

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
 Data File : VX031227.D
 Acq On : 08 Sep 2022 21:22
 Operator : JC/MD
 Sample : N4505-08
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 CLI-77

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\82X090722W.M
 Title : SW846 8260

Signal : TIC: VX031227.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	54	60	66	rBV	38453	46599	1.05%	0.287%
2	2.087	154	164	184	rBV	323964	775820	17.56%	4.775%
3	2.386	206	213	231	rBV	2649974	4417647	100.00%	27.190%
4	2.550	232	240	254	rVB	135460	302005	6.84%	1.859%
5	3.117	324	333	343	rBV2	35475	81421	1.84%	0.501%
6	4.562	560	570	584	rBV	30543	88266	2.00%	0.543%
7	5.385	695	705	723	rBV2	67303	198702	4.50%	1.223%
8	5.556	723	733	747	rVB2	78812	220576	4.99%	1.358%
9	5.964	788	800	806	rBV	73752	198620	4.50%	1.222%
10	6.038	806	812	823	rVB2	60037	158461	3.59%	0.975%
11	6.763	922	931	943	rBV2	110445	271056	6.14%	1.668%
12	8.653	1234	1241	1246	rVV	331509	533738	12.08%	3.285%
13	8.720	1246	1252	1271	rVB	1461433	2226867	50.41%	13.706%
14	10.055	1466	1471	1479	rVB	234593	312449	7.07%	1.923%
15	10.195	1488	1494	1500	rBV	215008	274675	6.22%	1.691%
16	10.299	1504	1511	1518	rBV	717181	965024	21.84%	5.940%
17	10.640	1562	1567	1579	rVB	539193	722701	16.36%	4.448%
18	11.079	1634	1639	1647	rBV	297026	387924	8.78%	2.388%
19	11.378	1683	1688	1696	rBV	119632	202091	4.57%	1.244%
20	11.451	1696	1700	1712	rVB	64447	82241	1.86%	0.506%
21	11.616	1721	1727	1732	rBV	85273	110165	2.49%	0.678%
22	11.750	1744	1749	1755	rBV	382817	485160	10.98%	2.986%
23	12.024	1789	1794	1800	rVB	255661	304703	6.90%	1.875%
24	12.085	1800	1804	1810	rBV	205248	257977	5.84%	1.588%
25	12.244	1822	1830	1838	rBV	195759	260943	5.91%	1.606%
26	12.616	1887	1891	1894	rBV	37405	45450	1.03%	0.280%
27	12.701	1900	1905	1912	rVB2	38034	53238	1.21%	0.328%
28	12.921	1935	1941	1945	rBV	43940	58453	1.32%	0.360%
29	12.963	1945	1948	1953	rVB	74997	85829	1.94%	0.528%
30	13.170	1979	1982	1987	rVB	66803	79014	1.79%	0.486%
31	13.292	1991	2002	2007	rBV2	169278	232498	5.26%	1.431%
32	13.420	2019	2023	2033	rVB	39771	51803	1.17%	0.319%
33	13.774	2076	2081	2091	rBV	673784	851941	19.28%	5.244%
34	14.231	2149	2156	2160	rBV2	32658	64476	1.46%	0.397%
35	14.481	2192	2197	2209	rBV3	22778	48685	1.10%	0.300%
36	14.640	2215	2223	2227	rBV	362678	464454	10.51%	2.859%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Title : SW846 8260

37	14.780	2240	2246	2251	rBV	228248	280558	6.35%	1.727%
38	15.615	2377	2383	2387	rBV	27809	45188	1.02%	0.278%

