LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060723\
Data File : VN078110.D
Acq On : 07 Jun 2023 17:51
Operator : JC\MD
Sample : 03074-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GT-GW-1

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\82N060623W.M
Title : SW846 8260

Signal : TIC: VN078110.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.089	19	23	32	rVB2	33464	52322	1.16%	0.226%
2	2.330	57	64	71	rBV	361643	524941	11.68%	2.270%
3	2.518	86	96	103	rBV	1111875	1787978	39.78%	7.732%
4	2.624	108	114	120	rVB3	64587	110551	2.46%	0.478%
5	2.753	129	136	142	rBV2	68304	117879	2.62%	0.510%
6	3.253	212	221	235	rVB	383950	851239	18.94%	3.681%
7	3.653	280	289	306	rVB4	64941	188041	4.18%	0.813%
8	3.865	316	325	335	rVB3	27092	68783	1.53%	0.297%
9	4.153	364	374	385	rVB3	59469	157385	3.50%	0.681%
10	4.436	414	422	436	rBV	79408	242109	5.39%	1.047%
11	5.171	539	547	557	rVB5	20201	63127	1.40%	0.273%
12	5.394	576	585	597	rVB4	38101	131659	2.93%	0.569%
13	5.530	597	608	622	rVB2	29681	108573	2.42%	0.470%
14	7.277	895	905	910	rBV3	24508	72595	1.62%	0.314%
15	7.336	910	915	924	rVB2	33464	83561	1.86%	0.361%
16	8.177	1047	1058	1062	rBV	312839	739720	16.46%	3.199%
17	8.235	1062	1068	1084	rVB	532787	1287784	28.65%	5.569%
18	8.612	1119	1132	1149	rBV2	1735355	4495045	100.00%	19.439%
19	9.106	1207	1216	1229	rBV	798163	1637222	36.42%	7.080%
20	10.571	1457	1465	1471	rBV	1202374	2238971	49.81%	9.682%
21	10.635	1471	1476	1492	rVB	1596383	2910909	64.76%	12.588%
22	11.871	1679	1686	1698	rVB	1021072	1882706	41.88%	8.142%
23	11.971	1698	1703	1709	rVB	45484	80590	1.79%	0.349%
24	12.071	1714	1720	1727	rBV	133180	276699	6.16%	1.197%
25	12.406	1770	1777	1784	rBV	108515	195637	4.35%	0.846%
26	12.853	1847	1853	1863	rVB	726175	1287207	28.64%	5.566%
27	13.488	1950	1961	1975	rBV	52000	221467	4.93%	0.958%
28	13.800	2007	2014	2022	rVB	708188	1248515	27.78%	5.399%
29	14.388	2107	2114	2115	rBV5	37574	60962	1.36%	0.264%

