

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
 Data File : VX023006.D
 Acq On : 29 Jun 2021 16:19
 Operator : JC/MD
 Sample : M2875-16
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-3

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\82X062321W.M
 Title : SW846 8260

Signal : TIC: VX023006.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.313	24	37	55	rBV2	76629	570717	4.09%	0.834%
2	3.105	321	331	345	rVB	71441	162460	1.16%	0.238%
3	4.312	520	529	540	rVB	74748	215326	1.54%	0.315%
4	5.397	693	707	714	rBV	46299	141629	1.01%	0.207%
5	5.501	714	724	729	rBV5	48467	187580	1.34%	0.274%
6	5.629	739	745	764	rVB2	102481	330254	2.37%	0.483%
7	5.830	767	778	791	rBV3	83266	252501	1.81%	0.369%
8	5.964	791	800	806	rVV2	56970	154270	1.11%	0.226%
9	6.044	806	813	824	rVV	255094	680941	4.88%	0.996%
10	6.172	824	834	842	rVV5	64341	301230	2.16%	0.440%
11	6.257	842	848	858	rVV2	147727	447453	3.21%	0.654%
12	6.769	923	932	939	rBV	128054	328601	2.35%	0.480%
13	6.854	940	946	957	rVB3	55965	167281	1.20%	0.245%
14	7.379	1020	1032	1045	rBV4	122009	350108	2.51%	0.512%
15	7.988	1122	1132	1144	rVB2	95857	249096	1.78%	0.364%
16	8.110	1144	1152	1162	rBV2	134188	350135	2.51%	0.512%
17	8.513	1212	1218	1226	rVB5	94897	218008	1.56%	0.319%
18	8.610	1226	1234	1236	rBV2	93752	171730	1.23%	0.251%
19	8.653	1236	1241	1247	rVB	280011	467758	3.35%	0.684%
20	8.726	1247	1253	1258	rBV	245581	409137	2.93%	0.598%
21	9.104	1309	1315	1321	rVB	86518	146671	1.05%	0.214%
22	9.165	1321	1325	1330	rBV	105724	148355	1.06%	0.217%
