LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061024\
Data File : VX041809.D
Acq On : 10 Jun 2024 14:44
Operator : JC/MD
Sample : P2767-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-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_X\Method\82X052924W.M
Title : SW846 8260

Signal : TIC: VX041809.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	23	25	27	rBV	9363	10045	1.47%	0.193%
2	1.264	27	29	43	rVB2	8893	12306	1.80%	0.237%
3	1.374	43	47	52	rBV	49142	49415	7.21%	0.951%
4	1.605	65	85	86	rBV8	8612	33891	4.95%	0.652%
5	1.660	92	94	98	rVB2	7451	7306	1.07%	0.141%
6	1.721	98	104	115	rVB	355462	466446	68.10%	8.973%
7	1.934	134	139	148	rVB	96070	128777	18.80%	2.477%
8	2.325	194	203	210	rBV	12238	24842	3.63%	0.478%
9	2.770	269	276	280	rBV	27051	62771	9.16%	1.208%
10	2.812	280	283	294	rVV	41389	86477	12.63%	1.664%
11	3.093	319	329	341	rBV	43177	95783	13.98%	1.843%
12	3.434	375	385	397	rBV2	8998	20276	2.96%	0.390%
13	4.294	516	526	538	rVB2	41495	121109	17.68%	2.330%
14	5.385	694	705	713	rBV	76809	227196	33.17%	4.371%
15	5.464	713	718	724	rVV2	17044	52640	7.69%	1.013%
16	5.550	724	732	756	rVB2	130548	393774	57.49%	7.575%
17	5.836	768	779	789	rBV6	9048	30107	4.40%	0.579%
18	5.952	789	798	817	rVV	81481	222578	32.50%	4.282%
19	6.153	821	831	840	rVV6	10085	32094	4.69%	0.617%
20	6.251	840	847	855	rVV3	10054	28077	4.10%	0.540%
21	6.354	855	864	875	rVB3	13370	38335	5.60%	0.737%
22	6.757	920	930	942	rBV	201666	488738	71.36%	9.402%
23	7.379	1021	1032	1043	rBV3	39072	97950	14.30%	1.884%
24	7.653	1071	1077	1084	rBV2	4089	7960	1.16%	0.153%
25	8.604	1227	1233	1234	rBV2	5161	8460	1.24%	0.163%
26	8.647	1234	1240	1255	rVV	434972	684938	100.00%	13.176%
27	8.769	1255	1260	1266	rVB2	5500	8987	1.31%	0.173%
28	8.976	1289	1294	1300	rVB2	10795	17938	2.62%	0.345%
29	9.098	1307	1314	1320	rBV4	3714	7067	1.03%	0.136%
30	9.159	1320	1324	1335	rVB	6583	10720	1.57%	0.206%
31	10.055	1465	1471	1479	rBV	453027	625523	91.33%	12.033%
32	11.079	1634	1639	1654	rBV	373435	497914	72.69%	9.578%
33	12.018	1788	1793	1804	rBV	458328	597852	87.29%	11.501%

