LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032680.D
Acq On : 09 Nov 2022 15:31
Operator : JC/MD
Sample : N5551-13 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-8I

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\82X102622W.M
Title : SW846 8260

Signal : TIC: VX032680.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	41	rBV	25682	24464	3.41%	0.331%
2	1.368	41	46	53	rVV	63131	65820	9.17%	0.891%
3	1.660	89	94	102	rVB2	5169	8533	1.19%	0.116%
4	1.746	103	108	119	rVB	93707	129310	18.01%	1.751%
5	1.971	138	145	155	rVB3	72434	138586	19.30%	1.877%
6	2.069	155	161	169	rVV	39132	53354	7.43%	0.722%
7	2.166	171	177	180	rVV	24485	36519	5.09%	0.495%
8	2.215	180	185	198	rVB	180019	268778	37.43%	3.640%
9	2.751	260	273	281	rBV2	22732	59054	8.22%	0.800%
10	2.825	281	285	287	rVV2	11580	19617	2.73%	0.266%
11	2.867	287	292	304	rVB2	38784	89394	12.45%	1.210%
12	3.105	323	331	343	rVB	9751	21189	2.95%	0.287%
13	3.318	359	366	374	rVB3	7216	16580	2.31%	0.225%
14	3.446	381	387	395	rVB2	4704	10469	1.46%	0.142%
15	3.575	402	408	416	rBV4	3738	8940	1.25%	0.121%
16	3.733	426	434	443	rVB	22667	53364	7.43%	0.723%
17	3.837	443	451	457	rVV4	12077	31076	4.33%	0.421%
18	3.904	457	462	471	rVV3	7287	21015	2.93%	0.285%
19	3.989	471	476	486	rVB3	3646	9480	1.32%	0.128%
20	4.105	486	495	507	rBV2	17659	45949	6.40%	0.622%
21	4.306	517	528	539	rBV3	36730	105783	14.73%	1.432%
22	4.428	539	548	558	rVB4	6189	17185	2.39%	0.233%
23	5.196	662	674	690	rBV2	25789	78971	11.00%	1.069%
24	5.385	693	705	714	rBV2	70863	209749	29.21%	2.840%
25	5.477	714	720	724	rVV3	11826	33217	4.63%	0.450%
26	5.550	724	732	753	rVB	119142	347794	48.44%	4.709%
27	5.958	787	799	806	rBV	77679	207467	28.89%	2.809%
28	6.037	806	812	824	rVV2	32112	89122	12.41%	1.207%
29	6.202	824	839	844	rVV8	8483	29202	4.07%	0.395%
30	6.257	844	848	857	rVV4	3164	7718	1.07%	0.105%
31	6.763	920	931	942	rBV	183155	459539	64.00%	6.223%
32	6.842	942	944	953	rVB7	8397	20402	2.84%	0.276%
33	7.171	991	998	1006	rBV2	7223	15742	2.19%	0.213%
34	7.379	1022	1032	1042	rVB5	9458	24948	3.47%	0.338%
35	7.885	1105	1115	1123	rVB5	2602	7855	1.09%	0.106%
36	8.141	1152	1157	1163	rVB	11770	19591	2.73%	0.265%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032680.D
Acq On : 09 Nov 2022 15:31
Operator : JC/MD
Sample : N5551-13 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-8I

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\82X102622W.M
Title : SW846 8260

37	8.507	1211	1217	1227	rVB2	8544	13726	1.91%	0.186%
38	8.647	1234	1240	1247	rBV	378160	610883	85.07%	8.272%
39	8.720	1247	1252	1261	rVB	72021	111549	15.53%	1.510%
40	8.958	1281	1291	1299	rBV2	13610	23656	3.29%	0.320%
41	9.049	1299	1306	1312	rBV	15439	23994	3.34%	0.325%
42	10.055	1465	1471	1484	rBV	396537	526891	73.38%	7.135%
43	10.195	1488	1494	1502	rVV	564553	718054	100.00%	9.723%
44	10.299	1505	1511	1522	rVB	312799	417640	58.16%	5.655%
45	10.640	1562	1567	1577	rBV	72470	95875	13.35%	1.298%
46	10.963	1615	1620	1625	rBV	28142	35202	4.90%	0.477%
47	11.079	1634	1639	1654	rBV	363940	463931	64.61%	6.282%
48	11.305	1671	1676	1684	rBV	75280	90692	12.63%	1.228%
49	11.402	1684	1692	1696	rVV	17054	27593	3.84%	0.374%
50	11.451	1696	1700	1707	rVB	15488	19757	2.75%	0.268%
51	11.610	1721	1726	1733	rBV	66122	86550	12.05%	1.172%
52	11.750	1744	1749	1757	rBV	74121	93641	13.04%	1.268%
53	12.024	1788	1794	1800	rBV	408194	516356	71.91%	6.992%
54	12.085	1800	1804	1810	rVB	125626	157352	21.91%	2.131%
55	12.244	1825	1830	1837	rBV	141670	176683	24.61%	2.392%
56	12.317	1837	1842	1849	rVB2	7773	13312	1.85%	0.180%
57	12.414	1853	1858	1862	rBV3	6510	8954	1.25%	0.121%
58	12.463	1862	1866	1871	rVB	6329	7694	1.07%	0.104%
59	12.609	1886	1890	1894	rBV	25096	32460	4.52%	0.440%
60	12.701	1900	1905	1912	rVB2	21371	28380	3.95%	0.384%
61	12.847	1925	1929	1934	rVV	6387	7524	1.05%	0.102%
62	12.920	1936	1941	1945	rBV	15277	18621	2.59%	0.252%
63	13.170	1978	1982	1987	rVB	21381	24755	3.45%	0.335%
64	13.292	1993	2002	2007	rBV2	43052	54661	7.61%	0.740%
65	13.426	2020	2024	2029	rBV2	5787	7288	1.01%	0.099%
66	13.774	2076	2081	2091	rBV	129093	162537	22.64%	2.201%
67	14.640	2219	2223	2229	rVB	11852	14373	2.00%	0.195%
68	14.780	2240	2246	2251	rVB	6955	8651	1.20%	0.117%

