LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033042.D
Acq On : 24 Nov 2022 06:27
Operator : JC/MD
Sample : N5741-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

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: VX033042.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	42	rBV	209471	325563	20.09%	4.425%
2	1.374	43	47	52	rVB	19212	22275	1.37%	0.303%
3	1.752	104	109	118	rVB	46051	63010	3.89%	0.856%
4	2.215	180	185	196	rVB	20687	32672	2.02%	0.444%
5	2.752	266	273	276	rBV2	8050	16408	1.01%	0.223%
6	2.867	282	292	302	rVB	26696	57738	3.56%	0.785%
7	2.989	302	312	325	rVV	36793	152118	9.39%	2.067%
8	3.111	325	332	345	rVB	82106	196337	12.11%	2.668%
9	3.764	426	439	446	rBV3	16720	49678	3.07%	0.675%
10	4.312	518	529	540	rVB3	29823	86250	5.32%	1.172%
11	5.385	694	705	714	rBV	66472	193863	11.96%	2.635%
12	5.471	714	719	724	rVV2	15794	44487	2.74%	0.605%
13	5.550	724	732	758	rVB	140194	410976	25.36%	5.585%
14	5.958	788	799	804	rBV	73251	187079	11.54%	2.543%
15	6.038	804	812	829	rVB	612560	1620784	100.00%	22.028%
16	6.208	829	840	843	rBV5	8743	25496	1.57%	0.347%
17	6.763	922	931	942	rBV	213425	507303	31.30%	6.895%
18	7.373	1023	1031	1040	rVB4	6812	19822	1.22%	0.269%
19	8.507	1210	1217	1224	rVB4	10053	19260	1.19%	0.262%
20	8.647	1234	1240	1248	rBV	345877	531035	32.76%	7.217%
21	8.958	1281	1291	1298	rBV	23460	39561	2.44%	0.538%
22	9.049	1300	1306	1311	rBV	24394	37796	2.33%	0.514%
23	9.458	1365	1373	1387	rVB	32124	55520	3.43%	0.755%
24	10.055	1465	1471	1485	rVV	442553	600135	37.03%	8.156%
25	10.195	1489	1494	1500	rVB	81987	104733	6.46%	1.423%
26	10.305	1505	1512	1518	rVB	12372	19145	1.18%	0.260%
27	10.963	1614	1620	1625	rBV	35782	44462	2.74%	0.604%
28	11.079	1634	1639	1649	rBV	294032	374572	23.11%	5.091%
29	11.305	1671	1676	1685	rVB	28171	36118	2.23%	0.491%
30	11.616	1722	1727	1734	rVB	21744	28021	1.73%	0.381%
31	11.750	1746	1749	1754	rVB	23336	29038	1.79%	0.395%
32	12.024	1788	1794	1801	rBV	448652	573101	35.36%	7.789%
33	12.244	1824	1830	1838	rBV2	172631	222563	13.73%	3.025%
34	12.311	1838	1841	1848	rVB3	12389	19002	1.17%	0.258%
35	12.463	1862	1866	1872	rVB	21816	25609	1.58%	0.348%
36	12.616	1886	1891	1893	rBV	18732	22661	1.40%	0.308%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033042.D
Acq On : 24 Nov 2022 06:27
Operator : JC/MD
Sample : N5741-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

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	12.646	1893	1896	1900	rVV	21299	25175	1.55%	0.342%
38	12.701	1900	1905	1913	rVV2	76685	104200	6.43%	1.416%
39	12.847	1924	1929	1934	rVB2	16103	23528	1.45%	0.320%
40	12.920	1934	1941	1945	rBV	31917	43121	2.66%	0.586%
41	12.963	1945	1948	1953	rVV	45457	51450	3.17%	0.699%
42	13.292	1997	2002	2007	rVB2	70456	89982	5.55%	1.223%
43	13.426	2019	2024	2029	rVB	21430	29590	1.83%	0.402%
44	13.542	2039	2043	2046	rVV2	12700	17508	1.08%	0.238%
45	13.585	2046	2050	2054	rVV3	13922	26181	1.62%	0.356%
46	13.640	2056	2059	2061	rVV2	13870	20043	1.24%	0.272%
47	13.664	2061	2063	2070	rVB2	19199	24100	1.49%	0.328%
48	13.774	2074	2081	2090	rVB	25824	38500	2.38%	0.523%
49	13.926	2100	2106	2110	rBV3	14182	18496	1.14%	0.251%
50	14.213	2149	2153	2159	rBV3	11571	19459	1.20%	0.264%
51	14.780	2241	2246	2250	rBV	24283	32409	2.00%	0.440%

