LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032923\
Data File : VX034834.D
Acq On : 29 Mar 2023 17:31
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 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\82X032923W.M
Title : SW846 8260

Signal : TIC: VX034834.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	35	rBV	36289	32009	1.99%	0.265%
2	1.367	43	46	51	rBV	192425	202536	12.62%	1.674%
3	1.416	51	54	58	rVB	17803	19374	1.21%	0.160%
4	1.751	103	109	127	rVB	1212874	1604699	100.00%	13.265%
5	1.953	137	142	152	rBV	179352	255013	15.89%	2.108%
6	2.343	197	206	217	rBV	59802	122133	7.61%	1.010%
7	2.782	270	278	282	rBV2	124337	267812	16.69%	2.214%
8	2.824	282	285	291	rVB	111100	194945	12.15%	1.612%
9	3.105	319	331	343	rBV	161174	367918	22.93%	3.041%
10	3.446	377	387	397	rVB2	17511	39150	2.44%	0.324%
11	3.836	443	451	461	rBV5	8099	22123	1.38%	0.183%
12	4.208	504	512	519	rBV4	8385	23928	1.49%	0.198%
13	4.306	519	528	539	rVB	106771	297277	18.53%	2.457%
14	5.123	648	662	663	rBV7	6674	17068	1.06%	0.141%
15	5.385	693	705	713	rBV	151415	441609	27.52%	3.651%
16	5.470	713	719	724	rVV	31670	73480	4.58%	0.607%
17	5.549	724	732	741	rVV3	233048	626697	39.05%	5.181%
18	5.842	769	780	789	rBV4	29178	96903	6.04%	0.801%
19	5.952	789	798	813	rVV	182637	478625	29.83%	3.957%
20	6.159	816	832	841	rVV5	31249	109625	6.83%	0.906%
21	6.257	841	848	856	rVV4	32325	92246	5.75%	0.763%
22	6.360	856	865	877	rVB3	39188	113962	7.10%	0.942%
23	6.763	920	931	941	rBV	406793	1005259	62.64%	8.310%
24	7.177	991	999	1007	rVB4	10947	24664	1.54%	0.204%
25	7.378	1020	1032	1041	rVB3	80829	215435	13.43%	1.781%
26	7.659	1071	1078	1089	rVB5	9781	21083	1.31%	0.174%
27	7.775	1089	1097	1104	rVB2	29863	57095	3.56%	0.472%
28	7.958	1121	1127	1141	rVB6	12616	40243	2.51%	0.333%
29	8.098	1141	1150	1156	rBV4	9001	21913	1.37%	0.181%
30	8.317	1178	1186	1193	rBV4	22314	49439	3.08%	0.409%
31	8.506	1208	1217	1226	rVB5	11084	27095	1.69%	0.224%
32	8.604	1226	1233	1235	rBV2	21364	40373	2.52%	0.334%
33	8.646	1235	1240	1250	rVB	872335	1352818	84.30%	11.183%
34	8.774	1256	1261	1265	rVB2	23758	37165	2.32%	0.307%
35	8.921	1280	1285	1289	rBV2	10386	16100	1.00%	0.133%
36	8.976	1289	1294	1300	rVB	71879	113795	7.09%	0.941%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032923\
Data File : VX034834.D
Acq On : 29 Mar 2023 17:31
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 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\82X032923W.M
Title : SW846 8260

37	9.098	1306	1314	1320	rBV3	17398	32512	2.03%	0.269%
38	9.159	1320	1324	1335	rVB	33455	62166	3.87%	0.514%
39	9.506	1376	1381	1386	rVB3	19445	34096	2.12%	0.282%
40	9.658	1402	1406	1416	rVB6	12774	27672	1.72%	0.229%
41	9.762	1416	1423	1430	rBV5	11442	24204	1.51%	0.200%
42	9.835	1430	1435	1444	rVV3	13180	25611	1.60%	0.212%
43	10.055	1465	1471	1478	rVV	870112	1167067	72.73%	9.648%
44	10.128	1480	1483	1486	rVB	11794	17080	1.06%	0.141%
45	10.274	1503	1507	1509	rBV3	16783	25675	1.60%	0.212%
46	10.299	1509	1511	1518	rVB5	20566	31406	1.96%	0.260%
47	10.457	1531	1537	1546	rVB4	14027	27920	1.74%	0.231%
48	10.591	1550	1559	1565	rBV8	16396	45570	2.84%	0.377%
49	10.780	1580	1590	1593	rBV2	14352	28861	1.80%	0.239%
50	10.853	1598	1602	1612	rVV6	6531	16523	1.03%	0.137%
51	11.079	1634	1639	1645	rBV	703620	892550	55.62%	7.378%
52	12.024	1788	1794	1804	rBV	818773	1077779	67.16%	8.910%
53	12.317	1838	1842	1849	rVB8	7994	19700	1.23%	0.163%
54	12.920	1933	1941	1947	rBV3	8886	18787	1.17%	0.155%

