LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
Data File : VN078915.D
Acq On : 16 Aug 2023 20:08
Operator : JC\MD
Sample : 03983-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1673

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\82N081523W.M
Title : SW846 8260

Signal : TIC: VN078915.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.694	792	806	816	rBV5	35027	170888	1.39%	0.162%
2	8.171	1046	1057	1060	rBV2	147887	341693	2.78%	0.323%
3	8.224	1060	1066	1076	rVB2	299831	696845	5.67%	0.659%
4	8.441	1094	1103	1114	rBV3	87051	202105	1.64%	0.191%
5	8.577	1117	1126	1136	rBV2	163460	367278	2.99%	0.348%
6	8.971	1184	1193	1201	rBV	157888	315929	2.57%	0.299%
7	9.106	1207	1216	1229	rVB	388981	811523	6.60%	0.768%
8	10.571	1457	1465	1471	rBV	629793	1175716	9.56%	1.113%
9	10.629	1471	1475	1482	rVB	60938	129752	1.05%	0.123%
10	11.871	1679	1686	1697	rVB	561212	998624	8.12%	0.945%
11	11.971	1697	1703	1707	rBV	102412	191338	1.56%	0.181%
12	12.076	1712	1721	1726	rBV	647428	1223830	9.95%	1.158%
13	12.153	1731	1734	1740	rVB3	96727	170209	1.38%	0.161%
14	12.400	1764	1776	1784	rBV3	311549	1006450	8.18%	0.952%
15	12.482	1784	1790	1796	rVB4	166102	303827	2.47%	0.288%
16	12.623	1802	1814	1822	rVV6	266643	1102693	8.96%	1.043%
17	12.700	1822	1827	1830	rVV3	130546	249930	2.03%	0.237%
18	12.776	1832	1840	1842	rVV2	208613	497815	4.05%	0.471%
19	12.800	1842	1844	1848	rVV3	173846	207566	1.69%	0.196%
20	12.853	1848	1853	1862	rVV2	471172	947612	7.70%	0.897%
21	12.941	1862	1868	1872	rVV6	87730	149992	1.22%	0.142%
22	13.035	1878	1884	1889	rVB3	351915	710235	5.77%	0.672%
23	13.100	1889	1895	1899	rBV	996333	1770979	14.40%	1.676%
24	13.165	1899	1906	1914	rVV2	1669033	3915526	31.83%	3.705%
25	13.229	1914	1917	1923	rVB2	244046	401228	3.26%	0.380%
26	13.341	1923	1936	1942	rBV	607830	1686995	13.71%	1.596%
27	13.400	1942	1946	1955	rVB2	482947	982981	7.99%	0.930%
28	13.488	1955	1961	1966	rBV	1900281	3123357	25.39%	2.956%
29	13.576	1973	1976	1980	rBV3	153362	219347	1.78%	0.208%
30	13.618	1980	1983	1987	rBV2	247223	312755	2.54%	0.296%
31	13.676	1987	1993	1998	rBV3	909471	1931452	15.70%	1.828%
32	13.723	1998	2001	2004	rVV2	422122	557914	4.54%	0.528%
33	13.823	2008	2018	2031	rVB7	3101313	12300575	100.00%	11.640%
34	13.953	2032	2040	2042	rBV7	506247	1148778	9.34%	1.087%
35	13.988	2042	2046	2049	rBV2	1023408	1626166	13.22%	1.539%
36	14.023	2050	2052	2057	rVB3	560121	865900	7.04%	0.819%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
Data File : VN078915.D
Acq On : 16 Aug 2023 20:08
Operator : JC\MD
Sample : 03983-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1673

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\82N081523W.M
Title : SW846 8260

37	14.112	2062	2067	2074	rBV3	5077371	9336785	75.91%	8.835%
38	14.188	2078	2080	2083	rVB	338157	357937	2.91%	0.339%
39	14.276	2088	2095	2100	rVV4	825995	2226022	18.10%	2.106%
40	14.335	2101	2105	2109	rVB	941999	1412850	11.49%	1.337%
41	14.447	2118	2124	2129	rBV3	1451725	2719240	22.11%	2.573%
42	14.512	2131	2135	2141	rVB5	455111	883758	7.18%	0.836%
43	14.576	2141	2146	2151	rBV5	1339766	2681248	21.80%	2.537%
44	14.629	2151	2155	2159	rVV	2018940	2979753	24.22%	2.820%
45	14.665	2159	2161	2164	rVB3	550587	512937	4.17%	0.485%
46	14.700	2164	2167	2170	rVB	968116	1209638	9.83%	1.145%
47	14.735	2170	2173	2176	rBV	1040902	1424414	11.58%	1.348%
48	14.770	2176	2179	2182	rBV2	803861	1177516	9.57%	1.114%
49	14.882	2189	2198	2202	rBV4	827813	2191738	17.82%	2.074%
50	14.965	2202	2212	2218	rBV4	3068543	6437691	52.34%	6.092%
51	15.041	2219	2225	2234	rBV4	2227788	6754237	54.91%	6.391%
52	15.217	2250	2255	2261	rVB	860060	1601029	13.02%	1.515%
53	15.282	2262	2266	2268	rBV4	195541	292556	2.38%	0.277%
54	15.323	2268	2273	2278	rBV4	695146	1318734	10.72%	1.248%
55	15.441	2287	2293	2300	rVB4	859677	2078000	16.89%	1.966%
56	15.594	2315	2319	2323	rBV6	218042	411990	3.35%	0.390%
57	15.706	2332	2338	2342	rBV	440256	868738	7.06%	0.822%
58	15.753	2342	2346	2349	rVV2	252522	396120	3.22%	0.375%
59	15.947	2371	2379	2387	rBV3	375384	943557	7.67%	0.893%
60	16.023	2389	2392	2399	rVV6	95218	221016	1.80%	0.209%
61	16.123	2402	2409	2412	rVV4	221567	572938	4.66%	0.542%
62	16.170	2412	2417	2426	rVB	787700	1602589	13.03%	1.516%
63	16.264	2428	2433	2439	rBV8	93815	187923	1.53%	0.178%
64	16.341	2441	2446	2453	rVB3	139804	332918	2.71%	0.315%
65	16.482	2461	2470	2487	rBV	3773886	8775072	71.34%	8.304%
66	16.717	2501	2510	2516	rBV2	410612	953795	7.75%	0.903%