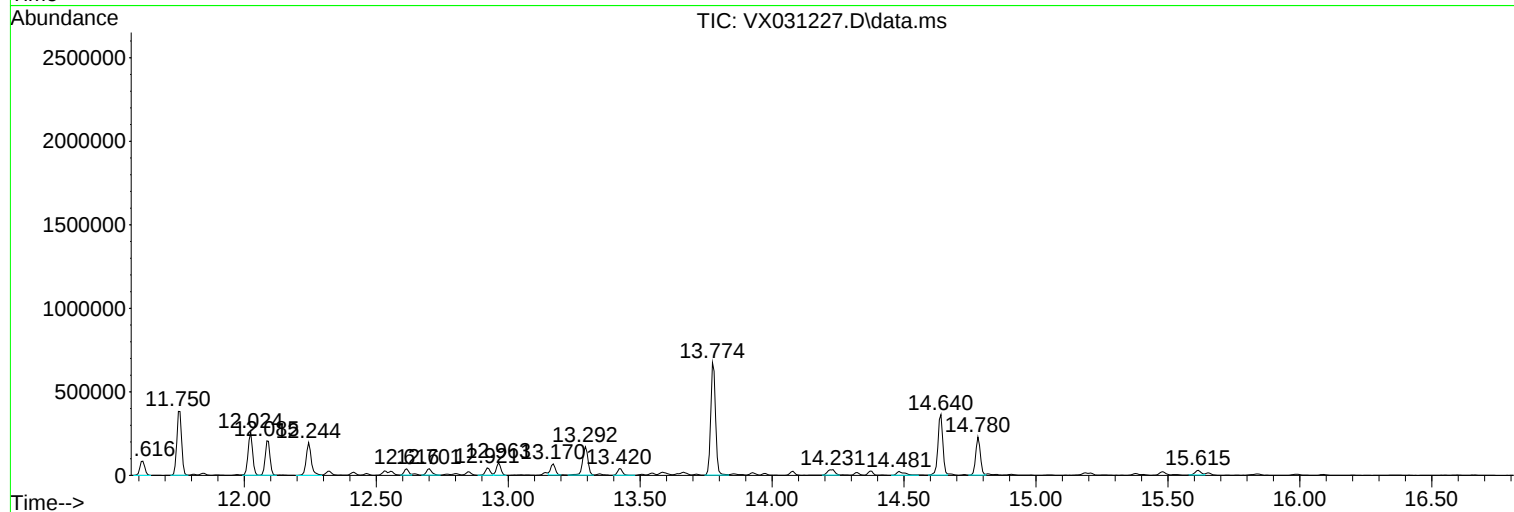
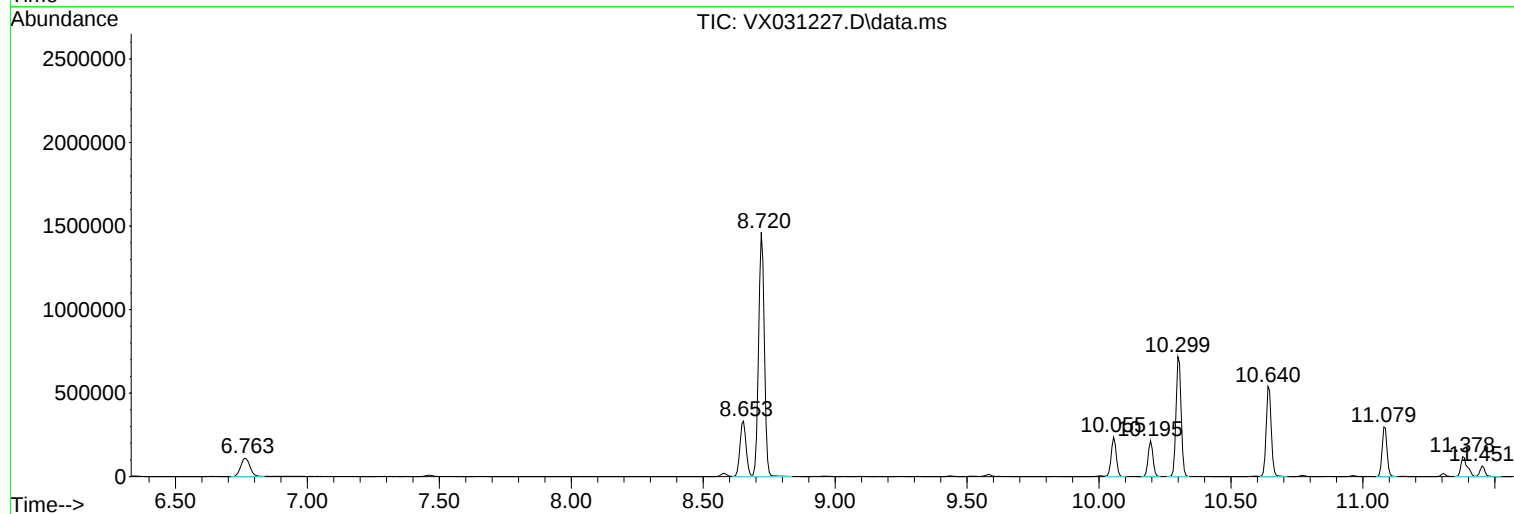
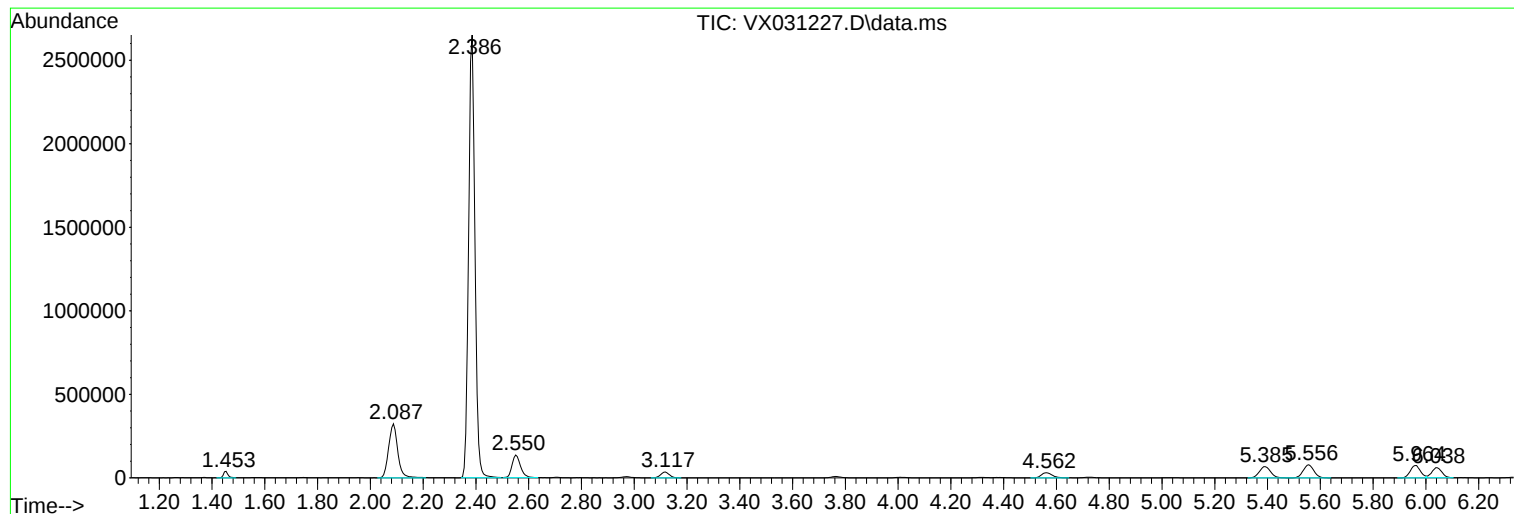
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