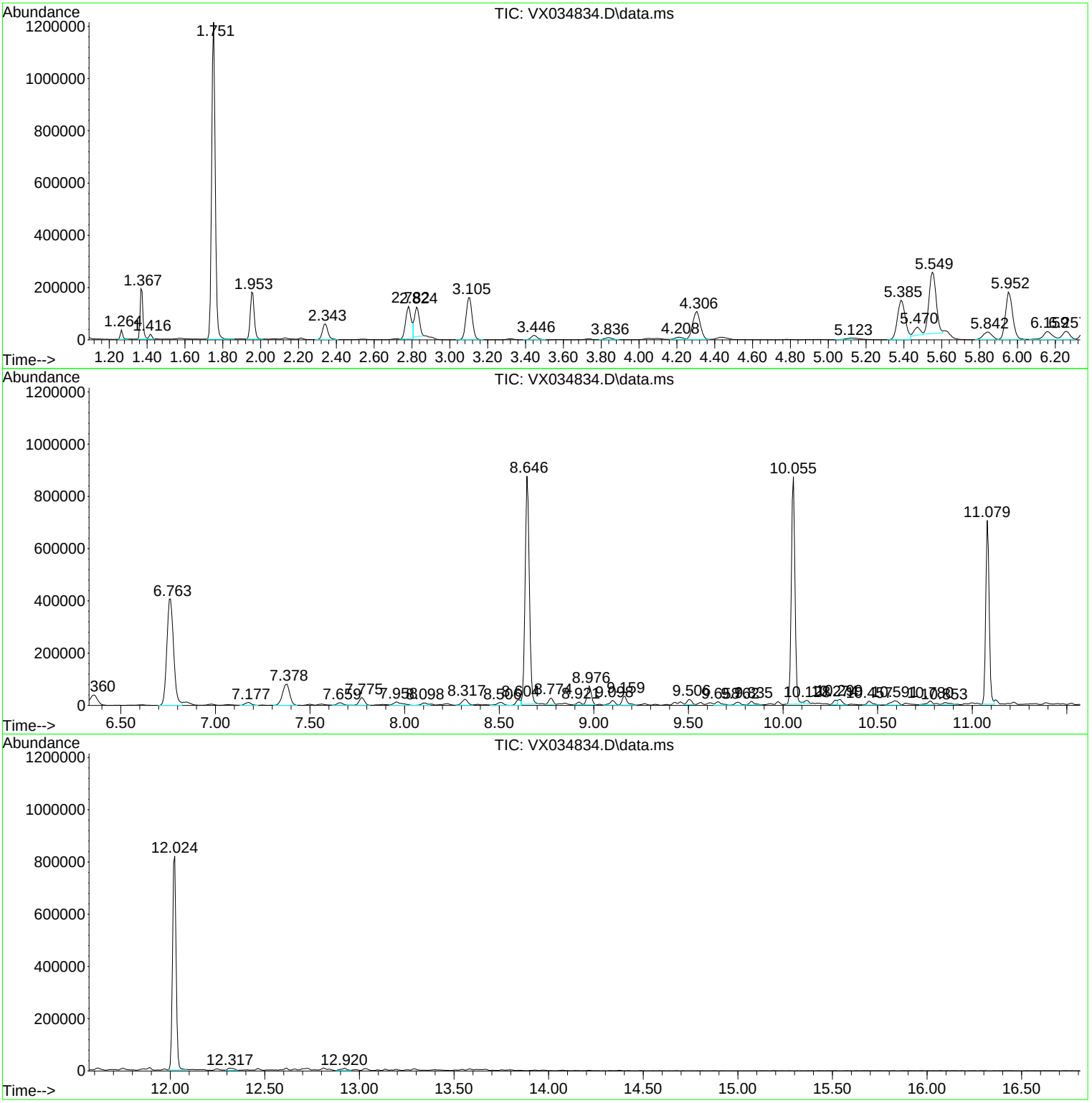
Sum of corrected areas: 12096788

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032923\
Data File : VX034834.D
Acq On : 29 Mar 2023 17:31
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032923\
Data File : VX034834.D
Acq On : 29 Mar 2023 17:31
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

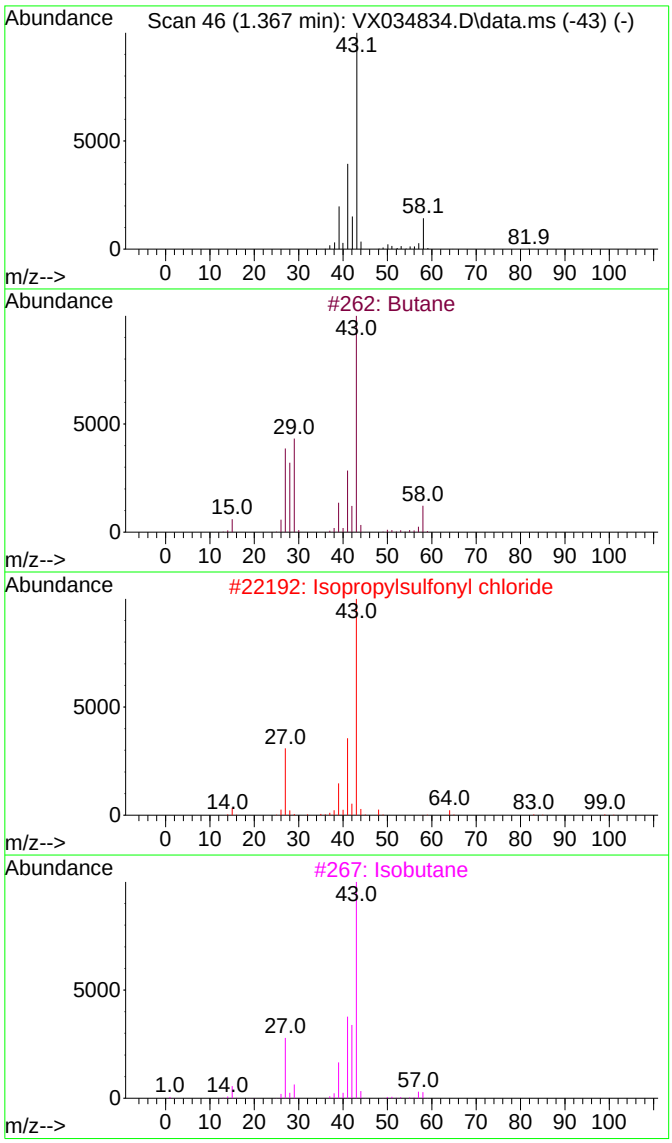
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

