

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
 Data File : VX027250.D
 Acq On : 01 Mar 2022 15:53
 Operator : JC/MD
 Sample : N1688-14
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-31

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\82X022322W.M
 Title : SW846 8260

Signal : TIC: VX027250.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.282	23	32	45	rBV	57322	213068	51.36%	5.076%
2	1.374	45	47	51	rVB	7903	10098	2.43%	0.241%
3	1.752	105	109	124	rVB2	9374	16801	4.05%	0.400%
4	1.959	139	143	149	rVB3	3445	6624	1.60%	0.158%
5	2.221	181	186	196	rVB	7103	11379	2.74%	0.271%
6	2.538	230	238	243	rBV2	2062	4693	1.13%	0.112%
7	2.751	262	273	276	rBV3	3435	7308	1.76%	0.174%
8	2.873	287	293	301	rVB3	9162	19098	4.60%	0.455%
9	2.959	301	307	321	rVB	21189	46722	11.26%	1.113%
10	3.117	323	333	345	rVB	32412	76978	18.56%	1.834%
11	3.770	427	440	447	rBV4	5364	19134	4.61%	0.456%
12	3.843	447	452	458	rVV4	2166	5414	1.31%	0.129%
13	4.105	489	495	504	rVB4	2127	5514	1.33%	0.131%
14	4.312	519	529	540	rBV2	11363	32588	7.86%	0.776%
15	4.428	540	548	558	rVB2	2314	5830	1.41%	0.139%
16	5.196	666	674	687	rVB3	3425	9629	2.32%	0.229%
17	5.391	694	706	715	rBV	49099	141789	34.18%	3.378%
18	5.483	716	721	725	rVV4	5253	13725	3.31%	0.327%
19	5.562	725	734	754	rVB	83372	238623	57.53%	5.684%
20	5.964	787	800	806	rBV	51174	135934	32.77%	3.238%
21	6.044	806	813	827	rVV	70573	186547	44.97%	4.444%
22	6.202	827	839	856	rVB5	4682	17974	4.33%	0.428%
23	6.769	921	932	943	rBV	128330	309194	74.54%	7.365%
24	6.854	943	946	954	rVB5	2114	4243	1.02%	0.101%
25	7.171	993	998	1006	rVB4	2283	4974	1.20%	0.118%
26	7.379	1023	1032	1040	rBV6	4322	11177	2.69%	0.266%
27	8.141	1147	1157	1163	rBV	5893	12356	2.98%	0.294%
28	8.427	1195	1204	1210	rBV	4739	8226	1.98%	0.196%
29	8.506	1210	1217	1222	rVB2	5781	9468	2.28%	0.226%
30	8.653	1234	1241	1248	rBV	257130	414812	100.00%	9.881%
31	8.720	1248	1252	1258	rVB	4948	7830	1.89%	0.187%
32	8.958	1284	1291	1300	rVB	13701	23409	5.64%	0.558%
33	9.049	1300	1306	1313	rBV	14813	22861	5.51%	0.545%
34	9.458	1364	1373	1377	rBV5	2105	4538	1.09%	0.108%
35	10.055	1466	1471	1482	rBV	262871	346445	83.52%	8.253%
36	10.195	1489	1494	1500	rBV	34640	44060	10.62%	1.050%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

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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	10.305	1506	1512	1518	rVB	35622	46777	11.28%	1.114%
38	10.640	1563	1567	1573	rVB	7713	10263	2.47%	0.244%
39	10.963	1615	1620	1625	rBV	38746	47750	11.51%	1.137%
40	11.079	1634	1639	1650	rBV	206440	267442	64.47%	6.371%
41	11.305	1668	1676	1684	rBV	40473	50188	12.10%	1.196%
42	11.402	1684	1692	1697	rVV	6153	8689	2.09%	0.207%
43	11.451	1697	1700	1707	rVB	7277	8784	2.12%	0.209%
44	11.616	1722	1727	1733	rBV	34408	41181	9.93%	0.981%
45	11.756	1746	1750	1755	rVB	15180	18762	4.52%	0.447%
46	11.890	1770	1772	1777	rVB2	5169	5699	1.37%	0.136%
47	12.024	1789	1794	1800	rBV	254381	307178	74.05%	7.317%
48	12.091	1800	1805	1810	rVB	21409	27257	6.57%	0.649%
49	12.244	1823	1830	1838	rBV	184306	235914	56.87%	5.620%
50	12.317	1838	1842	1850	rVB3	5947	10097	2.43%	0.241%
51	12.414	1853	1858	1862	rBV3	9897	13928	3.36%	0.332%
52	12.469	1862	1867	1871	rVB2	3666	5084	1.23%	0.121%
53	12.616	1886	1891	1894	rBV	29248	36659	8.84%	0.873%
54	12.646	1894	1896	1900	rVV	10035	10525	2.54%	0.251%
55	12.701	1900	1905	1912	rVB2	51181	72600	17.50%	1.729%
56	12.841	1923	1928	1935	rVB2	5300	7965	1.92%	0.190%
57	12.920	1935	1941	1945	rBV	24011	31919	7.69%	0.760%
58	12.963	1945	1948	1955	rVB	10766	12765	3.08%	0.304%
59	13.030	1955	1959	1964	rBV3	3837	5245	1.26%	0.125%
60	13.170	1978	1982	1990	rVB	21862	28339	6.83%	0.675%
61	13.292	1990	2002	2007	rBV2	62510	89740	21.63%	2.138%
62	13.347	2007	2011	2014	rBV3	7723	9801	2.36%	0.233%
63	13.426	2020	2024	2029	rVB2	16790	22449	5.41%	0.535%
64	13.548	2040	2044	2047	rVV2	11016	15406	3.71%	0.367%
65	13.585	2047	2050	2054	rVV3	8248	13304	3.21%	0.317%
66	13.646	2054	2060	2061	rVV3	6843	12349	2.98%	0.294%
67	13.664	2061	2063	2070	rVV2	10912	15801	3.81%	0.376%
68	13.774	2074	2081	2090	rVB	37992	56450	13.61%	1.345%
69	13.859	2090	2095	2100	rBV3	4418	8396	2.02%	0.200%
70	13.932	2100	2107	2110	rBV3	8344	12213	2.94%	0.291%
71	14.079	2126	2131	2134	rBV2	6020	8812	2.12%	0.210%
72	14.219	2149	2154	2160	rBV4	10811	19941	4.81%	0.475%
73	14.323	2167	2171	2176	rBV2	6819	8407	2.03%	0.200%
74	14.377	2176	2180	2184	rVB	9357	12882	3.11%	0.307%
75	14.487	2193	2198	2202	rBV3	9145	13740	3.31%	0.327%
76	14.615	2210	2219	2220	rBV3	4049	8622	2.08%	0.205%

