LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042523\
Data File : VN077477.D
Acq On : 25 Apr 2023 18:21
Operator : JC\MD
Sample : 02460-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

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: VN077477.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.825	144	151	158	rBV2	34769	79202	2.41%	0.435%
2	3.254	215	224	239	rVB2	114831	323735	9.84%	1.777%
3	4.431	412	424	436	rBV4	28633	100020	3.04%	0.549%
4	5.284	553	569	572	rBV4	44576	118674	3.61%	0.651%
5	5.354	575	581	592	rVB4	58105	194982	5.93%	1.070%
6	5.819	648	660	673	rBV3	60995	205531	6.25%	1.128%
7	6.331	736	747	757	rBV6	12278	39154	1.19%	0.215%
8	7.236	891	901	908	rBV5	14530	43488	1.32%	0.239%
9	7.331	908	917	928	rVB3	32836	89280	2.71%	0.490%
10	8.172	1050	1060	1065	rBV	452722	1116512	33.93%	6.128%
11	8.231	1065	1070	1081	rVV	813362	1874450	56.97%	10.288%
12	8.330	1081	1087	1098	rVB4	37044	98739	3.00%	0.542%
13	8.448	1100	1107	1114	rBV4	22367	49515	1.50%	0.272%
14	8.583	1122	1130	1141	rBV	448248	1010923	30.72%	5.549%
15	8.730	1146	1155	1157	rBV6	19843	48328	1.47%	0.265%
16	8.854	1172	1176	1187	rVB5	16112	40841	1.24%	0.224%
17	9.107	1209	1219	1233	rBV	1161434	2427416	73.77%	13.323%
18	9.607	1299	1304	1310	rVB3	29156	61346	1.86%	0.337%
19	10.572	1458	1468	1480	rBV	1742094	3290346	100.00%	18.059%
20	10.983	1532	1538	1548	rVB7	18408	47793	1.45%	0.262%
21	11.866	1680	1688	1701	rBV	1523489	2776775	84.39%	15.241%
22	12.695	1822	1829	1836	rBV2	19816	38184	1.16%	0.210%
23	12.854	1847	1856	1865	rBV	1071005	1904642	57.89%	10.454%
24	13.036	1882	1887	1895	rVB	41269	73115	2.22%	0.401%
25	13.795	2009	2016	2028	rVB	1221582	2112893	64.21%	11.597%
26	14.454	2123	2128	2134	rVB	32141	53680	1.63%	0.295%

Sum of corrected areas: 18219564

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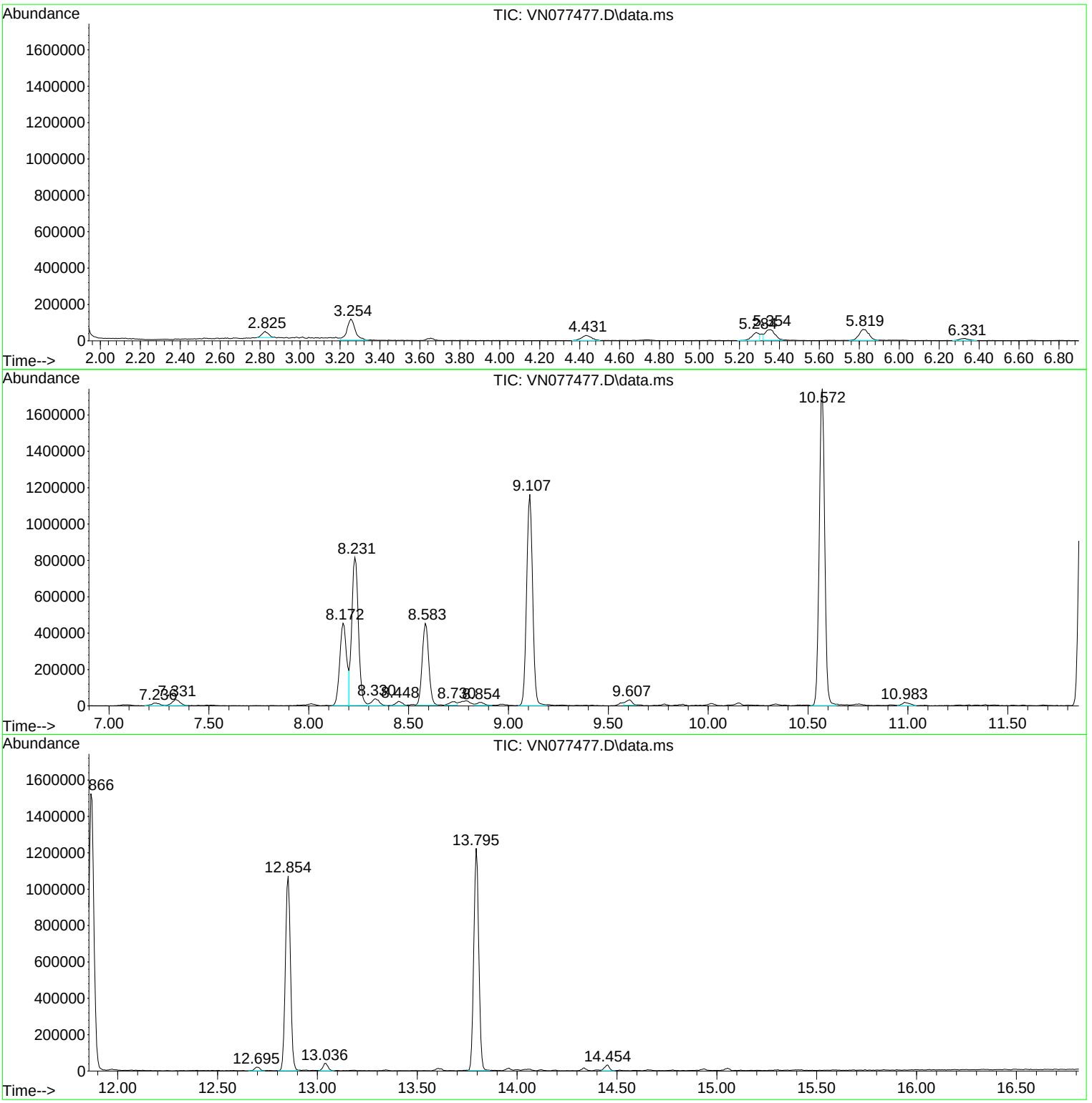
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