Sum of corrected areas: 7357933

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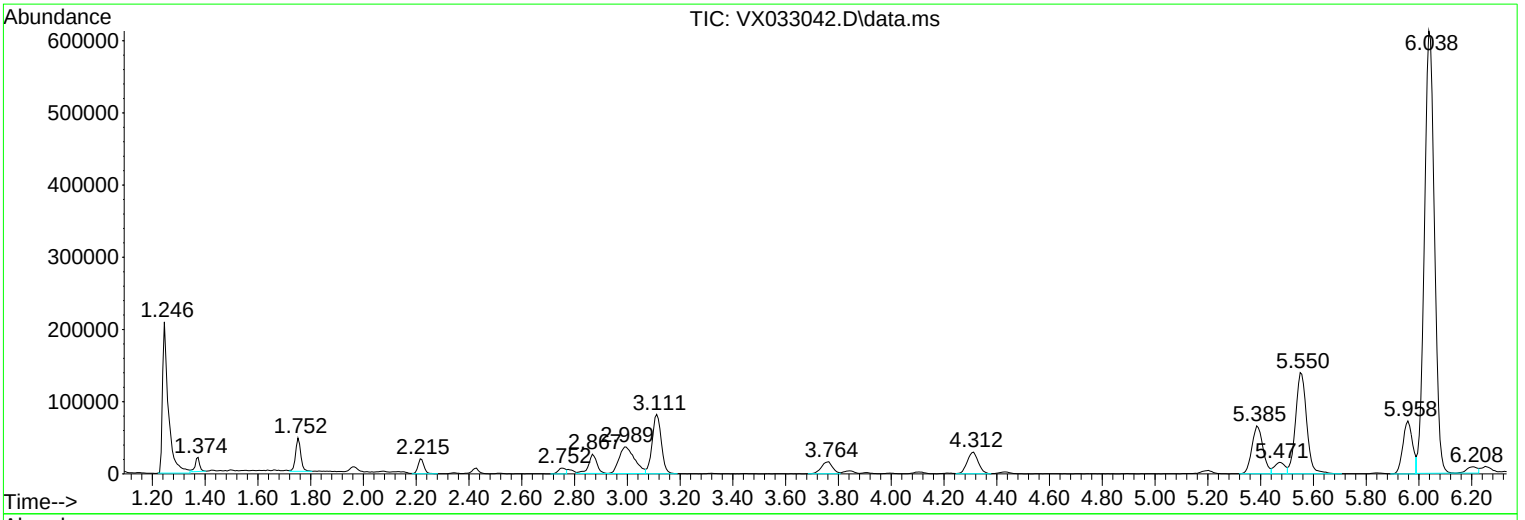
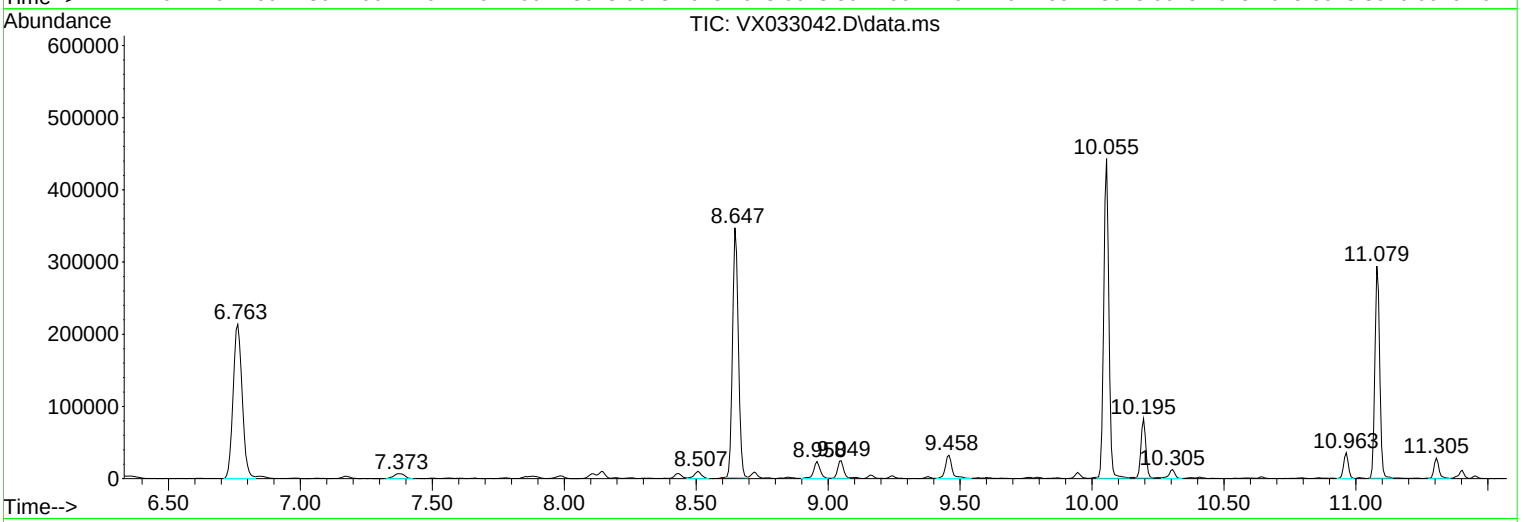
ALS Vial : 37 Sample Multiplier: 1

