LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074968.D
Acq On : 21 Oct 2022 17:48
Operator : JC\MD
Sample : N5222-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

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\82N102022W.M
Title : SW846 8260

Signal : TIC: VN074968.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.524	71	80	89	rBV	1337312	2277517	2.56%	0.322%
2	3.248	193	203	219	rVB	3864850	9320506	10.48%	1.319%
3	3.659	262	273	290	rVB3	849709	2865950	3.22%	0.406%
4	3.865	298	308	321	rVB	353595	890149	1.00%	0.126%
5	4.153	348	357	371	rVB2	852865	2430776	2.73%	0.344%
6	4.442	392	406	419	rBV4	262519	906704	1.02%	0.128%
7	5.165	514	529	539	rBV2	372488	1330461	1.50%	0.188%
8	5.289	539	550	552	rVV2	491203	1317529	1.48%	0.186%
9	5.359	553	562	589	rVB5	1672467	9240197	10.39%	1.308%
10	5.824	624	641	659	rBV2	1772481	6163865	6.93%	0.872%
11	6.318	714	725	741	rVB3	329573	1052199	1.18%	0.149%
12	6.671	775	785	796	rVB2	321236	1013051	1.14%	0.143%
13	7.094	847	857	872	rVB3	324185	936592	1.05%	0.133%
14	7.336	888	898	918	rVV	2309008	6917643	7.78%	0.979%
15	8.012	1006	1013	1022	rVB3	464398	1134524	1.28%	0.161%
16	8.177	1030	1041	1045	rBV2	895470	2249491	2.53%	0.318%
17	8.230	1045	1050	1062	rVV4	1747419	6356856	7.15%	0.900%
18	8.336	1062	1068	1076	rVB2	881750	2181664	2.45%	0.309%
19	8.453	1076	1088	1095	rBV2	1128977	2690243	3.02%	0.381%
20	8.612	1103	1115	1126	rBV2	38667537	88965205	100.00%	12.592%
21	8.783	1126	1144	1153	rVV	13410536	33970002	38.18%	4.808%
22	8.859	1153	1157	1166	rVB2	657017	1343366	1.51%	0.190%
23	8.971	1166	1176	1189	rVB4	389557	1207712	1.36%	0.171%
24	9.106	1189	1199	1206	rBV3	2112852	4957565	5.57%	0.702%
25	9.606	1264	1284	1301	rBV3	2492657	8142805	9.15%	1.153%
26	9.782	1307	1314	1321	rVB	616366	1176102	1.32%	0.166%
27	10.018	1349	1354	1362	rVB2	674141	1396001	1.57%	0.198%
28	10.153	1372	1377	1383	rVB3	805739	1550495	1.74%	0.219%
29	10.347	1399	1410	1412	rBV5	389498	904864	1.02%	0.128%
30	10.412	1416	1421	1425	rVV	932443	1792889	2.02%	0.254%
31	10.571	1440	1448	1453	rBV	4719925	8777405	9.87%	1.242%
32	10.635	1453	1459	1468	rVV	3314425	7210102	8.10%	1.021%
33	10.735	1470	1476	1487	rVB4	826788	2279275	2.56%	0.323%
34	11.006	1513	1522	1528	rVB5	566717	1583886	1.78%	0.224%
35	11.865	1658	1668	1674	rBV2	2363316	4493686	5.05%	0.636%
36	11.965	1674	1685	1694	rVV2	36101338	61824910	69.49%	8.751%

LSC Area Percent Report

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Operator : JC\MD
Sample : N5222-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

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\82N102022W.M
Title : SW846 8260

37	12.076	1694	1704	1715	rVB2	44249984	85728578	96.36%	12.134%
38	12.400	1748	1759	1768	rBV	13729273	23255656	26.14%	3.292%
39	12.700	1804	1810	1816	rVB	2554432	4387648	4.93%	0.621%
40	12.847	1828	1835	1847	rBV	3221881	5795749	6.51%	0.820%
41	13.035	1861	1867	1873	rBV	3987649	6561771	7.38%	0.929%
42	13.100	1873	1878	1880	rVV	4350037	6757747	7.60%	0.957%
43	13.129	1880	1883	1887	rVV	5263766	8863722	9.96%	1.255%
44	13.176	1887	1891	1898	rVB	5702554	9064287	10.19%	1.283%
45	13.335	1910	1918	1928	rVB	13042729	21735370	24.43%	3.076%
46	13.482	1936	1943	1957	rVB2	45141386	73961630	83.14%	10.469%
47	13.612	1957	1965	1971	rBV3	424729	1111581	1.25%	0.157%
48	13.823	1990	2001	2008	rBV2	9263169	21162291	23.79%	2.995%
49	13.953	2017	2023	2025	rBV	3167782	4625105	5.20%	0.655%
50	13.994	2025	2030	2046	rVB2	16848431	36049818	40.52%	5.103%
51	14.117	2046	2051	2056	rBV2	638012	1002400	1.13%	0.142%
52	14.182	2056	2062	2067	rVV2	1873716	3206645	3.60%	0.454%
53	14.247	2067	2073	2076	rVV	4194651	7424493	8.35%	1.051%
54	14.276	2076	2078	2082	rVV	2646039	3269071	3.67%	0.463%
55	14.329	2082	2087	2093	rVB	7534107	11838970	13.31%	1.676%
56	14.400	2093	2099	2102	rBV	1491749	2493657	2.80%	0.353%
57	14.447	2102	2107	2115	rVB	5603100	9317393	10.47%	1.319%
58	14.576	2125	2129	2135	rVB2	957405	1550828	1.74%	0.220%
59	14.653	2135	2142	2146	rBV	4802120	8275760	9.30%	1.171%
60	14.694	2146	2149	2154	rVV	5604254	8370007	9.41%	1.185%
61	14.929	2184	2189	2194	rVV	3758475	6249825	7.03%	0.885%
62	15.053	2201	2210	2216	rBV3	5159043	12331363	13.86%	1.745%
63	15.117	2216	2221	2230	rVB3	664834	1524718	1.71%	0.216%
64	15.212	2231	2237	2244	rBV3	630981	1280748	1.44%	0.181%
65	15.317	2244	2255	2261	rBV3	1721203	4513322	5.07%	0.639%
66	15.441	2268	2276	2284	rVB3	1141704	2922122	3.28%	0.414%
67	15.641	2302	2310	2318	rVB	7579664	14380408	16.16%	2.035%
68	15.747	2322	2328	2334	rVV3	672547	1338106	1.50%	0.189%
69	15.947	2354	2362	2369	rBV	513567	1044945	1.17%	0.148%
70	16.129	2383	2393	2404	rBV3	244190	922913	1.04%	0.131%
71	16.782	2497	2504	2505	rBV2	903368	1334325	1.50%	0.189%

