

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111824\
 Data File : VN084917.D
 Acq On : 18 Nov 2024 14:04
 Operator : JC\MD
 Sample : P4857-01
 Misc : 5.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 ETGI-328

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\82N103024W.M

Title : SW846 8260

Signal : TIC: VN084917.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.295	51	58	67	rBV	54478	98480	11.11%	1.441%
2	2.830	135	149	152	rBV5	14647	46748	5.27%	0.684%
3	2.953	152	170	172	rBV10	15714	73396	8.28%	1.074%
4	7.241	891	899	908	rBV	3892	10998	1.24%	0.161%
5	8.159	1044	1055	1060	rBV2	126378	309168	34.88%	4.524%
6	8.218	1060	1065	1074	rVB	225195	486664	54.90%	7.122%
7	8.577	1116	1126	1136	rBV	139114	314586	35.49%	4.603%
8	9.100	1204	1215	1230	rBV	317651	656848	74.10%	9.612%
9	10.565	1455	1464	1473	rBV	494770	886420	100.00%	12.971%
10	11.865	1677	1685	1696	rBV	443077	788985	89.01%	11.546%
11	12.071	1714	1720	1724	rBV4	6729	12992	1.47%	0.190%
12	12.400	1771	1776	1782	rBV5	5372	11347	1.28%	0.166%
13	12.706	1820	1828	1836	rBV2	47777	90984	10.26%	1.331%
14	12.847	1842	1852	1861	rBV	352001	628050	70.85%	9.191%
15	13.165	1902	1906	1911	rVB8	8411	17429	1.97%	0.255%
16	13.265	1919	1923	1926	rVB4	9070	13995	1.58%	0.205%
17	13.488	1956	1961	1962	rBV3	7164	9781	1.10%	0.143%
18	13.617	1979	1983	1987	rBV5	7507	14822	1.67%	0.217%
19	13.706	1989	1998	1999	rBV6	18927	37288	4.21%	0.546%
20	13.788	2006	2012	2021	rVB	423663	747305	84.31%	10.936%
21	13.917	2031	2034	2036	rBV4	6583	9119	1.03%	0.133%
22	13.982	2042	2045	2048	rBV4	6684	9988	1.13%	0.146%
23	14.106	2061	2066	2077	rBV3	55429	111374	12.56%	1.630%
24	14.435	2118	2122	2127	rBV6	12121	19886	2.24%	0.291%
25	14.506	2127	2134	2139	rBV9	23580	56713	6.40%	0.830%
26	14.623	2150	2154	2157	rBV3	42999	64827	7.31%	0.949%
27	14.664	2157	2161	2169	rVB2	53850	105468	11.90%	1.543%
28	14.729	2169	2172	2175	rBV3	23571	36311	4.10%	0.531%
29	14.770	2175	2179	2186	rVV3	38628	109930	12.40%	1.609%
30	14.841	2187	2191	2200	rVB9	31305	76099	8.58%	1.114%
31	14.959	2206	2211	2217	rVB4	65471	113525	12.81%	1.661%
32	15.035	2219	2224	2227	rBV6	54834	115161	12.99%	1.685%
33	15.264	2259	2263	2268	rBV3	59746	95287	10.75%	1.394%
34	15.329	2268	2274	2279	rBV6	50153	129115	14.57%	1.889%
35	15.429	2281	2291	2297	rVV6	75558	247379	27.91%	3.620%
36	15.917	2370	2374	2377	rBV4	71489	134230	15.14%	1.964%

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ClientSampleId :
ETGI-328

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\82N103024W.M
Title : SW846 8260