Sum of corrected areas: 23124177

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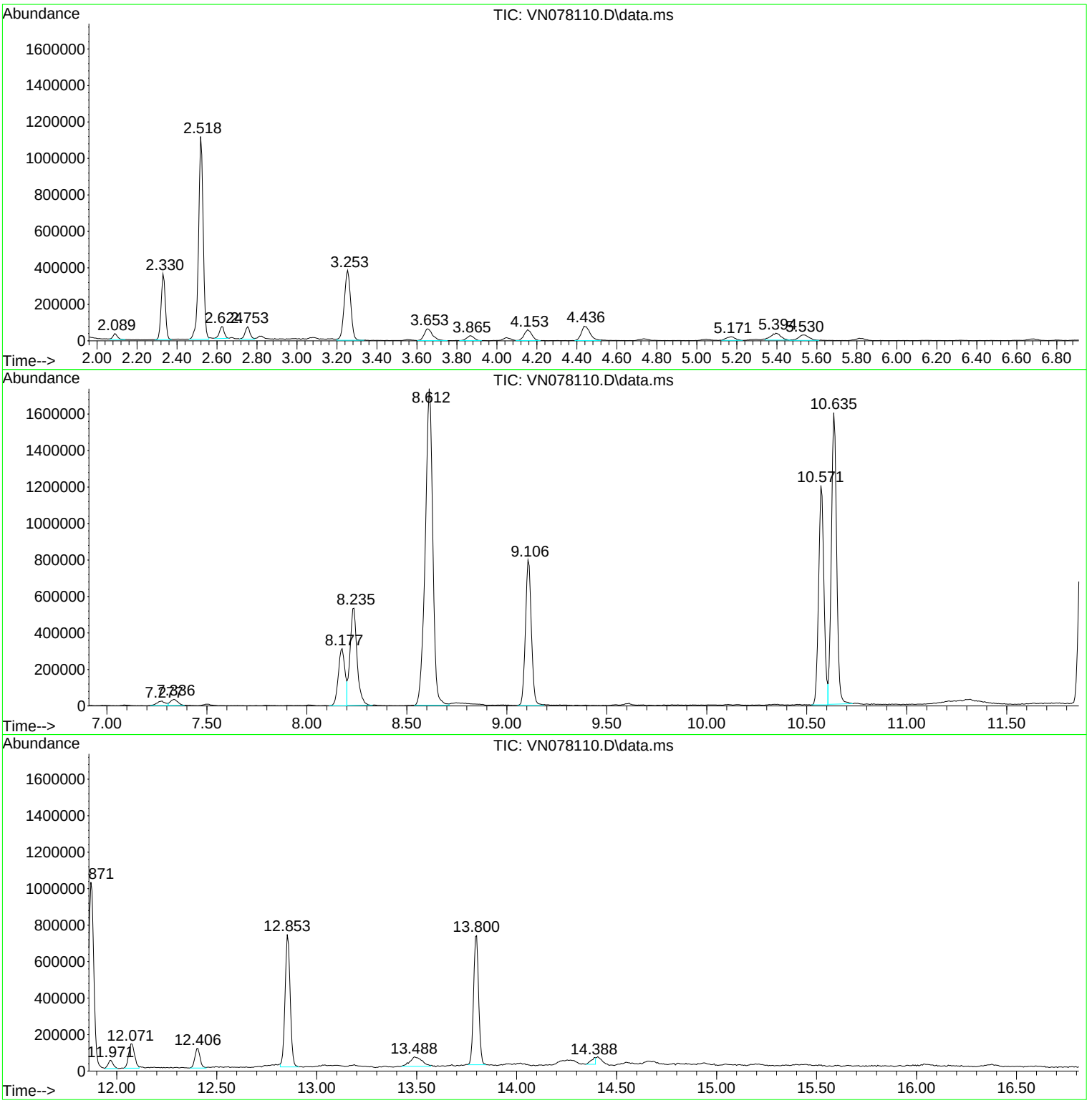
ClientSampleId :
GT-GW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

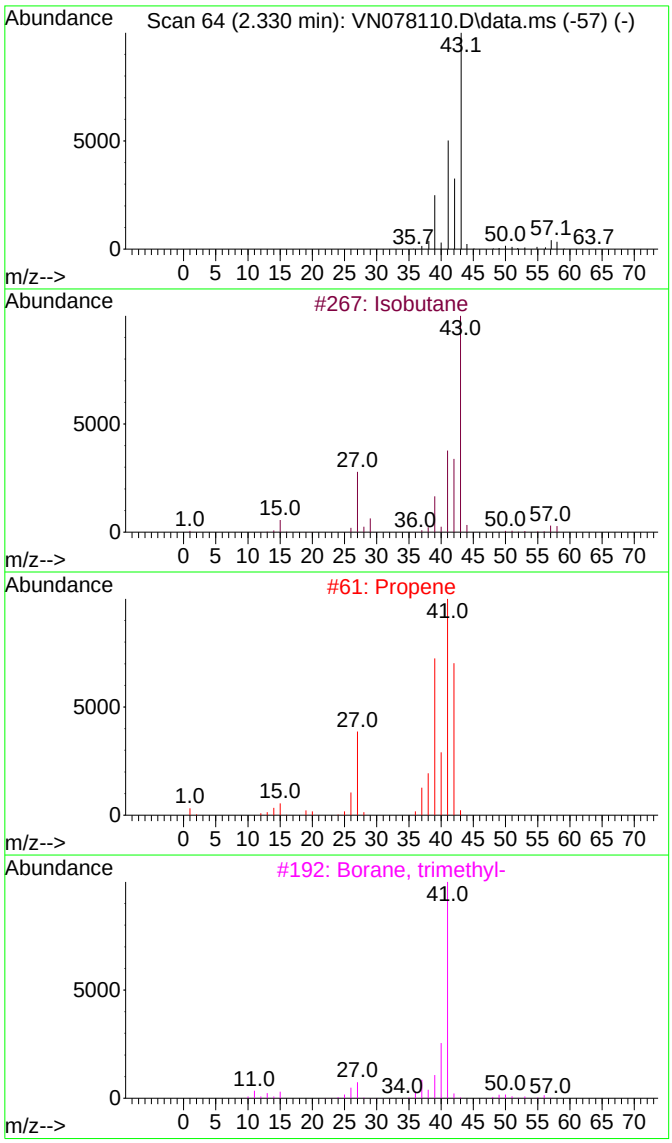
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

