

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
 Data File : VX027251.D
 Acq On : 01 Mar 2022 16:17
 Operator : JC/MD
 Sample : N1688-15
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-32

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: VX027251.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	43	rBV	42614	88072	7.04%	1.214%
2	3.111	324	332	342	rVB2	6980	17334	1.39%	0.239%
3	4.312	519	529	539	rVB3	8622	24958	2.00%	0.344%
4	5.391	695	706	716	rBV2	50988	147395	11.79%	2.032%
5	5.556	724	733	755	rVB	88551	260096	20.80%	3.586%
6	5.964	790	800	810	rBV	54225	141179	11.29%	1.947%
7	6.257	837	848	858	rVB	8584	27712	2.22%	0.382%
8	6.769	922	932	942	rBV	133534	322244	25.77%	4.443%
9	7.379	1023	1032	1043	rVB4	7561	19620	1.57%	0.271%
10	7.982	1123	1131	1139	rBV2	8071	16297	1.30%	0.225%
11	8.104	1144	1151	1156	rBV2	13777	29392	2.35%	0.405%
12	8.653	1234	1241	1248	rVB	272662	433475	34.67%	5.977%
13	10.055	1465	1471	1479	rBV	283922	382347	30.58%	5.272%
14	10.195	1488	1494	1502	rBV	416132	524245	41.93%	7.228%
15	10.305	1506	1512	1522	rBV	355413	444001	35.51%	6.122%
16	10.963	1614	1620	1626	rBV	36613	44419	3.55%	0.612%
17	11.079	1634	1639	1653	rVB	226155	300333	24.02%	4.141%
18	11.305	1671	1676	1684	rVB	101499	120610	9.65%	1.663%
19	11.402	1684	1692	1697	rVV	171414	221325	17.70%	3.052%
20	11.451	1697	1700	1707	rVB	13307	16349	1.31%	0.225%
21	11.616	1721	1727	1734	rVB	65182	81493	6.52%	1.124%
22	11.756	1744	1750	1756	rBV	1013444	1250430	100.00%	17.241%
23	12.024	1789	1794	1799	rBV	312194	385528	30.83%	5.316%
24	12.091	1799	1805	1810	rVB	242913	313382	25.06%	4.321%
25	12.244	1825	1830	1837	rBV	323026	394423	31.54%	5.438%
26	12.311	1837	1841	1849	rVB3	26069	43454	3.48%	0.599%
27	12.414	1852	1858	1862	rBV3	17217	24120	1.93%	0.333%
28	12.463	1862	1866	1872	rVB	22383	26807	2.14%	0.370%
29	12.530	1872	1877	1879	rBV	43720	52219	4.18%	0.720%
30	12.555	1879	1881	1886	rVB	35486	41125	3.29%	0.567%
31	12.615	1886	1891	1894	rBV	74097	88946	7.11%	1.226%
32	12.646	1894	1896	1901	rVV	17821	19146	1.53%	0.264%
33	12.701	1901	1905	1913	rVB2	52969	77708	6.21%	1.071%
34	12.847	1925	1929	1935	rVB	17667	22726	1.82%	0.313%
35	12.926	1935	1942	1945	rBV	41000	54368	4.35%	0.750%
36	12.963	1945	1948	1955	rVB	74966	86068	6.88%	1.187%

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Title : SW846 8260

37	13.170	1978	1982	1986	rVB	45651	53017	4.24%	0.731%
38	13.292	1997	2002	2007	rVB2	106882	137336	10.98%	1.894%
39	13.426	2019	2024	2029	rVB	34162	44154	3.53%	0.609%
40	13.585	2046	2050	2056	rVV3	10911	20576	1.65%	0.284%
41	13.664	2060	2063	2070	rVB2	10485	16852	1.35%	0.232%
42	13.774	2074	2081	2090	rBV	218758	288445	23.07%	3.977%
43	13.871	2090	2097	2101	rVB2	8170	13235	1.06%	0.182%
44	14.219	2149	2154	2160	rBV3	10274	19898	1.59%	0.274%
45	14.640	2211	2223	2227	rBV	26849	40086	3.21%	0.553%
46	14.780	2241	2246	2255	rBV	44319	58150	4.65%	0.802%
47	15.615	2377	2383	2387	rBV	11143	17497	1.40%	0.241%

