

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122023\
 Data File : VN080558.D
 Acq On : 20 Dec 2023 19:40
 Operator : JC\MD
 Sample : 05896-03
 Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1218

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\82N121223W.M
 Title : SW846 8260

Signal : TIC: VN080558.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.895	140	160	161	rBV5	29387	114167	1.20%	0.375%
2	4.430	411	421	438	rBV2	108181	337191	3.53%	1.109%
3	8.000	1016	1028	1040	rBV2	42124	117139	1.23%	0.385%
4	8.165	1046	1056	1059	rBV2	183470	431361	4.52%	1.419%
5	8.218	1059	1065	1075	rVV2	791779	1835181	19.24%	6.035%
6	8.324	1075	1083	1093	rVB2	163619	392551	4.12%	1.291%
7	8.441	1093	1103	1112	rBV	624675	1441988	15.12%	4.742%
8	8.577	1118	1126	1135	rVB2	176200	401892	4.21%	1.322%
9	8.700	1138	1147	1156	rBV3	70691	187509	1.97%	0.617%
10	8.965	1183	1192	1207	rBV	320503	628204	6.59%	2.066%
11	9.100	1207	1215	1225	rVB	462868	936390	9.82%	3.079%
12	9.600	1285	1300	1305	rBV2	46956	126506	1.33%	0.416%
13	10.565	1456	1464	1469	rBV	688411	1294218	13.57%	4.256%
14	10.630	1469	1475	1489	rVB	5261365	9538953	100.00%	31.368%
15	11.865	1678	1685	1696	rVB	722405	1272374	13.34%	4.184%
16	12.071	1713	1720	1731	rBV2	42874	97359	1.02%	0.320%
17	12.853	1846	1853	1861	rVB	573799	965845	10.13%	3.176%
18	13.159	1898	1905	1914	rBV2	110209	219368	2.30%	0.721%
19	13.394	1941	1945	1949	rBV3	79740	113412	1.19%	0.373%
20	13.682	1985	1994	1997	rBV6	104778	276974	2.90%	0.911%
21	13.794	2007	2013	2017	rBV	977725	2034878	21.33%	6.692%
22	14.006	2043	2049	2053	rBV7	49968	107133	1.12%	0.352%
23	14.106	2061	2066	2072	rBV	1064057	1775320	18.61%	5.838%
24	14.218	2081	2085	2089	rBV5	73719	111236	1.17%	0.366%
25	14.265	2089	2093	2097	rVV3	79713	123709	1.30%	0.407%
26	14.370	2108	2111	2117	rVB5	164041	260730	2.73%	0.857%
27	14.435	2117	2122	2126	rBV8	69507	151924	1.59%	0.500%
28	14.506	2130	2134	2139	rVV6	109027	221470	2.32%	0.728%
29	14.582	2140	2147	2150	rVV6	207400	495055	5.19%	1.628%
30	14.629	2150	2155	2159	rVV	446673	817500	8.57%	2.688%
31	14.665	2159	2161	2165	rVV2	161373	222882	2.34%	0.733%
32	14.735	2169	2173	2176	rVV3	136549	204161	2.14%	0.671%
33	14.794	2176	2183	2188	rVB6	206207	438956	4.60%	1.443%
34	14.959	2206	2211	2220	rBV	536439	848806	8.90%	2.791%
35	15.041	2221	2225	2228	rBV5	84484	153274	1.61%	0.504%
36	15.223	2245	2256	2267	rVB10	137227	581029	6.09%	1.911%

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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\82N121223W.M
Title : SW846 8260

37	15.670	2327	2332	2340	rBV	125343	256263	2.69%	0.843%
38	15.747	2340	2345	2351	rVV2	102302	218176	2.29%	0.717%
39	15.835	2354	2360	2371	rVB5	166194	447575	4.69%	1.472%
40	16.476	2463	2469	2479	rBV	76006	210769	2.21%	0.693%

