LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
Data File : VX028250.D
Acq On : 21 Apr 2022 18:42
Operator : JC/MD
Sample : N2459-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31579

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\82X041922W.M
Title : SW846 8260

Signal : TIC: VX028250.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	18	rVB	221354	187606	2.14%	0.255%
2	1.264	26	29	40	rBV	829537	768368	8.77%	1.043%
3	1.373	40	47	53	rBV	4991462	5574872	63.64%	7.569%
4	1.428	53	56	63	rVB	484785	484496	5.53%	0.658%
5	1.495	63	67	72	rBV	431746	414193	4.73%	0.562%
6	1.751	103	109	121	rVB	1553694	2125150	24.26%	2.885%
7	1.910	130	135	138	rBV	108524	146751	1.68%	0.199%
8	1.959	138	143	153	rVV2	767454	1396668	15.94%	1.896%
9	2.068	153	161	170	rVV2	551551	1023977	11.69%	1.390%
10	2.166	170	177	181	rVV	250974	400543	4.57%	0.544%
11	2.215	181	185	195	rVB	776580	1136757	12.98%	1.543%
12	2.751	259	273	281	rBV	183220	440653	5.03%	0.598%
13	2.830	281	286	288	rVV	98620	194158	2.22%	0.264%
14	2.867	288	292	303	rVB	250639	510425	5.83%	0.693%
15	3.105	321	331	345	rBV2	72238	174129	1.99%	0.236%
16	3.446	379	387	397	rBV	49176	110538	1.26%	0.150%
17	4.306	518	528	541	rVB	153813	444851	5.08%	0.604%
18	5.196	663	674	687	rVB	37606	115707	1.32%	0.157%
19	5.391	691	706	714	rBV2	301456	888258	10.14%	1.206%
20	5.470	714	719	725	rVV2	86841	258685	2.95%	0.351%
21	5.556	725	733	752	rVB	429801	1237752	14.13%	1.680%
22	5.958	788	799	805	rBV	295338	783506	8.94%	1.064%
23	6.043	805	813	827	rVV	1433649	3805119	43.44%	5.166%
24	6.226	827	843	856	rVB7	28572	146040	1.67%	0.198%
25	6.763	921	931	943	rBV	667486	1580391	18.04%	2.146%
26	7.378	1023	1032	1041	rVB2	40289	99519	1.14%	0.135%
27	8.653	1234	1241	1246	rBV	1580879	2449322	27.96%	3.325%
28	8.720	1246	1252	1264	rVB	5718543	8759660	100.00%	11.892%
29	10.055	1460	1471	1482	rBV	1452390	1964720	22.43%	2.667%
30	10.195	1489	1494	1500	rBV	520416	674684	7.70%	0.916%
31	10.305	1505	1512	1522	rBV	5510481	7574636	86.47%	10.284%
32	10.646	1562	1568	1583	rVB	3252115	4291798	49.00%	5.827%
33	11.085	1634	1640	1653	rBV	1384097	1816631	20.74%	2.466%
34	11.304	1667	1676	1683	rBV	82089	112431	1.28%	0.153%
35	11.378	1683	1688	1696	rVV	1993501	3425350	39.10%	4.650%
36	11.451	1696	1700	1710	rVB	919381	1140488	13.02%	1.548%

LSC Area Percent Report

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Data File : VX028250.D
Acq On : 21 Apr 2022 18:42
Operator : JC/MD
Sample : N2459-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31579

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\82X041922W.M
Title : SW846 8260

37	11.615	1721	1727	1736	rVB	935768	1123447	12.83%	1.525%
38	11.756	1744	1750	1755	rBV	3286808	4042282	46.15%	5.488%
39	11.969	1779	1785	1789	rBV	75194	95810	1.09%	0.130%
40	12.024	1789	1794	1800	rVV	1674777	2040573	23.30%	2.770%
41	12.091	1800	1805	1810	rVB	1029766	1268229	14.48%	1.722%
42	12.243	1822	1830	1833	rBV2	1020867	1405300	16.04%	1.908%
43	12.317	1838	1842	1851	rVV2	444320	627300	7.16%	0.852%
44	12.463	1862	1866	1872	rVB	117952	140329	1.60%	0.191%
45	12.530	1872	1877	1879	rBV	258094	316051	3.61%	0.429%
46	12.554	1879	1881	1886	rVB	239522	265422	3.03%	0.360%
47	12.615	1886	1891	1894	rBV	439749	519973	5.94%	0.706%
48	12.646	1894	1896	1900	rVB	113565	116901	1.33%	0.159%
49	12.701	1900	1905	1913	rBV2	301507	436932	4.99%	0.593%
50	12.847	1925	1929	1935	rVB	124578	164122	1.87%	0.223%
51	12.920	1935	1941	1945	rVV	242378	319454	3.65%	0.434%
52	12.963	1945	1948	1954	rVB	376738	439245	5.01%	0.596%
53	13.170	1978	1982	1986	rVB	326316	411214	4.69%	0.558%
54	13.292	1998	2002	2008	rVB2	629912	815757	9.31%	1.108%
55	13.420	2019	2023	2028	rVB	216829	281606	3.21%	0.382%
56	13.542	2040	2043	2046	rVV	92561	127156	1.45%	0.173%
57	13.585	2046	2050	2057	rVV4	113504	225121	2.57%	0.306%
58	13.664	2060	2063	2069	rVB2	89622	140761	1.61%	0.191%
59	13.780	2076	2082	2087	rBV	368398	488672	5.58%	0.663%
60	13.926	2100	2106	2110	rBV2	76779	109715	1.25%	0.149%
61	14.078	2127	2131	2140	rVB	81528	113175	1.29%	0.154%
62	14.225	2147	2155	2160	rBV4	118547	266749	3.05%	0.362%
63	14.371	2175	2179	2184	rVB	68501	89529	1.02%	0.122%
64	14.481	2192	2197	2202	rBV2	75775	104340	1.19%	0.142%
65	14.639	2215	2223	2227	rBV	234098	354698	4.05%	0.482%
66	14.779	2241	2246	2250	rBV	114692	148625	1.70%	0.202%