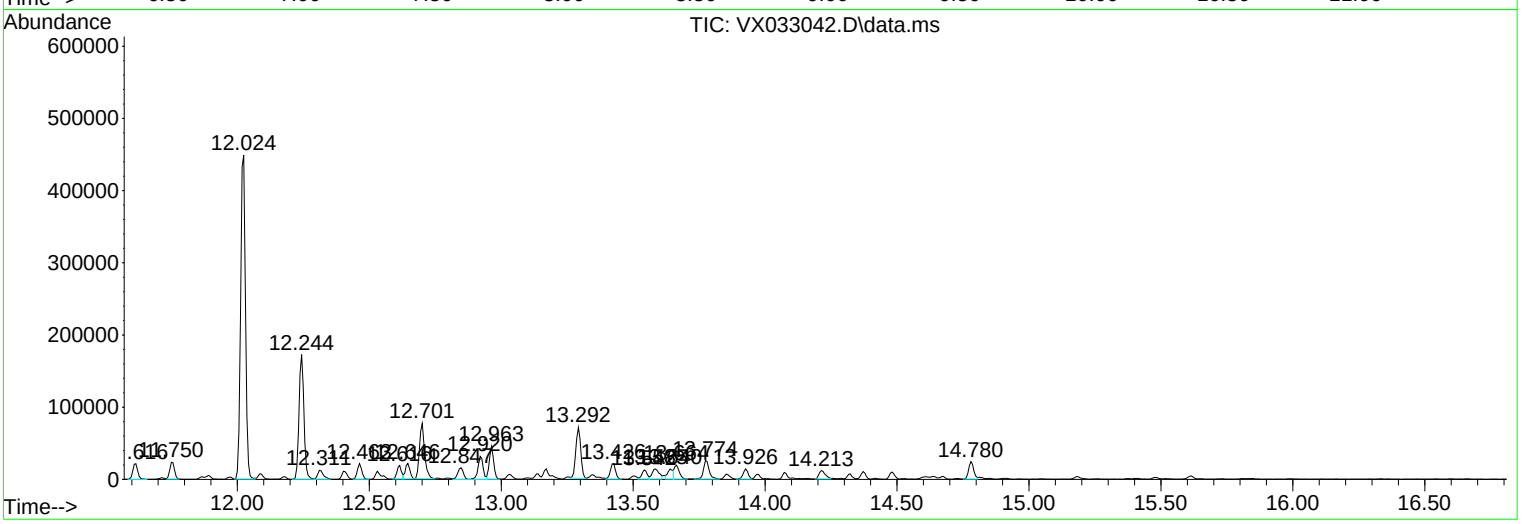
Instrument :
MSVOA_X
ClientSampleId :
MW-34

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\VX112322\
Data File : VX033042.D
Acq On : 24 Nov 2022 06:27
Operator : JC/MD
Sample : N5741-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

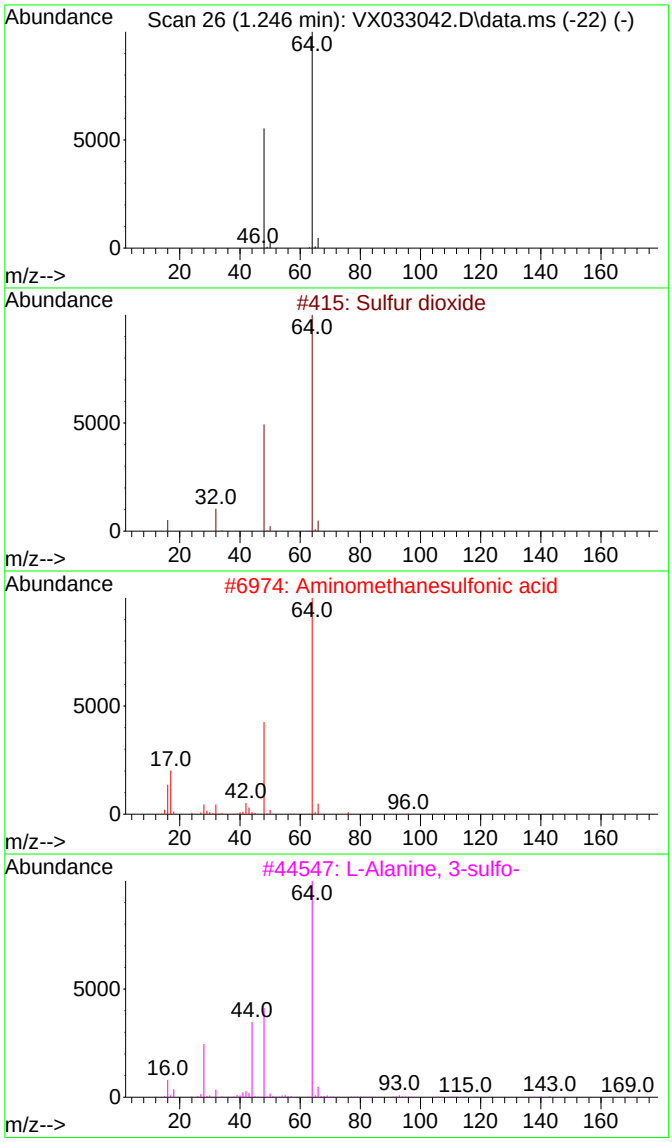
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

