LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121422\
Data File : VN075788.D
Acq On : 15 Dec 2022 00:28
Operator : JC\MD
Sample : N5990-07 40X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-41

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\82N121422W.M
Title : SW846 8260

Signal : TIC: VN075788.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.295	35	41	44	rBV2	15031	28500	1.91%	0.210%
2	2.336	44	48	56	rVB	33490	57782	3.87%	0.427%
3	2.524	72	80	88	rBV	83221	142083	9.52%	1.049%
4	2.630	94	98	103	rVB3	11552	19212	1.29%	0.142%
5	2.759	115	120	125	rBV4	12731	25567	1.71%	0.189%
6	2.824	125	131	143	rVB3	15326	50951	3.42%	0.376%
7	3.259	196	205	219	rVB	154679	368812	24.72%	2.723%
8	3.559	249	256	263	rBV2	8397	19725	1.32%	0.146%
9	3.659	263	273	288	rVB4	41407	129699	8.69%	0.958%
10	3.865	302	308	320	rVB3	25424	64240	4.31%	0.474%
11	4.059	331	341	349	rBV2	16388	42180	2.83%	0.311%
12	4.159	349	358	368	rVB2	33033	88805	5.95%	0.656%
13	5.165	519	529	530	rBV4	9038	19375	1.30%	0.143%
14	5.295	540	551	553	rBV5	6225	16718	1.12%	0.123%
15	5.359	555	562	563	rBV3	9478	15018	1.01%	0.111%
16	5.824	632	641	652	rBV6	10770	34346	2.30%	0.254%
17	6.606	762	774	778	rBV4	5918	17287	1.16%	0.128%
18	6.659	778	783	793	rVB3	6876	20365	1.37%	0.150%
19	7.089	850	856	864	rVB4	7487	19176	1.29%	0.142%
20	7.336	888	898	906	rBV3	29110	81240	5.45%	0.600%
21	7.424	908	913	915	rVV4	9887	15491	1.04%	0.114%
22	8.012	1004	1013	1023	rBV2	11404	25901	1.74%	0.191%
23	8.171	1029	1040	1045	rBV	198760	499685	33.49%	3.689%
24	8.230	1045	1050	1063	rVV	416541	952194	63.82%	7.030%
25	8.606	1101	1114	1128	rBV3	278277	957882	64.20%	7.072%
26	9.106	1189	1199	1214	rBV	545534	1118281	74.96%	8.257%
27	9.600	1279	1283	1288	rVB3	11773	22368	1.50%	0.165%
28	10.571	1439	1448	1454	rBV	817494	1491928	100.00%	11.016%
29	10.635	1454	1459	1467	rVB	361790	657407	44.06%	4.854%
30	11.865	1660	1668	1679	rBV	693067	1259078	84.39%	9.296%
31	11.965	1679	1685	1694	rVB	161868	272859	18.29%	2.015%
32	12.071	1694	1703	1712	rBV	324248	645252	43.25%	4.764%
33	12.400	1752	1759	1771	rVB	300504	497581	33.35%	3.674%
34	12.700	1801	1810	1816	rBV2	10907	18056	1.21%	0.133%
35	12.853	1828	1836	1847	rBV	551387	932243	62.49%	6.883%
36	13.041	1862	1868	1872	rBV	27666	44549	2.99%	0.329%

LSC Area Percent Report

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Instrument :
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ClientSampleId :
MW-41

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
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Title : SW846 8260

