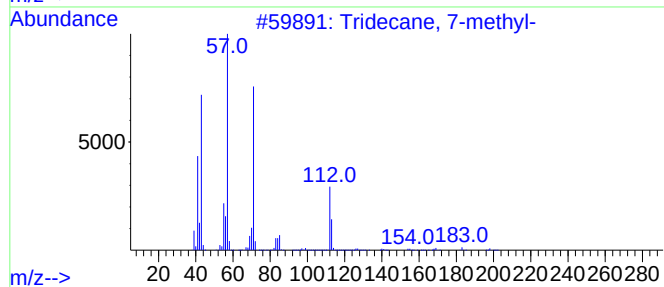
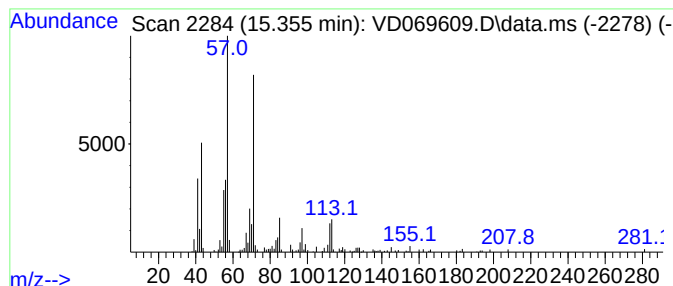
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D062121S.M
Quant Title : SW846 8260

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

Peak Number 7 Tridecane, 7-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.355	18.11 ug/l	269645	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 7-methyl-	198	C14H30	026730-14-3	76
2			Nonane, 3-methyl-	142	C10H22	005911-04-6	72
3			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	59
4			Oxalic acid, ethyl neopentyl ester	188	C9H16O4	1000309-72-4	50
5			Octane, 2-iodo-	240	C8H17I	000557-36-8	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD070721\