Sum of corrected areas: 706505159

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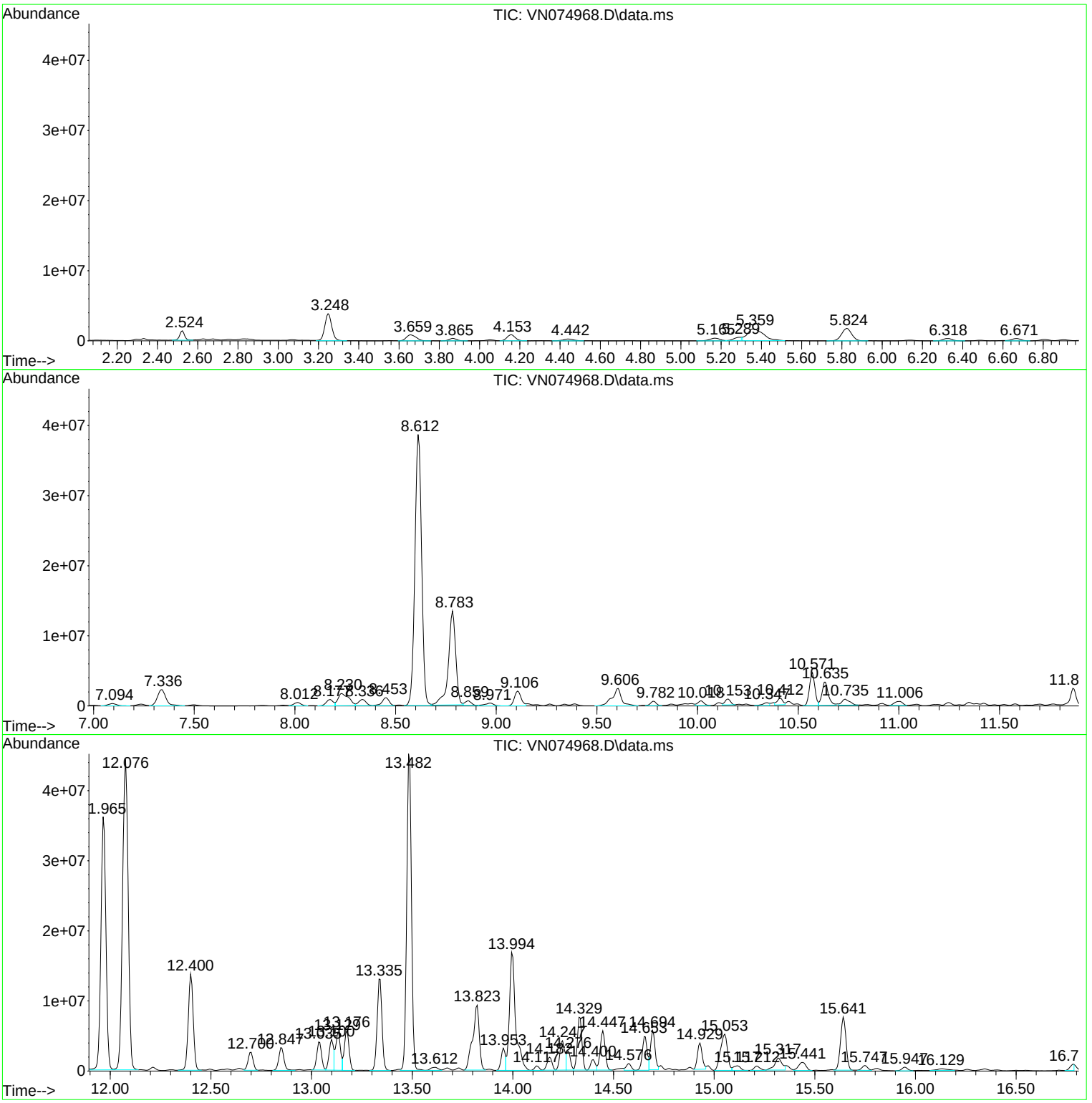
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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



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Data File : VN074968.D
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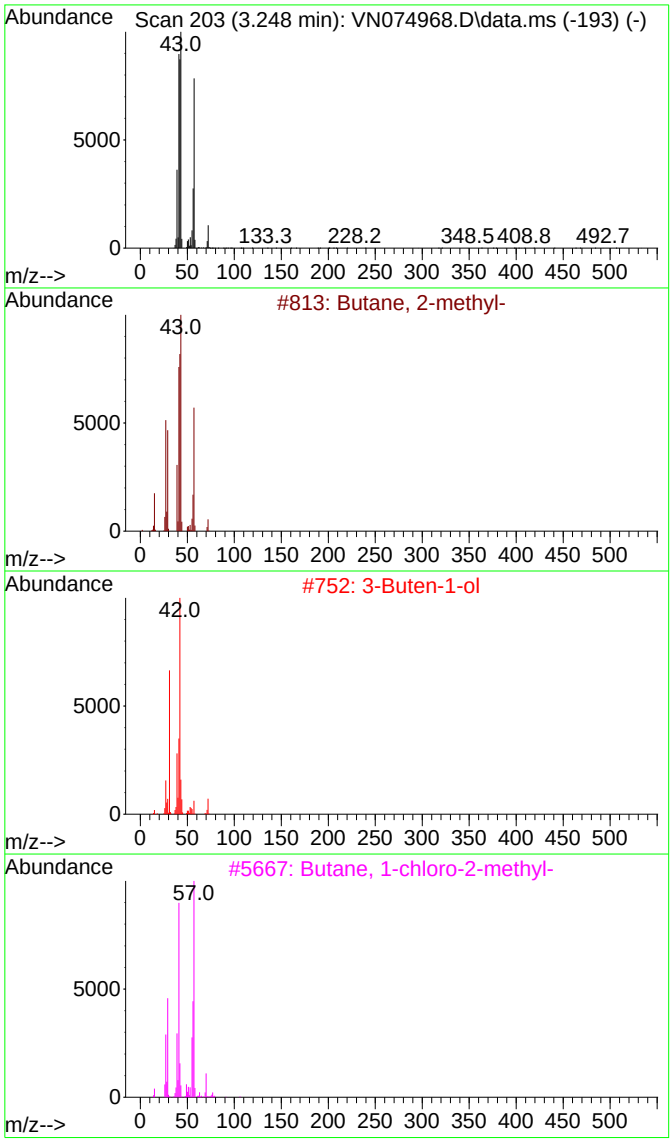
Quant Title : SW846 8260

