LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042423\
Data File : VN077464.D
Acq On : 25 Apr 2023 11:43
Operator : JC\MD
Sample : 02460-04 40X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-5

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\82N042423W.M
Title : SW846 8260

Signal : TIC: VN077464.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.519	94	99	105	rBV	73729	117050	2.89%	0.399%
2	2.837	144	153	158	rBV6	39094	112969	2.79%	0.385%
3	3.254	214	224	234	rVB2	764585	1789791	44.27%	6.098%
4	3.648	282	291	305	rVB	145560	386546	9.56%	1.317%
5	4.154	368	377	390	rVB3	21432	58721	1.45%	0.200%
6	4.431	412	424	439	rBV4	52397	190976	4.72%	0.651%
7	5.290	555	570	573	rBV4	85173	269462	6.66%	0.918%
8	5.354	574	581	611	rVB4	187464	835821	20.67%	2.848%
9	5.825	646	661	675	rBV	154268	523109	12.94%	1.782%
10	6.325	734	746	758	rBV3	53490	158461	3.92%	0.540%
11	6.666	793	804	813	rVB4	27569	84798	2.10%	0.289%
12	6.801	817	827	838	rVB7	20141	61152	1.51%	0.208%
13	7.083	866	875	884	rBV5	24911	75039	1.86%	0.256%
14	7.225	891	899	907	rBV5	18771	49999	1.24%	0.170%
15	7.336	907	918	931	rBV2	196686	561545	13.89%	1.913%
16	8.013	1026	1033	1040	rVB5	33808	86553	2.14%	0.295%
17	8.172	1050	1060	1064	rBV	544190	1266997	31.34%	4.317%
18	8.230	1064	1070	1082	rVV	1011971	2528681	62.54%	8.616%
19	8.336	1082	1088	1098	rVB4	69822	183908	4.55%	0.627%
20	8.454	1098	1108	1114	rBV3	40252	96185	2.38%	0.328%
21	8.583	1122	1130	1146	rVB3	541535	1237133	30.60%	4.215%
22	8.725	1146	1154	1159	rVV6	52658	143533	3.55%	0.489%
23	8.795	1161	1166	1171	rVV6	54506	138784	3.43%	0.473%
24	8.860	1172	1177	1186	rVB7	42355	102956	2.55%	0.351%
25	9.107	1209	1219	1235	rBV	1451654	3077689	76.12%	10.486%
26	9.389	1261	1267	1277	rVB3	25488	54672	1.35%	0.186%
27	9.601	1288	1303	1313	rBV3	131584	363916	9.00%	1.240%
28	9.783	1323	1334	1341	rBV6	23770	53204	1.32%	0.181%
29	10.101	1384	1388	1392	rBV3	32543	62937	1.56%	0.214%
30	10.148	1393	1396	1403	rVB6	21093	44887	1.11%	0.153%
31	10.454	1441	1448	1453	rBV2	27141	55098	1.36%	0.188%
32	10.572	1460	1468	1489	rBV	2103840	4043185	100.00%	13.776%
33	10.989	1533	1539	1548	rVB5	28583	72392	1.79%	0.247%
34	11.866	1680	1688	1699	rBV	1863995	3397608	84.03%	11.577%
35	11.966	1699	1705	1712	rVB	167591	296743	7.34%	1.011%
36	12.077	1718	1724	1732	rVB2	49138	91415	2.26%	0.311%

LSC Area Percent Report

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Operator : JC\MD
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ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-5

