

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX093023\
 Data File : VX038012.D
 Acq On : 30 Sep 2023 18:22
 Operator : JC/MD
 Sample : 04639-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1035

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\82X091523W.M
 Title : SW846 8260

Signal : TIC: VX038012.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.374	205	211	225	rBV	79744	133411	3.74%	0.579%
2	5.385	694	705	719	rBV2	109388	325368	9.13%	1.412%
3	5.550	722	732	747	rVB	175619	508207	14.26%	2.206%
4	5.958	786	799	806	rBV	125100	339655	9.53%	1.474%
5	6.038	806	812	828	rVB	214142	564106	15.83%	2.448%
6	6.763	919	931	946	rBV	296099	706512	19.83%	3.066%
7	8.647	1234	1240	1246	rBV	613047	956272	26.84%	4.150%
8	8.720	1246	1252	1265	rVB	923559	1374354	38.58%	5.965%
9	10.055	1465	1471	1480	rBV	688482	922154	25.88%	4.002%
10	10.305	1504	1512	1520	rVB	37430	57327	1.61%	0.249%
11	10.640	1561	1567	1573	rBV	2838042	3562704	100.00%	15.463%
12	11.079	1634	1639	1651	rBV	607075	764931	21.47%	3.320%
13	11.396	1682	1691	1696	rBV	271632	362599	10.18%	1.574%
14	11.451	1696	1700	1710	rVB	382604	464892	13.05%	2.018%
15	11.610	1720	1726	1733	rBV	534229	649273	18.22%	2.818%
16	12.018	1788	1793	1799	rVV	823885	1050905	29.50%	4.561%
17	12.085	1799	1804	1810	rVV	1084481	1252088	35.14%	5.434%
18	12.244	1822	1830	1838	rBV2	629125	857775	24.08%	3.723%
19	12.317	1838	1842	1852	rVV2	206403	254119	7.13%	1.103%
20	12.408	1852	1857	1862	rVV2	38974	55317	1.55%	0.240%
21	12.463	1862	1866	1872	rVB	60307	73049	2.05%	0.317%
22	12.610	1885	1890	1894	rBV	244770	298761	8.39%	1.297%
23	12.701	1900	1905	1912	rBV2	149013	229109	6.43%	0.994%
24	12.847	1924	1929	1935	rVB	121920	150025	4.21%	0.651%
25	12.920	1935	1941	1944	rBV	247155	287935	8.08%	1.250%
26	12.963	1944	1948	1953	rVB	402235	476336	13.37%	2.067%
27	13.048	1953	1962	1968	rBV4	28891	76444	2.15%	0.332%
28	13.164	1977	1981	1986	rVB	263554	317580	8.91%	1.378%
29	13.292	1996	2002	2007	rVB2	837216	1126958	31.63%	4.891%
30	13.420	2018	2023	2031	rVB2	131384	166862	4.68%	0.724%
31	13.500	2031	2036	2039	rBV2	32975	46239	1.30%	0.201%
32	13.542	2039	2043	2046	rVV	77528	106448	2.99%	0.462%
33	13.579	2046	2049	2056	rVV4	96156	190287	5.34%	0.826%
34	13.640	2056	2059	2060	rVV	44108	53297	1.50%	0.231%
35	13.664	2060	2063	2069	rVB2	90376	138762	3.89%	0.602%
36	13.774	2075	2081	2090	rBV	1781231	2127626	59.72%	9.234%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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	13.926	2100	2106	2110	rBV2	56051	82565	2.32%	0.358%
38	13.969	2110	2113	2117	rVB	55019	63296	1.78%	0.275%
39	14.073	2125	2130	2136	rBV	92965	114180	3.20%	0.496%
40	14.213	2148	2153	2162	rBV2	88913	159626	4.48%	0.693%
41	14.317	2166	2170	2174	rVV	51568	61876	1.74%	0.269%
42	14.371	2174	2179	2183	rVB	71009	86742	2.43%	0.376%
43	14.634	2213	2222	2228	rBV	617858	765891	21.50%	3.324%
44	14.780	2240	2246	2250	rBV	452373	585547	16.44%	2.541%
45	15.475	2353	2360	2372	rVB	24482	40110	1.13%	0.174%
46	15.609	2377	2382	2386	rBV	32442	53013	1.49%	0.230%

