LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122023\
Data File : VN080556.D
Acq On : 20 Dec 2023 18:53
Operator : JC\MD
Sample : 05896-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1104

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: VN080556.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.424	410	420	440	rBV	187399	566784	1.55%	0.593%
2	8.165	1046	1056	1058	rBV2	186639	388531	1.06%	0.406%
3	8.218	1058	1065	1076	rVV2	1473527	3420707	9.33%	3.577%
4	8.324	1076	1083	1093	rVB	435888	1025409	2.80%	1.072%
5	8.441	1093	1103	1112	rBV	1800296	4072065	11.11%	4.258%
6	8.577	1119	1126	1138	rVB2	182309	422578	1.15%	0.442%
7	8.700	1138	1147	1155	rVV4	254269	751719	2.05%	0.786%
8	8.782	1155	1161	1167	rVV4	136172	391760	1.07%	0.410%
9	8.965	1183	1192	1205	rVV	1812672	3527841	9.62%	3.689%
10	9.100	1207	1215	1236	rVB	463157	972850	2.65%	1.017%
11	9.600	1285	1300	1305	rBV2	498271	1314760	3.59%	1.375%
12	10.206	1398	1403	1417	rVB2	210785	505569	1.38%	0.529%
13	10.341	1417	1426	1439	rVB2	190984	437082	1.19%	0.457%
14	10.565	1457	1464	1469	rBV2	909222	1777312	4.85%	1.859%
15	10.629	1469	1475	1484	rVB	19555803	36661562	100.00%	38.338%
16	10.747	1489	1495	1503	rVB	509691	947495	2.58%	0.991%
17	11.006	1530	1539	1548	rBV2	188104	420228	1.15%	0.439%
18	11.418	1600	1609	1614	rVV	294056	663852	1.81%	0.694%
19	11.471	1614	1618	1624	rVB2	220579	398656	1.09%	0.417%
20	11.641	1640	1647	1651	rBV3	313989	662444	1.81%	0.693%
21	11.747	1660	1665	1670	rVB	291753	467357	1.27%	0.489%
22	11.865	1679	1685	1695	rVV	642254	1167457	3.18%	1.221%
23	11.965	1695	1702	1707	rVV	1344949	2292548	6.25%	2.397%
24	12.070	1711	1720	1731	rVV	4904533	10215778	27.87%	10.683%
25	12.153	1731	1734	1740	rVB	246218	411143	1.12%	0.430%
26	12.400	1764	1776	1785	rBV	1542174	3451176	9.41%	3.609%
27	12.618	1802	1813	1822	rBV8	259105	923302	2.52%	0.966%
28	12.853	1847	1853	1861	rBV2	592254	1129565	3.08%	1.181%
29	13.035	1877	1884	1889	rVB	339633	638077	1.74%	0.667%
30	13.100	1889	1895	1898	rBV	824642	1387364	3.78%	1.451%
31	13.165	1898	1906	1913	rVV5	830122	2362836	6.44%	2.471%
32	13.335	1923	1935	1941	rBV2	341639	877853	2.39%	0.918%
33	13.482	1954	1960	1969	rBV	995233	1667730	4.55%	1.744%
34	13.676	1987	1993	1998	rBV4	345192	741883	2.02%	0.776%
35	13.794	2007	2013	2022	rBV2	733893	1548147	4.22%	1.619%
36	13.988	2041	2046	2050	rBV2	318543	567652	1.55%	0.594%

LSC Area Percent Report

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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

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Peak separation: 5

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

37	14.112	2062	2067	2076	rBV6	651447	1398979	3.82%	1.463%
38	14.629	2150	2155	2159	rBV2	424787	641132	1.75%	0.670%
39	14.764	2174	2178	2188	rVB	521125	1103742	3.01%	1.154%
40	14.959	2202	2211	2215	rBV3	435521	859672	2.34%	0.899%
41	15.059	2220	2228	2233	rVV6	254398	725889	1.98%	0.759%
42	15.835	2355	2360	2370	rVB	242733	468734	1.28%	0.490%
43	16.482	2462	2470	2486	rVB2	476873	1250811	3.41%	1.308%

