

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
 Data File : VX029573.D
 Acq On : 18 Jun 2022 16:36
 Operator : JC/MD
 Sample : N3325-06
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-17

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\82X061822W.M
 Title : SW846 8260

Signal : TIC: VX029573.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	23	28	30	rBV	349514	588027	14.93%	1.987%
2	1.752	104	109	128	rVB2	112086	204626	5.20%	0.691%
3	1.953	138	142	149	rBV	45867	63825	1.62%	0.216%
4	2.562	230	242	249	rBV2	18100	84943	2.16%	0.287%
5	2.782	262	278	281	rBV3	48016	126592	3.21%	0.428%
6	2.825	281	285	290	rVB	73356	127981	3.25%	0.432%
7	3.105	323	331	342	rVB2	96116	226239	5.74%	0.765%
8	3.446	380	387	401	rVB3	31285	73113	1.86%	0.247%
9	4.306	519	528	541	rVB2	130927	376506	9.56%	1.272%
10	5.391	694	706	714	rBV2	150105	442234	11.23%	1.494%
11	5.477	714	720	725	rVV4	33743	90124	2.29%	0.305%
12	5.556	725	733	743	rVV	252632	687779	17.46%	2.324%
13	5.830	766	778	789	rVB4	25084	80755	2.05%	0.273%
14	5.958	789	799	806	rBV	160434	425162	10.80%	1.437%
15	6.043	806	813	824	rVV2	253759	688250	17.48%	2.326%
16	6.165	824	833	839	rVV4	27172	95536	2.43%	0.323%
17	6.251	840	847	857	rVV4	55749	185811	4.72%	0.628%
18	6.361	857	865	877	rVB6	21866	66303	1.68%	0.224%
19	6.763	922	931	941	rBV	416424	999330	25.38%	3.377%
20	7.379	1019	1032	1046	rBV3	99876	268618	6.82%	0.908%
21	7.659	1072	1078	1087	rVB2	21530	43004	1.09%	0.145%
22	7.988	1123	1132	1144	rVB2	31956	69293	1.76%	0.234%
23	8.110	1144	1152	1156	rBV	61910	126532	3.21%	0.428%
24	8.506	1212	1217	1225	rVB3	25346	46653	1.18%	0.158%
25	8.653	1235	1241	1247	rVB	832186	1290725	32.78%	4.362%
26	8.720	1247	1252	1258	rVB	117924	181537	4.61%	0.613%
27	10.055	1460	1471	1477	rBV	839386	1146129	29.10%	3.873%
28	10.195	1489	1494	1500	rBV	944818	1199970	30.47%	4.055%
29	10.305	1506	1512	1518	rVB	570355	807731	20.51%	2.730%
30	10.646	1562	1568	1579	rVB	1386964	1876186	47.64%	6.340%
31	10.963	1614	1620	1625	rBV	166772	204833	5.20%	0.692%
32	11.085	1634	1640	1645	rBV	642285	831614	21.12%	2.810%
33	11.305	1667	1676	1683	rBV	382756	476567	12.10%	1.610%
34	11.378	1683	1688	1696	rVV	452853	672713	17.08%	2.273%
35	11.451	1696	1700	1707	rVB	100591	131308	3.33%	0.444%
36	11.616	1721	1727	1736	rBV	736212	893937	22.70%	3.021%

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37	11.756	1745	1750	1764	rVB	3277236	3938080	100.00%	13.308%
38	11.890	1770	1772	1778	rVB	36210	44246	1.12%	0.150%
39	11.969	1781	1785	1789	rBV	39610	50233	1.28%	0.170%
40	12.024	1789	1794	1800	rVB	892899	1059531	26.90%	3.580%
41	12.091	1800	1805	1810	rBV	676057	846831	21.50%	2.862%
42	12.244	1823	1830	1838	rBV2	1212818	1621198	41.17%	5.478%
43	12.317	1838	1842	1852	rVB3	147080	243742	6.19%	0.824%
44	12.408	1852	1857	1862	rBV2	60534	82854	2.10%	0.280%
45	12.463	1862	1866	1872	rVB	115749	143782	3.65%	0.486%
46	12.530	1872	1877	1879	rBV	242089	302231	7.67%	1.021%
47	12.555	1879	1881	1886	rVB	215104	242486	6.16%	0.819%
48	12.616	1886	1891	1894	rBV	459344	545960	13.86%	1.845%
49	12.646	1894	1896	1900	rVB	97279	102981	2.62%	0.348%
50	12.701	1900	1905	1913	rBV2	313377	451463	11.46%	1.526%
51	12.847	1925	1929	1934	rVB2	72973	94051	2.39%	0.318%
52	12.920	1934	1941	1945	rBV	227097	296539	7.53%	1.002%
53	12.963	1945	1948	1954	rVB	349150	398515	10.12%	1.347%
54	13.024	1954	1958	1965	rBV3	32470	57462	1.46%	0.194%
55	13.170	1974	1982	1986	rBV	271767	348099	8.84%	1.176%
56	13.256	1992	1996	1998	rBV2	36957	49946	1.27%	0.169%
57	13.292	1998	2002	2008	rVB2	280237	381242	9.68%	1.288%
58	13.426	2019	2024	2032	rVB	103056	137505	3.49%	0.465%
59	13.506	2032	2037	2040	rBV2	37811	52594	1.34%	0.178%
60	13.542	2040	2043	2046	rVV	69829	94660	2.40%	0.320%
61	13.579	2046	2049	2056	rVV3	68895	151242	3.84%	0.511%
62	13.664	2060	2063	2069	rVB2	70807	118610	3.01%	0.401%
63	13.774	2075	2081	2091	rBV	686230	903169	22.93%	3.052%
64	13.865	2091	2096	2101	rVB2	60277	100249	2.55%	0.339%
65	13.926	2101	2106	2111	rBV2	49225	71013	1.80%	0.240%
66	14.079	2126	2131	2135	rBV	61975	79710	2.02%	0.269%
67	14.219	2149	2154	2163	rBV3	67573	135844	3.45%	0.459%
68	14.371	2176	2179	2184	rVB3	46527	63116	1.60%	0.213%
69	14.481	2192	2197	2202	rBV3	24665	40278	1.02%	0.136%
70	14.603	2210	2217	2219	rBV	33761	58861	1.49%	0.199%
71	14.640	2219	2223	2227	rVB	71372	98605	2.50%	0.333%
72	14.780	2241	2246	2251	rBV2	177683	240232	6.10%	0.812%
73	15.188	2306	2313	2320	rBV2	23906	44874	1.14%	0.152%

