

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
 Data File : VX036972.D
 Acq On : 14 Aug 2023 18:12
 Operator : JC/MD
 Sample : 03986-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1771

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\82X072123W.M
 Title : SW846 8260

Signal : TIC: VX036972.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.380	203	212	229	rBV	70559	115454	6.18%	0.829%
2	5.385	694	705	722	rBV2	76744	225169	12.05%	1.617%
3	5.556	722	733	746	rVV	122333	346101	18.52%	2.485%
4	5.958	789	799	805	rBV	82770	213728	11.44%	1.535%
5	6.037	805	812	826	rVB	155974	425616	22.77%	3.056%
6	6.763	921	931	943	rBV	206072	485135	25.96%	3.483%
7	8.647	1234	1240	1246	rBV	413104	671654	35.94%	4.823%
8	8.720	1246	1252	1265	rVB	1092542	1690792	90.46%	12.140%
9	10.055	1465	1471	1490	rVB	457095	617139	33.02%	4.431%
10	10.305	1506	1512	1522	rBV	243696	341737	18.28%	2.454%
11	10.640	1561	1567	1581	rBV	1467650	1869034	100.00%	13.420%
12	11.079	1632	1639	1654	rBV	385915	490830	26.26%	3.524%
13	11.378	1683	1688	1690	rBV	133990	182155	9.75%	1.308%
14	11.451	1696	1700	1708	rVB	226043	264102	14.13%	1.896%
15	11.610	1721	1726	1734	rBV	267763	335354	17.94%	2.408%
16	11.750	1744	1749	1756	rVB	28350	35270	1.89%	0.253%
17	12.024	1788	1794	1799	rBV	457067	605843	32.41%	4.350%
18	12.085	1799	1804	1814	rVB	586160	706655	37.81%	5.074%
19	12.244	1822	1830	1838	rBV	407056	537441	28.76%	3.859%
20	12.317	1838	1842	1851	rVB2	73100	91549	4.90%	0.657%
21	12.408	1851	1857	1862	rBV2	14774	21715	1.16%	0.156%
22	12.463	1862	1866	1871	rVB	19017	23860	1.28%	0.171%
23	12.530	1871	1877	1879	rBV	17886	24022	1.29%	0.172%
24	12.555	1879	1881	1886	rVV	30718	30964	1.66%	0.222%
25	12.609	1886	1890	1894	rVV	102475	127703	6.83%	0.917%
26	12.640	1894	1895	1900	rVV	18417	19407	1.04%	0.139%
27	12.701	1900	1905	1914	rVB2	92413	134615	7.20%	0.967%
28	12.847	1925	1929	1934	rVB	54165	65642	3.51%	0.471%
29	12.920	1934	1941	1944	rBV	106087	122864	6.57%	0.882%
30	12.963	1944	1948	1953	rVB	174608	203797	10.90%	1.463%
31	13.170	1977	1982	1987	rVB	131044	162617	8.70%	1.168%
32	13.292	1992	2002	2007	rBV2	432699	587994	31.46%	4.222%
33	13.420	2019	2023	2029	rVB	64635	79251	4.24%	0.569%
34	13.542	2039	2043	2046	rVV	28596	38957	2.08%	0.280%
35	13.585	2046	2050	2056	rVV3	34502	69167	3.70%	0.497%
36	13.640	2056	2059	2060	rVV	19686	22383	1.20%	0.161%

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Peak Location: TOP

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37	13.664	2060	2063	2069	rVB2	35922	54179	2.90%	0.389%
38	13.774	2076	2081	2089	rVB	852623	1061174	56.78%	7.619%
39	13.926	2100	2106	2110	rBV2	22161	32122	1.72%	0.231%
40	13.969	2110	2113	2121	rVB	23326	27508	1.47%	0.198%
41	14.073	2126	2130	2135	rBV	36604	44965	2.41%	0.323%
42	14.213	2149	2153	2159	rBV2	40541	67309	3.60%	0.483%
43	14.316	2166	2170	2175	rBV	22971	28665	1.53%	0.206%
44	14.371	2175	2179	2183	rVB	33634	39253	2.10%	0.282%
45	14.481	2191	2197	2201	rBV2	19942	28509	1.53%	0.205%
46	14.633	2214	2222	2227	rBV	206597	266532	14.26%	1.914%
47	14.780	2239	2246	2250	rBV	193904	240005	12.84%	1.723%
48	15.481	2353	2361	2365	rBV3	14079	24693	1.32%	0.177%
49	15.609	2377	2382	2386	rBV	17058	26570	1.42%	0.191%

