LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031418.D
Acq On : 16 Sep 2022 18:22
Operator : JC/MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF-0907

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\82X091422W.M
Title : SW846 8260

Signal : TIC: VX031418.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	28	rBV	17110	20262	2.78%	0.321%
2	1.368	43	46	52	rVB	14326	14702	2.02%	0.233%
3	1.605	72	85	86	rBV6	13032	34428	4.73%	0.545%
4	1.746	103	108	116	rVB	99936	129833	17.82%	2.057%
5	1.953	137	142	154	rVB2	41073	66732	9.16%	1.057%
6	2.069	157	161	166	rVB2	7360	11067	1.52%	0.175%
7	2.160	172	176	180	rBV4	5758	9524	1.31%	0.151%
8	2.215	180	185	193	rVB	27156	42395	5.82%	0.672%
9	2.782	266	278	281	rBV7	10383	31697	4.35%	0.502%
10	2.825	281	285	288	rVV	16386	31897	4.38%	0.505%
11	2.867	288	292	299	rVV2	19767	42720	5.86%	0.677%
12	2.947	299	305	315	rVB	11558	28058	3.85%	0.444%
13	3.099	319	330	344	rVB2	13054	31212	4.28%	0.494%
14	3.440	379	386	393	rBV4	4571	10428	1.43%	0.165%
15	3.733	425	434	441	rBV3	8291	19975	2.74%	0.316%
16	3.837	444	451	457	rBV4	4603	11189	1.54%	0.177%
17	3.898	457	461	472	rVB2	3280	7329	1.01%	0.116%
18	4.099	487	494	504	rVB3	5295	13704	1.88%	0.217%
19	4.306	519	528	542	rVB	30801	86132	11.82%	1.364%
20	5.196	663	674	684	rVB3	5895	18779	2.58%	0.297%
21	5.391	693	706	715	rBV	86556	253341	34.78%	4.013%
22	5.471	715	719	724	rVV4	10267	27686	3.80%	0.439%
23	5.556	724	733	754	rVB	86897	264498	36.31%	4.190%
24	5.830	768	778	788	rBV7	2693	8580	1.18%	0.136%
25	5.958	788	799	806	rVV	95224	254673	34.96%	4.034%
26	6.044	806	813	826	rVV	140982	368843	50.63%	5.842%
27	6.196	826	838	843	rVV	5796	22249	3.05%	0.352%
28	6.251	845	847	855	rVV7	4613	10015	1.37%	0.159%
29	6.355	857	864	874	rVB5	2984	8522	1.17%	0.135%
30	6.763	921	931	941	rBV	133580	322613	44.29%	5.110%
31	6.848	941	945	955	rVB4	4511	11303	1.55%	0.179%
32	7.373	1019	1031	1040	rBV6	9183	25954	3.56%	0.411%
33	8.507	1210	1217	1224	rBV3	7486	11874	1.63%	0.188%
34	8.653	1234	1241	1247	rBV	468092	728444	100.00%	11.539%
35	8.720	1247	1252	1259	rVB	60754	92941	12.76%	1.472%
36	10.055	1465	1471	1481	rVB	288842	379008	52.03%	6.003%

LSC Area Percent Report

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Data File : VX031418.D
Acq On : 16 Sep 2022 18:22
Operator : JC/MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF-0907

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\82X091422W.M
Title : SW846 8260

37	10.195	1489	1494	1501	rBV	179334	232792	31.96%	3.687%
38	10.305	1506	1512	1521	rVB	423396	582136	79.91%	9.221%
39	10.640	1562	1567	1576	rBV	22415	31719	4.35%	0.502%
40	10.963	1615	1620	1625	rBV	27665	34483	4.73%	0.546%
41	11.079	1634	1639	1653	rVB	399427	507034	69.61%	8.031%
42	11.305	1671	1676	1682	rVB	54453	65362	8.97%	1.035%
43	11.402	1682	1692	1696	rBV	53516	94350	12.95%	1.495%
44	11.451	1696	1700	1707	rVB	52532	64729	8.89%	1.025%
45	11.616	1721	1727	1734	rVB	48429	61481	8.44%	0.974%
46	11.756	1744	1750	1756	rVB	193033	242226	33.25%	3.837%
47	12.024	1789	1794	1800	rBV	296320	359423	49.34%	5.693%
48	12.091	1800	1805	1810	rVB	103310	128360	17.62%	2.033%
49	12.244	1825	1830	1837	rBV	137576	168293	23.10%	2.666%
50	12.317	1837	1842	1850	rVB3	13051	20532	2.82%	0.325%
51	12.463	1862	1866	1872	rVB	7513	8689	1.19%	0.138%
52	12.530	1872	1877	1880	rBV	9369	12956	1.78%	0.205%
53	12.616	1886	1891	1894	rBV	22888	29579	4.06%	0.469%
54	12.701	1900	1905	1911	rBV2	25024	33225	4.56%	0.526%
55	12.920	1936	1941	1945	rBV	16266	19485	2.67%	0.309%
56	12.963	1945	1948	1953	rVB	13663	16324	2.24%	0.259%
57	13.170	1978	1982	1986	rVB	18484	22238	3.05%	0.352%
58	13.292	1997	2002	2007	rVB2	37036	48743	6.69%	0.772%
59	13.774	2077	2081	2087	rBV	52672	69055	9.48%	1.094%
60	14.640	2219	2223	2230	rVB	6060	7315	1.00%	0.116%