Sum of corrected areas: 95628031

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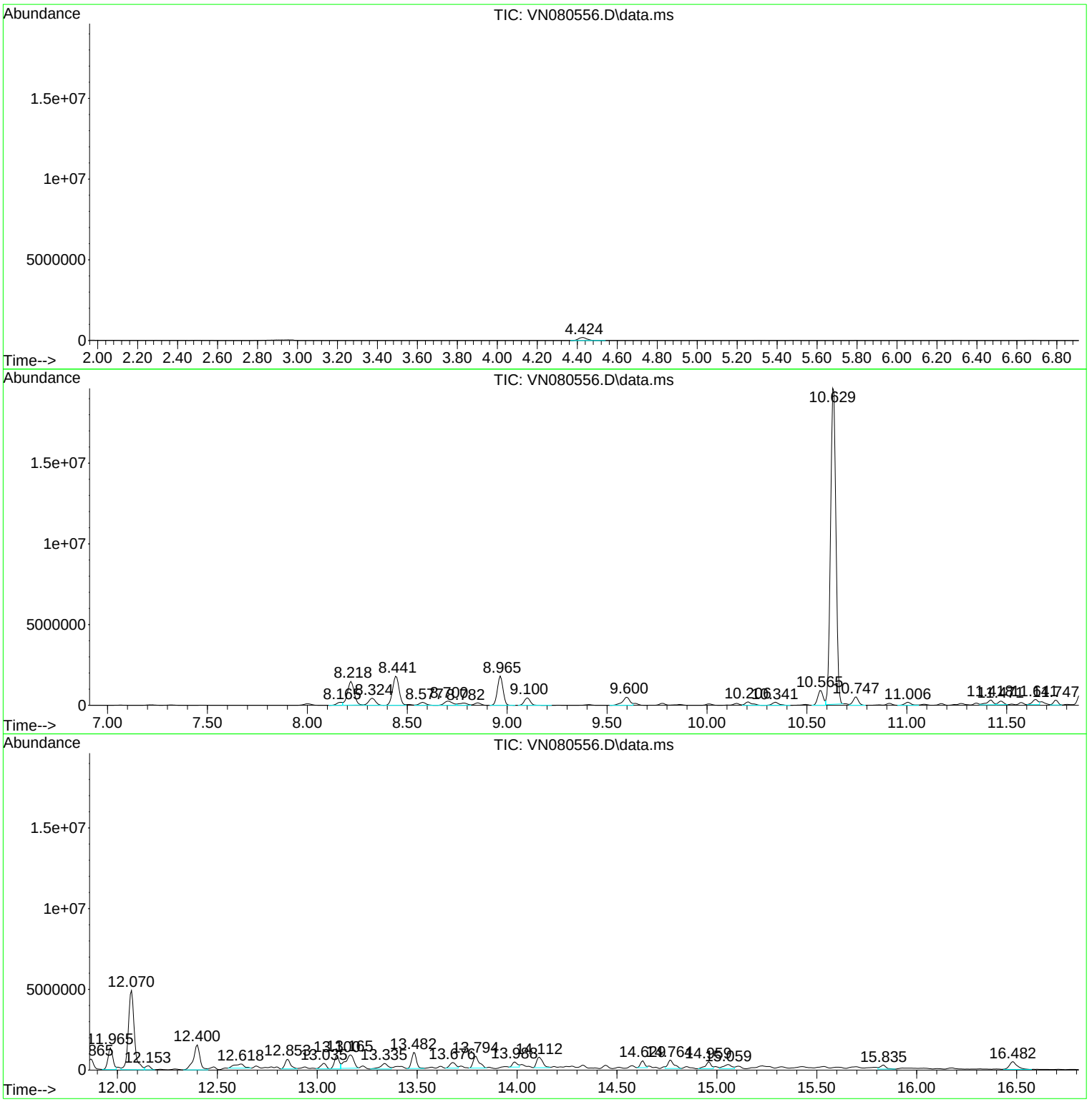
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

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



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Data File : VN080556.D
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MSVOA_N
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

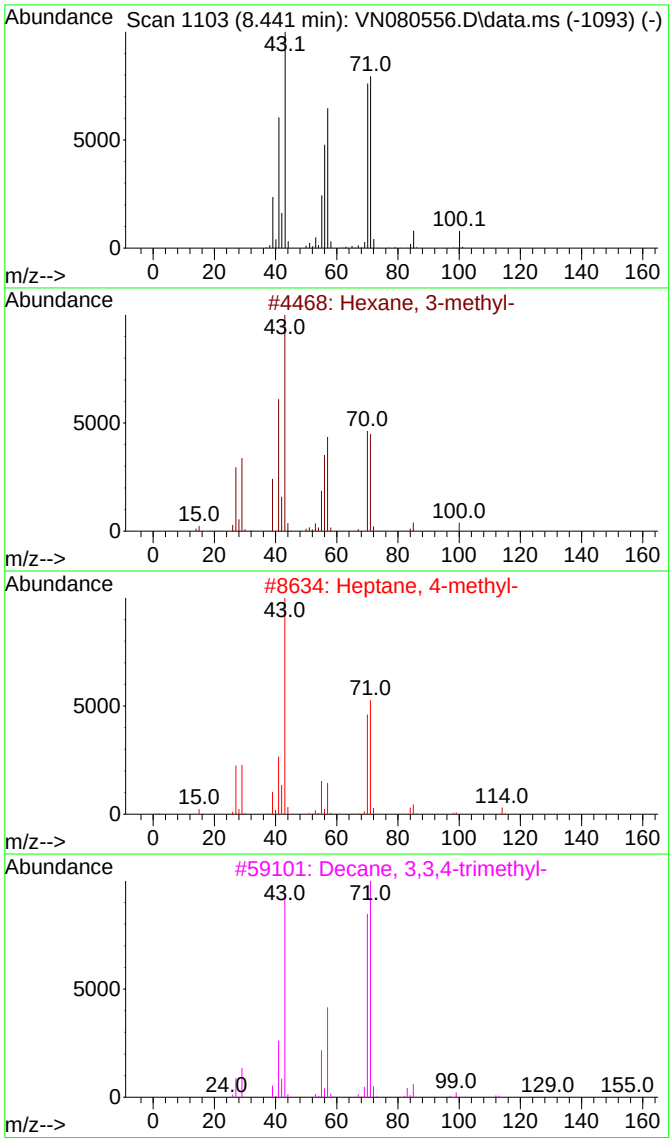
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

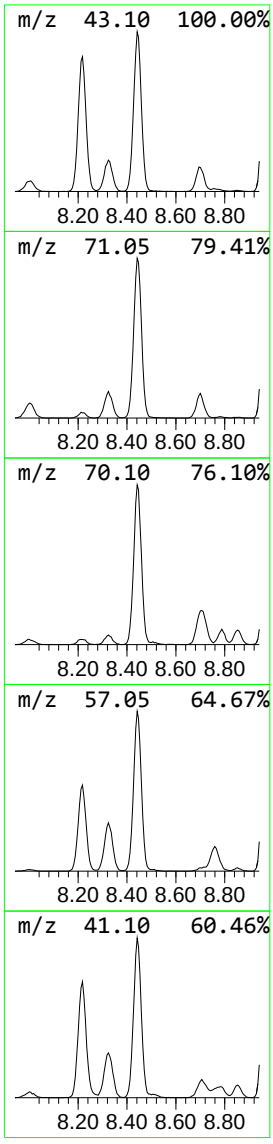
****

Peak Number 1 Hexane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.441	59.52 ug/l	4072070	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64
4	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59





