

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
 Data File : VX021223.D
 Acq On : 16 Mar 2021 01:08
 Operator : JC/MD
 Sample : M1647-21
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMP5-30811:15

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\82X031521W.M
 Title : SW846 8260

Signal : TIC: VX021223.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.470	62	65	81	rVB	9898759	11211913	100.00%	54.817%
2	5.464	733	744	756	rBV	57542	164768	1.47%	0.806%
3	5.629	760	772	785	rBV	86255	242309	2.16%	1.185%
4	6.029	829	840	846	rBV	64811	166833	1.49%	0.816%
5	6.111	846	854	880	rVB	245372	651009	5.81%	3.183%
6	6.829	965	976	990	rBV	147928	344588	3.07%	1.685%
7	8.694	1286	1293	1299	rBV	300123	470014	4.19%	2.298%
8	8.765	1299	1305	1322	rVB	550842	847262	7.56%	4.142%
9	10.094	1521	1531	1542	rBV	319416	455593	4.06%	2.227%
10	10.235	1551	1555	1565	rVB	80721	113062	1.01%	0.553%
11	10.341	1565	1573	1584	rVB2	508483	743393	6.63%	3.635%
12	10.683	1626	1631	1640	rVB2	472101	669042	5.97%	3.271%
13	11.118	1699	1705	1710	rBV	251405	332124	2.96%	1.624%
14	11.789	1814	1819	1824	rBV	230015	277409	2.47%	1.356%
15	12.059	1861	1865	1871	rVB	306614	386249	3.44%	1.888%
16	12.253	1889	1898	1910	rBV2	293873	491553	4.38%	2.403%
17	12.453	1926	1932	1937	rBV	267977	324544	2.89%	1.587%
18	13.818	2156	2164	2170	rBV	1569419	2003299	17.87%	9.794%
19	14.677	2305	2310	2320	rVB	269579	337155	3.01%	1.648%
20	14.818	2329	2334	2345	rVB	169512	221295	1.97%	1.082%

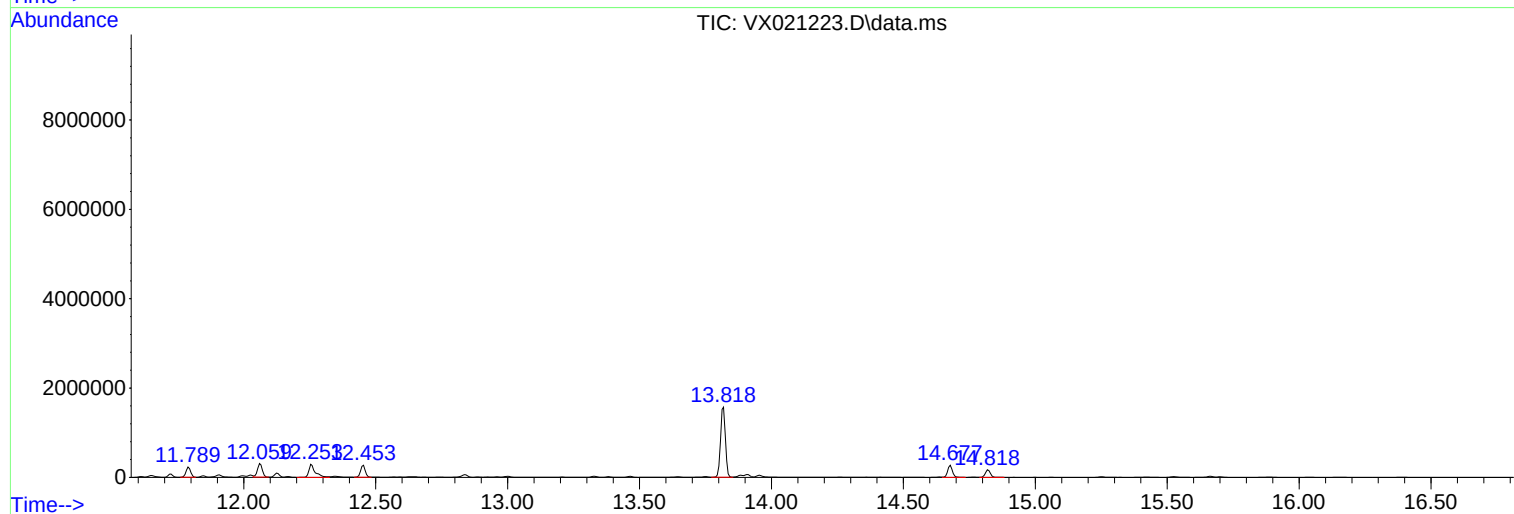
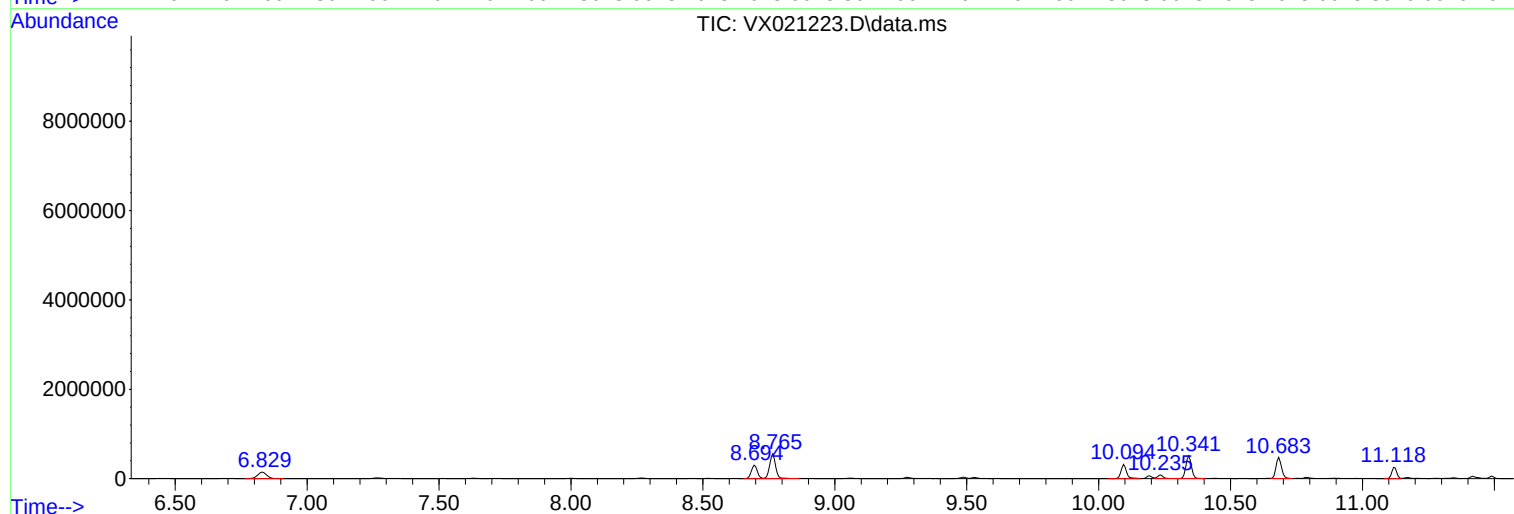