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



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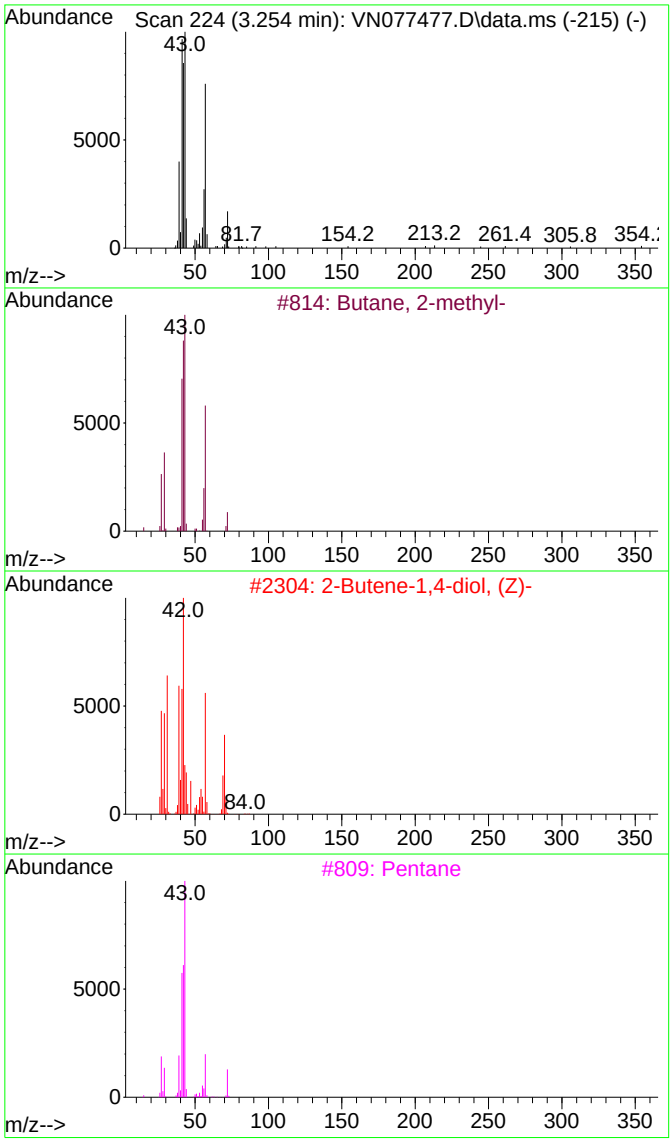
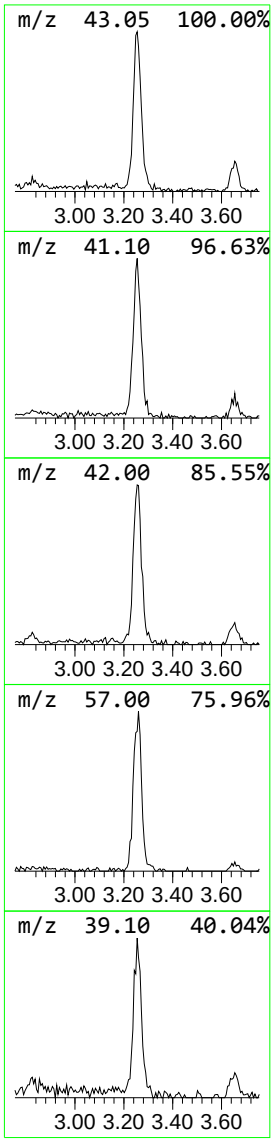
****
Peak Number 1 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.254	8.64 ug/l	323735	Pentafluorobenzene	8.236

