

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
 Data File : VN086319.D
 Acq On : 17 Apr 2025 14:05
 Operator : JC\MD
 Sample : Q1818-01
 Misc : 1.14g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 3822

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\82N041525W.M
 Title : SW846 8260

Signal : TIC: VN086319.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.165	1045	1056	1057	rBV	107572	208636	1.25%	0.598%
2	8.212	1057	1064	1074	rVV2	609488	1431791	8.57%	4.104%
3	8.318	1074	1082	1091	rVB	92593	228356	1.37%	0.655%
4	8.435	1091	1102	1111	rBV	485650	1085364	6.50%	3.111%
5	8.571	1117	1125	1135	rVB	164683	372788	2.23%	1.069%
6	8.700	1135	1147	1154	rBV4	61007	181430	1.09%	0.520%
7	8.959	1182	1191	1201	rBV	468192	901515	5.40%	2.584%
8	9.094	1206	1214	1228	rBV	430356	887392	5.31%	2.544%
9	9.594	1286	1299	1310	rBV2	101054	226839	1.36%	0.650%
10	10.565	1457	1464	1468	rBV	681372	1284574	7.69%	3.682%
11	10.624	1468	1474	1490	rVB	9233075	16710063	100.00%	47.898%
12	11.865	1677	1685	1693	rBV	569261	1054230	6.31%	3.022%
13	11.959	1695	1701	1710	rBV	168921	280404	1.68%	0.804%
14	12.065	1711	1719	1729	rBV	696608	1340704	8.02%	3.843%
15	12.394	1765	1775	1781	rBV	211071	450228	2.69%	1.291%
16	12.847	1846	1852	1861	rVB	435840	785516	4.70%	2.252%
17	13.153	1898	1904	1912	rVB	332597	581303	3.48%	1.666%
18	13.476	1954	1959	1964	rVV	126012	205594	1.23%	0.589%
19	13.665	1986	1991	1996	rBV6	90919	178358	1.07%	0.511%
20	13.788	2007	2012	2020	rBV	572886	1068064	6.39%	3.062%
21	13.982	2040	2045	2049	rBV3	94699	210670	1.26%	0.604%
22	14.100	2060	2065	2072	rBV	543946	900163	5.39%	2.580%
23	14.759	2174	2177	2186	rVB	138728	267490	1.60%	0.767%
24	14.953	2201	2210	2217	rBV2	608804	1015026	6.07%	2.910%
25	15.053	2218	2227	2228	rBV4	134340	341053	2.04%	0.978%
26	15.206	2249	2253	2259	rVB2	102522	203676	1.22%	0.584%
27	15.500	2300	2303	2312	rVB4	90260	218603	1.31%	0.627%
28	15.588	2313	2318	2322	rBV3	97099	194355	1.16%	0.557%
29	15.823	2353	2358	2369	rVB	401203	830608	4.97%	2.381%
30	15.941	2370	2378	2384	rBV5	69224	202251	1.21%	0.580%
31	16.158	2411	2415	2423	rVB2	102563	204064	1.22%	0.585%
32	16.470	2460	2468	2476	rBV	346326	835437	5.00%	2.395%

