

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051023\
 Data File : VX035596.D
 Acq On : 10 May 2023 19:06
 Operator : JC/MD
 Sample : 02742-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 14-051023

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\82X042523W.M
 Title : SW846 8260

Signal : TIC: VX035596.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.007	632	643	652	rBV	160889	504972	19.41%	2.501%
2	5.093	652	657	667	rVB	34404	102271	3.93%	0.507%
3	5.385	691	705	720	rBV	180560	525330	20.19%	2.602%
4	5.550	722	732	748	rVB	320405	902008	34.67%	4.468%
5	5.952	787	798	812	rBV	175769	471860	18.14%	2.337%
6	6.757	919	930	942	rBV	478532	1153885	44.35%	5.715%
7	8.647	1233	1240	1247	rBV	1019118	1577042	60.62%	7.811%
8	8.720	1247	1252	1260	rVB	70958	112969	4.34%	0.560%
9	9.275	1338	1343	1349	rVB	22244	32988	1.27%	0.163%
10	10.055	1465	1471	1481	rVB	983648	1387911	53.35%	6.874%
11	10.299	1506	1511	1517	rVB	57483	76827	2.95%	0.381%
12	10.640	1560	1567	1574	rBV	56467	78986	3.04%	0.391%
13	10.963	1614	1620	1623	rBV	32729	43857	1.69%	0.217%
14	11.079	1634	1639	1650	rVB	917853	1146962	44.08%	5.681%
15	11.305	1670	1676	1682	rBV	202242	248898	9.57%	1.233%
16	11.378	1682	1688	1696	rVV	995036	1701610	65.40%	8.428%
17	11.451	1696	1700	1708	rVB	581031	711383	27.34%	3.523%
18	11.610	1721	1726	1733	rVB	442751	549314	21.11%	2.721%
19	11.750	1744	1749	1755	rVB	1958287	2284419	87.80%	11.315%
20	11.890	1761	1772	1777	rBV2	75116	132890	5.11%	0.658%
21	11.969	1777	1785	1788	rVV	103591	133880	5.15%	0.663%
22	12.018	1788	1793	1800	rVV	1143381	1556245	59.82%	7.708%
23	12.085	1800	1804	1816	rVB	337177	409803	15.75%	2.030%
24	12.244	1822	1830	1832	rBV	214452	292909	11.26%	1.451%
25	12.268	1832	1834	1838	rVV	112399	119738	4.60%	0.593%
26	12.317	1838	1842	1850	rVB3	160135	240590	9.25%	1.192%
27	12.414	1850	1858	1862	rBV5	17070	34461	1.32%	0.171%
28	12.463	1862	1866	1870	rVB	30918	38574	1.48%	0.191%
29	12.530	1871	1877	1879	rBV	55272	71139	2.73%	0.352%
30	12.555	1879	1881	1885	rVV	44872	45914	1.76%	0.227%
31	12.609	1886	1890	1894	rVB	68293	79618	3.06%	0.394%
32	12.920	1935	1941	1944	rBV2	17785	27068	1.04%	0.134%
33	12.963	1944	1948	1955	rVB	27054	34682	1.33%	0.172%
34	13.164	1967	1981	1995	rBV	1453873	2601735	100.00%	12.886%
35	13.774	2078	2081	2087	rVB	22345	29346	1.13%	0.145%
36	14.195	2146	2150	2160	rBV10	15230	39008	1.50%	0.193%

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ClientSampleId :
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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\82X042523W.M
Title : SW846 8260

37	15.182	2304	2312	2316	rBV9	23240	56338	2.17%	0.279%
38	15.542	2365	2371	2379	rBV	212729	322741	12.40%	1.599%
39	16.469	2516	2523	2535	rBV	170295	309992	11.91%	1.535%