Sum of corrected areas: 7385011

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
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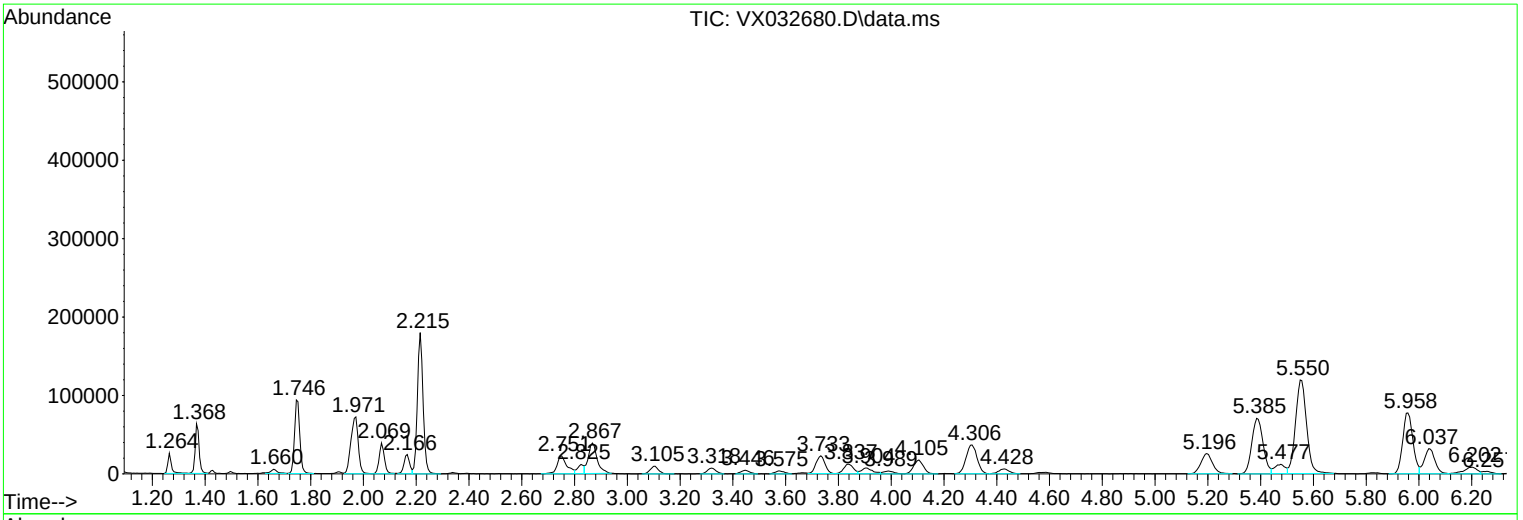
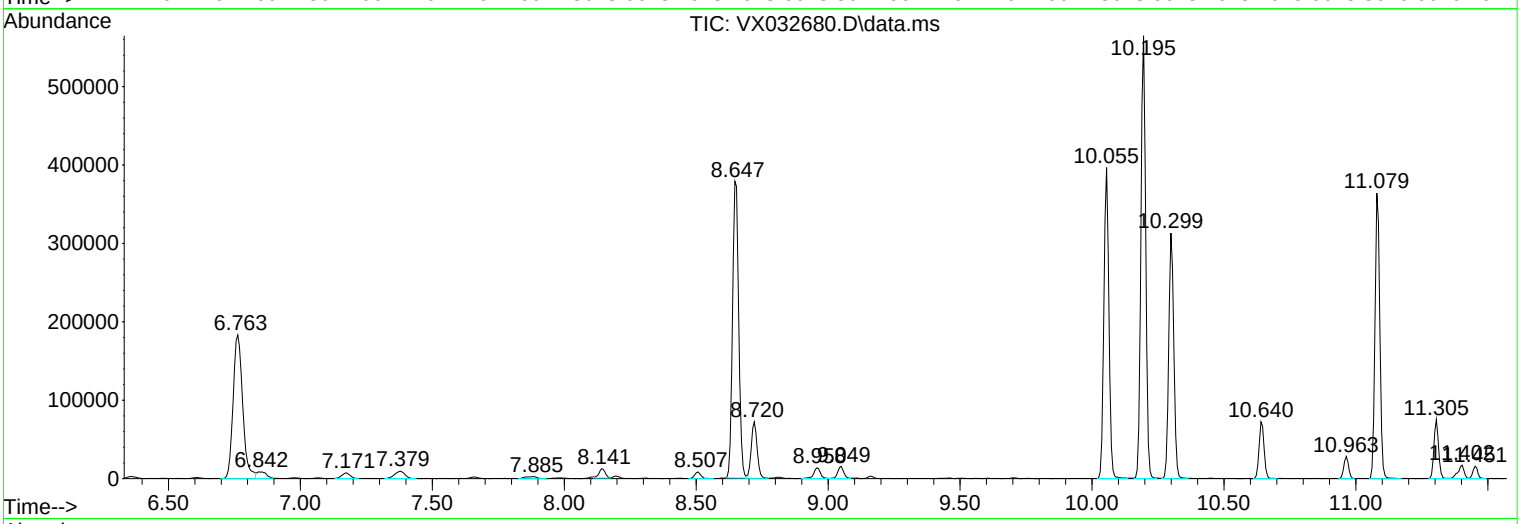
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

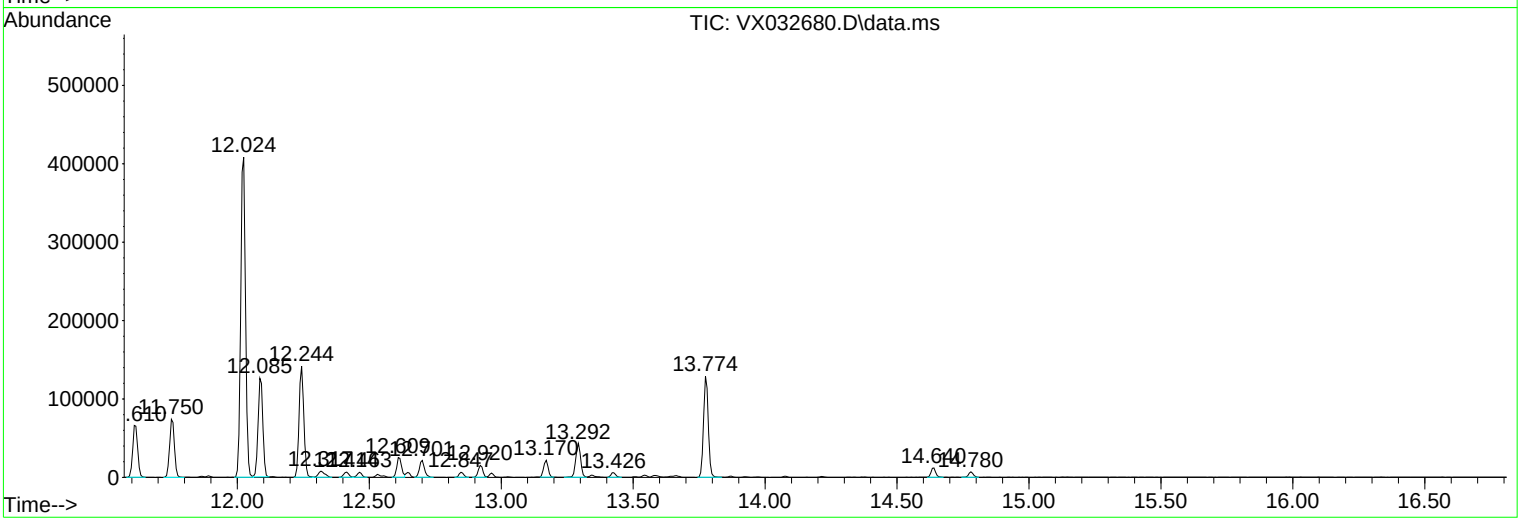
Instrument :
MSVOA_X
ClientSampleId :
MW-8I