Sum of corrected areas: 6313136

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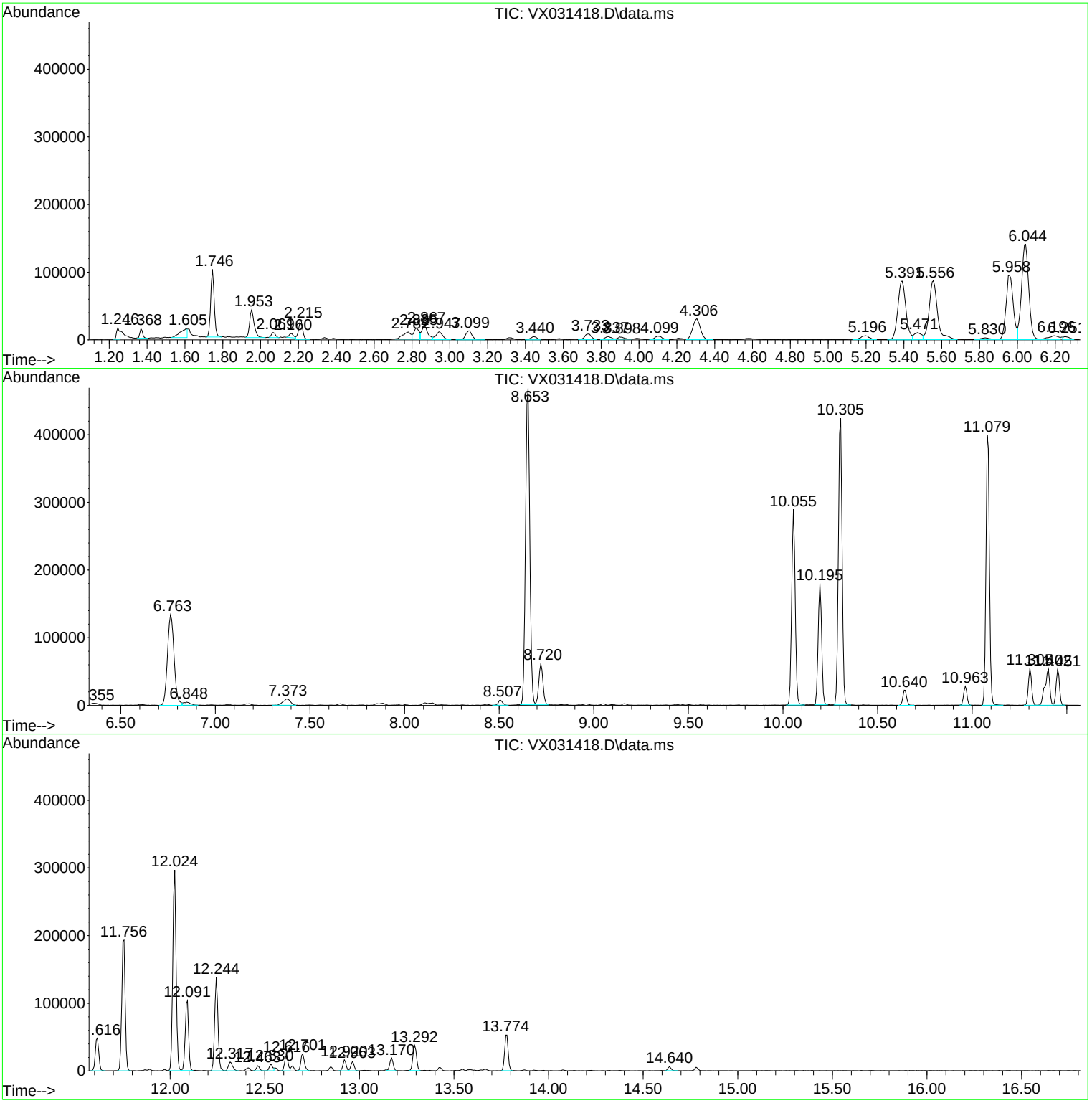
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF-0907

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031418.D
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Operator : JC/MD
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Instrument :
MSVOA_X
ClientSampleId :
INF-0907

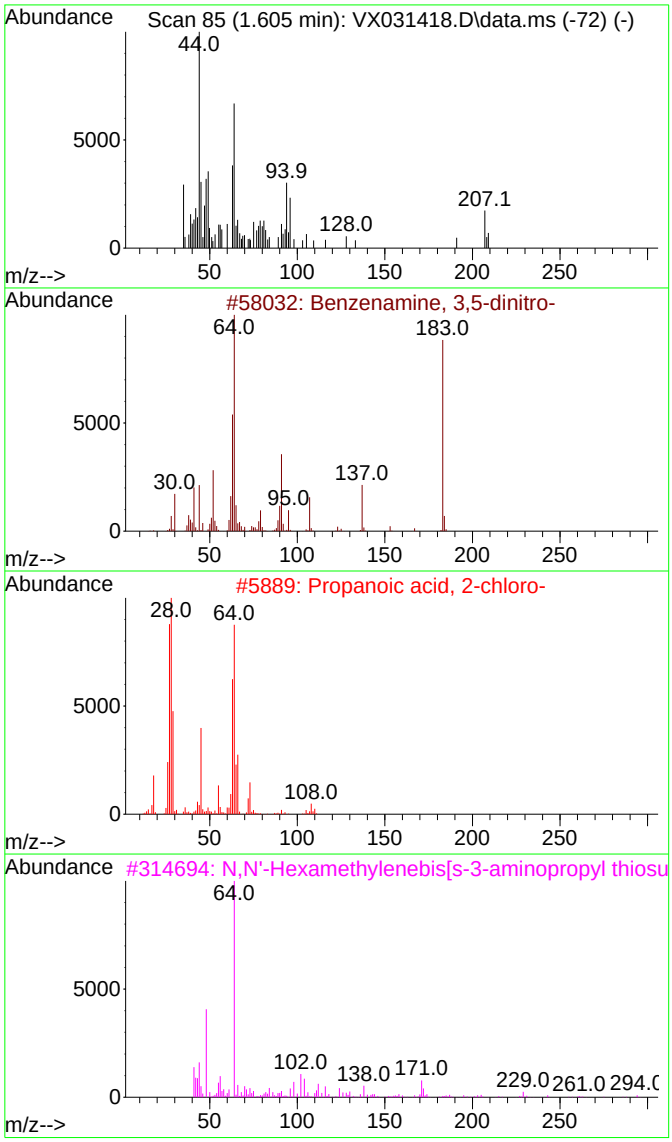
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