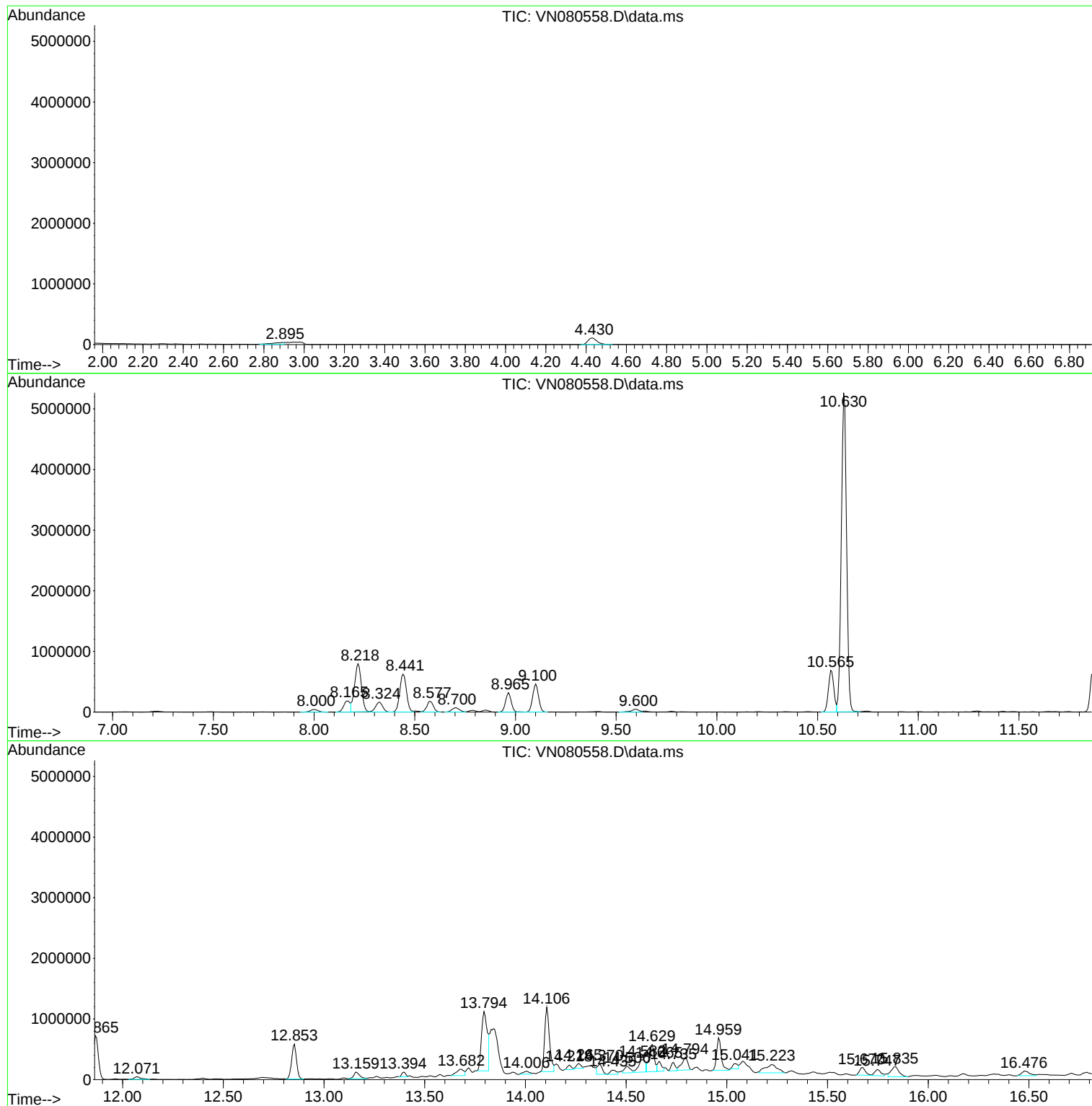
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

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



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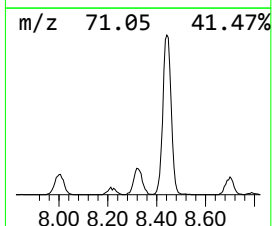
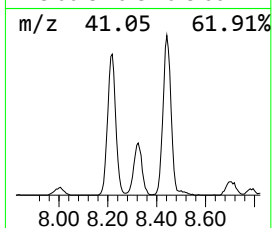
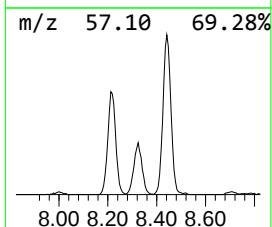
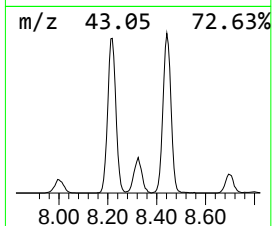
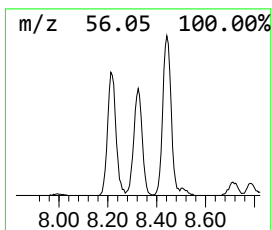
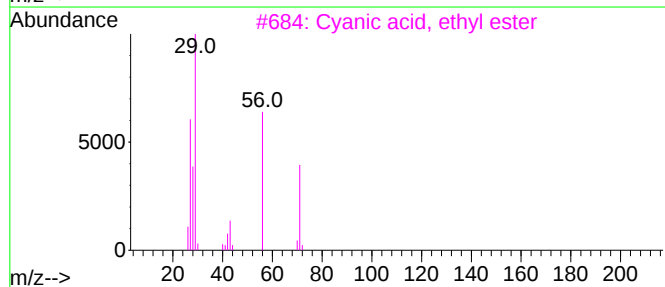
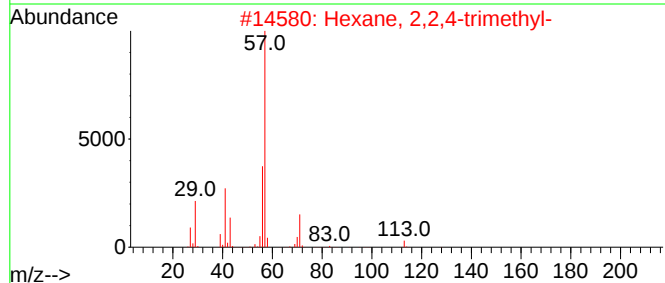
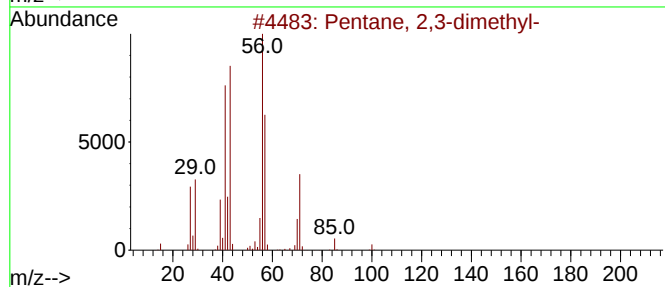
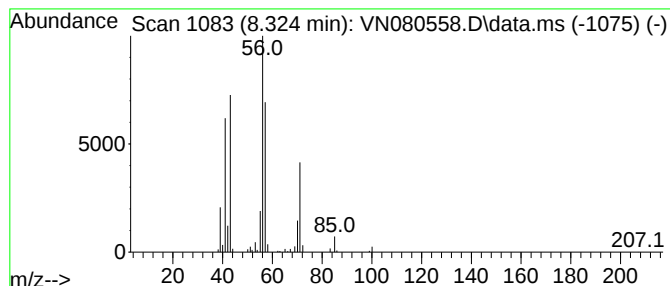
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.324	10.70 ug/l	392551	Pentafluorobenzene	8.218