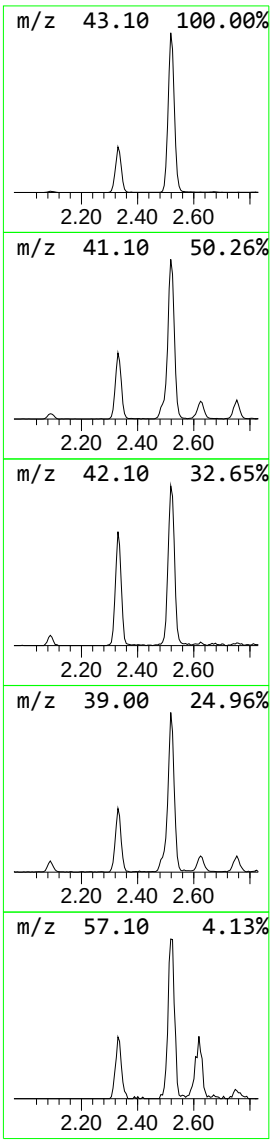
****

Peak Number 1 Isobutane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.330	20.38 ug/l	524941	Pentafluorobenzene	8.235

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	64
2	Propene	42	C3H6	000115-07-1	5
3	Borane, trimethyl-	56	C3H9B	000593-90-8	5
4	Hydrogen isocyanate	43	CHNO	000075-13-8	4
5	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	4





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Instrument :
MSVOA_N
ClientSampleId :
GT-GW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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

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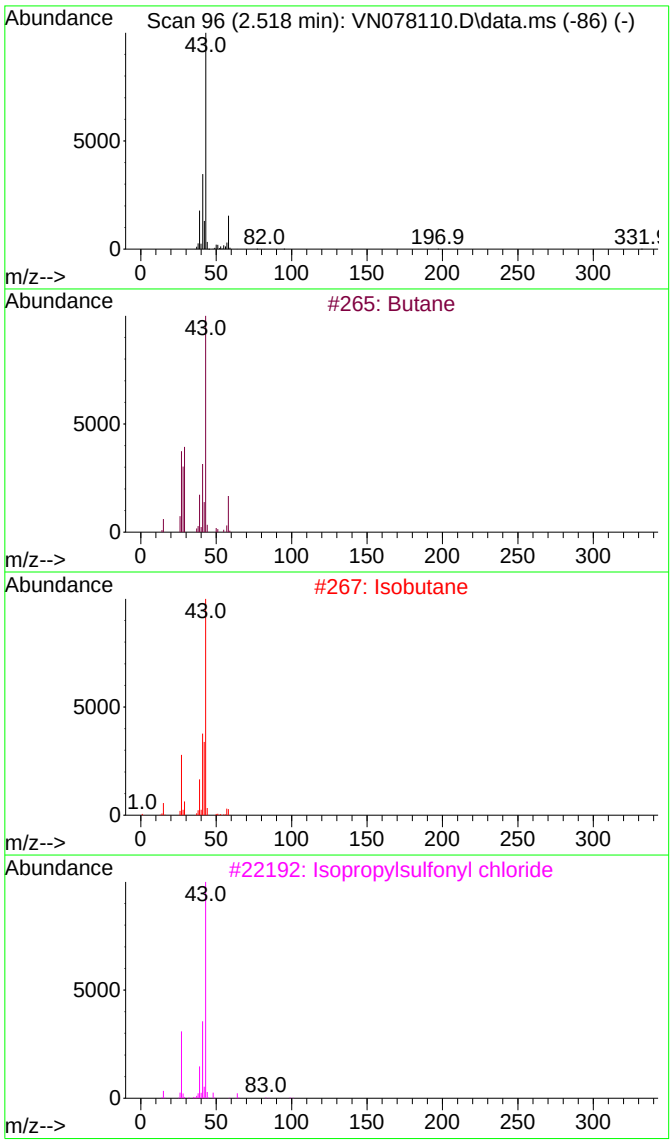
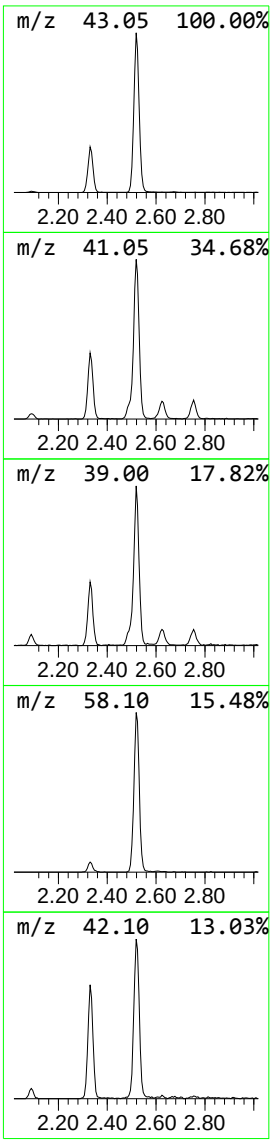
Peak Number 2 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.518	69.42 ug/l	1787980	Pentafluorobenzene	8.235

