LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033138.D
Acq On : 30 Nov 2022 17:37
Operator : JC/MD
Sample : N5815-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

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\82X112222W.M
Title : SW846 8260

Signal : TIC: VX033138.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	37	rBV	49782	50128	7.29%	0.630%
2	1.374	43	47	51	rBV	249052	260054	37.83%	3.267%
3	1.416	51	54	63	rVB	35430	44158	6.42%	0.555%
4	1.752	104	109	120	rVB	387487	502561	73.11%	6.313%
5	1.959	136	143	152	rVB	39841	58122	8.46%	0.730%
6	2.215	180	185	195	rVB	31917	48865	7.11%	0.614%
7	2.343	197	206	219	rBV	101267	195596	28.45%	2.457%
8	2.782	268	278	287	rBV	209257	471434	68.58%	5.922%
9	2.867	287	292	304	rVB	64298	135612	19.73%	1.703%
10	3.105	322	331	348	rVB2	52752	122302	17.79%	1.536%
11	3.733	426	434	445	rBV5	3912	10956	1.59%	0.138%
12	4.056	478	487	491	rBV5	2384	7051	1.03%	0.089%
13	4.099	491	494	502	rVV3	3150	7189	1.05%	0.090%
14	4.215	502	513	520	rVV2	31910	95067	13.83%	1.194%
15	4.306	520	528	539	rVV2	46988	134268	19.53%	1.687%
16	4.428	539	548	564	rVB5	15604	48964	7.12%	0.615%
17	5.135	651	664	668	rBV4	5497	18841	2.74%	0.237%
18	5.196	668	674	687	rVB3	9375	28791	4.19%	0.362%
19	5.391	694	706	714	rBV2	62236	179390	26.10%	2.253%
20	5.477	714	720	724	rVV4	14394	40675	5.92%	0.511%
21	5.556	724	733	740	rVV	133173	398232	57.93%	5.002%
22	5.623	740	744	757	rVB3	50722	135954	19.78%	1.708%
23	5.842	772	780	790	rVV7	4642	14373	2.09%	0.181%
24	5.958	790	799	806	rVV	66573	174032	25.32%	2.186%
25	6.044	806	813	824	rVV2	51619	140070	20.38%	1.759%
26	6.172	825	834	835	rVV3	6812	14797	2.15%	0.186%
27	6.251	837	847	858	rVV	51164	162879	23.69%	2.046%
28	6.361	858	865	873	rVB5	4687	12933	1.88%	0.162%
29	6.763	920	931	944	rBV	198414	473970	68.95%	5.954%
30	7.172	992	998	1005	rVB3	7879	16431	2.39%	0.206%
31	7.367	1022	1030	1039	rVB4	10561	27421	3.99%	0.344%
32	7.495	1045	1051	1057	rBV3	5242	10292	1.50%	0.129%
33	7.775	1088	1097	1104	rBV3	4353	8950	1.30%	0.112%
34	7.982	1123	1131	1140	rVB	24674	50254	7.31%	0.631%
35	8.104	1142	1151	1156	rBV	48661	103112	15.00%	1.295%
36	8.318	1178	1186	1192	rBV4	3842	7375	1.07%	0.093%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033138.D
Acq On : 30 Nov 2022 17:37
Operator : JC/MD
Sample : N5815-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

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\82X112222W.M
Title : SW846 8260

37	8.507	1209	1217	1225	rBV3	10434	19594	2.85%	0.246%
38	8.647	1228	1240	1248	rBV	301816	481996	70.12%	6.055%
39	8.720	1248	1252	1257	rVB	9256	13981	2.03%	0.176%
40	9.104	1310	1315	1320	rVB2	5617	9080	1.32%	0.114%
41	9.159	1320	1324	1335	rVB	8975	14935	2.17%	0.188%
42	10.055	1459	1471	1477	rBV	411926	549618	79.96%	6.904%
43	10.195	1489	1494	1502	rVV	531148	687407	100.00%	8.635%
44	10.305	1504	1512	1518	rVB	12624	20665	3.01%	0.260%
45	10.964	1615	1620	1626	rBV	52476	65158	9.48%	0.818%
46	11.079	1634	1639	1651	rBV	266086	341527	49.68%	4.290%
47	11.305	1671	1676	1686	rVB	52965	68584	9.98%	0.862%
48	11.610	1722	1726	1734	rVB	21648	27768	4.04%	0.349%
49	11.866	1764	1768	1771	rBV	8103	11005	1.60%	0.138%
50	12.024	1788	1794	1801	rBV	413316	524737	76.34%	6.591%
51	12.085	1801	1804	1810	rVB	8481	10546	1.53%	0.132%
52	12.244	1824	1830	1837	rVV2	319017	397814	57.87%	4.997%
53	12.311	1837	1841	1851	rVB	37037	48614	7.07%	0.611%
54	12.402	1851	1856	1862	rBV2	30212	39116	5.69%	0.491%
55	12.463	1862	1866	1873	rVB	27030	34203	4.98%	0.430%
56	12.701	1900	1905	1912	rBV2	40002	63640	9.26%	0.799%
57	12.920	1934	1941	1946	rBV	68073	86842	12.63%	1.091%
58	13.024	1953	1958	1966	rVB2	7030	10404	1.51%	0.131%
59	13.170	1978	1982	1989	rVB	19048	26336	3.83%	0.331%
60	13.292	1996	2002	2007	rBV2	39688	51615	7.51%	0.648%
61	13.341	2007	2010	2017	rVV4	6972	10467	1.52%	0.131%
62	13.420	2020	2023	2030	rVB2	11599	15831	2.30%	0.199%
63	13.579	2046	2049	2053	rVB2	8177	9460	1.38%	0.119%
64	13.664	2053	2063	2069	rVB2	15364	32460	4.72%	0.408%
65	13.774	2074	2081	2090	rVB	35557	46267	6.73%	0.581%
66	14.213	2148	2153	2158	rBV2	7813	10817	1.57%	0.136%
67	14.323	2166	2171	2175	rBV	5509	6959	1.01%	0.087%
68	14.780	2241	2246	2255	rBV2	9168	12409	1.81%	0.156%