37	16.170	2413	2417	2421	rbV4	82588	142980	16.13%	2.092%
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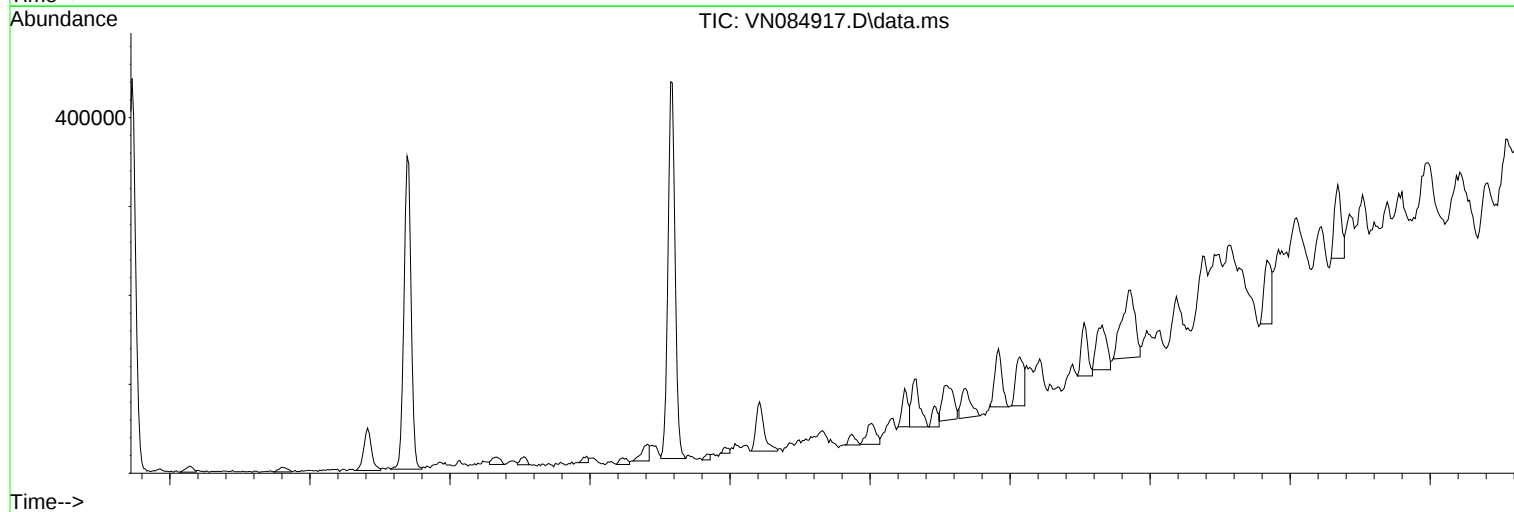
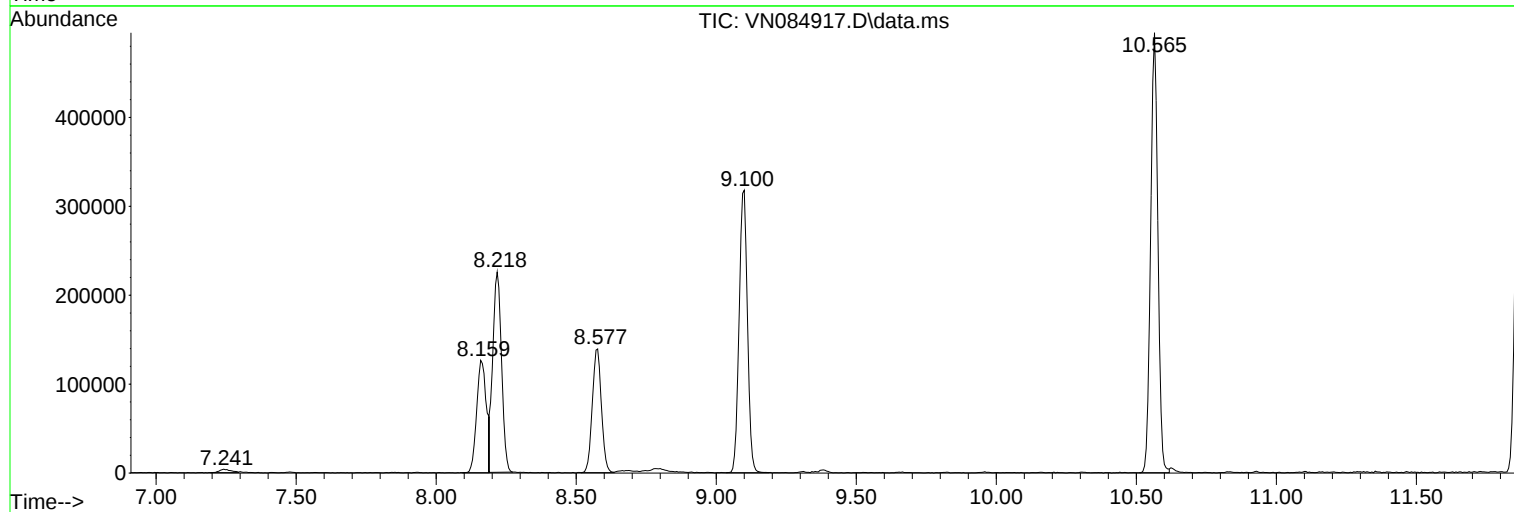
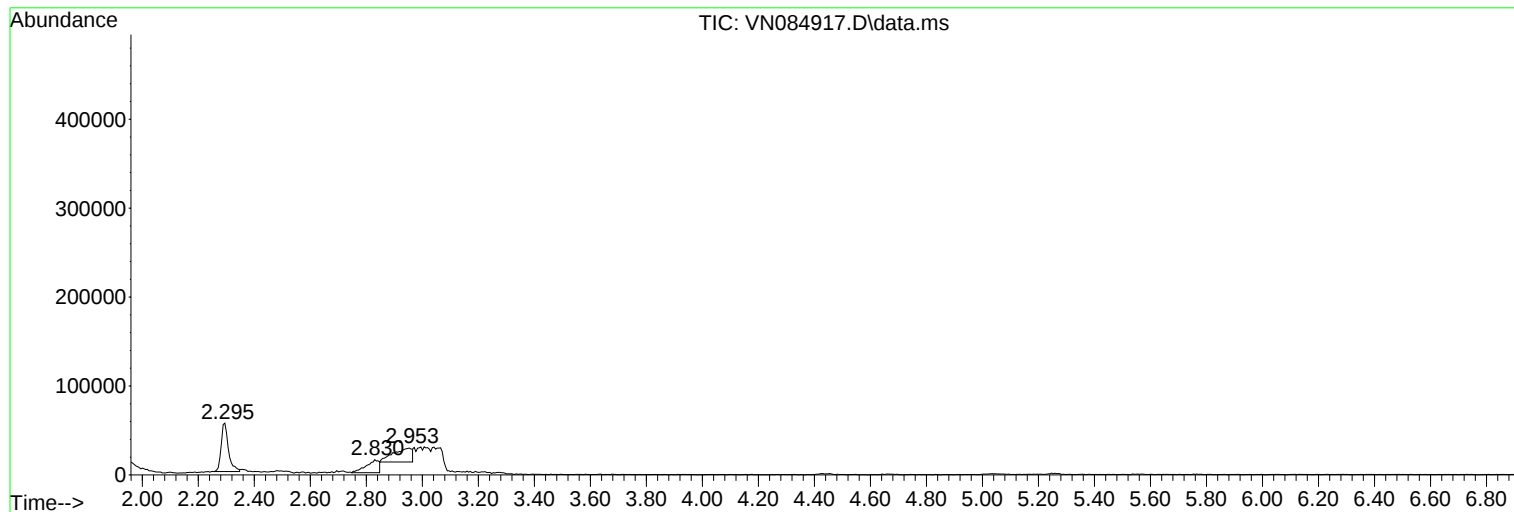
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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



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ALS Vial : 10 Sample Multiplier: 1

