LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042022\
Data File : VN072108.D
Acq On : 21 Apr 2022 04:18
Operator : JC\MD
Sample : N2482-13
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-15

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: VN072108.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	38	46	60	rVB5	45833	160282	4.71%	0.463%
2	2.440	72	77	84	rVB2	42390	70220	2.06%	0.203%
3	3.134	184	195	216	rVB	764077	1760530	51.72%	5.083%
4	3.510	248	259	272	rBV	115897	294790	8.66%	0.851%
5	3.993	331	341	357	rBV3	44747	126646	3.72%	0.366%
6	4.281	376	390	409	rBV4	33536	145405	4.27%	0.420%
7	4.575	432	440	453	rBV2	19774	66543	1.96%	0.192%
8	5.081	513	526	532	rBV3	79020	289974	8.52%	0.837%
9	5.157	533	539	567	rVB7	84020	507444	14.91%	1.465%
10	5.622	605	618	635	rBV3	70315	242845	7.13%	0.701%
11	6.463	751	761	772	rVB2	52038	156172	4.59%	0.451%
12	6.604	774	785	794	rBV3	35580	111473	3.28%	0.322%
13	6.898	826	835	852	rBV4	34112	107131	3.15%	0.309%
14	7.145	863	877	886	rBV2	302096	882874	25.94%	2.549%
15	7.216	886	889	900	rVB3	38805	86521	2.54%	0.250%
16	7.416	915	923	934	rVB3	15036	40631	1.19%	0.117%
17	7.839	988	995	1005	rVB3	27968	70332	2.07%	0.203%
18	8.016	1015	1025	1030	rBV	400983	954692	28.05%	2.756%
19	8.081	1030	1036	1047	rVB3	854354	2039643	59.92%	5.889%
20	8.434	1087	1096	1109	rBV	413779	988145	29.03%	2.853%
21	8.581	1109	1121	1125	rBV	28153	91237	2.68%	0.263%
22	8.963	1177	1186	1200	rBV	1157866	2426106	71.28%	7.004%
23	9.457	1255	1270	1278	rBV5	34567	102218	3.00%	0.295%
24	9.969	1349	1357	1362	rBV	46281	86668	2.55%	0.250%
25	10.439	1428	1437	1444	rBV	1811564	3387562	99.53%	9.780%
26	10.498	1444	1447	1453	rVB	87133	144281	4.24%	0.417%
27	10.639	1465	1471	1478	rVB2	34909	62709	1.84%	0.181%
28	10.710	1478	1483	1491	rVB2	28999	50022	1.47%	0.144%
29	11.739	1650	1658	1668	rBV	1794333	3194753	93.86%	9.223%
30	11.839	1668	1675	1686	rVV	1509522	2579651	75.79%	7.448%
31	11.951	1686	1694	1706	rVB	1409450	2577876	75.74%	7.442%
32	12.274	1741	1749	1757	rBV	74769	124238	3.65%	0.359%
33	12.574	1790	1800	1810	rBV	156460	259851	7.63%	0.750%
34	12.727	1818	1826	1840	rBV	1411235	2440947	71.71%	7.047%
35	12.916	1852	1858	1864	rBV	254346	412698	12.12%	1.191%
36	12.980	1864	1869	1870	rVV	139189	191224	5.62%	0.552%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042022\
Data File : VN072108.D
Acq On : 21 Apr 2022 04:18
Operator : JC\MD
Sample : N2482-13
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-15

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	13.010	1870	1874	1878	rVV	392661	654197	19.22%	1.889%
38	13.051	1878	1881	1894	rVB	147006	250268	7.35%	0.723%
39	13.216	1902	1909	1917	rBV	156493	253777	7.46%	0.733%
40	13.363	1923	1934	1944	rBV	1134220	1797207	52.80%	5.189%
41	13.668	1979	1986	1998	rBV2	1567049	3403721	100.00%	9.827%
42	13.763	1999	2002	2009	rVV2	21179	35396	1.04%	0.102%
43	13.868	2015	2020	2037	rVB	240519	471467	13.85%	1.361%
44	14.127	2058	2064	2073	rBV2	28625	61511	1.81%	0.178%
45	14.210	2073	2078	2083	rBV	41047	63670	1.87%	0.184%
46	14.321	2092	2097	2105	rVB3	41984	74459	2.19%	0.215%
47	14.533	2127	2133	2137	rVV	27055	47126	1.38%	0.136%
48	14.574	2137	2140	2145	rVB2	33604	46869	1.38%	0.135%
49	14.804	2174	2179	2186	rVB2	29507	42044	1.24%	0.121%
50	14.927	2192	2200	2206	rBV2	48043	97330	2.86%	0.281%
51	15.504	2288	2298	2307	rBV	51280	103904	3.05%	0.300%

