LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060623\
Data File : VN078068.D
Acq On : 06 Jun 2023 14:01
Operator : JC\MD
Sample : 02907-01
Misc : 5.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WASTE

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\82N051523W.M
Title : SW846 8260

Signal : TIC: VN078068.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.171	1047	1057	1062	rBV	268685	677231	1.16%	0.081%
2	8.230	1062	1067	1078	rVB	484600	1070140	1.83%	0.128%
3	8.582	1118	1127	1140	rVB	285242	632460	1.08%	0.076%
4	9.106	1206	1216	1231	rVB	671680	1409086	2.41%	0.168%
5	9.600	1287	1300	1317	rBV	260756	689219	1.18%	0.082%
6	10.212	1398	1404	1417	rVB2	281287	698293	1.19%	0.084%
7	10.347	1417	1427	1441	rBV2	259899	606389	1.04%	0.073%
8	10.571	1458	1465	1471	rBV	1542518	2978882	5.09%	0.356%
9	10.635	1471	1476	1482	rVB2	356482	772429	1.32%	0.092%
10	10.747	1489	1495	1505	rVB	910003	1730885	2.96%	0.207%
11	11.012	1531	1540	1547	rBV2	424250	897214	1.53%	0.107%
12	11.423	1601	1610	1614	rVV	944912	1997643	3.42%	0.239%
13	11.476	1614	1619	1625	rVB	817890	1569502	2.68%	0.188%
14	11.576	1631	1636	1640	rBV2	452311	689035	1.18%	0.082%
15	11.647	1640	1648	1652	rBV2	1069902	2243752	3.84%	0.268%
16	11.747	1660	1665	1671	rVB	1063522	1743543	2.98%	0.208%
17	11.870	1681	1686	1692	rBV	886927	1591126	2.72%	0.190%
18	11.970	1697	1703	1707	rBV	1122014	1978583	3.38%	0.237%
19	12.076	1712	1721	1726	rBV	9264514	17459565	29.86%	2.088%
20	12.159	1731	1735	1741	rVB2	1137137	2061700	3.53%	0.247%
21	12.406	1764	1777	1785	rBV2	4595618	12393495	21.19%	1.482%
22	12.488	1785	1791	1795	rVB2	973010	1823335	3.12%	0.218%
23	12.541	1795	1800	1802	rBV2	621554	1015332	1.74%	0.121%
24	12.623	1802	1814	1823	rVV6	1880385	7512689	12.85%	0.898%
25	12.700	1823	1827	1832	rVV	1284555	2449942	4.19%	0.293%
26	12.747	1832	1835	1837	rVV3	582031	963851	1.65%	0.115%
27	12.776	1837	1840	1842	rVV2	929277	1358210	2.32%	0.162%
28	12.800	1842	1844	1849	rVB2	1066437	1372249	2.35%	0.164%
29	12.859	1849	1854	1856	rBV2	1109474	1909771	3.27%	0.228%
30	12.882	1856	1858	1863	rVB	823319	980257	1.68%	0.117%
31	12.941	1863	1868	1872	rBV3	639718	993769	1.70%	0.119%
32	13.041	1877	1885	1889	rBV	3540071	6574845	11.24%	0.786%
33	13.100	1889	1895	1899	rBV	12005952	20015861	34.23%	2.393%
34	13.135	1899	1901	1903	rVV	3958744	5327691	9.11%	0.637%
35	13.170	1903	1907	1914	rVV3	10281306	21228664	36.30%	2.538%
36	13.229	1914	1917	1923	rVB2	1156565	1847161	3.16%	0.221%

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Integrator: RTE
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Title : SW846 8260

37	13.341	1923	1936	1942	rBV	6908793	13878466	23.73%	1.660%
38	13.423	1943	1950	1955	rVB4	1212119	3254179	5.56%	0.389%
39	13.488	1955	1961	1971	rBV	24980495	39134285	66.92%	4.680%
40	13.623	1979	1984	1988	rVB2	2706900	4420985	7.56%	0.529%
41	13.676	1988	1993	1999	rBV2	5195294	9642071	16.49%	1.153%
42	13.729	1999	2002	2009	rVB3	1795549	3210500	5.49%	0.384%
43	13.823	2009	2018	2023	rBV	8767480	16472015	28.17%	1.970%
44	13.959	2031	2041	2042	rBV4	4021330	7503883	12.83%	0.897%
45	13.988	2042	2046	2050	rVV2	12496438	22308105	38.15%	2.668%
46	14.029	2050	2053	2058	rVB2	6641767	11103191	18.99%	1.328%
47	14.117	2063	2068	2075	rBV4	7042071	13957575	23.87%	1.669%
48	14.188	2075	2080	2085	rBV	6065191	8951867	15.31%	1.070%
49	14.247	2085	2090	2093	rBV	6605955	10857119	18.57%	1.298%
50	14.282	2093	2096	2100	rVB	7024090	9808099	16.77%	1.173%
51	14.335	2100	2105	2111	rVB	11145978	17125736	29.28%	2.048%
52	14.400	2111	2116	2119	rBV	2240655	3907150	6.68%	0.467%
53	14.447	2119	2124	2130	rVB2	13406621	22258087	38.06%	2.662%
54	14.523	2133	2137	2142	rVB2	2242819	3450984	5.90%	0.413%
55	14.582	2142	2147	2151	rBV2	4392529	6693544	11.45%	0.800%
56	14.635	2151	2156	2158	rBV	4941985	8223538	14.06%	0.983%
57	14.659	2158	2160	2164	rVV2	3980837	5026796	8.60%	0.601%
58	14.700	2164	2167	2171	rVB	7445821	9102161	15.56%	1.088%
59	14.741	2171	2174	2178	rVB	6383061	7461856	12.76%	0.892%
60	14.782	2178	2181	2189	rVB3	4653640	9482679	16.21%	1.134%
61	14.882	2189	2198	2202	rBV3	9622811	19309924	33.02%	2.309%
62	14.941	2202	2208	2219	rVB4	12551923	40636787	69.49%	4.859%
63	15.058	2219	2228	2233	rBV4	22374427	58481070	100.00%	6.993%
64	15.111	2233	2237	2247	rVB2	4745478	10448301	17.87%	1.249%
65	15.217	2249	2255	2262	rVB	15196089	25601789	43.78%	3.061%
66	15.288	2262	2267	2269	rBV4	3783319	6617876	11.32%	0.791%
67	15.323	2269	2273	2278	rBV3	7285534	12820220	21.92%	1.533%
68	15.447	2287	2294	2300	rVB3	11724501	27149366	46.42%	3.246%
69	15.606	2315	2321	2324	rBV4	3876082	8120587	13.89%	0.971%
70	15.641	2324	2327	2332	rVB3	4711994	7347516	12.56%	0.879%
71	15.706	2332	2338	2342	rBV	11187144	21835831	37.34%	2.611%
72	15.753	2342	2346	2350	rVV2	6698587	11831811	20.23%	1.415%
73	15.794	2350	2353	2358	rVB3	3052859	5659557	9.68%	0.677%
74	15.953	2371	2380	2387	rBV3	9910213	23685294	40.50%	2.832%
75	16.029	2388	2393	2398	rVV	2039003	3861417	6.60%	0.462%
76	16.135	2399	2411	2412	rVV3	5998891	15071748	25.77%	1.802%