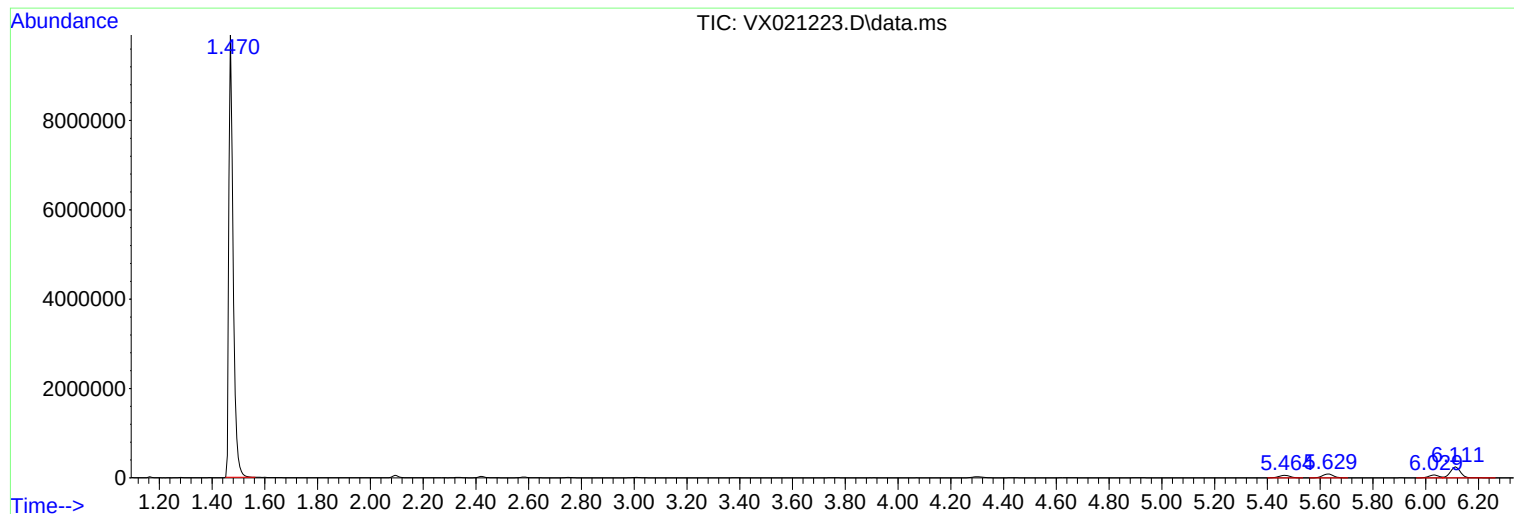
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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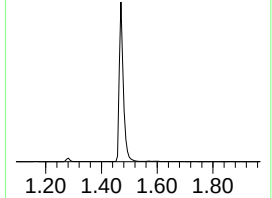
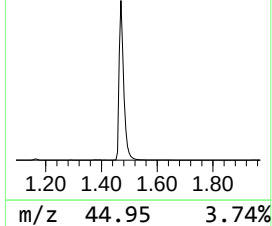
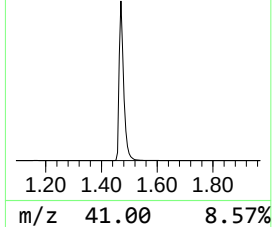
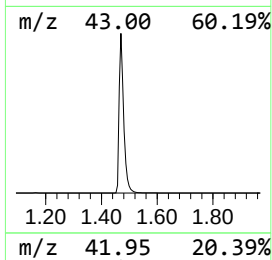
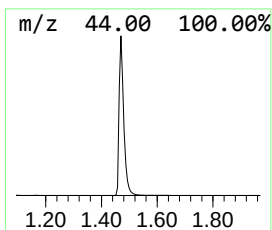
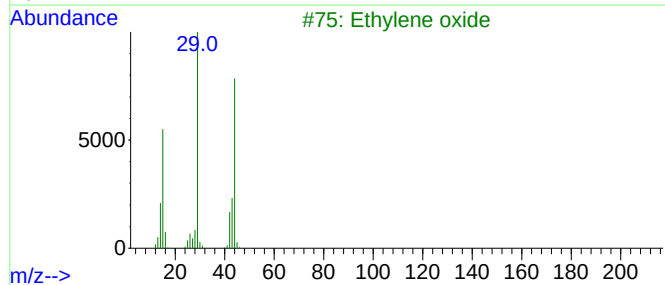
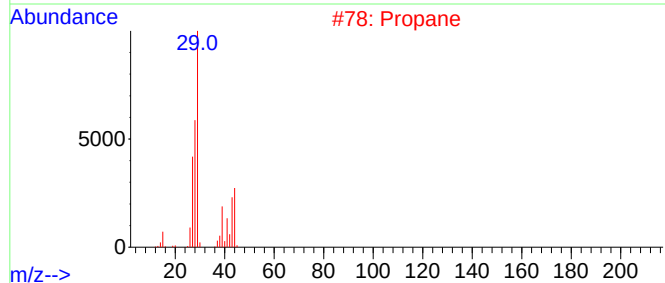
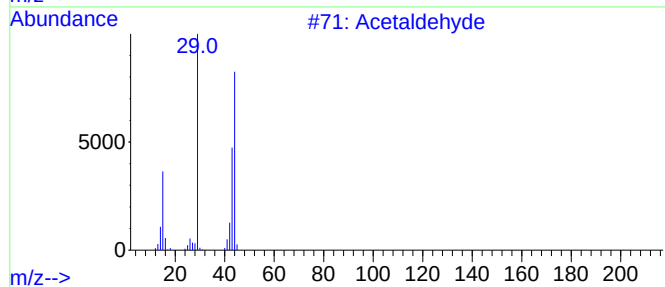
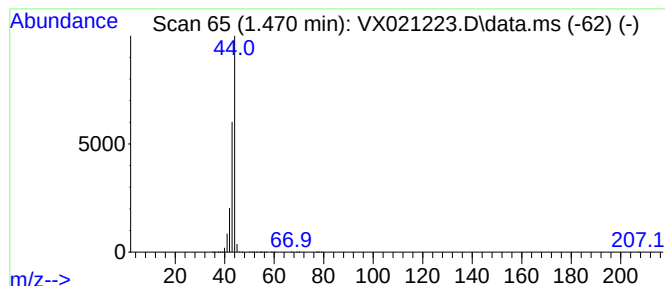
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.470	2313.56 ug/l	11211900	Pentafluorobenzene	5.635

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Carbon dioxide	44	CO2	000124-38-9	3



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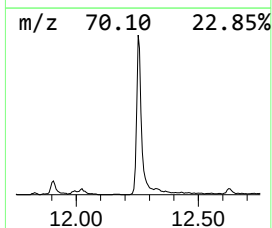