Sum of corrected areas: 105678542

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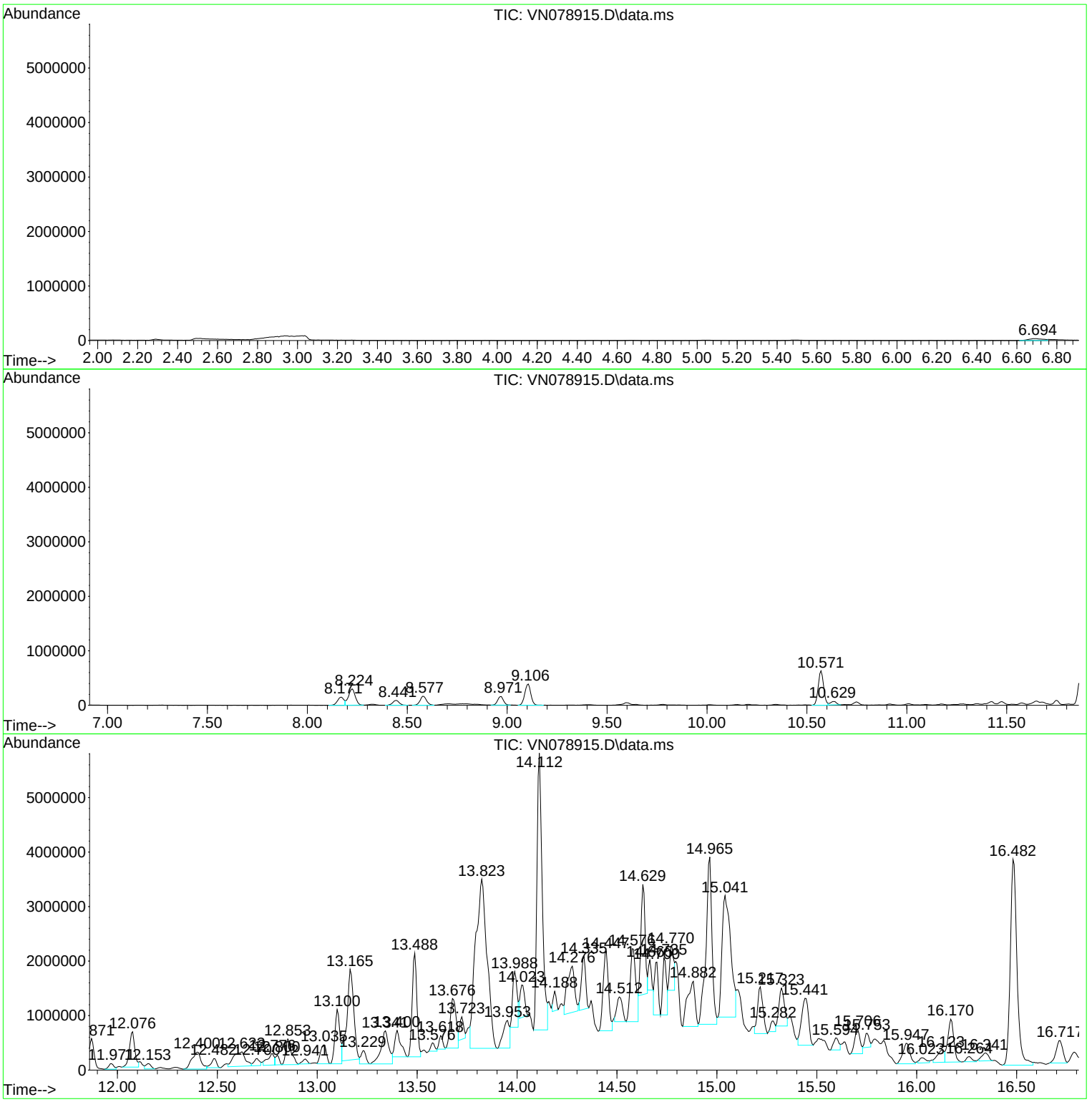
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1673

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
Data File : VN078915.D
Acq On : 16 Aug 2023 20:08
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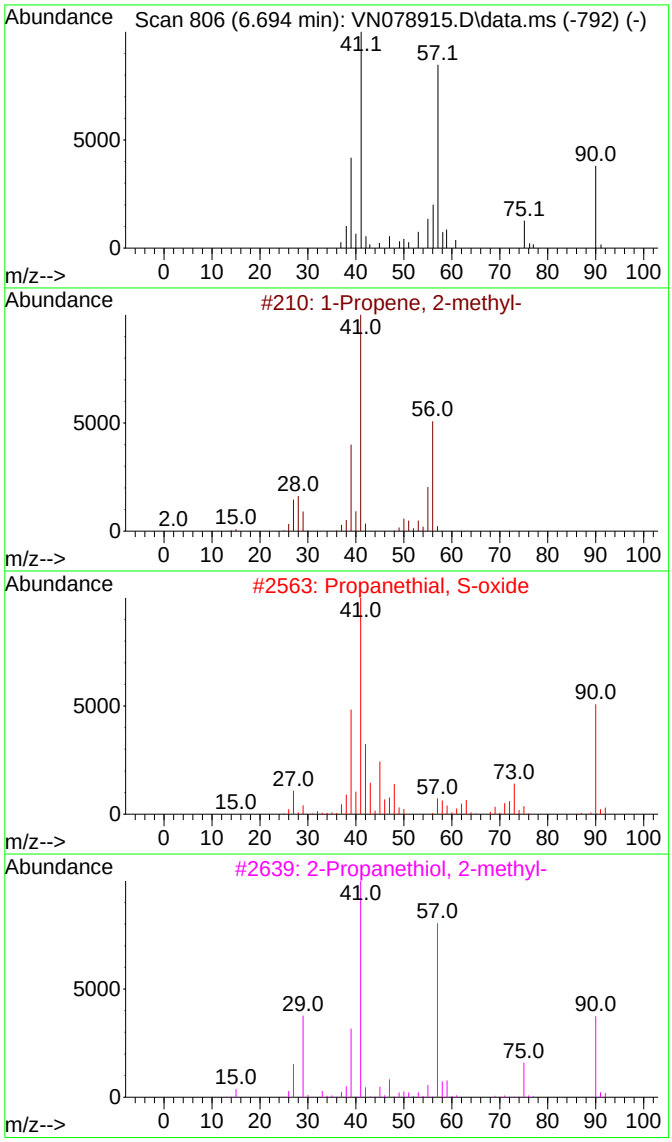
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