Sum of corrected areas: 5198292

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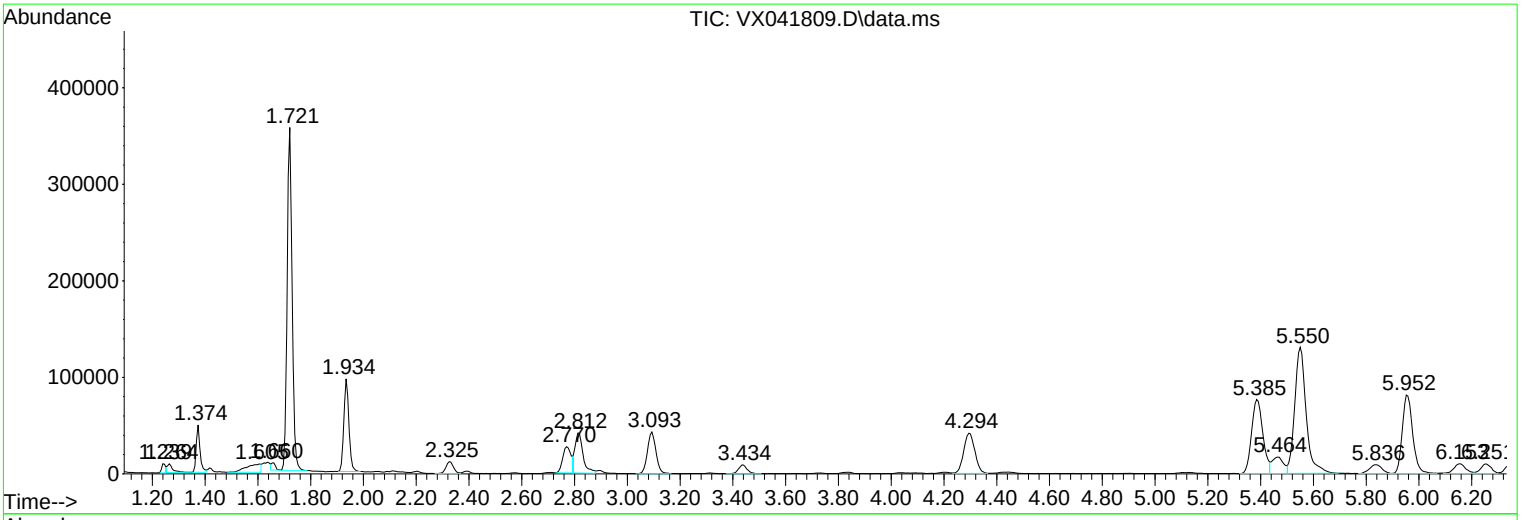
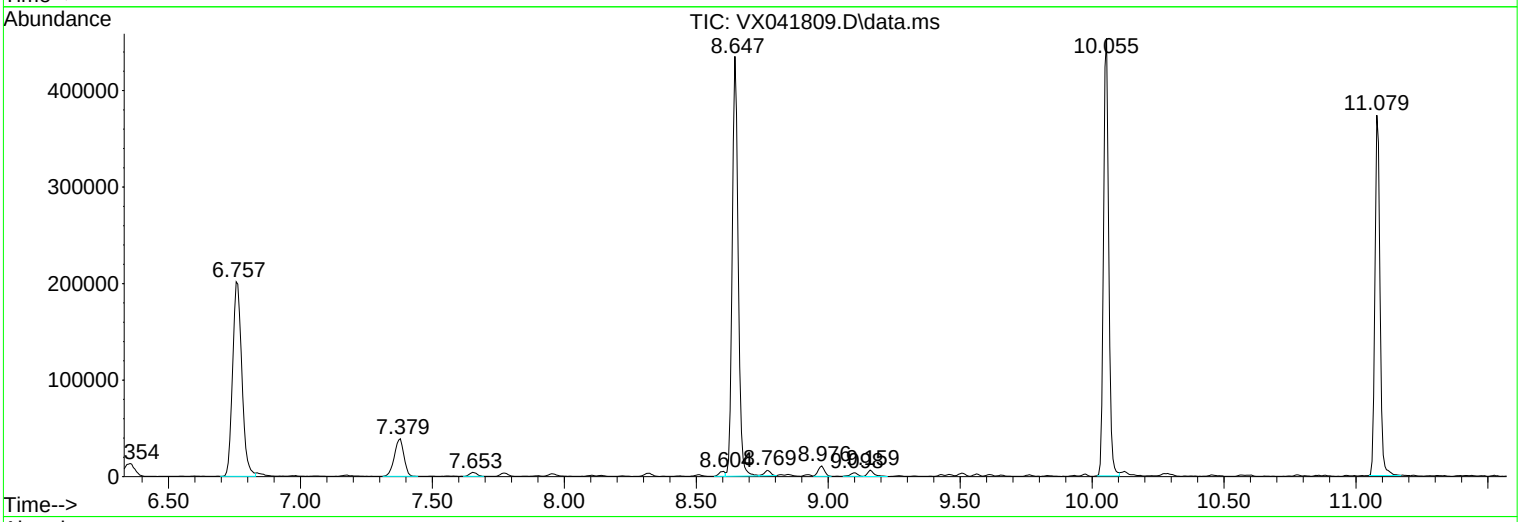
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