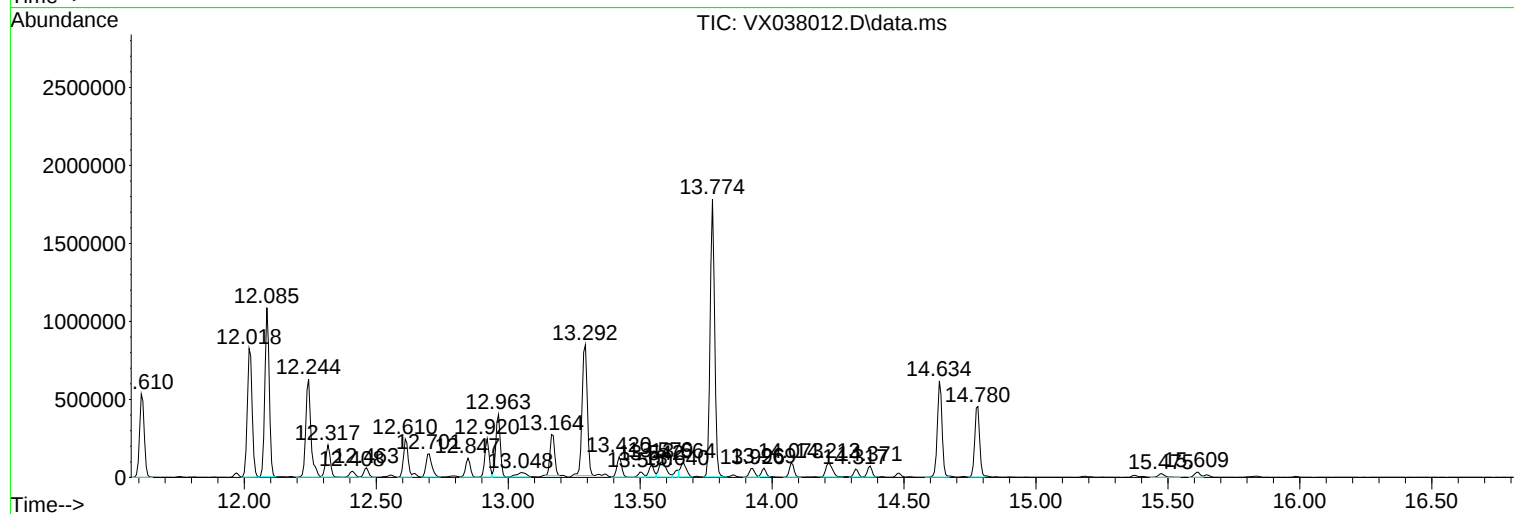
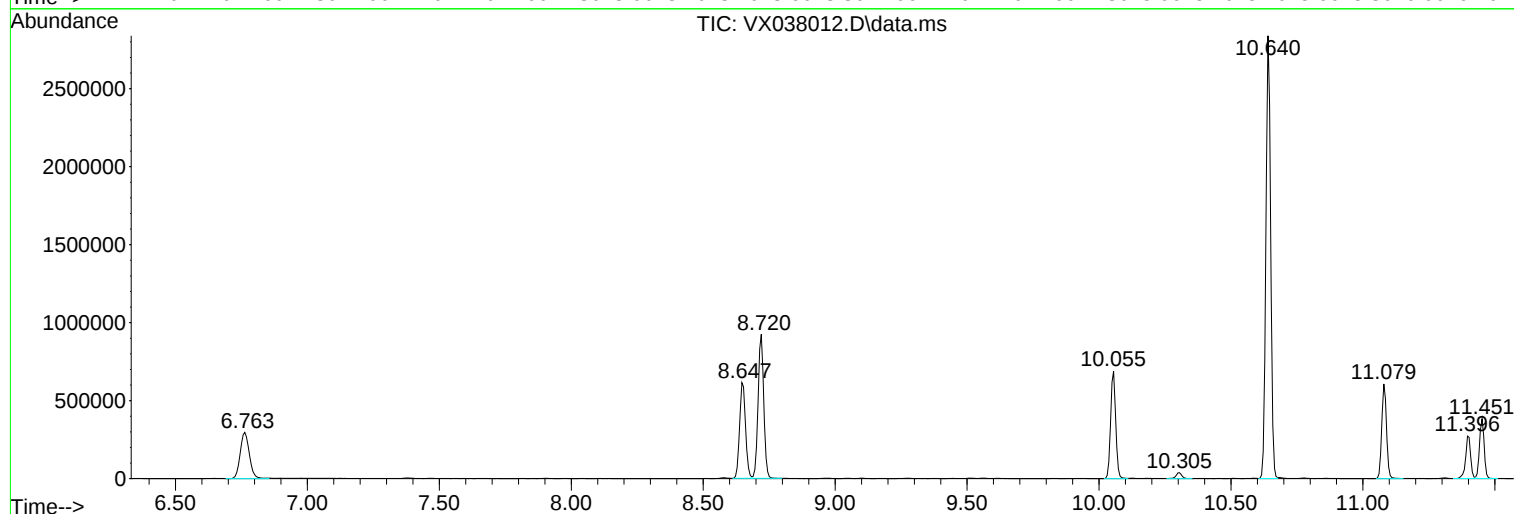
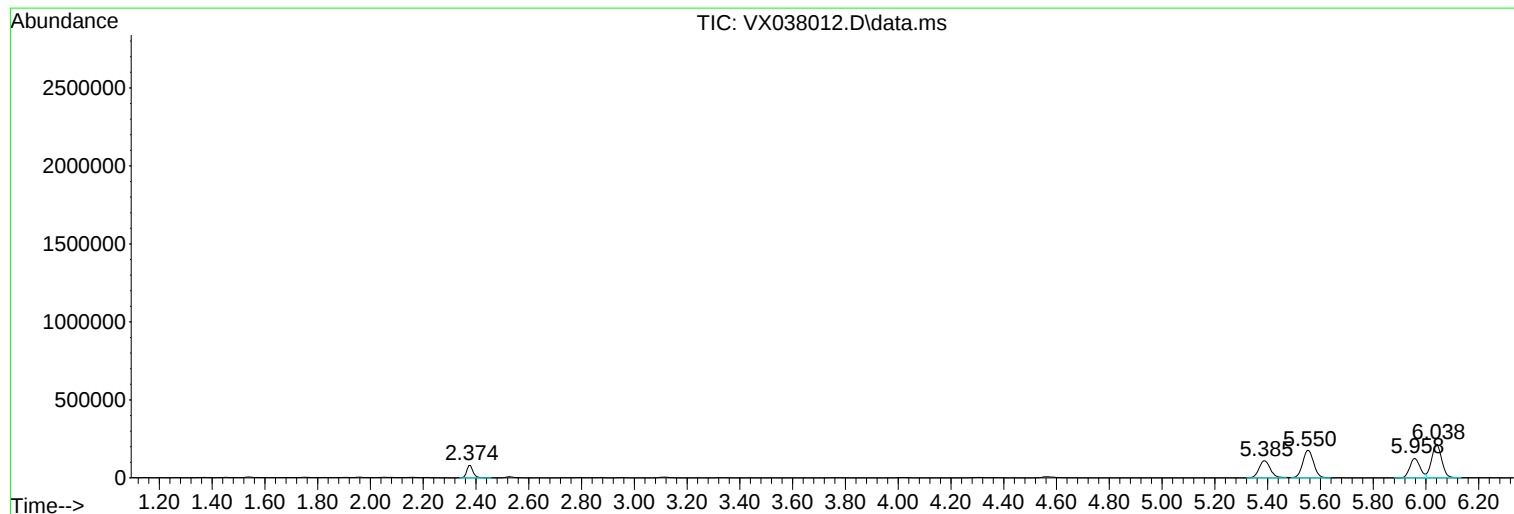
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

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



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Instrument :
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1035