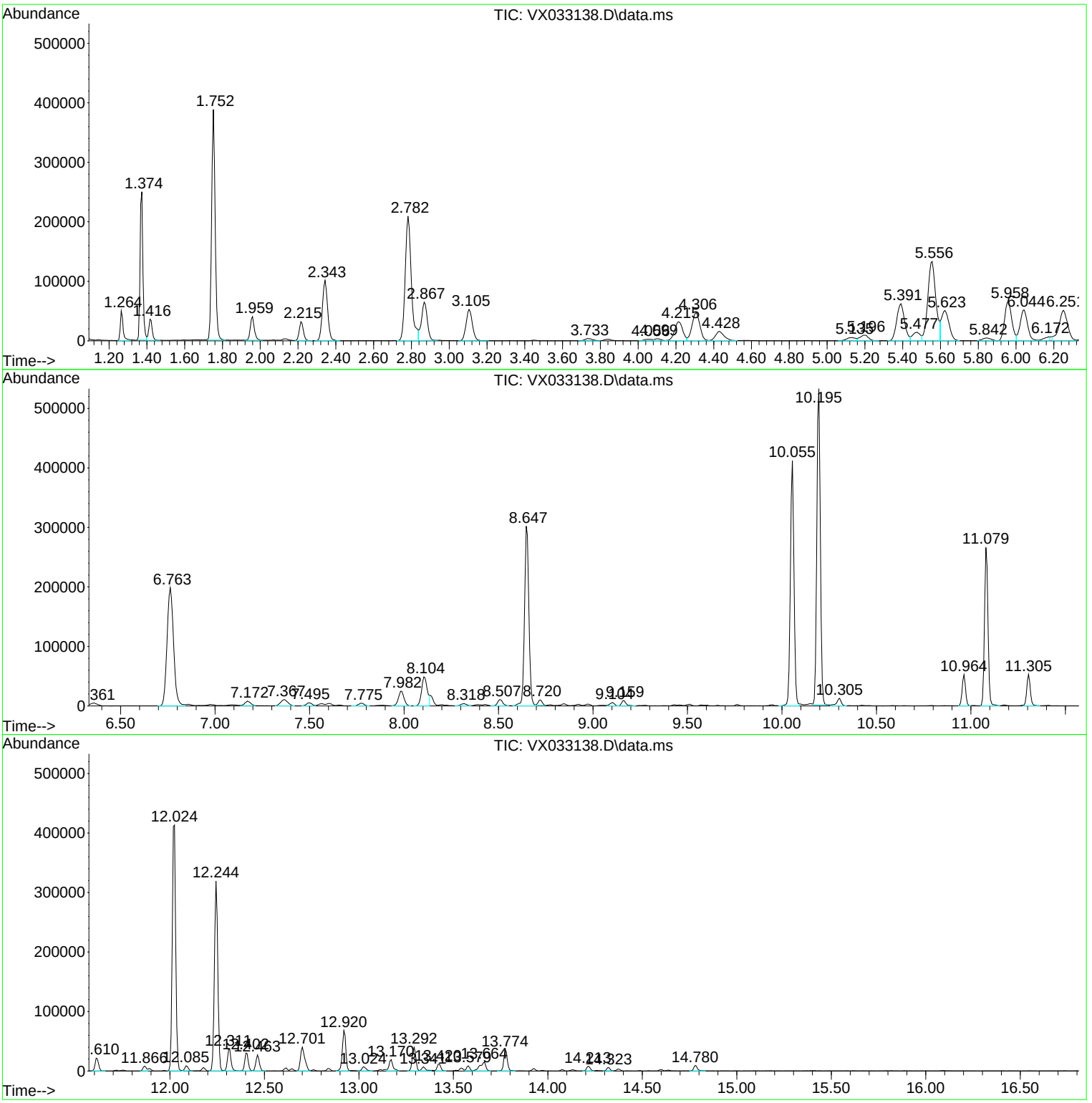
Sum of corrected areas: 7960954

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033138.D
Acq On : 30 Nov 2022 17:37
Operator : JC/MD
Sample : N5815-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033138.D
Acq On : 30 Nov 2022 17:37
Operator : JC/MD
Sample : N5815-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

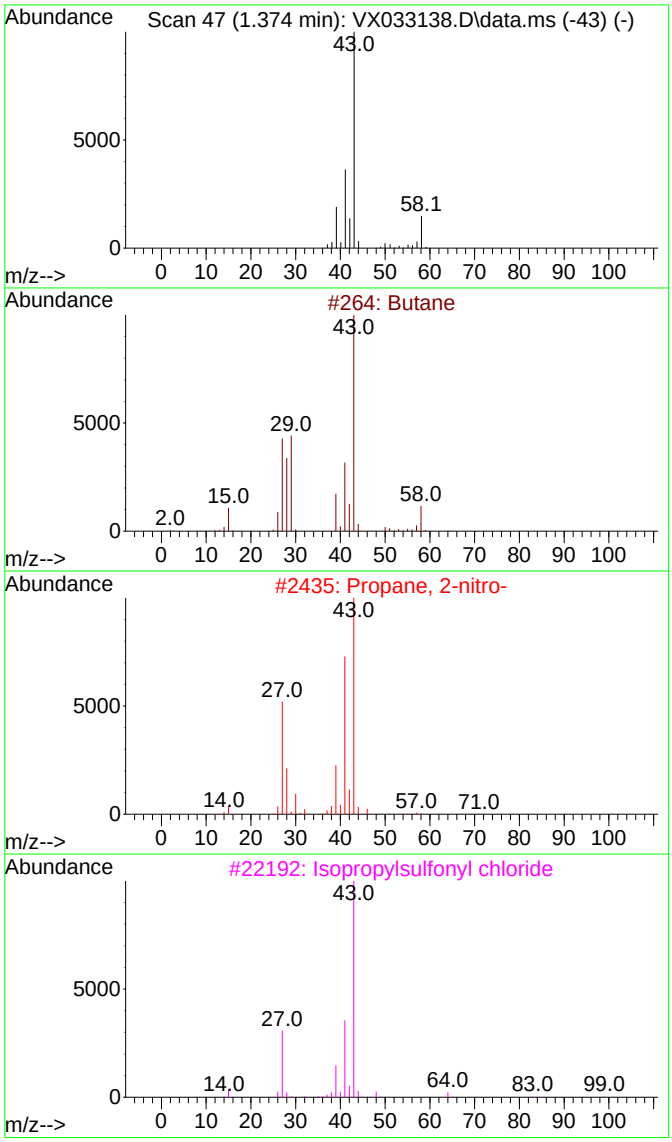
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