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Title : SW846 8260

37	12.701	1823	1830	1838	rBV2	92316	162539	4.02%	0.554%
38	12.854	1846	1856	1867	rBV	1351431	2352926	58.19%	8.017%
39	13.042	1880	1888	1897	rBV	233709	397721	9.84%	1.355%
40	13.136	1897	1904	1908	rVV2	54224	93906	2.32%	0.320%
41	13.342	1931	1939	1945	rBV2	39097	68526	1.69%	0.233%
42	13.489	1958	1964	1972	rVB	75192	126781	3.14%	0.432%
43	13.607	1976	1984	1992	rBV6	22216	53206	1.32%	0.181%
44	13.795	2007	2016	2026	rBV	1519677	2647833	65.49%	9.022%
45	13.954	2038	2043	2046	rBV3	45750	74721	1.85%	0.255%
46	14.001	2046	2051	2056	rVB	105430	178164	4.41%	0.607%
47	14.336	2101	2108	2113	rBV3	54674	91506	2.26%	0.312%
48	14.401	2113	2119	2122	rVV2	25622	44656	1.10%	0.152%
49	14.448	2122	2127	2134	rVB2	95898	166303	4.11%	0.567%
50	14.930	2204	2209	2215	rVB2	39518	63717	1.58%	0.217%
51	15.054	2221	2230	2235	rBV3	58250	102765	2.54%	0.350%
52	15.589	2314	2321	2327	rBV2	27035	49881	1.23%	0.170%

Sum of corrected areas: 29349066

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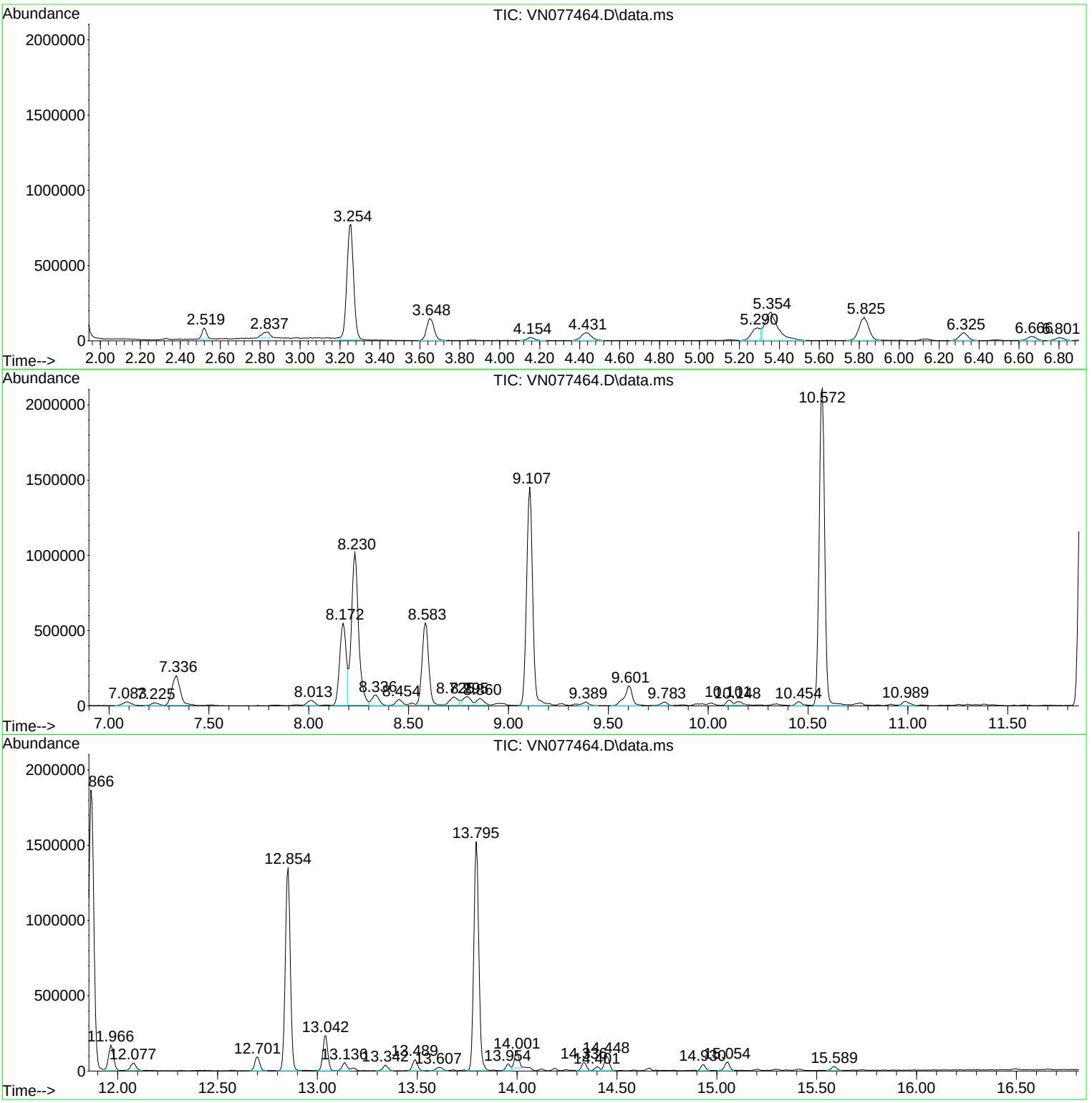
Instrument :
MSVOA_N
ClientSampleId :
MW-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042423\
Data File : VN077464.D
Acq On : 25 Apr 2023 11:43
Operator : JC\MD
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Instrument :
MSVOA_N
ClientSampleId :
MW-5

