LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042022\
Data File : VN072106.D
Acq On : 21 Apr 2022 03:30
Operator : JC\MD
Sample : N2482-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

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: VN072106.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.263	38	47	61	rBV	3610351	6022253	34.89%	3.875%
2	2.440	67	77	88	rBV	4871124	7672441	44.46%	4.937%
3	2.540	88	94	106	rVV	388501	654789	3.79%	0.421%
4	2.657	108	114	124	rVB	244590	415015	2.40%	0.267%
5	2.969	159	167	180	rVB	154798	337779	1.96%	0.217%
6	3.134	184	195	222	rBV	7464809	17258743	100.00%	11.105%
7	3.422	236	244	251	rBV2	124352	287925	1.67%	0.185%
8	3.516	251	260	283	rVB3	1566435	4937444	28.61%	3.177%
9	3.722	283	295	308	rBV	818693	2032922	11.78%	1.308%
10	3.898	310	325	332	rVV	484091	1314555	7.62%	0.846%
11	3.992	332	341	363	rVB	1502026	4148040	24.03%	2.669%
12	4.257	371	386	404	rVB4	65201	270706	1.57%	0.174%
13	4.963	491	506	515	rBV3	145843	527300	3.06%	0.339%
14	5.087	515	527	530	rVV3	253687	833285	4.83%	0.536%
15	5.163	531	540	571	rVB7	501545	3382702	19.60%	2.177%
16	5.622	602	618	634	rBV	399501	1381872	8.01%	0.889%
17	5.934	659	671	689	rVB2	98815	327170	1.90%	0.211%
18	6.122	691	703	718	rBV2	89029	274094	1.59%	0.176%
19	6.469	752	762	774	rVB	326509	962186	5.58%	0.619%
20	6.604	774	785	794	rVV	199128	618337	3.58%	0.398%
21	6.692	794	800	812	rVV3	78355	318012	1.84%	0.205%
22	6.904	826	836	851	rVB	217371	634135	3.67%	0.408%
23	7.145	865	877	887	rBV	1134608	3382970	19.60%	2.177%
24	7.839	988	995	1005	rVB	185577	462753	2.68%	0.298%
25	8.022	1016	1026	1030	rBV	447732	1076080	6.23%	0.692%
26	8.086	1030	1037	1047	rVV2	1181953	3006046	17.42%	1.934%
27	8.175	1047	1052	1065	rVB4	86237	239950	1.39%	0.154%
28	8.439	1088	1097	1107	rBV2	572046	1739631	10.08%	1.119%
29	8.527	1107	1112	1116	rVV2	119965	290347	1.68%	0.187%
30	8.575	1116	1120	1126	rVV6	129779	355042	2.06%	0.228%
31	8.633	1126	1130	1137	rVV3	115849	302722	1.75%	0.195%
32	8.704	1137	1142	1152	rVB5	79960	208055	1.21%	0.134%
33	8.963	1176	1186	1199	rBV	1389615	3083729	17.87%	1.984%
34	9.457	1256	1270	1279	rBV3	189663	584940	3.39%	0.376%
35	9.969	1349	1357	1362	rBV	202133	379685	2.20%	0.244%
36	10.439	1429	1437	1442	rBV	1944068	3538726	20.50%	2.277%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042022\
Data File : VN072106.D
Acq On : 21 Apr 2022 03:30
Operator : JC\MD
Sample : N2482-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

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	10.504	1442	1448	1463	rVV	1877610	3549369	20.57%	2.284%
38	11.739	1650	1658	1667	rBV	2052021	3603567	20.88%	2.319%
39	11.839	1668	1675	1685	rVV	8176269	13721244	79.50%	8.829%
40	11.951	1685	1694	1706	rVB	7729944	15040499	87.15%	9.678%
41	12.274	1741	1749	1759	rBV	2627275	4416036	25.59%	2.841%
42	12.574	1789	1800	1808	rBV	756341	1250401	7.25%	0.805%
43	12.727	1818	1826	1839	rBV	1608352	2720896	15.77%	1.751%
44	12.915	1851	1858	1864	rBV	1796596	2823216	16.36%	1.817%
45	13.010	1864	1874	1878	rVV	1264286	2365058	13.70%	1.522%
46	13.057	1878	1882	1891	rVB	1251051	1996400	11.57%	1.285%
47	13.215	1901	1909	1922	rBV	1350584	2164175	12.54%	1.393%
48	13.362	1926	1934	1948	rVV	7456705	11849608	68.66%	7.624%
49	13.668	1980	1986	1988	rBV	1904296	2970033	17.21%	1.911%
50	13.698	1988	1991	1999	rVB	2561317	4145059	24.02%	2.667%
51	13.833	2008	2014	2016	rBV	323513	488828	2.83%	0.315%
52	13.874	2016	2021	2037	rVV2	1089286	2476744	14.35%	1.594%
53	14.062	2047	2053	2058	rVV2	151671	251373	1.46%	0.162%
54	14.127	2058	2064	2066	rVV	324167	530842	3.08%	0.342%
55	14.151	2066	2068	2073	rVV	224947	341363	1.98%	0.220%
56	14.209	2073	2078	2084	rVV	665100	1059830	6.14%	0.682%
57	14.321	2092	2097	2107	rVB2	352179	603714	3.50%	0.388%
58	14.451	2113	2119	2126	rBV	197342	318796	1.85%	0.205%
59	14.533	2127	2133	2136	rBV	302522	487064	2.82%	0.313%
60	14.574	2136	2140	2145	rVB	365873	578569	3.35%	0.372%
61	14.804	2173	2179	2185	rBV	251342	406241	2.35%	0.261%
62	14.921	2191	2199	2207	rBV3	517996	1099977	6.37%	0.708%
63	15.498	2285	2297	2310	rBV	447794	893778	5.18%	0.575%

