LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078182.D
Acq On : 13 Jun 2023 13:36
Operator : JC\MD
Sample : 03172-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1578

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\82N060623W.M
Title : SW846 8260

Signal : TIC: VN078182.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.542	95	100	121	rVB2	248957	1257632	2.46%	0.465%
2	4.441	411	423	447	rBV	5957964	19366350	37.93%	7.154%
3	6.700	791	807	835	rBV4	214244	1443435	2.83%	0.533%
4	8.171	1044	1057	1061	rBV	457379	1117856	2.19%	0.413%
5	8.224	1061	1066	1076	rVB2	1078920	2472896	4.84%	0.913%
6	8.447	1094	1104	1113	rBV	482766	1073182	2.10%	0.396%
7	8.582	1117	1127	1139	rVB	461374	1098723	2.15%	0.406%
8	8.971	1184	1193	1203	rVB	396559	807391	1.58%	0.298%
9	9.106	1207	1216	1232	rVV	1090967	2284719	4.48%	0.844%
10	9.600	1284	1300	1309	rBV	244924	602809	1.18%	0.223%
11	10.459	1438	1446	1457	rBV	280073	570201	1.12%	0.211%
12	10.570	1457	1465	1470	rBV	1617041	3058718	5.99%	1.130%
13	10.635	1470	1476	1490	rVB	16025944	28868747	56.55%	10.664%
14	11.870	1678	1686	1697	rBV	1547521	2751352	5.39%	1.016%
15	12.076	1712	1721	1731	rBV	779761	1600400	3.13%	0.591%
16	12.400	1765	1776	1783	rBV2	395140	942516	1.85%	0.348%
17	12.853	1847	1853	1863	rVB2	1275144	2400879	4.70%	0.887%
18	13.100	1889	1895	1899	rBV	1031081	1833079	3.59%	0.677%
19	13.164	1899	1906	1914	rVB3	1386523	3412649	6.68%	1.261%
20	13.264	1914	1923	1930	rBV	34388730	51053350	100.00%	18.859%
21	13.341	1931	1936	1942	rVB	401085	652420	1.28%	0.241%
22	13.506	1954	1964	1973	rBV2	12025640	22262205	43.61%	8.224%
23	13.611	1977	1982	1988	rVB4	726907	1257693	2.46%	0.465%
24	13.676	1988	1993	1997	rBV3	638017	1274326	2.50%	0.471%
25	13.729	1999	2002	2008	rVB3	465054	873288	1.71%	0.323%
26	13.794	2008	2013	2021	rBV2	1716374	4144639	8.12%	1.531%
27	13.876	2021	2027	2033	rVB	2606009	4485918	8.79%	1.657%
28	13.953	2034	2040	2042	rBV5	465782	801109	1.57%	0.296%
29	13.988	2042	2046	2049	rBV2	1089308	1621170	3.18%	0.599%
30	14.023	2049	2052	2062	rVB3	1464748	3345822	6.55%	1.236%
31	14.111	2062	2067	2073	rBV3	1645852	2896866	5.67%	1.070%
32	14.188	2076	2080	2084	rVB	486988	643348	1.26%	0.238%
33	14.247	2085	2090	2093	rBV	1810054	2824372	5.53%	1.043%
34	14.335	2100	2105	2113	rBV	1509526	2340305	4.58%	0.865%
35	14.447	2118	2124	2129	rVB2	1460337	2423787	4.75%	0.895%
36	14.576	2140	2146	2151	rBV3	622136	1146311	2.25%	0.423%

LSC Area Percent Report

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Data File : VN078182.D
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Operator : JC\MD
Sample : 03172-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1578

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\82N060623W.M
Title : SW846 8260

37	14.629	2151	2155	2158	rBV	1120418	1845718	3.62%	0.682%
38	14.658	2158	2160	2163	rVB2	676314	713149	1.40%	0.263%
39	14.700	2163	2167	2170	rVB	1235327	1673318	3.28%	0.618%
40	14.770	2170	2179	2188	rVB2	4799604	9941391	19.47%	3.672%
41	14.876	2188	2197	2202	rBV3	3034121	5494632	10.76%	2.030%
42	14.941	2202	2208	2210	rBV3	1875381	3754657	7.35%	1.387%
43	15.058	2218	2228	2233	rBV3	2954960	8352548	16.36%	3.085%
44	15.105	2233	2236	2246	rVB3	927301	1926154	3.77%	0.712%
45	15.217	2249	2255	2261	rVB	1764273	3178628	6.23%	1.174%
46	15.282	2262	2266	2268	rBV4	453313	681772	1.34%	0.252%
47	15.323	2268	2273	2278	rBV3	1414577	2720993	5.33%	1.005%
48	15.464	2287	2297	2304	rBV5	2519689	7253850	14.21%	2.680%
49	15.605	2316	2321	2323	rBV5	559875	985342	1.93%	0.364%
50	15.641	2324	2327	2332	rVB3	683641	987933	1.94%	0.365%
51	15.705	2332	2338	2342	rBV	1130743	2217765	4.34%	0.819%
52	15.752	2342	2346	2350	rBV2	1072994	1650876	3.23%	0.610%
53	15.952	2371	2380	2387	rBV4	1452685	3653031	7.16%	1.349%
54	16.029	2388	2393	2397	rVV	264130	512265	1.00%	0.189%
55	16.129	2403	2410	2412	rBV5	688238	1481636	2.90%	0.547%
56	16.170	2412	2417	2427	rVB	2681073	5541057	10.85%	2.047%
57	16.264	2428	2433	2438	rVB3	356132	609734	1.19%	0.225%
58	16.341	2439	2446	2453	rBV4	726436	1978308	3.87%	0.731%
59	16.488	2462	2471	2481	rBV	7245982	17940402	35.14%	6.627%
60	16.717	2500	2510	2516	rBV2	1845824	4604704	9.02%	1.701%