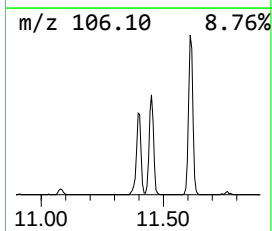
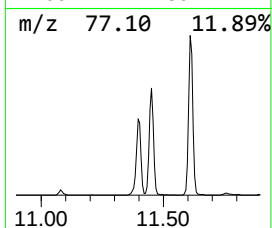
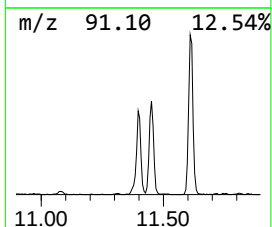
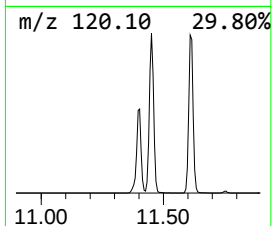
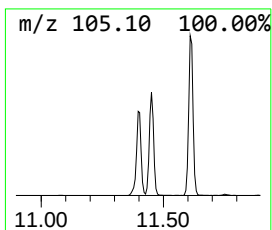
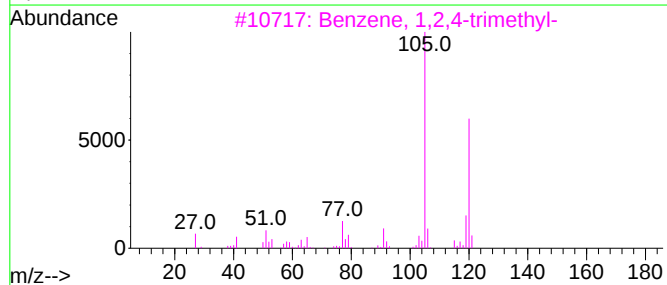
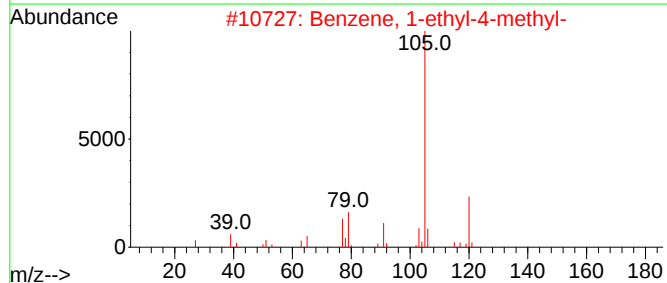
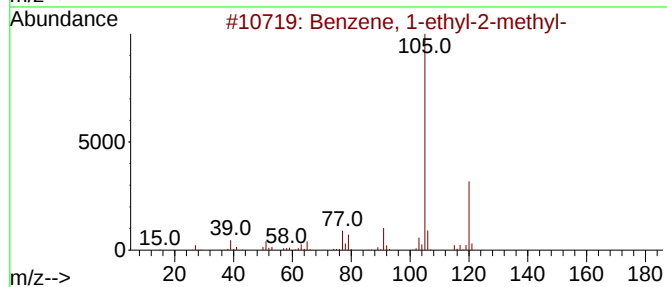
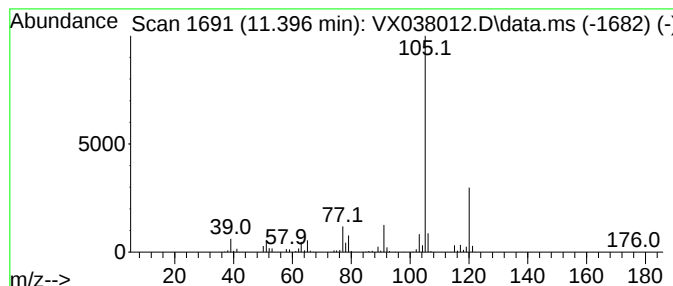
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.396	17.25 ug/l	362599	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			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Mesitylene	120	C9H12	000108-67-8	90
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



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Instrument :
MSVOA_X
ClientSampleId :
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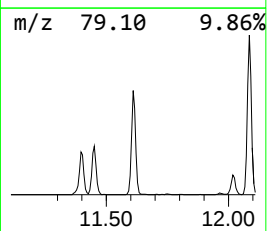
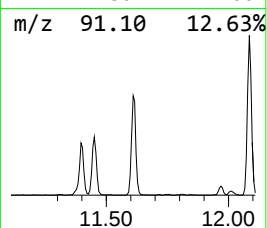
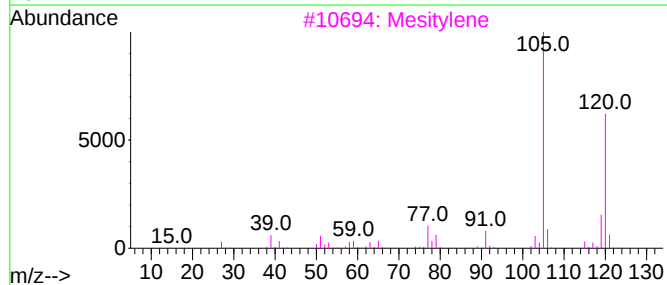
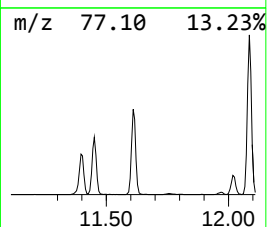
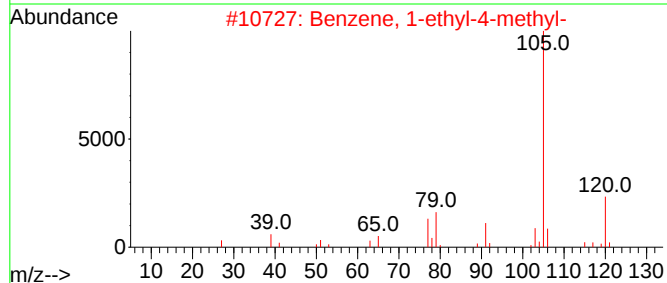
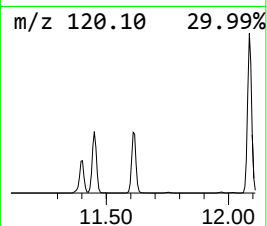
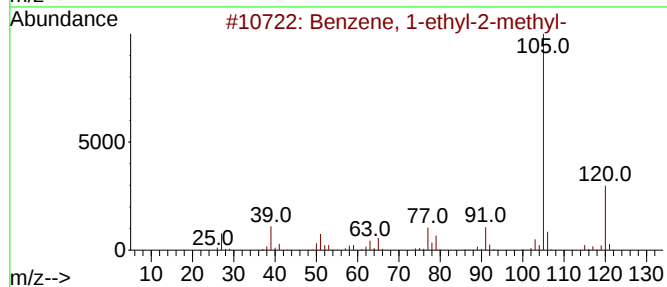
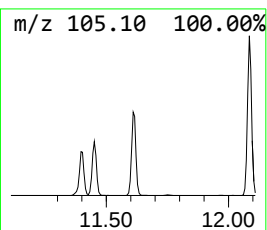
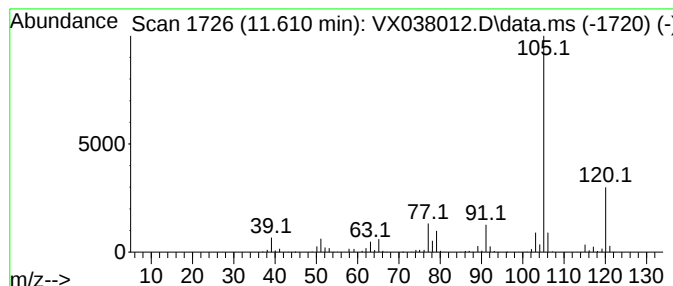
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethyl-4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	30.89 ug/l	649273	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	93
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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Instrument :
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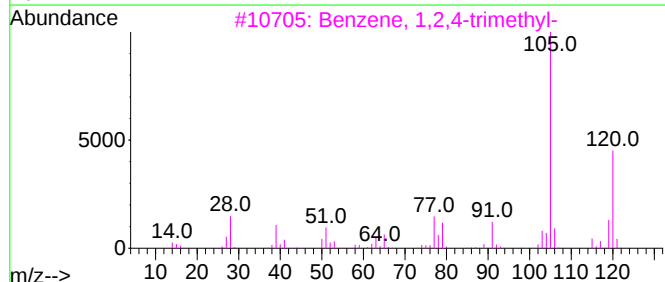
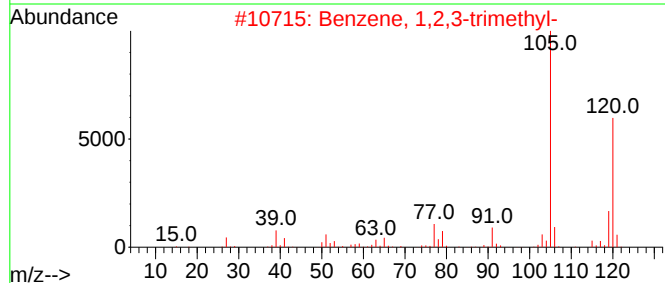
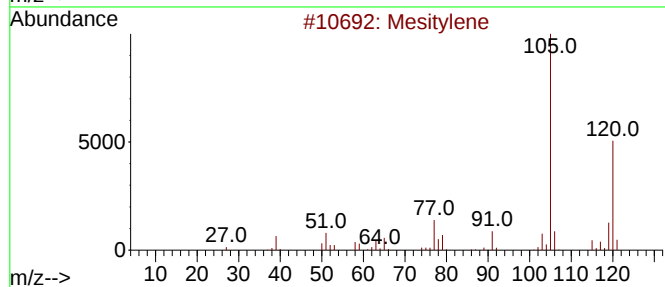
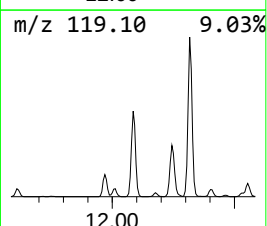
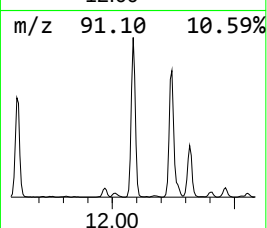
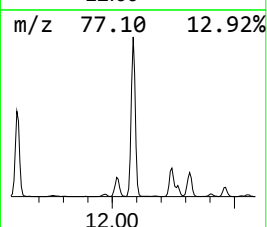
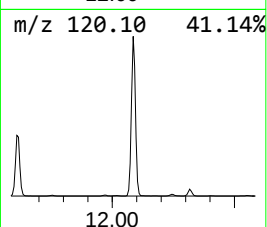
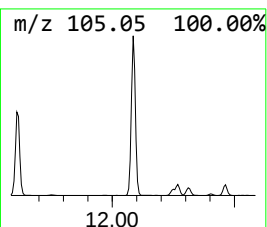
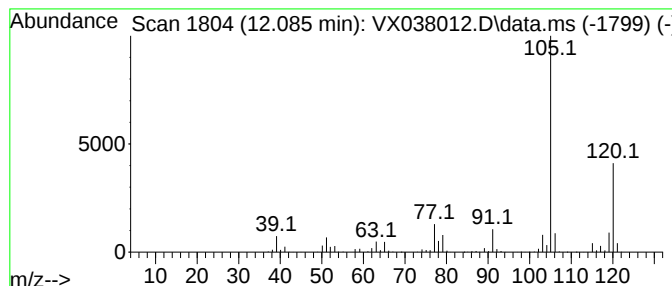
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	59.57 ug/l	1252090	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	94
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87