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



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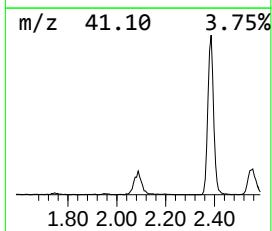
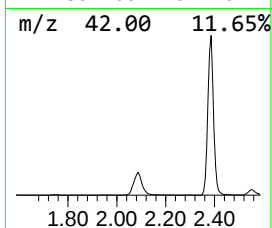
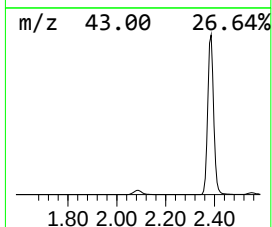
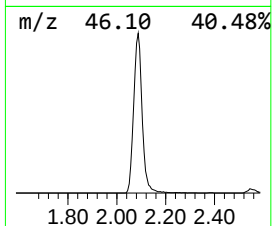
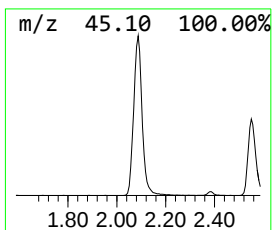
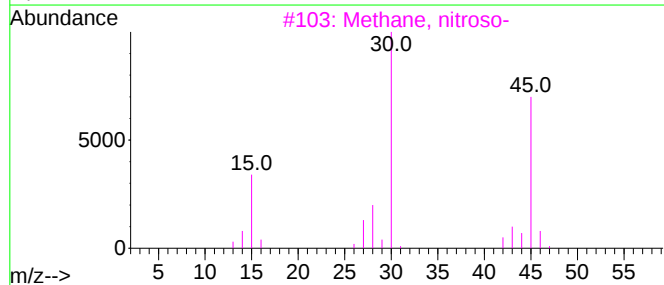
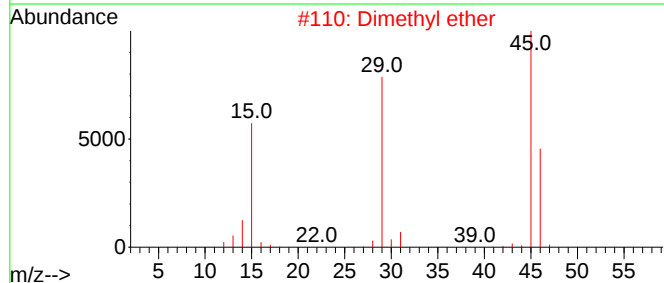
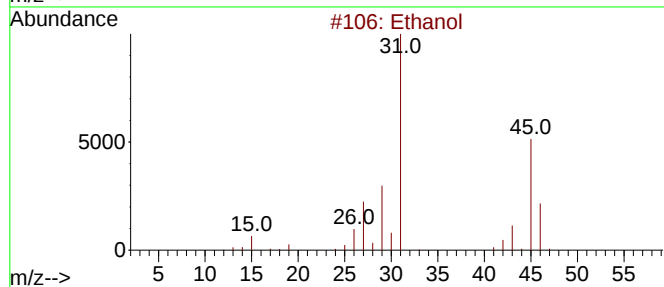
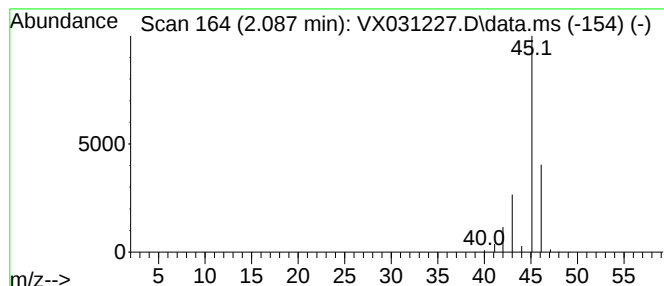
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.087	175.86 ug/l	775820	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	74
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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Instrument :
MSVOA_X
ClientSampleId :
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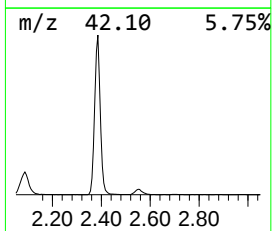
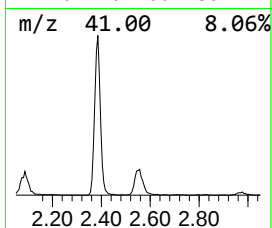
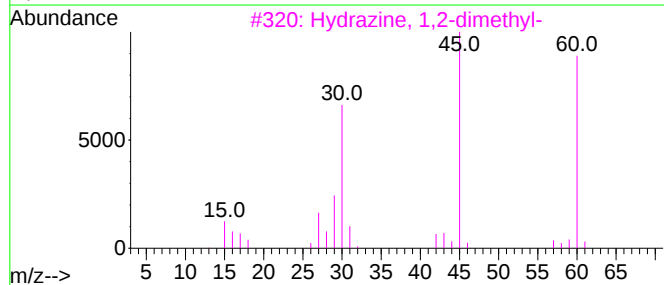
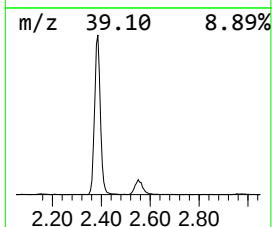
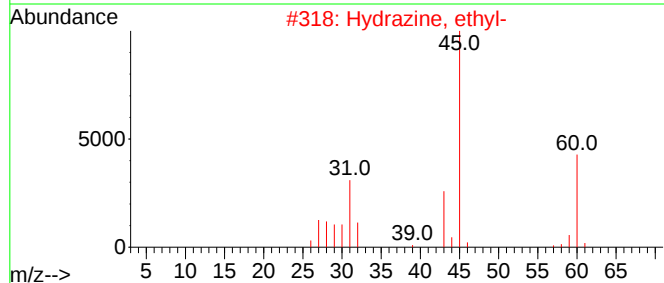
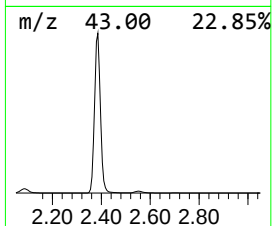
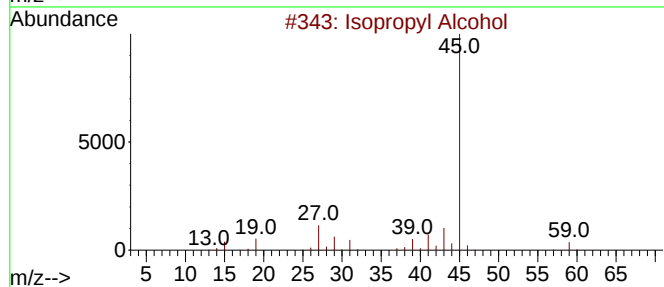
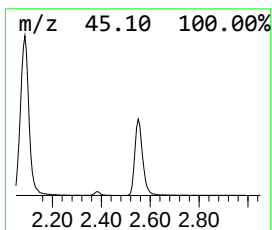
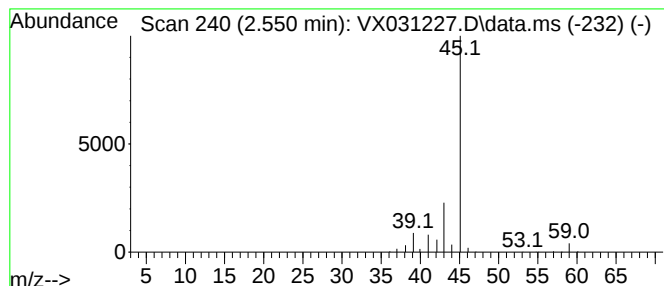
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.550	68.46 ug/l	302005	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
3			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4			Ethylamine	45	C2H7N	000075-04-7	4
5			Formamide	45	CH3NO	000075-12-7	4