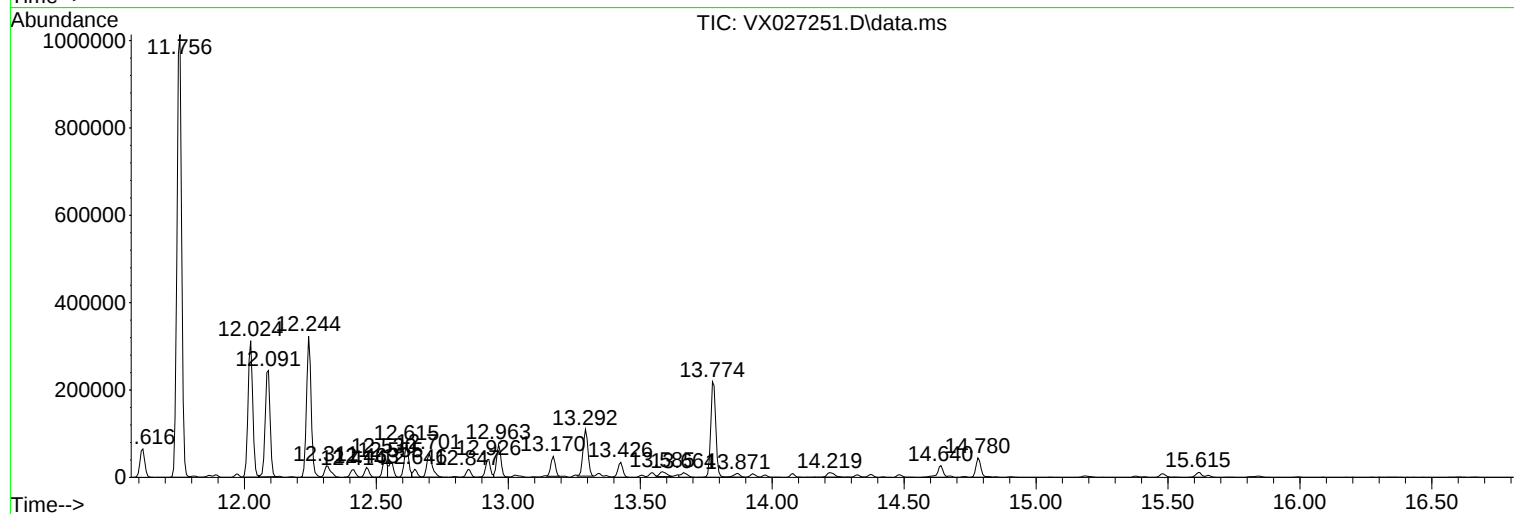
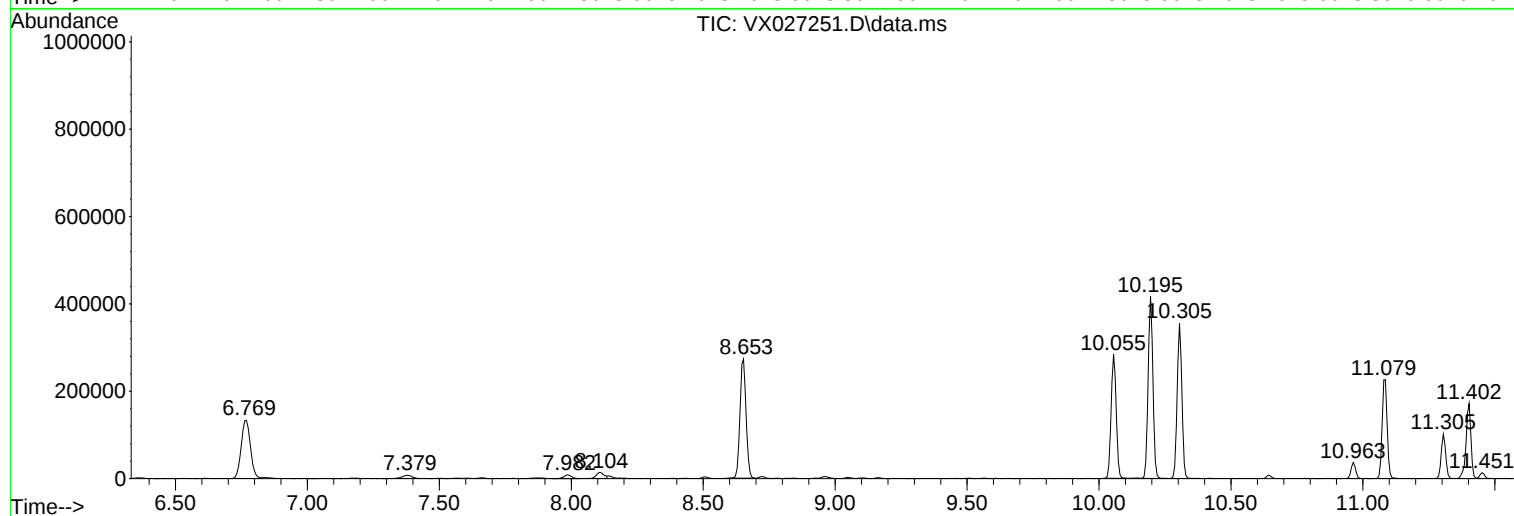
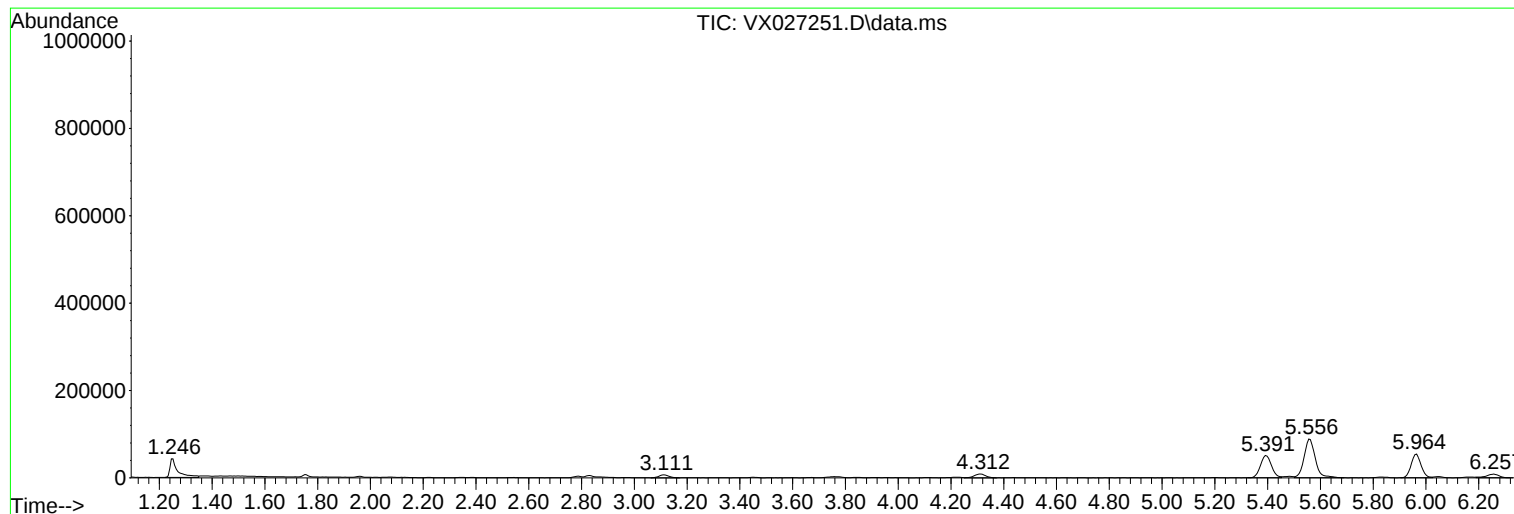
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
MW-32

