LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040222\
Data File : VN071817.D
Acq On : 02 Apr 2022 22:59
Operator : JC\MD
Sample : N2242-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

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\82N033022W.M
Title : SW846 8260

Signal : TIC: VN071817.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.134	185	195	221	rVB	4845139	11036763	8.26%	2.168%
2	3.516	250	260	281	rVB2	1962190	5110646	3.82%	1.004%
3	3.999	333	342	359	rVB	730021	1985738	1.49%	0.390%
4	4.263	373	387	410	rVB2	419860	1504020	1.13%	0.295%
5	5.093	515	528	529	rVV2	631390	1789104	1.34%	0.351%
6	5.152	530	538	567	rVB3	1909637	8415667	6.30%	1.653%
7	5.616	600	617	639	rBV2	3282649	11621376	8.70%	2.282%
8	6.122	689	703	719	rBV	671861	2056237	1.54%	0.404%
9	6.469	755	762	774	rVB	514505	1545300	1.16%	0.303%
10	6.904	825	836	851	rVB	562983	1625045	1.22%	0.319%
11	7.146	868	877	886	rBV	1449707	4125604	3.09%	0.810%
12	7.846	988	996	1005	rVB	1342533	3189796	2.39%	0.626%
13	8.081	1029	1036	1045	rVV5	1418538	4213362	3.15%	0.828%
14	8.175	1045	1052	1063	rVB	915828	2357109	1.76%	0.463%
15	8.298	1063	1073	1080	rBV	734424	1687708	1.26%	0.331%
16	8.457	1089	1100	1111	rBV	11966330	28559855	21.37%	5.609%
17	8.628	1112	1129	1138	rVV6	1687585	7076079	5.30%	1.390%
18	8.963	1177	1186	1193	rBV3	1926282	4467475	3.34%	0.877%
19	9.457	1253	1270	1276	rBV2	925314	2967276	2.22%	0.583%
20	10.016	1361	1365	1371	rVB2	780136	1470648	1.10%	0.289%
21	10.440	1429	1437	1441	rBV	2393856	4523842	3.39%	0.888%
22	10.504	1441	1448	1461	rVV2	31395005	59480636	44.52%	11.682%
23	11.128	1548	1554	1564	rVB	759229	1422781	1.06%	0.279%
24	11.739	1649	1658	1668	rBV	2121332	4085225	3.06%	0.802%
25	11.839	1668	1675	1685	rVV	20554574	34473194	25.80%	6.771%
26	11.945	1685	1693	1707	rVB3	65192914	133614429	100.00%	26.242%
27	12.275	1737	1749	1759	rBV	18233028	30861847	23.10%	6.061%
28	12.575	1794	1800	1808	rVB	1833742	2951217	2.21%	0.580%
29	12.728	1819	1826	1833	rBV	1668856	2860949	2.14%	0.562%
30	12.916	1851	1858	1863	rBV	1899730	3027496	2.27%	0.595%
31	12.981	1863	1869	1872	rVV	10682095	17835837	13.35%	3.503%
32	13.010	1872	1874	1878	rVV	4482545	6240733	4.67%	1.226%
33	13.057	1878	1882	1889	rVB	5429933	8473448	6.34%	1.664%
34	13.216	1901	1909	1919	rBV	4726788	7749470	5.80%	1.522%
35	13.363	1919	1934	1948	rVB	21983682	35451756	26.53%	6.963%
36	13.698	1987	1991	2007	rVB	5985326	10350489	7.75%	2.033%

LSC Area Percent Report

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Operator : JC\MD
Sample : N2242-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

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\82N033022W.M
Title : SW846 8260

37	13.875	2015	2021	2037	rVB3	6782993	15146154	11.34%	2.975%
38	14.128	2058	2064	2066	rBV	1229599	1964183	1.47%	0.386%
39	14.151	2066	2068	2073	rVV	1084763	1620376	1.21%	0.318%
40	14.210	2073	2078	2084	rVB	1818948	2875991	2.15%	0.565%
41	14.322	2092	2097	2106	rVB2	1390461	2274113	1.70%	0.447%
42	14.533	2125	2133	2136	rBV	1064170	1683930	1.26%	0.331%
43	14.575	2136	2140	2145	rVB	1448368	2077566	1.55%	0.408%
44	14.804	2174	2179	2184	rBV	1217079	1856997	1.39%	0.365%
45	14.927	2191	2200	2206	rBV3	1942562	4061540	3.04%	0.798%
46	15.498	2284	2297	2309	rBV	2814342	5393336	4.04%	1.059%