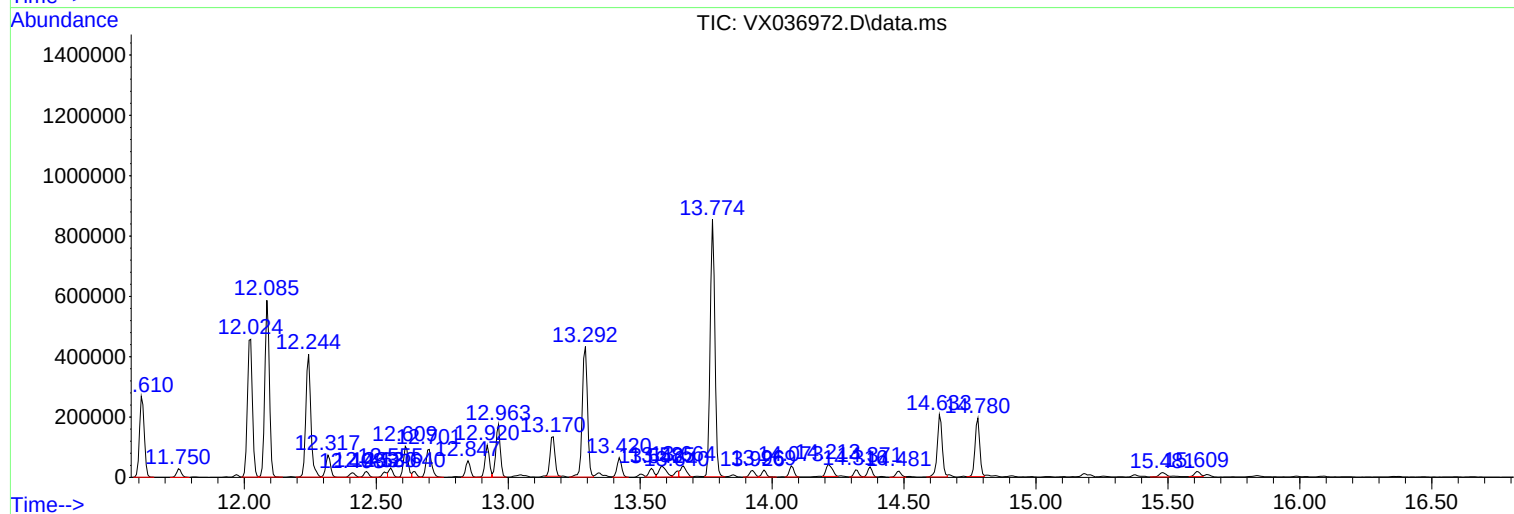
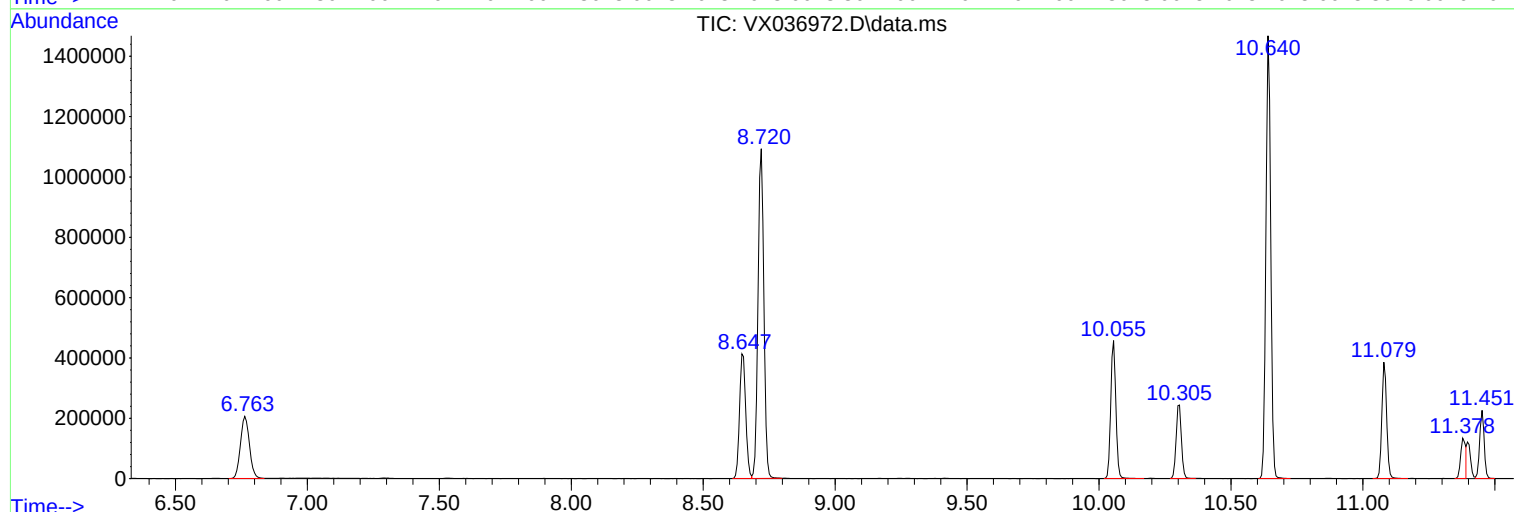
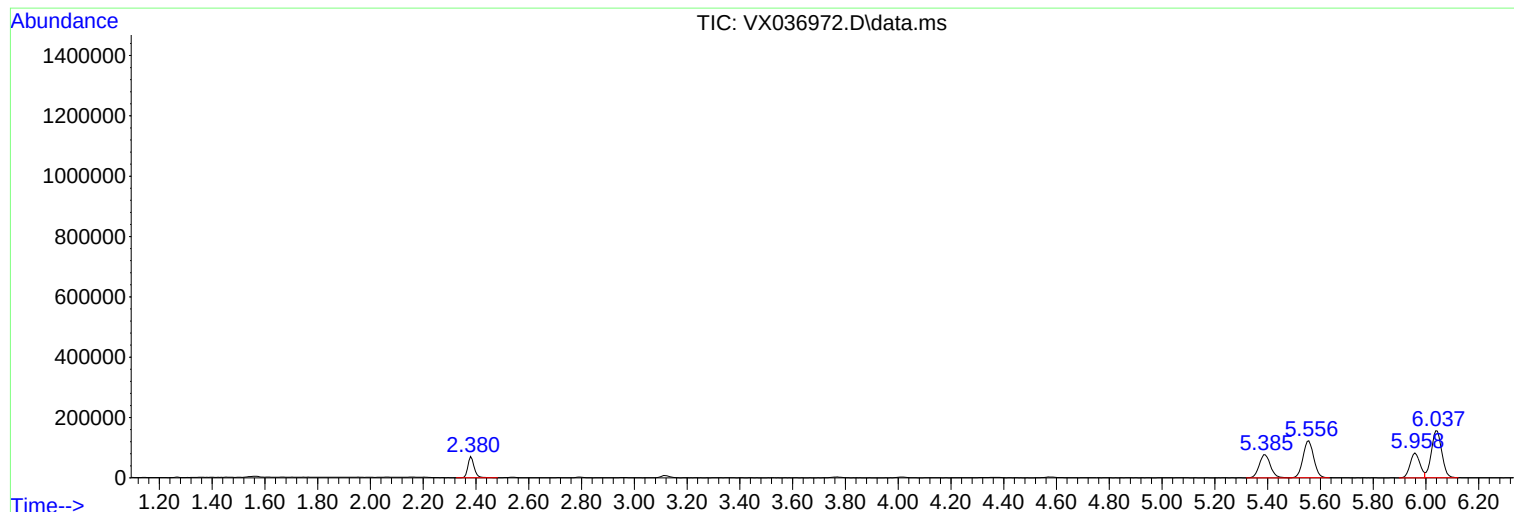
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