23	10.055	1467	1471	1476	rBV	241103	327676	2.35%	0.479%
24	10.201	1489	1495	1505	rBV	9082160	12017569	86.09%	17.569%
25	10.305	1509	1512	1518	rVB	116828	169448	1.21%	0.248%
26	10.646	1563	1568	1573	rVB	220609	280677	2.01%	0.410%
27	10.963	1615	1620	1628	rBV	549654	705134	5.05%	1.031%
28	11.085	1635	1640	1644	rBV	205240	258369	1.85%	0.378%
29	11.305	1666	1676	1682	rBV	1096268	1390298	9.96%	2.033%
30	11.616	1722	1727	1736	rVB	2251305	2736127	19.60%	4.000%
31	11.762	1745	1751	1756	rVB	11064211	13959871	100.00%	20.409%
32	12.024	1789	1794	1798	rBV2	273064	377715	2.71%	0.552%
33	12.091	1801	1805	1809	rVB	188995	220690	1.58%	0.323%
34	12.250	1825	1831	1837	rBV	7532204	9195622	65.87%	13.444%
35	12.311	1837	1841	1850	rVB2	509388	777718	5.57%	1.137%
36	12.414	1852	1858	1863	rBV	1220998	1538334	11.02%	2.249%

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37	12.469	1863	1867	1873	rVB2	313226	440878	3.16%	0.645%
38	12.536	1873	1878	1880	rBV	778312	1029363	7.37%	1.505%
39	12.555	1880	1881	1886	rVB	467426	460569	3.30%	0.673%
40	12.616	1886	1891	1894	rBV	1137005	1335075	9.56%	1.952%
41	12.646	1894	1896	1900	rVV	351356	399846	2.86%	0.585%
42	12.701	1900	1905	1913	rVV	1398520	1874849	13.43%	2.741%
43	12.926	1933	1942	1945	rBV	1059318	1286702	9.22%	1.881%
44	12.963	1945	1948	1954	rVV	1311497	1643538	11.77%	2.403%
45	13.024	1954	1958	1967	rVB2	152507	246991	1.77%	0.361%
46	13.170	1978	1982	1987	rVB	1159640	1355837	9.71%	1.982%
47	13.256	1992	1996	1998	rBV2	124954	167241	1.20%	0.245%
48	13.292	1998	2002	2007	rVV2	831142	1104855	7.91%	1.615%