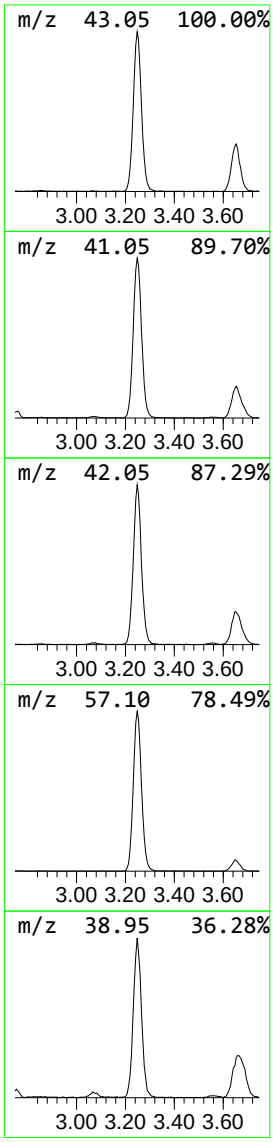
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.248	73.31 ug/l	9320510	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	3-Buten-1-ol	72	C4H8O	000627-27-0	43
3	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	35
4	1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	33
5	Pentane	72	C5H12	000109-66-0	28





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Operator : JC\MD
Sample : N5222-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

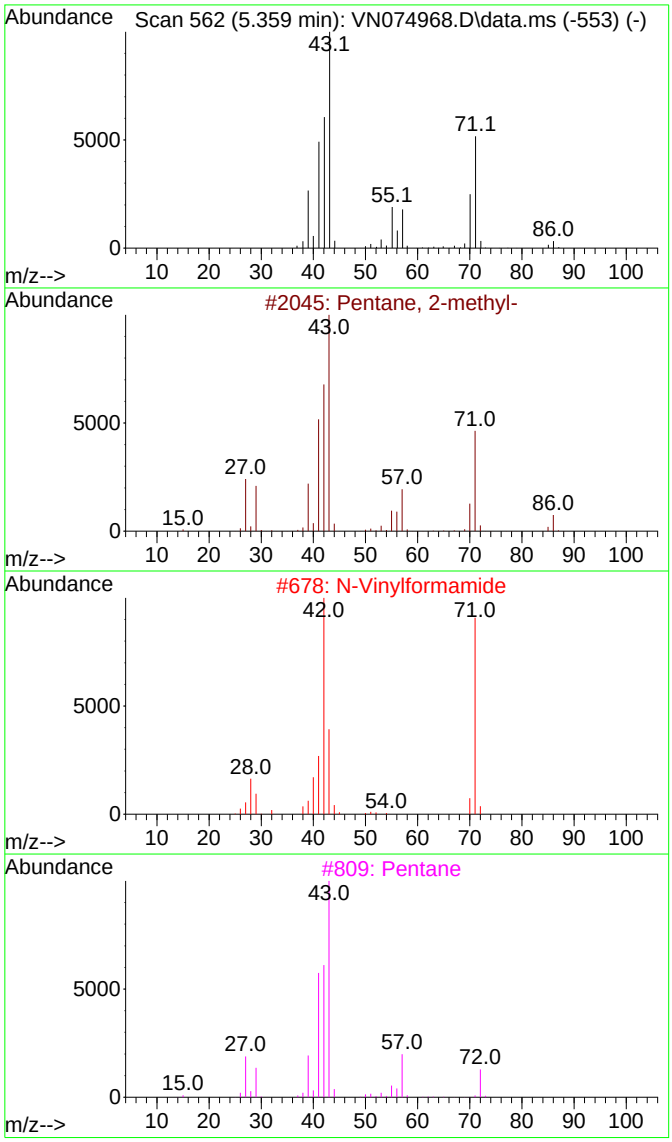
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

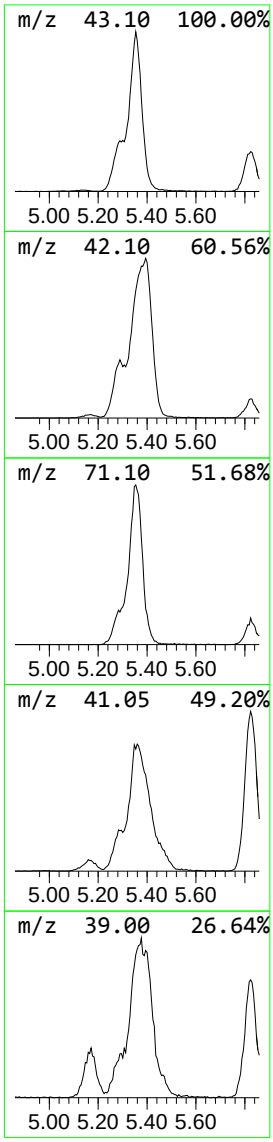
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.359	72.68 ug/l	9240200	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	90
2	N-Vinylformamide	71	C3H5NO	013162-05-5	47
3	Pentane	72	C5H12	000109-66-0	43
4	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	42
5	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	40





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Data File : VN074968.D
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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