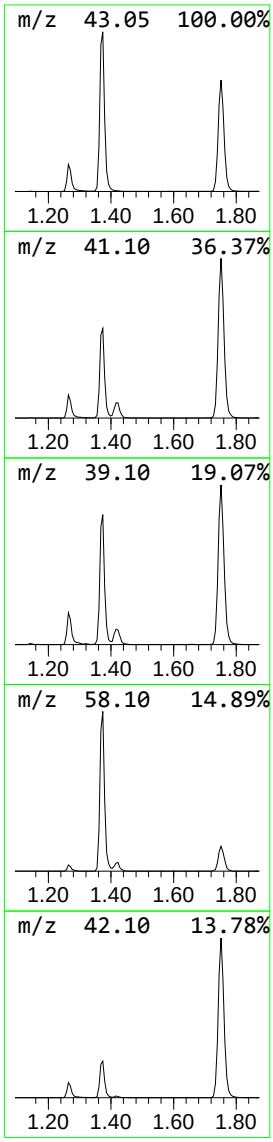
****

Peak Number 1 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	32.65 ug/l	260054	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	64
2	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
3	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4	Isobutane	58	C4H10	000075-28-5	9
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033138.D
Acq On : 30 Nov 2022 17:37
Operator : JC/MD
Sample : N5815-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

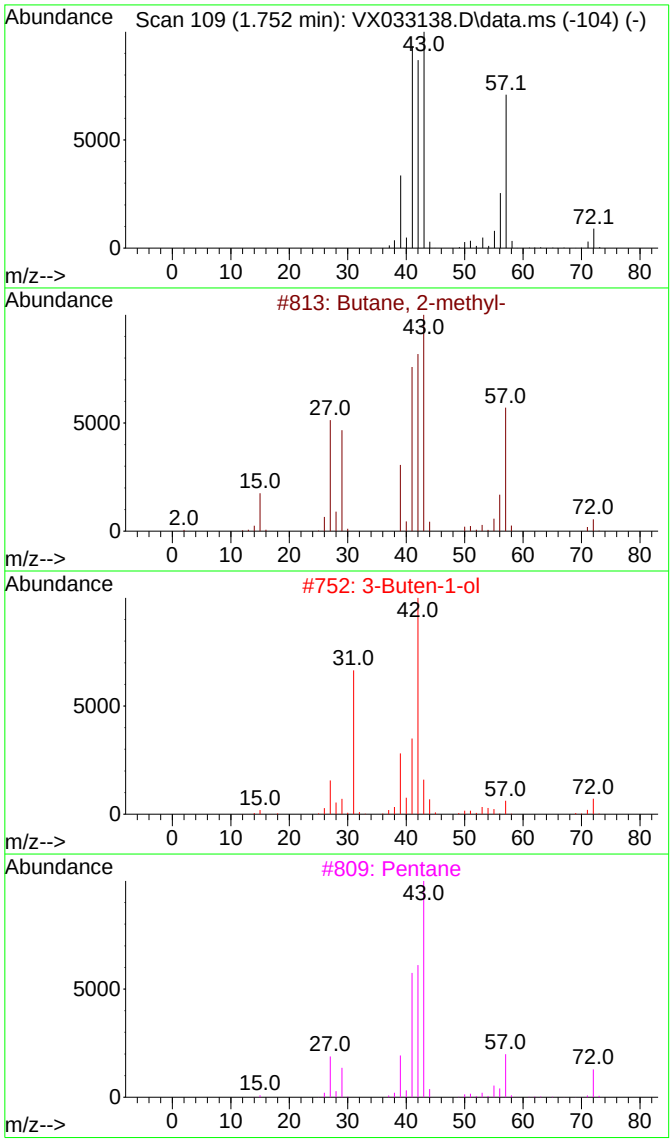
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

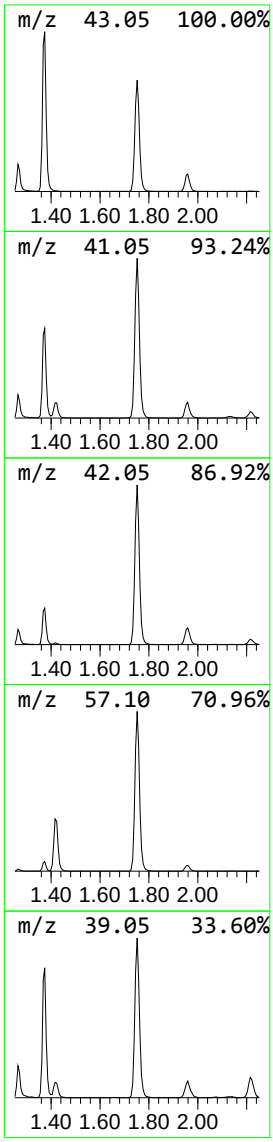
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	63.10 ug/l	502561	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	80
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	36
4	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10
5	1-Butene	56	C4H8	000106-98-9	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033138.D
Acq On : 30 Nov 2022 17:37
Operator : JC/MD
Sample : N5815-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