Data File : VD069609.D
Acq On : 07 Jul 2021 15:36
Operator : VA/SY
Sample : M2936-01
Misc : 5.08G/5.00ml/MSVOA_D/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
TR-05-070221

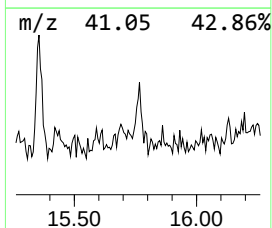
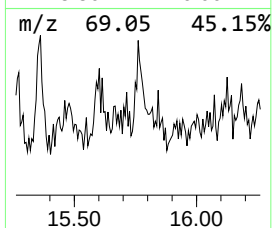
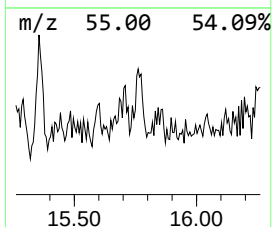
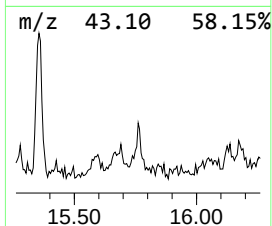
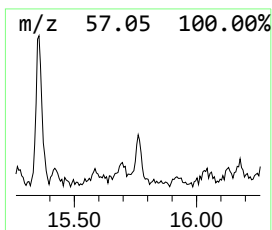
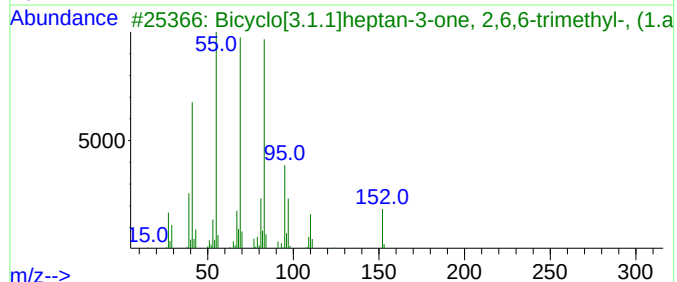
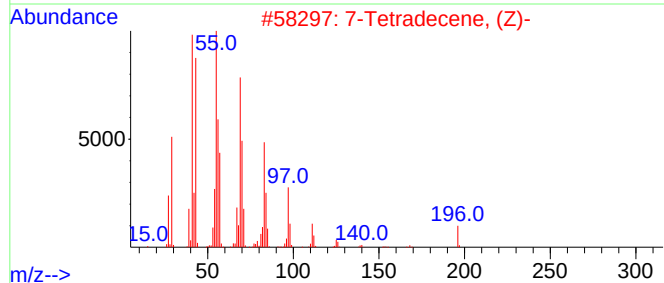
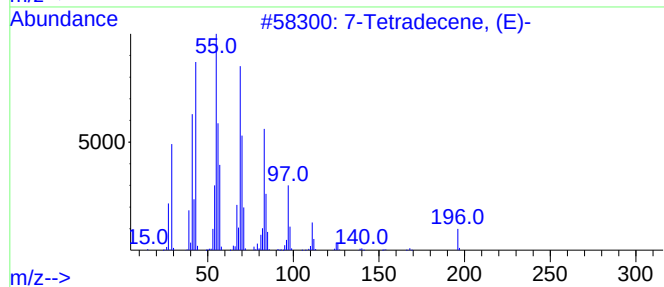
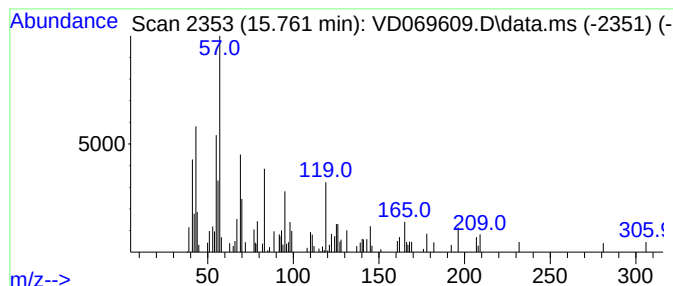
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D062121S.M
Quant Title : SW846 8260