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032680.D
Acq On : 09 Nov 2022 15:31
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MSVOA_X
ClientSampleId :
MW-8I

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

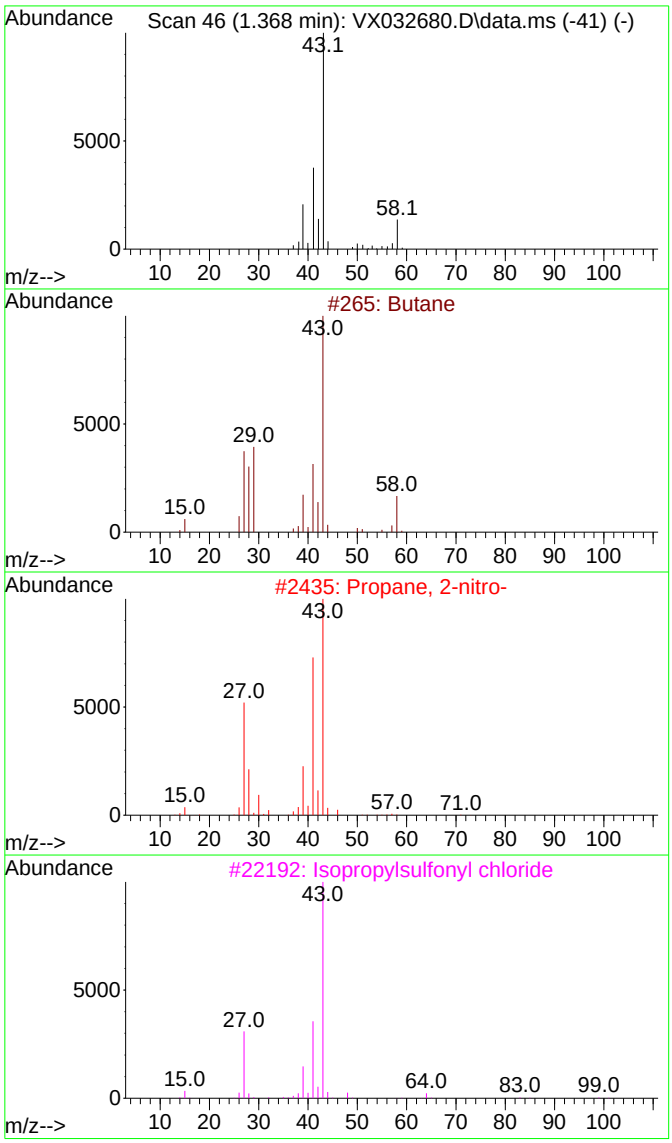
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

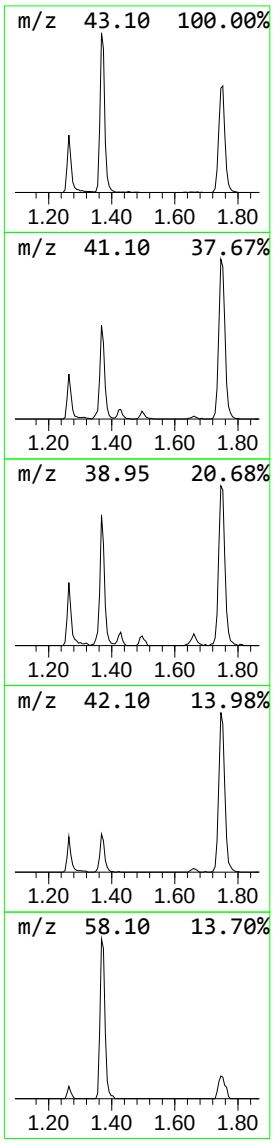
****

Peak Number 1 Butane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	9.46 ug/l	65820	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	72
2	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
3	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5	Isobutane	58	C4H10	000075-28-5	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032680.D
Acq On : 09 Nov 2022 15:31
Operator : JC/MD
Sample : N5551-13 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-8I

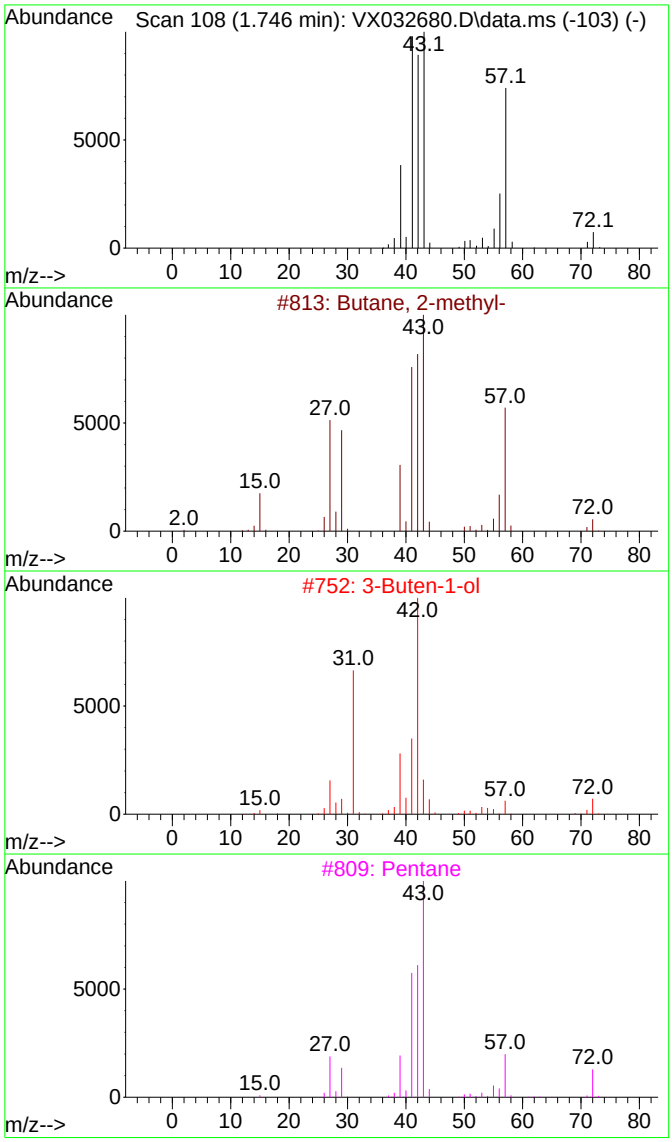
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

