LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072462.D
Acq On : 12 May 2022 18:57
Operator : JC\MD
Sample : N2800-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP051022

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\82N051022W.M
Title : SW846 8260

Signal : TIC: VN072462.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.440	70	77	86	rVB	197648	309105	2.05%	0.296%
2	3.122	182	193	214	rBV	1686533	3900076	25.87%	3.735%
3	3.510	249	259	276	rBV	1192005	2906284	19.28%	2.783%
4	3.716	284	294	306	rVB	139905	344541	2.29%	0.330%
5	3.993	332	341	354	rVB	95346	253308	1.68%	0.243%
6	4.257	374	386	402	rBV3	128845	453549	3.01%	0.434%
7	4.957	487	505	514	rBV6	49402	215361	1.43%	0.206%
8	5.081	514	526	528	rBV2	285512	763074	5.06%	0.731%
9	5.151	530	538	553	rVB5	813907	3394230	22.51%	3.250%
10	5.622	603	618	638	rBV	677147	2369168	15.71%	2.269%
11	6.122	689	703	718	rBV2	384896	1188653	7.88%	1.138%
12	6.469	756	762	774	rVB3	57368	170582	1.13%	0.163%
13	6.604	774	785	793	rBV3	60167	194534	1.29%	0.186%
14	6.698	793	801	812	rVV3	98417	380222	2.52%	0.364%
15	6.904	826	836	846	rVV4	61968	188167	1.25%	0.180%
16	7.045	850	860	867	rBV2	80427	226081	1.50%	0.216%
17	7.145	867	877	898	rVB	1081685	3174138	21.05%	3.039%
18	7.839	989	995	1004	rVB6	57935	159275	1.06%	0.153%
19	8.022	1016	1026	1029	rBV2	162522	389896	2.59%	0.373%
20	8.086	1029	1037	1045	rVV4	761086	2305701	15.29%	2.208%
21	8.175	1045	1052	1063	rVB2	266527	721726	4.79%	0.691%
22	8.292	1063	1072	1079	rBV	290667	677560	4.49%	0.649%
23	8.433	1089	1096	1106	rBV2	192565	472935	3.14%	0.453%
24	8.569	1106	1119	1125	rBV7	240354	820047	5.44%	0.785%
25	8.704	1137	1142	1152	rVB2	139402	313799	2.08%	0.300%
26	8.828	1152	1163	1177	rVB3	57686	153262	1.02%	0.147%
27	8.963	1177	1186	1200	rBV	453411	1042747	6.92%	0.998%
28	9.457	1253	1270	1277	rBV2	523784	1463156	9.70%	1.401%
29	9.639	1295	1301	1308	rVB	114885	220712	1.46%	0.211%
30	9.880	1337	1342	1350	rVB	98275	205577	1.36%	0.197%
31	9.969	1350	1357	1360	rBV	147859	269341	1.79%	0.258%
32	10.010	1360	1364	1371	rVB	170015	344182	2.28%	0.330%
33	10.227	1388	1401	1410	rBV4	109292	392985	2.61%	0.376%
34	10.439	1429	1437	1442	rBV	713612	1310481	8.69%	1.255%
35	10.504	1442	1448	1453	rVV	1215446	2211429	14.67%	2.118%
36	10.545	1453	1455	1461	rVB	114514	185887	1.23%	0.178%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072462.D
Acq On : 12 May 2022 18:57
Operator : JC\MD
Sample : N2800-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP051022

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\82N051022W.M
Title : SW846 8260

37	10.863	1502	1509	1517	rVB4	85312	210127	1.39%	0.201%
38	11.739	1650	1658	1667	rBV	624246	1133249	7.52%	1.085%
39	11.839	1667	1675	1685	rVV	3701302	6289064	41.71%	6.022%
40	11.945	1685	1693	1706	rVV	7691641	15077652	100.00%	14.438%
41	12.274	1737	1749	1759	rBV	4668736	7839322	51.99%	7.507%
42	12.574	1794	1800	1808	rVB	467355	737265	4.89%	0.706%
43	12.727	1819	1826	1836	rBV	498374	829345	5.50%	0.794%
44	12.915	1850	1858	1863	rBV	830883	1331844	8.83%	1.275%
45	12.980	1863	1869	1872	rVV	2499226	4270844	28.33%	4.090%
46	13.010	1872	1874	1878	rVV	1602323	2201349	14.60%	2.108%
47	13.057	1878	1882	1901	rVB	1500734	2419948	16.05%	2.317%
48	13.215	1901	1909	1919	rBV	2126909	3447527	22.87%	3.301%
49	13.363	1925	1934	1941	rBV	5106466	8138485	53.98%	7.793%
50	13.492	1948	1956	1962	rVB3	91738	223644	1.48%	0.214%
51	13.698	1980	1991	2001	rBV2	1730811	3771237	25.01%	3.611%
52	13.833	2008	2014	2016	rBV	361284	551037	3.65%	0.528%
53	13.868	2016	2020	2024	rVV2	1092618	1949539	12.93%	1.867%
54	13.910	2024	2027	2037	rVV4	515558	1025667	6.80%	0.982%
55	14.062	2046	2053	2058	rVV2	231825	408168	2.71%	0.391%
56	14.127	2058	2064	2067	rVV	374579	657630	4.36%	0.630%
57	14.151	2067	2068	2073	rVV	243367	287261	1.91%	0.275%
58	14.210	2073	2078	2085	rVV	791720	1237570	8.21%	1.185%
59	14.321	2092	2097	2106	rVB2	463803	773578	5.13%	0.741%
60	14.457	2114	2120	2126	rVB	141873	224861	1.49%	0.215%
61	14.533	2126	2133	2137	rBV	423341	705556	4.68%	0.676%
62	14.574	2137	2140	2145	rVB	353719	489592	3.25%	0.469%
63	14.804	2174	2179	2184	rBV	253492	404118	2.68%	0.387%
64	14.921	2191	2199	2206	rBV3	461160	1017993	6.75%	0.975%
65	14.986	2206	2210	2218	rVB4	75165	152524	1.01%	0.146%
66	15.080	2218	2226	2233	rBV2	104706	198699	1.32%	0.190%
67	15.192	2233	2245	2257	rVV3	112986	362804	2.41%	0.347%
68	15.304	2257	2264	2275	rVB4	94370	226457	1.50%	0.217%
69	15.498	2289	2297	2310	rVB	746491	1378679	9.14%	1.320%
70	16.609	2479	2486	2498	rVB	159348	367475	2.44%	0.352%