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





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Instrument :
MSVOA_N
ClientSampleId :
GT-GW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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

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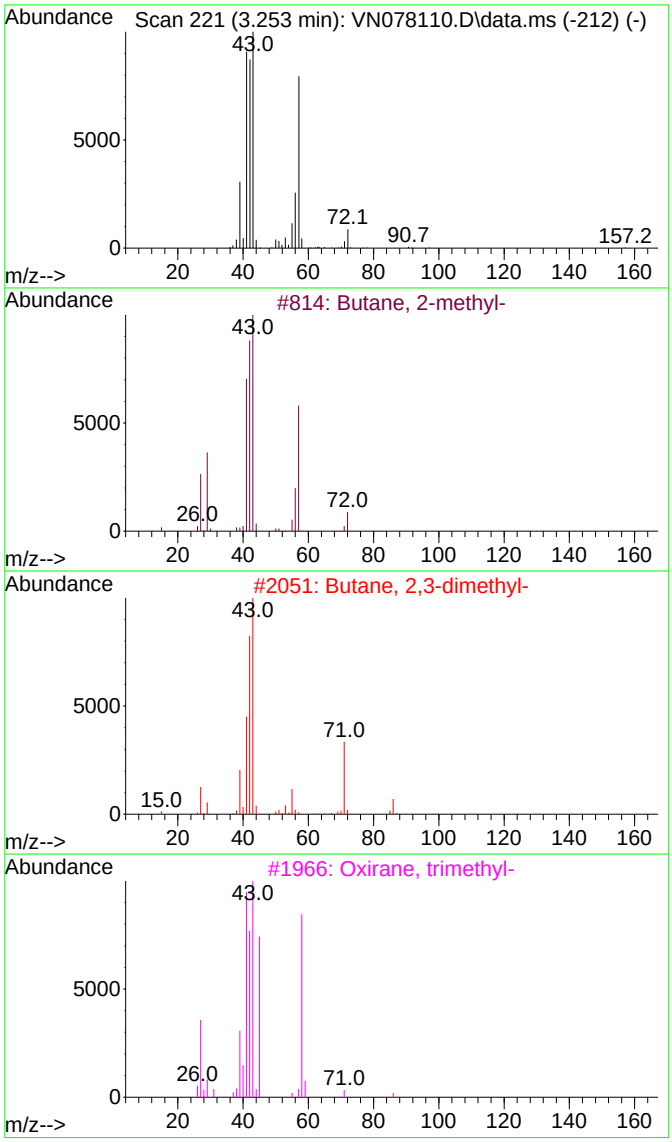
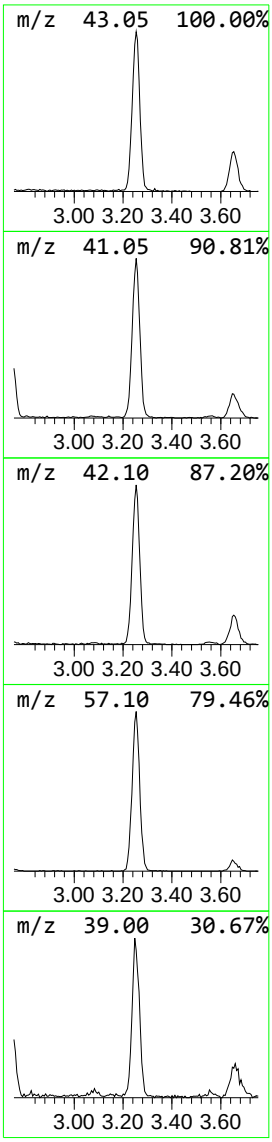
Peak Number 3 Butane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.253	33.05 ug/l	851239	Pentafluorobenzene	8.235