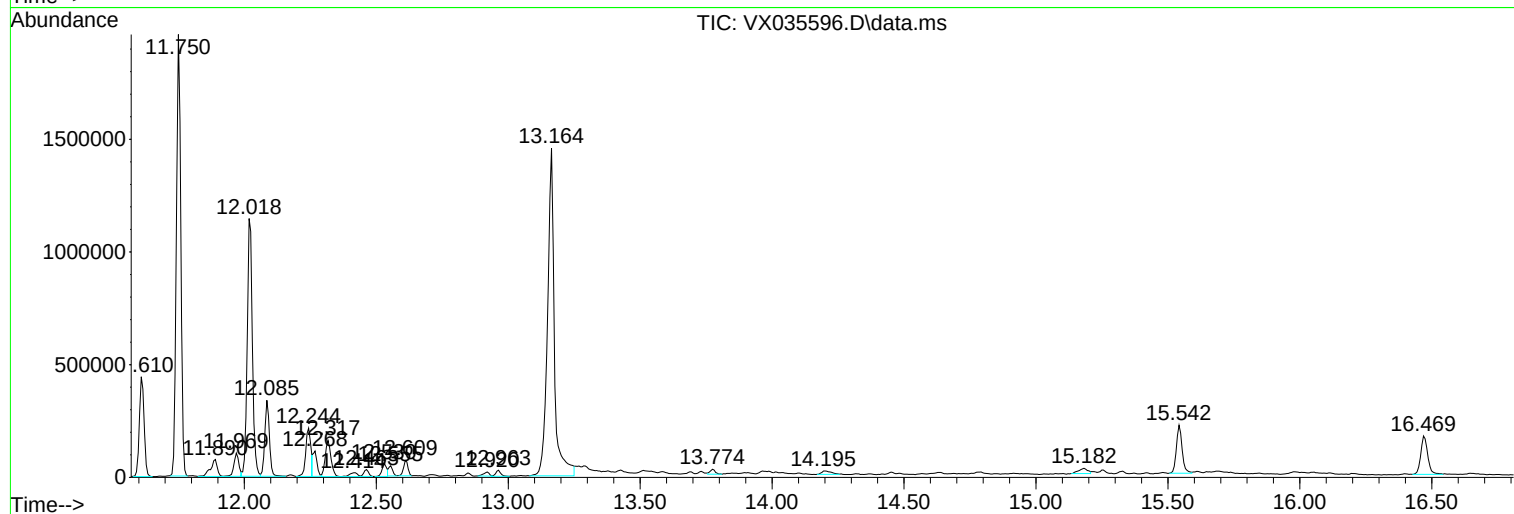
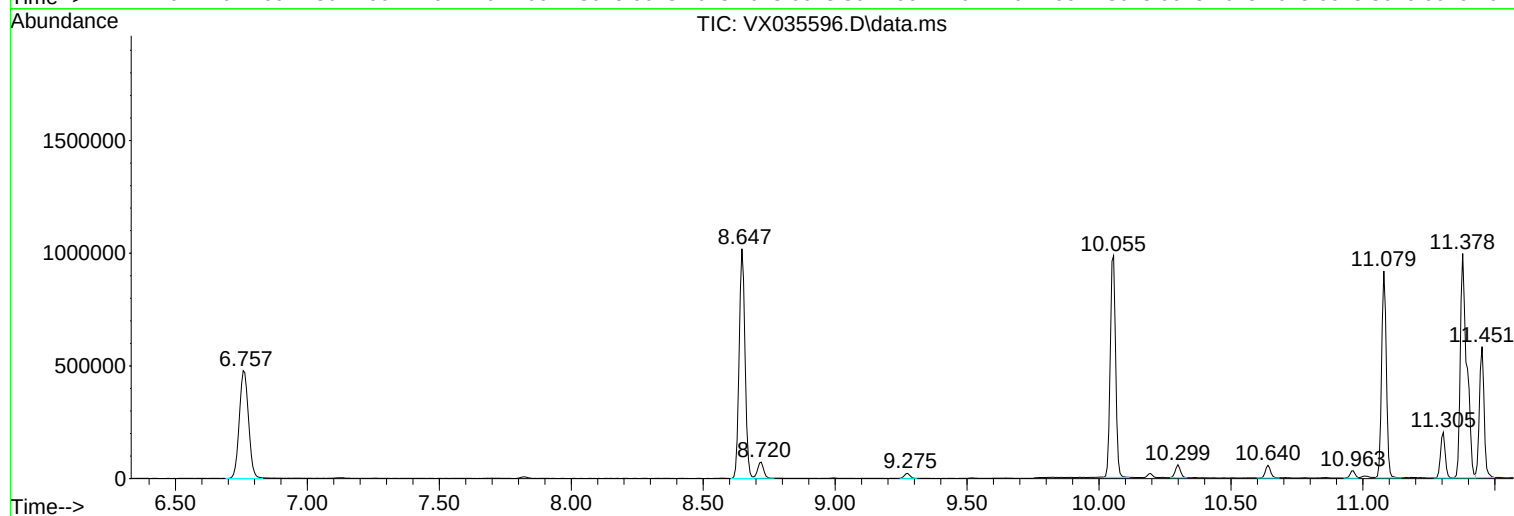
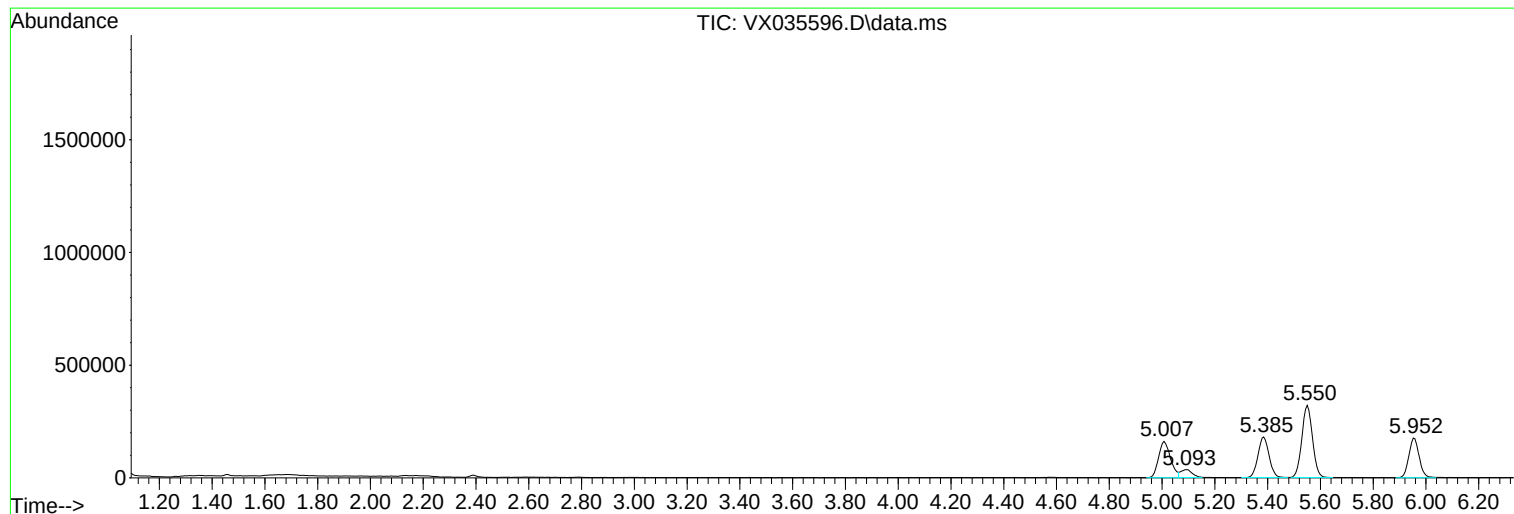
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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