Sum of corrected areas: 155415061

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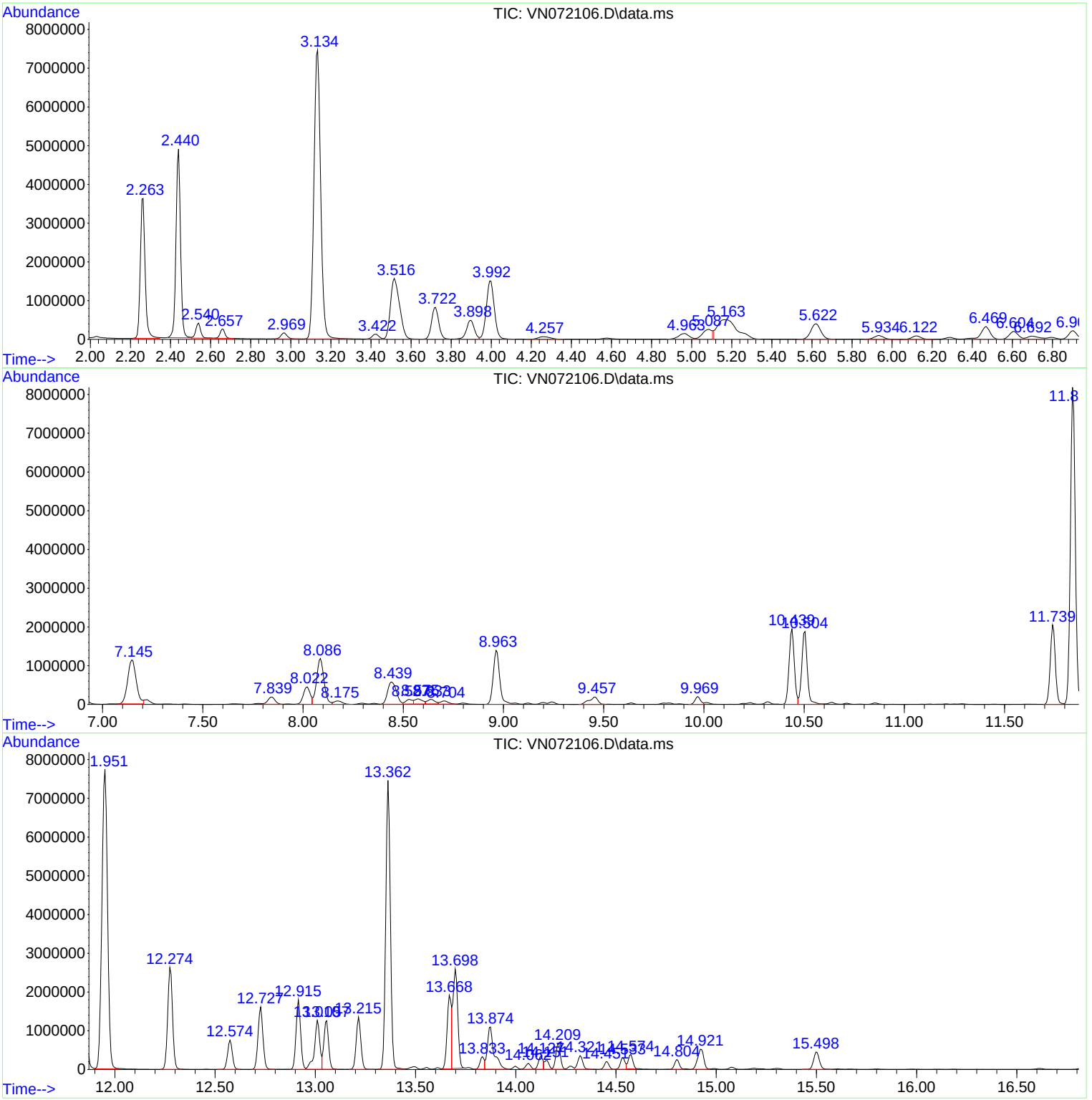
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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



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

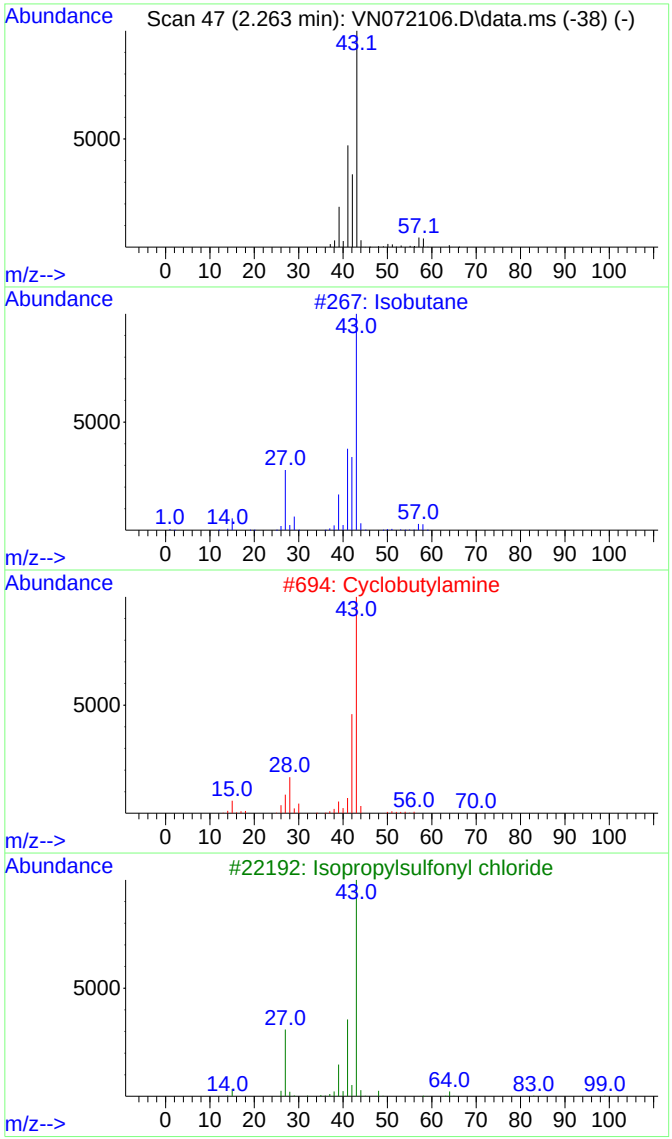
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