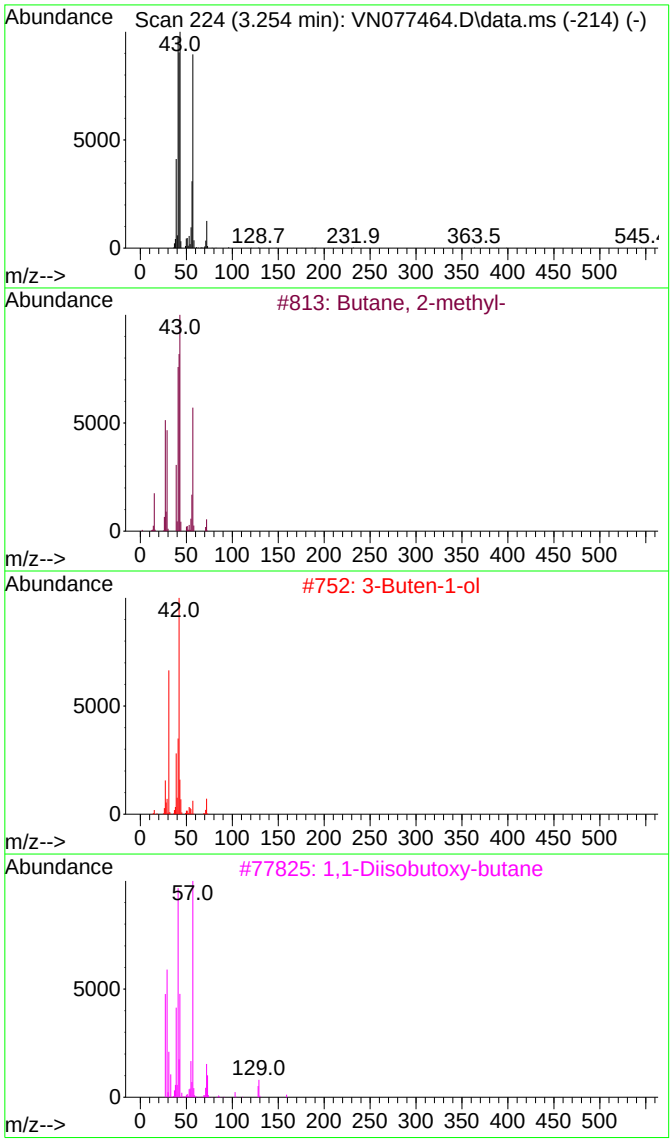
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