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	90
2			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	56
3			Cyanoic acid, ethyl ester	71	C3H5NO	000627-48-5	50
4			1-Hexene, 2-methyl-	98	C7H14	006094-02-6	47
5			1-Hexene, 5-methyl-	98	C7H14	003524-73-0	40



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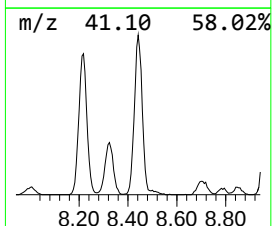
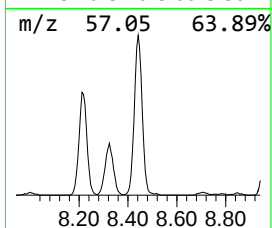
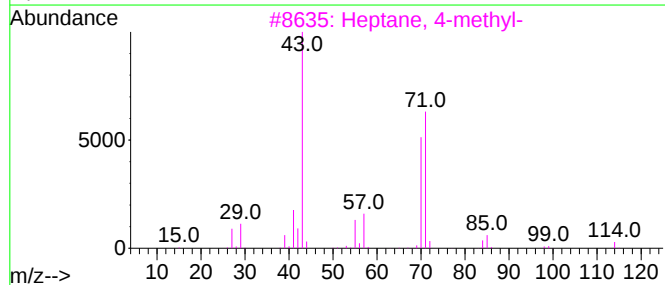
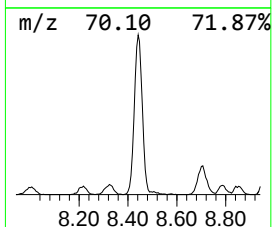
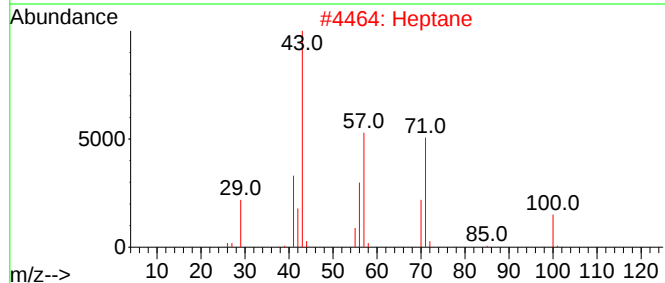
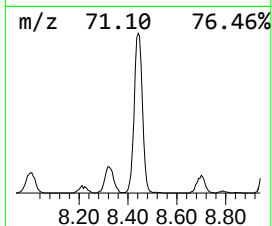
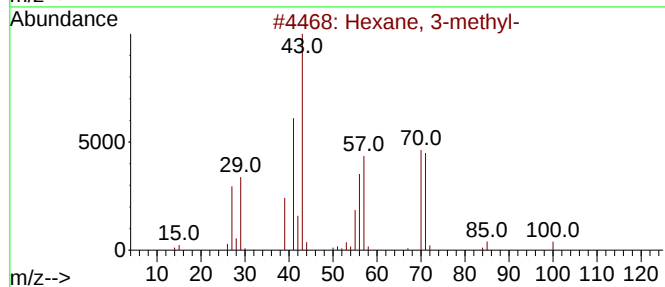
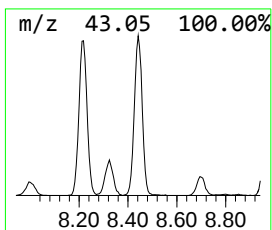
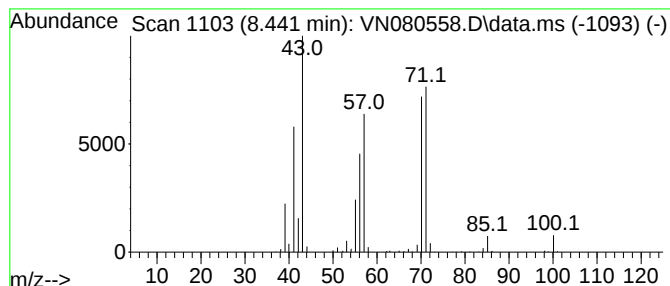
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Peak Number 2 Hexane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.441	39.29 ug/l	1441990	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	64
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	59
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59