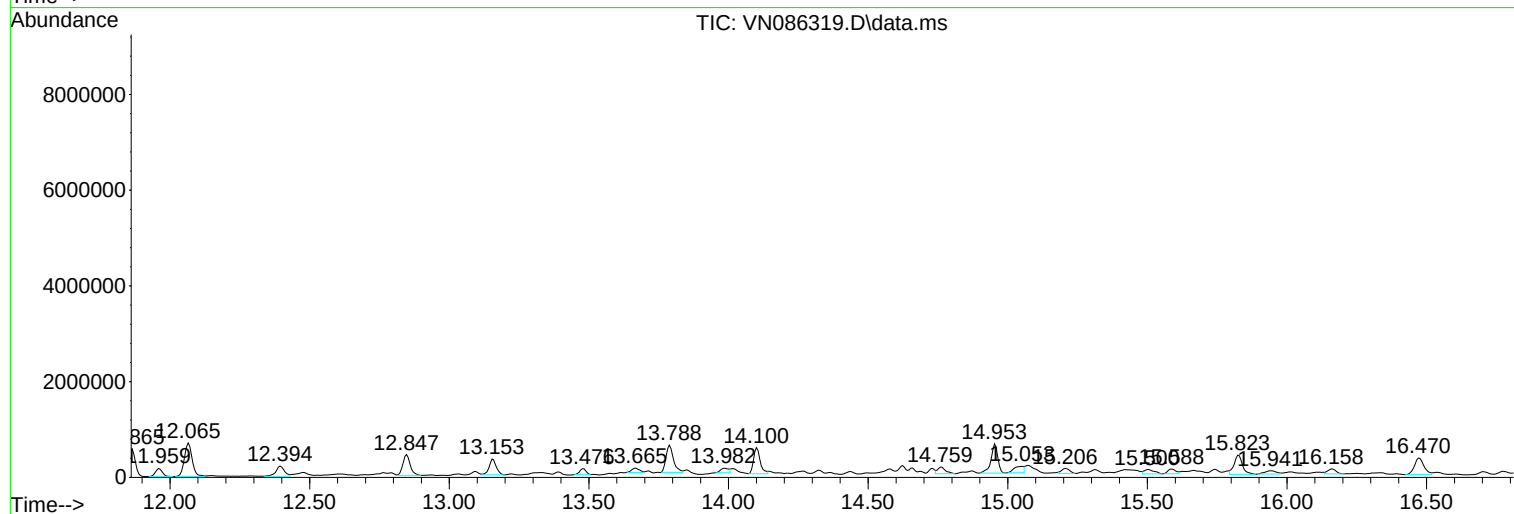
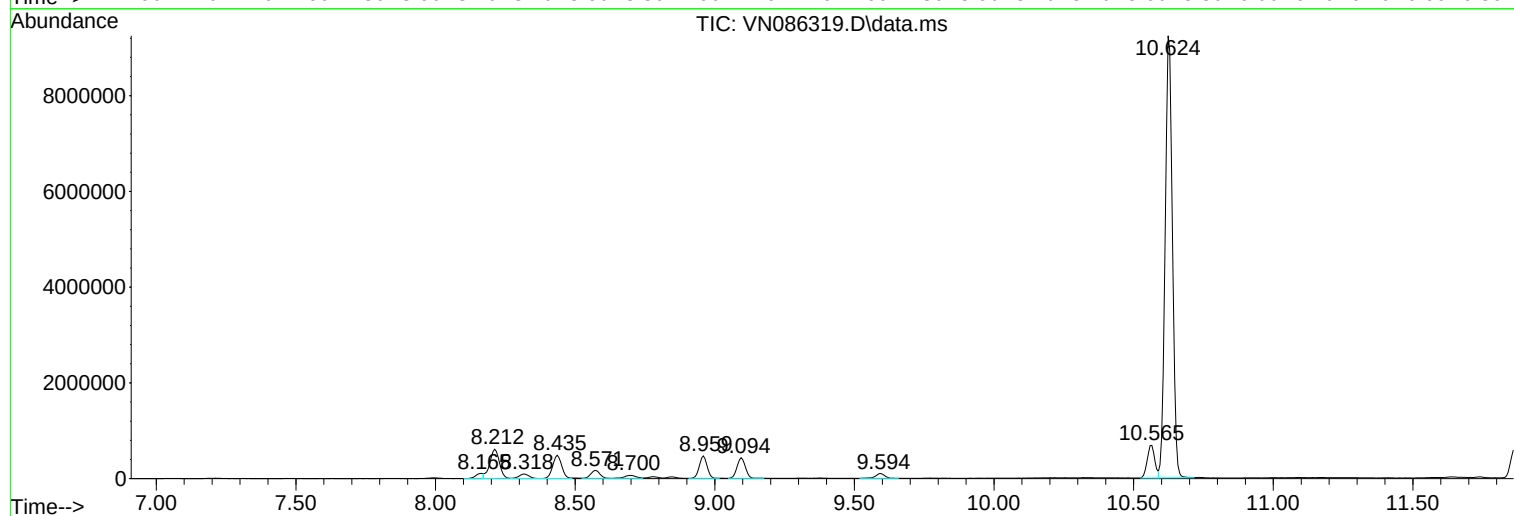
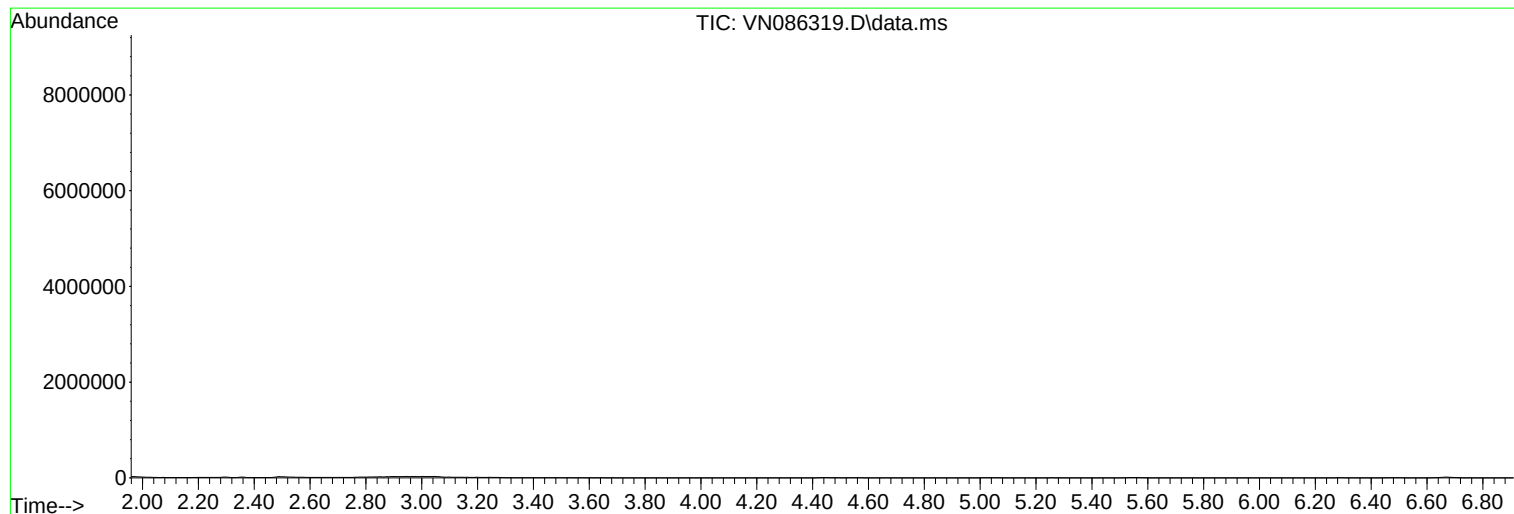
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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



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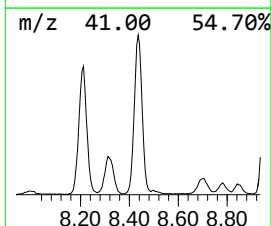
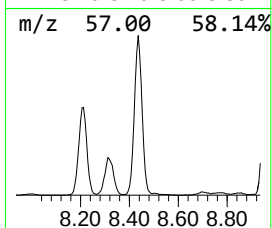
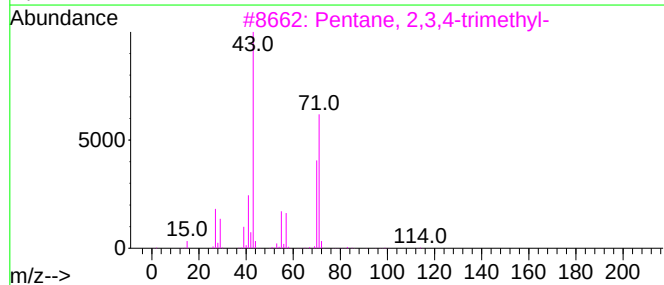
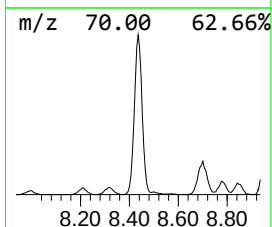
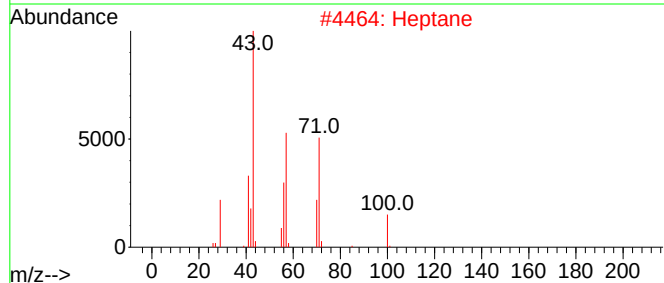
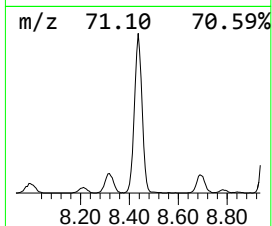
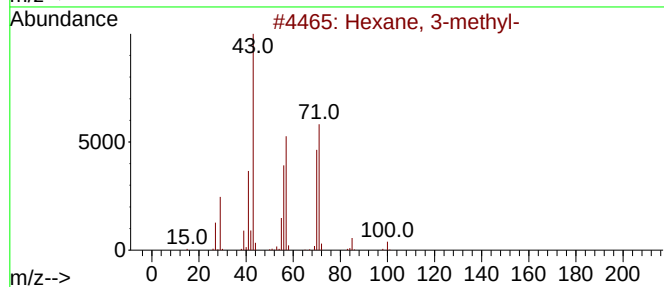
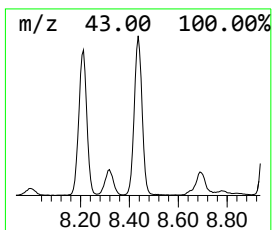
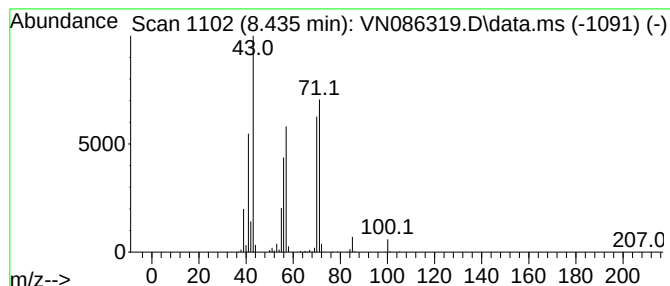
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.435	37.90 ug/l	1085360	Pentafluorobenzene	8.218

