

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040125\
 Data File : VN086197.D
 Acq On : 01 Apr 2025 15:37
 Operator : JC\MD
 Sample : Q1659-02 50X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 3809

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_N\methods\82N031825W.M
 Title : SW846 8260

Signal : TIC: VN086197.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.677	270	293	294	rBV	31000	84972	1.16%	0.310%
2	3.718	296	300	302	rBV5	160936	154154	2.10%	0.562%
3	3.789	306	312	315	rBV6	502099	1009110	13.74%	3.676%
4	3.812	315	316	317	rVB	878990	310283	4.23%	1.130%
5	3.830	317	319	329	rBV	341966	487003	6.63%	1.774%
6	5.594	615	619	621	rVB	105058	111958	1.52%	0.408%
7	5.647	621	628	632	rBV	3156650	4289381	58.42%	15.627%
8	8.794	1153	1163	1172	rBV2	568266	1313304	17.89%	4.785%
9	9.094	1208	1214	1219	rBV	134929	313998	4.28%	1.144%
10	9.182	1219	1229	1251	rVB	812013	2090575	28.47%	7.617%
11	9.506	1276	1284	1296	rVB	737489	1472957	20.06%	5.366%
12	10.771	1491	1499	1510	rBV	1003929	1798981	24.50%	6.554%
13	11.959	1694	1701	1707	rBV	869164	1600613	21.80%	5.832%
14	12.888	1852	1859	1869	rVB	496828	848788	11.56%	3.092%
15	13.717	1995	2000	2009	rBV5	40716	83564	1.14%	0.304%
16	13.812	2009	2016	2021	rVV	402503	689449	9.39%	2.512%
17	13.876	2021	2027	2034	rVV3	60776	125523	1.71%	0.457%
18	14.241	2081	2089	2108	rBV	4534800	7342297	100.00%	26.750%
19	14.488	2126	2131	2140	rVB	344948	577089	7.86%	2.103%
20	15.370	2269	2281	2288	rBV3	102172	253274	3.45%	0.923%
21	15.506	2292	2304	2319	rVV2	392442	898413	12.24%	3.273%
22	15.647	2321	2328	2341	rVB6	65735	193260	2.63%	0.704%
23	15.823	2346	2358	2364	rBV3	71152	173201	2.36%	0.631%
24	15.882	2364	2368	2376	rVB5	35657	75895	1.03%	0.277%
25	16.006	2379	2389	2406	rBV	473026	983433	13.39%	3.583%
26	16.411	2451	2458	2467	rBV3	78754	166212	2.26%	0.606%