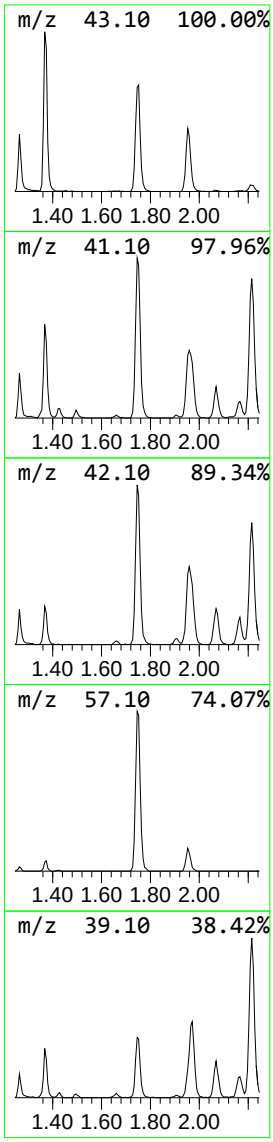
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	18.59 ug/l	129310	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	64
2	3-Buten-1-ol	72	C4H8O	000627-27-0	38
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	16





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032680.D
Acq On : 09 Nov 2022 15:31
Operator : JC/MD
Sample : N5551-13 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-8I

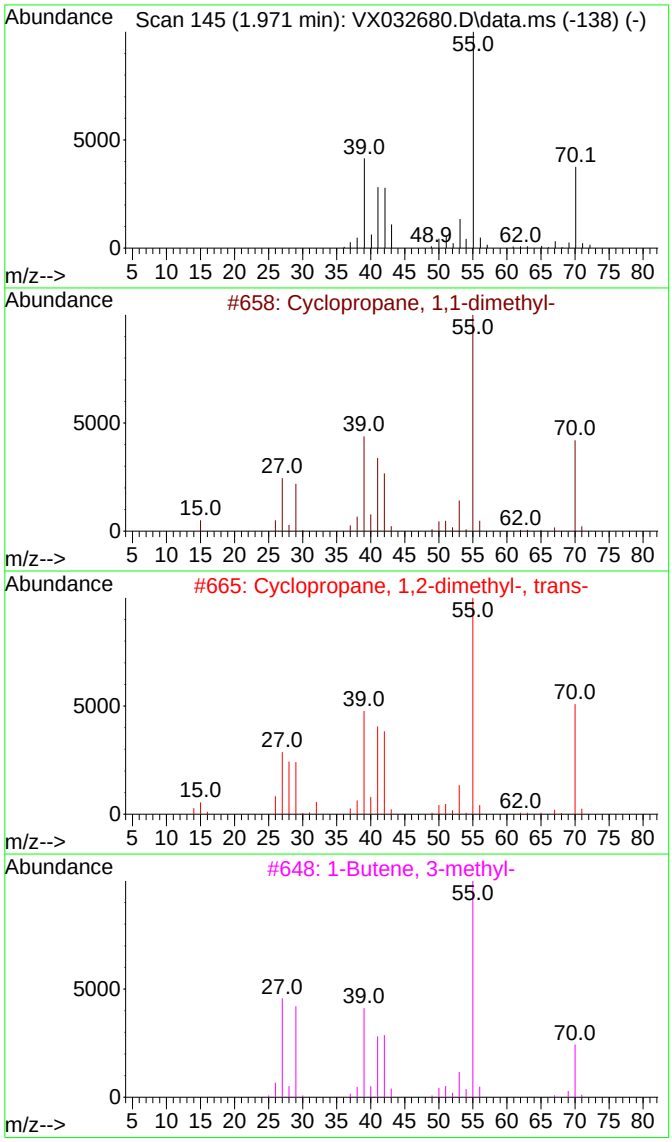
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

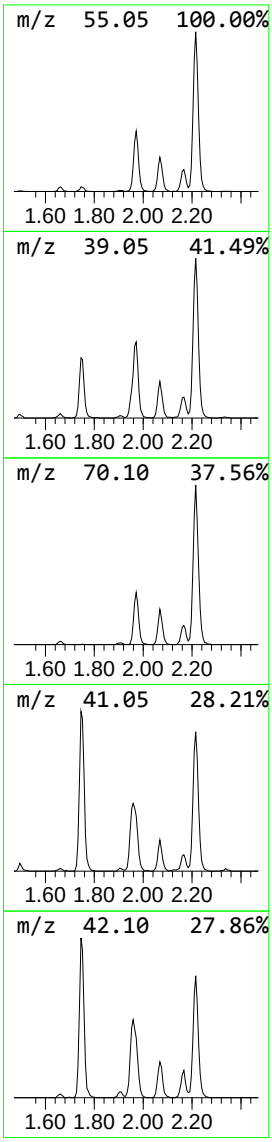
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopropane, 1,1-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.971	19.92 ug/l	138586	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	90
2	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	90
3	1-Butene, 3-methyl-	70	C5H10	000563-45-1	83
4	2-Pentene, (Z)-	70	C5H10	000627-20-3	81
5	2-Butene, 2-methyl-	70	C5H10	000513-35-9	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032680.D
Acq On : 09 Nov 2022 15:31
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-8I