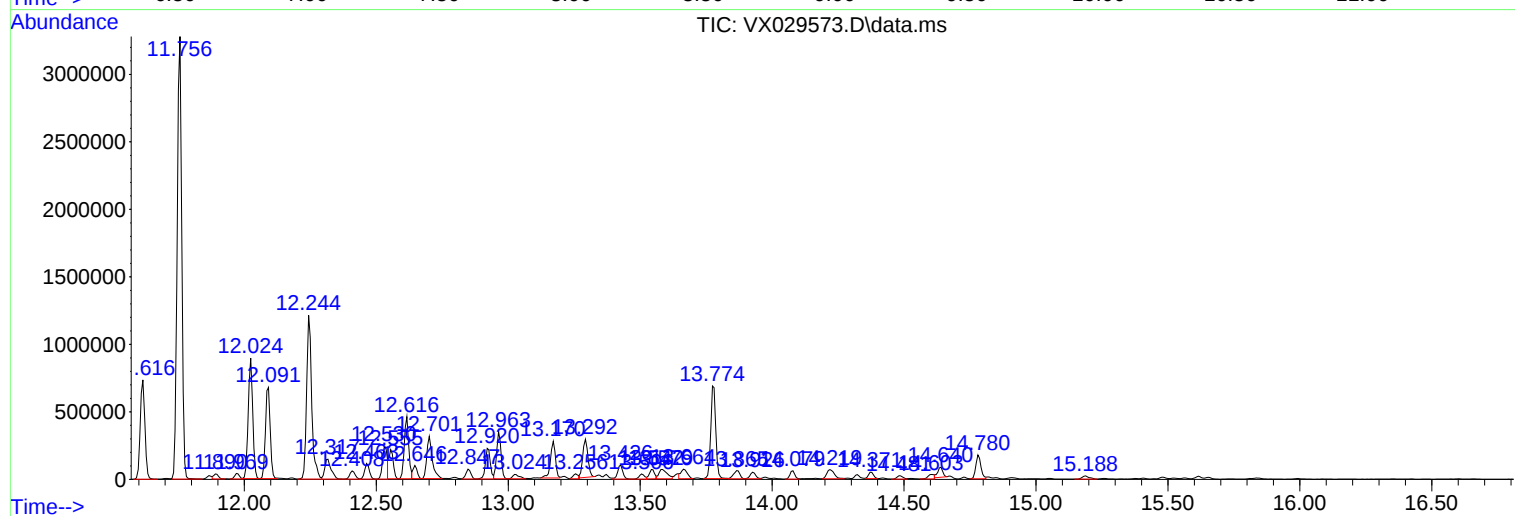
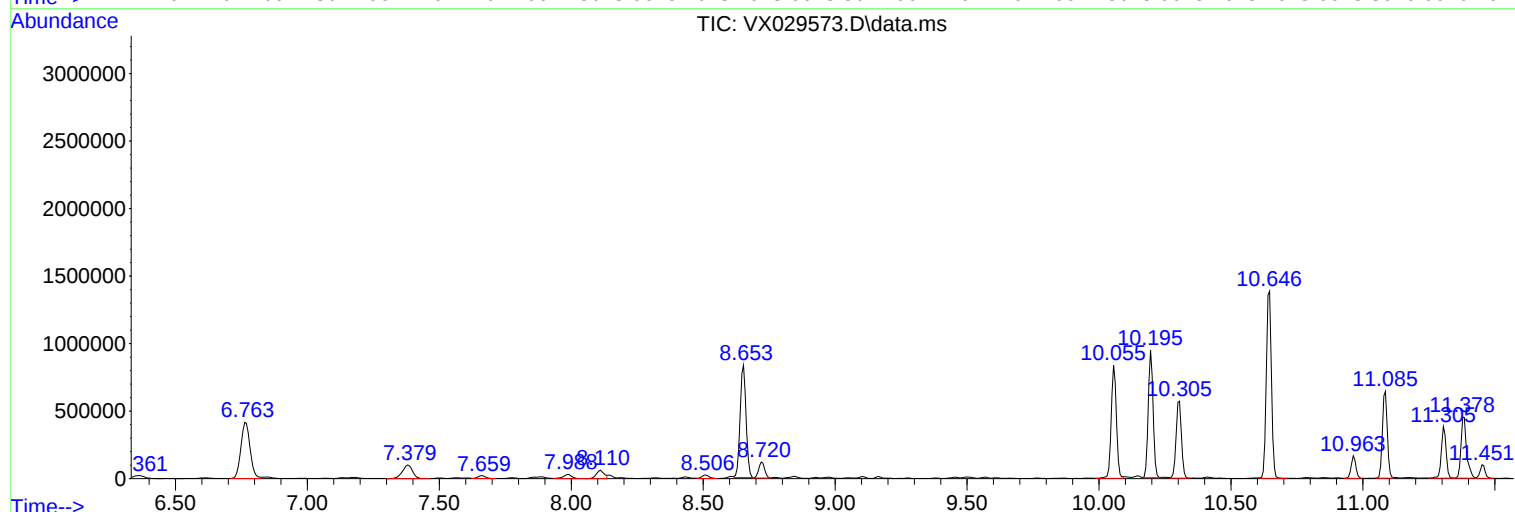
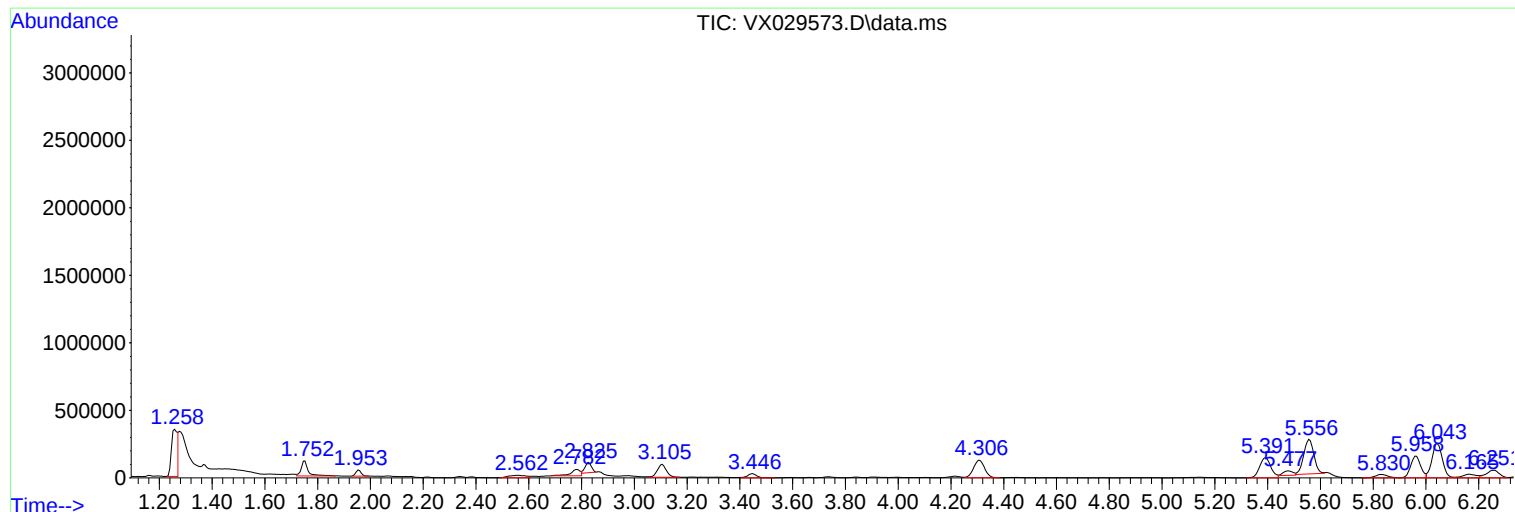
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