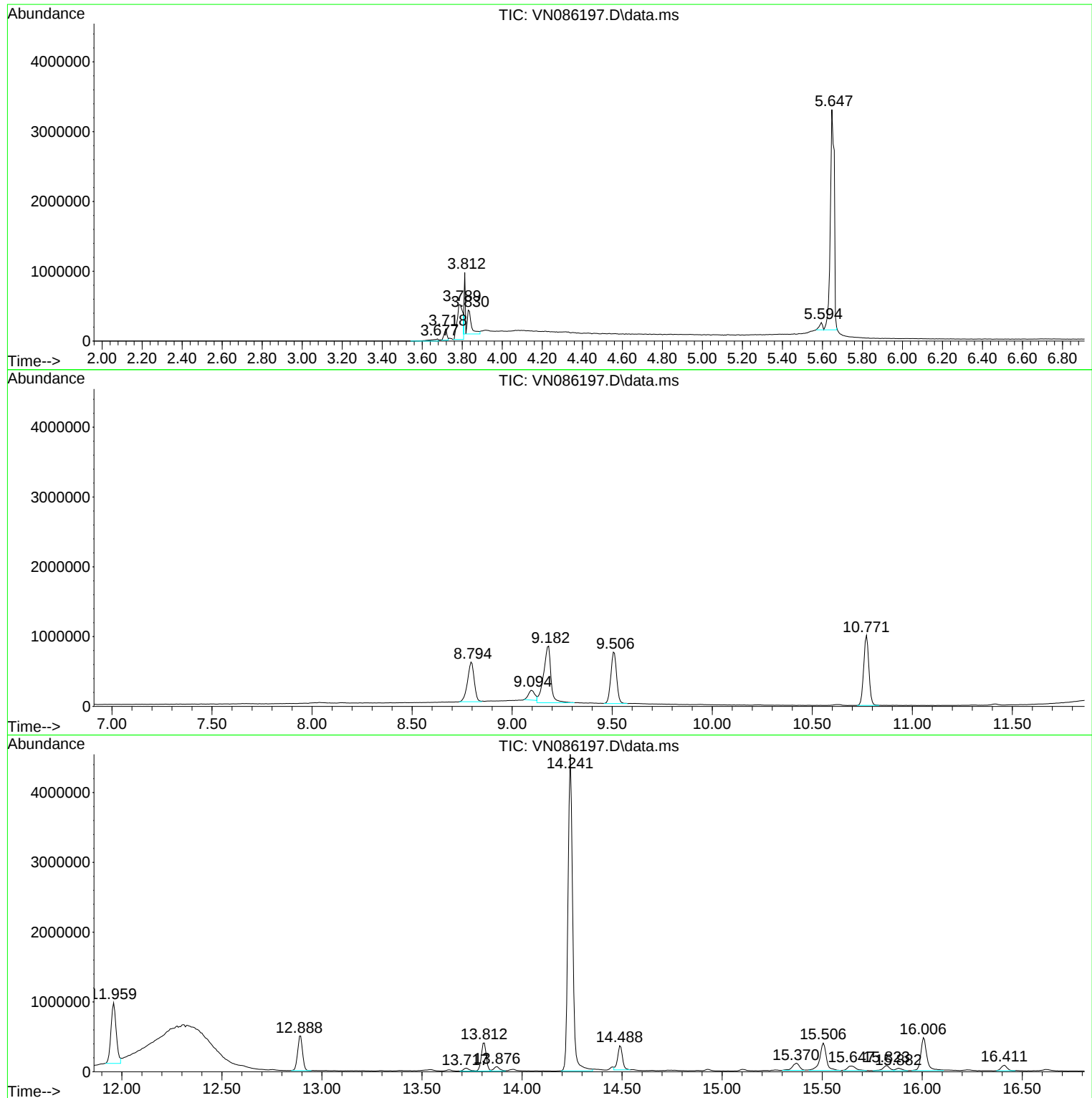
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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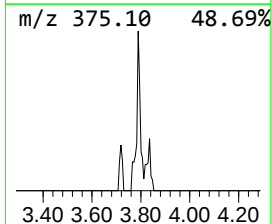
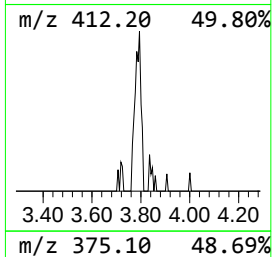
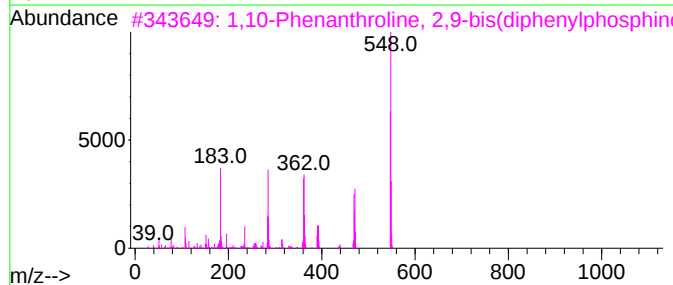
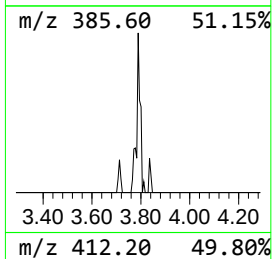
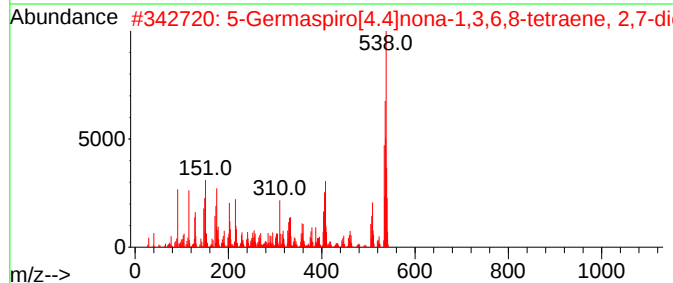
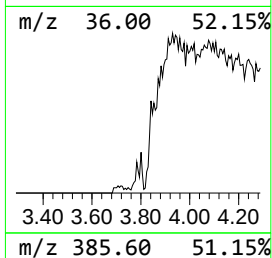
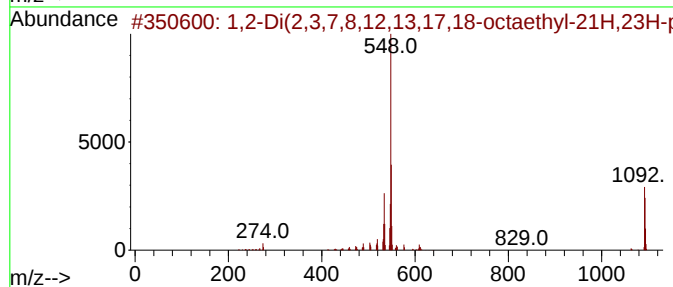
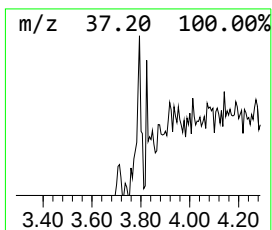
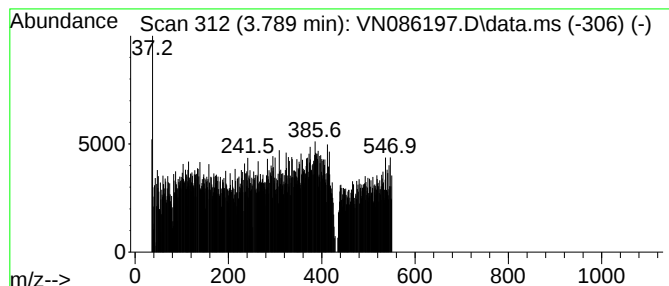
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown3.789 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.789	38.42 ug/l	1009110	Pentafluorobenzene	8.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Di(2,3,7,8,12,13,17,18-octae...	1093	C74H92N8	106085-73-8	11		
2	5-Germaspiro[4.4]nona-1,3,6,8-te...	538	C36H32Ge	150479-95-1	11		
3	1,10-Phenanthroline, 2,9-bis(dip...	548	C36H26N2P2	122768-46-1	10		
4	Ferrocene, 1,1'-bis[(pentafluoro...	546	C24H12F10Fe	055494-16-1	9		
5	Indomethacin, dodecyl ester	525	C31H40ClN04	1000405-10-7	9		