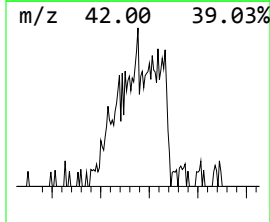
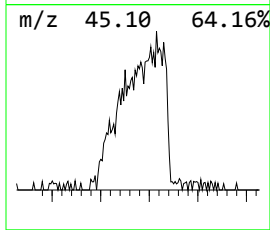
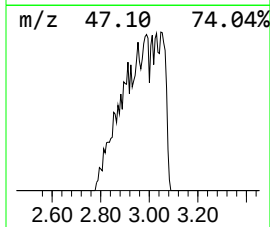
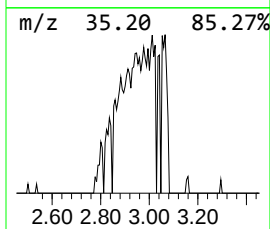
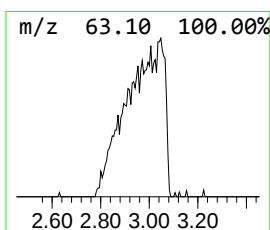
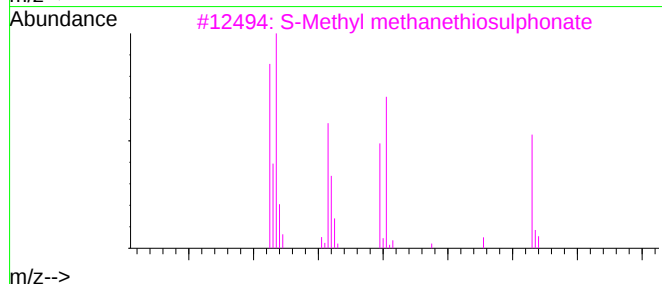
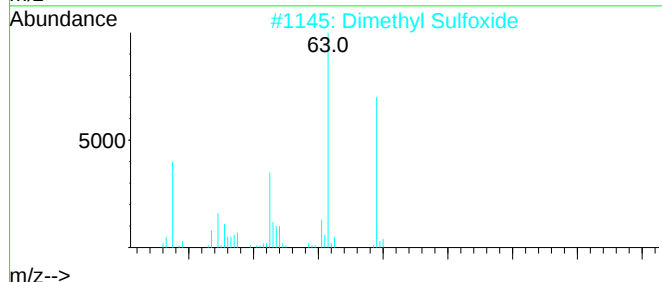
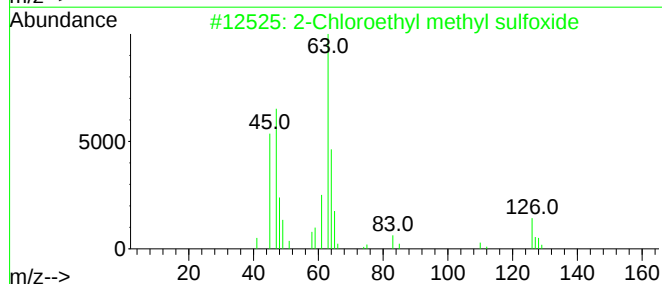
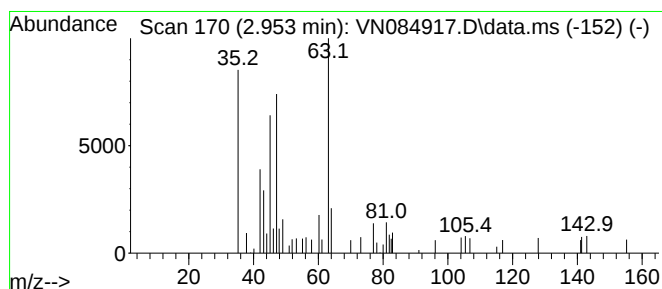
Instrument :
MSVOA_N
ClientSampleId :
ETGI-328

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Chloroethyl methyl sulfoxide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.953	7.54 ug/l	73396	Pentafluorobenzene	8.218	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloroethyl methyl sulfoxide	126	C3H7ClOS	005331-57-7	50
2	Dimethyl Sulfoxide	78	C2H6OS	000067-68-5	12
3	S-Methyl methanethiosulphonate	126	C2H6O2S2	002949-92-0	12
4	Ethene, (methylsulfonyl)-	106	C3H6O2S	003680-02-2	9
5	(Z)-1-Chloro-2-(methylsulfonyl)e...	140	C3H5ClO2S	115584-12-8	9



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ETGI-328

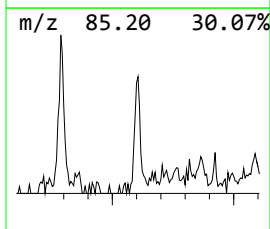
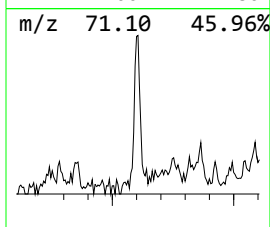
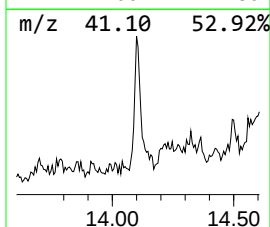
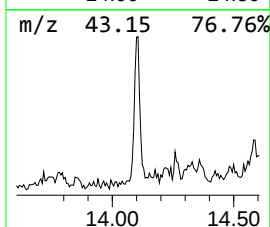
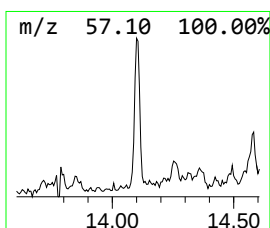
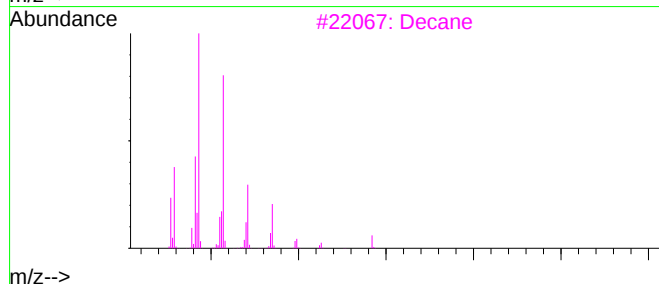
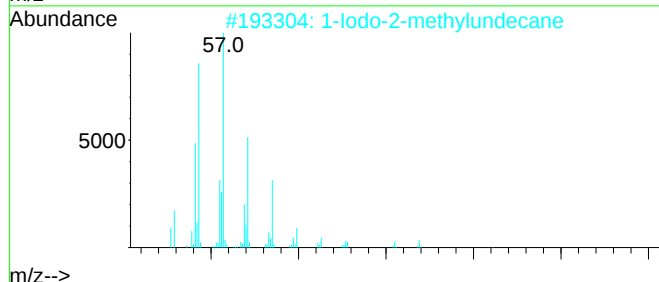
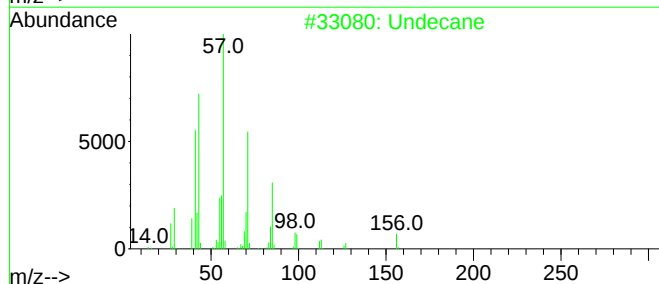
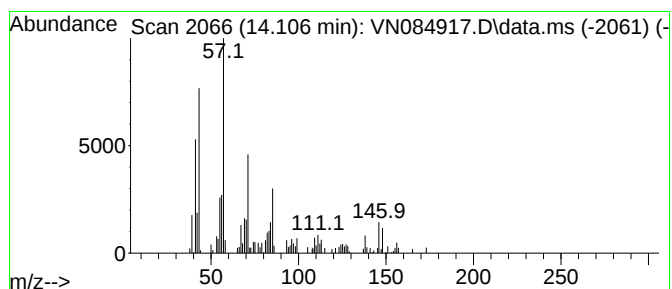
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Undecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.106	7.45 ug/l	111374	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	81
2	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	64
3	Decane	142	C10H22	000124-18-5	59
4	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	58
5	Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1010309-37-4	52



