

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD121923\
 Data File : VD077981.D
 Acq On : 19 Dec 2023 18:27
 Operator : RP/MD
 Sample : 05765-03
 Misc : 5.06G/5.0ml/MSVOA_D/SOIL/B
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 RT-SB-03-9.5-10.5

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\82D120823S.M
 Title : SW846 8260

Signal : TIC: VD077981.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.734	20	25	32	rVB	54712	85662	9.18%	1.421%
2	2.258	108	114	117	rBV3	7105	10815	1.16%	0.179%
3	4.810	537	548	561	rVB6	11249	36798	3.94%	0.610%
4	5.857	716	726	734	rBV5	6145	18116	1.94%	0.300%
5	7.057	921	930	938	rBV2	11674	35723	3.83%	0.592%
6	7.810	1043	1058	1064	rBV	120386	305145	32.70%	5.061%
7	7.881	1064	1070	1079	rVB	213688	470433	50.41%	7.802%
8	8.234	1120	1130	1139	rBV2	96954	224028	24.01%	3.715%
9	8.781	1213	1223	1231	rBV	322025	679726	72.84%	11.273%
10	10.269	1468	1476	1488	rBV	523292	933152	100.00%	15.476%
11	10.663	1537	1543	1549	rBV2	6320	11229	1.20%	0.186%
12	11.581	1692	1699	1707	rBV	458597	764826	81.96%	12.684%
13	12.575	1861	1868	1875	rBV	295352	484395	51.91%	8.033%
14	12.845	1909	1914	1919	rVB5	7546	11571	1.24%	0.192%
15	13.157	1963	1967	1973	rBV8	5513	11244	1.20%	0.186%
16	13.304	1987	1992	1995	rVB6	6659	10345	1.11%	0.172%
17	13.516	2017	2028	2036	rBV	301498	539250	57.79%	8.943%
18	13.651	2047	2051	2057	rVB8	7946	14987	1.61%	0.249%
19	13.710	2057	2061	2063	rBV5	8316	13769	1.48%	0.228%
20	13.839	2076	2083	2086	rBV7	15170	30256	3.24%	0.502%
21	13.875	2086	2089	2094	rVB6	8878	13665	1.46%	0.227%
22	14.057	2115	2120	2124	rBV7	17014	30917	3.31%	0.513%
23	14.157	2134	2137	2138	rBV2	9887	9480	1.02%	0.157%
24	14.222	2143	2148	2157	rVV2	17826	48406	5.19%	0.803%
25	14.298	2157	2161	2166	rVB8	12494	22736	2.44%	0.377%
26	14.381	2166	2175	2182	rBV3	47733	127976	13.71%	2.122%
27	14.486	2184	2193	2197	rBV	66983	136973	14.68%	2.272%
28	14.551	2201	2204	2214	rVB6	29744	74631	8.00%	1.238%
29	14.675	2220	2225	2229	rBV8	16067	42089	4.51%	0.698%
30	14.969	2272	2275	2280	rVB4	63344	100755	10.80%	1.671%
31	15.033	2282	2286	2291	rBV3	57138	97086	10.40%	1.610%
32	15.098	2291	2297	2299	rBV2	75533	135723	14.54%	2.251%
33	15.375	2340	2344	2346	rBV3	63633	99953	10.71%	1.658%
34	16.222	2485	2488	2492	rBV5	39192	60629	6.50%	1.005%
35	16.586	2546	2550	2558	rVB4	157830	337308	36.15%	5.594%

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RT-SB-03-9.5-10.5

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\82D120823S.M
Title : SW846 8260

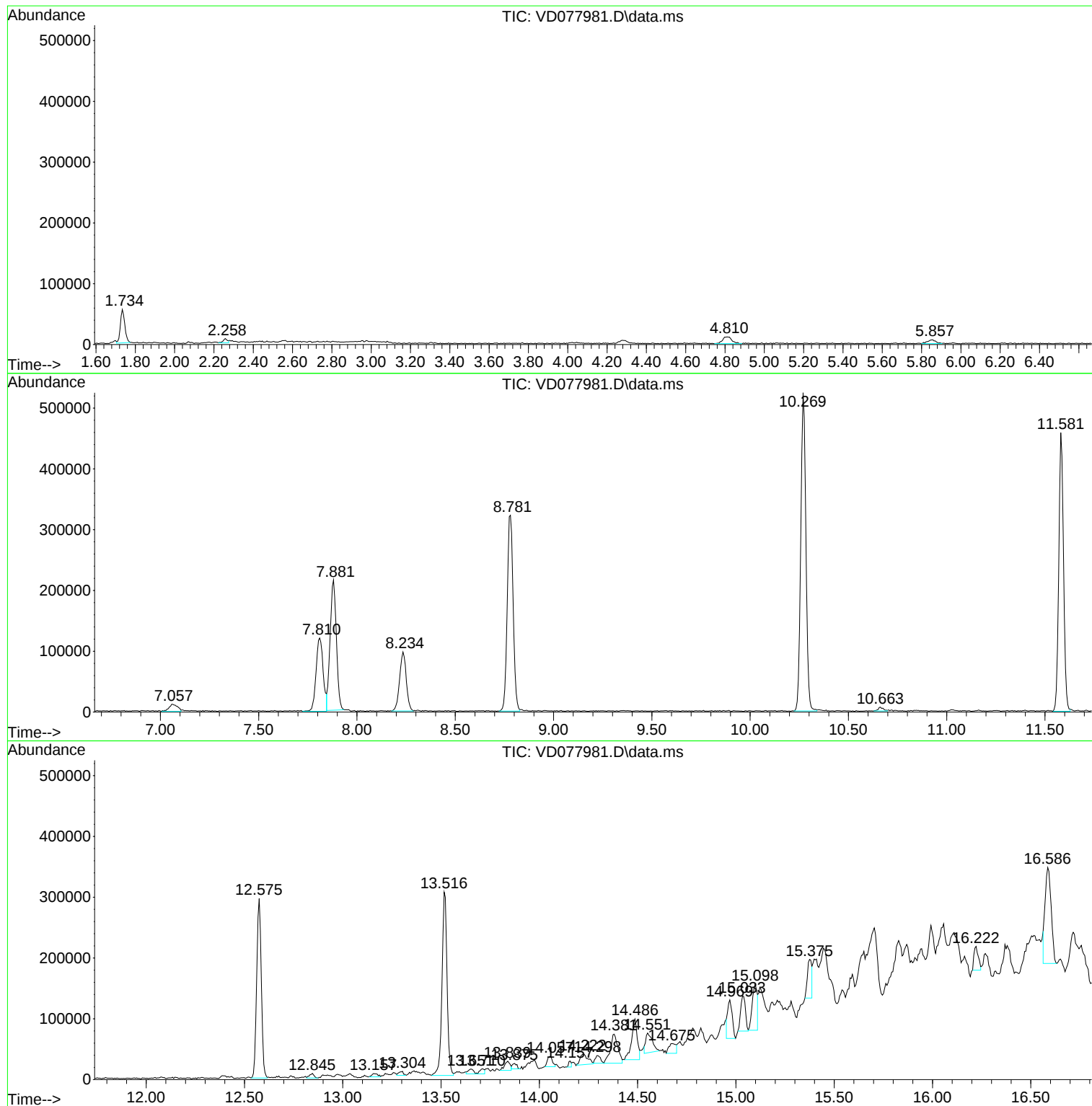
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D120823S.M
Quant Title : SW846 8260