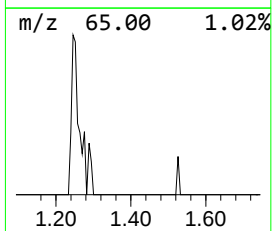
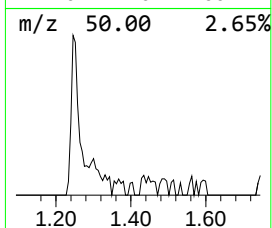
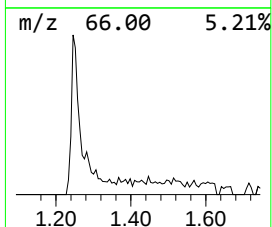
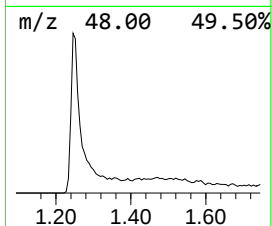
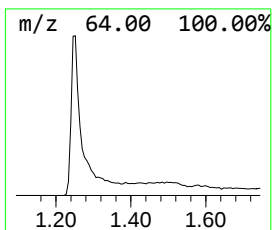
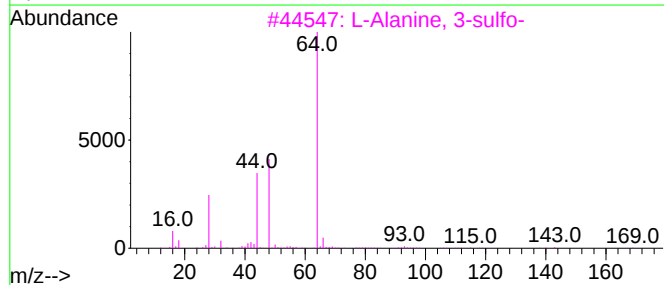
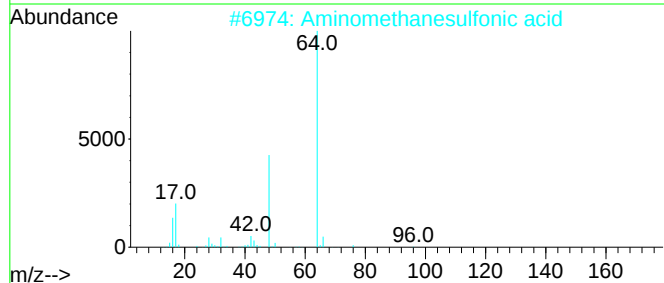
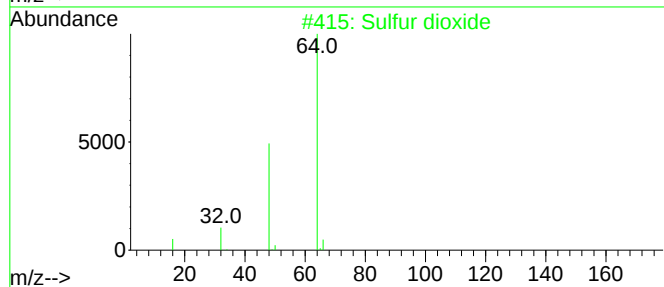
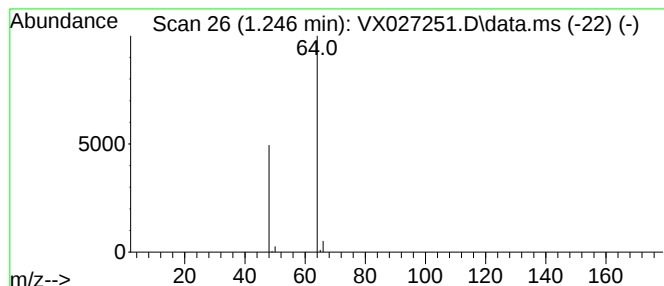
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	16.93 ug/l	88072	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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Instrument :
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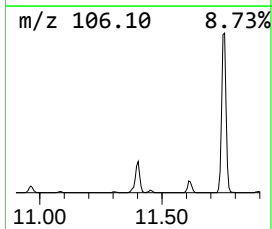
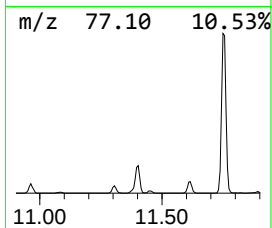
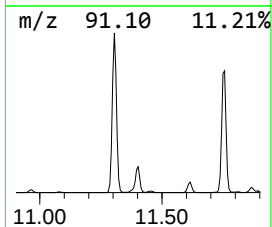
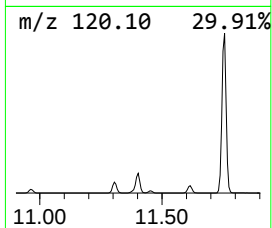
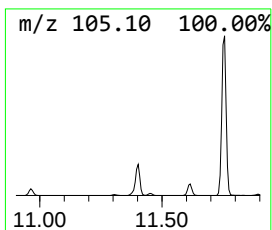
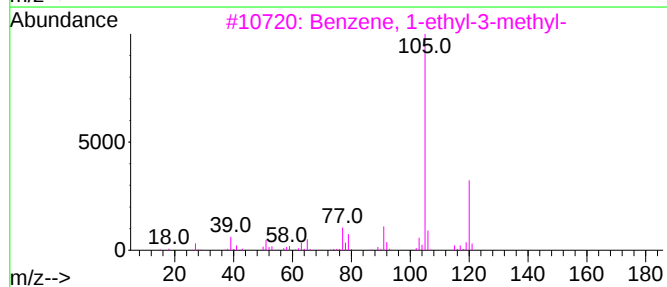
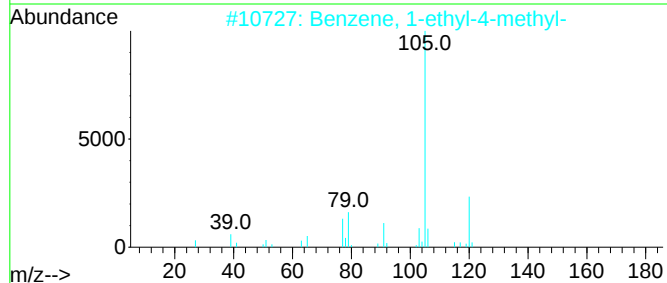
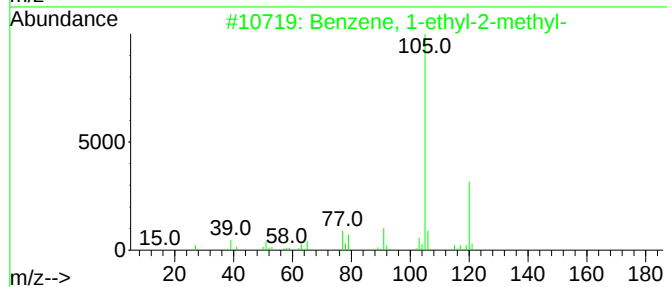
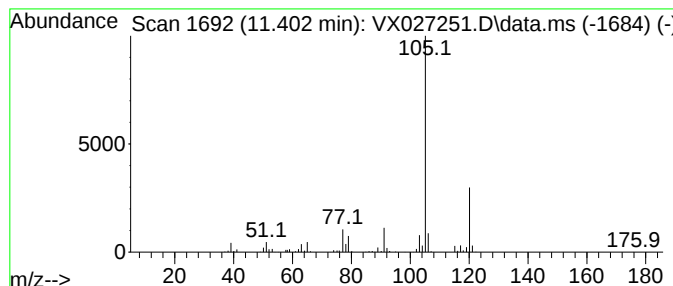
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.402	28.70 ug/l	221325	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	95
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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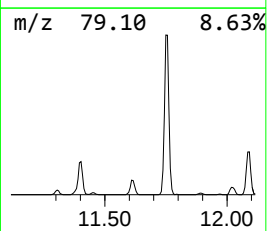
