LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032687.D
Acq On : 09 Nov 2022 18:11
Operator : JC/MD
Sample : N5551-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12I

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: VX032687.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	578894	625069	4.81%	0.824%
2	1.368	41	46	53	rVV	1165988	1363402	10.49%	1.797%
3	1.429	53	56	64	rVB2	119194	147531	1.13%	0.194%
4	1.660	90	94	103	rVB	109043	132242	1.02%	0.174%
5	1.752	103	109	123	rVB	2621472	3475960	26.74%	4.582%
6	1.910	130	135	138	rBV	140972	186225	1.43%	0.246%
7	1.959	138	143	155	rVV2	850802	1779875	13.69%	2.346%
8	2.069	155	161	169	rVV	980279	1331888	10.25%	1.756%
9	2.166	171	177	181	rVV	561048	825870	6.35%	1.089%
10	2.215	181	185	195	rVB	1252231	1846247	14.20%	2.434%
11	2.752	258	273	281	rBV2	313129	1027297	7.90%	1.354%
12	2.825	281	285	288	rVV	299143	586926	4.52%	0.774%
13	2.867	288	292	315	rVB2	466999	1117720	8.60%	1.474%
14	3.105	320	331	345	rVB	275787	631255	4.86%	0.832%
15	3.319	356	366	378	rBV	87781	200860	1.55%	0.265%
16	3.447	378	387	399	rVB	76745	171698	1.32%	0.226%
17	3.587	399	410	416	rBV3	61487	160322	1.23%	0.211%
18	3.666	416	423	428	rBV	54589	130588	1.00%	0.172%
19	3.733	428	434	443	rVB	174959	405518	3.12%	0.535%
20	3.837	443	451	457	rBV	115615	295880	2.28%	0.390%
21	3.904	457	462	473	rBV2	83333	219712	1.69%	0.290%
22	4.105	486	495	505	rBV	132343	340184	2.62%	0.448%
23	4.306	518	528	540	rVB	459682	1299774	10.00%	1.714%
24	4.428	540	548	563	rVB2	47501	139546	1.07%	0.184%
25	5.196	663	674	688	rVB	123136	384435	2.96%	0.507%
26	5.385	693	705	712	rVV	78028	240840	1.85%	0.318%
27	5.471	712	719	726	rVV2	121153	396493	3.05%	0.523%
28	5.550	727	732	739	rVV	126864	383806	2.95%	0.506%
29	5.623	739	744	764	rVB3	83690	278945	2.15%	0.368%
30	5.958	790	799	804	rBV	80370	203011	1.56%	0.268%
31	6.038	804	812	824	rVV	584673	1582402	12.17%	2.086%
32	6.202	824	839	842	rVV4	101007	413386	3.18%	0.545%
33	6.251	843	847	857	rVV3	154171	422873	3.25%	0.557%
34	6.763	923	931	938	rBV	187839	486963	3.75%	0.642%
35	6.848	941	945	956	rVB4	63023	168695	1.30%	0.222%
36	7.379	1018	1032	1044	rBV5	106804	312463	2.40%	0.412%

LSC Area Percent Report

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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12I

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	7.982	1121	1131	1143	rVB	64885	150299	1.16%	0.198%
38	8.110	1143	1152	1155	rBV	123502	255038	1.96%	0.336%
39	8.507	1210	1217	1223	rBV2	81785	139830	1.08%	0.184%
40	8.647	1235	1240	1246	rVB	384908	617586	4.75%	0.814%
41	8.720	1246	1252	1258	rVB	822378	1236160	9.51%	1.630%
42	8.958	1280	1291	1298	rBV	173206	281781	2.17%	0.371%
43	9.049	1298	1306	1311	rBV	178629	275529	2.12%	0.363%
44	10.055	1461	1471	1477	rBV	408961	543091	4.18%	0.716%
45	10.195	1488	1494	1500	rBV	9790032	12944377	99.58%	17.065%
46	10.305	1505	1512	1518	rVV	10032147	12998461	100.00%	17.136%
47	10.640	1562	1567	1578	rVB	2532362	3310359	25.47%	4.364%
48	10.963	1614	1620	1628	rVB	369840	456082	3.51%	0.601%
49	11.079	1634	1639	1645	rBV	398837	510495	3.93%	0.673%
50	11.305	1671	1676	1683	rVB	935493	1081483	8.32%	1.426%
51	11.402	1683	1692	1696	rVV	699980	926211	7.13%	1.221%
52	11.451	1696	1700	1707	rVB	746811	900743	6.93%	1.187%
53	11.616	1721	1727	1736	rVB	1448590	1811112	13.93%	2.388%
54	11.756	1744	1750	1755	rBV	3426298	4329100	33.30%	5.707%
55	12.024	1788	1794	1799	rVB	488593	603708	4.64%	0.796%
56	12.085	1799	1804	1809	rBV	1408912	1780101	13.69%	2.347%
57	12.244	1824	1830	1837	rBV	1964433	2406623	18.51%	3.173%
58	12.317	1837	1842	1852	rVV3	215645	324601	2.50%	0.428%
59	12.408	1852	1857	1862	rVV2	135324	185679	1.43%	0.245%
60	12.530	1872	1877	1879	rBV	137571	167602	1.29%	0.221%
61	12.616	1886	1891	1894	rBV	274392	359431	2.77%	0.474%
62	12.701	1900	1905	1912	rVB	364887	478919	3.68%	0.631%
63	12.920	1934	1941	1945	rBV	272003	323972	2.49%	0.427%
64	12.963	1945	1948	1954	rVB	189080	219286	1.69%	0.289%
65	13.170	1978	1982	1992	rVB	237222	304401	2.34%	0.401%
66	13.292	1997	2002	2007	rVB2	363028	460063	3.54%	0.607%
67	13.774	2075	2081	2088	rBV	1312584	1598684	12.30%	2.108%
68	14.640	2218	2223	2234	rVB	118912	157521	1.21%	0.208%