Sum of corrected areas: 73657320

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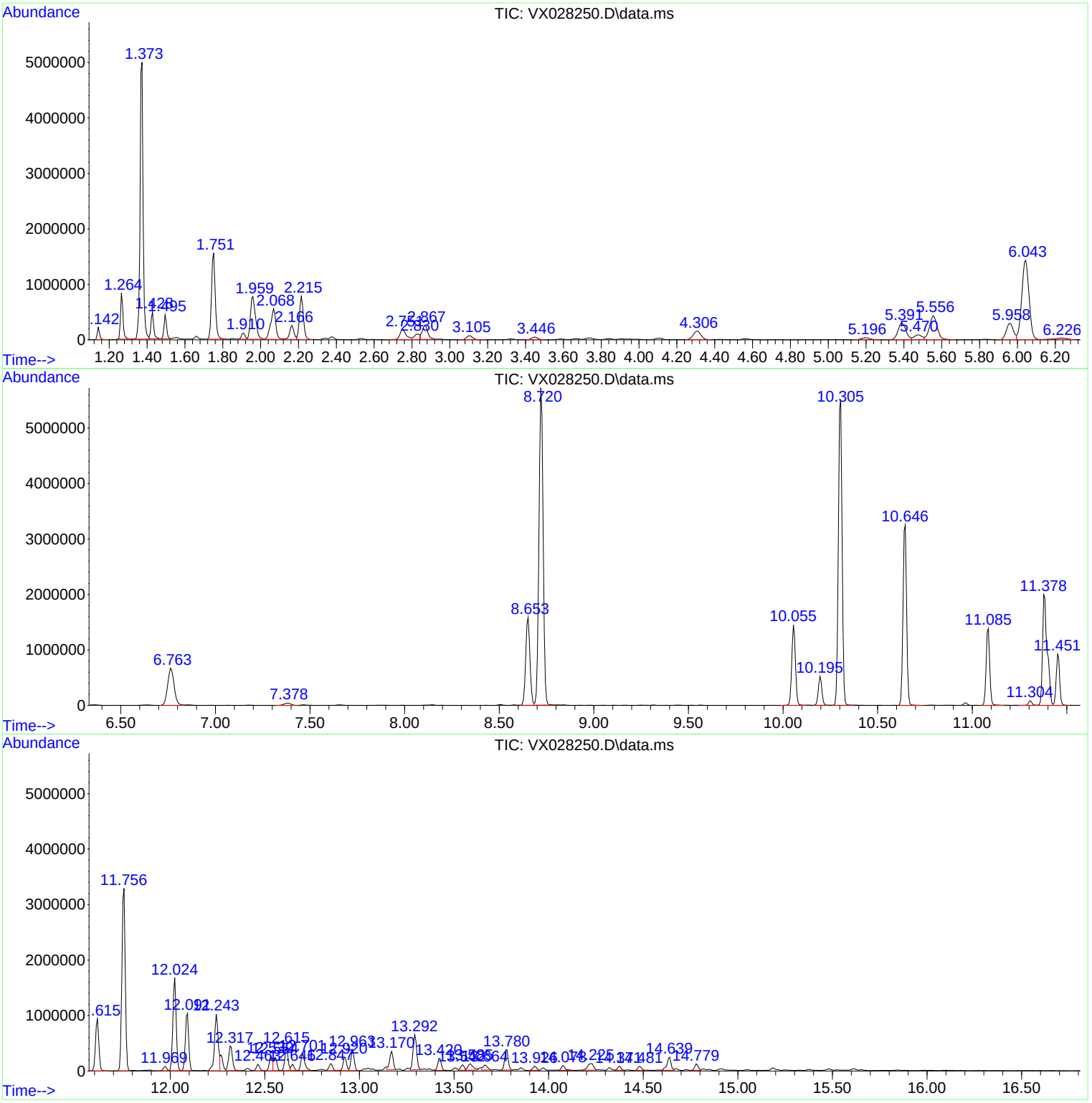
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31579

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
Data File : VX028250.D
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Quant Title : SW846 8260

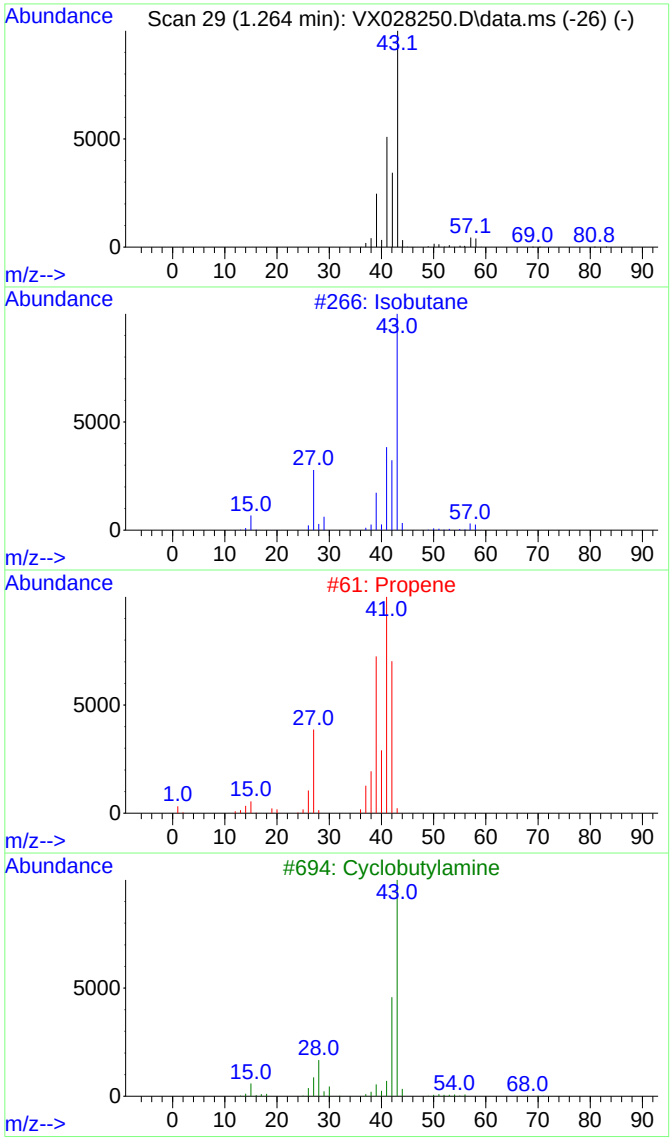
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