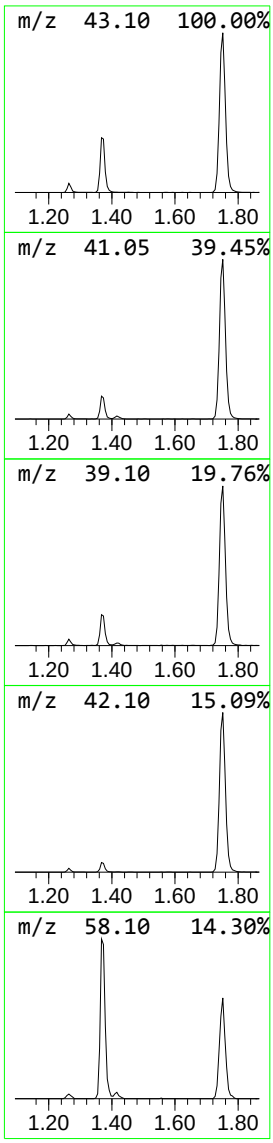
****

Peak Number 1 Butane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.367	16.16 ug/l	202536	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	72
2	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3	Isobutane	58	C4H10	000075-28-5	9
4	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5	Diazene, dimethyl-	58	C2H6N2	000503-28-6	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032923\
Data File : VX034834.D
Acq On : 29 Mar 2023 17:31
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

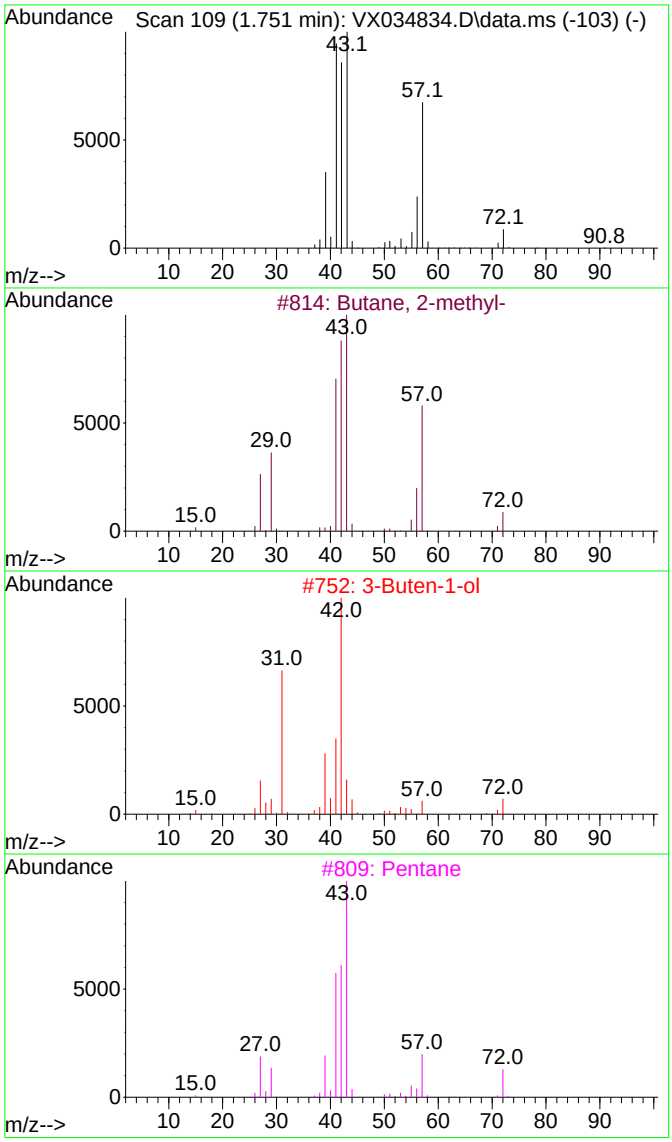
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

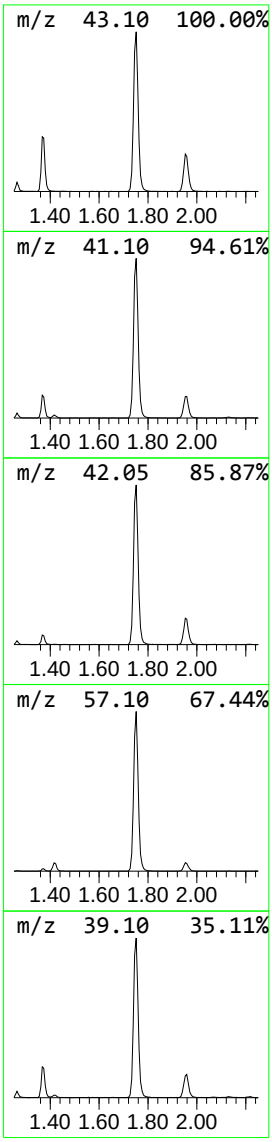
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.751	128.03 ug/l	1604700	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	36
4	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	33
5	1-Butene	56	C4H8	000106-98-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032923\
Data File : VX034834.D
Acq On : 29 Mar 2023 17:31
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

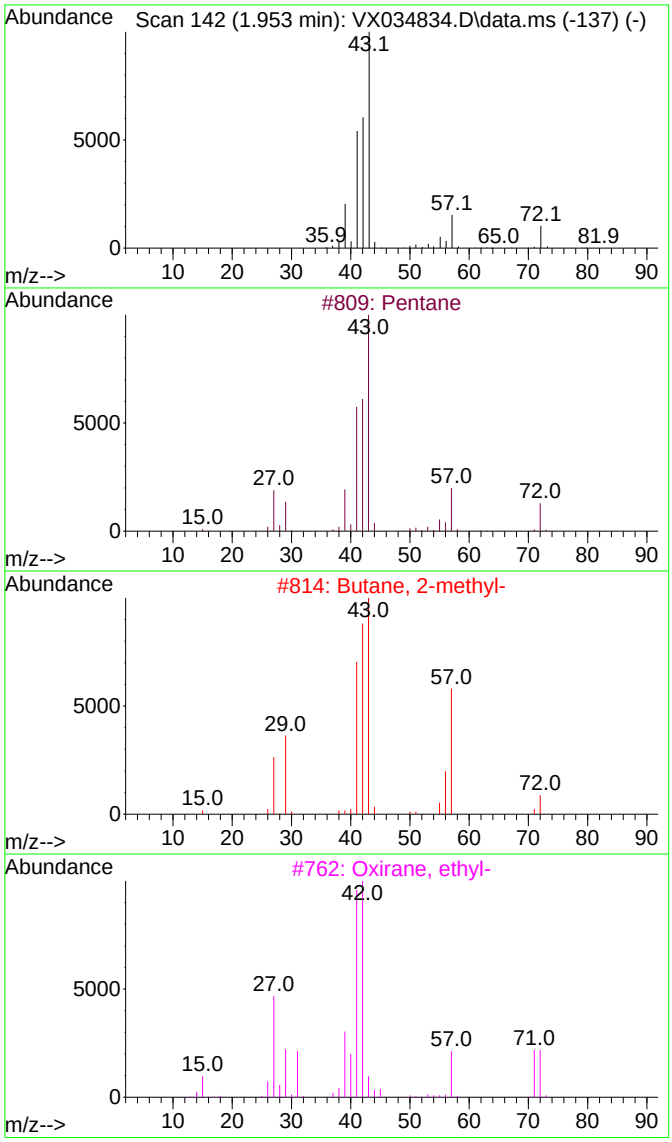
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

