

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110122\
 Data File : VX032523.D
 Acq On : 01 Nov 2022 19:04
 Operator : JC/MD
 Sample : N5414-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW3

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\82X102622W.M
 Title : SW846 8260

Signal : TIC: VX032523.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.746	103	108	125	rVB	1075477	1457547	5.33%	1.240%
2	1.953	137	142	155	rVB	356234	500965	1.83%	0.426%
3	2.782	271	278	281	rBV	223842	451361	1.65%	0.384%
4	2.825	281	285	290	rVB	219489	391480	1.43%	0.333%
5	3.105	320	331	345	rBV2	329285	760750	2.78%	0.647%
6	4.306	519	528	540	rVB	385276	1086604	3.97%	0.924%
7	5.623	738	744	764	rVB2	155413	513391	1.88%	0.437%
8	6.251	839	847	857	rVB2	187868	582342	2.13%	0.495%
9	6.763	923	931	938	rBV	203469	503232	1.84%	0.428%
10	7.379	1016	1032	1044	rBV4	109776	331076	1.21%	0.282%
11	8.110	1142	1152	1155	rBV	173549	345989	1.27%	0.294%
12	8.653	1235	1241	1247	rVB	408255	658945	2.41%	0.560%
13	10.055	1461	1471	1476	rBV	419361	575784	2.11%	0.490%
14	10.201	1489	1495	1500	rBV	8840253	11864975	43.39%	10.092%
15	10.311	1505	1513	1518	rBV	20372810	27348073	100.00%	23.261%
16	10.640	1562	1567	1578	rVB	246238	331510	1.21%	0.282%
17	10.963	1614	1620	1626	rBV	984103	1196497	4.38%	1.018%
18	11.079	1632	1639	1645	rBV	392212	522920	1.91%	0.445%
19	11.305	1671	1676	1683	rVB	2372252	2772204	10.14%	2.358%
20	11.384	1683	1689	1696	rBV	6722297	12084665	44.19%	10.279%
21	11.457	1696	1701	1706	rVB	3884374	4919513	17.99%	4.184%
22	11.616	1721	1727	1738	rBV	3955017	4798574	17.55%	4.082%
23	11.756	1744	1750	1755	rBV	15731214	19837114	72.54%	16.873%
24	12.024	1789	1794	1799	rVB2	558403	728389	2.66%	0.620%
25	12.091	1799	1805	1810	rBV	3853430	4712546	17.23%	4.008%
26	12.244	1824	1830	1838	rBV2	3518249	4867244	17.80%	4.140%
27	12.317	1838	1842	1852	rVB2	1156849	1604685	5.87%	1.365%
28	12.463	1862	1866	1872	rVB	286066	350902	1.28%	0.298%
29	12.530	1872	1877	1879	rBV	705222	852933	3.12%	0.725%
30	12.555	1879	1881	1886	rVB	557386	615716	2.25%	0.524%
31	12.616	1886	1891	1894	rBV	1351844	1600097	5.85%	1.361%
32	12.701	1900	1905	1913	rBV2	611356	861000	3.15%	0.732%
33	12.847	1924	1929	1934	rVB	265914	326269	1.19%	0.278%
34	12.920	1934	1941	1945	rBV	774954	973534	3.56%	0.828%
35	12.963	1945	1948	1954	rVB	1029048	1163438	4.25%	0.990%
36	13.170	1978	1982	1987	rVB	616054	705364	2.58%	0.600%

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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\82X102622W.M
Title : SW846 8260

37	13.292	1998	2002	2007	rVB2	1171643	1512963	5.53%	1.287%
38	13.774	2075	2081	2091	rBV	1499780	1898877	6.94%	1.615%
39	14.640	2218	2223	2233	rVB	362328	465747	1.70%	0.396%
40	14.780	2241	2246	2254	rBV	402193	492843	1.80%	0.419%