37	13.100	1872	1878	1881	rVV	119533	199387	13.36%	1.472%
38	13.135	1881	1884	1887	rVV	67056	104596	7.01%	0.772%
39	13.176	1887	1891	1897	rVB	89774	141035	9.45%	1.041%
40	13.335	1912	1918	1927	rBV	75162	126101	8.45%	0.931%
41	13.482	1931	1943	1954	rVV	284871	475044	31.84%	3.507%
42	13.794	1989	1996	2009	rVB2	688467	1288136	86.34%	9.511%
43	13.953	2018	2023	2025	rBV2	12212	17349	1.16%	0.128%
44	13.994	2025	2030	2033	rBV2	46749	84678	5.68%	0.625%
45	14.182	2056	2062	2068	rBV2	11396	17332	1.16%	0.128%
46	14.247	2068	2073	2076	rVV	21295	36573	2.45%	0.270%
47	14.276	2076	2078	2082	rVV2	18598	23209	1.56%	0.171%
48	14.335	2082	2088	2094	rVV	32450	50244	3.37%	0.371%
49	14.447	2102	2107	2113	rVB2	26145	42276	2.83%	0.312%
50	14.659	2136	2143	2146	rBV	18996	30038	2.01%	0.222%
51	14.694	2146	2149	2154	rVB2	26987	39617	2.66%	0.293%
52	14.929	2184	2189	2194	rBV2	17825	30857	2.07%	0.228%
53	15.053	2201	2210	2217	rBV4	41228	93195	6.25%	0.688%
54	15.647	2303	2311	2318	rBV	38033	72262	4.84%	0.534%

Sum of corrected areas: 13543765

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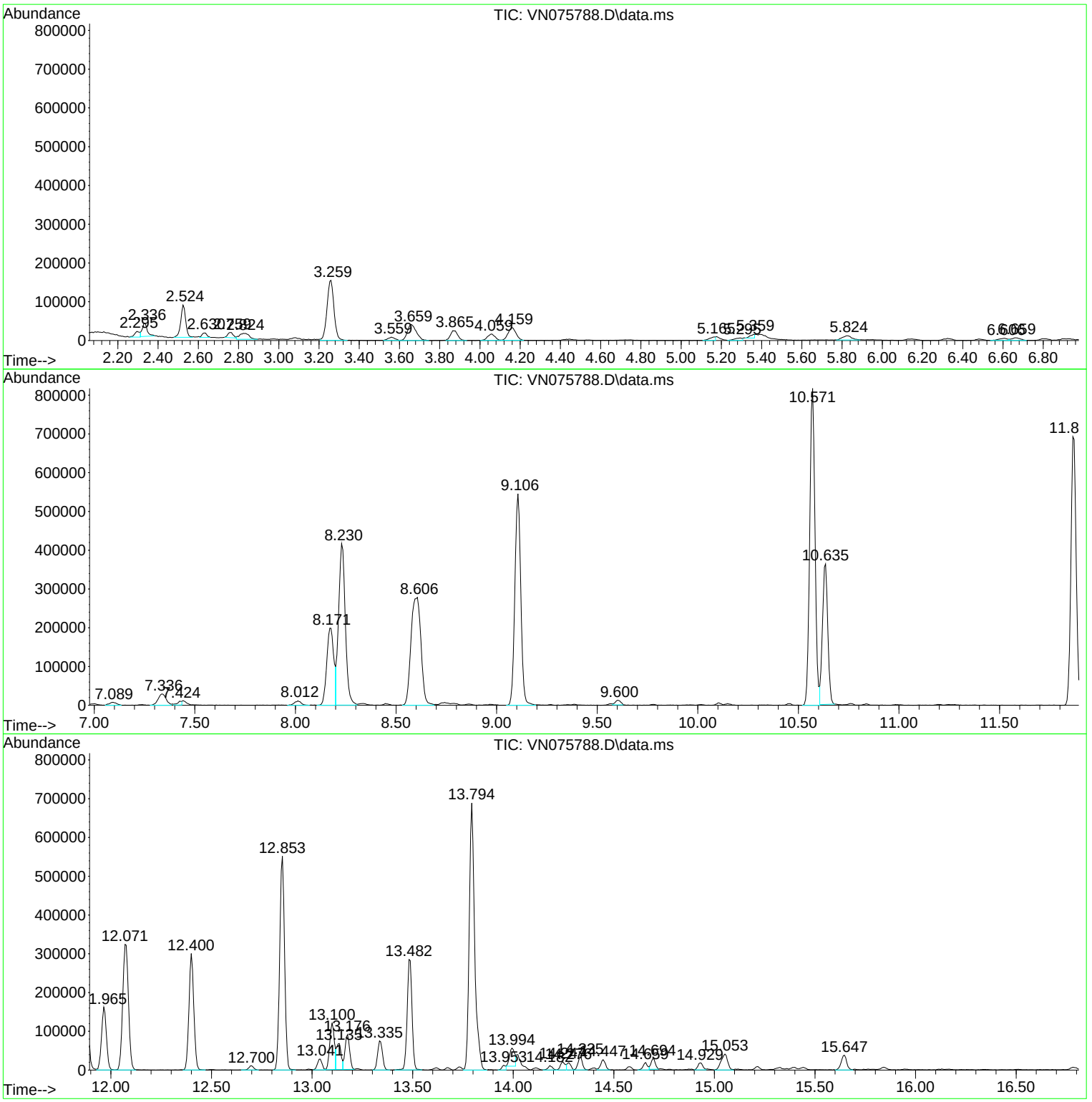
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