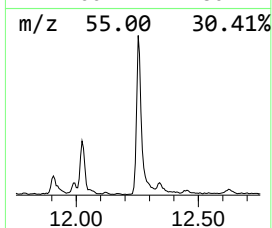
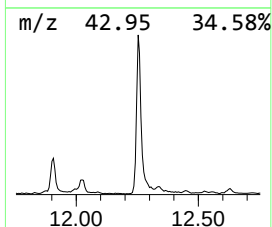
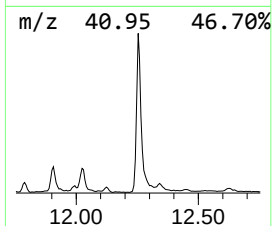
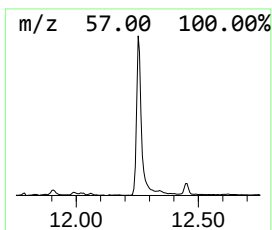
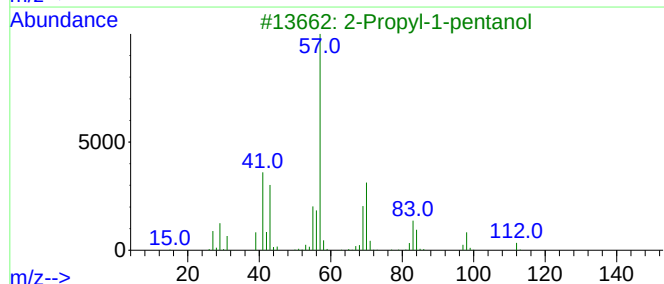
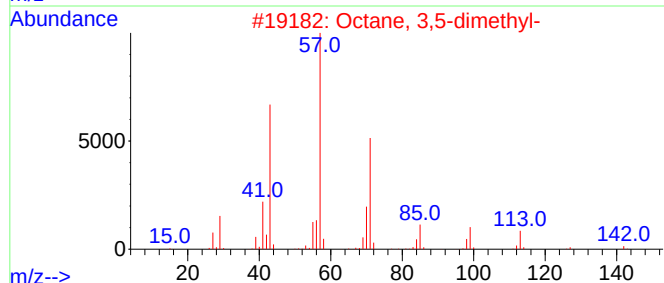
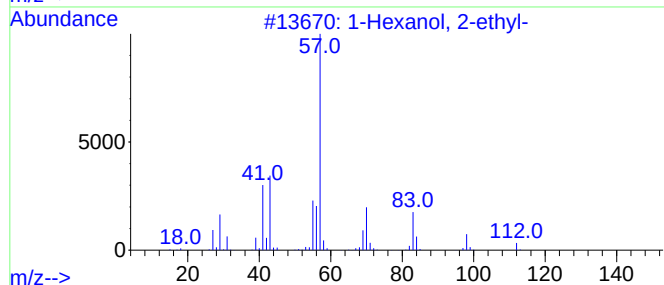
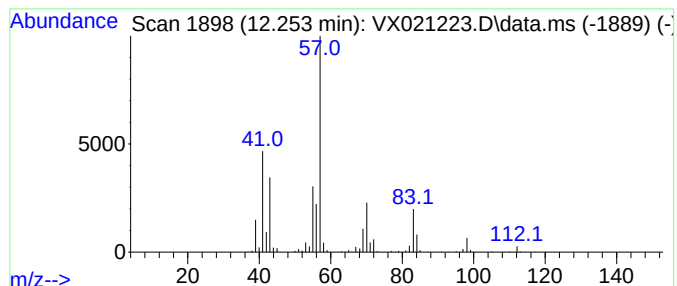
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.253	63.63 ug/l	491553	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	50
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	45
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	42



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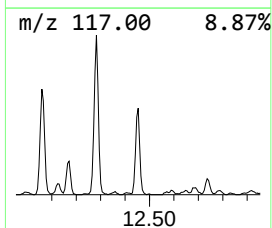
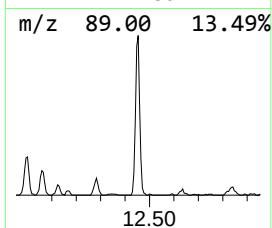