Sum of corrected areas: 104431881

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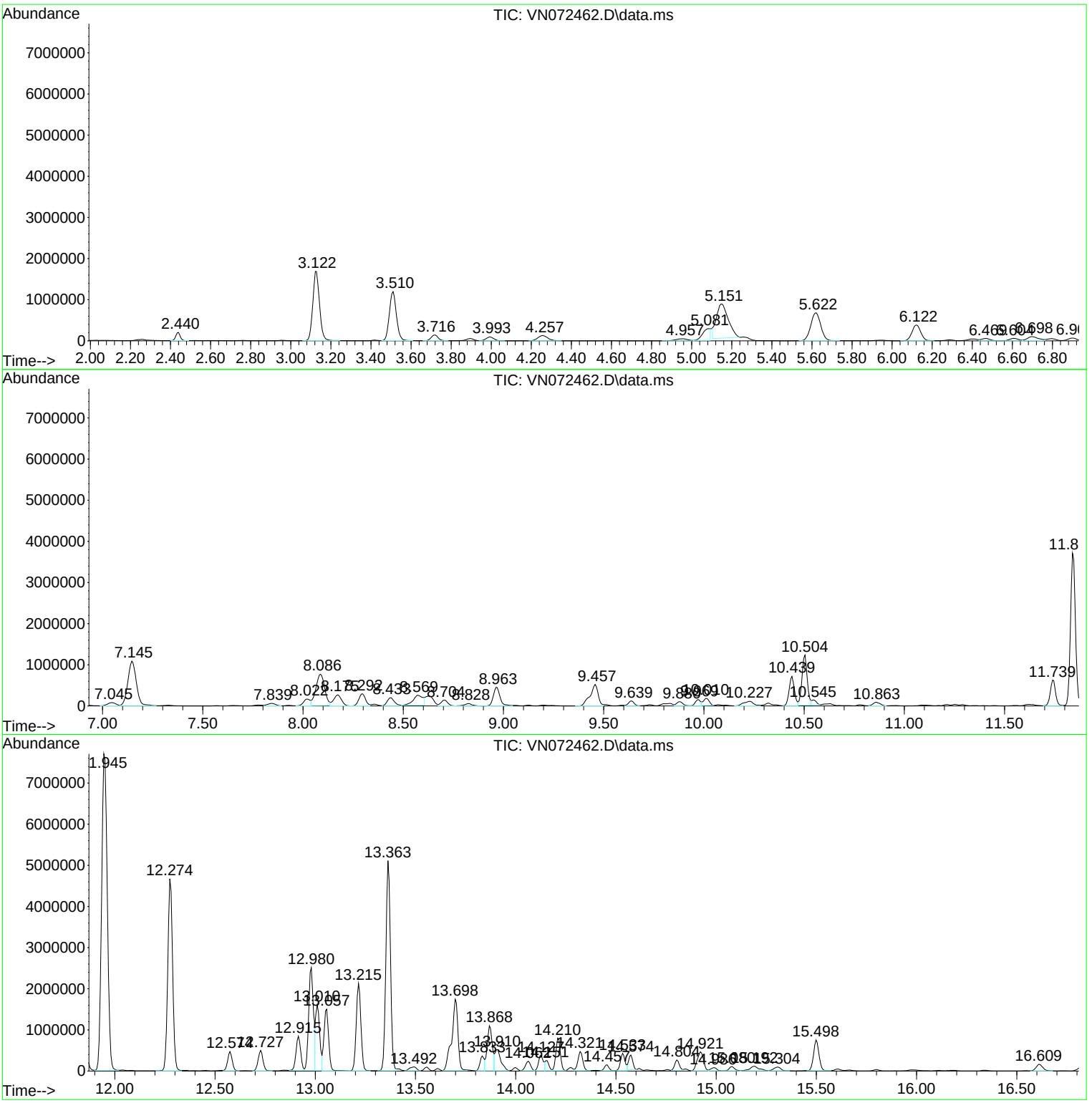
Acq On : 12 May 2022 18:57
Operator : JC\MD
Sample : N2800-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP051022

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072462.D
Acq On : 12 May 2022 18:57
Operator : JC\MD
Sample : N2800-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP051022

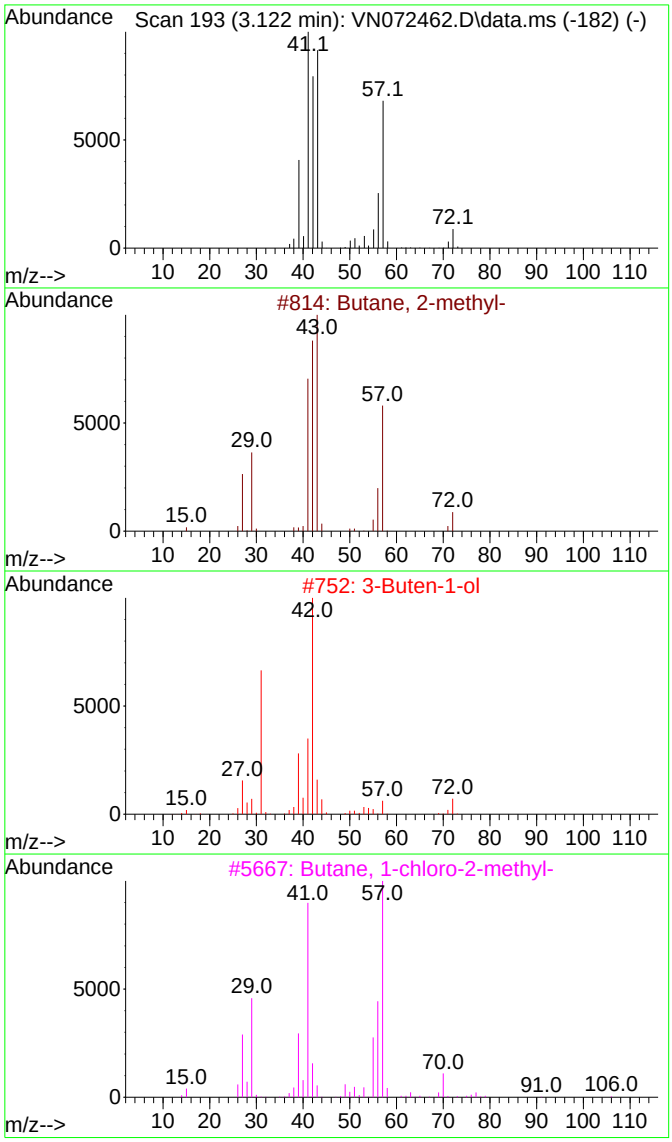
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