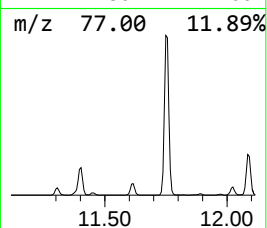
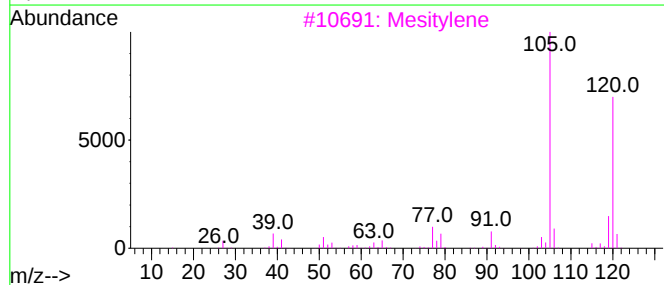
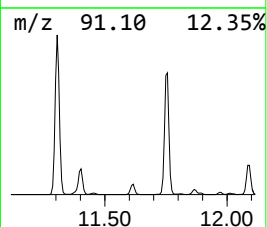
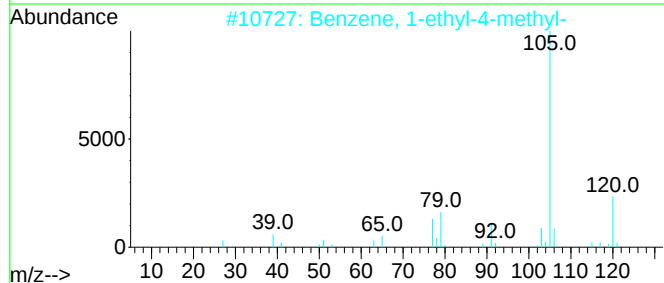
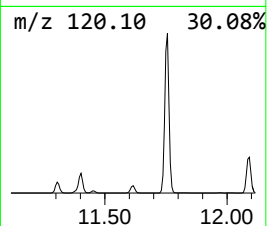
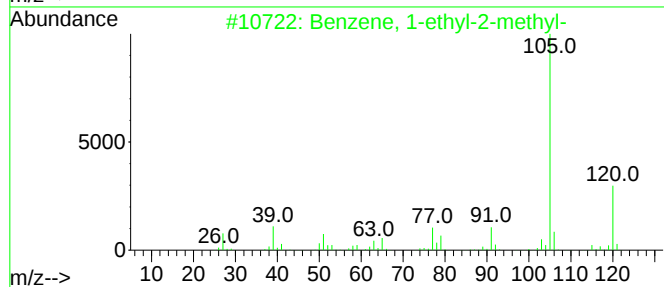
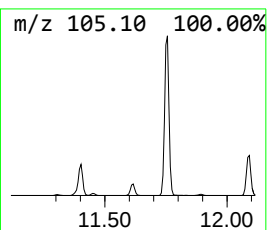
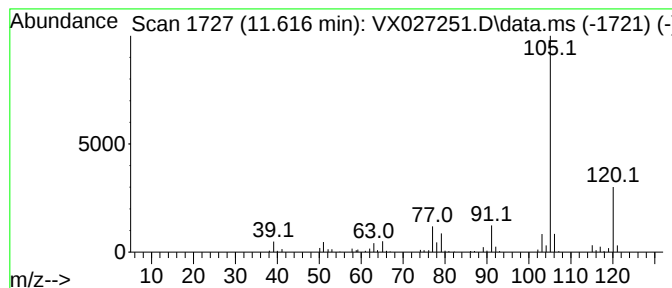
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethyl-4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	10.57 ug/l	81493	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	95
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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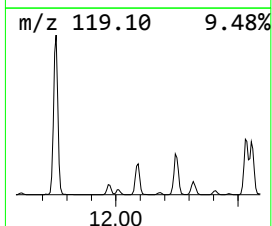
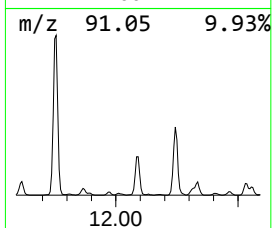
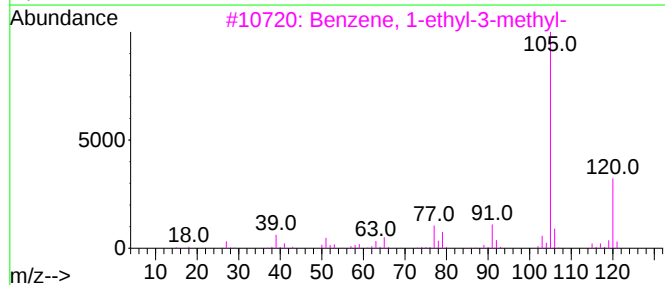
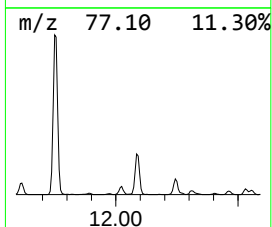
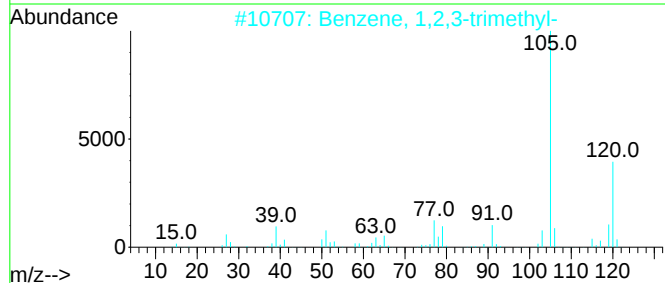
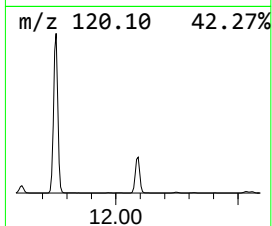
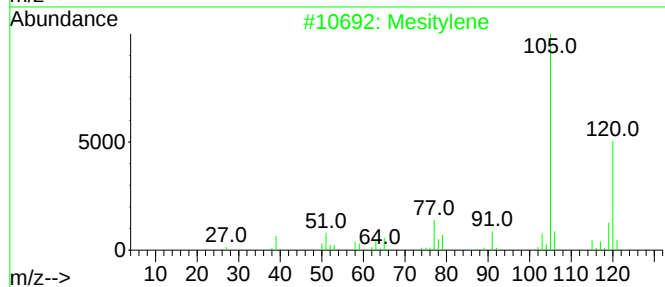
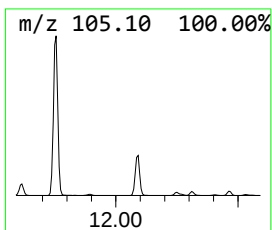
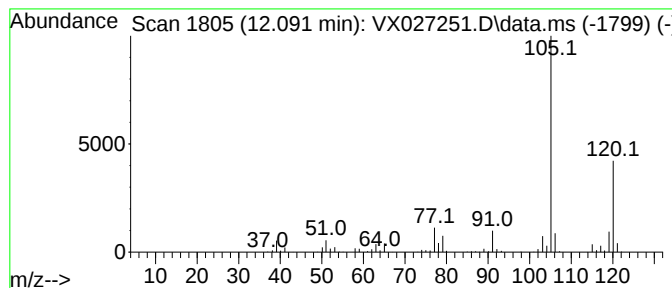
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Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1,2,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	40.64 ug/l	313382	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-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