Sum of corrected areas: 34637280

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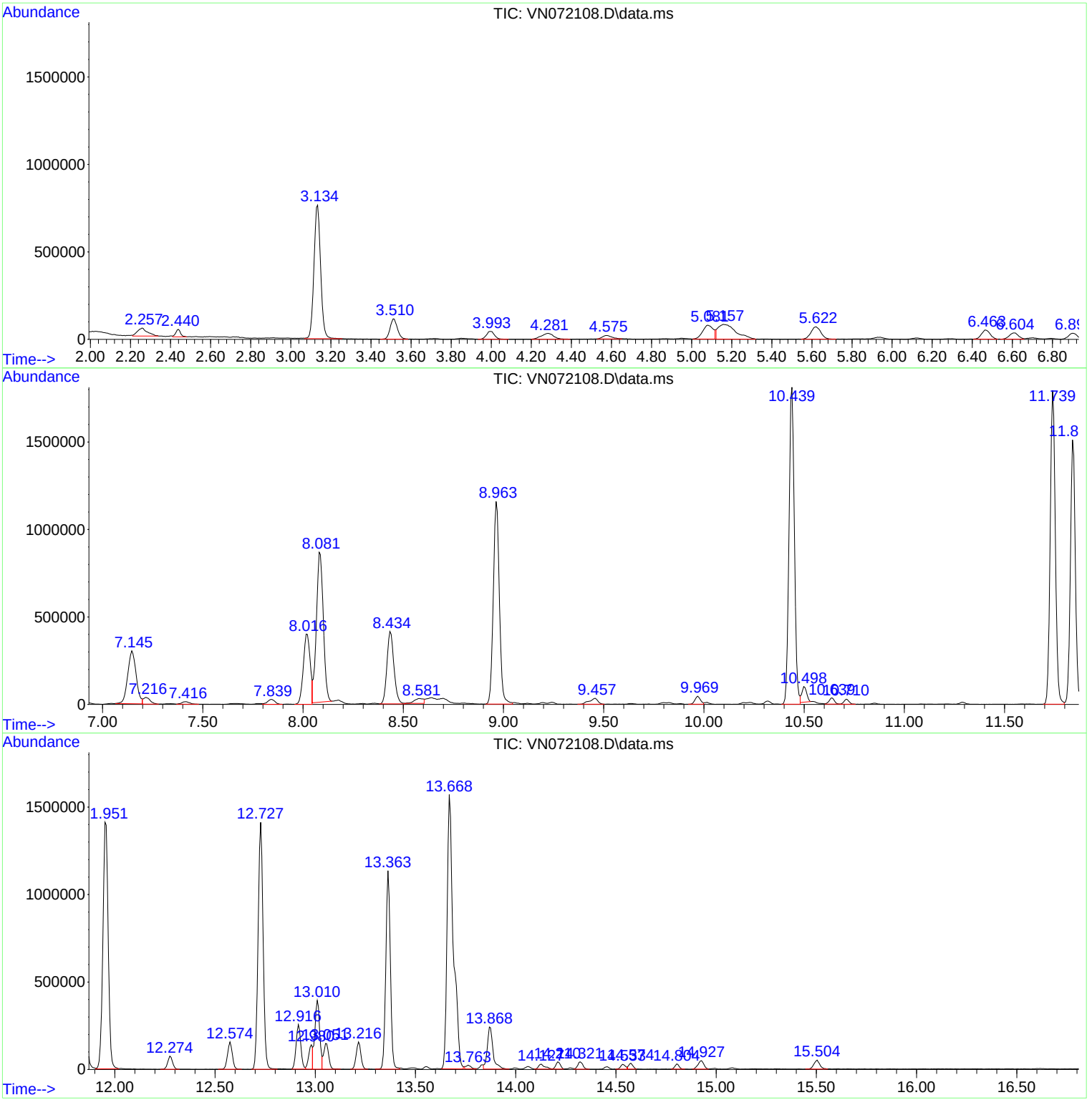
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-15

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042022\
Data File : VN072108.D
Acq On : 21 Apr 2022 04:18
Operator : JC\MD
Sample : N2482-13
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-15