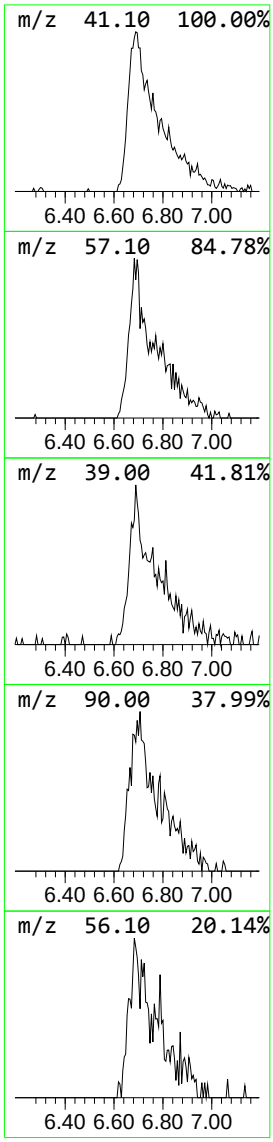
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown6.694 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.694	12.26 ug/l	170888	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	43
2	Propanethial, S-oxide	90	C3H6OS	032157-29-2	43
3	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	38
4	Propane, 2-methyl-1-nitro-	103	C4H9NO2	000625-74-1	33
5	Butane, 2-nitro-	103	C4H9NO2	000600-24-8	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
Data File : VN078915.D
Acq On : 16 Aug 2023 20:08
Operator : JC\MD
Sample : 03983-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1673

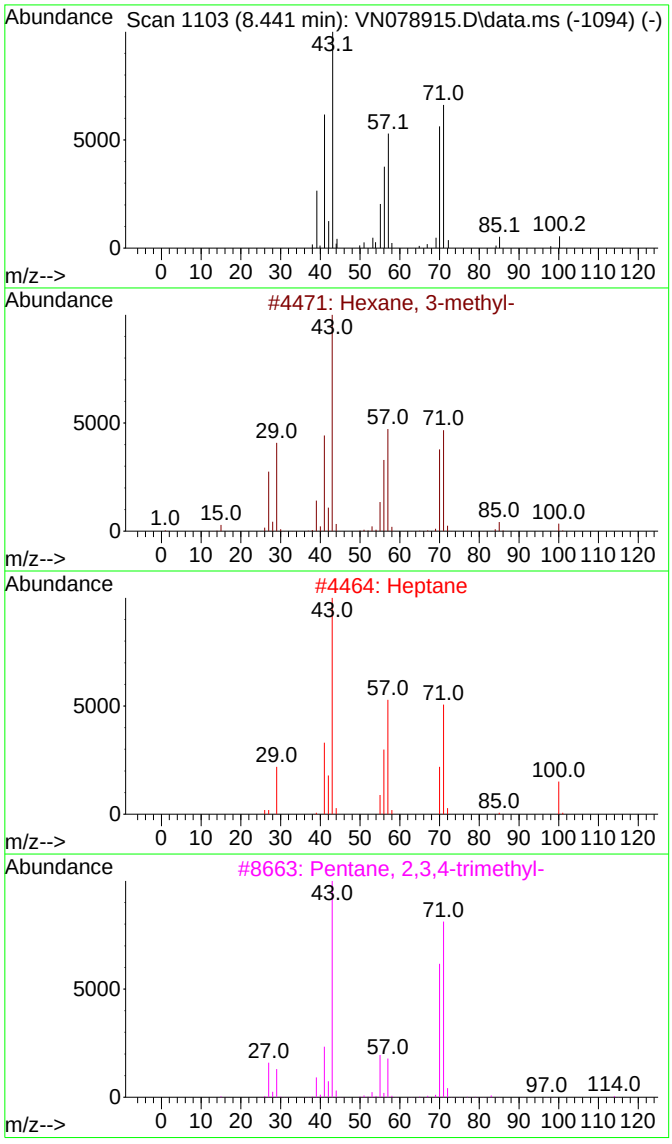
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

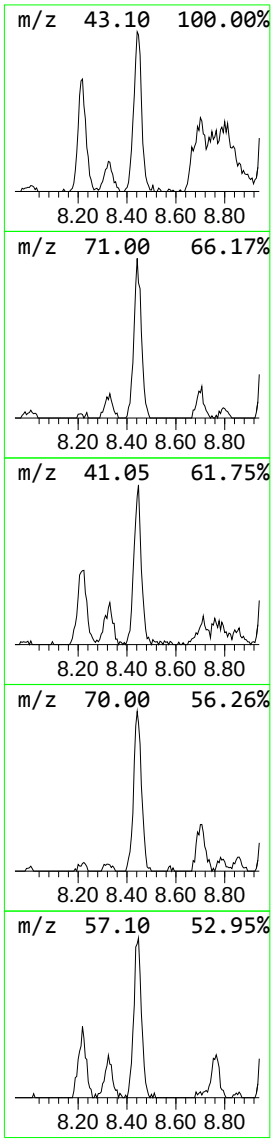
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.441	14.50 ug/l	202105	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2	Heptane	100	C7H16	000142-82-5	72
3	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	64
4	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64
5	Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
Data File : VN078915.D
Acq On : 16 Aug 2023 20:08
Operator : JC\MD
Sample : 03983-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1673