Sum of corrected areas: 270710326

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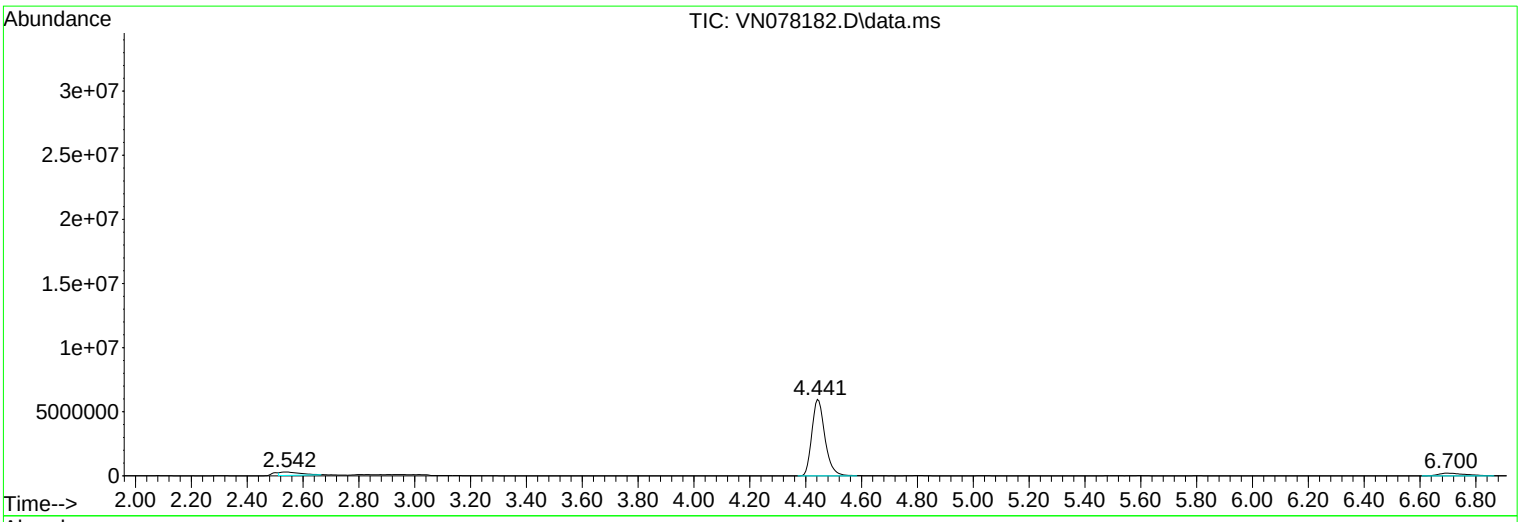
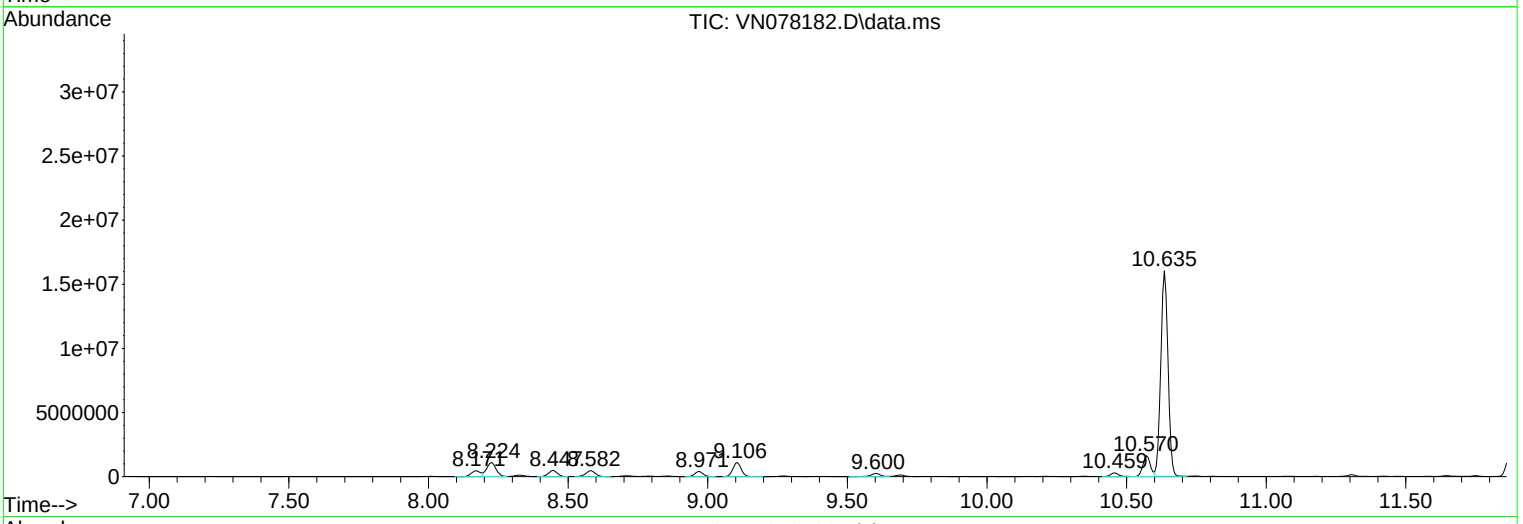
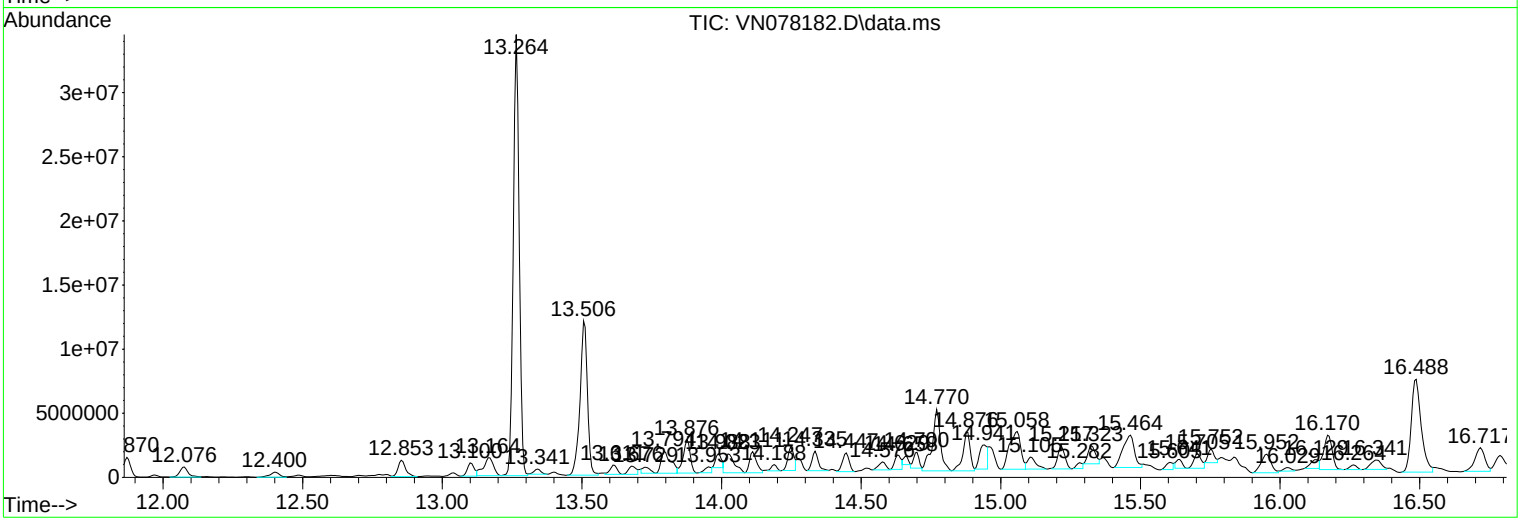
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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