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WASTE

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Title : SW846 8260

77	16.176	2412	2418	2427	rVB	21570855	45079877	77.08%	5.391%
78	16.264	2428	2433	2439	rBV4	2722361	5293372	9.05%	0.633%
79	16.347	2439	2447	2454	rBV3	5054861	13616719	23.28%	1.628%
80	16.511	2464	2475	2493	rBV3	12424570	37291050	63.77%	4.459%
81	16.723	2499	2511	2517	rBV2	14338861	38011599	65.00%	4.545%

Sum of corrected areas: 836270381

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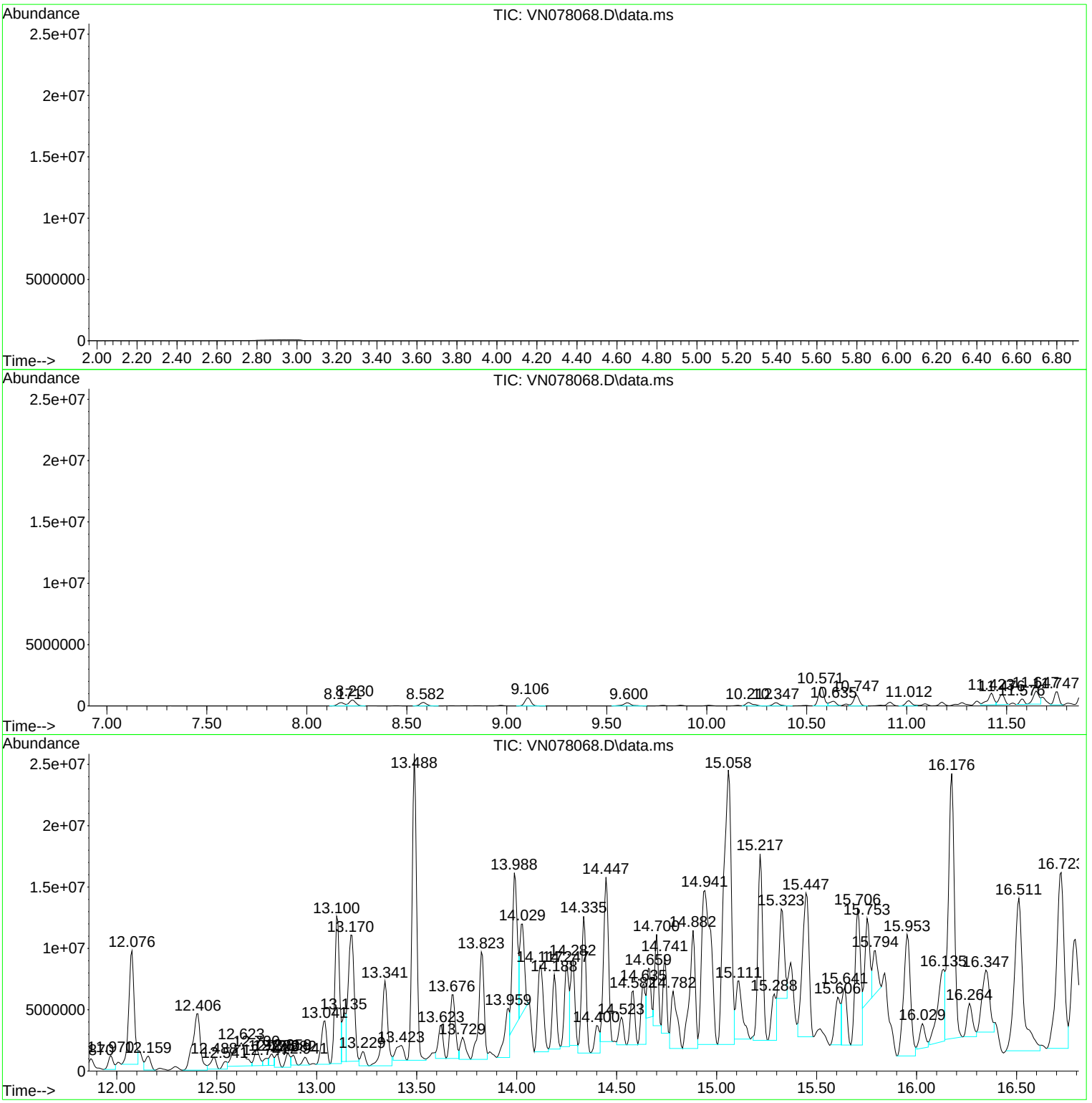
WASTE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060623\
Data File : VN078068.D
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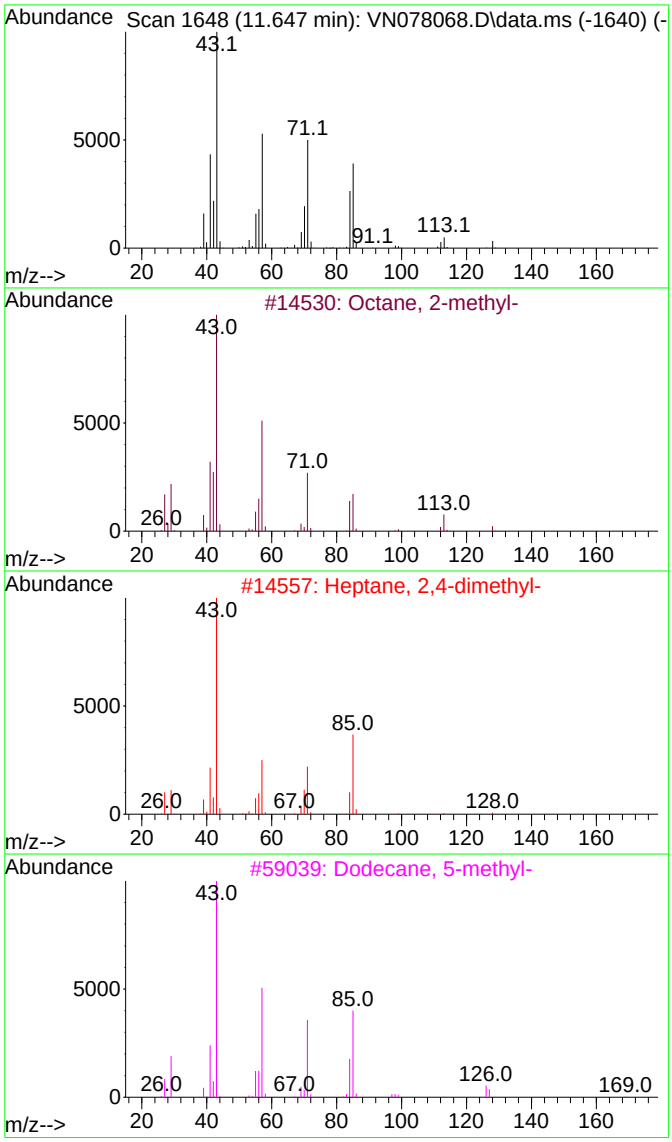
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