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Data File : VX029573.D
Acq On : 18 Jun 2022 16:36
Operator : JC/MD
Sample : N3325-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-17

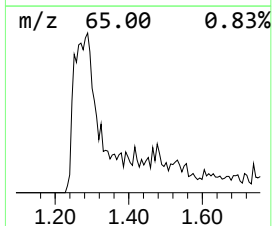
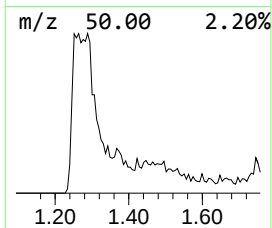
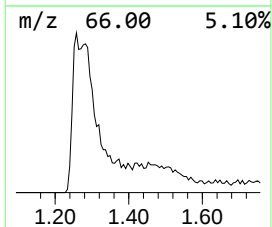
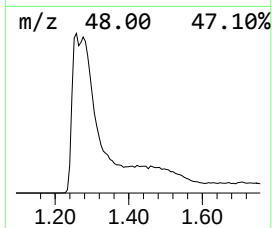
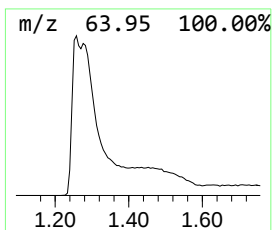
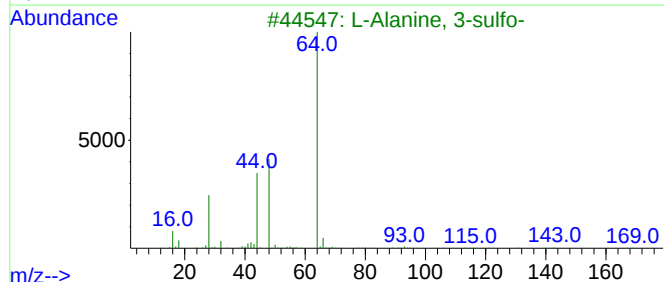
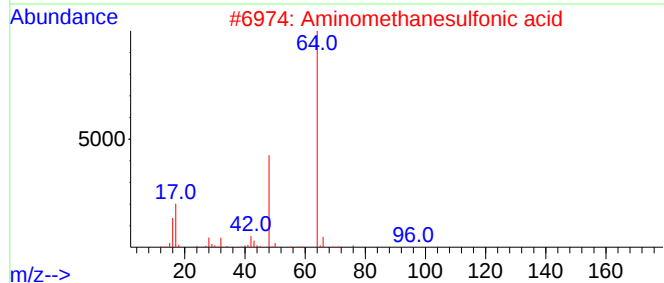
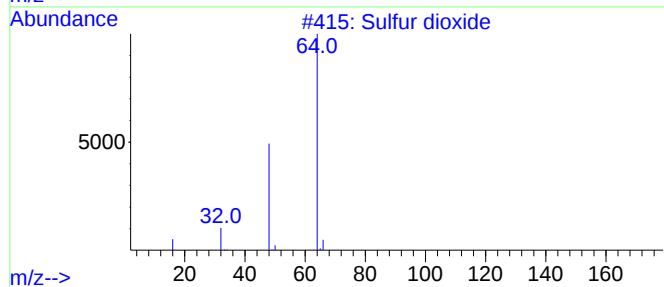
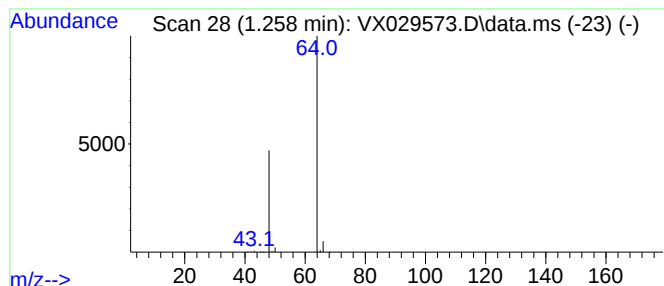
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	42.75 ug/l	588027	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			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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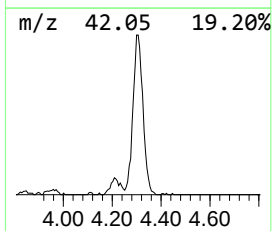
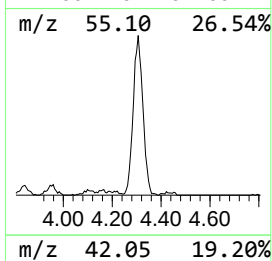
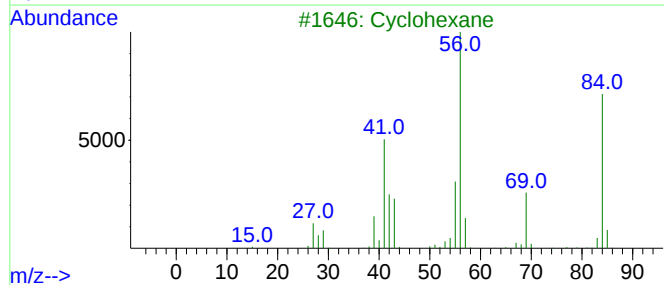
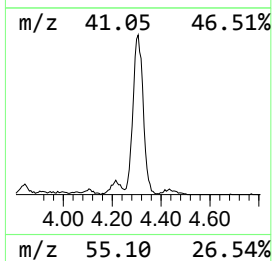
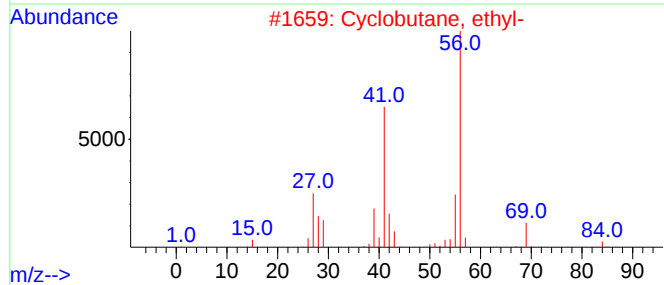
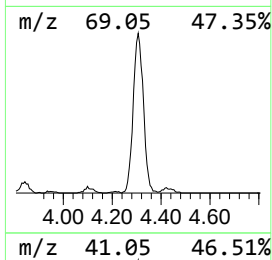
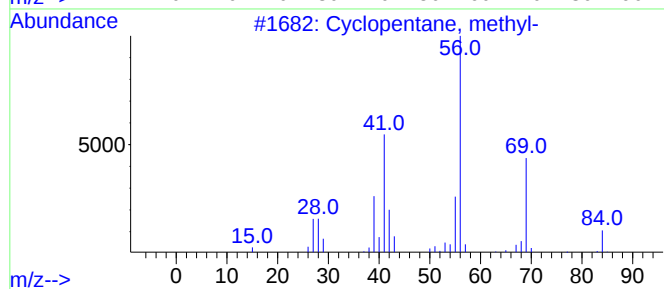
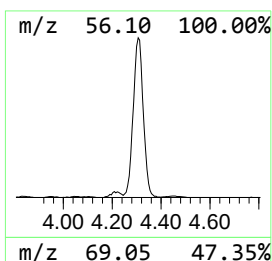
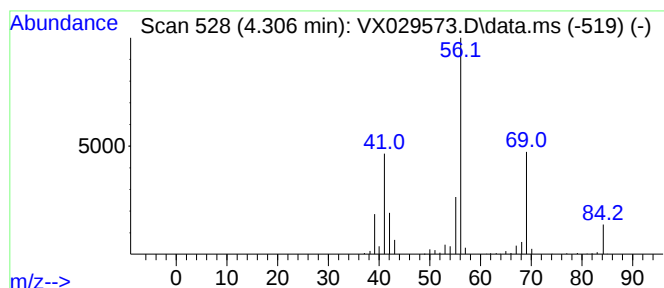
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	27.37 ug/l	376506	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	64
3			Cyclohexane	84	C6H12	000110-82-7	64
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43