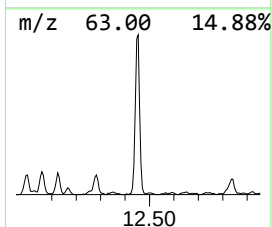
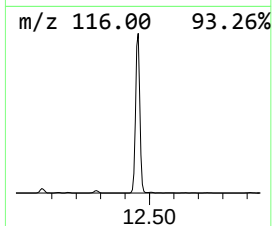
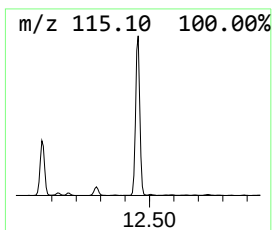
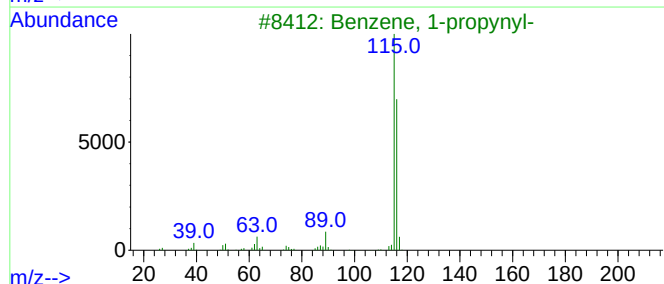
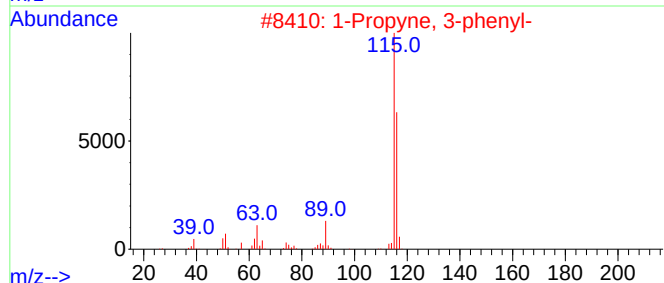
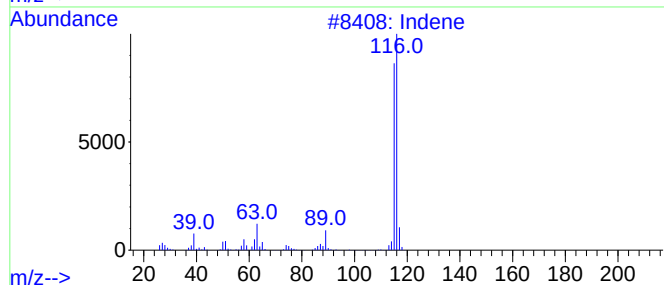
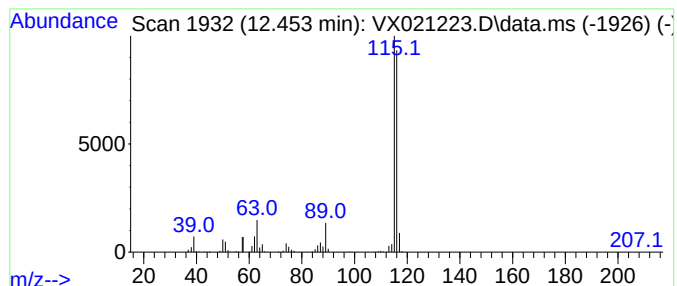
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Indene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.453	42.01 ug/l	324544	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	95
2			1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	94
3			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
4			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP5-30811:15

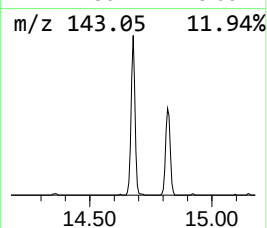
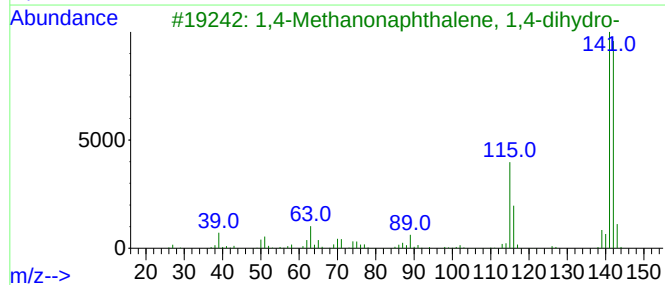
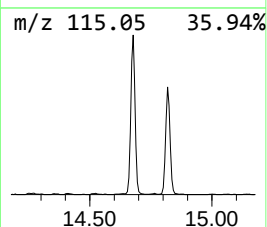