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Misc : 5.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ETGI-328

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

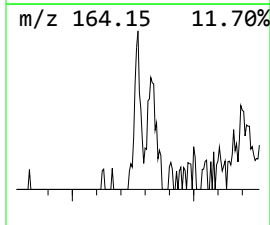
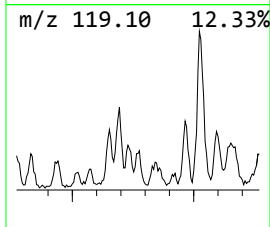
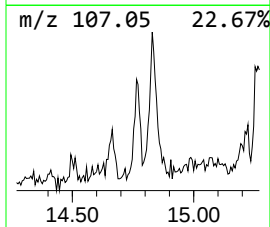
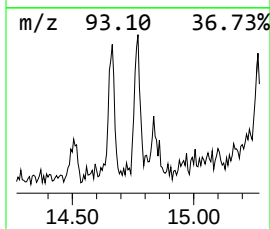
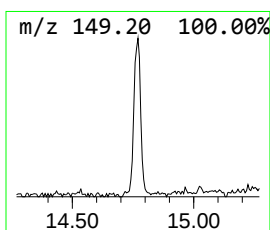
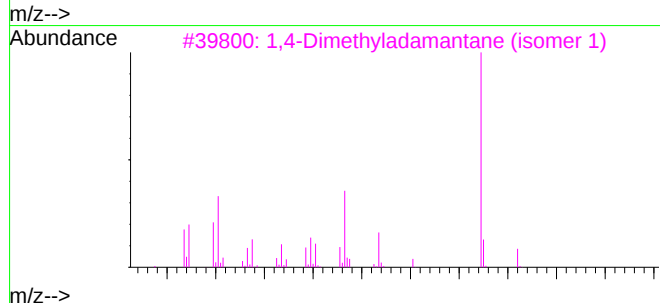
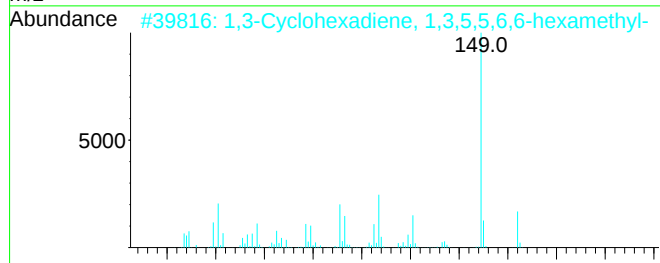
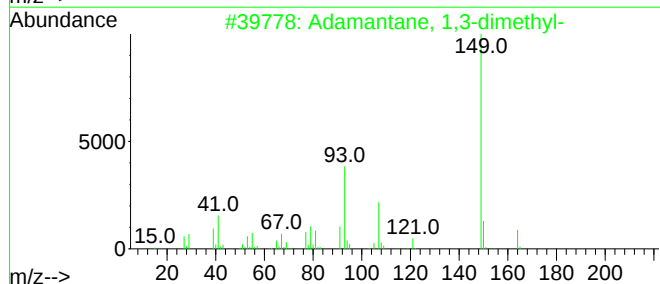
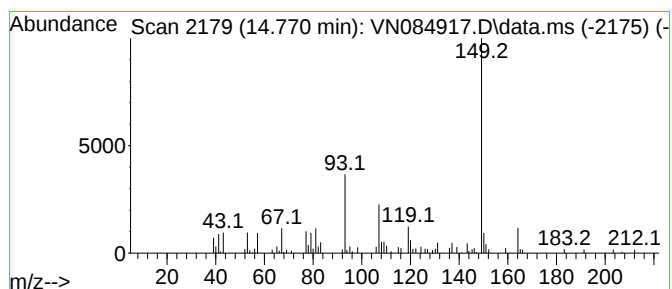
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Adamantane, 1,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.770	7.36 ug/l	109930	1,4-Dichlorobenzene-d4	13.794

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	76
2		1,3-Cyclohexadiene, 1,3,5,5,6,6-...	164	C12H20	1000150-39-4	74
3		1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	64
4		1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	59
5		Added stereo to name	164	C12H20	024145-88-8	59