Sum of corrected areas: 509162343

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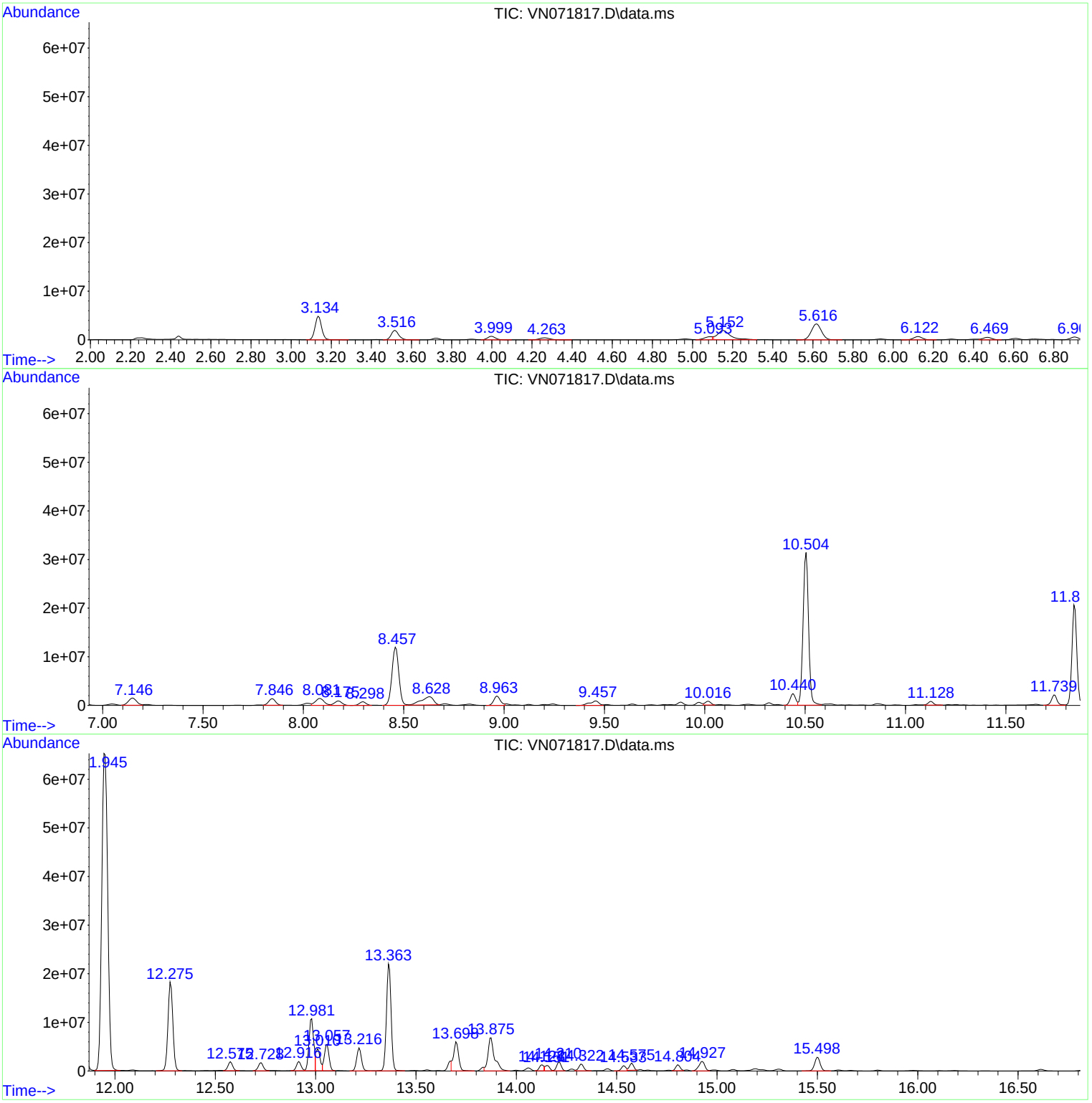
MSVOA_N
ClientSampleId :
MW-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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



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Data File : VN071817.D
Acq On : 02 Apr 2022 22:59
Operator : JC\MD
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

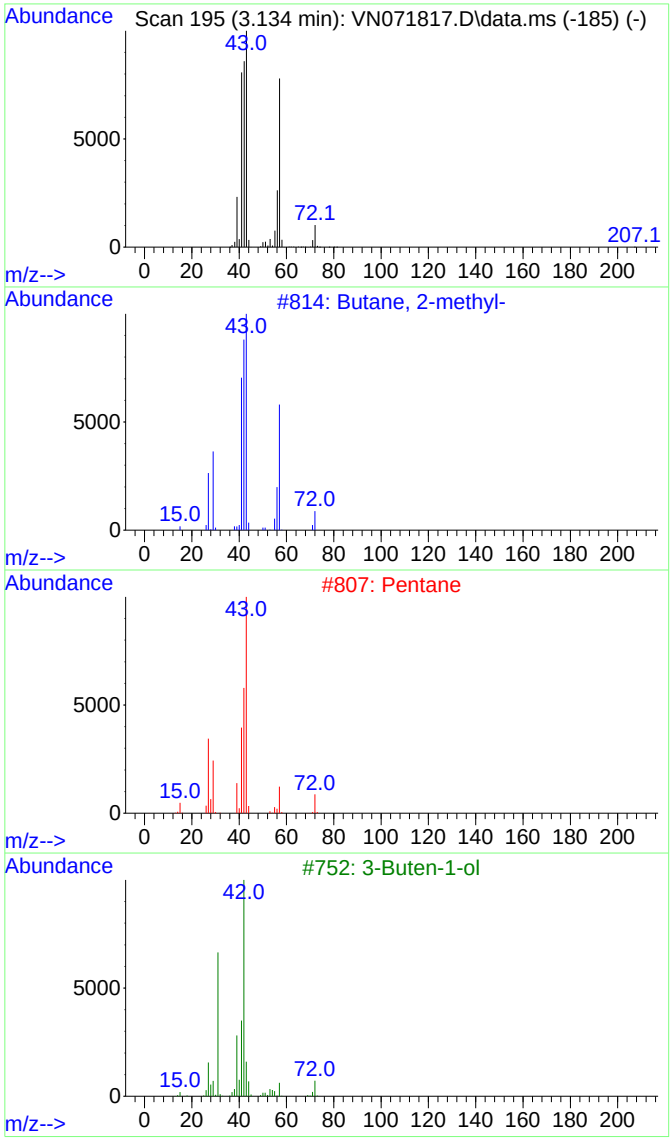
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

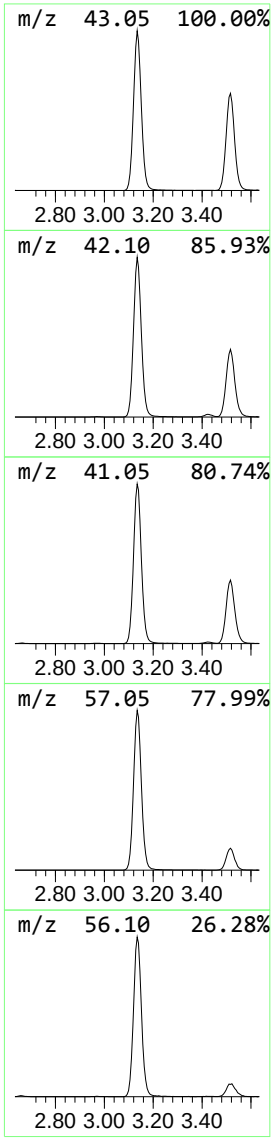
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.134	130.97 ug/l	11036800	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	87
2	Pentane	72	C5H12	000109-66-0	42
3	3-Buten-1-ol	72	C4H8O	000627-27-0	25
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	12
5	Butane, 2-nitro-	103	C4H9NO2	000600-24-8	10