Sum of corrected areas: 75854229

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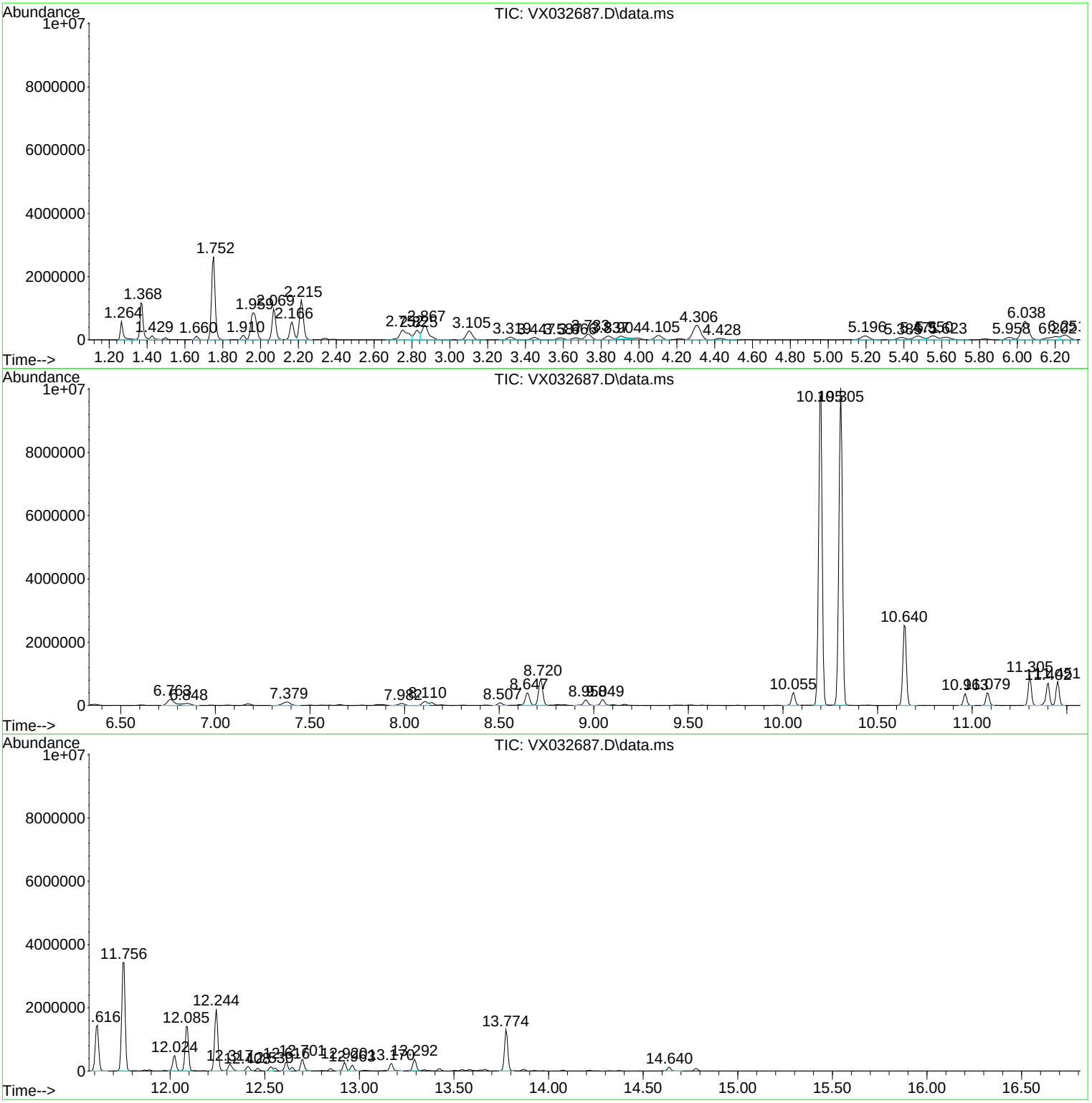
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12I

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 : VX032687.D
Acq On : 09 Nov 2022 18:11
Operator : JC/MD
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MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

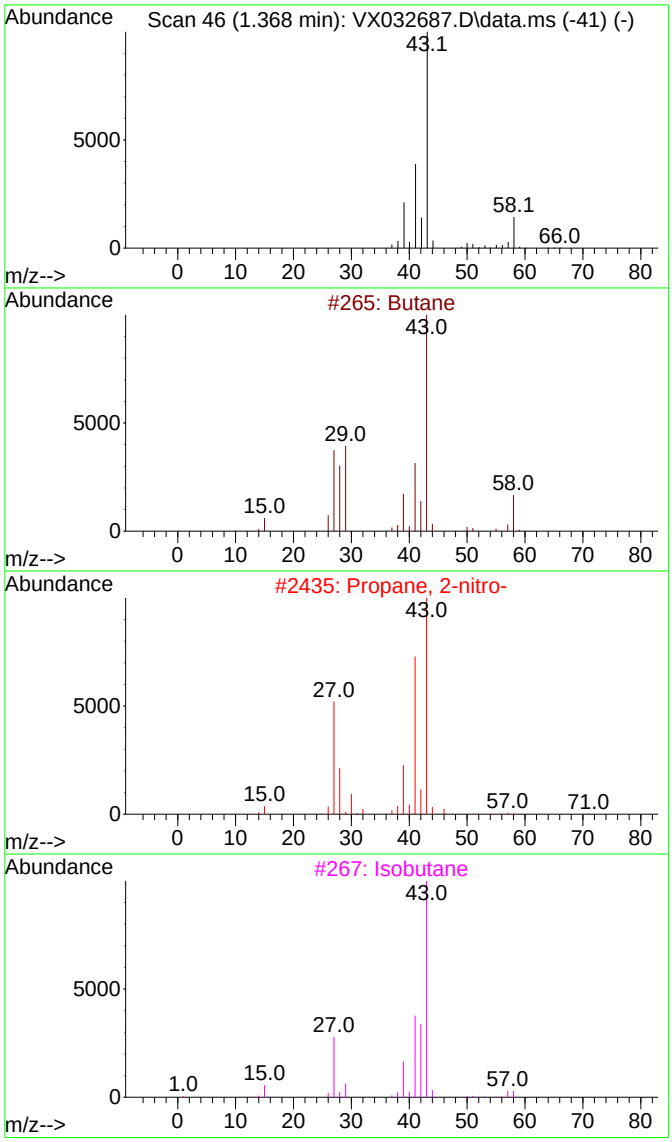
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