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Instrument :
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ClientSampleId :
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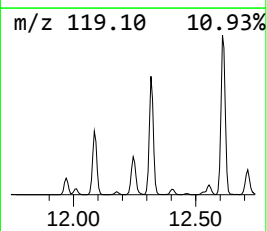
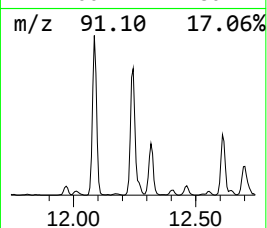
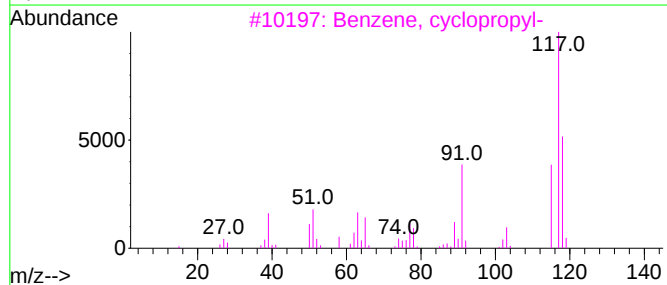
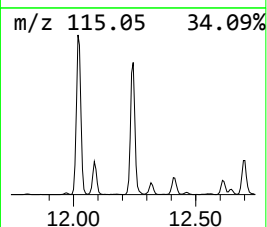
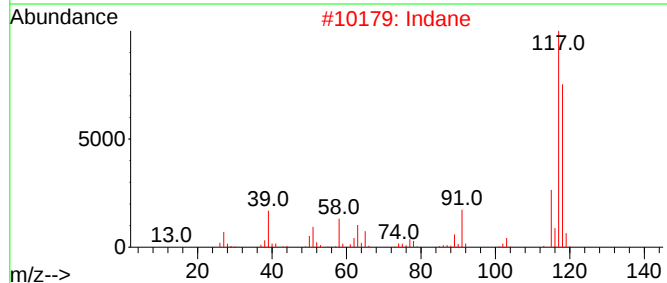
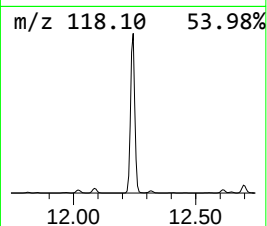
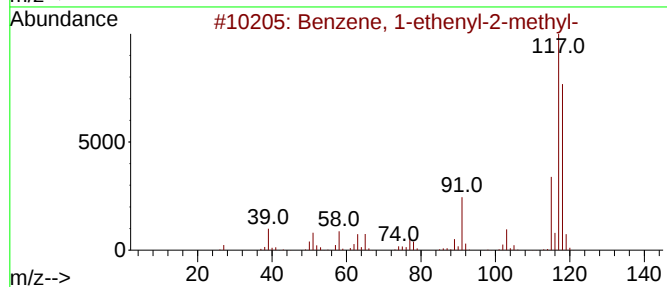
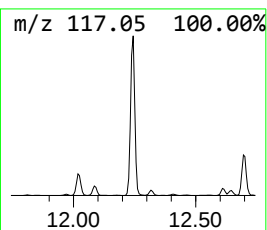
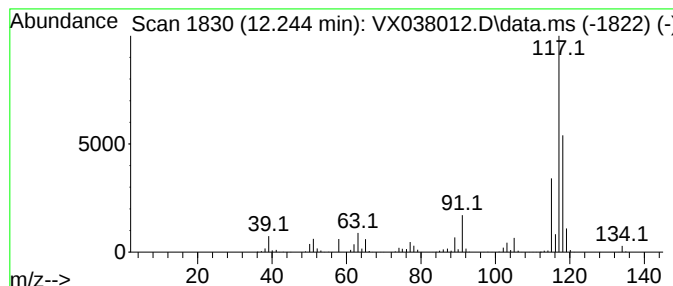
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	40.81 ug/l	857775	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	90
2			Indane	118	C9H10	000496-11-7	87
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
5			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	49