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14-051023

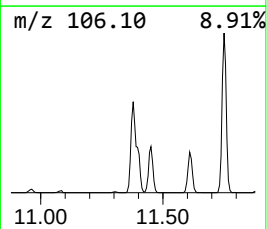
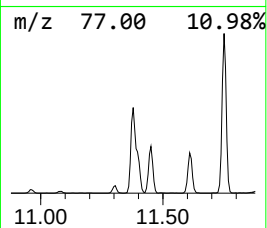
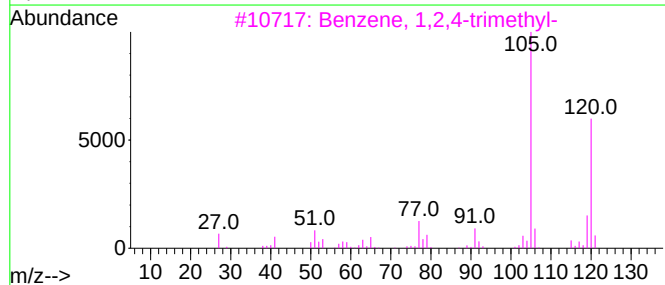
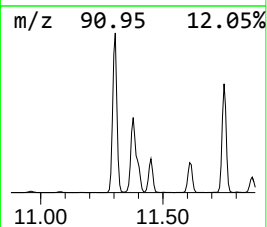
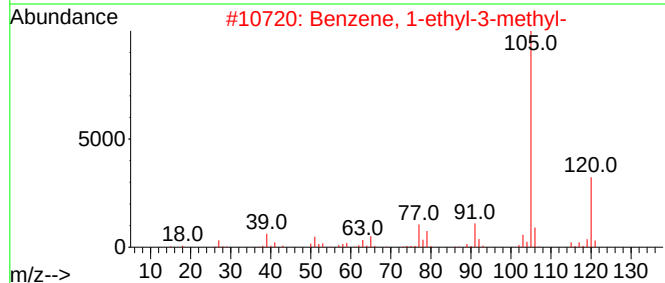
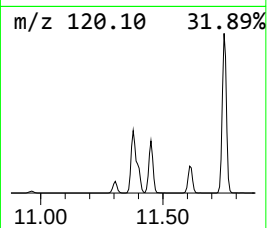
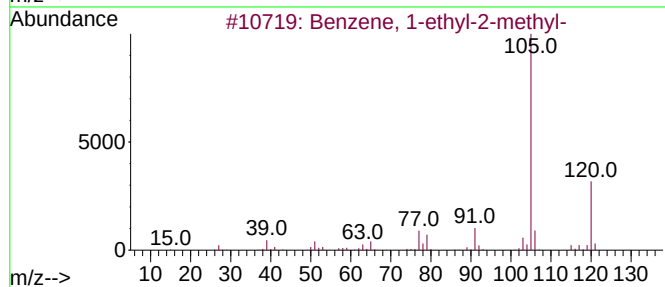
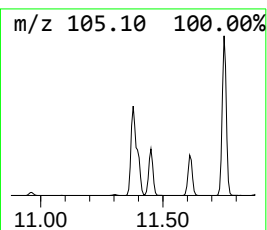
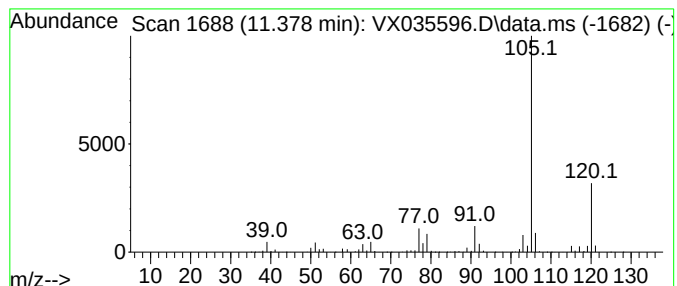
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	54.67 ug/l	1701610	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, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