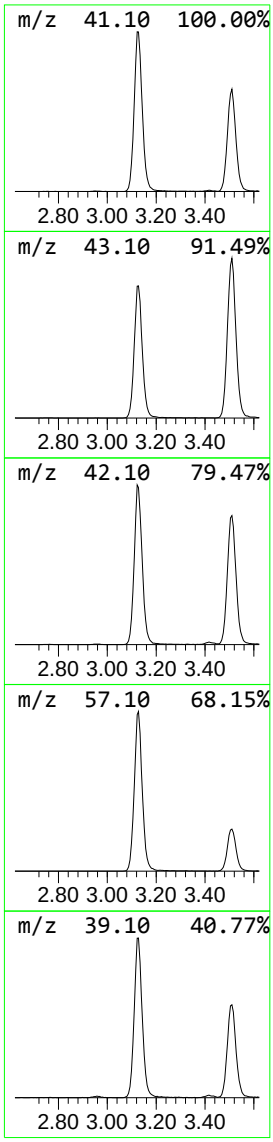
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.122	84.57 ug/l	3900080	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	58
2	3-Buten-1-ol	72	C4H8O	000627-27-0	38
3	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10
4	1-Butene	56	C4H8	000106-98-9	9
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072462.D
Acq On : 12 May 2022 18:57
Operator : JC\MD
Sample : N2800-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP051022

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

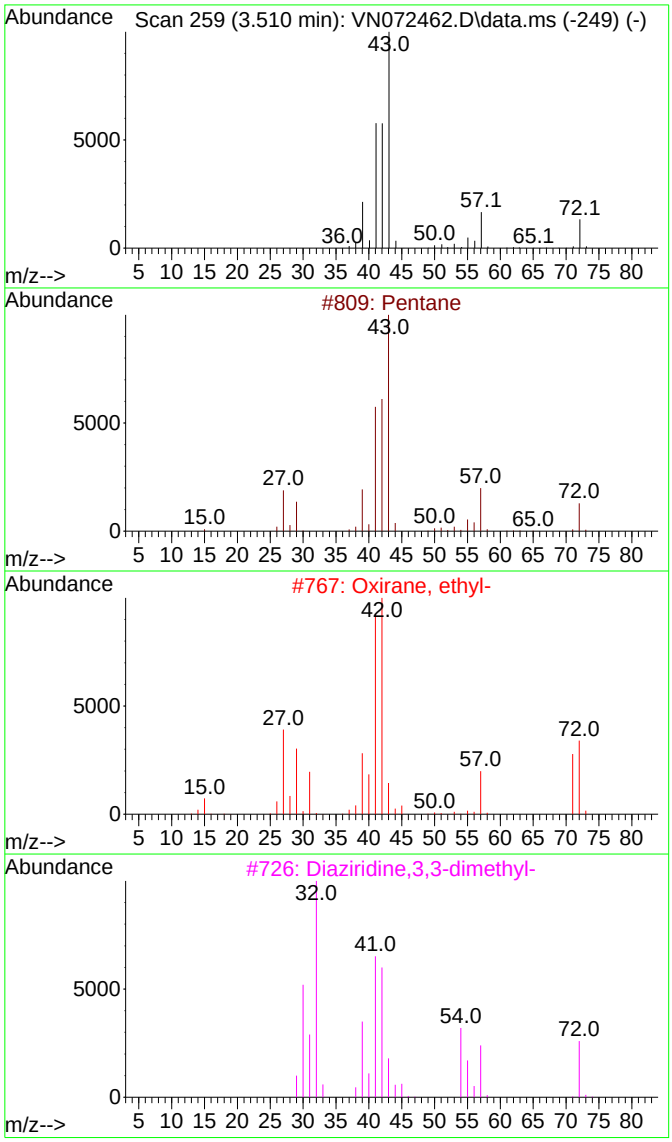
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

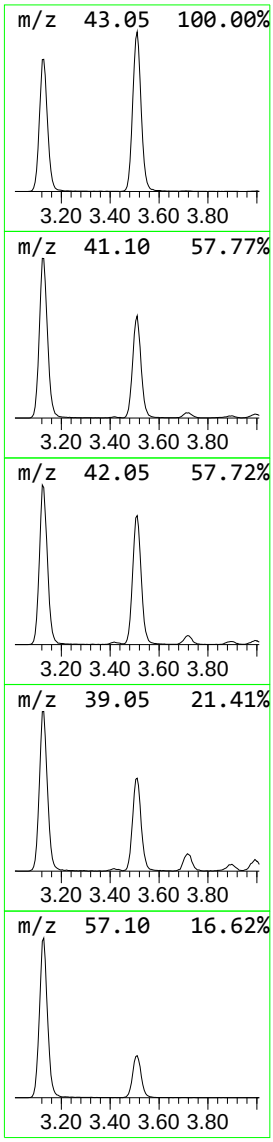
****

Peak Number 2 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.510	63.02 ug/l	2906280	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	35
4	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	25
5	Butane, 2-methyl-	72	C5H12	000078-78-4	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072462.D
Acq On : 12 May 2022 18:57
Operator : JC\MD
Sample : N2800-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP051022