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

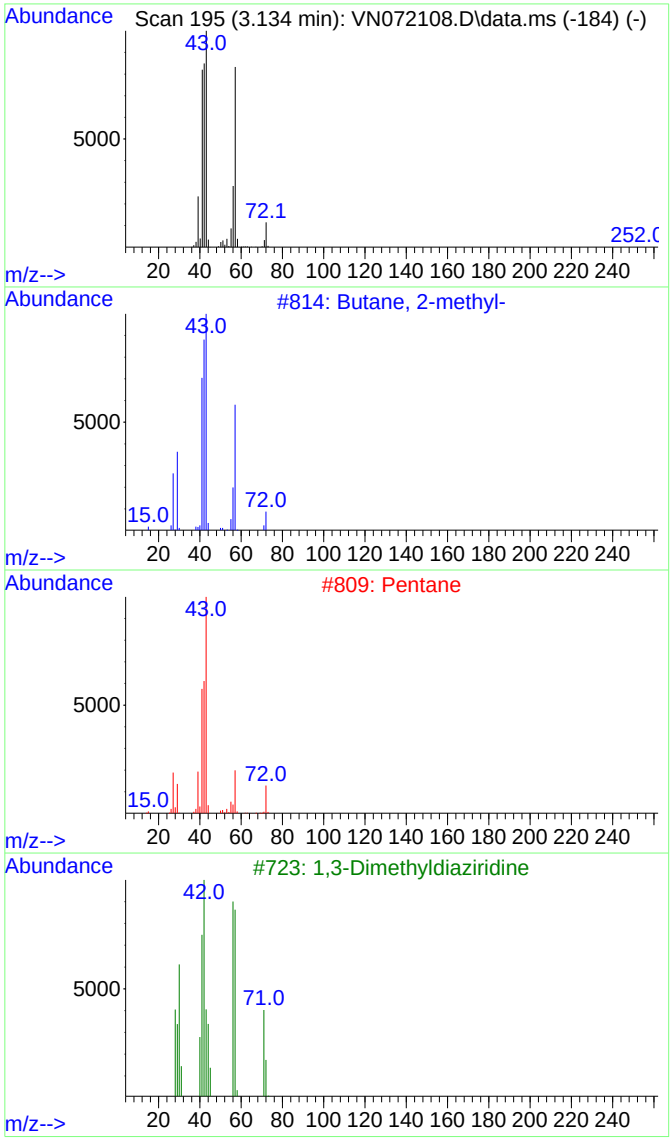
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

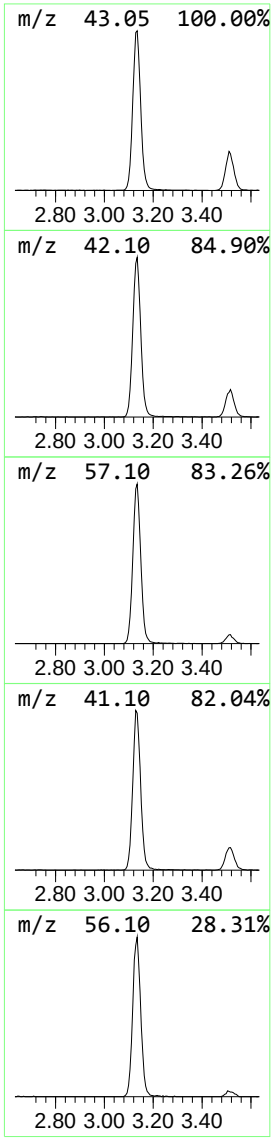
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.134	43.16 ug/l	1760530	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	46
3	1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	36
4	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	36
5	3-Buten-1-ol	72	C4H8O	000627-27-0	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042022\
Data File : VN072108.D
Acq On : 21 Apr 2022 04:18
Operator : JC\MD
Sample : N2482-13
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-15