49	13.347	2007	2011	2019	rVB4	387677	566677	4.06%	0.828%
50	13.426	2019	2024	2032	rVB	677736	851716	6.10%	1.245%
51	13.506	2032	2037	2040	rBV2	178398	240865	1.73%	0.352%
52	13.548	2040	2044	2047	rVV	364284	478347	3.43%	0.699%
53	13.585	2047	2050	2056	rVV2	293289	519032	3.72%	0.759%
54	13.646	2056	2060	2061	rVV	145035	202004	1.45%	0.295%
55	13.664	2061	2063	2070	rVB2	333715	496406	3.56%	0.726%
56	13.780	2074	2082	2091	rBV	297101	432456	3.10%	0.632%
57	13.871	2091	2097	2101	rBV	376343	490652	3.51%	0.717%
58	13.926	2101	2106	2110	rBV2	159165	210686	1.51%	0.308%
59	14.079	2126	2131	2137	rBV	294613	369541	2.65%	0.540%
60	14.219	2149	2154	2159	rBV	229179	361055	2.59%	0.528%
61	14.323	2167	2171	2176	rBV	127356	177520	1.27%	0.260%
62	14.377	2176	2180	2185	rVB2	167747	213943	1.53%	0.313%
63	14.780	2241	2246	2256	rBV	776777	1037189	7.43%	1.516%

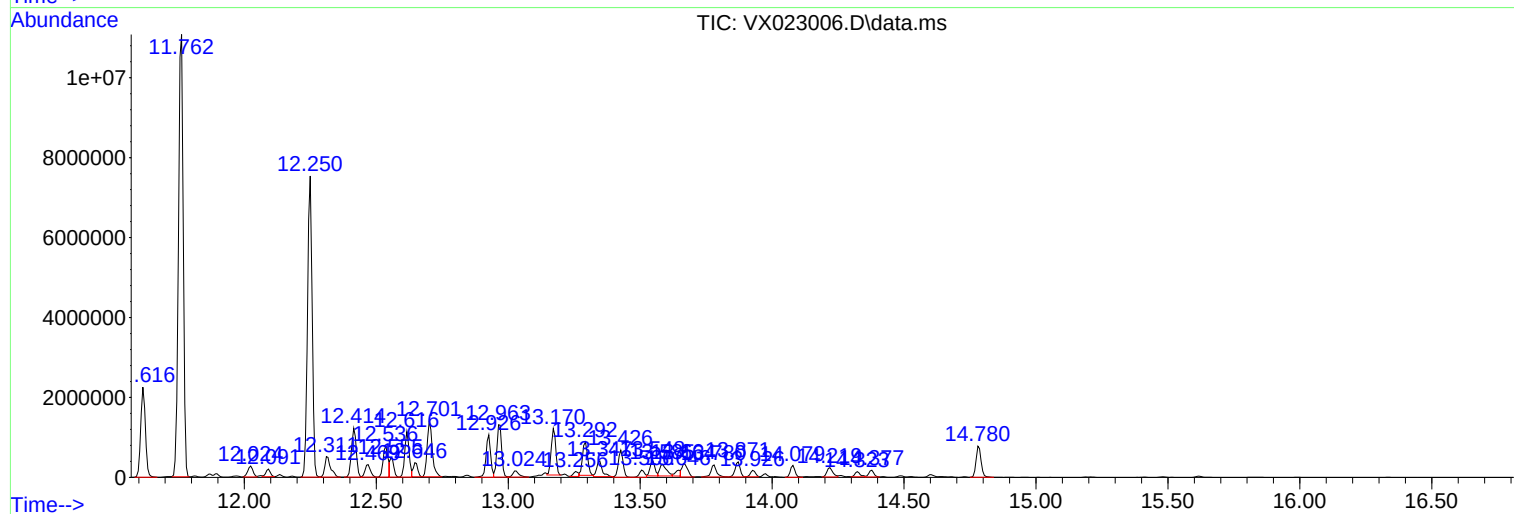
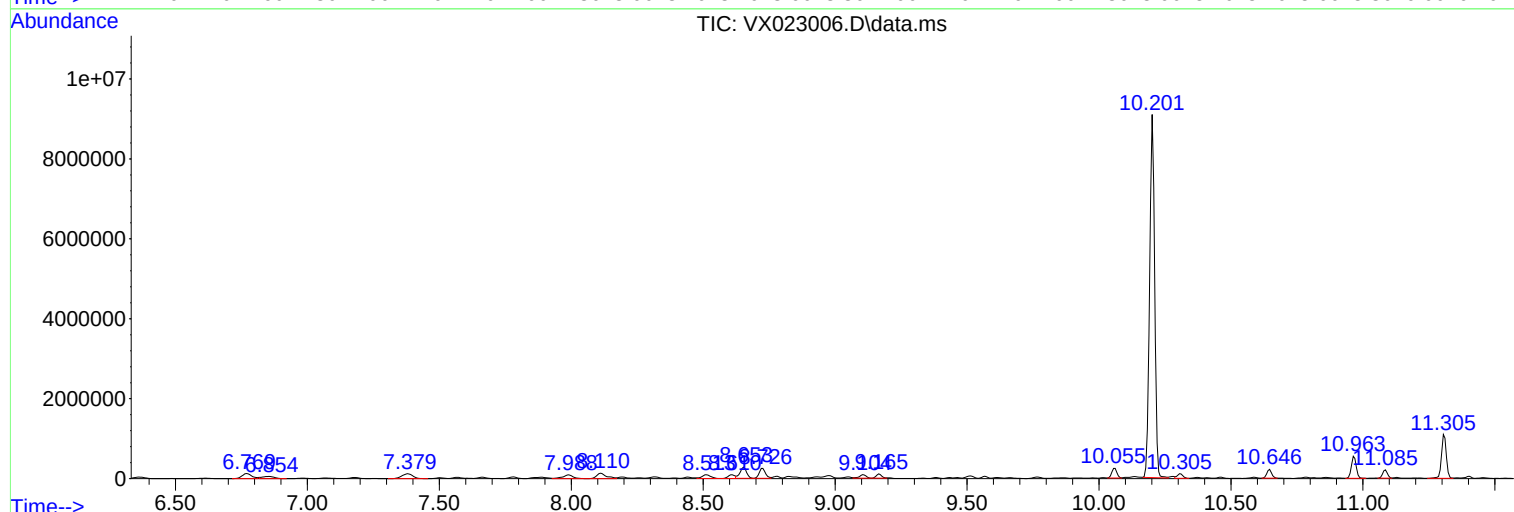
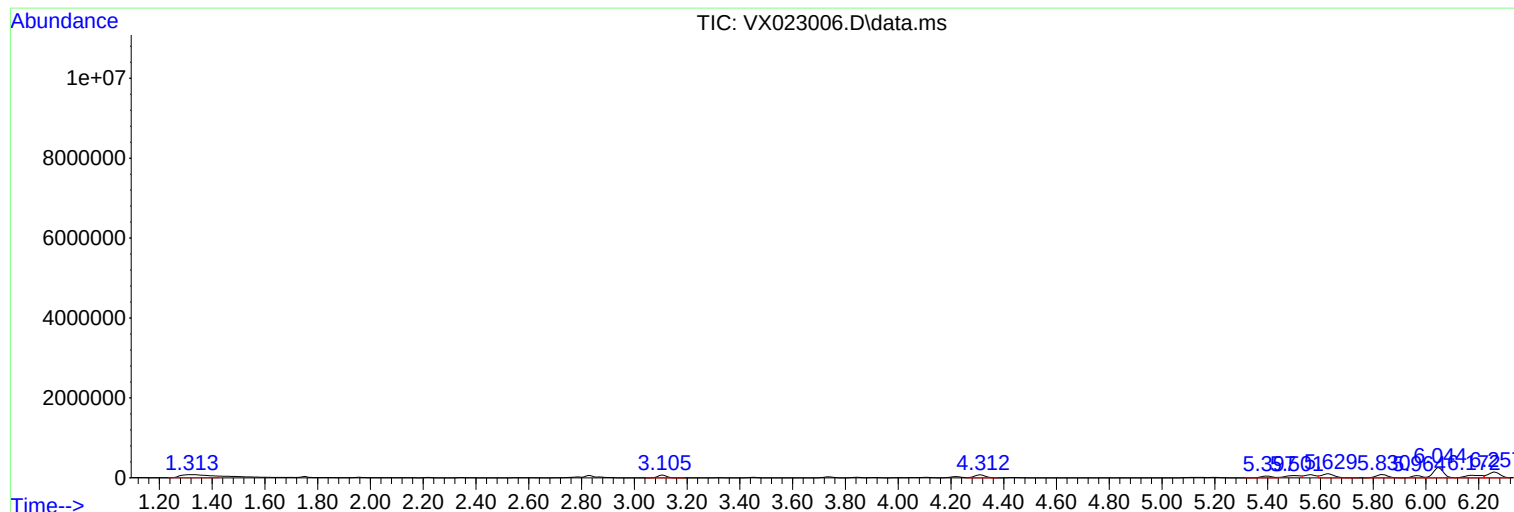
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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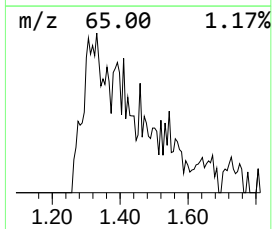
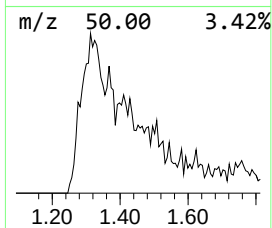
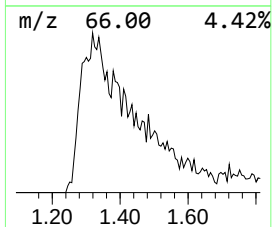
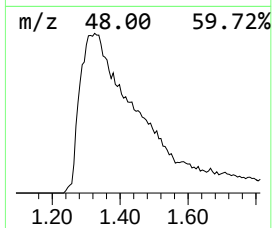
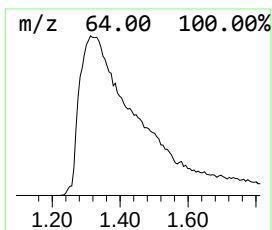
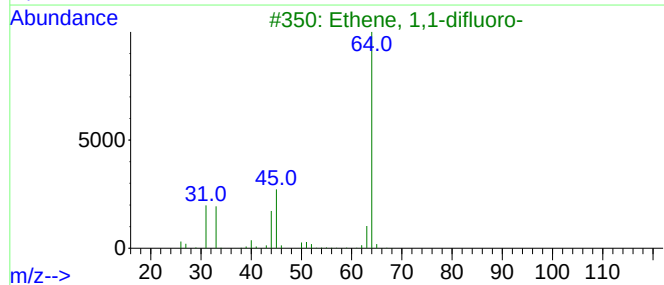
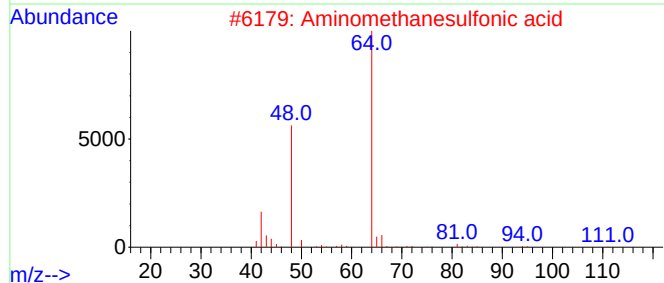
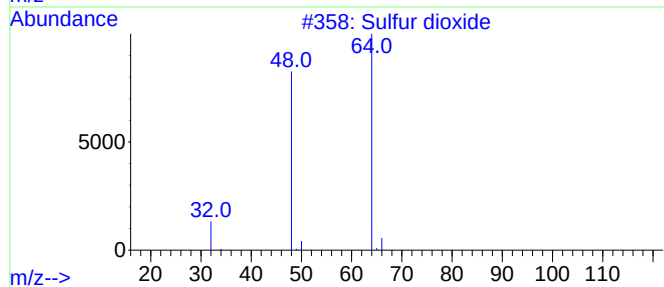
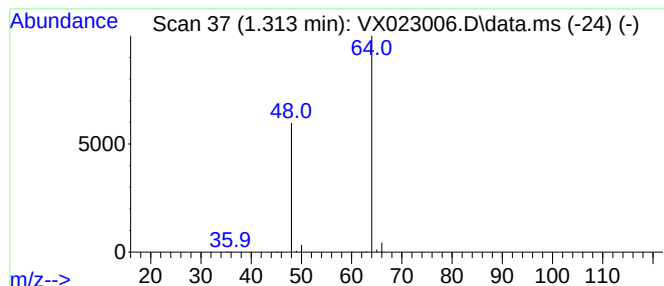
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.313	152.13 ug/l	570717	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	9