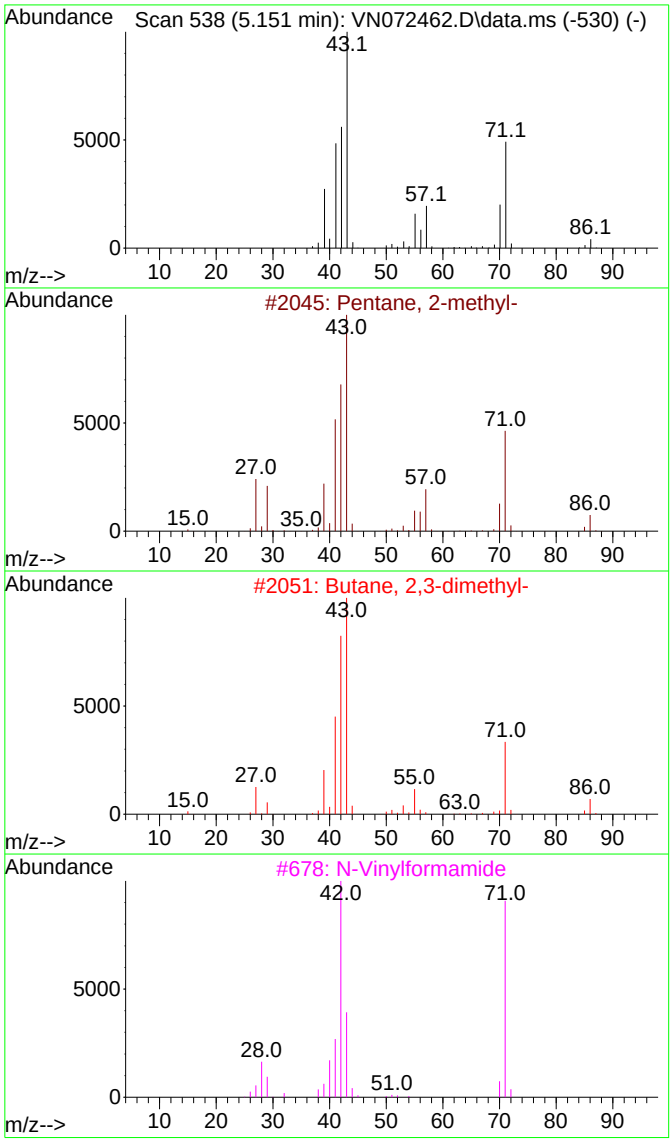
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

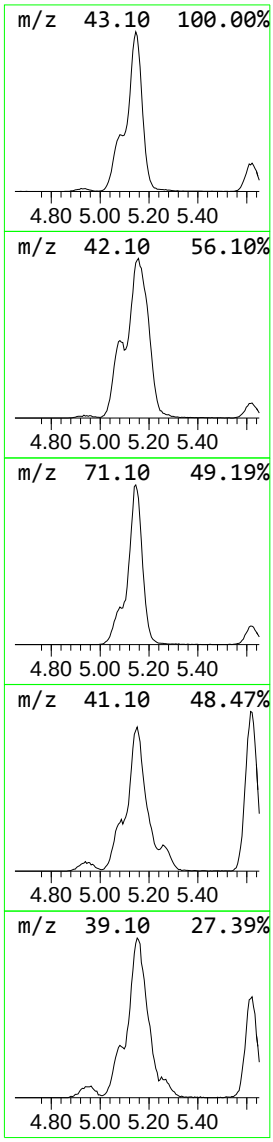
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.151	73.61 ug/l	3394230	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	90
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	47
3	N-Vinylformamide	71	C3H5NO	013162-05-5	47
4	Pentane	72	C5H12	000109-66-0	38
5	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072462.D
Acq On : 12 May 2022 18:57
Operator : JC\MD
Sample : N2800-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP051022

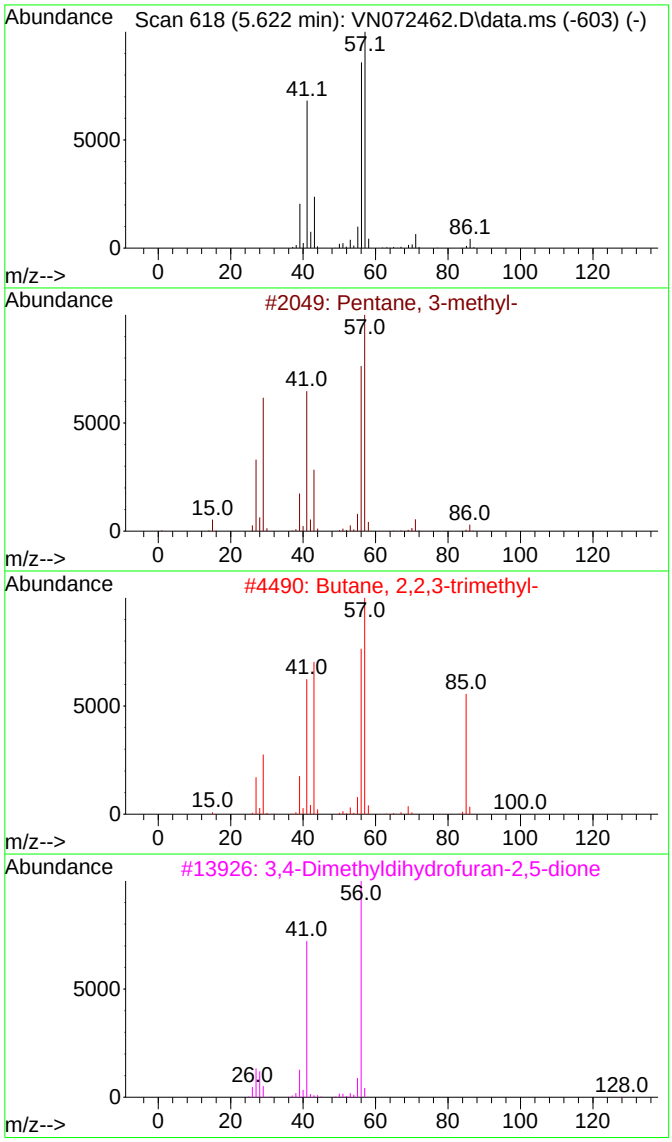
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