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2			Heptane	100	C7H16	000142-82-5	80
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
4			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	53
5			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	53



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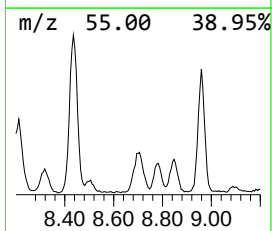
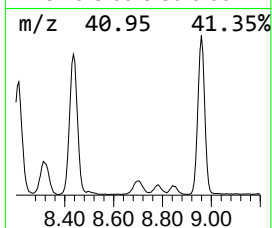
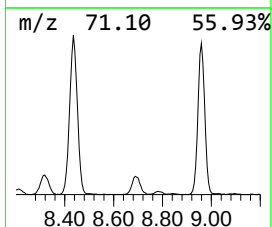
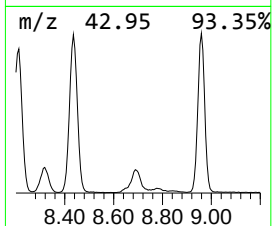
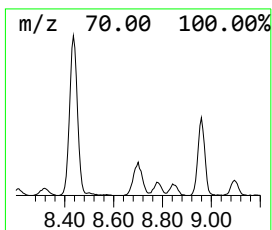
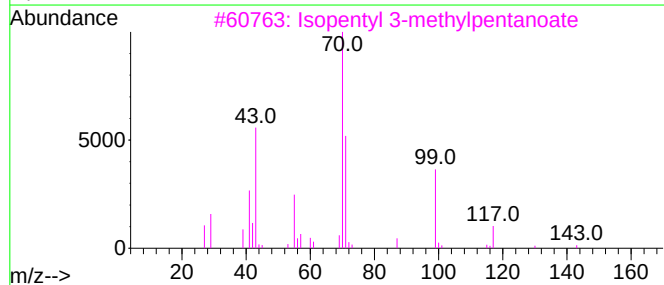
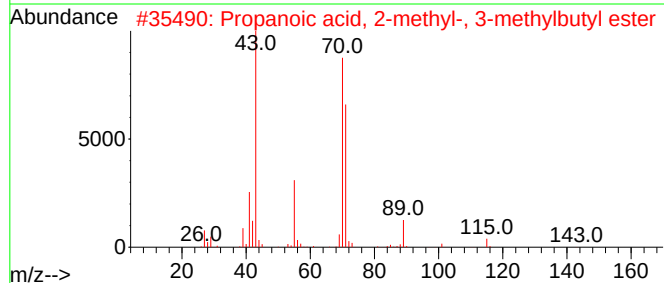
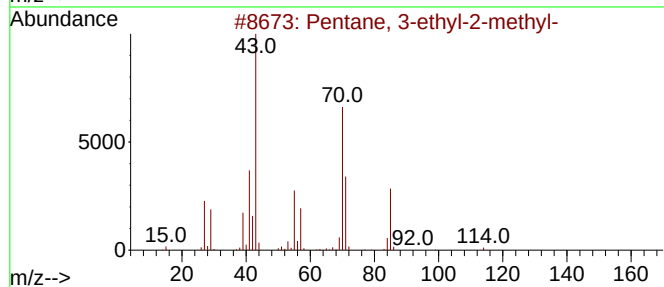
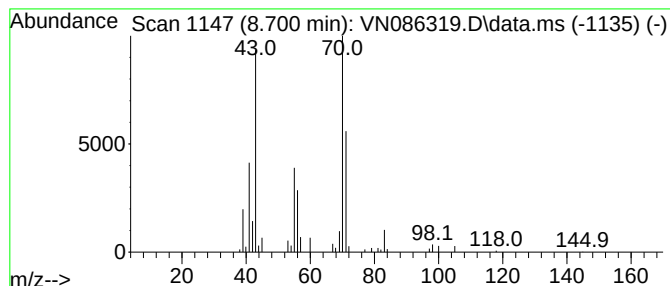
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 3-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.700	10.22 ug/l	181430	1,4-Difluorobenzene	9.094

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	64
2			Propanoic acid, 2-methyl-, 3-met...	158	C9H18O2	002050-01-3	64
3			Isopentyl 3-methylpentanoate	186	C11H22O2	1000433-23-1	53
4			Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	50
5			1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	50