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Instrument :
MSVOA_X
ClientSampleId :
14-051023

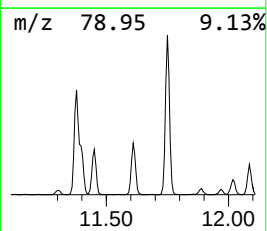
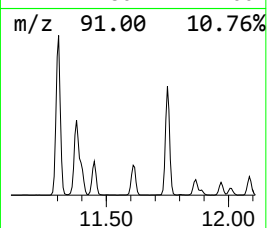
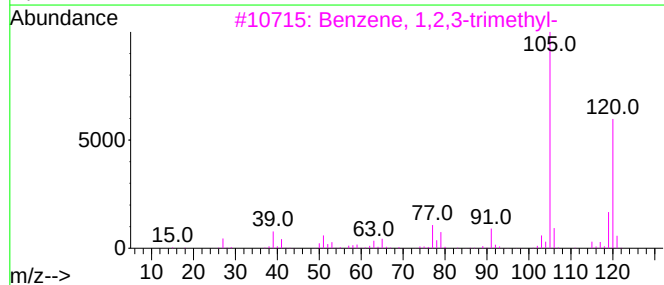
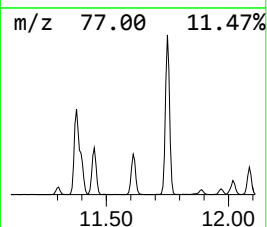
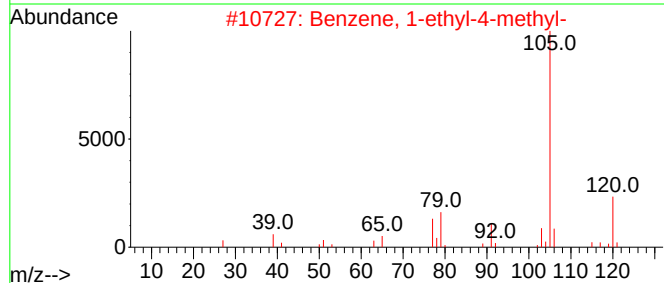
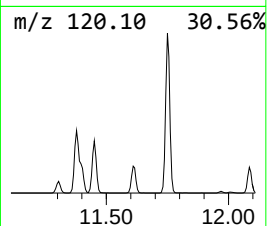
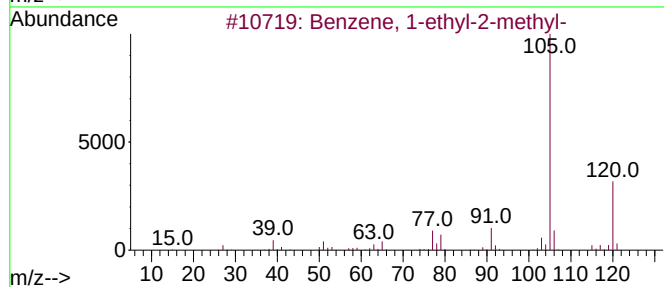
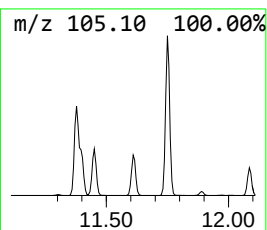
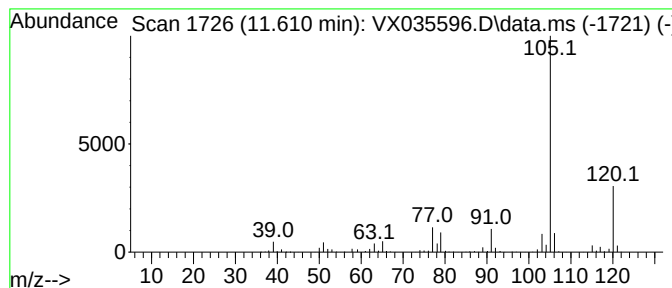
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	17.65 ug/l	549314	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	94
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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Instrument :
MSVOA_X
ClientSampleId :
14-051023