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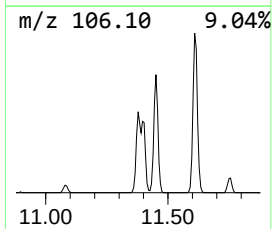
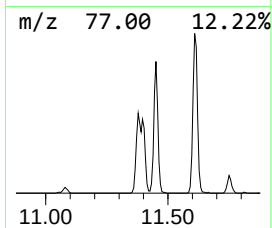
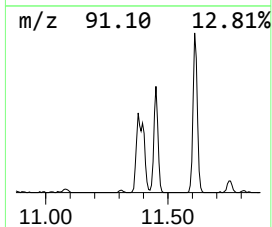
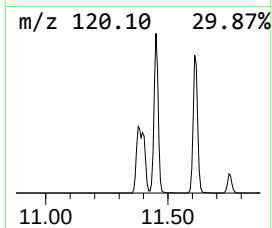
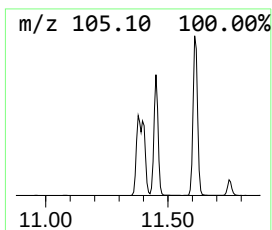
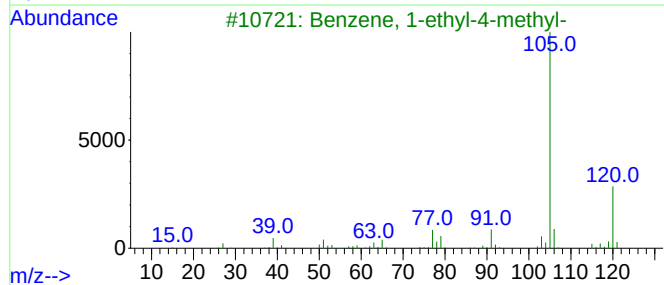
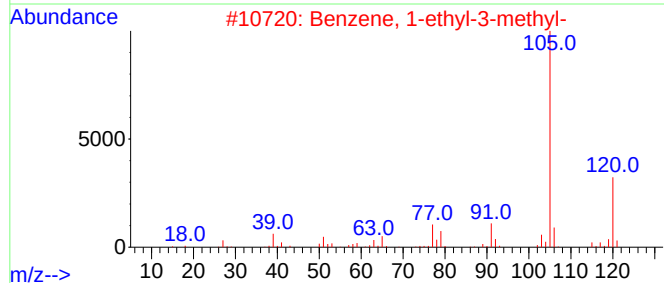
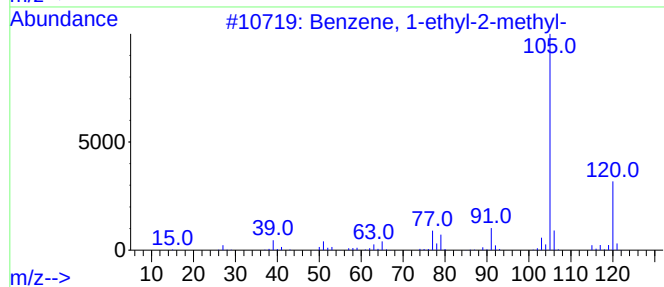
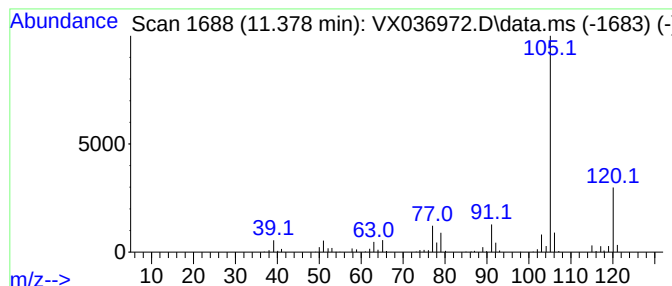
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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.
11.378	15.03 ug/l	182155	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-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	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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Instrument :
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ClientSampleId :
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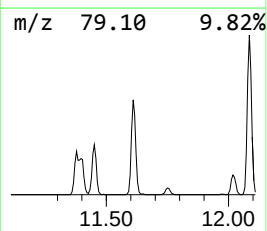
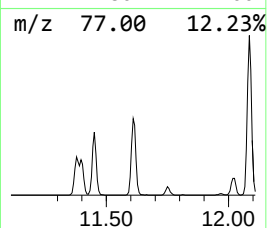
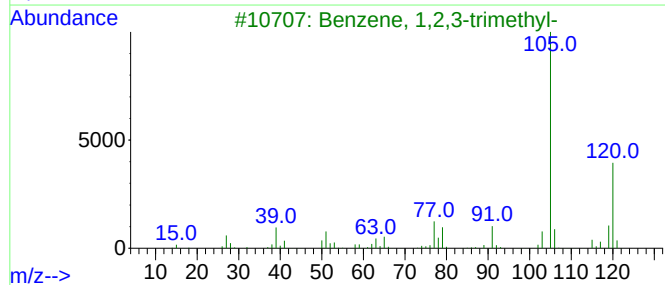
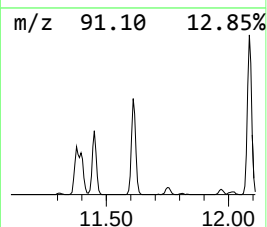
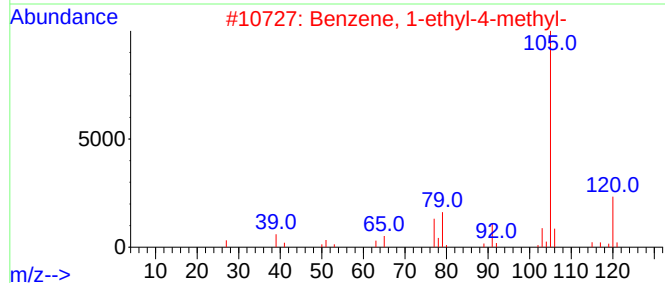
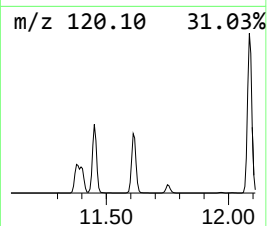
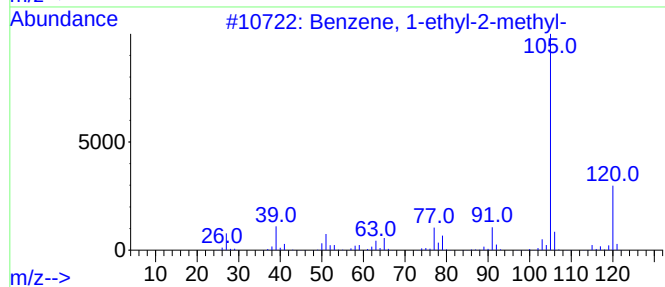
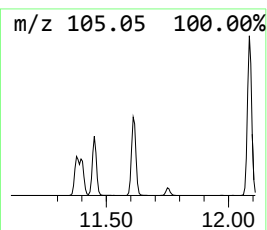
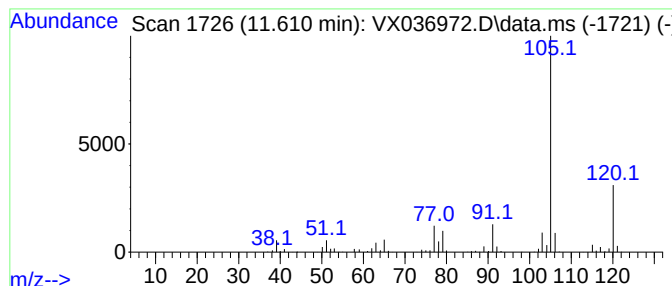
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	27.68 ug/l	335354	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			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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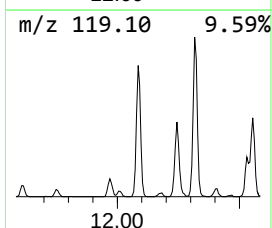
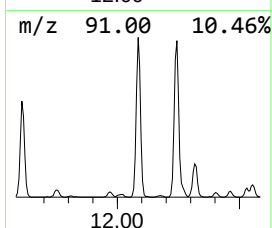
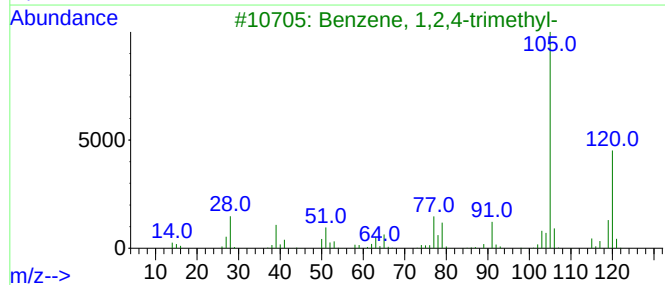
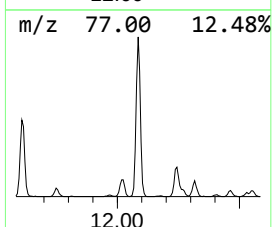
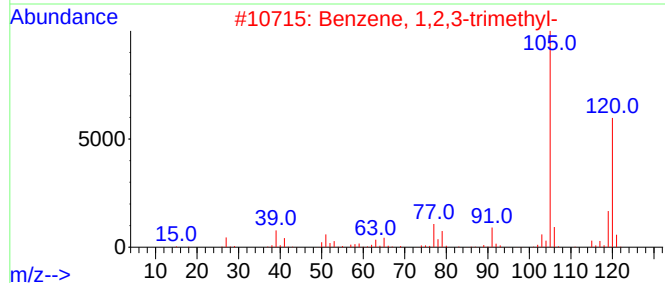
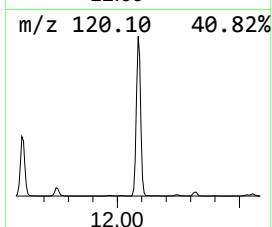
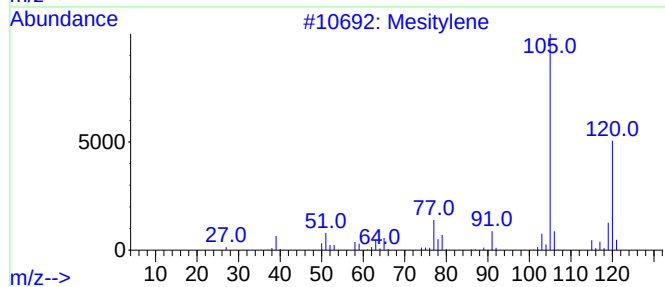
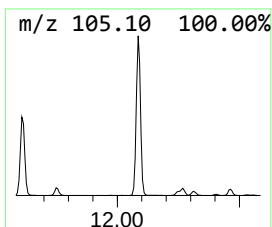
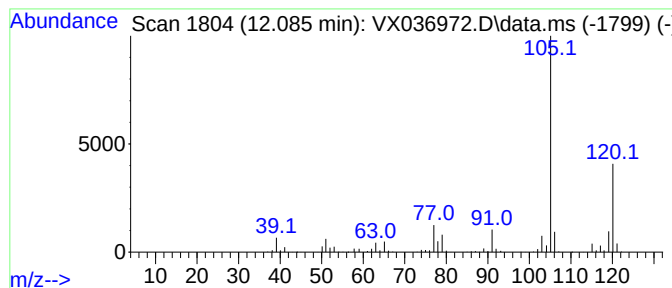
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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	58.32 ug/l	706655	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-4-methyl-	120	C9H12	000622-96-8	90
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