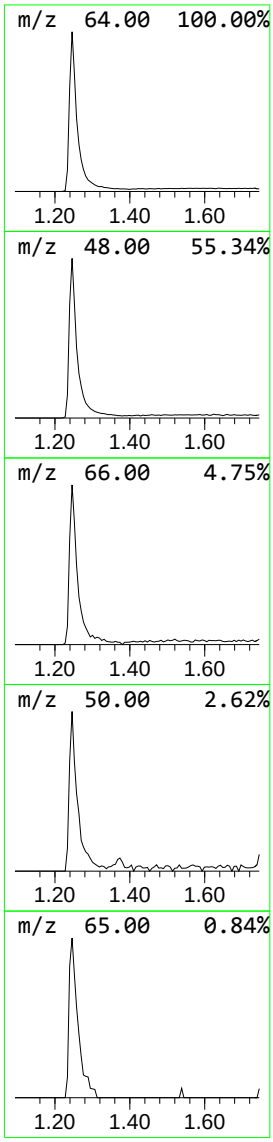
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	39.61 ug/l	325563	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033042.D
Acq On : 24 Nov 2022 06:27
Operator : JC/MD
Sample : N5741-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

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

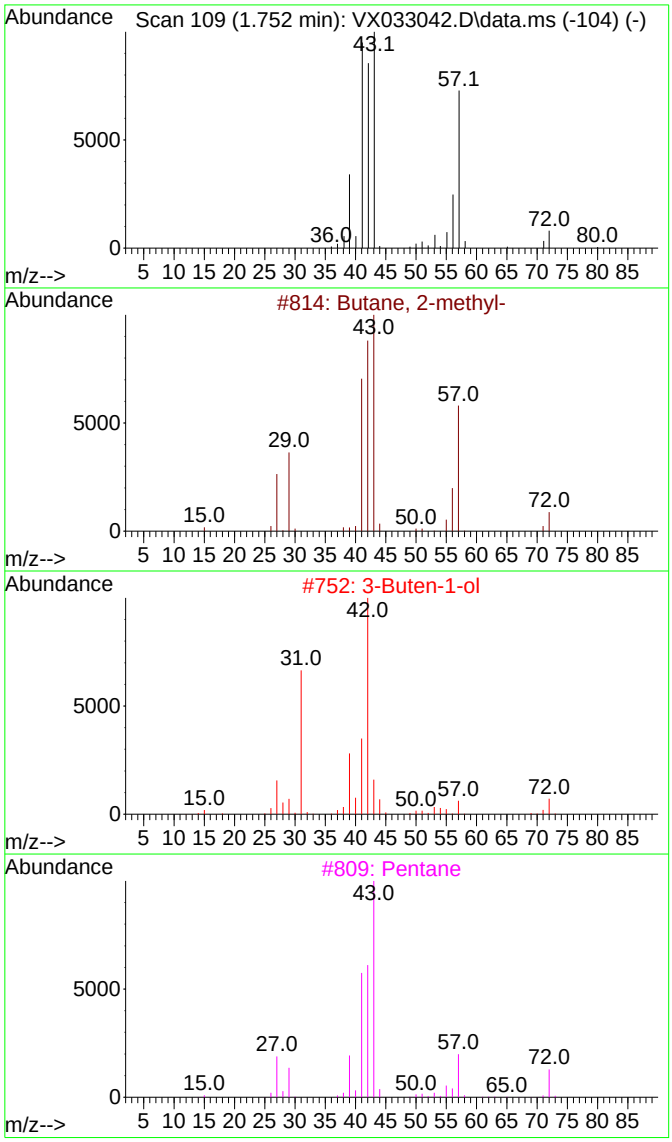
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

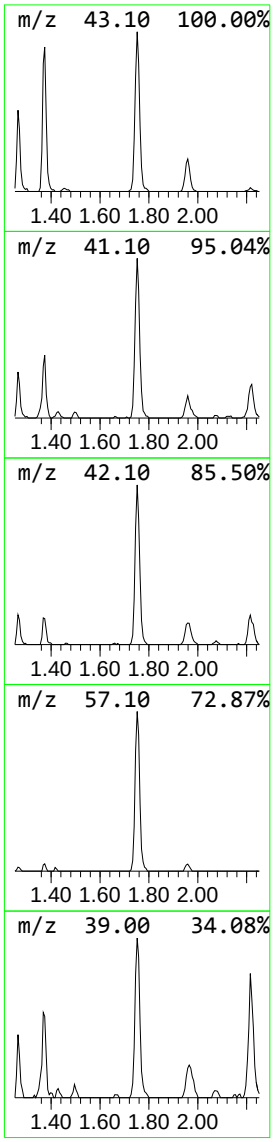
****

Peak Number 2 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	7.67 ug/l	63010	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	36
4	Oxirane, trimethyl-	86	C5H10O	005076-19-7	36
5	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	33