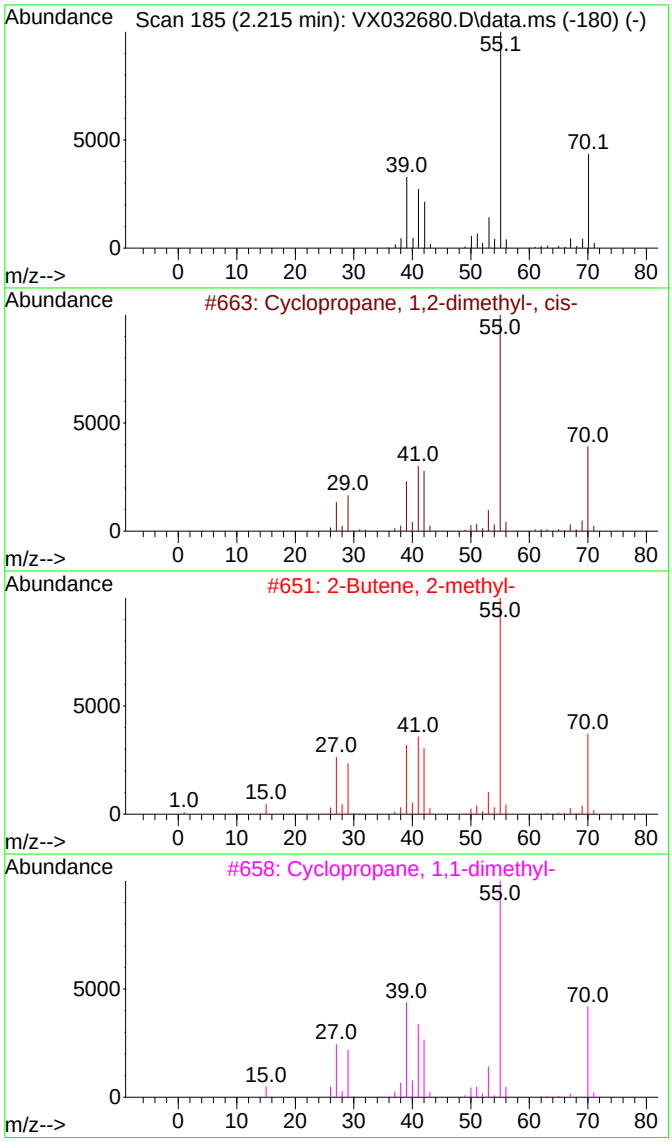
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

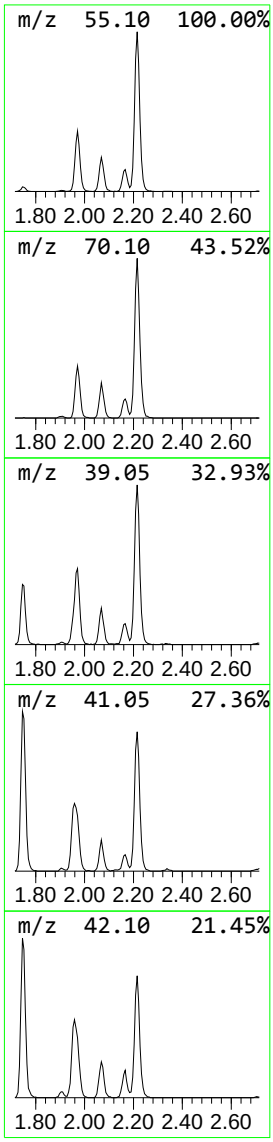
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopropane, 1,2-dimethyl-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	38.64 ug/l	268778	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
2	2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
3	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
4	1-Butene, 3-methyl-	70	C5H10	000563-45-1	80
5	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	74





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
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Acq On : 09 Nov 2022 15:31
Operator : JC/MD
Sample : N5551-13 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-8I

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

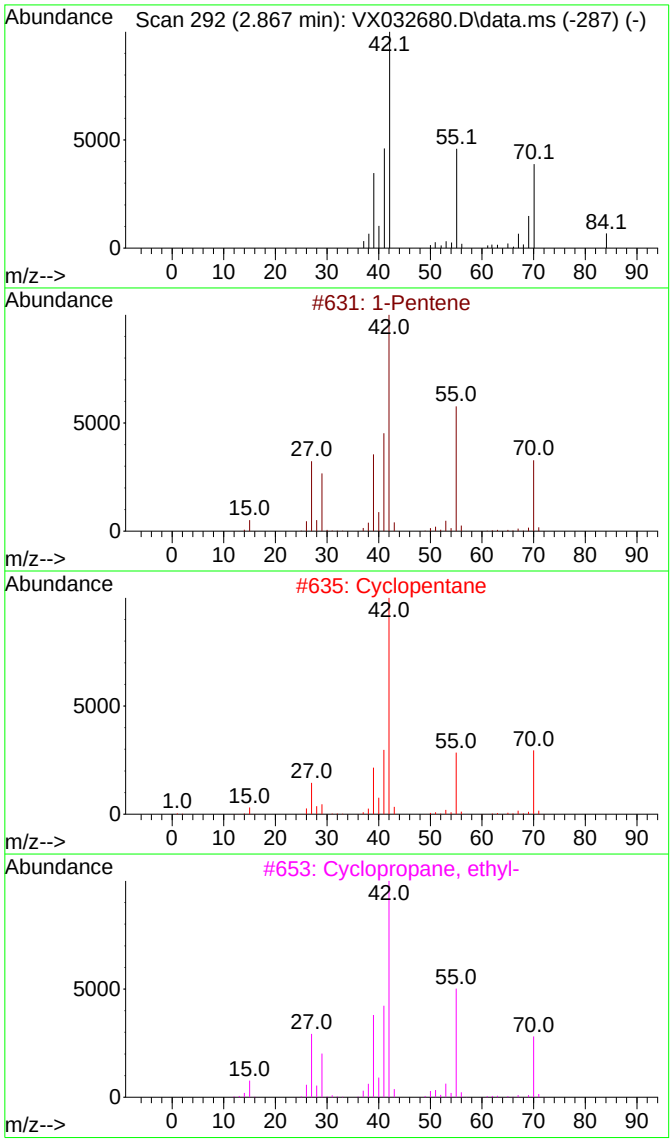
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

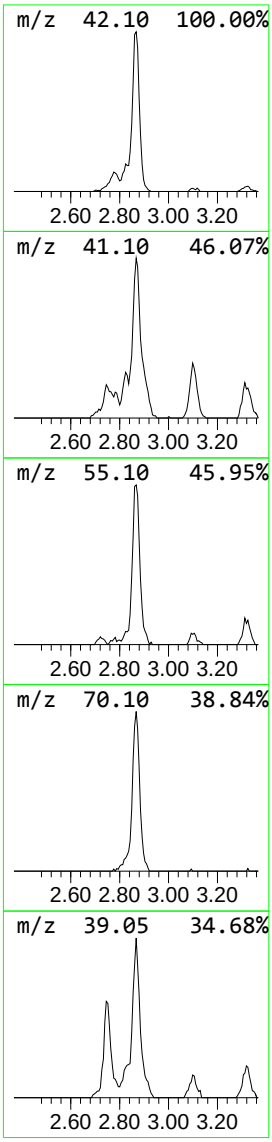
****

Peak Number 5 1-Pentene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	12.85 ug/l	89394	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	64
2	Cyclopentane	70	C5H10	000287-92-3	64
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	64
4	Cyclobutane, methyl-	70	C5H10	000598-61-8	50
5	2-Butene-1,4-diol, (Z)-	88	C4H8O2	006117-80-2	40