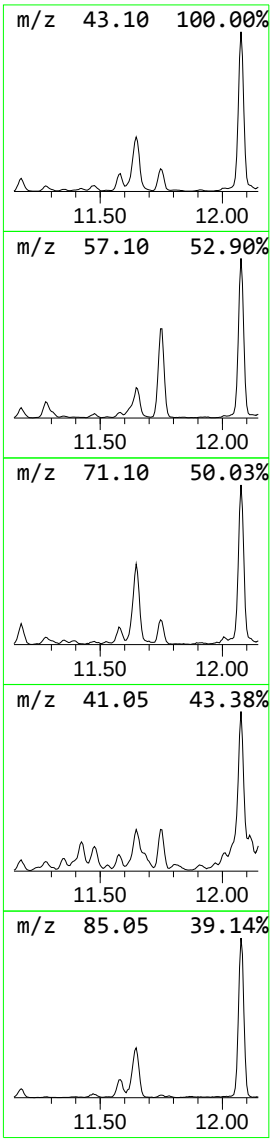
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Octane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.647	70.51 ug/l	2243750	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-	128	C9H20	003221-61-2	76
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72
3	Dodecane, 5-methyl-	184	C13H28	017453-93-9	59
4	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5	Octane	114	C8H18	000111-65-9	58





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Instrument :
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ClientSampleId :
WASTE

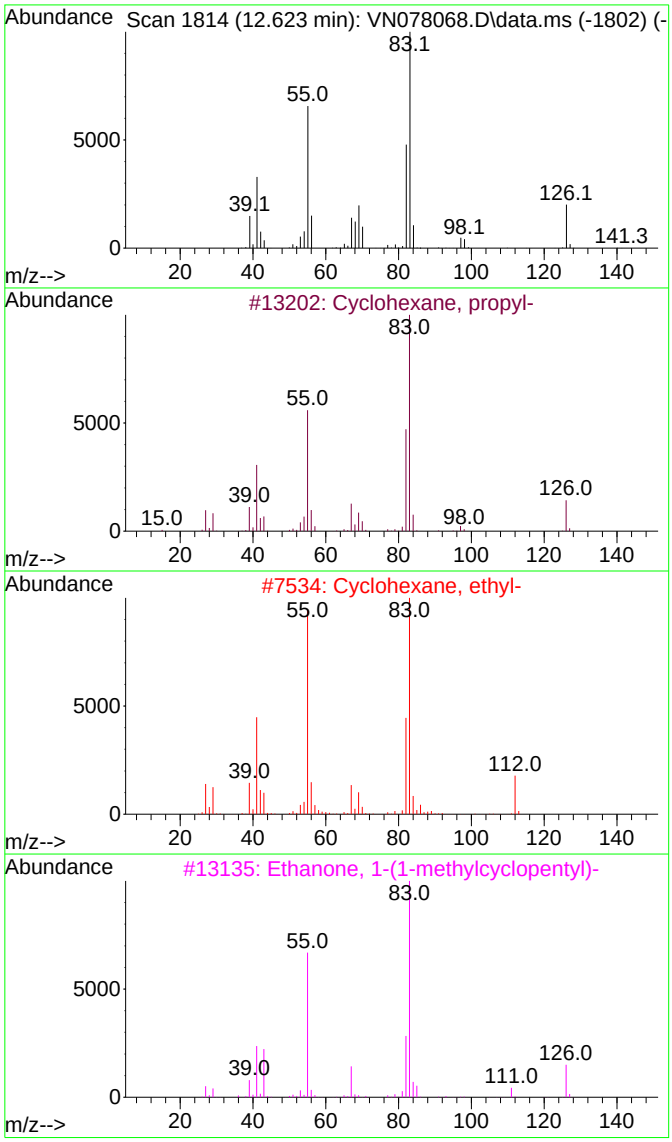
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

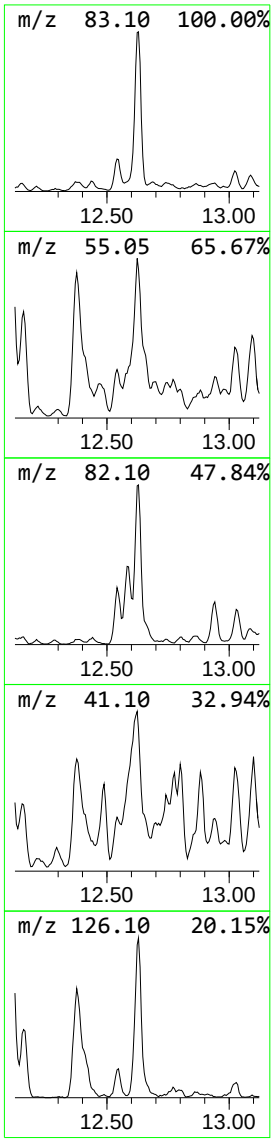
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclohexane, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.623	236.08 ug/l	7512690	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	90
2	Cyclohexane, ethyl-	112	C8H16	001678-91-7	59
3	Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	58
4	Cyclohexanone, 2,3-dimethyl-	126	C8H14O	013395-76-1	52
5	Cyclohexane, octyl-	196	C14H28	001795-15-9	50