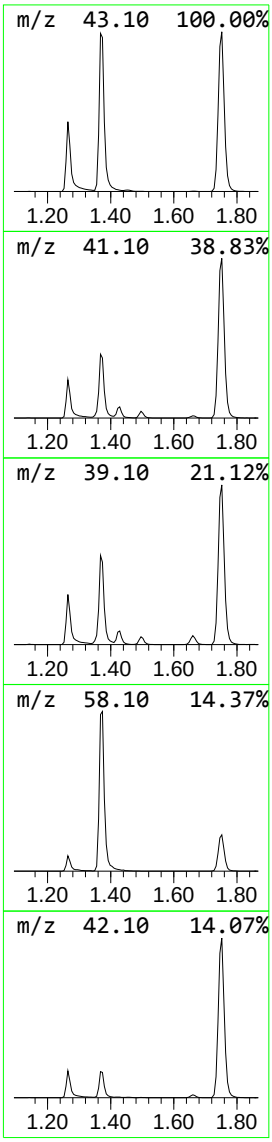
****

Peak Number 1 Butane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	177.62 ug/l	1363400	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	80
2	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
3	Isobutane	58	C4H10	000075-28-5	9
4	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032687.D
Acq On : 09 Nov 2022 18:11
Operator : JC/MD
Sample : N5551-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12I

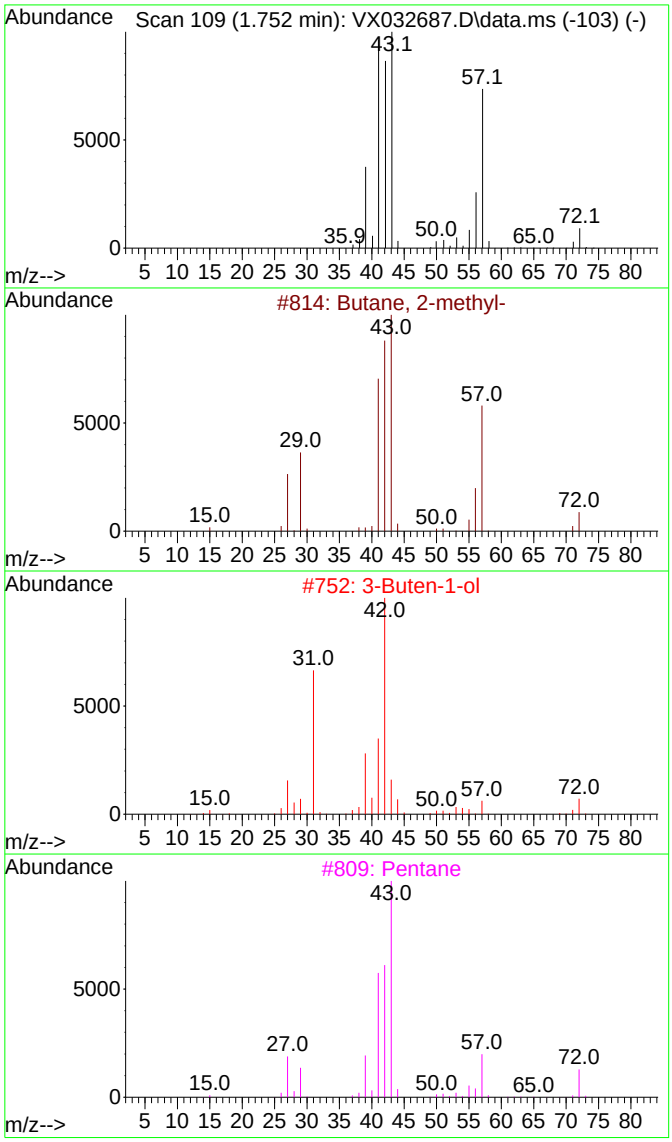
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

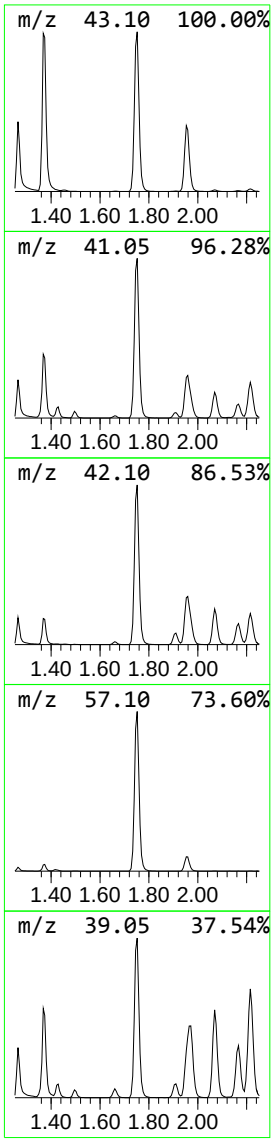
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	452.83 ug/l	3475960	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	3-Buten-1-ol	72	C4H8O	000627-27-0	43
3	Pentane	72	C5H12	000109-66-0	28
4	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	16
5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032687.D
Acq On : 09 Nov 2022 18:11
Operator : JC/MD
Sample : N5551-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12I