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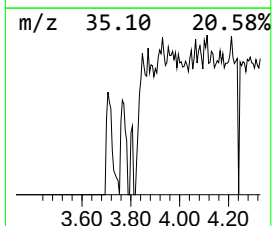
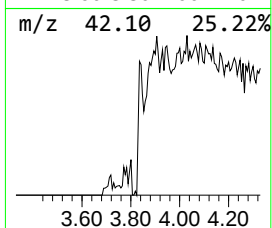
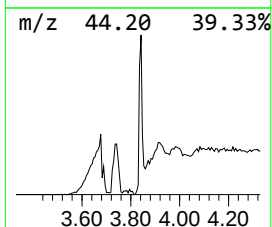
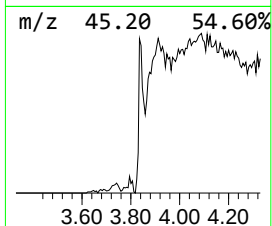
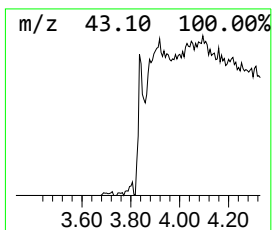
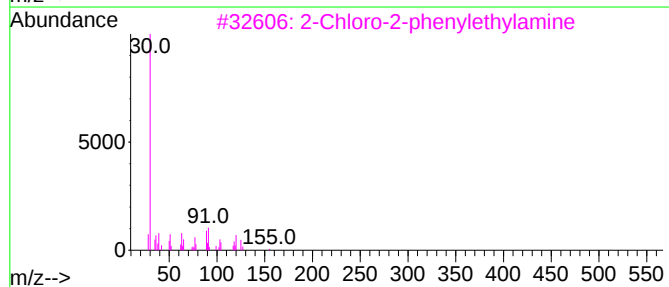
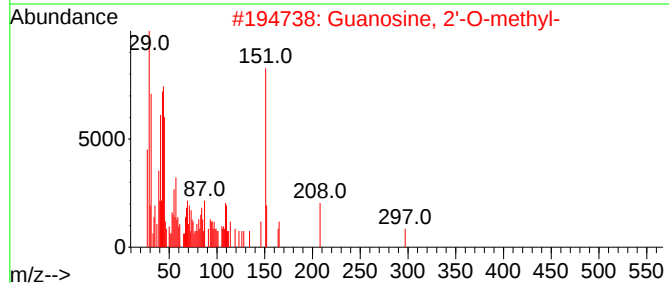
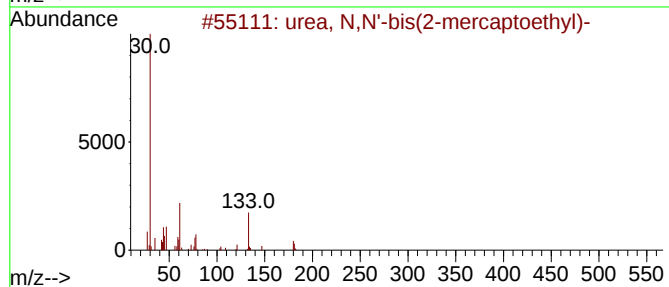
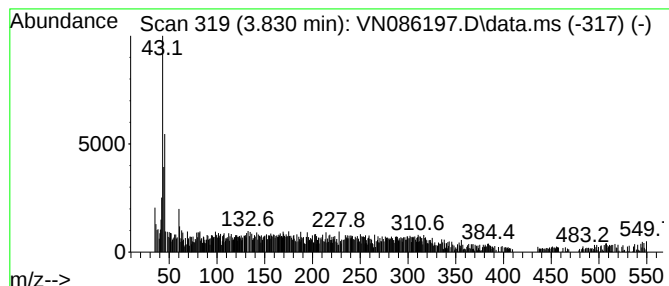
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

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Peak Number 2 unknown3.830 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.830	18.54 ug/l	487003	Pentafluorobenzene	8.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	urea, N,N'-bis(2-mercaptoethyl)-	180	C5H12N2OS2	1000404-84-9	47		
2	Guanosine, 2'-O-methyl-	297	C11H15N5O5	002140-71-8	38		
3	2-Chloro-2-phenylethylamine	155	C8H10ClN	004633-92-5	28		
4	2-Propenoyl chloride	90	C3H3ClO	000814-68-6	28		
5	Ethanedial,1,2-dichloro-, bis(0-...	240	C6H6Cl2N2O4	089715-76-4	25		



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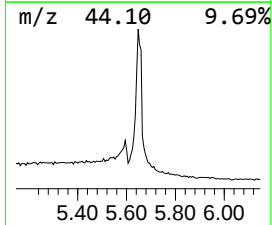
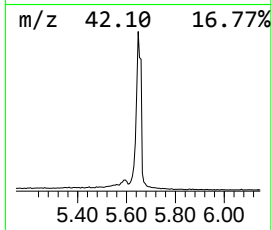
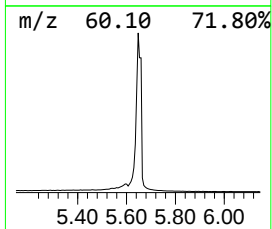
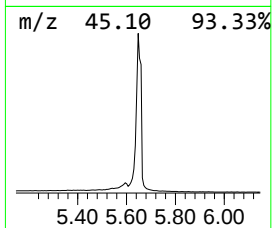
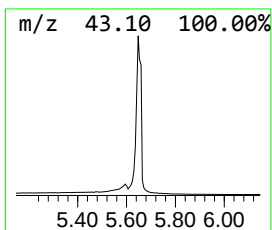
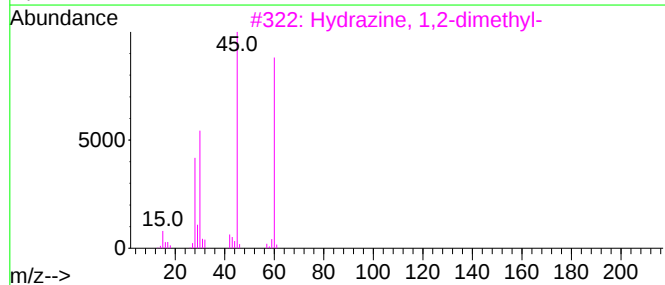
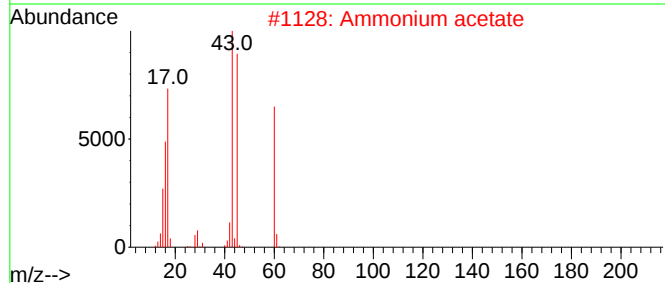
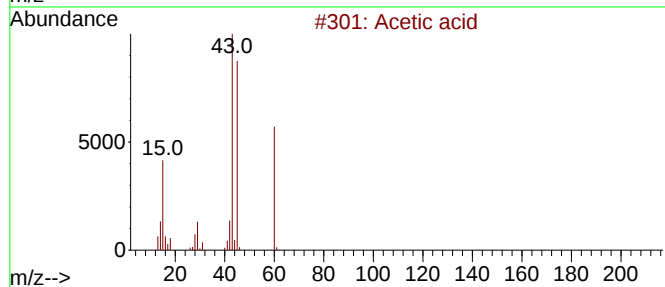
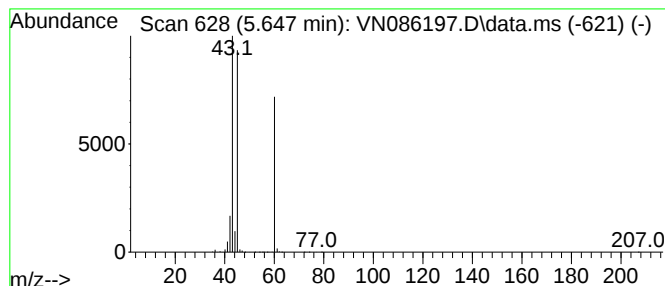
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Quant Title : SW846 8260