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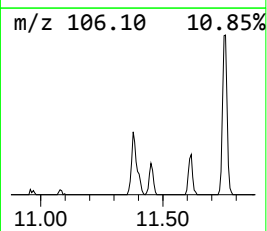
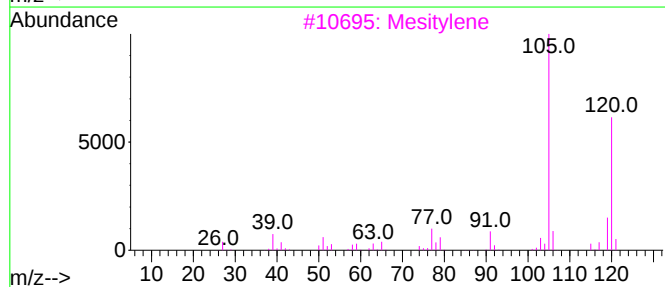
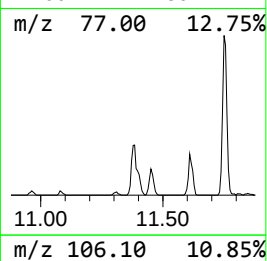
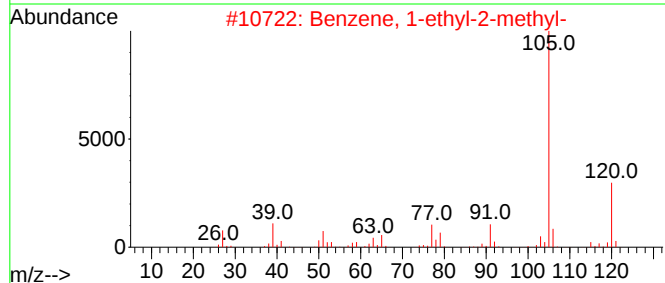
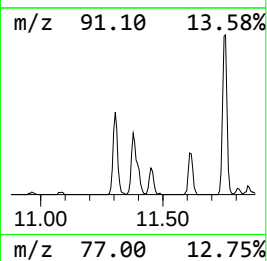
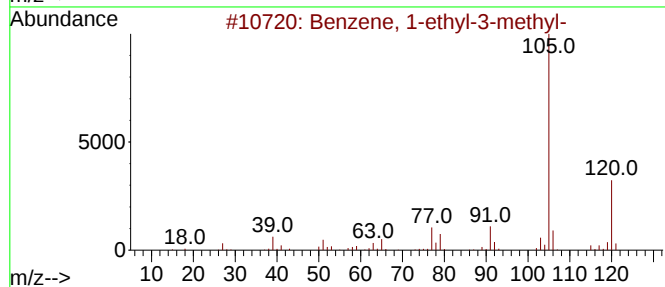
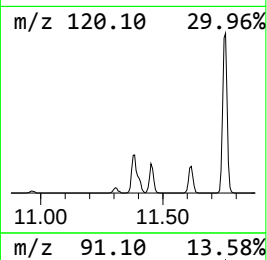
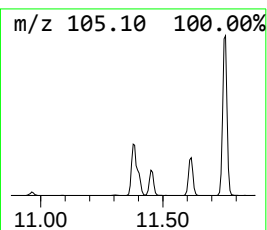
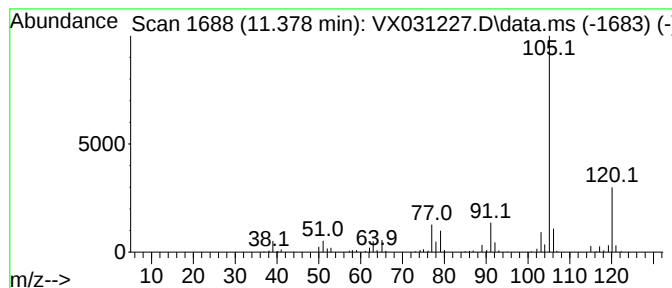
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	33.16 ug/l	202091	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-77

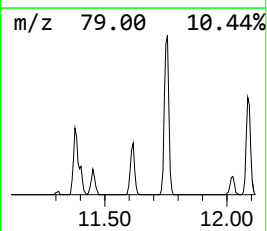
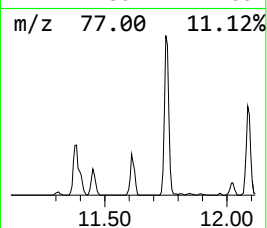
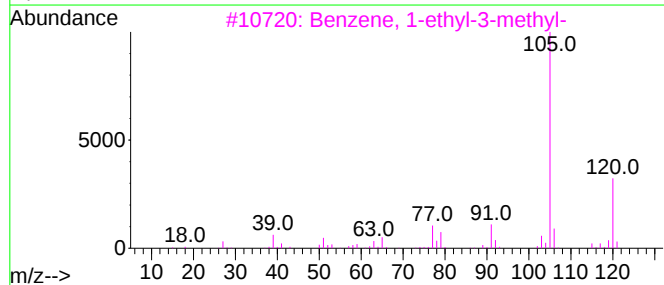
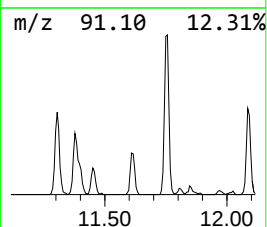
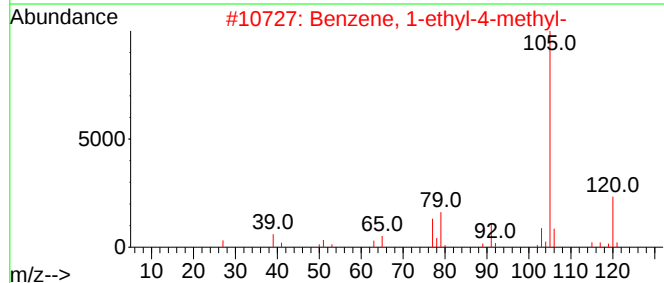
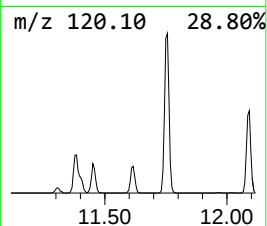
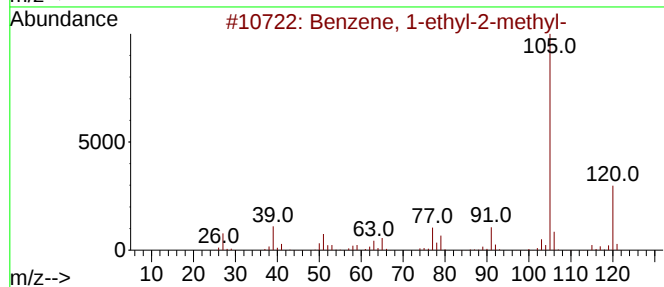
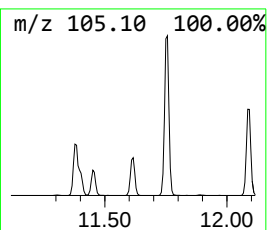
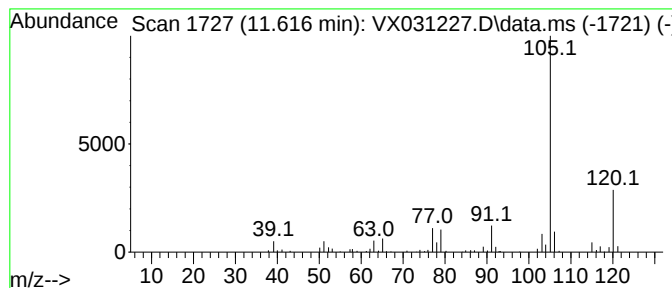
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	18.08 ug/l	110165	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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Instrument :
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ClientSampleId :
CLI-77