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ClientSampleId :
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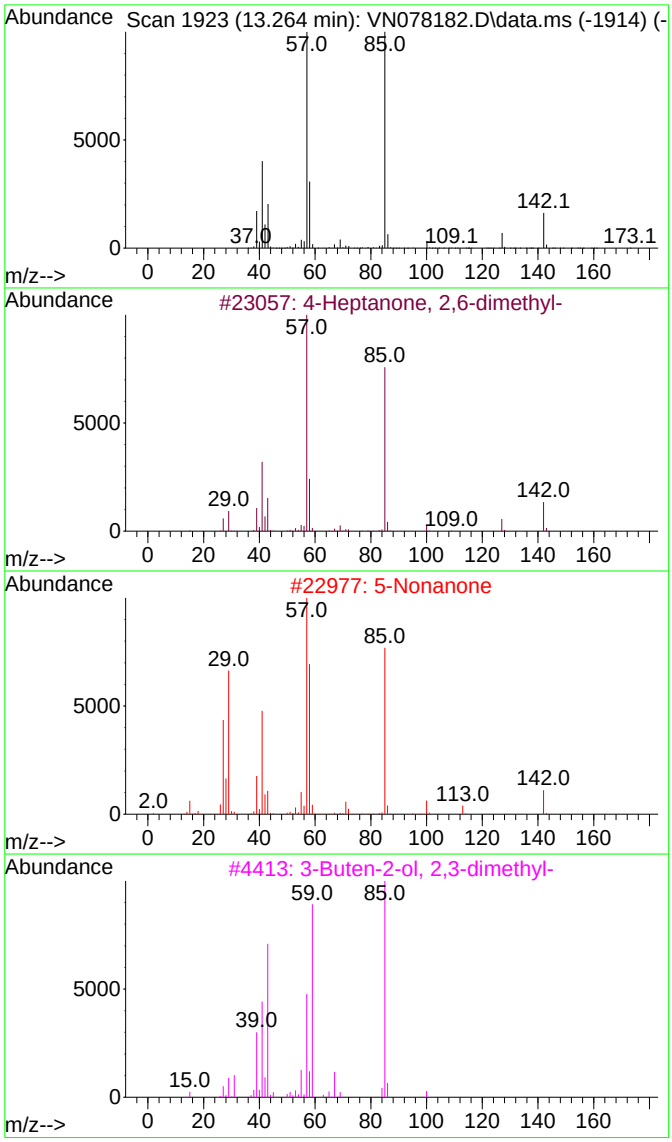
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

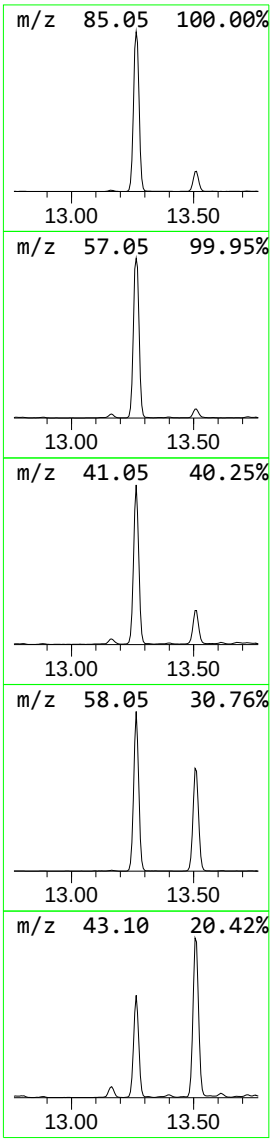
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.264	615.90 ug/l	51053400	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2	5-Nonanone	142	C9H18O	000502-56-7	64
3	3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	59
4	t-Butyl isobutyl ketone	142	C9H18O	014705-50-1	50
5	2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	50





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Instrument :
MSVOA_N
ClientSampleId :
BUR-1578

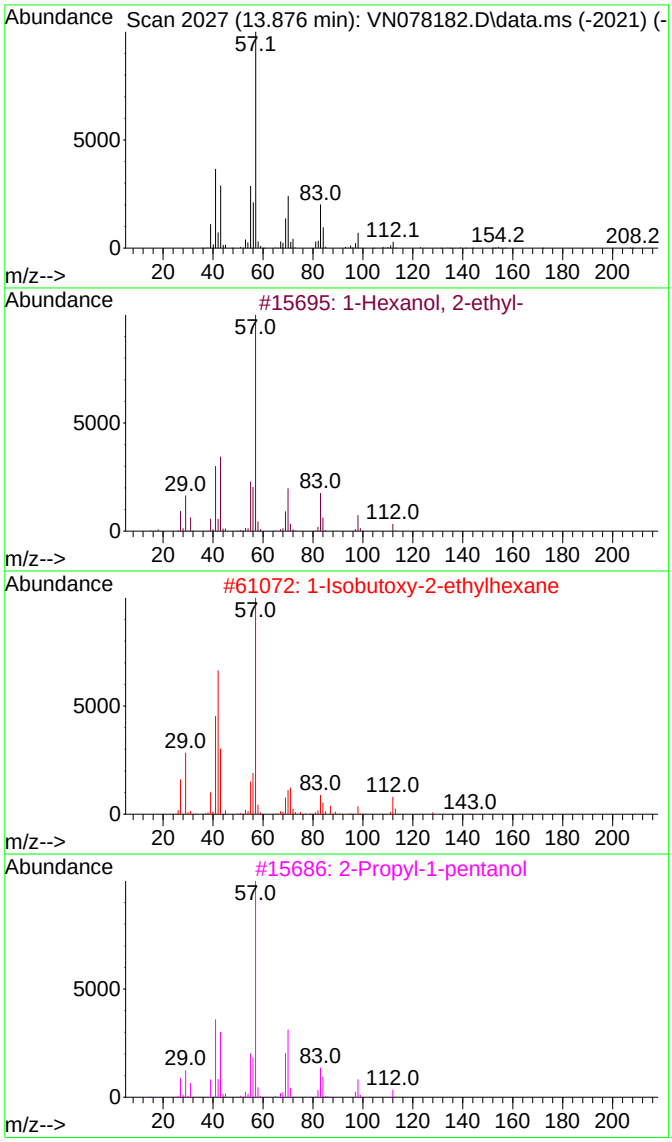
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