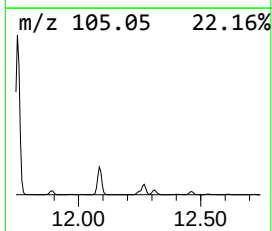
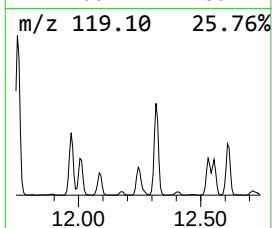
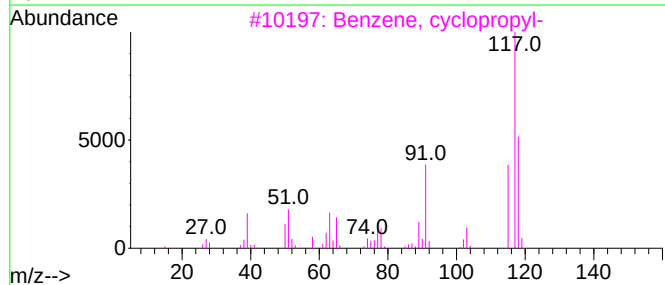
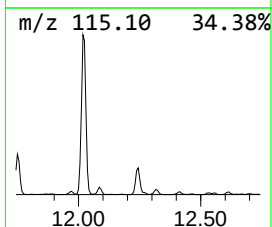
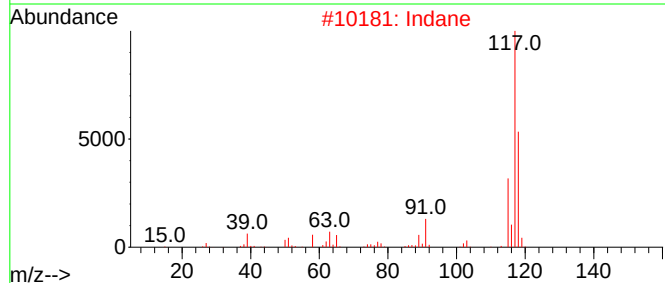
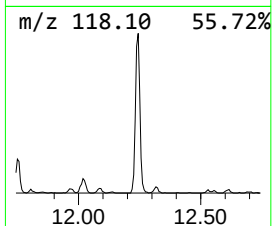
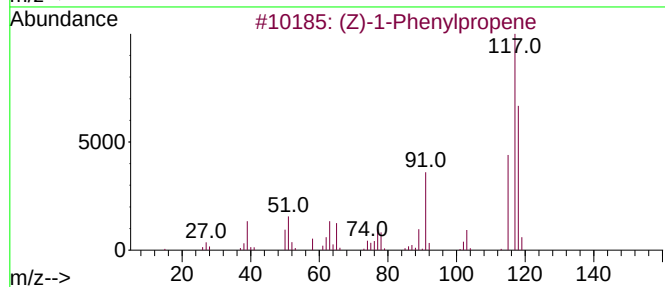
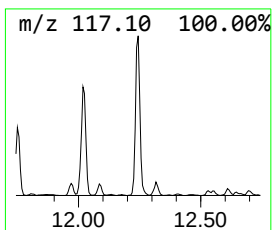
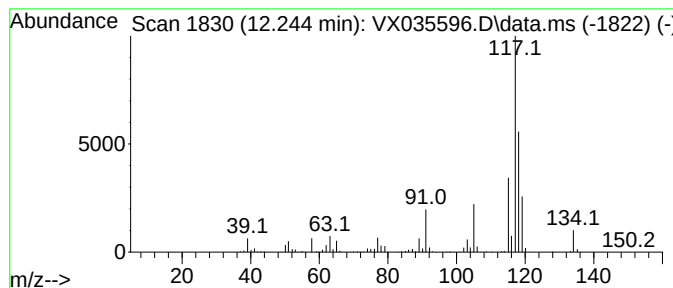
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 3 (Z)-1-Phenylpropene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	9.41 ug/l	292909	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	64
2			Indane	118	C9H10	000496-11-7	64
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	64