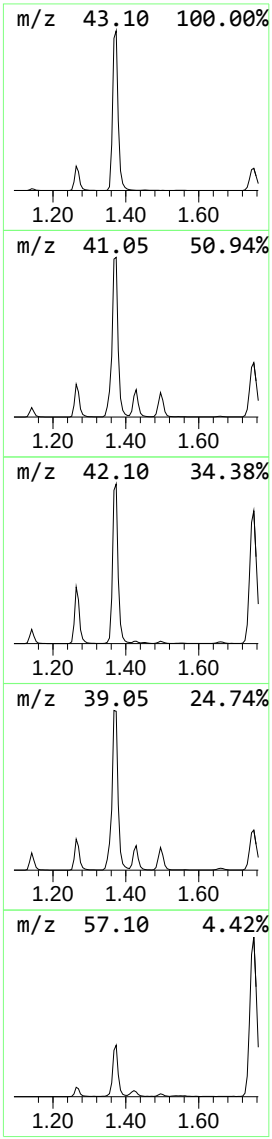
****

Peak Number 1 Isobutane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	31.04 ug/l	768368	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	72
2	Propene	42	C3H6	000115-07-1	5
3	Cyclobutylamine	71	C4H9N	002516-34-9	4
4	5-Methyloxazolidine	87	C4H9NO	058328-22-6	4
5	Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
Data File : VX028250.D
Acq On : 21 Apr 2022 18:42
Operator : JC/MD
Sample : N2459-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31579

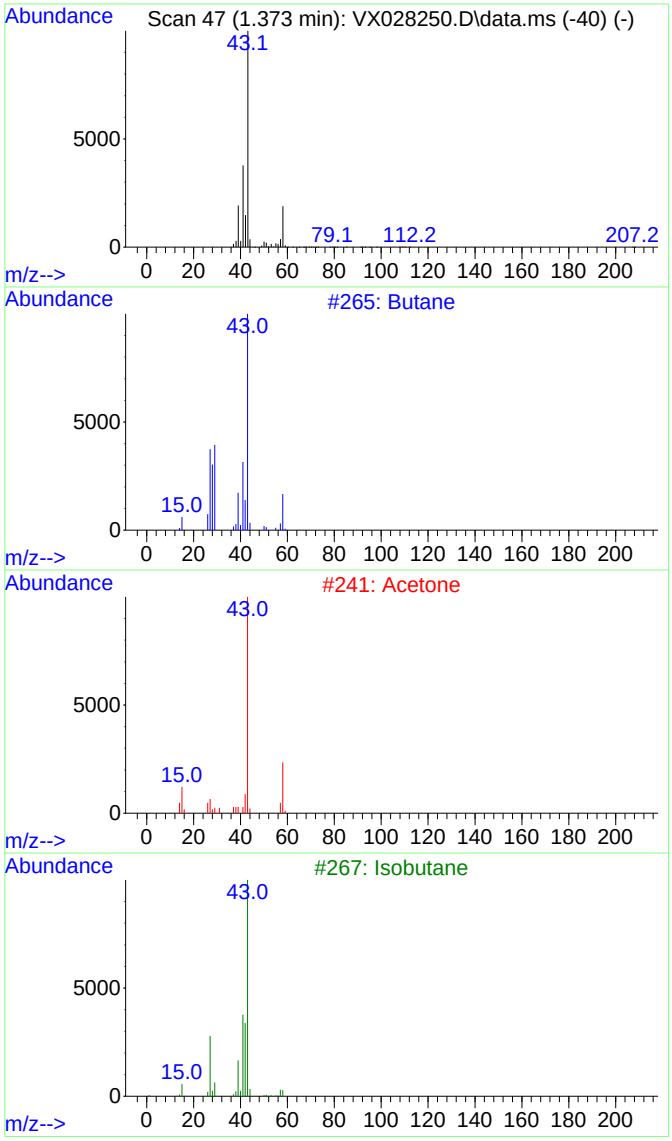
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

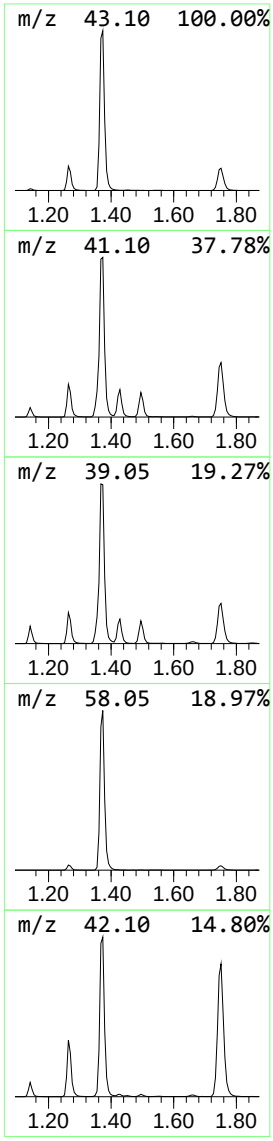
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.373	225.20 ug/l	5574870	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	80
2	Acetone	58	C3H6O	000067-64-1	9
3	Isobutane	58	C4H10	000075-28-5	9
4	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
Data File : VX028250.D
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Operator : JC/MD
Sample : N2459-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31579