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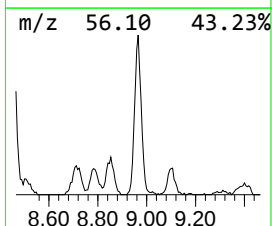
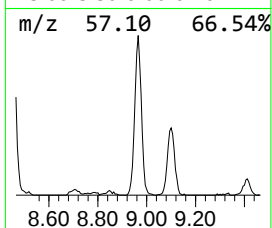
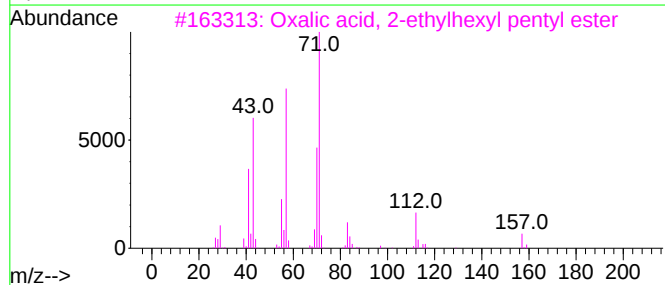
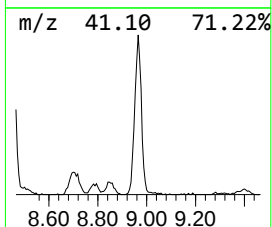
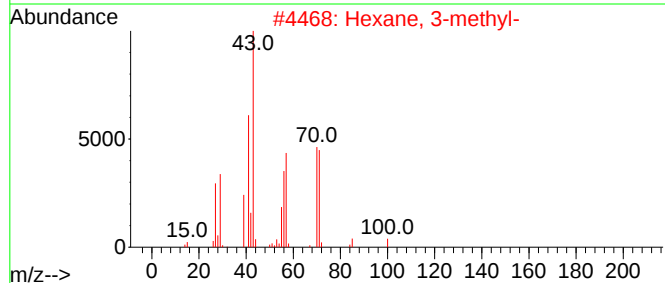
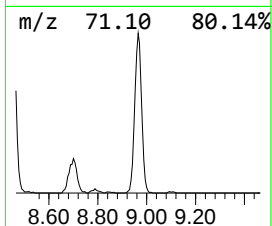
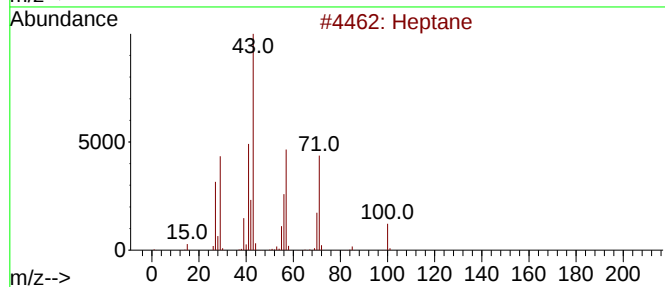
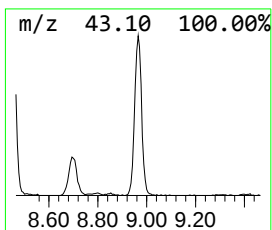
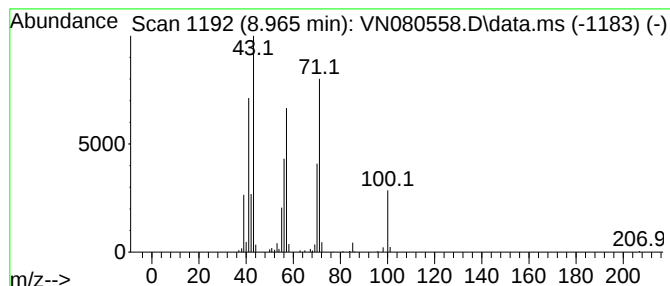
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

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

Peak Number 3 Heptane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.965	33.54 ug/l	628204	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	53
3			Oxalic acid, 2-ethylhexyl pentyl...	272	C15H28O4	1000309-38-7	50
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	47
5			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	43



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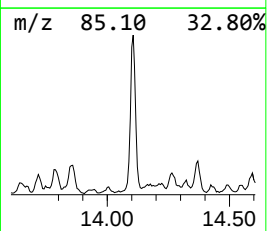
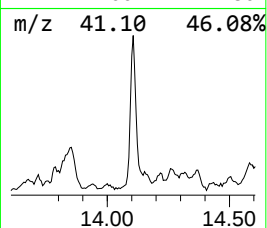
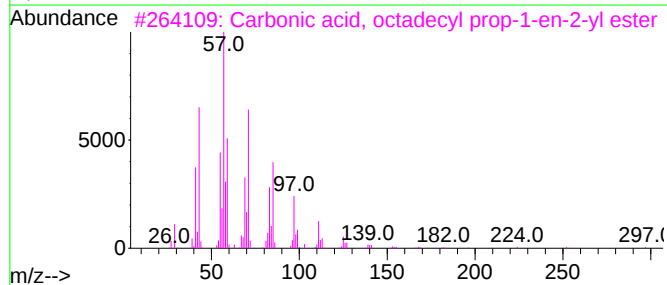
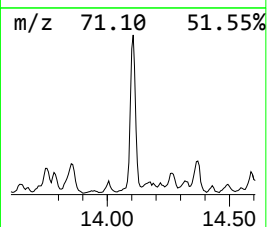
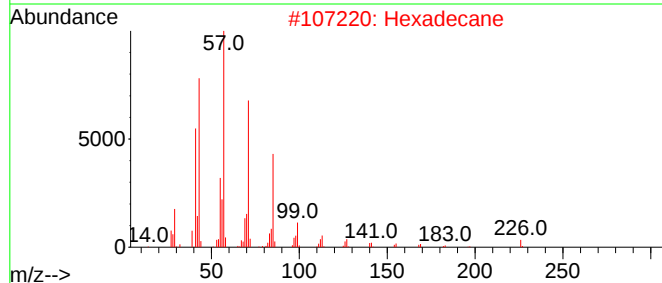
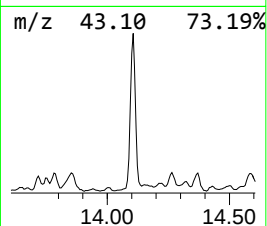
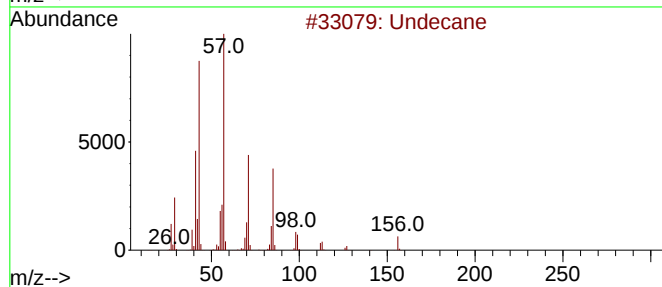
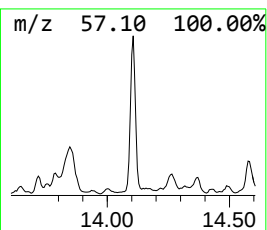
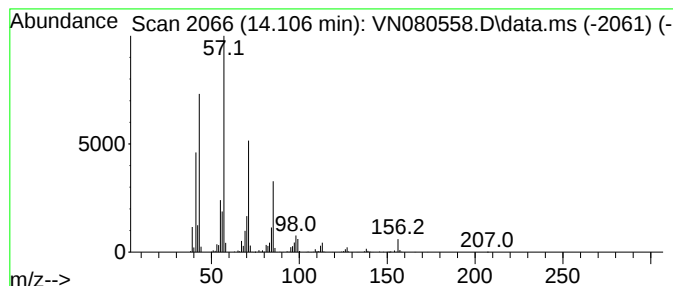
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.106	43.62 ug/l	1775320	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	97
2	Hexadecane			226	C16H34	000544-76-3	86
3	Carbonic acid, octadecyl prop-1-...			354	C22H42O3	1000383-11-5	86
4	Tetradecane			198	C14H30	000629-59-4	80
5	1-Decene, 4-methyl-			154	C11H22	013151-29-6	64