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Peak Number 3 Acetic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.647	163.31 ug/l	4289380	Pentafluorobenzene	8.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid	60	C2H4O2	000064-19-7	90
2			Ammonium acetate	77	C2H7NO2	000631-61-8	64
3			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	45
4			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	25
5			Carbonyl sulfide	60	COS	000463-58-1	5



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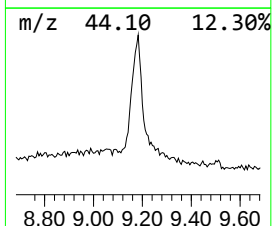
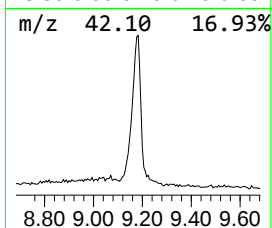
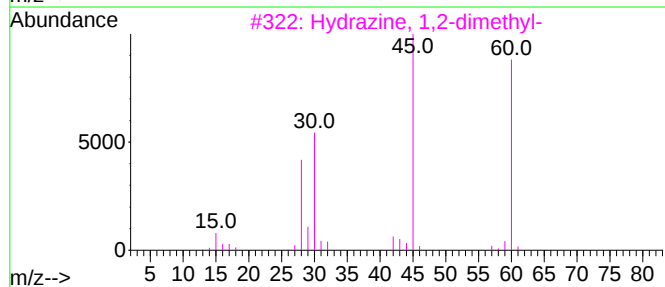
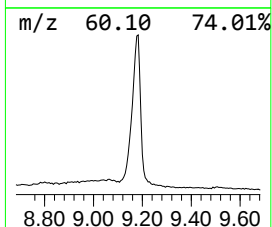
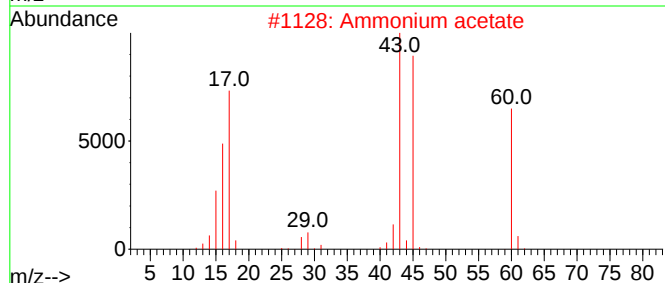
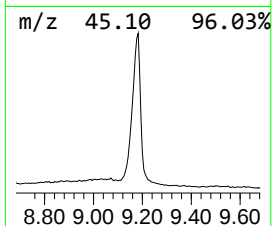
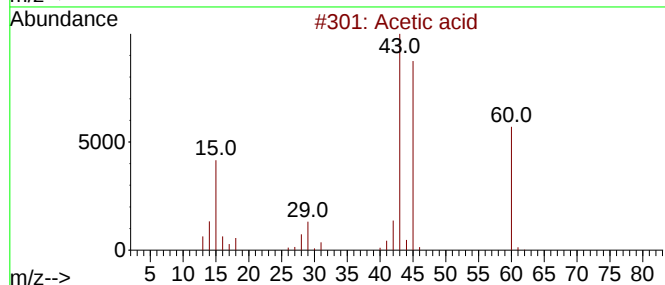
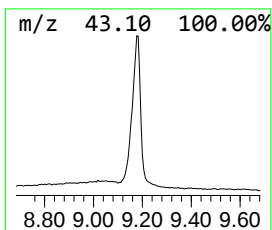
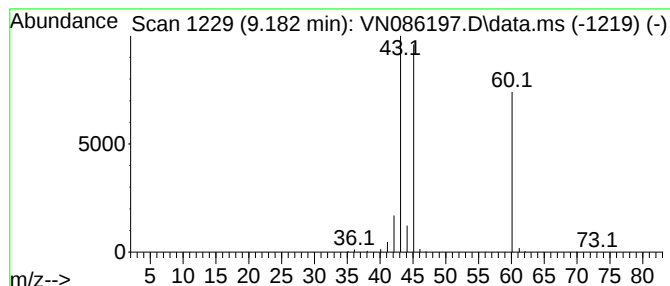
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Peak Number 4 Ammonium acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.182	70.97 ug/l	2090580	1,4-Difluorobenzene	9.506

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid	60	C2H4O2	000064-19-7	90
2			Ammonium acetate	77	C2H7NO2	000631-61-8	64
3			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	50
4			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	37
5			Formic acid hydrazide	60	CH4N2O	000624-84-0	9