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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

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Title : SW846 8260

77	14.640	2220	2223	2226	rVV2	6967	10255	2.47%	0.244%
78	14.676	2226	2229	2234	rVB2	4985	6676	1.61%	0.159%
79	14.780	2241	2246	2251	rBV	40432	54982	13.25%	1.310%
80	14.902	2261	2266	2274	rBV6	2058	4284	1.03%	0.102%
81	15.188	2305	2313	2320	rVB3	6172	11789	2.84%	0.281%
82	15.481	2357	2361	2365	rVV2	3513	4759	1.15%	0.113%
83	15.615	2377	2383	2387	rBV2	8024	12387	2.99%	0.295%
84	15.816	2410	2416	2417	rBV4	2924	4366	1.05%	0.104%

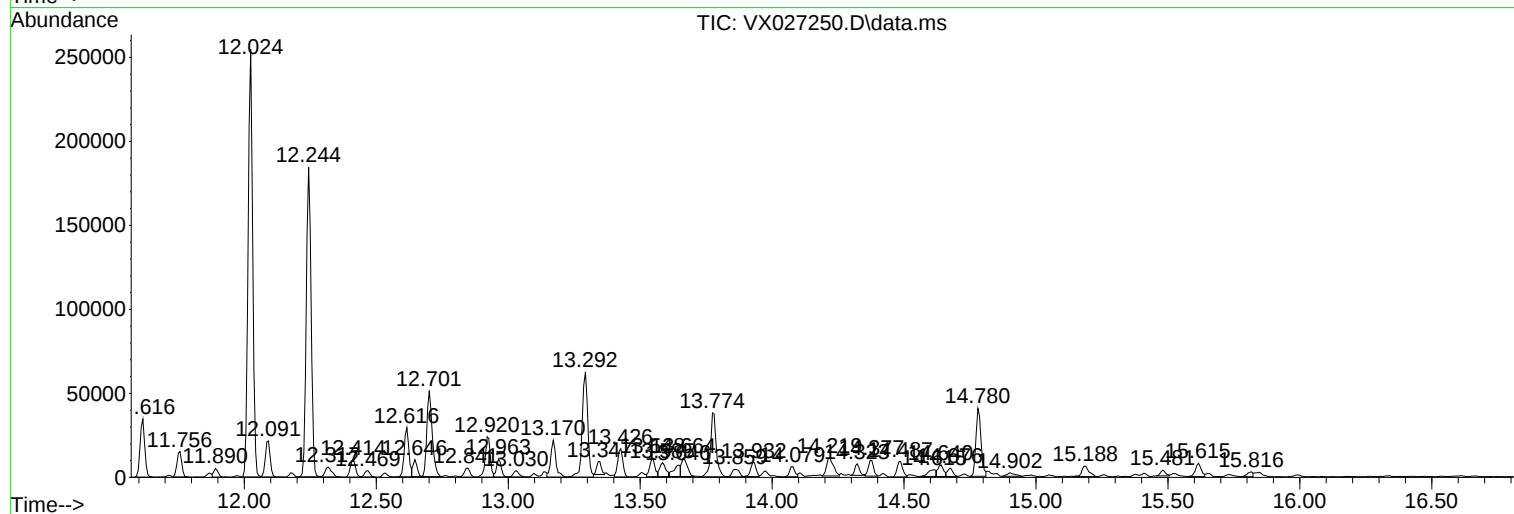
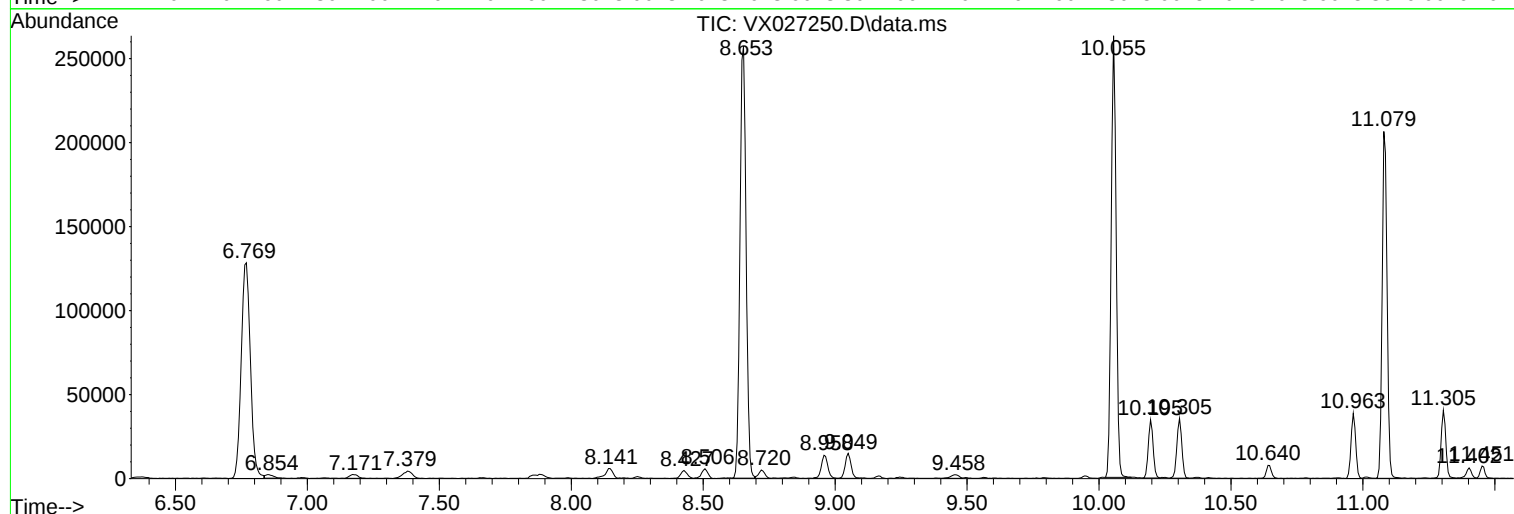
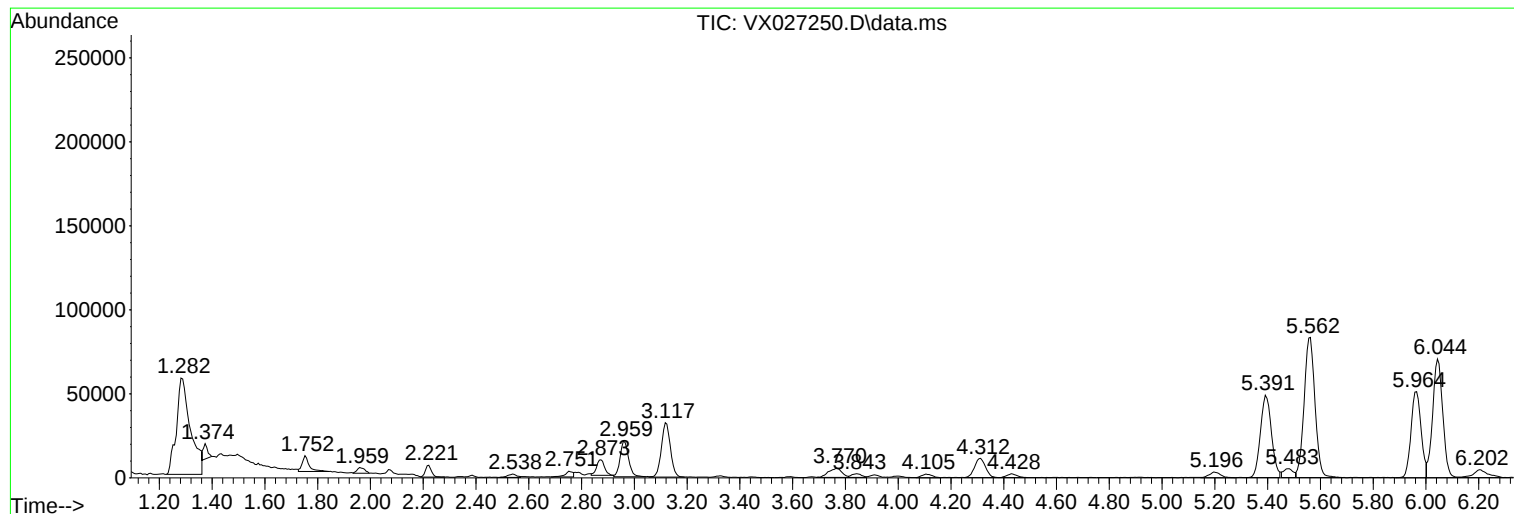
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MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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