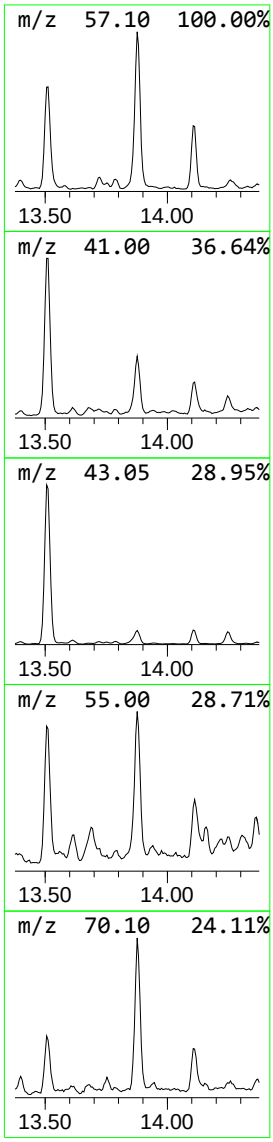
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	54.12 ug/l	4485920	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	72
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4	Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	50
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50





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Operator : JC\MD
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1578

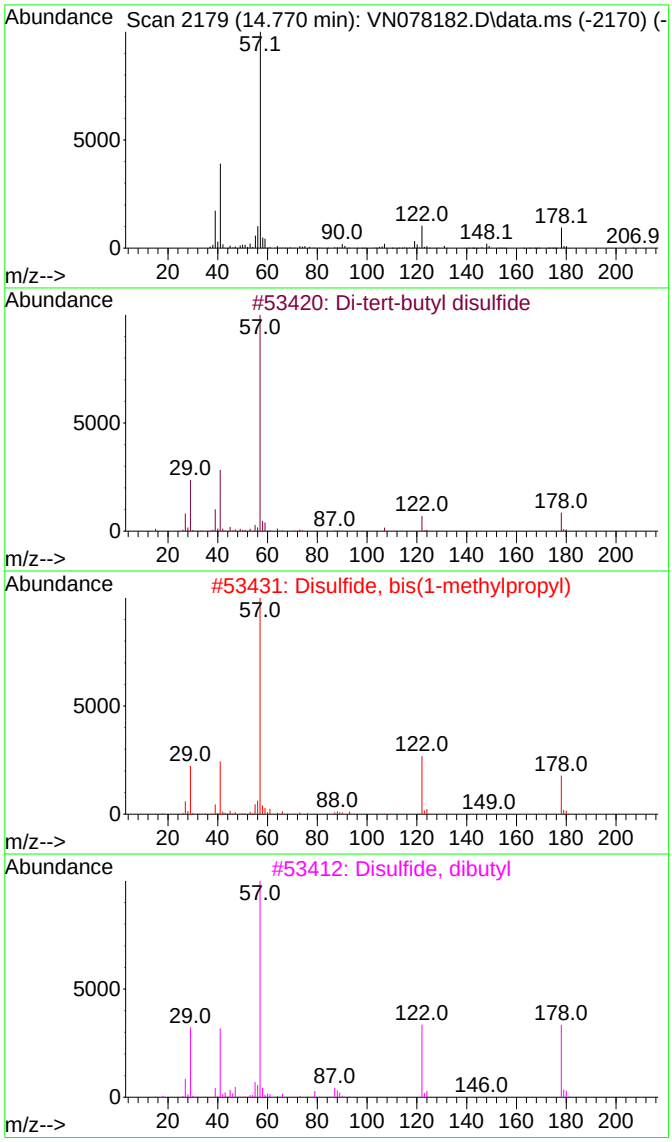
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

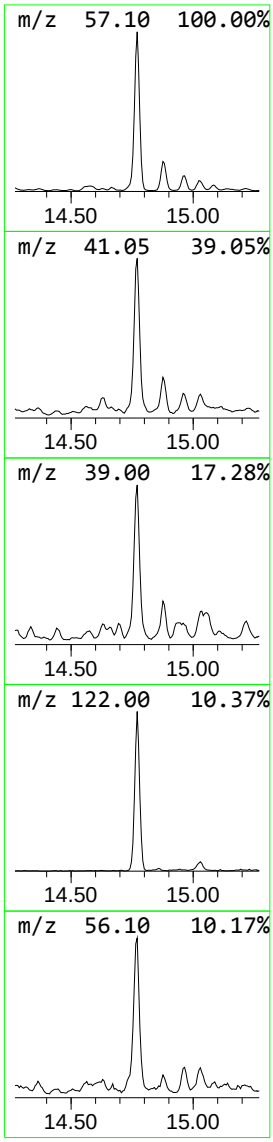
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Di-tert-butyl disulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.770	119.93 ug/l	9941390	1,4-Dichlorobenzene-d4	13.800

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	64
3	Disulfide, dibutyl	178	C8H18S2	000629-45-8	49
4	Disulfide, bis(2-methylpropyl)	178	C8H18S2	001518-72-5	47
5	Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	43





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Instrument :
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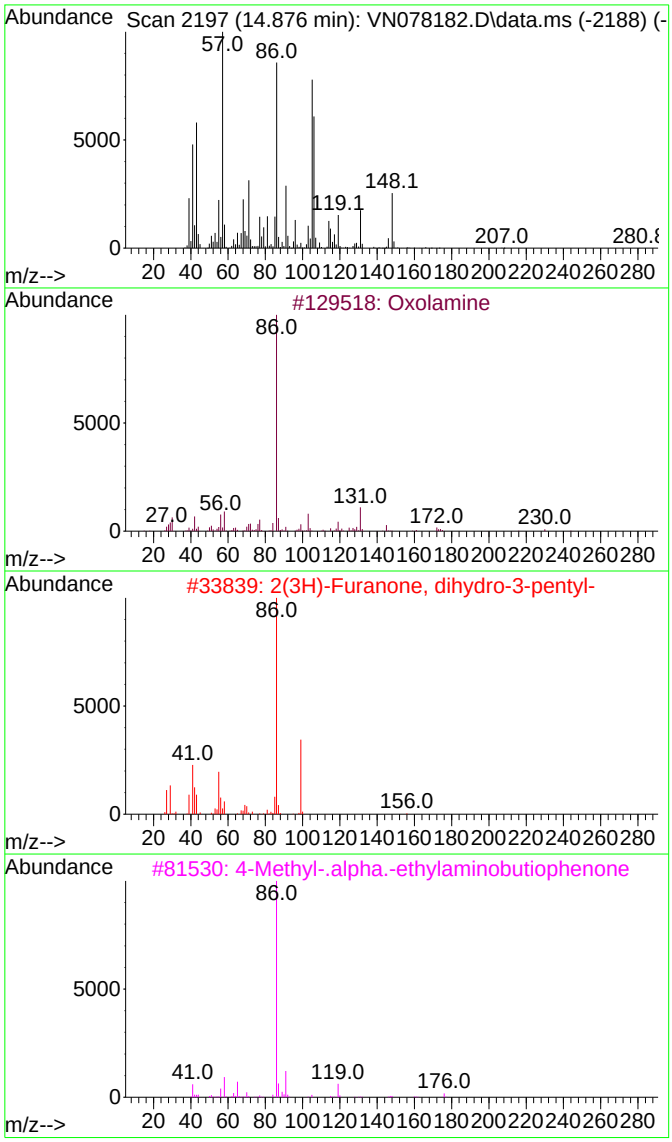
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