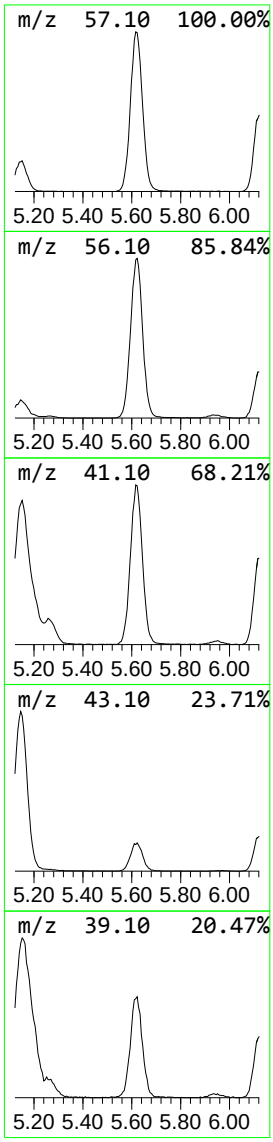
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.622	51.38 ug/l	2369170	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
3	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	53
4	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	45
5	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
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Acq On : 12 May 2022 18:57
Operator : JC\MD
Sample : N2800-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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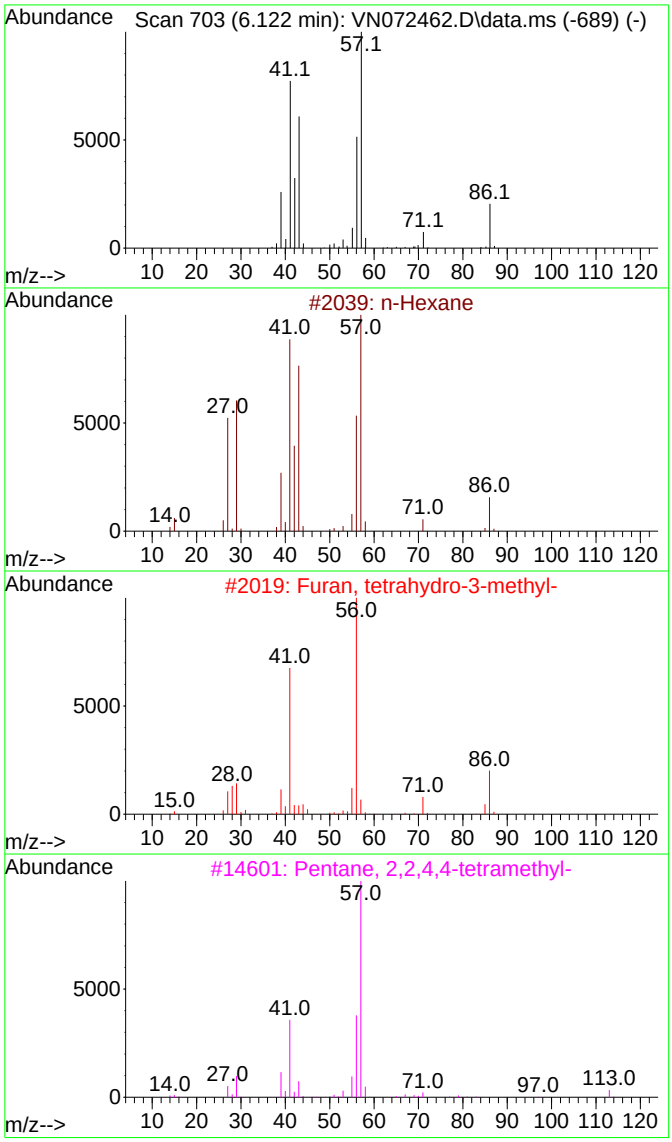
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

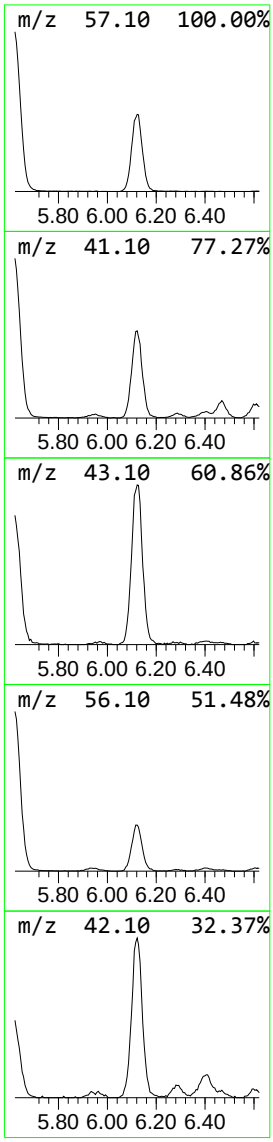
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 n-Hexane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.122	25.78 ug/l	1188650	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	78
2	Furan, tetrahydro-3-methyl-	86	C5H10O	013423-15-9	50
3	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	50
4	2-Ethyl-oxetane	86	C5H10O	1010386-40-2	45
5	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072462.D
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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP051022

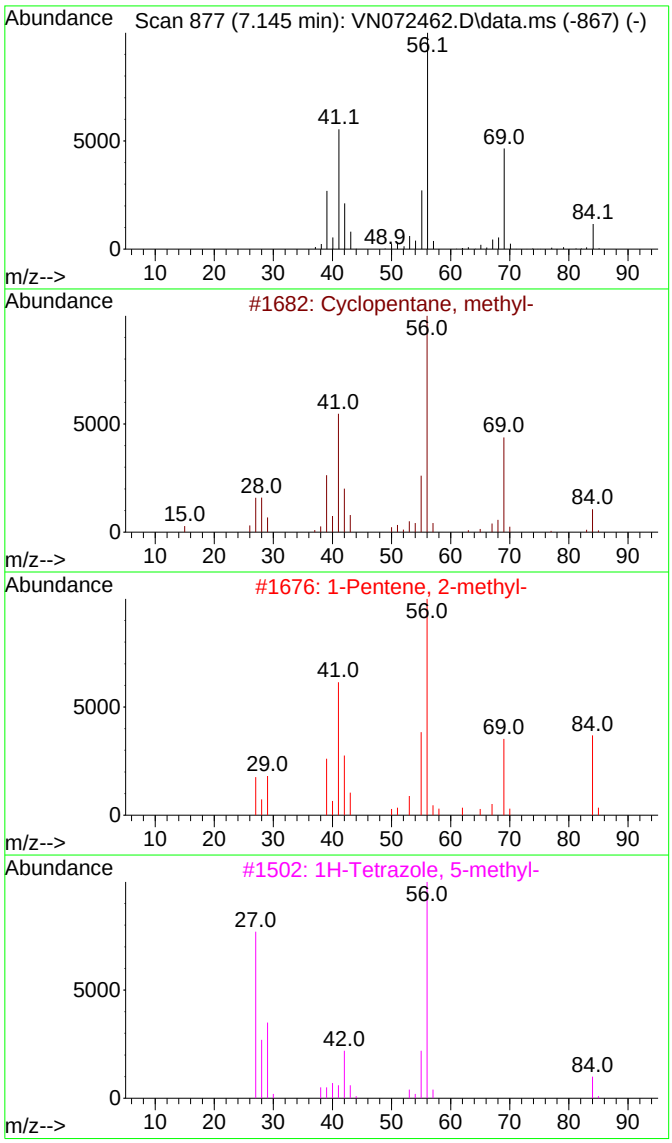
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