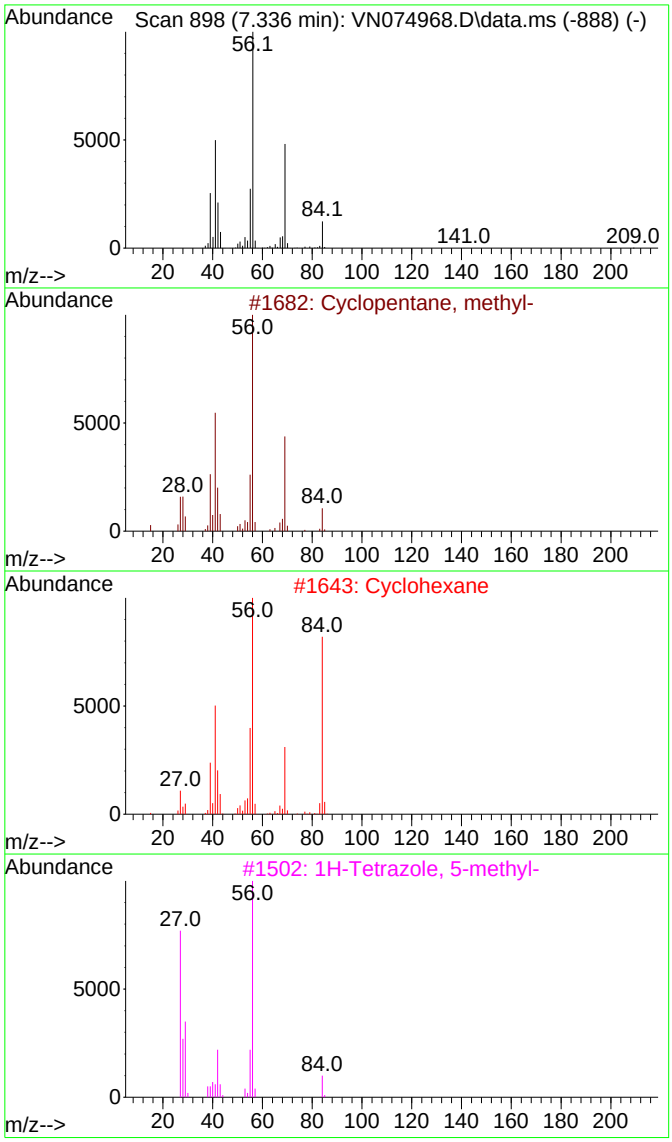
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

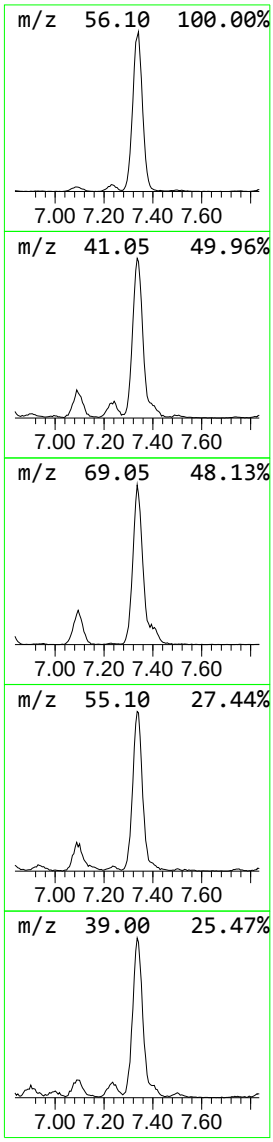
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.336	54.41 ug/l	6917640	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclohexane	84	C6H12	000110-82-7	78
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5	Cyclopropane, propyl-	84	C6H12	002415-72-7	56