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033042.D
Acq On : 24 Nov 2022 06:27
Operator : JC/MD
Sample : N5741-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

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

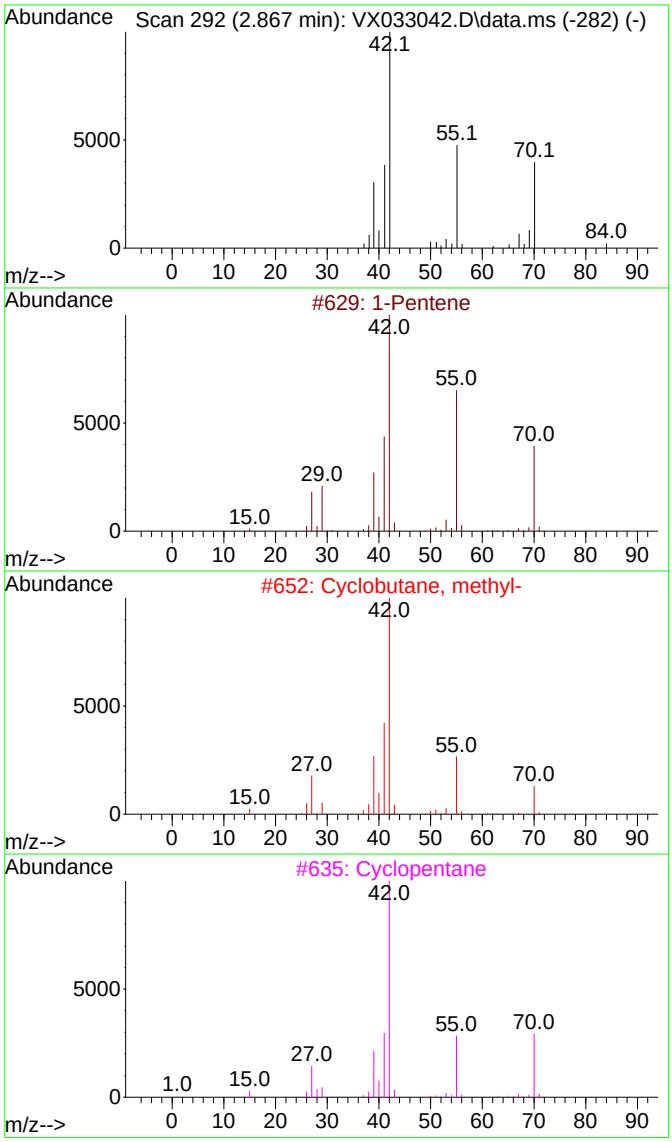
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

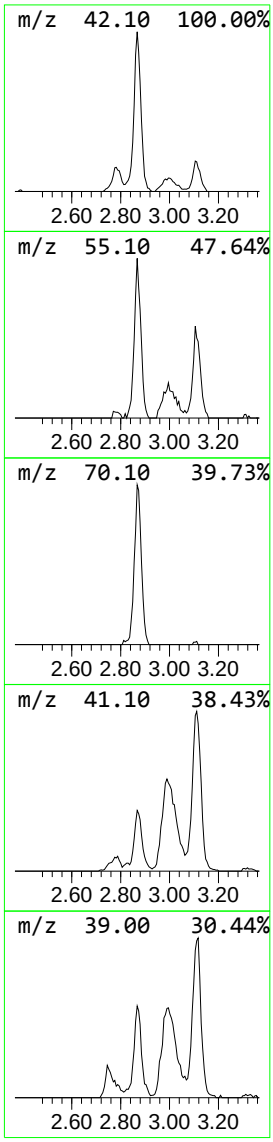
****

Peak Number 3 1-Pentene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	7.02 ug/l	57738	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	78
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	78
3	Cyclopentane	70	C5H10	000287-92-3	78
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	59
5	1-Pentanol	88	C5H12O	000071-41-0	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033042.D
Acq On : 24 Nov 2022 06:27
Operator : JC/MD
Sample : N5741-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