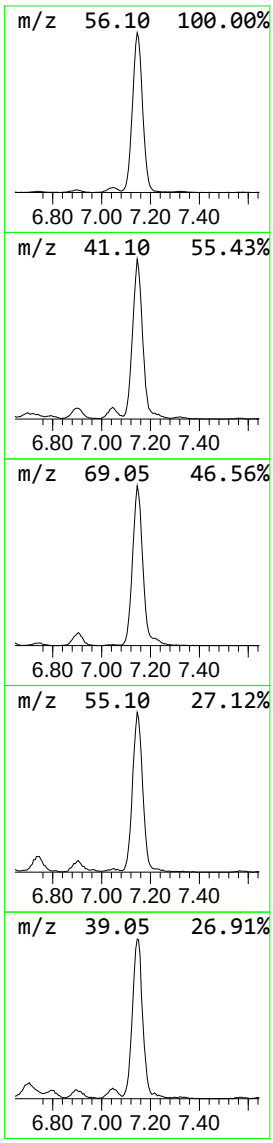
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	68.83 ug/l	3174140	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	86
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4	Cyclohexane	84	C6H12	000110-82-7	64
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072462.D
Acq On : 12 May 2022 18:57
Operator : JC\MD
Sample : N2800-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP051022

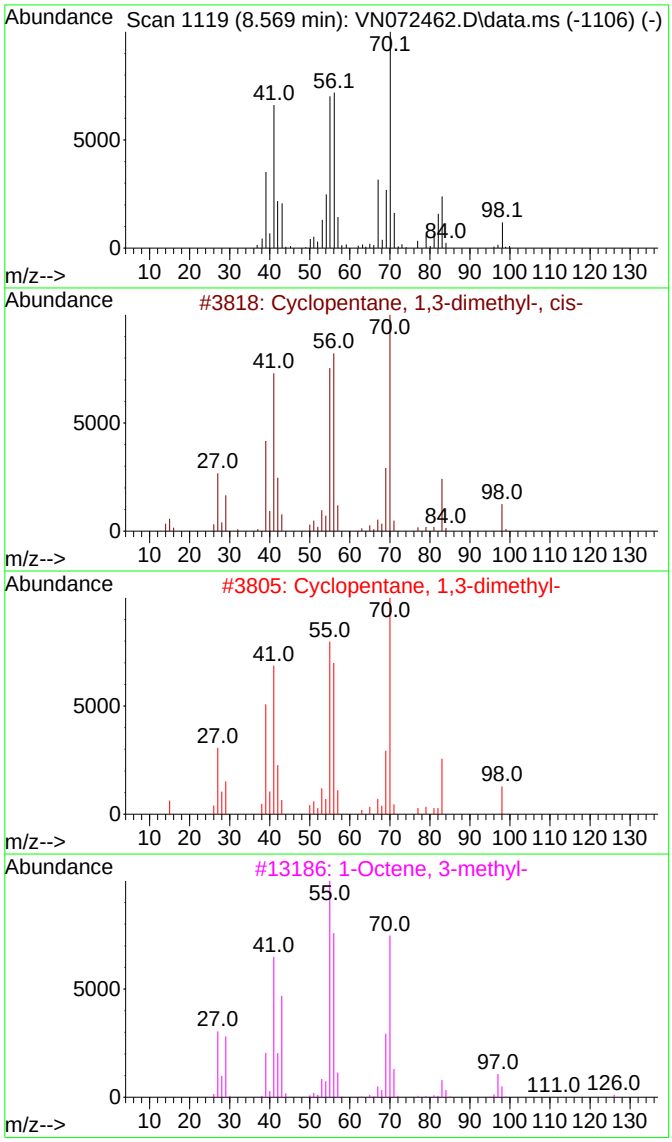
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

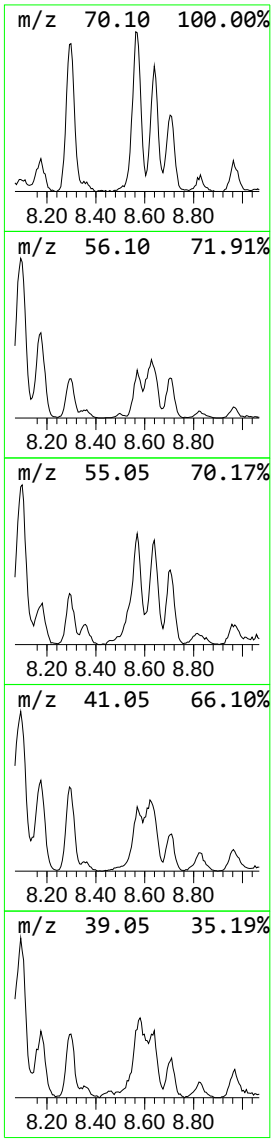
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclopentane, 1,3-dimethyl-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.569	39.32 ug/l	820047	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	94
2	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	93
3	1-Octene, 3-methyl-	126	C9H18	013151-08-1	53
4	Cyclobutanone, 2,2-dimethyl-	98	C6H10O	001192-14-9	50
5	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	46