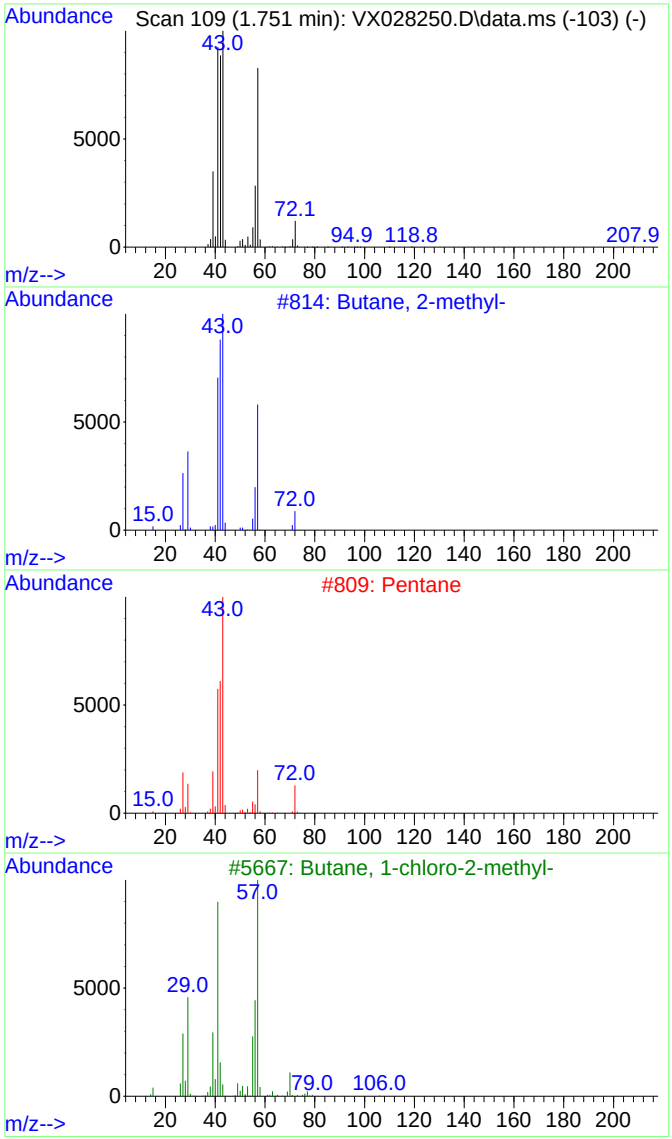
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

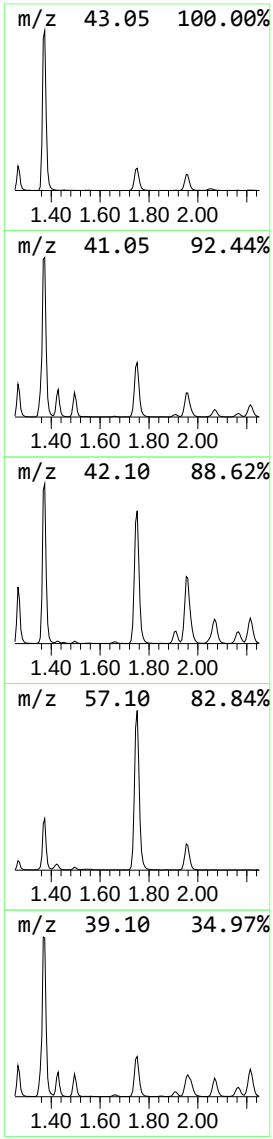
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.751	85.85 ug/l	2125150	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	87
2	Pentane	72	C5H12	000109-66-0	38
3	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	35
4	1-Butene	56	C4H8	000106-98-9	10
5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
Data File : VX028250.D
Acq On : 21 Apr 2022 18:42
Operator : JC/MD
Sample : N2459-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31579

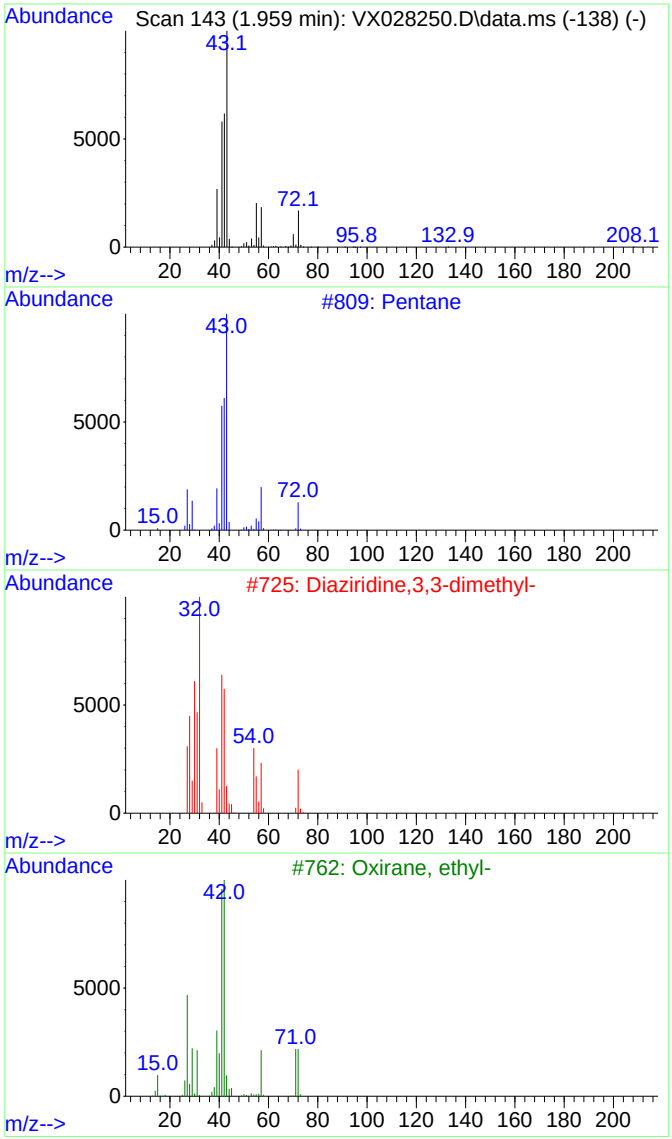
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