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

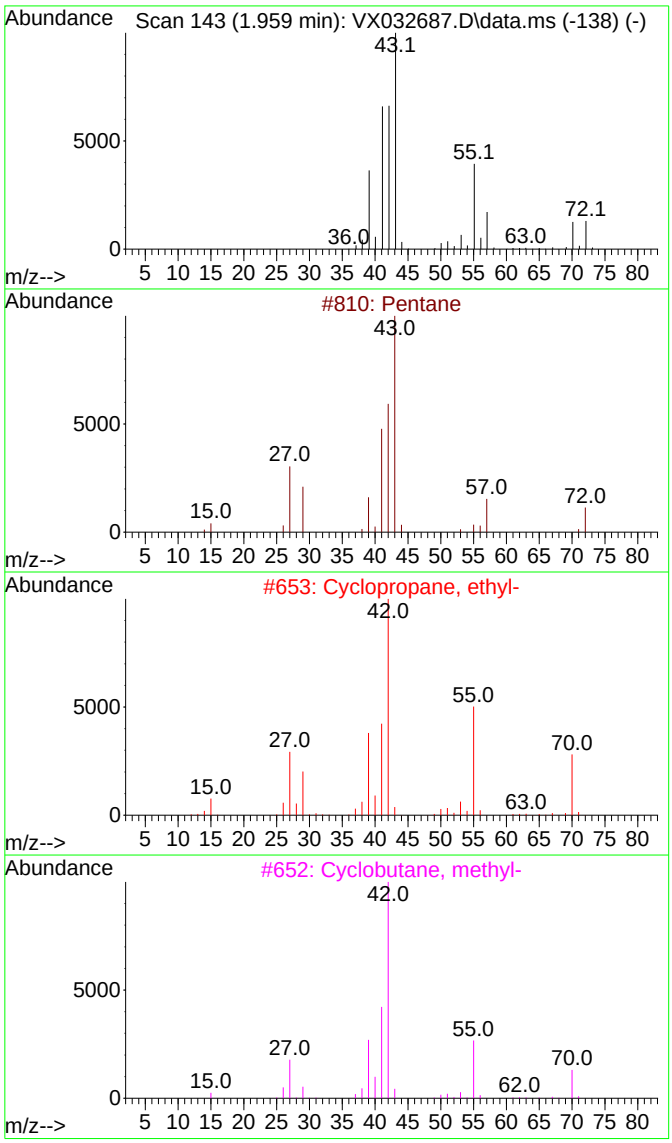
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

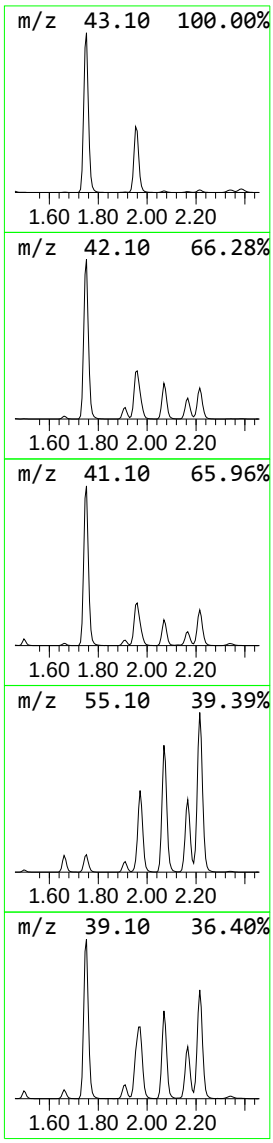
****

Peak Number 3 Pentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	231.87 ug/l	1779880	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	64
2	Cyclopropane, ethyl-	70	C5H10	001191-96-4	47
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	47
4	1-Pentene	70	C5H10	000109-67-1	46
5	Cyclobutanone	70	C4H6O	001191-95-3	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032687.D
Acq On : 09 Nov 2022 18:11
Operator : JC/MD
Sample : N5551-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12I

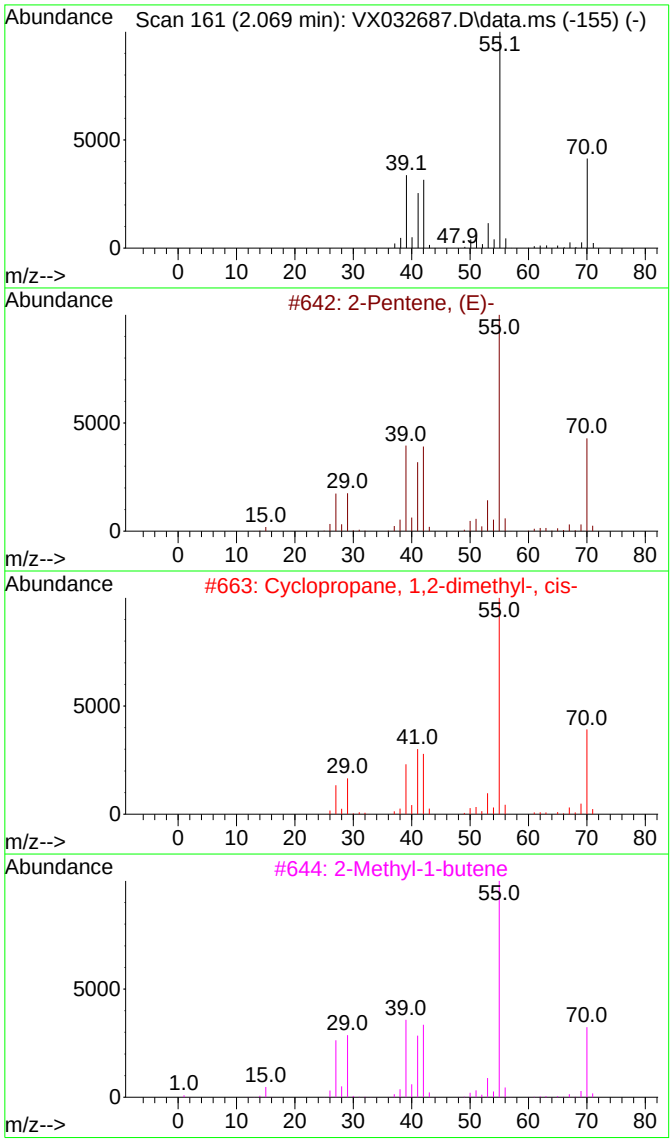
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