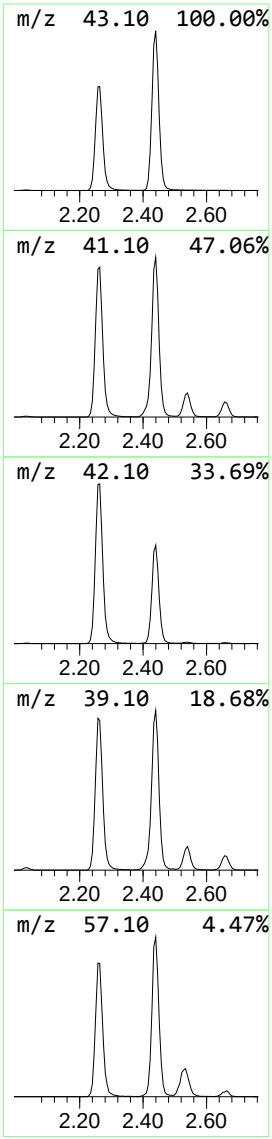
****

Peak Number 1 Isobutane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.263	100.17 ug/l	6022250	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	80
2	Cyclobutylamine	71	C4H9N	002516-34-9	9
3	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4	Hydrogen isocyanate	43	CHNO	000075-13-8	4
5	Isobutyl nitrite	103	C4H9NO2	000542-56-3	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042022\
Data File : VN072106.D
Acq On : 21 Apr 2022 03:30
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

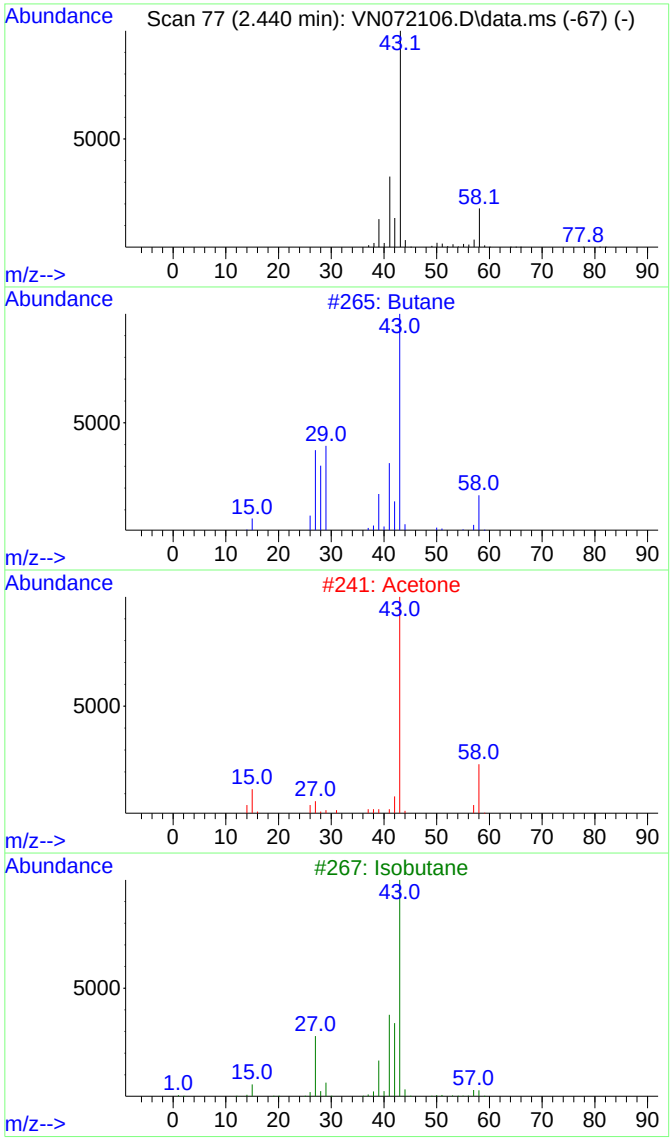
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

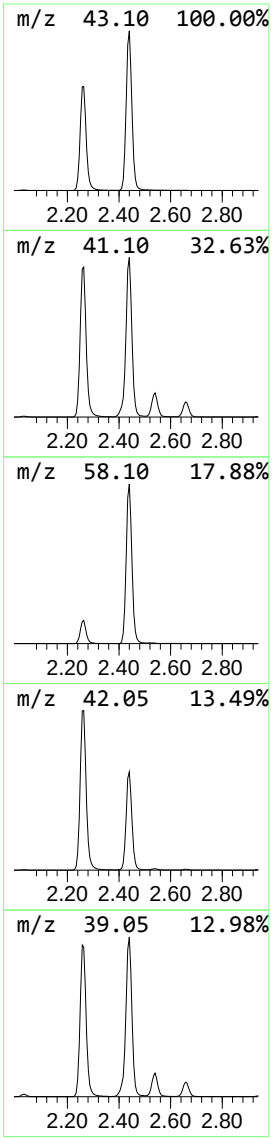
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.440	127.62 ug/l	7672440	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	72
2	Acetone	58	C3H6O	000067-64-1	50
3	Isobutane	58	C4H10	000075-28-5	9
4	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9





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Data File : VN072106.D
Acq On : 21 Apr 2022 03:30
Operator : JC\MD
Sample : N2482-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