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

Instrument :
MSVOA_X
ClientSampleId :
MW-31

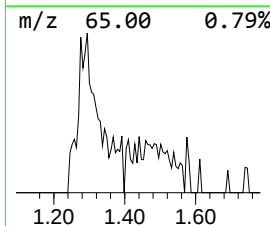
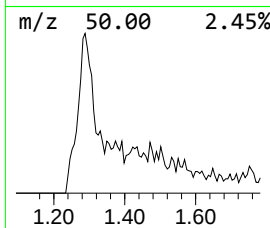
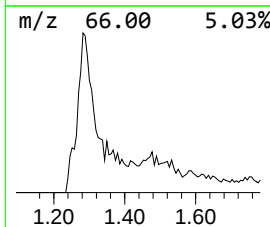
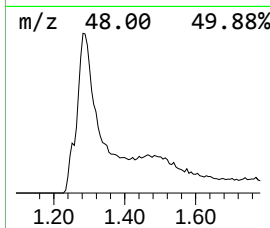
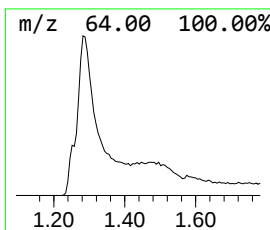
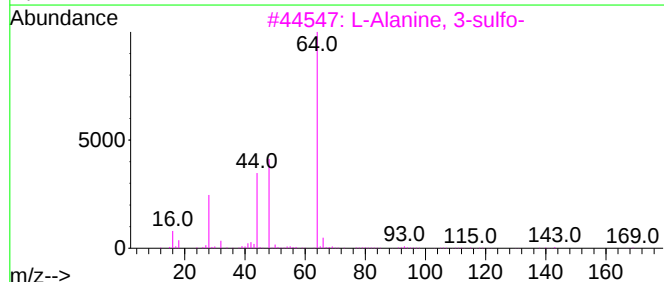
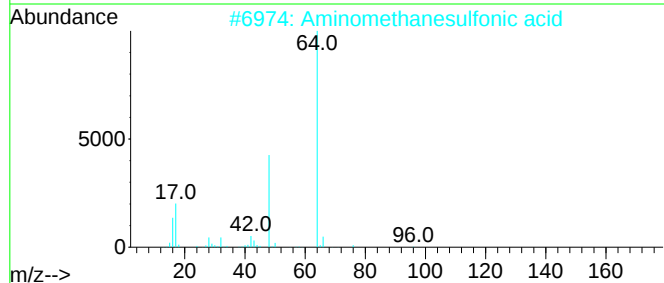
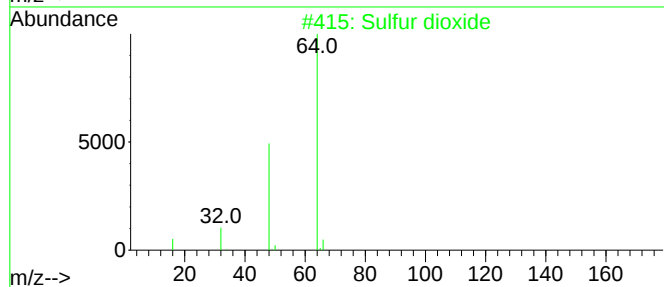
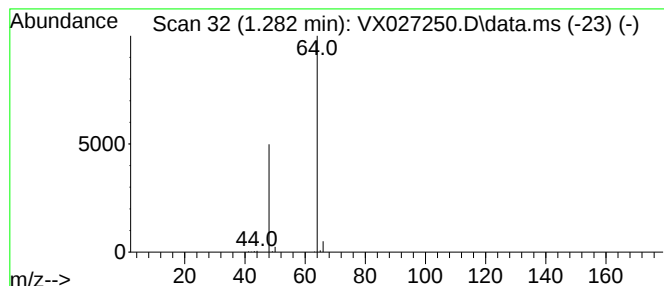
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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.
1.282	44.65 ug/l	213068	Pentafluorobenzene	5.562