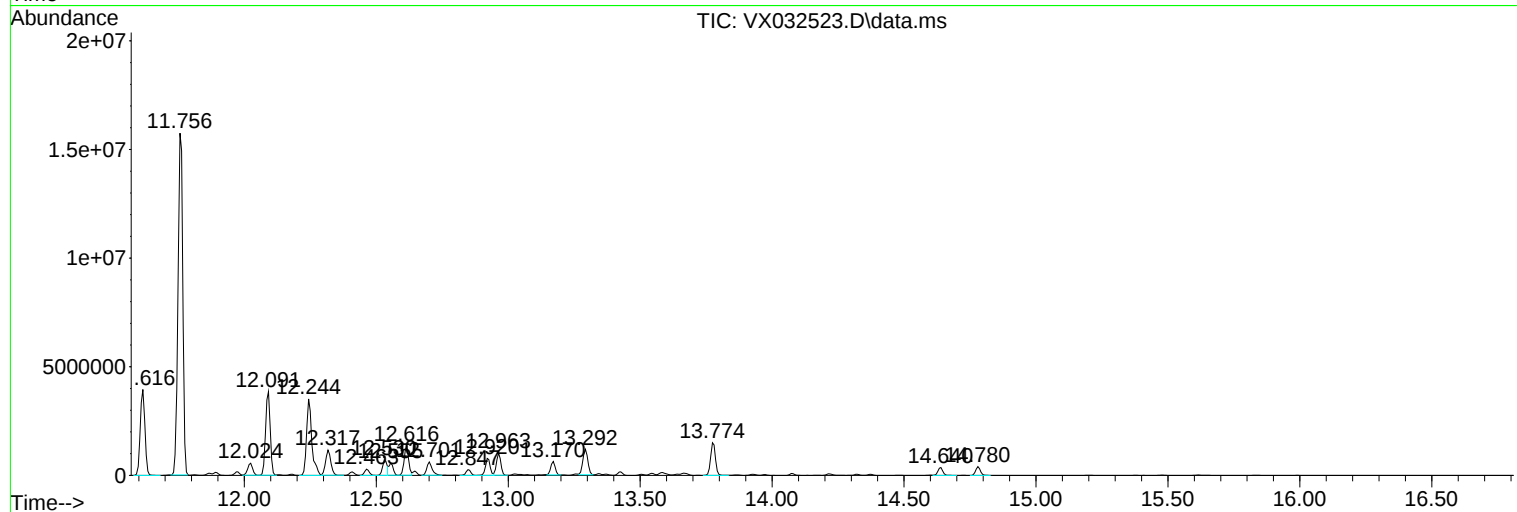
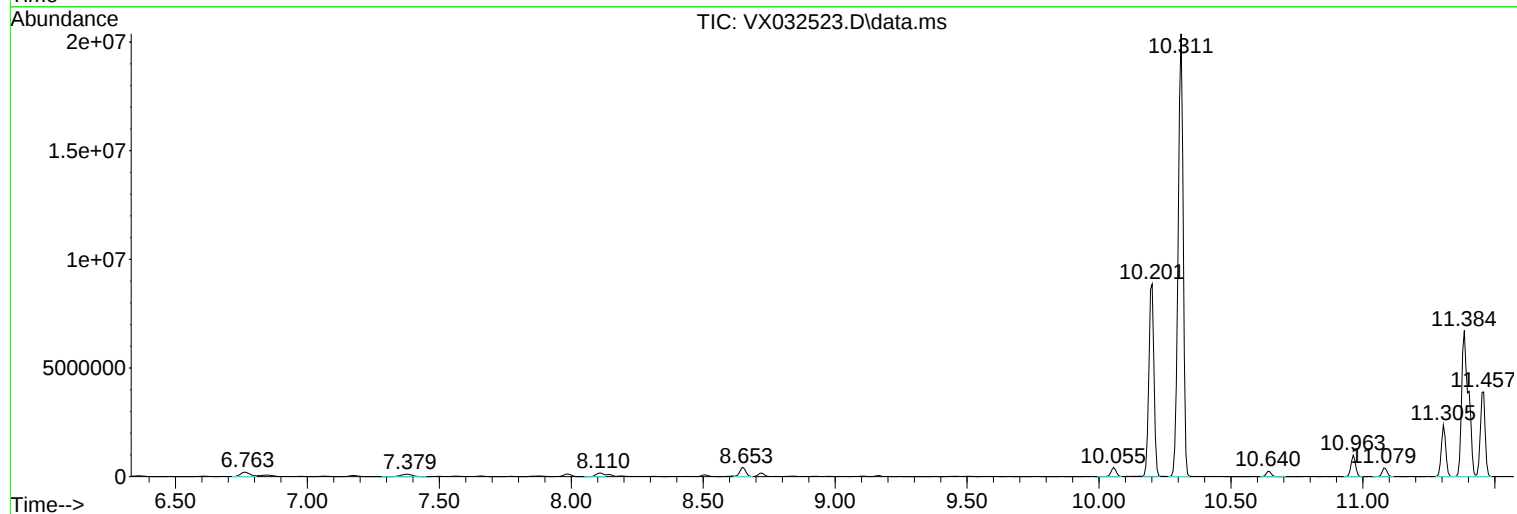
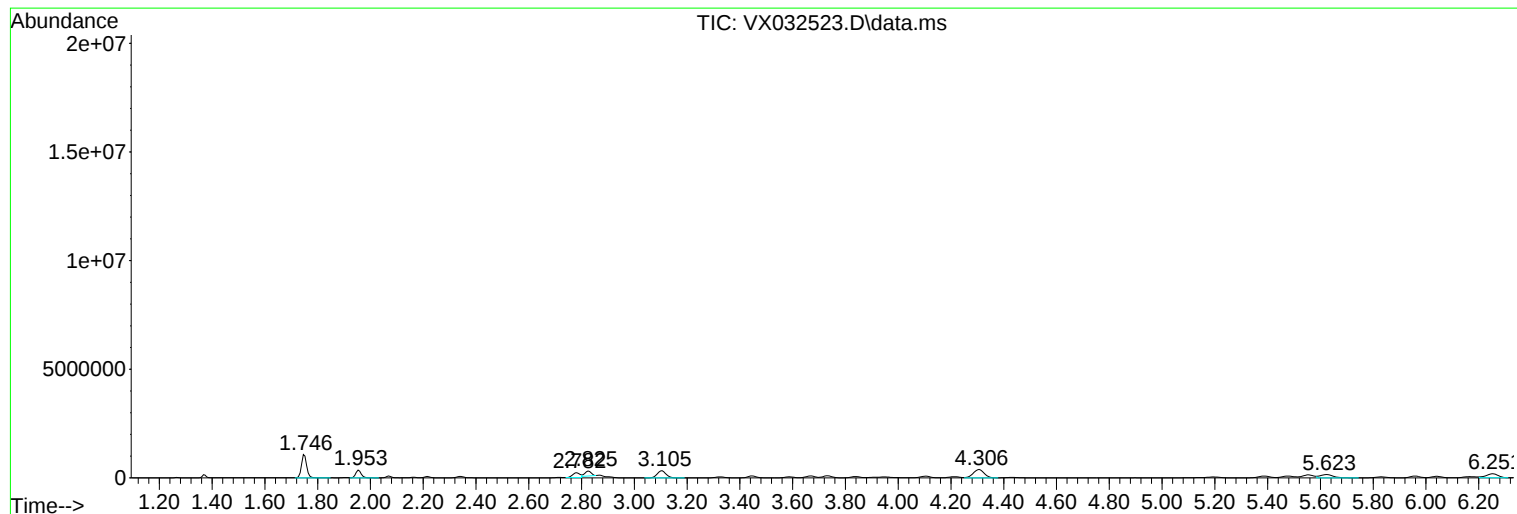
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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