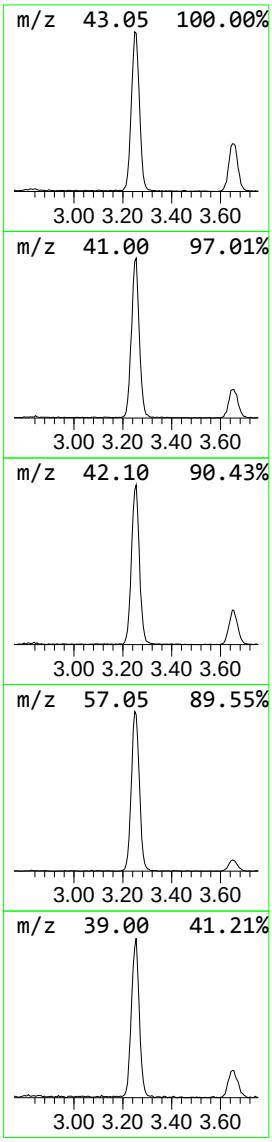
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.254	35.39 ug/l	1789790	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	59
2	3-Buten-1-ol	72	C4H8O	000627-27-0	38
3	1,1-Diisobutoxy-butane	202	C12H26O2	013002-16-9	38
4	Oxirane, trimethyl-	86	C5H10O	005076-19-7	37
5	Pentane	72	C5H12	000109-66-0	36





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ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

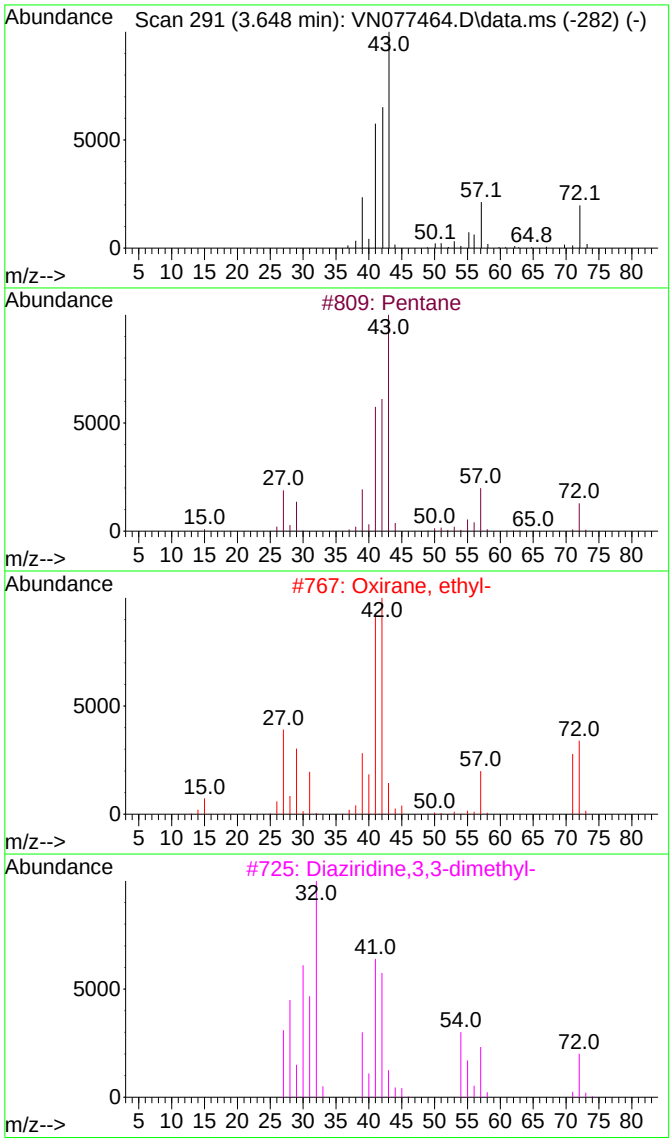
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

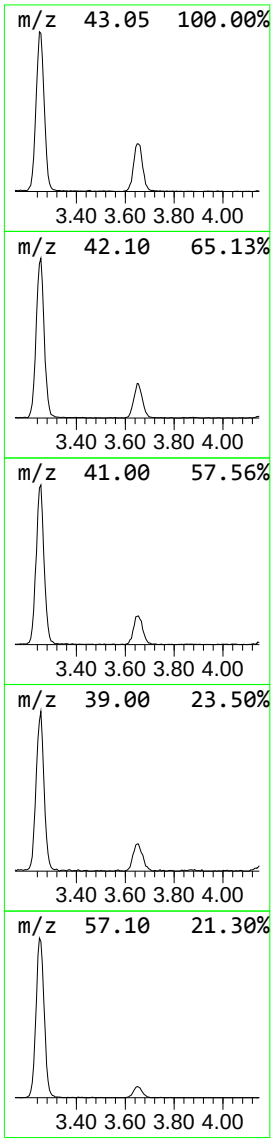
****

Peak Number 2 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.648	7.64 ug/l	386546	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	86
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	59
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	58
4	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	37
5	Butane, 2-methyl-	72	C5H12	000078-78-4	36





