LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050322\
Data File : VX028515.D
Acq On : 03 May 2022 20:32
Operator : JC/MD
Sample : N2643-03
Misc : 1.20g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31487

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_X\Method\82X041922W.M
Title : SW846 8260

Signal : TIC: VX028515.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.386	41	49	97	rBV	1366009	8719267	9.15%	1.178%
2	3.733	413	434	477	rBV3	1279607	9128685	9.58%	1.233%
3	5.495	712	723	735	rVV2	2613535	9168399	9.62%	1.238%
4	5.605	736	741	760	rVB	946075	2869988	3.01%	0.388%
5	5.818	760	776	790	rBV	3747356	10972010	11.51%	1.482%
6	6.178	819	835	842	rBV5	420888	1725801	1.81%	0.233%
7	6.605	895	905	921	rVB	1654568	3989191	4.18%	0.539%
8	6.763	921	931	952	rVB	708983	1726578	1.81%	0.233%
9	7.373	1019	1031	1043	rBV	992739	2293257	2.41%	0.310%
10	8.598	1225	1232	1236	rBV2	582827	1128889	1.18%	0.152%
11	8.653	1236	1241	1246	rVB	1378326	2334479	2.45%	0.315%
12	8.732	1246	1254	1260	rBV	40318821	76816831	80.58%	10.376%
13	8.915	1278	1284	1289	rBV	1222934	1768883	1.86%	0.239%
14	9.385	1352	1361	1370	rBV2	568928	968987	1.02%	0.131%
15	9.506	1375	1381	1386	rBV3	796219	1650796	1.73%	0.223%
16	9.561	1386	1390	1395	rVB	1088015	1564672	1.64%	0.211%
17	9.622	1395	1400	1404	rBV	826730	1452373	1.52%	0.196%
18	9.830	1427	1434	1438	rBV3	986063	2001861	2.10%	0.270%
19	9.903	1442	1446	1451	rVB	1958866	2865556	3.01%	0.387%
20	10.012	1457	1464	1467	rBV	1983666	2875493	3.02%	0.388%
21	10.055	1467	1471	1476	rVB	1386716	1952762	2.05%	0.264%
22	10.195	1487	1494	1499	rBV2	1685779	2910035	3.05%	0.393%
23	10.305	1499	1512	1517	rVV2	5026237	11428985	11.99%	1.544%
24	10.360	1517	1521	1532	rVB2	8477638	11833205	12.41%	1.598%
25	10.586	1552	1558	1562	rBV2	2422463	3969812	4.16%	0.536%
26	10.647	1562	1568	1571	rBV	2275337	3249896	3.41%	0.439%
27	10.781	1582	1590	1594	rBV2	4361804	6716247	7.05%	0.907%
28	10.860	1594	1603	1607	rVV3	4084709	7539408	7.91%	1.018%
29	10.896	1607	1609	1614	rVB	1737768	2159067	2.26%	0.292%
30	10.951	1614	1618	1623	rBV3	1015336	2106176	2.21%	0.284%
31	11.031	1628	1631	1634	rVV	1636355	2124603	2.23%	0.287%
32	11.085	1634	1640	1643	rVV3	5362574	9320456	9.78%	1.259%
33	11.110	1643	1644	1651	rVB2	4139870	4415707	4.63%	0.596%
34	11.195	1651	1658	1661	rBV2	4770577	7409018	7.77%	1.001%
35	11.220	1661	1662	1667	rVB3	2329154	2245489	2.36%	0.303%
36	11.311	1673	1677	1679	rBV	2076855	2640615	2.77%	0.357%

LSC Area Percent Report

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Instrument :
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ClientSampleId :
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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_X\Method\82X041922W.M
Title : SW846 8260

37	11.342	1679	1682	1685	rVV2	1206954	1931504	2.03%	0.261%
38	11.384	1685	1689	1695	rVV	8471650	15980255	16.76%	2.159%
39	11.433	1695	1697	1699	rVV	4854371	6203857	6.51%	0.838%
40	11.457	1699	1701	1702	rVV	5111601	5240987	5.50%	0.708%
41	11.482	1702	1705	1710	rVB	22499075	27533246	28.88%	3.719%
42	11.579	1717	1721	1723	rBV	1002596	1183896	1.24%	0.160%
43	11.622	1723	1728	1735	rVB4	5774540	10777170	11.31%	1.456%
44	11.689	1735	1739	1741	rBV2	1812359	2313456	2.43%	0.312%
45	11.719	1741	1744	1747	rVV	6003239	6753412	7.08%	0.912%
46	11.756	1747	1750	1760	rVB	15911923	24760121	25.97%	3.344%
47	11.841	1760	1764	1766	rBV2	1834047	2604395	2.73%	0.352%
48	11.896	1766	1773	1777	rVB2	4274355	6968672	7.31%	0.941%
49	11.951	1777	1782	1784	rBV	5338874	7064993	7.41%	0.954%
50	11.976	1784	1786	1790	rVB2	3259356	3362713	3.53%	0.454%
51	12.043	1790	1797	1800	rBV3	3458504	6705143	7.03%	0.906%
52	12.097	1800	1806	1811	rBV3	6567008	13973003	14.66%	1.887%
53	12.177	1816	1819	1826	rVB4	4144633	6706609	7.04%	0.906%
54	12.250	1826	1831	1833	rBV	6641359	9520101	9.99%	1.286%
55	12.274	1833	1835	1838	rVB	6770790	6864770	7.20%	0.927%
56	12.323	1838	1843	1849	rVB3	11863167	21984002	23.06%	2.969%
57	12.433	1849	1861	1864	rBV2	20482145	30063505	31.54%	4.061%
58	12.469	1864	1867	1873	rVB2	6668403	9259507	9.71%	1.251%
59	12.536	1874	1878	1880	rBV	4659739	6472930	6.79%	0.874%
60	12.561	1880	1882	1886	rVB	4009765	3639446	3.82%	0.492%
61	12.616	1888	1891	1894	rVB	4049885	4636589	4.86%	0.626%
62	12.646	1894	1896	1900	rVB3	1971835	2381761	2.50%	0.322%
63	12.707	1900	1906	1907	rBV2	3834522	6727261	7.06%	0.909%
64	12.823	1919	1925	1928	rBV4	4442431	6442863	6.76%	0.870%
65	12.896	1933	1937	1940	rBV3	4090722	7128375	7.48%	0.963%
66	13.000	1946	1954	1958	rBV2	22710227	36068144	37.84%	4.872%
67	13.049	1959	1962	1965	rVV2	3220479	3775533	3.96%	0.510%
68	13.170	1975	1982	1986	rBV4	5669596	9573953	10.04%	1.293%
69	13.219	1986	1990	1993	rVV	3649152	4319202	4.53%	0.583%
70	13.268	1993	1998	2000	rVV2	10232539	14579978	15.30%	1.969%
71	13.298	2000	2003	2007	rVV2	12285236	16470117	17.28%	2.225%
72	13.335	2007	2009	2013	rVV	1346241	1783910	1.87%	0.241%
73	13.384	2013	2017	2020	rVV2	1294640	2264562	2.38%	0.306%
74	13.426	2020	2024	2032	rVB	8141848	13906216	14.59%	1.878%
75	13.506	2032	2037	2040	rBV2	2025855	2942116	3.09%	0.397%
76	13.548	2040	2044	2047	rBV	1651109	2021168	2.12%	0.273%