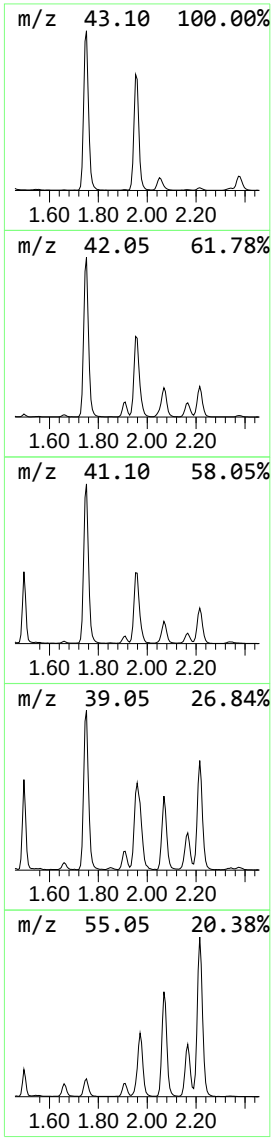
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	56.42 ug/l	1396670	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	90
2	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	50
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	43
4	Isobutylene epoxide	72	C4H8O	000558-30-5	38
5	1-Propene, 2-methoxy-	72	C4H8O	000116-11-0	37





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Sample : N2459-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31579

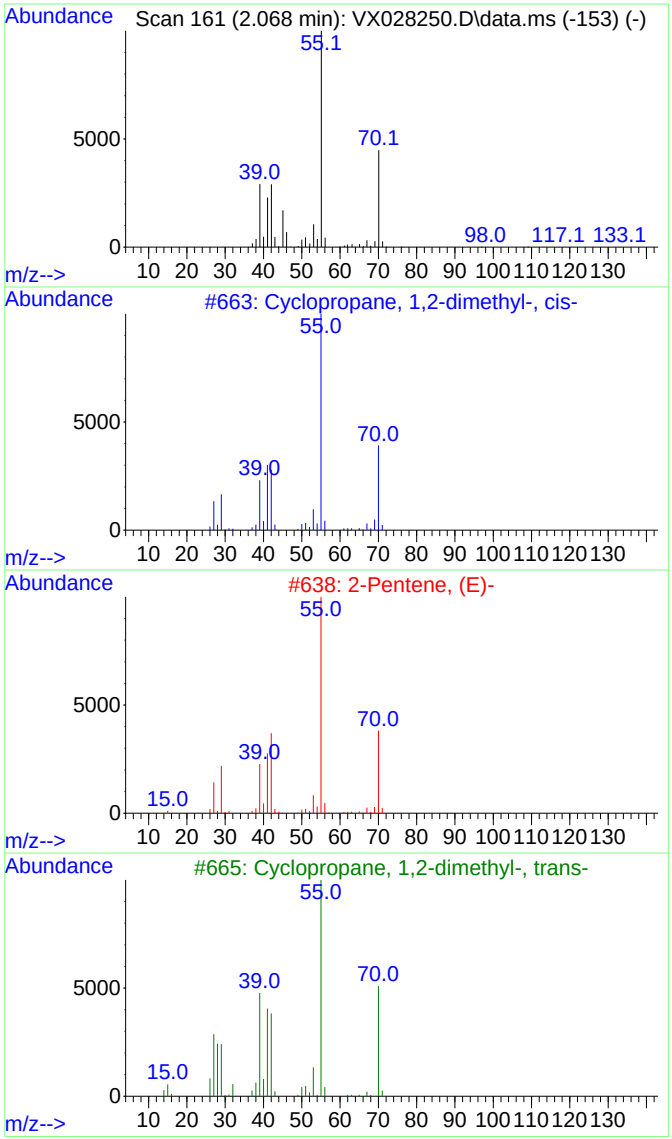
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

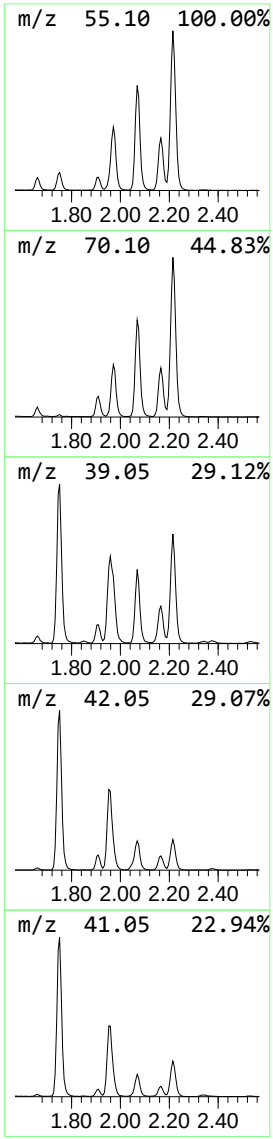
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopropane, 1,2-dimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.068	41.36 ug/l	1023980	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	87
2	2-Pentene, (E)-	70	C5H10	000646-04-8	74
3	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	74
4	2-Methyl-1-butene	70	C5H10	000563-46-2	74
5	2-Butene, 2-methyl-	70	C5H10	000513-35-9	72





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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31579

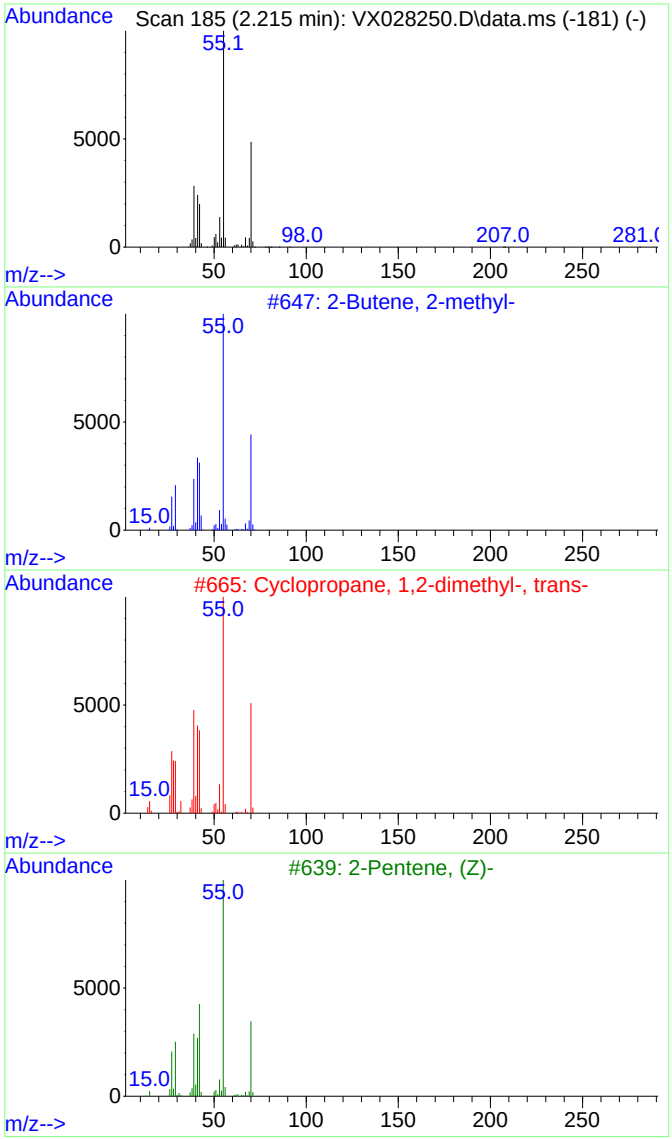
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