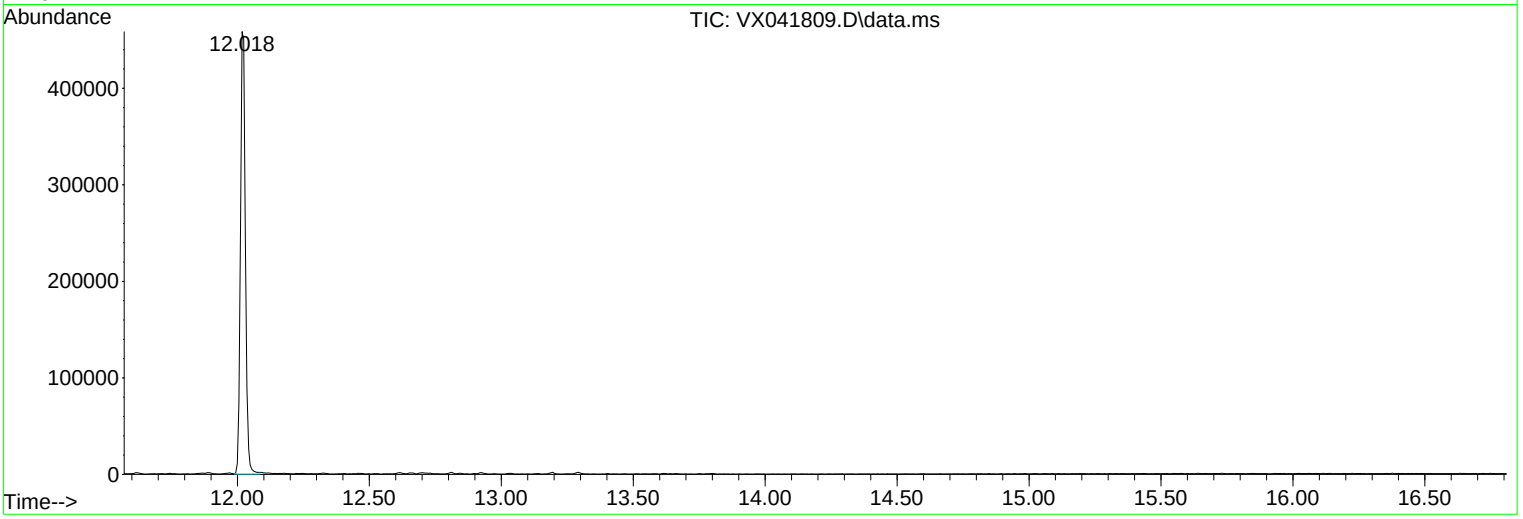
Instrument :
MSVOA_X
ClientSampleId :
PMW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061024\
Data File : VX041809.D
Acq On : 10 Jun 2024 14:44
Operator : JC/MD
Sample : P2767-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

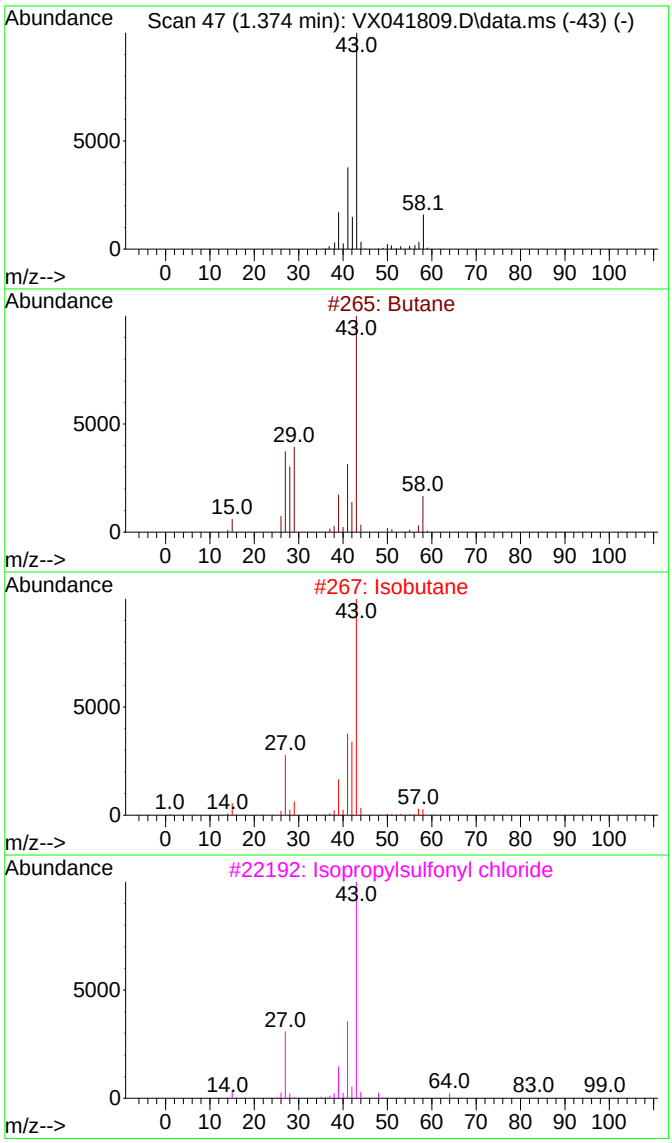
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

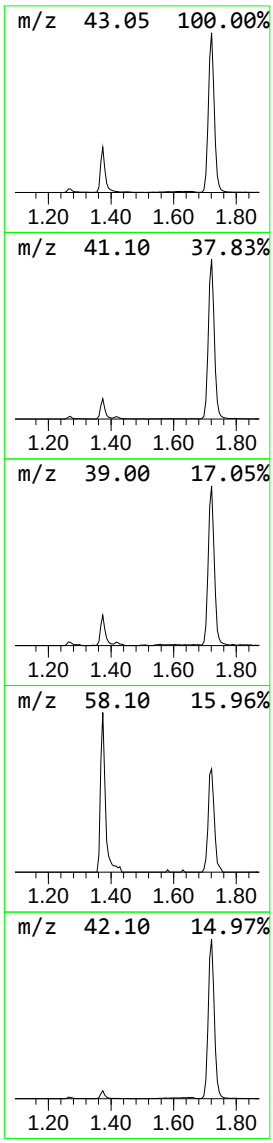
****

Peak Number 1 Butane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	6.27 ug/l	49415	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	80
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	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061024\
Data File : VX041809.D
Acq On : 10 Jun 2024 14:44
Operator : JC/MD
Sample : P2767-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