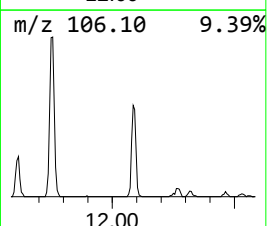
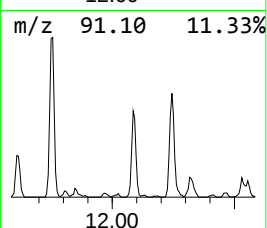
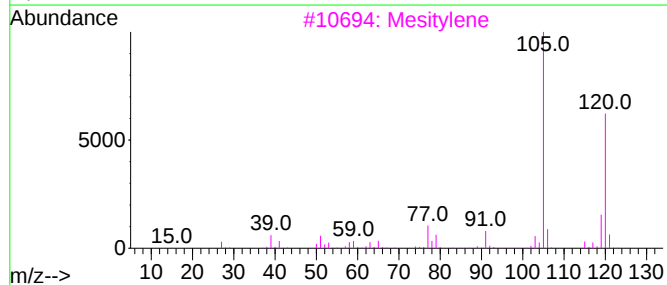
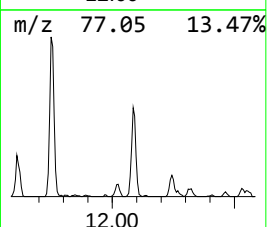
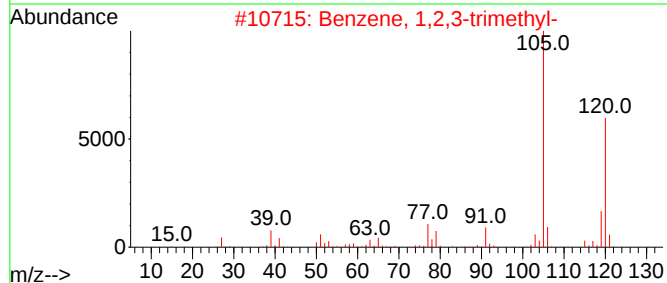
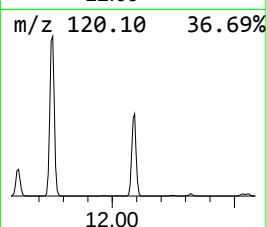
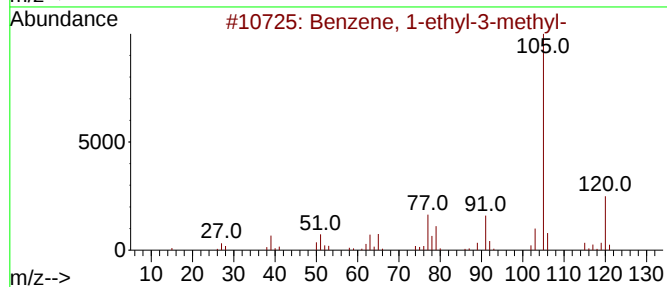
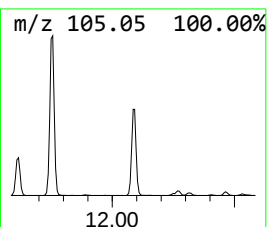
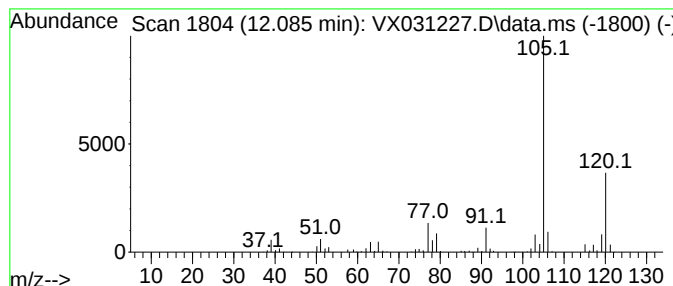
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	42.33 ug/l	257977	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031227.D
Acq On : 08 Sep 2022 21:22
Operator : JC/MD
Sample : N4505-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