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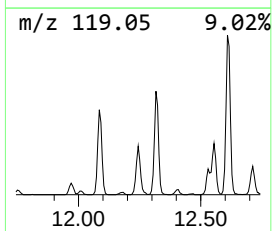
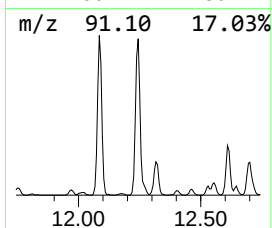
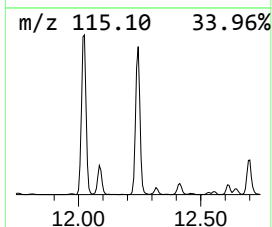
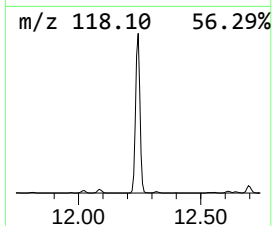
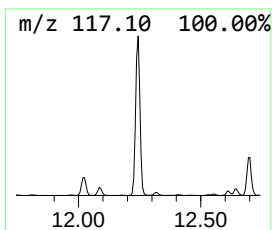
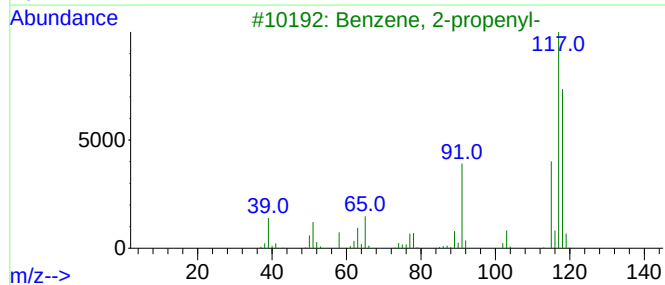
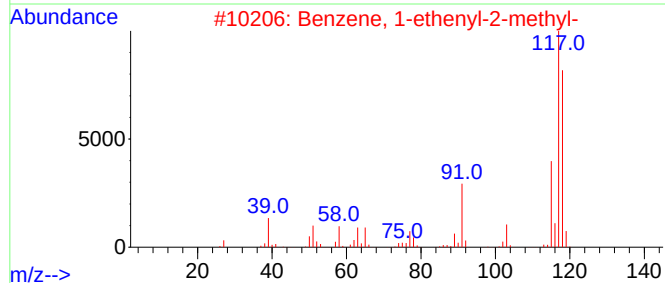
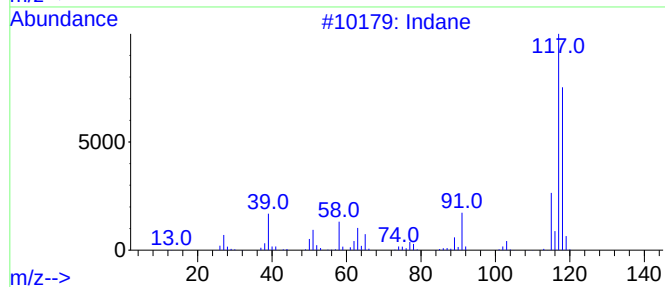
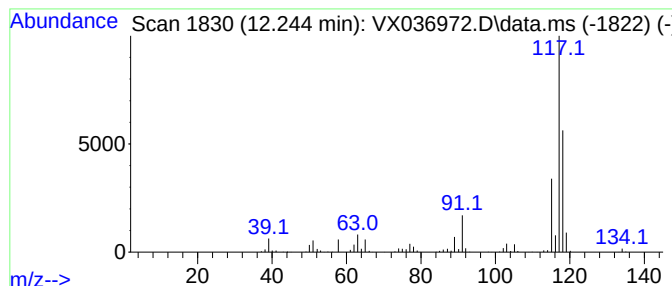
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Quant Title : SW846 8260