3			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
4			Ethyl Chloride	64	C2H5Cl	000075-00-3	3
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3



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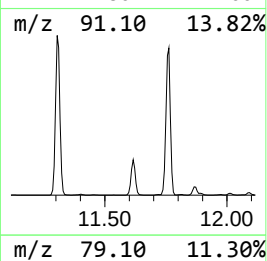
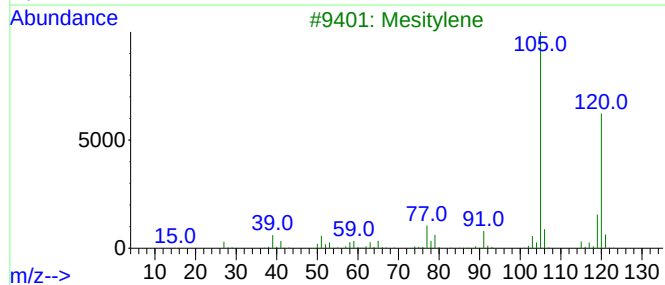
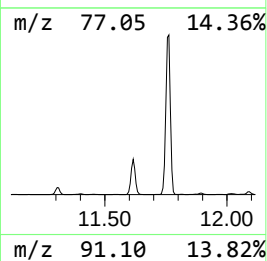
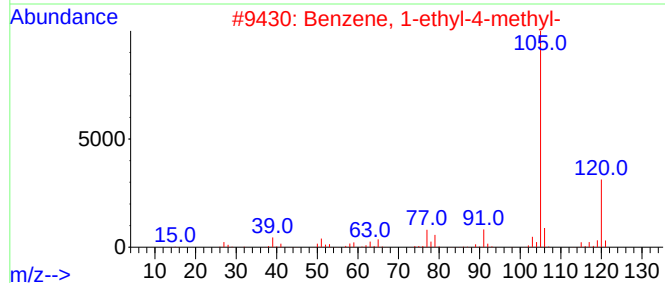
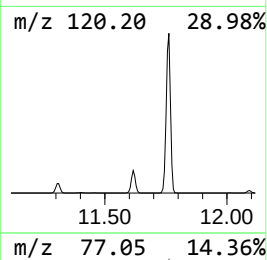
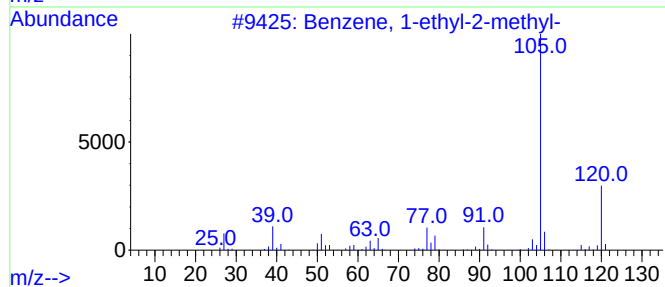
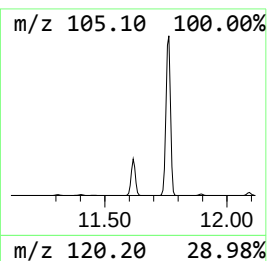
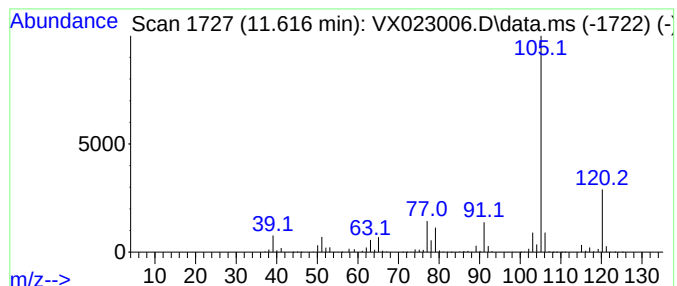
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	362.19 ug/l	2736130	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	91
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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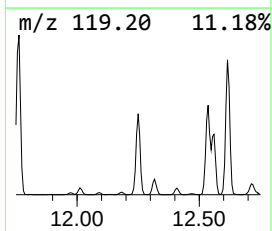
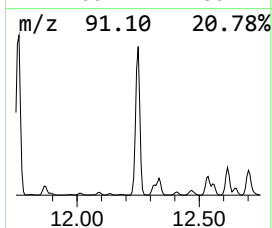
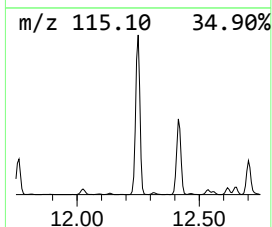
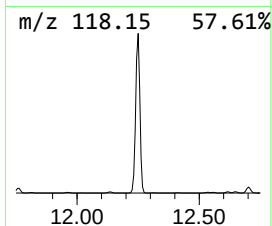
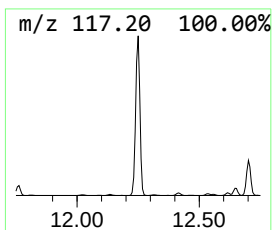
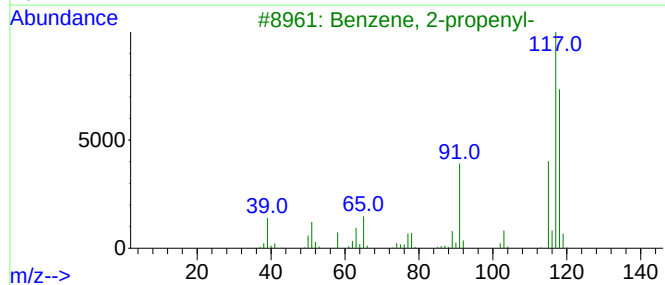
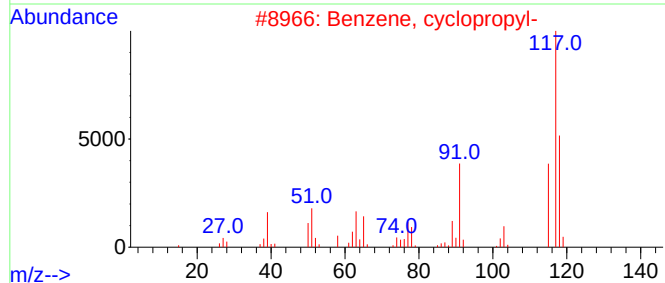
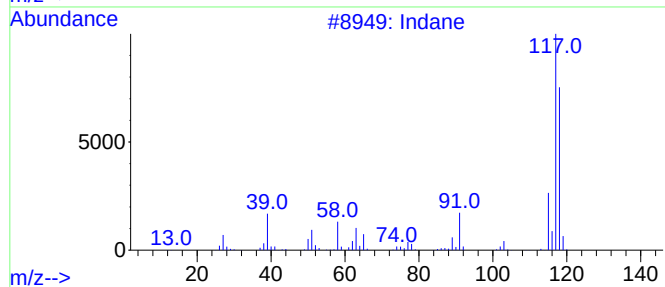
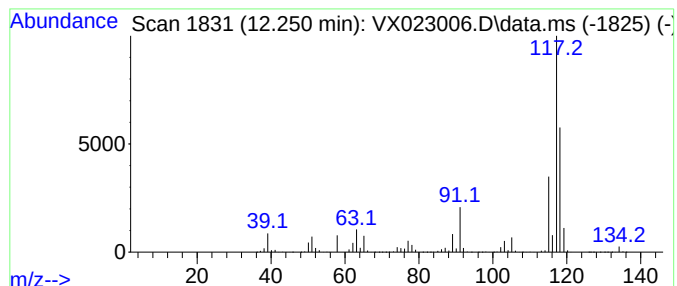
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.250	1217.27 ug/l	9195620	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	87
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	60
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	53



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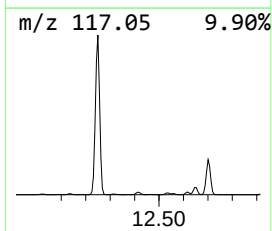
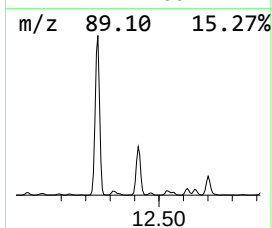