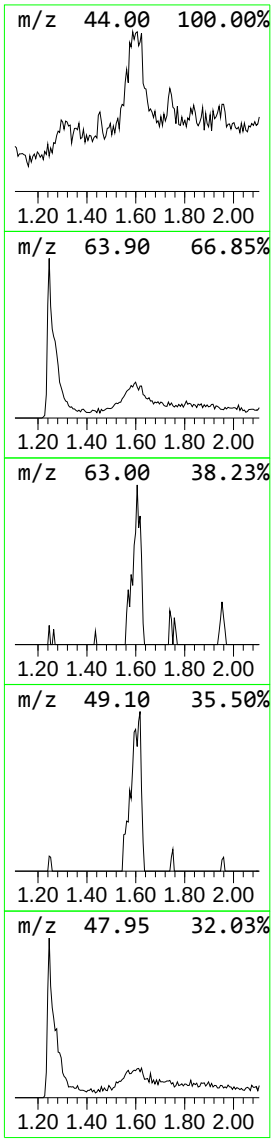
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown1.605 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.605	6.51 ug/l	34428	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 3,5-dinitro-	183	C6H5N3O4	000618-87-1	32
2	Propanoic acid, 2-chloro-	108	C3H5ClO2	000598-78-7	23
3	N,N'-Hexamethylenebis[s-3-aminop...	424	C12H28N2O6S4	035871-55-7	22
4	1-Selenopropanesulfonic acid, 3-...	205	C2H7NO3SSe	1010400-46-3	12
5	S-2-[2-Succinimidoethylamino]eth...	282	C8H14N2O5S2	031701-74-3	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031418.D
Acq On : 16 Sep 2022 18:22
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF-0907

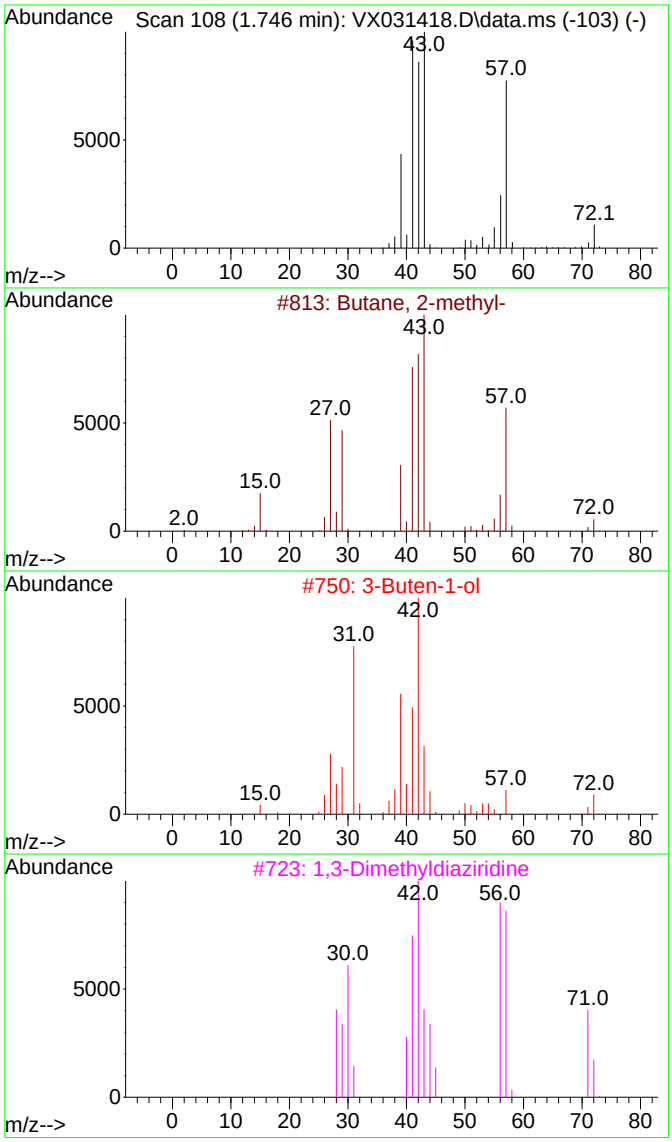
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

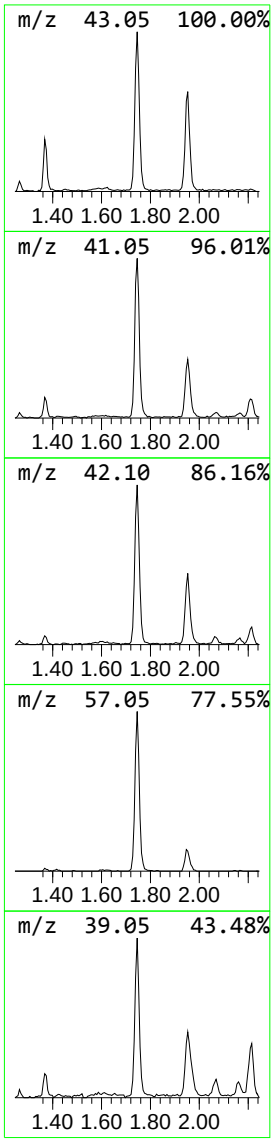
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	24.54 ug/l	129833	Pentafluorobenzene	5.556

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	33
3	1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	25
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	22
5	Pentane	72	C5H12	000109-66-0	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031418.D
Acq On : 16 Sep 2022 18:22
Operator : JC/MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF-0907