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

Peak Number 4 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	44.35 ug/l	537441	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
5			Benzeneethanol, .beta.-ethenyl-....	162	C11H14O	040596-14-3	50



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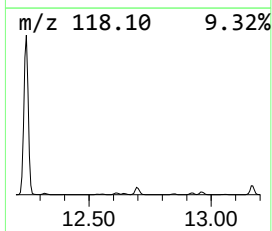
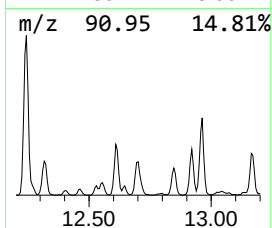
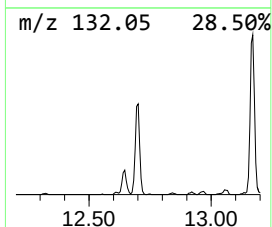
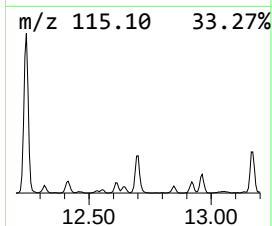
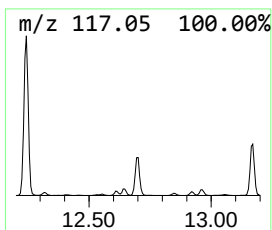
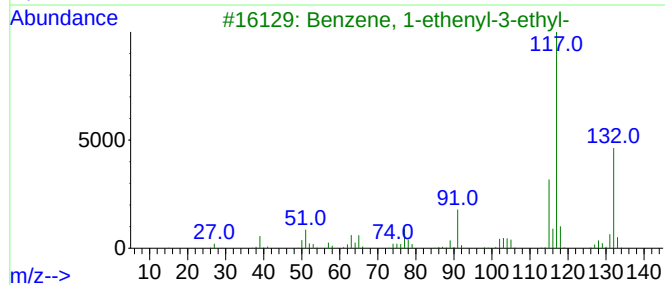
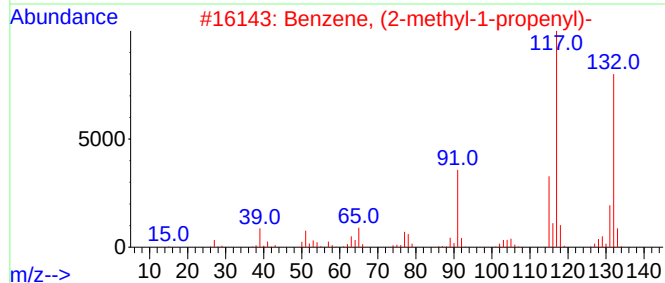
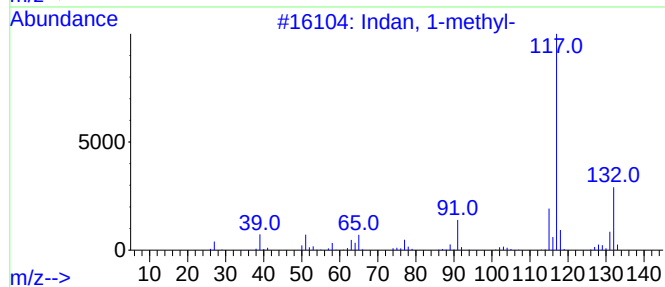
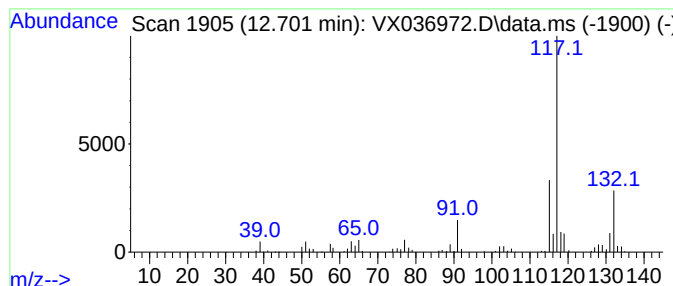
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Quant Title : SW846 8260

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

Peak Number 5 Indan, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	11.11 ug/l	134615	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	93
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
4			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	83
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
Data File : VX036972.D
Acq On : 14 Aug 2023 18:12
Operator : JC/MD
Sample : 03986-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1771

