LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032681.D
Acq On : 09 Nov 2022 15:54
Operator : JC/MD
Sample : N5514-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6I

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: VX032681.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	42	rVB	121077	115627	11.50%	1.069%
2	1.367	42	46	51	rBV	97222	110399	10.98%	1.021%
3	1.751	103	109	119	rVB	743006	1005766	100.00%	9.300%
4	1.953	138	142	150	rVB2	23951	39555	3.93%	0.366%
5	2.129	167	171	180	rVB3	12625	31513	3.13%	0.291%
6	2.215	180	185	192	rVB	29905	45196	4.49%	0.418%
7	2.343	198	206	220	rVB	41582	84873	8.44%	0.785%
8	2.782	268	278	282	rBV	76956	168558	16.76%	1.559%
9	2.824	282	285	288	rVV	65002	117979	11.73%	1.091%
10	2.867	288	292	300	rVV	95874	193516	19.24%	1.789%
11	2.971	300	309	322	rVV	145318	406803	40.45%	3.762%
12	3.111	322	332	351	rVB2	358096	855369	85.05%	7.909%
13	3.739	424	435	444	rBV5	6227	22215	2.21%	0.205%
14	3.836	444	451	461	rVB2	8084	19521	1.94%	0.181%
15	4.105	488	495	502	rVB2	7648	17866	1.78%	0.165%
16	4.214	504	513	519	rVV3	8416	24399	2.43%	0.226%
17	4.306	519	528	539	rVV2	93931	265800	26.43%	2.458%
18	4.428	539	548	561	rVB4	18637	57207	5.69%	0.529%
19	5.196	665	674	685	rVB4	8163	30463	3.03%	0.282%
20	5.385	694	705	713	rBV2	72291	212719	21.15%	1.967%
21	5.470	713	719	725	rVV2	36002	110091	10.95%	1.018%
22	5.556	725	733	741	rVV	118515	352895	35.09%	3.263%
23	5.617	741	743	760	rVB4	22448	58239	5.79%	0.539%
24	5.836	766	779	789	rBV4	7986	26007	2.59%	0.240%
25	5.958	789	799	806	rVV	78704	211037	20.98%	1.951%
26	6.037	806	812	826	rVV	97250	273957	27.24%	2.533%
27	6.159	826	832	840	rVV5	12860	47786	4.75%	0.442%
28	6.251	840	847	856	rVV3	29127	94162	9.36%	0.871%
29	6.360	856	865	876	rVB3	16240	49964	4.97%	0.462%
30	6.763	921	931	942	rBV	184498	450032	44.75%	4.161%
31	6.854	942	946	955	rVV5	8294	19412	1.93%	0.179%
32	7.177	989	999	1007	rBB2	14518	32679	3.25%	0.302%
33	7.372	1021	1031	1042	rVB5	24463	71155	7.07%	0.658%
34	7.884	1104	1115	1121	rBV4	4586	14068	1.40%	0.130%
35	7.982	1121	1131	1140	rVB3	13161	34064	3.39%	0.315%
36	8.110	1143	1152	1156	rBV	29036	61197	6.08%	0.566%

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-6I

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

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Title : SW846 8260

37	8.506	1210	1217	1225	rVB4	17686	32363	3.22%	0.299%
38	8.646	1235	1240	1248	rVV	375720	608097	60.46%	5.623%
39	8.720	1248	1252	1258	rVB	13743	20864	2.07%	0.193%
40	8.957	1282	1291	1300	rVB	152620	234976	23.36%	2.173%
41	9.049	1300	1306	1312	rVV	143902	221602	22.03%	2.049%
42	9.104	1312	1315	1321	rVV	7215	10800	1.07%	0.100%
43	9.159	1321	1324	1335	rVB	8139	13834	1.38%	0.128%
44	10.055	1460	1471	1477	rBV	389615	513157	51.02%	4.745%
45	10.305	1505	1512	1518	rVB	46161	64085	6.37%	0.593%
46	10.963	1615	1620	1625	rBV	90664	111235	11.06%	1.029%
47	11.079	1634	1639	1645	rBV	343565	449911	44.73%	4.160%
48	11.305	1667	1676	1686	rBV	106606	135618	13.48%	1.254%
49	11.402	1686	1692	1696	rVB	8059	10246	1.02%	0.095%
50	11.615	1722	1727	1732	rVB	34388	45319	4.51%	0.419%
51	11.865	1764	1768	1770	rBV	12436	17529	1.74%	0.162%
52	11.890	1770	1772	1779	rVB	26866	30283	3.01%	0.280%
53	12.024	1788	1794	1802	rVB	396320	501152	49.83%	4.634%
54	12.176	1814	1819	1824	rBV	10880	13181	1.31%	0.122%
55	12.243	1824	1830	1837	rVV	748519	911004	90.58%	8.424%
56	12.317	1837	1842	1851	rVV2	36533	57518	5.72%	0.532%
57	12.408	1852	1857	1862	rVV	18250	23160	2.30%	0.214%
58	12.463	1862	1866	1872	rVB	31101	38635	3.84%	0.357%
59	12.615	1886	1891	1893	rBV	35364	43649	4.34%	0.404%
60	12.646	1893	1896	1900	rVV	46750	55916	5.56%	0.517%
61	12.701	1900	1905	1912	rVV	210182	261339	25.98%	2.417%
62	12.841	1924	1928	1934	rVB2	10504	13228	1.32%	0.122%
63	12.920	1934	1941	1946	rBV	86267	108362	10.77%	1.002%
64	13.030	1953	1959	1964	rBV3	11695	17074	1.70%	0.158%
65	13.170	1978	1982	1992	rVB	66753	87306	8.68%	0.807%
66	13.292	1992	2002	2007	rBV2	128050	176496	17.55%	1.632%
67	13.347	2007	2011	2020	rVV5	11058	19562	1.94%	0.181%
68	13.420	2020	2023	2028	rVB2	14418	18836	1.87%	0.174%
69	13.548	2040	2044	2046	rBV	17370	21717	2.16%	0.201%
70	13.585	2046	2050	2053	rVV2	14008	19871	1.98%	0.184%
71	13.640	2053	2059	2061	rVV2	19297	31661	3.15%	0.293%
72	13.664	2061	2063	2071	rVB2	17584	21975	2.18%	0.203%
73	13.774	2074	2081	2090	rBV	32059	44709	4.45%	0.413%
74	14.072	2127	2130	2135	rBV	10946	13547	1.35%	0.125%
75	14.371	2175	2179	2186	rVB2	9035	11562	1.15%	0.107%
76	14.780	2241	2246	2255	rVB	40026	51265	5.10%	0.474%