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

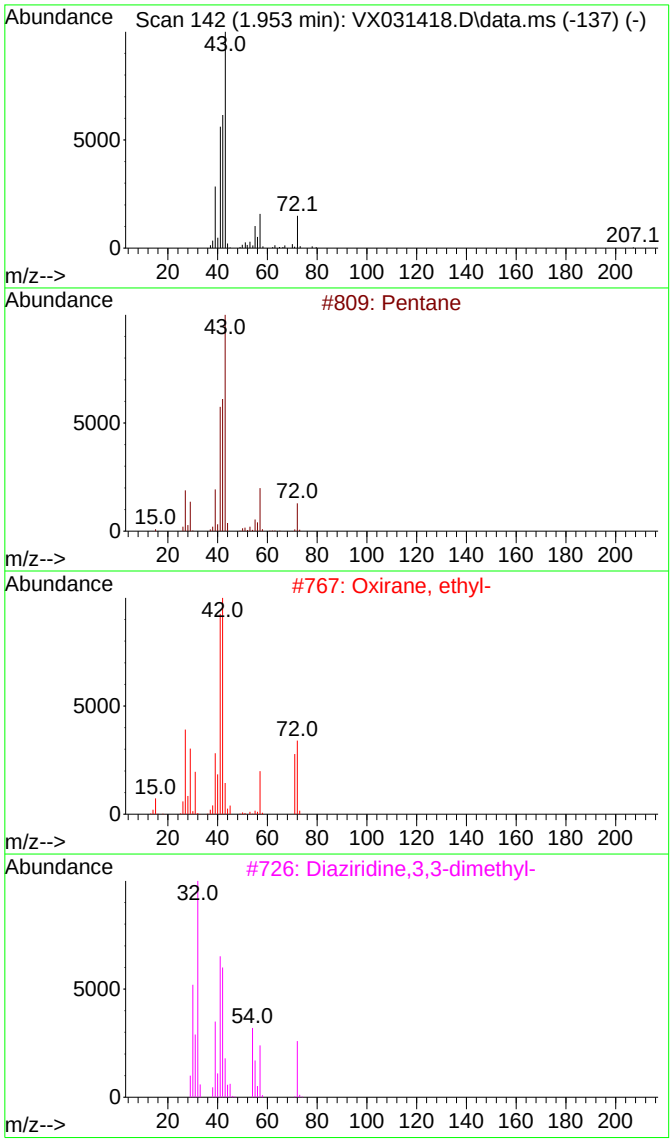
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

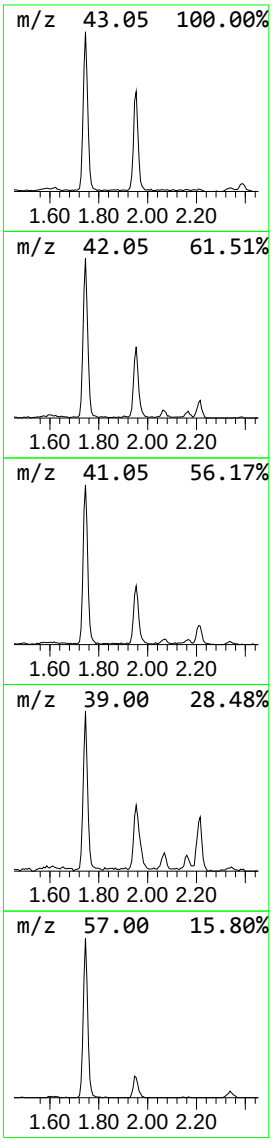
****

Peak Number 3 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	12.61 ug/l	66732	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	80
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	53
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	43
4	Tetrahydrofuran	72	C4H8O	000109-99-9	37
5	Propanal, 2-methyl-	72	C4H8O	000078-84-2	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031418.D
Acq On : 16 Sep 2022 18:22
Operator : JC/MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF-0907

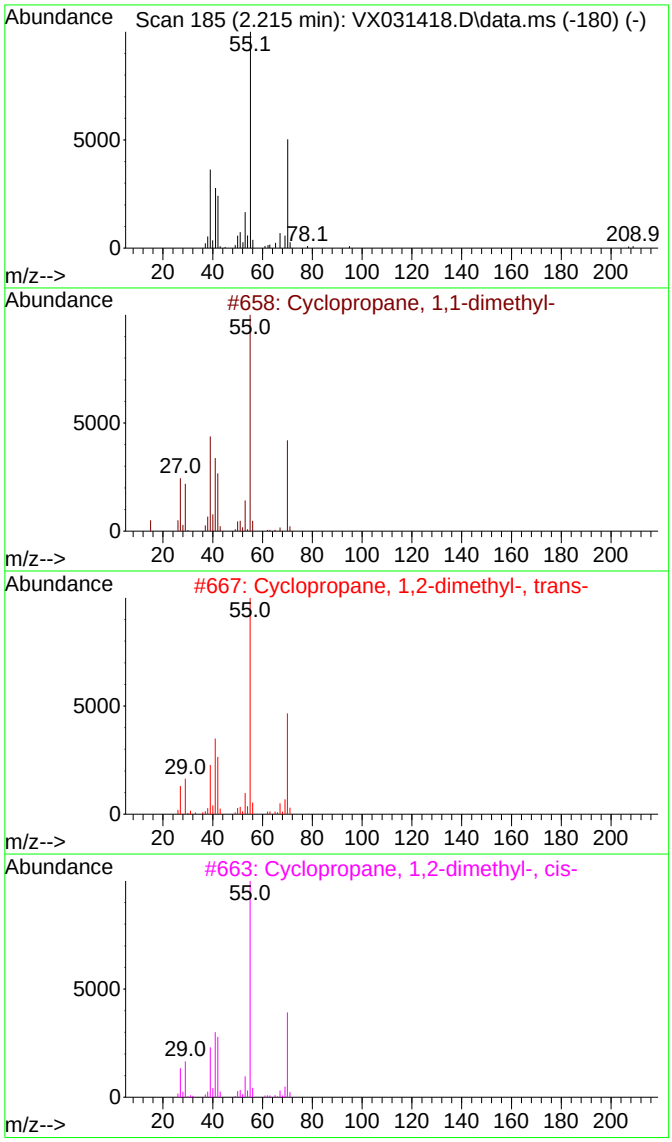
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