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020122\
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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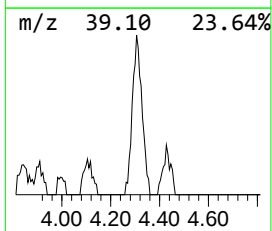
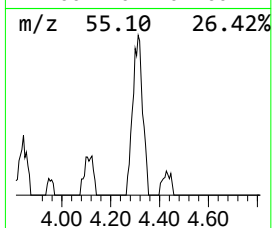
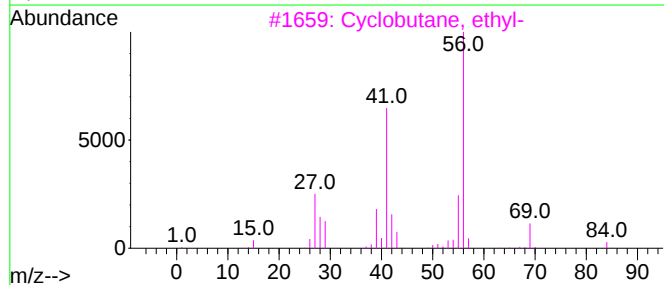
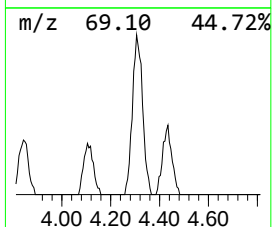
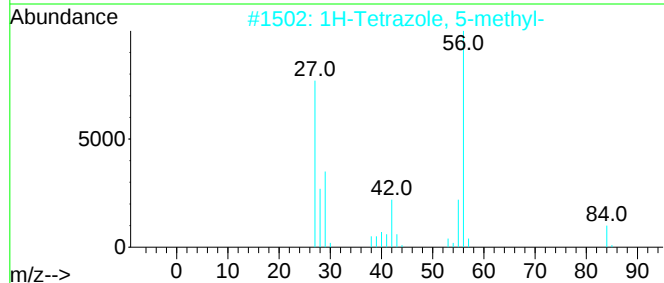
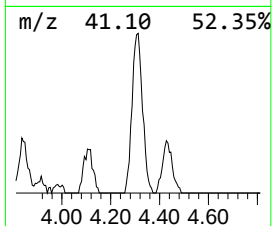
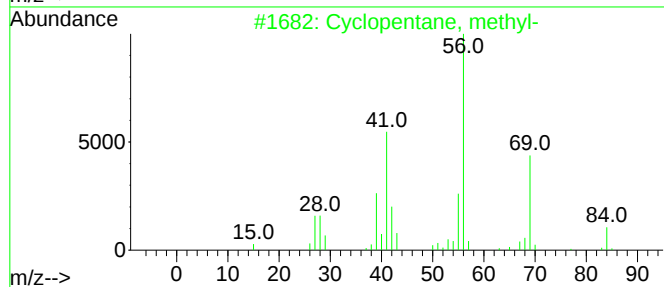
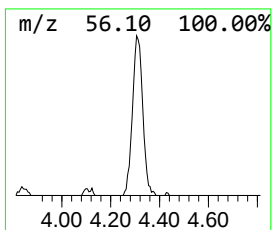
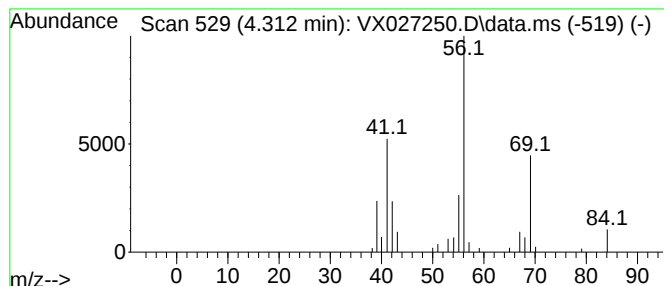
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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.
4.312	6.83 ug/l	32588	Pentafluorobenzene	5.562

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	72
3		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4		Cyclobutane	56	C4H8	000287-23-0	47
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43



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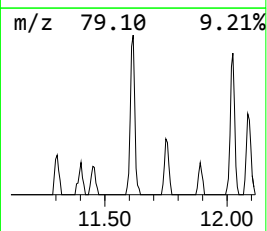
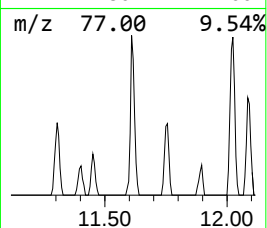
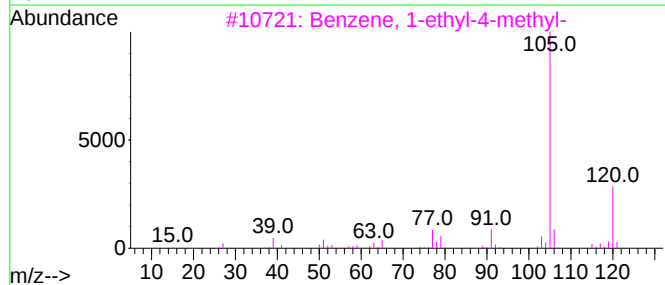
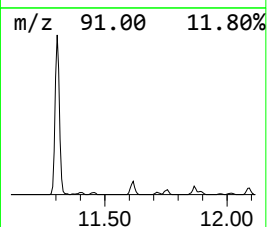
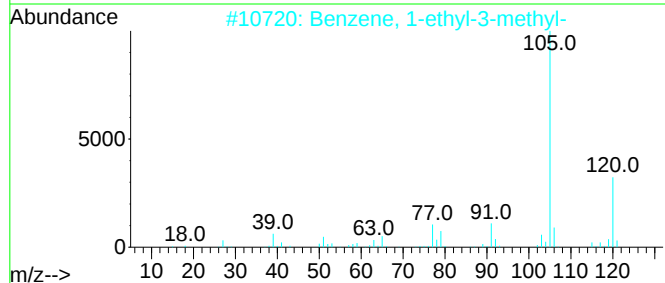
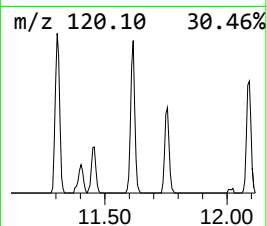
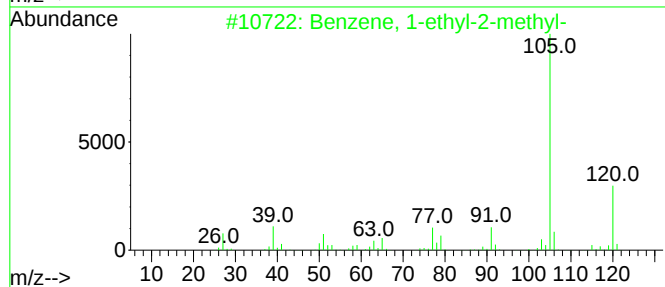
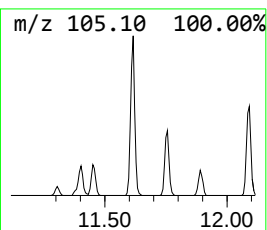
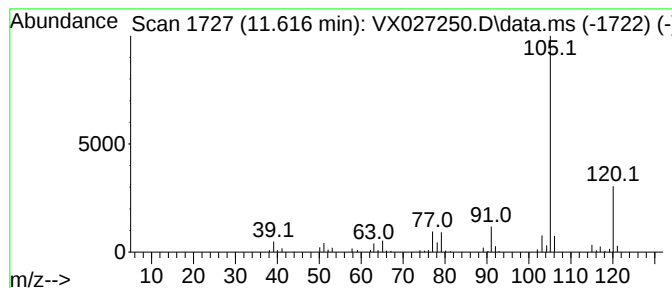
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	6.70 ug/l	41181	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-3-methyl-	120	C9H12	000620-14-4	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