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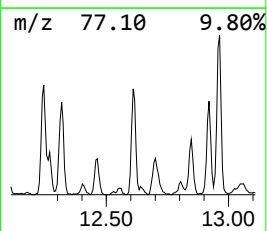
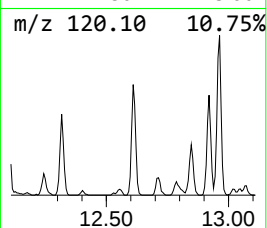
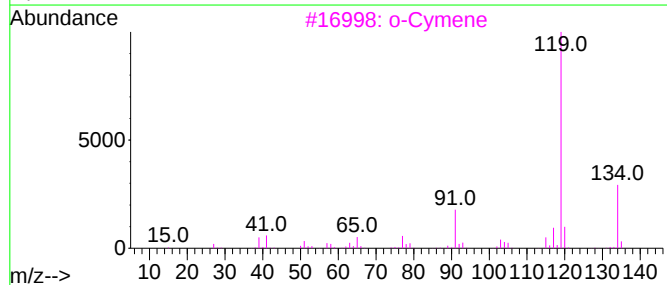
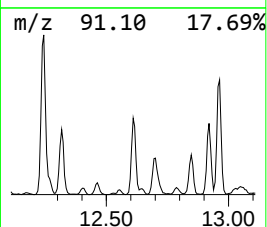
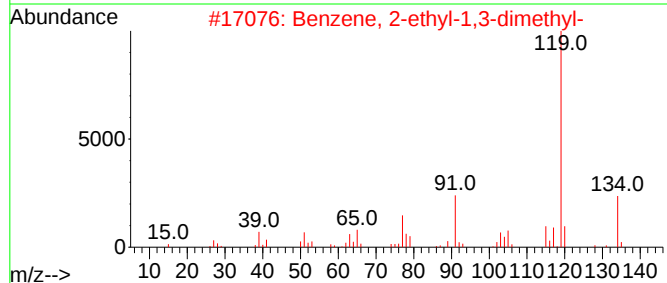
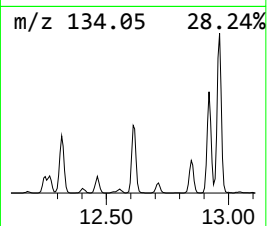
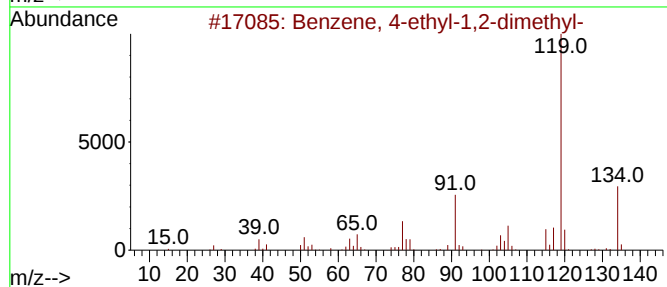
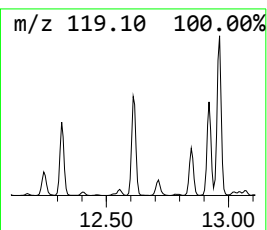
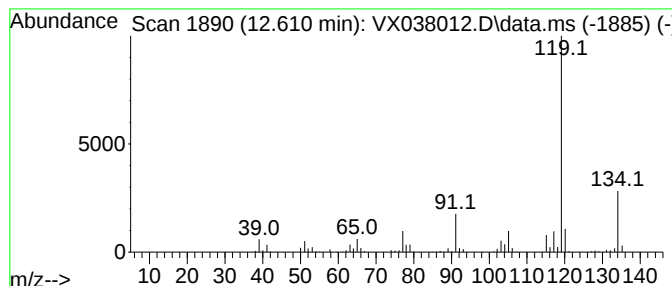
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	14.21 ug/l	298761	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	96
2			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3			o-Cymene	134	C10H14	000527-84-4	95
4			p-Cymene	134	C10H14	000099-87-6	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX093023\
Data File : VX038012.D
Acq On : 30 Sep 2023 18:22
Operator : JC/MD
Sample : 04639-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