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Instrument :
MSVOA_N
ClientSampleId :
MW-5

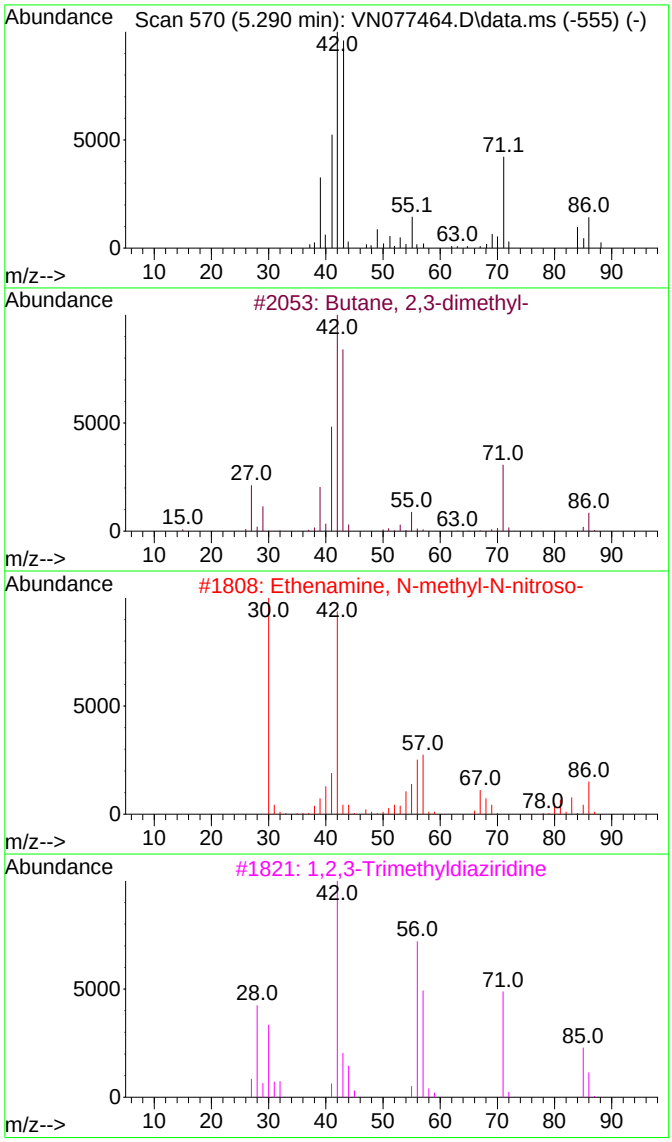
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

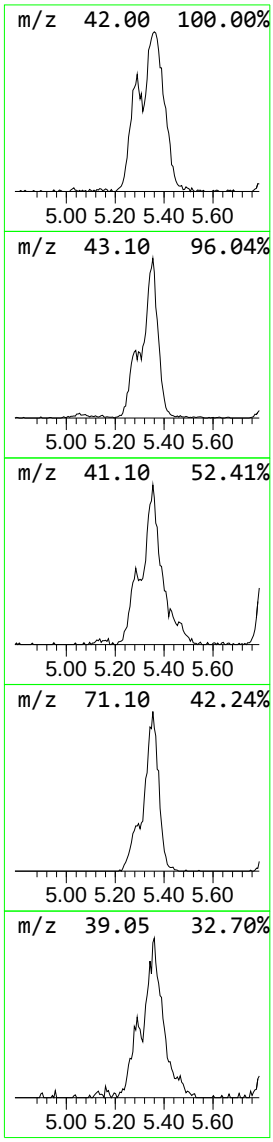
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.290	5.33 ug/l	269462	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	83
2	Ethenamine, N-methyl-N-nitroso-	86	C3H6N2O	004549-40-0	37
3	1,2,3-Trimethyldiaziridine	86	C4H10N2	113604-56-1	36
4	Pentane, 2-methyl-	86	C6H14	000107-83-5	28
5	1,6-Heptadien-4-ol	112	C7H12O	002883-45-6	27