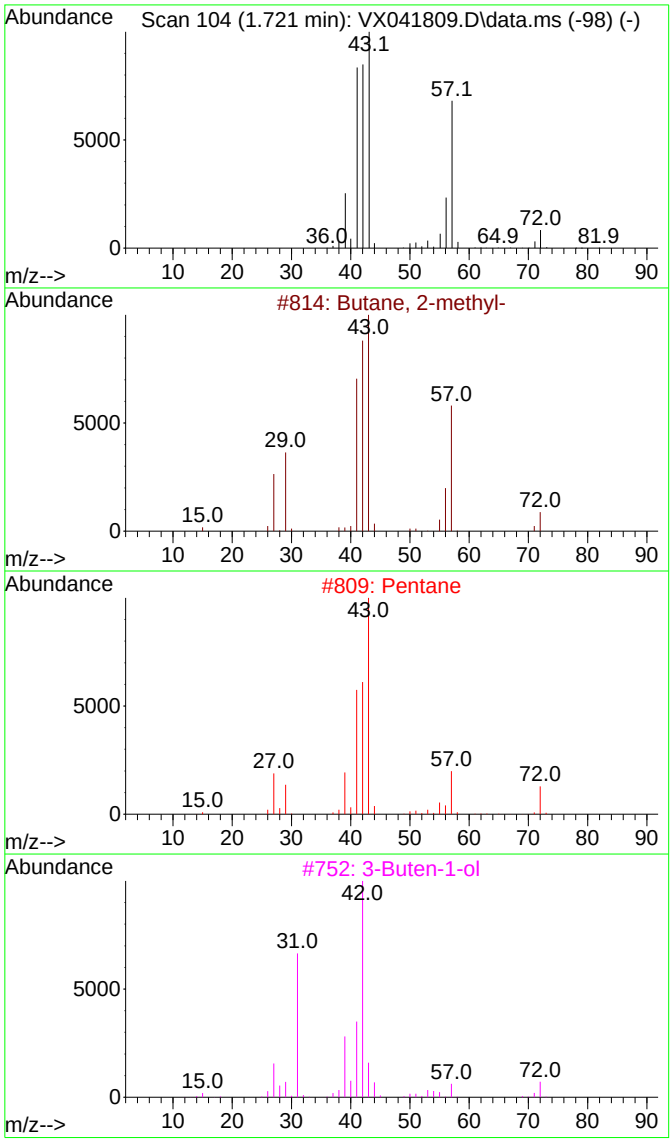
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

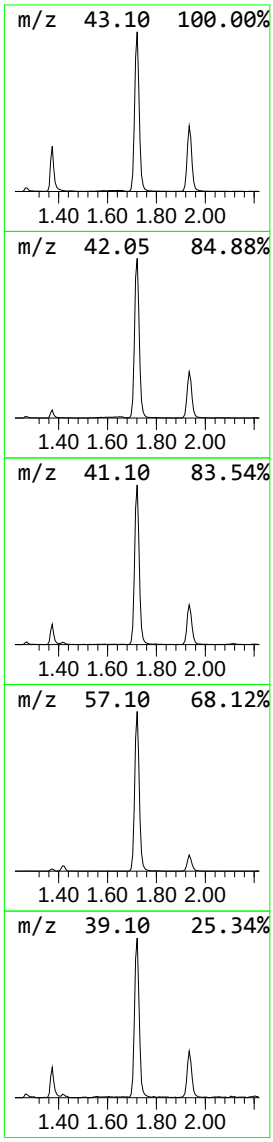
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.721	59.23 ug/l	466446	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	Pentane	72	C5H12	000109-66-0	36
3	3-Buten-1-ol	72	C4H8O	000627-27-0	28
4	1-Butene	56	C4H8	000106-98-9	10
5	3-Buten-2-ol	72	C4H8O	000598-32-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061024\
Data File : VX041809.D
Acq On : 10 Jun 2024 14:44
Operator : JC/MD
Sample : P2767-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