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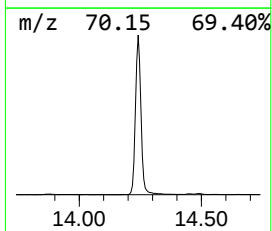
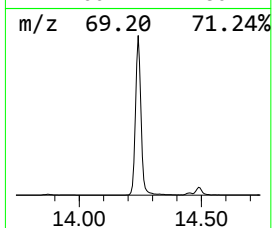
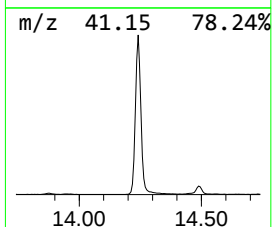
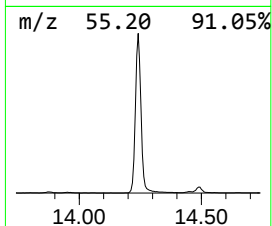
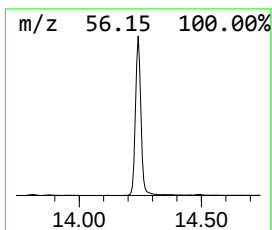
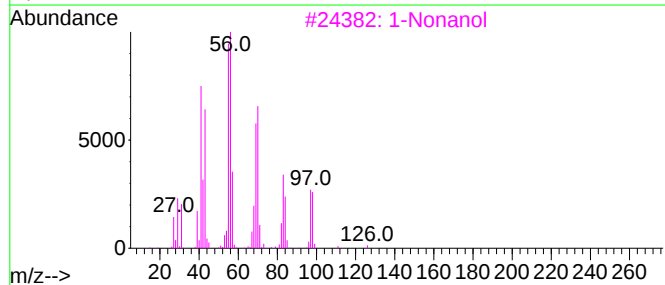
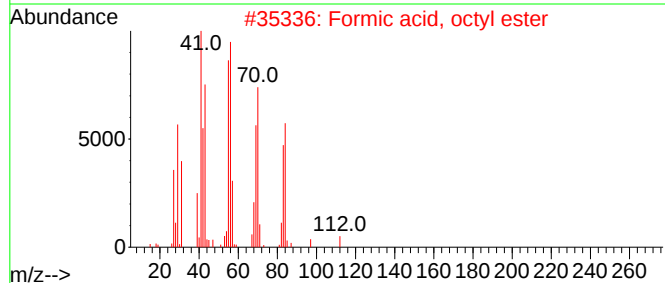
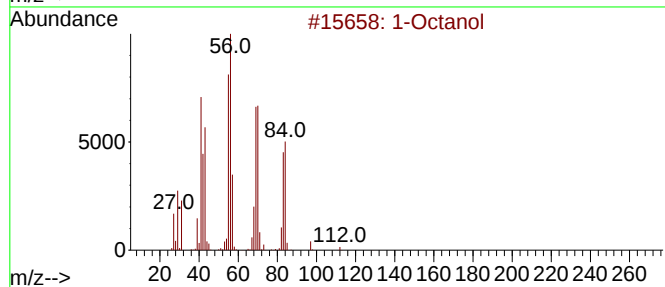
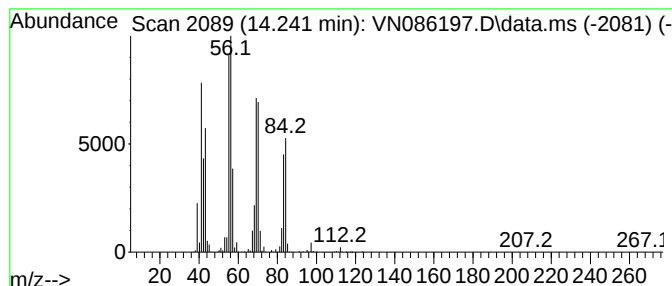
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Peak Number 5 1-Octanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.241	532.48 ug/l	7342300	1,4-Dichlorobenzene-d4	13.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol	130	C8H18O	000111-87-5	91
2			Formic acid, octyl ester	158	C9H18O2	000112-32-3	90
3			1-Nonanol	144	C9H20O	000143-08-8	86
4			Cyclooctane	112	C8H16	000292-64-8	80
5			1-Heptene	98	C7H14	000592-76-7	47



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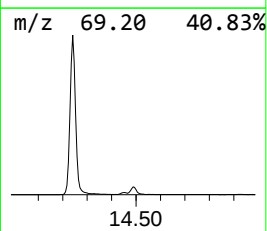
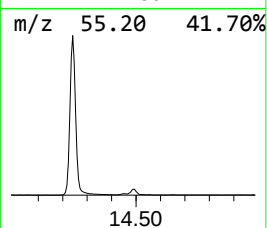
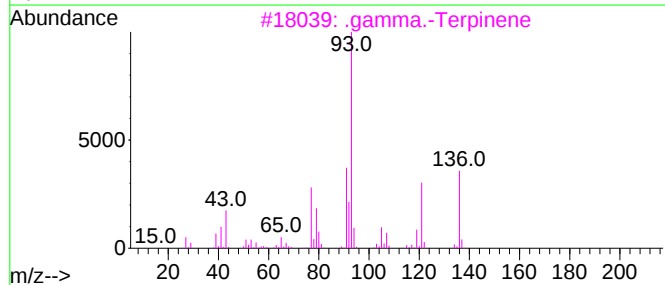
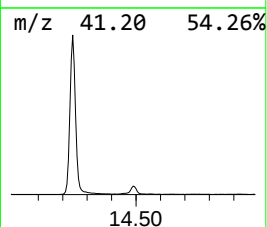
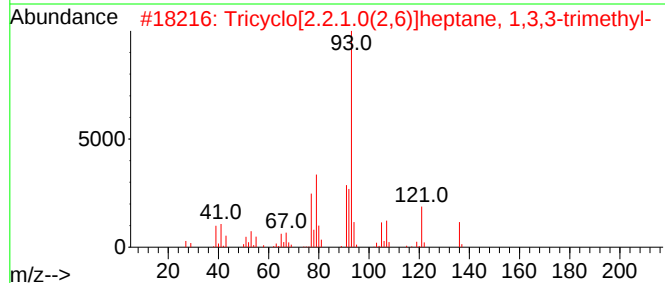
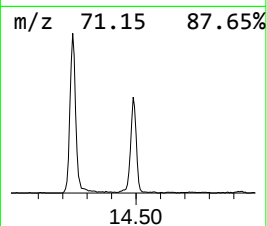
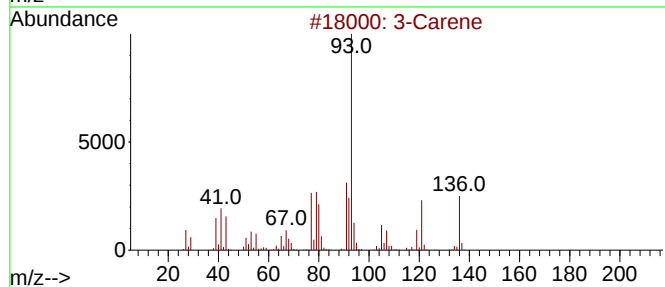
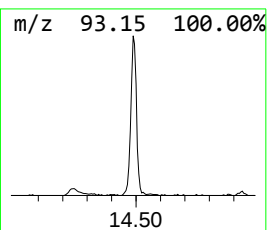
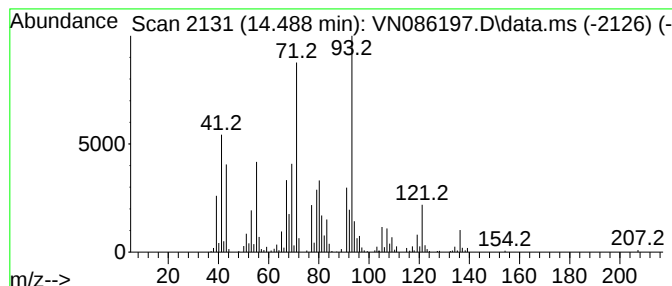
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Quant Title : SW846 8260