LSC Area Percent Report

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ClientSampleId :
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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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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Title : SW846 8260

77	13.591	2047	2051	2055	rBV3	2974809	4910888	5.15%	0.663%
78	13.670	2061	2064	2068	rVB2	1705485	2358133	2.47%	0.319%
79	13.853	2088	2094	2100	rVB4	3863609	6920963	7.26%	0.935%
80	13.926	2100	2106	2112	rBV4	2932036	5924173	6.21%	0.800%
81	14.048	2122	2126	2128	rVV2	1604358	1792513	1.88%	0.242%
82	14.079	2128	2131	2134	rVB2	1316412	1396488	1.46%	0.189%
83	14.231	2149	2156	2164	rVV2	4278051	7124861	7.47%	0.962%
84	14.378	2177	2180	2186	rVV4	813054	1763280	1.85%	0.238%
85	14.463	2186	2194	2198	rVV2	53862802	95324581	100.00%	12.876%
86	14.493	2198	2199	2206	rVV2	2701730	3020741	3.17%	0.408%
87	14.560	2206	2210	2216	rVV5	403795	957369	1.00%	0.129%
88	14.615	2216	2219	2222	rVV	1905732	2824165	2.96%	0.381%
89	14.640	2222	2223	2226	rVV2	1550664	1431746	1.50%	0.193%
90	14.676	2226	2229	2233	rVB3	917724	1191442	1.25%	0.161%
91	14.981	2275	2279	2285	rVB	1875701	2462212	2.58%	0.333%

Sum of corrected areas: 740336473

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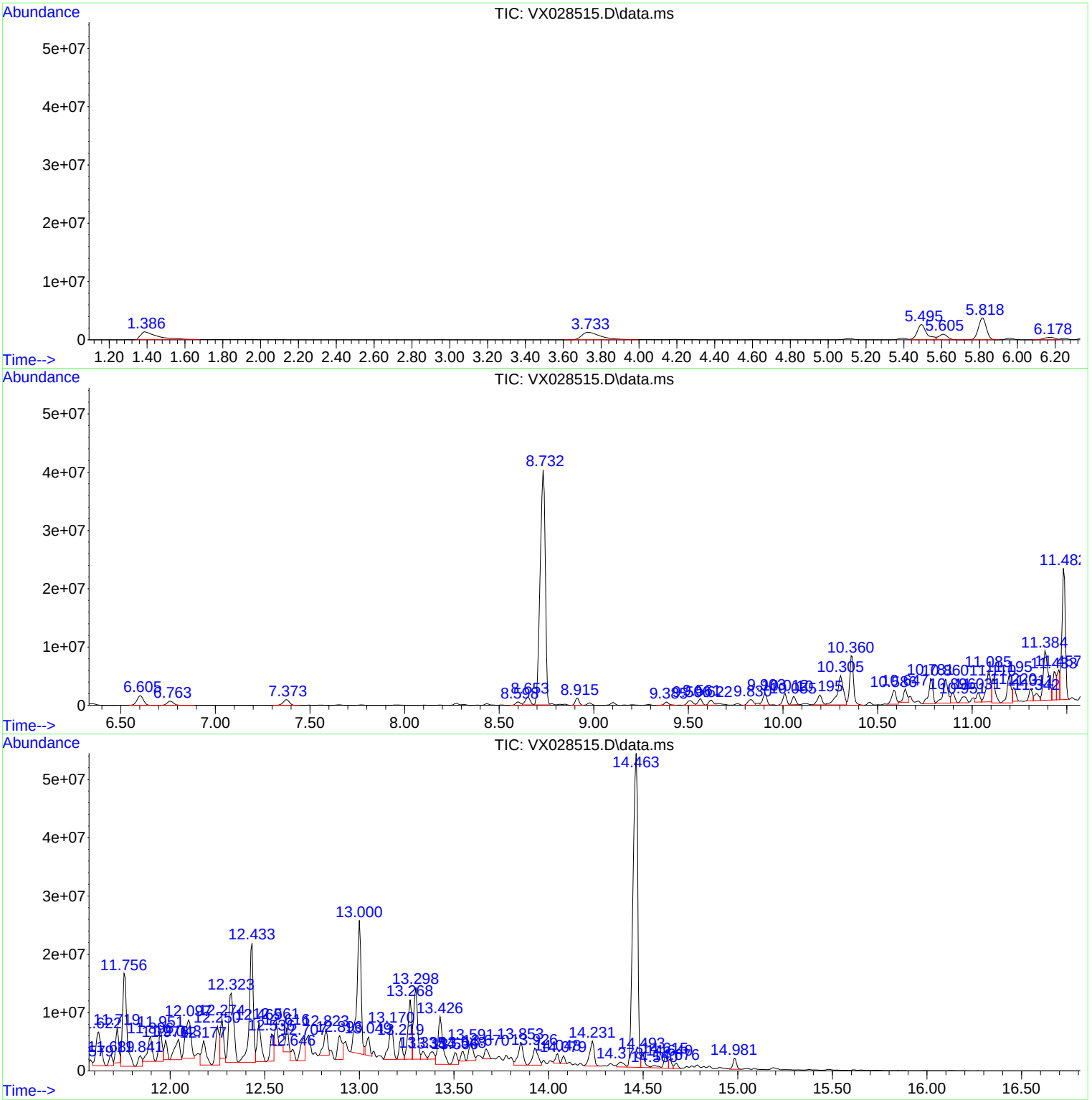
Instrument :
MSVOA_X
ClientSampleId :
31487

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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



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MSVOA_X
ClientSampleId :
31487