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MSVOA_N
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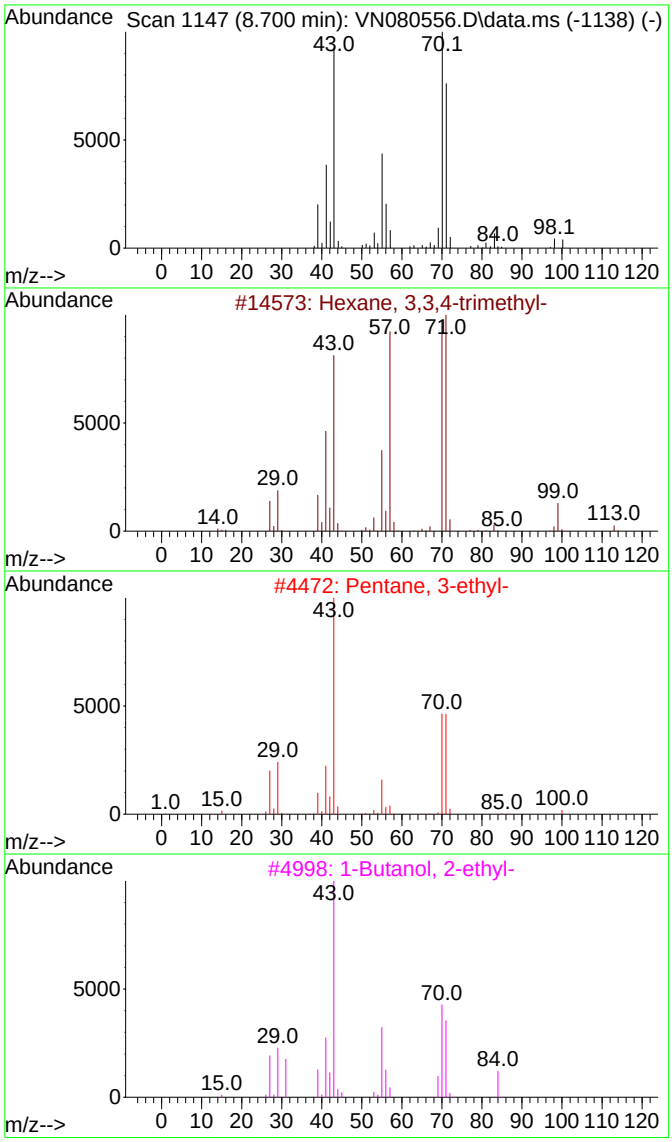
Quant Title : SW846 8260

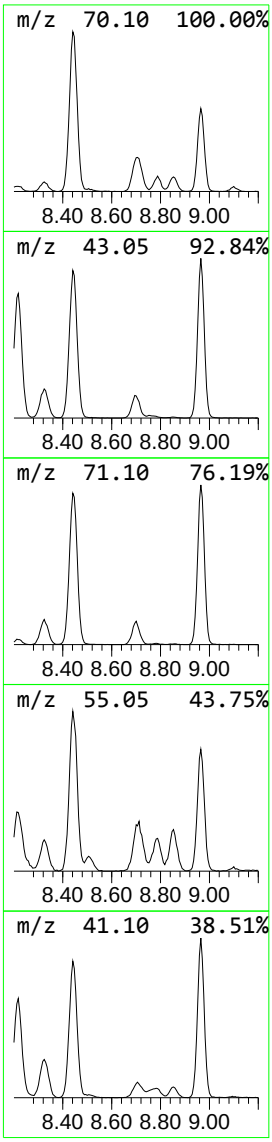
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexane, 3,3,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.700	38.63 ug/l	751719	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	72
2	Pentane, 3-ethyl-	100	C7H16	000617-78-7	72
3	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	64
4	1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	50
5	Hexane, 3-methyl-	100	C7H16	000589-34-4	50





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

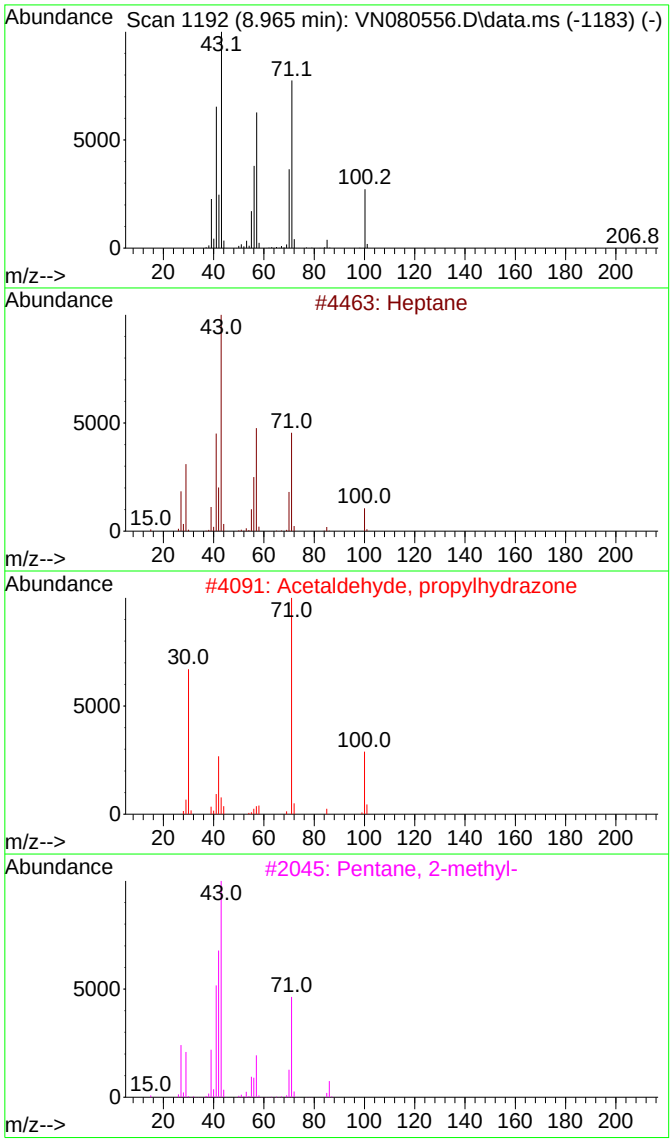
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