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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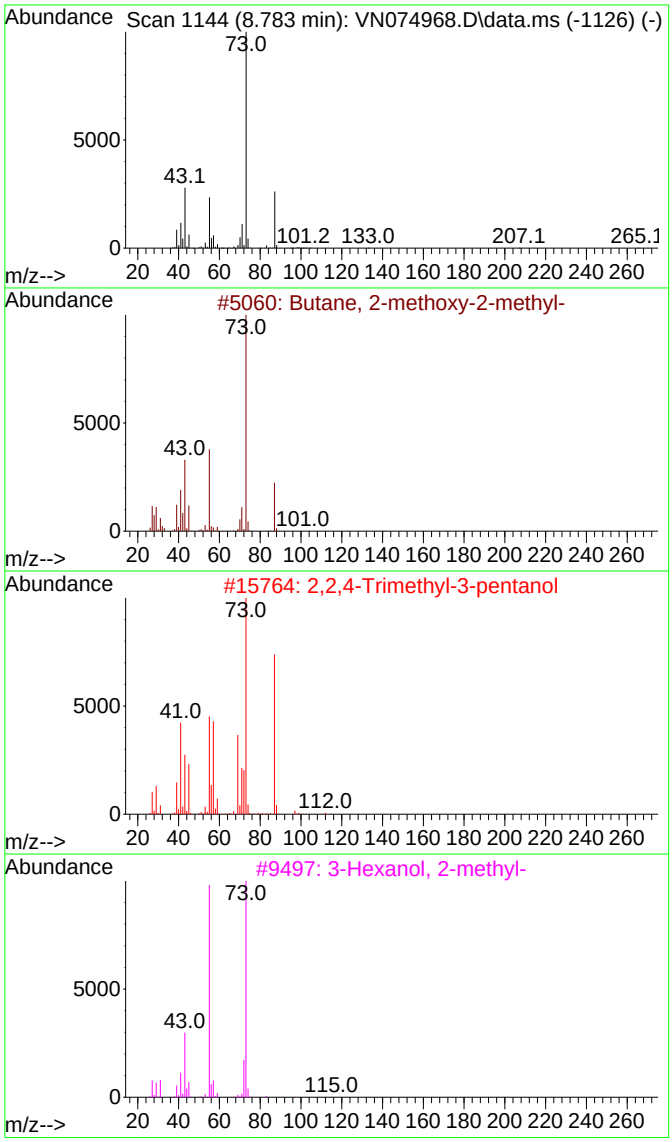
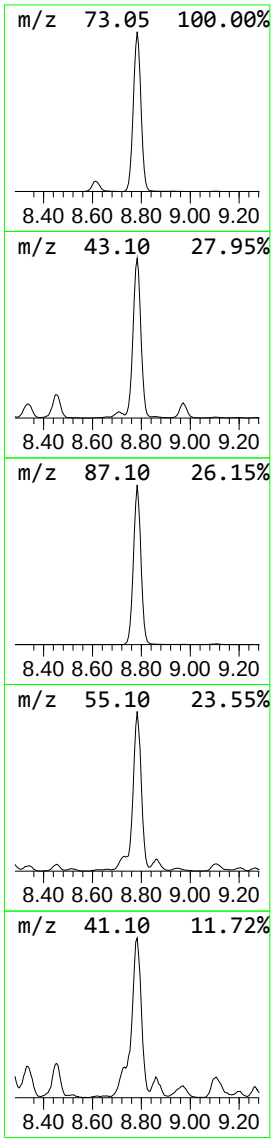
****
Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.783	342.61 ug/l	33970000	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	23
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	17
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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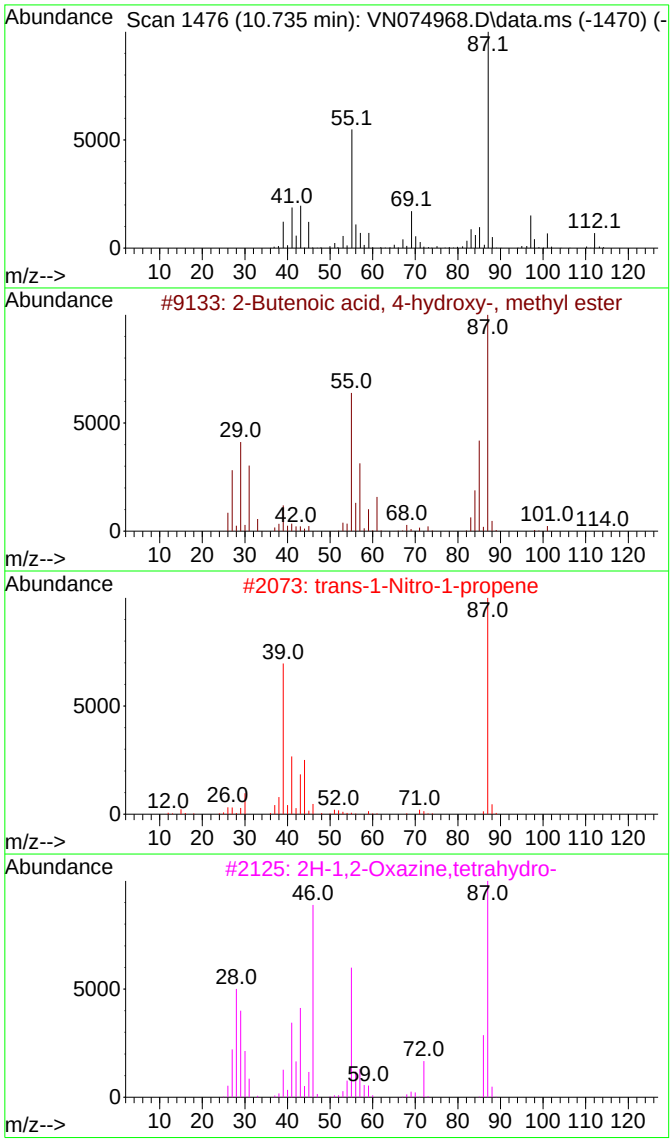
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

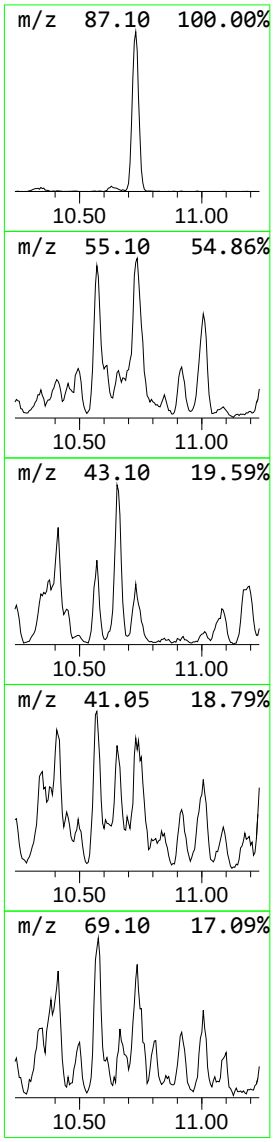
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Butenoic acid, 4-hydroxy-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.735	25.36 ug/l	2279280	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 4-hydroxy-, met...	116	C5H8O3	004508-99-0	50
2	trans-1-Nitro-1-propene	87	C3H5NO2	017082-05-2	49
3	2H-1,2-Oxazine,tetrahydro-	87	C4H9NO	036652-42-3	40
4	4,4-Ethylenedioxy-1-pentylamine	145	C7H15NO2	066442-97-5	36
5	3-Pentanol, 2,3,4-trimethyl-	130	C8H18O	003054-92-0	33





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Instrument :
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ClientSampleId :
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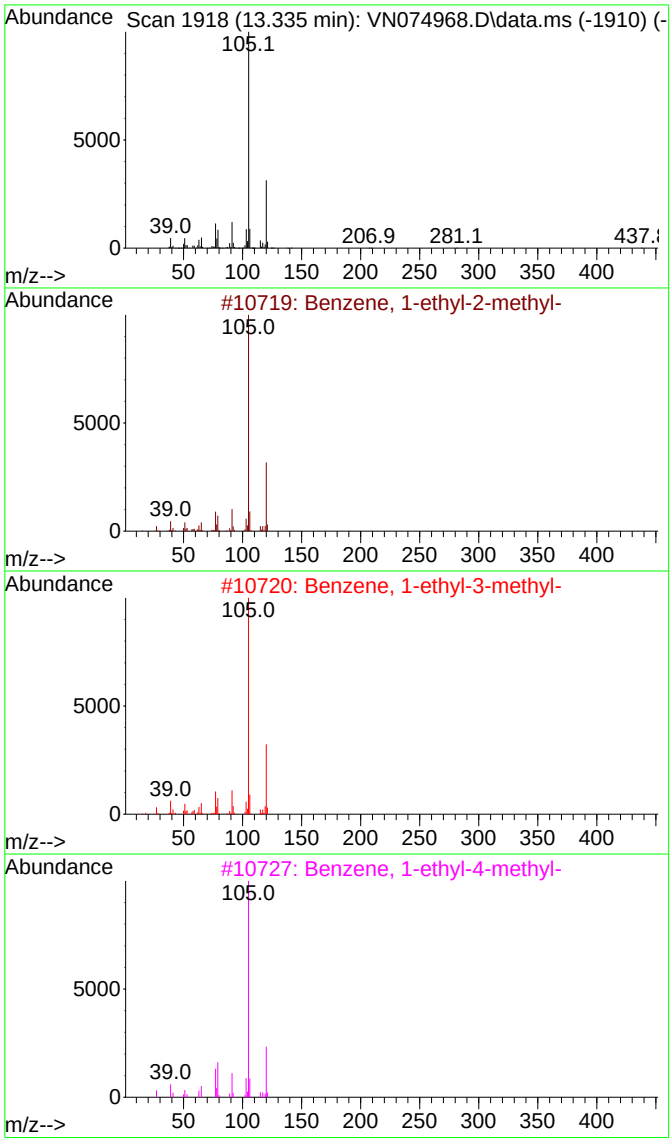
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