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MW-6I

Integration Parameters: RTEINT.P
Integrator: RTE
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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Title : SW846 8260

Sum of corrected areas: 10814733

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032681.D
Acq On : 09 Nov 2022 15:54
Operator : JC/MD
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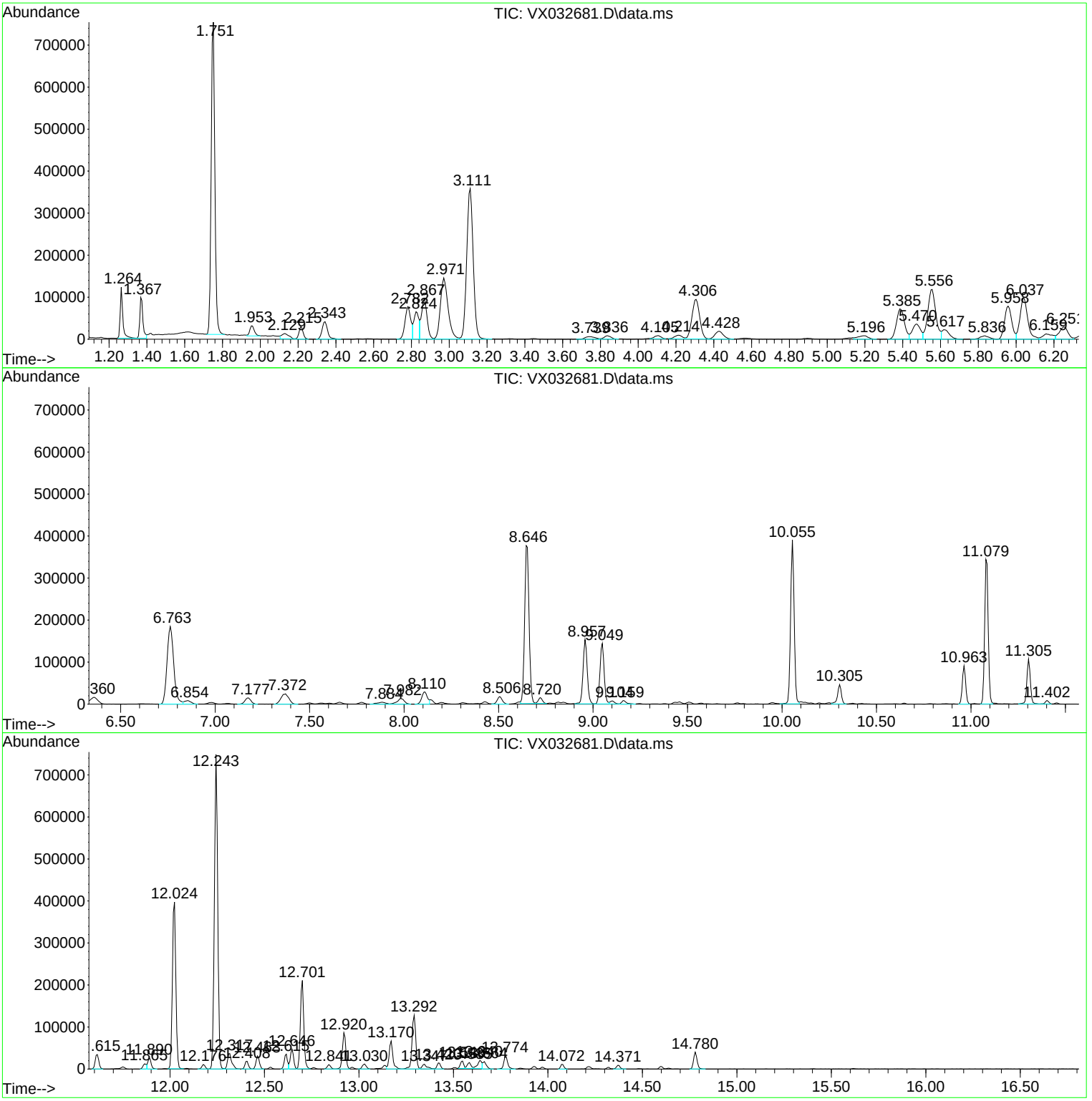
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6I

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 : VX032681.D
Acq On : 09 Nov 2022 15:54
Operator : JC/MD
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ALS Vial : 14 Sample Multiplier: 1

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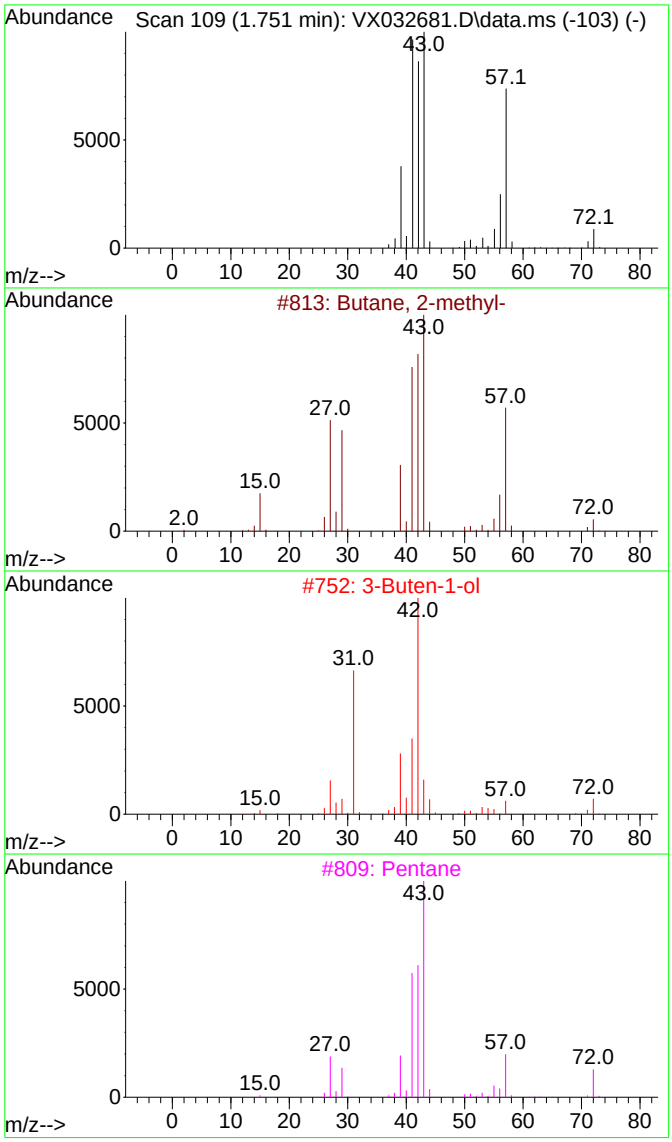
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