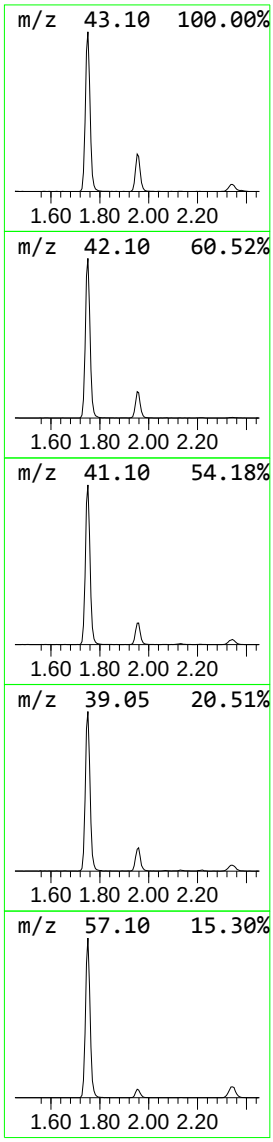
****

Peak Number 3 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	20.35 ug/l	255013	Pentafluorobenzene	5.556

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	64
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	42
4	Isobutyl nitrite	103	C4H9NO2	000542-56-3	17
5	Isobutylene epoxide	72	C4H8O	000558-30-5	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032923\
Data File : VX034834.D
Acq On : 29 Mar 2023 17:31
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

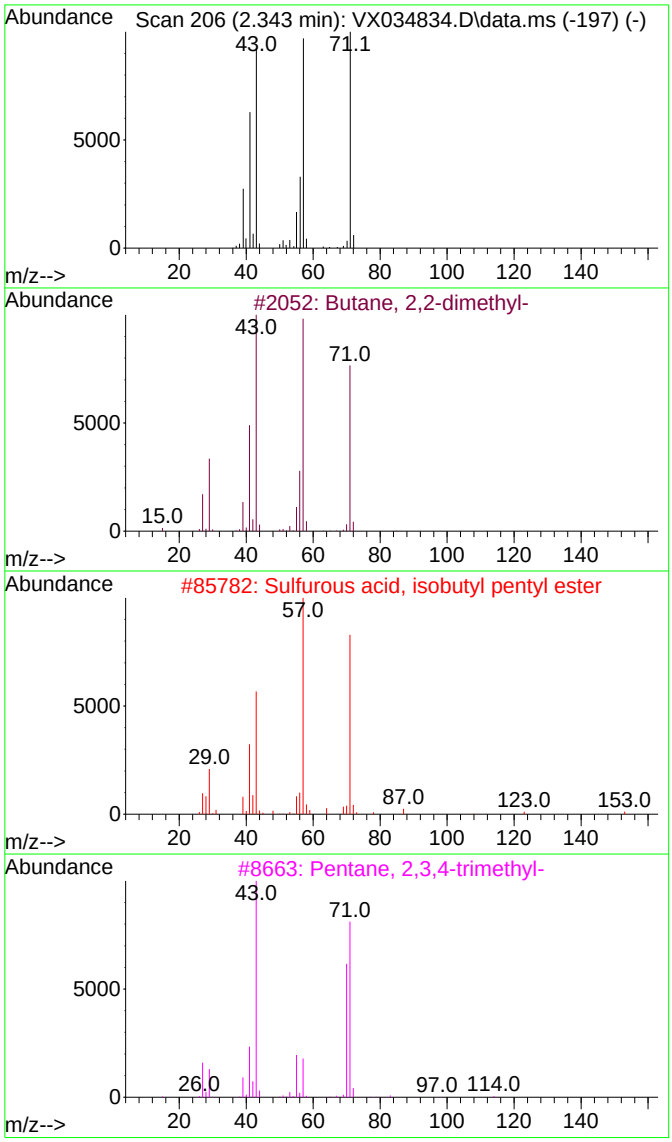
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

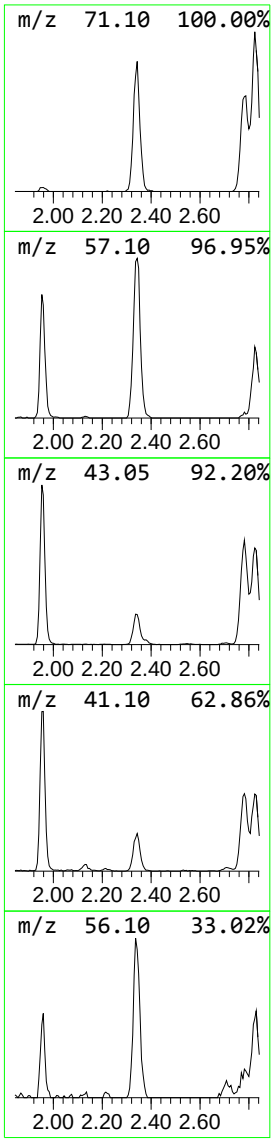
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butane, 2,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.343	9.74 ug/l	122133	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	83
2	Sulfurous acid, isobutyl pentyl ...	208	C9H20O3S	1000309-13-8	50
3	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	45
4	Butane, 2-iodo-3-methyl-	198	C5H11I	018295-27-7	42
5	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032923\
Data File : VX034834.D
Acq On : 29 Mar 2023 17:31
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