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

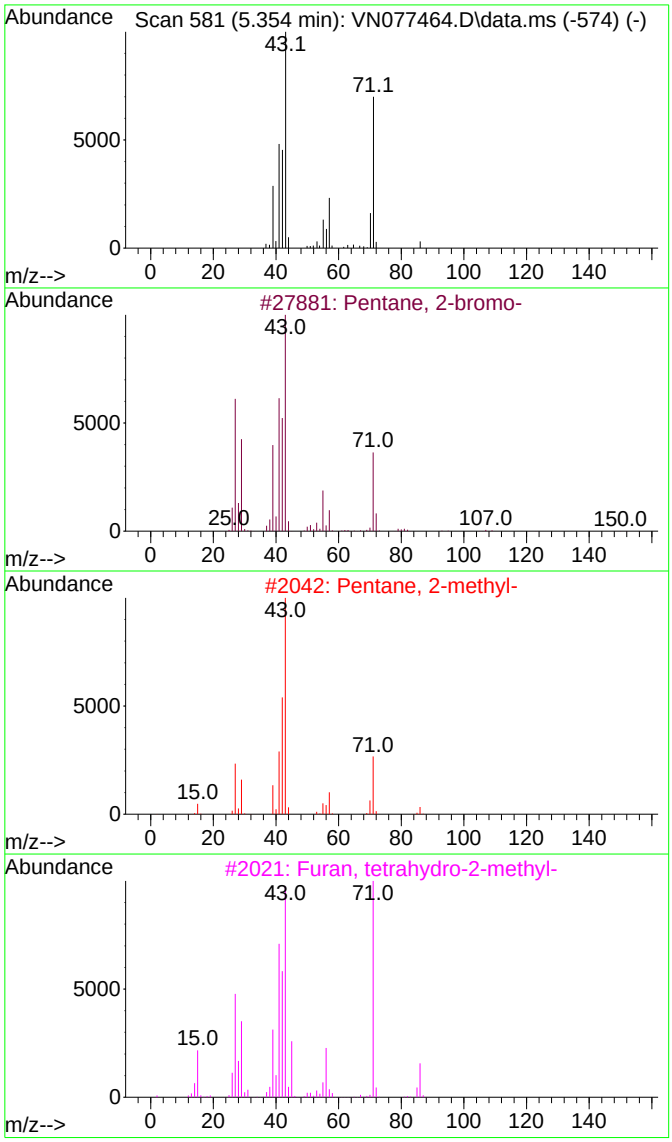
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

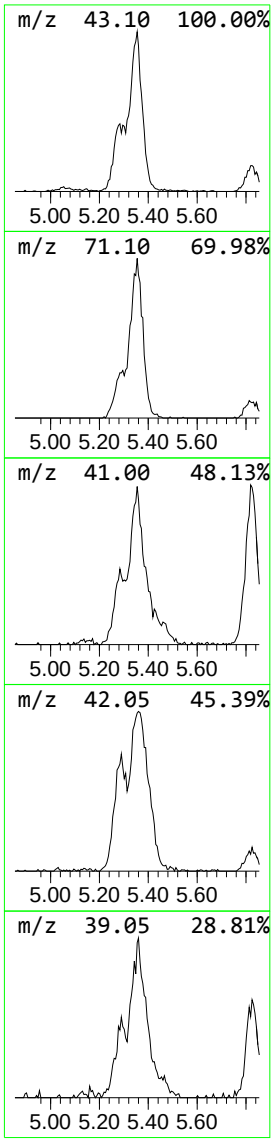
****

Peak Number 4 Pentane, 2-bromo- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.354	16.53 ug/l	835821	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	78
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	74
3	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	40
4	Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	40
5	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	38