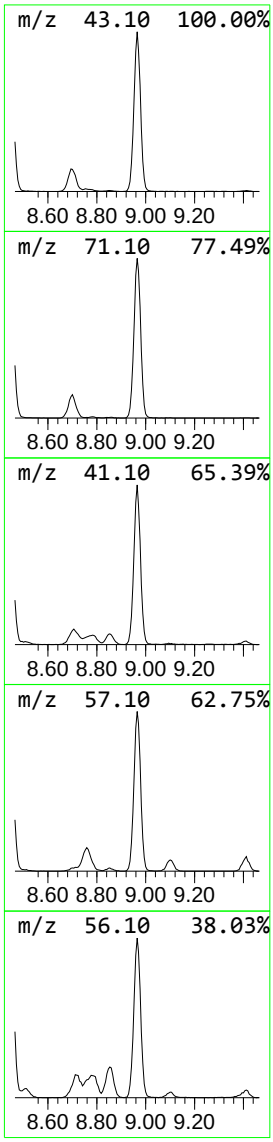
****

Peak Number 3 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.965	181.32 ug/l	3527840	1,4-Difluorobenzene	9.100

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	53
3	Pentane, 2-methyl-	86	C6H14	000107-83-5	53
4	Oxirane, butyl-	100	C6H12O	001436-34-6	47
5	Hexane, 3-methyl-	100	C7H16	000589-34-4	47





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

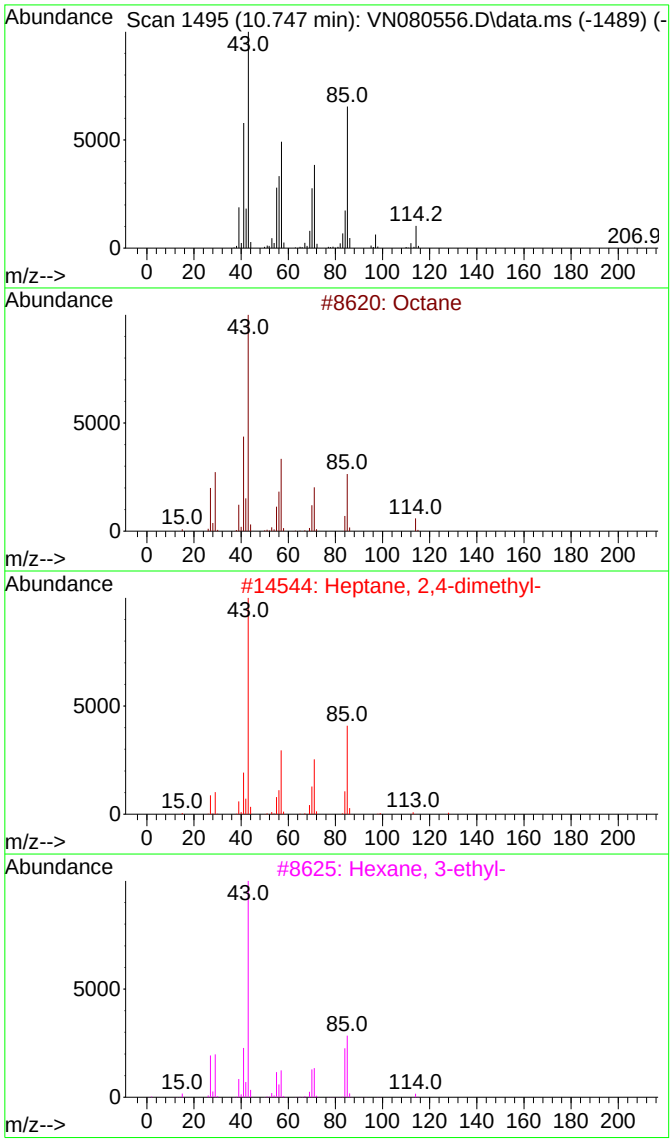
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

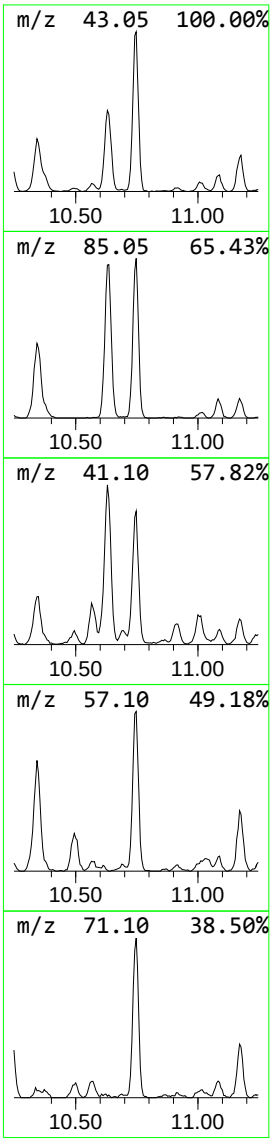
****

Peak Number 4 Octane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.747	40.58 ug/l	947495	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane	114	C8H18	000111-65-9	91
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72
3	Hexane, 3-ethyl-	114	C8H18	000619-99-8	59
4	Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	47
5	1-Trifluoroacetoxy-2-methylpentane	198	C8H13F3O2	155089-96-6	47