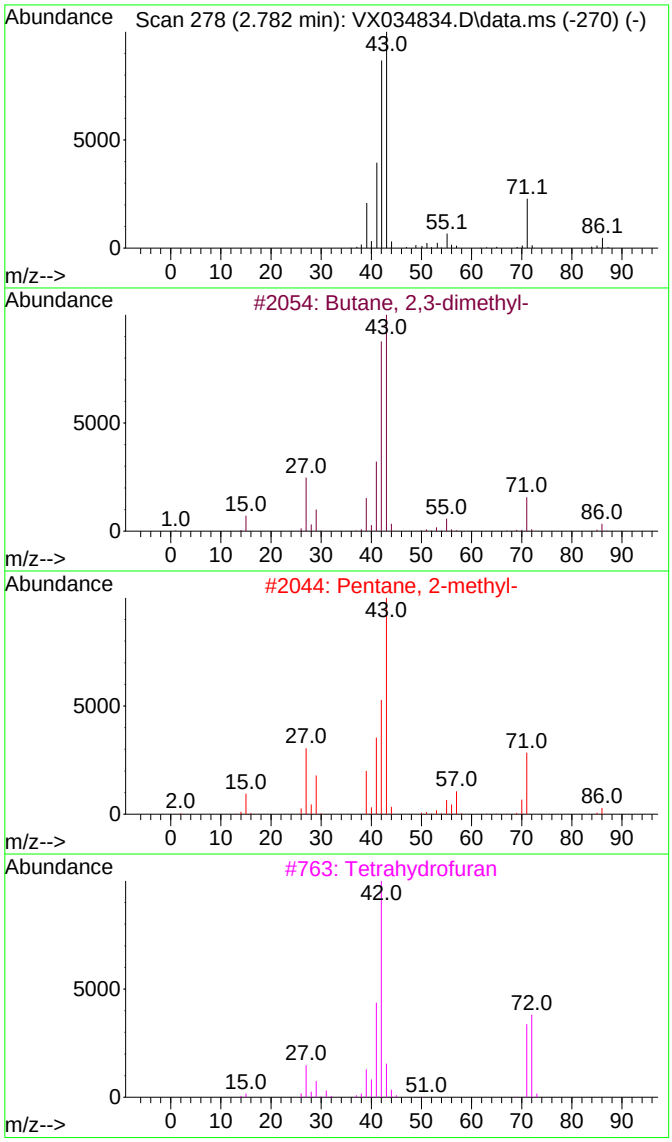
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

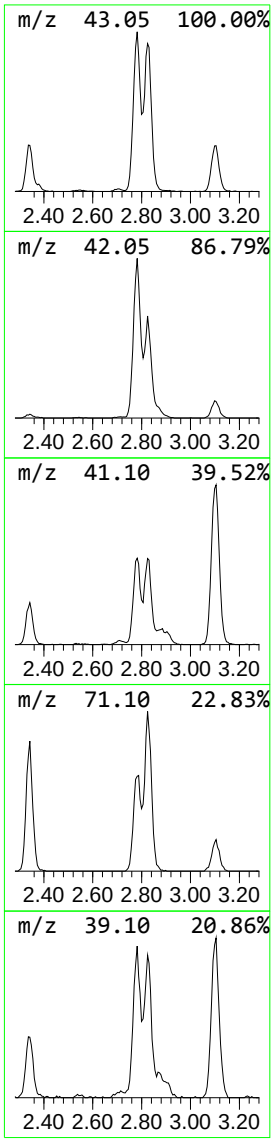
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	21.37 ug/l	267812	Pentafluorobenzene	5.556

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	Tetrahydrofuran	72	C4H8O	000109-99-9	38
4	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	12
5	Pyrrolidine	71	C4H9N	000123-75-1	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032923\
Data File : VX034834.D
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Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

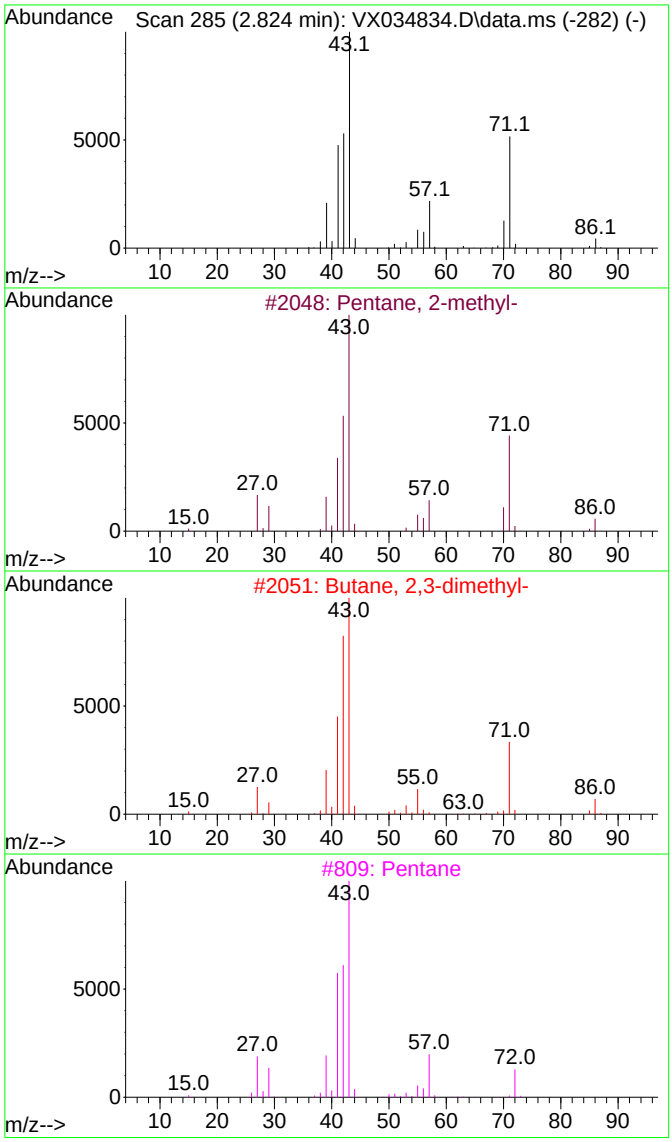
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