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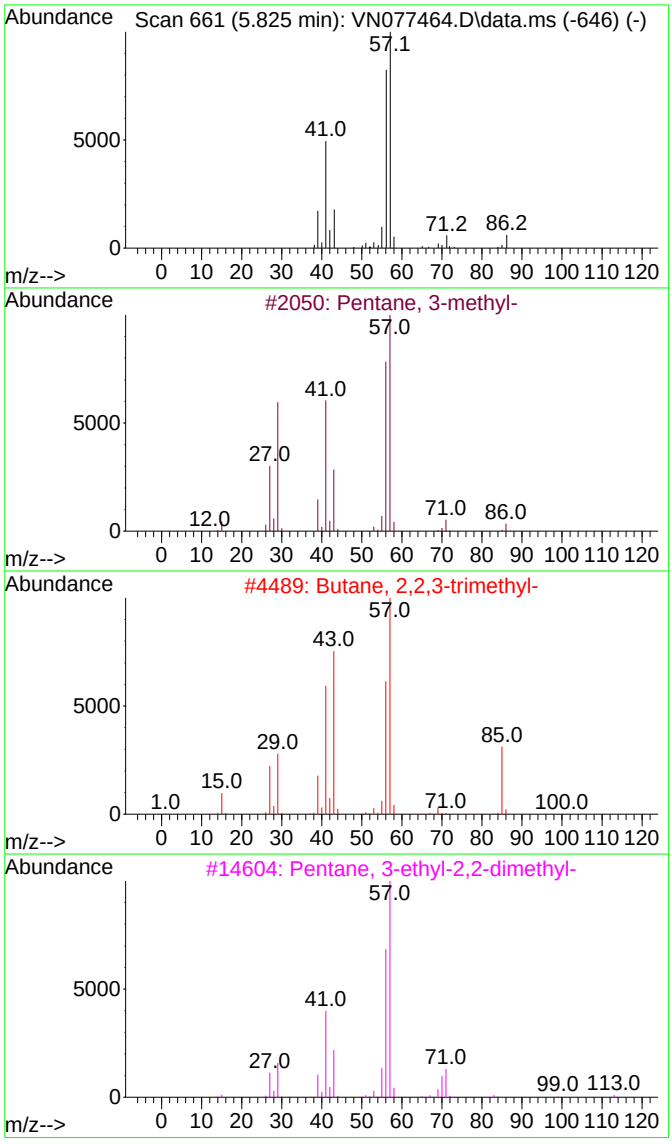
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

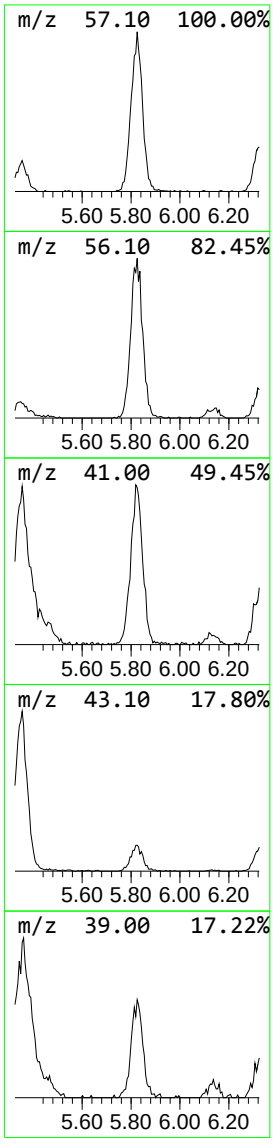
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.825	10.34 ug/l	523109	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	80
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	72
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
4	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
5	Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	56