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
14-051023

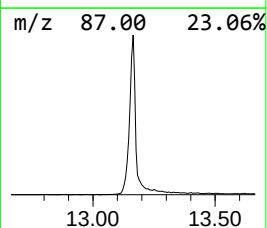
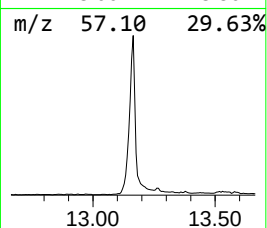
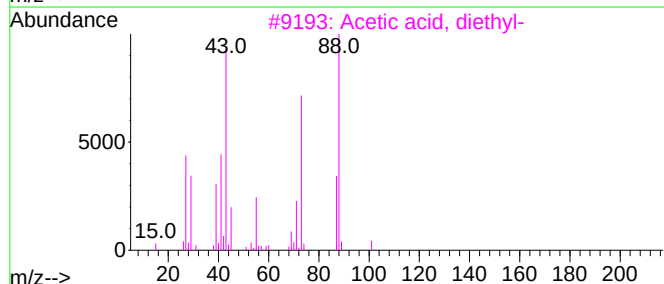
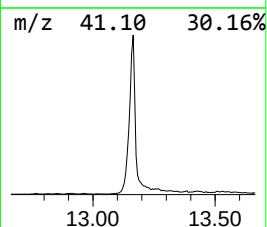
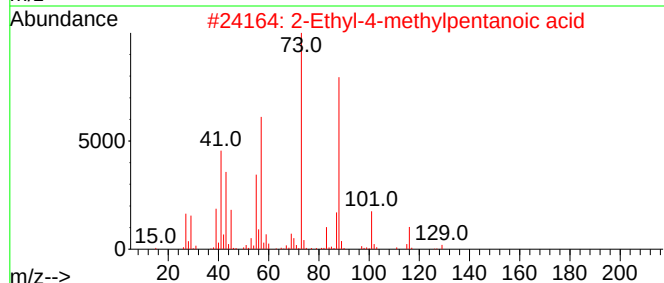
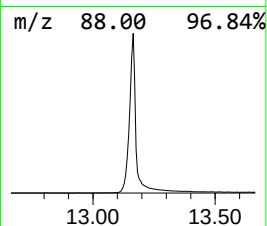
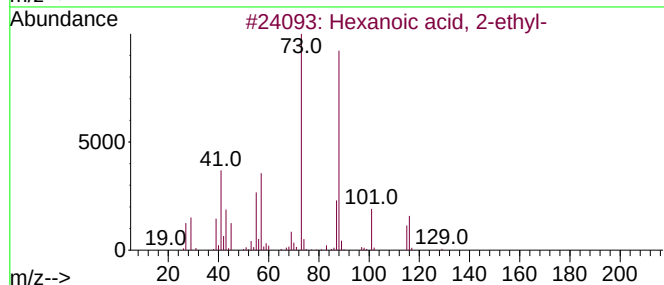
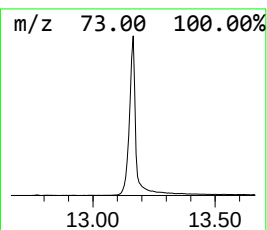
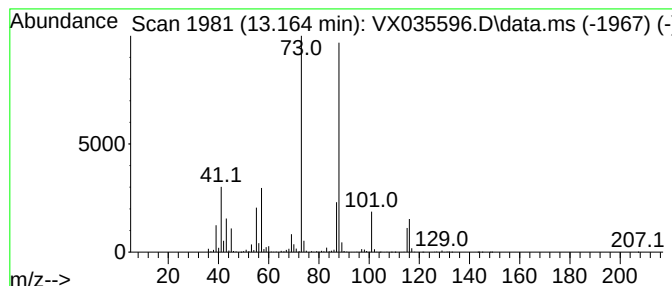
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.164	83.59 ug/l	2601740	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	91
2			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	50
3			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	42
4			Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40
5			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	38