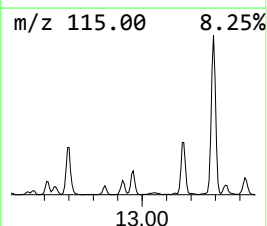
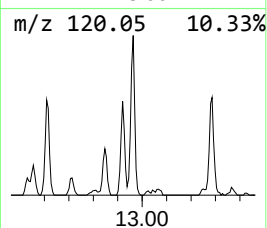
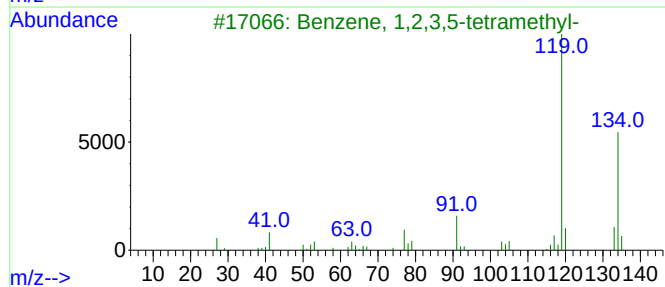
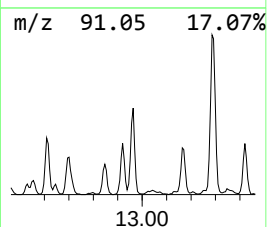
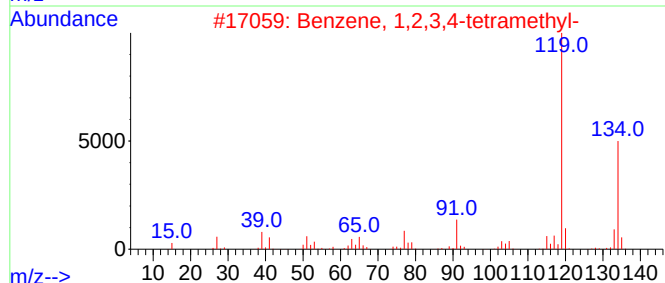
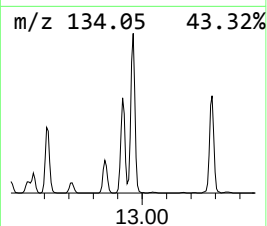
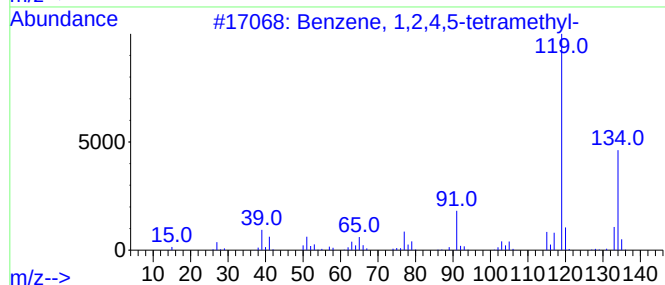
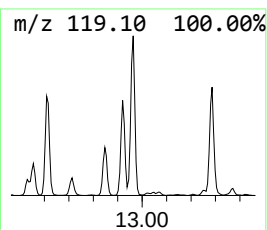
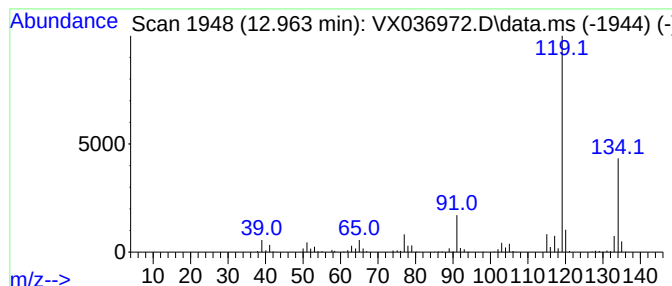
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Quant Title : SW846 8260