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

TIC Library : C:\Database\NIST20.L
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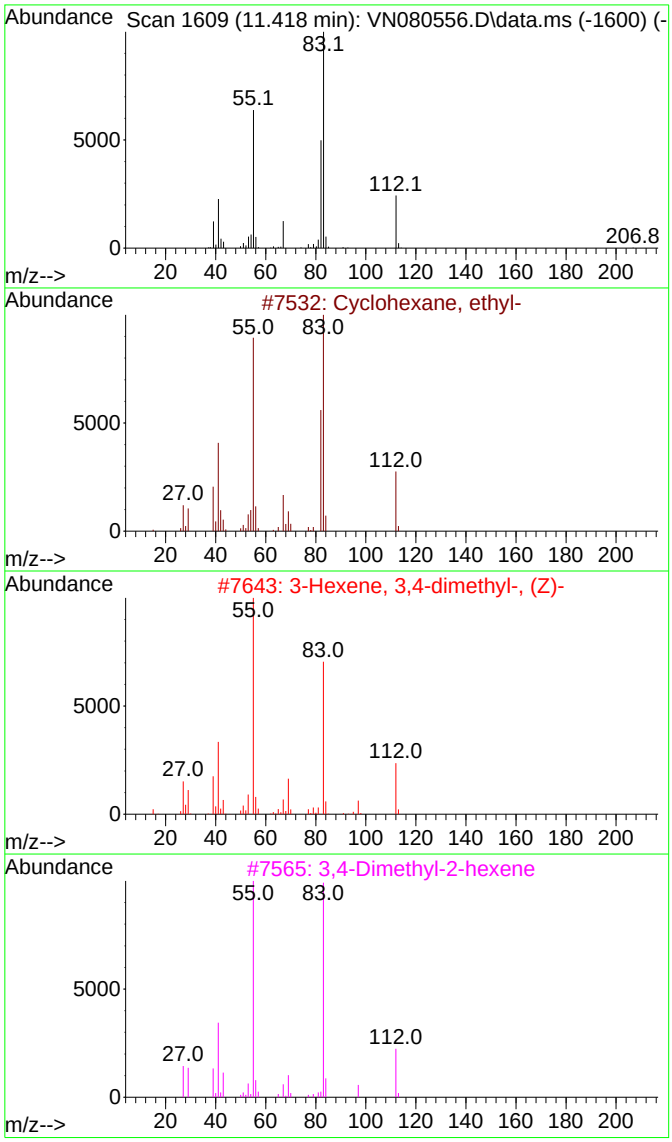
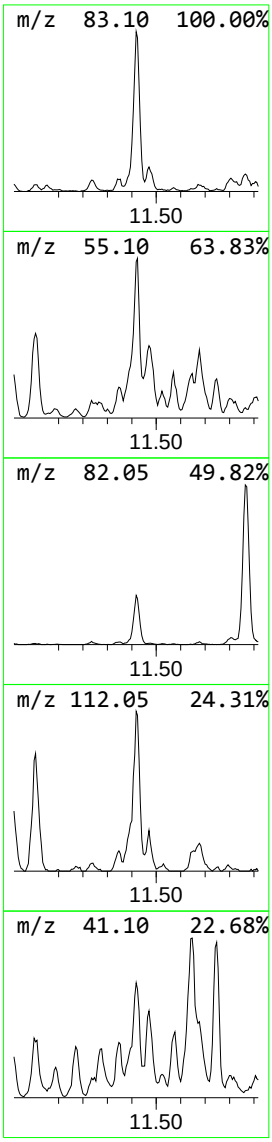
****
Peak Number 5 Cyclohexane, ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.418	28.43 ug/l	663852	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, ethyl-	112	C8H16	001678-91-7	86
2	3-Hexene, 3,4-dimethyl-, (Z)-	112	C8H16	019550-87-9	53
3	3,4-Dimethyl-2-hexene	112	C8H16	002213-37-8	53
4	3-Hexene, 3,4-dimethyl-	112	C8H16	030951-95-2	53
5	2-Hexene, 2,3-dimethyl-	112	C8H16	007145-20-2	53





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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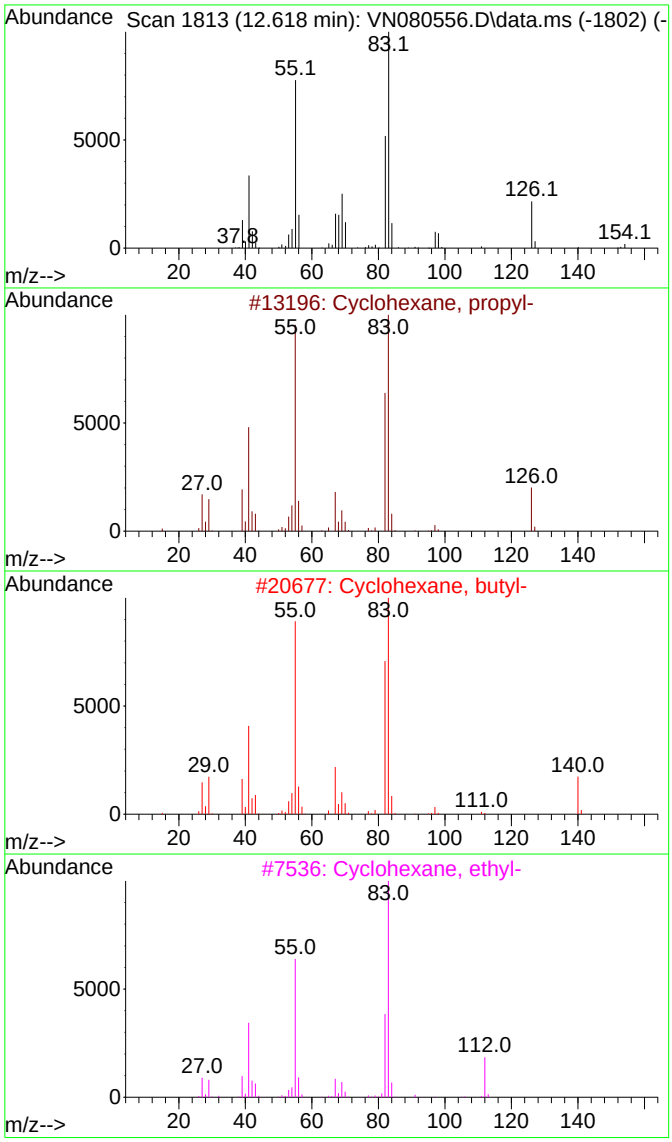
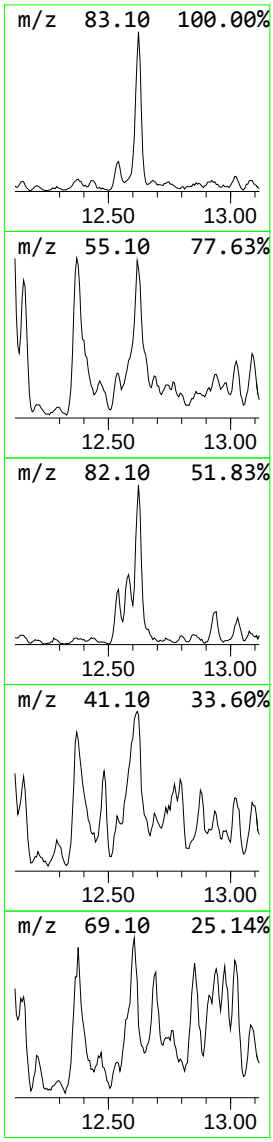
Peak Number 6 Cyclohexane, propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.618	39.54 ug/l	923302	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	90
2	Cyclohexane, butyl-	140	C10H20	001678-93-9	64
3	Cyclohexane, ethyl-	112	C8H16	001678-91-7	59
4	Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	59
5	Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	59