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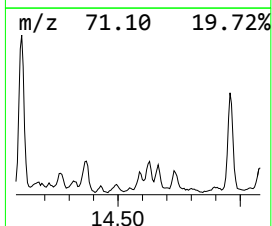
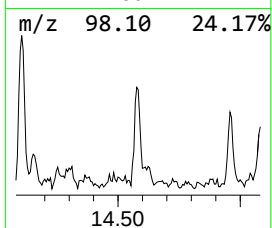
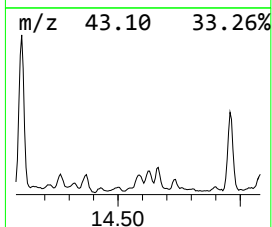
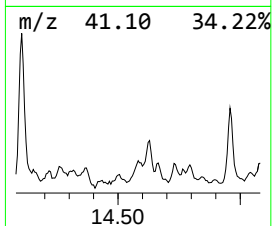
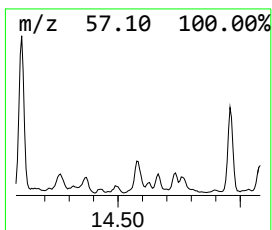
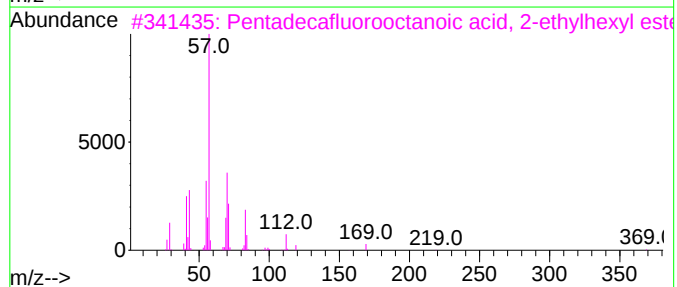
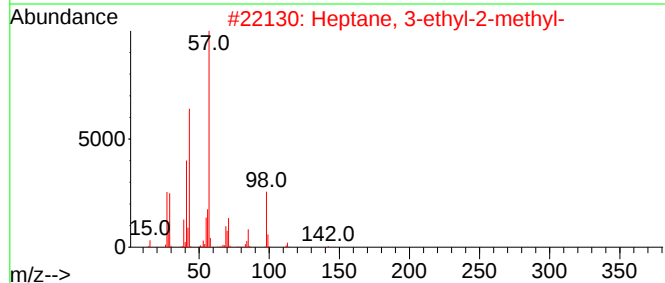
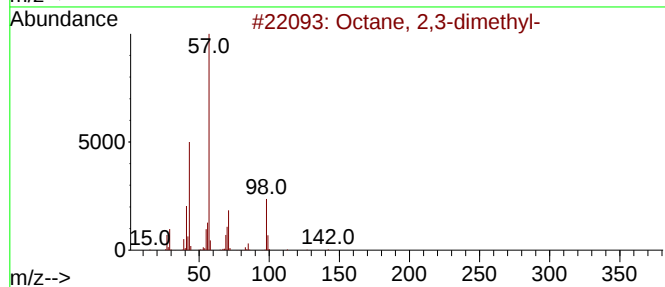
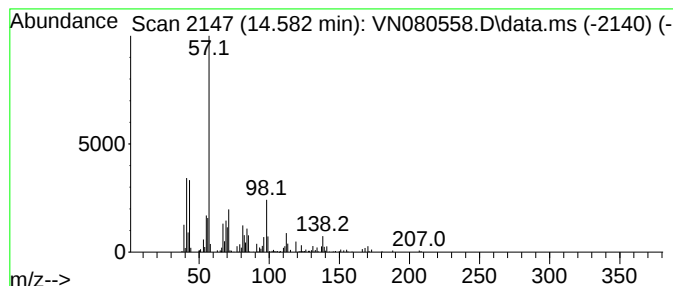
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

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

Peak Number 5 unknown14.582 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.582	12.16 ug/l	495055	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	47
2			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	43
3			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	43
4			Undecane, 6-methyl-	170	C12H26	017302-33-9	38
5			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122023\
Data File : VN080558.D
Acq On : 20 Dec 2023 19:40
Operator : JC\MD
Sample : 05896-03
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1218