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Quant Title : SW846 8260

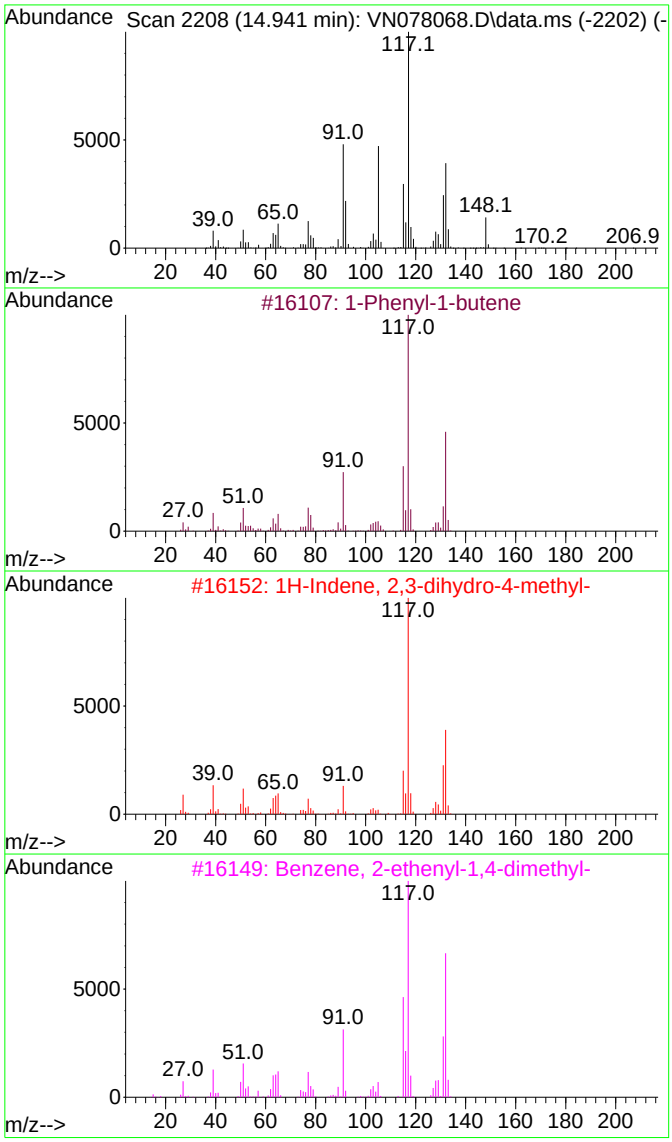
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

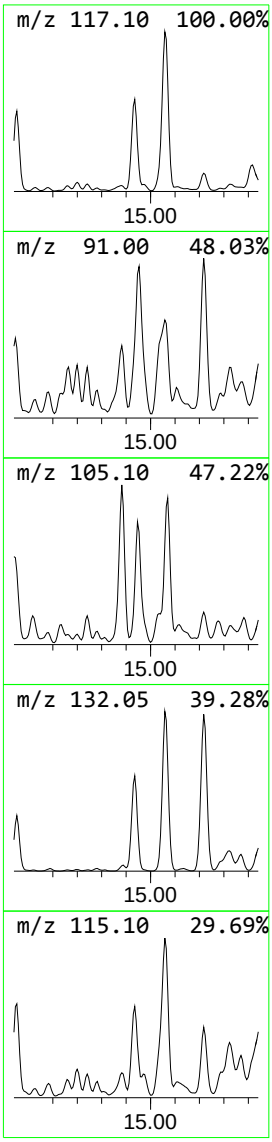
****

Peak Number 3 1-Phenyl-1-butene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.941	123.35 ug/l	40636800	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	93
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	91
3	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
4	Azulene, 1,2,3,3a-tetrahydro-	132	C10H12	033877-87-1	83
5	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	81





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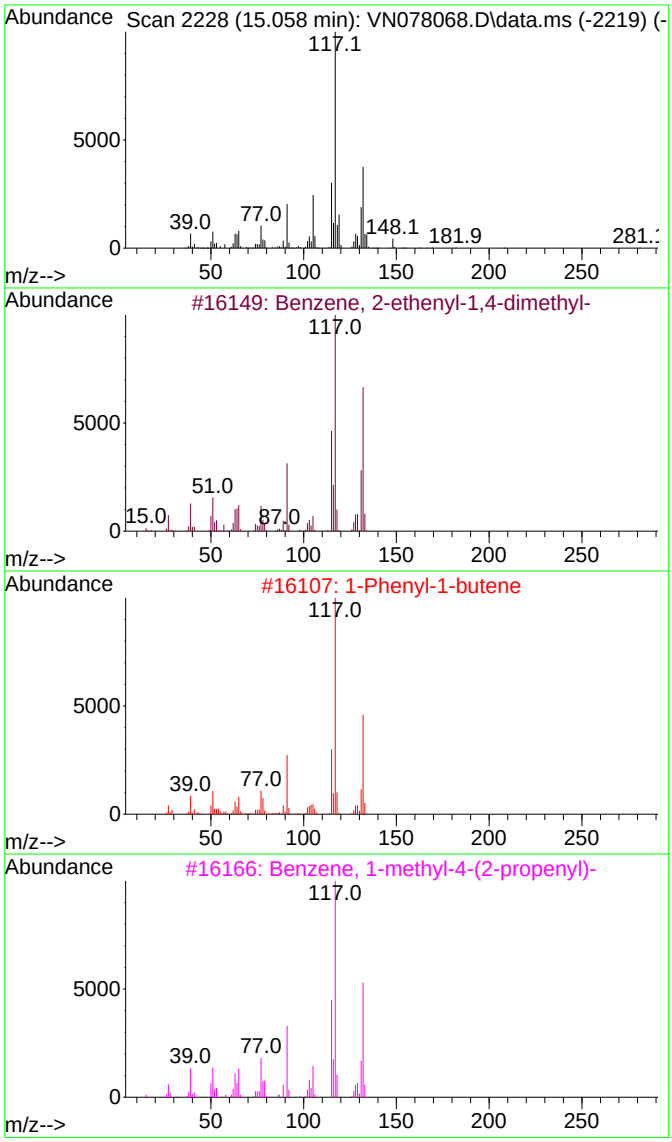
Quant Title : SW846 8260