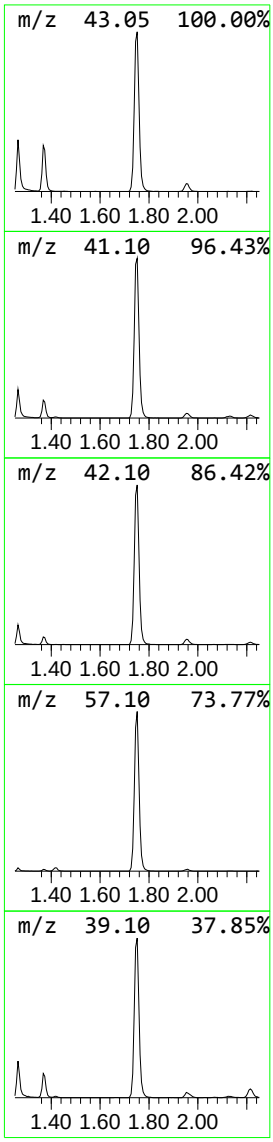
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.751	142.50 ug/l	1005770	Pentafluorobenzene	5.556

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	33
4	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	28
5	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	16





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Instrument :
MSVOA_X
ClientSampleId :
MW-6I

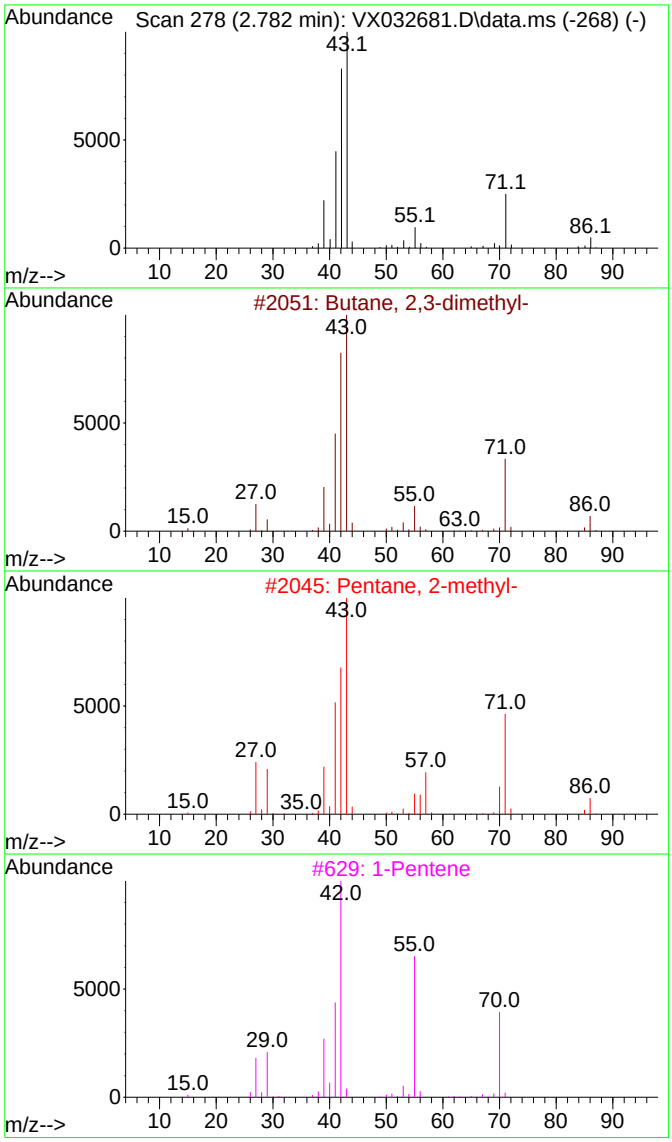
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

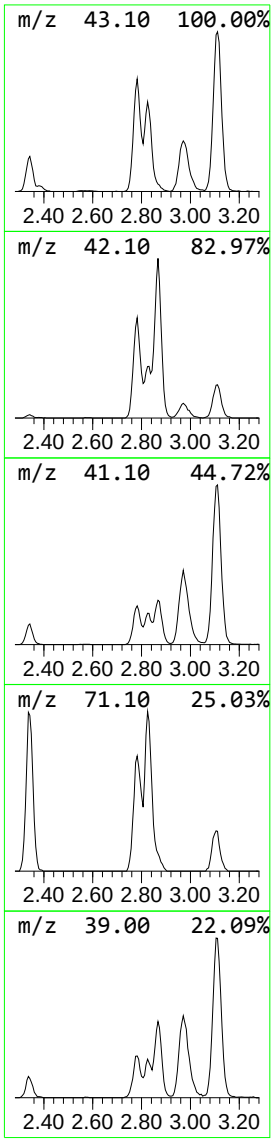
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	23.88 ug/l	168558	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	78
3	1-Pentene	70	C5H10	000109-67-1	50
4	Tetrahydrofuran	72	C4H8O	000109-99-9	38
5	Pentane	72	C5H12	000109-66-0	36





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032681.D
Acq On : 09 Nov 2022 15:54
Operator : JC/MD
Sample : N5514-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6I