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	33
3	Oxirane, trimethyl-	86	C5H10O	005076-19-7	33
4	Pentane	72	C5H12	000109-66-0	33
5	3-Buten-1-ol	72	C4H8O	000627-27-0	25





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Instrument :
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ClientSampleId :
GT-GW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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

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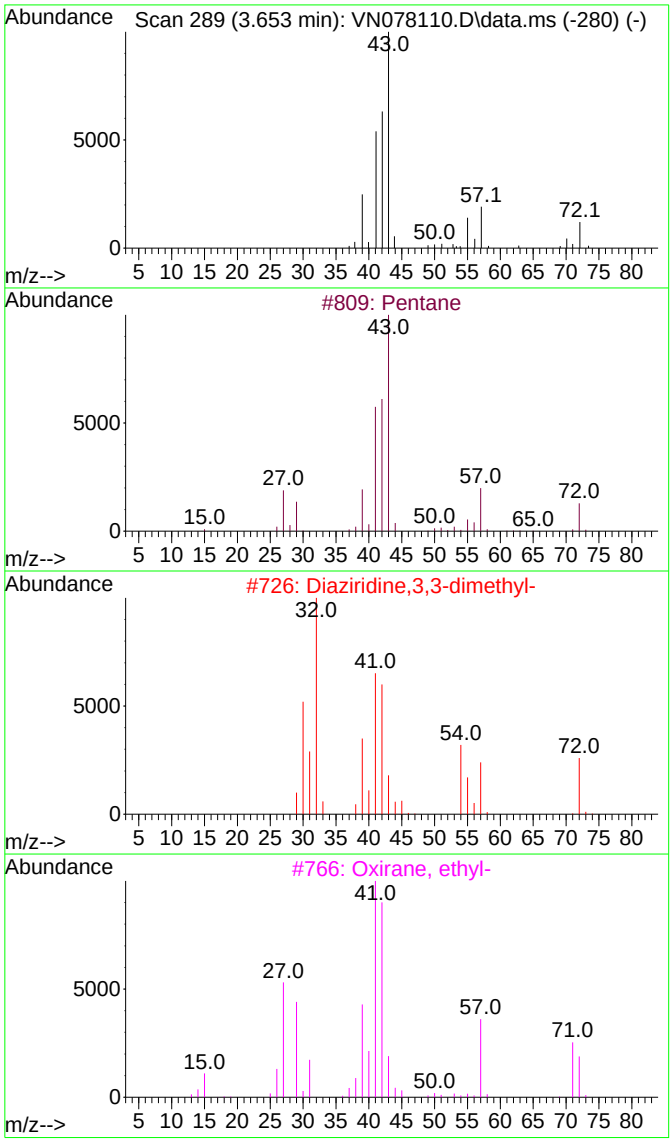
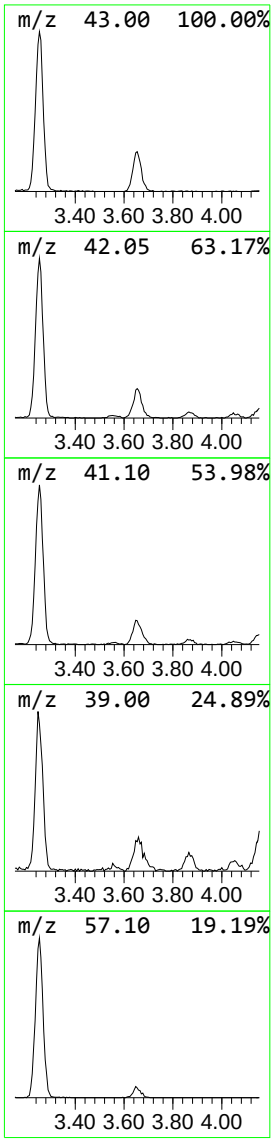
Peak Number 4 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.653	7.30 ug/l	188041	Pentafluorobenzene	8.235