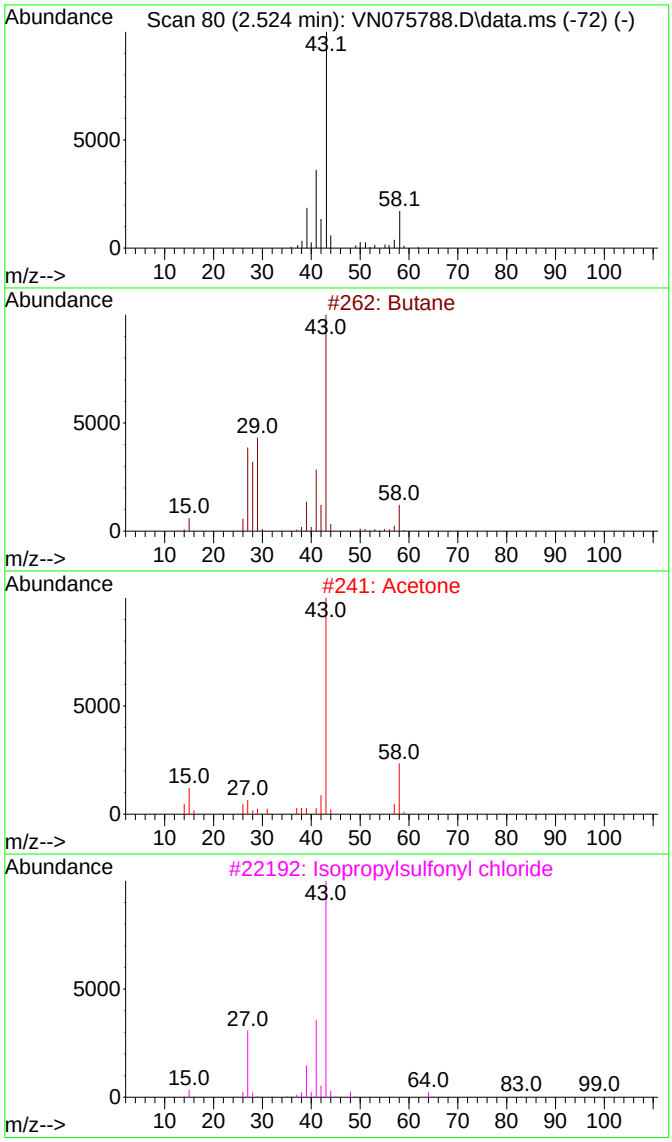
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

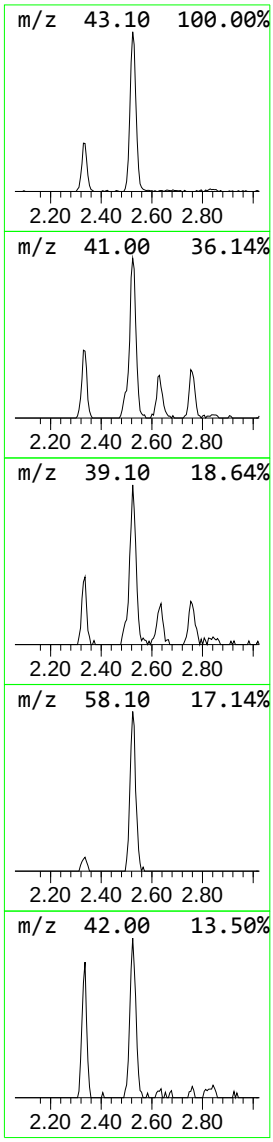
****

Peak Number 1 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.524	7.46 ug/l	142083	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	80
2	Acetone	58	C3H6O	000067-64-1	9
3	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4	Isobutane	58	C4H10	000075-28-5	9
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9