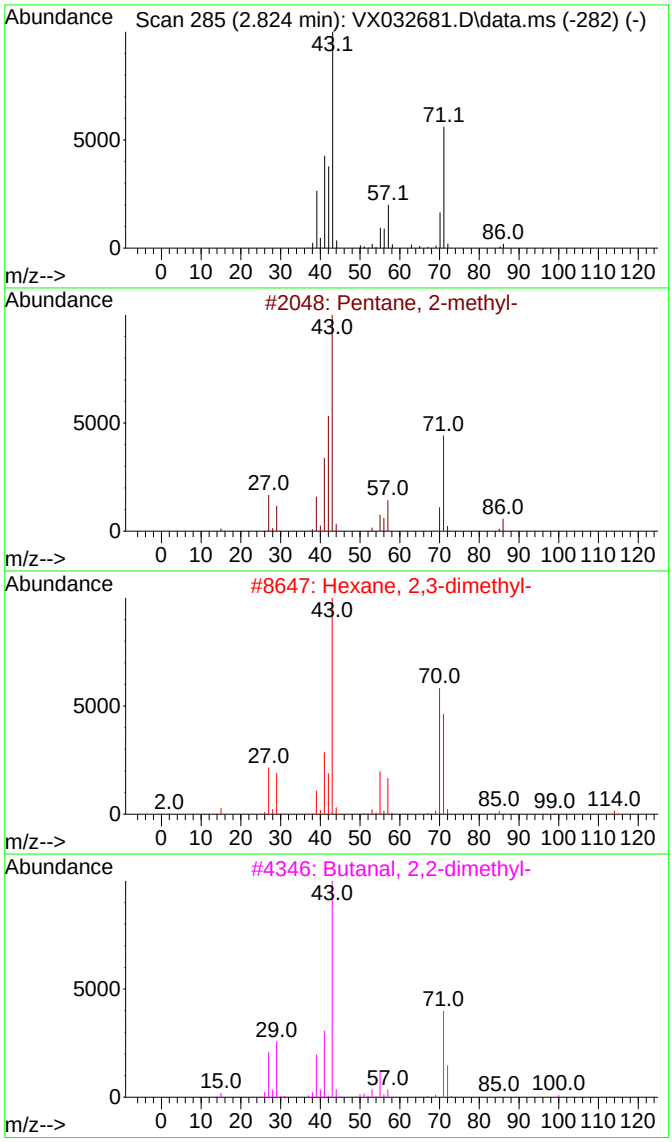
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

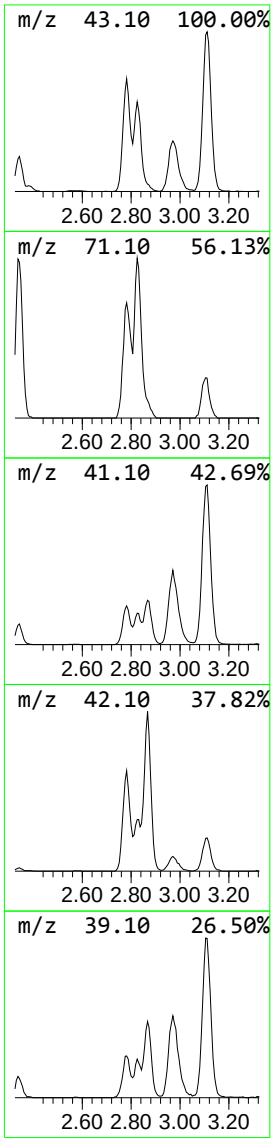
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.824	16.72 ug/l	117979	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	78
2	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38
3	Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	33
4	Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	28
5	Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	23





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Instrument :
MSVOA_X
ClientSampleId :
MW-6I

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

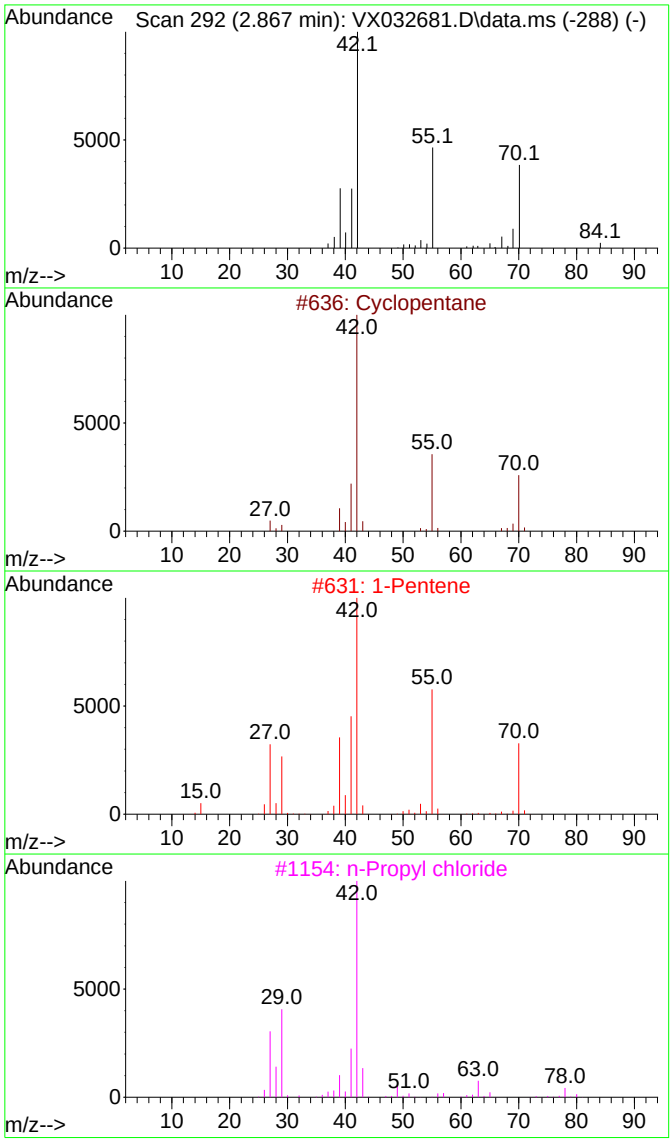
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