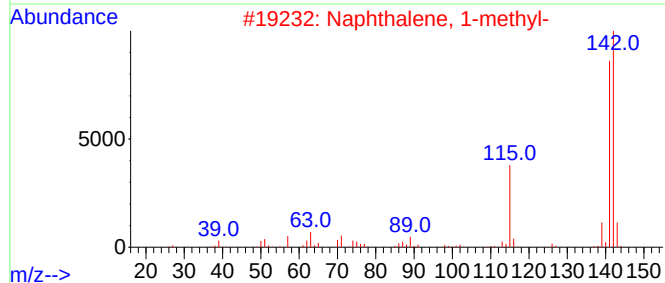
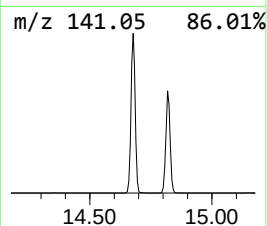
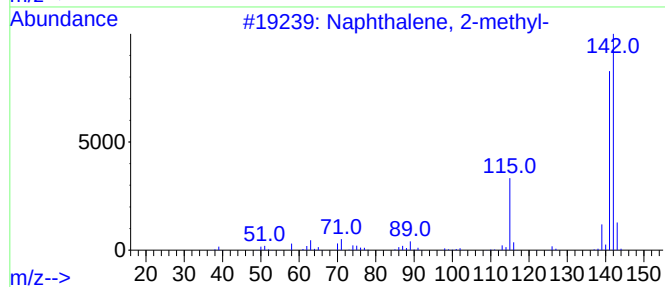
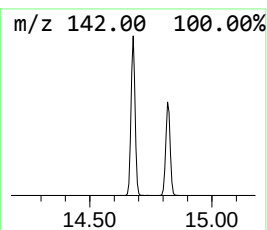
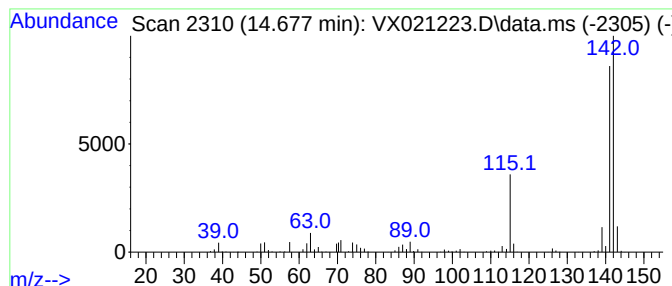
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.677	43.64 ug/l	337155	1,4-Dichlorobenzene-d4	12.059

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	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			3,4-Difluorobenzaldehyde	142	C7H4F2O	034036-07-2	59



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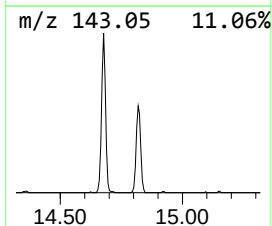
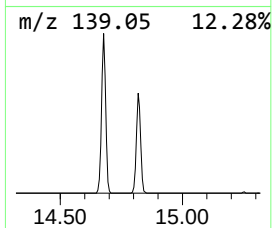
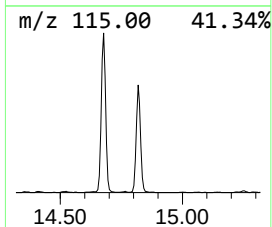
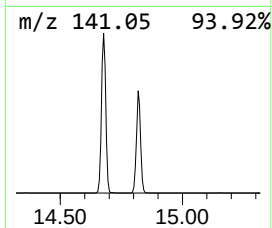
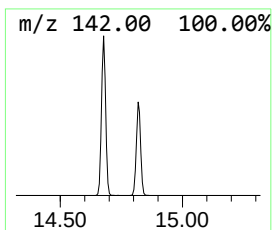
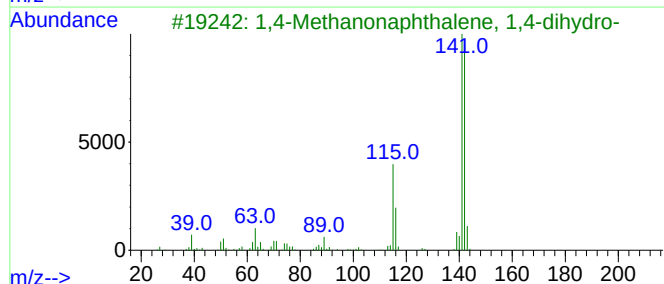