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	64
2	2-Butene-1,4-diol, (Z)-	88	C4H8O2	006117-80-2	47
3	Pentane	72	C5H12	000109-66-0	47
4	Oxirane, ethyl-	72	C4H8O	000106-88-7	36
5	1-Hexene	84	C6H12	000592-41-6	33





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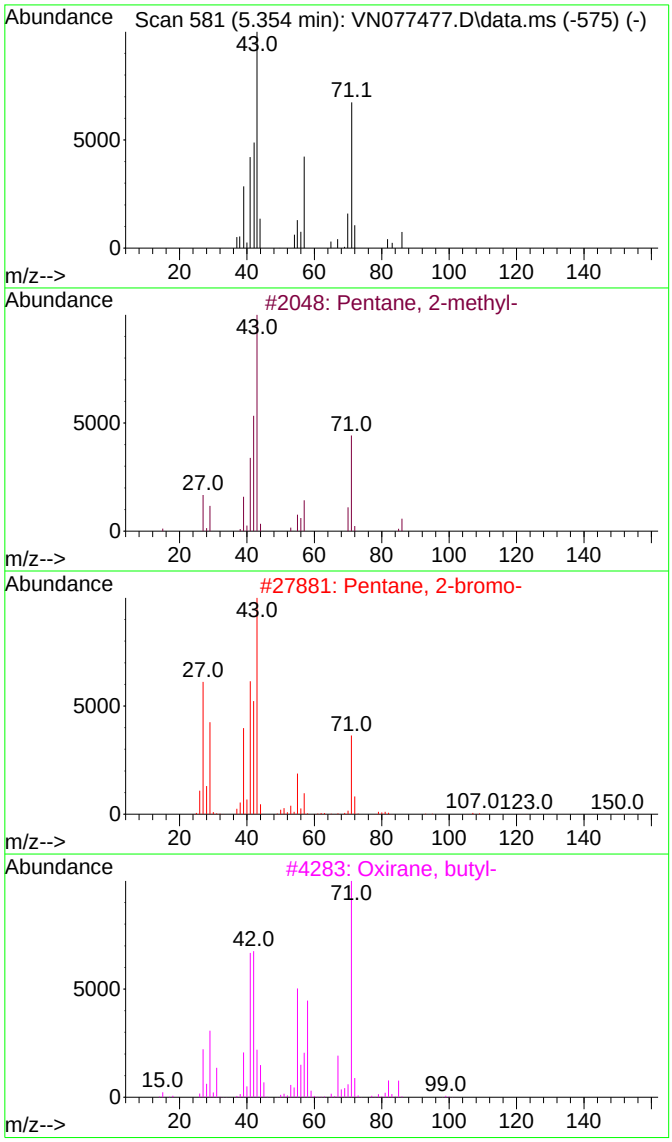
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042423W.M
Quant Title : SW846 8260

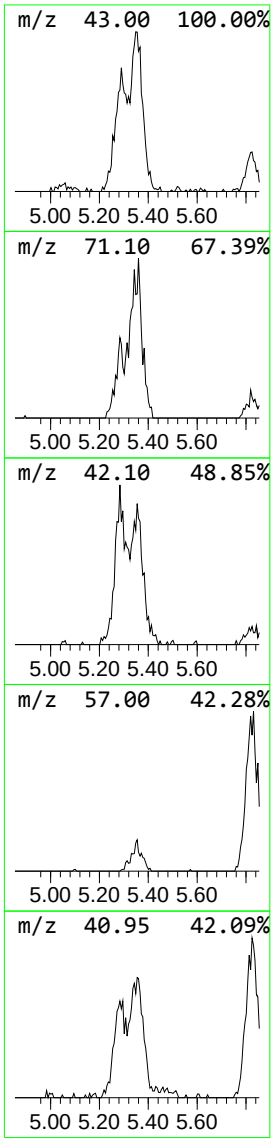
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.354	5.20 ug/l	194982	Pentafluorobenzene	8.236