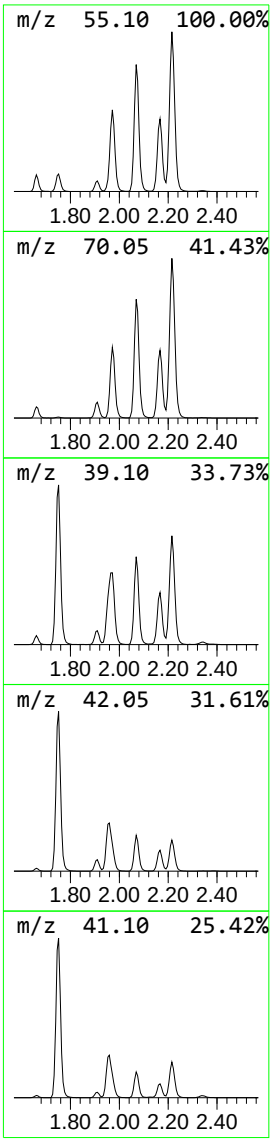
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.069	173.51 ug/l	1331890	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (E)-	70	C5H10	000646-04-8	93
2	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
3	2-Methyl-1-butene	70	C5H10	000563-46-2	90
4	2-Butene, 2-methyl-	70	C5H10	000513-35-9	87
5	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12I

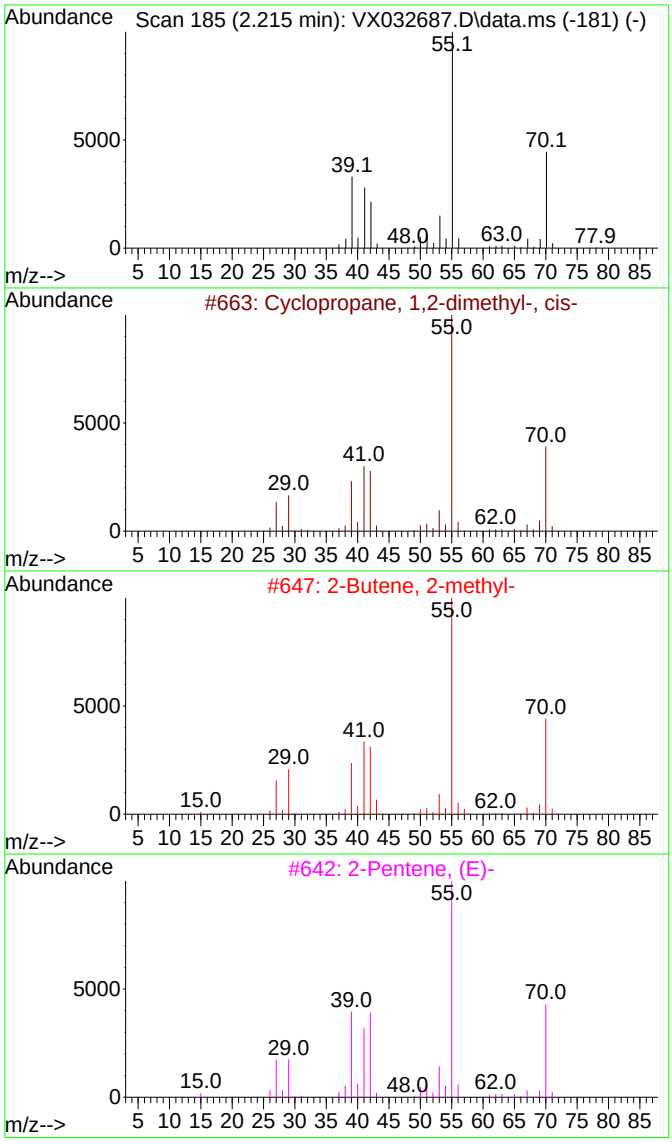
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

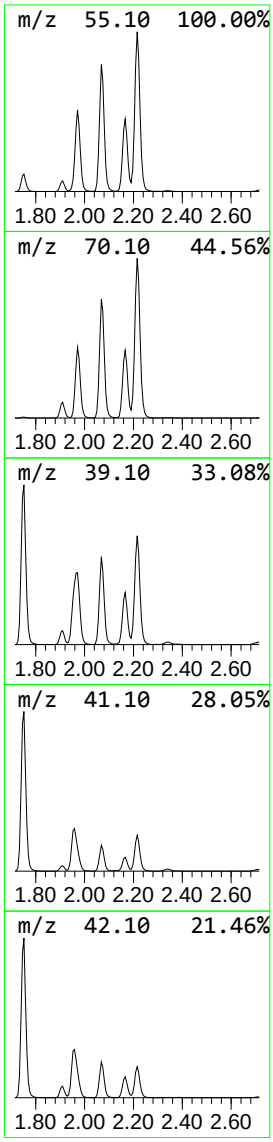
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopropane, 1,2-dimethyl-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	240.52 ug/l	1846250	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2	2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
3	2-Pentene, (E)-	70	C5H10	000646-04-8	86
4	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
5	1-Butene, 3-methyl-	70	C5H10	000563-45-1	78





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12I

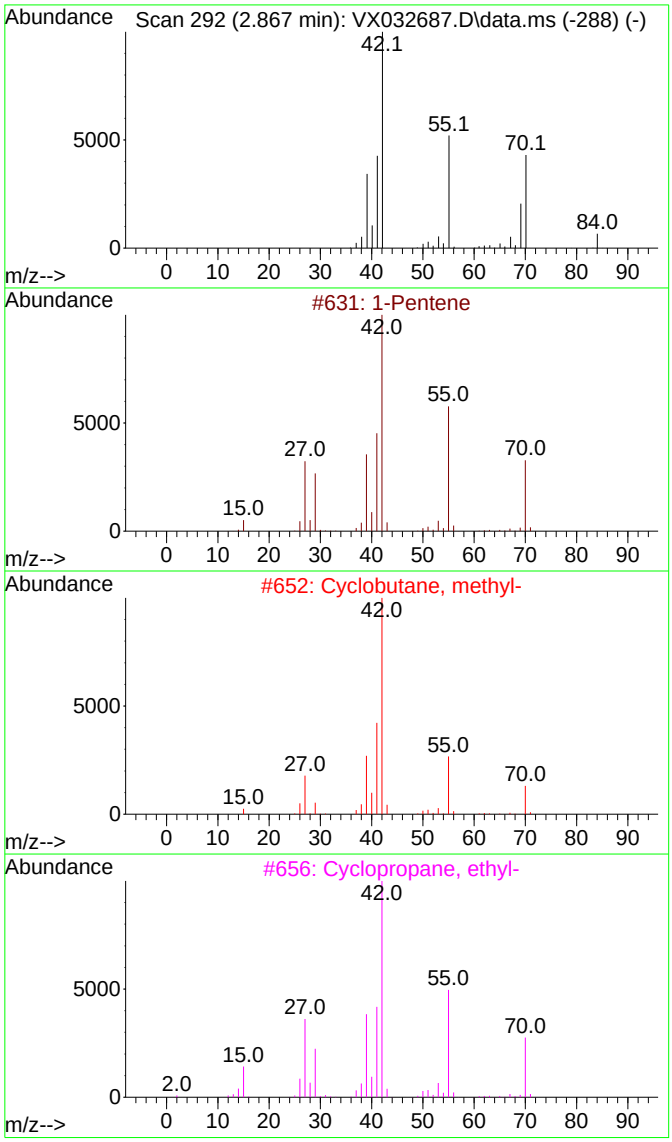
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