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

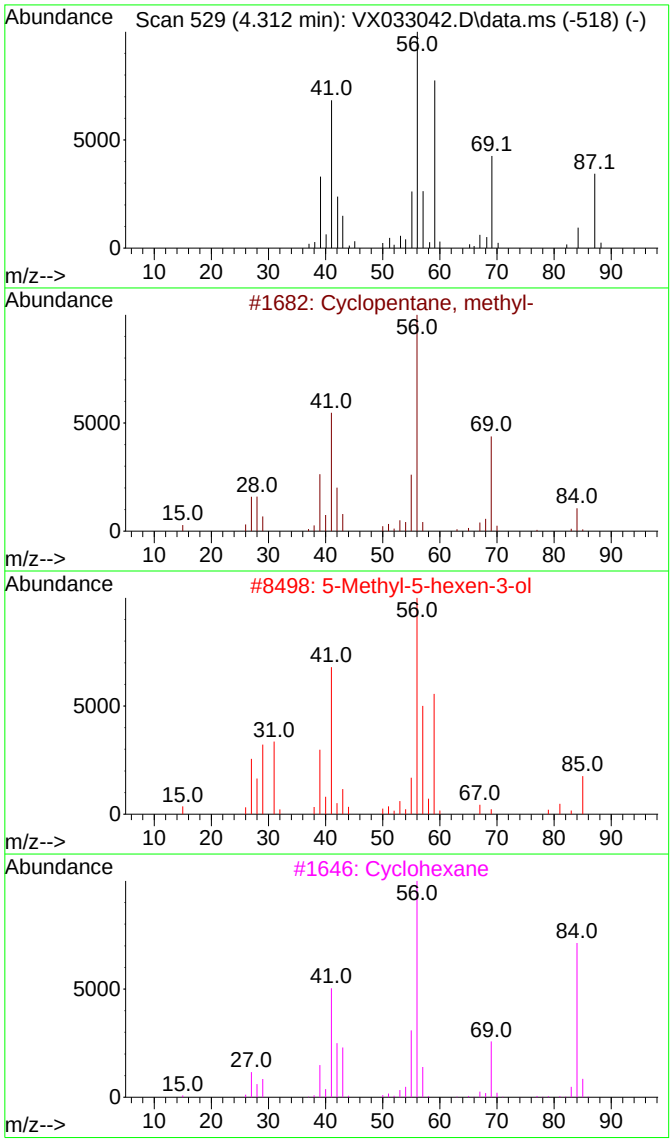
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

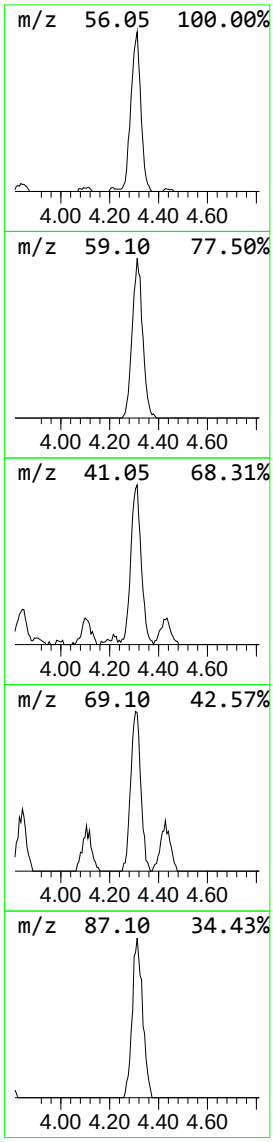
****

Peak Number 4 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	10.49 ug/l	86250	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	55
2	5-Methyl-5-hexen-3-ol	114	C7H14O	067760-89-8	42
3	Cyclohexane	84	C6H12	000110-82-7	38
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	35
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033042.D
Acq On : 24 Nov 2022 06:27
Operator : JC/MD
Sample : N5741-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

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

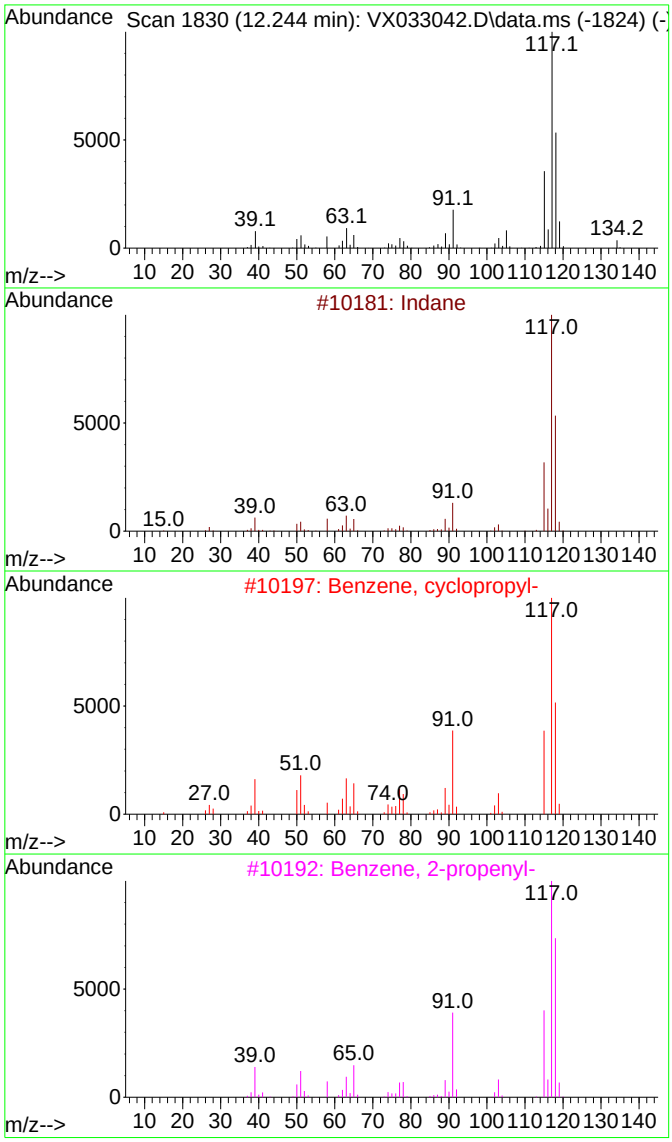
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