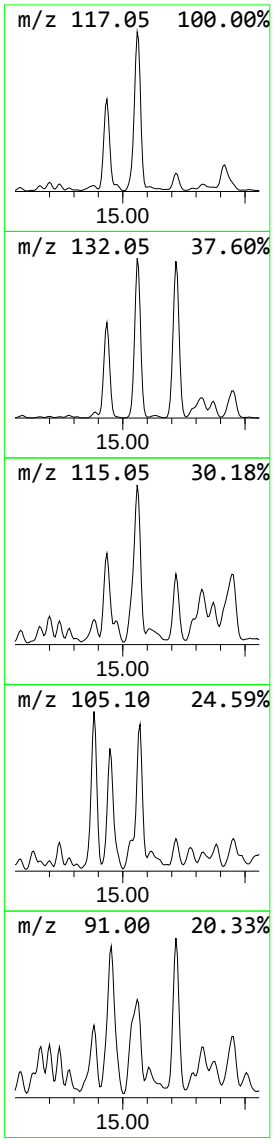
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.059	177.52 ug/l	58481100	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	94
3	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	90
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	89
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	81





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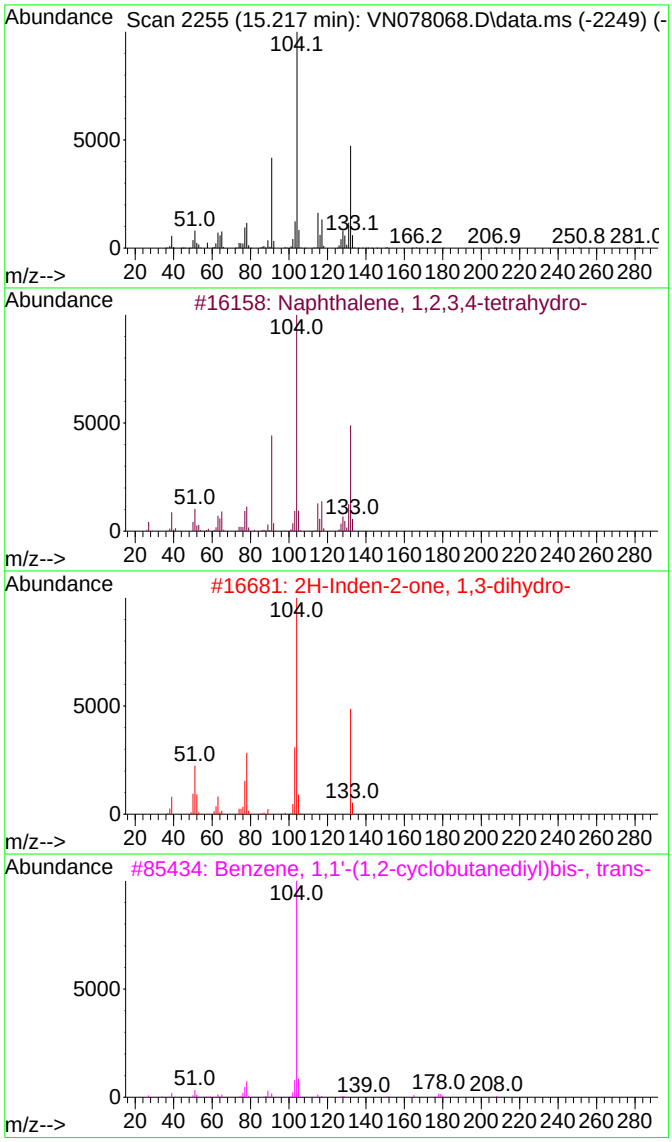
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

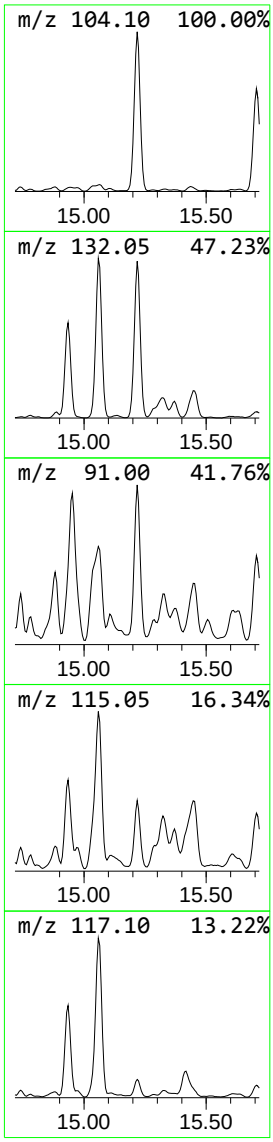
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.217	77.71 ug/l	25601800	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	97
2	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	58
3	Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	020071-09-4	38
4	Benzoic acid, 2-phenylethyl ester	226	C15H14O2	000094-47-3	38
5	Benzene, 3-cyclohexen-1-yl-	158	C12H14	004994-16-5	38