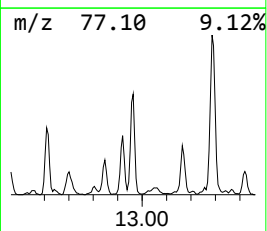
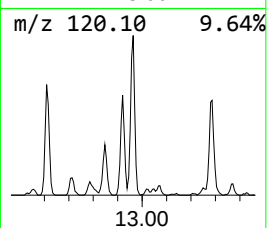
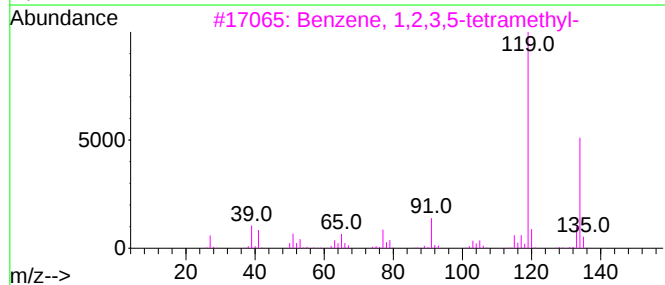
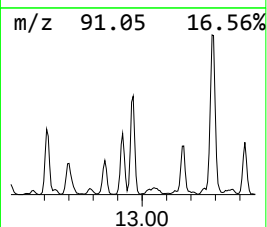
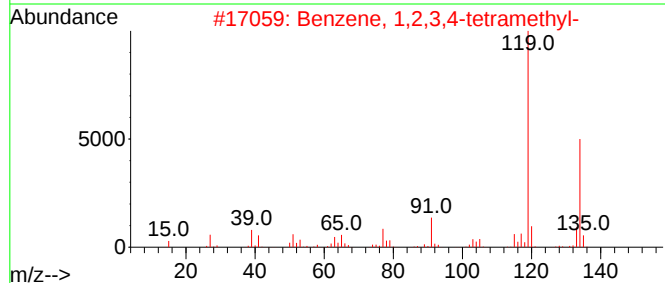
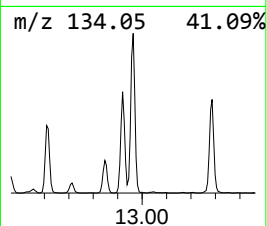
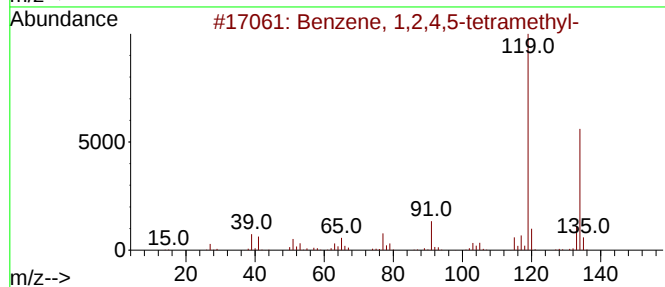
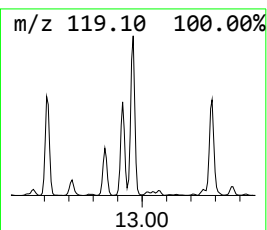
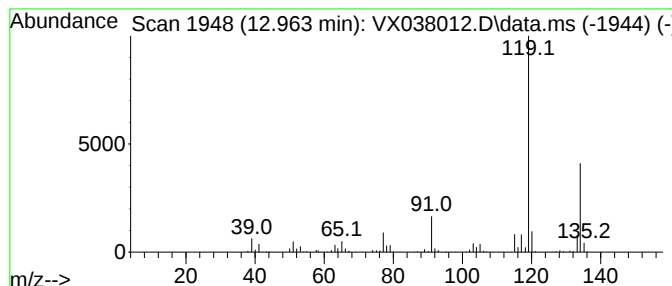
Instrument :
MSVOA_X
ClientSampleId :
1035

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.963	22.66 ug/l	476336	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\VX093023\
Data File : VX038012.D
Acq On : 30 Sep 2023 18:22
Operator : JC/MD
Sample : 04639-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1035

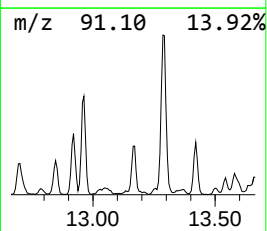
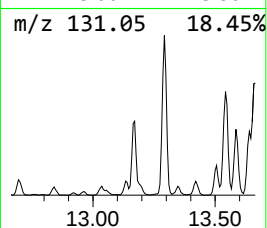
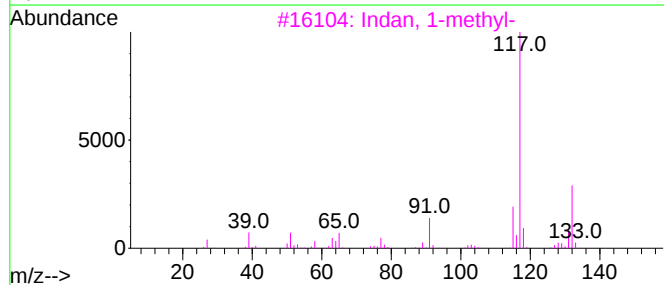
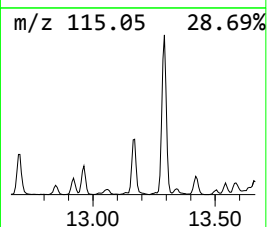
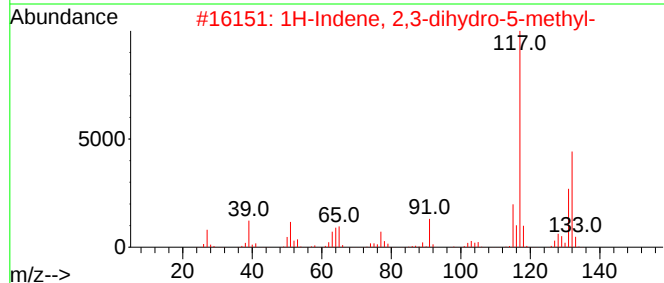
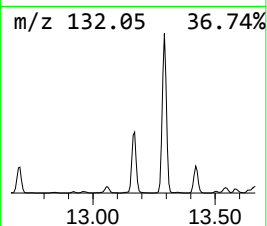
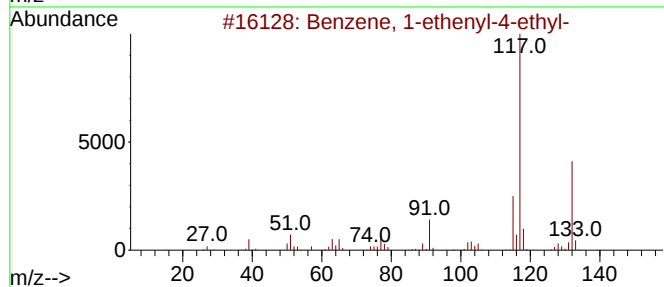
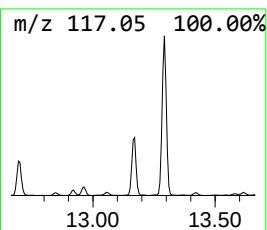
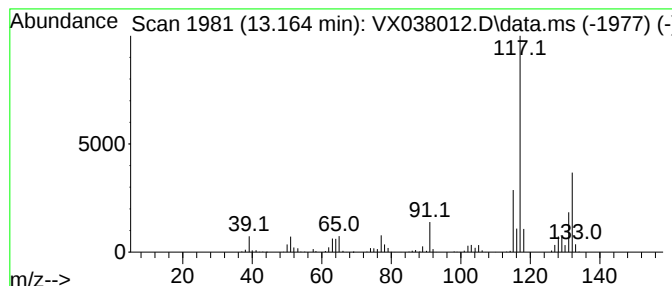
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.164	15.11 ug/l	317580	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	94
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
3			Indan, 1-methyl-	132	C10H12	000767-58-8	90
4			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX093023\
Data File : VX038012.D
Acq On : 30 Sep 2023 18:22
Operator : JC/MD
Sample : 04639-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1035