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



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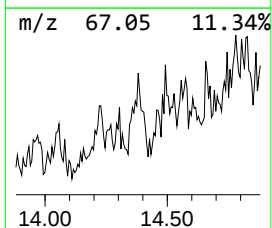
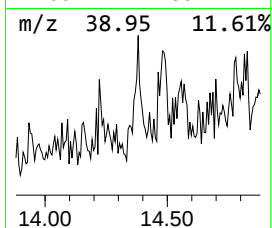
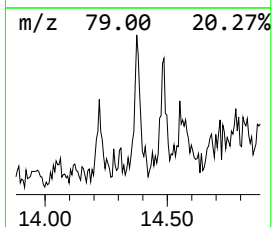
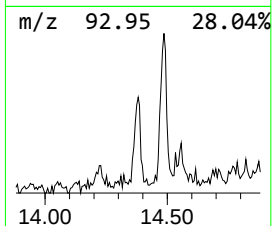
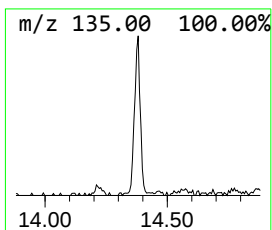
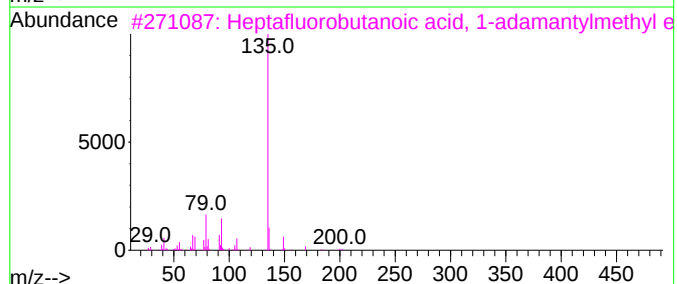
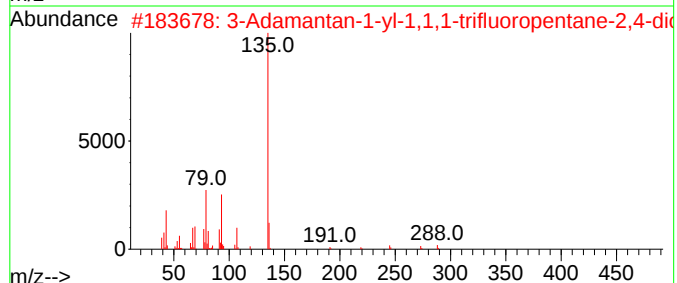
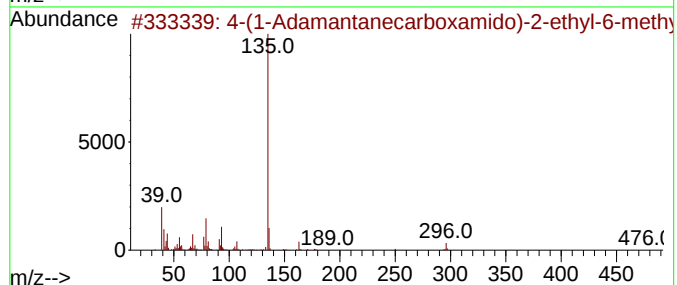
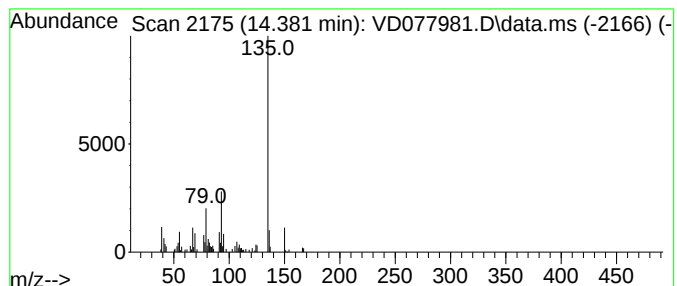
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Quant Title : SW846 8260

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

Peak Number 2 4-(1-Adamantanecarboxamido)... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.381	11.87 ug/l	127976	1,4-Dichlorobenzene-d4	13.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(1-Adamantanecarboxamido)-2-et...	476	C30H40N2O3	143413-39-2	64
2			3-Adamantan-1-yl-1,1,1-trifluoro...	288	C15H19F3O2	1000311-44-8	64
3			Heptafluorobutanoic acid, 1-adam...	362	C15H17F7O2	1000282-96-9	64
4			1-Adamantanecarboxylic acid, 3,5...	292	C17H18F2O2	1000293-75-1	64
5			Benzenesulfonamide, N-adamantan...	384	C17H21ClN2O4S	1000303-35-0	64



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Instrument :
MSVOA_D
ClientSampleId :
RT-SB-03-9.5-10.5