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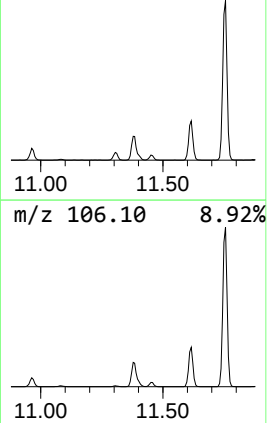
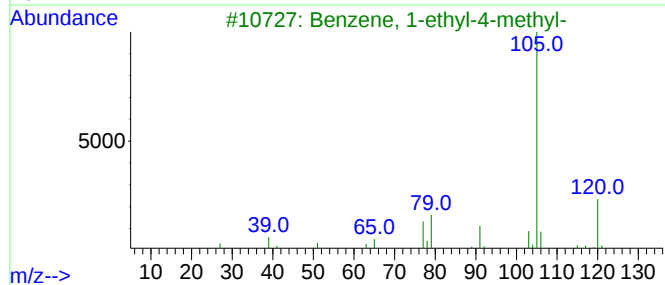
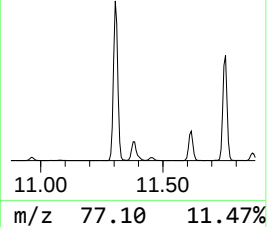
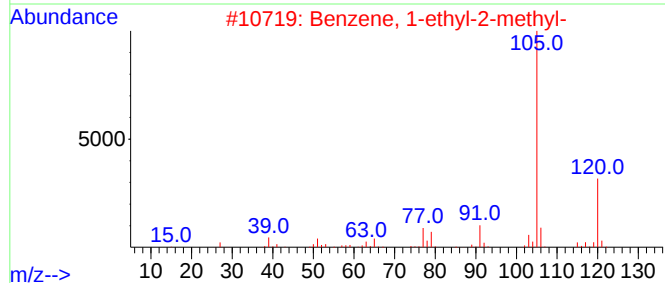
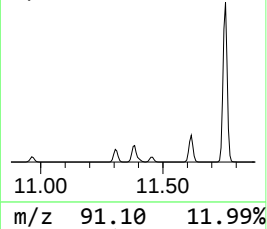
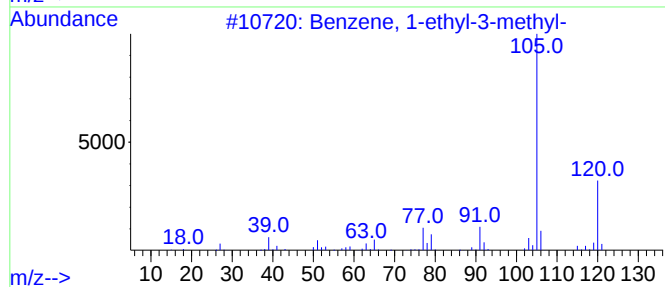
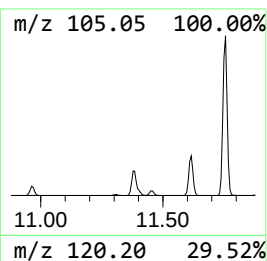
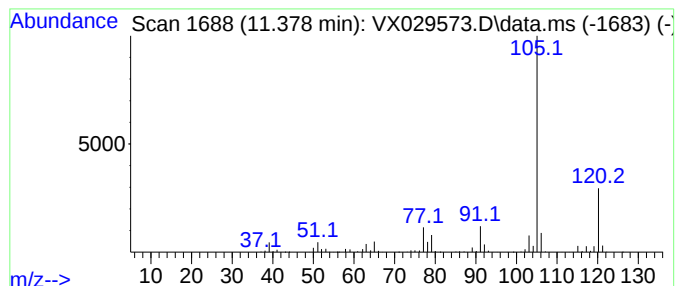
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	31.75 ug/l	672713	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			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