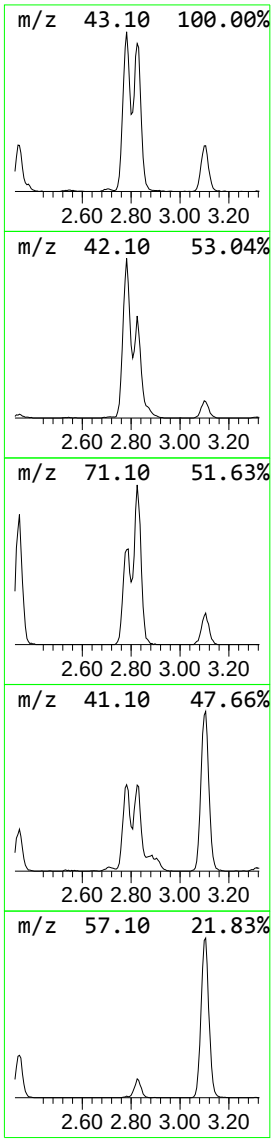
****

Peak Number 6 Pentane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.824	15.55 ug/l	194945	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	90
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	52
3	Pentane	72	C5H12	000109-66-0	43
4	Propanoic acid, 2-methyl-, 2-pro...	128	C7H12O2	015727-77-2	25
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032923\
Data File : VX034834.D
Acq On : 29 Mar 2023 17:31
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

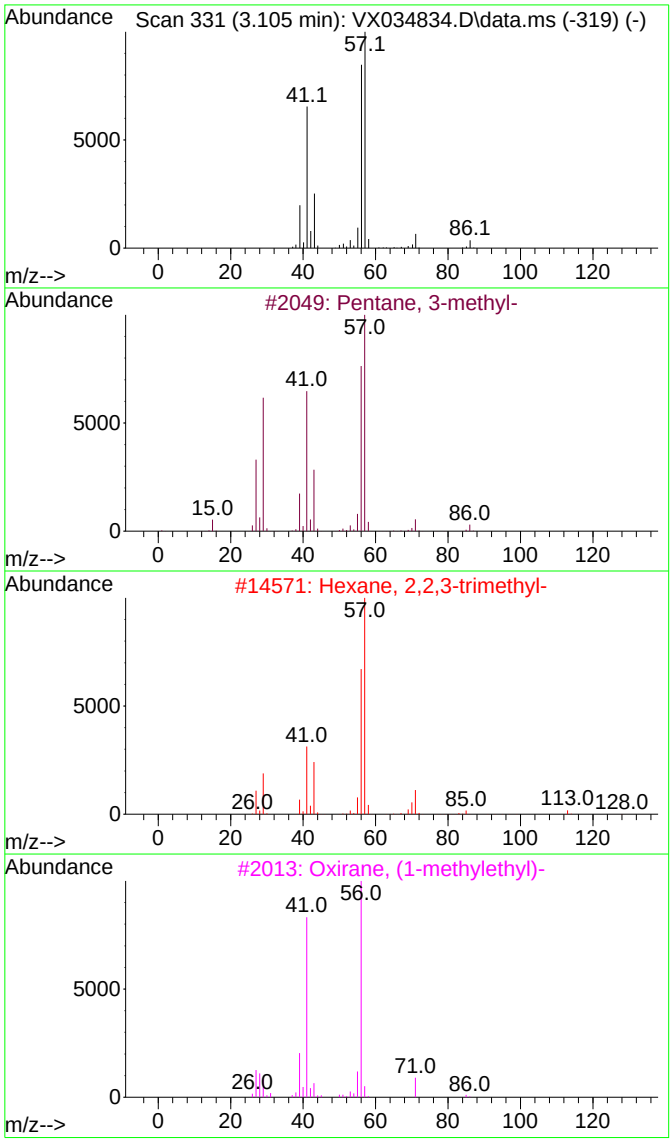
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

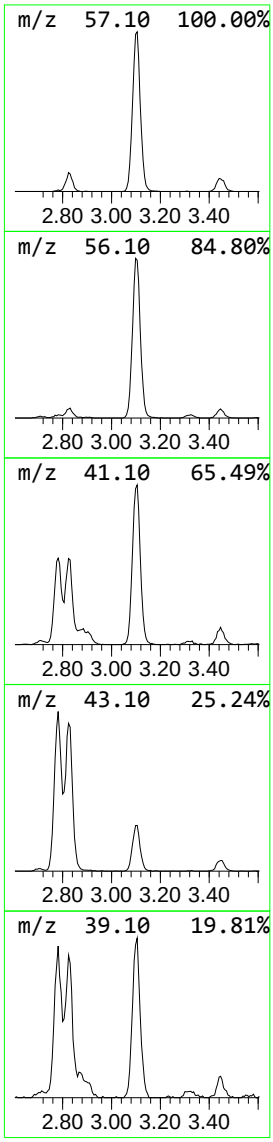
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pentane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	29.35 ug/l	367918	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
3	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45
4	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
5	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032923\
Data File : VX034834.D
Acq On : 29 Mar 2023 17:31
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