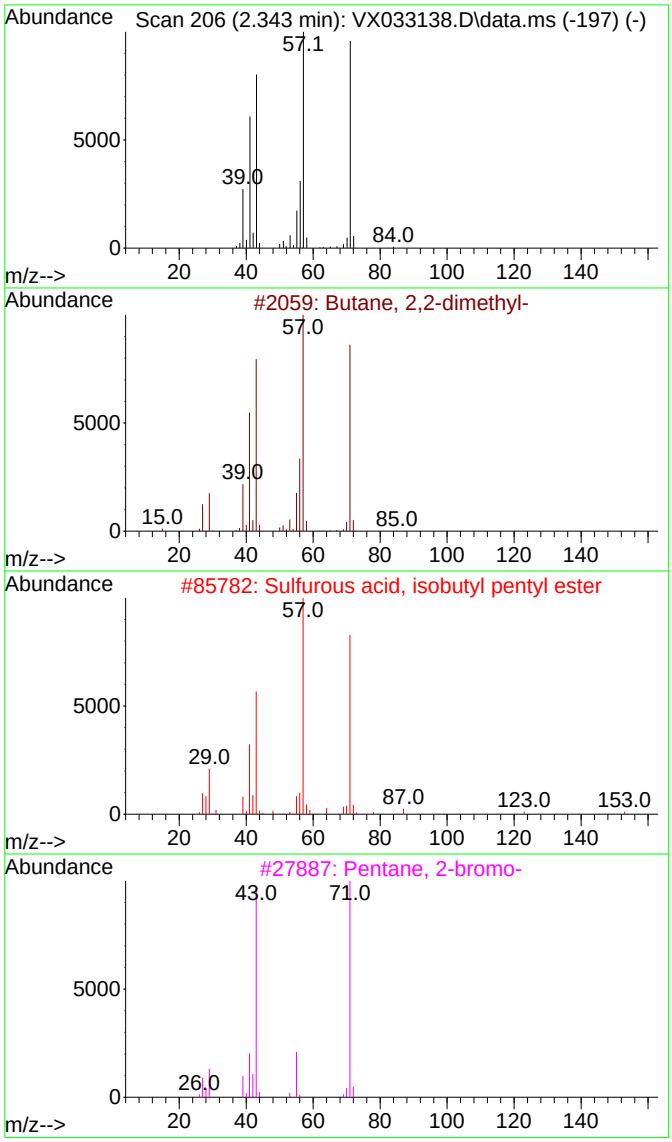
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

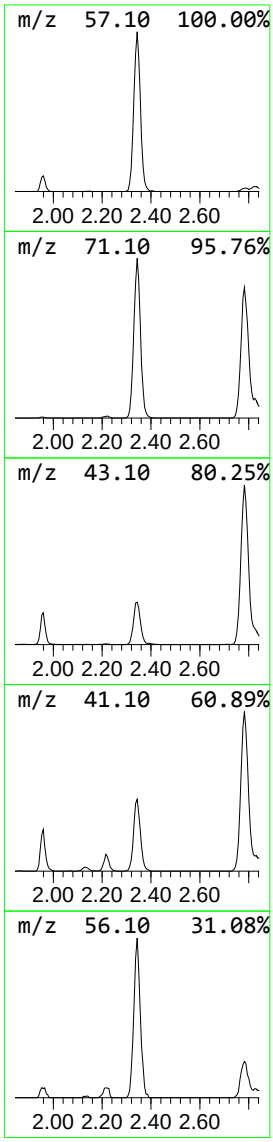
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.343	24.56 ug/l	195596	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	90
2	Sulfurous acid, isobutyl pentyl ...	208	C9H20O3S	1000309-13-8	64
3	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	50
4	1,6-Heptadien-4-ol	112	C7H12O	002883-45-6	47
5	Oxirane, propyl-	86	C5H10O	001003-14-1	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033138.D
Acq On : 30 Nov 2022 17:37
Operator : JC/MD
Sample : N5815-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

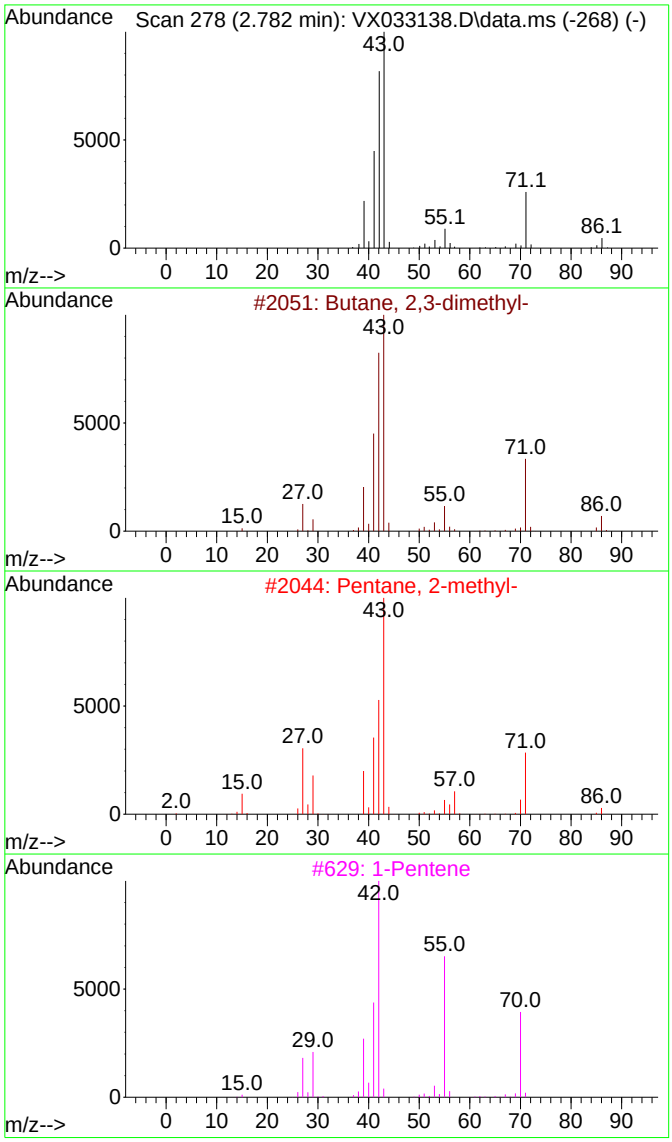
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