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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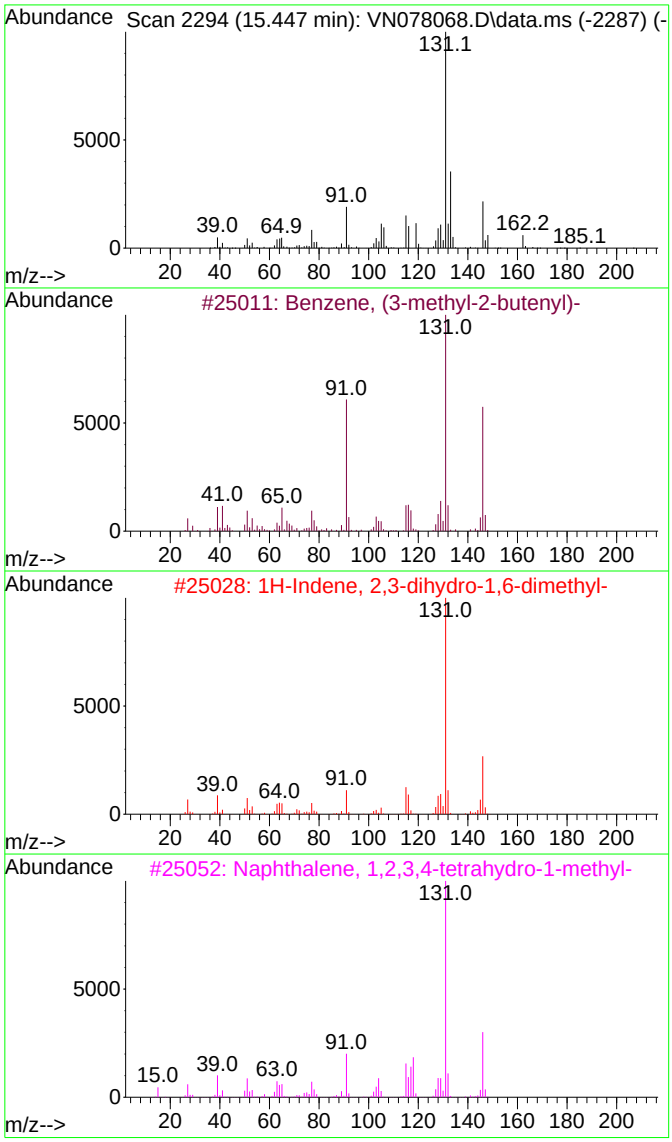
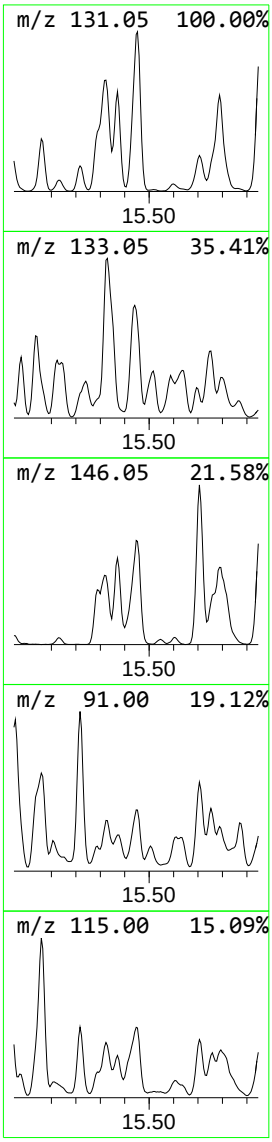
****
Peak Number 6 Benzene, (3-methyl-2-butenyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.447	82.41 ug/l	27149400	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	76
2	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	76
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	76
4	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	76
5	1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	76





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Data File : VN078068.D
Acq On : 06 Jun 2023 14:01
Operator : JC\MD
Sample : 02907-01
Misc : 5.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WASTE

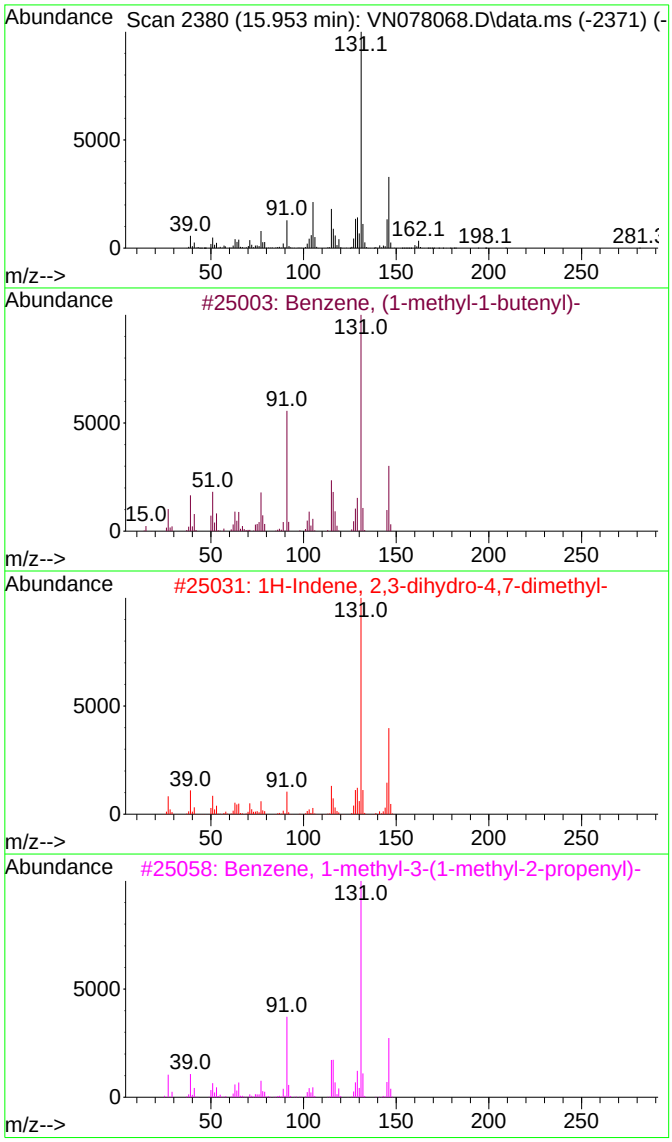
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

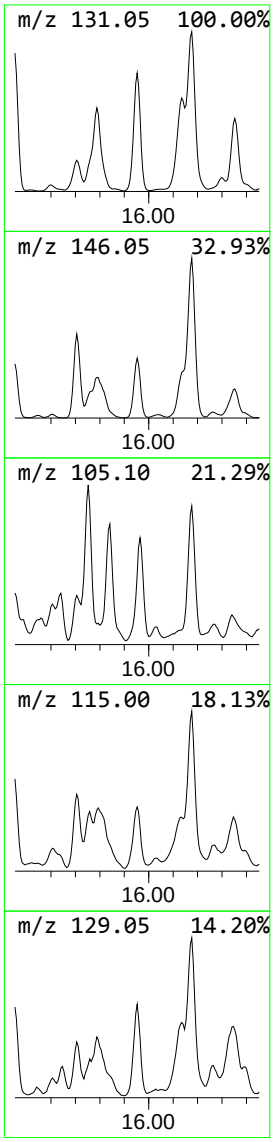
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, (1-methyl-1-butenyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.953	71.90 ug/l	23685300	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	93
2	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	91
3	Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	87
4	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	87
5	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	87