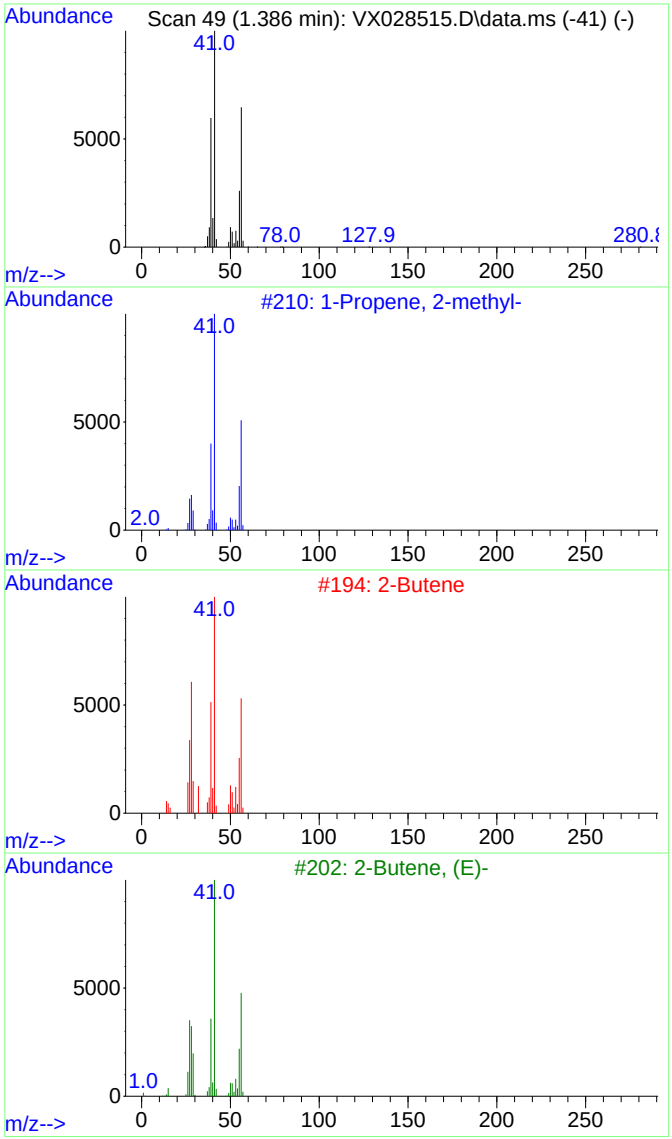
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

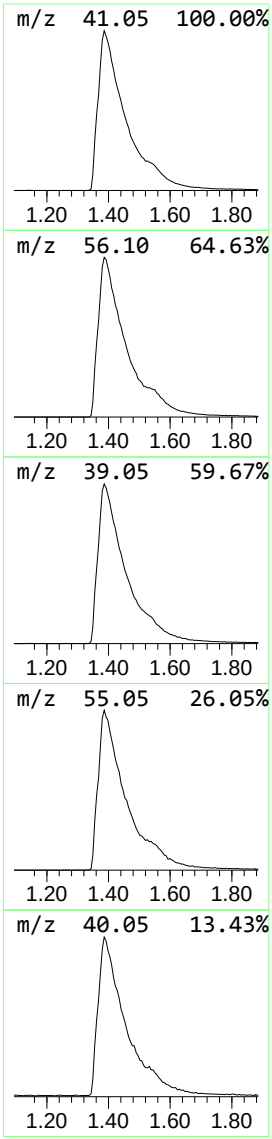
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Propene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.386	151.90 ug/l	8719270	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	90
2	2-Butene	56	C4H8	000107-01-7	80
3	2-Butene, (E)-	56	C4H8	000624-64-6	53
4	2-Butene, (Z)-	56	C4H8	000590-18-1	47
5	1-Butene	56	C4H8	000106-98-9	46





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Operator : JC/MD
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Misc : 1.20g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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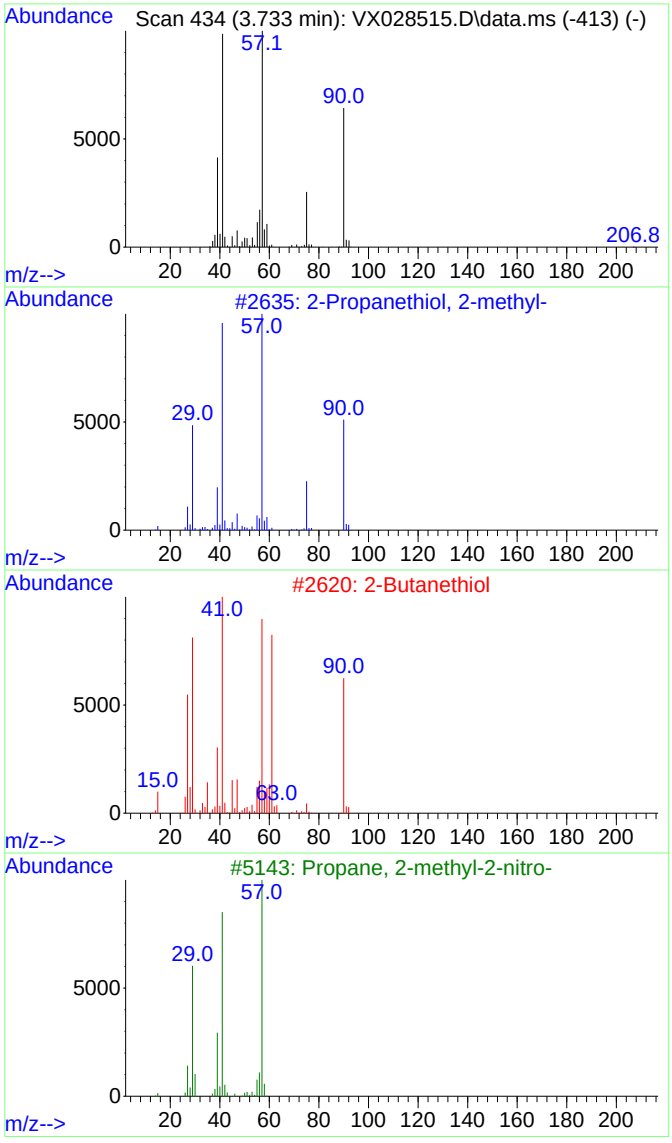
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