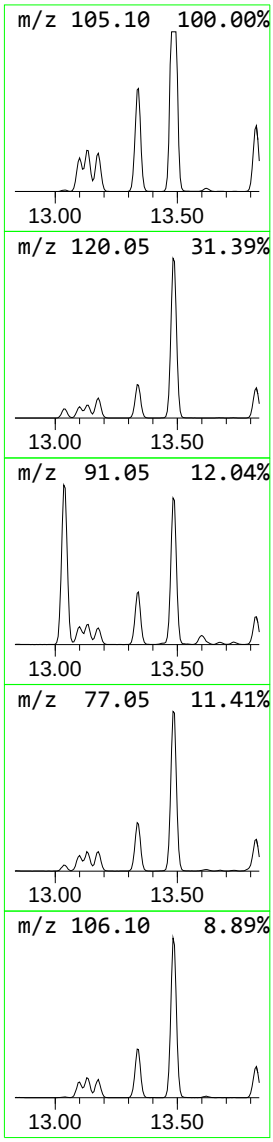
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	51.35 ug/l	21735400	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	93
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
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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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

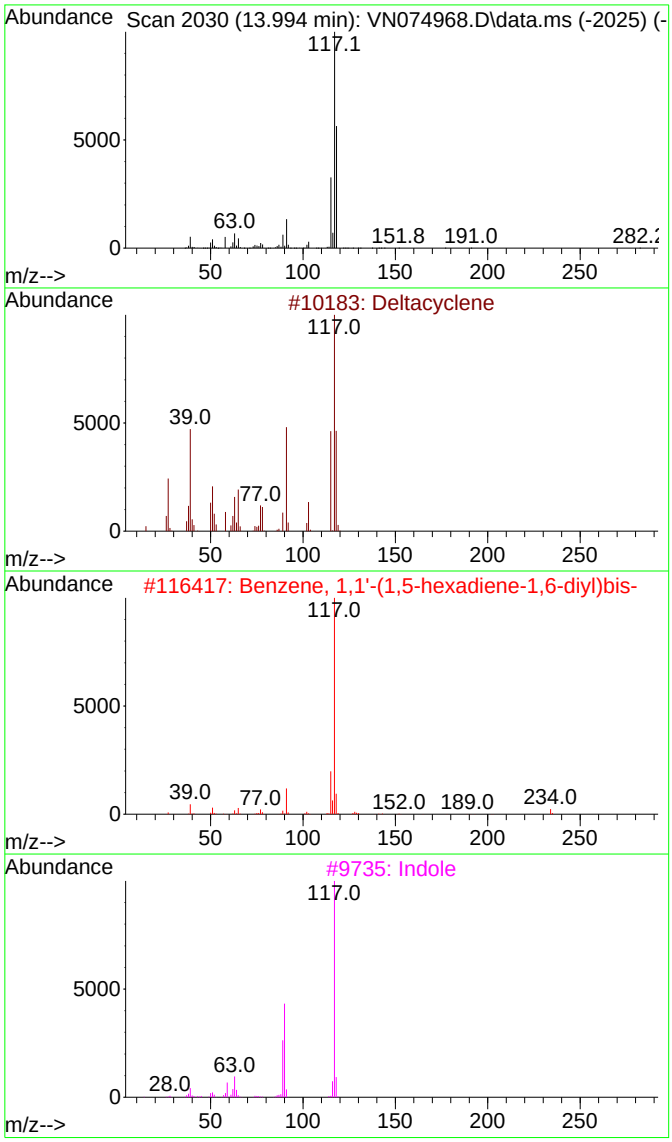
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

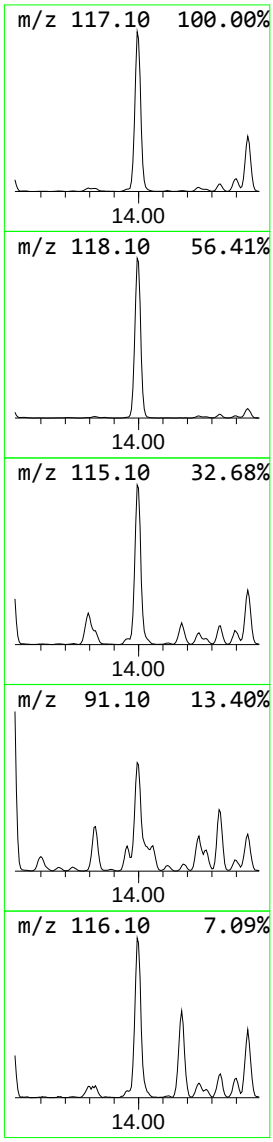
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	85.17 ug/l	36049800	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Deltacyclene	118	C9H10	007785-10-6	59
2	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
3	Indole	117	C8H7N	000120-72-9	46
4	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45
5	m-Aminophenylacetylene	117	C8H7N	054060-30-9	43





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Data File : VN074968.D
Acq On : 21 Oct 2022 17:48
Operator : JC\MD
Sample : N5222-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