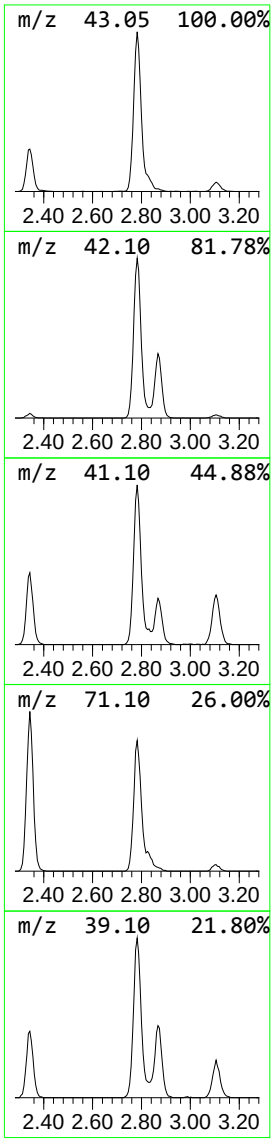
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	59.19 ug/l	471434	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	38
3	1-Pentene	70	C5H10	000109-67-1	28
4	Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	16
5	Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033138.D
Acq On : 30 Nov 2022 17:37
Operator : JC/MD
Sample : N5815-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

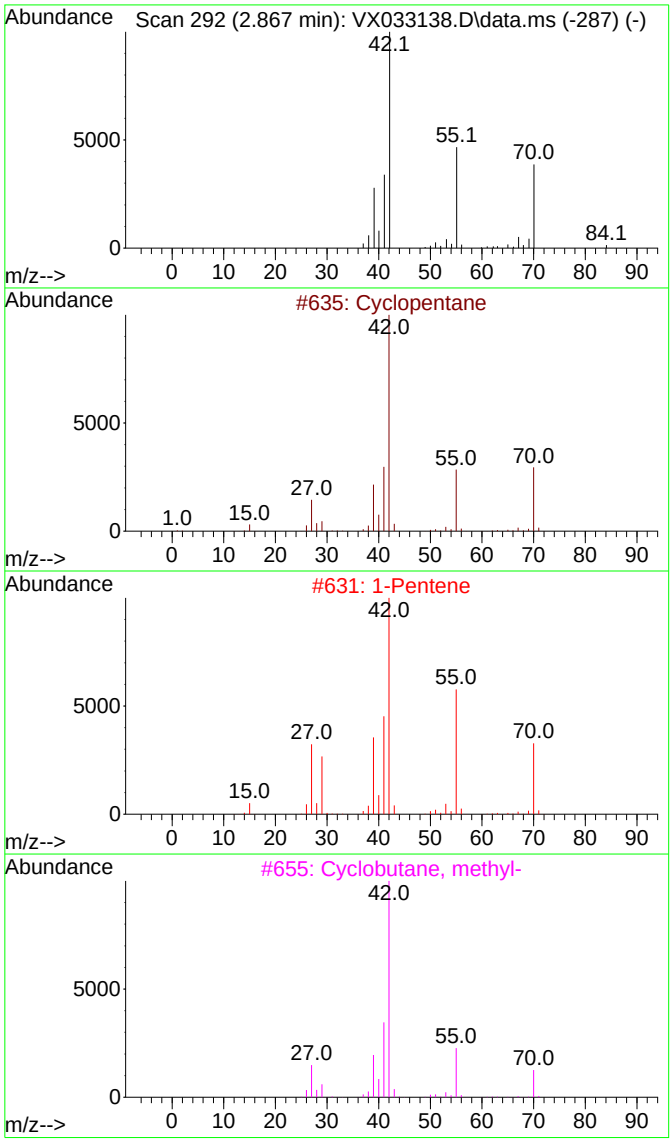
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

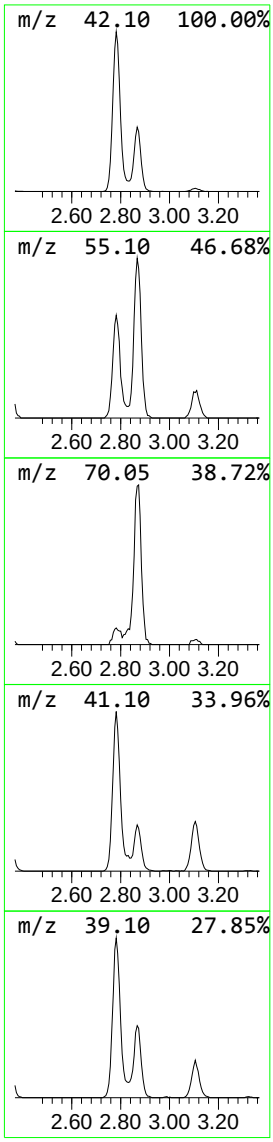
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	17.03 ug/l	135612	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	86
2	1-Pentene	70	C5H10	000109-67-1	72
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
4	1-Pentanol	88	C5H12O	000071-41-0	40
5	3-Buten-1-ol	72	C4H8O	000627-27-0	28





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033138.D
Acq On : 30 Nov 2022 17:37
Operator : JC/MD
Sample : N5815-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

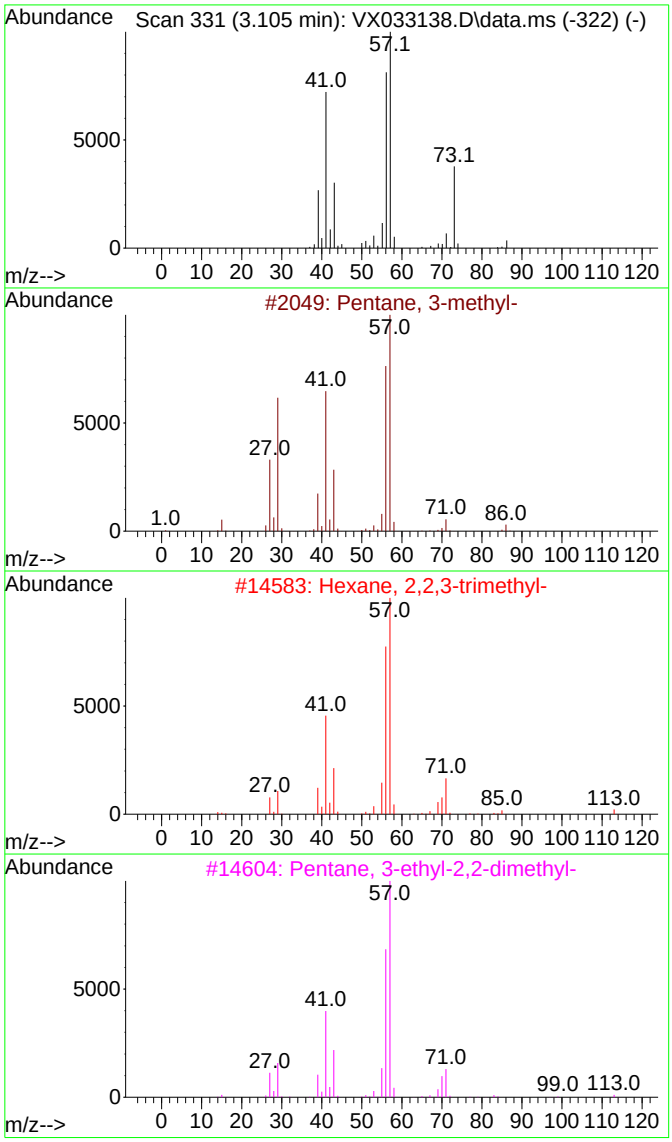
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