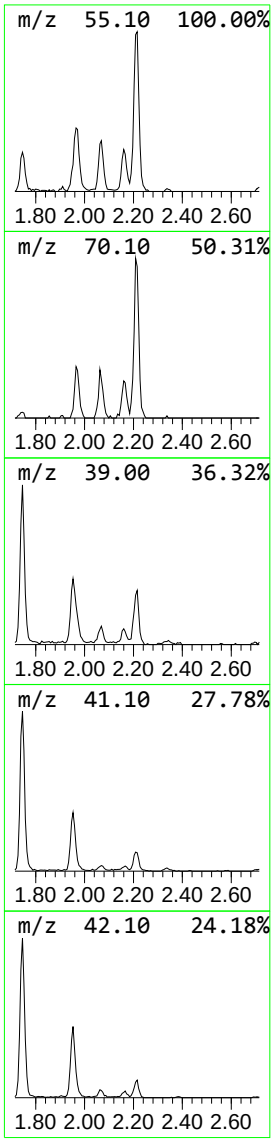
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopropane, 1,1-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	8.01 ug/l	42395	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	87
2	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	86
3	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	86
4	2-Pentene	70	C5H10	000109-68-2	80
5	2-Butene, 2-methyl-	70	C5H10	000513-35-9	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031418.D
Acq On : 16 Sep 2022 18:22
Operator : JC/MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF-0907

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

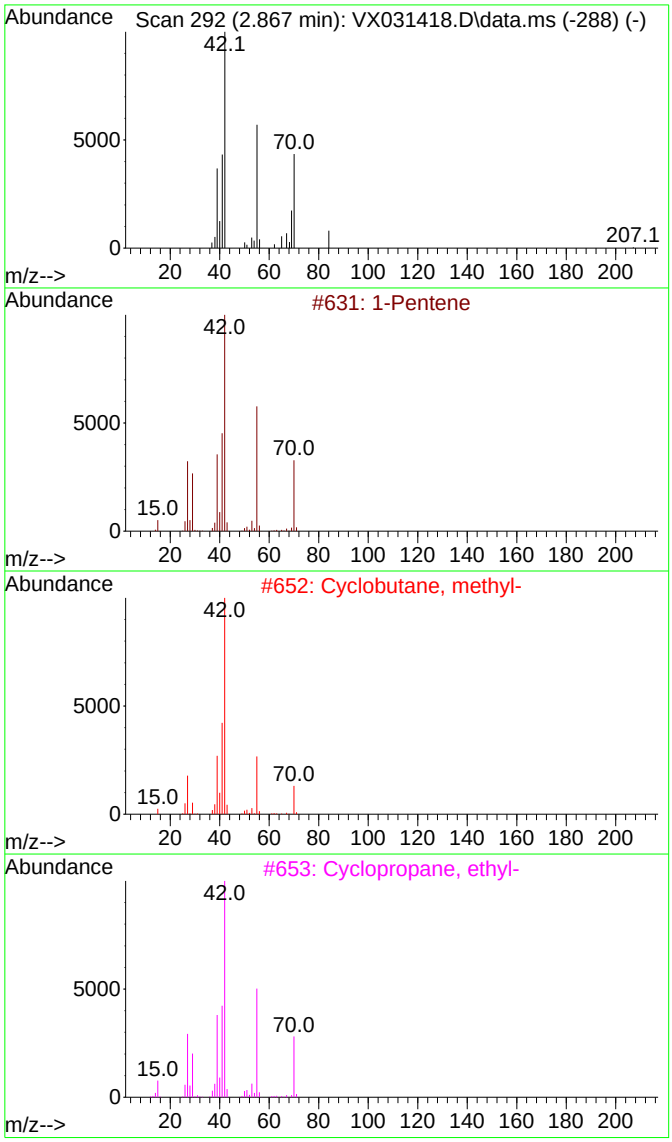
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

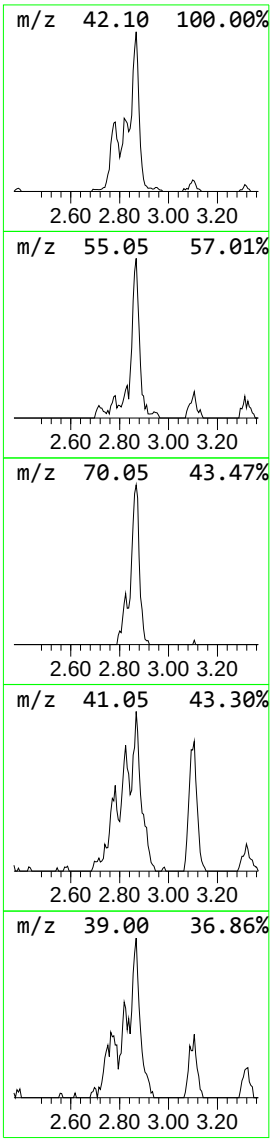
****

Peak Number 5 1-Pentene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	8.08 ug/l	42720	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	80
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	59
4	Carbonochloridic acid, pentyl ester	150	C6H11ClO2	000638-41-5	40
5	Formic acid, pentyl ester	116	C6H12O2	000638-49-3	39