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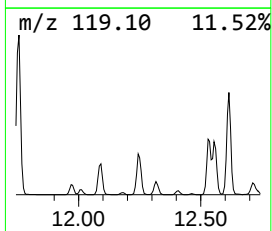
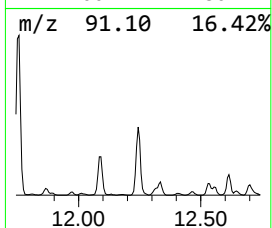
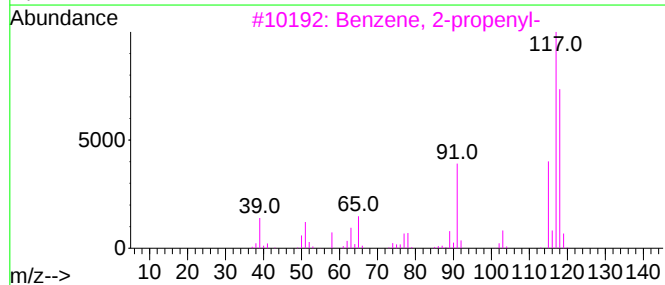
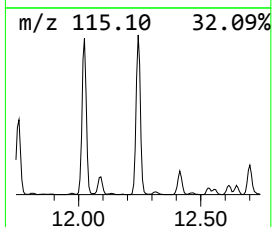
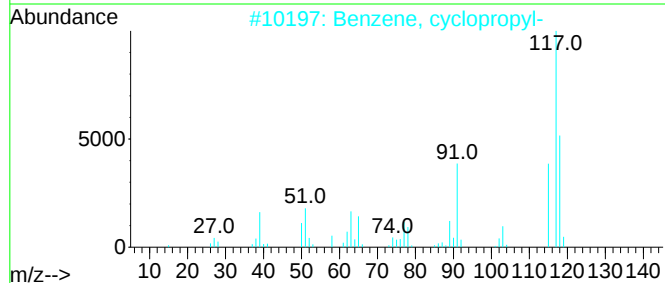
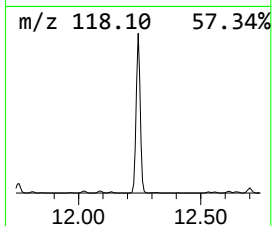
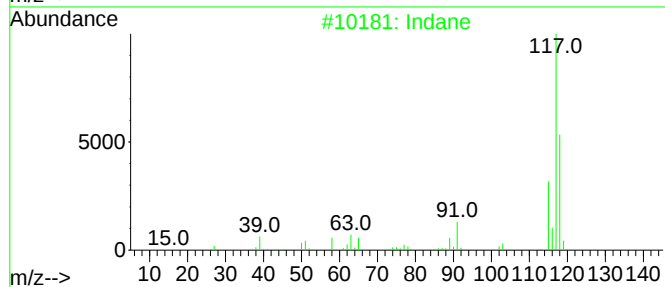
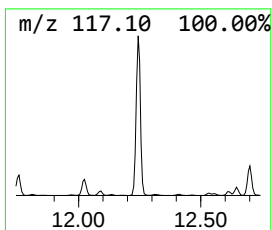
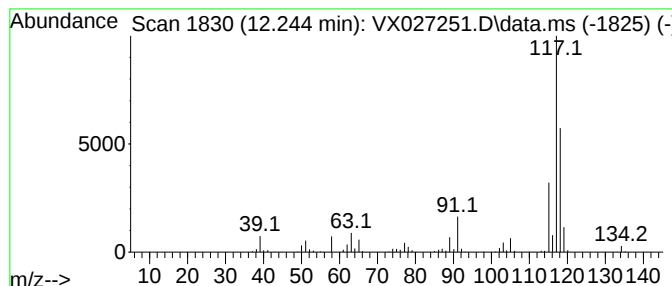
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Quant Title : SW846 8260