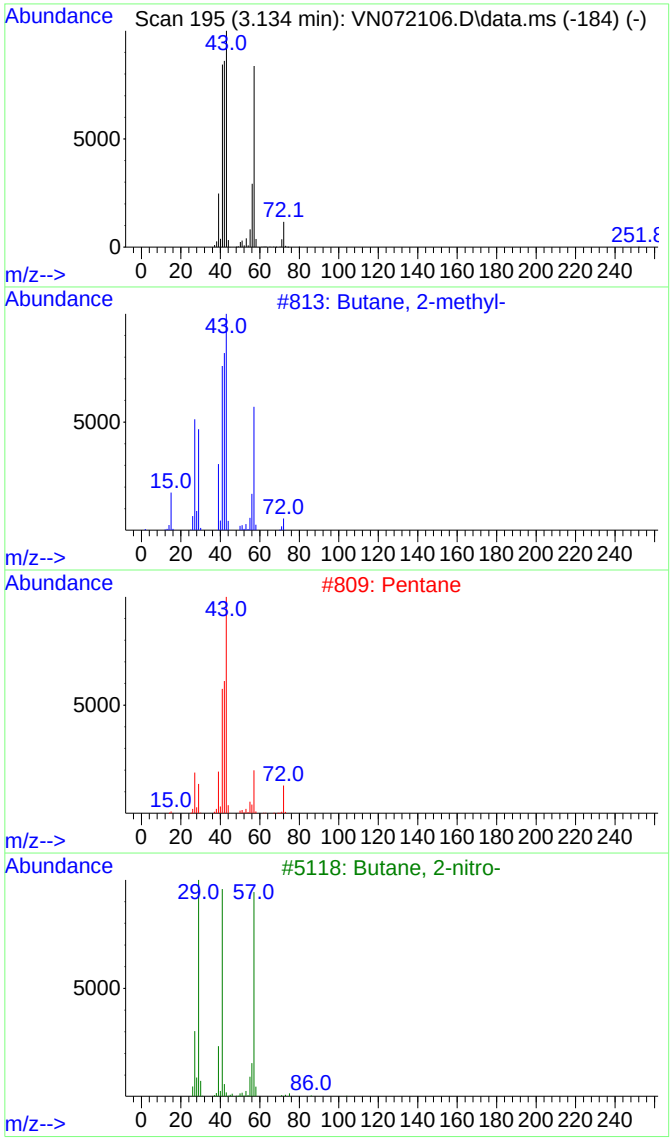
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

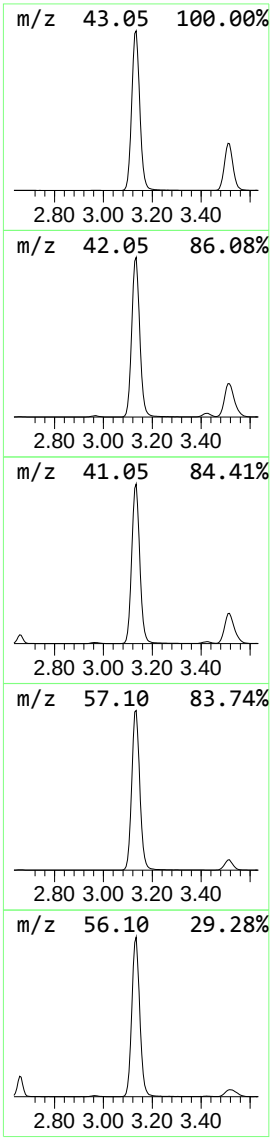
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.134	287.07 ug/l	17258700	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	Pentane	72	C5H12	000109-66-0	38
3	Butane, 2-nitro-	103	C4H9NO2	000600-24-8	10
4	1-Butene	56	C4H8	000106-98-9	10
5	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042022\
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ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

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

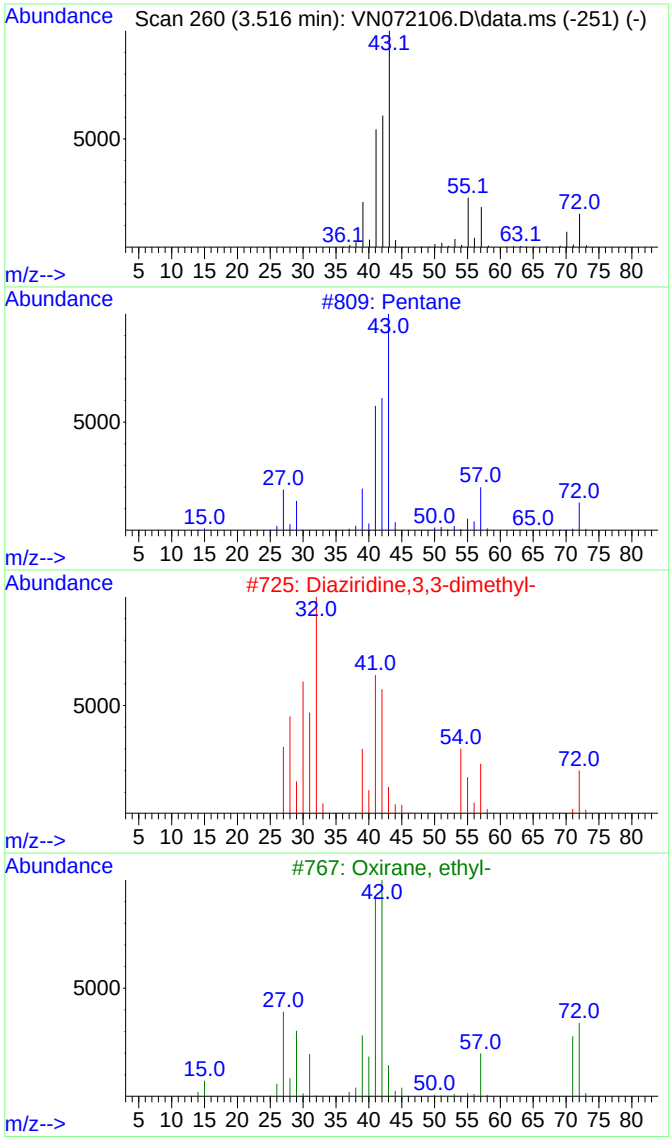
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