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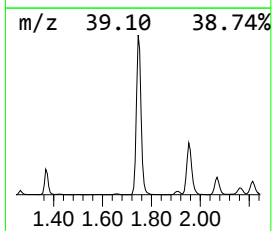
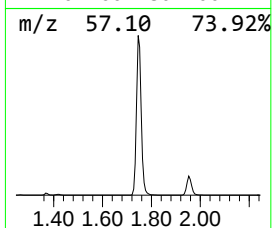
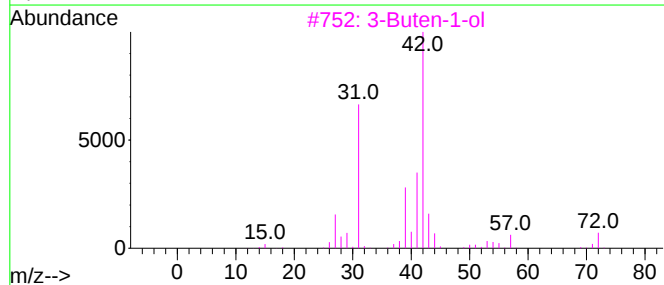
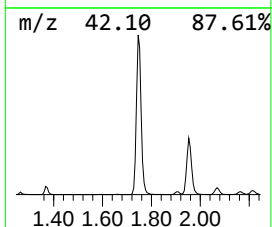
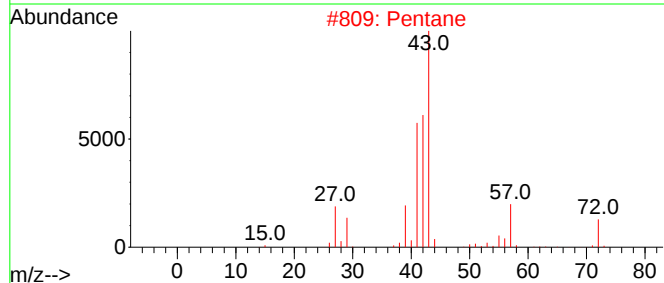
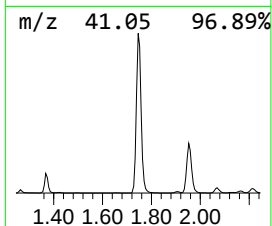
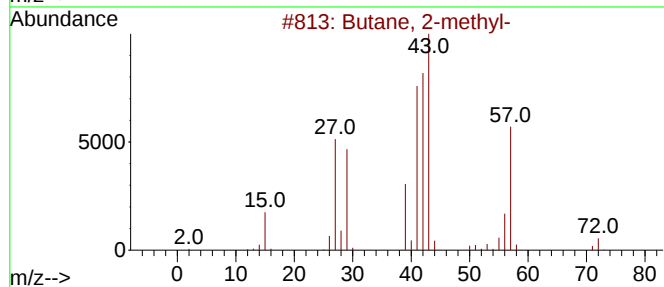
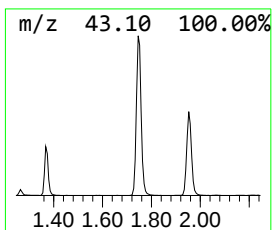
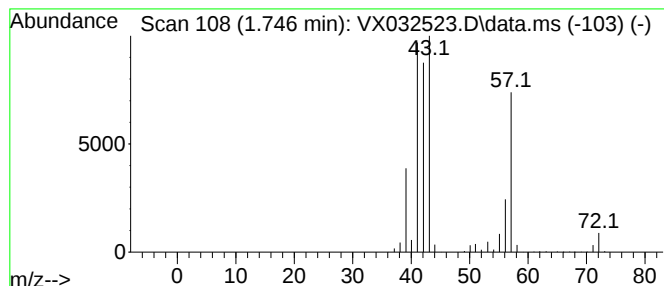
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	141.95 ug/l	1457550	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	64
2			Pentane	72	C5H12	000109-66-0	36
3			3-Buten-1-ol	72	C4H8O	000627-27-0	35
4			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	12
5			1-Butene	56	C4H8	000106-98-9	10



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Instrument :
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ClientSampleId :
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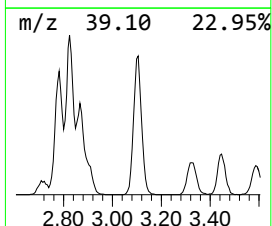
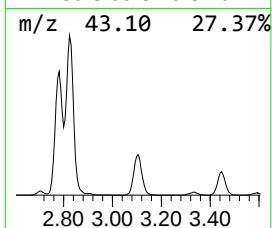
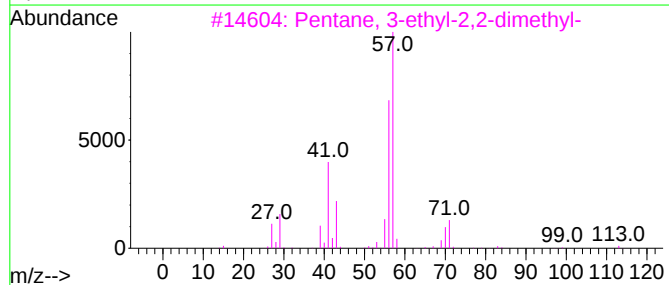
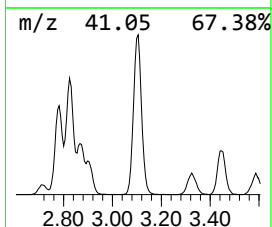
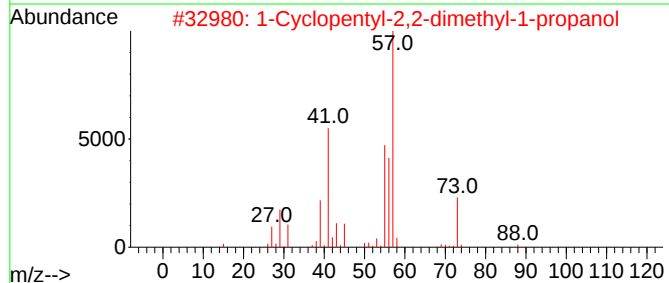
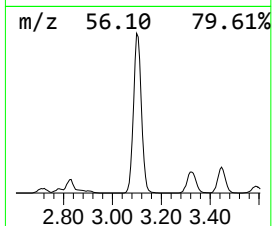
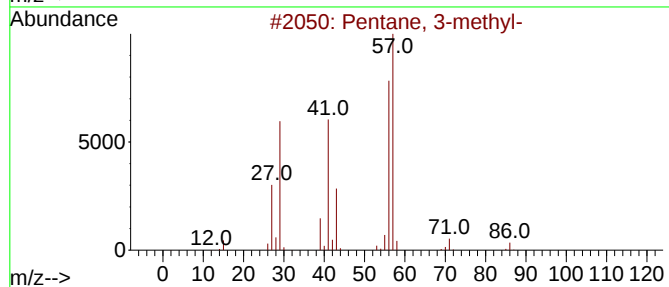
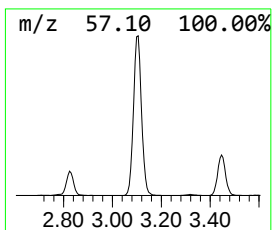
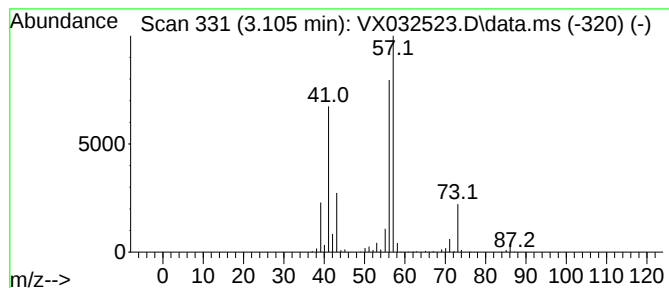
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	74.09 ug/l	760750	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	83
2			1-Cyclopentyl-2,2-dimethyl-1-pro...	156	C10H20O	337966-85-5	50
3			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	50
4			Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	38
5			1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110122\
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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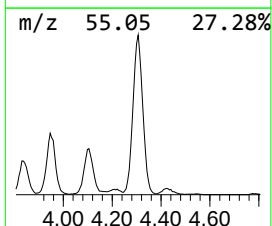
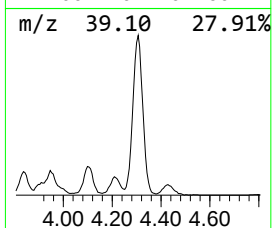
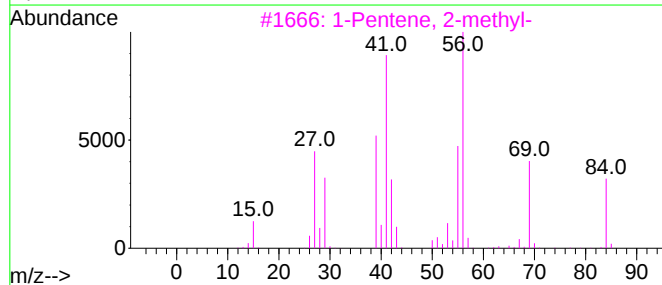
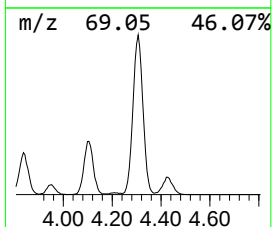
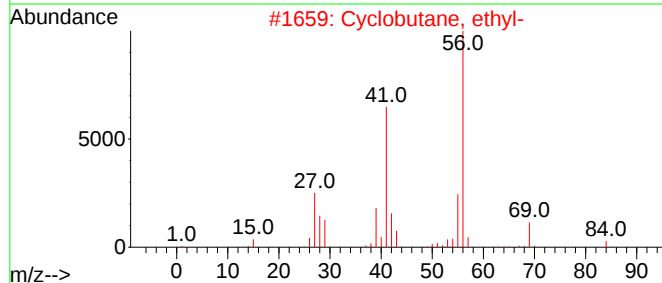
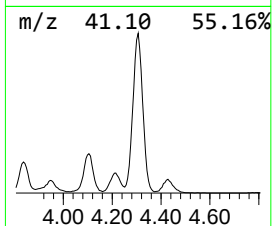
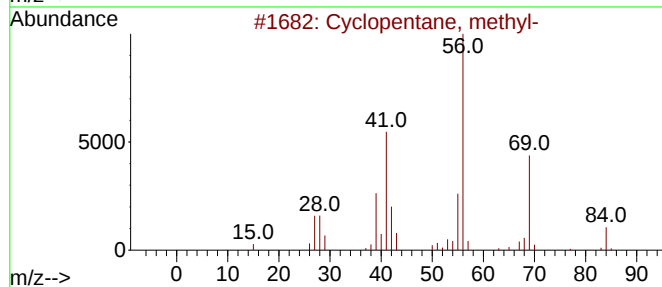
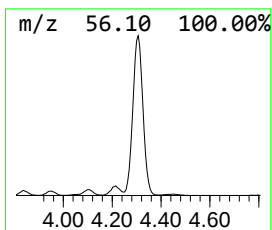
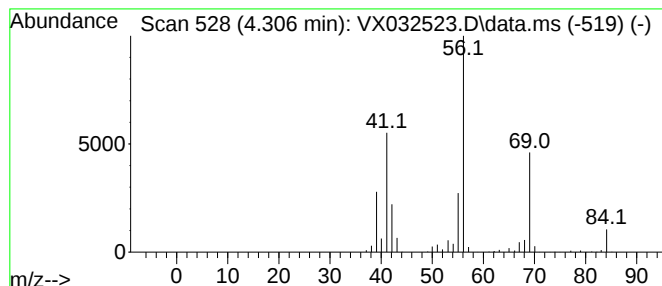
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	105.83 ug/l	1086600	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2		Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
4		Cyclopropane, propyl-	84	C6H12	002415-72-7	64
5		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50