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

Peak Number 5 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	51.15 ug/l	394423	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, cyclopropyl-	118	C9H10	000873-49-4	81
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	64
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027251.D
Acq On : 01 Mar 2022 16:17
Operator : JC/MD
Sample : N1688-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

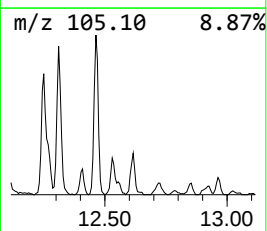
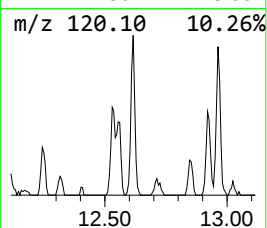
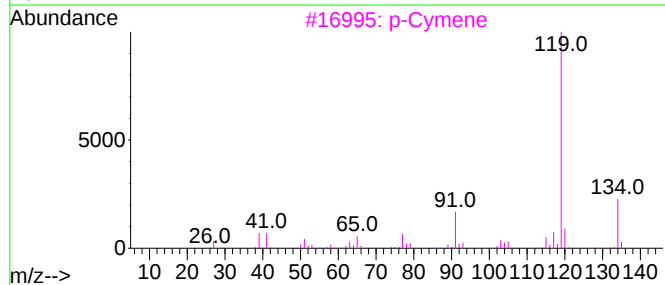
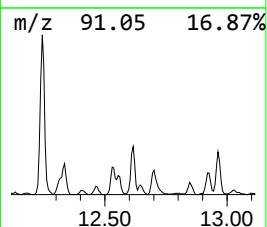
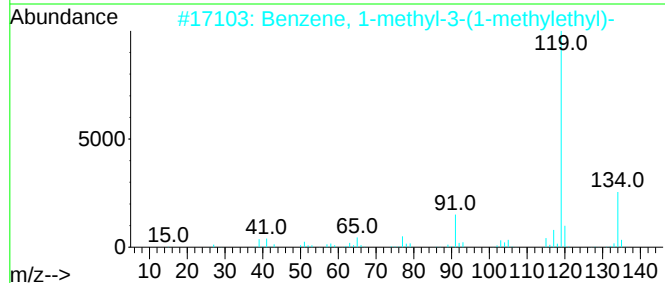
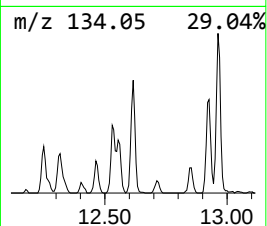
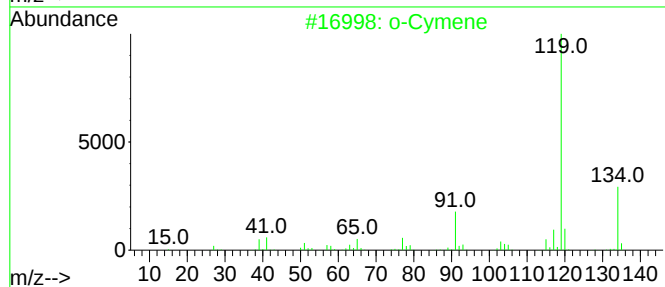
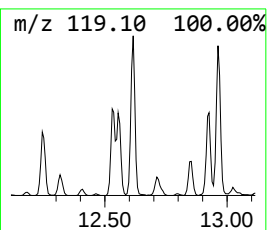
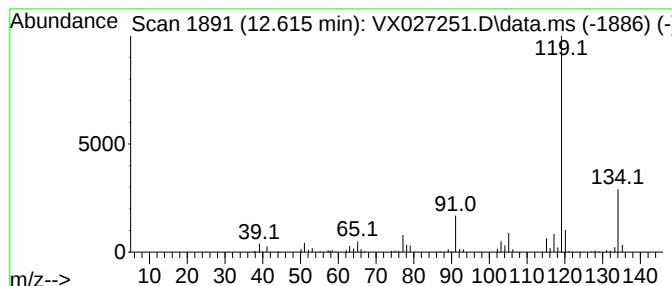
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Quant Title : SW846 8260

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

Peak Number 6 o-Cymene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	11.54 ug/l	88946	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, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
3			p-Cymene	134	C10H14	000099-87-6	95
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	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 : VX027251.D
Acq On : 01 Mar 2022 16:17
Operator : JC/MD
Sample : N1688-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

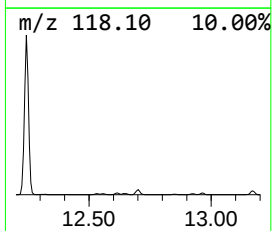
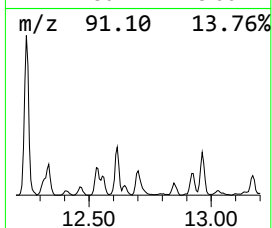
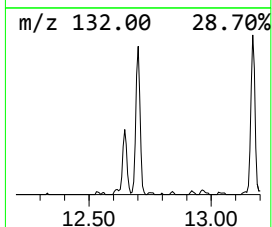
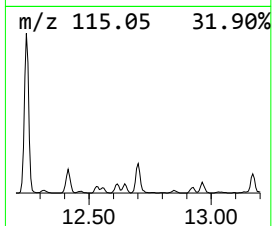
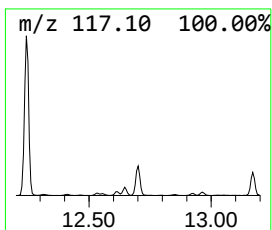
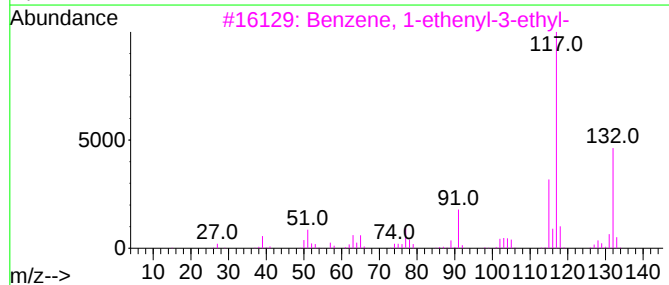
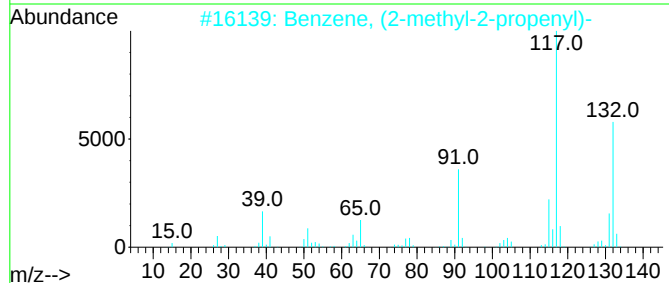
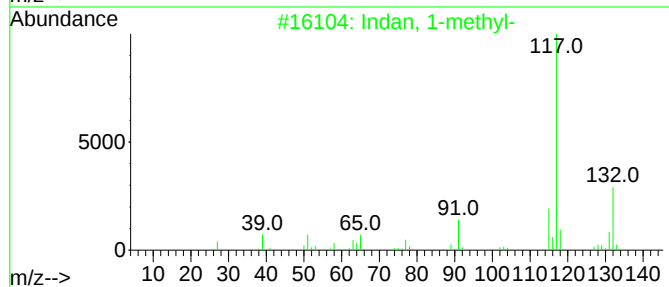
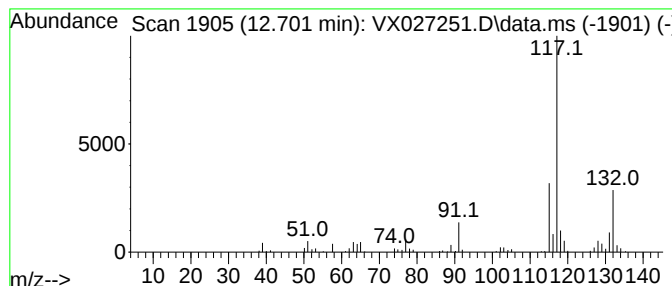
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Quant Title : SW846 8260