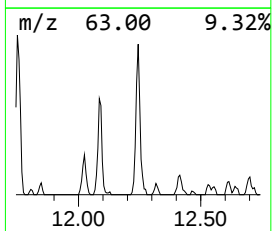
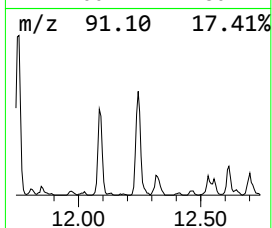
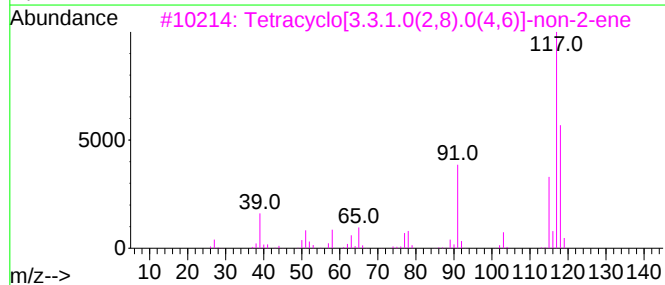
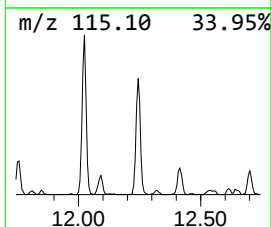
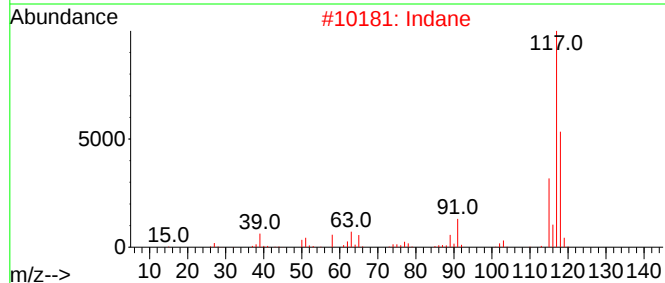
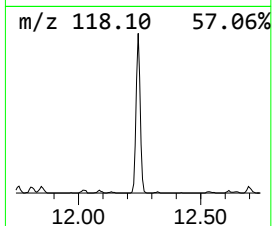
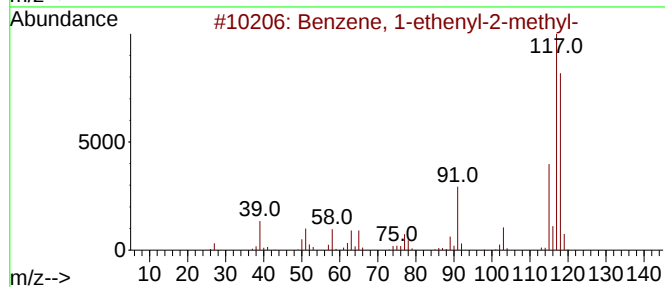
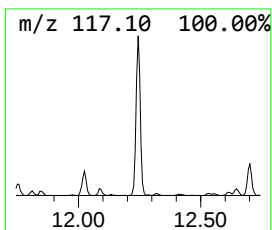
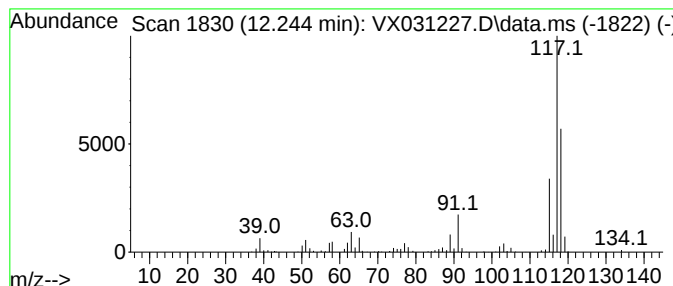
Instrument :
MSVOA_X
ClientSampleId :
CLI-77

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethenyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.244	42.82 ug/l	260943	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	87
2	Indane	118	C9H10	000496-11-7	87
3	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031227.D
Acq On : 08 Sep 2022 21:22
Operator : JC/MD
Sample : N4505-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-77

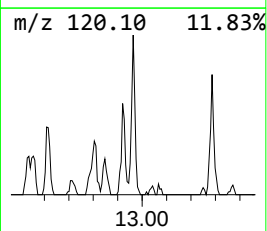
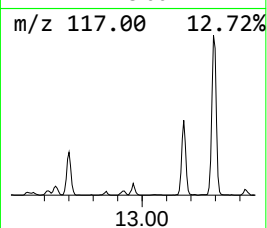
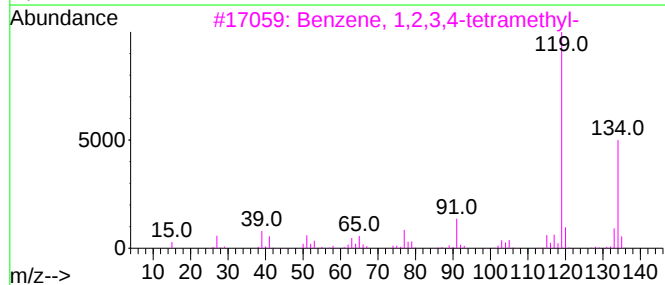
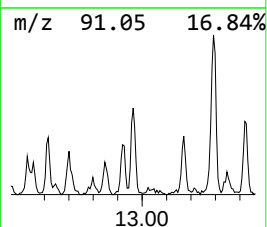
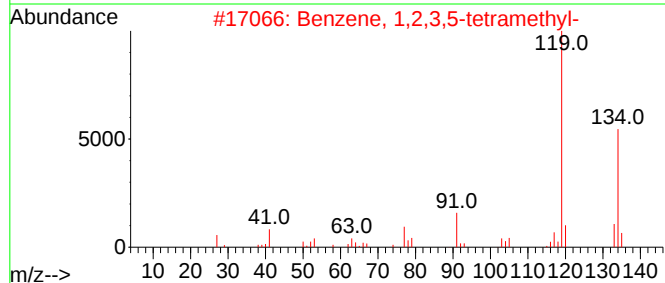
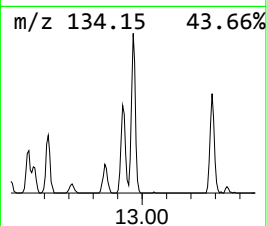
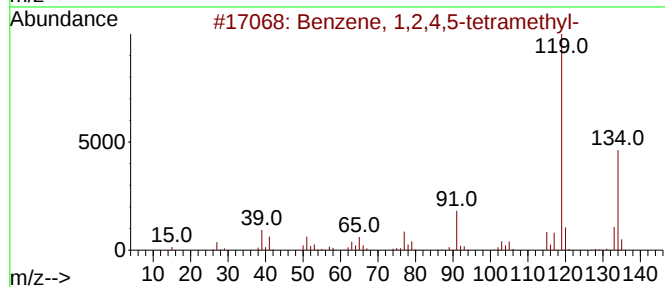
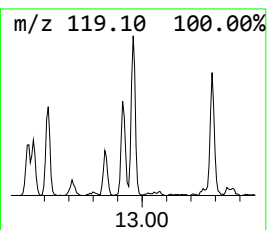
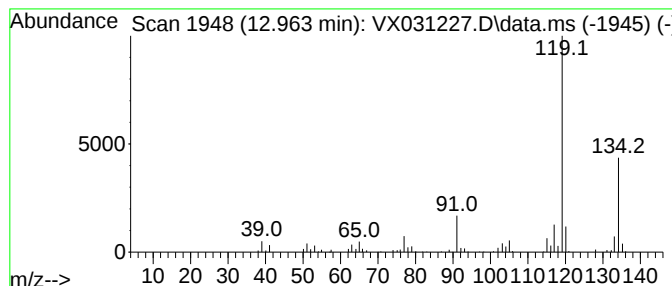
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	14.08 ug/l	85829	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	94
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031227.D
Acq On : 08 Sep 2022 21:22
Operator : JC/MD
Sample : N4505-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-77