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Quant Title : SW846 8260

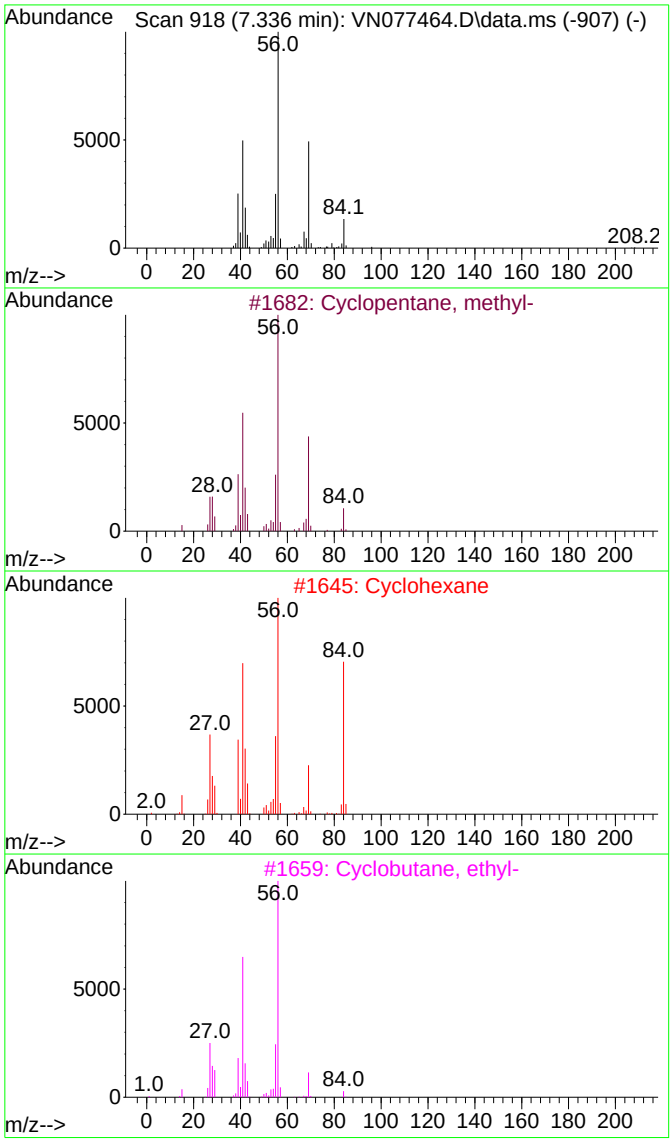
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

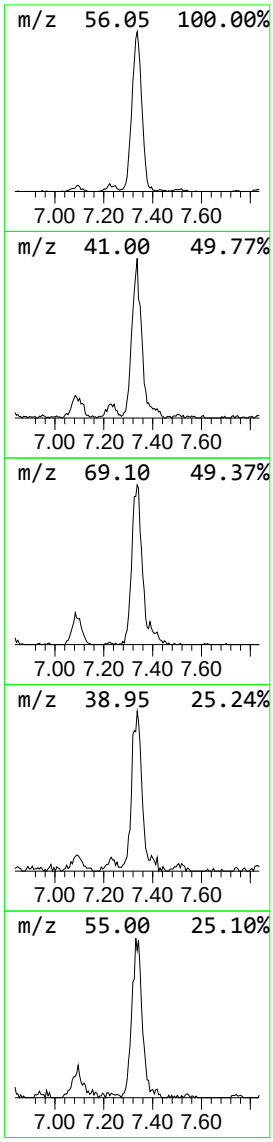
****

Peak Number 6 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.336	11.10 ug/l	561545	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclohexane	84	C6H12	000110-82-7	86
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	64





Tentatively Identified Compound (LSC) summary

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MSVOA_N
ClientSampleId :
MW-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.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-	3.254	35.4	ug/l	1789790	1	8.230	2528680	50.0
Pentane	3.648	7.6	ug/l	386546	1	8.230	2528680	50.0
Butane, 2,3-dim...	5.290	5.3	ug/l	269462	1	8.230	2528680	50.0
Pentane, 2-bromo-	5.354	16.5	ug/l	835821	1	8.230	2528680	50.0
Pentane, 3-methyl-	5.825	10.3	ug/l	523109	1	8.230	2528680	50.0
Cyclopentane, m...	7.336	11.1	ug/l	561545	1	8.230	2528680	50.0