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

Instrument :
MSVOA_X
ClientSampleId :
INF-0907

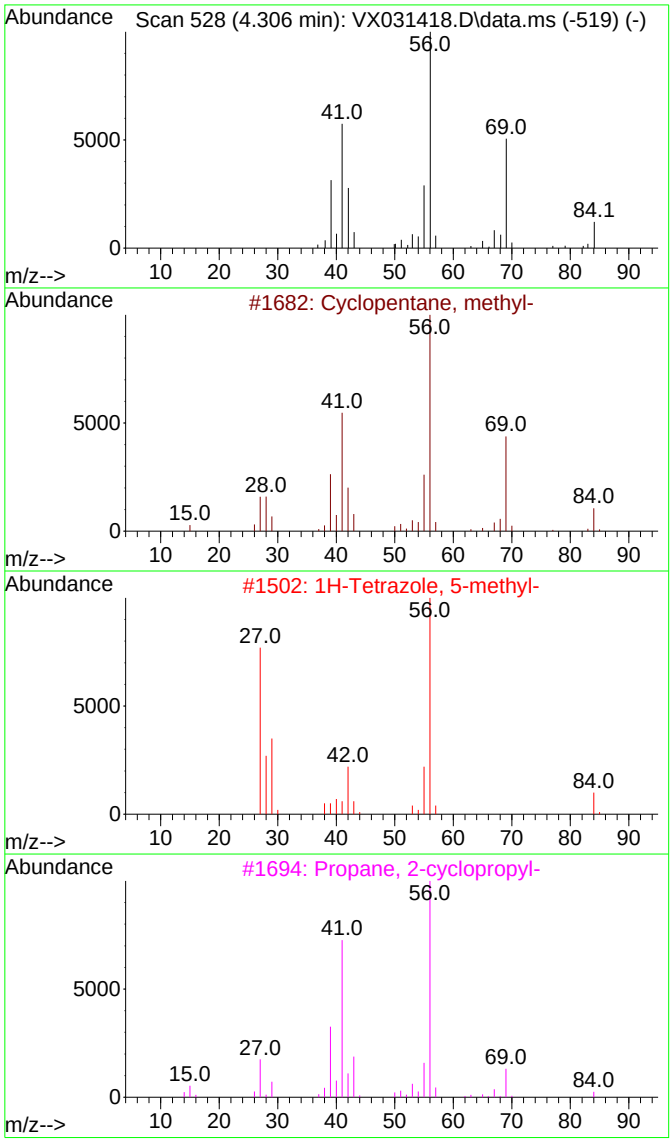
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

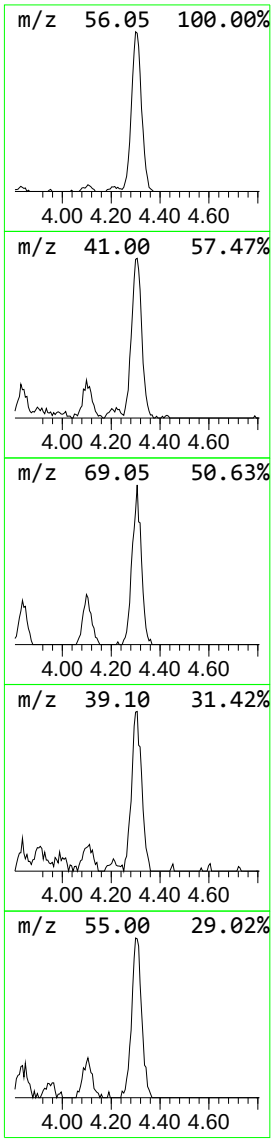
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	16.28 ug/l	86132	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	80
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	72
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF-0907

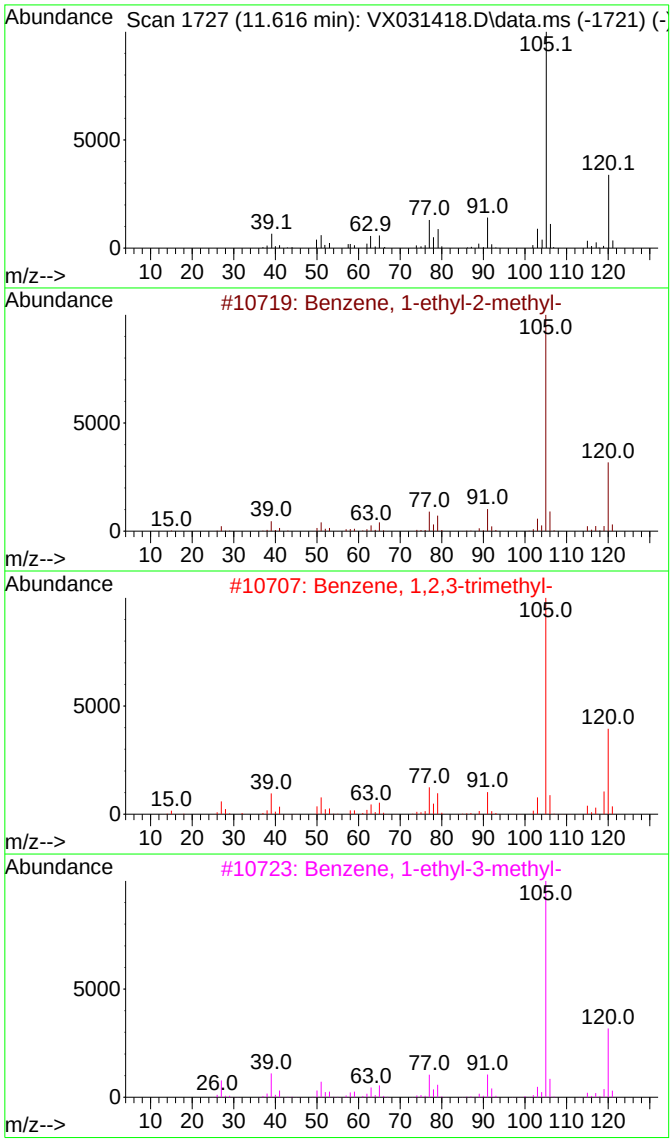
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

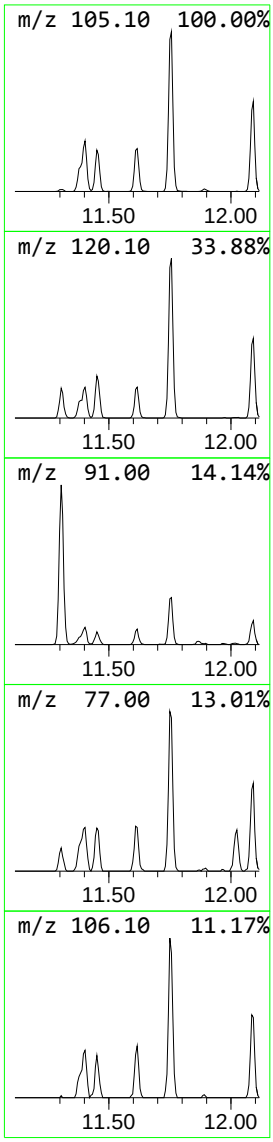
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	8.55 ug/l	61481	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, 1,2,3-trimethyl-	120	C9H12	000526-73-8	93
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031418.D
Acq On : 16 Sep 2022 18:22
Operator : JC/MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF-0907