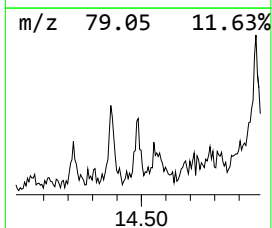
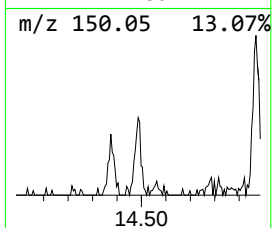
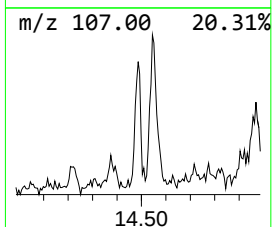
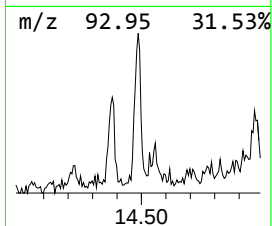
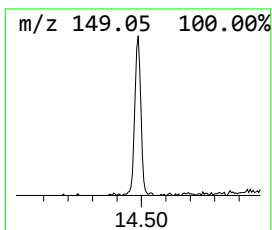
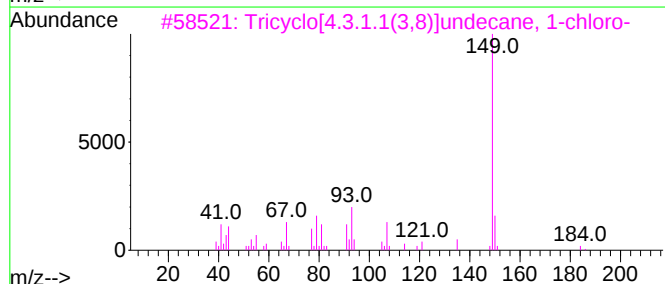
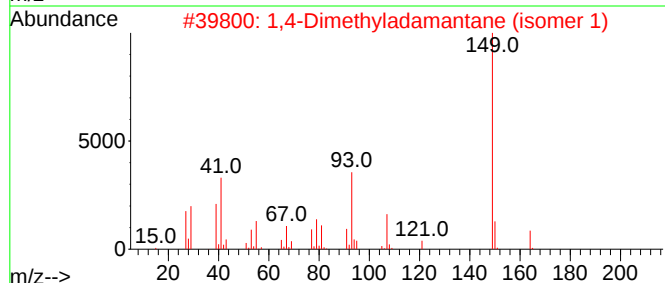
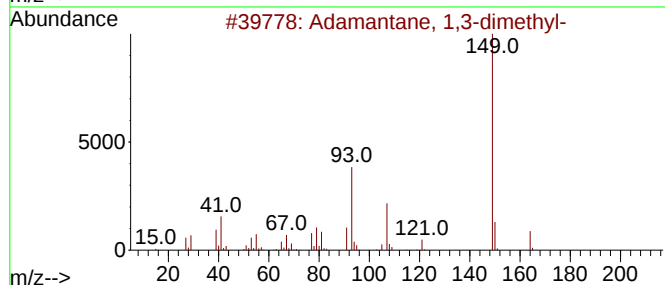
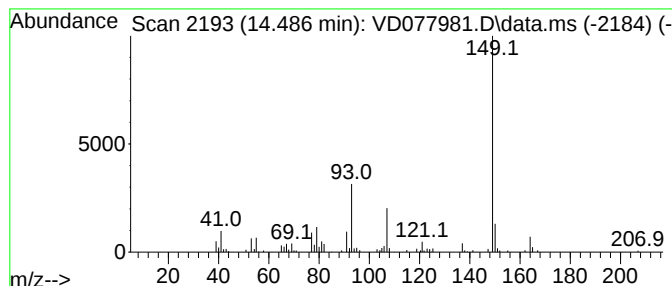
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D120823S.M
Quant Title : SW846 8260

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

Peak Number 3 Adamantane, 1,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.486	12.70 ug/l	136973	1,4-Dichlorobenzene-d4	13.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	90
2			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	78
3			Tricyclo[4.3.1.1(3,8)]undecane, ...	184	C11H17Cl	027011-46-7	64
4			1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	56
5			3-Methyl-1-adamantanecarboxylic ...	194	C12H18O2	1000504-38-9	53



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Instrument :
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ClientSampleId :
RT-SB-03-9.5-10.5

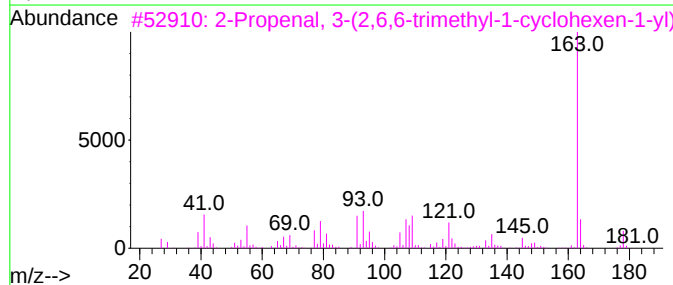
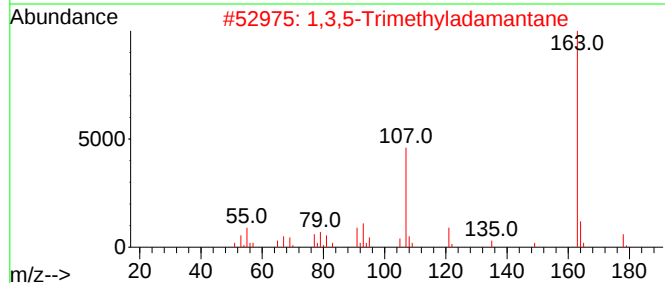
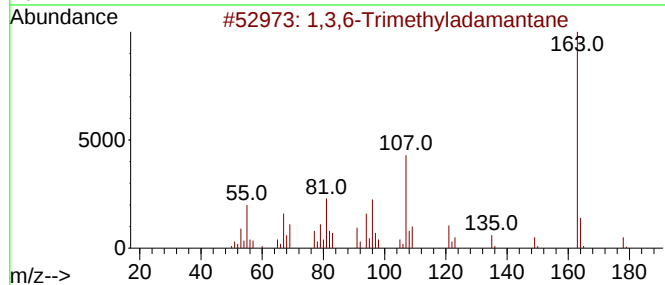
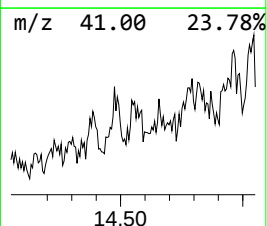
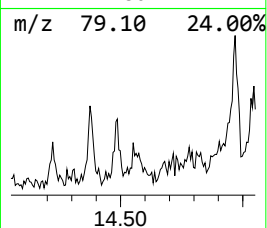
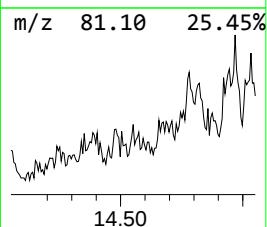
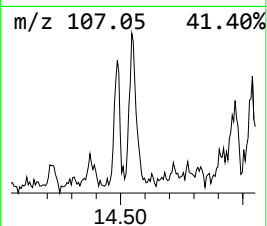
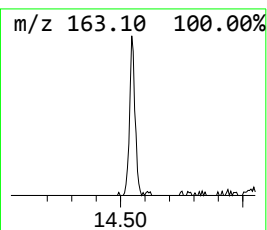
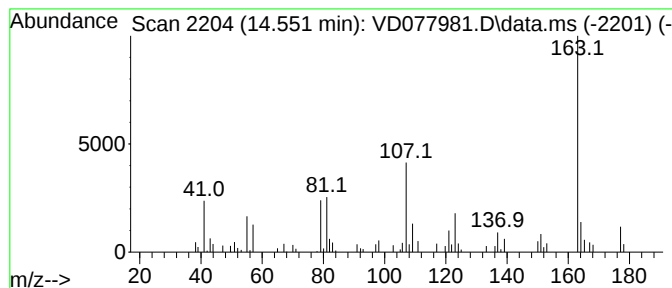
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Quant Title : SW846 8260