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Data File : VN072462.D
Acq On : 12 May 2022 18:57
Operator : JC\MD
Sample : N2800-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP051022

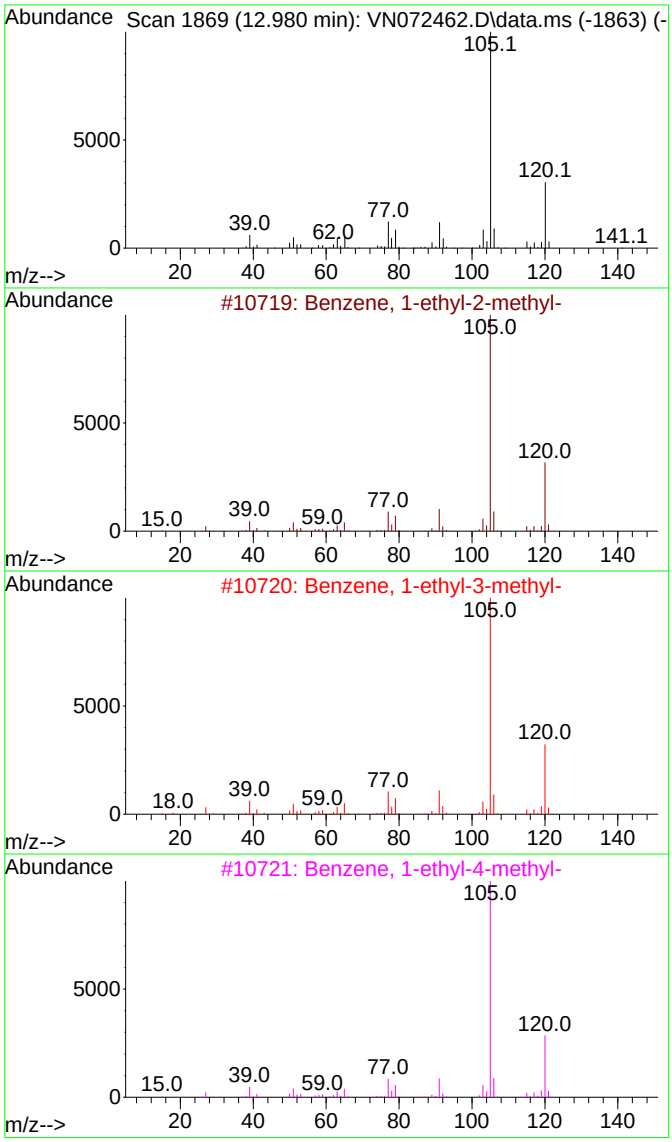
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

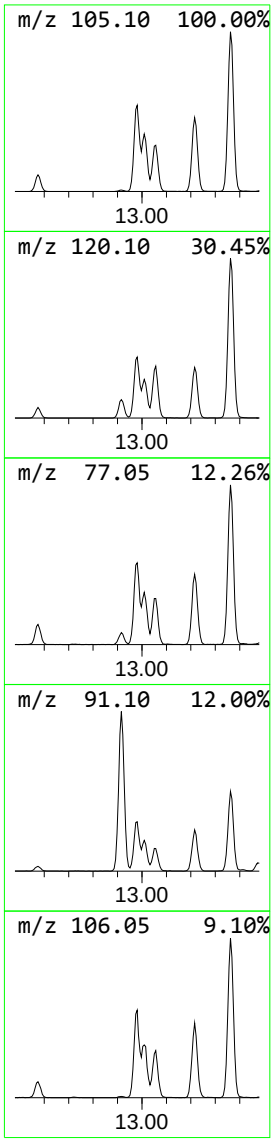
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	56.62 ug/l	4270840	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072462.D
Acq On : 12 May 2022 18:57
Operator : JC\MD
Sample : N2800-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP051022

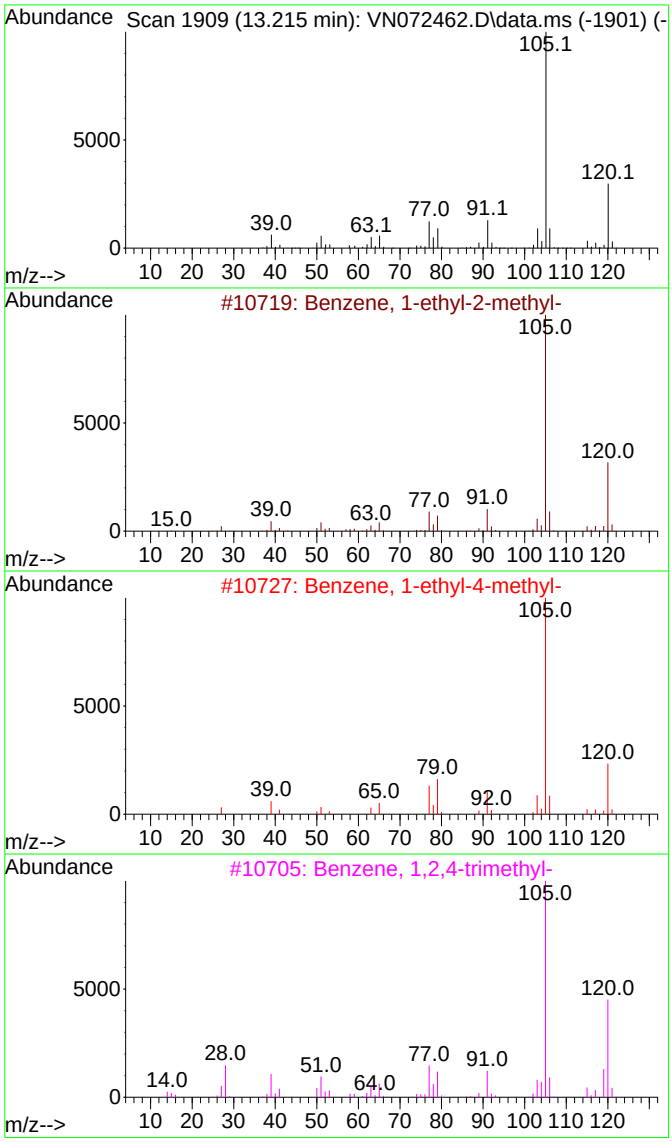
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