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Data File : VN071817.D
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Operator : JC\MD
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

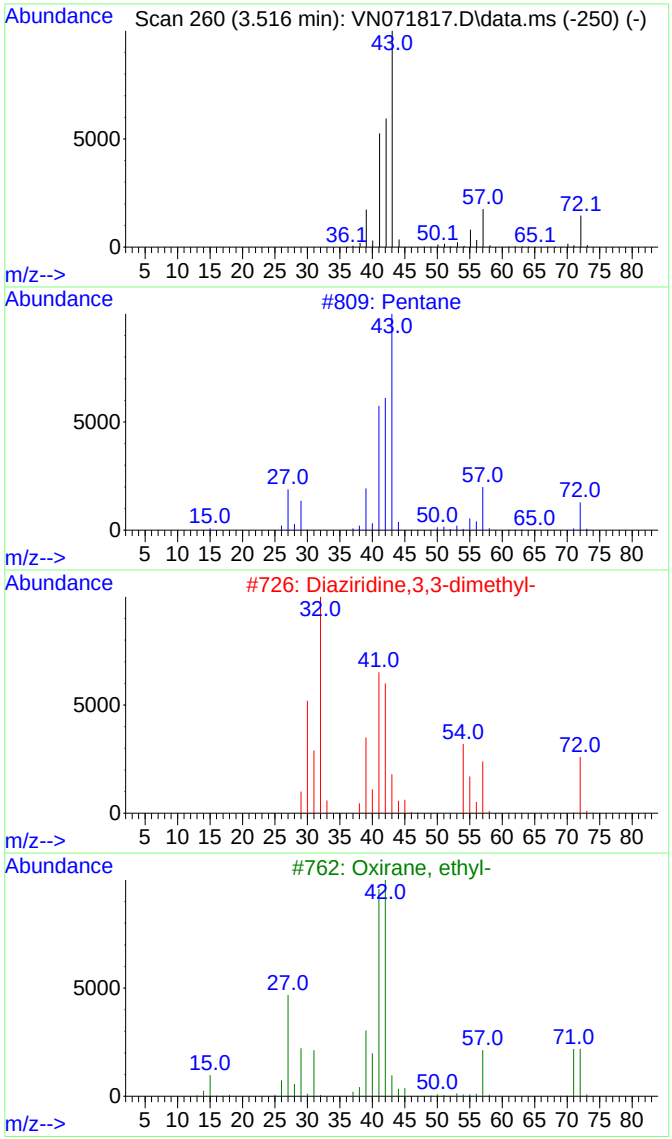
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

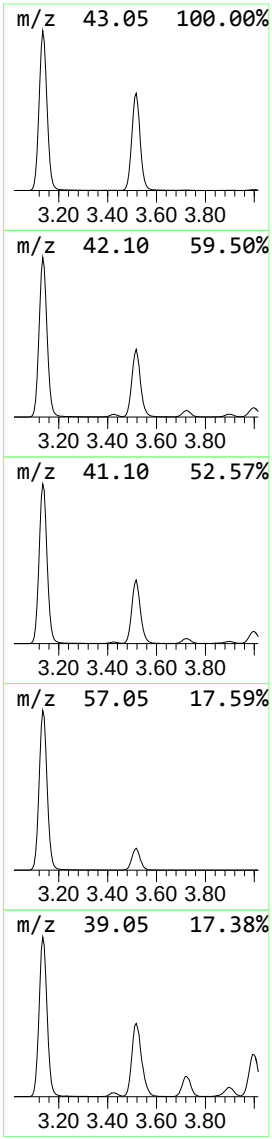
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.516	60.65 ug/l	5110650	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	9
4	Butane, 2-methyl-	72	C5H12	000078-78-4	9
5	Butanal, 2-ethyl-	100	C6H12O	000097-96-1	9





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Data File : VN071817.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 :
MW-3

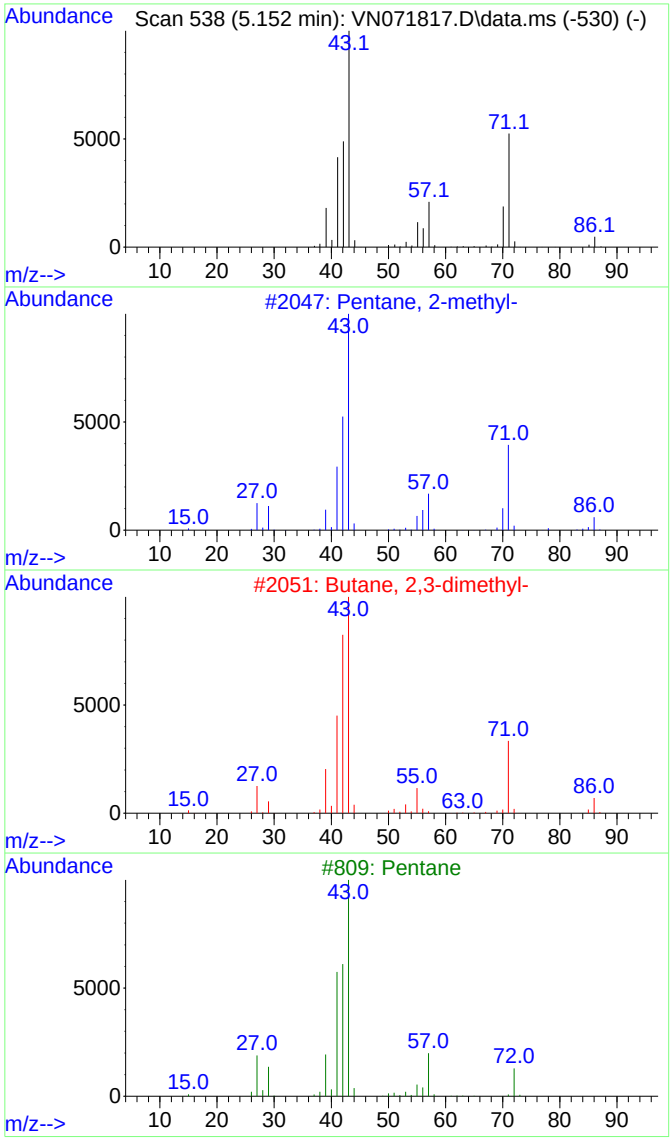
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