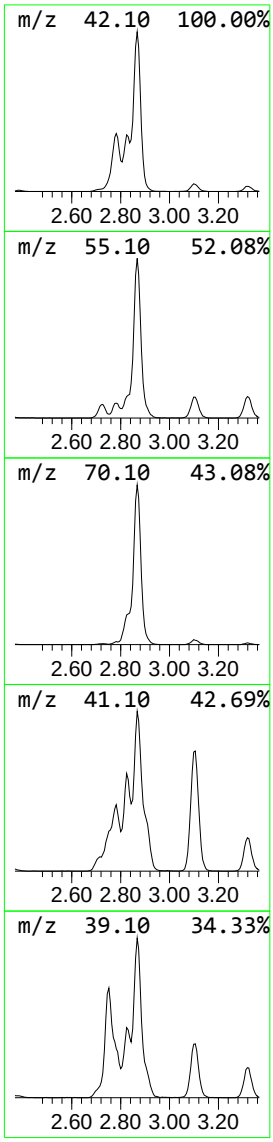
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Pentene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	145.61 ug/l	1117720	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	86
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	80
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	64
4	2-Pentene	70	C5H10	000109-68-2	43
5	2-Butene-1,4-diol, (Z)-	88	C4H8O2	006117-80-2	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032687.D
Acq On : 09 Nov 2022 18:11
Operator : JC/MD
Sample : N5551-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12I

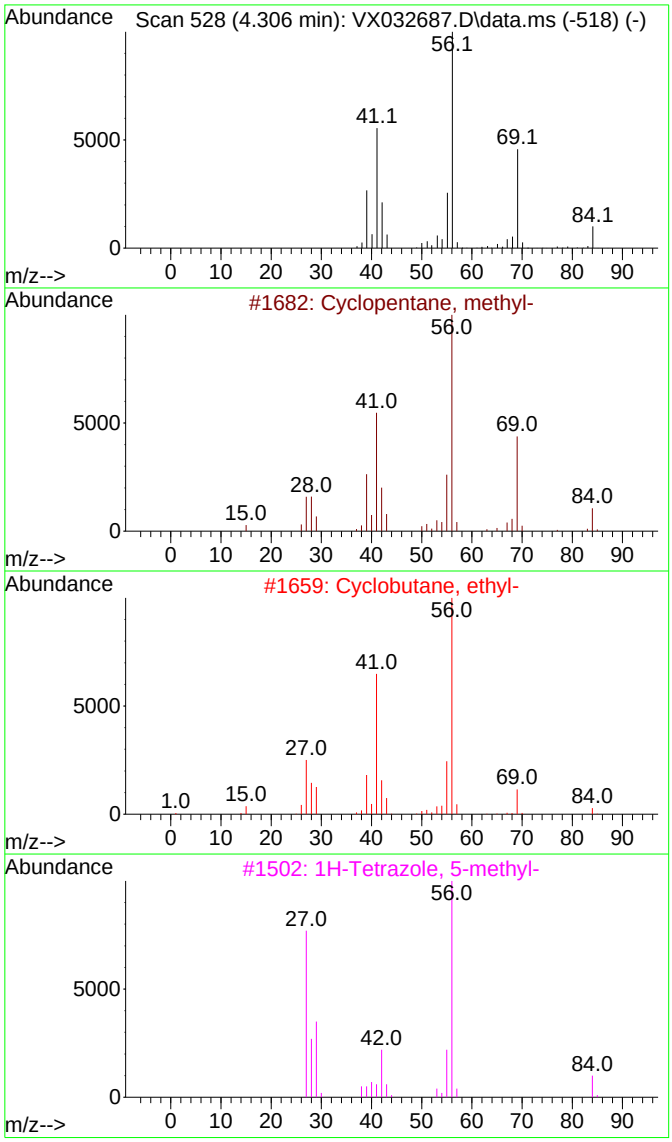
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

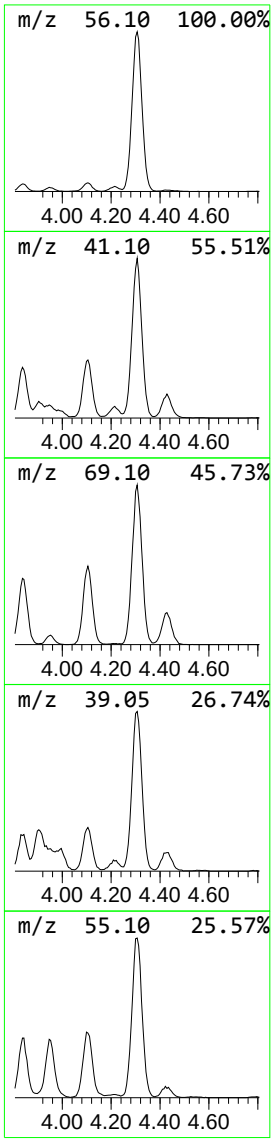
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	169.33 ug/l	1299770	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	72
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	56
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	49
5	Cyclopropane, 1-ethyl-2-methyl-,...	84	C6H12	019781-68-1	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032687.D
Acq On : 09 Nov 2022 18:11
Operator : JC/MD
Sample : N5551-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12I