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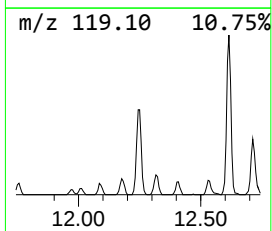
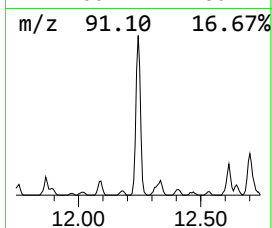
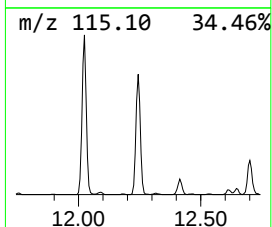
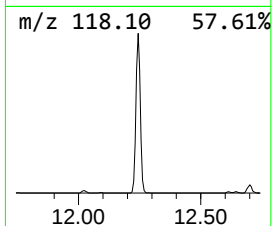
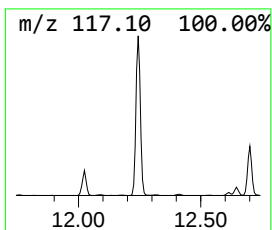
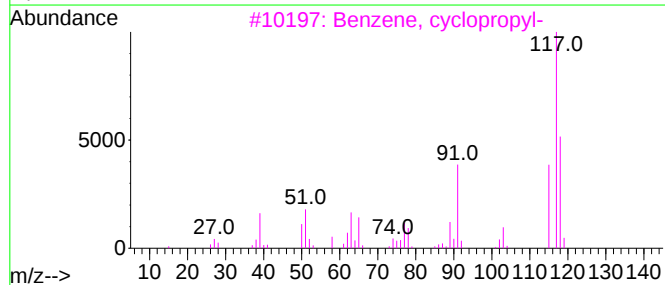
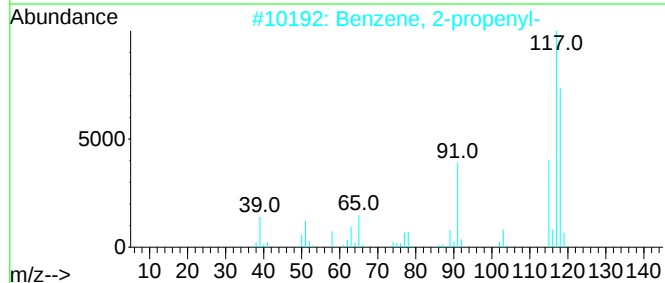
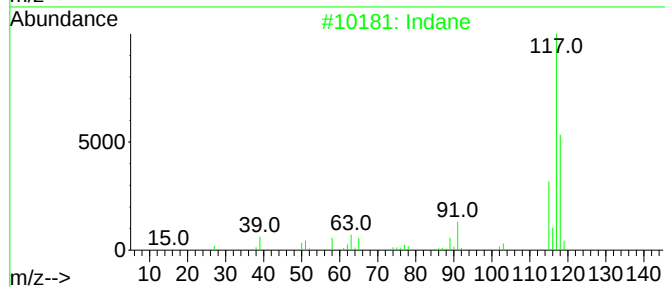
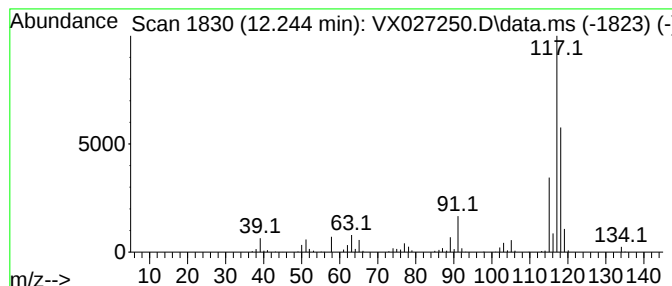
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Quant Title : SW846 8260

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

Peak Number 4 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	38.40 ug/l	235914	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	90
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5			Deltacyclene	118	C9H10	007785-10-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027250.D
Acq On : 01 Mar 2022 15:53
Operator : JC/MD
Sample : N1688-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-31