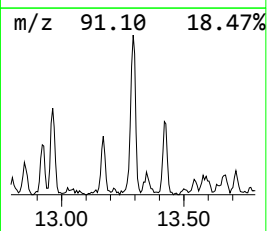
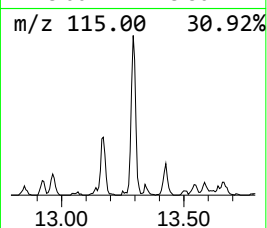
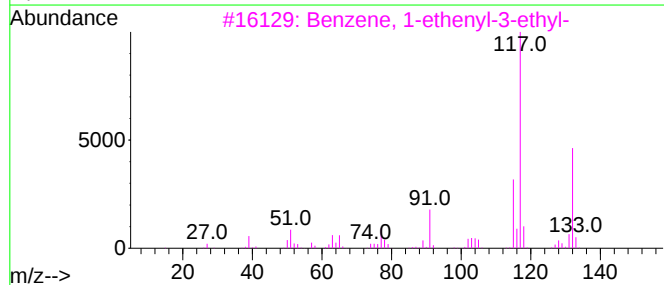
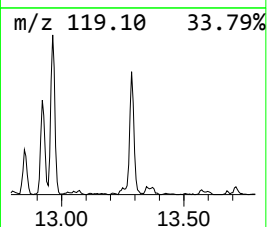
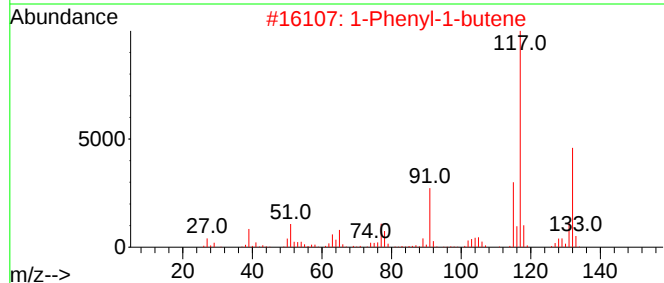
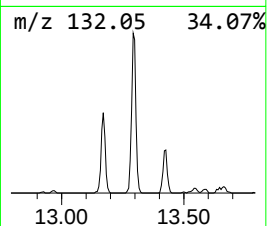
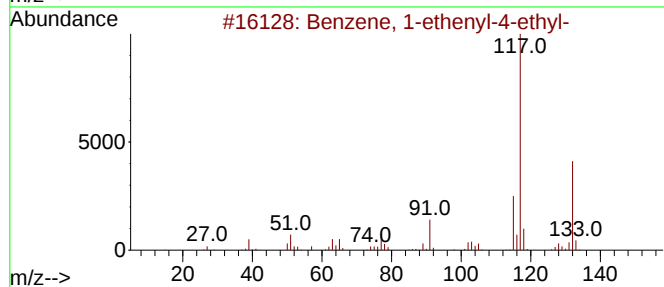
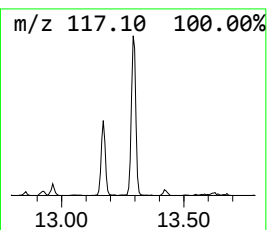
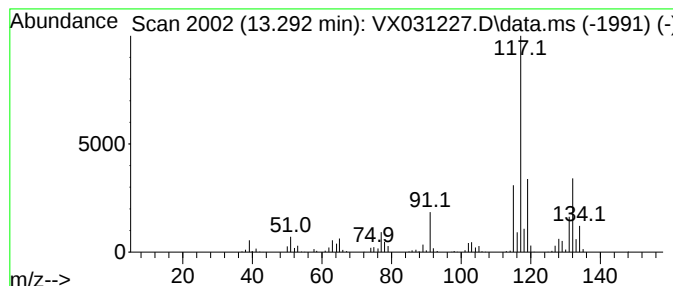
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	38.15 ug/l	232498	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			1-Phenyl-1-butene	132	C10H12	000824-90-8	91
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
4			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031227.D
Acq On : 08 Sep 2022 21:22
Operator : JC/MD
Sample : N4505-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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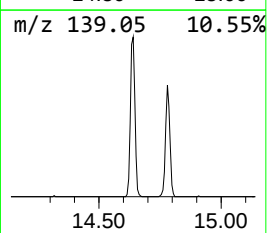
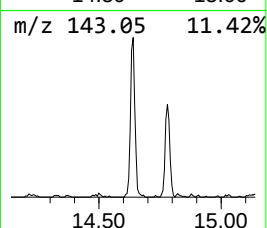
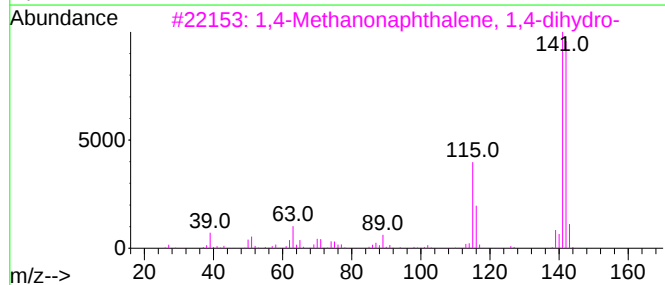
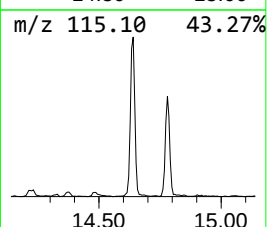
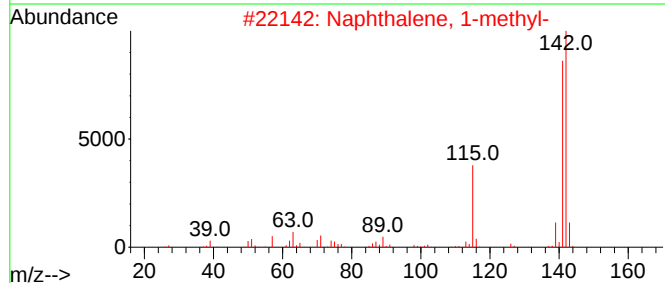
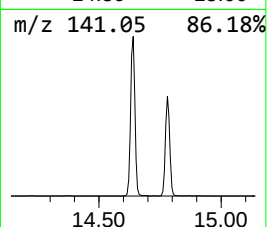
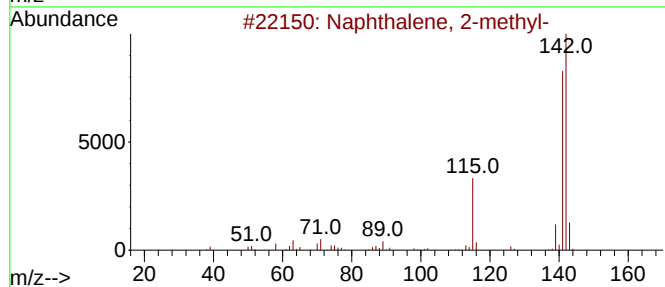
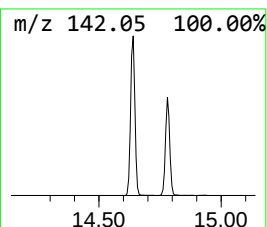
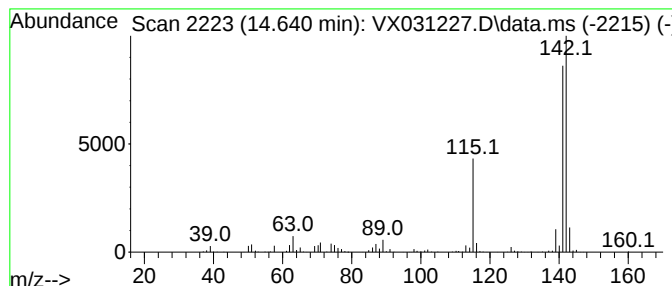
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	76.21 ug/l	464454	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	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031227.D
Acq On : 08 Sep 2022 21:22
Operator : JC/MD