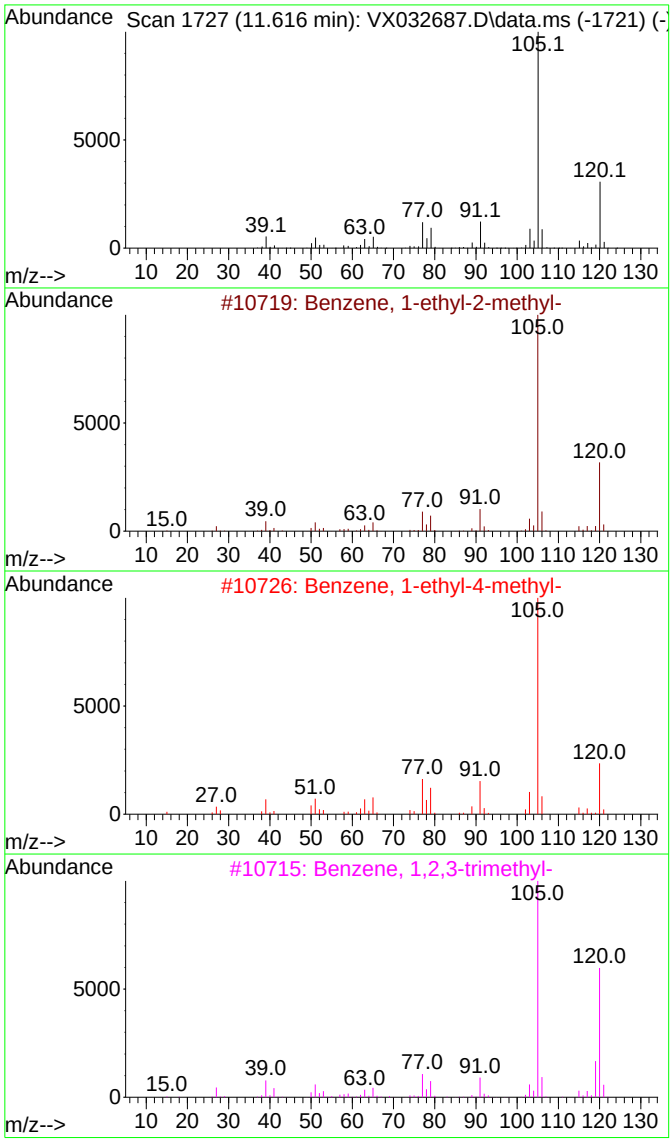
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

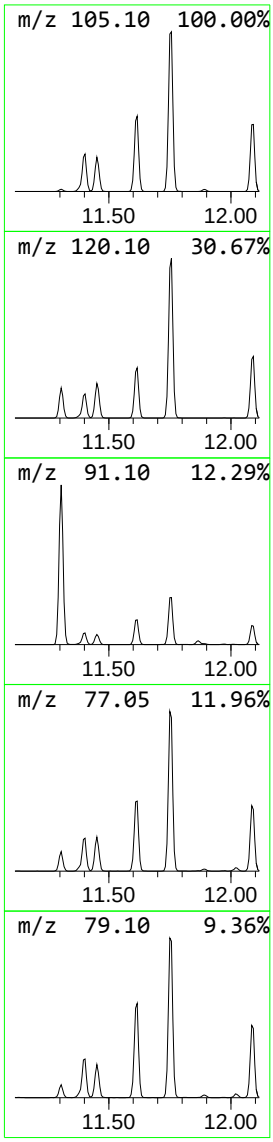
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	150.00 ug/l	1811110	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	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032687.D
Acq On : 09 Nov 2022 18:11
Operator : JC/MD
Sample : N5551-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12I

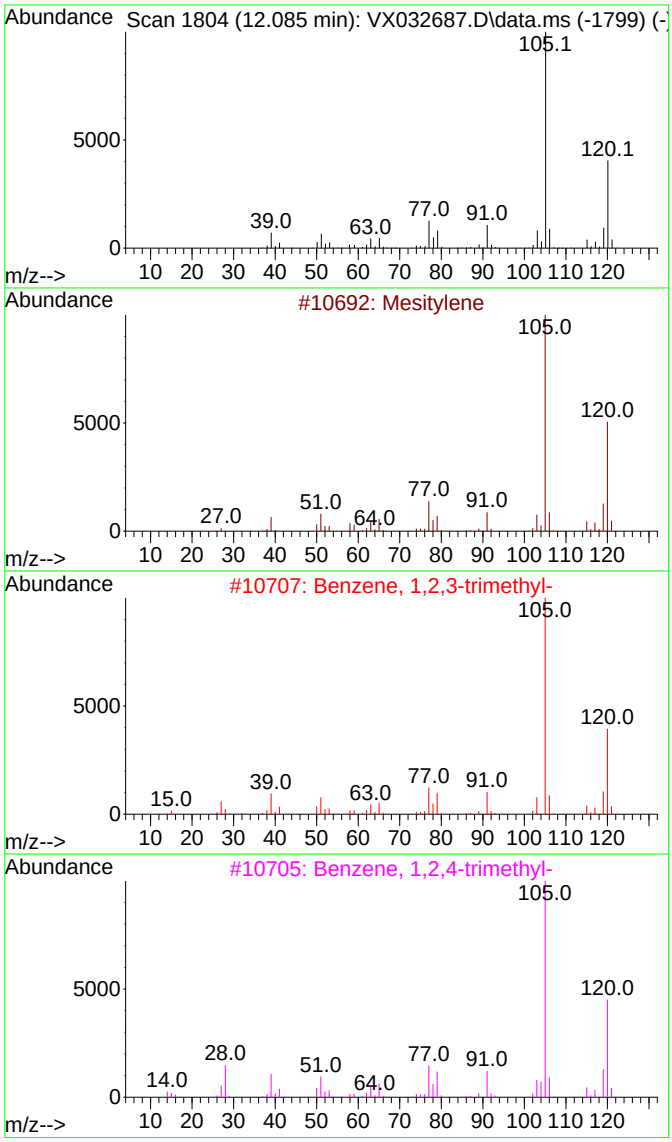
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