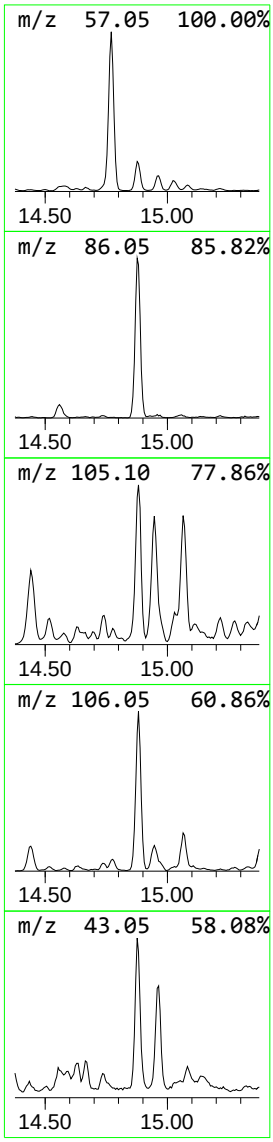
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 unknown14.876 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.876	66.29 ug/l	5494630	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxolamine	245	C14H19N3O	000959-14-8	35
2	2(3H)-Furanone, dihydro-3-pentyl-	156	C9H16O2	051849-71-9	30
3	4-Methyl-.alpha.-ethylaminobutio...	205	C13H19NO	018268-19-4	27
4	N,N-Diethyl-2-aminoethanol	117	C6H15NO	000100-37-8	25
5	1,2-Ethanediamine, N,N-diethyl-	116	C6H16N2	000100-36-7	22





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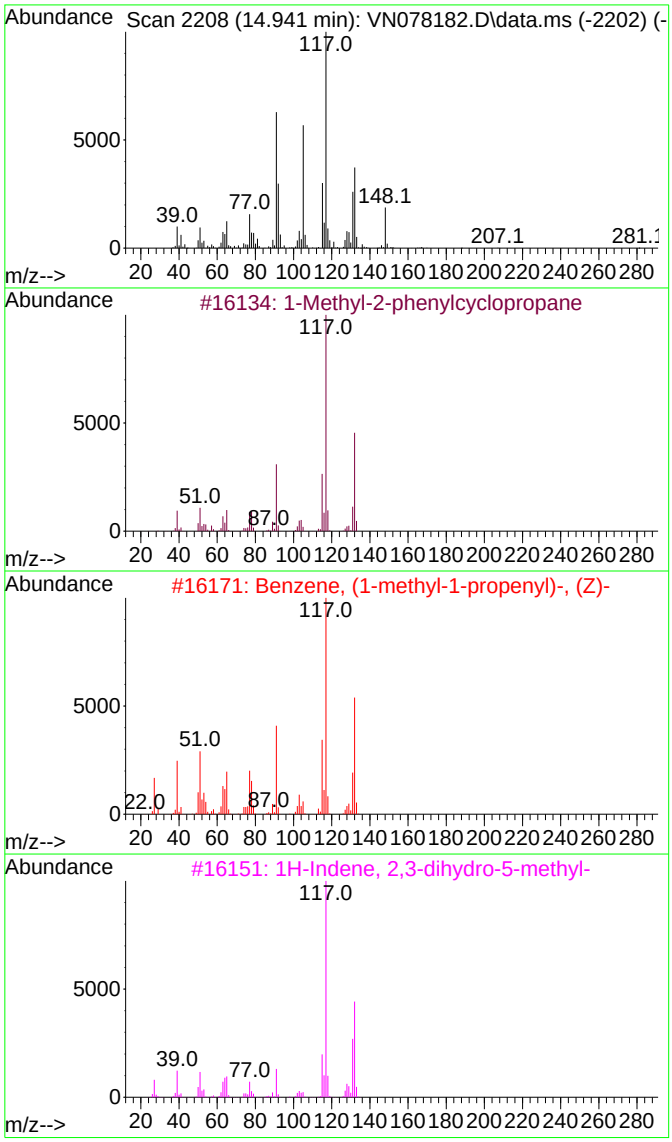
Quant Title : SW846 8260

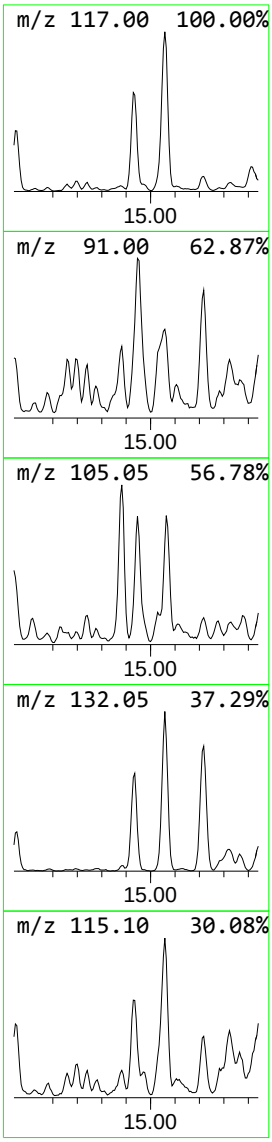
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Methyl-2-phenylcyclopropane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.941	45.30 ug/l	3754660	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	93
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	90
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	81
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	76
5	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	76





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Instrument :
MSVOA_N
ClientSampleId :
BUR-1578