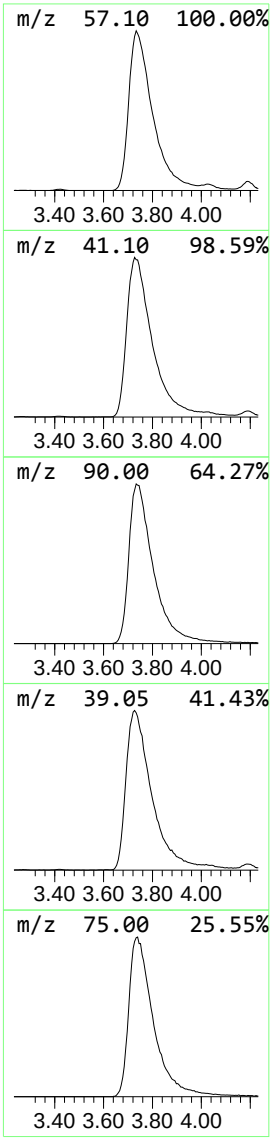
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Propanethiol, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.733	159.04 ug/l	9128690	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	70
2	2-Butanethiol	90	C4H10S	000513-53-1	47
3	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	38
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	30
5	Allyl chloride	76	C3H5Cl	000107-05-1	27





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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

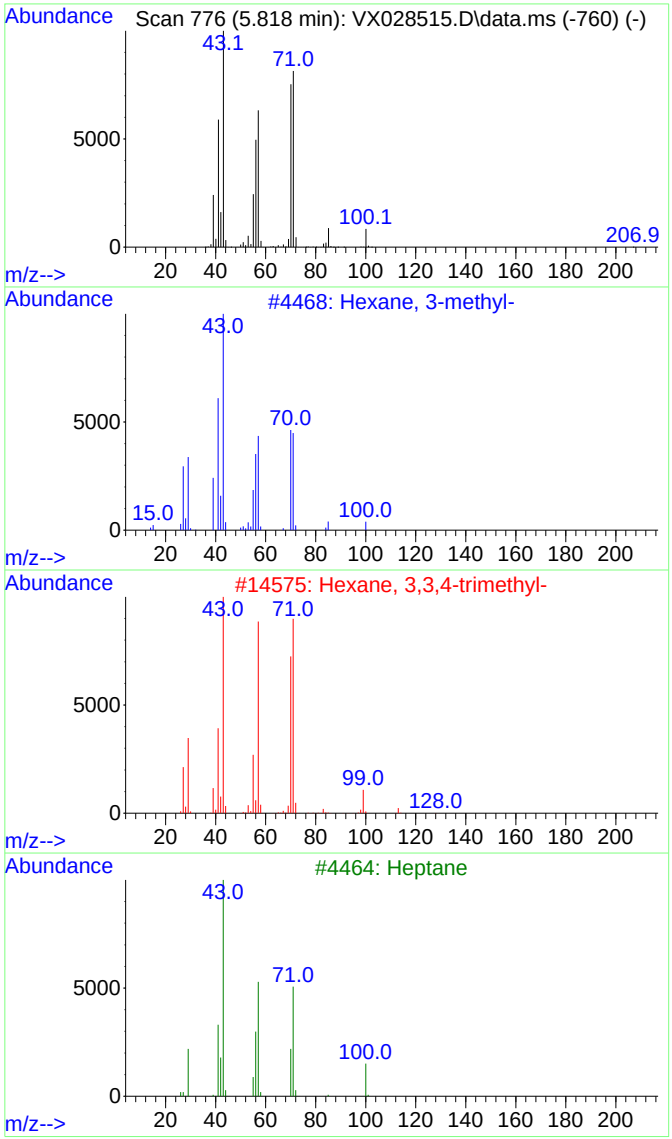
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

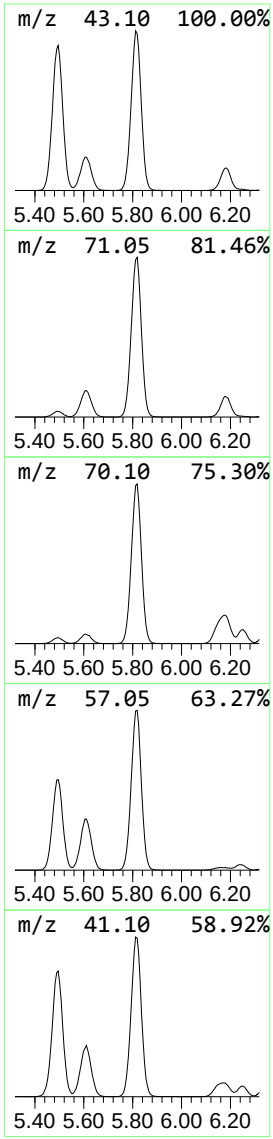
****

Peak Number 3 Hexane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.818	191.15 ug/l	10972000	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64
3	Heptane	100	C7H16	000142-82-5	62
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
5	Pentane, 3-ethyl-	100	C7H16	000617-78-7	59





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Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

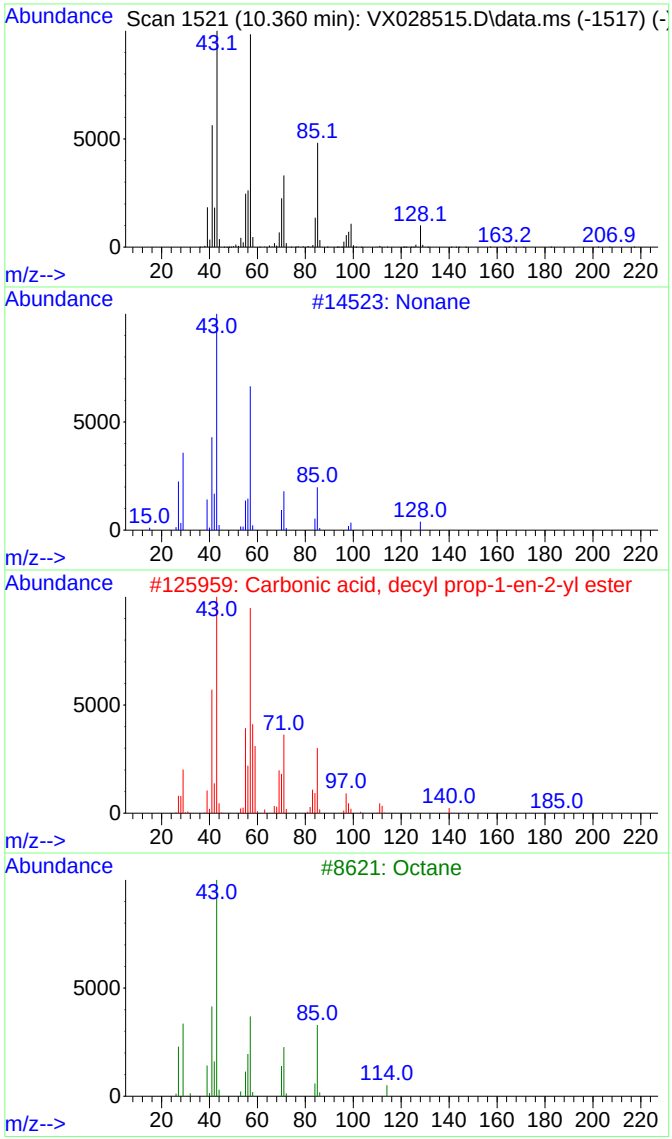
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