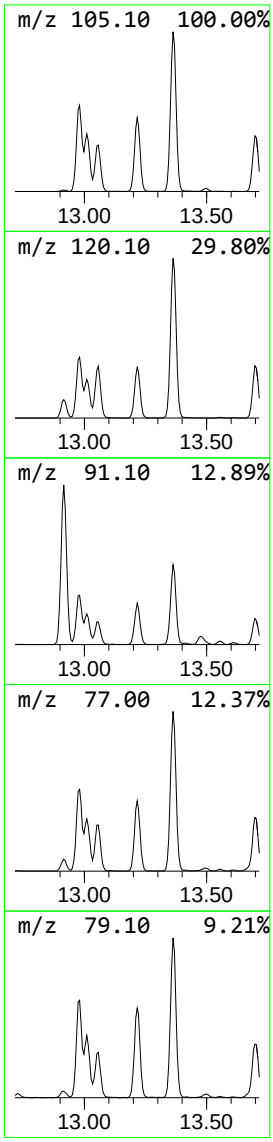
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	45.71 ug/l	3447530	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072462.D
Acq On : 12 May 2022 18:57
Operator : JC\MD
Sample : N2800-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP051022

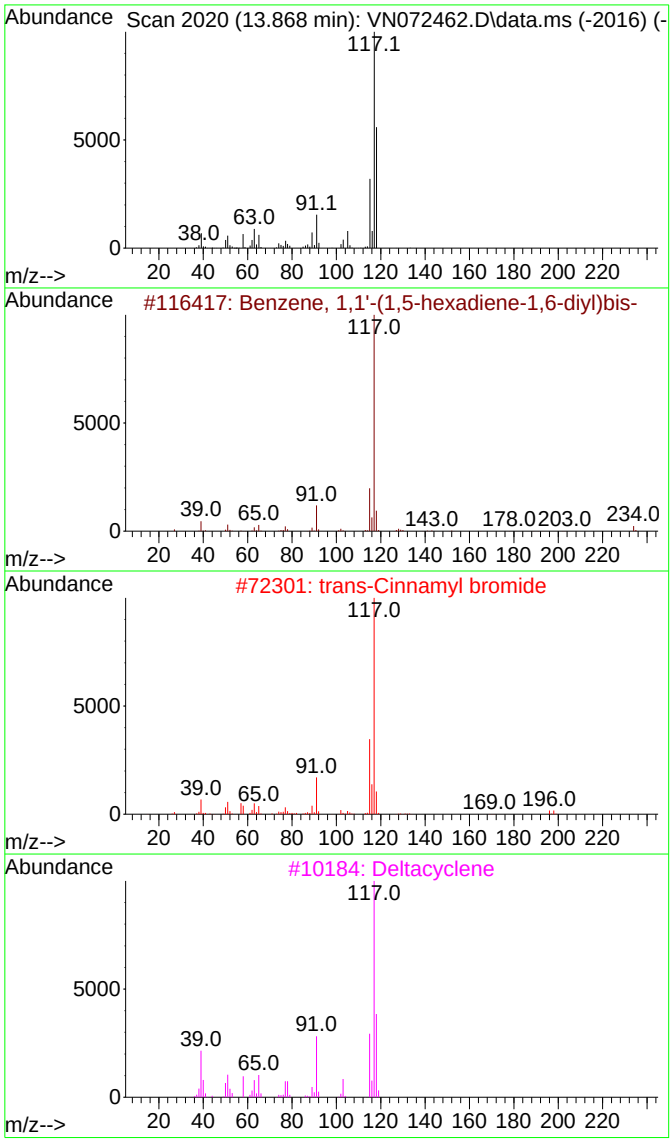
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

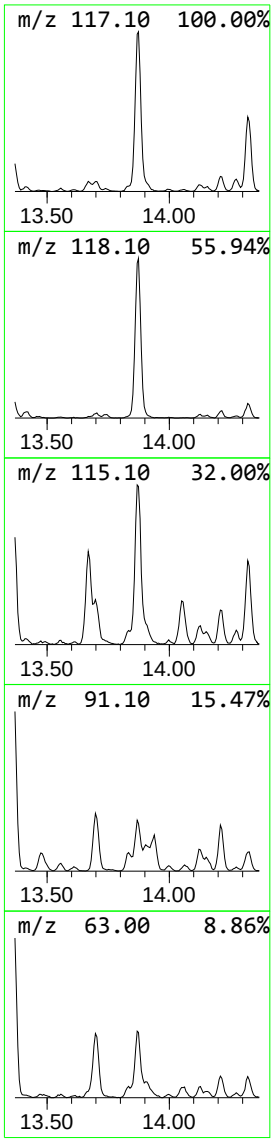
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	25.85 ug/l	1949540	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
2	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59
3	Deltacyclene	118	C9H10	007785-10-6	59
4	Indole	117	C8H7N	000120-72-9	49
5	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072462.D
Acq On : 12 May 2022 18:57
Operator : JC\MD
Sample : N2800-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP051022

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.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-	3.122	84.6	ug/l	3900080	1	8.086	2305700	50.0
Pentane	3.510	63.0	ug/l	2906280	1	8.086	2305700	50.0
Pentane, 2-methyl-	5.151	73.6	ug/l	3394230	1	8.086	2305700	50.0
Pentane, 3-methyl-	5.622	51.4	ug/l	2369170	1	8.086	2305700	50.0
n-Hexane	6.122	25.8	ug/l	1188650	1	8.086	2305700	50.0
Cyclopentane, m...	7.145	68.8	ug/l	3174140	1	8.086	2305700	50.0
Cyclopentane, 1...	8.569	39.3	ug/l	820047	2	8.963	1042750	50.0
Benzene, 1-ethy...	12.980	56.6	ug/l	4270840	4	13.668	3771240	50.0
Benzene, 1-ethy...	13.216	45.7	ug/l	3447530	4	13.668	3771240	50.0
Benzene, 1,1'-(...	13.868	25.9	ug/l	1949540	4	13.668	3771240	50.0