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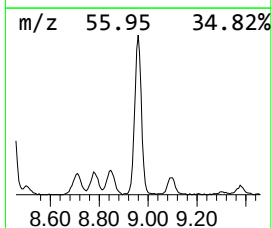
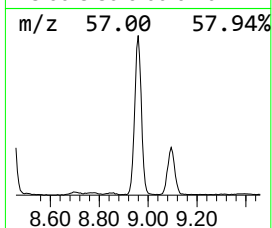
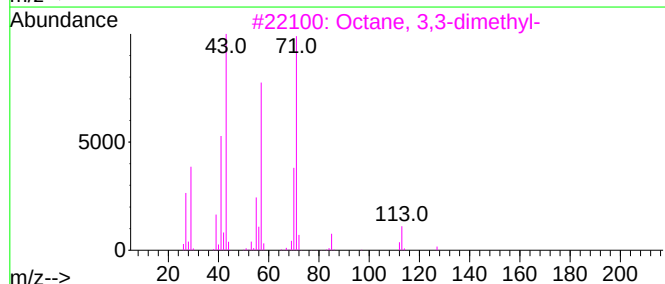
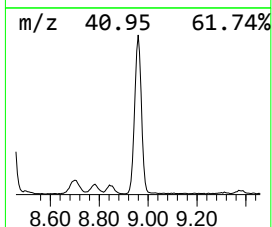
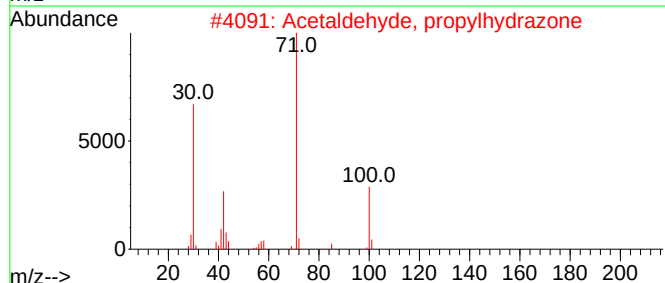
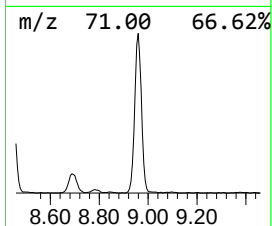
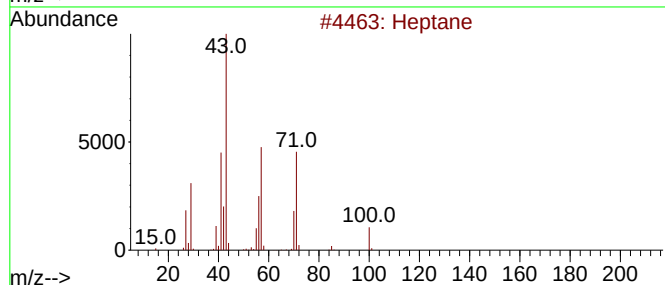
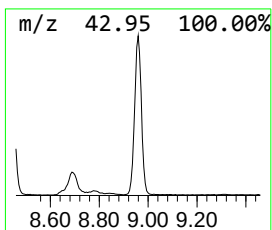
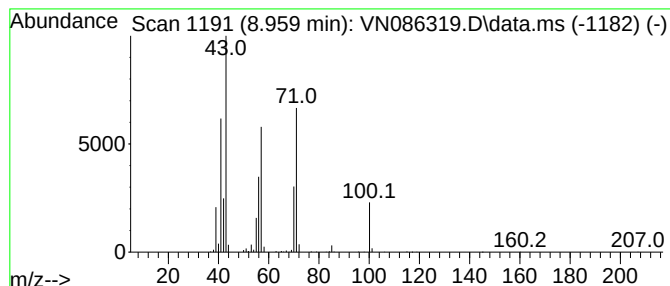
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.959	50.80 ug/l	901515	1,4-Difluorobenzene	9.094	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	49
3	Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	43
4	Decane, 4-methyl-	156	C11H24	002847-72-5	42
5	Hexane, 3-methyl-	100	C7H16	000589-34-4	40



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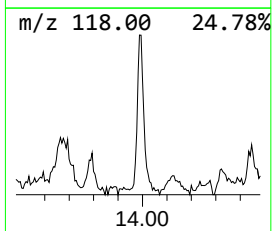
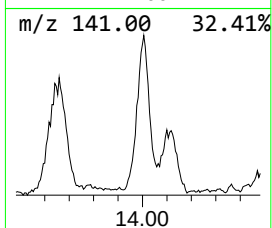
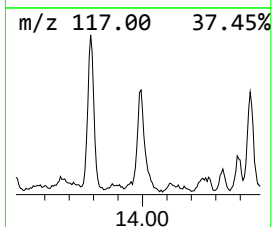
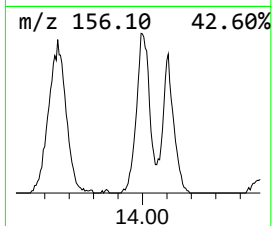
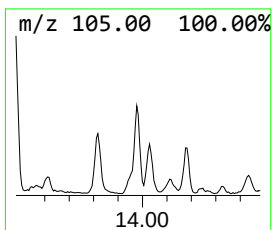
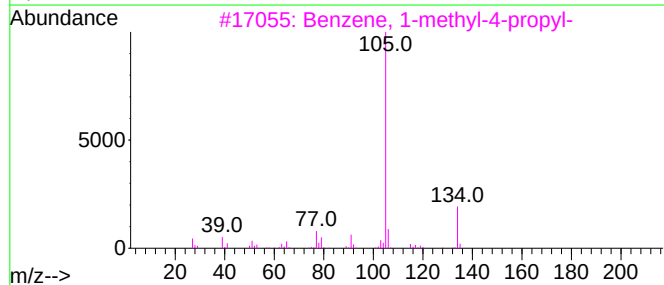
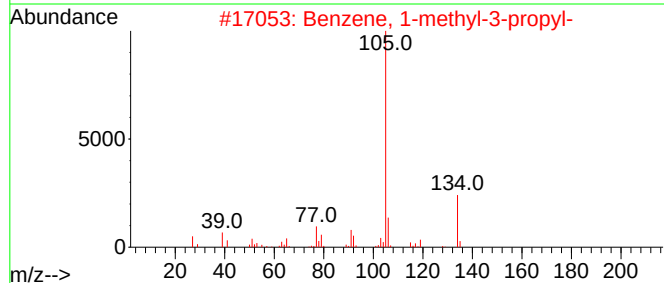
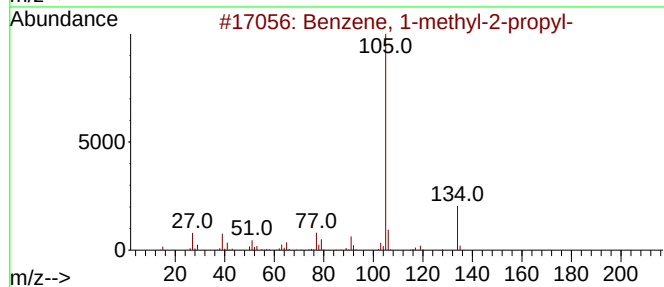
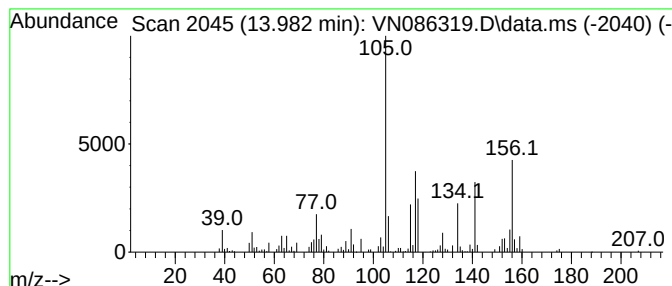
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown13.982 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.982	9.86 ug/l	210670	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	25
2			Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	25
3			Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	18
4			Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	18
5			2-Indanol	134	C9H10O	004254-29-9	14