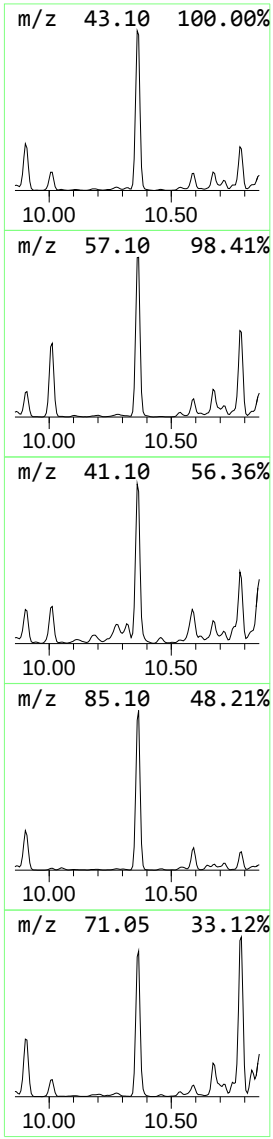
****

Peak Number 4 Nonane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.360	302.99 ug/l	11833200	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane	128	C9H20	000111-84-2	94
2	Carbonic acid, decyl prop-1-en-2...	242	C14H26O3	1000382-90-5	72
3	Octane	114	C8H18	000111-65-9	64
4	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	59
5	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	50





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Operator : JC/MD
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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31487

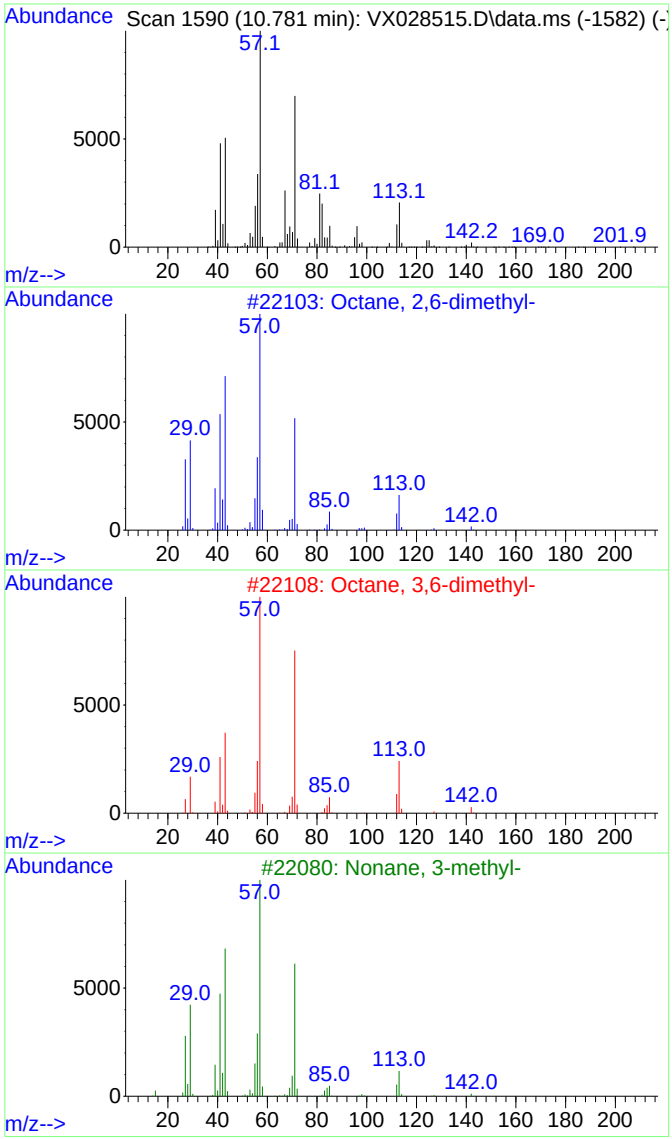
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

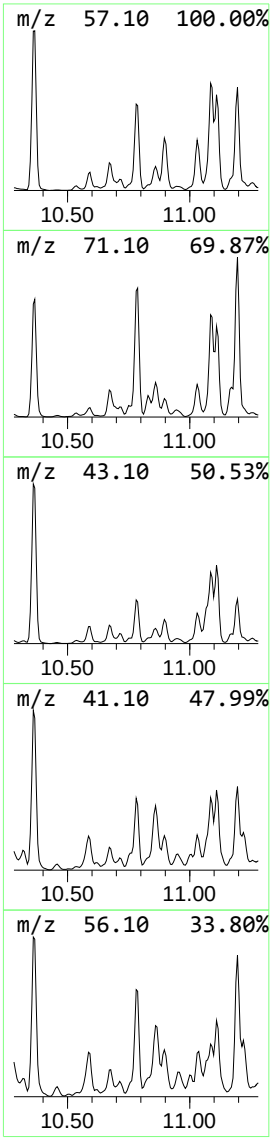
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Octane, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.781	171.97 ug/l	6716250	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	70
2	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	64
3	Nonane, 3-methyl-	142	C10H22	005911-04-6	60
4	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	49
5	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050322\
Data File : VX028515.D
Acq On : 03 May 2022 20:32
Operator : JC/MD
Sample : N2643-03
Misc : 1.20g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31487