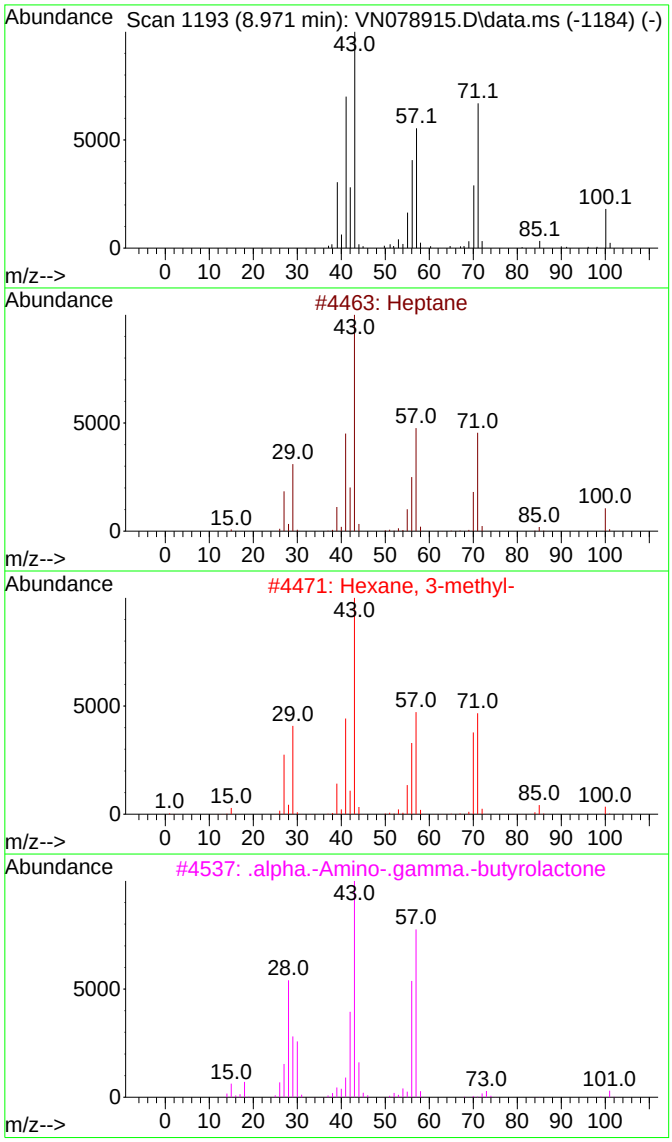
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

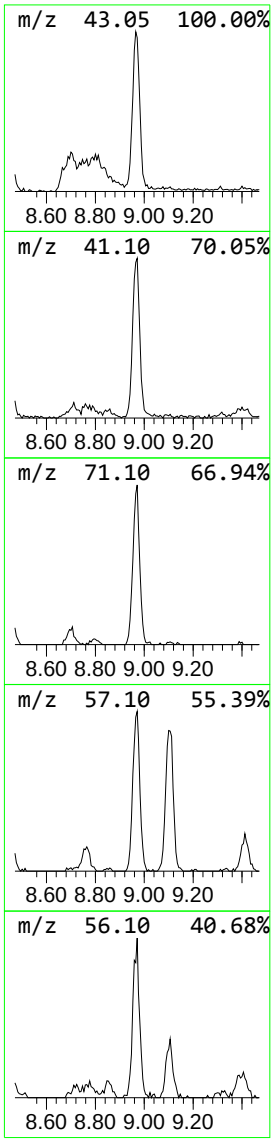
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Heptane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.971	19.47 ug/l	315929	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	87
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	59
3	.alpha.-Amino-.gamma.-butyrolactone	101	C4H7NO2	001192-20-7	43
4	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	38
5	Pentane, 2-methyl-	86	C6H14	000107-83-5	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
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Acq On : 16 Aug 2023 20:08
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Sample : 03983-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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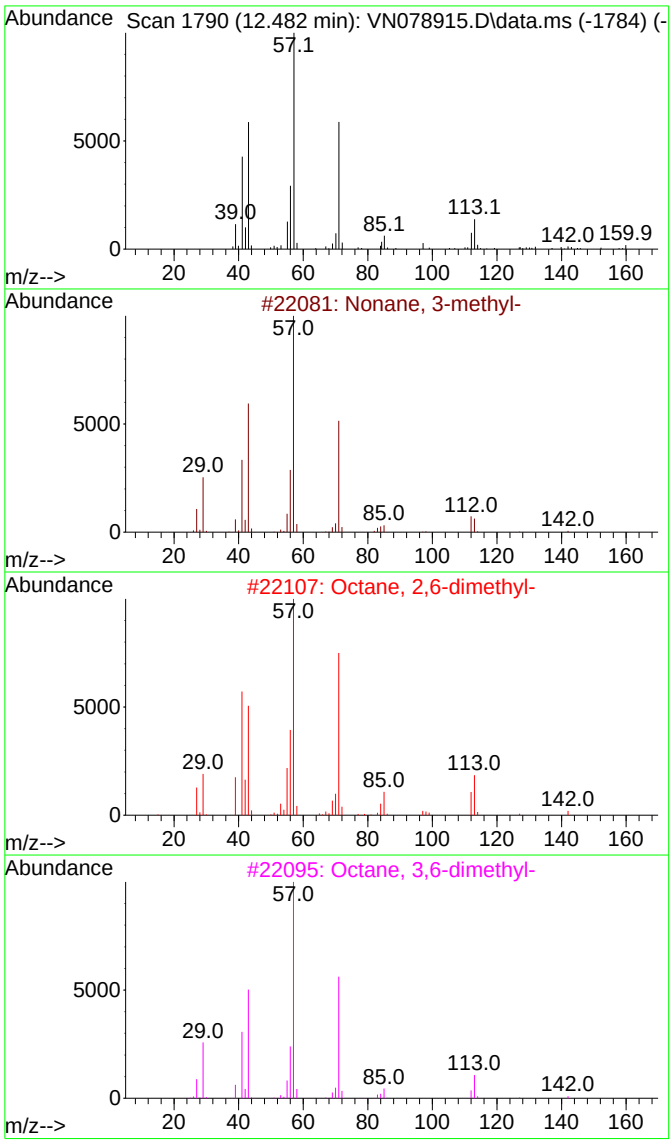
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