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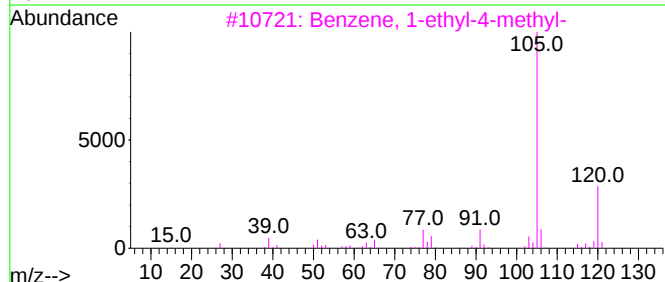
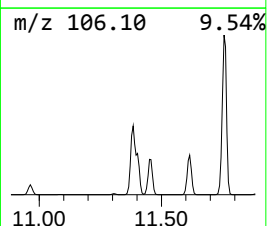
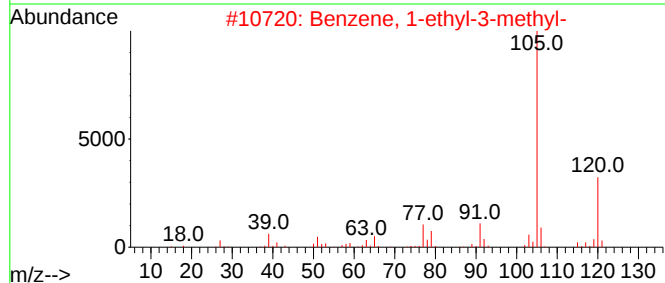
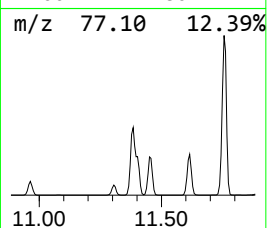
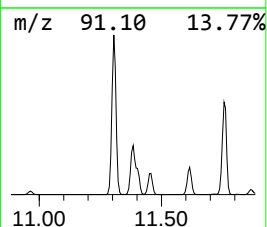
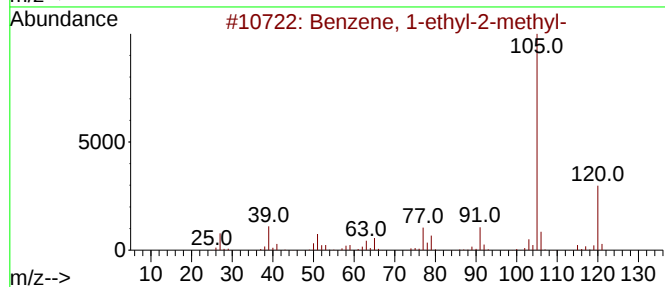
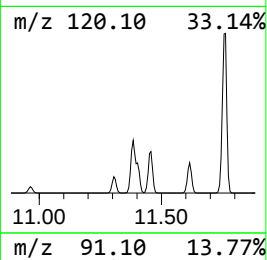
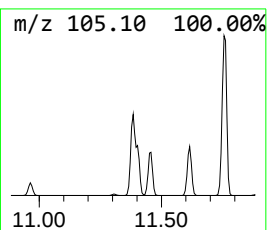
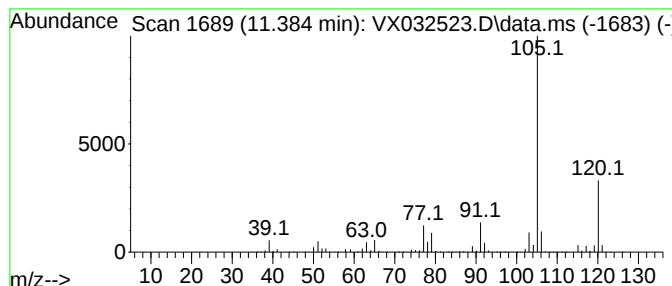
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	829.55 ug/l	12084700	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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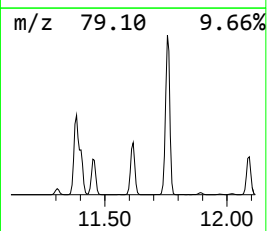
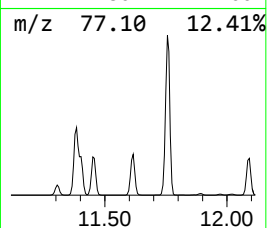
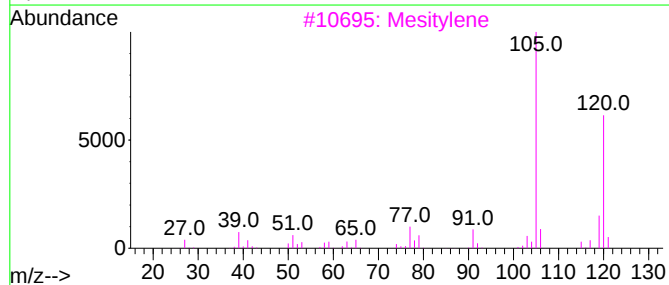
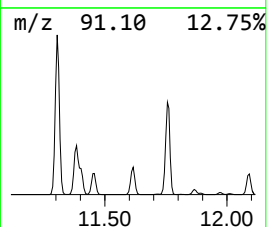
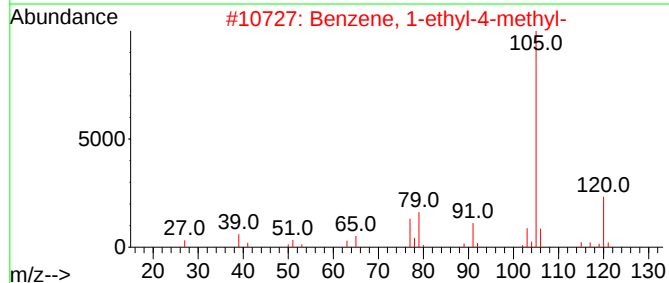
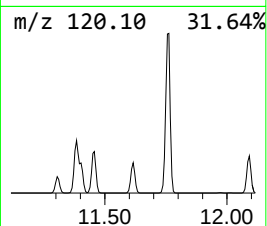
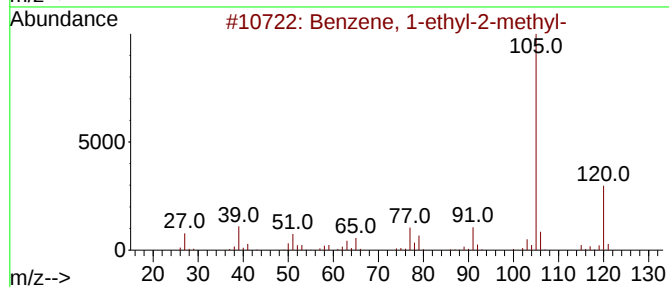
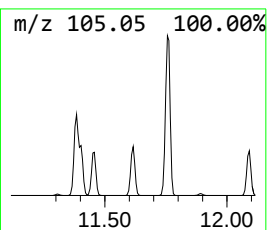
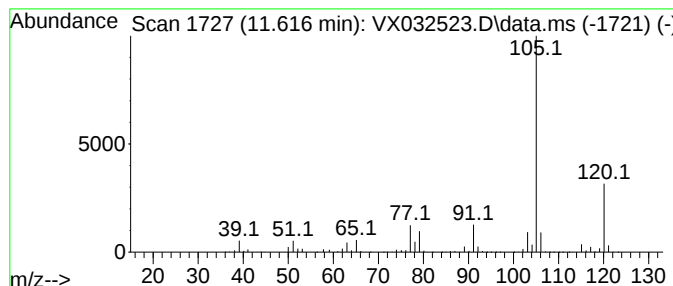
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	329.40 ug/l	4798570	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, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110122\
Data File : VX032523.D
Acq On : 01 Nov 2022 19:04
Operator : JC/MD
Sample : N5414-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW3