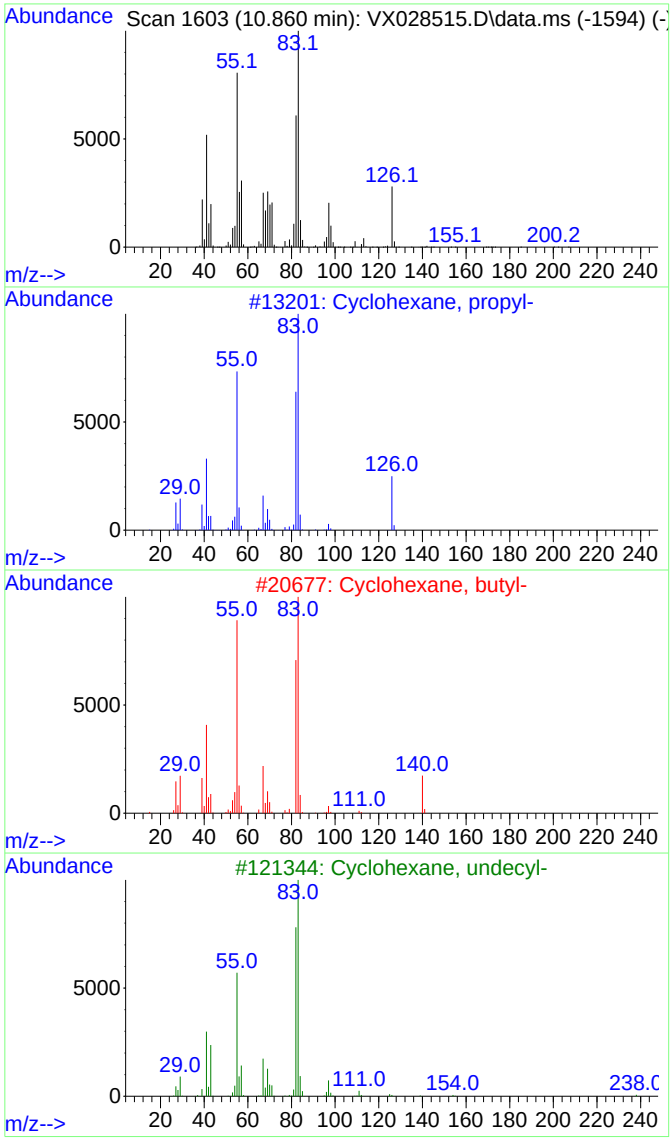
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

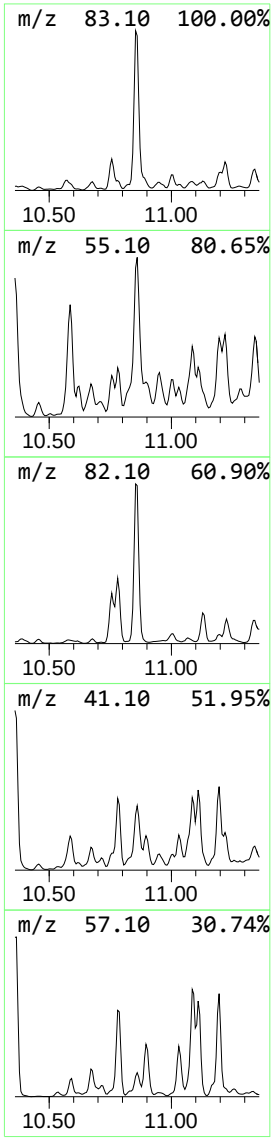
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclohexane, propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.860	193.04 ug/l	7539410	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	58
2	Cyclohexane, butyl-	140	C10H20	001678-93-9	50
3	Cyclohexane, undecyl-	238	C17H34	054105-66-7	50
4	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	47
5	Cyclohexane, methyl-	98	C7H14	000108-87-2	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050322\
Data File : VX028515.D
Acq On : 03 May 2022 20:32
Operator : JC/MD
Sample : N2643-03
Misc : 1.20g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31487

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

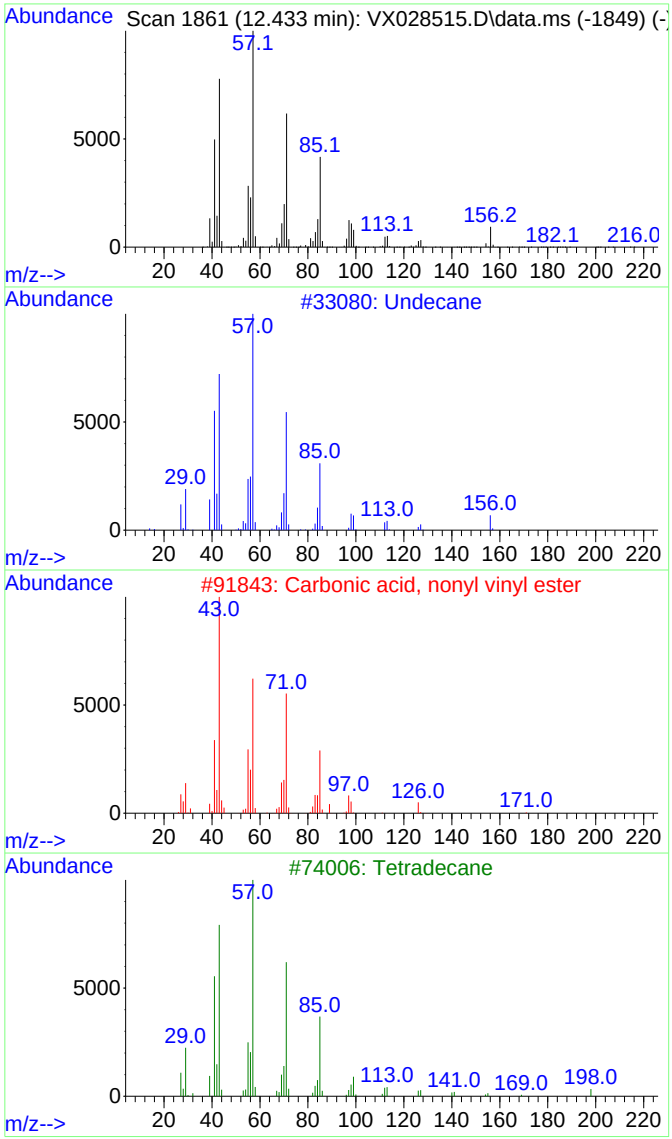
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

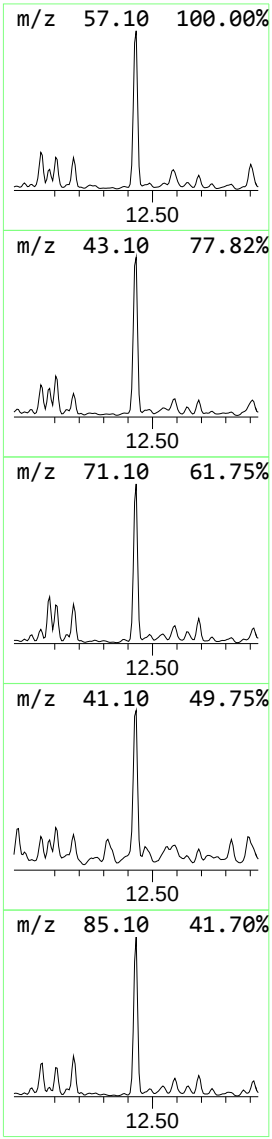
****

Peak Number 7 Undecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.433	224.18 ug/l	30063500	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	95
2	Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	86
3	Tetradecane	198	C14H30	000629-59-4	72
4	Hexadecane	226	C16H34	000544-76-3	72
5	Nonane	128	C9H20	000111-84-2	70