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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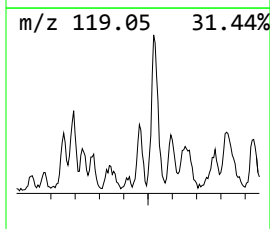
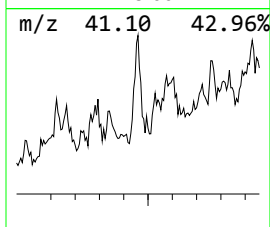
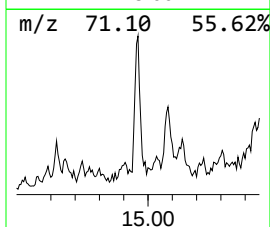
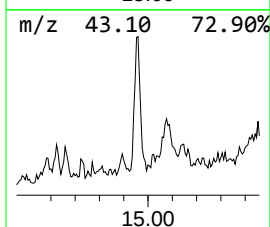
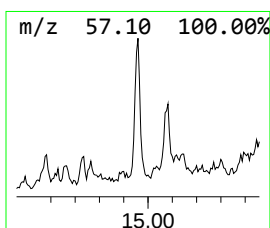
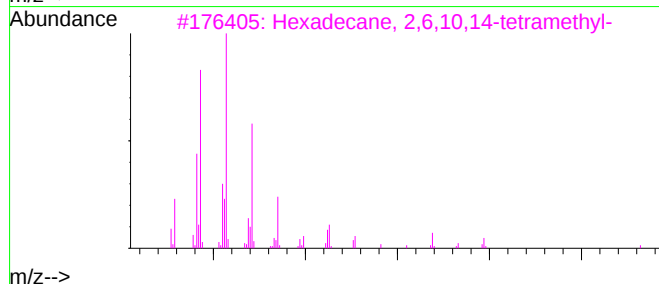
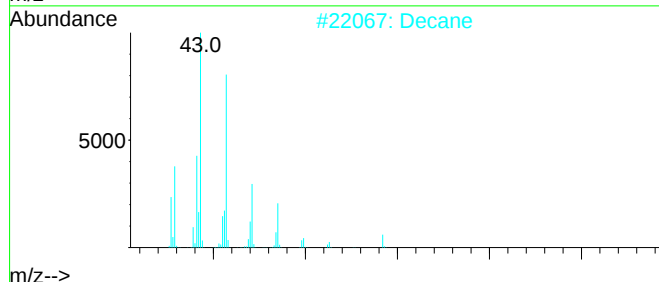
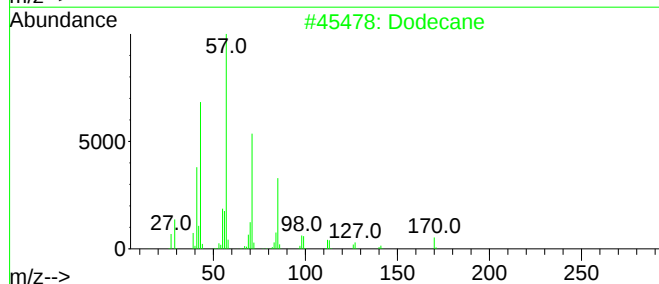
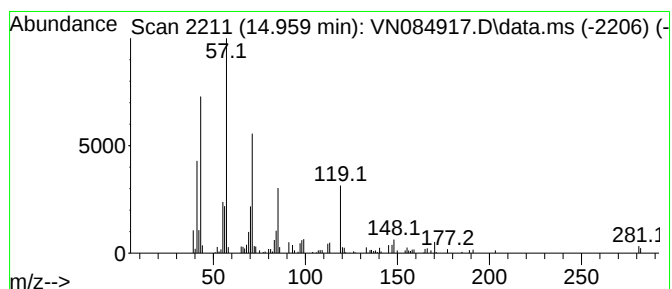
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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

Peak Number 5 Dodecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	7.60 ug/l	113525	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	76
2	Decane	142	C10H22	000124-18-5	72
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	64
4	Hexadecane	226	C16H34	000544-76-3	64
5	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64



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MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

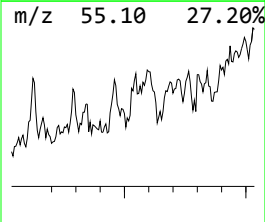
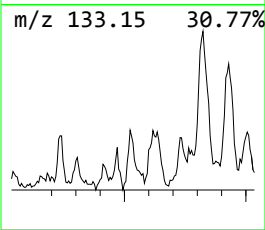
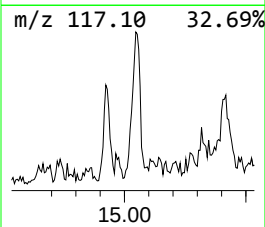
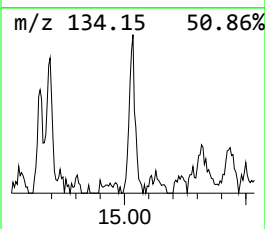
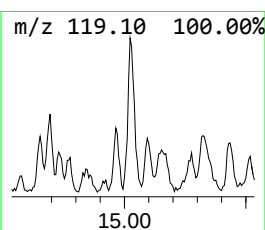
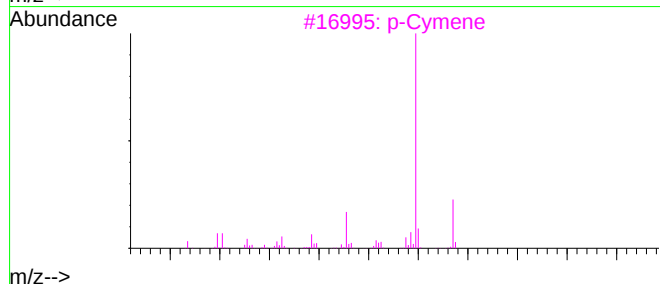
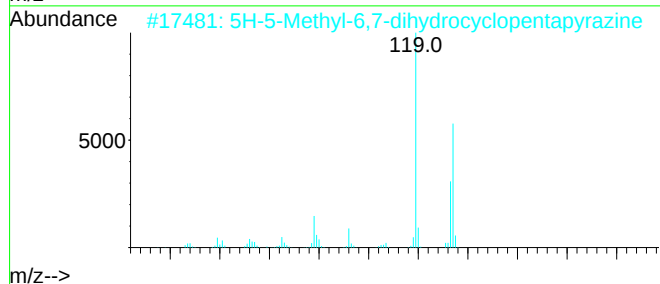
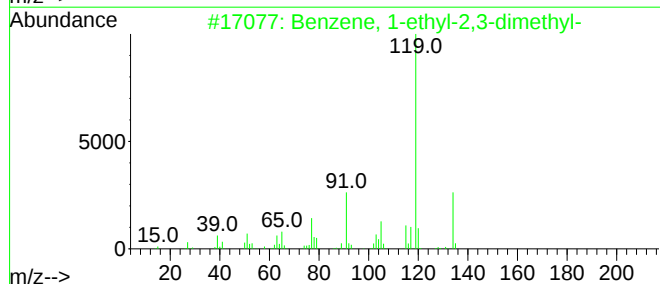
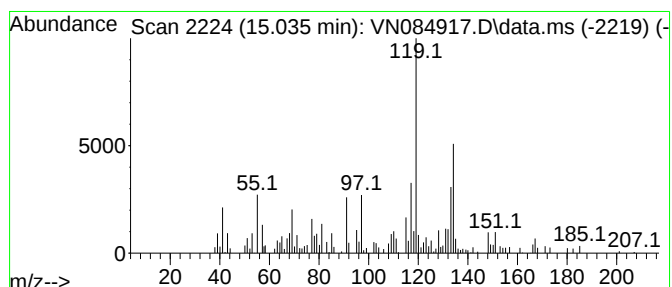
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.035	7.71 ug/l	115161	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	55
2	5H-5-Methyl-6,7-dihydrocyclopent...	134	C8H10N2	023747-48-0	53
3	p-Cymene	134	C10H14	000099-87-6	49
4	o-Cymene	134	C10H14	000527-84-4	49
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111824\
Data File : VN084917.D
Acq On : 18 Nov 2024 14:04
Operator : JC\MD
Sample : P4857-01
Misc : 5.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