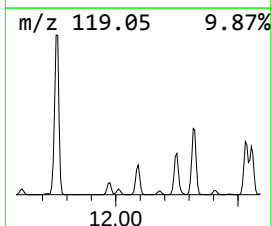
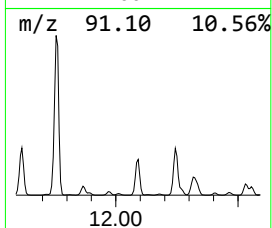
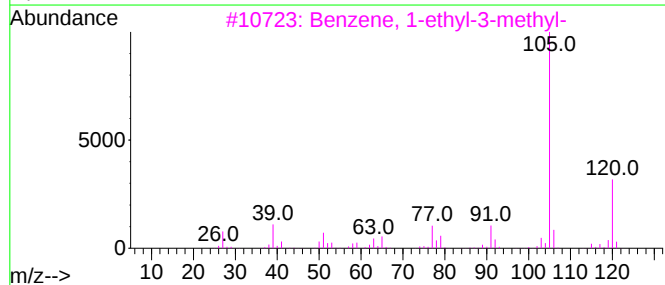
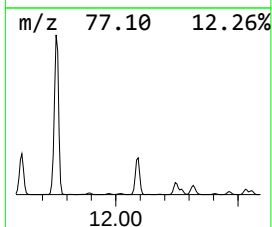
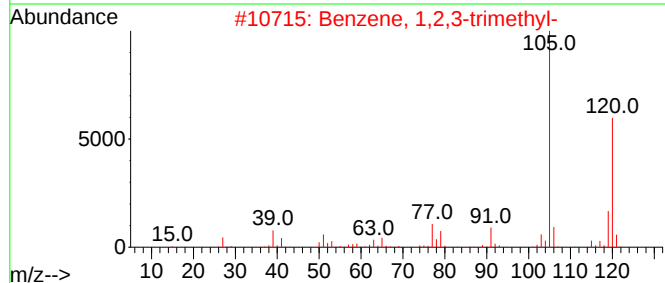
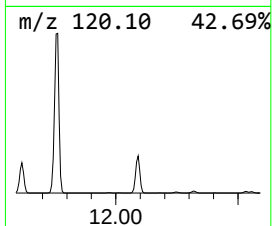
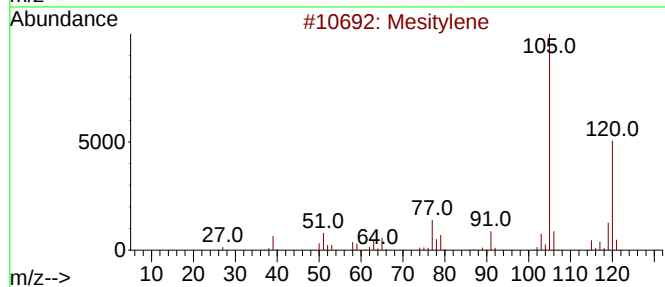
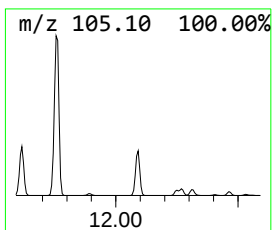
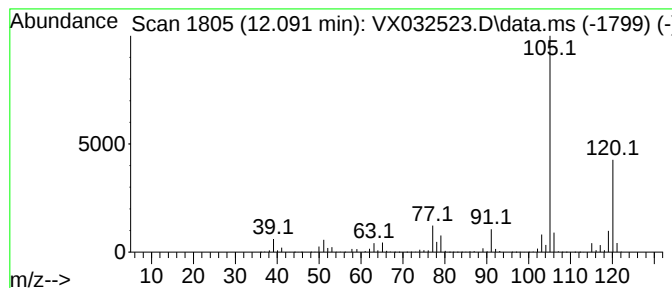
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	323.49 ug/l	4712550	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110122\
Data File : VX032523.D
Acq On : 01 Nov 2022 19:04
Operator : JC/MD
Sample : N5414-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW3