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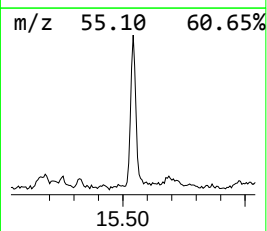
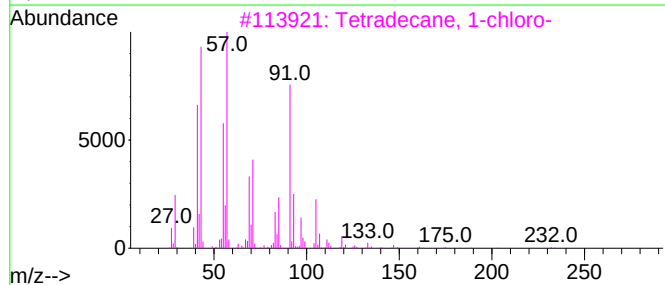
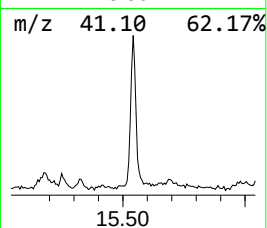
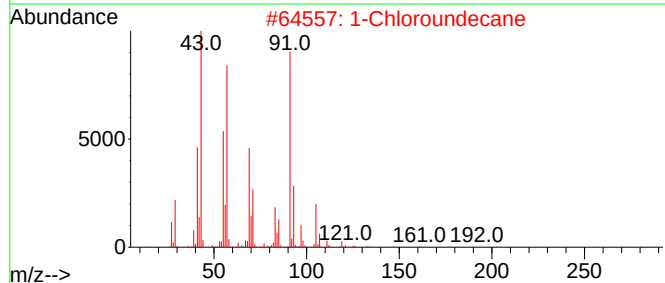
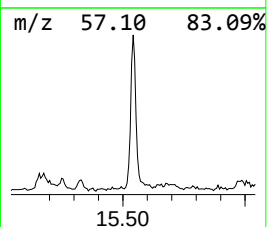
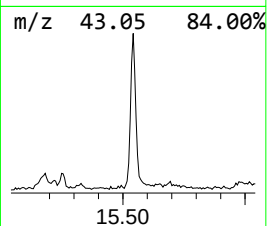
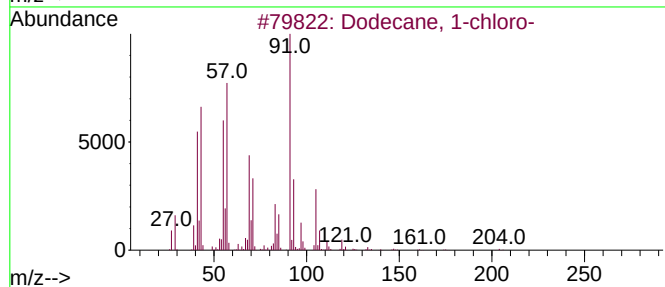
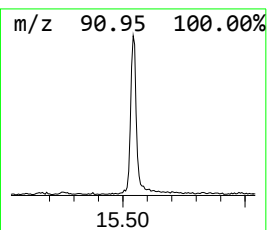
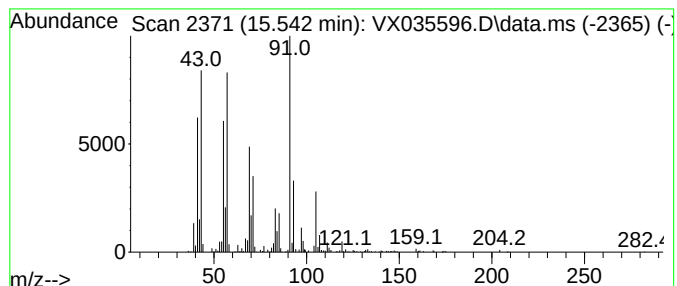
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 5 Dodecane, 1-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.542	10.37 ug/l	322741	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	98
2			1-Chloroundecane	190	C11H23Cl	002473-03-2	90
3			Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	72
4			Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	46
5			Vinyl lauryl ether	212	C14H28O	000765-14-0	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051023\
Data File : VX035596.D
Acq On : 10 May 2023 19:06
Operator : JC/MD
Sample : 02742-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