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	64
2	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	40
3	Oxirane, butyl-	100	C6H12O	001436-34-6	33
4	Pentane	72	C5H12	000109-66-0	32
5	3-Penten-2-ol	86	C5H10O	001569-50-2	27





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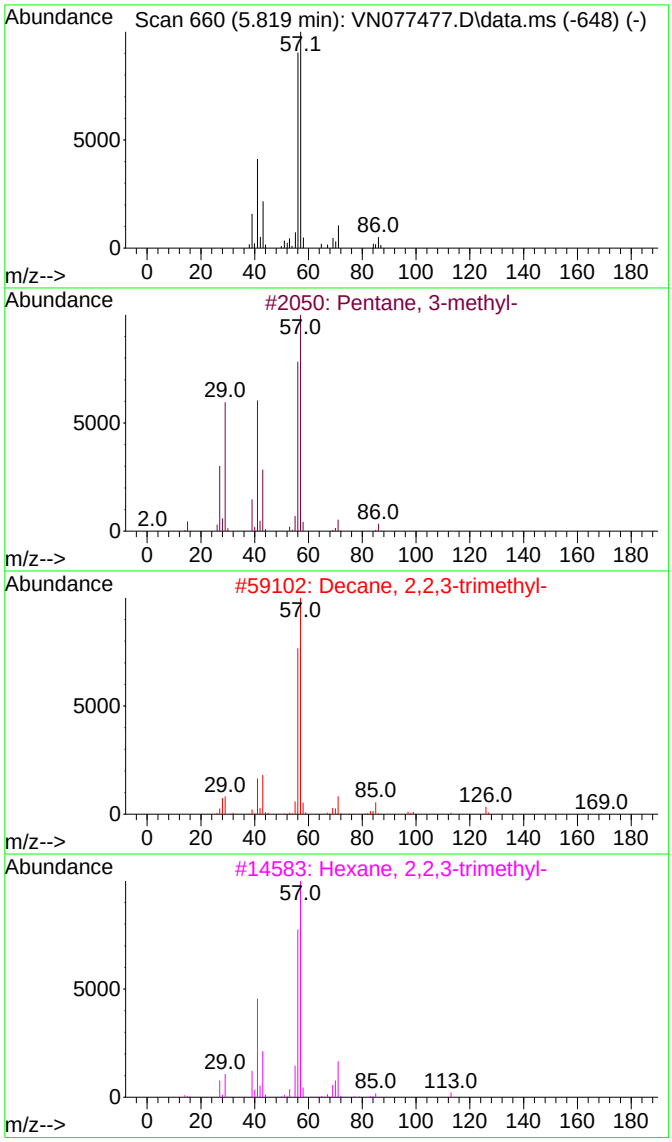
Quant Title : SW846 8260

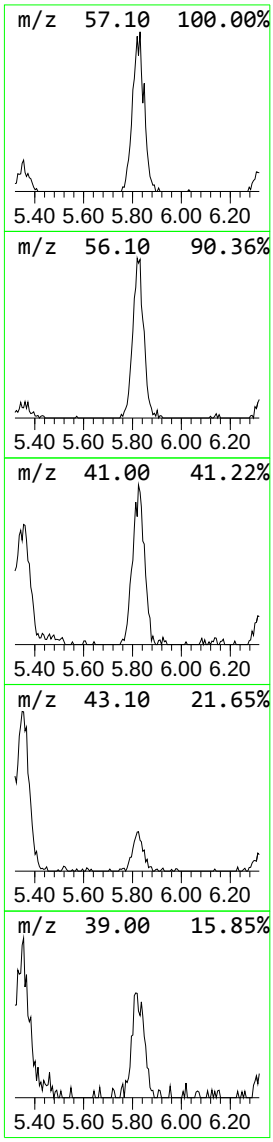
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.819	5.48 ug/l	205531	Pentafluorobenzene	8.236

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	86
2	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	78
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	72
4	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
5	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	56





Tentatively Identified Compound (LSC) summary

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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	8.6	ug/l	323735	1	8.236	1874450	50.0
Pentane, 2-methyl-	5.354	5.2	ug/l	194982	1	8.236	1874450	50.0
Pentane, 3-methyl-	5.819	5.5	ug/l	205531	1	8.236	1874450	50.0