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

Peak Number 4 1,3,6-Trimethyladamantane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.551	6.92 ug/l	74631	1,4-Dichlorobenzene-d4	13.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,6-Trimethyladamantane	178	C13H22	024139-37-5	64		
2	1,3,5-Trimethyladamantane	178	C13H22	000707-35-7	53		
3	2-Propenal, 3-(2,6,6-trimethyl-1...	178	C12H18O	004951-40-0	47		
4	1,3-Dimethyl-5-ethyladamantane	192	C14H24	001687-35-0	42		
5	1,2-Hexanediol, 1,2-diphenyl-	270	C18H22O2	080475-19-0	38		



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Instrument :
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ClientSampleId :
RT-SB-03-9.5-10.5

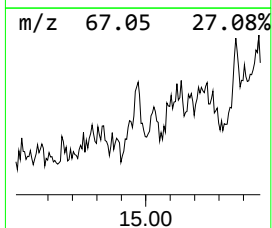
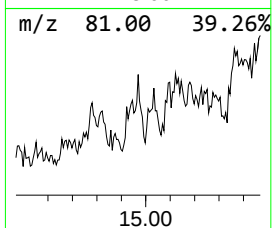
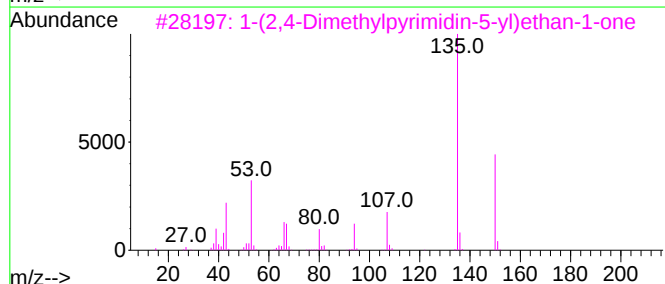
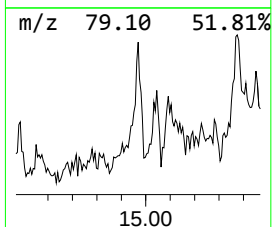
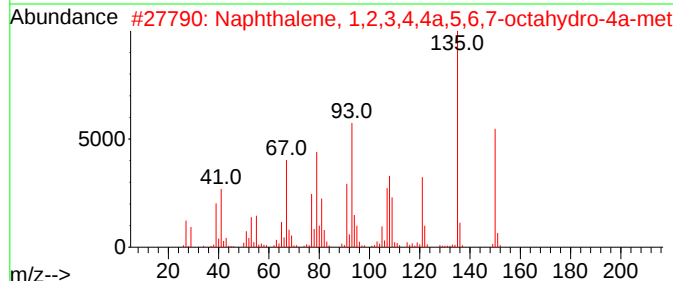
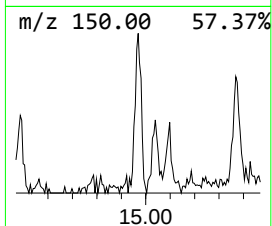
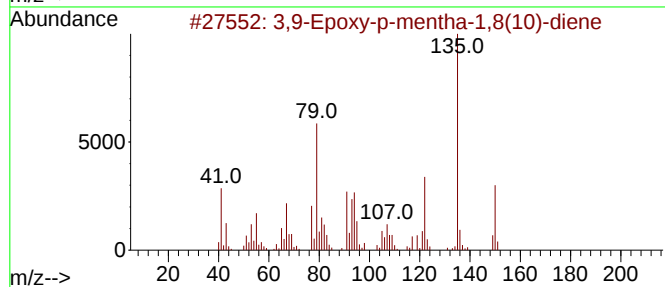
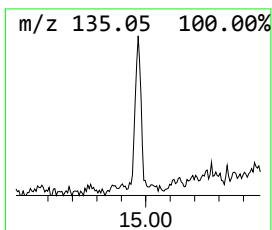
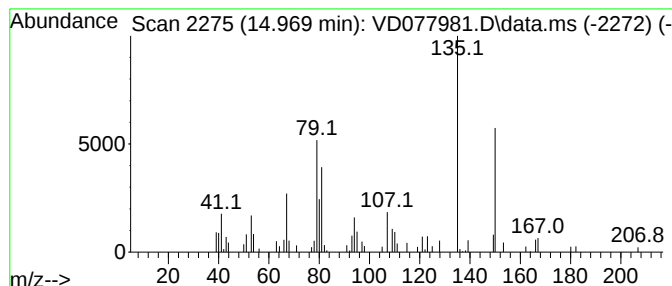
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Quant Title : SW846 8260