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	53
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	50
4	Butane, 2-methyl-	72	C5H12	000078-78-4	38
5	1-Pentene	70	C5H10	000109-67-1	17





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Sample : 03074-08
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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GT-GW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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

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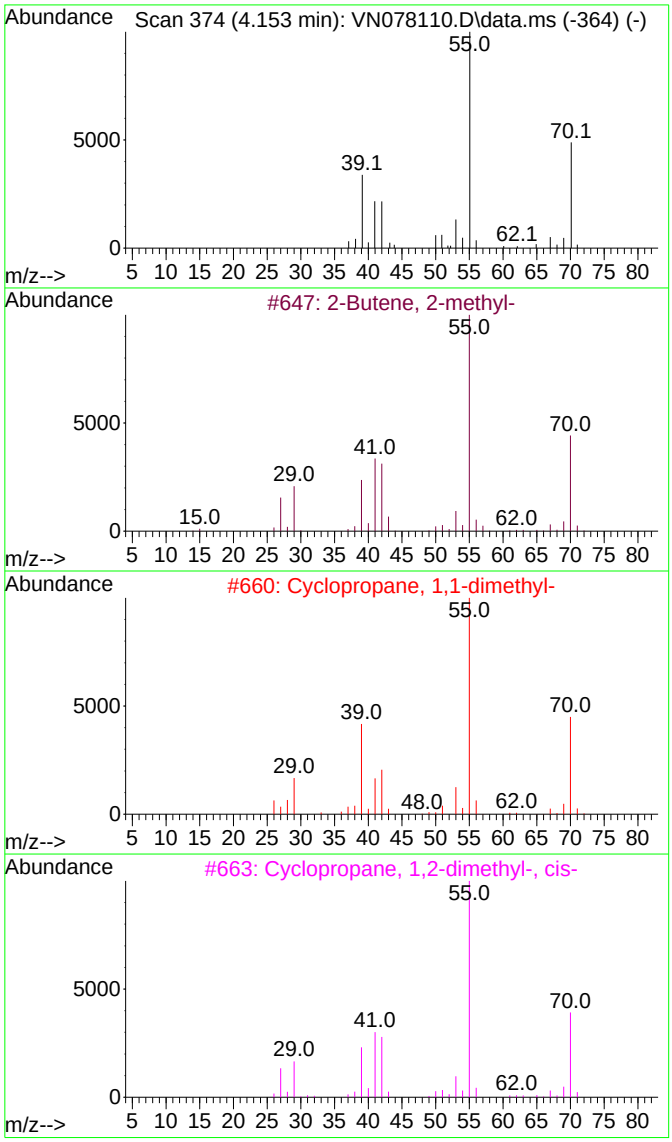
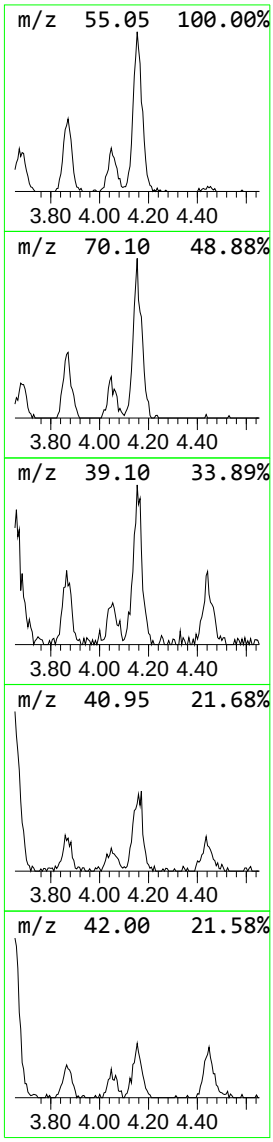
Peak Number 5 2-Butene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.153	6.11 ug/l	157385	Pentafluorobenzene	8.235

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-methyl-	70	C5H10	000513-35-9	78
2	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	72
3	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	72
4	2-Methyl-1-butene	70	C5H10	000563-46-2	72
5	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	64





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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GT-GW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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