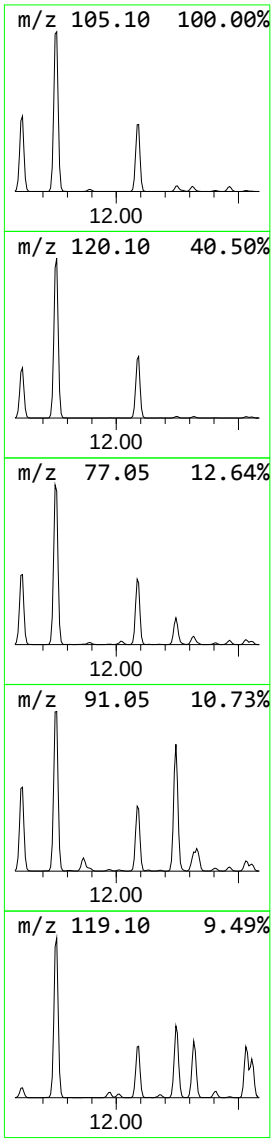
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	147.43 ug/l	1780100	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, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032687.D
Acq On : 09 Nov 2022 18:11
Operator : JC/MD
Sample : N5551-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12I

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

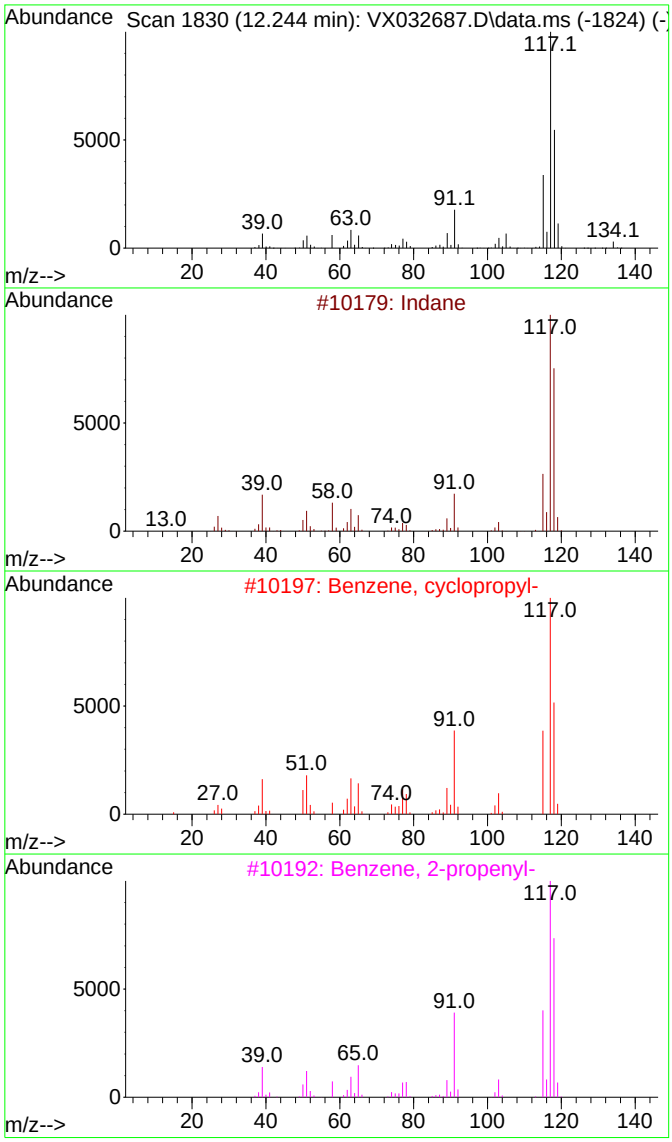
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

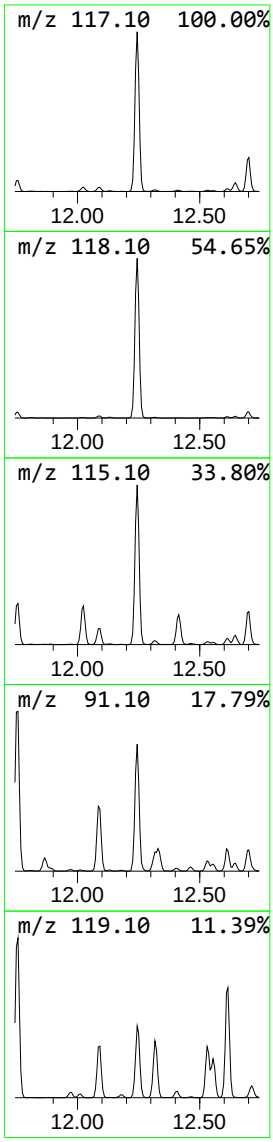
****

Peak Number 10 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	199.32 ug/l	2406620	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
4	Deltacyclene	118	C9H10	007785-10-6	64
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032687.D
Acq On : 09 Nov 2022 18:11
Operator : JC/MD
Sample : N5551-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12I

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	177.6	ug/l	1363400	1	5.550	383806	50.0
Butane, 2-methyl-	1.752	452.8	ug/l	3475960	1	5.550	383806	50.0
Pentane	1.959	231.9	ug/l	1779880	1	5.550	383806	50.0
2-Pentene, (E)-	2.069	173.5	ug/l	1331890	1	5.550	383806	50.0
Cyclopropane, 1...	2.215	240.5	ug/l	1846250	1	5.550	383806	50.0
1-Pentene	2.867	145.6	ug/l	1117720	1	5.550	383806	50.0
Cyclopentane, m...	4.306	169.3	ug/l	1299770	1	5.550	383806	50.0
Benzene, 1-ethy...	11.616	150.0	ug/l	1811110	4	12.024	603708	50.0
Benzene, 1,2,3-...	12.085	147.4	ug/l	1780100	4	12.024	603708	50.0
Indane	12.244	199.3	ug/l	2406620	4	12.024	603708	50.0