Sample : N4505-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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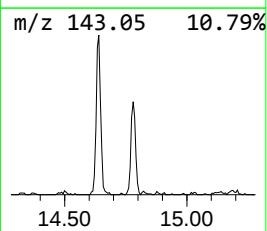
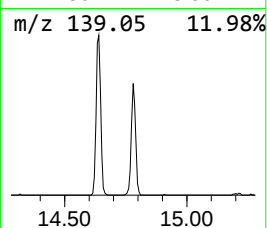
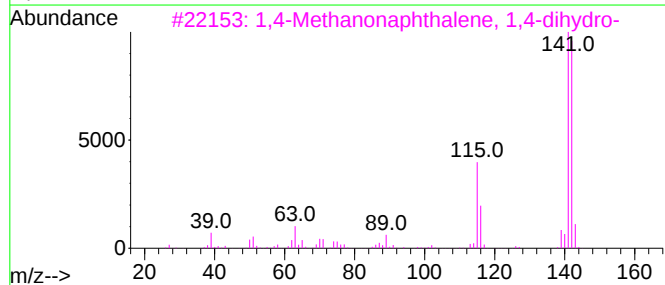
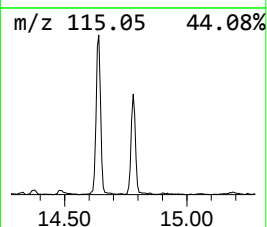
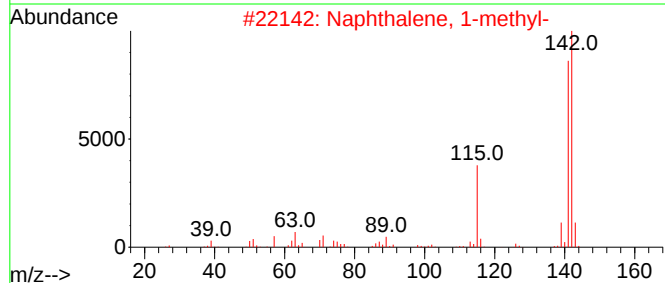
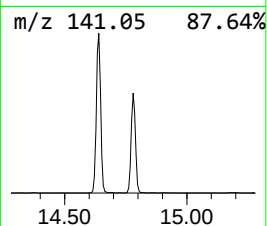
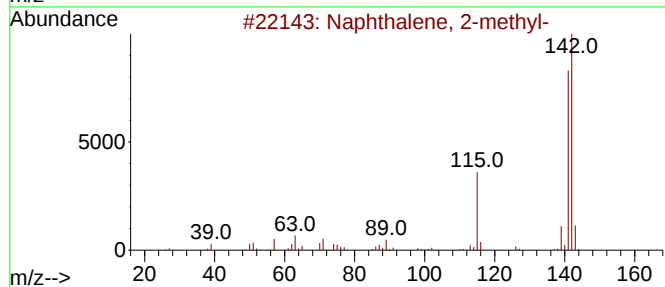
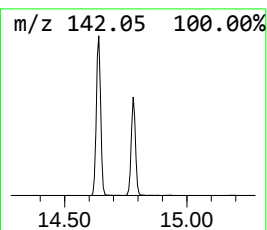
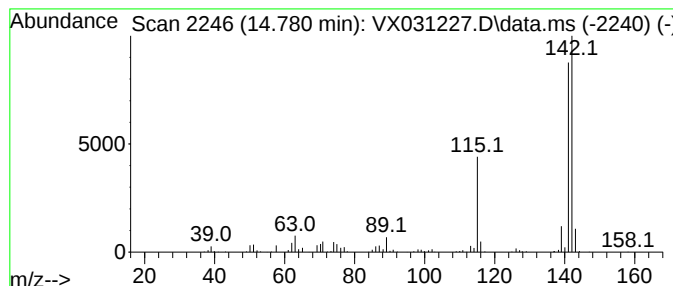
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	46.04 ug/l	280558	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	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031227.D
Acq On : 08 Sep 2022 21:22
Operator : JC/MD
Sample : N4505-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-77

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.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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Isopropyl Alcohol	2.550	68.5	ug/l	302005	1	5.556	220576	50.0
Benzene, 1-ethy...	11.378	33.2	ug/l	202091	4	12.024	304703	50.0
Benzene, 1-ethy...	11.616	18.1	ug/l	110165	4	12.024	304703	50.0
Benzene, 1,2,3-...	12.085	42.3	ug/l	257977	4	12.024	304703	50.0
Benzene, 1-ethe...	12.244	42.8	ug/l	260943	4	12.024	304703	50.0
Benzene, 1,2,4,...	12.963	14.1	ug/l	85829	4	12.024	304703	50.0
Benzene, 1-ethe...	13.292	38.1	ug/l	232498	4	12.024	304703	50.0
Naphthalene, 2-...	14.640	76.2	ug/l	464454	4	12.024	304703	50.0
Naphthalene, 1-...	14.780	46.0	ug/l	280558	4	12.024	304703	50.0