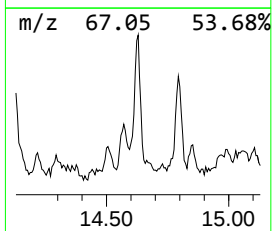
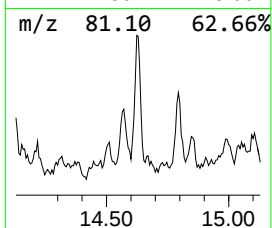
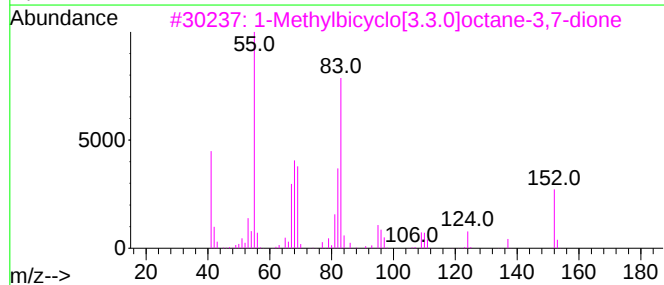
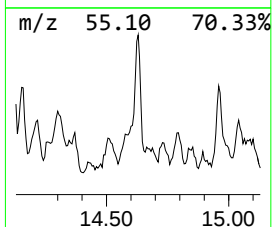
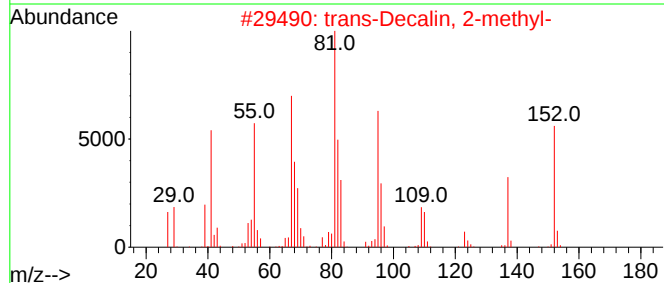
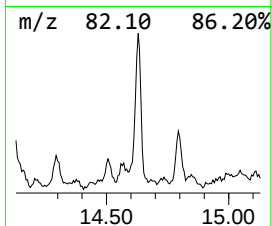
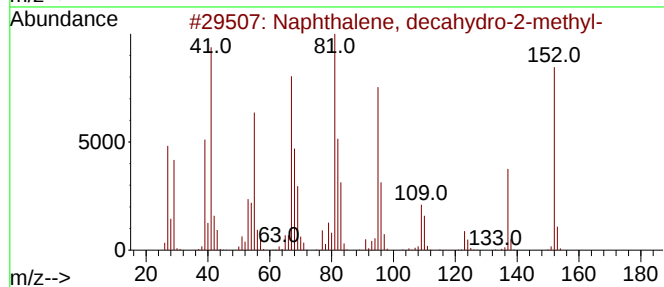
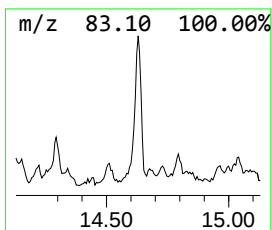
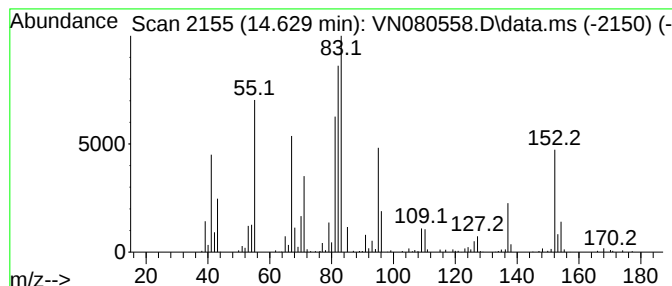
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, decahydro-2-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.629	20.09 ug/l	817500	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	87
2			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	55
3			1-Methylbicyclo[3.3.0]octane-3,7...	152	C9H12O2	021170-08-1	53
4			(Z)-(Z)-Hex-3-en-1-yl 2-methylbu...	182	C11H18O2	084060-80-0	43
5			Cyclohexane, pentyl-	154	C11H22	004292-92-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122023\
Data File : VN080558.D
Acq On : 20 Dec 2023 19:40
Operator : JC\MD
Sample : 05896-03
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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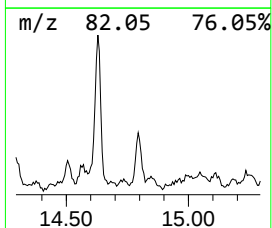
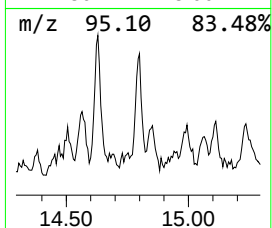
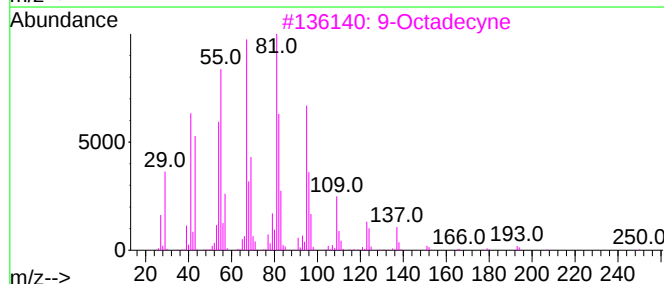
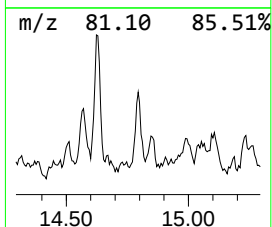
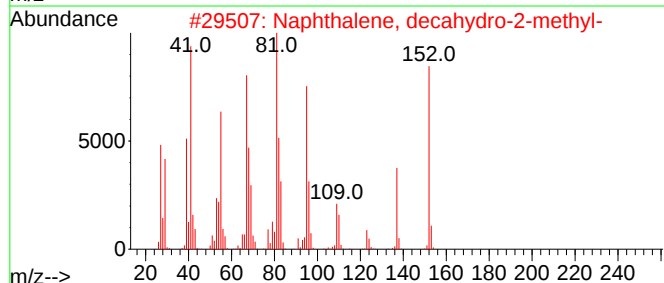
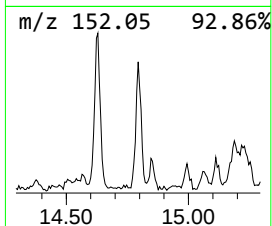
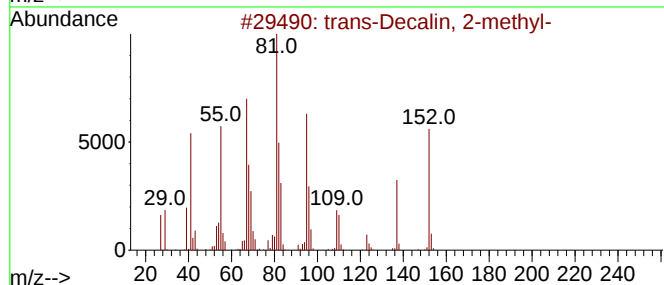
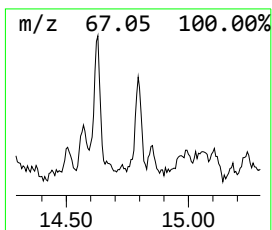
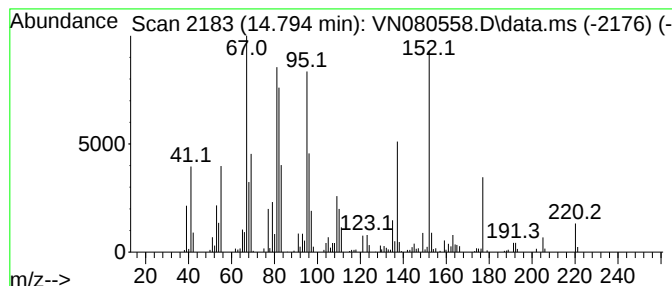
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Quant Title : SW846 8260