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

Peak Number 6 3-Carene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.488	41.85 ug/l	577089	1,4-Dichlorobenzene-d4	13.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Carene	136	C10H16	013466-78-9	60
2			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	60
3			.gamma.-Terpinene	136	C10H16	000099-85-4	55
4			Linalool	154	C10H18O	000078-70-6	53
5			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040125\
Data File : VN086197.D
Acq On : 01 Apr 2025 15:37
Operator : JC\MD
Sample : Q1659-02 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3809

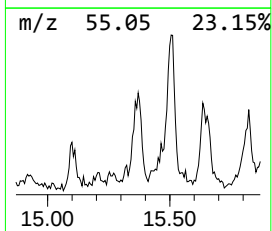
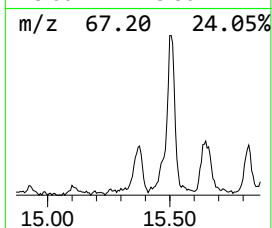
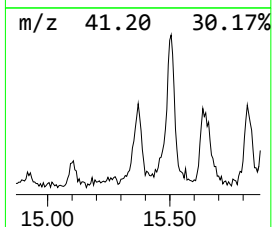
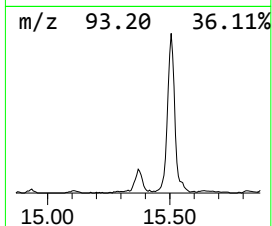
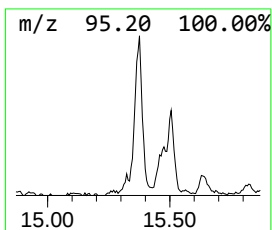
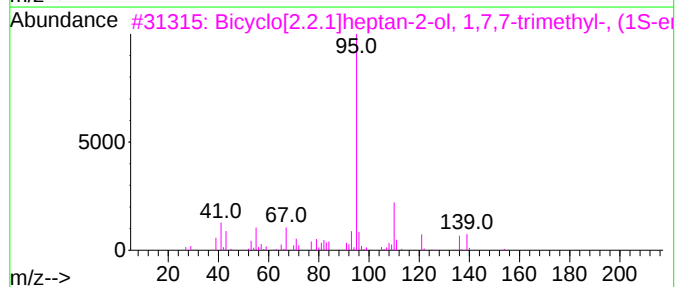
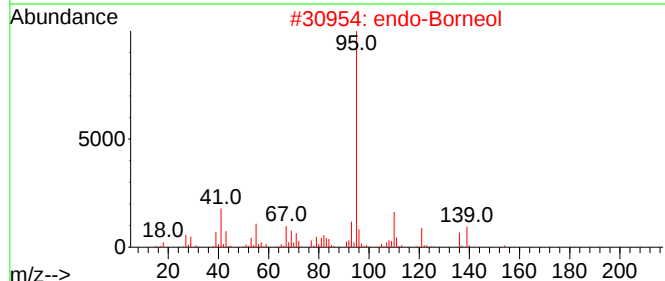
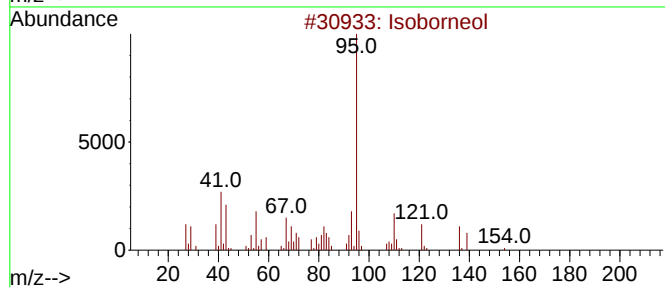
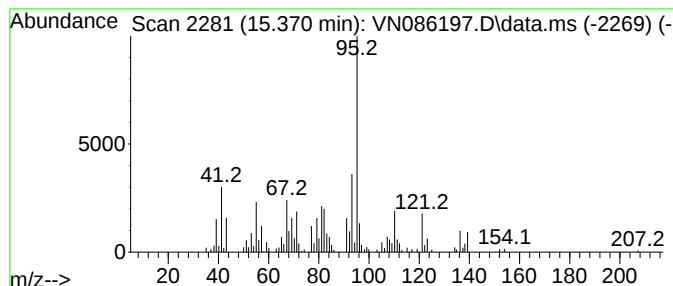
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Quant Title : SW846 8260

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

Peak Number 7 Isoborneol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.370	18.37 ug/l	253274	1,4-Dichlorobenzene-d4	13.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isoborneol	154	C10H18O	000124-76-5	81
2			endo-Borneol	154	C10H18O	000507-70-0	76
3			Bicyclo[2.2.1]heptan-2-ol, 1,7,7...	154	C10H18O	000464-45-9	70
4			1,7,7-Trimethylbicyclo[2.2.1]hep...	154	C10H18O	010385-78-1	60
5			Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040125\
Data File : VN086197.D
Acq On : 01 Apr 2025 15:37
Operator : JC\MD
Sample : Q1659-02 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3809