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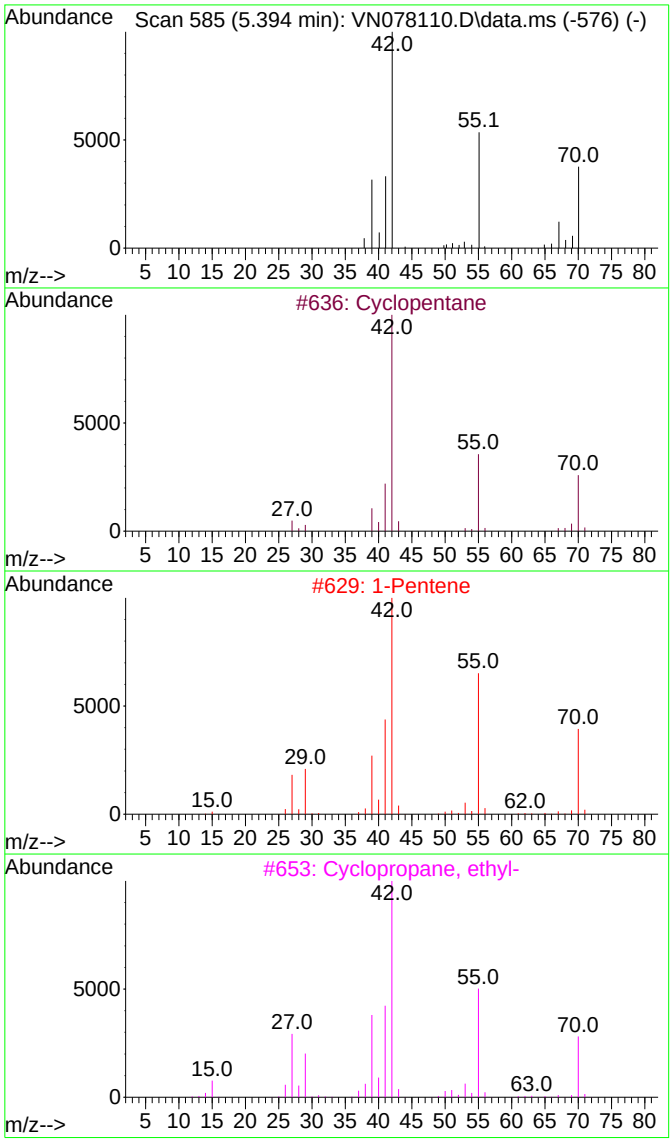
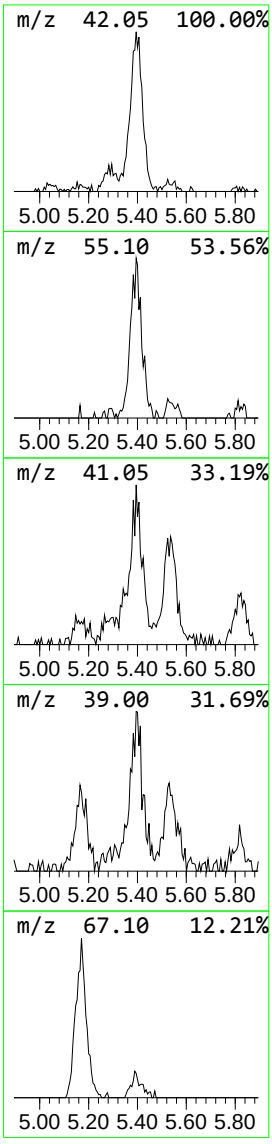
Peak Number 6 Cyclopentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.394	5.11 ug/l	131659	Pentafluorobenzene	8.235

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	72
2	1-Pentene	70	C5H10	000109-67-1	45
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	39
4	2-Pentene	70	C5H10	000109-68-2	23
5	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	12





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
Isobutane	2.330	20.4	ug/l	524941	1	8.235	1287780	50.0
Butane	2.518	69.4	ug/l	1787980	1	8.235	1287780	50.0
Butane, 2-methyl-	3.253	33.0	ug/l	851239	1	8.235	1287780	50.0
Pentane	3.653	7.3	ug/l	188041	1	8.235	1287780	50.0
2-Butene, 2-met...	4.153	6.1	ug/l	157385	1	8.235	1287780	50.0
Cyclopentane	5.394	5.1	ug/l	131659	1	8.235	1287780	50.0