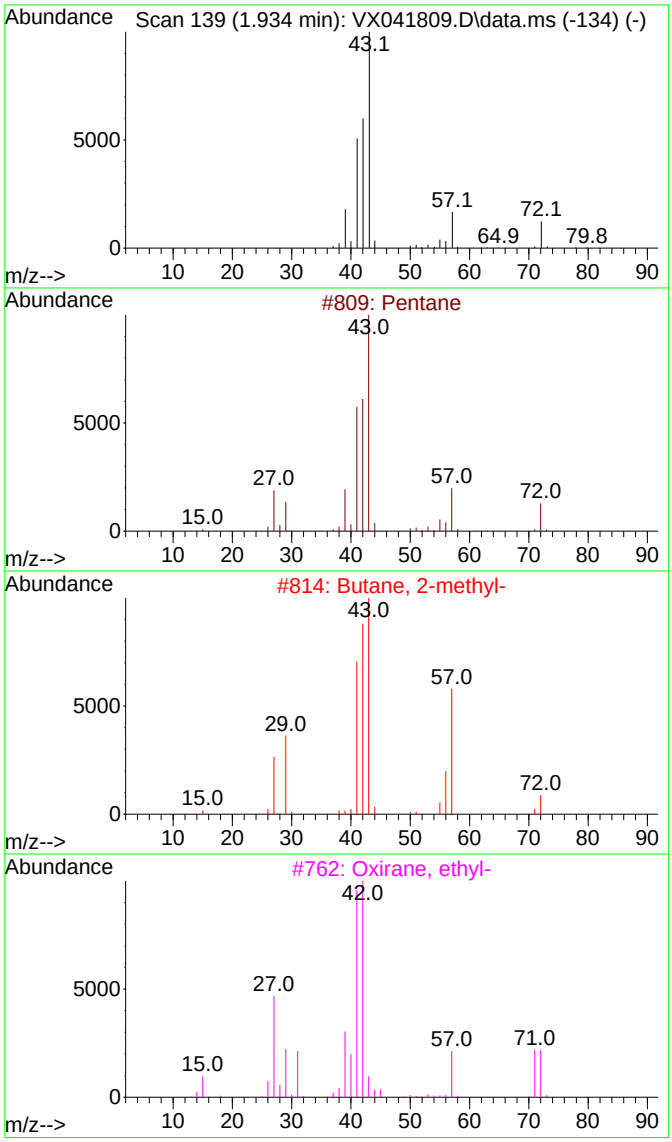
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

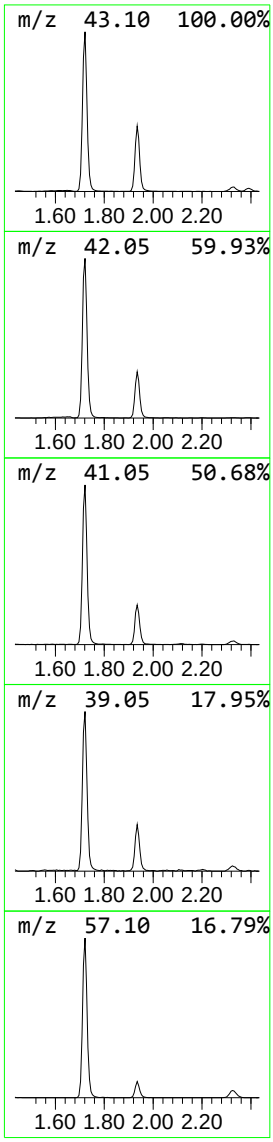
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.934	16.35 ug/l	128777	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Butane, 2-methyl-	72	C5H12	000078-78-4	50
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	40
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	35
5	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061024\
Data File : VX041809.D
Acq On : 10 Jun 2024 14:44
Operator : JC/MD
Sample : P2767-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

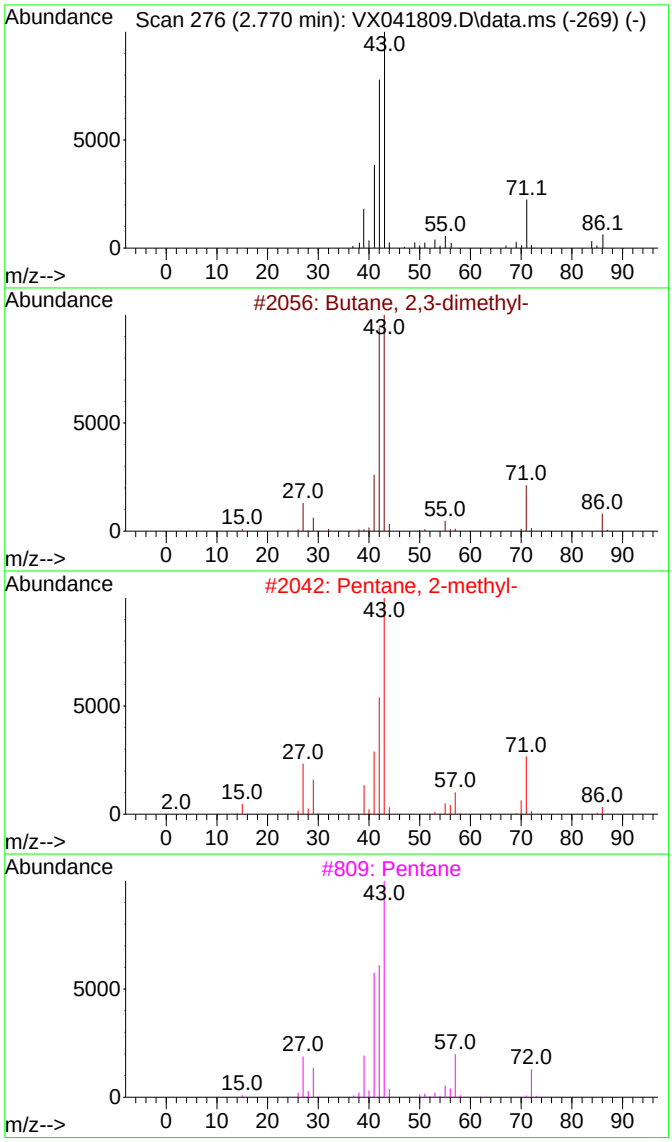
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