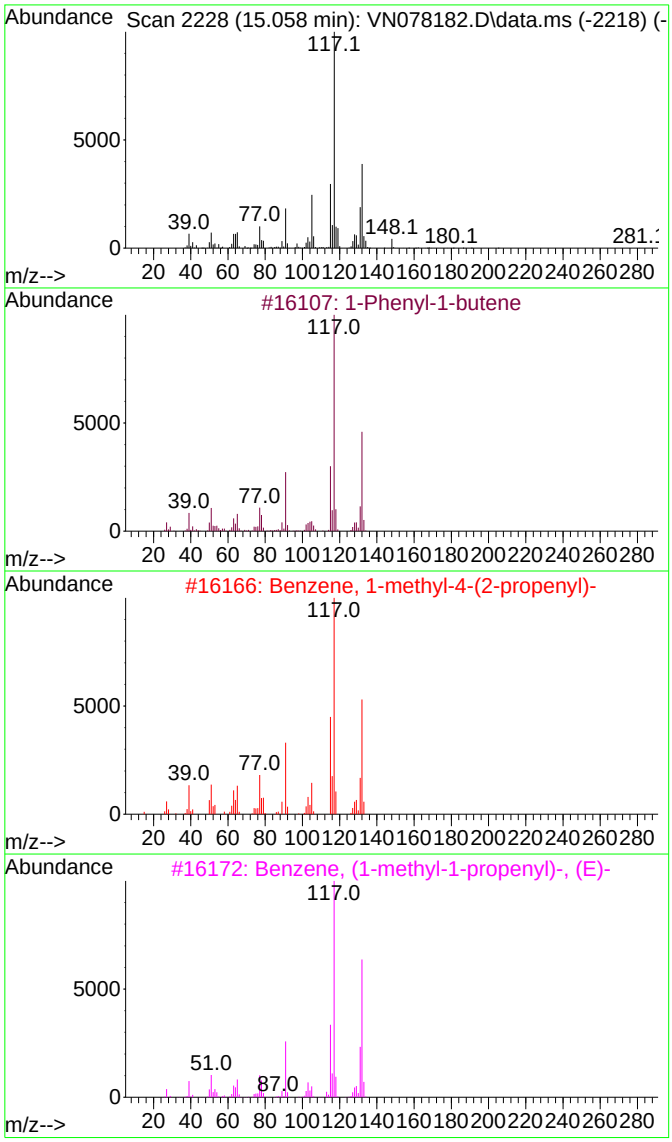
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

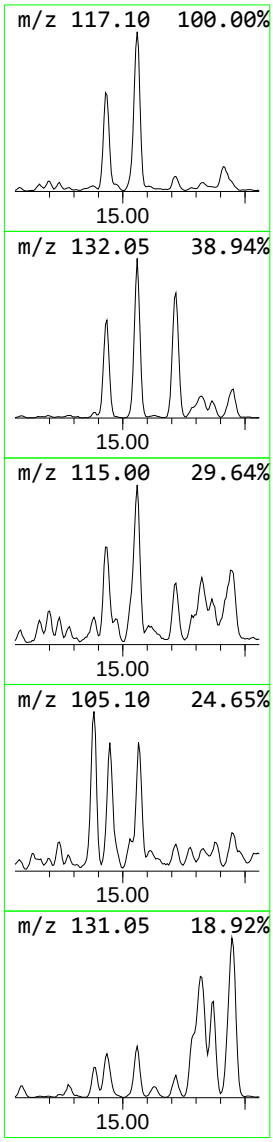
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Phenyl-1-butene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.058	100.76 ug/l	8352550	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	94
2	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	91
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90
4	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
5	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	89





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
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Quant Title : SW846 8260

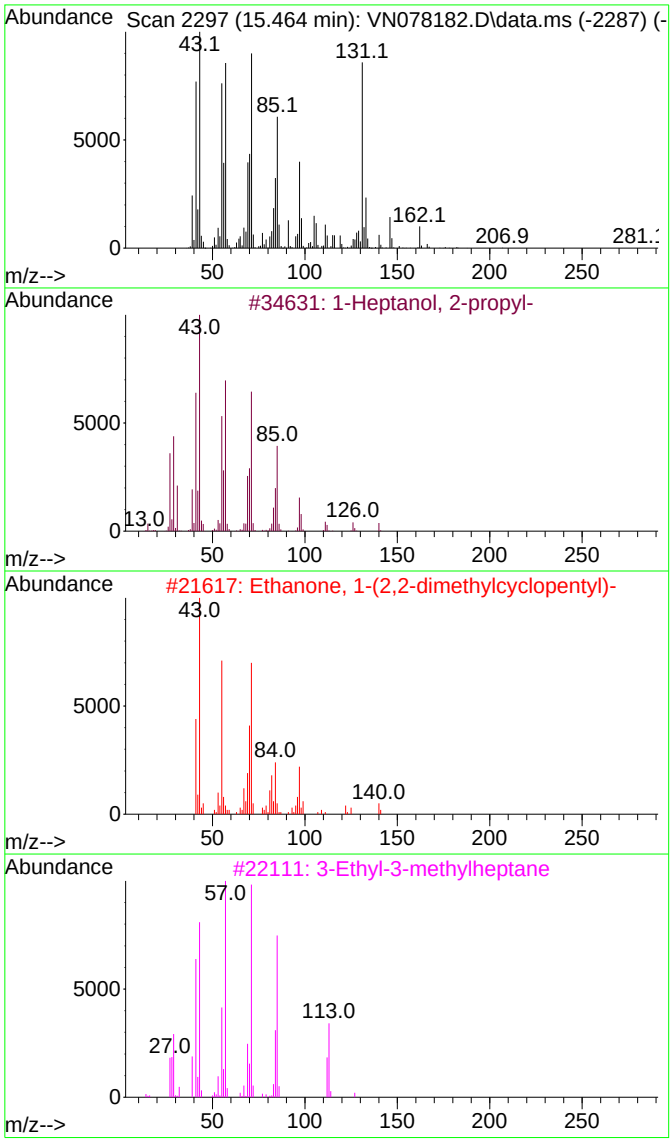
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

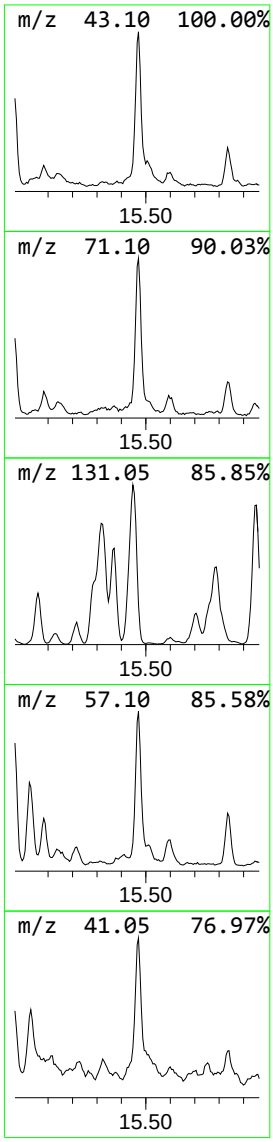
****

Peak Number 7 unknown15.464 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.464	87.51 ug/l	7253850	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	49
2	Ethanone, 1-(2,2-dimethylcyclope...	140	C9H16O	003664-75-3	30
3	3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	27
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	27
5	Cycloheptane, methyl-	112	C8H16	004126-78-7	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078182.D
Acq On : 13 Jun 2023 13:36
Operator : JC\MD
Sample : 03172-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1578