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

Peak Number 7 trans-Decalin, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.794	10.79 ug/l	438956	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	68
2			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	62
3			9-Octadecyne	250	C18H34	035365-59-4	58
4			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	58
5			9-Eicosyne	278	C20H38	071899-38-2	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122023\
Data File : VN080558.D
Acq On : 20 Dec 2023 19:40
Operator : JC\MD
Sample : 05896-03
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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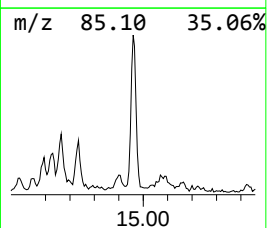
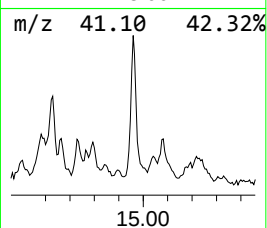
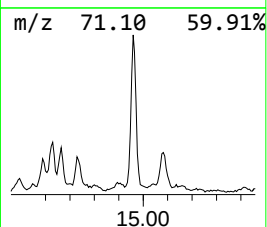
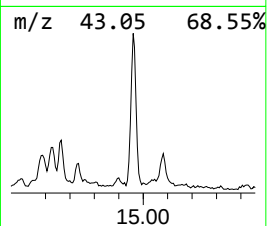
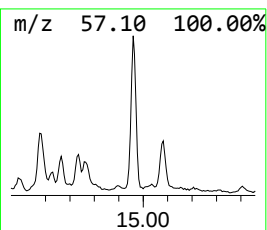
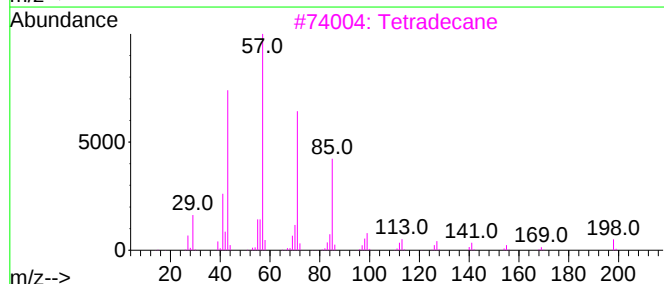
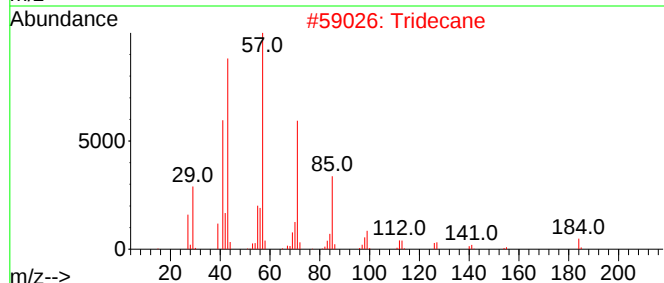
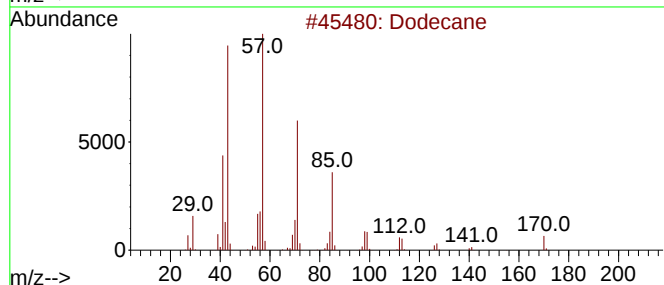
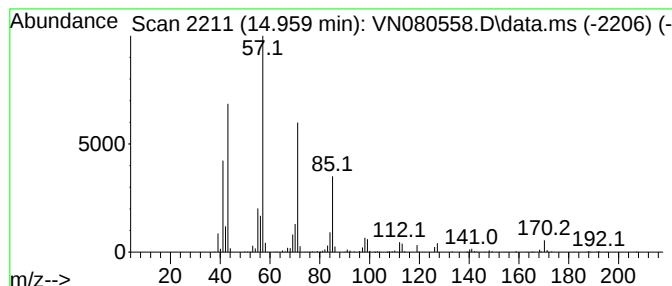
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Quant Title : SW846 8260