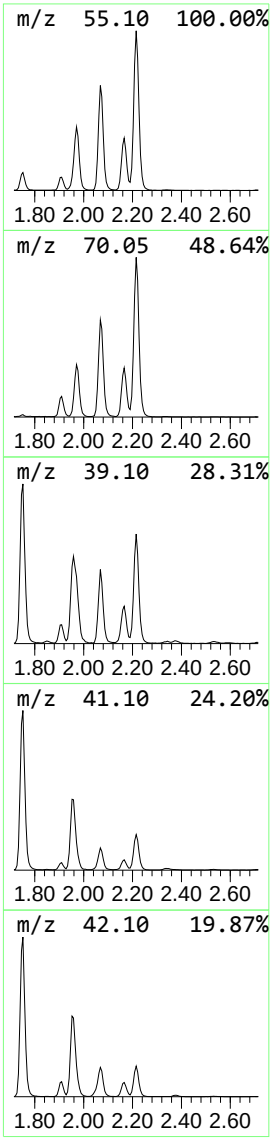
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Butene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	45.92 ug/l	1136760	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
2	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	83
3	2-Pentene, (Z)-	70	C5H10	000627-20-3	80
4	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
5	2-Methyl-1-butene	70	C5H10	000563-46-2	78





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Data File : VX028250.D
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31579

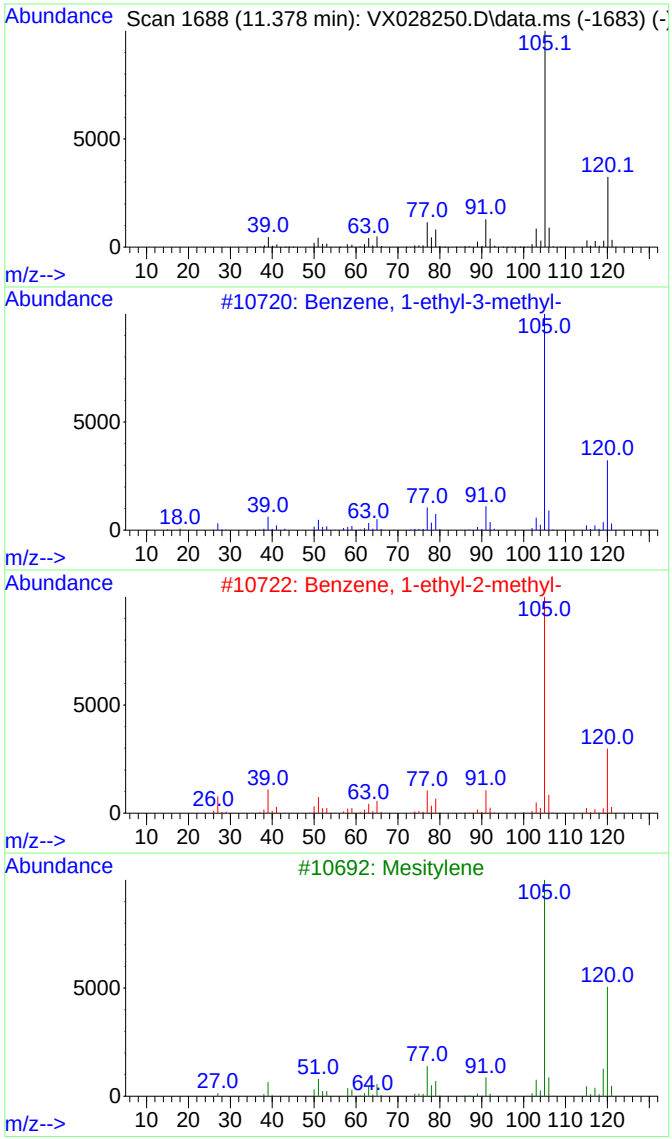
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

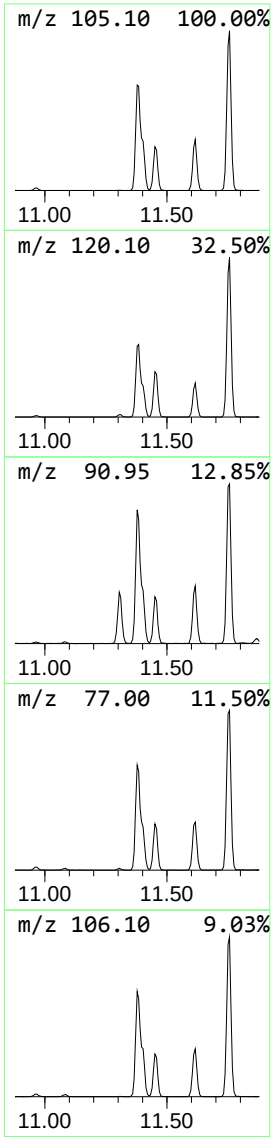
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	83.93 ug/l	3425350	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
Data File : VX028250.D
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ALS Vial : 21 Sample Multiplier: 1

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MSVOA_X
ClientSampleId :
31579