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

Peak Number 7 Indan, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	10.08 ug/l	77708	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, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	86
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	86
4			1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	83
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027251.D
Acq On : 01 Mar 2022 16:17
Operator : JC/MD
Sample : N1688-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

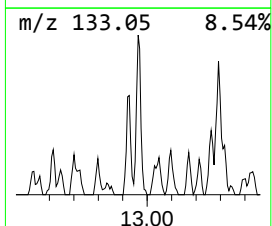
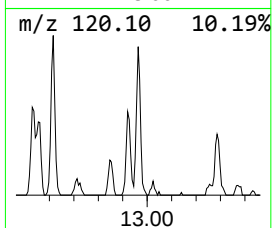
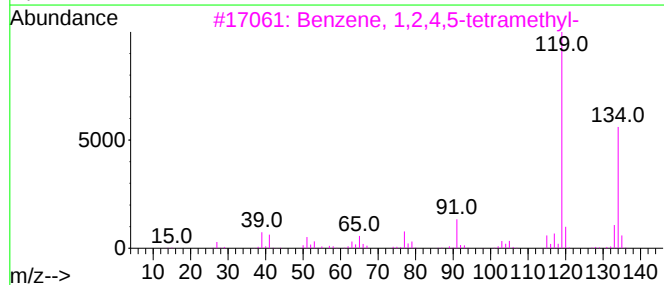
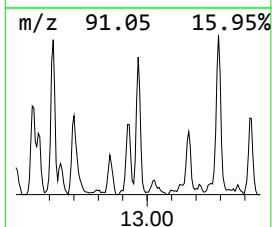
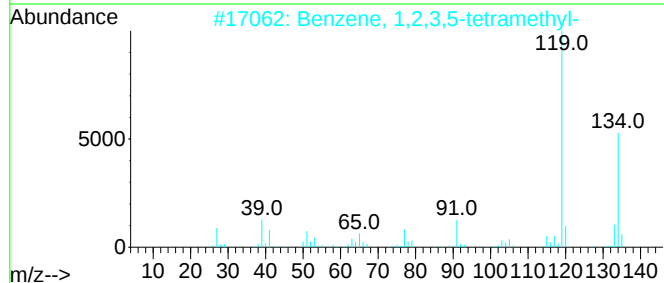
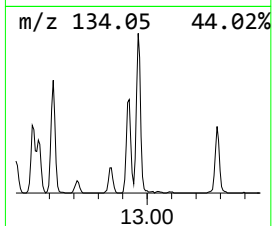
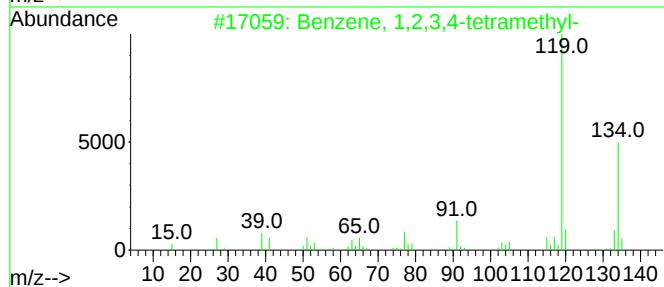
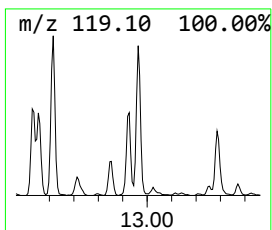
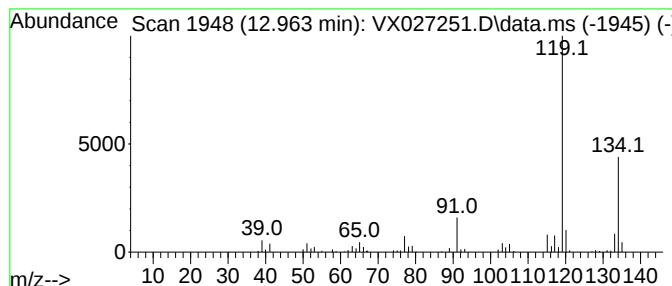
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	11.16 ug/l	86068	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
4			o-Cymene	134	C10H14	000527-84-4	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 : VX027251.D
Acq On : 01 Mar 2022 16:17
Operator : JC/MD
Sample : N1688-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

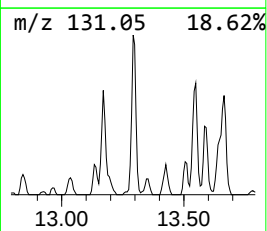
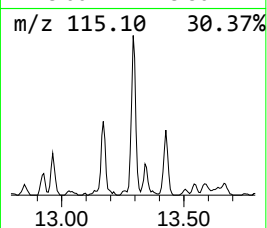
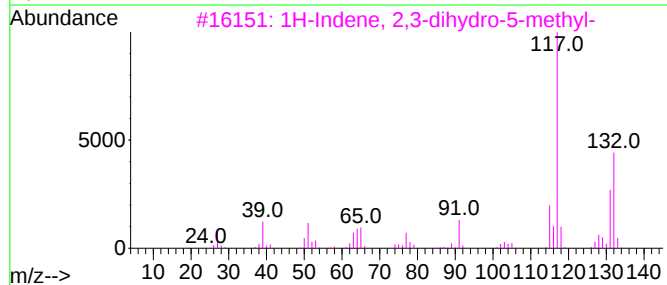
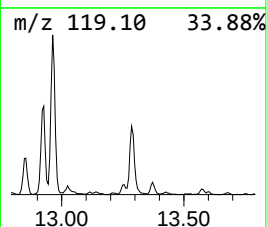
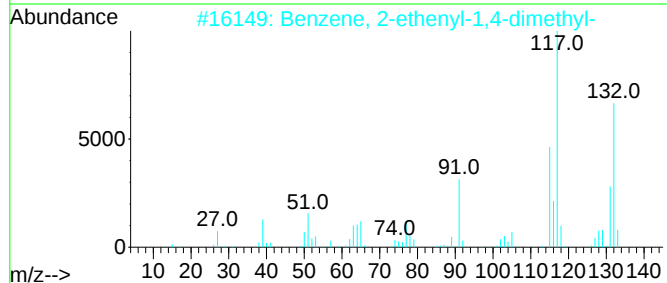
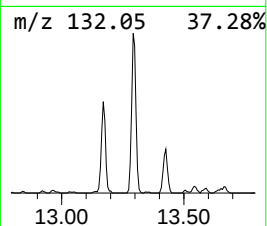
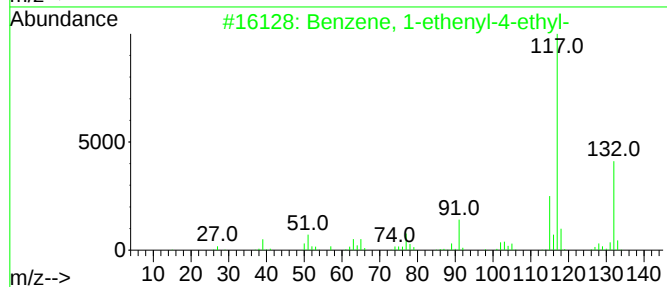
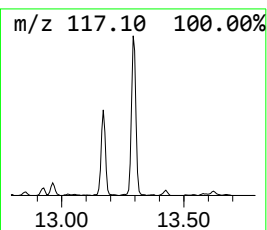
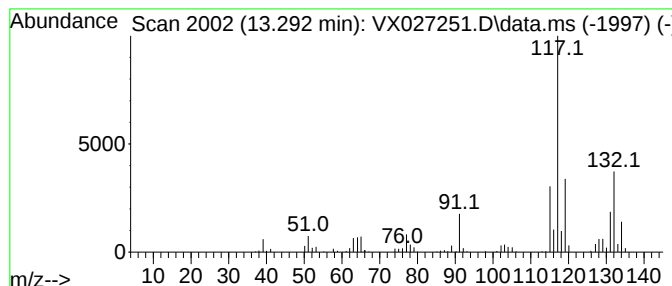
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	17.81 ug/l	137336	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VO030122\
Data File : VX027251.D
Acq On : 01 Mar 2022 16:17
Operator : JC/MD
Sample : N1688-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