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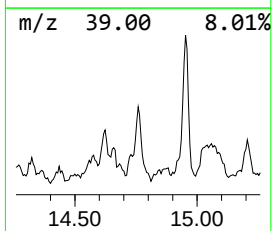
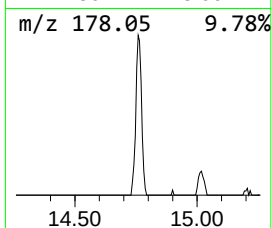
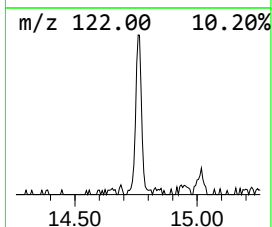
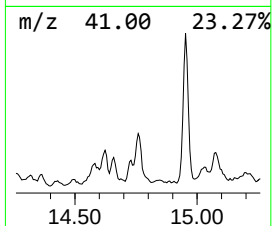
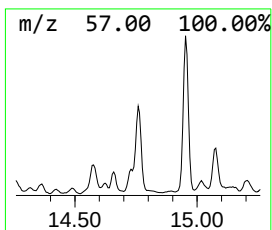
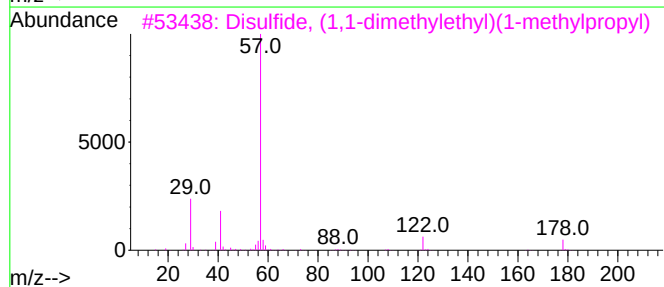
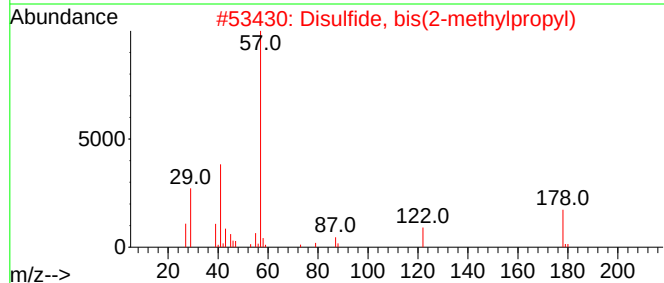
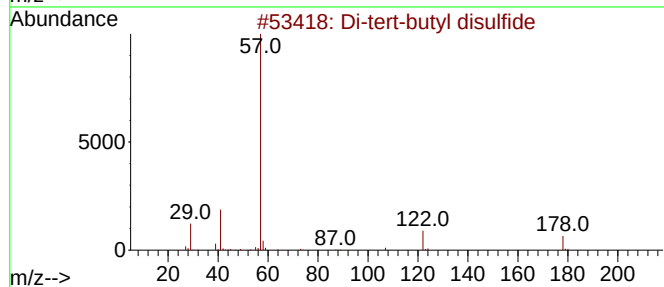
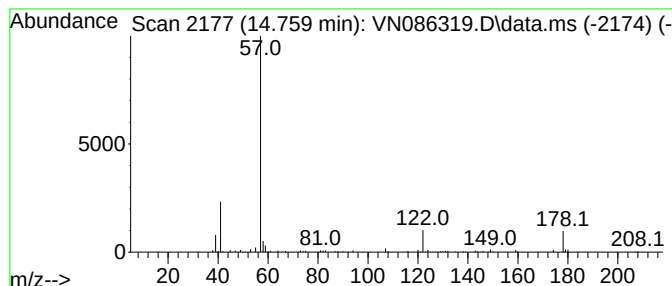
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 5 Di-tert-butyl disulfide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.759	12.52 ug/l	267490	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	80
2			Disulfide, bis(2-methylpropyl)	178	C8H18S2	001518-72-5	58
3			Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	53
4			Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	52
5			Disulfide, dibutyl	178	C8H18S2	000629-45-8	37



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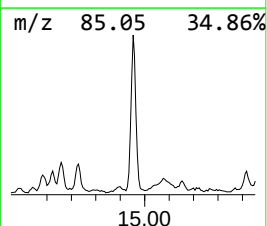
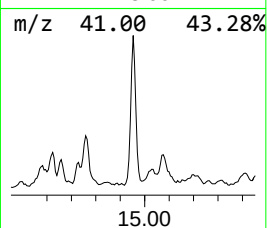
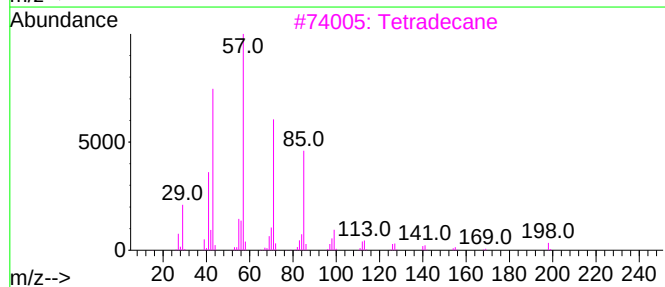
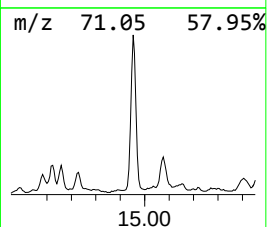
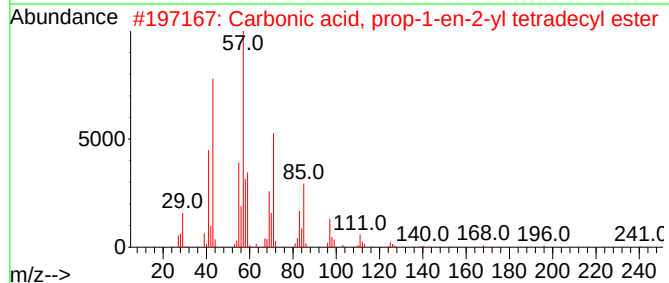
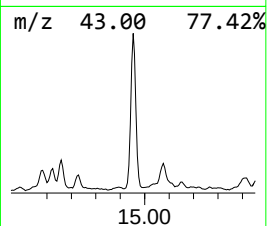
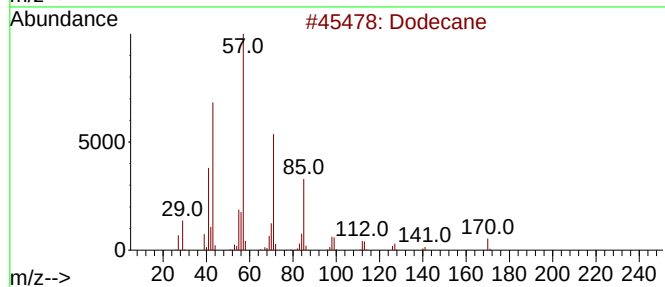
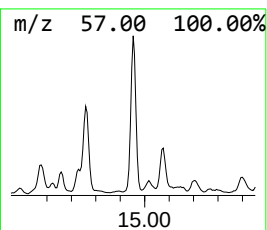
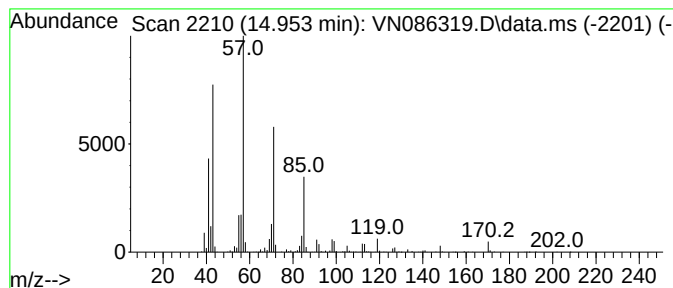
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Quant Title : SW846 8260