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Data File : VN078068.D
Acq On : 06 Jun 2023 14:01
Operator : JC\MD
Sample : 02907-01
Misc : 5.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WASTE

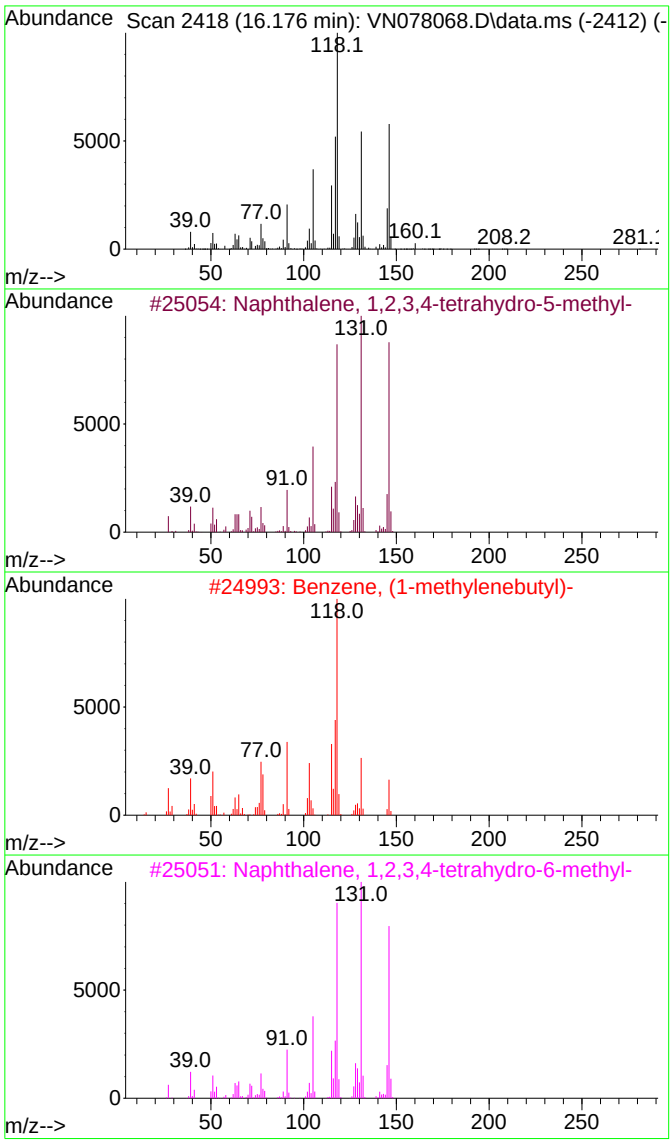
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

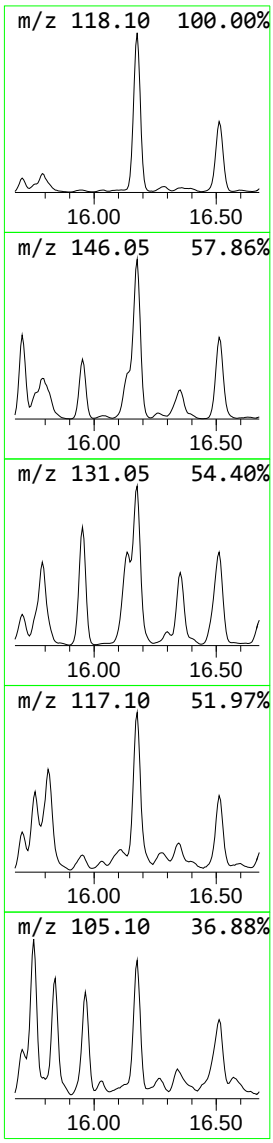
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.176	136.84 ug/l	45079900	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	90
2	Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	86
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	64
4	5H-Benzocycloheptene,6,7,8,9-tet...	146	C11H14	001075-16-7	58
5	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	55





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Data File : VN078068.D
Acq On : 06 Jun 2023 14:01
Operator : JC\MD
Sample : 02907-01
Misc : 5.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WASTE

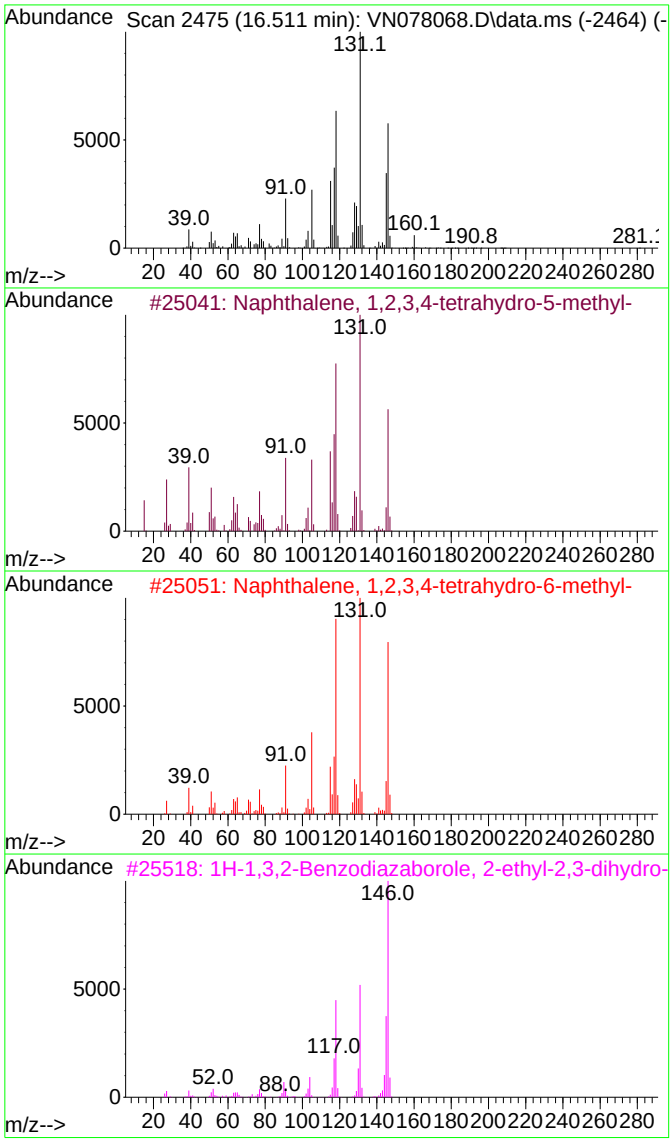
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