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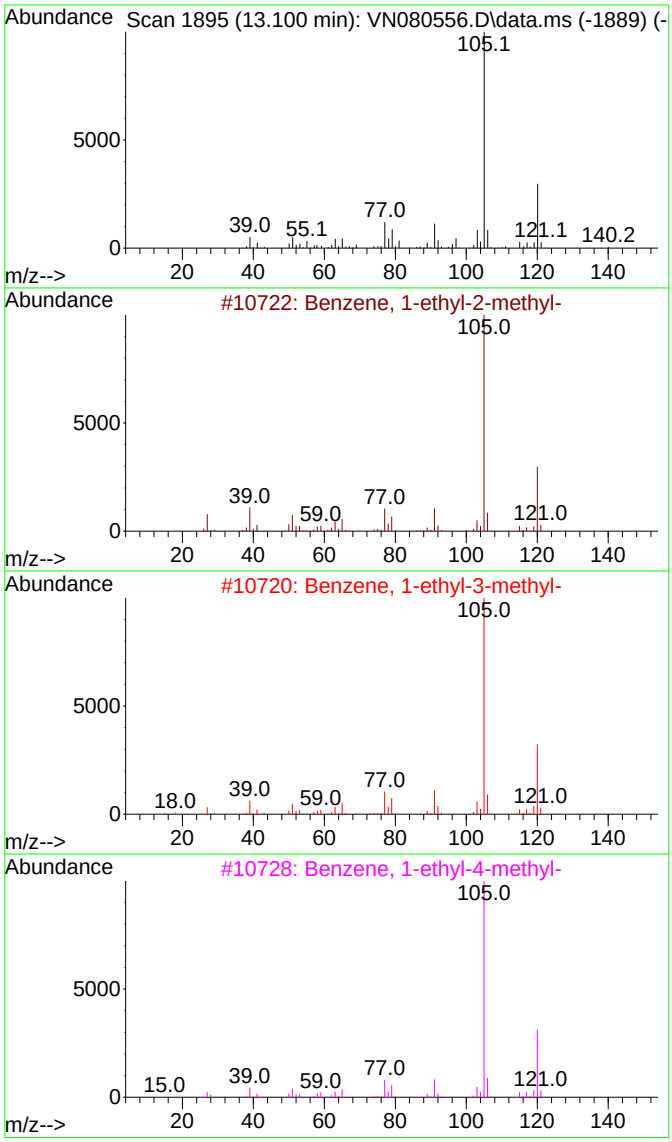
Quant Title : SW846 8260

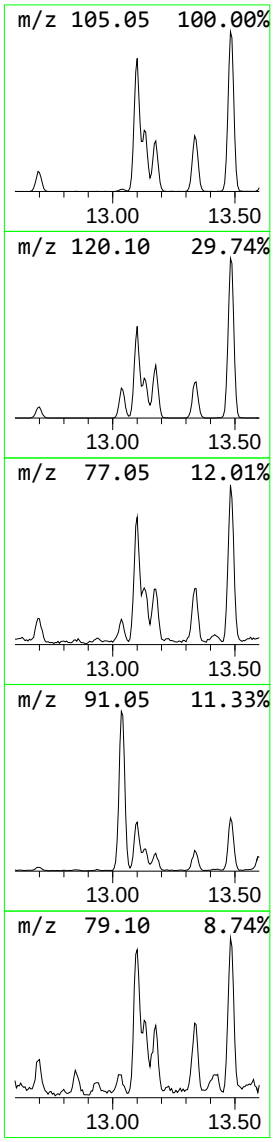
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	44.81 ug/l	1387360	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
4	Mesitylene	120	C9H12	000108-67-8	90
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90





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Data File : VN080556.D
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Quant Title : SW846 8260