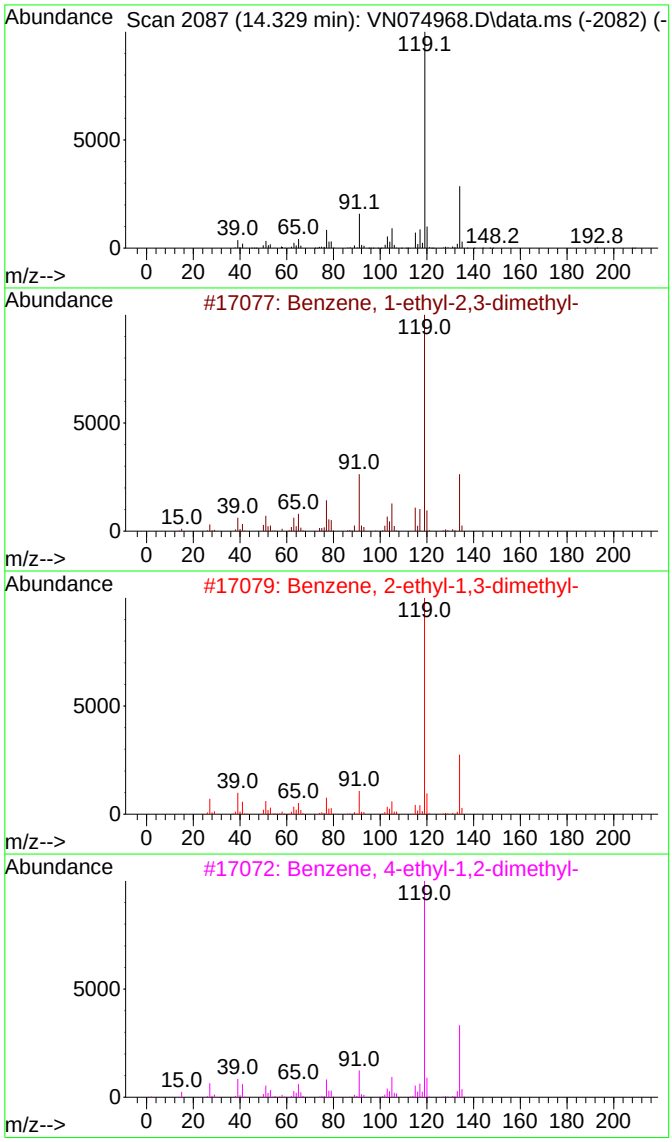
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

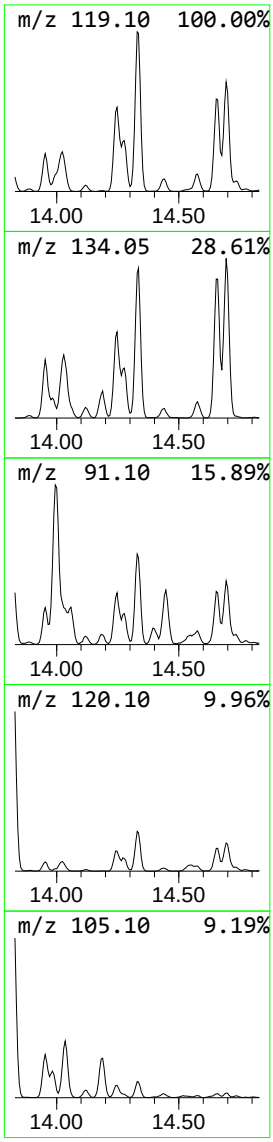
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	27.97 ug/l	11839000	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
2	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5	o-Cymene	134	C10H14	000527-84-4	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074968.D
Acq On : 21 Oct 2022 17:48
Operator : JC\MD
Sample : N5222-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

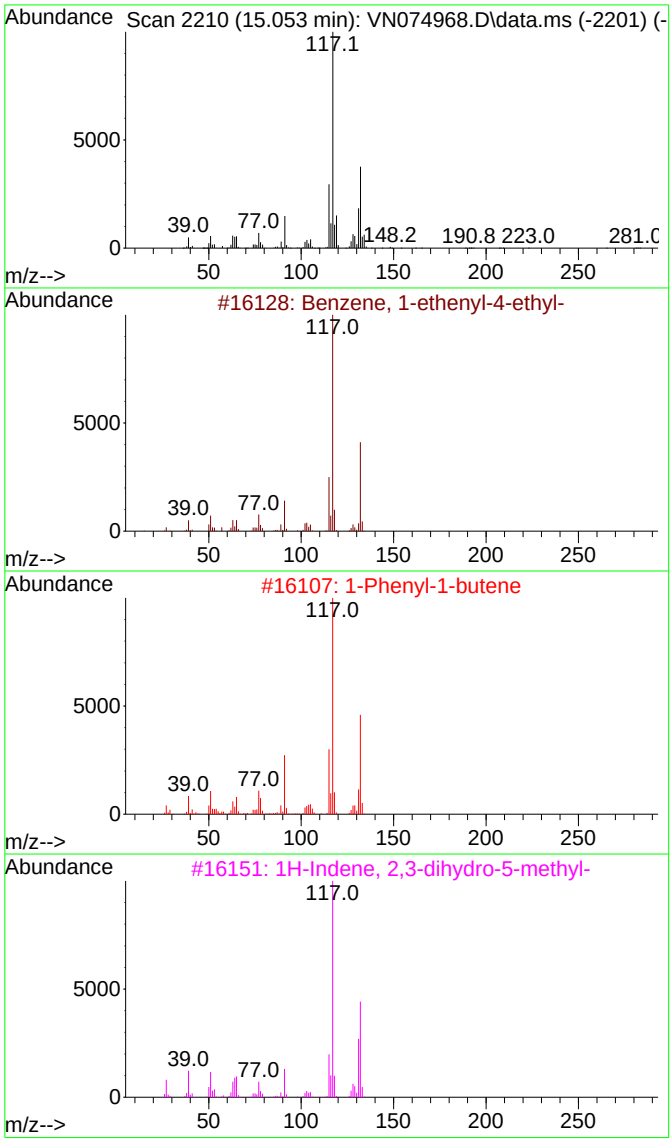
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