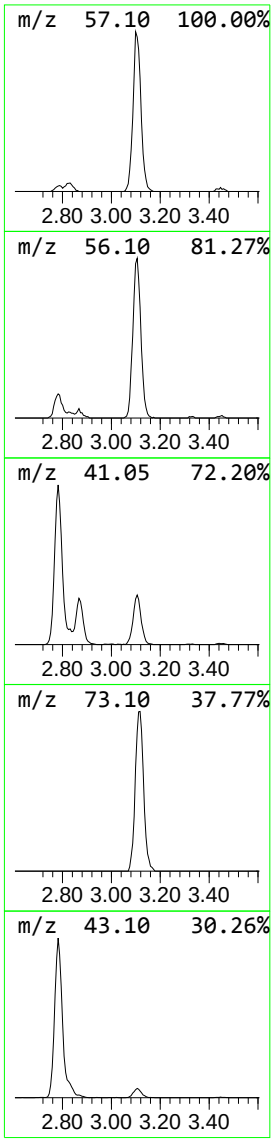
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Pentane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	15.36 ug/l	122302	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	80
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	50
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	50
4	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	40
5	1-Cyclopentyl-2,2-dimethyl-1-pro...	156	C10H20O	337966-85-5	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033138.D
Acq On : 30 Nov 2022 17:37
Operator : JC/MD
Sample : N5815-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

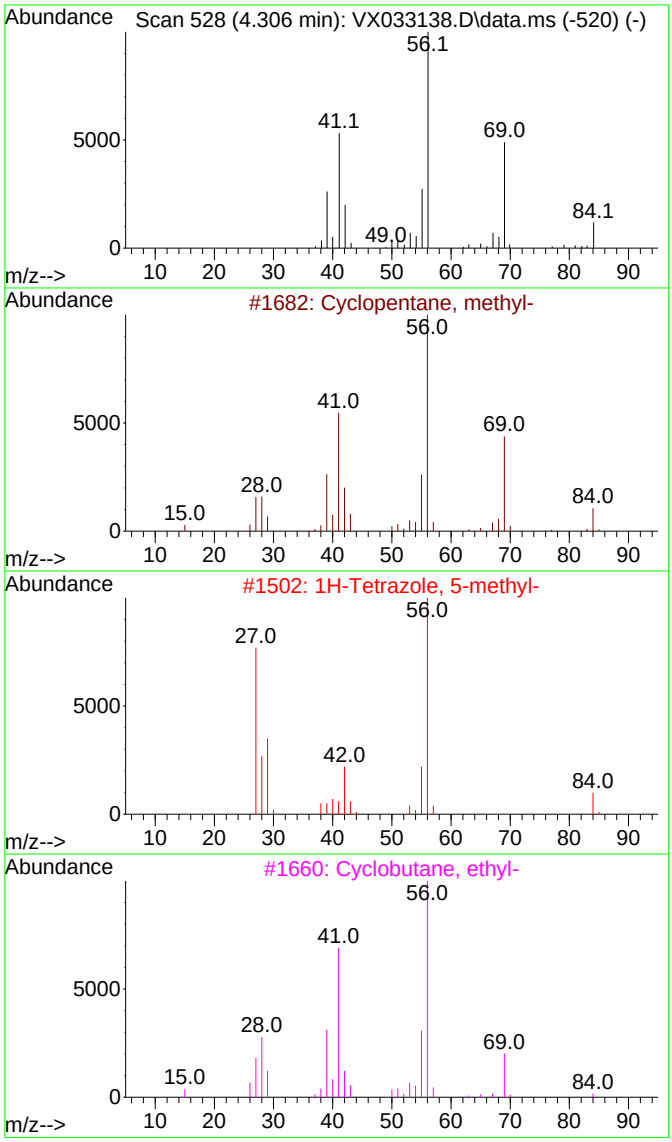
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

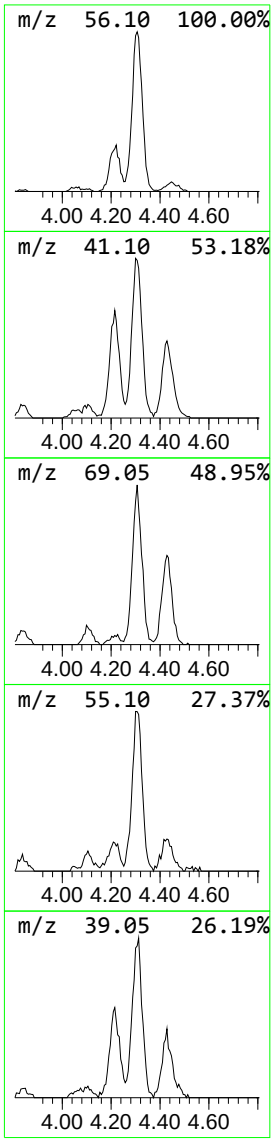
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	16.86 ug/l	134268	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
4	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	56
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	49





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Data File : VX033138.D
Acq On : 30 Nov 2022 17:37
Operator : JC/MD
Sample : N5815-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