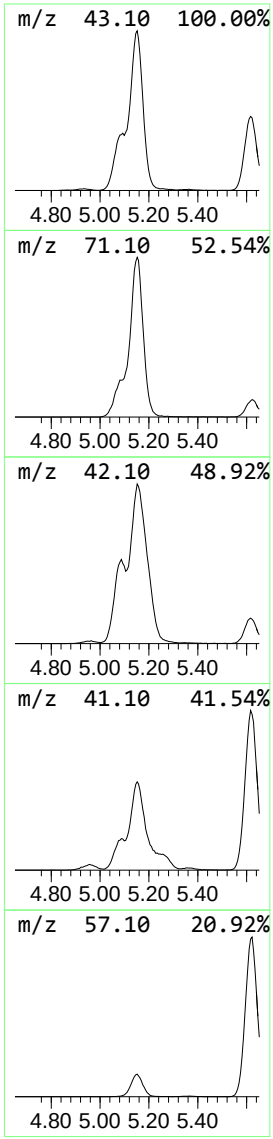
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.152	99.87 ug/l	8415670	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	47
3	Pentane	72	C5H12	000109-66-0	38
4	Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	38
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	38





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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 :
MW-3

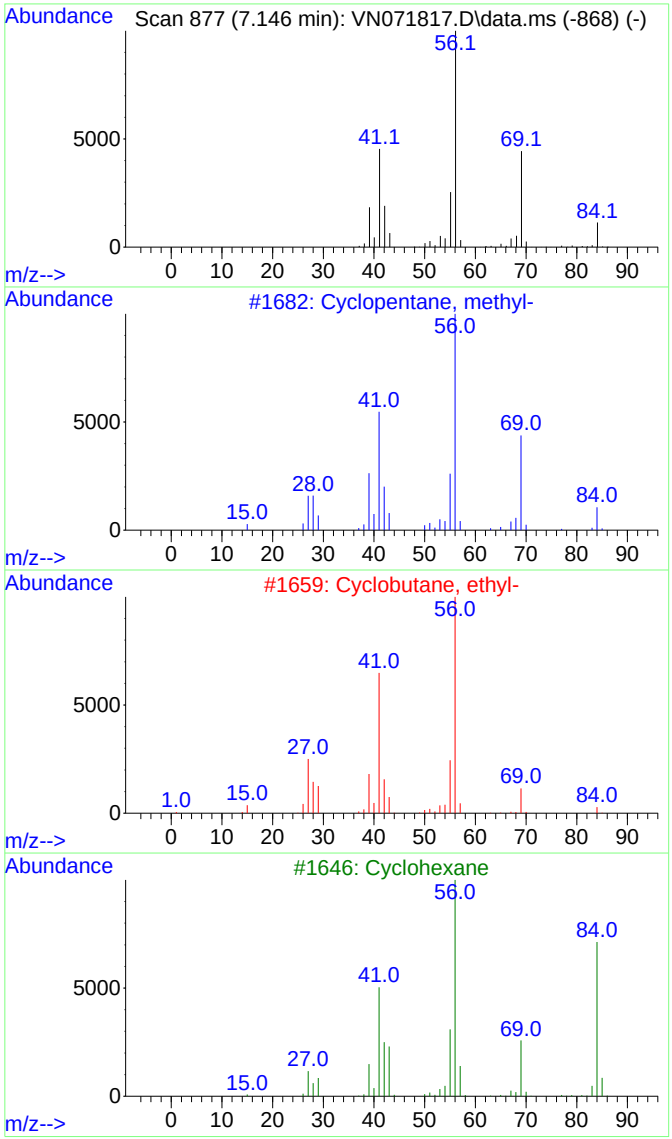
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

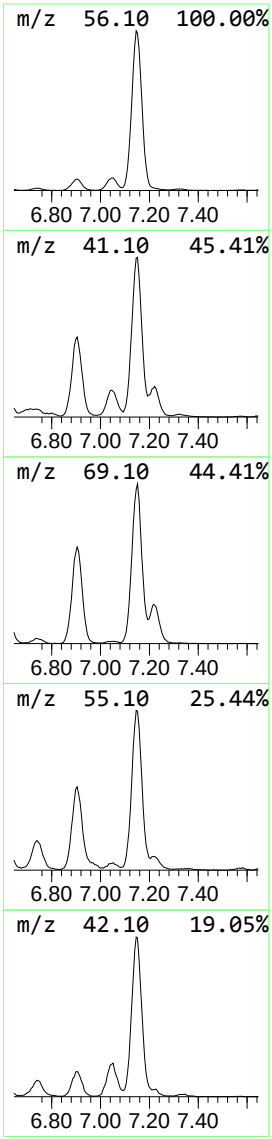
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.146	48.96 ug/l	4125600	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
3	Cyclohexane	84	C6H12	000110-82-7	64
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43