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

Peak Number 8 unknown15.761 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.761	6.84 ug/l	101783	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Tetradecene, (E)-	196	C14H28	041446-63-3	30
2			7-Tetradecene, (Z)-	196	C14H28	041446-60-0	22
3			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	22
4			2-Butenoic acid, 2-methyl-, 2-pr...	140	C8H12O2	007493-71-2	22
5			Ethanone, 1-cyclohexyl-	126	C8H14O	000823-76-7	18



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD070721\
Data File : VD069609.D
Acq On : 07 Jul 2021 15:36
Operator : VA/SY
Sample : M2936-01
Misc : 5.08G/5.00ml/MSVOA_D/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
TR-05-070221

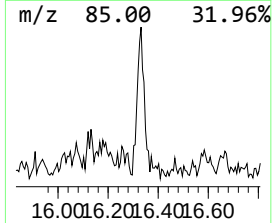
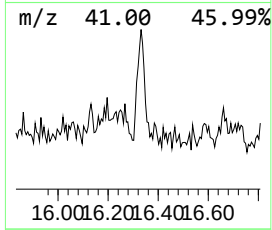
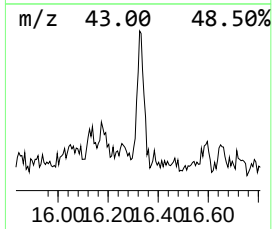
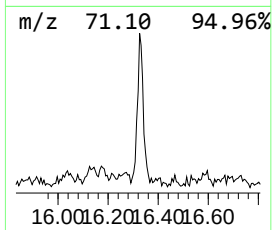
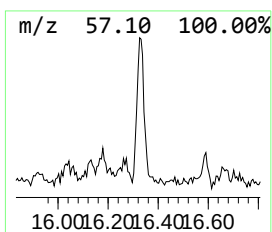
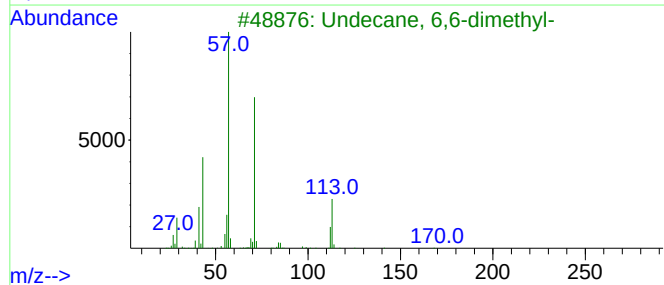
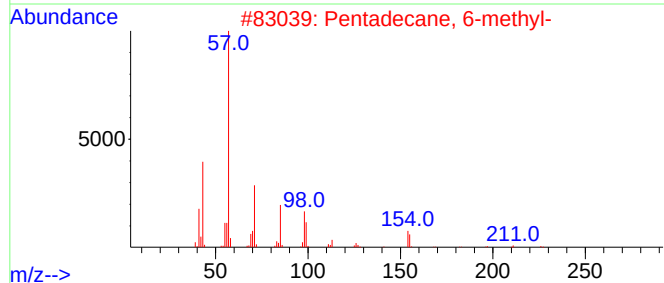
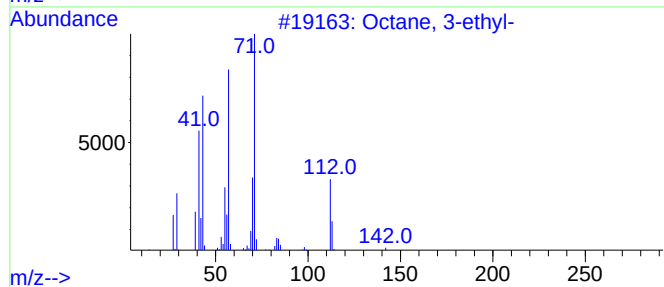
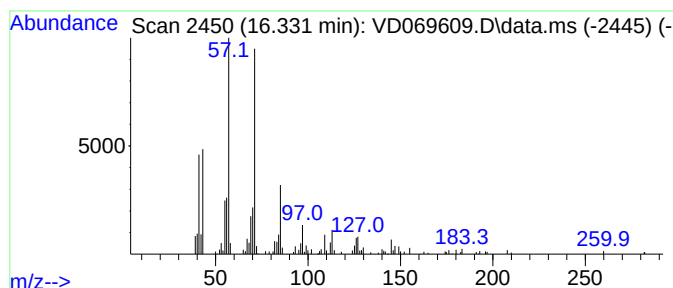
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Quant Title : SW846 8260

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

Peak Number 9 Octane, 3-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.331	15.11 ug/l	224908	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3-ethyl-	142	C10H22	005881-17-4	50
2			Pentadecane, 6-methyl-	226	C16H34	010105-38-1	50
3			Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	50
4			Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	50
5			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD070721\
Data File : VD069609.D
Acq On : 07 Jul 2021 15:36
Operator : VA/SY
Sample : M2936-01
Misc : 5.08G/5.00ml/MSVOA_D/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
TR-05-070221