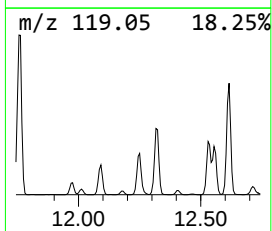
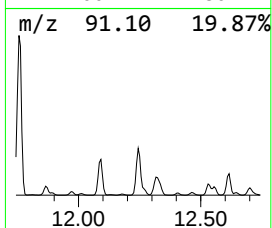
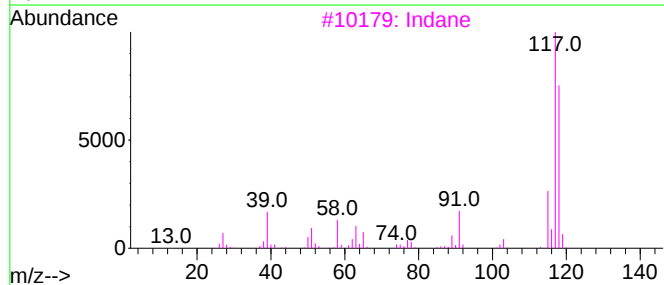
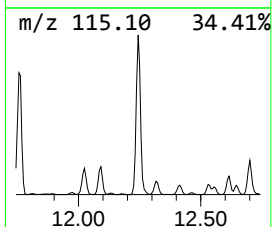
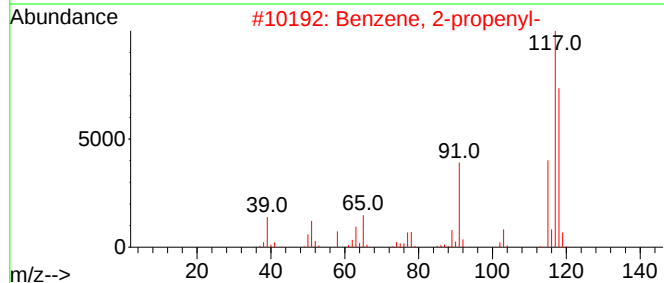
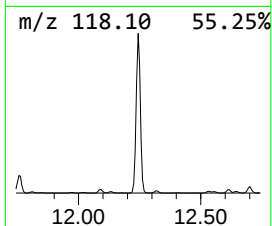
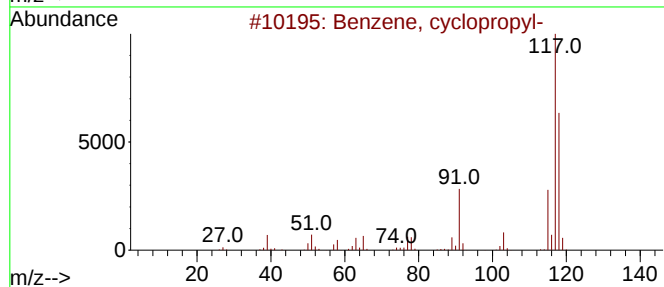
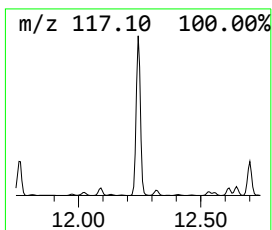
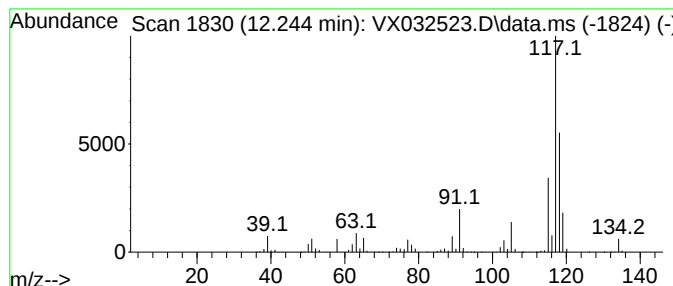
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, cyclopropyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	334.11 ug/l	4867240	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
3			Indane	118	C9H10	000496-11-7	76
4			Δtacyclene	118	C9H10	007785-10-6	58
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110122\
Data File : VX032523.D
Acq On : 01 Nov 2022 19:04
Operator : JC/MD
Sample : N5414-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW3