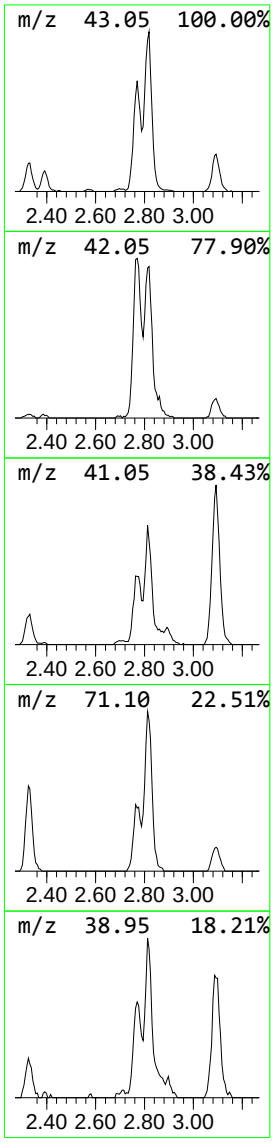
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.770	7.97 ug/l	62771	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3	Pentane	72	C5H12	000109-66-0	38
4	1-Pentene	70	C5H10	000109-67-1	38
5	Pyrrolidine	71	C4H9N	000123-75-1	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061024\
Data File : VX041809.D
Acq On : 10 Jun 2024 14:44
Operator : JC/MD
Sample : P2767-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

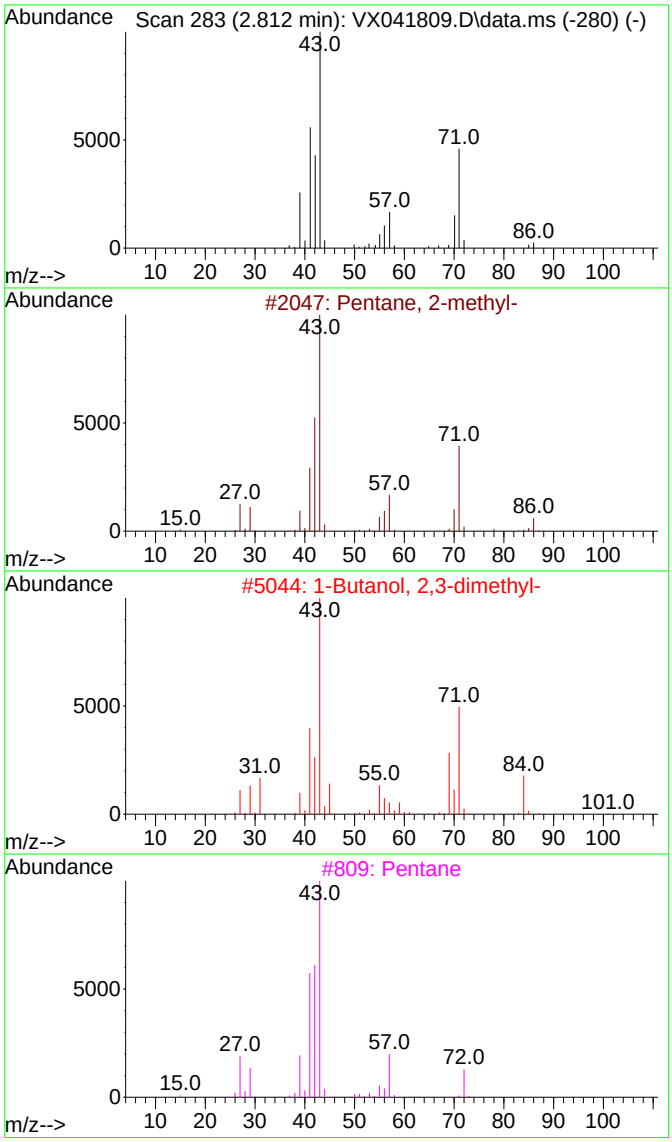
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