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

Peak Number 5 3,9-Epoxy-p-mentha-1,8(10)-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.969	9.34 ug/l	100755	1,4-Dichlorobenzene-d4	13.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,9-Epoxy-p-mentha-1,8(10)-diene	150	C10H14O	1000111-14-8	64
2			Naphthalene, 1,2,3,4,4a,5,6,7-oc...	150	C11H18	013943-77-6	59
3			1-(2,4-Dimethylpyrimidin-5-yl)et...	150	C8H10N2O	055933-85-2	47
4			Cyclopentanone, 2-cyclopentylidene-	150	C10H14O	000825-25-2	43
5			2,5-Dimethyl-3-isopropylpyrazine	150	C9H14N2	013610-20-3	43



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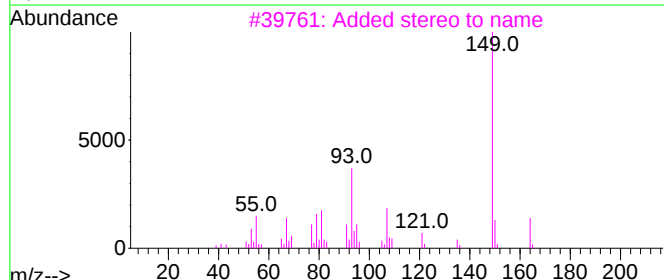
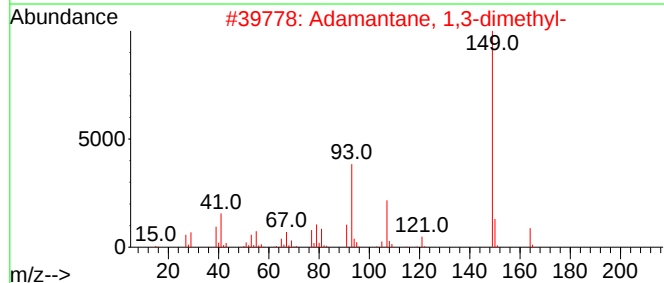
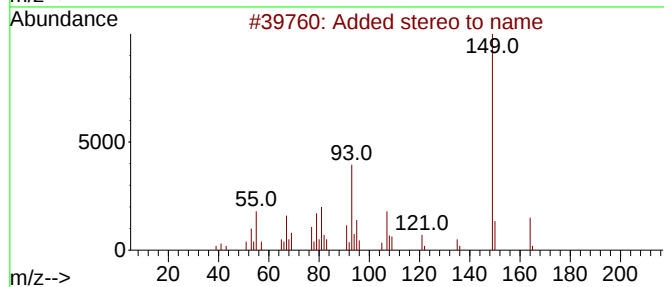
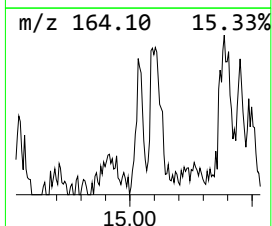
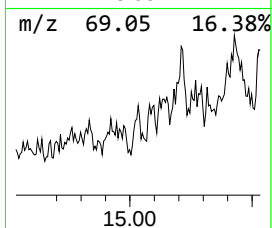
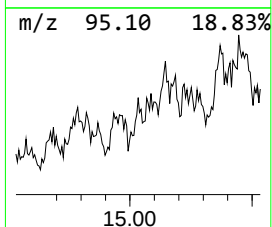
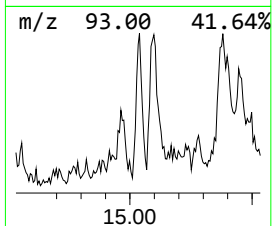
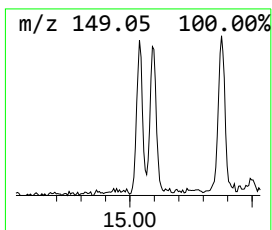
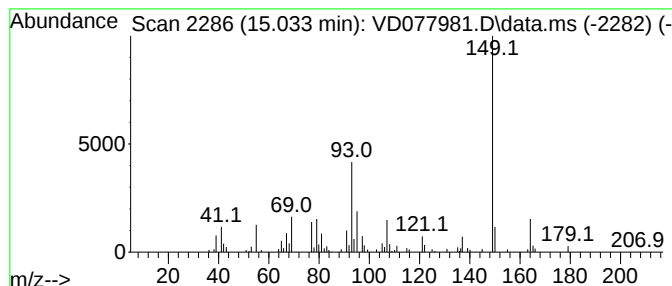
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Quant Title : SW846 8260

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

Peak Number 6 1,4-Dimethyladamantane (iso... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.034	9.00 ug/l	97086	1,4-Dichlorobenzene-d4	13.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Added stereo to name			164	C12H20	024145-88-8	90
2	Adamantane, 1,3-dimethyl-			164	C12H20	000702-79-4	87
3	Added stereo to name			164	C12H20	024145-89-9	81
4	1,4-Dimethyladamantane (isomer 1)			164	C12H20	1000460-67-0	72
5	1-Methyl-3-ethyladamantane			178	C13H22	001687-34-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD121923\
Data File : VD077981.D
Acq On : 19 Dec 2023 18:27
Operator : RP/MD
Sample : 05765-03
Misc : 5.06G/5.0ml/MSVOA_D/SOIL/B
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
RT-SB-03-9.5-10.5