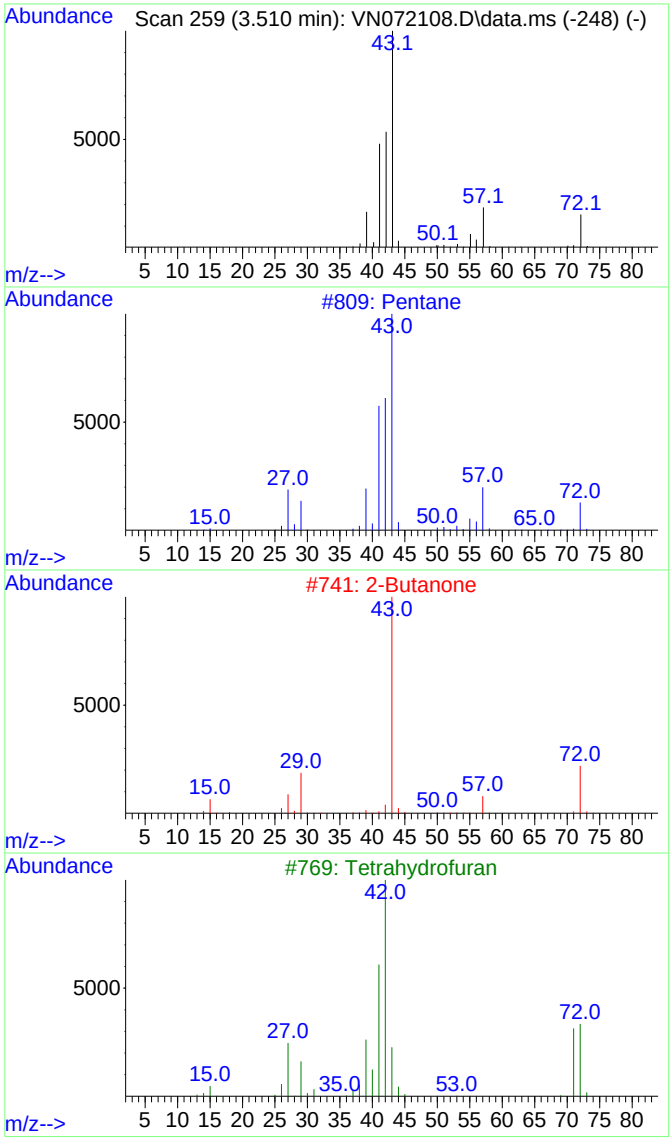
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

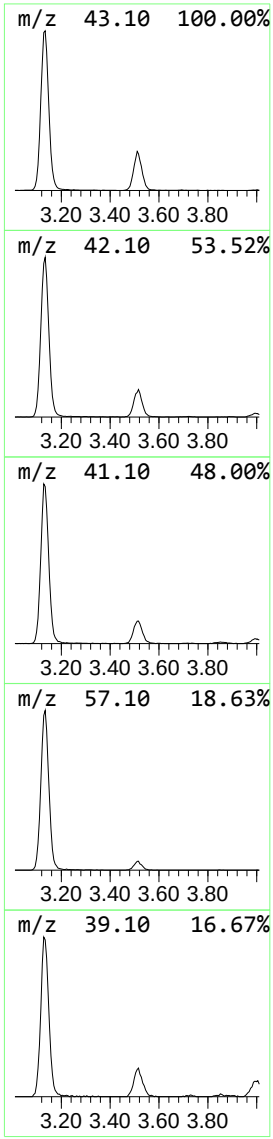
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.510	7.23 ug/l	294790	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	2-Butanone	72	C4H8O	000078-93-3	35
3	Tetrahydrofuran	72	C4H8O	000109-99-9	9
4	1-Propene, 2-methoxy-	72	C4H8O	000116-11-0	9
5	Oxirane, ethyl-	72	C4H8O	000106-88-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042022\
Data File : VN072108.D
Acq On : 21 Apr 2022 04:18
Operator : JC\MD
Sample : N2482-13
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-15

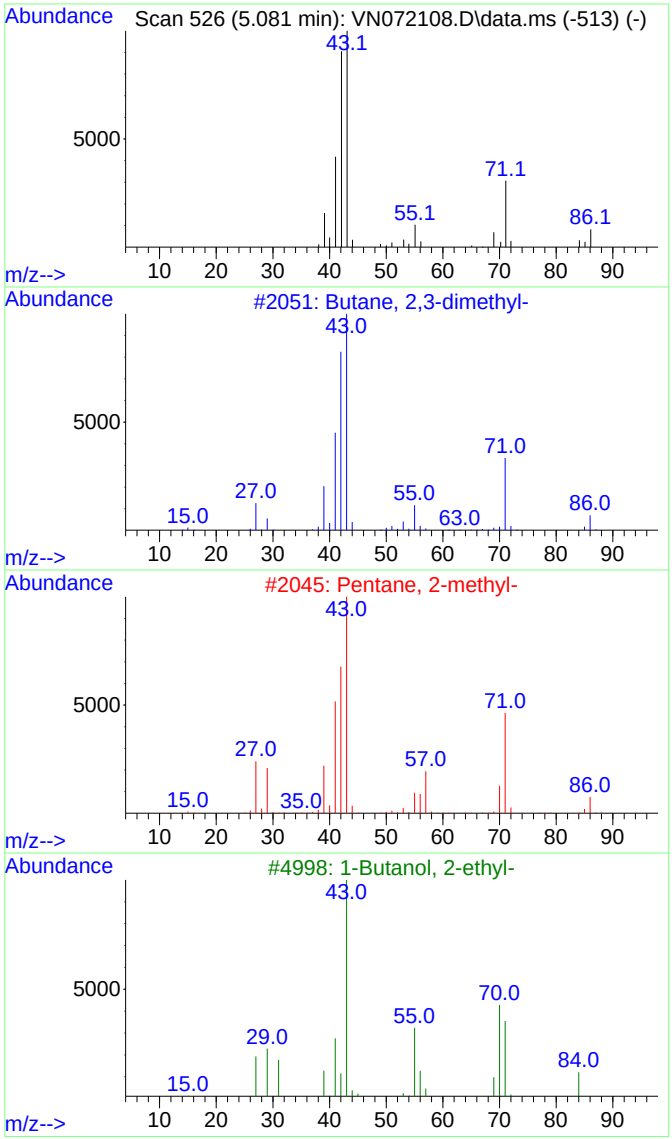
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