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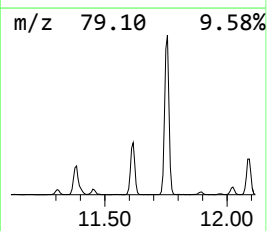
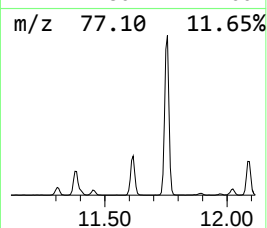
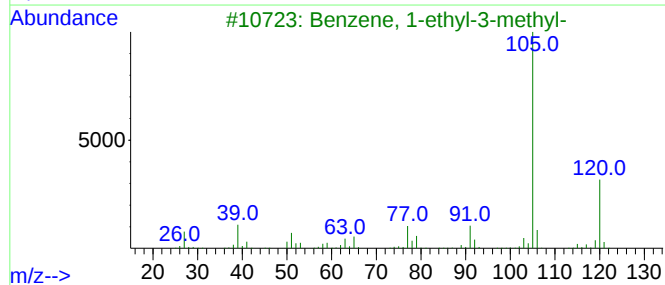
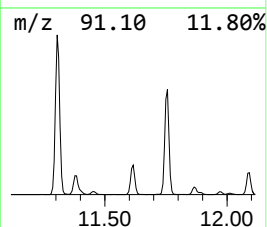
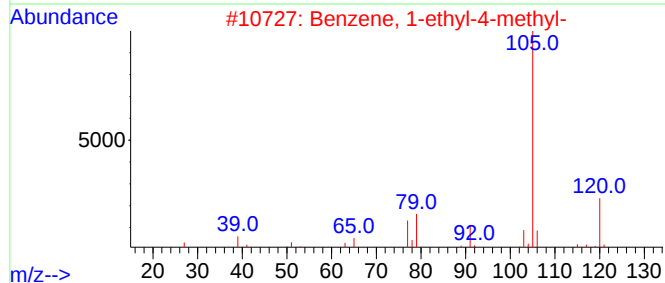
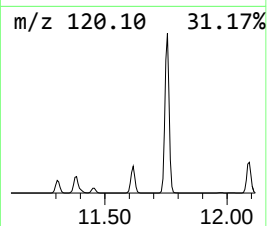
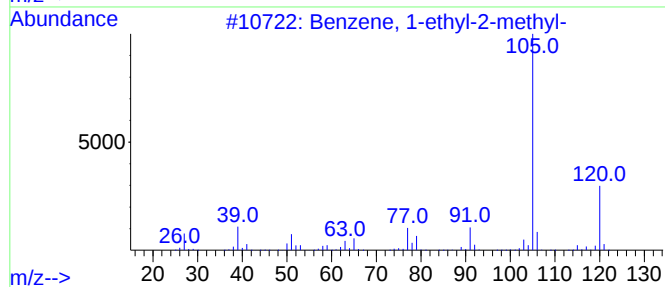
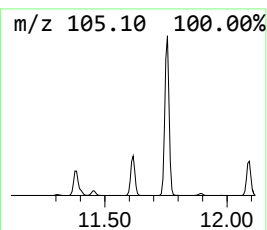
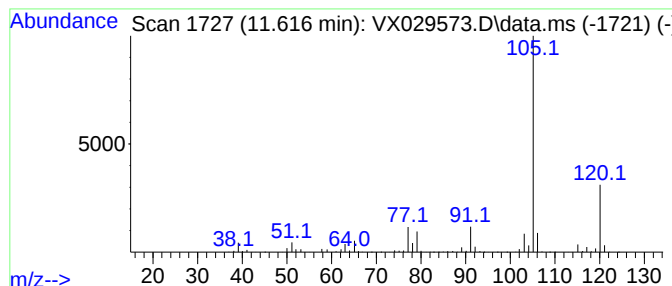
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	42.19 ug/l	893937	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	94
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029573.D
Acq On : 18 Jun 2022 16:36
Operator : JC/MD
Sample : N3325-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-17

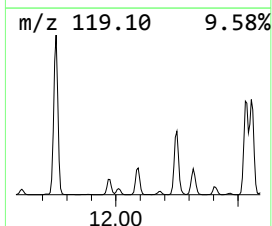
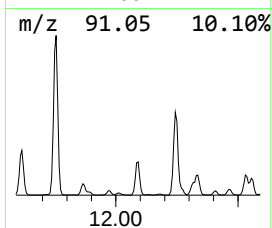
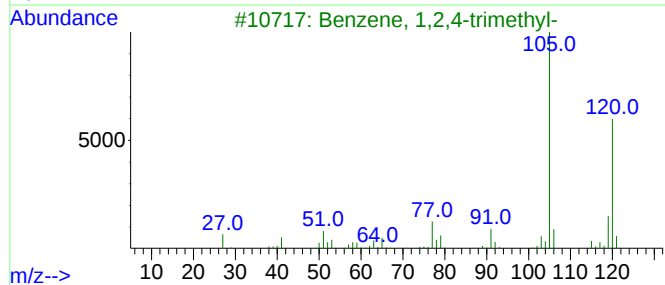
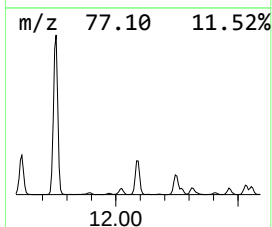
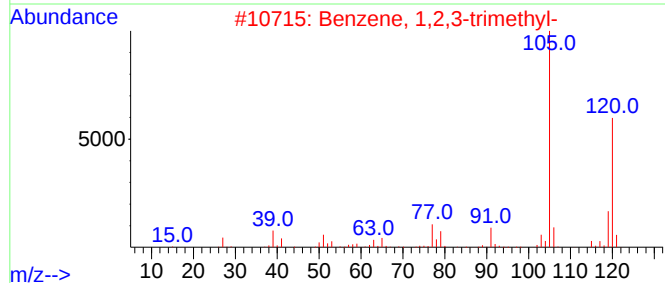
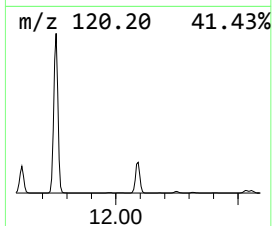
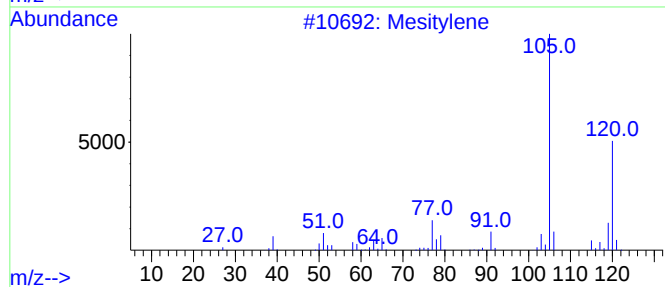
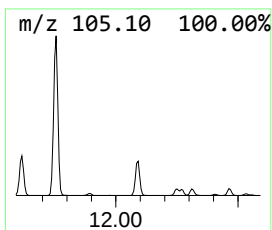
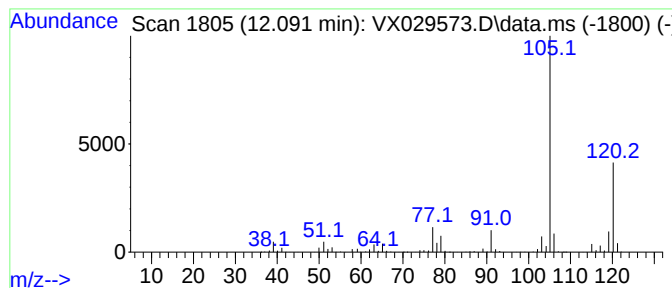
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	39.96 ug/l	846831	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-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029573.D
Acq On : 18 Jun 2022 16:36
Operator : JC/MD
Sample : N3325-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-17