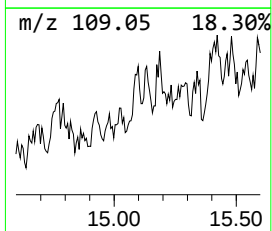
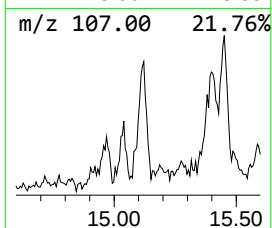
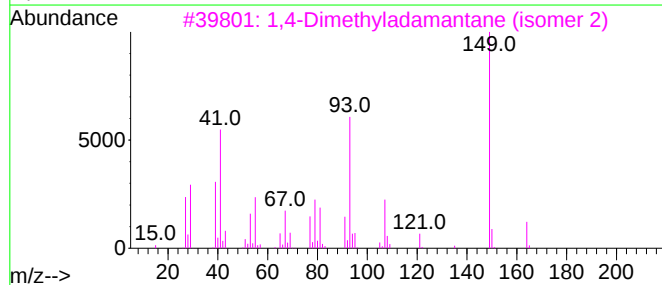
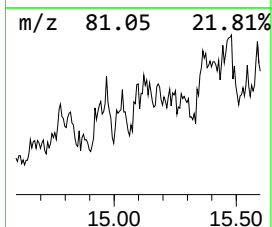
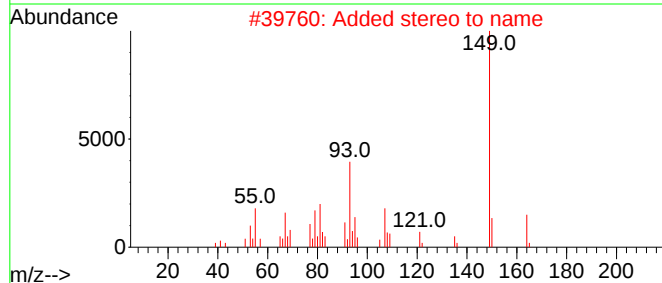
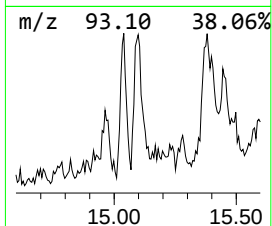
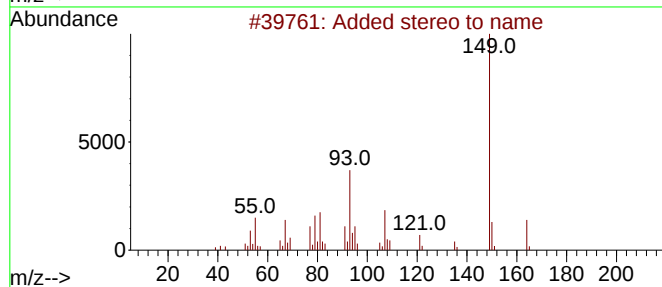
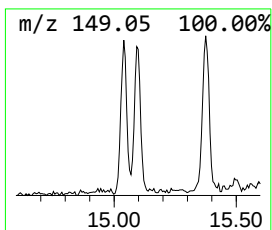
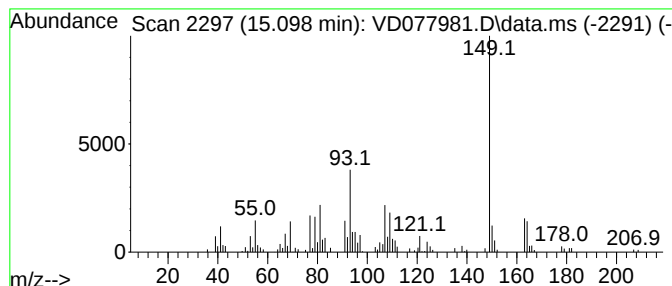
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Quant Title : SW846 8260

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

Peak Number 7 1,4-Dimethyladamantane (iso... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.098	12.58 ug/l	135723	1,4-Dichlorobenzene-d4	13.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Added stereo to name			164	C12H20	024145-89-9	93
2	Added stereo to name			164	C12H20	024145-88-8	91
3	1,4-Dimethyladamantane (isomer 2)			164	C12H20	1000460-67-1	83
4	1,4-Dimethyladamantane (isomer 1)			164	C12H20	1000460-67-0	81
5	Adamantane, 1,3-dimethyl-			164	C12H20	000702-79-4	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD121923\
Data File : VD077981.D
Acq On : 19 Dec 2023 18:27
Operator : RP/MD
Sample : 05765-03
Misc : 5.06G/5.0ml/MSVOA_D/SOIL/B
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
RT-SB-03-9.5-10.5

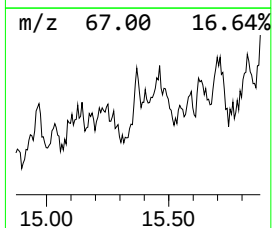
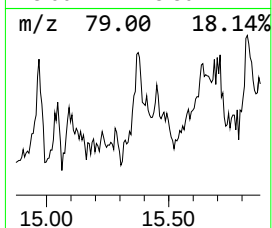
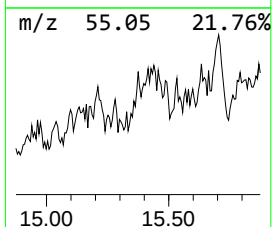
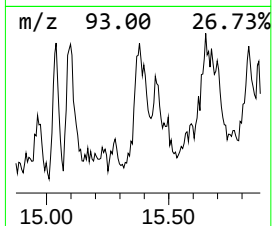
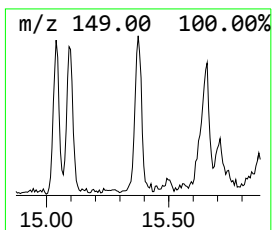
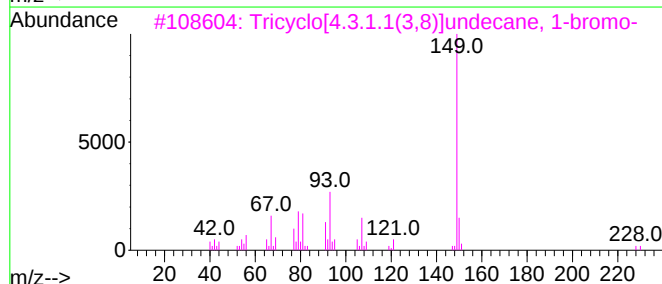
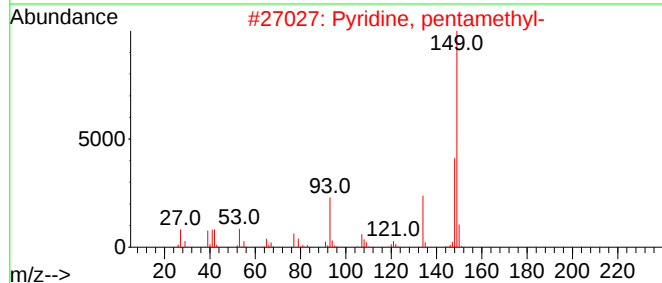
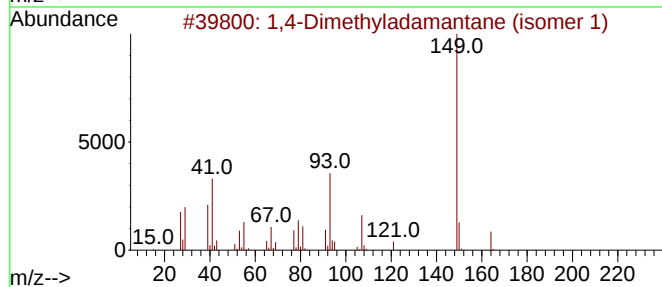
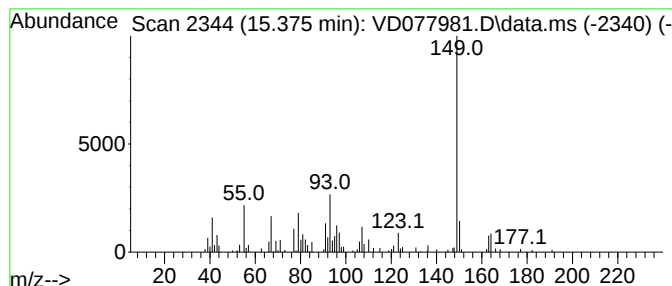
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Quant Title : SW846 8260