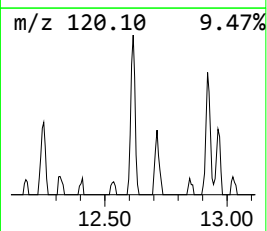
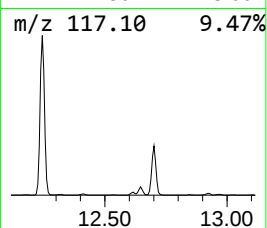
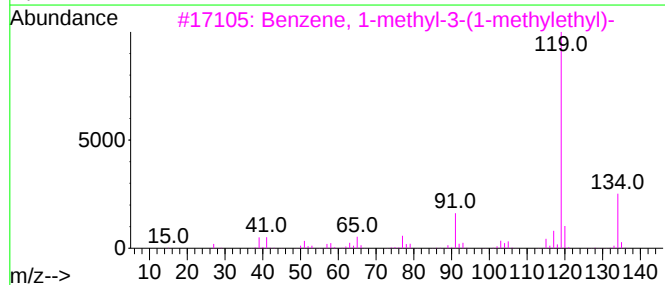
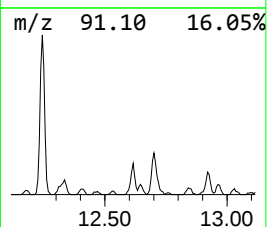
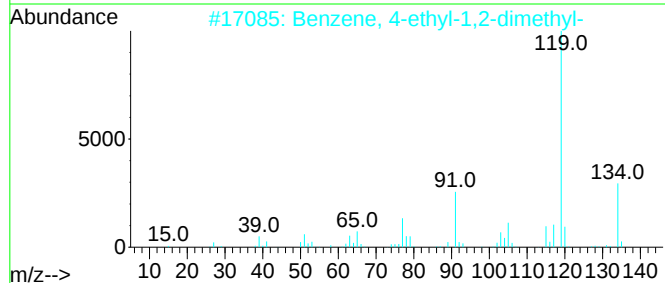
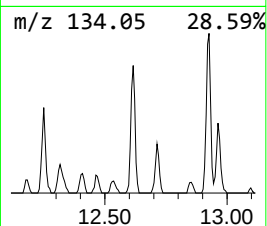
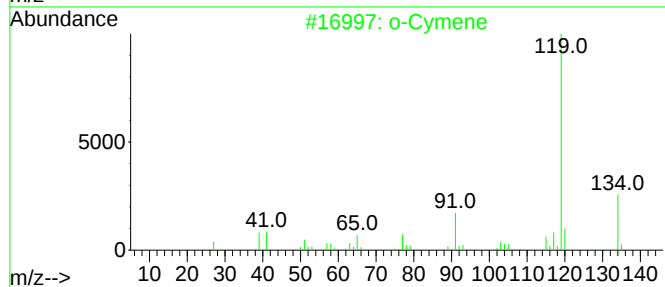
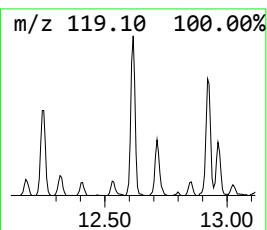
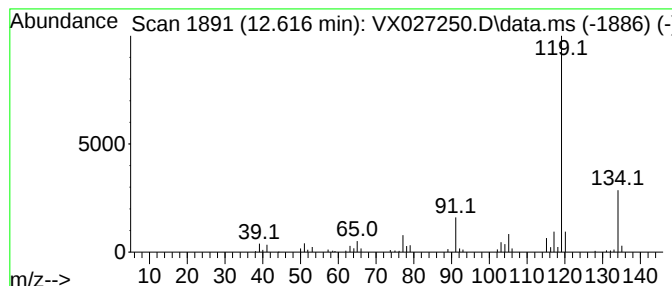
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Quant Title : SW846 8260

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

Peak Number 5 o-Cymene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	5.97 ug/l	36659	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	97
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
4			p-Cymene	134	C10H14	000099-87-6	95
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027250.D
Acq On : 01 Mar 2022 15:53
Operator : JC/MD
Sample : N1688-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-31

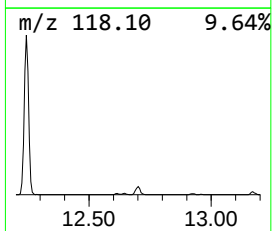
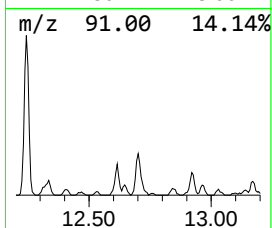
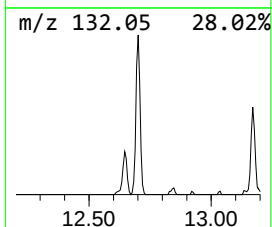
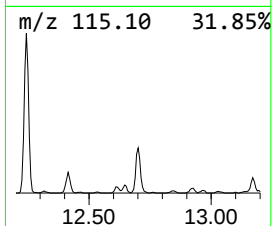
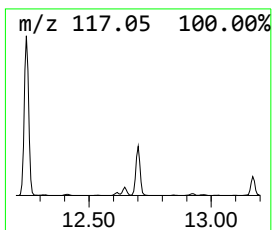
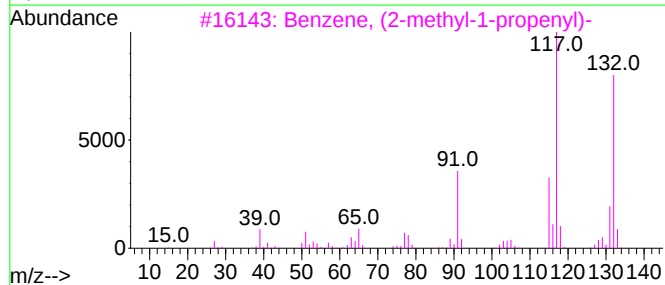
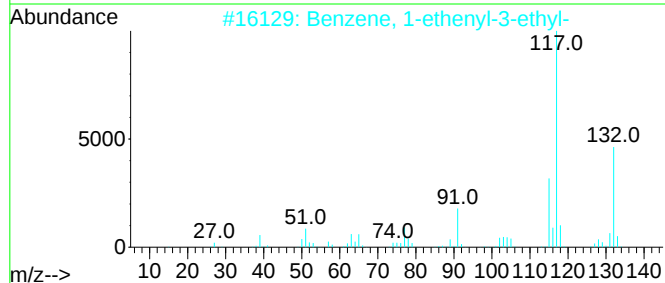
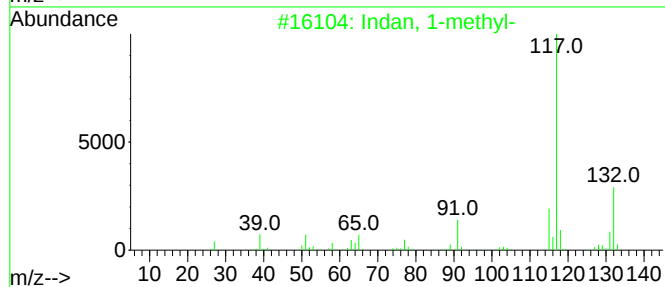
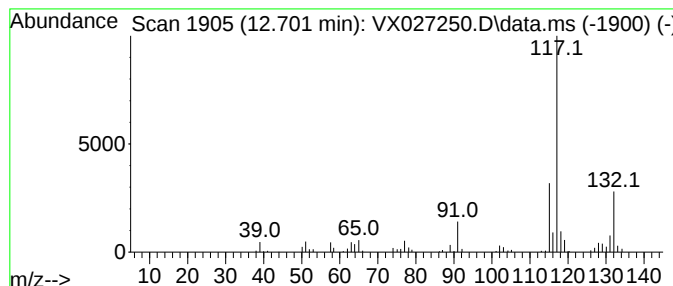
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Quant Title : SW846 8260