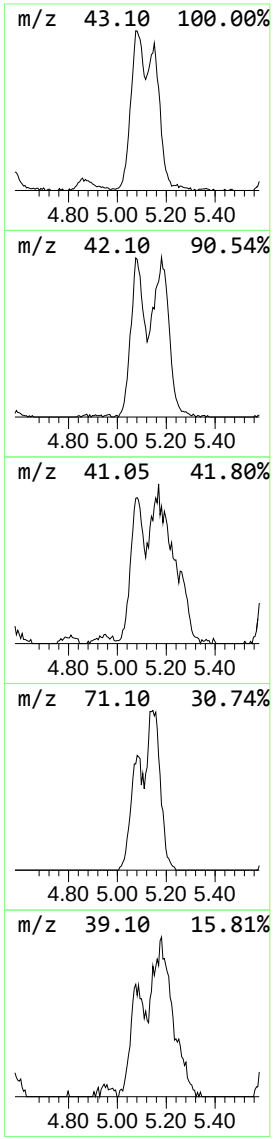
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	7.11 ug/l	289974	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	64
3	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	12
4	Propanoic acid, 2-methyl-, 2-pro...	128	C7H12O2	015727-77-2	9
5	Butanal, 2-ethyl-	100	C6H12O	000097-96-1	9





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-15

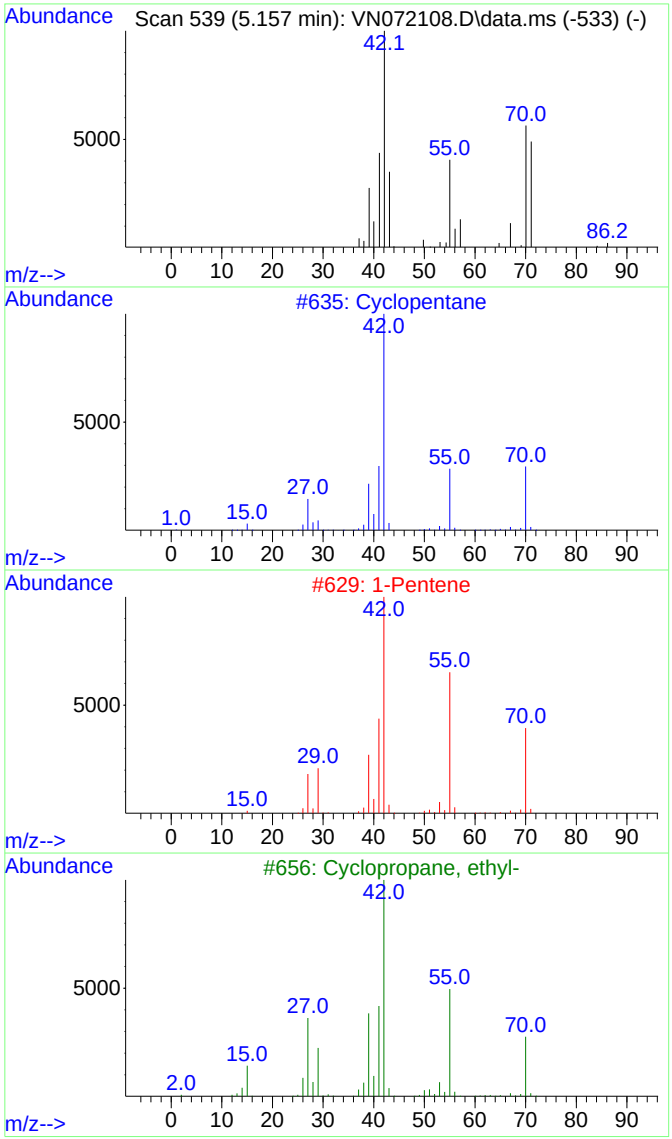
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