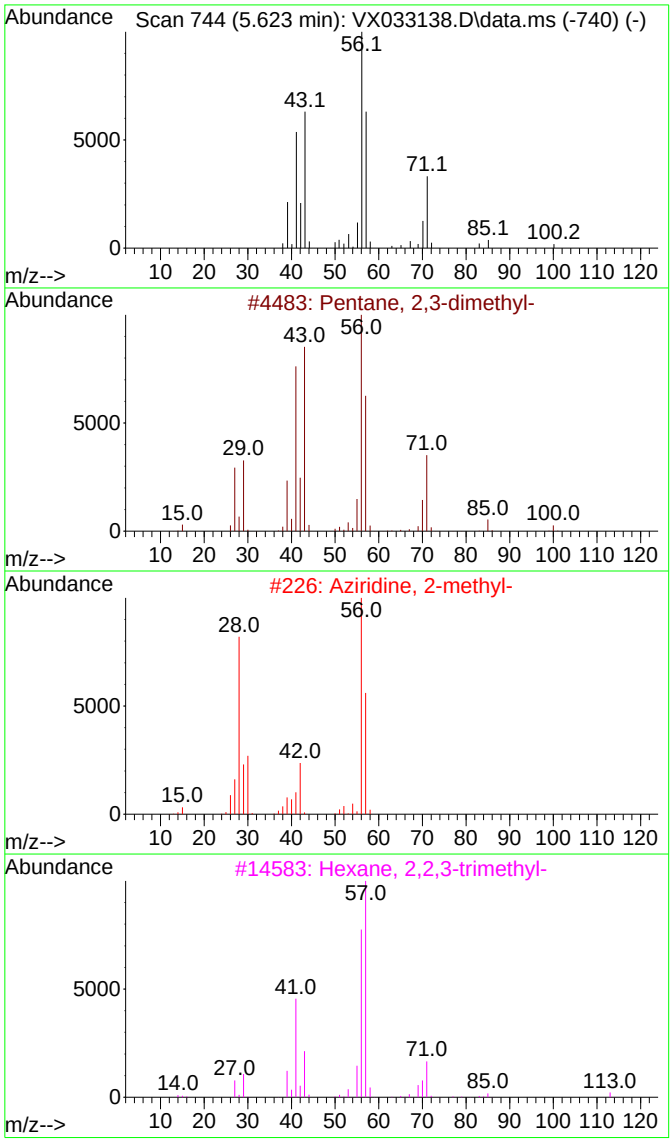
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

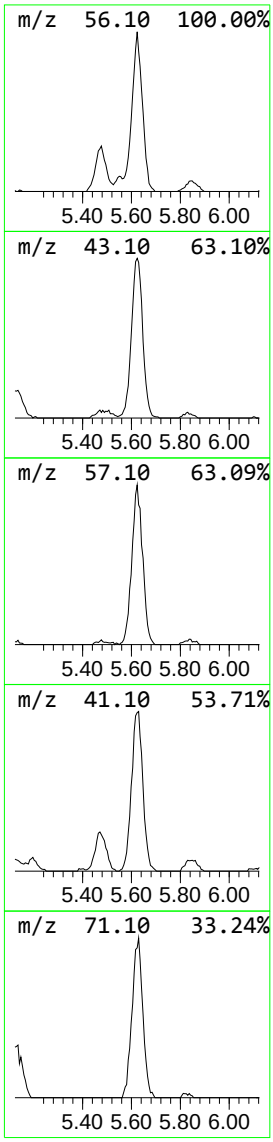
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Pentane, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.623	17.07 ug/l	135954	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	94
2	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	53
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	50
4	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	45
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033138.D
Acq On : 30 Nov 2022 17:37
Operator : JC/MD
Sample : N5815-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

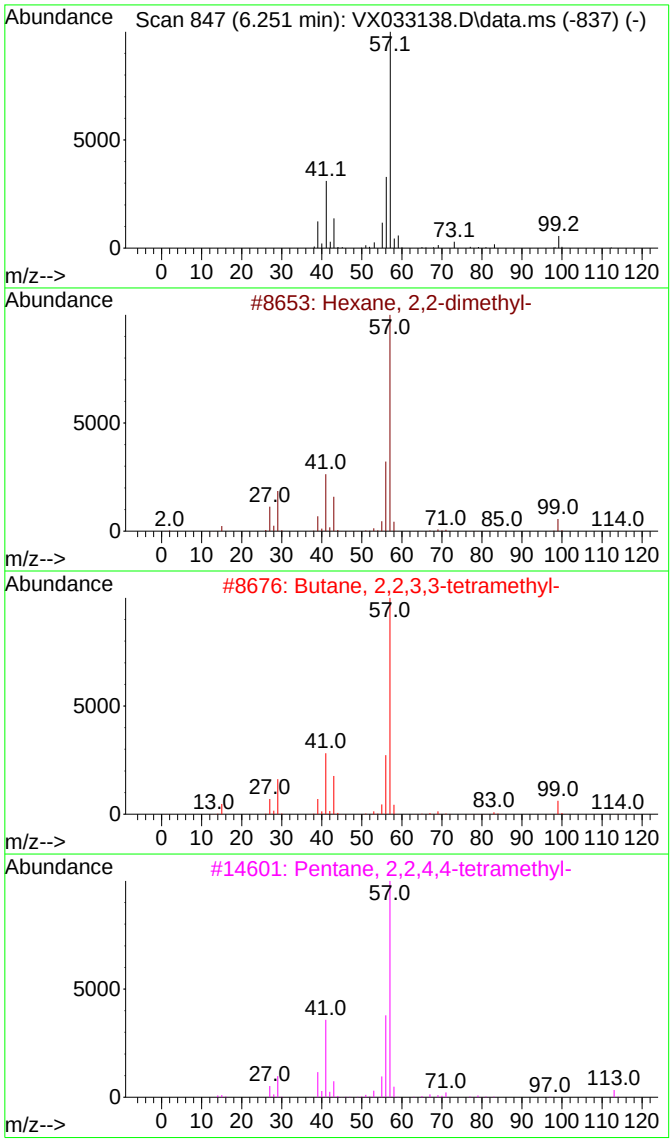
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