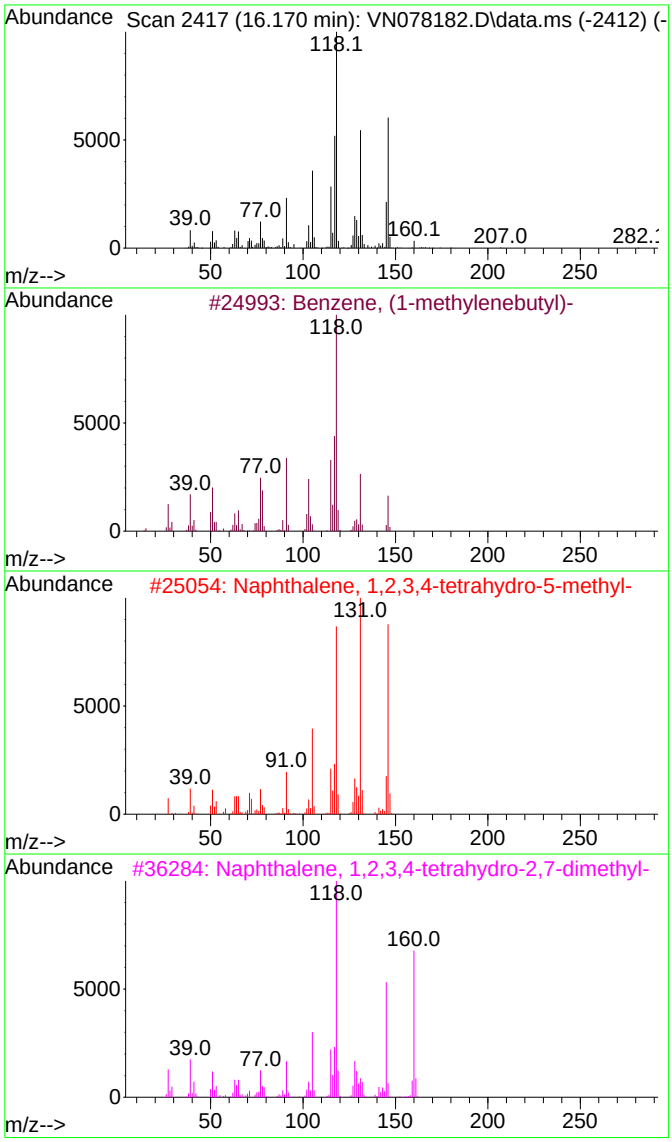
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

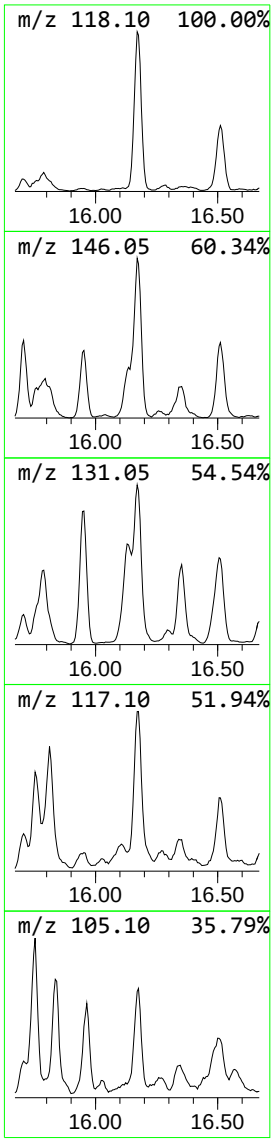
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, (1-methylenebutyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	66.85 ug/l	5541060	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	83
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	81
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	53
4	5H-Benzocycloheptene,6,7,8,9-tet...	146	C11H14	001075-16-7	53
5	3-Phenylcyclopentanecarboxylic acid	190	C12H14O2	091495-75-9	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078182.D
Acq On : 13 Jun 2023 13:36
Operator : JC\MD
Sample : 03172-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1578

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

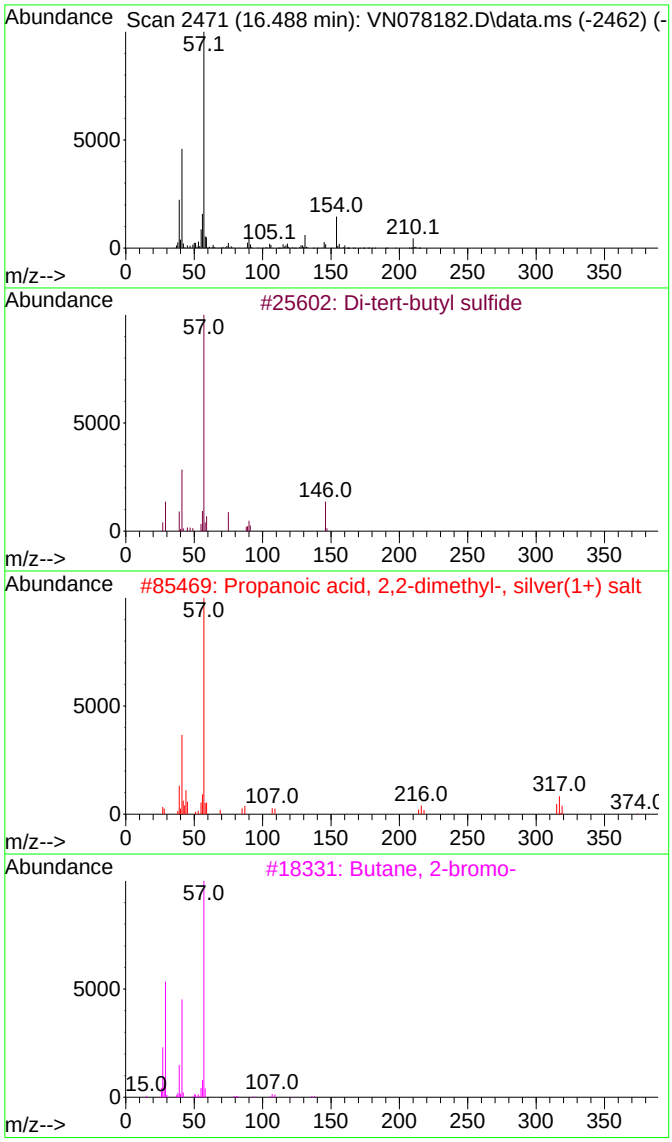
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