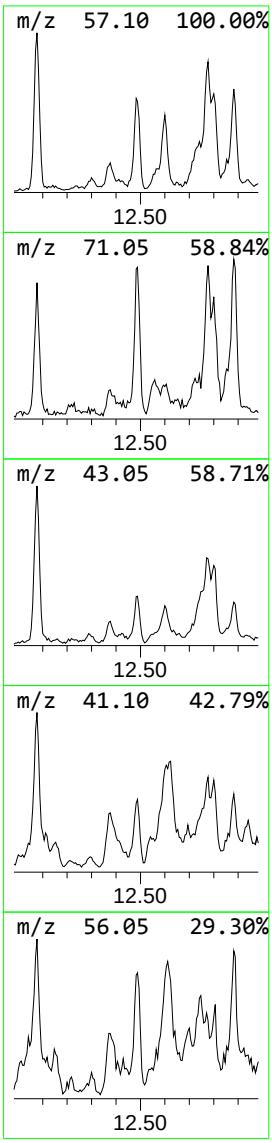
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Nonane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.482	15.21 ug/l	303827	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-	142	C10H22	005911-04-6	90
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	87
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	83
4	Tridecane, 7-methyl-	198	C14H30	026730-14-3	64
5	Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
Data File : VN078915.D
Acq On : 16 Aug 2023 20:08
Operator : JC\MD
Sample : 03983-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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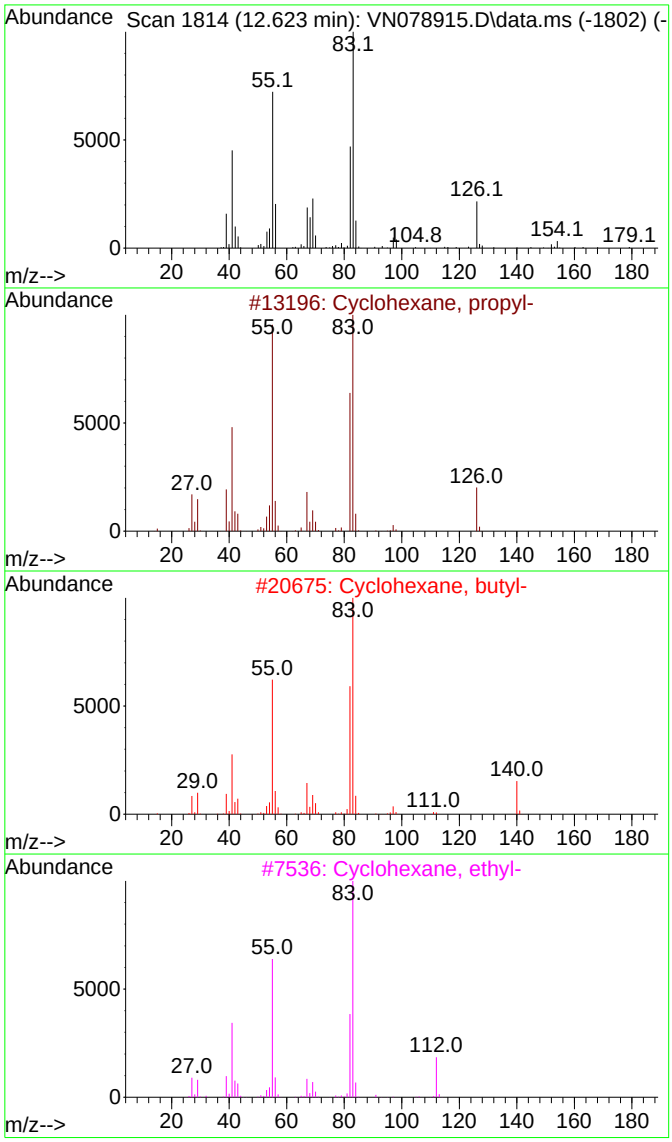
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

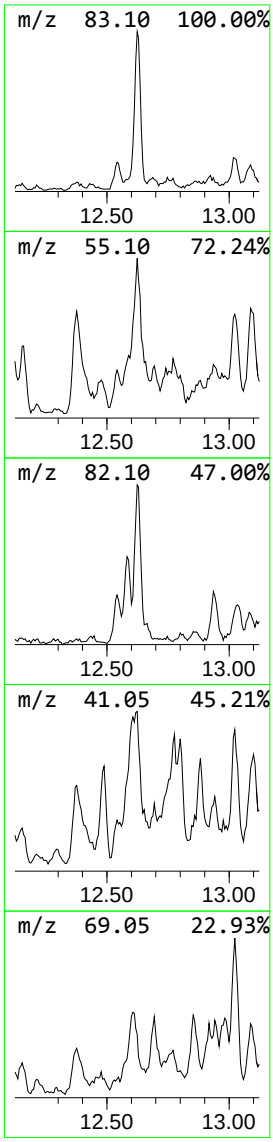
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclohexane, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.624	55.21 ug/l	1102690	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	87
2	Cyclohexane, butyl-	140	C10H20	001678-93-9	59
3	Cyclohexane, ethyl-	112	C8H16	001678-91-7	59
4	Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	58
5	3-Cyclohexyl-1-chloropropane	160	C9H17Cl	001124-62-5	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
Data File : VN078915.D
Acq On : 16 Aug 2023 20:08
Operator : JC\MD
Sample : 03983-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1673

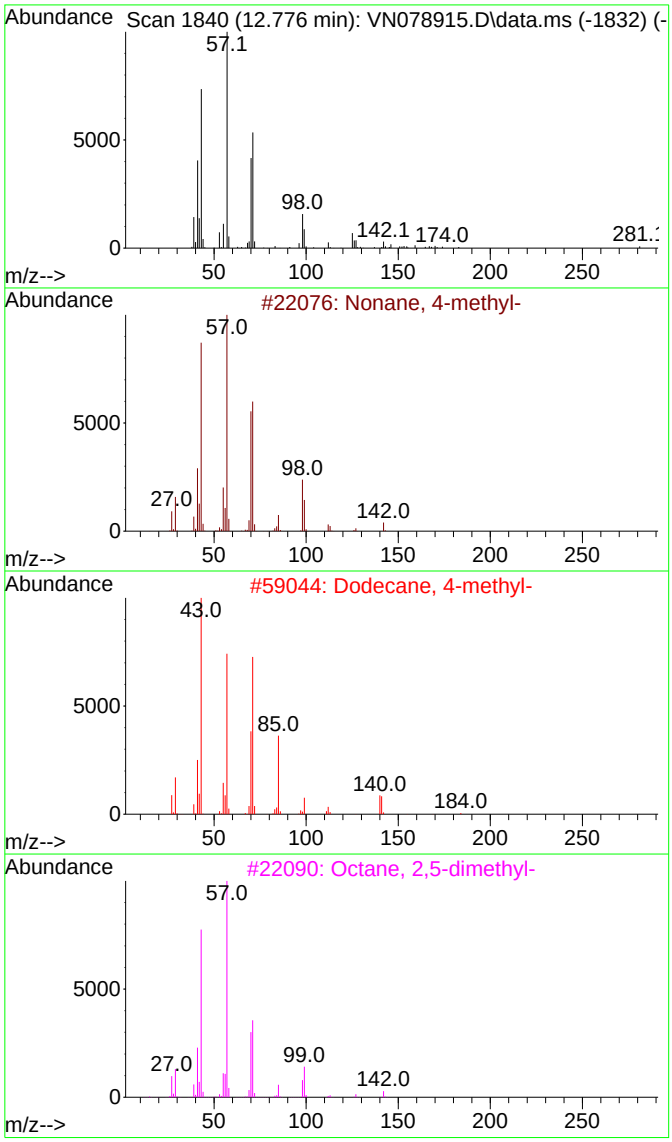
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