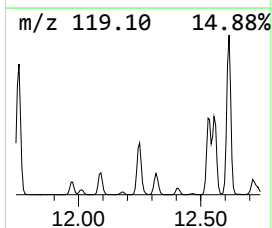
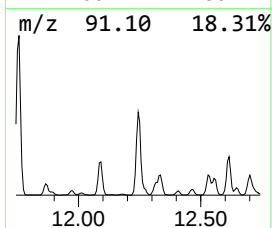
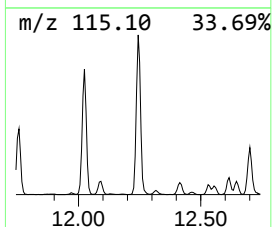
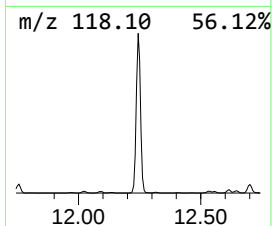
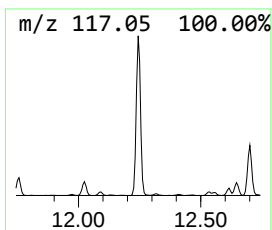
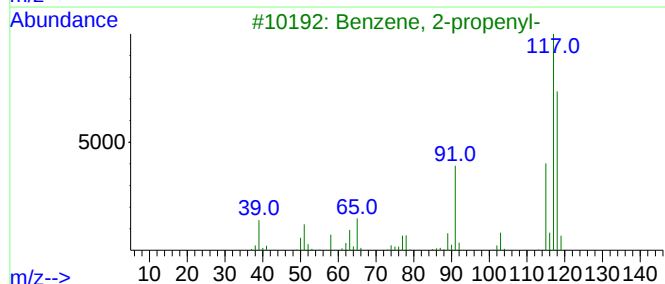
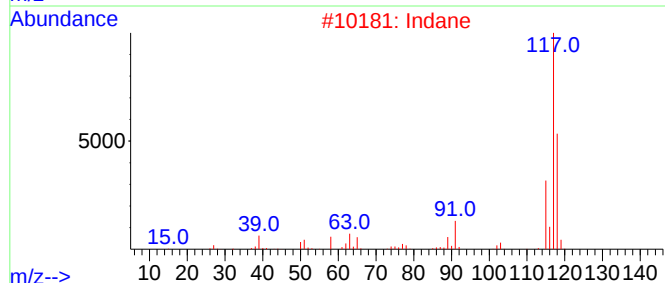
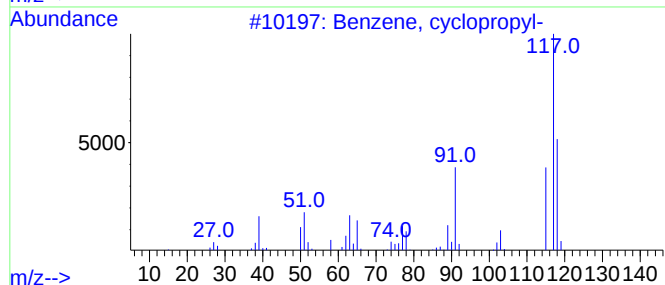
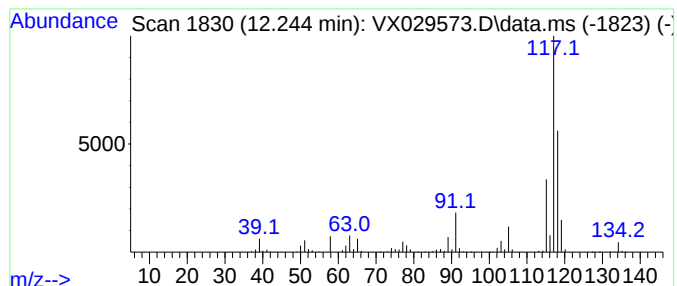
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, cyclopropyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	76.51 ug/l	1621200	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
2			Indane	118	C9H10	000496-11-7	76
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
4			Delatacyclene	118	C9H10	007785-10-6	58
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029573.D
Acq On : 18 Jun 2022 16:36
Operator : JC/MD
Sample : N3325-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

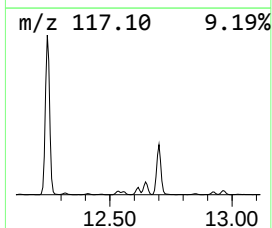
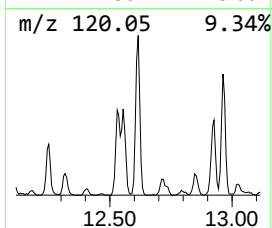
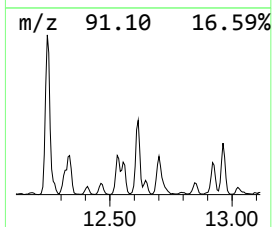
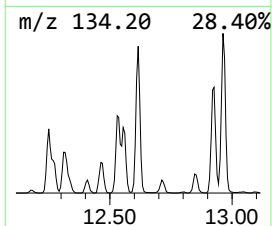
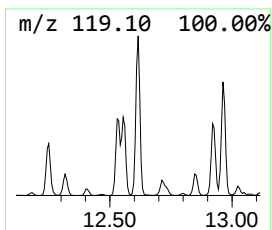
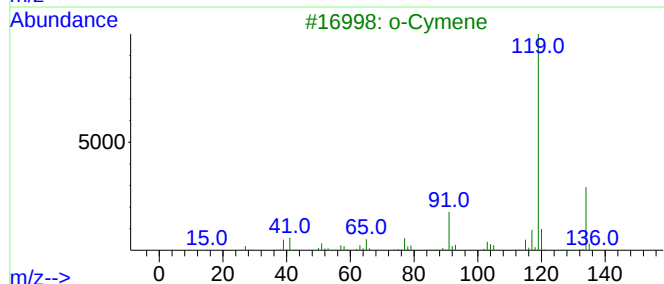
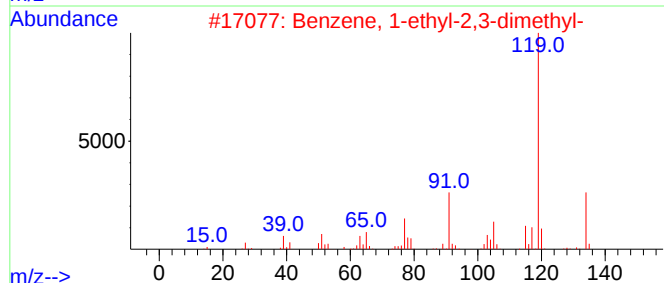
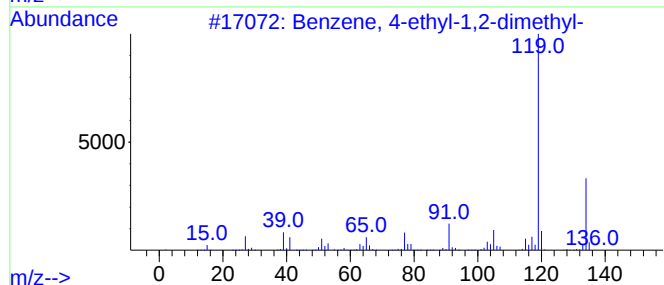
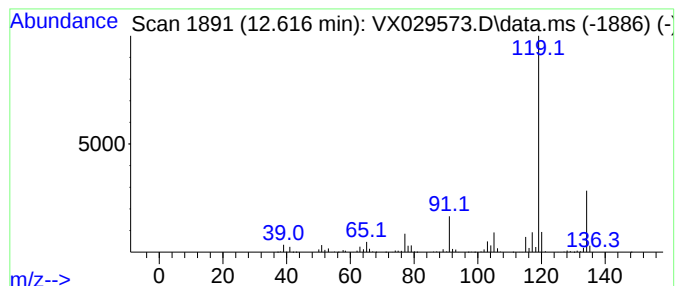
Instrument :
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ClientSampleId :
MW-17