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

Peak Number 6 Dodecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.953	47.52 ug/l	1015030	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	93
2			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	80
3			Tetradecane	198	C14H30	000629-59-4	80
4			Tridecane	184	C13H28	000629-50-5	80
5			Undecane	156	C11H24	001120-21-4	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
Data File : VN086319.D
Acq On : 17 Apr 2025 14:05
Operator : JC\MD
Sample : Q1818-01
Misc : 1.14g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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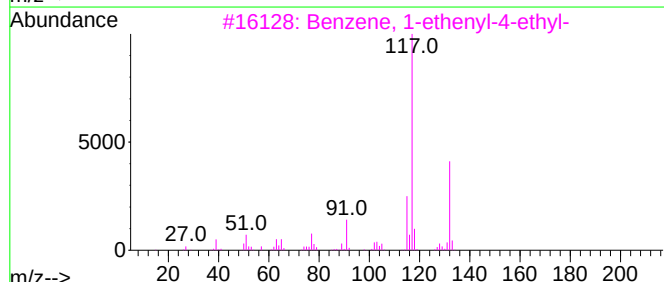
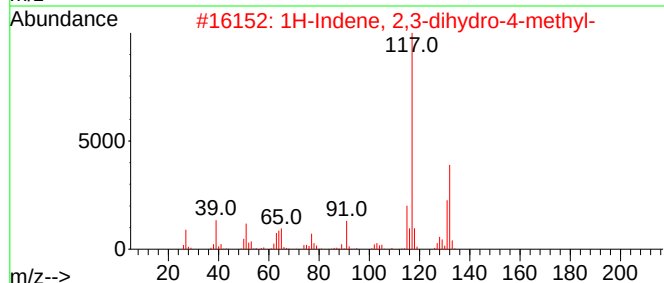
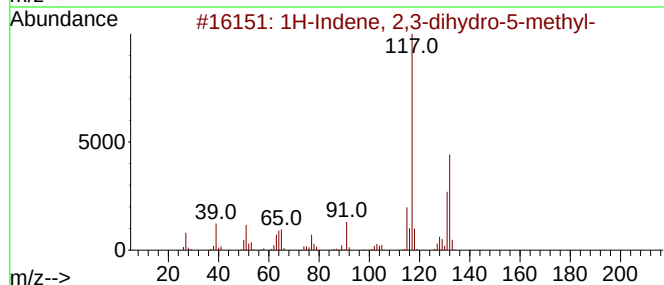
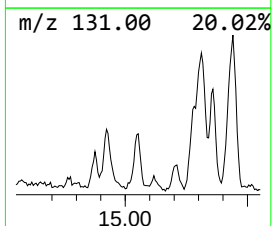
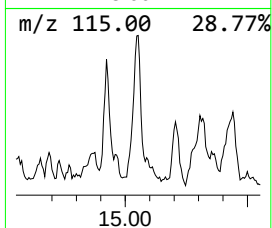
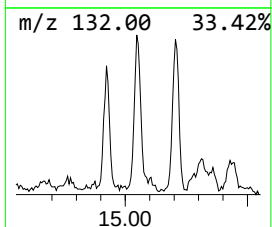
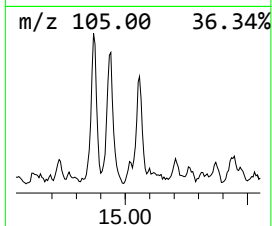
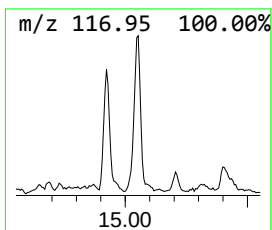
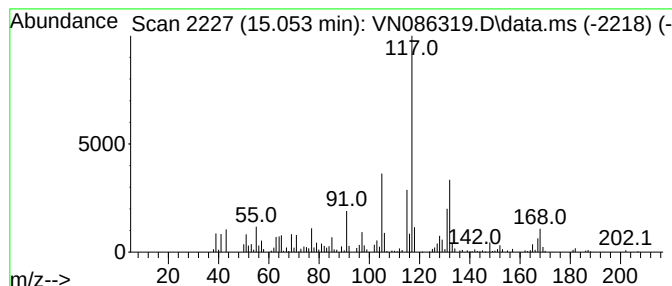
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Quant Title : SW846 8260