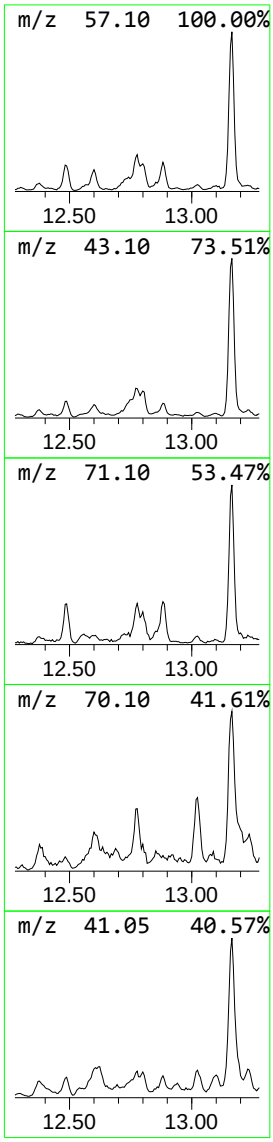
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Nonane, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.776	24.93 ug/l	497815	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 4-methyl-	142	C10H22	017301-94-9	72
2	Dodecane, 4-methyl-	184	C13H28	006117-97-1	59
3	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	58
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	53
5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
Data File : VN078915.D
Acq On : 16 Aug 2023 20:08
Operator : JC\MD
Sample : 03983-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1673

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

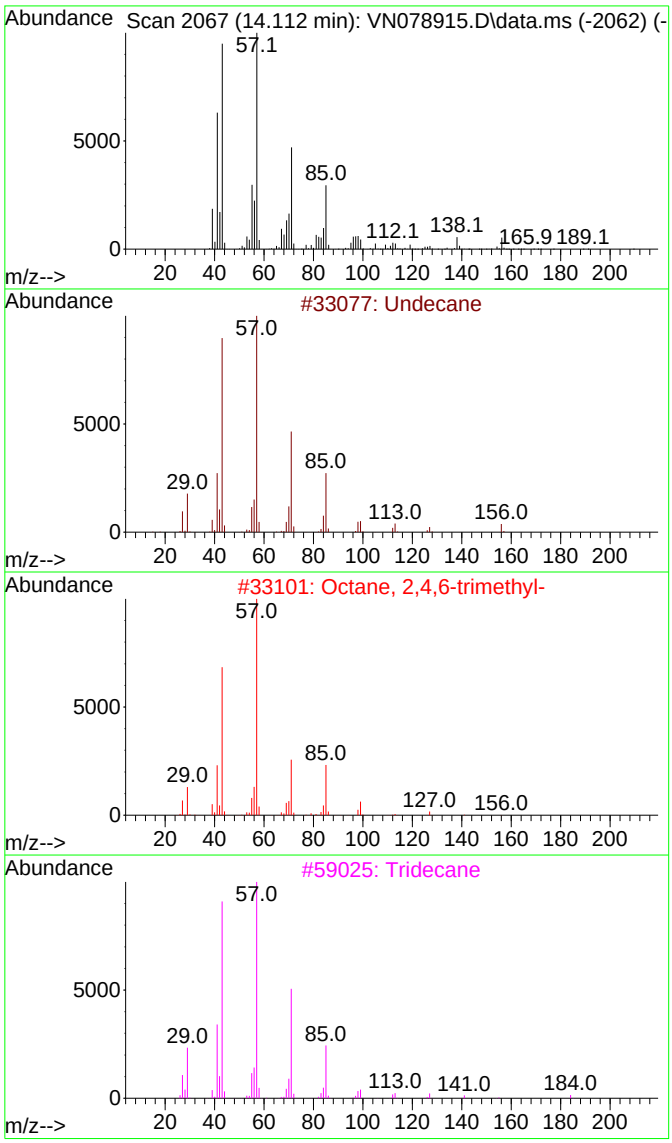
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

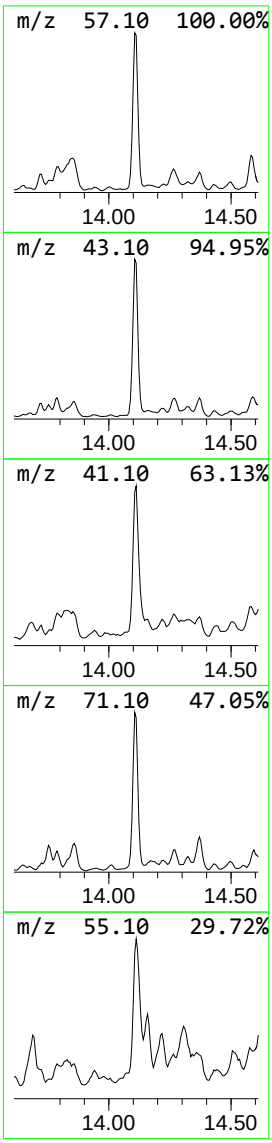
****

Peak Number 7 Undecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.112	37.95 ug/l	9336790	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	87
2	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	72
3	Tridecane	184	C13H28	000629-50-5	64
4	Decane	142	C10H22	000124-18-5	59
5	Heptadecane	240	C17H36	000629-78-7	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
Data File : VN078915.D
Acq On : 16 Aug 2023 20:08
Operator : JC\MD
Sample : 03983-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1673