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MSVOA_N
ClientSampleId :
MW-41

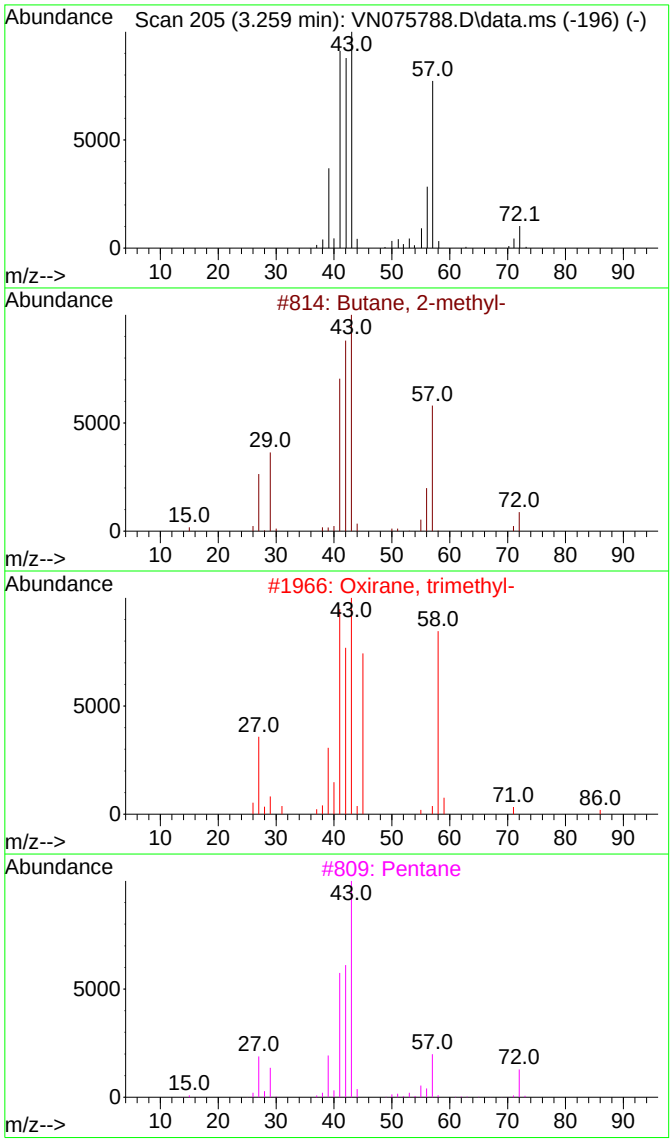
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

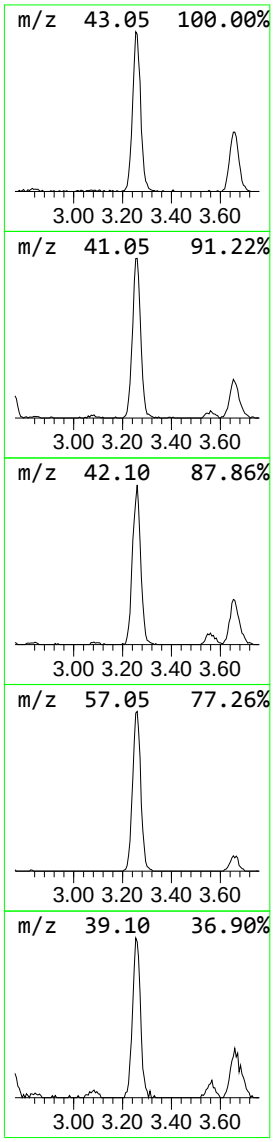
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.259	19.37 ug/l	368812	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	Oxirane, trimethyl-	86	C5H10O	005076-19-7	36
3	Pentane	72	C5H12	000109-66-0	33
4	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	27
5	3-Buten-1-ol	72	C4H8O	000627-27-0	25