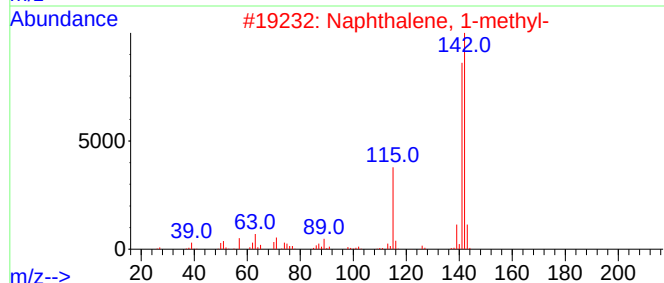
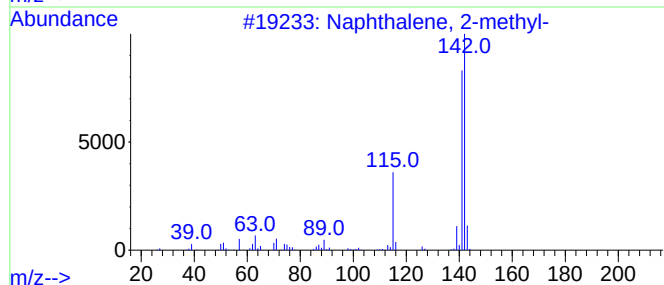
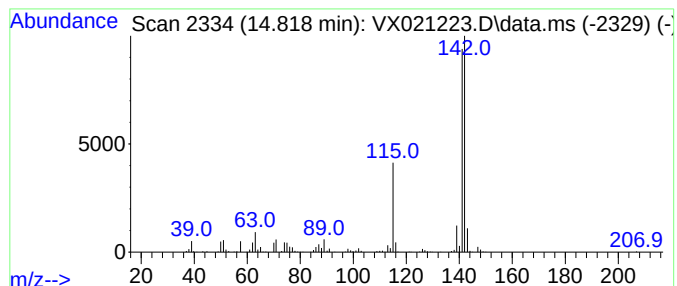
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Naphthalene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.818	28.65 ug/l	221295	1,4-Dichlorobenzene-d4	12.059

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	91



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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.470	2313.6	ug/l	11211900	1	5.635	242309	50.0
1-Hexanol, 2-et...	12.253	63.6	ug/l	491553	4	12.059	386249	50.0
Indene	12.453	42.0	ug/l	324544	4	12.059	386249	50.0
Naphthalene, 1-...	14.677	43.6	ug/l	337155	4	12.059	386249	50.0
Naphthalene, 2-...	14.818	28.6	ug/l	221295	4	12.059	386249	50.0