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

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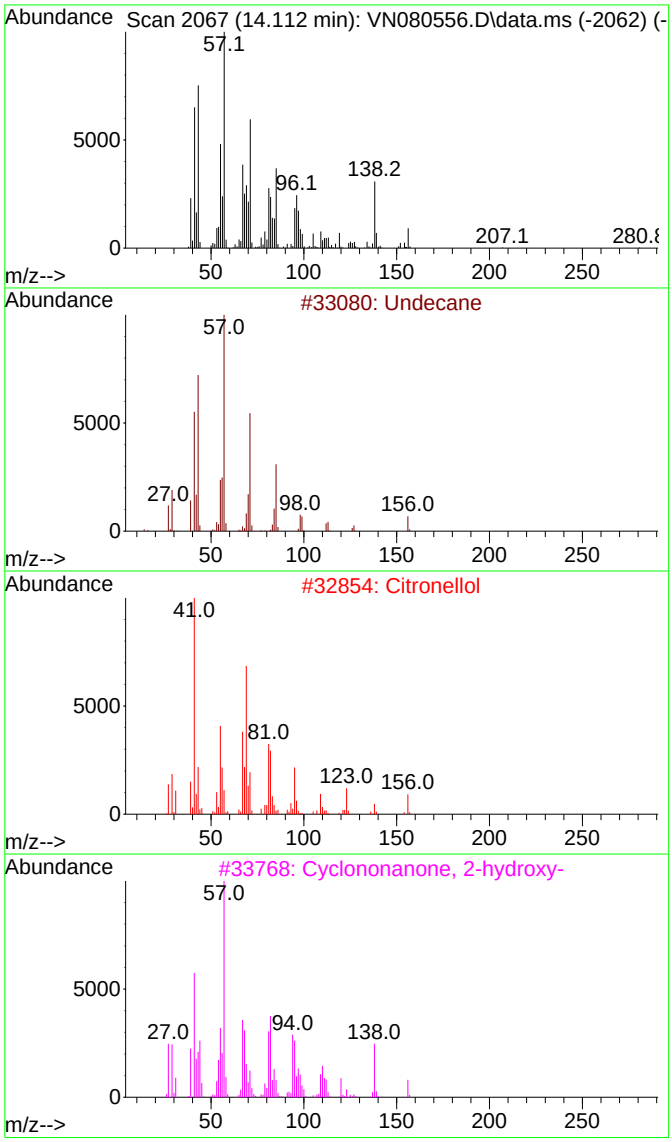
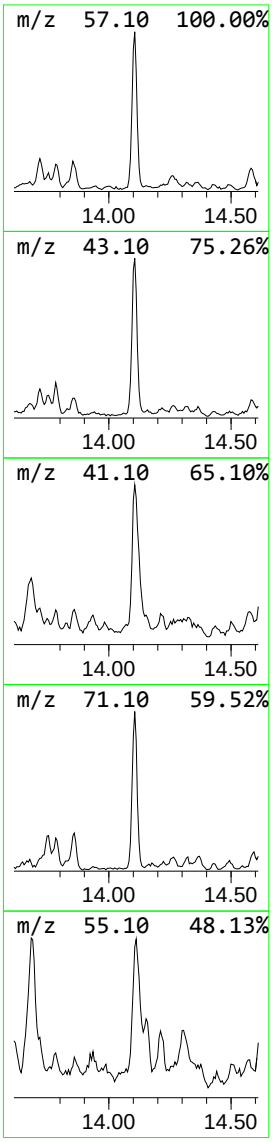
Peak Number 8 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.111	45.18 ug/l	1398980	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	93
2	Citronellol	156	C10H20O	000106-22-9	45
3	Cyclononanone, 2-hydroxy-	156	C9H16O2	000496-83-3	38
4	Carbonic acid, undecyl vinyl ester	242	C14H26O3	1000382-54-9	30
5	Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	30





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Data File : VN080556.D
Acq On : 20 Dec 2023 18:53
Operator : JC\MD
Sample : 05896-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1104

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

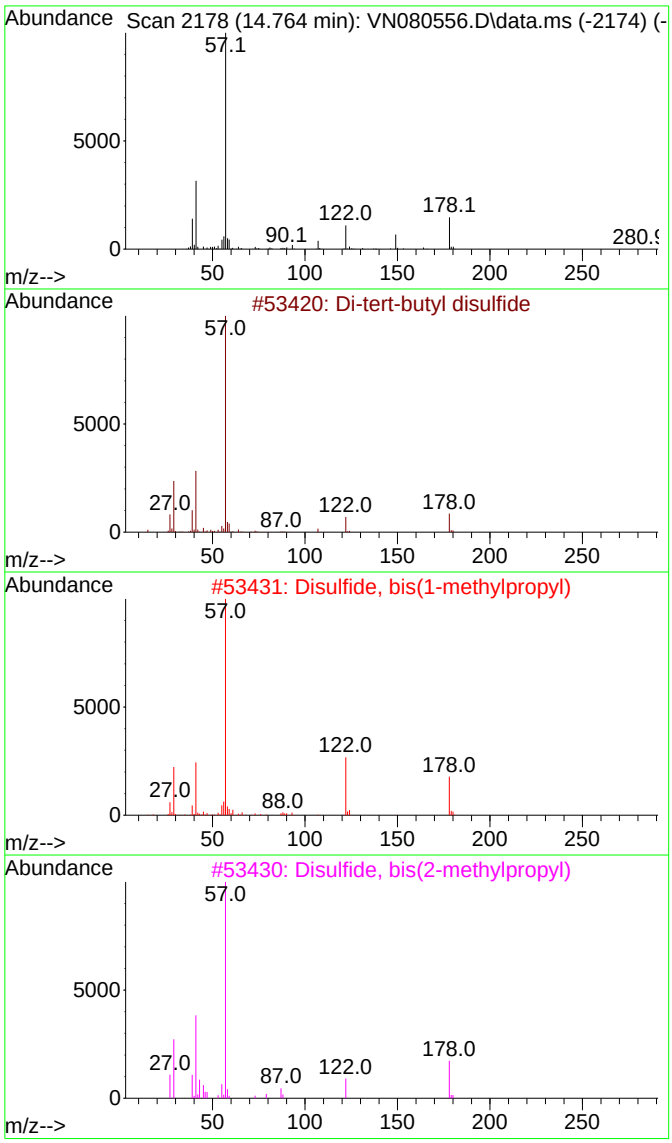
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