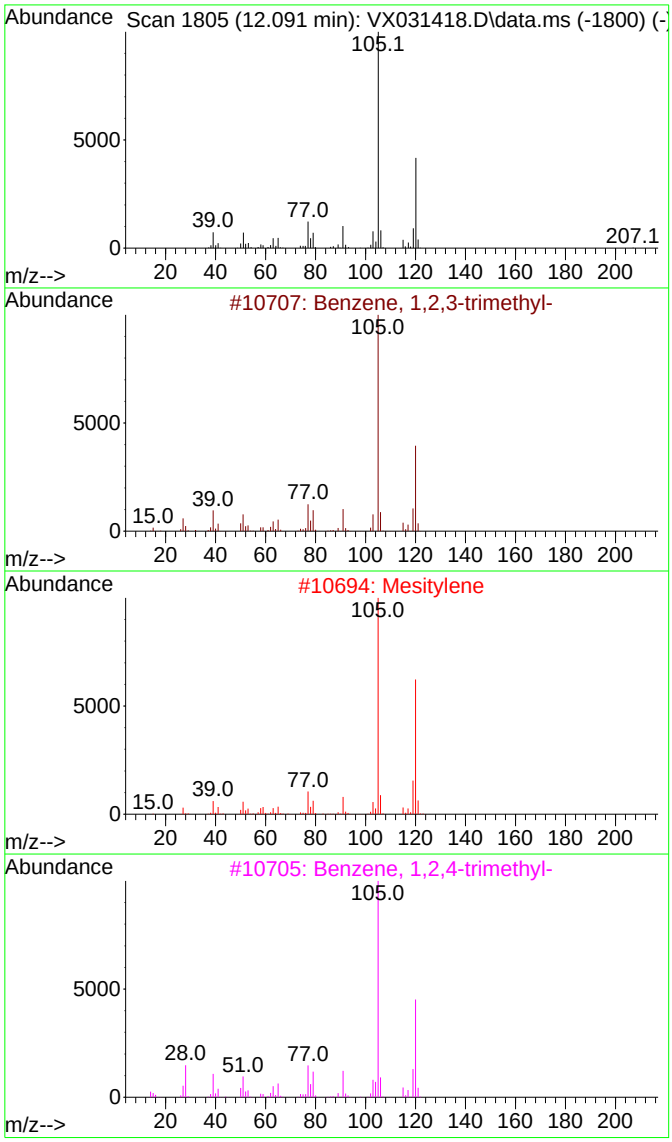
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

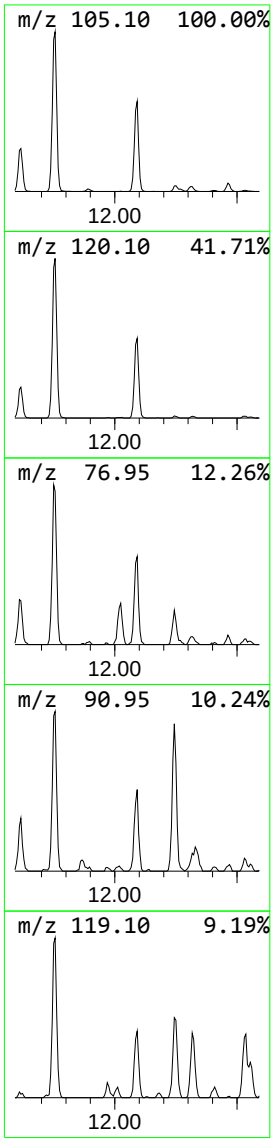
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	17.86 ug/l	128360	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2	Mesitylene	120	C9H12	000108-67-8	94
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





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Data File : VX031418.D
Acq On : 16 Sep 2022 18:22
Operator : JC/MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF-0907

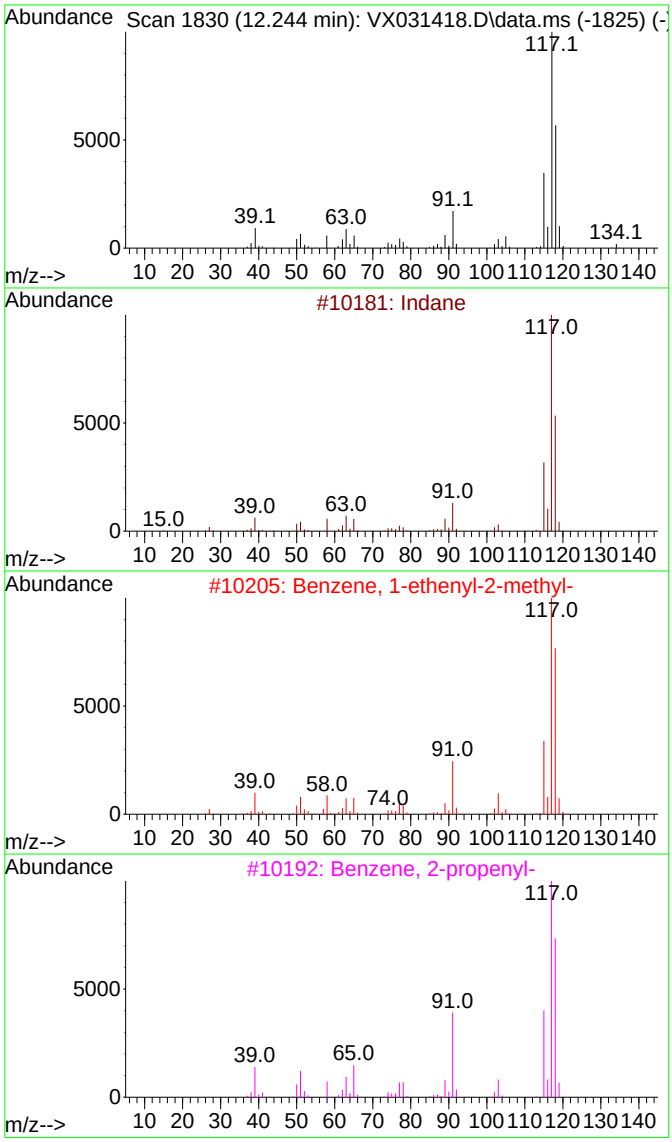
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