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

Peak Number 6 Indan, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	11.82 ug/l	72600	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-1-propenyl)-	132	C10H12	000768-49-0	83
4		Benzene, 2-butenyl-	132	C10H12	001560-06-1	80
5		1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027250.D
Acq On : 01 Mar 2022 15:53
Operator : JC/MD
Sample : N1688-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-31

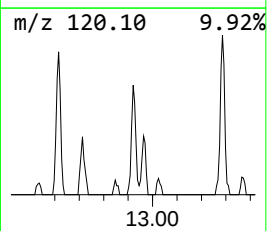
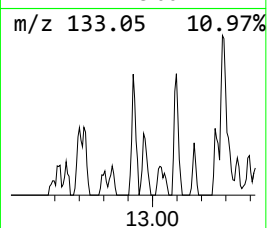
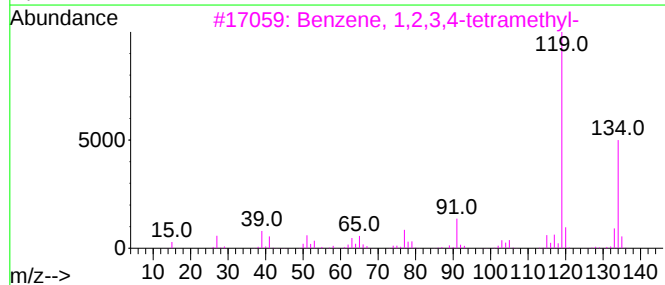
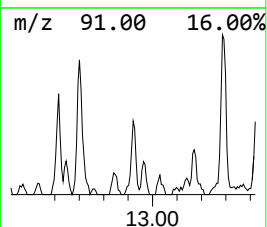
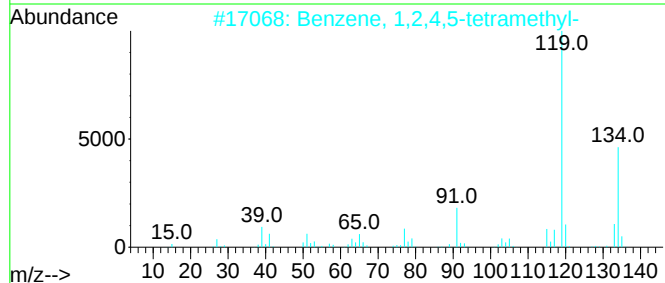
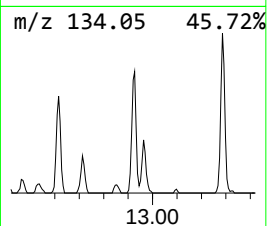
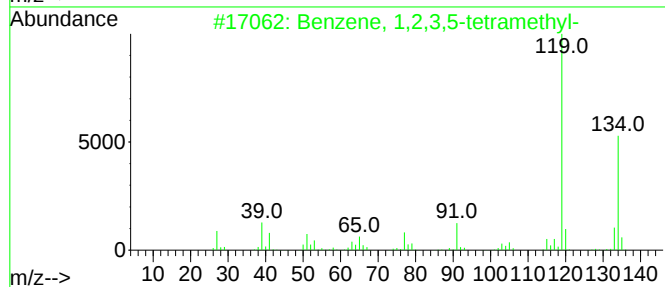
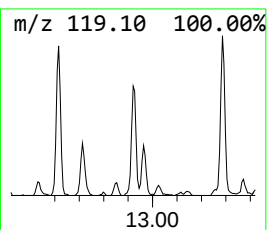
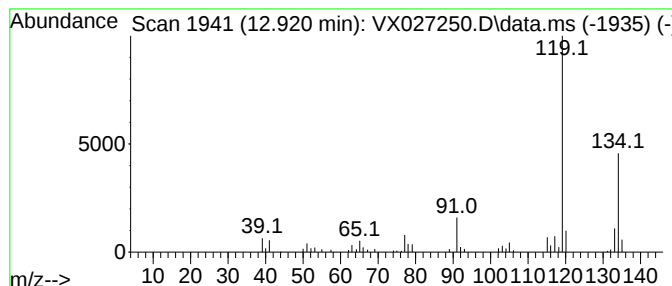
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.920	5.20 ug/l	31919	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027250.D
Acq On : 01 Mar 2022 15:53
Operator : JC/MD
Sample : N1688-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-31

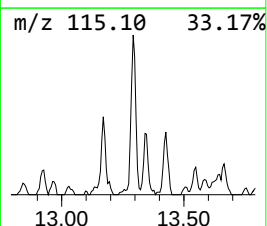
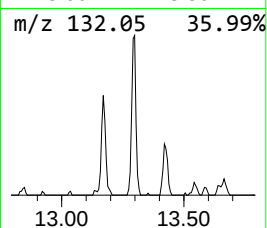
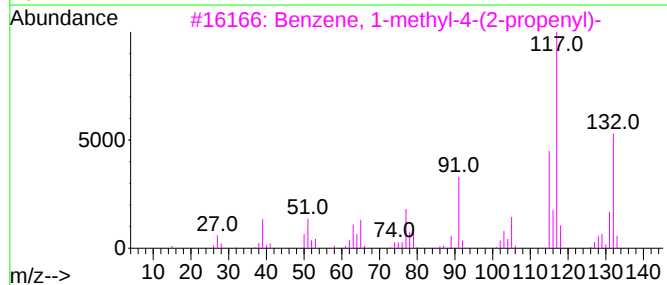
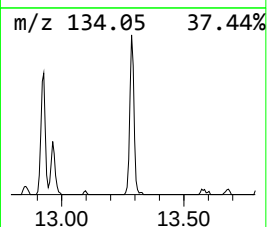
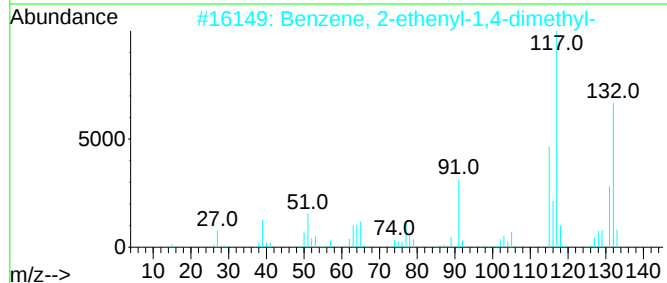
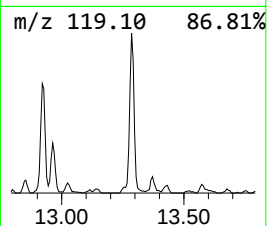
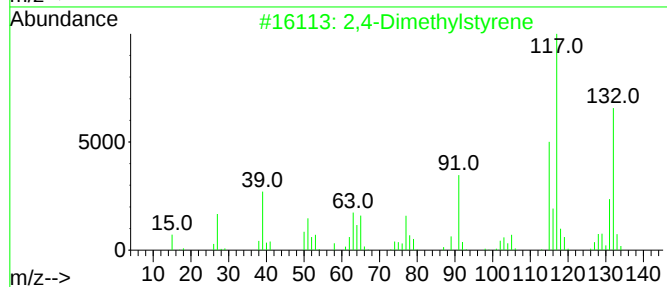
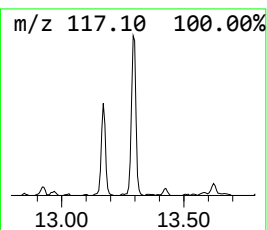
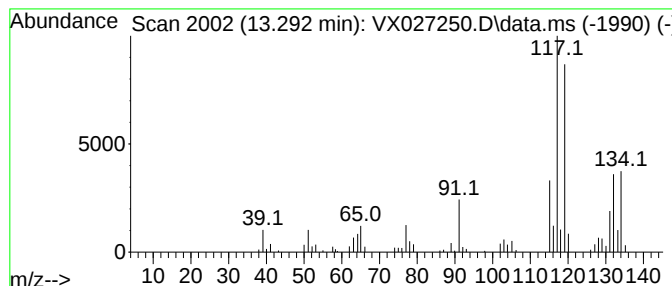
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Quant Title : SW846 8260