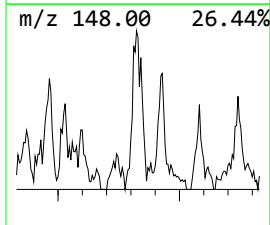
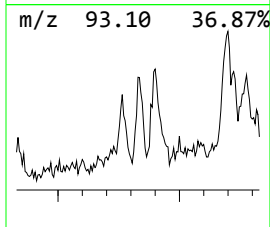
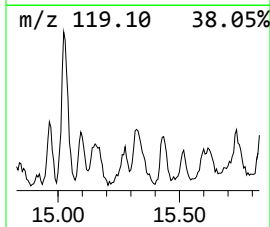
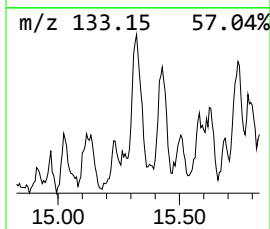
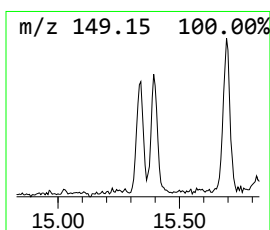
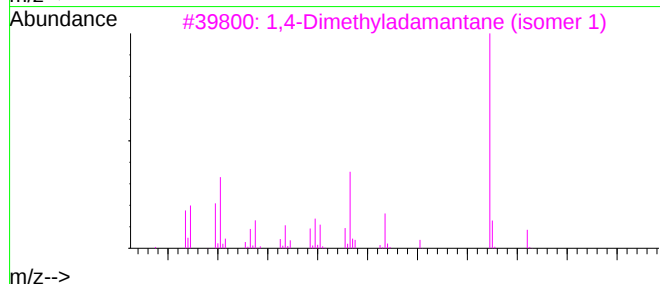
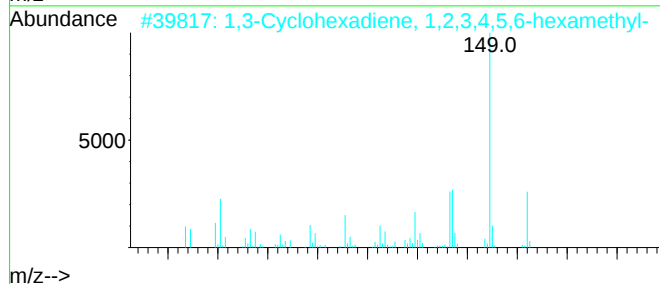
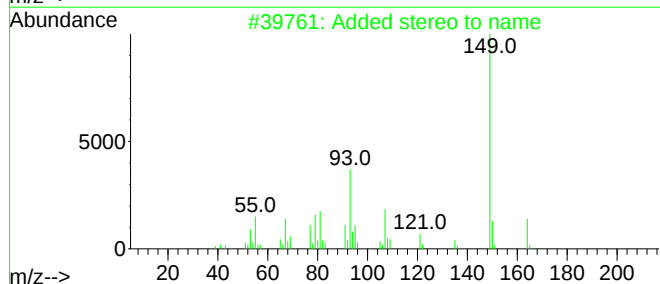
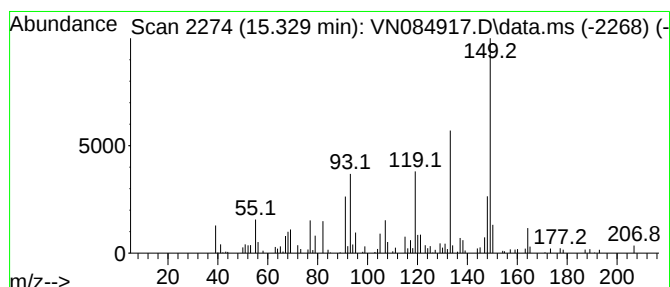
Instrument :
MSVOA_N
ClientSampleId :
ETGI-328

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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

Peak Number 7 Added stereo to name Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.329	8.64 ug/l	129115	1,4-Dichlorobenzene-d4	13.794	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Added stereo to name	164	C12H20	024145-89-9	55
2	1,3-Cyclohexadiene, 1,2,3,4,5,6-...	164	C12H20	1000152-09-6	53
3	1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	46
4	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	46
5	1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111824\
Data File : VN084917.D
Acq On : 18 Nov 2024 14:04
Operator : JC\MD
Sample : P4857-01
Misc : 5.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ETGI-328