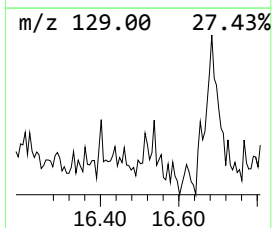
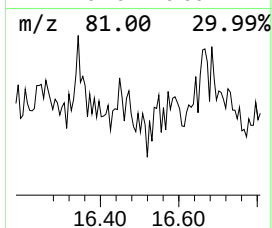
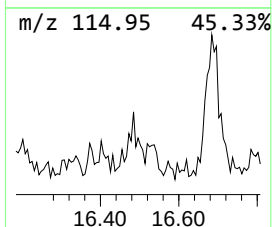
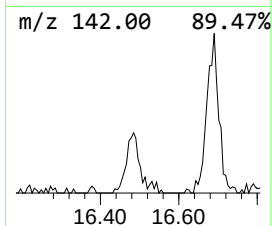
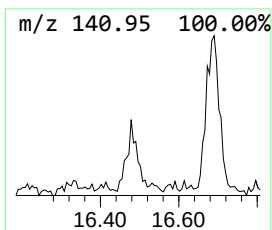
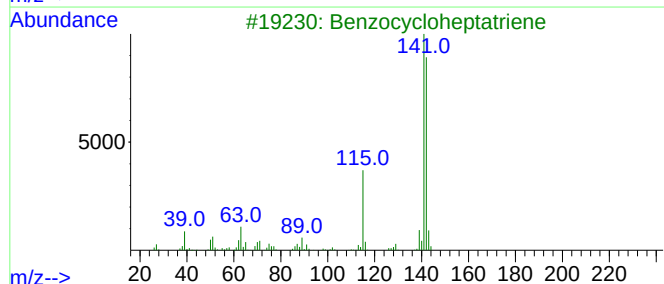
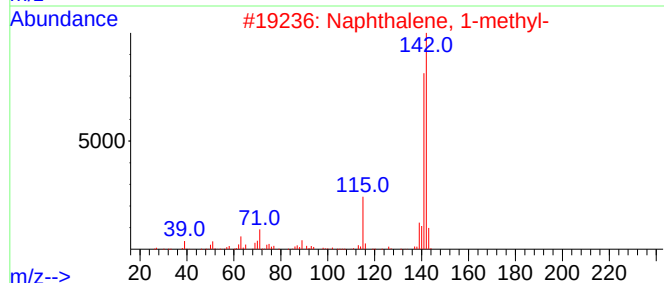
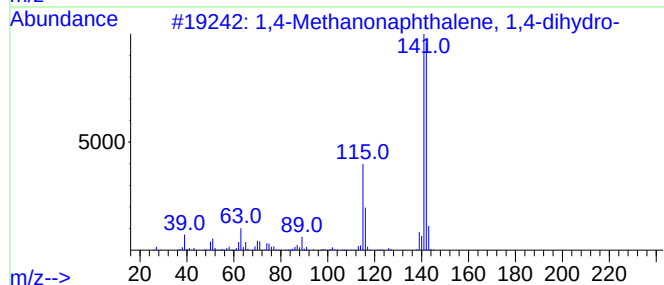
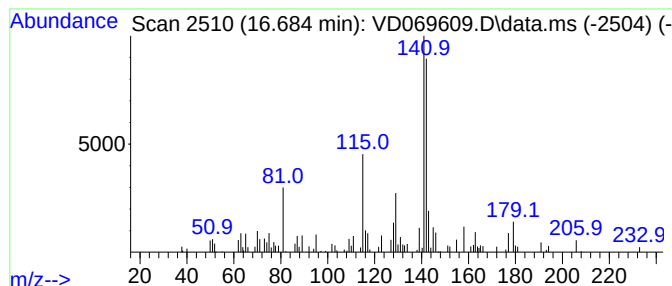
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D062121S.M
Quant Title : SW846 8260

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

Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.684	16.72 ug/l	248887	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	70
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	70
3			Benzocycloheptatriene	142	C11H10	000264-09-5	68
4			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	62
5			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD070721\
Data File : VD069609.D
Acq On : 07 Jul 2021 15:36
Operator : VA/SY
Sample : M2936-01
Misc : 5.08G/5.00ml/MSVOA_D/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
TR-05-070221

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D062121S.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1H-Pyrazole-3-c...	14.432	7.6	ug/l	112641	4	13.567	744365	50.0
Adamantane, 1,3...	14.532	8.8	ug/l	130726	4	13.567	744365	50.0
2-Ethylhexyl me...	14.861	8.8	ug/l	130807	4	13.567	744365	50.0
unknown15.267	15.267	5.8	ug/l	86441	4	13.567	744365	50.0
Tridecane, 7-me...	15.355	18.1	ug/l	269645	4	13.567	744365	50.0
unknown15.761	15.761	6.8	ug/l	101783	4	13.567	744365	50.0
Octane, 3-ethyl-	16.331	15.1	ug/l	224908	4	13.567	744365	50.0
1,4-Methanonaph...	16.684	16.7	ug/l	248887	4	13.567	744365	50.0