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

Peak Number 8 Dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	20.86 ug/l	848806	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	96
2			Tridecane	184	C13H28	000629-50-5	91
3			Tetradecane	198	C14H30	000629-59-4	90
4			Undecane	156	C11H24	001120-21-4	86
5			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122023\
Data File : VN080558.D
Acq On : 20 Dec 2023 19:40
Operator : JC\MD
Sample : 05896-03
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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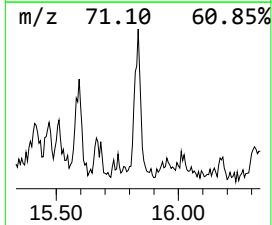
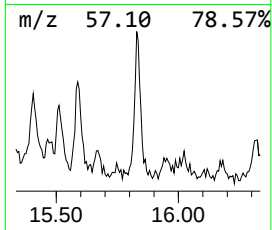
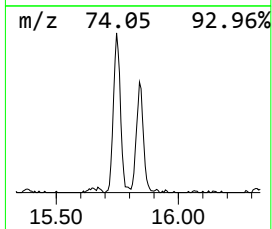
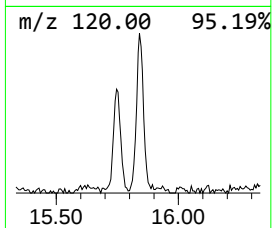
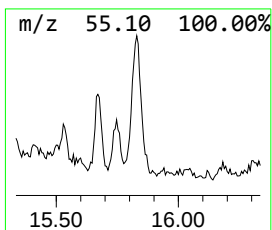
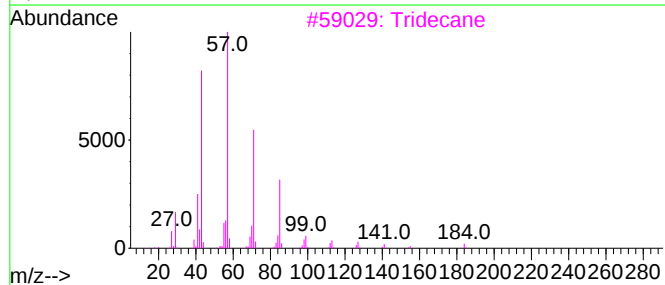
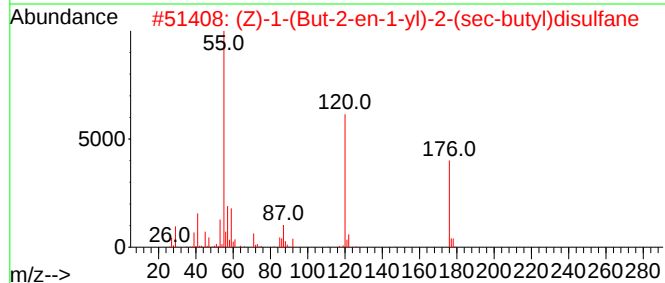
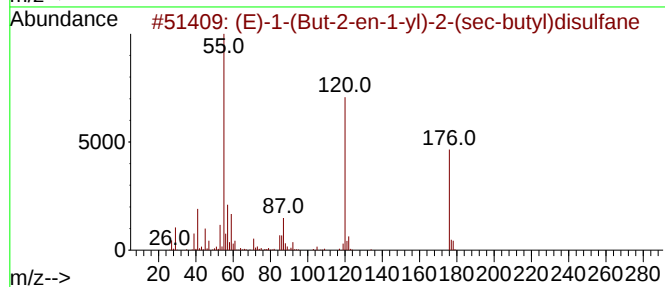
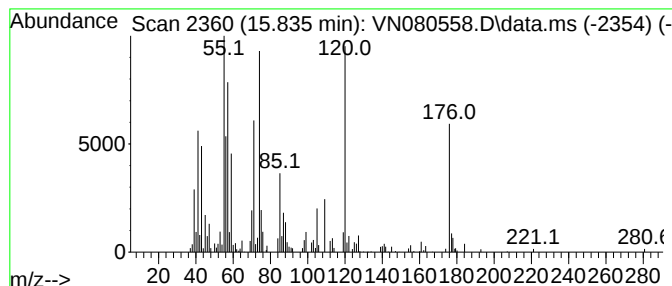
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Quant Title : SW846 8260

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

Peak Number 10 unknown15.835 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.835	11.00 ug/l	447575	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-1-(But-2-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-24-9	38		
2	(Z)-1-(But-2-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-23-8	30		
3	Tridecane	184	C13H28	000629-50-5	25		
4	Methanamine, 1,1-bis(2,2-dimethy...	231	C13H29NO2	004909-78-8	22		
5	(Z)-1-(But-1-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-21-6	22		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122023\
Data File : VN080558.D
Acq On : 20 Dec 2023 19:40
Operator : JC\MD
Sample : 05896-03
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1218

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.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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Hexane, 3-methyl-	8.441	39.3	ug/l	1441990	1	8.218	1835180	50.0
Heptane	8.965	33.5	ug/l	628204	2	9.100	936390	50.0
Undecane	14.106	43.6	ug/l	1775320	4	13.794	2034880	50.0
unknown14.582	14.582	12.2	ug/l	495055	4	13.794	2034880	50.0
Naphthalene, de...	14.629	20.1	ug/l	817500	4	13.794	2034880	50.0
trans-Decalin, ...	14.794	10.8	ug/l	438956	4	13.794	2034880	50.0
Dodecane	14.959	20.9	ug/l	848806	4	13.794	2034880	50.0
unknown15.223	15.223	14.3	ug/l	581029	4	13.794	2034880	50.0
unknown15.835	15.835	11.0	ug/l	447575	4	13.794	2034880	50.0