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050322\
Data File : VX028515.D
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Operator : JC/MD
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Instrument :
MSVOA_X
ClientSampleId :
31487

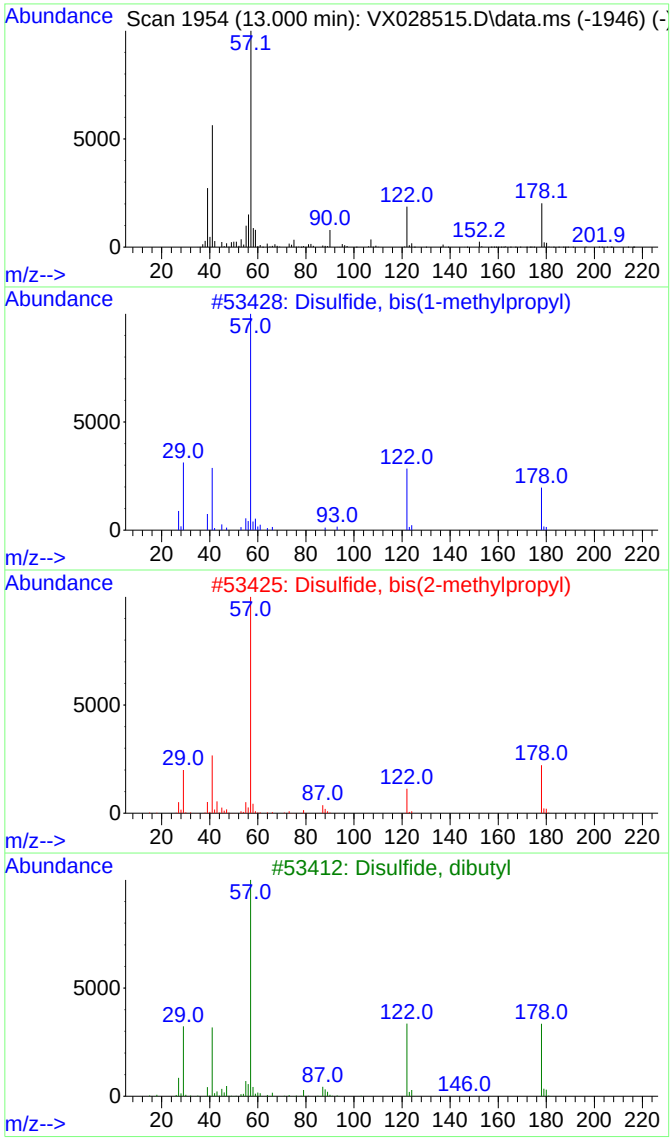
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

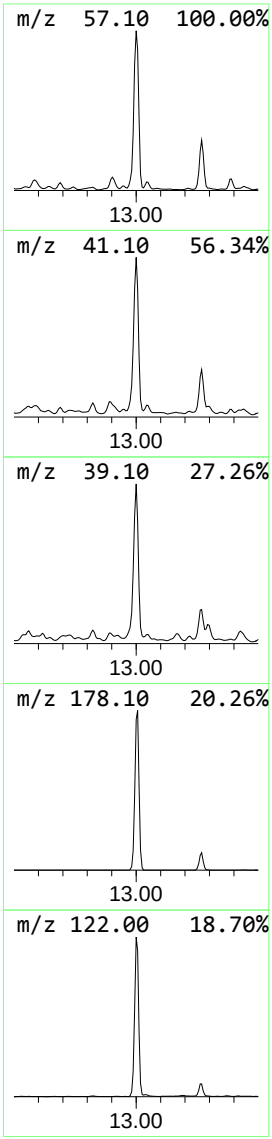
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Disulfide, bis(1-methylpropyl) Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.000	268.96 ug/l	36068100	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	59
2	Disulfide, bis(2-methylpropyl)	178	C8H18S2	001518-72-5	53
3	Disulfide, dibutyl	178	C8H18S2	000629-45-8	50
4	Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	49
5	Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050322\
Data File : VX028515.D
Acq On : 03 May 2022 20:32
Operator : JC/MD
Sample : N2643-03
Misc : 1.20g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31487

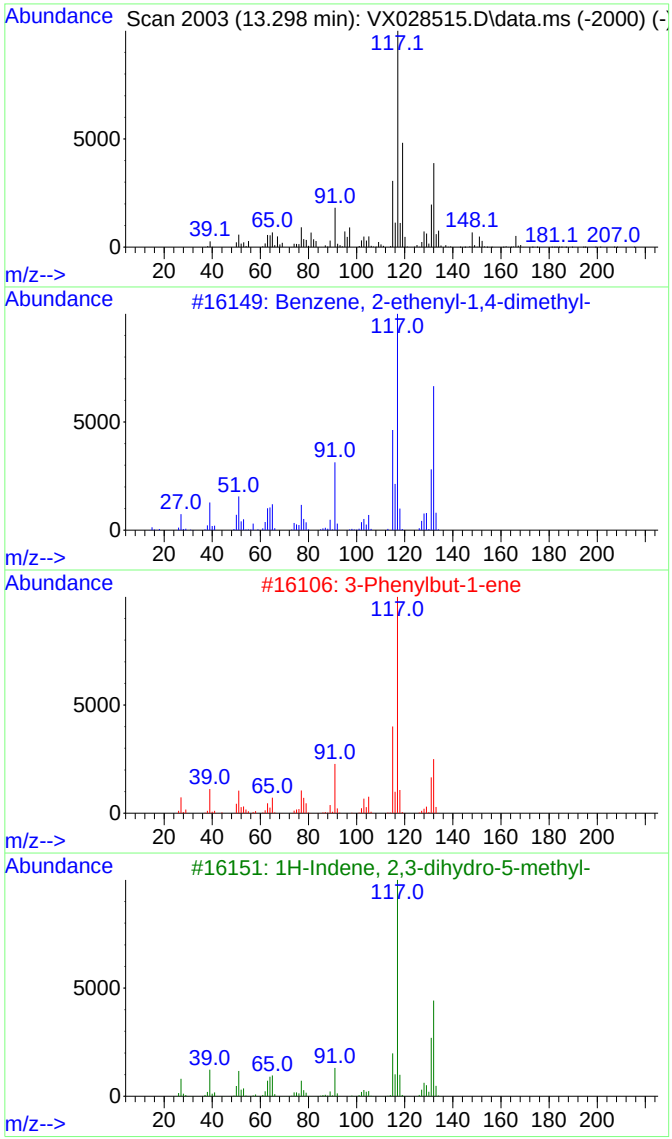
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