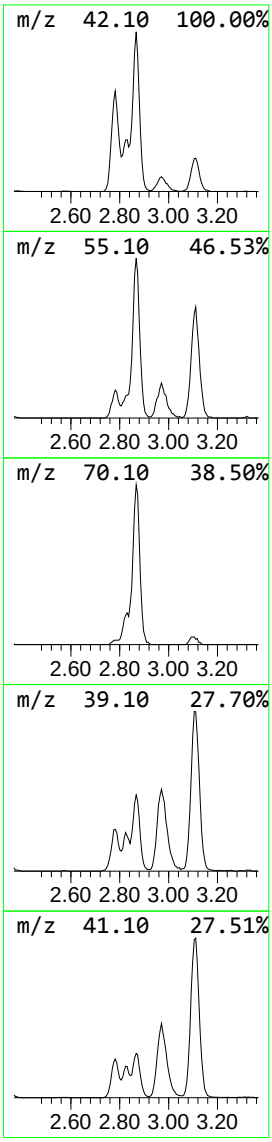
****

Peak Number 4 Cyclopentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	27.42 ug/l	193516	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	78
2	1-Pentene	70	C5H10	000109-67-1	64
3	n-Propyl chloride	78	C3H7Cl	000540-54-5	25
4	Cyclobutanone	70	C4H6O	001191-95-3	9
5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	9





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6I

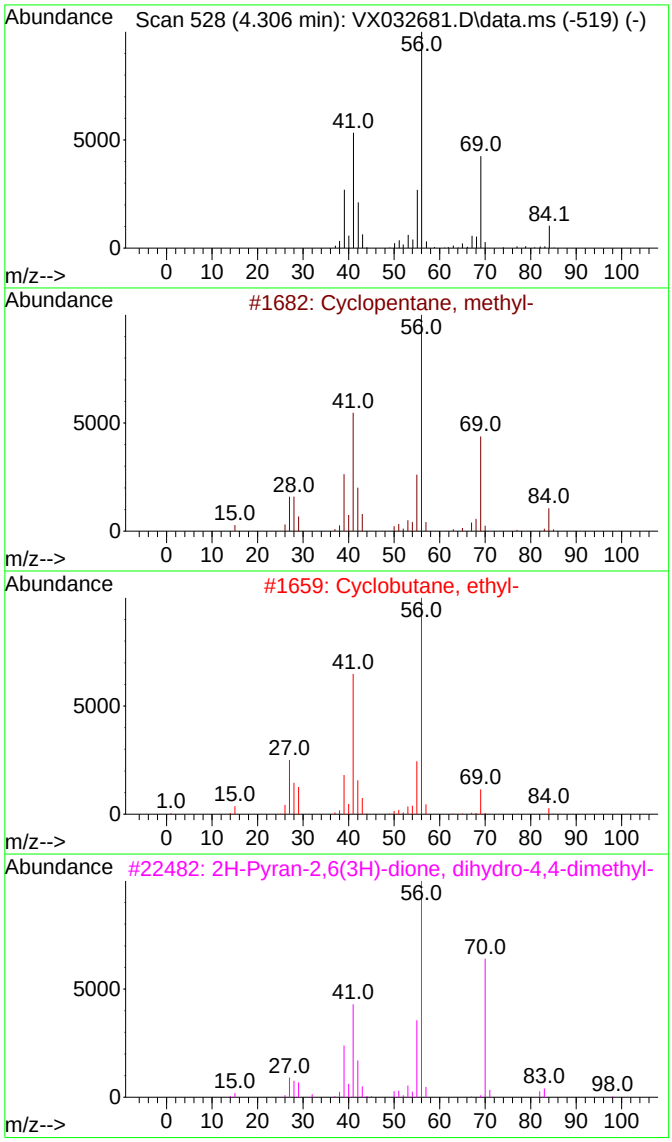
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

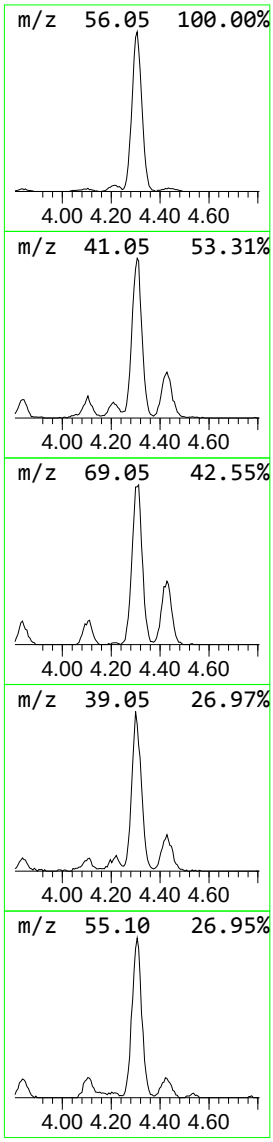
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	37.66 ug/l	265800	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	64
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	64
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6I

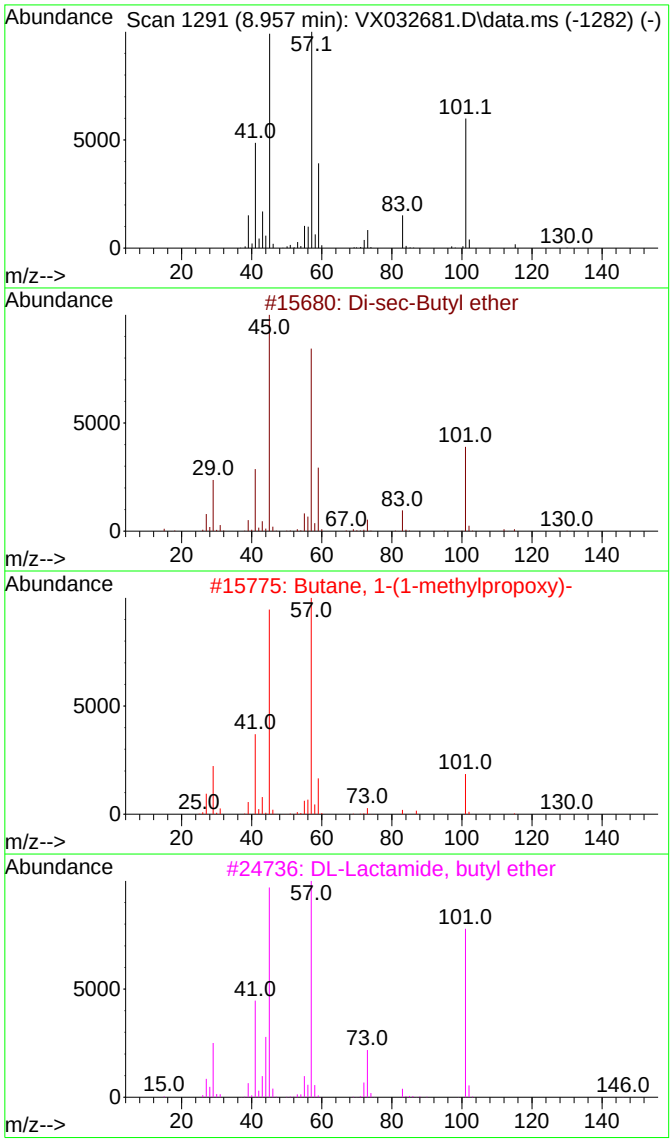
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