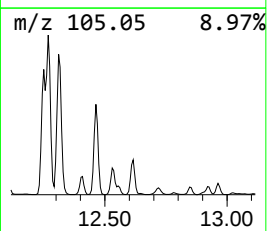
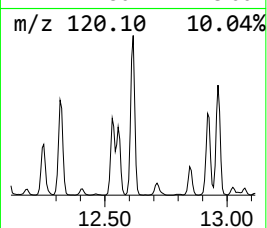
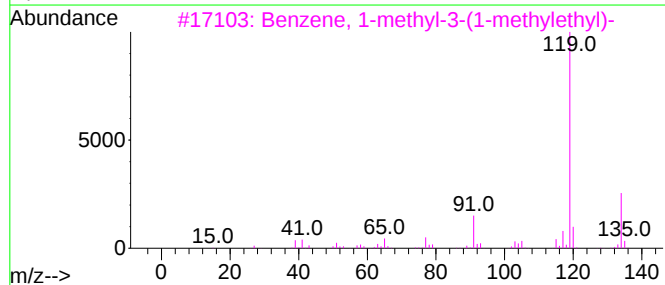
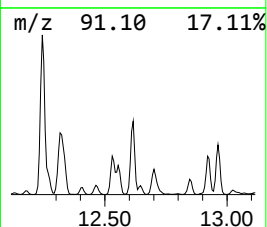
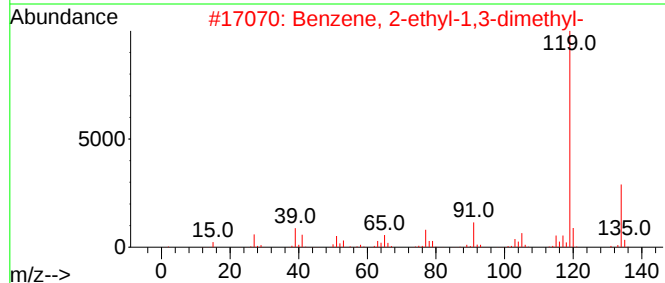
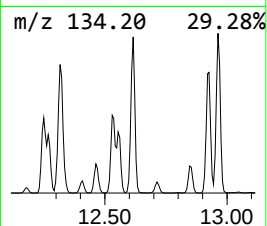
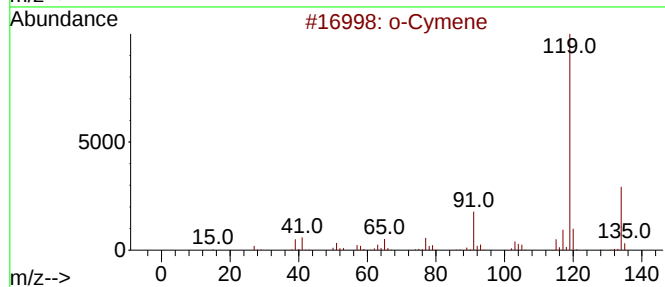
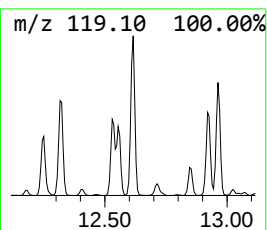
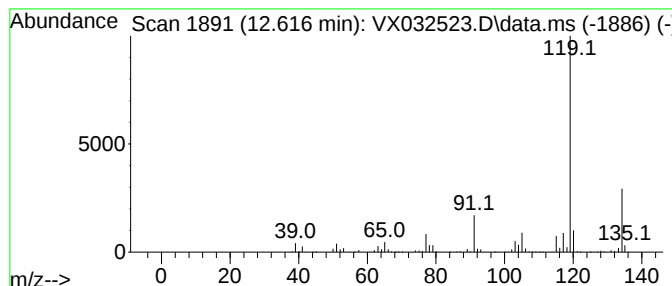
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Quant Title : SW846 8260

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

Peak Number 8 o-Cymene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	109.84 ug/l	1600100	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	97
2			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110122\
Data File : VX032523.D
Acq On : 01 Nov 2022 19:04
Operator : JC/MD
Sample : N5414-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW3

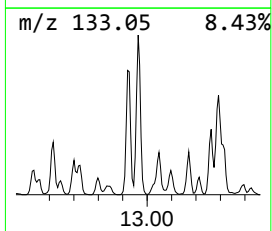
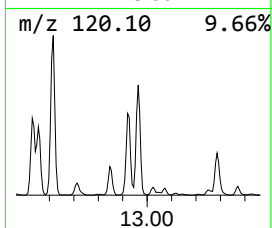
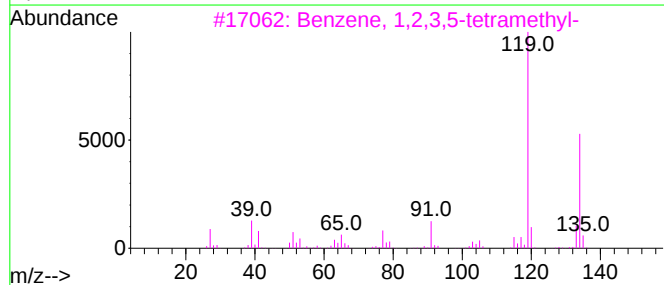
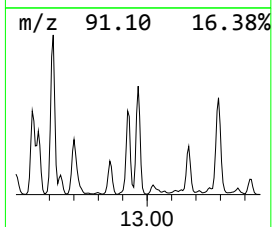
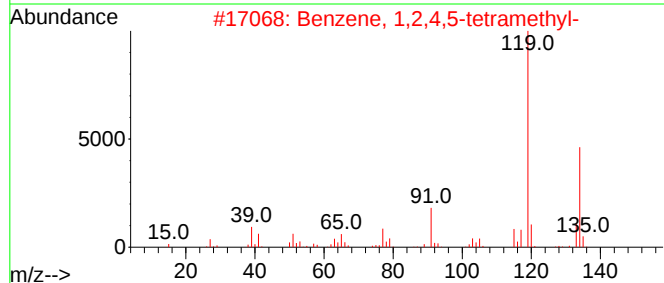
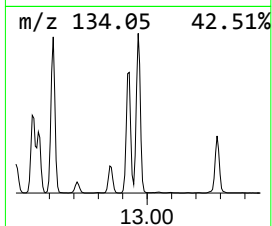
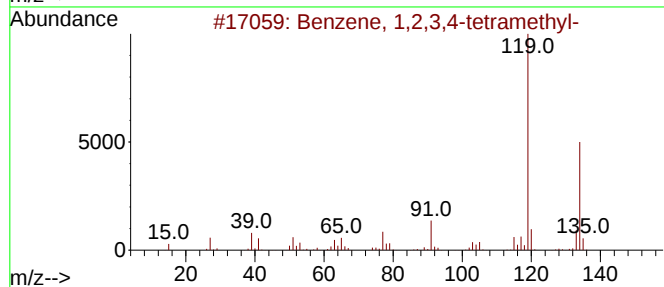
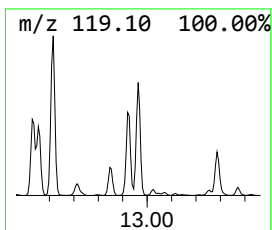
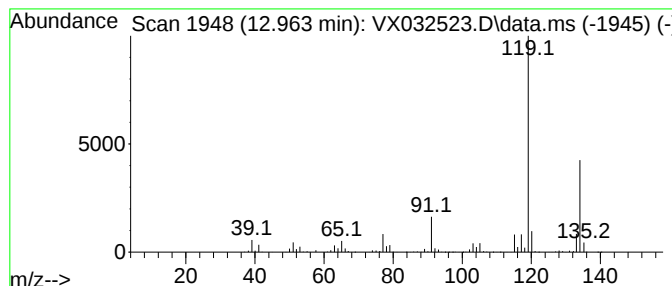
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	79.86 ug/l	1163440	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
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-2,3-dimethyl-	134	C10H14	000933-98-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110122\
Data File : VX032523.D
Acq On : 01 Nov 2022 19:04
Operator : JC/MD
Sample : N5414-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW3