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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 :
MW-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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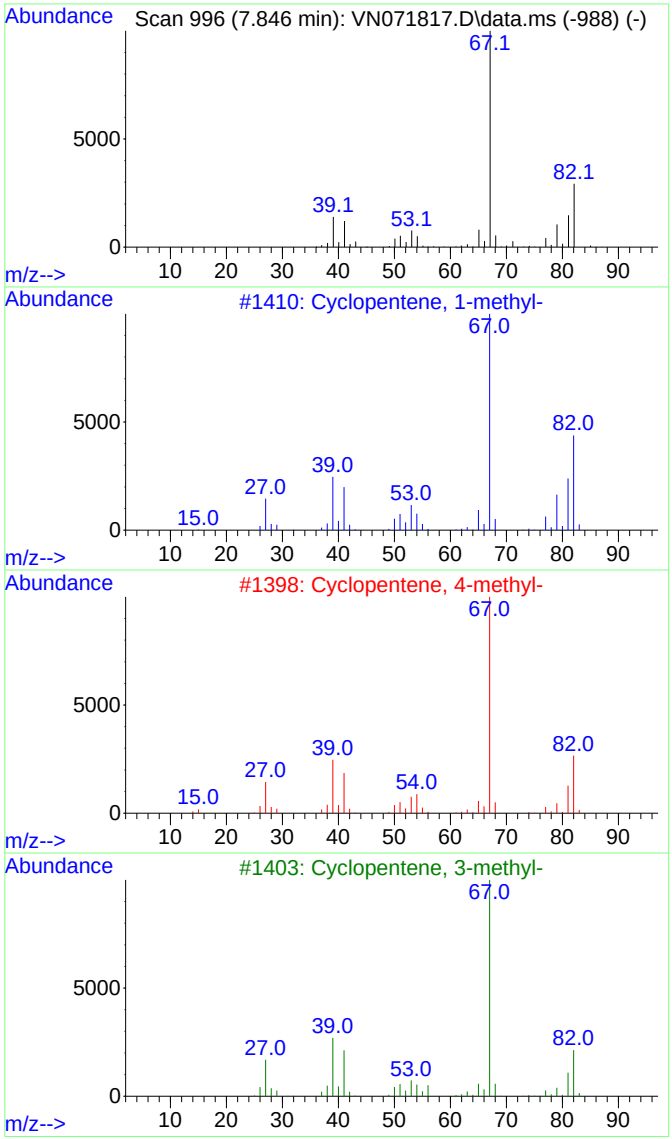
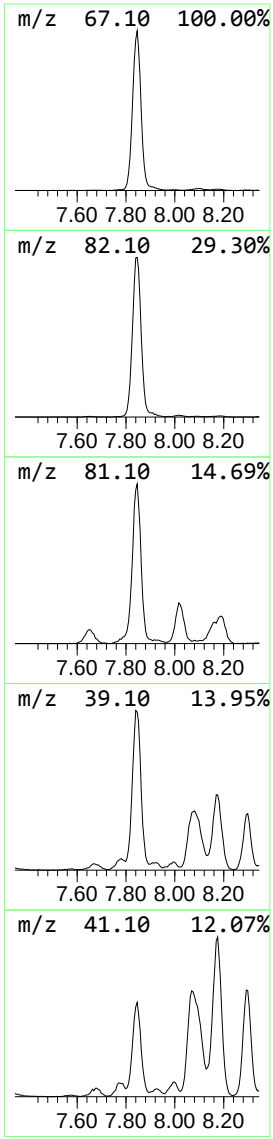
****
Peak Number 5 Cyclopentene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.846	37.85 ug/l	3189800	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 1-methyl-	82	C6H10	000693-89-0	90
2	Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	90
3	Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	87
4	1,4-Pentadiene, 2-methyl-	82	C6H10	000763-30-4	83
5	Cyclopentane, methylene-	82	C6H10	001528-30-9	80





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Instrument :
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ClientSampleId :
MW-3

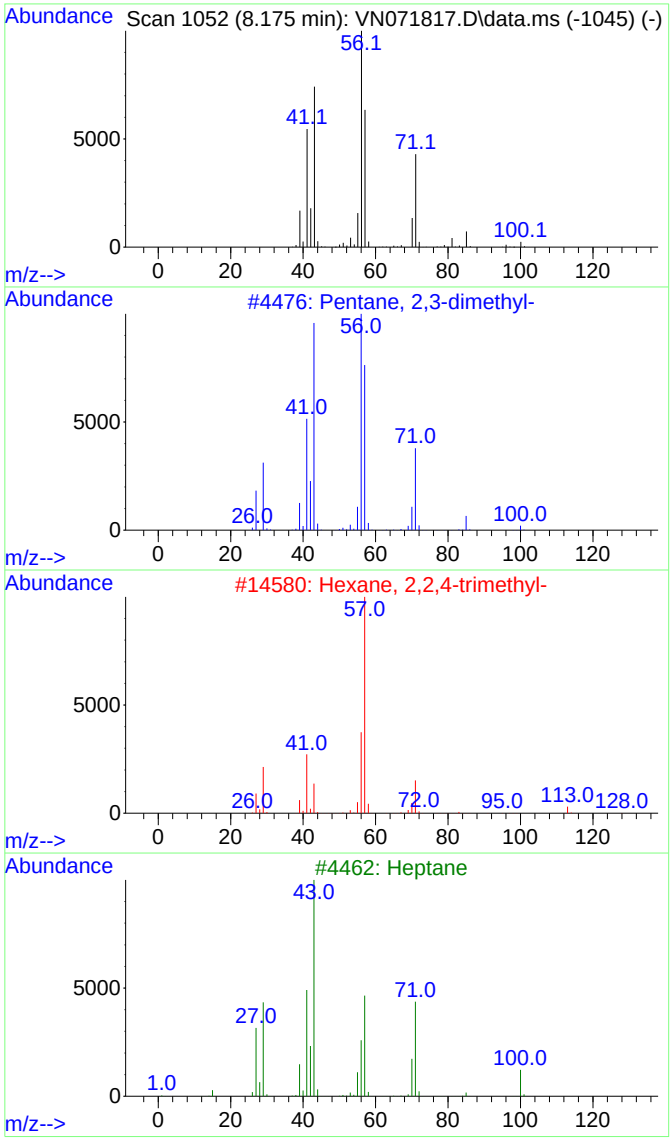
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