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

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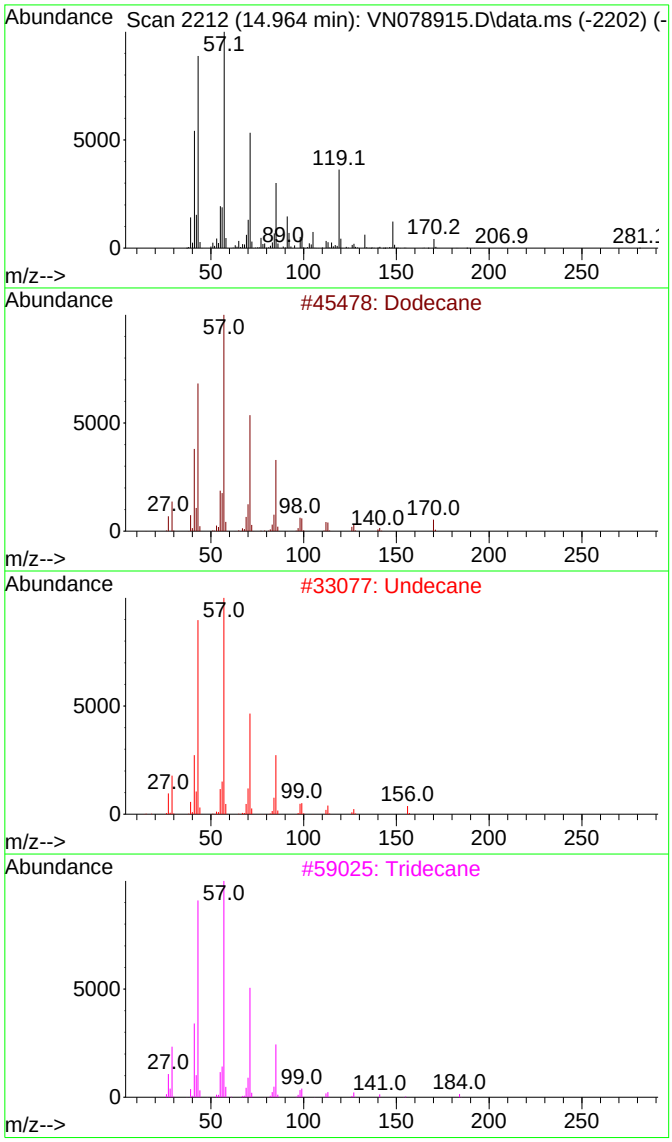
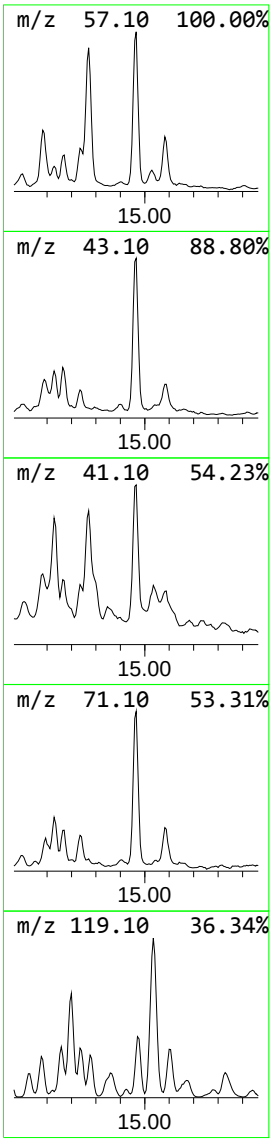
Peak Number 8 Dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.964	26.17 ug/l	6437690	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	92
2	Undecane	156	C11H24	001120-21-4	52
3	Tridecane	184	C13H28	000629-50-5	52
4	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	52
5	Hexadecane	226	C16H34	000544-76-3	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
Data File : VN078915.D
Acq On : 16 Aug 2023 20:08
Operator : JC\MD
Sample : 03983-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1673

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

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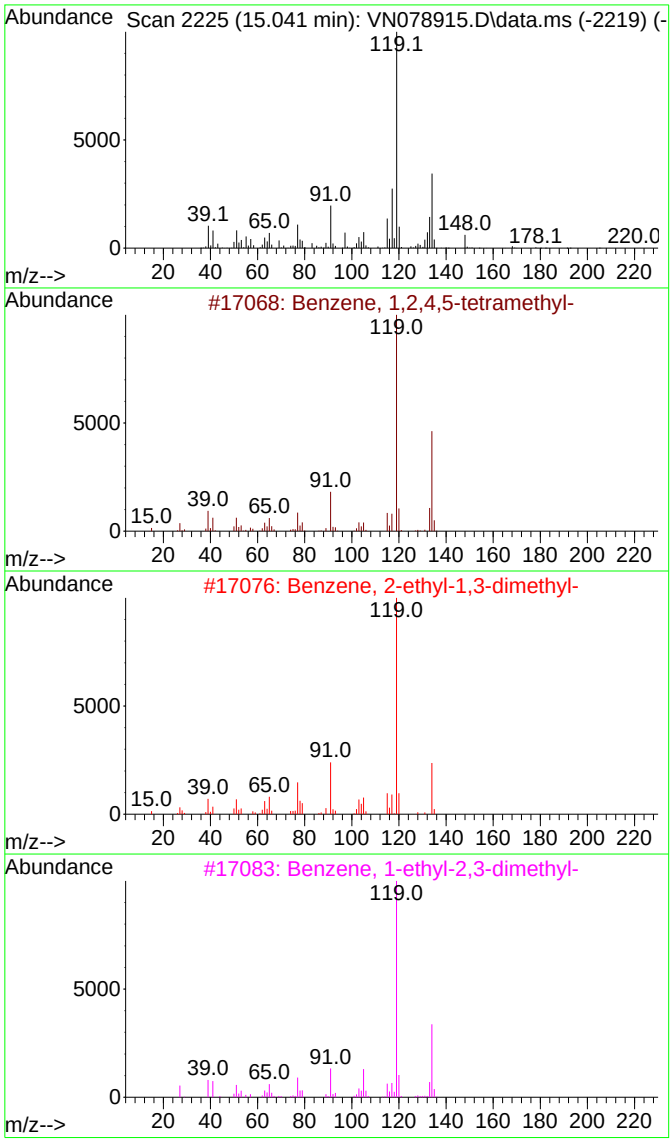
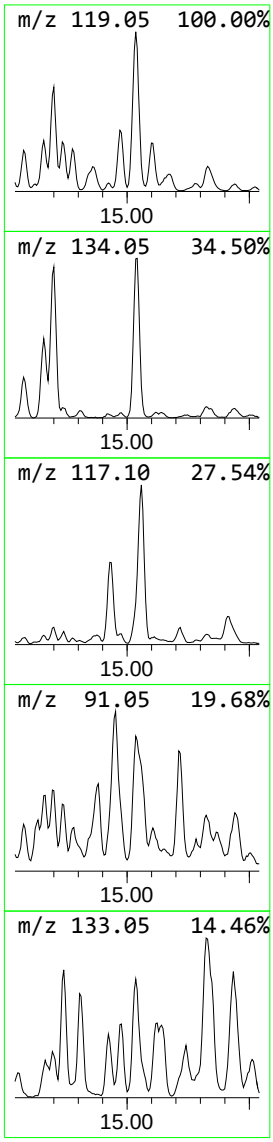
Peak Number 9 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.041	27.45 ug/l	6754240	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	93
2	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	92
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	81
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	81
5	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	81