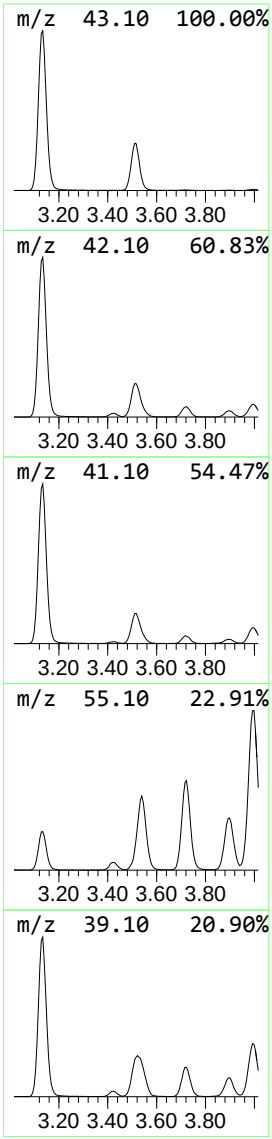
****

Peak Number 4 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.516	82.13 ug/l	4937440	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	90
2	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	38
4	Isobutylene epoxide	72	C4H8O	000558-30-5	25
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	23





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ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

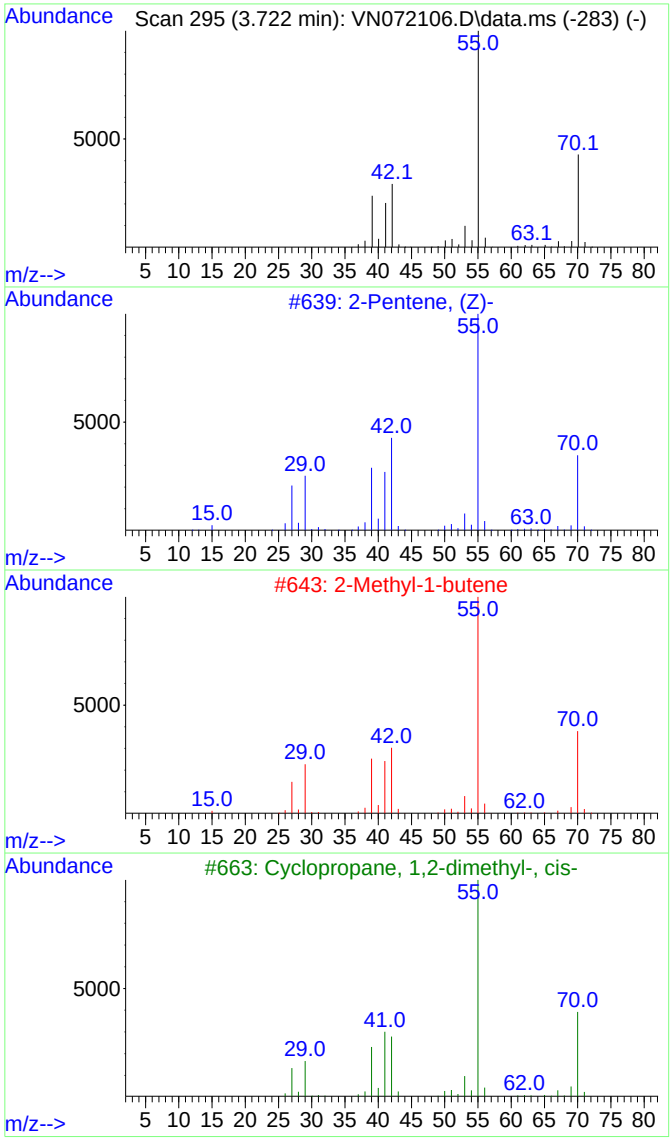
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

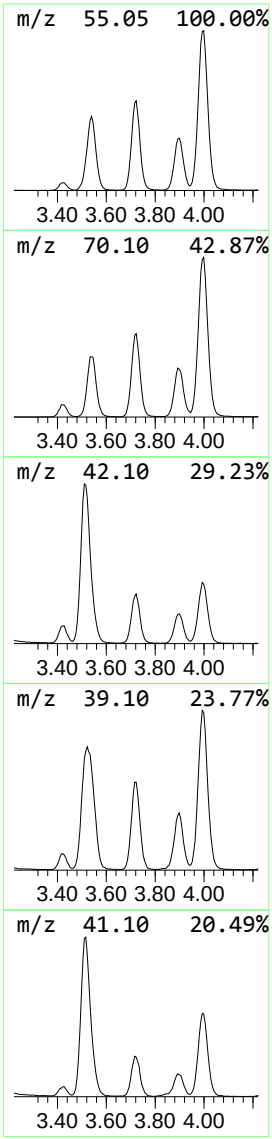
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Pentene, (Z)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.722	33.81 ug/l	2032920	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (Z)-	70	C5H10	000627-20-3	91
2	2-Methyl-1-butene	70	C5H10	000563-46-2	91
3	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
4	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	91
5	2-Butene, 2-methyl-	70	C5H10	000513-35-9	91





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ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

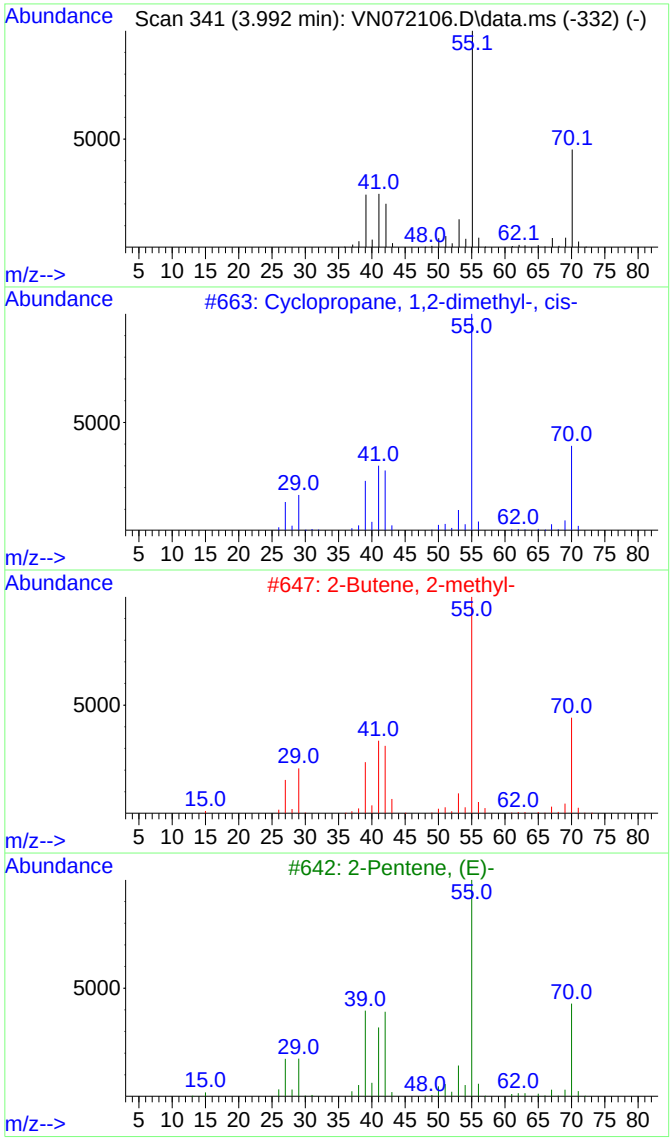
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