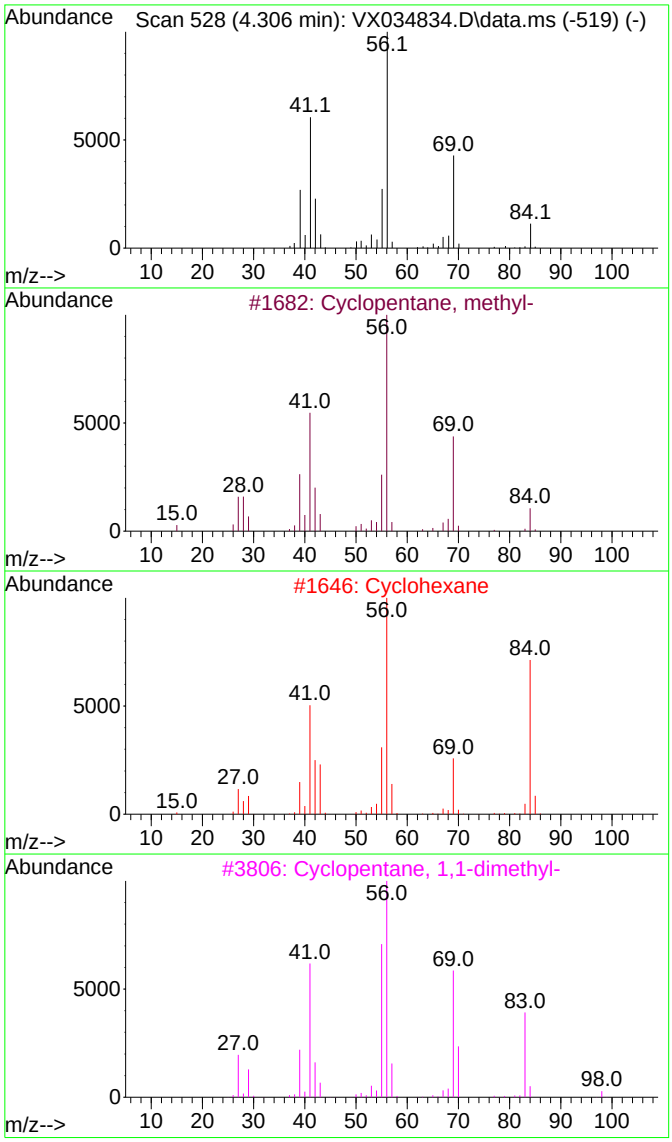
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

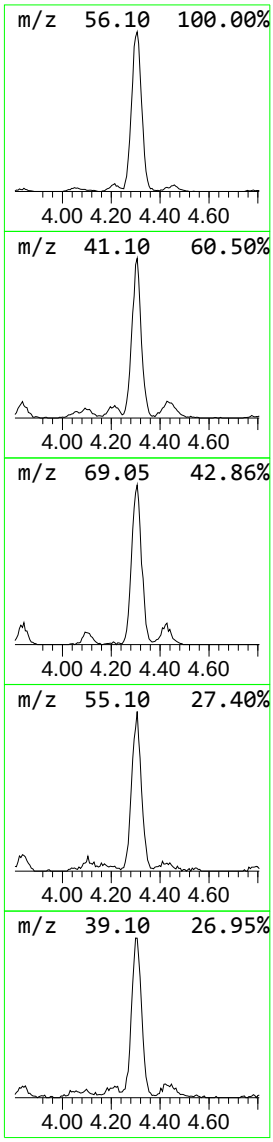
****

Peak Number 8 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	23.72 ug/l	297277	Pentafluorobenzene	5.556

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	78
3	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	72
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50





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Data File : VX034834.D
Acq On : 29 Mar 2023 17:31
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

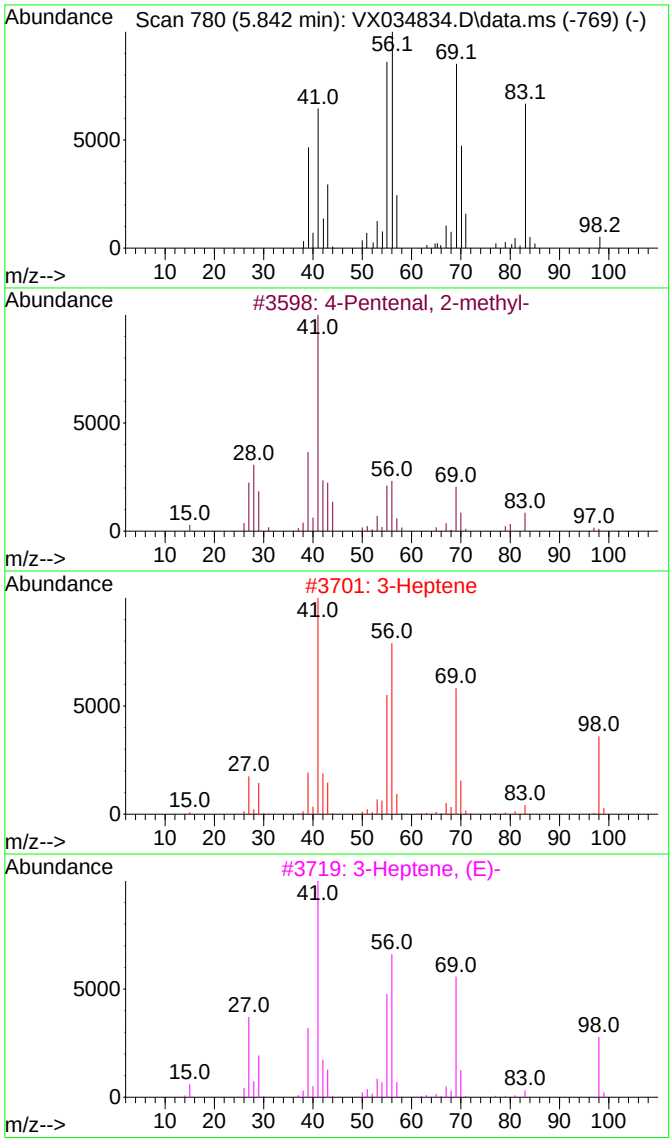
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