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Acq On : 09 Nov 2022 15:31
Operator : JC/MD
Sample : N5551-13 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-8I

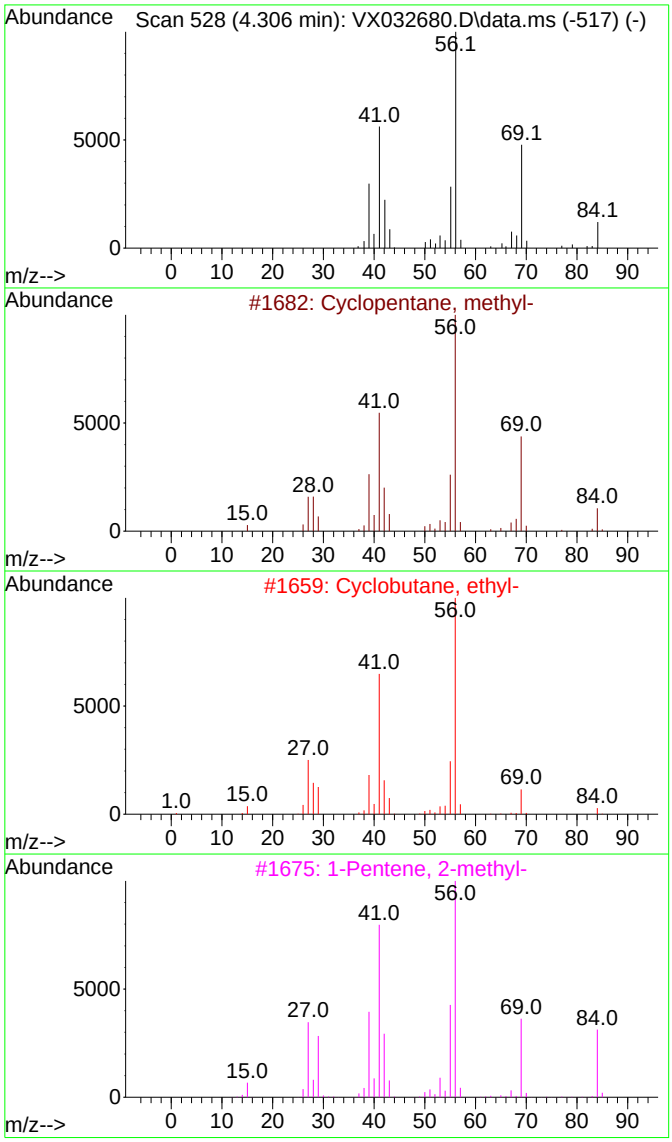
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

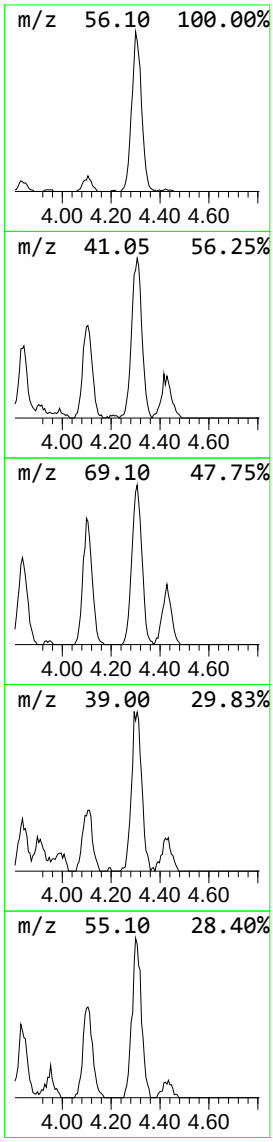
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	15.21 ug/l	105783	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
4	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	50
5	Cyclobutane	56	C4H8	000287-23-0	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032680.D
Acq On : 09 Nov 2022 15:31
Operator : JC/MD
Sample : N5551-13 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-8I

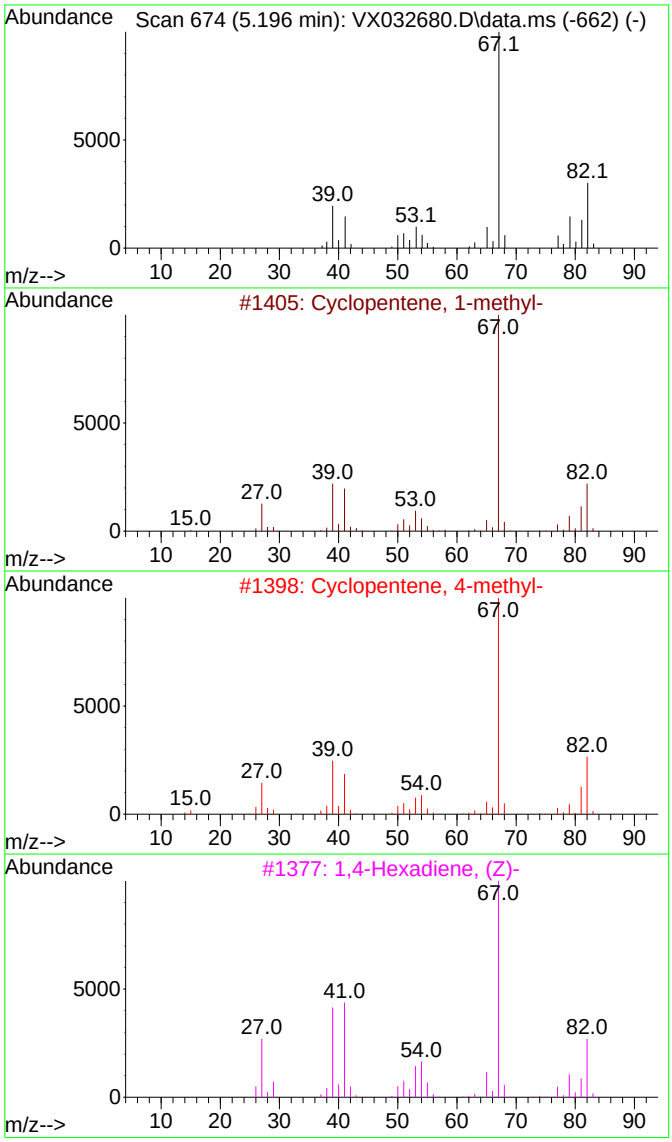
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