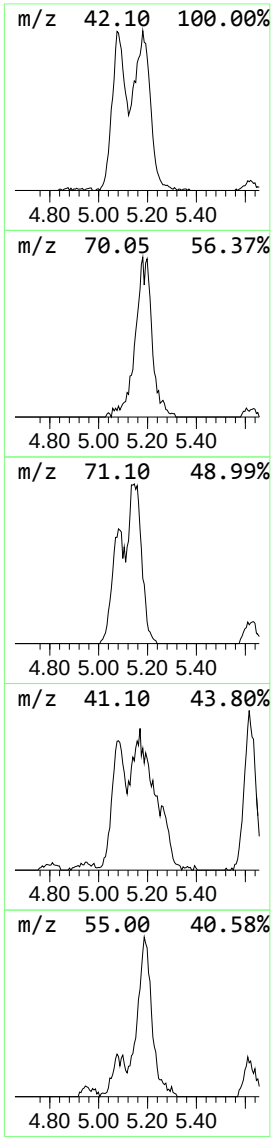
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 unknown5.157 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.157	12.44 ug/l	507444	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	40
2	1-Pentene	70	C5H10	000109-67-1	38
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	25
4	Diaziridine,1,3,3-trimethyl-	86	C4H10N2	040711-15-7	9
5	Aziridine, 2,2-dimethyl-	71	C4H9N	002658-24-4	9





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Acq On : 21 Apr 2022 04:18
Operator : JC\MD
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ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-15

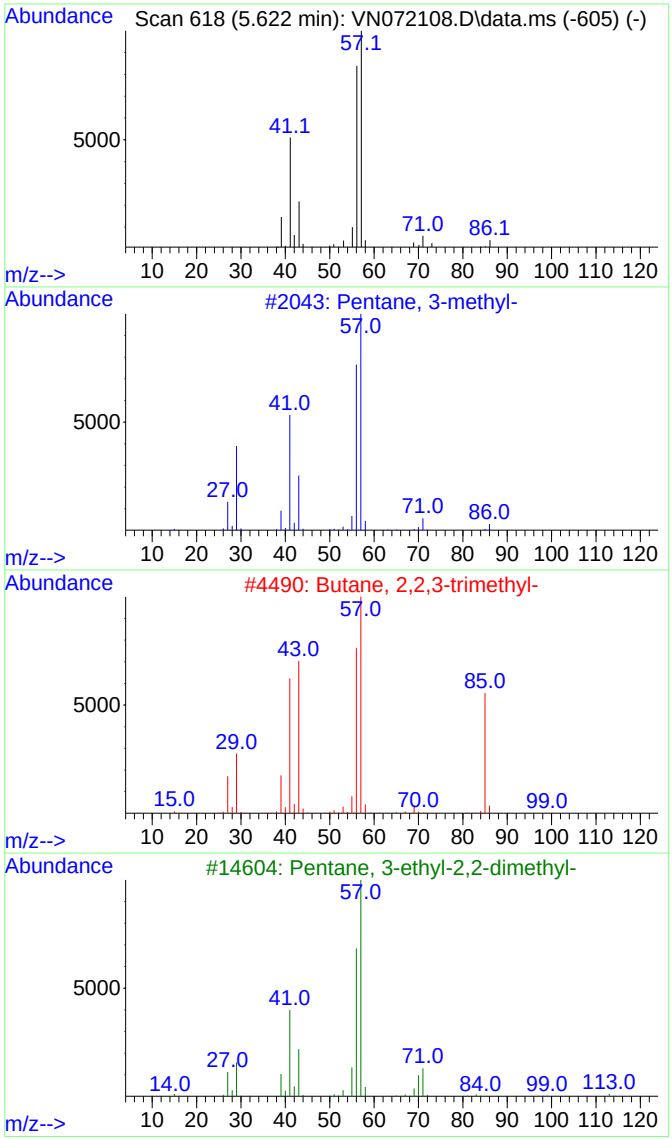
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