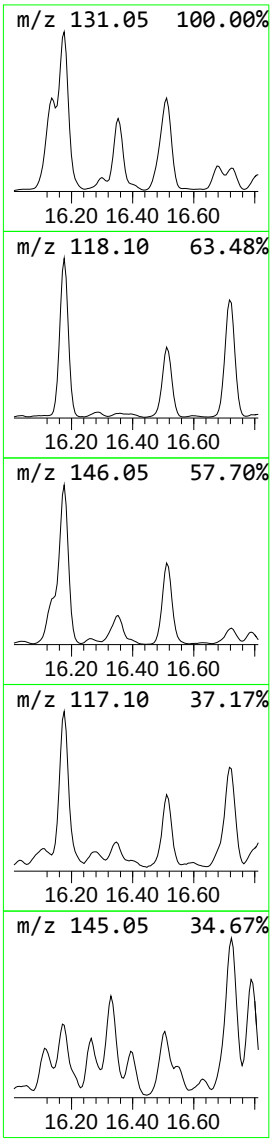
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.511	113.19 ug/l	37291100	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	90
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	83
3	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	74
4	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	70
5	Benzene, (1,1-dimethyl-2-propenyl)-	146	C11H14	018321-36-3	60





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Acq On : 06 Jun 2023 14:01
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Misc : 5.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WASTE

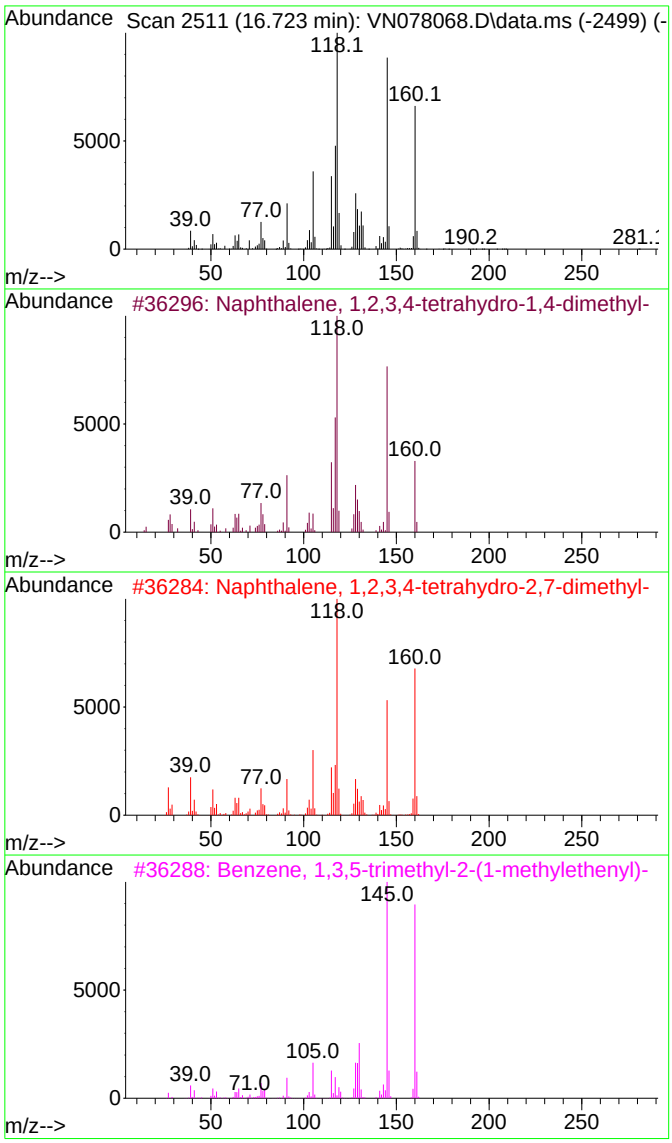
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

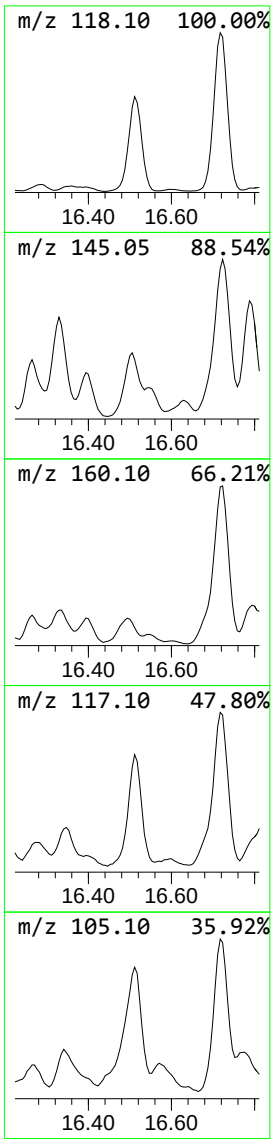
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.723	115.38 ug/l	38011600	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	97
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	90
3	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	70
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	70
5	Benzene, 1,2,4-trimethyl-5-(1-me...	160	C12H16	054340-84-0	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060623\
Data File : VN078068.D
Acq On : 06 Jun 2023 14:01
Operator : JC\MD
Sample : 02907-01
Misc : 5.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WASTE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.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
Octane, 2-methyl-	11.647	70.5	ug/l	2243750	3	11.871	1591130	50.0
Cyclohexane, pr...	12.623	236.1	ug/l	7512690	3	11.871	1591130	50.0
1-Phenyl-1-butene	14.941	123.3	ug/l	40636800	4	13.800	16472000	50.0
Benzene, 2-ethe...	15.059	177.5	ug/l	58481100	4	13.800	16472000	50.0
Naphthalene, 1,...	15.217	77.7	ug/l	25601800	4	13.800	16472000	50.0
Benzene, (3-met...	15.447	82.4	ug/l	27149400	4	13.800	16472000	50.0
Benzene, (1-met...	15.953	71.9	ug/l	23685300	4	13.800	16472000	50.0
Naphthalene, 1,...	16.176	136.8	ug/l	45079900	4	13.800	16472000	50.0
Naphthalene, 1,...	16.511	113.2	ug/l	37291100	4	13.800	16472000	50.0
Naphthalene, 1,...	16.723	115.4	ug/l	38011600	4	13.800	16472000	50.0