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

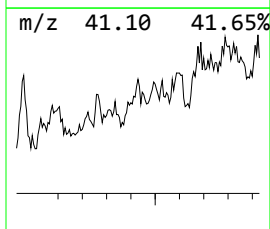
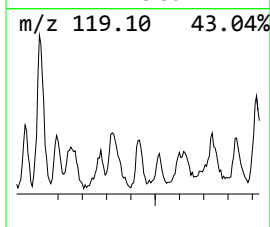
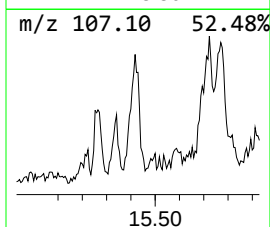
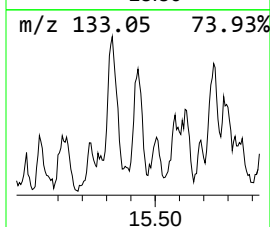
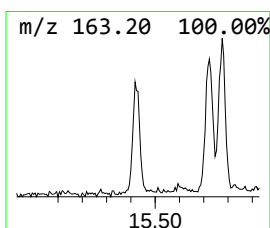
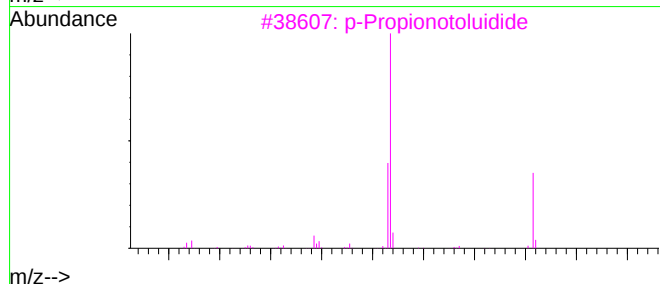
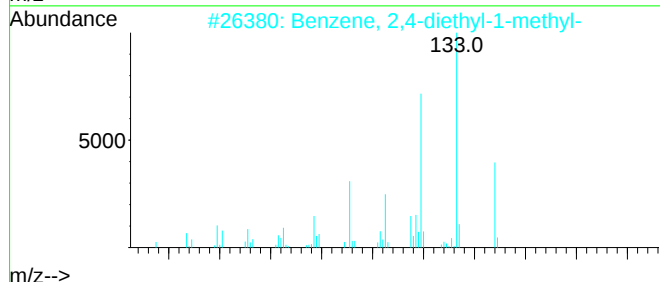
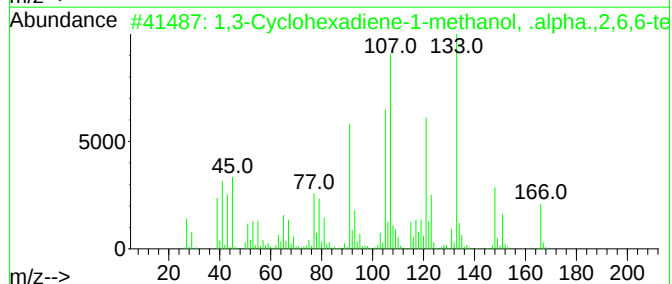
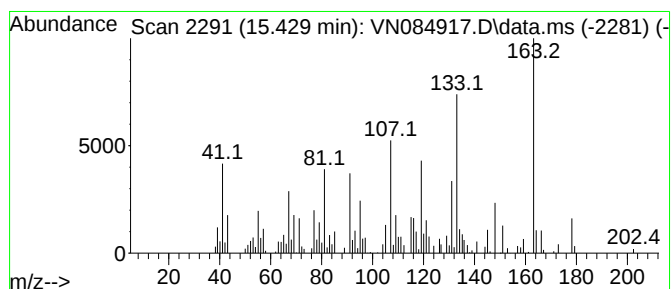
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown15.429 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.429	16.55 ug/l	247379	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Cyclohexadiene-1-methanol,	166	C11H18O	102676-97-1	41
2			Benzene, 2,4-diethyl-1-methyl-	148	C11H16	001758-85-6	38
3			p-Propionotoluidide	163	C10H13NO	002759-55-9	30
4			2-Propenal, 3-(2,6,6-trimethyl-1...	178	C12H18O	004951-40-0	25
5			Benzene, 1-ethyl-2,4,5-trimethyl-	148	C11H16	017851-27-3	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111824\
Data File : VN084917.D
Acq On : 18 Nov 2024 14:04
Operator : JC\MD
Sample : P4857-01
Misc : 5.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ETGI-328

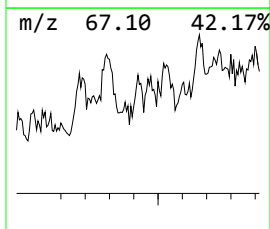
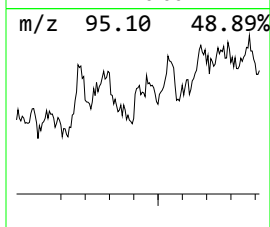
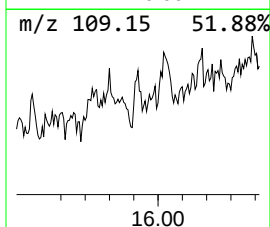
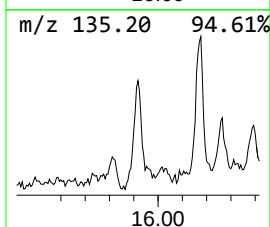
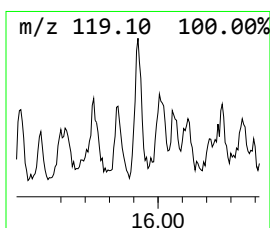
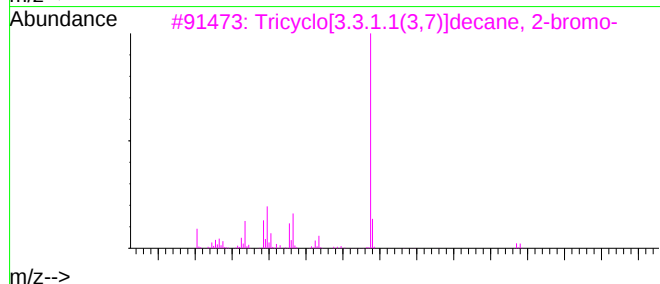
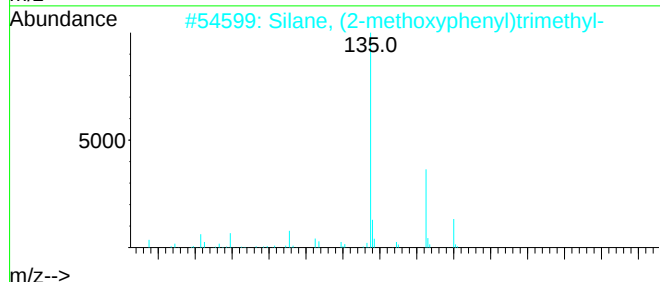
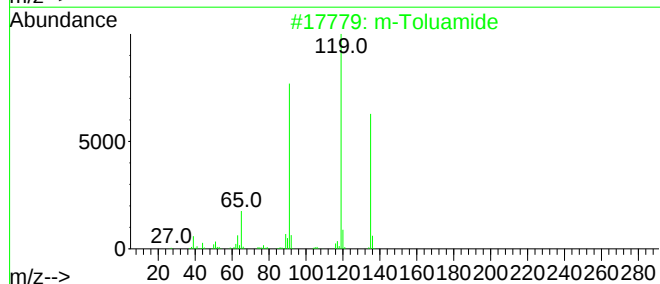
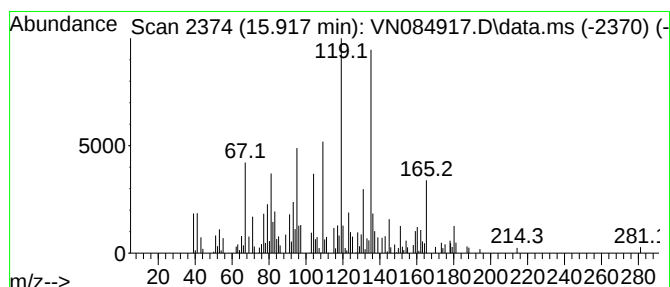
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Quant Title : SW846 8260