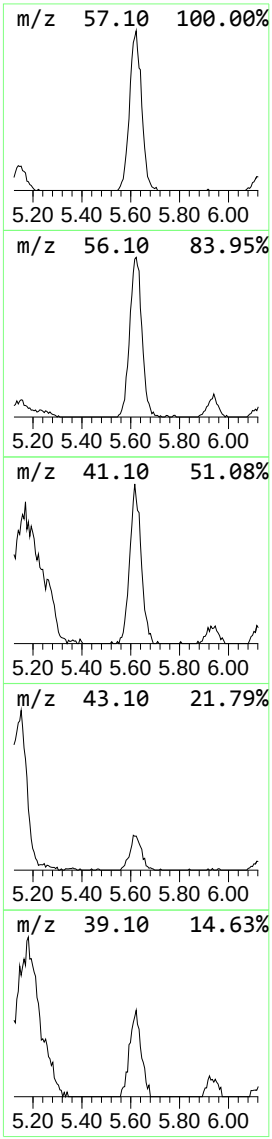
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.622	5.95 ug/l	242845	Pentafluorobenzene	8.081

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	78
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	78
4	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	72
5	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64





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ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
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SPN-15

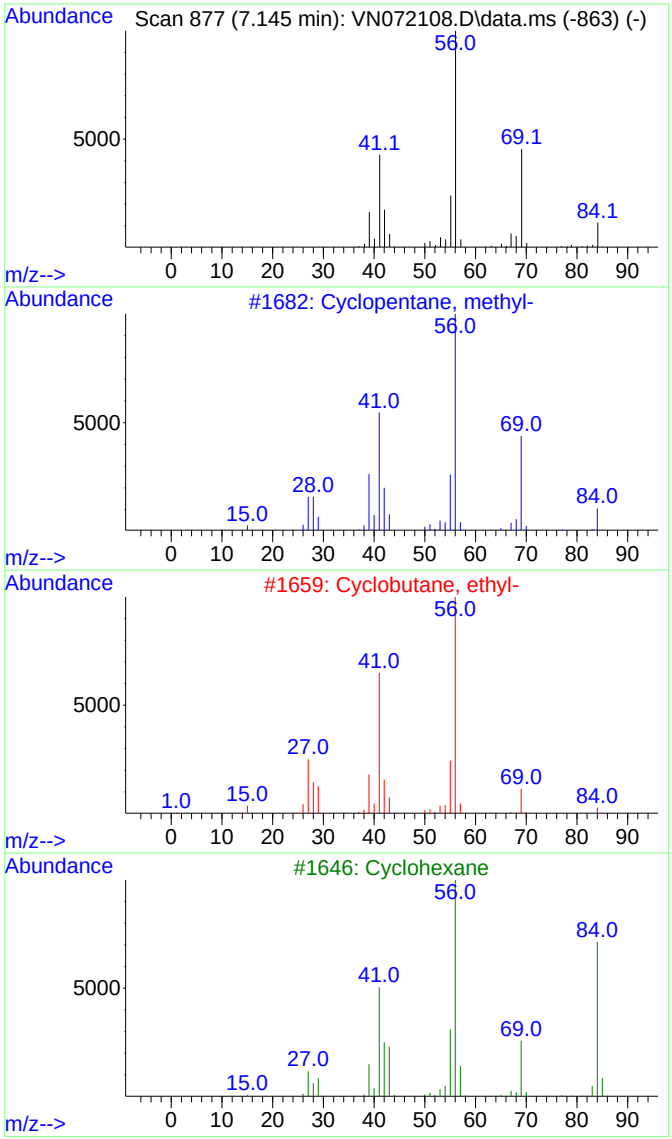
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

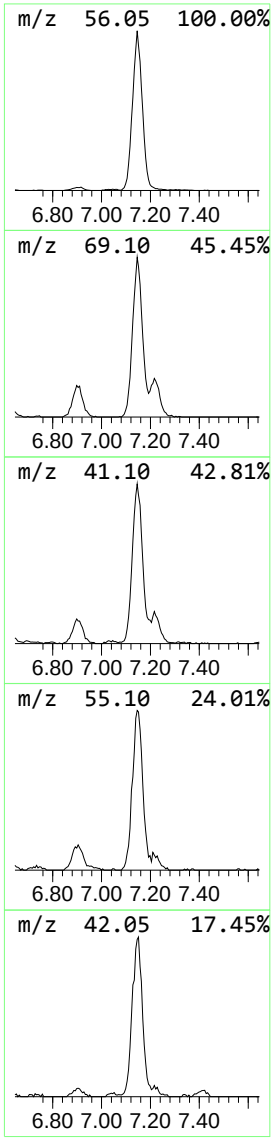
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	21.64 ug/l	882874	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	86
3	Cyclohexane	84	C6H12	000110-82-7	78
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	47