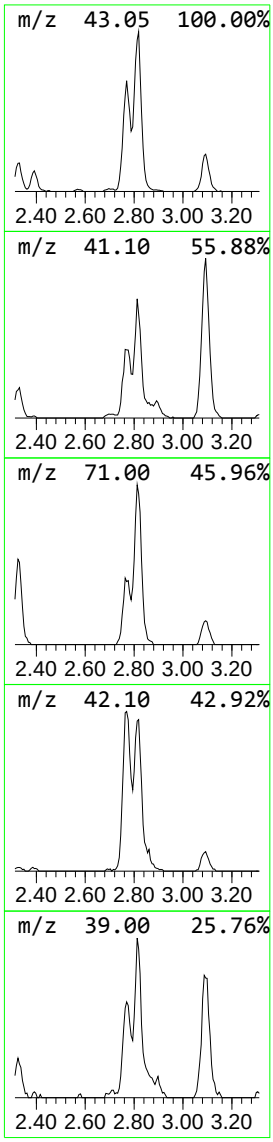
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.812	10.98 ug/l	86477	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	45
3	Pentane	72	C5H12	000109-66-0	43
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	28
5	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	28





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061024\
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Operator : JC/MD
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

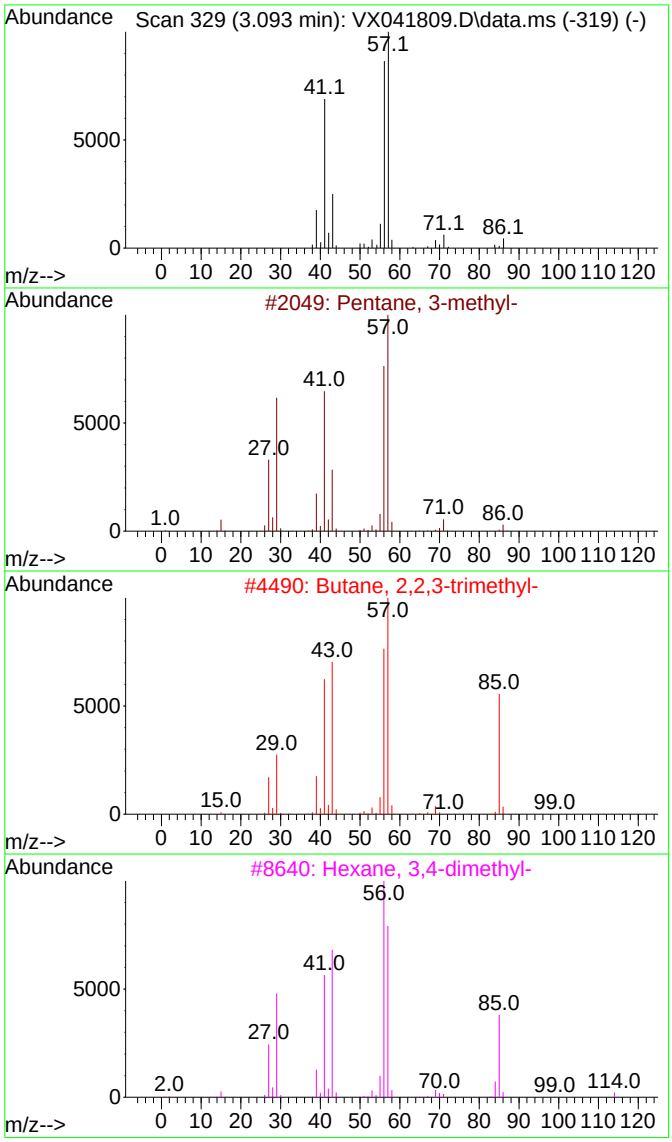
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

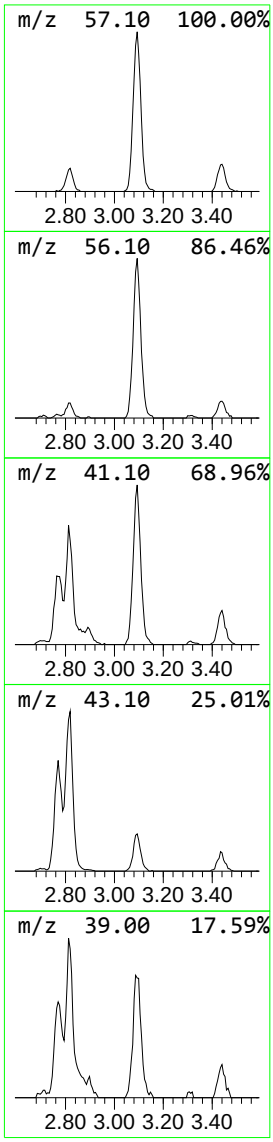
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Pentane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.093	12.16 ug/l	95783	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	87
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	83
3	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	78
4	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	59
5	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	56