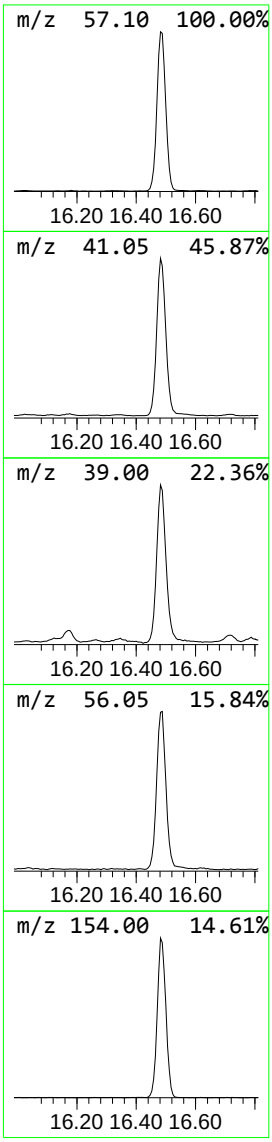
****

Peak Number 9 unknown16.488 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.488	216.43 ug/l	17940400	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-tert-butyl sulfide	146	C8H18S	000107-47-1	49
2	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	32
3	Butane, 2-bromo-	136	C4H9Br	000078-76-2	25
4	Butane, 1-bromo-	136	C4H9Br	000109-65-9	25
5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078182.D
Acq On : 13 Jun 2023 13:36
Operator : JC\MD
Sample : 03172-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1578

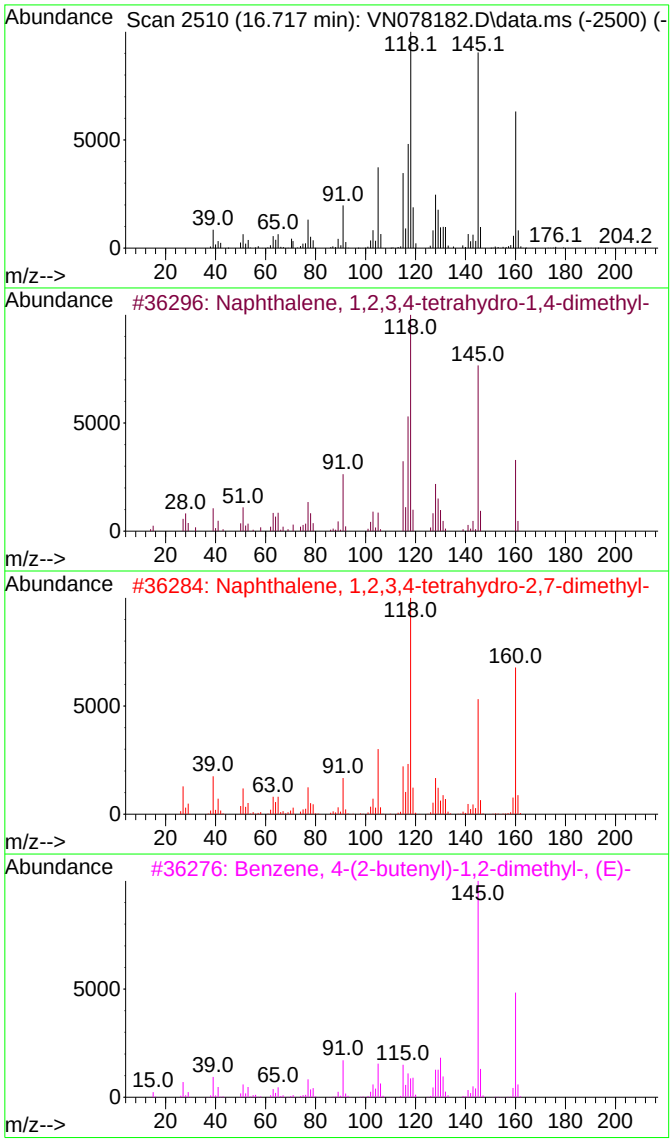
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

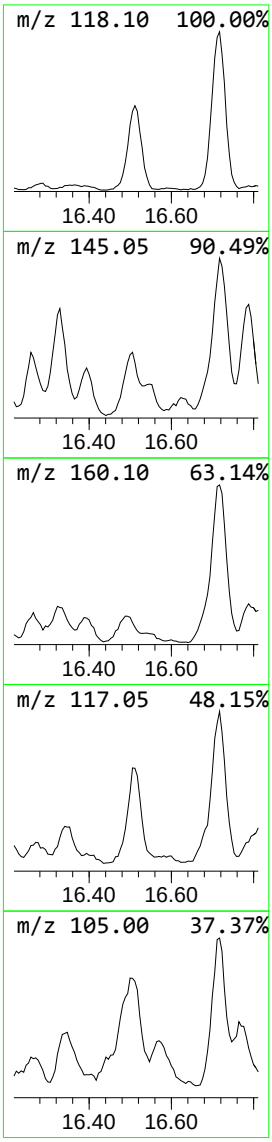
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.717	55.55 ug/l	4604700	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	95
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	81
3	Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	78
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	70
5	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078182.D
Acq On : 13 Jun 2023 13:36
Operator : JC\MD
Sample : 03172-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1578

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.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
4-Heptanone, 2,...	13.264	615.9	ug/l	51053400	4	13.800	4144640	50.0
1-Hexanol, 2-et...	13.876	54.1	ug/l	4485920	4	13.800	4144640	50.0
Di-tert-butyl d...	14.770	119.9	ug/l	9941390	4	13.800	4144640	50.0
unknown14.876	14.876	66.3	ug/l	5494630	4	13.800	4144640	50.0
1-Methyl-2-phen...	14.941	45.3	ug/l	3754660	4	13.800	4144640	50.0
1-Phenyl-1-butene	15.058	100.8	ug/l	8352550	4	13.800	4144640	50.0
unknown15.464	15.464	87.5	ug/l	7253850	4	13.800	4144640	50.0
Benzene, (1-met...	16.170	66.8	ug/l	5541060	4	13.800	4144640	50.0
unknown16.488	16.488	216.4	ug/l	17940400	4	13.800	4144640	50.0
Naphthalene, 1,...	16.717	55.5	ug/l	4604700	4	13.800	4144640	50.0