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

Peak Number 8 Pyridine, pentamethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.375	9.27 ug/l	99953	1,4-Dichlorobenzene-d4	13.522

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	76
2		Pyridine, pentamethyl-	149	C10H15N	003748-83-2	64
3		Tricyclo[4.3.1.1(3,8)]undecane, ...	228	C11H17Br	021898-96-4	64
4		Phthalic acid, hexadecyl 3-metho...	510	C32H46O5	1010377-98-9	50
5		1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD121923\
Data File : VD077981.D
Acq On : 19 Dec 2023 18:27
Operator : RP/MD
Sample : 05765-03
Misc : 5.06G/5.0ml/MSVOA_D/SOIL/B
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
RT-SB-03-9.5-10.5

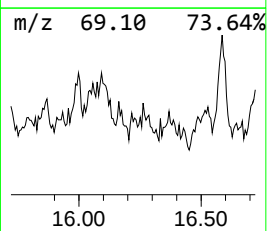
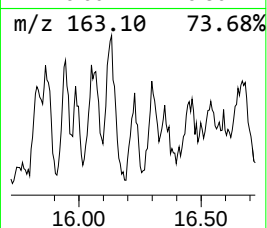
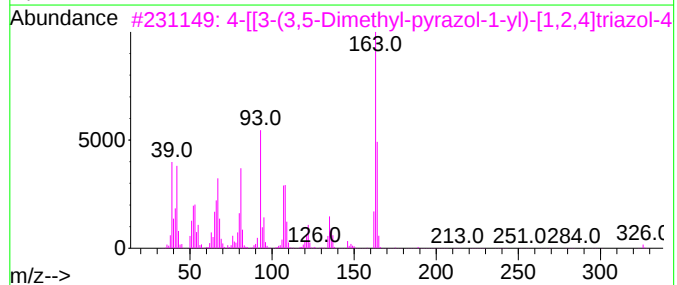
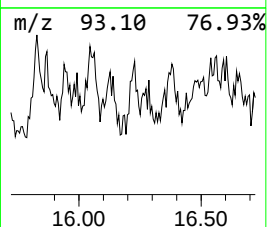
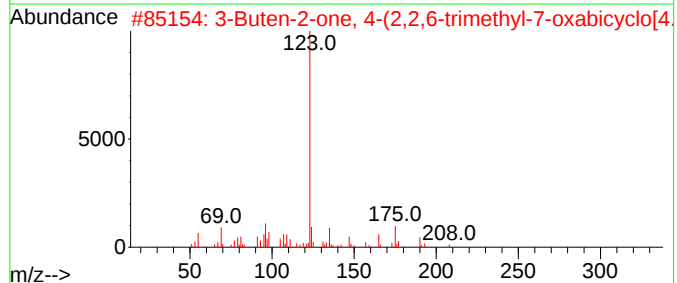
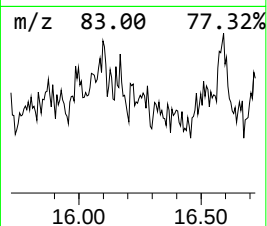
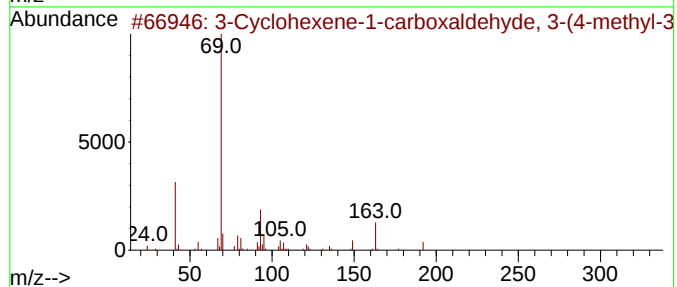
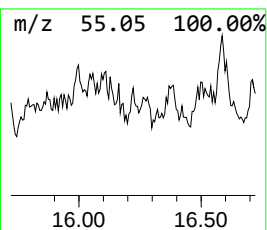
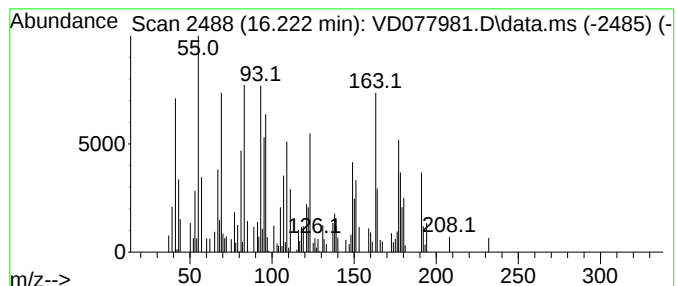
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Quant Title : SW846 8260