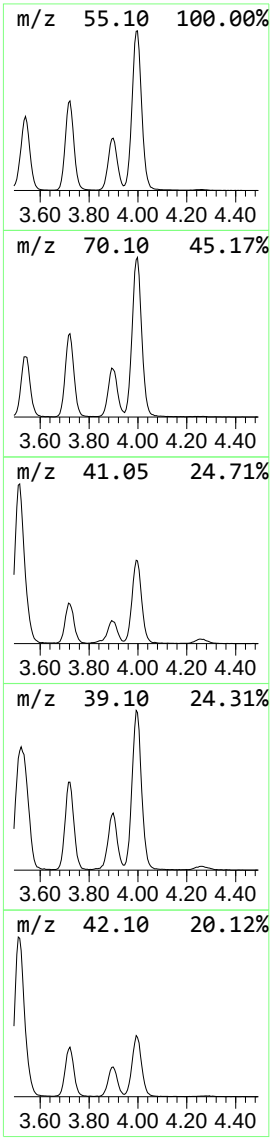
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopropane, 1,2-dimethyl-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.992	69.00 ug/l	4148040	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2	2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
3	2-Pentene, (E)-	70	C5H10	000646-04-8	86
4	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
5	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	80





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ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

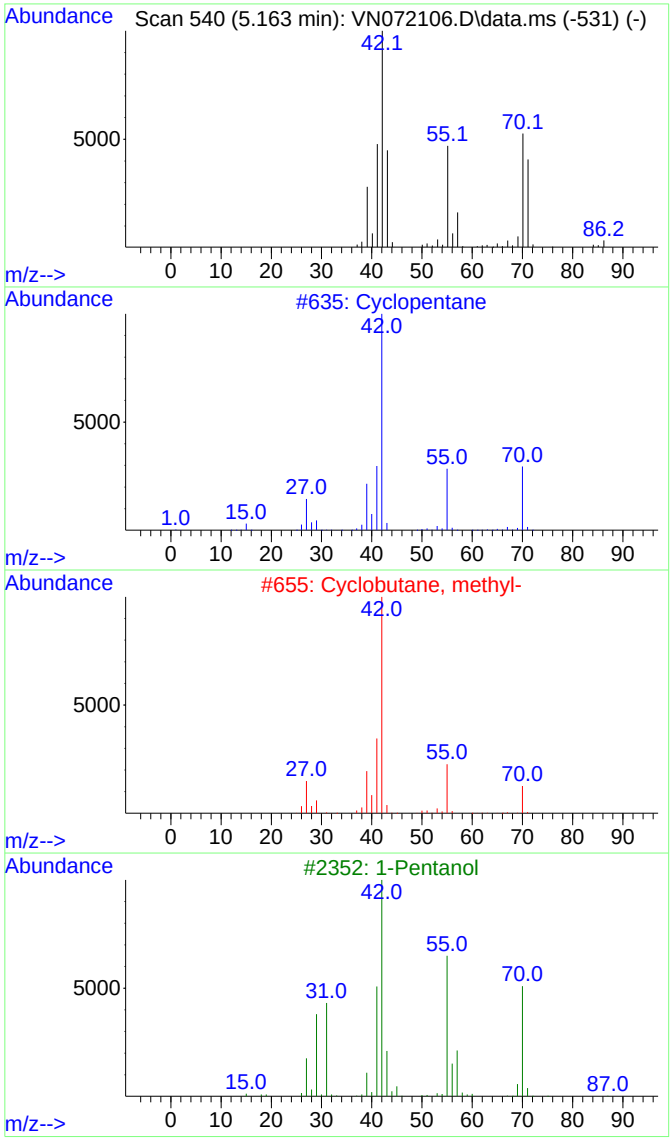
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

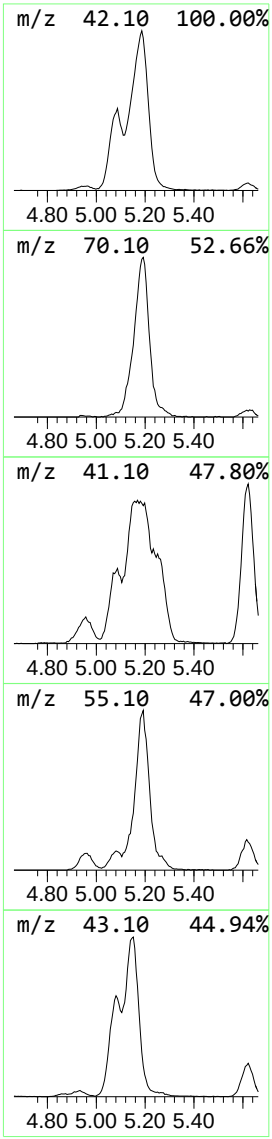
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclopentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.163	56.27 ug/l	3382700	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	58
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	52
3	1-Pentanol	88	C5H12O	000071-41-0	45
4	1-Pentene	70	C5H10	000109-67-1	40
5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	33





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042022\
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MSVOA_N
ClientSampleId :
MW-9R