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

Peak Number 9 unknown15.917 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.917	8.98 ug/l	134230	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	m-Toluamide	135	C8H9NO	000618-47-3	38
2	Silane, (2-methoxyphenyl)trimethyl-	180	C10H16OSi	000704-43-8	18
3	Tricyclo[3.3.1.1(3,7)]decane, 2-...	214	C10H15Br	007314-85-4	11
4	N-Benzylformamide	135	C8H9NO	006343-54-0	11
5	4'-Methylbutyrophenone	162	C11H14O	004160-52-5	11



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111824\
Data File : VN084917.D
Acq On : 18 Nov 2024 14:04
Operator : JC\MD
Sample : P4857-01
Misc : 5.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ETGI-328

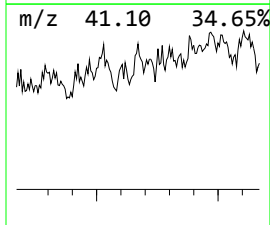
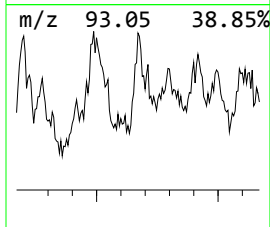
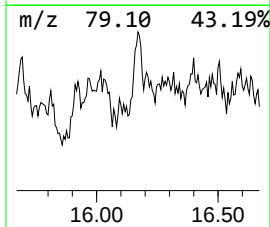
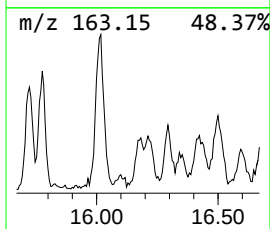
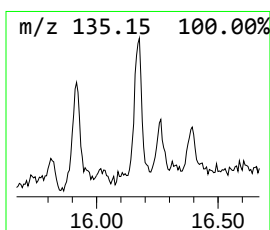
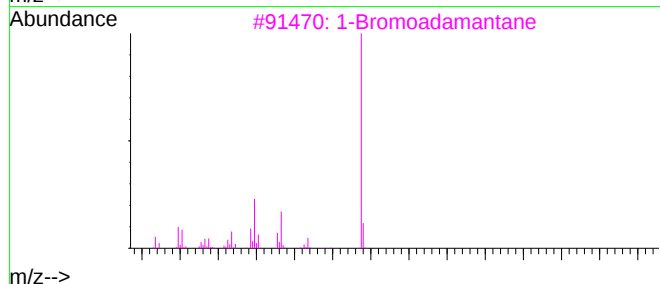
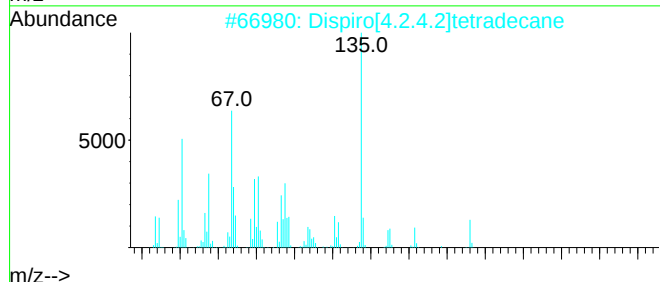
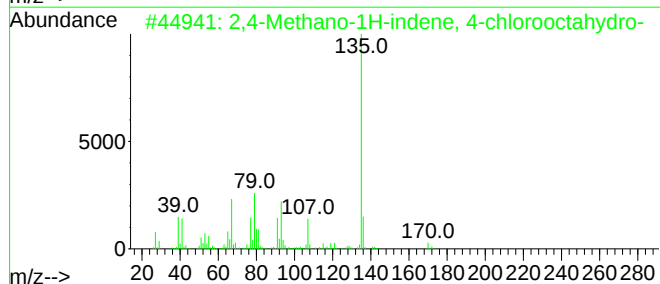
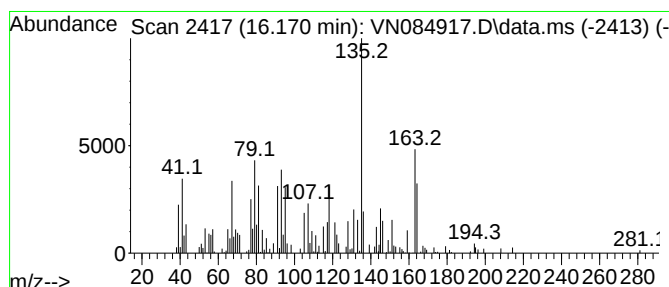
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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

Peak Number 10 unknown16.170 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	9.57 ug/l	142980	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Methano-1H-indene, 4-chloroo...	170	C10H15Cl	098640-25-6	38
2			Dispiro[4.2.4.2]tetradecane	192	C14H24	079273-13-5	38
3			1-Bromoadamantane	214	C10H15Br	000768-90-1	35
4			3-(Adamantan-1-yl)propanoic acid	208	C13H20O2	016269-16-2	35
5			1,4-Methanophthalazine, 1,4,4a,5...	178	C11H18N2	109746-13-6	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111824\
Data File : VN084917.D
Acq On : 18 Nov 2024 14:04
Operator : JC\MD
Sample : P4857-01
Misc : 5.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ETGI-328

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.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
2-Chloroethyl m...	2.953	7.5	ug/l	73396	1	8.218	486664	50.0
Undecane	14.106	7.5	ug/l	111374	4	13.794	747305	50.0
Adamantane, 1,3...	14.770	7.4	ug/l	109930	4	13.794	747305	50.0
Dodecane	14.959	7.6	ug/l	113525	4	13.794	747305	50.0
Benzene, 1-ethy...	15.035	7.7	ug/l	115161	4	13.794	747305	50.0
Added stereo to...	15.329	8.6	ug/l	129115	4	13.794	747305	50.0
unknown15.429	15.429	16.6	ug/l	247379	4	13.794	747305	50.0
unknown15.917	15.917	9.0	ug/l	134230	4	13.794	747305	50.0
unknown16.170	16.170	9.6	ug/l	142980	4	13.794	747305	50.0