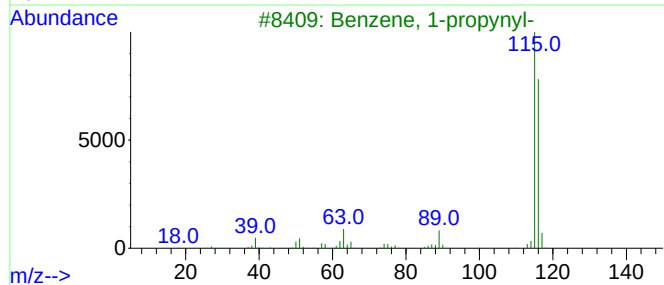
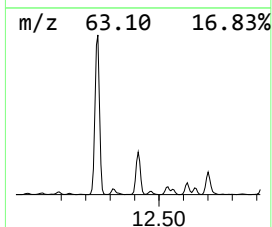
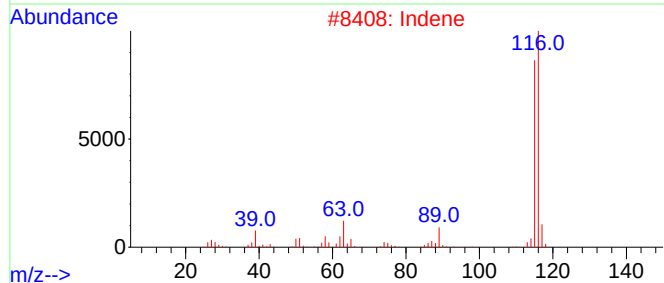
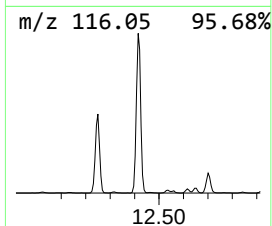
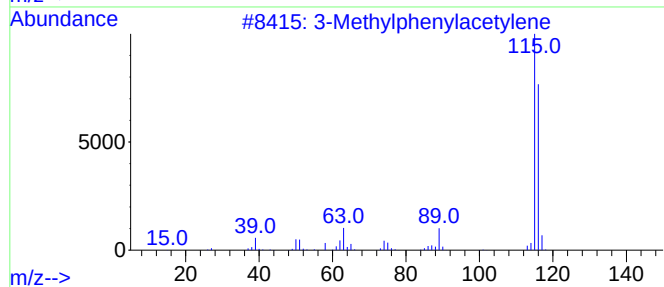
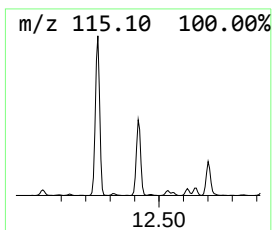
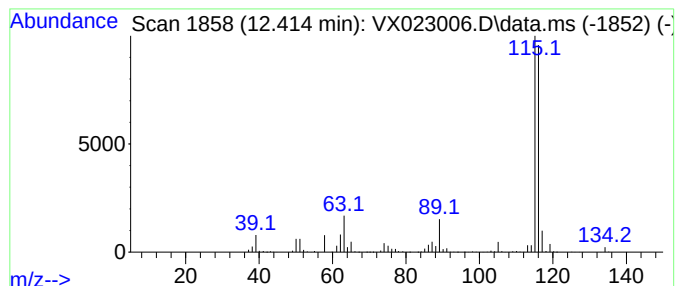
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Methylphenylacetylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	203.64 ug/l	1538330	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methylphenylacetylene	116	C9H8	000766-82-5	95
2			Indene	116	C9H8	000095-13-6	94
3			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
4			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	86
5			1-indanol trifluoroacetate ester	230	C11H9F3O2	1000376-43-6	64



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MW-3

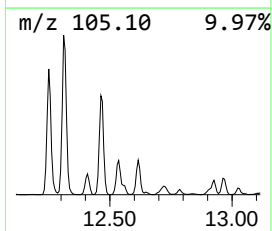
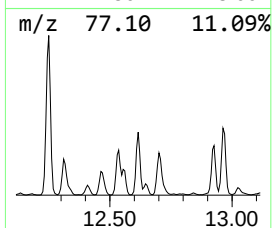
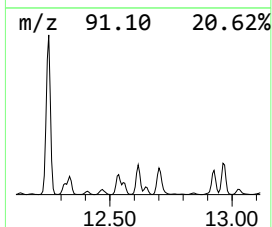
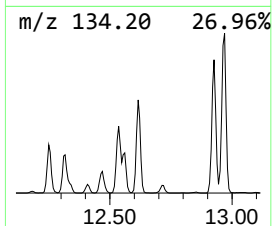
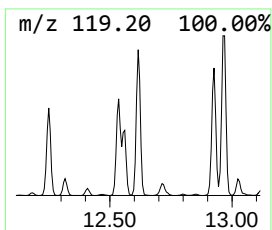
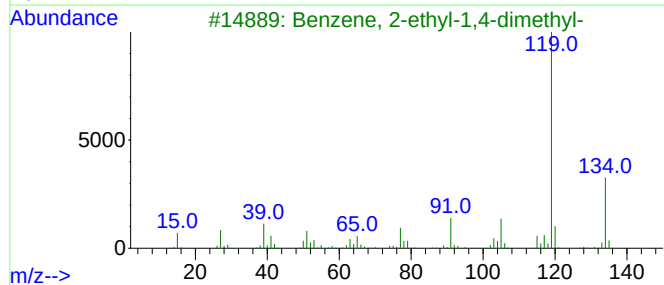
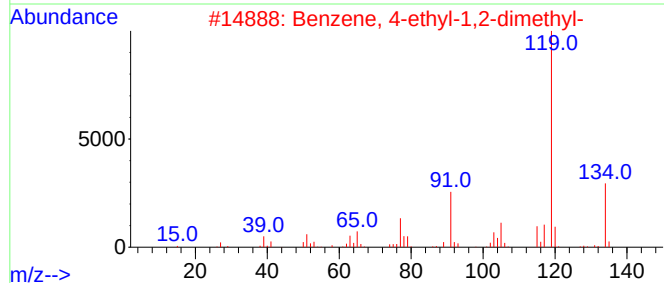
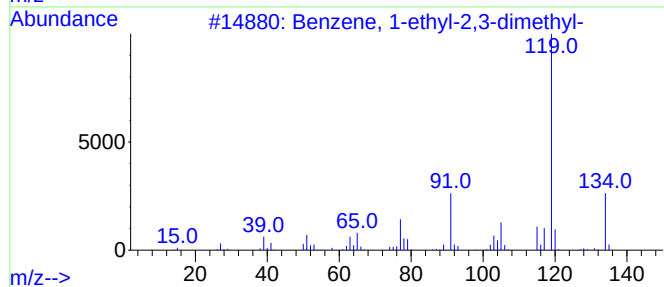
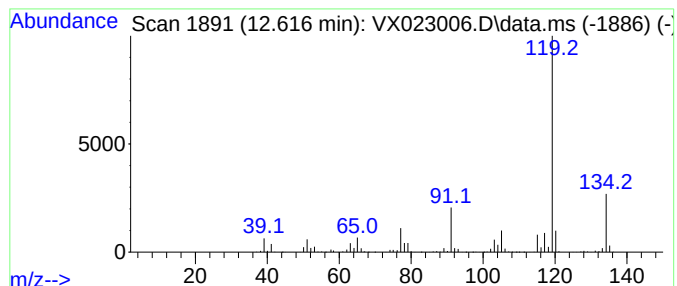
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	176.73 ug/l	1335080	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			p-Cymene	134	C10H14	000099-87-6	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023006.D
Acq On : 29 Jun 2021 16:19
Operator : JC/MD
Sample : M2875-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

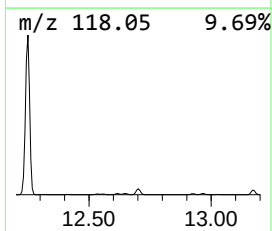