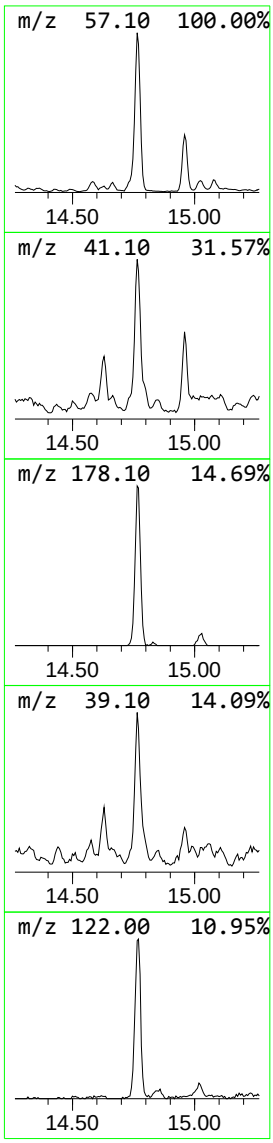
****

Peak Number 9 Di-tert-butyl disulfide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.764	35.65 ug/l	1103740	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	68
2	Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	59
3	Disulfide, bis(2-methylpropyl)	178	C8H18S2	001518-72-5	58
4	Disulfide, dibutyl	178	C8H18S2	000629-45-8	53
5	Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122023\
Data File : VN080556.D
Acq On : 20 Dec 2023 18:53
Operator : JC\MD
Sample : 05896-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1104

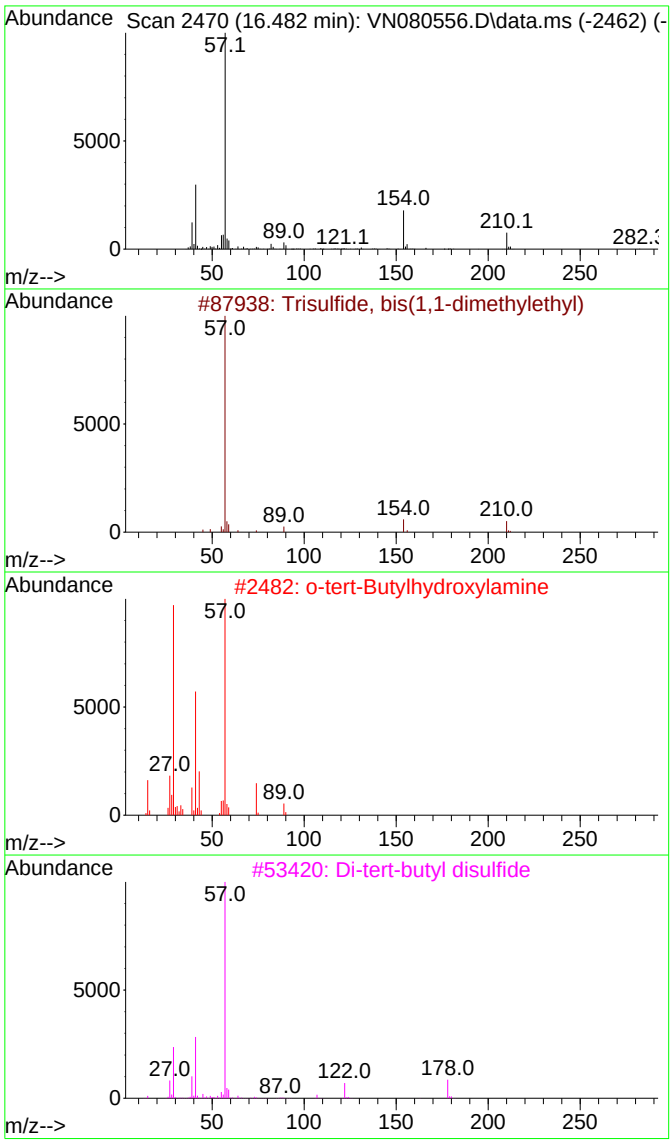
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

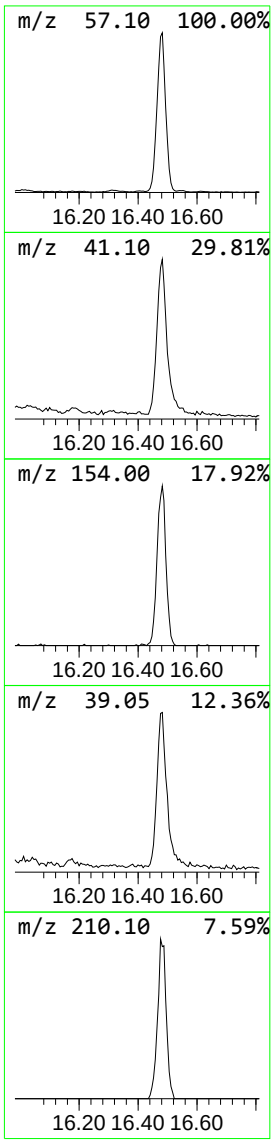
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Trisulfide, bis(1,1-dimethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.482	40.40 ug/l	1250810	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	58
2	o-tert-Butylhydroxylamine	89	C4H11NO	1000322-43-1	38
3	Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	38
4	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	35
5	Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	17





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122023\
Data File : VN080556.D
Acq On : 20 Dec 2023 18:53
Operator : JC\MD
Sample : 05896-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1104

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hexane, 3-methyl-	8.441	59.5	ug/l	4072070	1	8.224	3420710	50.0
Hexane, 3,3,4-t...	8.700	38.6	ug/l	751719	2	9.100	972850	50.0
Heptane	8.965	181.3	ug/l	3527840	2	9.100	972850	50.0
Octane	10.747	40.6	ug/l	947495	3	11.865	1167460	50.0
Cyclohexane, et...	11.418	28.4	ug/l	663852	3	11.865	1167460	50.0
Cyclohexane, pr...	12.618	39.5	ug/l	923302	3	11.865	1167460	50.0
Benzene, 1-ethy...	13.100	44.8	ug/l	1387360	4	13.794	1548150	50.0
Undecane	14.111	45.2	ug/l	1398980	4	13.794	1548150	50.0
Di-tert-butyl d...	14.764	35.6	ug/l	1103740	4	13.794	1548150	50.0
Trisulfide, bis...	16.482	40.4	ug/l	1250810	4	13.794	1548150	50.0