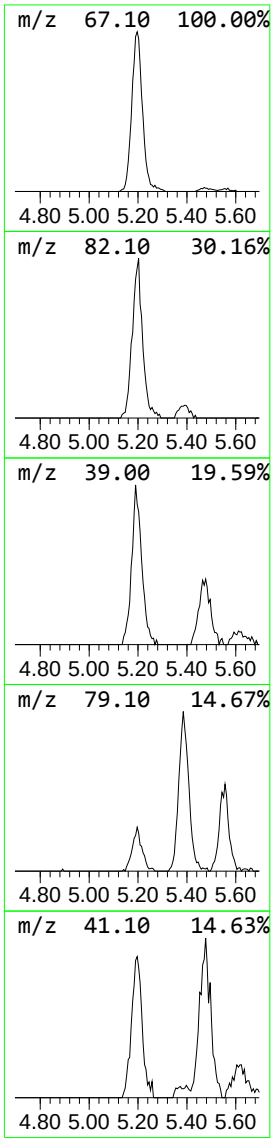
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclopentene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.196	11.35 ug/l	78971	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 1-methyl-	82	C6H10	000693-89-0	90
2	Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	87
3	1,4-Hexadiene, (Z)-	82	C6H10	007318-67-4	87
4	Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	86
5	1,3-Pentadiene, 2-methyl-, (E)-	82	C6H10	000926-54-5	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032680.D
Acq On : 09 Nov 2022 15:31
Operator : JC/MD
Sample : N5551-13 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-8I

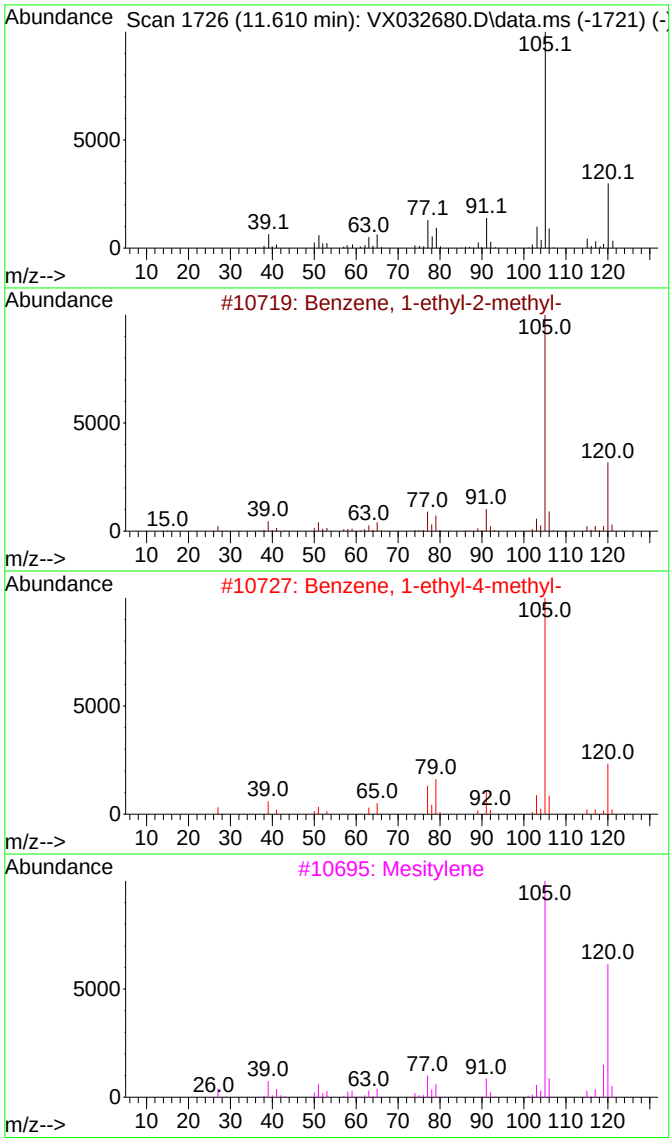
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

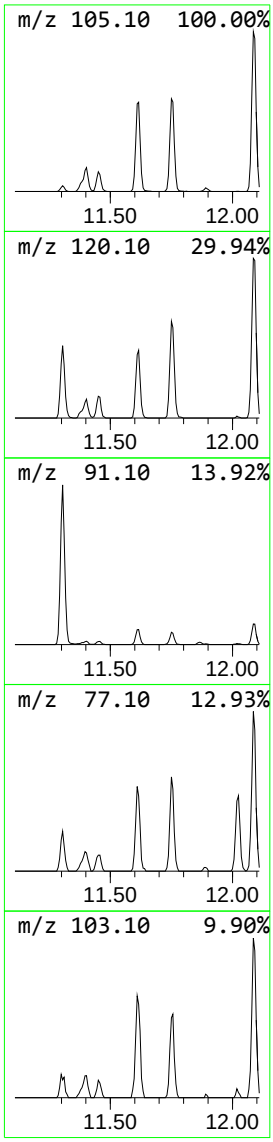
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	8.38 ug/l	86550	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032680.D
Acq On : 09 Nov 2022 15:31
Operator : JC/MD
Sample : N5551-13 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-8I

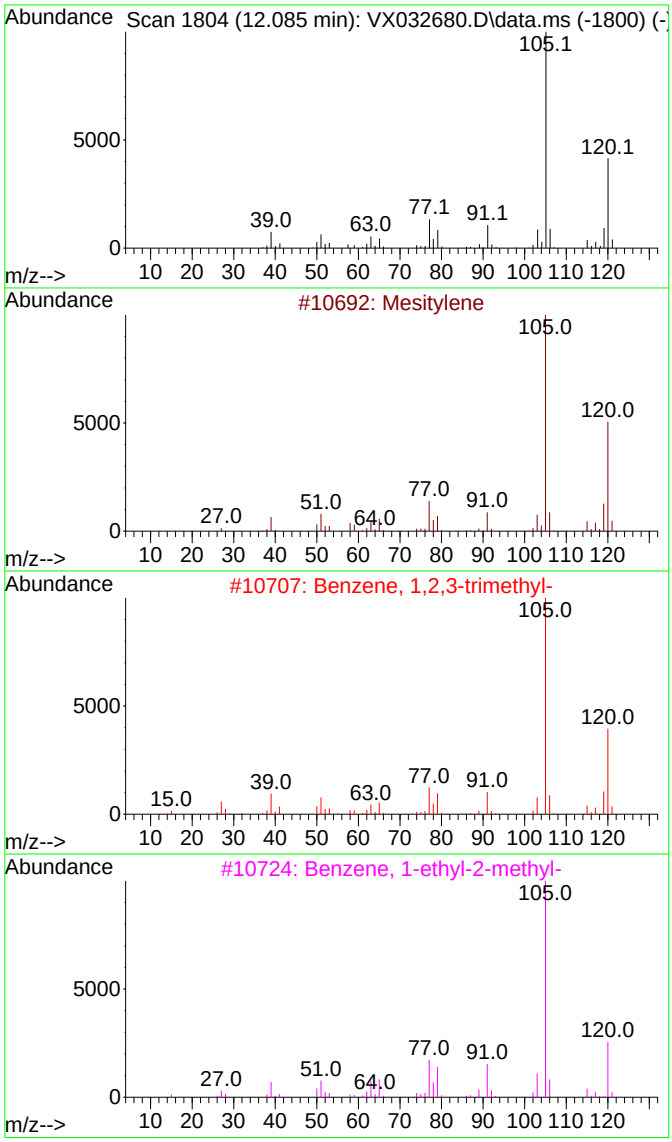
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