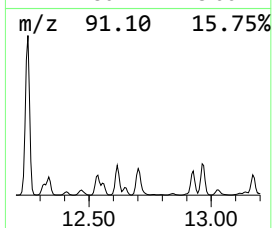
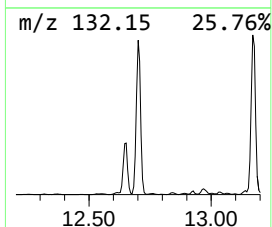
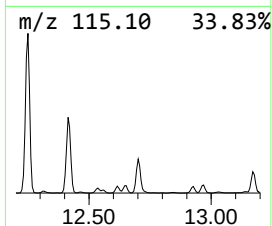
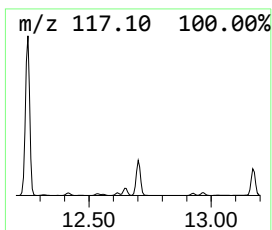
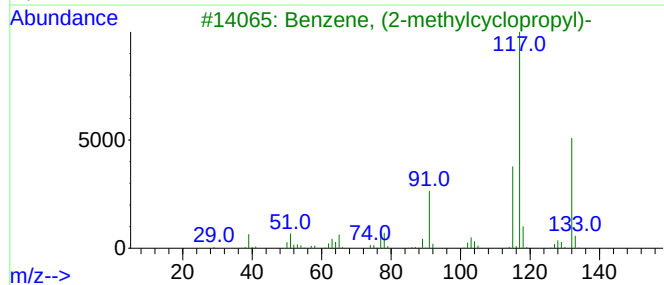
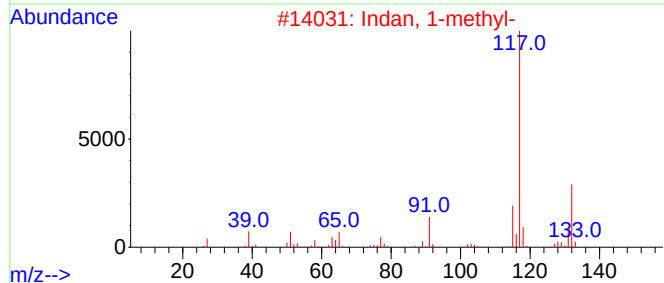
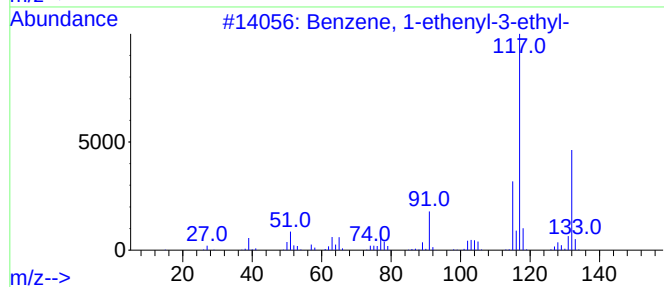
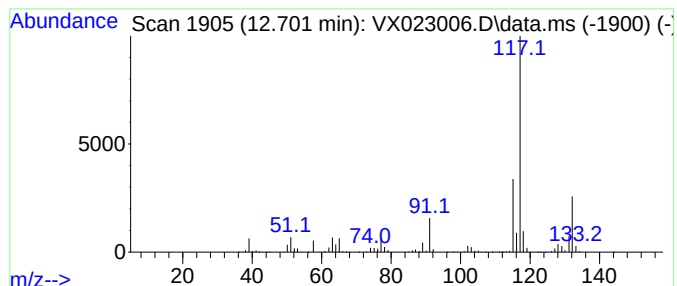
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	248.18 ug/l	1874850	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
2			Indan, 1-methyl-	132	C10H12	000767-58-8	87
3			Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	87
4			Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	83
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023006.D
Acq On : 29 Jun 2021 16:19
Operator : JC/MD
Sample : M2875-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

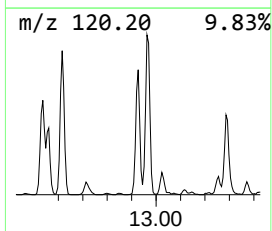
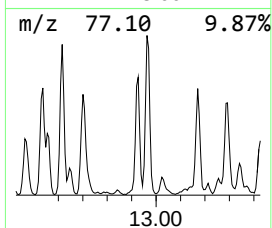
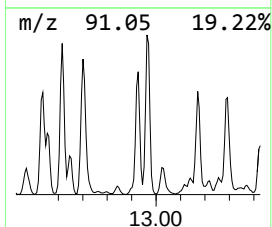
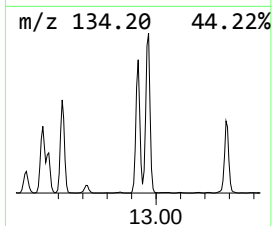
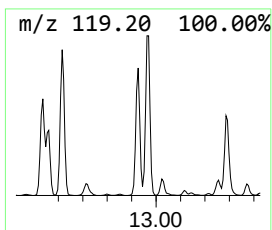
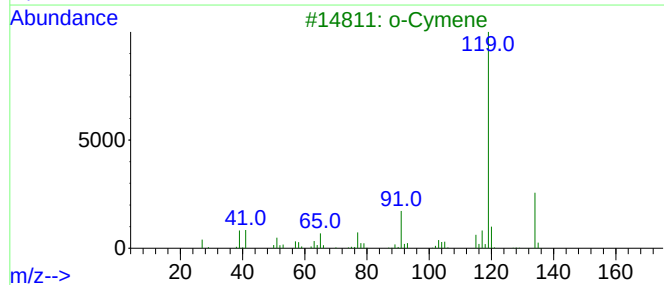
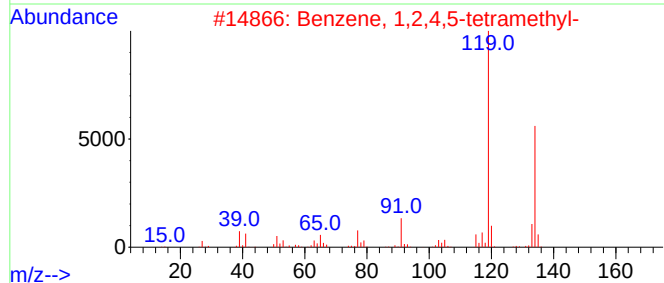
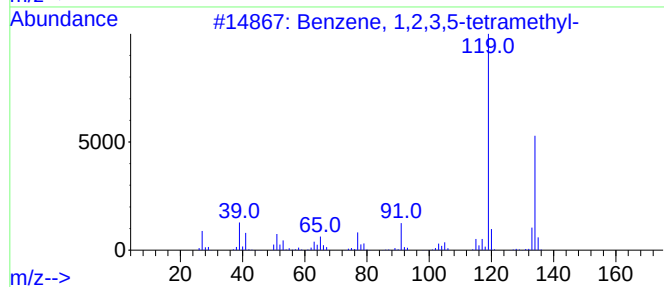
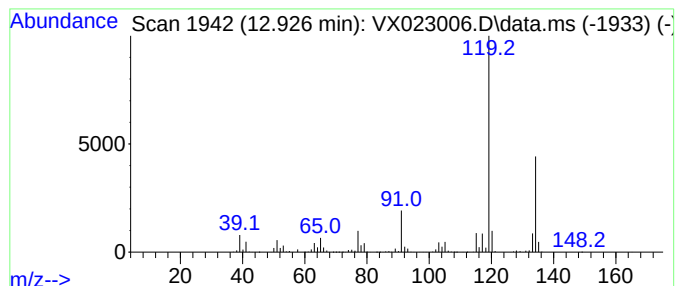
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.927	170.33 ug/l	1286700	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	96
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
3			o-Cymene	134	C10H14	000527-84-4	95
4			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023006.D
Acq On : 29 Jun 2021 16:19
Operator : JC/MD