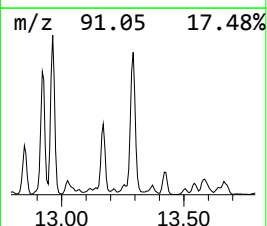
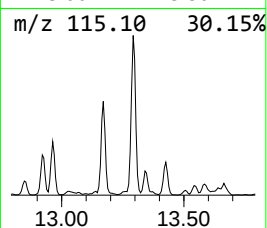
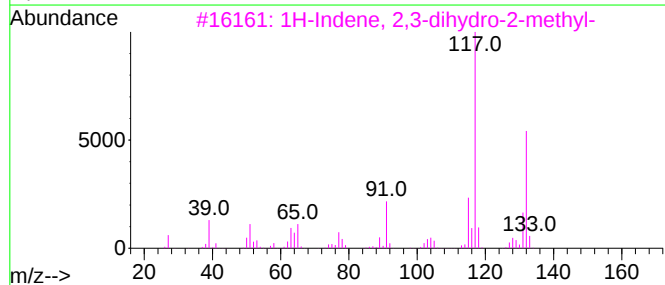
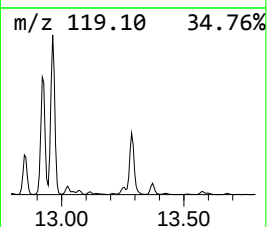
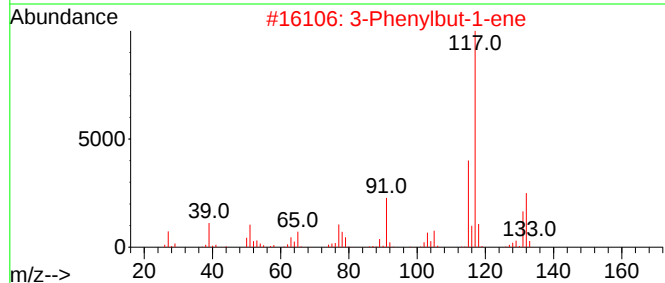
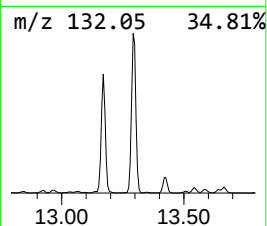
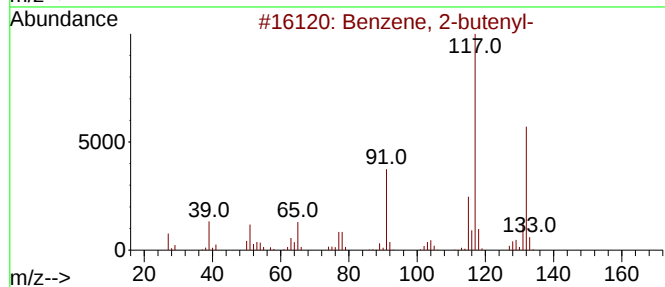
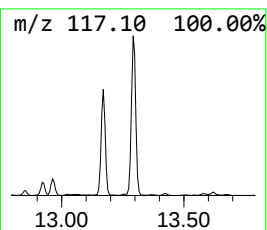
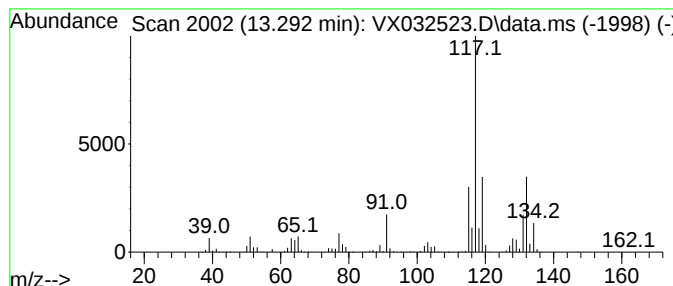
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-butenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	103.86 ug/l	1512960	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
3			1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	83
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110122\
Data File : VX032523.D
Acq On : 01 Nov 2022 19:04
Operator : JC/MD
Sample : N5414-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.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
Butane, 2-methyl-	1.746	141.9	ug/l	1457550	1	5.550	513391	50.0
Pentane, 3-methyl-	3.105	74.1	ug/l	760750	1	5.550	513391	50.0
Cyclopentane, m...	4.306	105.8	ug/l	1086600	1	5.550	513391	50.0
Benzene, 1-ethy...	11.384	829.5	ug/l	12084700	4	12.024	728389	50.0
Benzene, 1-ethy...	11.616	329.4	ug/l	4798570	4	12.024	728389	50.0
Benzene, 1,2,3-...	12.091	323.5	ug/l	4712550	4	12.024	728389	50.0
Benzene, cyclop...	12.244	334.1	ug/l	4867240	4	12.024	728389	50.0
o-Cymene	12.616	109.8	ug/l	1600100	4	12.024	728389	50.0
Benzene, 1,2,3,...	12.963	79.9	ug/l	1163440	4	12.024	728389	50.0
Benzene, 2-bute...	13.292	103.9	ug/l	1512960	4	12.024	728389	50.0