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Quant Title : SW846 8260

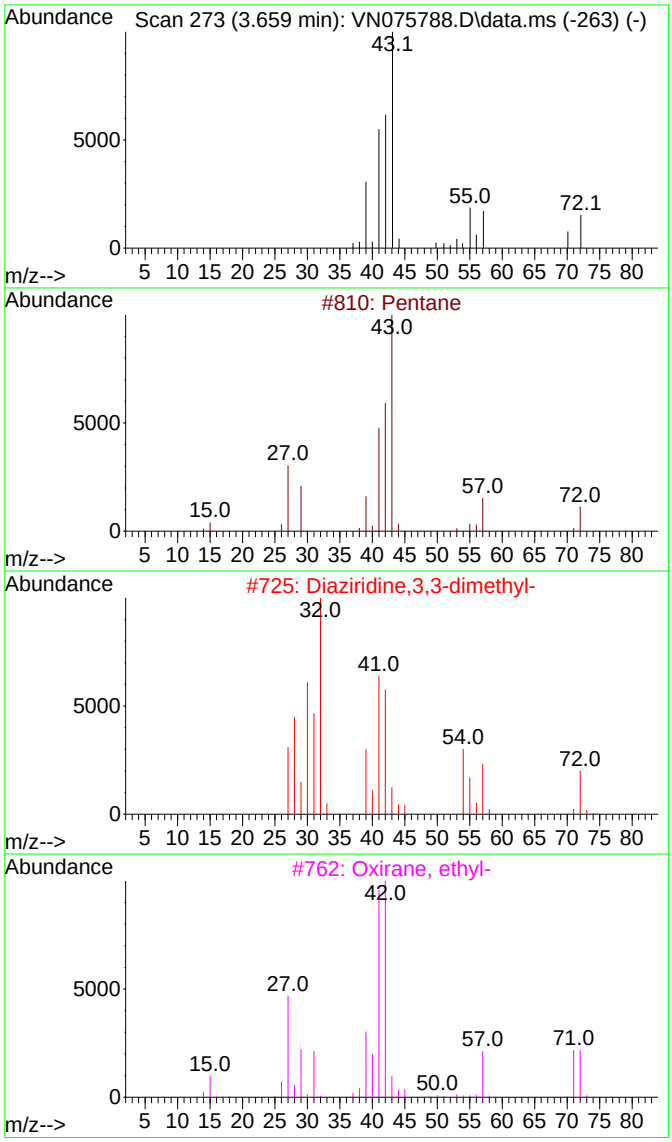
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

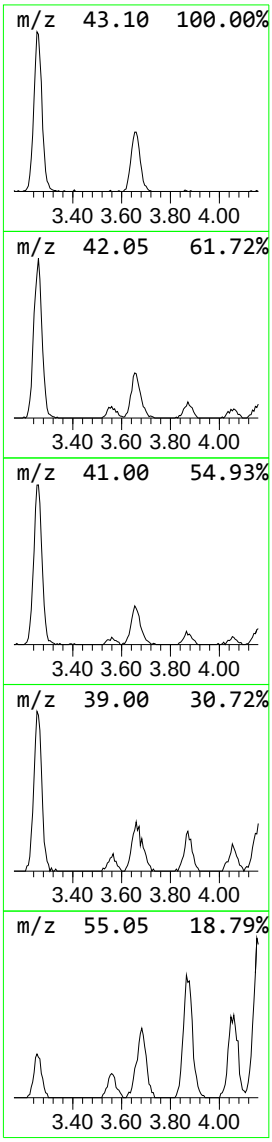
****

Peak Number 3 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.659	6.81 ug/l	129699	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	86
2	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	50
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	47
4	Isobutylene epoxide	72	C4H8O	000558-30-5	43
5	Cyclobutane, methyl-	70	C5H10	000598-61-8	38