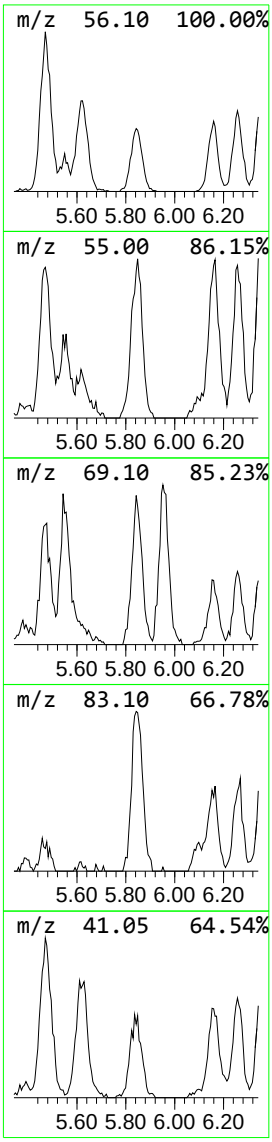
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 4-Pentenal, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.842	7.73 ug/l	96903	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Pentenal, 2-methyl-	98	C6H10O	005187-71-3	53
2	3-Heptene	98	C7H14	000592-78-9	52
3	3-Heptene, (E)-	98	C7H14	014686-14-7	49
4	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	43
5	Cyclopropane, 1,1-diethyl-	98	C7H14	001003-19-6	41





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032923\
Data File : VX034834.D
Acq On : 29 Mar 2023 17:31
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

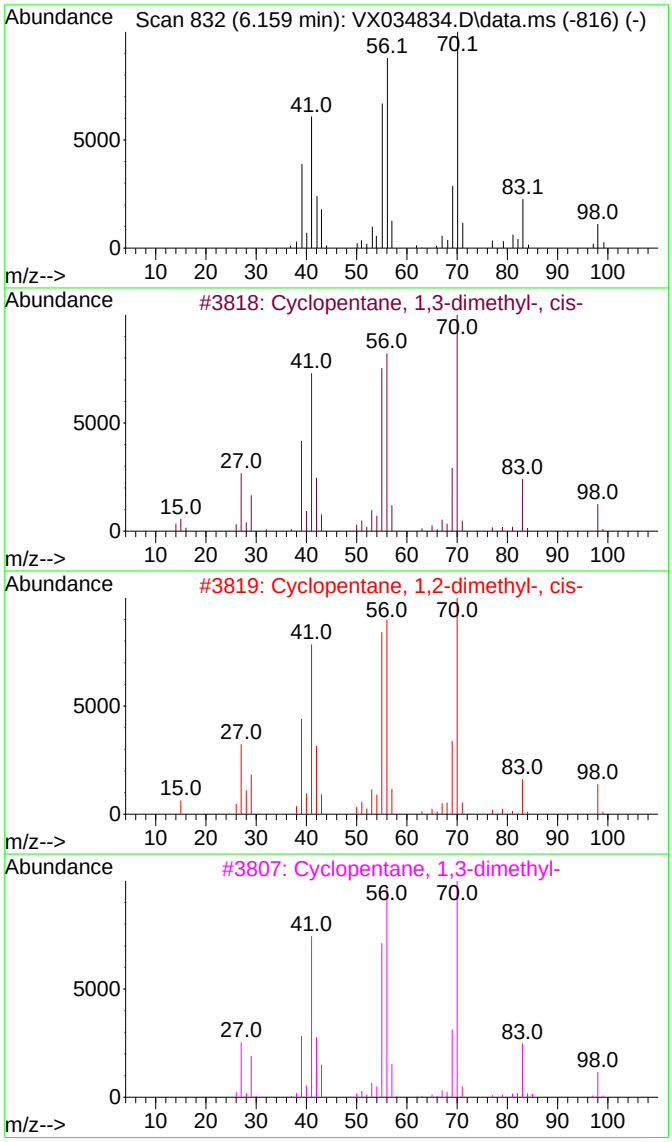
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

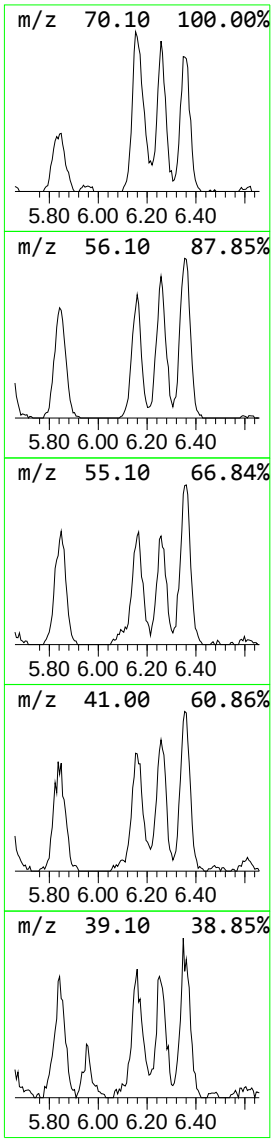
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Cyclopentane, 1,3-dimethyl-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.159	8.75 ug/l	109625	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	97
2	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	94
3	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	94
4	Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	93
5	Cyclobutanone, 2,2-dimethyl-	98	C6H10O	001192-14-9	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032923\
Data File : VX034834.D
Acq On : 29 Mar 2023 17:31
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.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	1.367	16.2	ug/l	202536	1	5.556	626697	50.0
Butane, 2-methyl-	1.751	128.0	ug/l	1604700	1	5.556	626697	50.0
Pentane	1.953	20.4	ug/l	255013	1	5.556	626697	50.0
Butane, 2,2-dim...	2.343	9.7	ug/l	122133	1	5.556	626697	50.0
Butane, 2,3-dim...	2.782	21.4	ug/l	267812	1	5.556	626697	50.0
Pentane, 2-methyl-	2.824	15.6	ug/l	194945	1	5.556	626697	50.0
Pentane, 3-methyl-	3.105	29.4	ug/l	367918	1	5.556	626697	50.0
Cyclopentane, m...	4.306	23.7	ug/l	297277	1	5.556	626697	50.0
4-Pentenal, 2-m...	5.842	7.7	ug/l	96903	1	5.556	626697	50.0
Cyclopentane, 1...	6.159	8.8	ug/l	109625	1	5.556	626697	50.0