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

Peak Number 7 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	15.97 ug/l	341053	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
2			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	70
3			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	64
4			Indan, 1-methyl-	132	C10H12	000767-58-8	58
5			1-Phenyl-1-butene	132	C10H12	000824-90-8	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
Data File : VN086319.D
Acq On : 17 Apr 2025 14:05
Operator : JC\MD
Sample : Q1818-01
Misc : 1.14g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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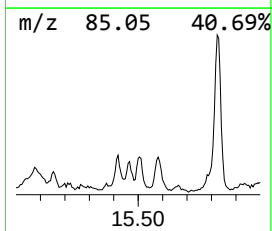
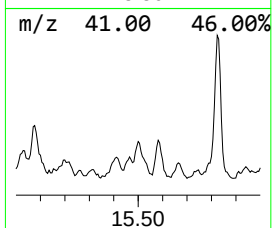
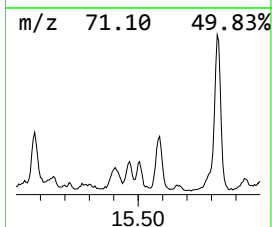
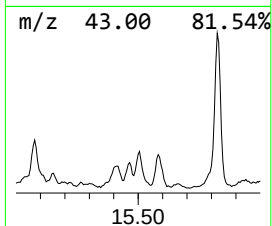
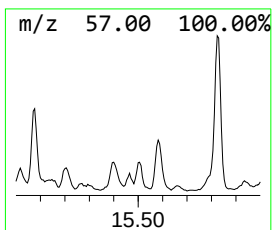
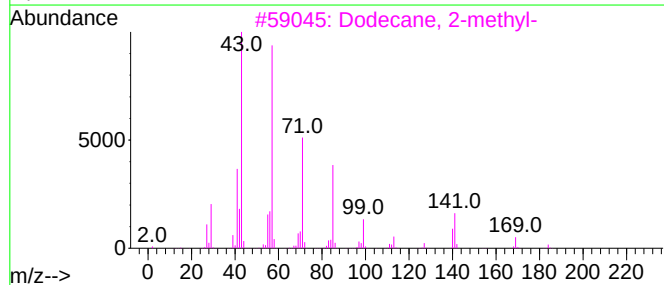
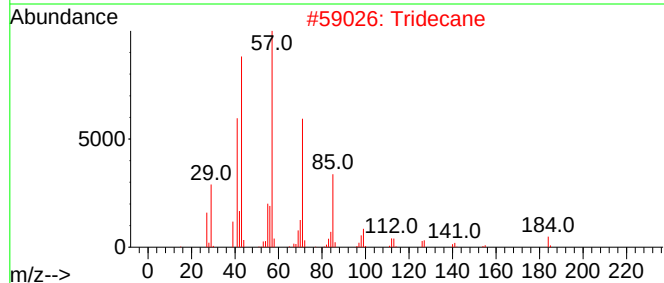
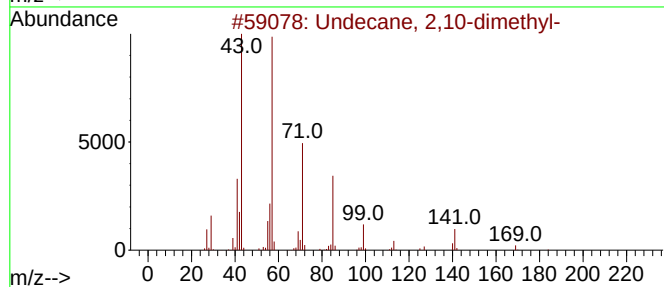
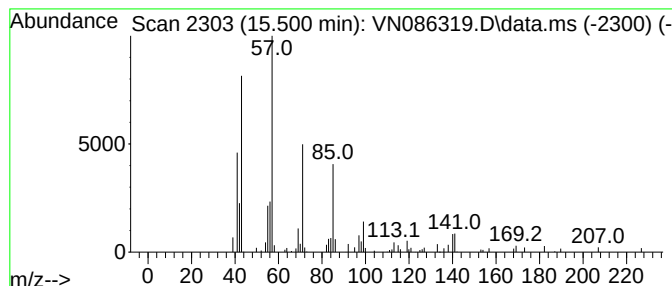
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Quant Title : SW846 8260

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

Peak Number 8 Undecane, 2,10-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.500	10.23 ug/l	218603	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,10-dimethyl-	184	C13H28	017301-27-8	80
2			Tridecane	184	C13H28	000629-50-5	72
3			Dodecane, 2-methyl-	184	C13H28	001560-97-0	64
4			Decane, 1-iodo-	268	C10H21I	002050-77-3	58
5			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
Data File : VN086319.D
Acq On : 17 Apr 2025 14:05
Operator : JC\MD
Sample : Q1818-01
Misc : 1.14g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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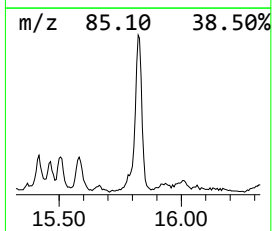
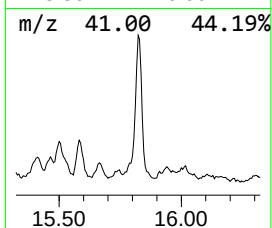
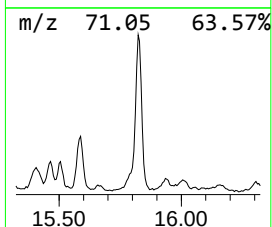
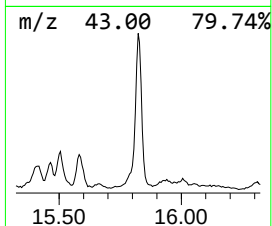
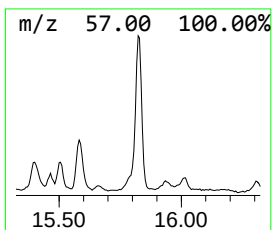
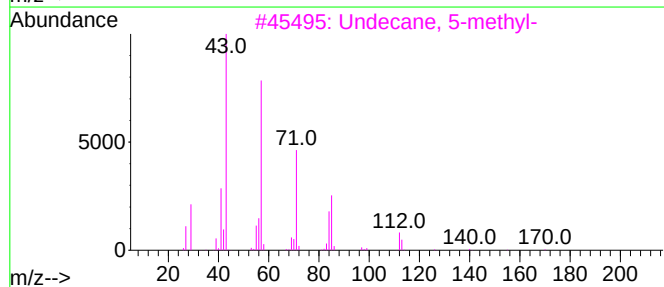
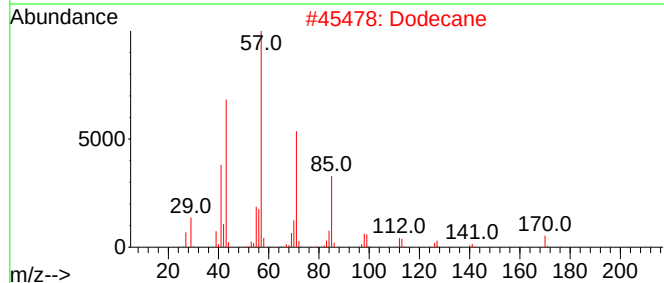
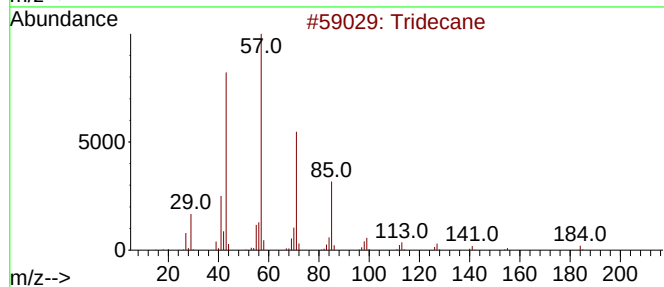
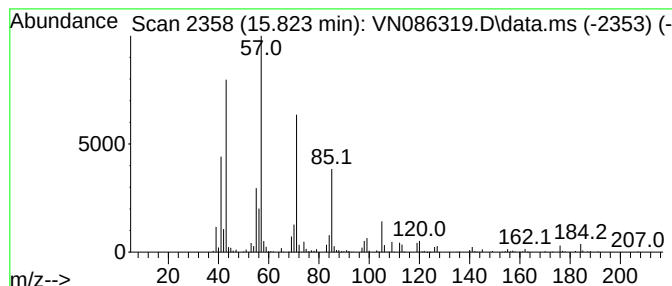
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Quant Title : SW846 8260