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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

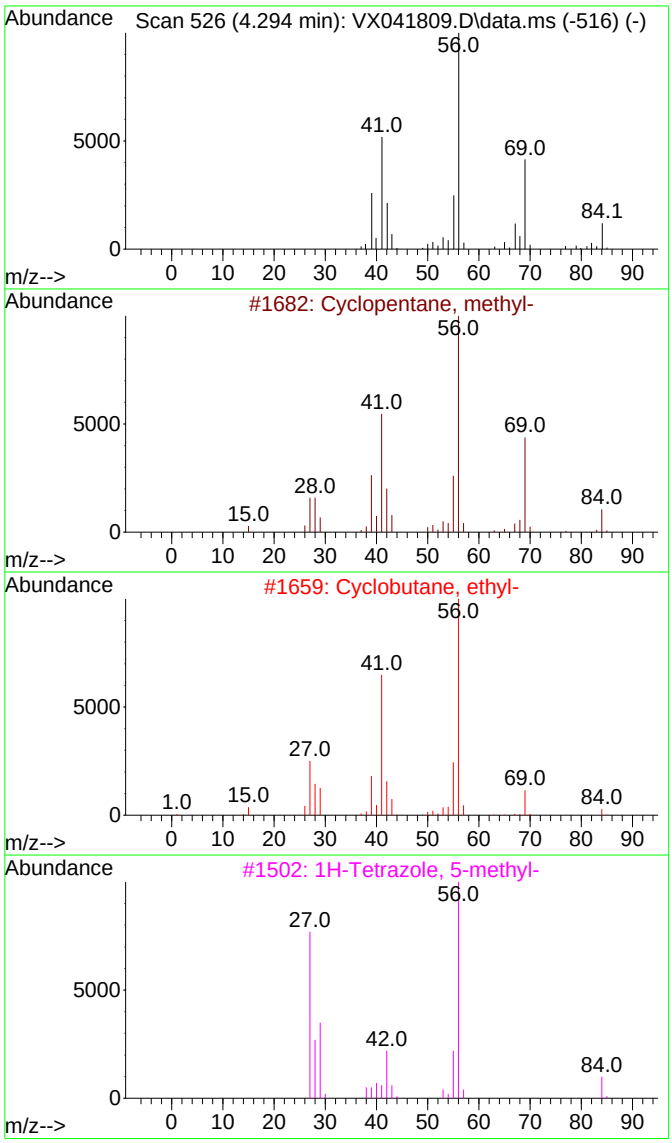
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

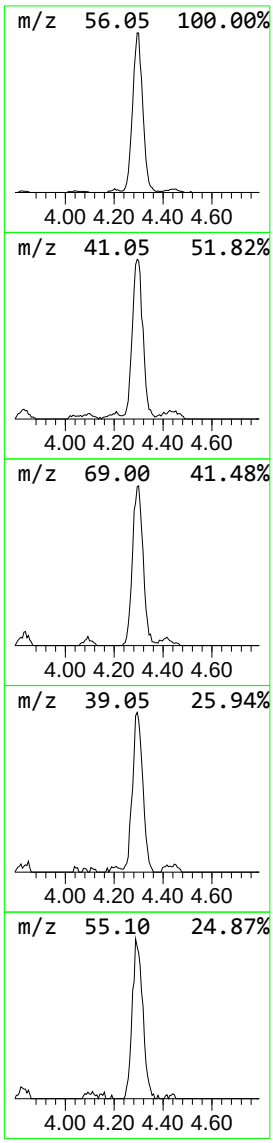
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.294	15.38 ug/l	121109	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	59
4	Cyclobutane	56	C4H8	000287-23-0	47
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	47





Tentatively Identified Compound (LSC) summary

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.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	1.374	6.3	ug/l	49415	1	5.550	393774	50.0
Butane, 2-methyl-	1.721	59.2	ug/l	466446	1	5.550	393774	50.0
Pentane	1.934	16.4	ug/l	128777	1	5.550	393774	50.0
Butane, 2,3-dim...	2.770	8.0	ug/l	62771	1	5.550	393774	50.0
Pentane, 2-methyl-	2.812	11.0	ug/l	86477	1	5.550	393774	50.0
Pentane, 3-methyl-	3.093	12.2	ug/l	95783	1	5.550	393774	50.0
Cyclopentane, m...	4.294	15.4	ug/l	121109	1	5.550	393774	50.0