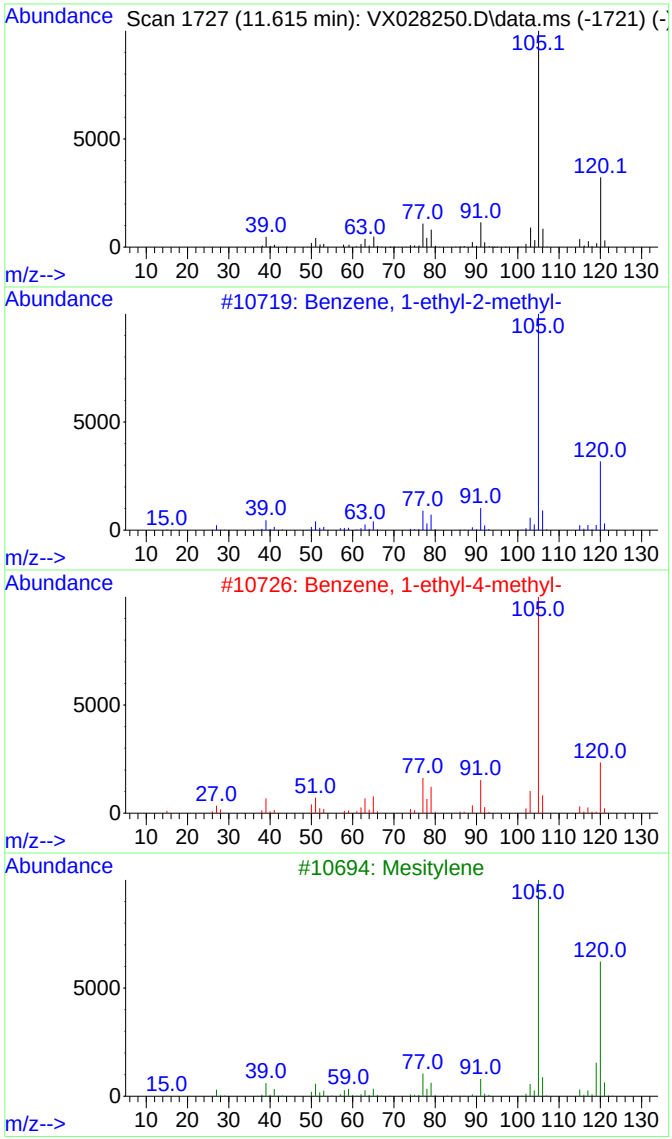
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

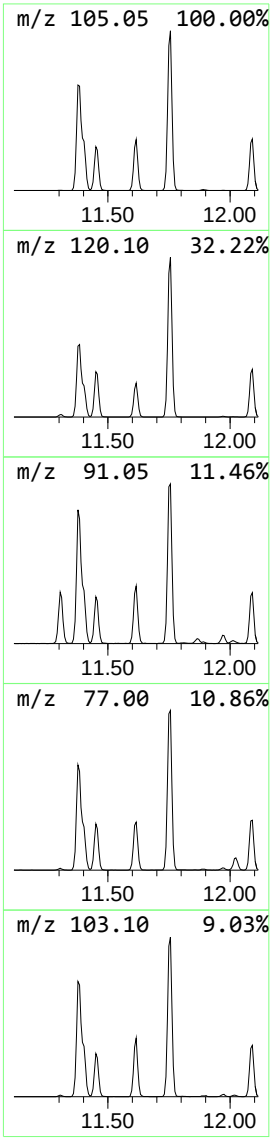
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.615	27.53 ug/l	1123450	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	93
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3	Mesitylene	120	C9H12	000108-67-8	90
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
Data File : VX028250.D
Acq On : 21 Apr 2022 18:42
Operator : JC/MD
Sample : N2459-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31579

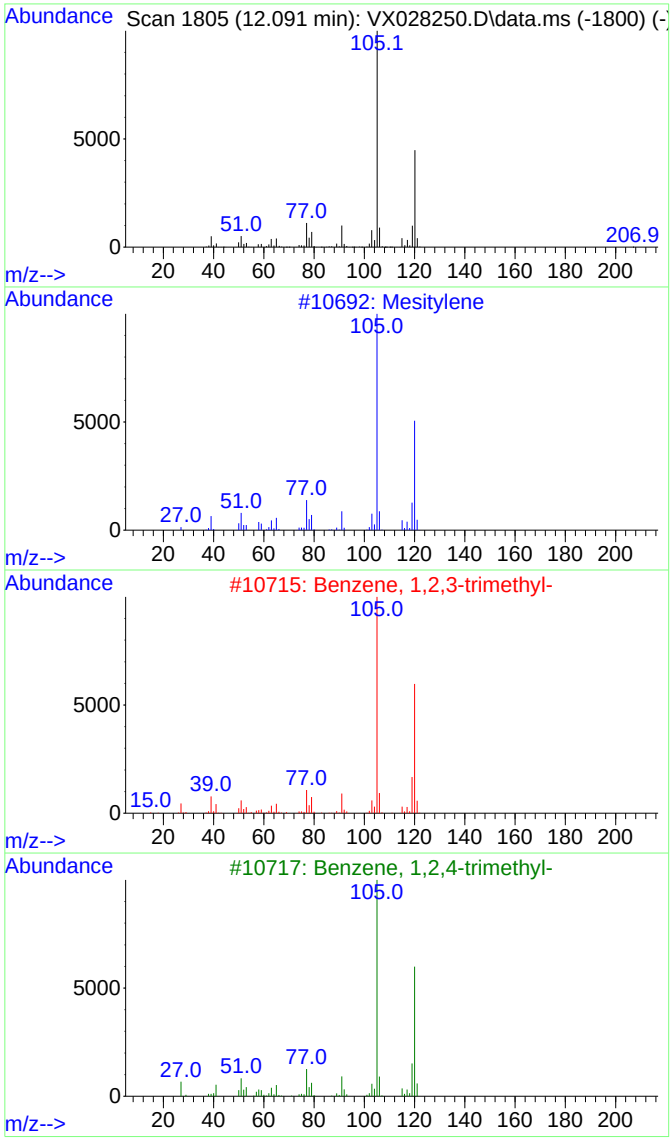
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