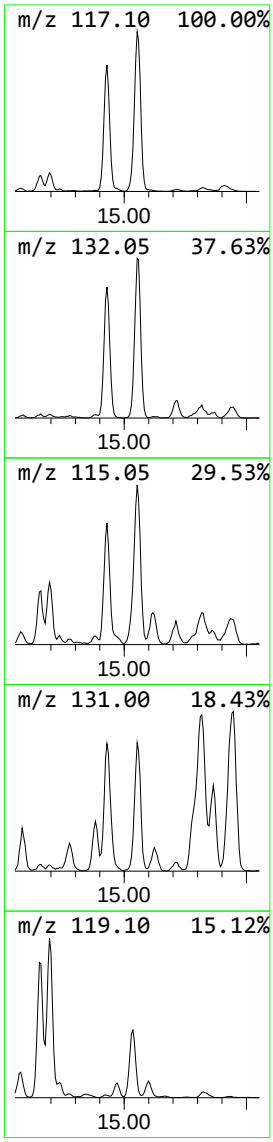
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	29.14 ug/l	12331400	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	93
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
4	Indan, 1-methyl-	132	C10H12	000767-58-8	90
5	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074968.D
Acq On : 21 Oct 2022 17:48
Operator : JC\MD
Sample : N5222-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

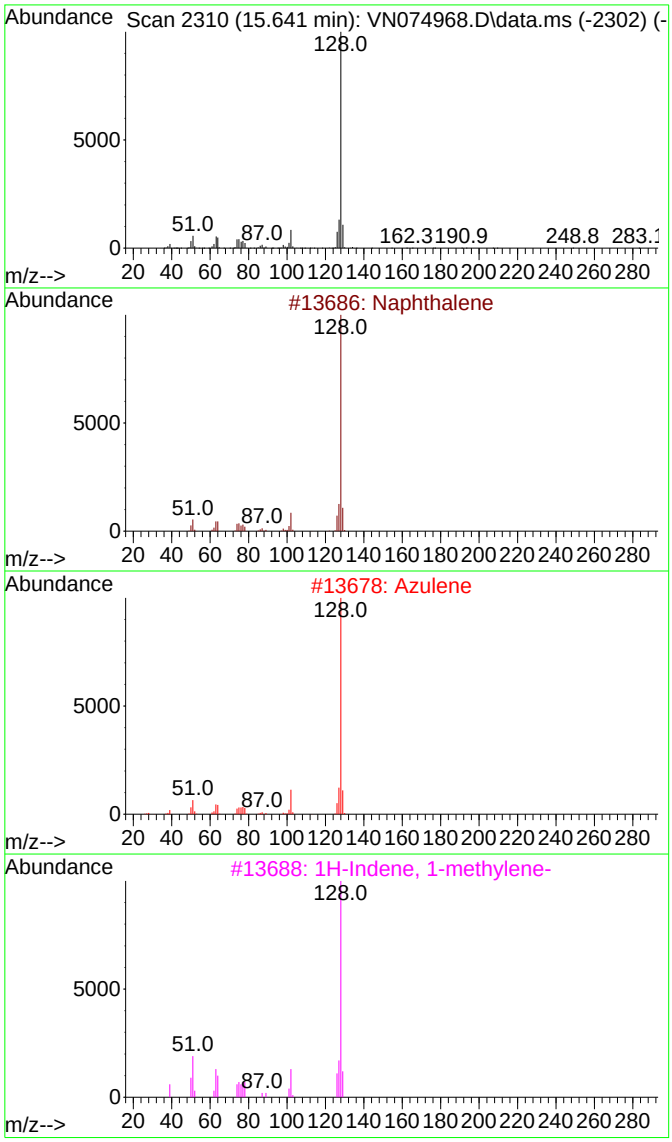
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

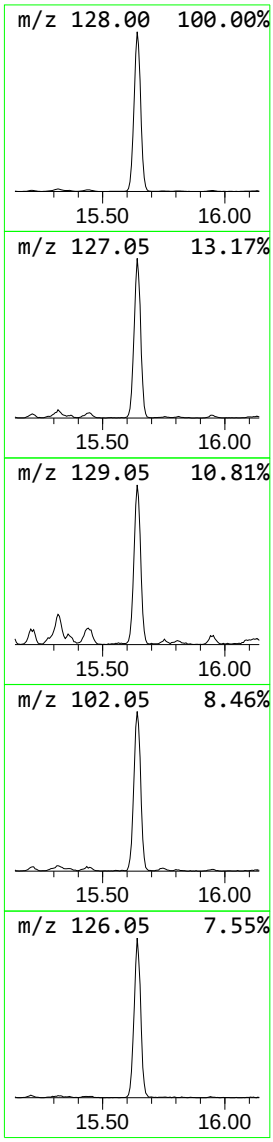
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Indene, 1-methylene- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.641	33.98 ug/l	14380400	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	Azulene	128	C10H8	000275-51-4	94
3	1H-Indene, 1-methylene-	128	C10H8	002471-84-3	91
4	4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	78
5	1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074968.D
Acq On : 21 Oct 2022 17:48
Operator : JC\MD
Sample : N5222-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.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
Butane, 2-methyl-	3.248	73.3	ug/l	9320510	1	8.230	6356860	50.0
Pentane, 2-methyl-	5.359	72.7	ug/l	9240200	1	8.230	6356860	50.0
Cyclopentane, m...	7.336	54.4	ug/l	6917640	1	8.230	6356860	50.0
Butane, 2-metho...	8.783	342.6	ug/l	33970000	2	9.106	4957570	50.0
2-Butenoic acid...	10.735	25.4	ug/l	2279280	3	11.865	4493690	50.0
Benzene, 1-ethy...	13.335	51.4	ug/l	21735400	4	13.794	21162300	50.0
Benzene, 1,1'-(...	13.994	85.2	ug/l	36049800	4	13.794	21162300	50.0
Benzene, 1-ethy...	14.329	28.0	ug/l	11839000	4	13.794	21162300	50.0
Benzene, 1-ethe...	15.053	29.1	ug/l	12331400	4	13.794	21162300	50.0
1H-Indene, 1-me...	15.641	34.0	ug/l	14380400	4	13.794	21162300	50.0