Sample : M2875-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

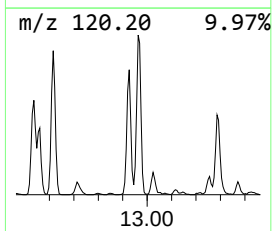
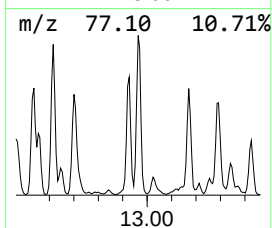
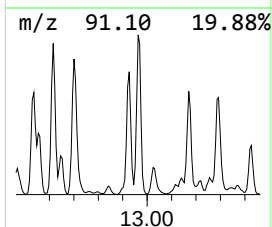
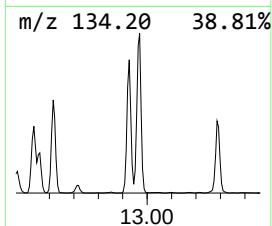
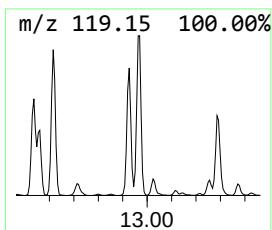
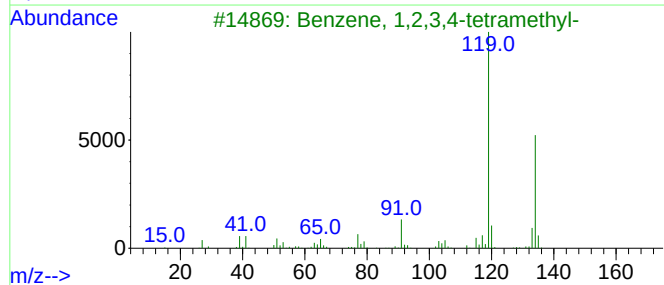
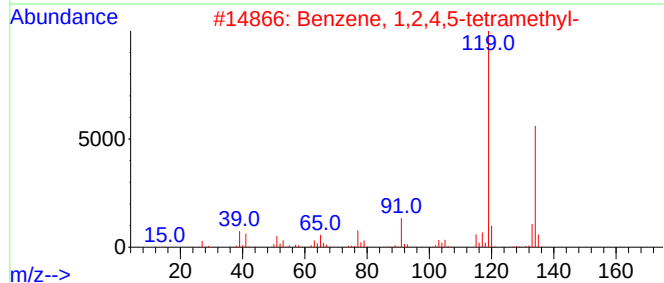
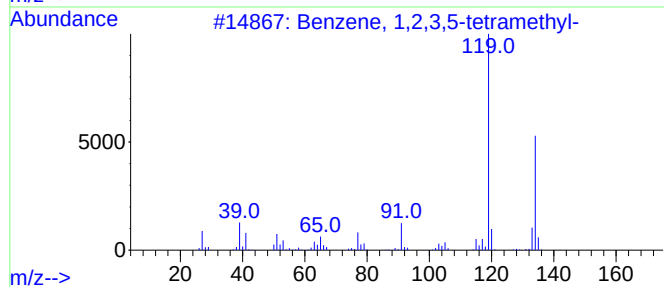
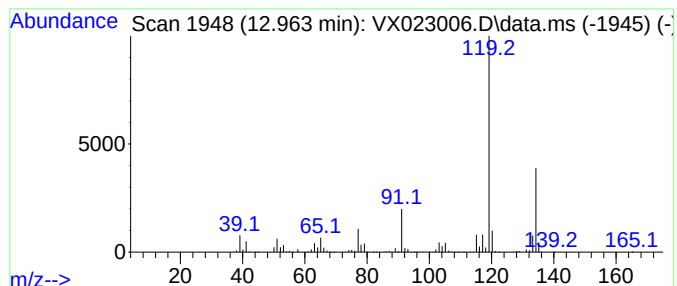
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	217.56 ug/l	1643540	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	96
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			p-Cymene	134	C10H14	000099-87-6	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023006.D
Acq On : 29 Jun 2021 16:19
Operator : JC/MD
Sample : M2875-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

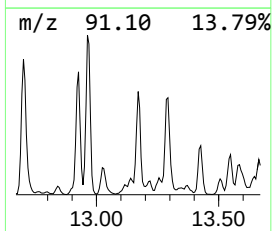
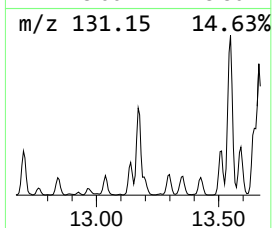
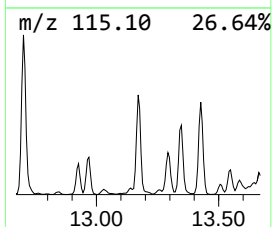
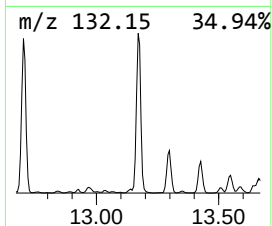
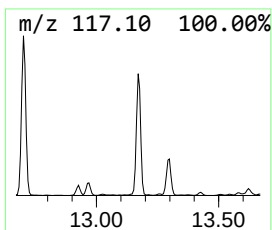
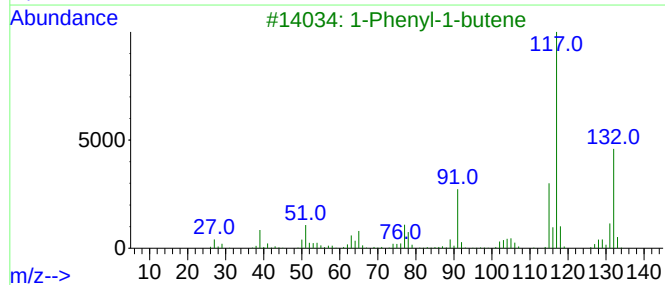
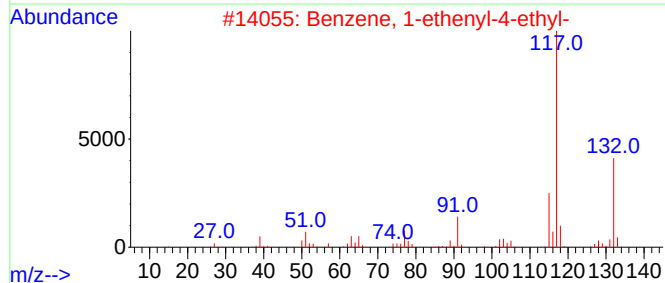
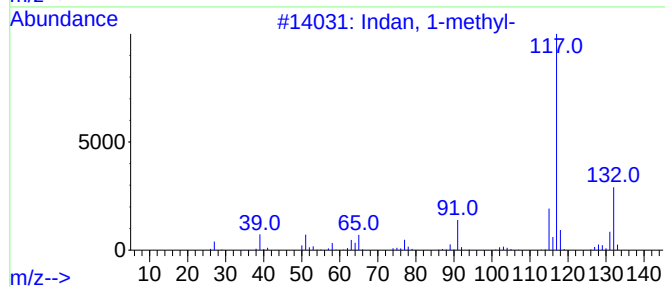
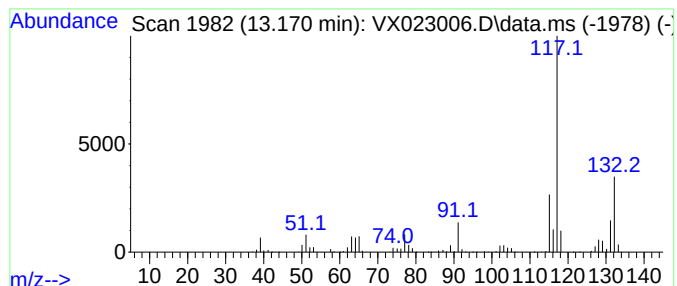
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Indan, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	179.48 ug/l	1355840	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	94
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	91
4			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023006.D
Acq On : 29 Jun 2021 16:19
Operator : JC/MD