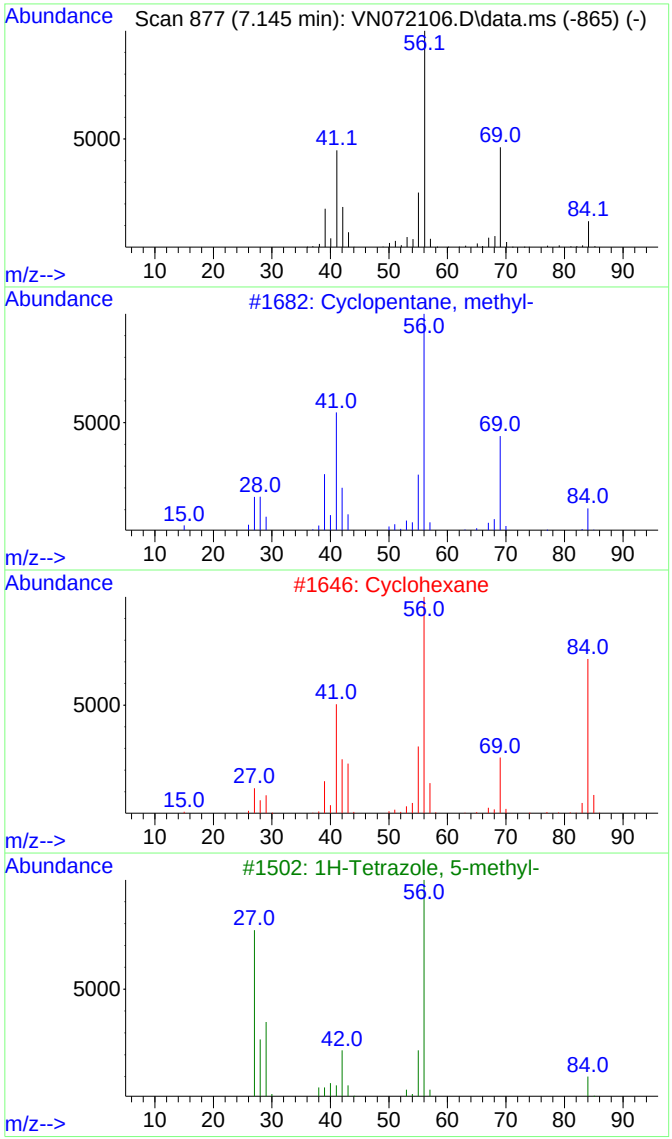
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

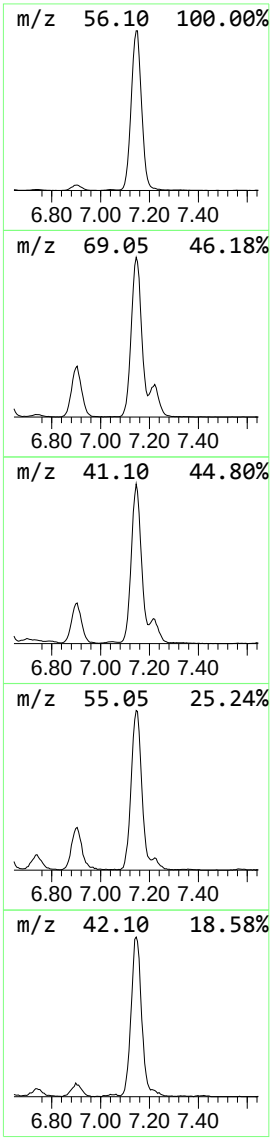
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	56.27 ug/l	3382970	Pentafluorobenzene	8.086

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	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	43





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Data File : VN072106.D
Acq On : 21 Apr 2022 03:30
Operator : JC\MD
Sample : N2482-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

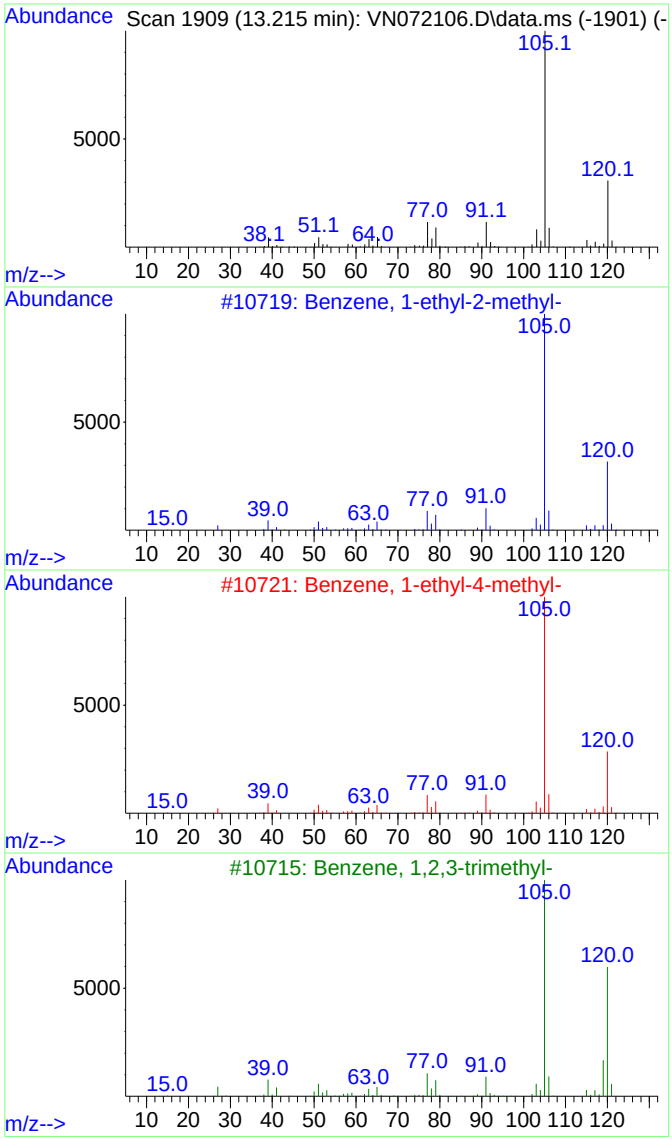
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