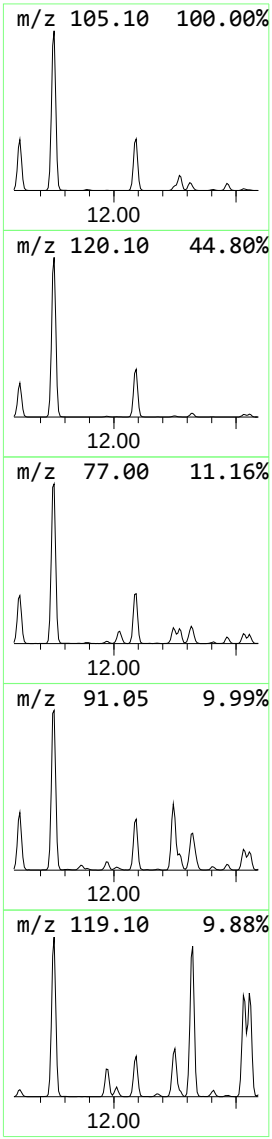
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	31.08 ug/l	1268230	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	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
Data File : VX028250.D
Acq On : 21 Apr 2022 18:42
Operator : JC/MD
Sample : N2459-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31579

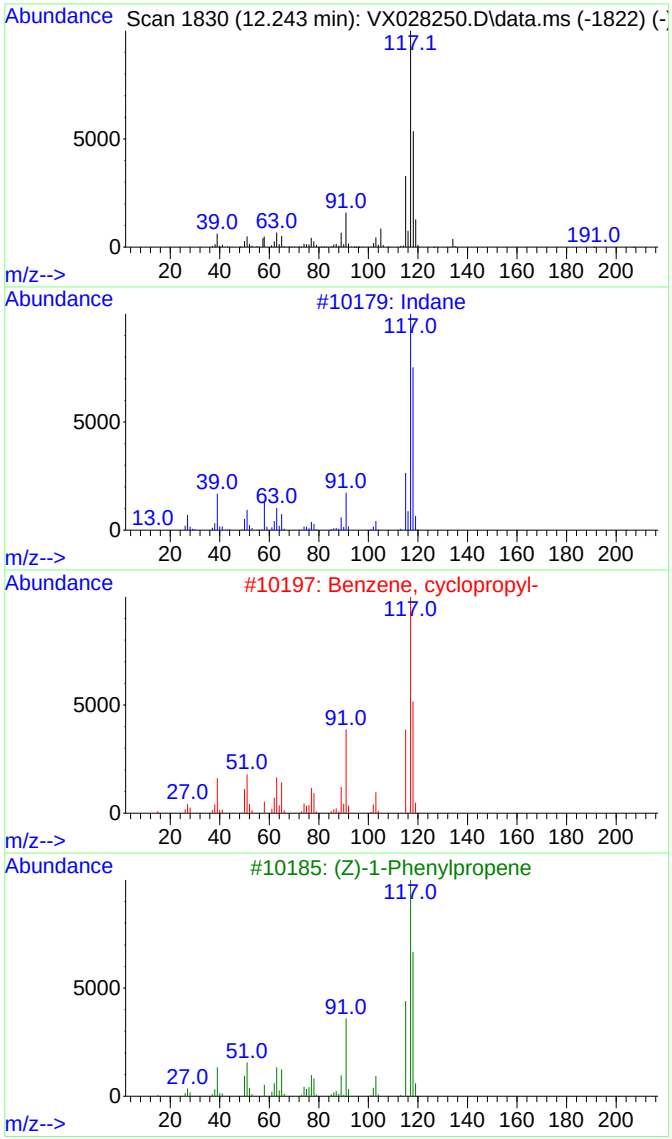
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

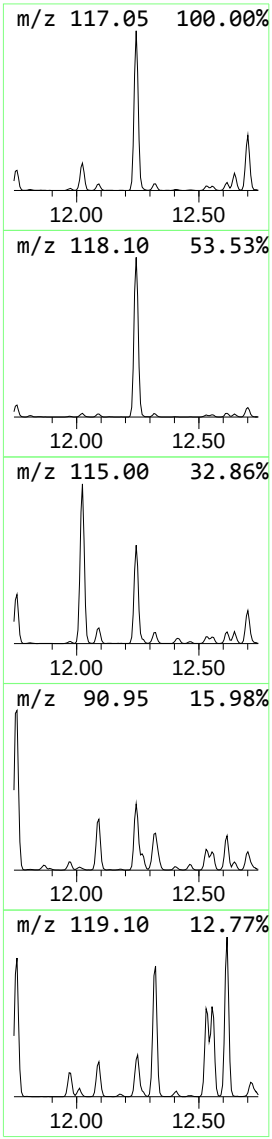
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Indane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	34.43 ug/l	1405300	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	81
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
3	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	81
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72
5	Benzene, 2-propenyl-	118	C9H10	000300-57-2	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
Data File : VX028250.D
Acq On : 21 Apr 2022 18:42
Operator : JC/MD
Sample : N2459-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31579

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.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
Isobutane	1.264	31.0	ug/l	768368	1	5.556	1237750	50.0
Butane	1.373	225.2	ug/l	5574870	1	5.556	1237750	50.0
Butane, 2-methyl-	1.751	85.8	ug/l	2125150	1	5.556	1237750	50.0
Pentane	1.959	56.4	ug/l	1396670	1	5.556	1237750	50.0
Cyclopropane, 1...	2.068	41.4	ug/l	1023980	1	5.556	1237750	50.0
2-Butene, 2-met...	2.215	45.9	ug/l	1136760	1	5.556	1237750	50.0
Benzene, 1-ethy...	11.378	83.9	ug/l	3425350	4	12.024	2040570	50.0
Benzene, 1-ethy...	11.615	27.5	ug/l	1123450	4	12.024	2040570	50.0
Benzene, 1,2,3-...	12.091	31.1	ug/l	1268230	4	12.024	2040570	50.0
Indane	12.243	34.4	ug/l	1405300	4	12.024	2040570	50.0