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ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-41

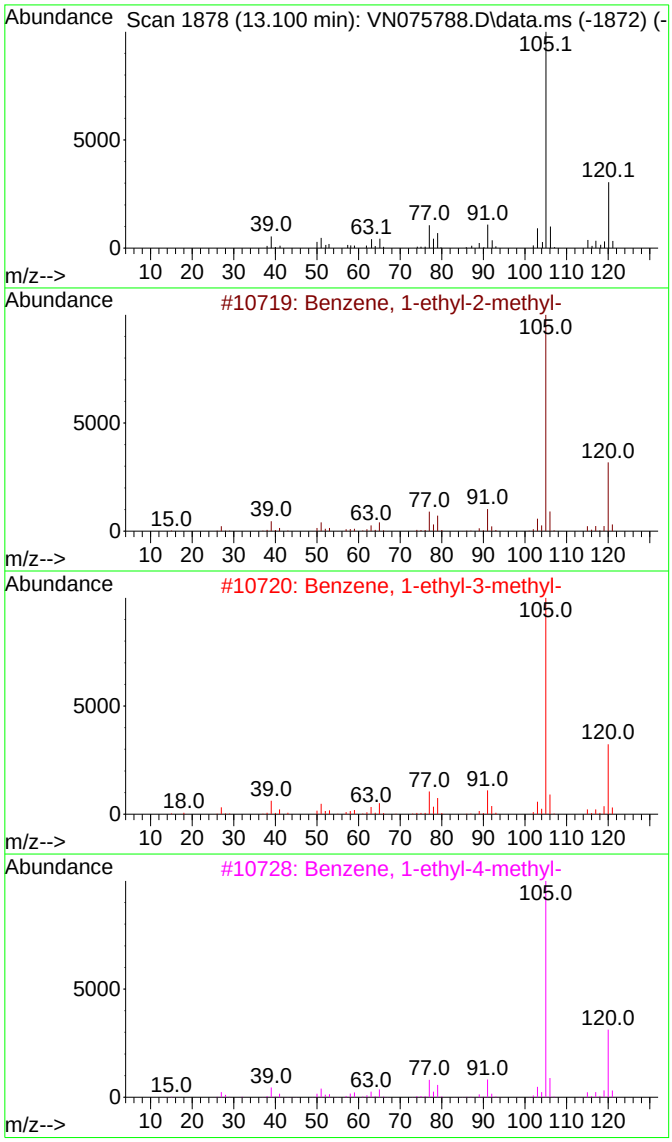
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

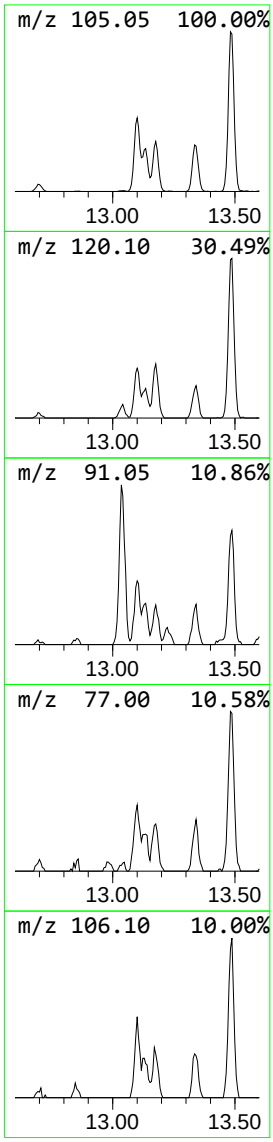
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	7.74 ug/l	199387	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	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
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





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane	2.524	7.5	ug/l	142083	1	8.230	952194	50.0
Butane, 2-methyl-	3.259	19.4	ug/l	368812	1	8.230	952194	50.0
Pentane	3.659	6.8	ug/l	129699	1	8.230	952194	50.0
Benzene, 1-ethy...	13.100	7.7	ug/l	199387	4	13.794	1288140	50.0