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-15

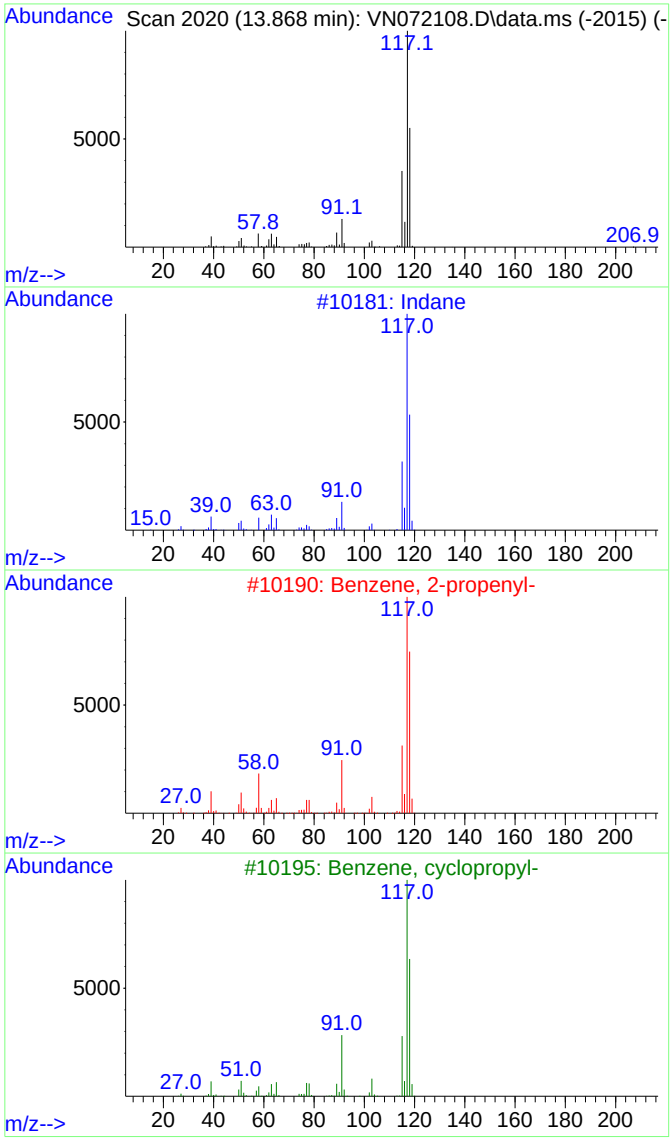
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

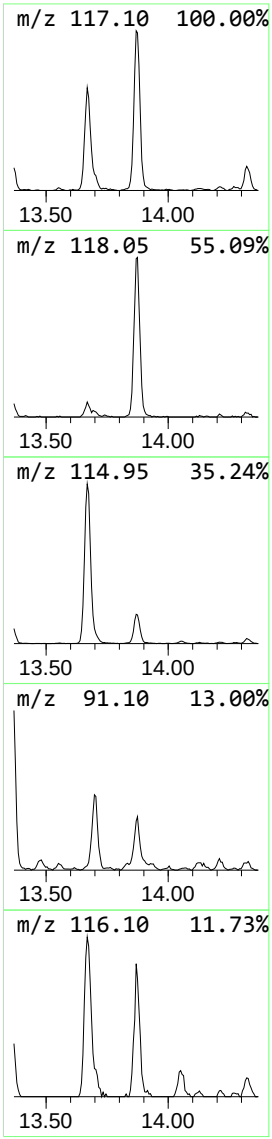
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Indane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	6.93 ug/l	471467	1,4-Dichlorobenzene-d4	13.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	91
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	64
5	Deltacyclene	118	C9H10	007785-10-6	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042022\
Data File : VN072108.D
Acq On : 21 Apr 2022 04:18
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-15

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	43.2	ug/l	1760530	1	8.081	2039640	50.0
Pentane	3.510	7.2	ug/l	294790	1	8.081	2039640	50.0
Butane, 2,3-dim...	5.081	7.1	ug/l	289974	1	8.081	2039640	50.0
unknown5.157	5.157	12.4	ug/l	507444	1	8.081	2039640	50.0
Pentane, 3-methyl-	5.622	6.0	ug/l	242845	1	8.081	2039640	50.0
Cyclopentane, m...	7.145	21.6	ug/l	882874	1	8.081	2039640	50.0
Indane	13.868	6.9	ug/l	471467	4	13.669	3403720	50.0