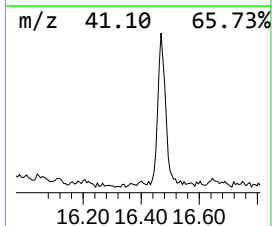
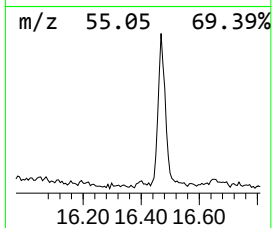
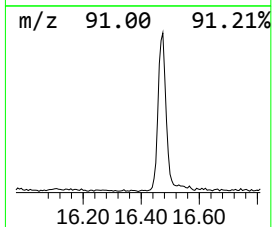
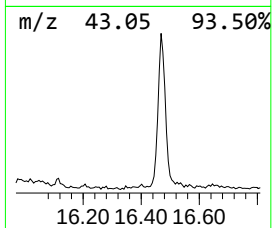
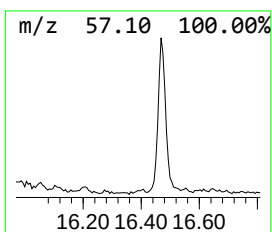
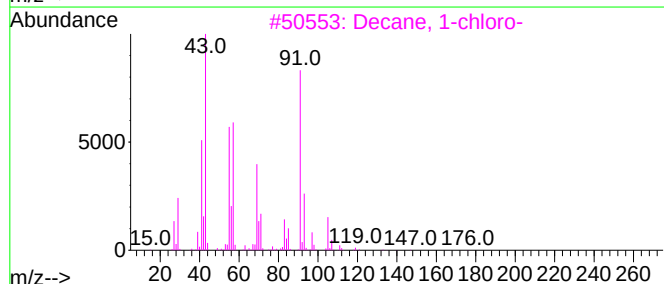
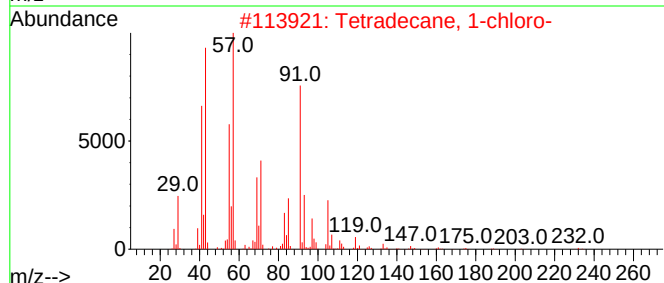
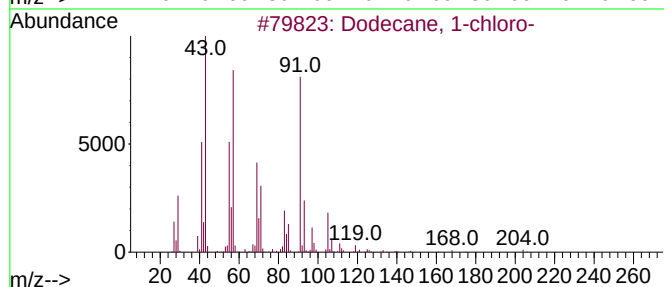
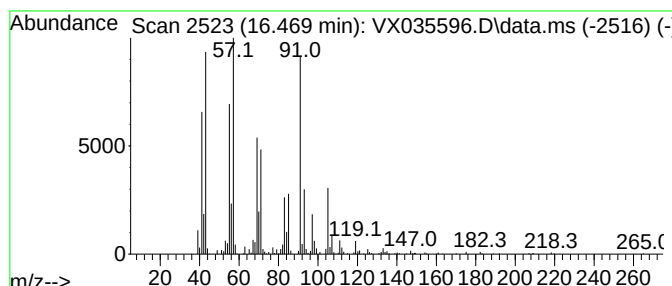
Instrument :
MSVOA_X
ClientSampleId :
14-051023

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 6 Tetradecane, 1-chloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.468	9.96 ug/l	309992	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	91
2	Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	87
3	Decane, 1-chloro-	176	C10H21Cl	001002-69-3	58
4	Oxalic acid, allyl dodecyl ester	298	C17H30O4	1000309-24-0	58
5	Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051023\
Data File : VX035596.D
Acq On : 10 May 2023 19:06
Operator : JC/MD
Sample : 02742-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
14-051023

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.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	54.7	ug/l	1701610	4	12.024	1556250	50.0
Benzene, 1-ethy...	11.610	17.6	ug/l	549314	4	12.024	1556250	50.0
(Z)-1-Phenylpro...	12.244	9.4	ug/l	292909	4	12.024	1556250	50.0
Hexanoic acid, ...	13.164	83.6	ug/l	2601740	4	12.024	1556250	50.0
Dodecane, 1-chl...	15.542	10.4	ug/l	322741	4	12.024	1556250	50.0
Tetradecane, 1-...	16.468	10.0	ug/l	309992	4	12.024	1556250	50.0