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

Peak Number 9 unknown16.222 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.222	5.62 ug/l	60629	1,4-Dichlorobenzene-d4	13.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	43
2			3-Buten-2-one, 4-(2,2,6-trimethy...	208	C13H20O2	023267-57-4	14
3			4-[[3-(3,5-Dimethyl-pyrazol-1-yl)...	326	C16H18N6O2	1000296-14-6	14
4			1-Cyclopentyl-4-(1-methylethyl)c...	194	C14H26	1000215-44-4	11
5			3-Amino-5-(furan-2-yl)cyclohex-2...	177	C10H11NO2	090921-87-2	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD121923\
Data File : VD077981.D
Acq On : 19 Dec 2023 18:27
Operator : RP/MD
Sample : 05765-03
Misc : 5.06G/5.0ml/MSVOA_D/SOIL/B
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
RT-SB-03-9.5-10.5

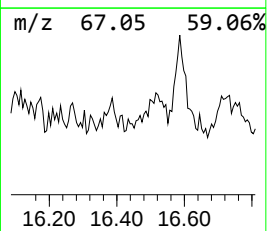
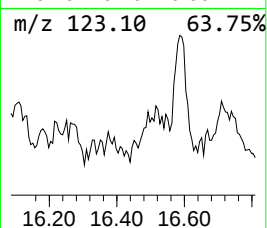
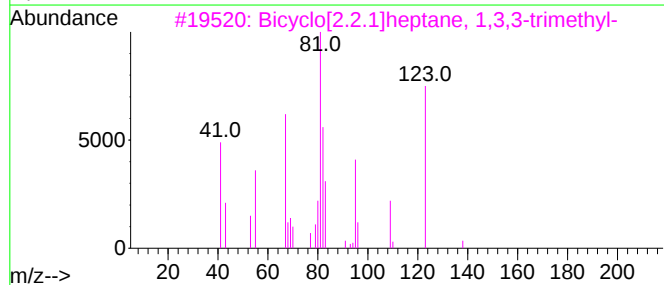
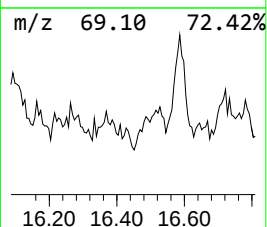
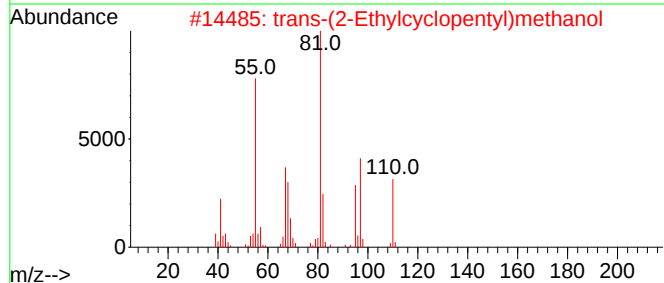
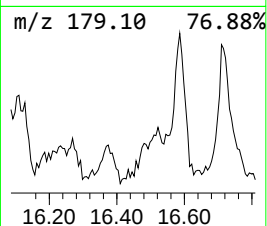
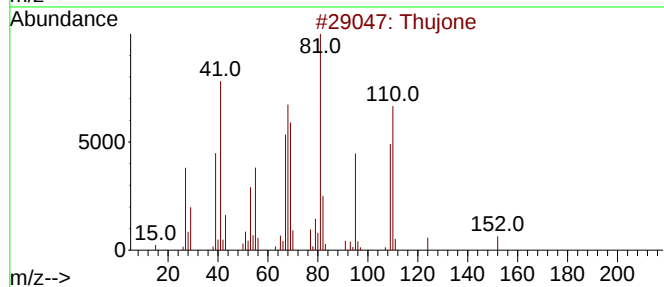
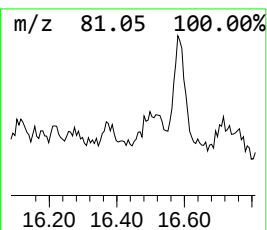
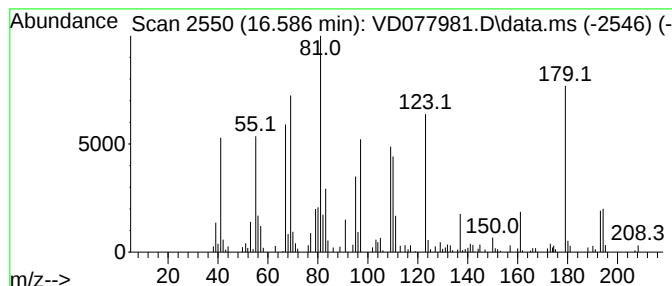
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Quant Title : SW846 8260

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

Peak Number 10 unknown16.586 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.586	31.28 ug/l	337308	1,4-Dichlorobenzene-d4	13.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thujone	152	C10H16O	000546-80-5	38
2			trans-(2-Ethylcyclopentyl)methanol	128	C8H16O	036258-08-9	35
3			Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	27
4			2(1H)-Naphthalenone, octahydro-4...	194	C13H22O	007056-56-6	22
5			2-Propenyl-3-vinylloxirane	110	C7H10O	070597-49-8	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD121923\
Data File : VD077981.D
Acq On : 19 Dec 2023 18:27
Operator : RP/MD
Sample : 05765-03
Misc : 5.06G/5.0ml/MSVOA_D/SOIL/B
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
RT-SB-03-9.5-10.5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D120823S.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
4-(1-Adamantane...	14.381	11.9	ug/l	127976	4	13.522	539250	50.0
Adamantane, 1,3...	14.486	12.7	ug/l	136973	4	13.522	539250	50.0
1,3,6-Trimethyl...	14.551	6.9	ug/l	74631	4	13.522	539250	50.0
3,9-Epoxy-p-men...	14.969	9.3	ug/l	100755	4	13.522	539250	50.0
1,4-Dimethylada...	15.034	9.0	ug/l	97086	4	13.522	539250	50.0
1,4-Dimethylada...	15.098	12.6	ug/l	135723	4	13.522	539250	50.0
Pyridine, penta...	15.375	9.3	ug/l	99953	4	13.522	539250	50.0
unknown16.222	16.222	5.6	ug/l	60629	4	13.522	539250	50.0
unknown16.586	16.586	31.3	ug/l	337308	4	13.522	539250	50.0