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
Data File : VN078915.D
Acq On : 16 Aug 2023 20:08
Operator : JC\MD
Sample : 03983-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1673

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

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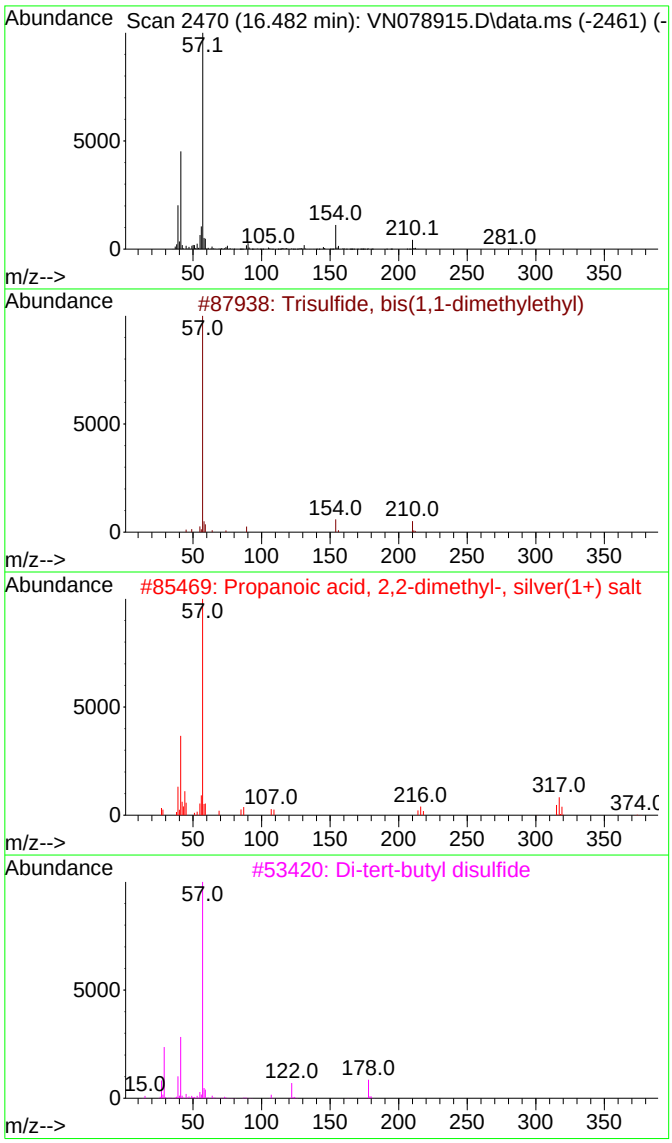
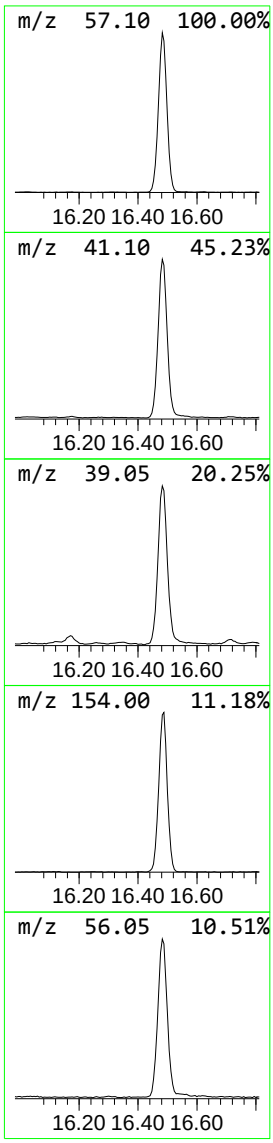
Peak Number 10 unknown16.482 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.482	35.67 ug/l	8775070	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	38
2	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	37
3	Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	32
4	tert-Butyl cyclopropylmethyl sul...	160	C8H16OS	131758-65-1	25
5	Butane, 2-bromo-	136	C4H9Br	000078-76-2	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
Data File : VN078915.D
Acq On : 16 Aug 2023 20:08
Operator : JC\MD
Sample : 03983-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1673

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.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
unknown6.694	6.694	12.3	ug/l	170888	1	8.224	696845	50.0
Hexane, 3-methyl-	8.441	14.5	ug/l	202105	1	8.224	696845	50.0
Heptane	8.971	19.5	ug/l	315929	2	9.106	811523	50.0
Nonane, 3-methyl-	12.482	15.2	ug/l	303827	3	11.871	998624	50.0
Cyclohexane, pr...	12.624	55.2	ug/l	1102690	3	11.871	998624	50.0
Nonane, 4-methyl-	12.776	24.9	ug/l	497815	3	11.871	998624	50.0
Undecane	14.112	38.0	ug/l	9336790	4	13.794	12300600	50.0
Dodecane	14.964	26.2	ug/l	6437690	4	13.794	12300600	50.0
Benzene, 1,2,4,...	15.041	27.4	ug/l	6754240	4	13.794	12300600	50.0
unknown16.482	16.482	35.7	ug/l	8775070	4	13.794	12300600	50.0