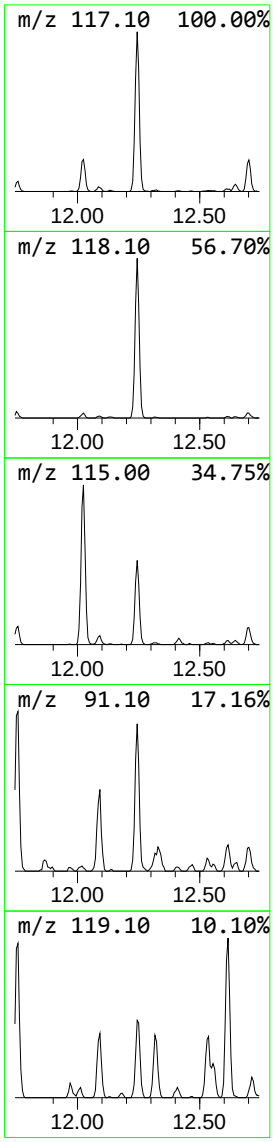
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	23.41 ug/l	168293	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	90
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	87
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	72
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031418.D
Acq On : 16 Sep 2022 18:22
Operator : JC/MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF-0907

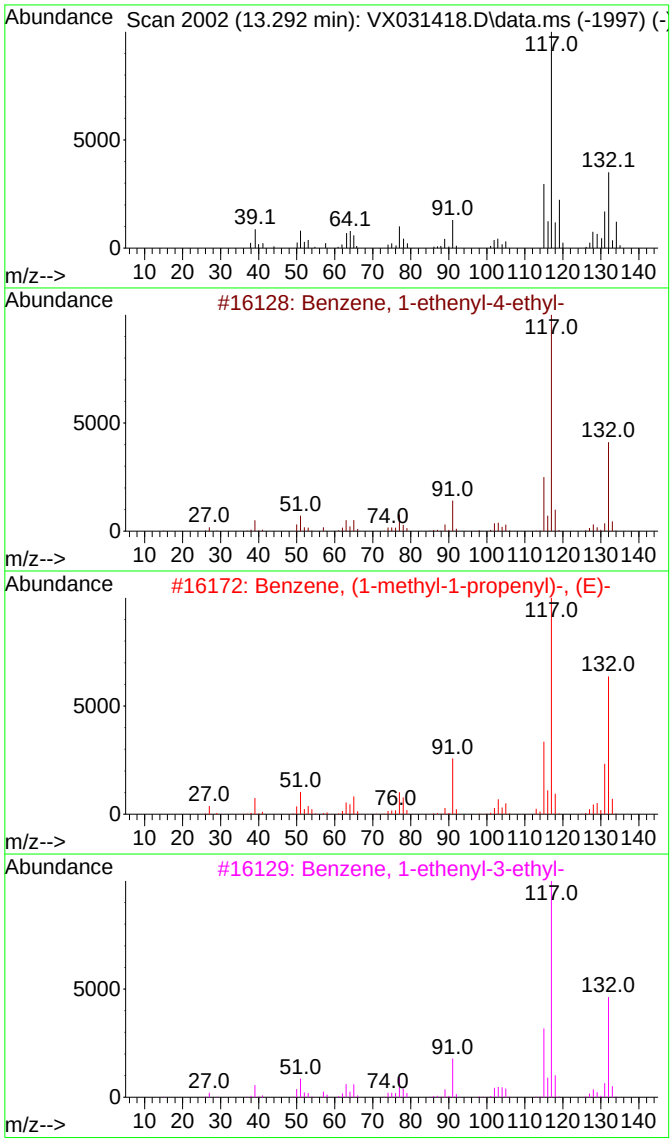
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

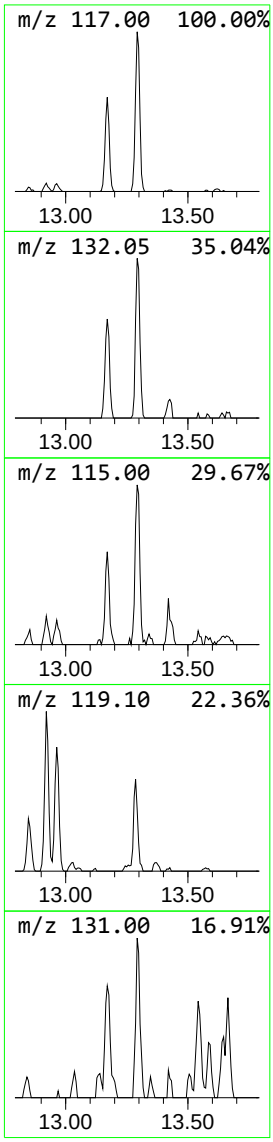
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	6.78 ug/l	48743	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90
3	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	89
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	81
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031418.D
Acq On : 16 Sep 2022 18:22
Operator : JC/MD
Sample : N4526-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
INF-0907

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.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
unknown1.605	1.605	6.5	ug/l	34428	1	5.556	264498	50.0
Butane, 2-methyl-	1.746	24.5	ug/l	129833	1	5.556	264498	50.0
Pentane	1.953	12.6	ug/l	66732	1	5.556	264498	50.0
Cyclopropane, 1...	2.215	8.0	ug/l	42395	1	5.556	264498	50.0
1-Pentene	2.867	8.1	ug/l	42720	1	5.556	264498	50.0
Cyclopentane, m...	4.306	16.3	ug/l	86132	1	5.556	264498	50.0
Benzene, 1-ethy...	11.616	8.6	ug/l	61481	4	12.024	359423	50.0
Benzene, 1,2,3-...	12.091	17.9	ug/l	128360	4	12.024	359423	50.0
Indane	12.244	23.4	ug/l	168293	4	12.024	359423	50.0
Benzene, 1-ethe...	13.292	6.8	ug/l	48743	4	12.024	359423	50.0