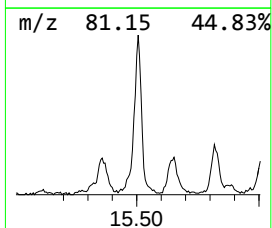
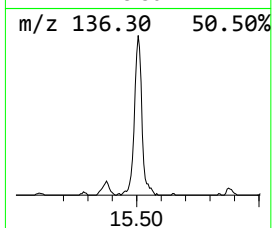
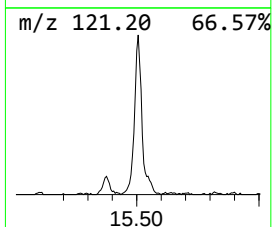
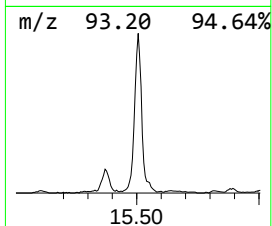
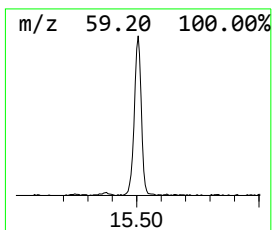
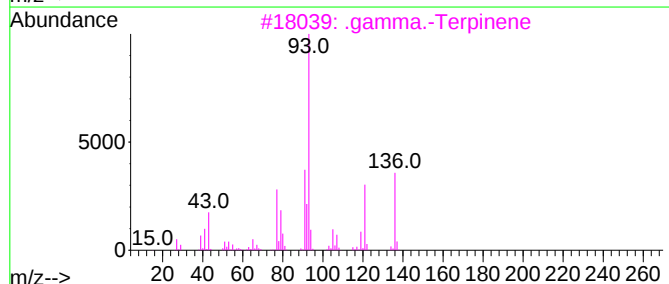
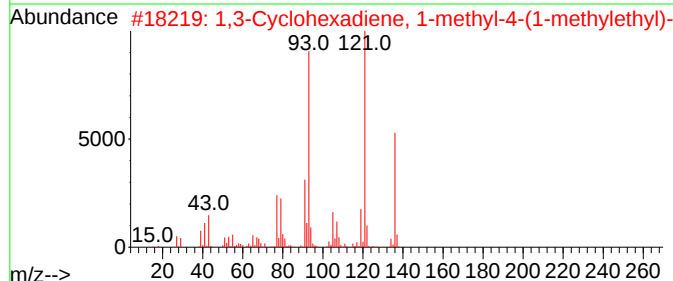
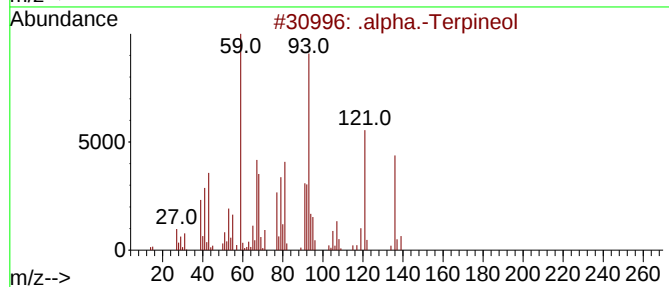
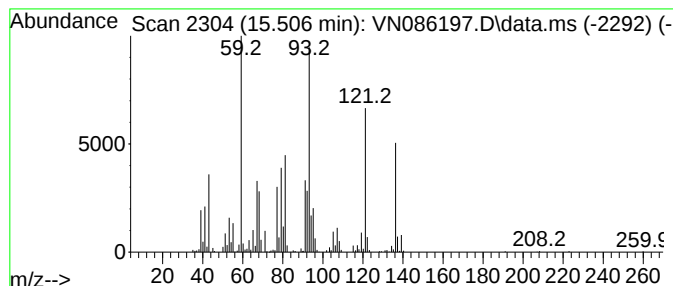
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Quant Title : SW846 8260

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

Peak Number 8 .alpha.-Terpineol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.506	65.15 ug/l	898413	1,4-Dichlorobenzene-d4	13.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Terpineol	154	C10H18O	000098-55-5	91
2			1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	90
3			.gamma.-Terpinene	136	C10H16	000099-85-4	87
4			(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	83
5			2-Carene	136	C10H16	000554-61-0	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040125\
Data File : VN086197.D
Acq On : 01 Apr 2025 15:37
Operator : JC\MD
Sample : Q1659-02 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3809

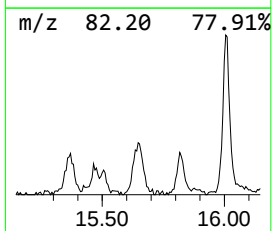
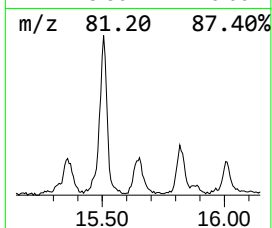
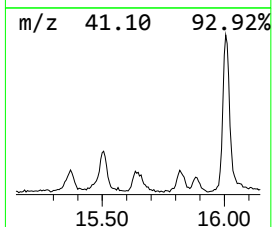
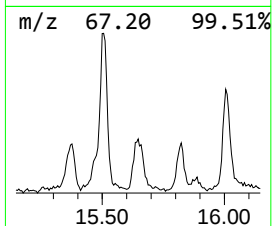
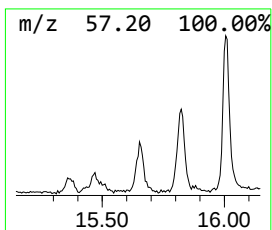
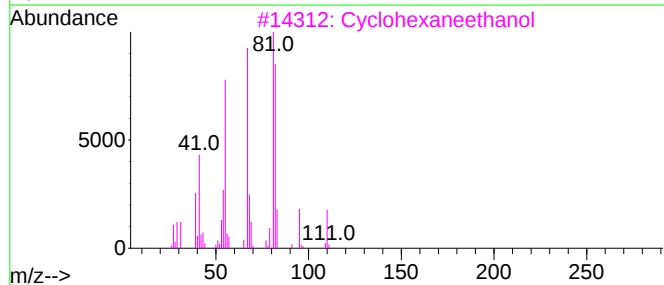
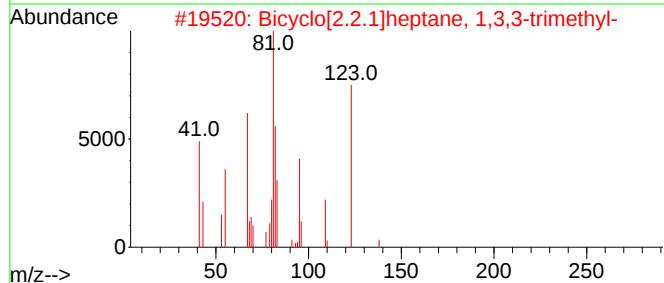
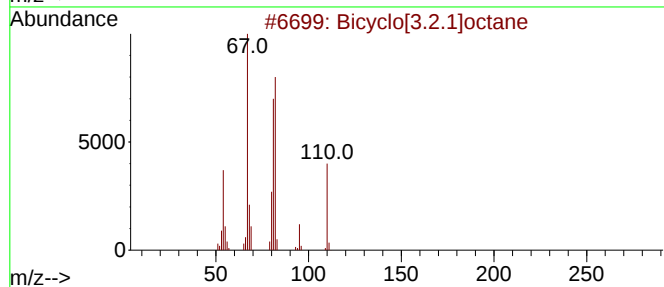
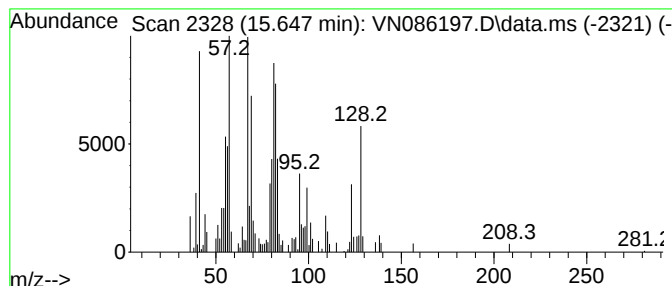
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Quant Title : SW846 8260