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 7 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.616	25.76 ug/l	545960	1,4-Dichlorobenzene-d4			12.024
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-		134	C10H14	000934-80-5	95
2	Benzene, 1-ethyl-2,3-dimethyl-		134	C10H14	000933-98-2	95
3	o-Cymene		134	C10H14	000527-84-4	95
4	Benzene, 1-ethyl-2,4-dimethyl-		134	C10H14	000874-41-9	94
5	Benzene, 2-ethyl-1,3-dimethyl-		134	C10H14	002870-04-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029573.D
Acq On : 18 Jun 2022 16:36
Operator : JC/MD
Sample : N3325-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-17

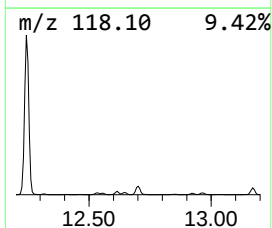
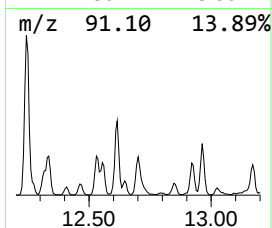
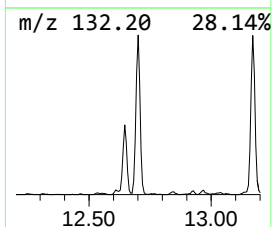
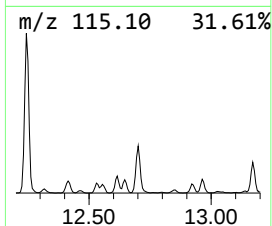
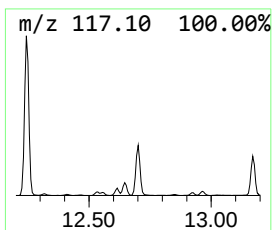
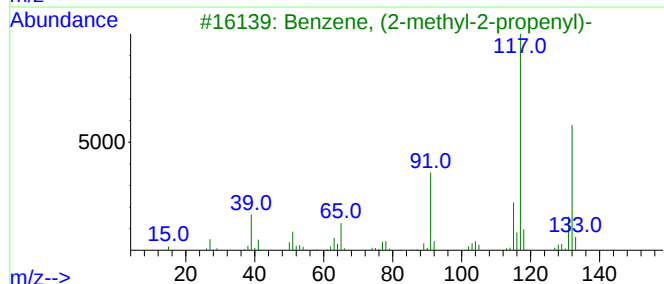
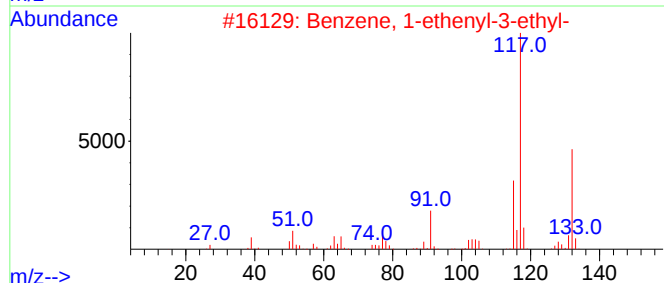
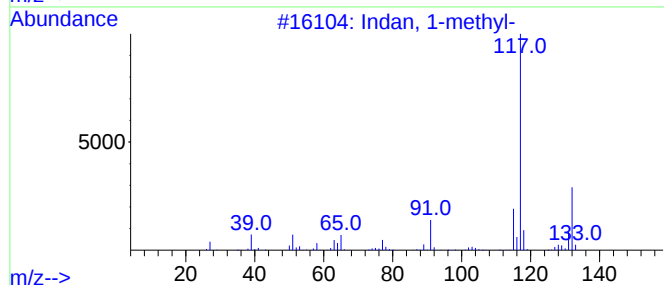
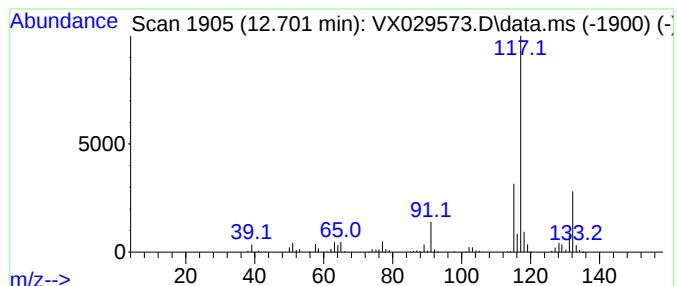
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Quant Title : SW846 8260

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

Peak Number 8 Indan, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	21.30 ug/l	451463	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	87
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
3			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	86
4			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	86
5			1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029573.D
Acq On : 18 Jun 2022 16:36
Operator : JC/MD
Sample : N3325-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-17

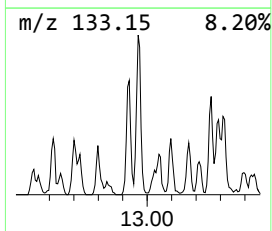
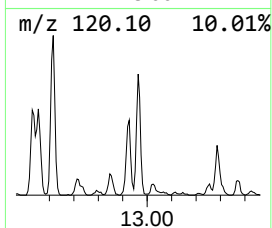
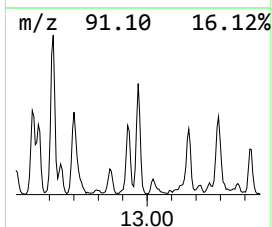
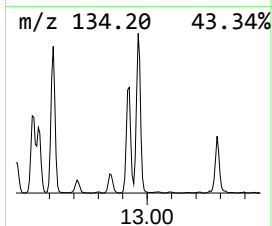
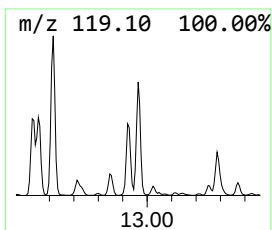
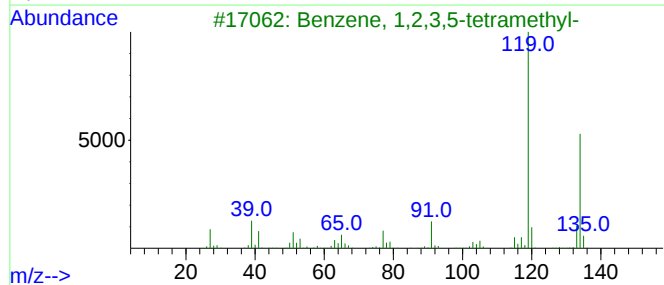
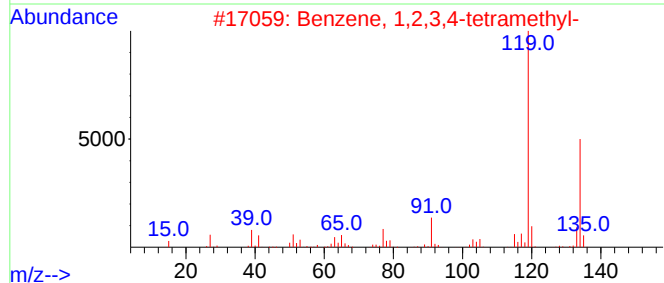
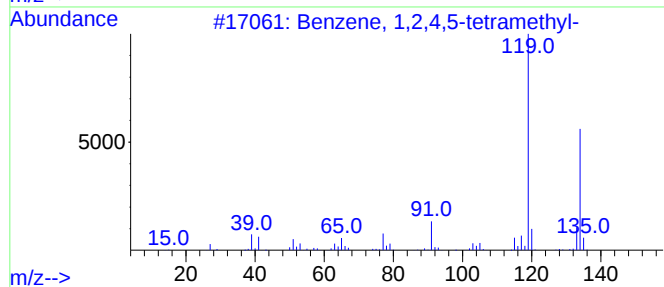
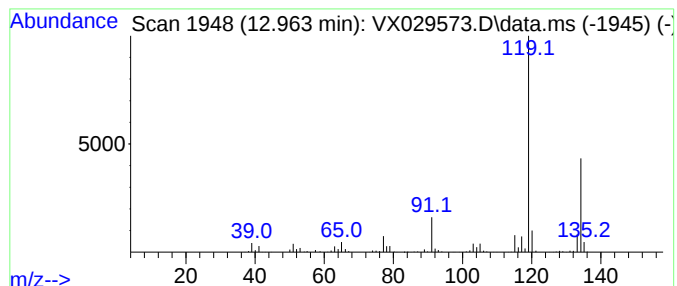
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	18.81 ug/l	398515	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029573.D
Acq On : 18 Jun 2022 16:36
Operator : JC/MD
Sample : N3325-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-17