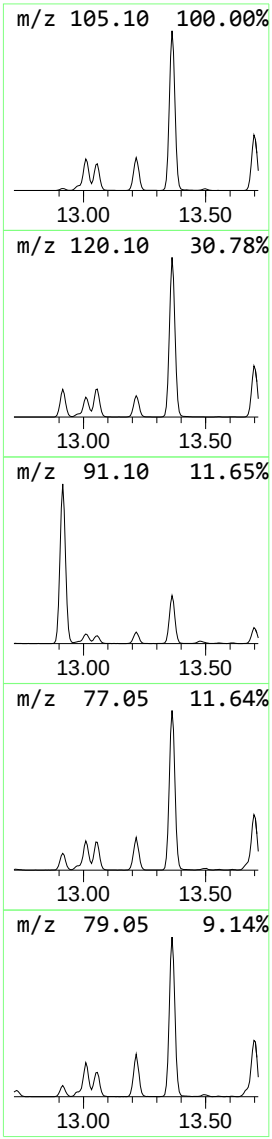
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.215	36.43 ug/l	2164180	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	91
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042022\
Data File : VN072106.D
Acq On : 21 Apr 2022 03:30
Operator : JC\MD
Sample : N2482-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

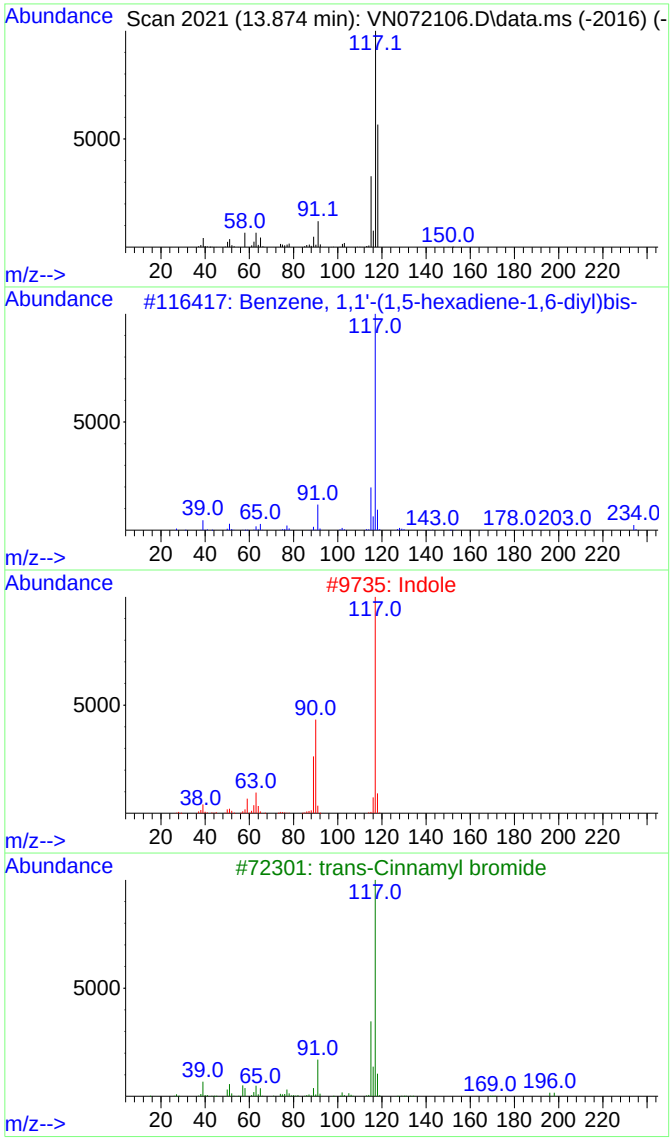
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

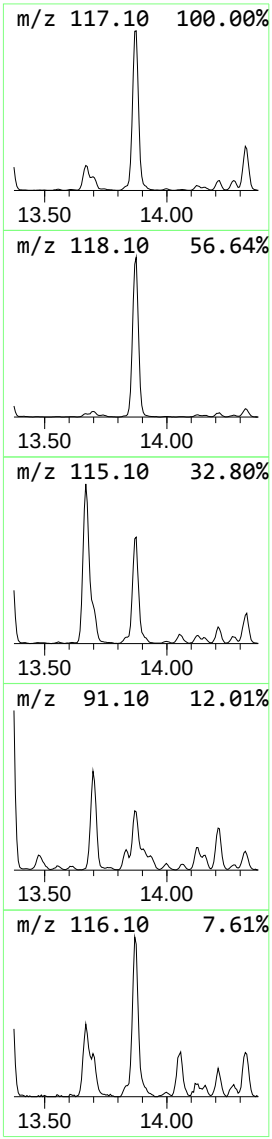
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	41.70 ug/l	2476740	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	53
2	Indole	117	C8H7N	000120-72-9	43
3	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	42
4	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	42
5	m-Aminophenylacetylene	117	C8H7N	054060-30-9	37





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042022\
Data File : VN072106.D
Acq On : 21 Apr 2022 03:30
Operator : JC\MD
Sample : N2482-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-9R

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
Isobutane	2.263	100.2	ug/l	6022250	1	8.086	3006050	50.0
Butane	2.440	127.6	ug/l	7672440	1	8.086	3006050	50.0
Butane, 2-methyl-	3.134	287.1	ug/l	17258700	1	8.086	3006050	50.0
Pentane	3.516	82.1	ug/l	4937440	1	8.086	3006050	50.0
2-Pentene, (Z)-	3.722	33.8	ug/l	2032920	1	8.086	3006050	50.0
Cyclopropane, 1...	3.992	69.0	ug/l	4148040	1	8.086	3006050	50.0
Cyclopentane	5.163	56.3	ug/l	3382700	1	8.086	3006050	50.0
Cyclopentane, m...	7.145	56.3	ug/l	3382970	1	8.086	3006050	50.0
Benzene, 1-ethy...	13.215	36.4	ug/l	2164180	4	13.668	2970030	50.0
Benzene, 1,1'-(...	13.874	41.7	ug/l	2476740	4	13.668	2970030	50.0