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	16.82 ug/l	203797	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	97
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-3,5-dimethyl-	134	C10H14	000934-74-7	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
Data File : VX036972.D
Acq On : 14 Aug 2023 18:12
Operator : JC/MD
Sample : 03986-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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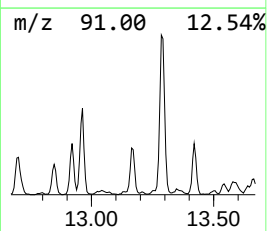
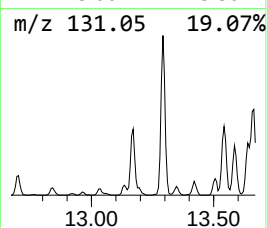
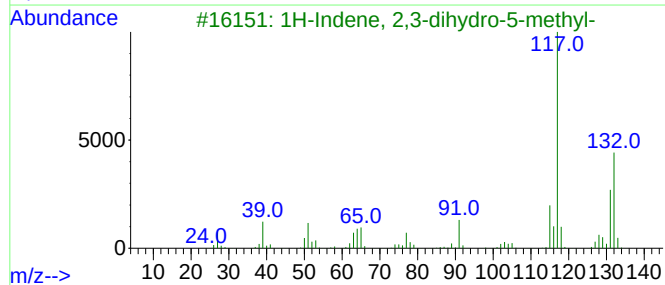
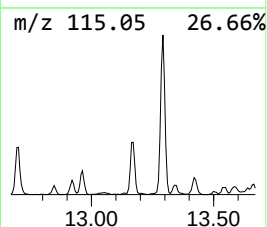
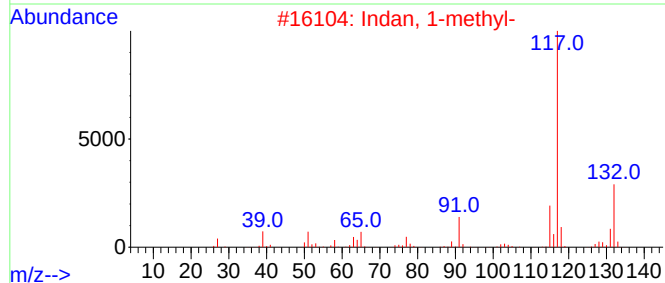
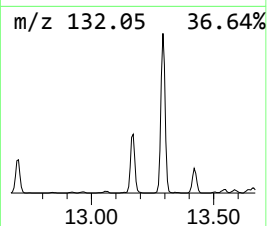
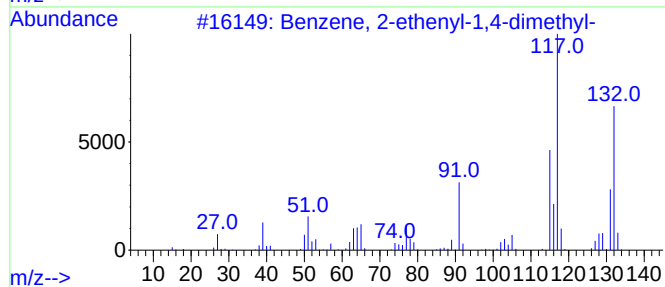
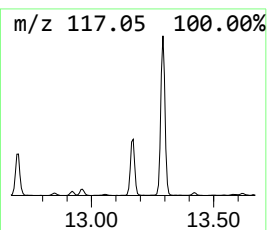
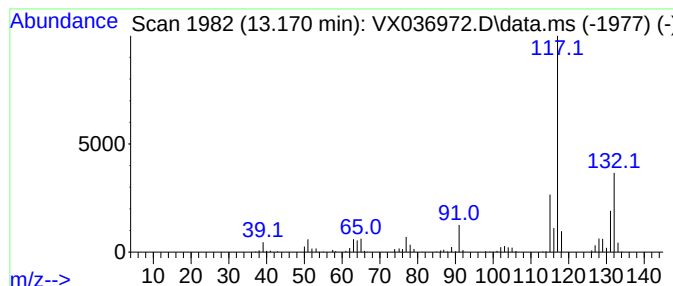
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	13.42 ug/l	162617	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
2			Indan, 1-methyl-	132	C10H12	000767-58-8	90
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
4			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
Data File : VX036972.D
Acq On : 14 Aug 2023 18:12
Operator : JC/MD
Sample : 03986-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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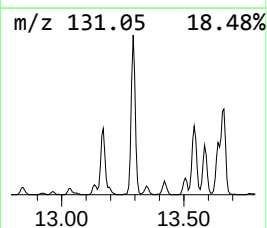
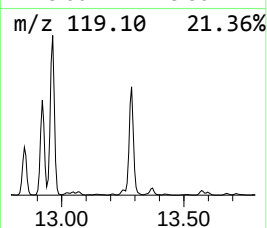
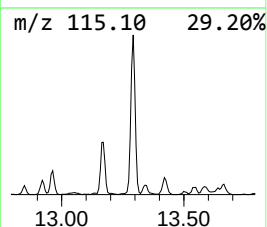
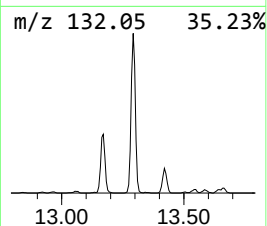
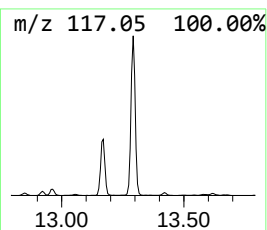
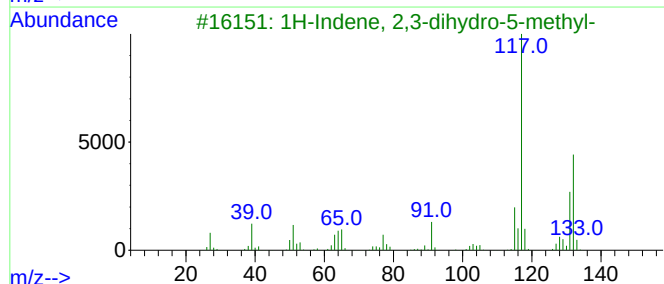
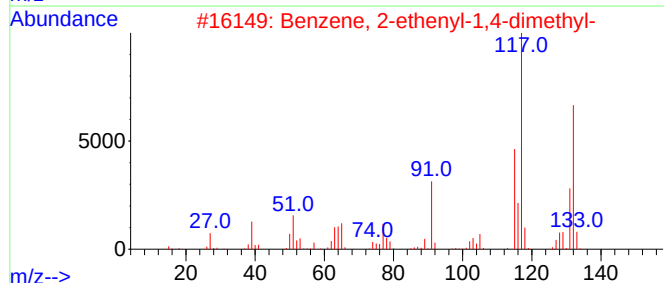
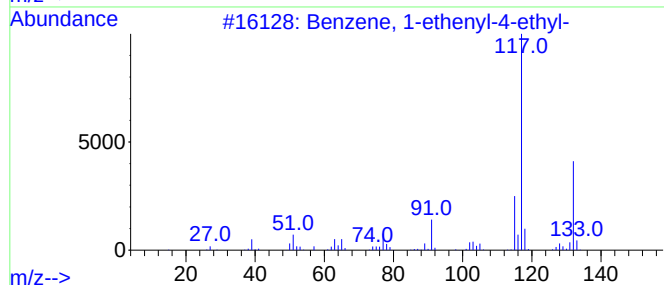
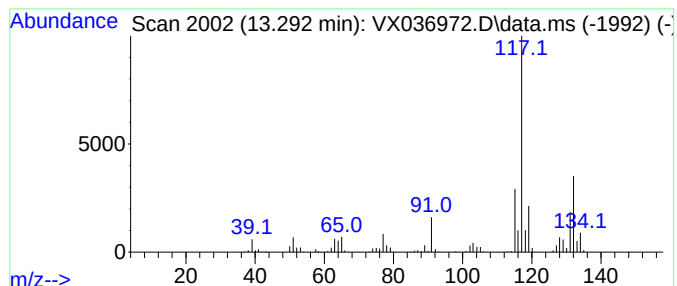
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	48.53 ug/l	587994	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			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
Data File : VX036972.D
Acq On : 14 Aug 2023 18:12
Operator : JC/MD
Sample : 03986-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

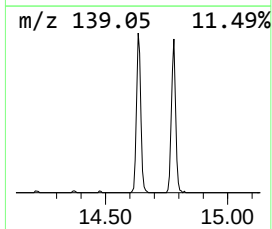
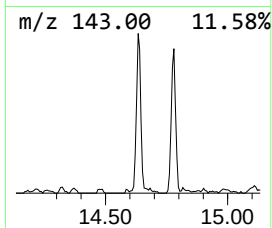
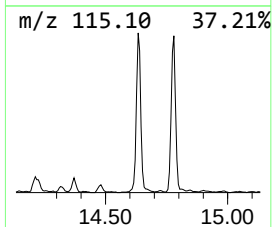
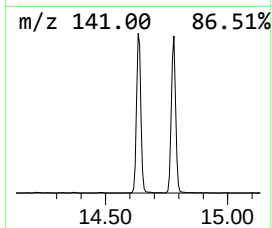
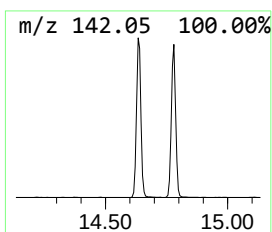
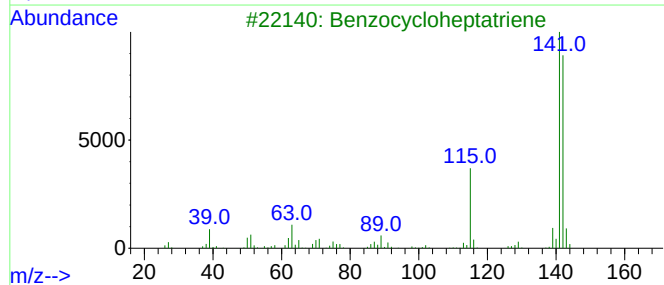
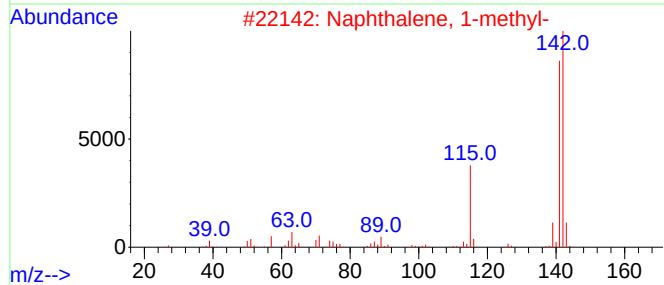
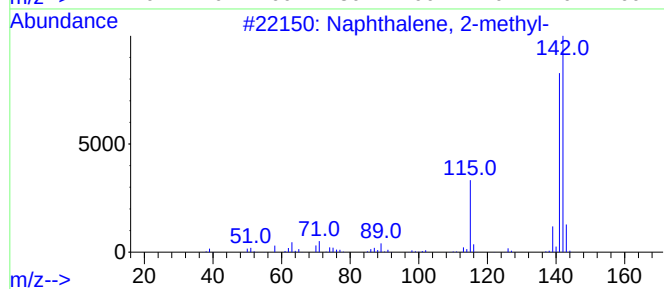
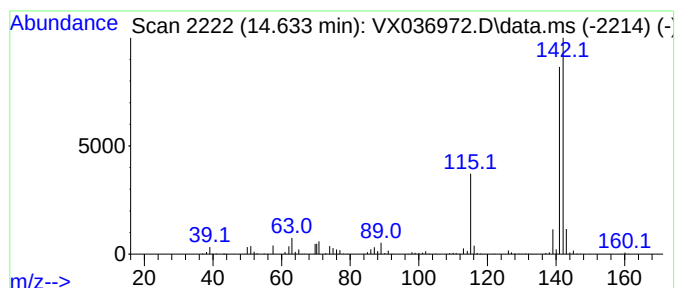
Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzocycloheptatriene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.633	22.00 ug/l	266532	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	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
Data File : VX036972.D
Acq On : 14 Aug 2023 18:12
Operator : JC/MD
Sample : 03986-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1771