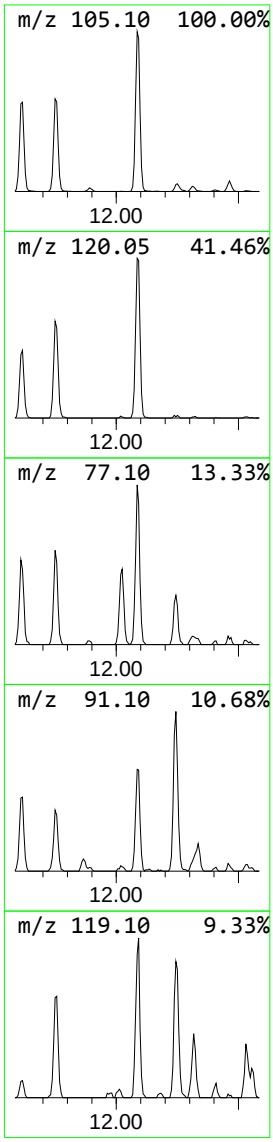
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	15.24 ug/l	157352	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	97
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032680.D
Acq On : 09 Nov 2022 15:31
Operator : JC/MD
Sample : N5551-13 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-8I

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

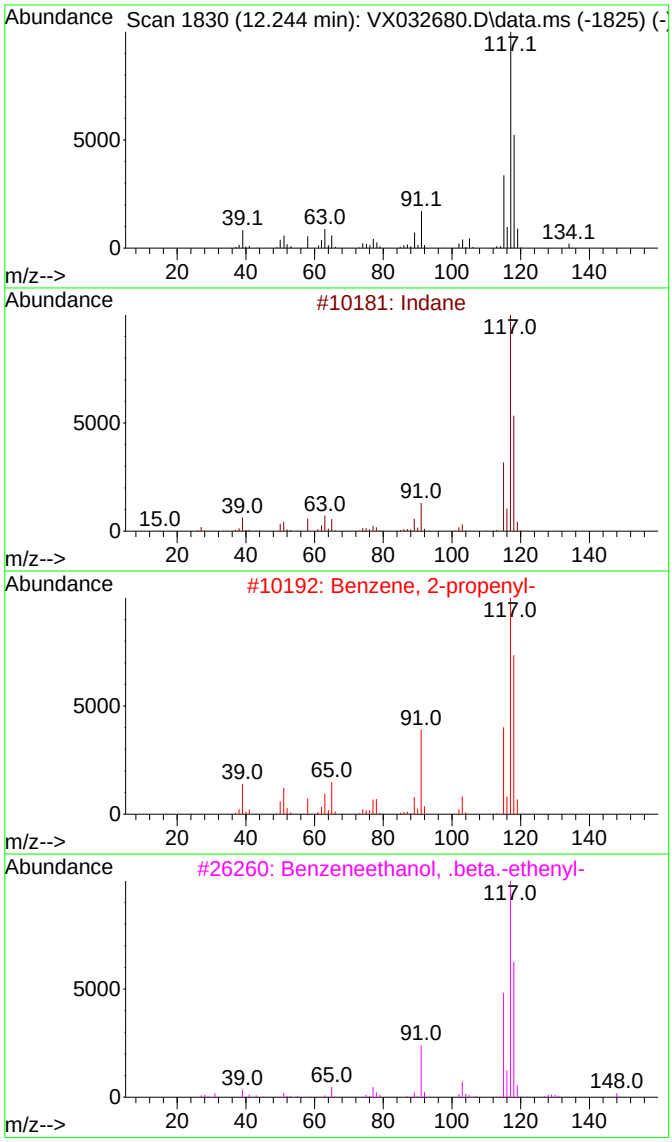
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

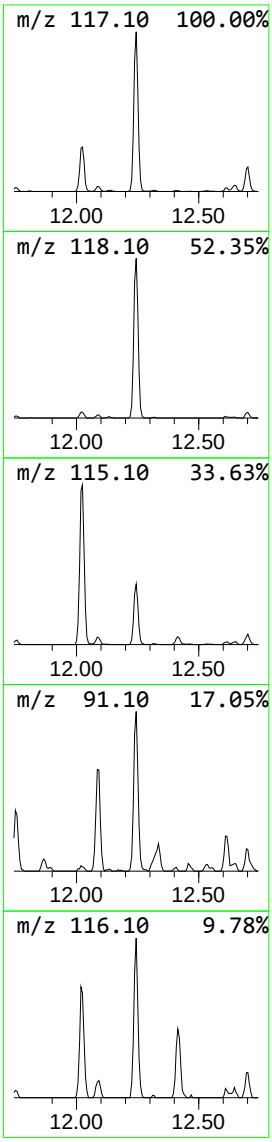
****

Peak Number 10 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	17.11 ug/l	176683	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	94
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3	Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	78
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
5	Deltacyclene	118	C9H10	007785-10-6	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032680.D
Acq On : 09 Nov 2022 15:31
Operator : JC/MD
Sample : N5551-13 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-8I

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.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	1.368	9.5	ug/l	65820	1	5.550	347794	50.0
Butane, 2-methyl-	1.746	18.6	ug/l	129310	1	5.550	347794	50.0
Cyclopropane, 1...	1.971	19.9	ug/l	138586	1	5.550	347794	50.0
Cyclopropane, 1...	2.215	38.6	ug/l	268778	1	5.550	347794	50.0
1-Pentene	2.867	12.9	ug/l	89394	1	5.550	347794	50.0
Cyclopentane, m...	4.306	15.2	ug/l	105783	1	5.550	347794	50.0
Cyclopentene, 1...	5.196	11.4	ug/l	78971	1	5.550	347794	50.0
Benzene, 1-ethy...	11.610	8.4	ug/l	86550	4	12.024	516356	50.0
Benzene, 1,2,3-...	12.085	15.2	ug/l	157352	4	12.024	516356	50.0
Indane	12.244	17.1	ug/l	176683	4	12.024	516356	50.0