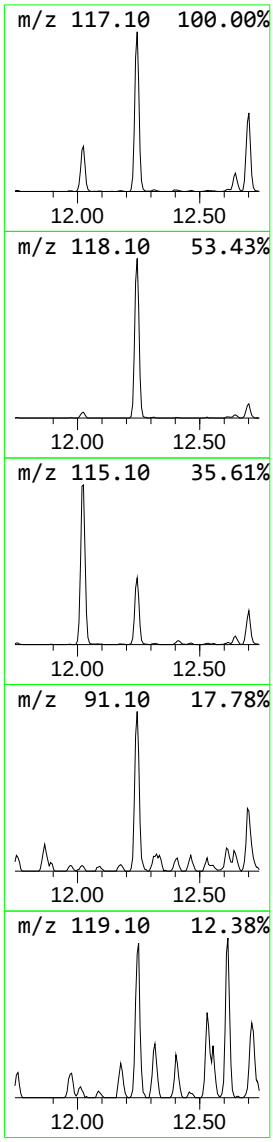
****

Peak Number 5 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	19.42 ug/l	222563	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, cyclopropyl-	118	C9H10	000873-49-4	81
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
4	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	68
5	Deltacyclene	118	C9H10	007785-10-6	68





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Data File : VX033042.D
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Operator : JC/MD
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ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

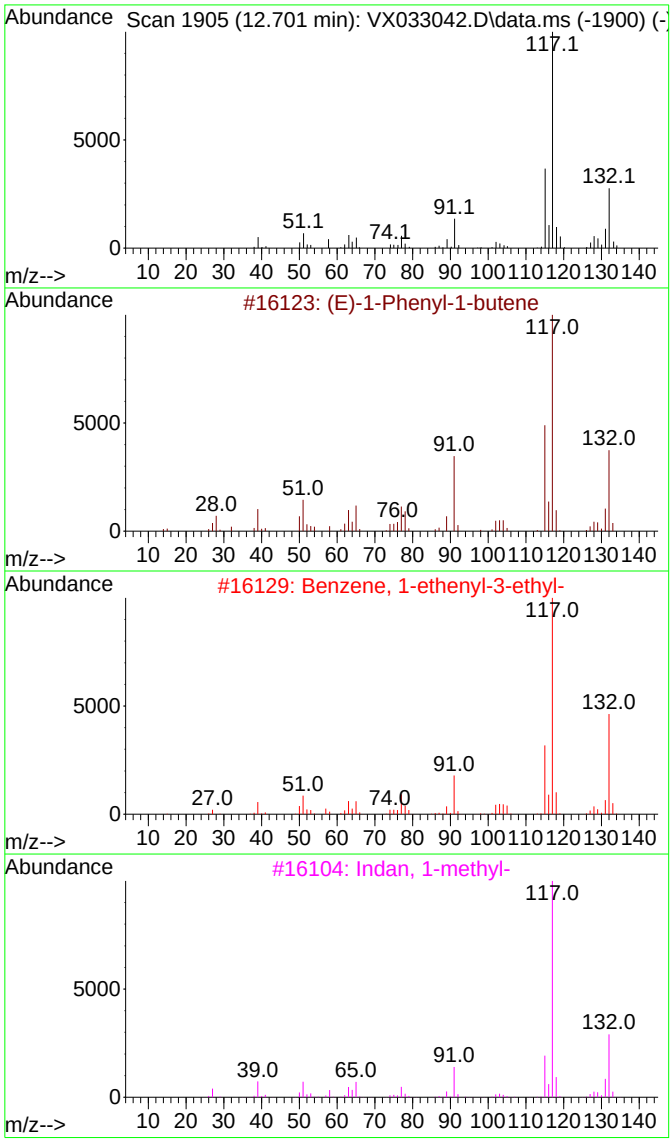
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

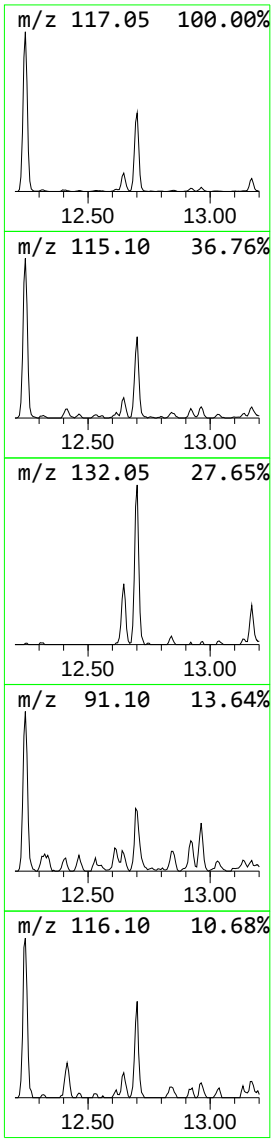
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (E)-1-Phenyl-1-butene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	9.09 ug/l	104200	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	87
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
3	Indan, 1-methyl-	132	C10H12	000767-58-8	87
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	86