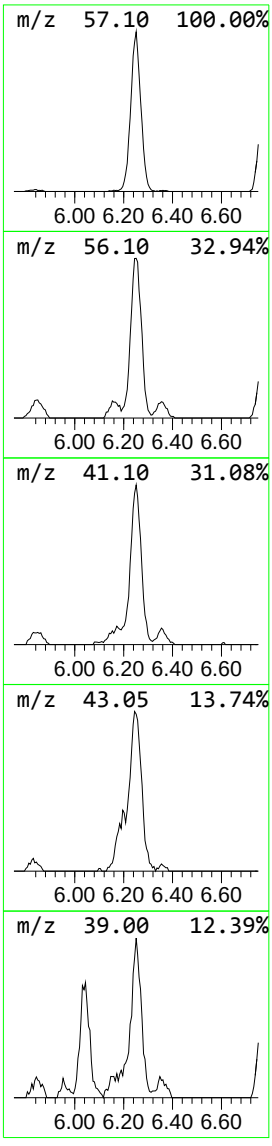
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Hexane, 2,2-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	17.18 ug/l	162879	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
2	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	59
3	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	50
4	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	45
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033138.D
Acq On : 30 Nov 2022 17:37
Operator : JC/MD
Sample : N5815-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

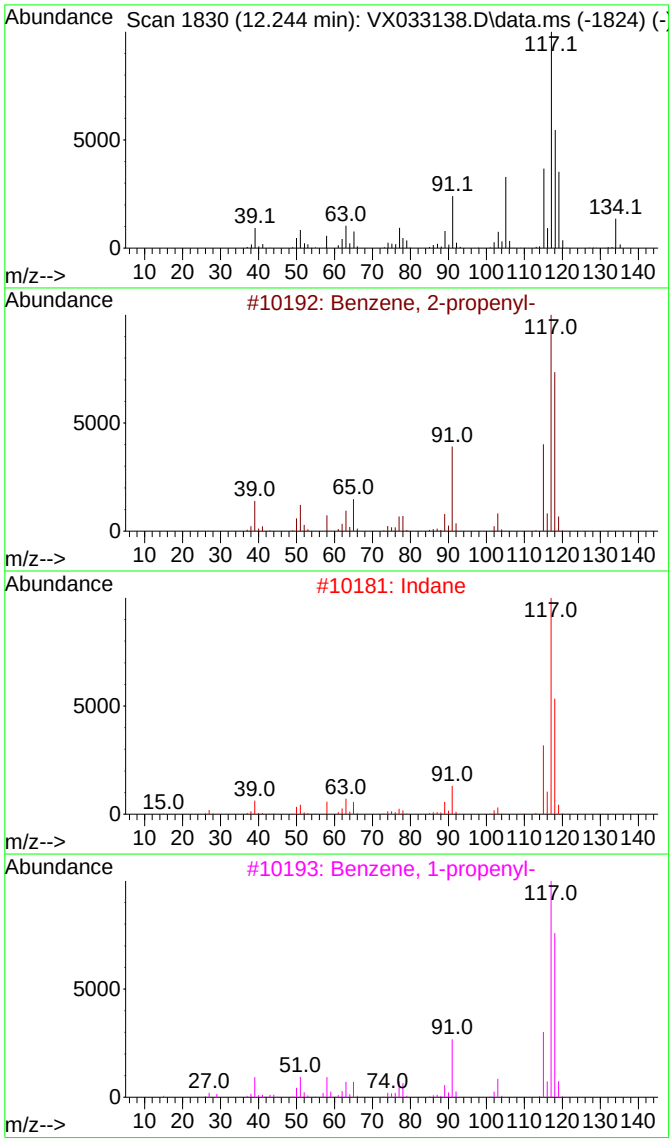
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

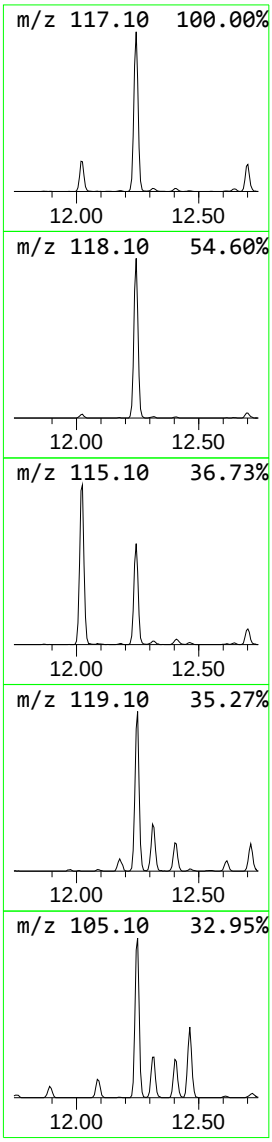
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-propenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	37.91 ug/l	397814	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
2	Indane	118	C9H10	000496-11-7	64
3	Benzene, 1-propenyl-	118	C9H10	000637-50-3	64
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033138.D
Acq On : 30 Nov 2022 17:37
Operator : JC/MD
Sample : N5815-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.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	32.6	ug/l	260054	1	5.556	398232	50.0
Butane, 2-methyl-	1.752	63.1	ug/l	502561	1	5.556	398232	50.0
Butane, 2,2-dim...	2.343	24.6	ug/l	195596	1	5.556	398232	50.0
Butane, 2,3-dim...	2.782	59.2	ug/l	471434	1	5.556	398232	50.0
Cyclopentane	2.867	17.0	ug/l	135612	1	5.556	398232	50.0
Pentane, 3-methyl-	3.105	15.4	ug/l	122302	1	5.556	398232	50.0
Cyclopentane, m...	4.306	16.9	ug/l	134268	1	5.556	398232	50.0
Pentane, 2,3-di...	5.623	17.1	ug/l	135954	1	5.556	398232	50.0
Hexane, 2,2-dim...	6.251	17.2	ug/l	162879	2	6.763	473970	50.0
Benzene, 2-prop...	12.244	37.9	ug/l	397814	4	12.024	524737	50.0