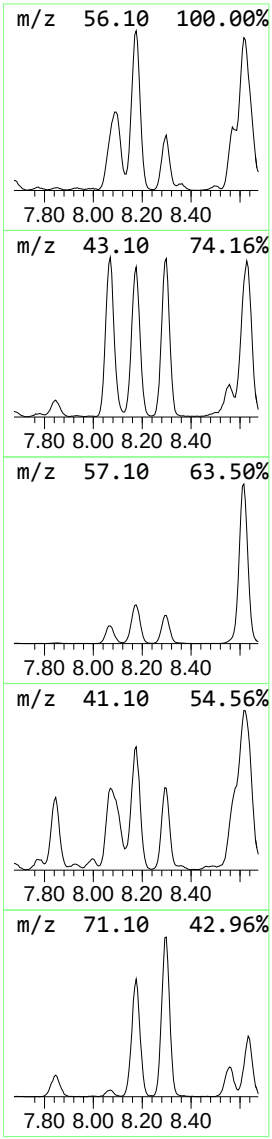
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Pentane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.175	27.97 ug/l	2357110	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
3	Heptane	100	C7H16	000142-82-5	37
4	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	37
5	Hexane, 3-methyl-	100	C7H16	000589-34-4	32





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

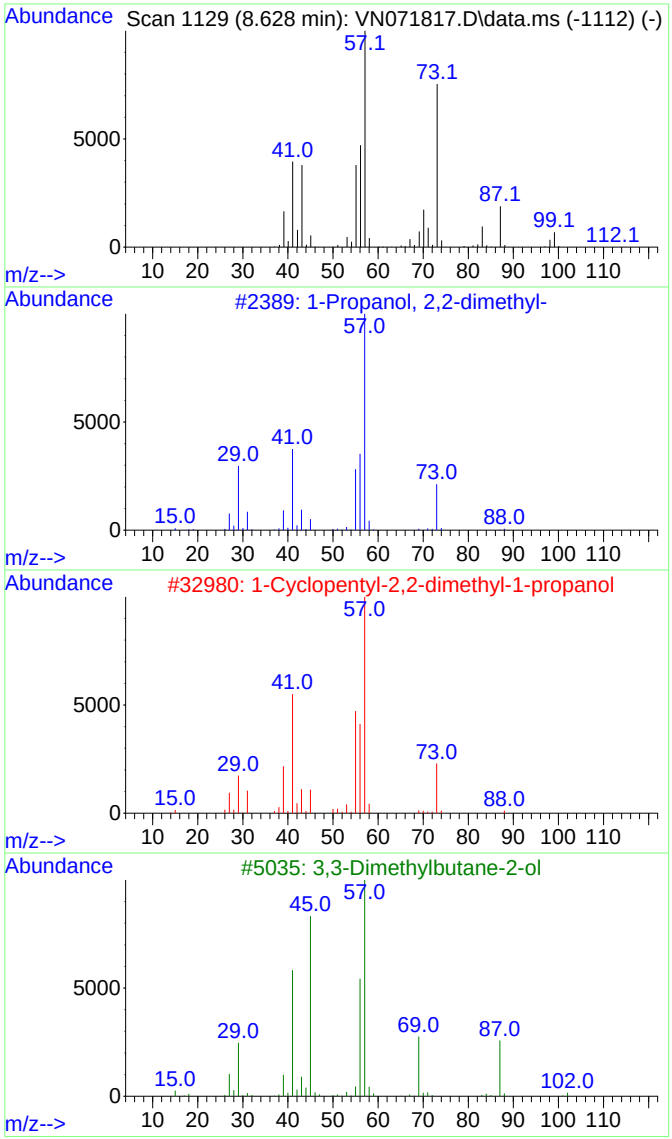
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

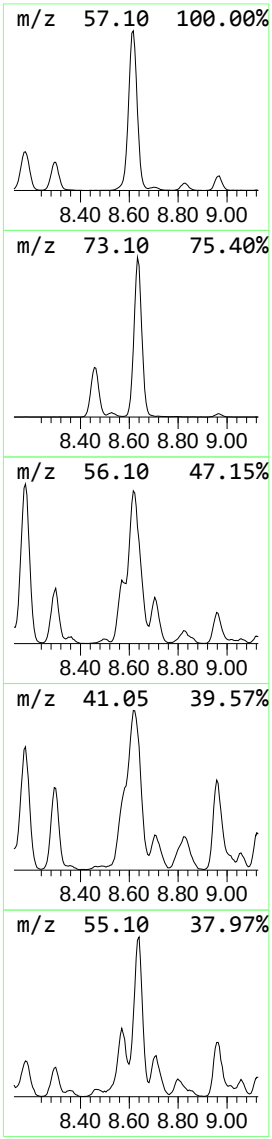
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Propanol, 2,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.628	79.20 ug/l	7076080	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2,2-dimethyl-	88	C5H12O	000075-84-3	50
2	1-Cyclopentyl-2,2-dimethyl-1-pro...	156	C10H20O	337966-85-5	40
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	37
4	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	35
5	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	32





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Data File : VN071817.D
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Operator : JC\MD
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