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

Peak Number 9 Tridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.823	38.88 ug/l	830608	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	96
2			Dodecane	170	C12H26	000112-40-3	80
3			Undecane, 5-methyl-	170	C12H26	001632-70-8	74
4			Tetradecane	198	C14H30	000629-59-4	72
5			Hexadecane	226	C16H34	000544-76-3	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
Data File : VN086319.D
Acq On : 17 Apr 2025 14:05
Operator : JC\MD
Sample : Q1818-01
Misc : 1.14g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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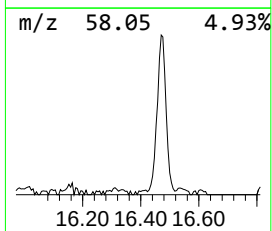
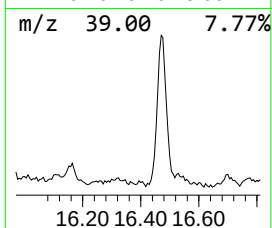
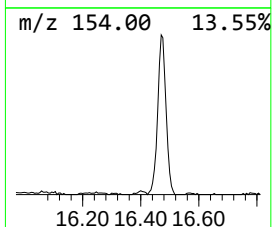
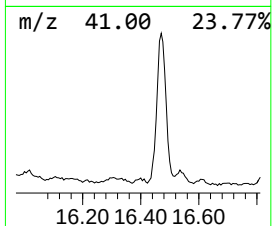
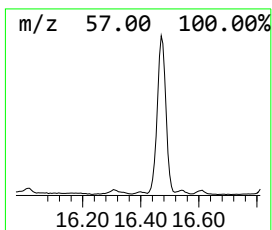
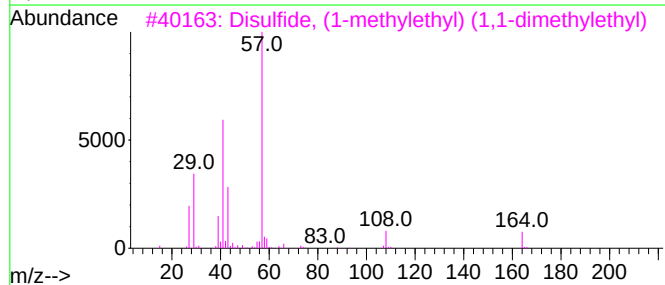
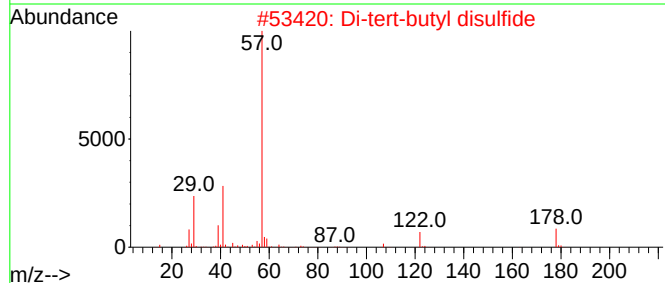
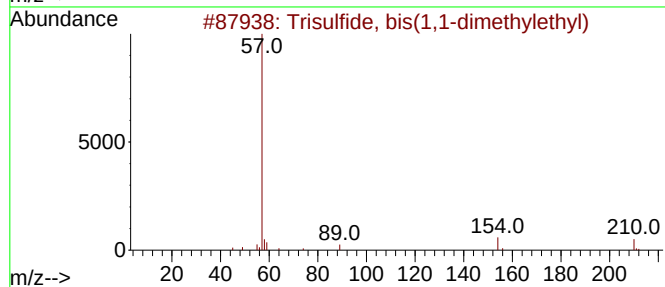
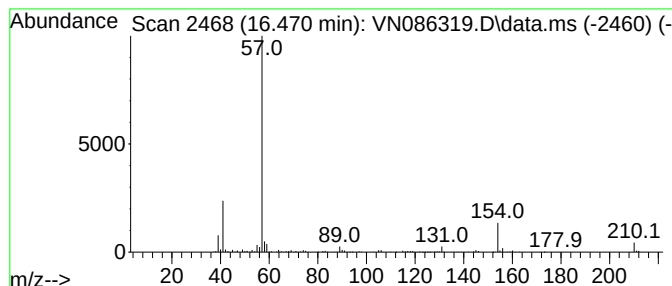
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 10 Trisulfide, bis(1,1-dimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.470	39.11 ug/l	835437	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	68
2			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	38
3			Disulfide, (1-methylethyl) (1,1-...	164	C7H16S2	043022-60-2	38
4			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	17
5			Phosphinous chloride, (chloromet...	172	C5H11Cl2P	078055-63-7	16



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
Data File : VN086319.D
Acq On : 17 Apr 2025 14:05
Operator : JC\MD
Sample : Q1818-01
Misc : 1.14g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3822

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.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
Hexane, 3-methyl-	8.435	37.9	ug/l	1085360	1	8.218	1431790	50.0
Pentane, 3-ethy...	8.700	10.2	ug/l	181430	2	9.094	887392	50.0
Heptane	8.959	50.8	ug/l	901515	2	9.094	887392	50.0
unknown13.982	13.982	9.9	ug/l	210670	4	13.788	1068060	50.0
Di-tert-butyl d...	14.759	12.5	ug/l	267490	4	13.788	1068060	50.0
Dodecane	14.953	47.5	ug/l	1015030	4	13.788	1068060	50.0
1H-Indene, 2,3-...	15.053	16.0	ug/l	341053	4	13.788	1068060	50.0
Undecane, 2,10-...	15.500	10.2	ug/l	218603	4	13.788	1068060	50.0
Tridecane	15.823	38.9	ug/l	830608	4	13.788	1068060	50.0
Trisulfide, bis...	16.470	39.1	ug/l	835437	4	13.788	1068060	50.0