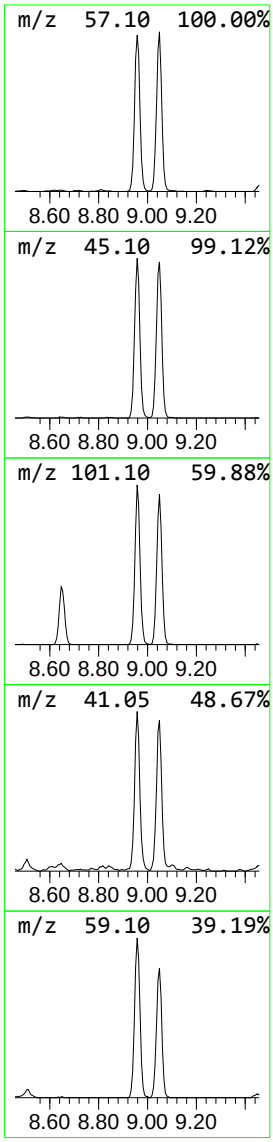
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Di-sec-Butyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.957	22.90 ug/l	234976	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	87
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
3	DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	42
4	Boronic acid, ethyl-, diethyl ester	130	C6H15BO2	053907-92-9	40
5	Sulfurous acid, di(2-methyl-4-me...	282	C12H26O5S	1000309-20-7	38





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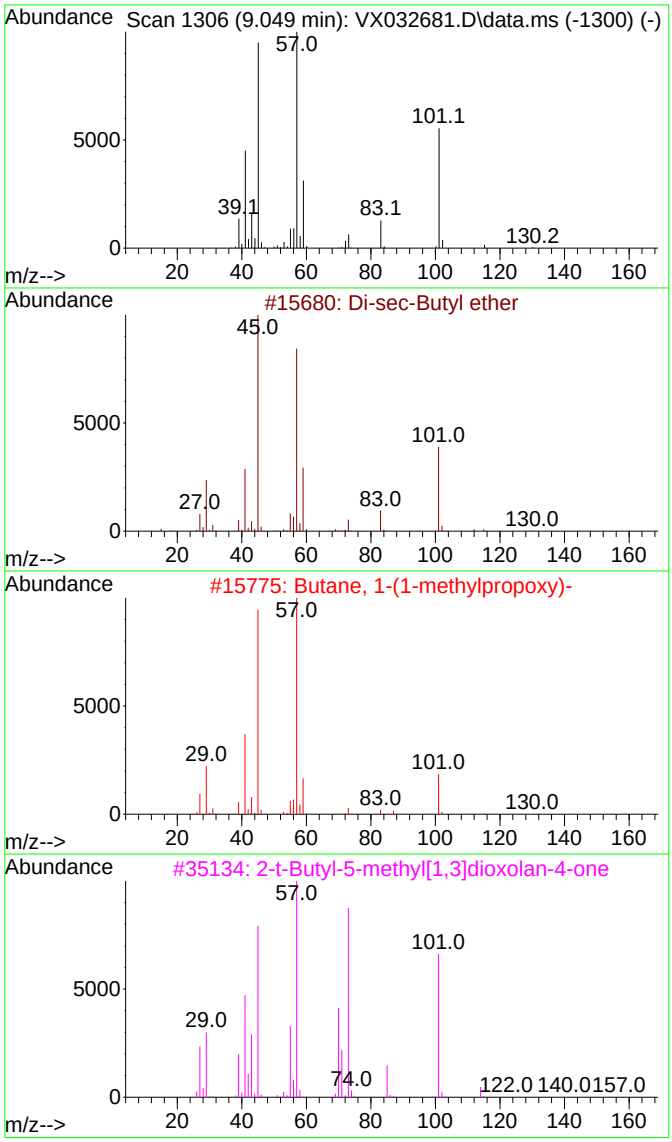
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

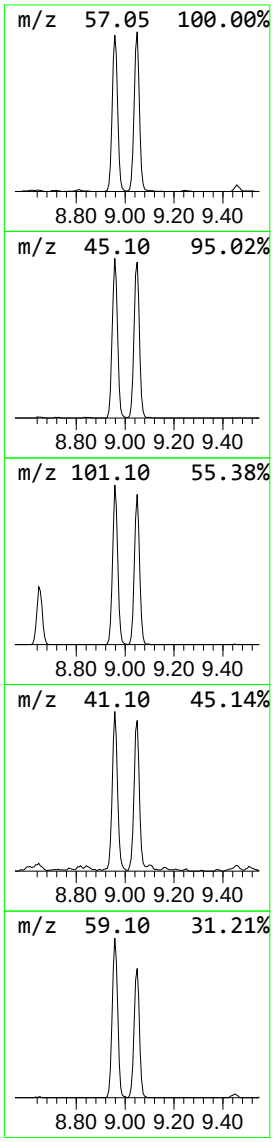
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Butane, 1-(1-methylpropoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.049	21.59 ug/l	221602	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	91
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
3	2-t-Butyl-5-methyl[1,3]dioxolan-...	158	C8H14O3	130930-47-1	50
4	Boronic acid, ethyl-, diethyl ester	130	C6H15BO2	053907-92-9	42
5	1-Octene, 3-(methoxymethoxy)-	172	C10H20O2	088738-34-5	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032681.D
Acq On : 09 Nov 2022 15:54
Operator : JC/MD
Sample : N5514-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6I