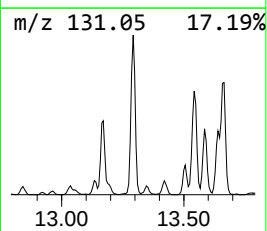
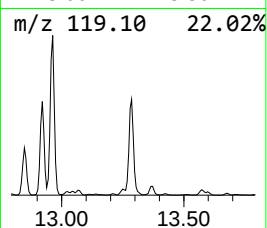
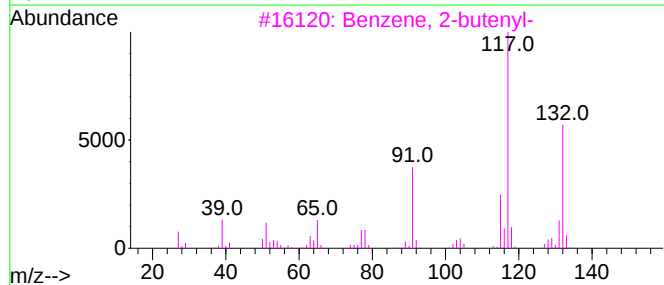
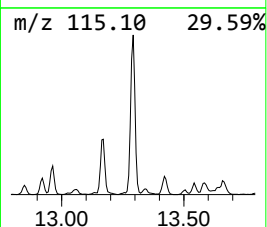
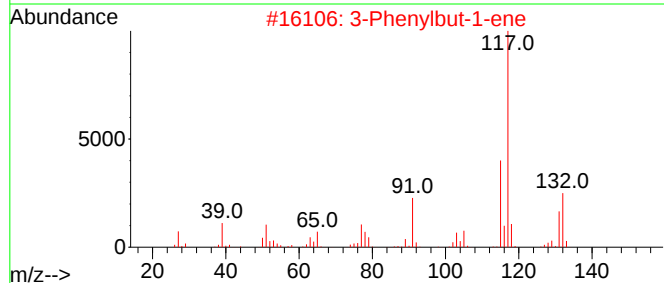
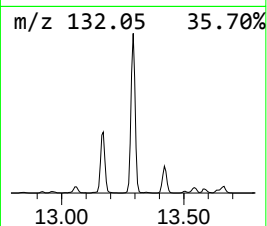
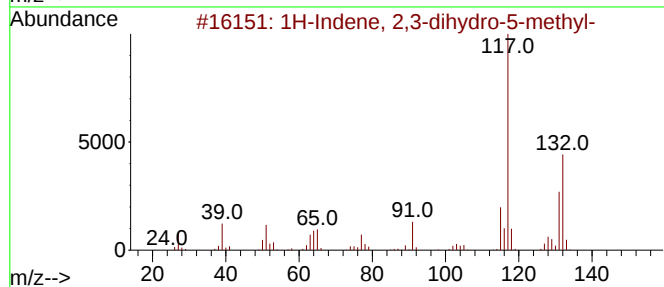
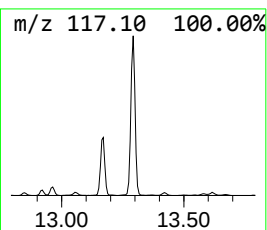
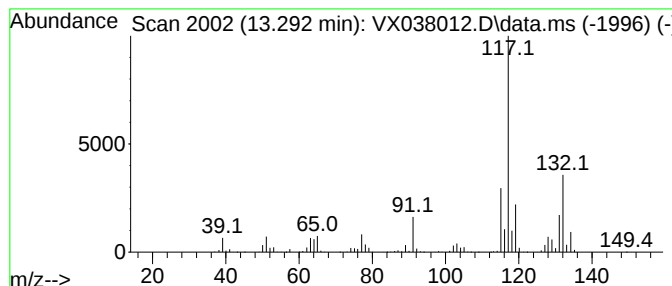
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Quant Title : SW846 8260

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

Peak Number 8 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	53.62 ug/l	1126960	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
2		3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
3		Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
4		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
5		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX093023\
Data File : VX038012.D
Acq On : 30 Sep 2023 18:22
Operator : JC/MD
Sample : 04639-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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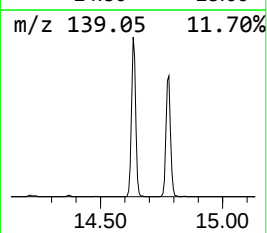
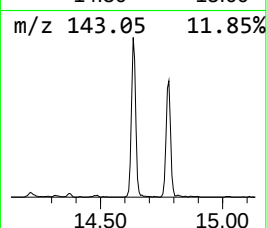
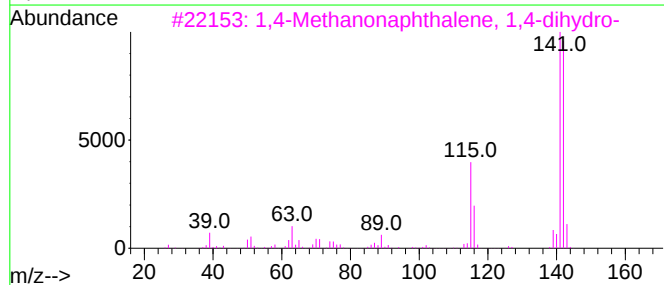
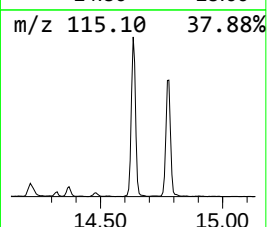
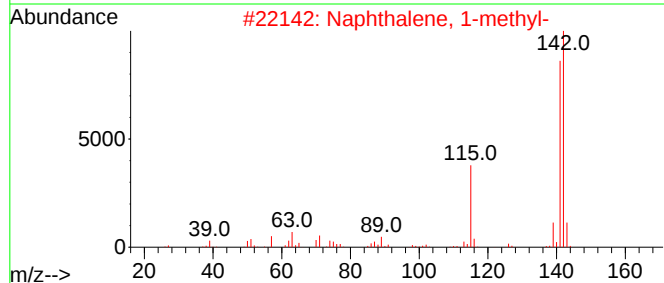
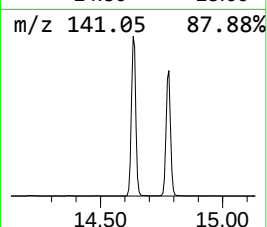
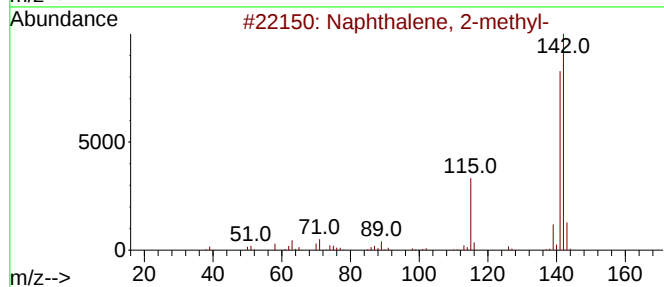
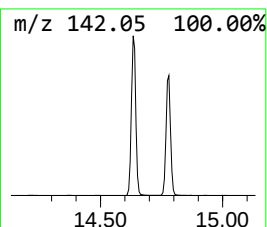
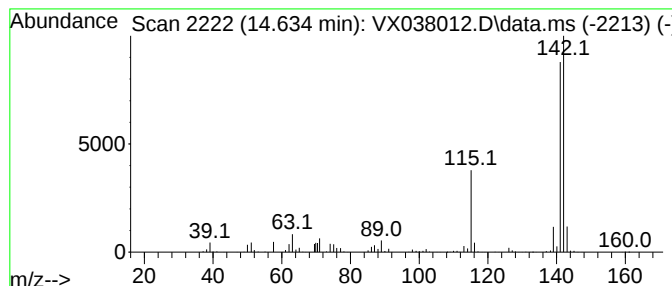
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	36.44 ug/l	765891	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX093023\
Data File : VX038012.D
Acq On : 30 Sep 2023 18:22
Operator : JC/MD
Sample : 04639-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1035