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

Peak Number 9 unknown15.647 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.647	14.02 ug/l	193260	1,4-Dichlorobenzene-d4	13.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.2.1]octane	110	C8H14	006221-55-2	49
2			Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	45
3			Cyclohexaneethanol	128	C8H16O	004442-79-9	43
4			Bicyclo[4.1.0]heptane, 2-methyl-	110	C8H14	041977-46-2	41
5			Hexenyl angelate, 4z-	182	C11H18O2	1000383-63-7	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040125\
Data File : VN086197.D
Acq On : 01 Apr 2025 15:37
Operator : JC\MD
Sample : Q1659-02 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3809

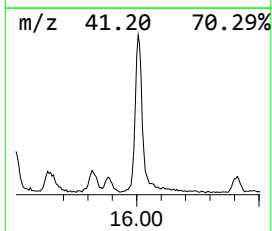
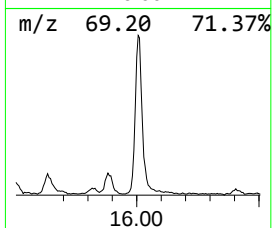
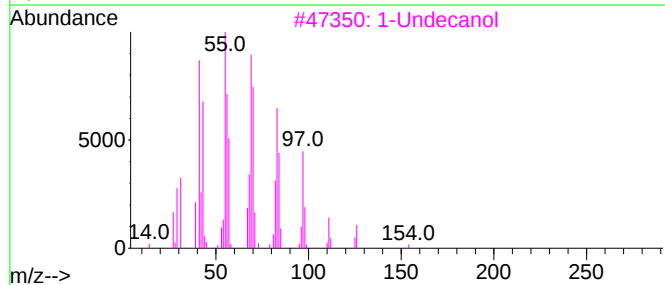
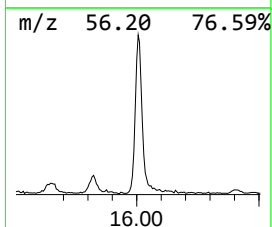
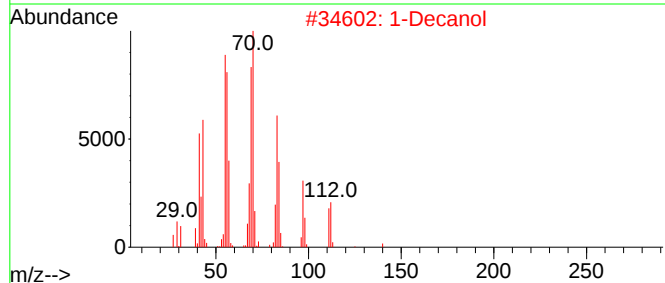
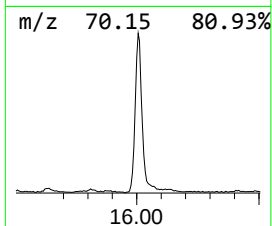
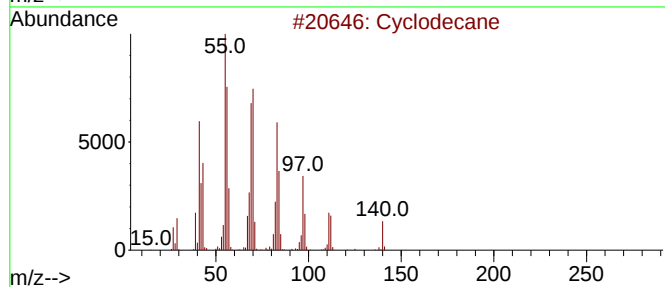
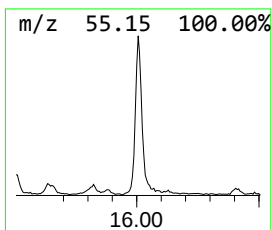
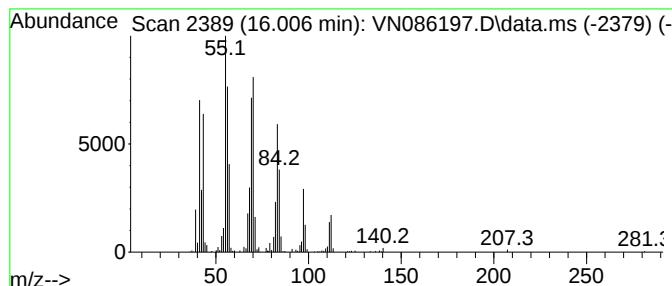
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

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

Peak Number 10 Cyclodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.006	71.32 ug/l	983433	1,4-Dichlorobenzene-d4	13.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclodecane	140	C10H20	000293-96-9	96
2			1-Decanol	158	C10H22O	000112-30-1	91
3			1-Undecanol	172	C11H24O	000112-42-5	91
4			Bromoacetic acid, decyl ester	278	C12H23BrO2	005436-93-1	90
5			E-11,13-Tetradecadien-1-ol	210	C14H26O	1000131-00-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040125\
Data File : VN086197.D
Acq On : 01 Apr 2025 15:37
Operator : JC\MD
Sample : Q1659-02 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3809

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.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
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unknown3.830	3.830	18.5	ug/l	487003	1	8.800	1313300	50.0
Acetic acid	5.647	163.3	ug/l	4289380	1	8.800	1313300	50.0
Ammonium acetate	9.182	71.0	ug/l	2090580	2	9.506	1472960	50.0
1-Octanol	14.241	532.5	ug/l	7342300	4	13.812	689449	50.0
3-Carene	14.488	41.9	ug/l	577089	4	13.812	689449	50.0
Isoborneol	15.370	18.4	ug/l	253274	4	13.812	689449	50.0
.alpha.-Terpineol	15.506	65.2	ug/l	898413	4	13.812	689449	50.0
unknown15.647	15.647	14.0	ug/l	193260	4	13.812	689449	50.0
Cyclodecane	16.006	71.3	ug/l	983433	4	13.812	689449	50.0