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Data File : VX033042.D
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

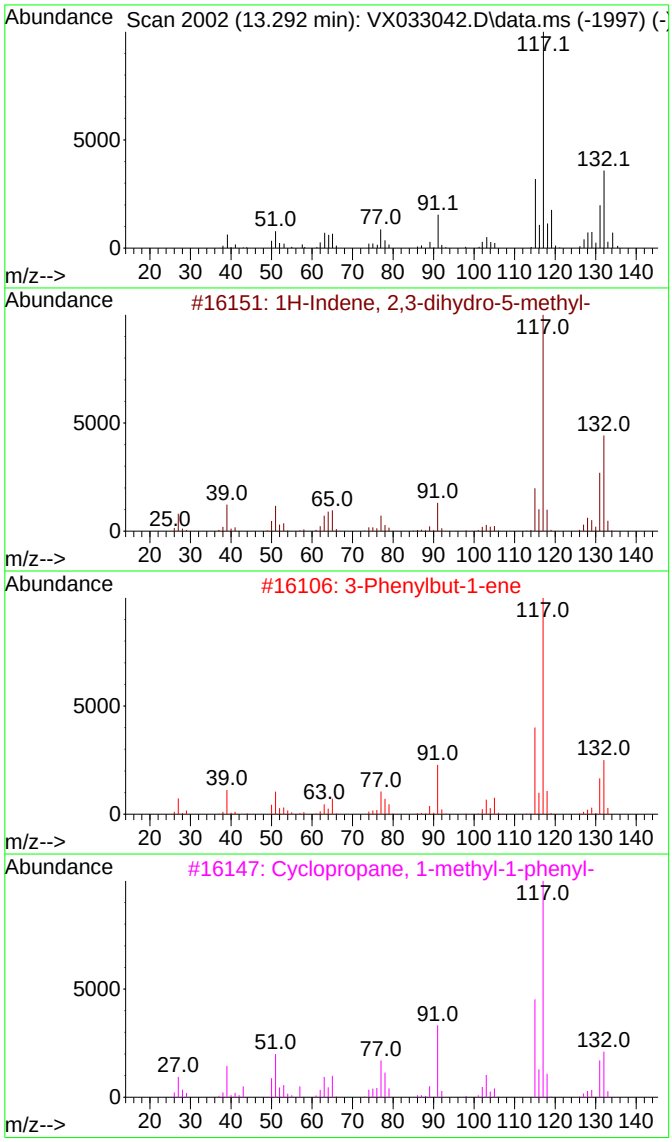
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

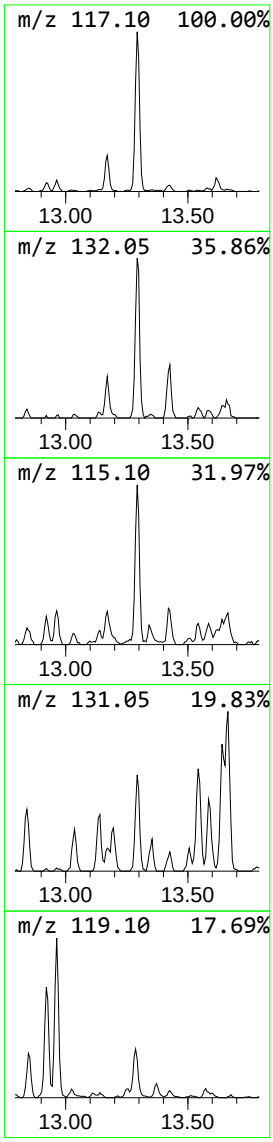
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	7.85 ug/l	89982	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
3	Cyclopropane, 1-methyl-1-phenyl-	132	C10H12	002214-14-4	87
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83
5	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033042.D
Acq On : 24 Nov 2022 06:27
Operator : JC/MD
Sample : N5741-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

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
Sulfur dioxide	1.246	39.6	ug/l	325563	1	5.556	410976	50.0
Butane, 2-methyl-	1.752	7.7	ug/l	63010	1	5.556	410976	50.0
1-Pentene	2.867	7.0	ug/l	57738	1	5.556	410976	50.0
Cyclopentane, m...	4.312	10.5	ug/l	86250	1	5.556	410976	50.0
Indane	12.244	19.4	ug/l	222563	4	12.024	573101	50.0
(E)-1-Phenyl-1-...	12.701	9.1	ug/l	104200	4	12.024	573101	50.0
1H-Indene, 2,3-...	13.292	7.8	ug/l	89982	4	12.024	573101	50.0