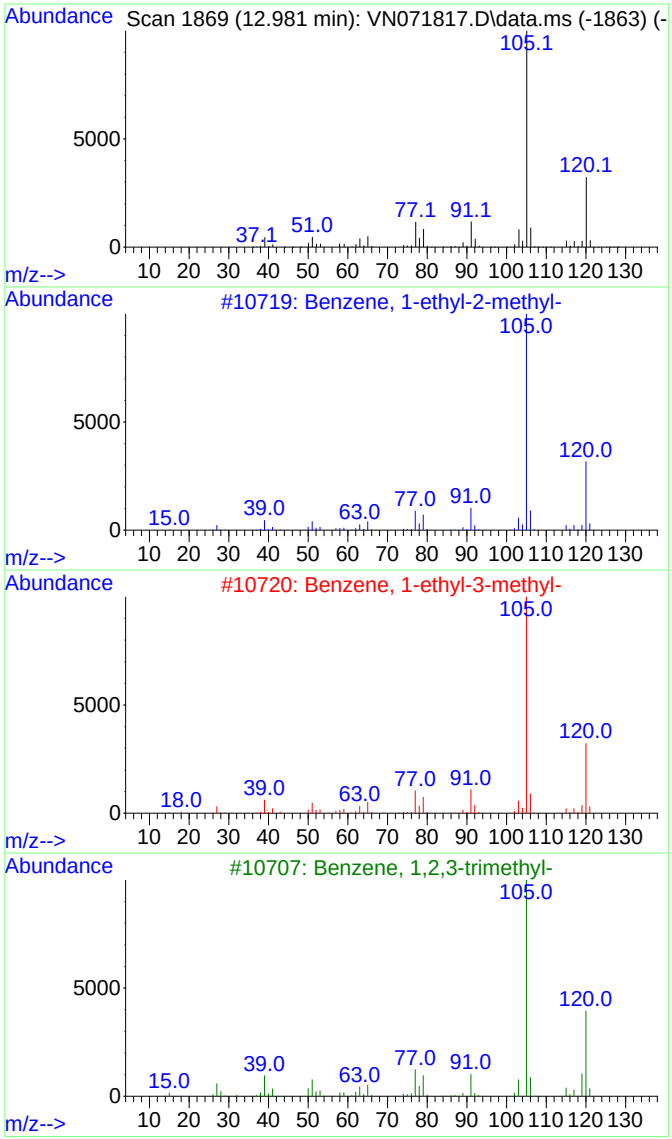
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

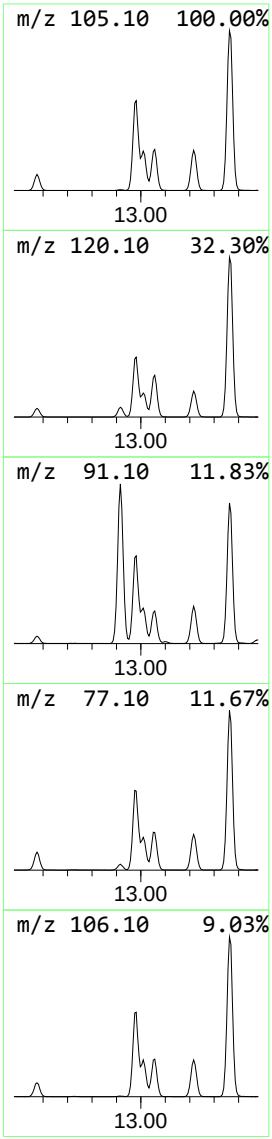
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	86.16 ug/l	17835800	1,4-Dichlorobenzene-d4	13.669

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	95
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040222\
Data File : VN071817.D
Acq On : 02 Apr 2022 22:59
Operator : JC\MD
Sample : N2242-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

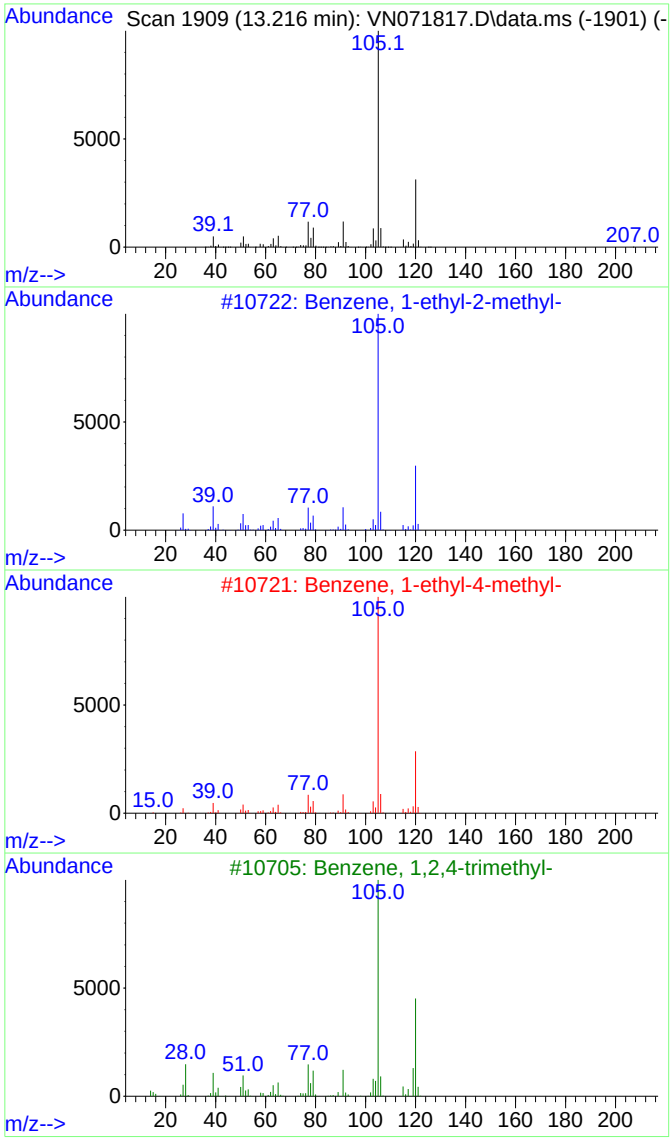
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

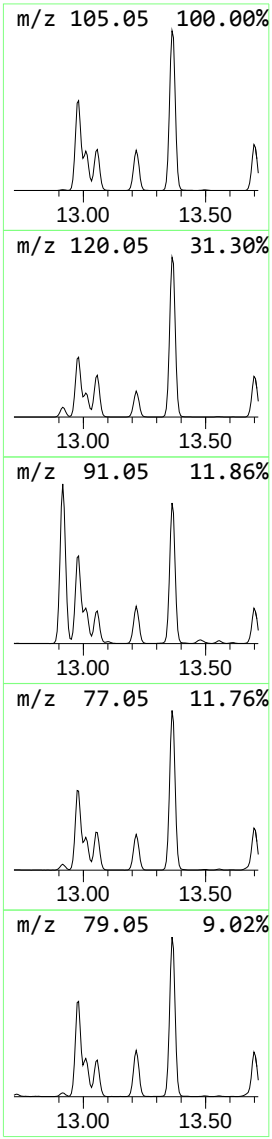
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	37.44 ug/l	7749470	1,4-Dichlorobenzene-d4	13.669