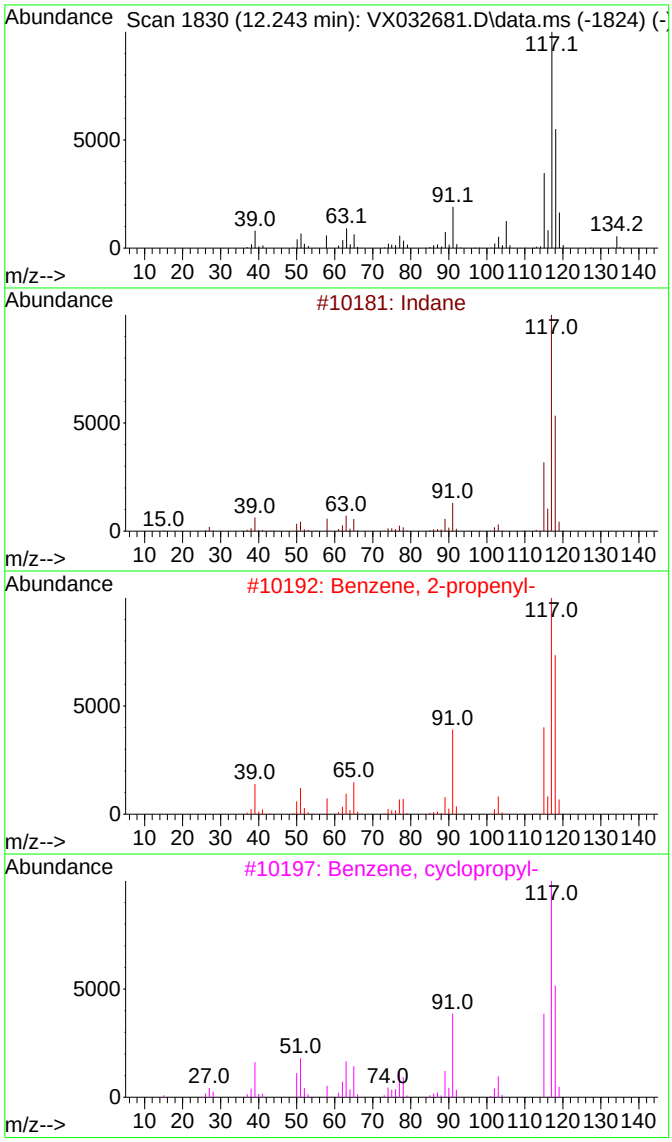
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

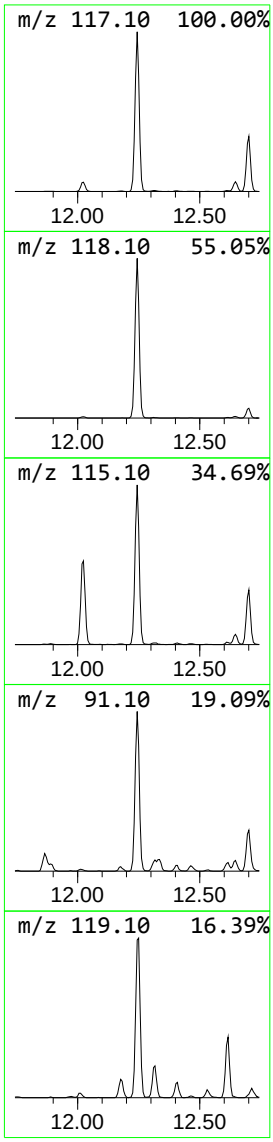
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	90.89 ug/l	911004	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, 2-propenyl-	118	C9H10	000300-57-2	76
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	55
5	Deltacyclene	118	C9H10	007785-10-6	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032681.D
Acq On : 09 Nov 2022 15:54
Operator : JC/MD
Sample : N5514-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6I

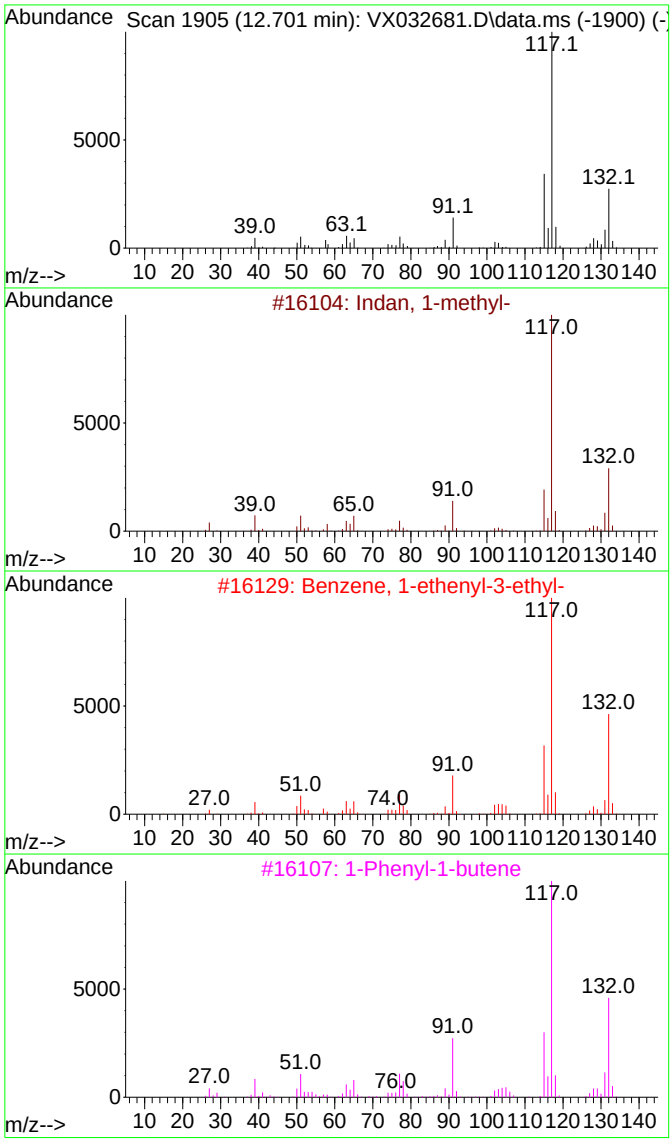
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