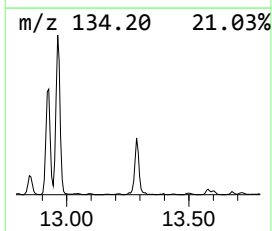
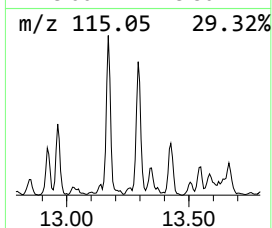
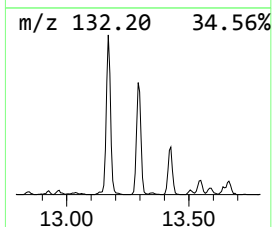
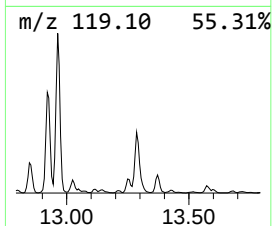
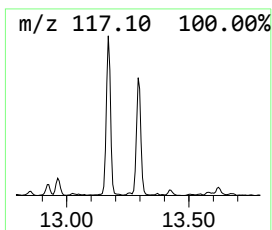
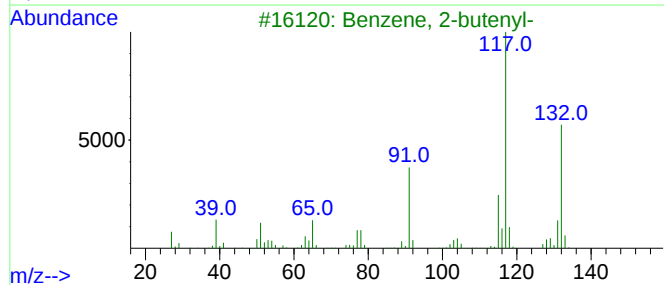
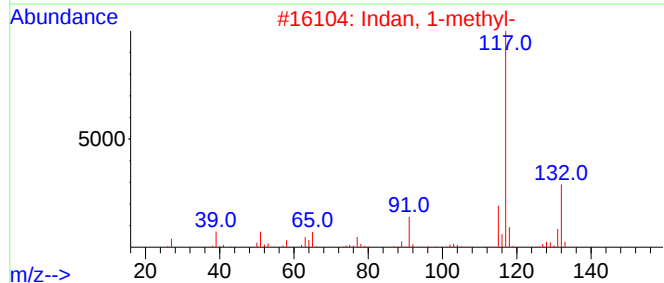
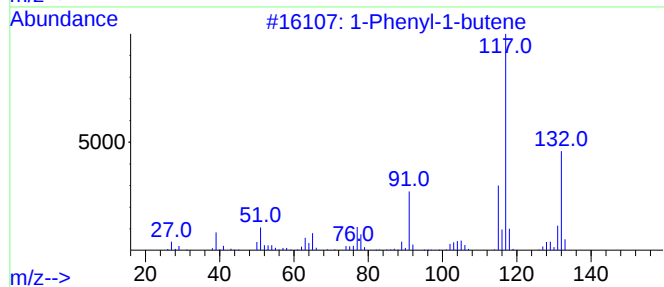
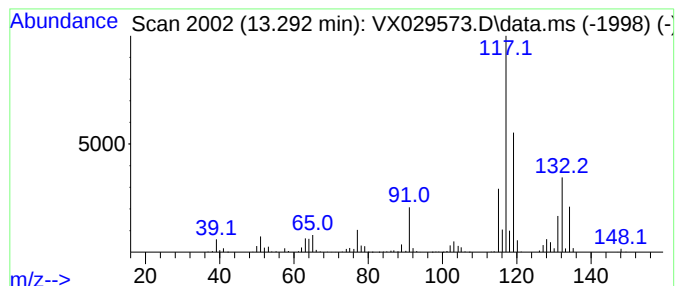
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Quant Title : SW846 8260

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

Peak Number 10 1-Phenyl-1-butene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	17.99 ug/l	381242	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenyl-1-butene	132	C10H12	000824-90-8	83
2		Indan, 1-methyl-	132	C10H12	000767-58-8	70
3		Benzene, 2-butenyl-	132	C10H12	001560-06-1	70
4		3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
5		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029573.D
Acq On : 18 Jun 2022 16:36
Operator : JC/MD
Sample : N3325-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-17

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Cyclopentane, m...	4.306	27.4	ug/l	376506	1	5.556	687779	50.0
Benzene, 1-ethy...	11.378	31.8	ug/l	672713	4	12.024	1059530	50.0
Benzene, 1-ethy...	11.616	42.2	ug/l	893937	4	12.024	1059530	50.0
Benzene, 1-ethy...	12.091	40.0	ug/l	846831	4	12.024	1059530	50.0
Benzene, cyclop...	12.244	76.5	ug/l	1621200	4	12.024	1059530	50.0
Benzene, 4-ethy...	12.616	25.8	ug/l	545960	4	12.024	1059530	50.0
Indan, 1-methyl-	12.701	21.3	ug/l	451463	4	12.024	1059530	50.0
Benzene, 1,2,4,...	12.963	18.8	ug/l	398515	4	12.024	1059530	50.0
1-Phenyl-1-butene	13.292	18.0	ug/l	381242	4	12.024	1059530	50.0