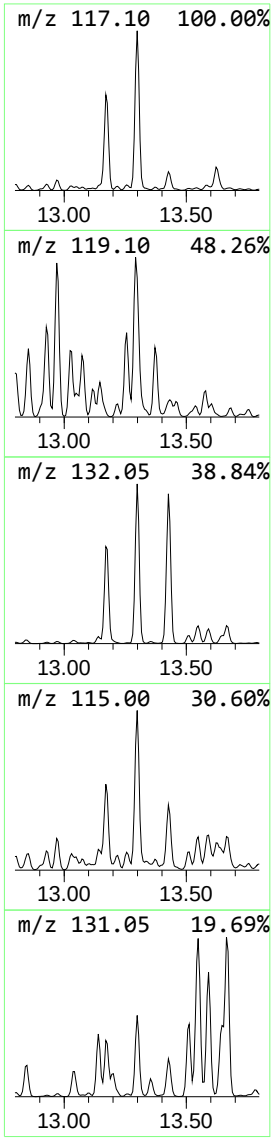
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.299	122.82 ug/l	16470100	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	76
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	70
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	70
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	70





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Operator : JC/MD
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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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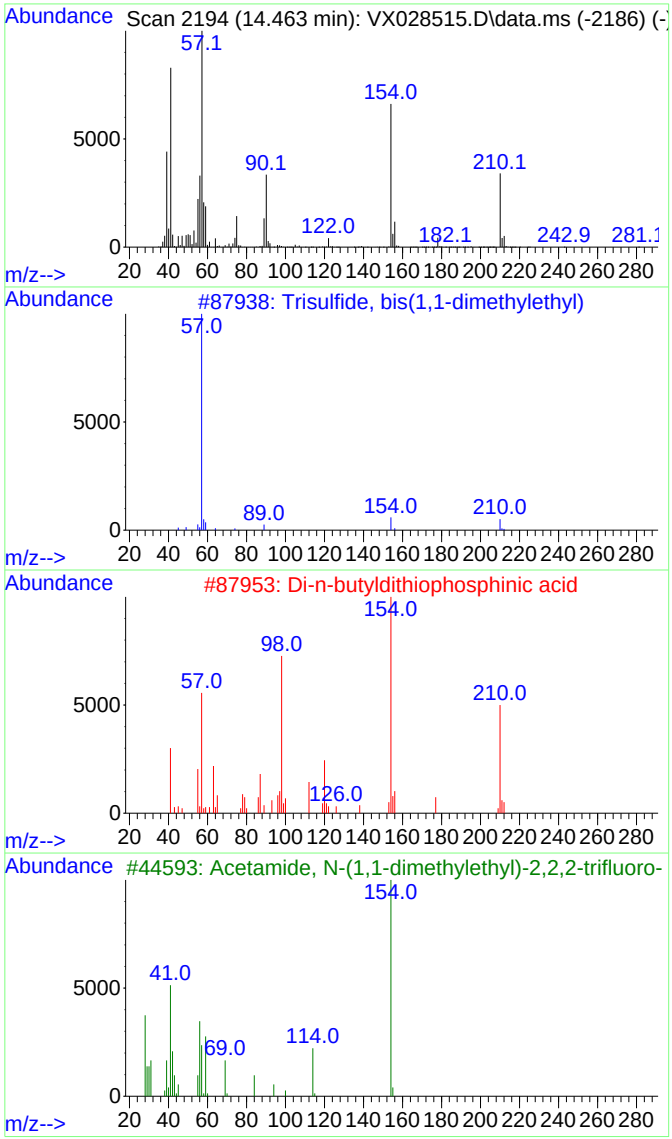
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

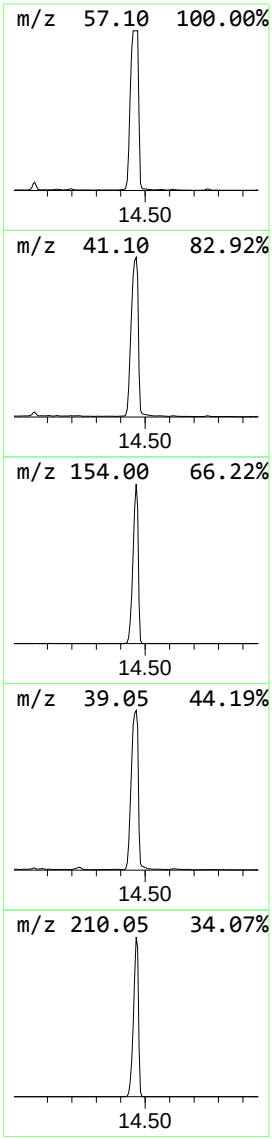
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.463	710.83 ug/l	95324600	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	50
2	Di-n-butyldithiophosphinic acid	210	C8H19PS2	032435-35-1	30
3	Acetamide, N-(1,1-dimethylethyl)...	169	C6H10F3NO	001960-29-8	17
4	1-Hexene, 1-iodo-, (Z)-	210	C6H11I	016538-47-9	12
5	3,4-Diethoxybenzoic acid	210	C11H14O4	005409-31-4	12





Tentatively Identified Compound (LSC) summary

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Data File : VX028515.D
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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
1-Propene, 2-me...	1.386	151.9	ug/l	8719270	1	5.550	2869990	50.0
2-Propanethiol,...	3.733	159.0	ug/l	9128690	1	5.550	2869990	50.0
Hexane, 3-methyl-	5.818	191.2	ug/l	10972000	1	5.550	2869990	50.0
Nonane	10.360	303.0	ug/l	11833200	3	10.055	1952760	50.0
Octane, 2,6-dim...	10.781	172.0	ug/l	6716250	3	10.055	1952760	50.0
Cyclohexane, pr...	10.860	193.0	ug/l	7539410	3	10.055	1952760	50.0
Undecane	12.433	224.2	ug/l	30063500	4	12.030	6705140	50.0
Disulfide, bis(...	13.000	269.0	ug/l	36068100	4	12.030	6705140	50.0
Benzene, 2-ethe...	13.299	122.8	ug/l	16470100	4	12.030	6705140	50.0
Trisulfide, bis...	14.463	710.8	ug/l	95324600	4	12.030	6705140	50.0