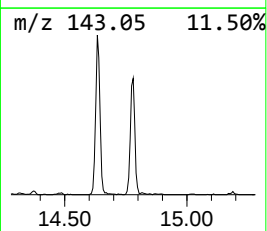
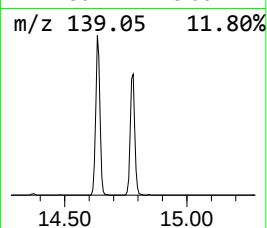
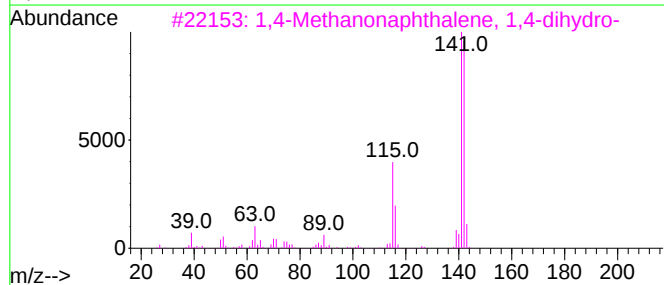
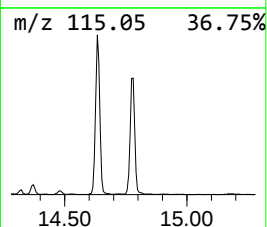
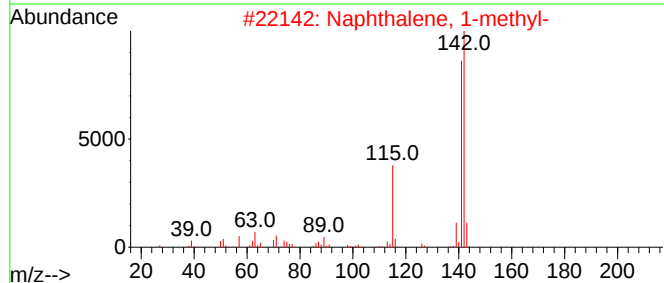
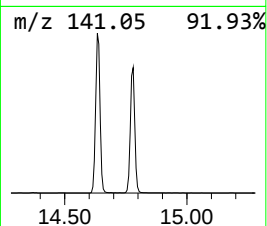
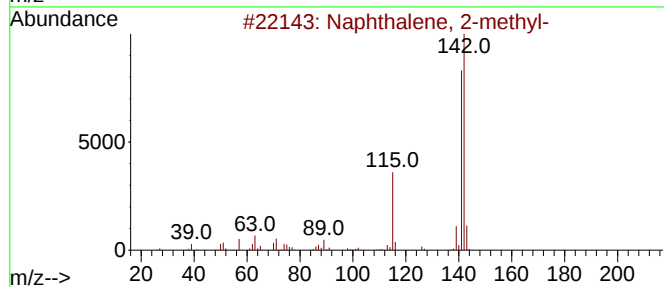
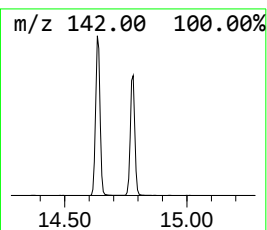
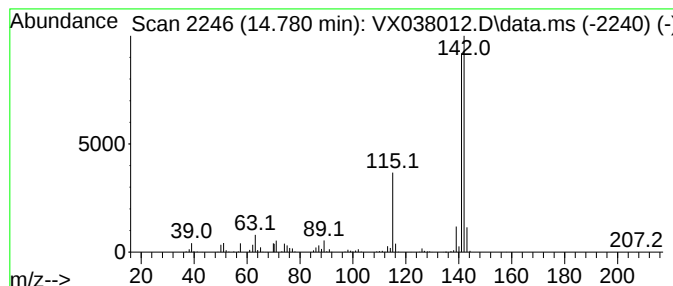
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	27.86 ug/l	585547	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX093023\
Data File : VX038012.D
Acq On : 30 Sep 2023 18:22
Operator : JC/MD
Sample : 04639-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1035

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.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
Benzene, 1-ethy...	11.396	17.3	ug/l	362599	4	12.024	1050910	50.0
Benzene, 1-ethy...	11.610	30.9	ug/l	649273	4	12.024	1050910	50.0
Benzene, 1,2,3-...	12.085	59.6	ug/l	1252090	4	12.024	1050910	50.0
Benzene, 1-ethe...	12.244	40.8	ug/l	857775	4	12.024	1050910	50.0
Benzene, 4-ethy...	12.610	14.2	ug/l	298761	4	12.024	1050910	50.0
Benzene, 1,2,4,...	12.963	22.7	ug/l	476336	4	12.024	1050910	50.0
Benzene, 1-ethe...	13.164	15.1	ug/l	317580	4	12.024	1050910	50.0
1H-Indene, 2,3-...	13.292	53.6	ug/l	1126960	4	12.024	1050910	50.0
Naphthalene, 2-...	14.634	36.4	ug/l	765891	4	12.024	1050910	50.0
Naphthalene, 1-...	14.780	27.9	ug/l	585547	4	12.024	1050910	50.0