Sample : M2875-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

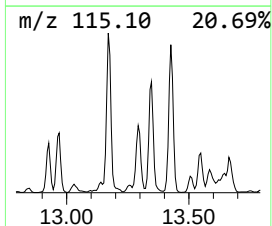
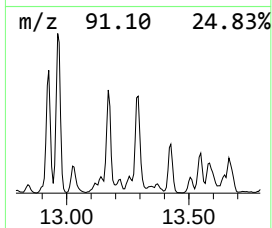
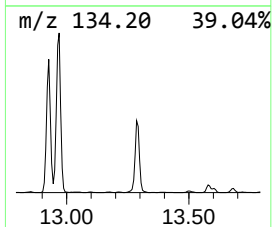
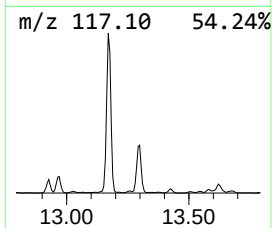
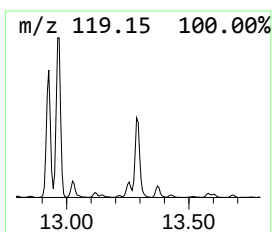
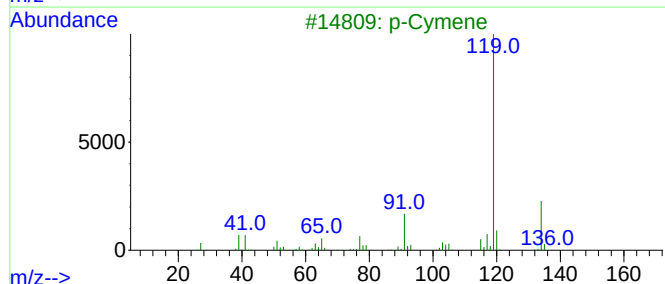
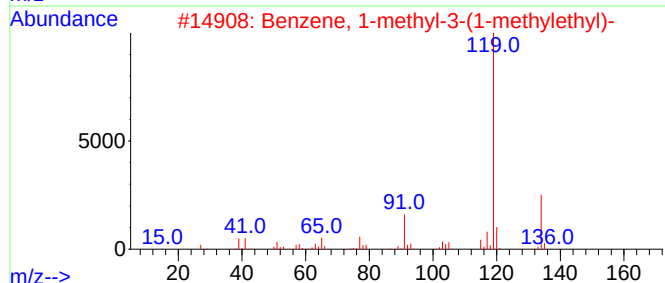
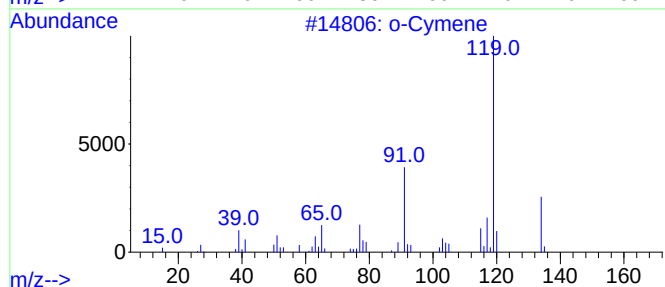
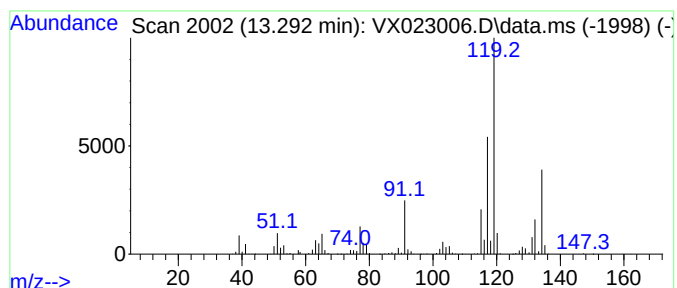
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 o-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	146.26 ug/l	1104860	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		o-Cymene	134	C10H14	000527-84-4	70
2		Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	64
3		p-Cymene	134	C10H14	000099-87-6	64
4		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	58
5		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023006.D
Acq On : 29 Jun 2021 16:19
Operator : JC/MD
Sample : M2875-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Benzene, 1-ethy...	11.616	362.2	ug/l	2736130	4	12.024	377715	50.0
Indane	12.250	1217.3	ug/l	9195620	4	12.024	377715	50.0
3-Methylphenyla...	12.414	203.6	ug/l	1538330	4	12.024	377715	50.0
Benzene, 1-ethy...	12.616	176.7	ug/l	1335080	4	12.024	377715	50.0
Benzene, 1-ethe...	12.701	248.2	ug/l	1874850	4	12.024	377715	50.0
Benzene, 1,2,3,...	12.927	170.3	ug/l	1286700	4	12.024	377715	50.0
Benzene, 1,2,4,...	12.963	217.6	ug/l	1643540	4	12.024	377715	50.0
Indan, 1-methyl-	13.170	179.5	ug/l	1355840	4	12.024	377715	50.0
o-Cymene	13.292	146.3	ug/l	1104860	4	12.024	377715	50.0