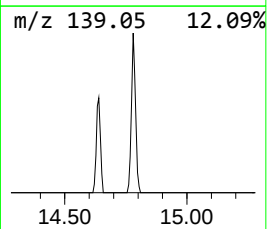
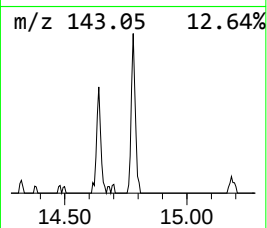
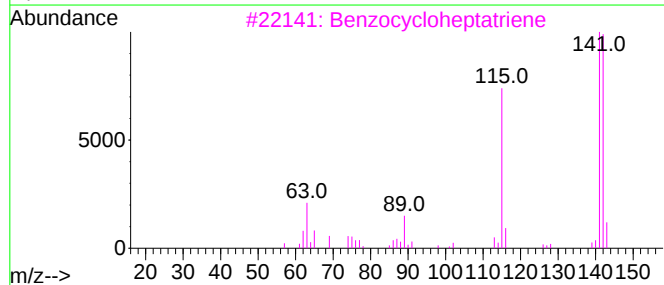
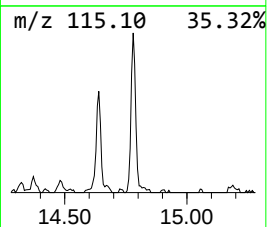
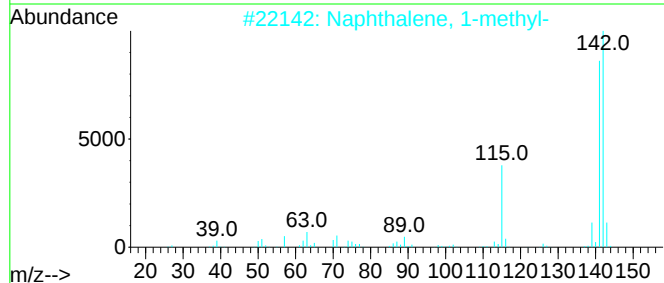
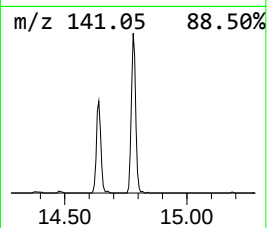
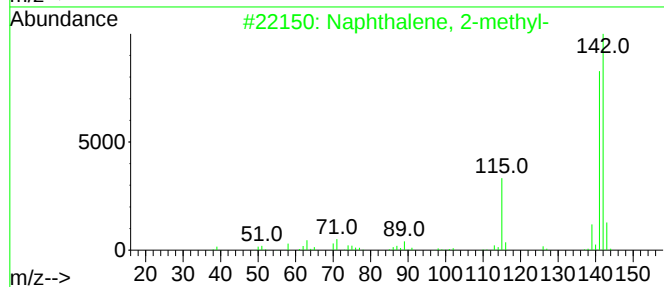
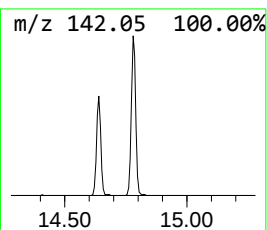
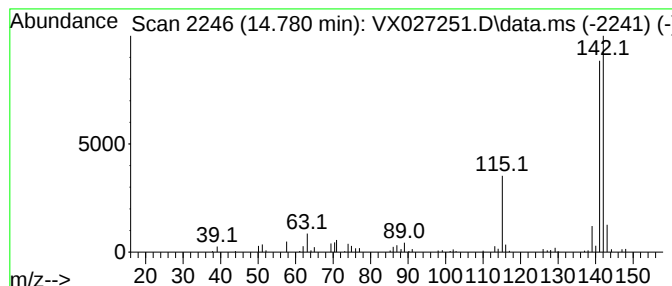
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Quant Title : SW846 8260

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

Peak Number 10 Benzocycloheptatriene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	7.54 ug/l	58150	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	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	87
5			1-Ethanone, 1-[4-(1-naphthalenyl)...	276	C19H16O2	1000338-30-5	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027251.D
Acq On : 01 Mar 2022 16:17
Operator : JC/MD
Sample : N1688-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

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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Benzene, 1-ethy...	11.402	28.7	ug/l	221325	4	12.024	385528	50.0
Benzene, 1-ethy...	11.616	10.6	ug/l	81493	4	12.024	385528	50.0
Benzene, 1,2,3-...	12.091	40.6	ug/l	313382	4	12.024	385528	50.0
Indane	12.244	51.1	ug/l	394423	4	12.024	385528	50.0
o-Cymene	12.616	11.5	ug/l	88946	4	12.024	385528	50.0
Indan, 1-methyl-	12.701	10.1	ug/l	77708	4	12.024	385528	50.0
Benzene, 1,2,3,...	12.963	11.2	ug/l	86068	4	12.024	385528	50.0
Benzene, 1-ethe...	13.292	17.8	ug/l	137336	4	12.024	385528	50.0
Benzocyclohepta...	14.780	7.5	ug/l	58150	4	12.024	385528	50.0