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

Peak Number 8 2,4-Dimethylstyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	14.61 ug/l	89740	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Dimethylstyrene	132	C10H12	002234-20-0	89
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	89
3			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	78
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	60
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027250.D
Acq On : 01 Mar 2022 15:53
Operator : JC/MD
Sample : N1688-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-31

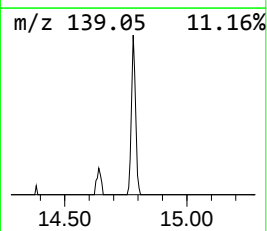
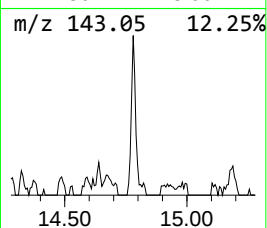
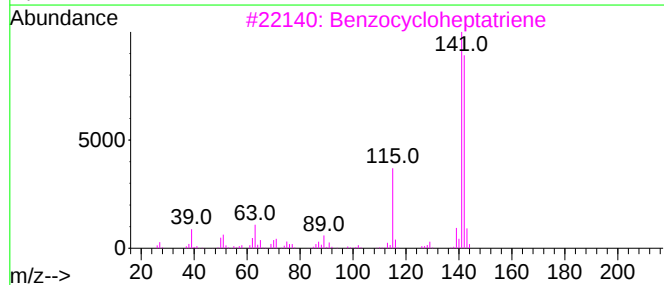
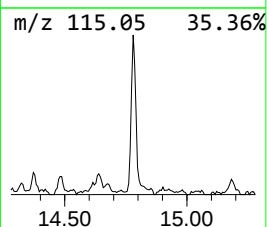
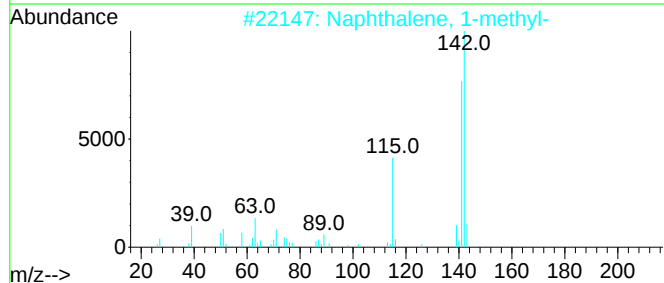
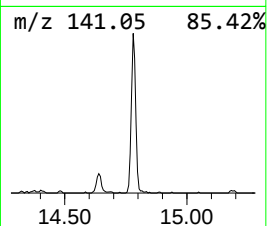
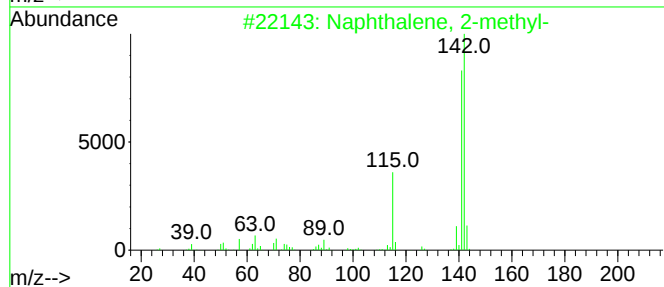
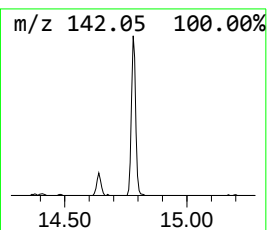
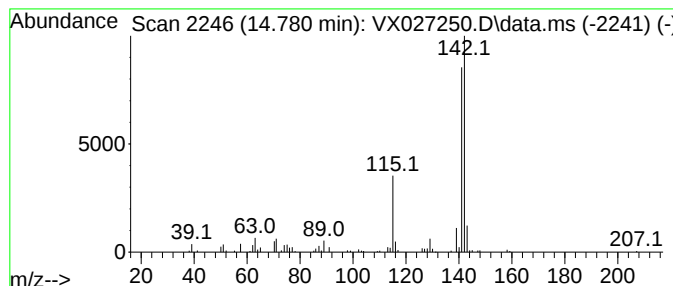
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Quant Title : SW846 8260

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

Peak Number 9 Benzocycloheptatriene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	8.95 ug/l	54982	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027250.D
Acq On : 01 Mar 2022 15:53
Operator : JC/MD
Sample : N1688-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-31

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.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...	4.312	6.8	ug/l	32588	1	5.562	238623	50.0
Benzene, 1-ethy...	11.616	6.7	ug/l	41181	4	12.024	307178	50.0
Indane	12.244	38.4	ug/l	235914	4	12.024	307178	50.0
o-Cymene	12.616	6.0	ug/l	36659	4	12.024	307178	50.0
Indan, 1-methyl-	12.701	11.8	ug/l	72600	4	12.024	307178	50.0
Benzene, 1,2,3,...	12.920	5.2	ug/l	31919	4	12.024	307178	50.0
2,4-Dimethylsty...	13.292	14.6	ug/l	89740	4	12.024	307178	50.0
Benzocyclohepta...	14.780	8.9	ug/l	54982	4	12.024	307178	50.0