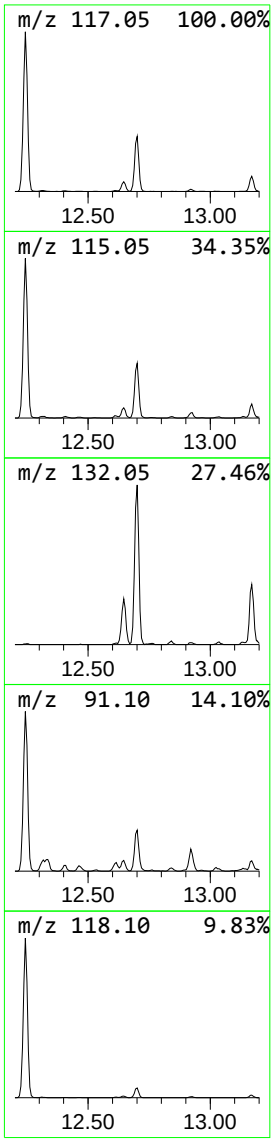
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Indan, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	26.07 ug/l	261339	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	90
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032681.D
Acq On : 09 Nov 2022 15:54
Operator : JC/MD
Sample : N5514-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6I

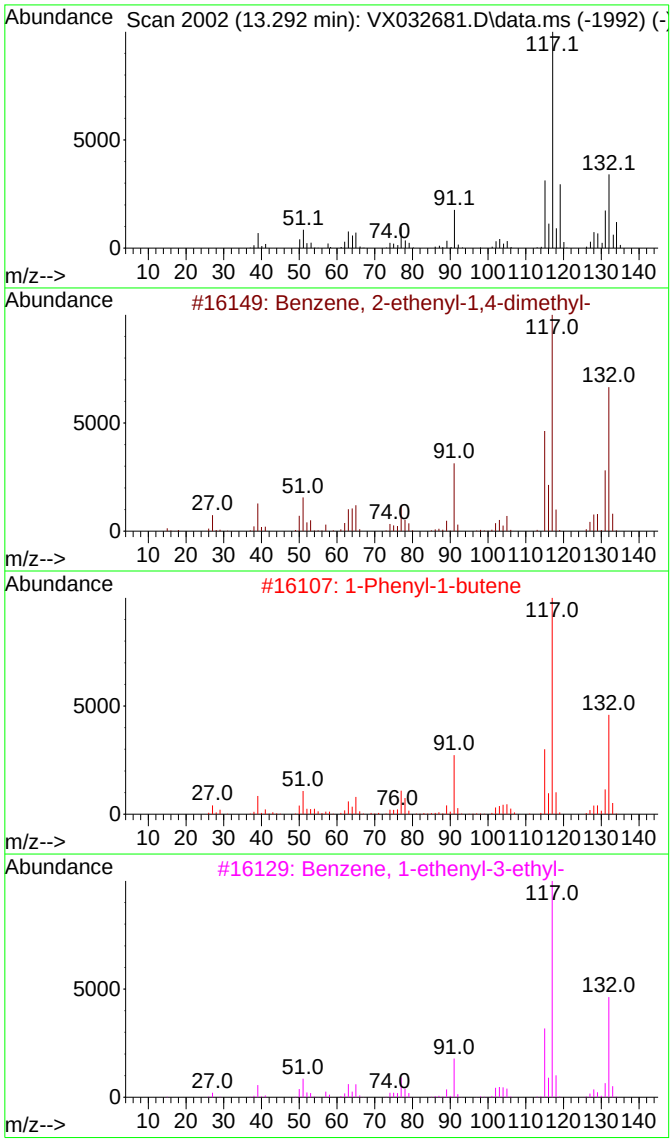
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

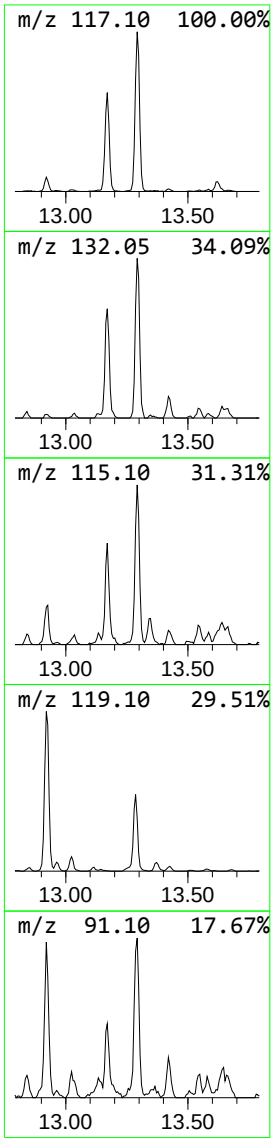
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	17.61 ug/l	176496	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	90
3	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032681.D
Acq On : 09 Nov 2022 15:54
Operator : JC/MD
Sample : N5514-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6I

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, 2-methyl-	1.751	142.5	ug/l	1005770	1	5.556	352895	50.0
Butane, 2,3-dim...	2.782	23.9	ug/l	168558	1	5.556	352895	50.0
Pentane, 2-methyl-	2.824	16.7	ug/l	117979	1	5.556	352895	50.0
Cyclopentane	2.867	27.4	ug/l	193516	1	5.556	352895	50.0
Cyclopentane, m...	4.306	37.7	ug/l	265800	1	5.556	352895	50.0
Di-sec-Butyl ether	8.957	22.9	ug/l	234976	3	10.055	513157	50.0
Butane, 1-(1-me...	9.049	21.6	ug/l	221602	3	10.055	513157	50.0
Indane	12.243	90.9	ug/l	911004	4	12.024	501152	50.0
Indan, 1-methyl-	12.701	26.1	ug/l	261339	4	12.024	501152	50.0
Benzene, 2-ethe...	13.292	17.6	ug/l	176496	4	12.024	501152	50.0