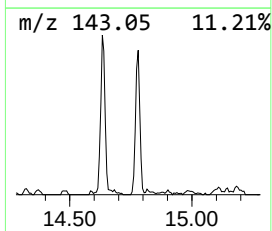
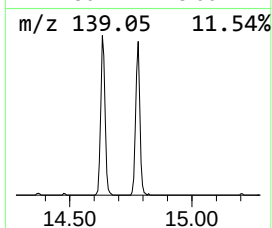
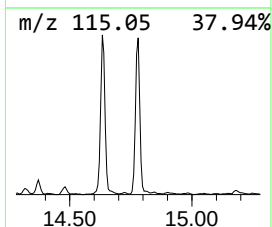
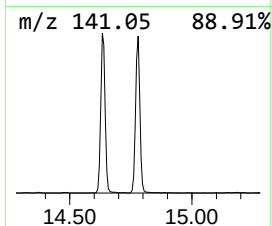
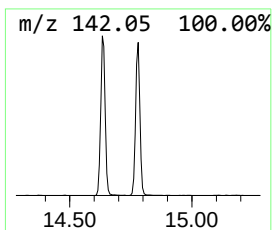
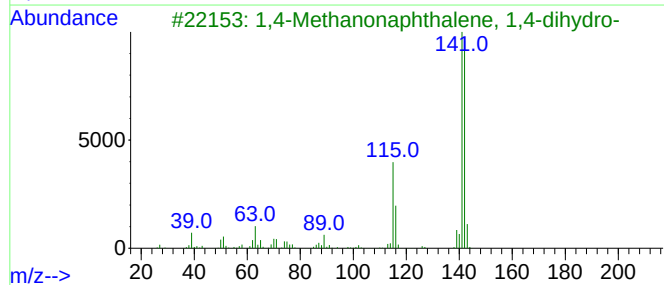
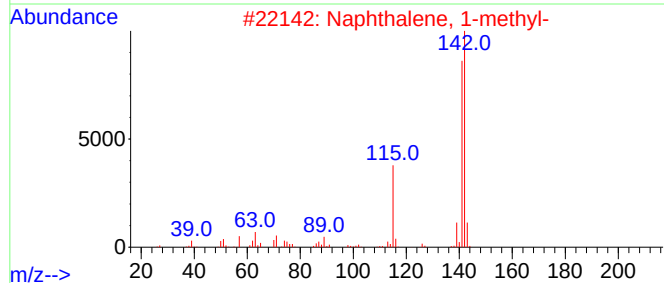
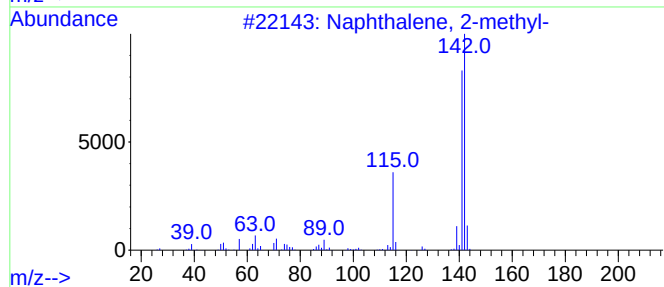
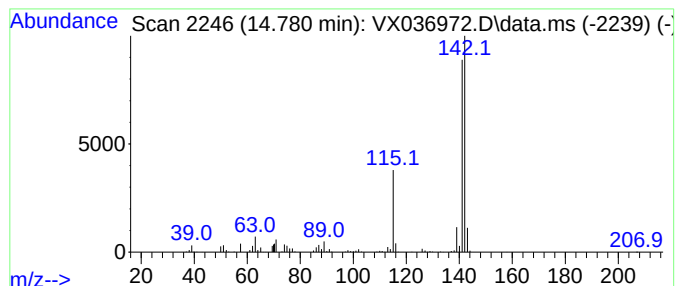
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	19.81 ug/l	240005	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	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
Data File : VX036972.D
Acq On : 14 Aug 2023 18:12
Operator : JC/MD
Sample : 03986-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1771

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.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...	11.378	15.0	ug/l	182155	4	12.024	605843	50.0
Benzene, 1-ethy...	11.610	27.7	ug/l	335354	4	12.024	605843	50.0
Benzene, 1,2,3-...	12.085	58.3	ug/l	706655	4	12.024	605843	50.0
Indane	12.244	44.4	ug/l	537441	4	12.024	605843	50.0
Indan, 1-methyl-	12.701	11.1	ug/l	134615	4	12.024	605843	50.0
Benzene, 1,2,4,...	12.963	16.8	ug/l	203797	4	12.024	605843	50.0
Benzene, 2-ethe...	13.170	13.4	ug/l	162617	4	12.024	605843	50.0
Benzene, 1-ethe...	13.292	48.5	ug/l	587994	4	12.024	605843	50.0
Benzocyclohepta...	14.633	22.0	ug/l	266532	4	12.024	605843	50.0
1,4-Methanonaph...	14.780	19.8	ug/l	240005	4	12.024	605843	50.0