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	91
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040222\
Data File : VN071817.D
Acq On : 02 Apr 2022 22:59
Operator : JC\MD
Sample : N2242-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

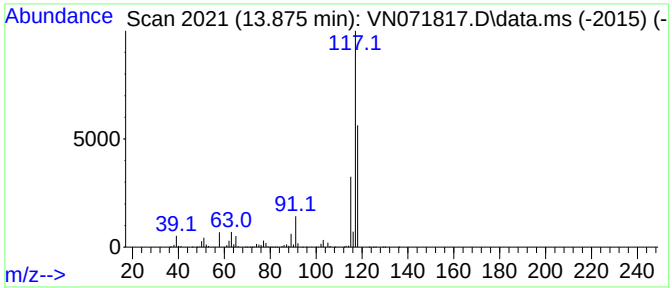
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

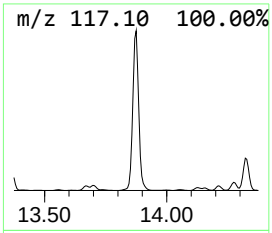
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

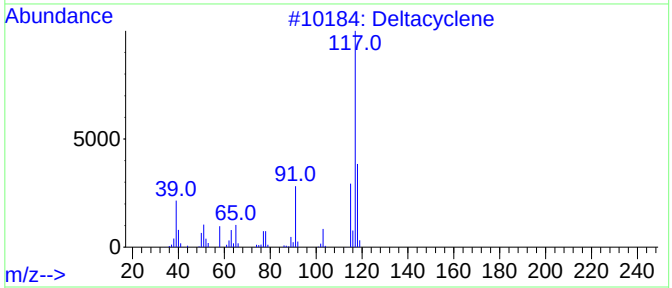
****
Peak Number 10 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 5

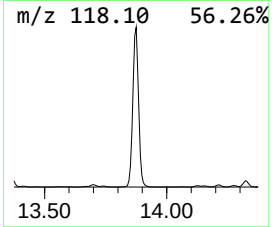
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.875	73.17 ug/l	15146200	1,4-Dichlorobenzene-d4	13.669

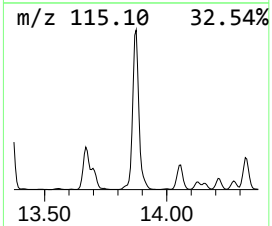
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Deltacyclene	118	C9H10	007785-10-6	64
2	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
3	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	53
4	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	53
5	Indole	117	C8H7N	000120-72-9	46

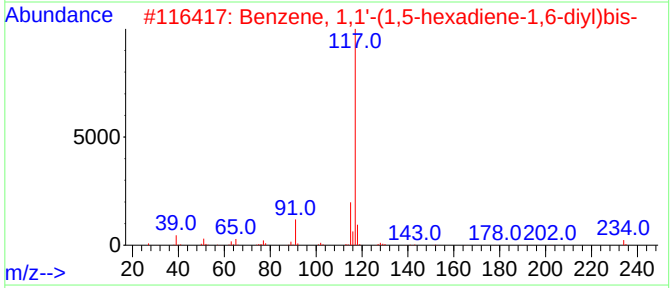


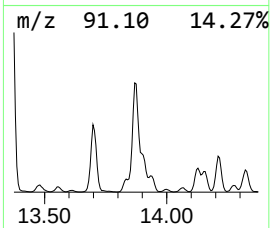


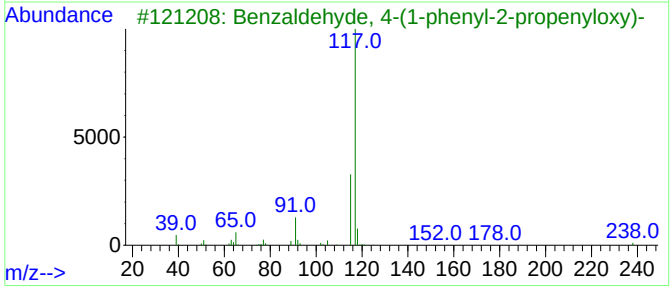


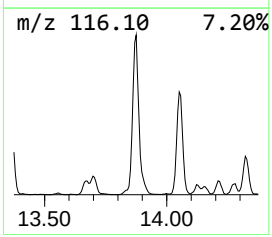












Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040222\
Data File : VN071817.D
Acq On : 02 Apr 2022 22:59
Operator : JC\MD
Sample : N2242-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.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-	3.134	131.0	ug/l	11036800	1	8.081	4213360	50.0
Pentane	3.516	60.6	ug/l	5110650	1	8.081	4213360	50.0
Pentane, 2-methyl-	5.152	99.9	ug/l	8415670	1	8.081	4213360	50.0
Cyclopentane, m...	7.146	49.0	ug/l	4125600	1	8.081	4213360	50.0
Cyclopentene, 1...	7.846	37.9	ug/l	3189800	1	8.081	4213360	50.0
Pentane, 2,3-di...	8.175	28.0	ug/l	2357110	1	8.081	4213360	50.0
1-Propanol, 2,2...	8.628	79.2	ug/l	7076080	2	8.963	4467480	50.0
Benzene, 1-ethy...	12.980	86.2	ug/l	17835800	4	13.669	10350500	50.0
Benzene, 1-ethy...	13.216	37.4	ug/l	7749470	4	13.669	10350500	50.0
Benzene, 1,1'-(...	13.875	73.2	ug/l	15146200	4	13.669	10350500	50.0