

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052125\
 Data File : VX046291.D
 Acq On : 21 May 2025 12:46
 Operator : JC/MD
 Sample : Q2093-14
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WATER-COMP

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\82X050525W.M
 Title : SW846 8260

Signal : TIC: VX046291.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.575	69	80	81	rBV3	3775	7977	1.73%	0.224%
2	2.380	205	212	223	rBV	29717	48890	10.59%	1.374%
3	2.544	230	239	244	rBV2	3369	6365	1.38%	0.179%
4	5.093	643	657	674	rBV2	60635	178483	38.67%	5.015%
5	5.379	694	704	721	rBV	53850	161992	35.10%	4.552%
6	5.550	721	732	750	rVB	75440	222416	48.19%	6.250%
7	5.952	788	798	810	rBV	62226	167119	36.21%	4.696%
8	6.757	921	930	946	rBV	136367	331159	71.75%	9.305%
9	7.824	1099	1105	1115	rVB	19446	36130	7.83%	1.015%
10	8.647	1234	1240	1256	rVV	291475	461516	100.00%	12.968%
11	9.519	1379	1383	1389	rBV5	3258	5200	1.13%	0.146%
12	10.049	1465	1470	1479	rBV	306907	423661	91.80%	11.904%
13	11.079	1634	1639	1650	rBV	254760	329127	71.31%	9.248%
14	11.969	1781	1785	1789	rBV2	24300	31672	6.86%	0.890%
15	12.018	1789	1793	1801	rVB	313655	388537	84.19%	10.917%
16	12.579	1881	1885	1888	rBV3	7705	11614	2.52%	0.326%
17	12.823	1921	1925	1929	rBV7	5290	10868	2.35%	0.305%
18	13.481	2030	2033	2035	rBV4	6487	6993	1.52%	0.196%
19	13.591	2046	2051	2069	rBV	193145	316878	68.66%	8.904%
20	14.451	2188	2192	2196	rVB	33237	40775	8.84%	1.146%
21	14.591	2212	2215	2220	rBV6	6537	9798	2.12%	0.275%
22	14.725	2233	2237	2241	rBV	25110	33143	7.18%	0.931%
23	14.786	2243	2247	2253	rBV2	26597	35213	7.63%	0.989%
24	14.987	2275	2280	2286	rBV	36772	52317	11.34%	1.470%
25	15.073	2290	2294	2300	rVB2	28125	39905	8.65%	1.121%
26	15.182	2308	2312	2313	rBV4	4119	5109	1.11%	0.144%
27	15.207	2313	2316	2320	rVB2	8278	11514	2.49%	0.324%
28	15.353	2335	2340	2346	rVB4	10063	16012	3.47%	0.450%
29	15.493	2357	2363	2373	rVB	14166	31648	6.86%	0.889%
30	15.993	2441	2445	2449	rBV4	4982	6556	1.42%	0.184%
31	16.097	2455	2462	2473	rBV3	48565	130309	28.23%	3.662%

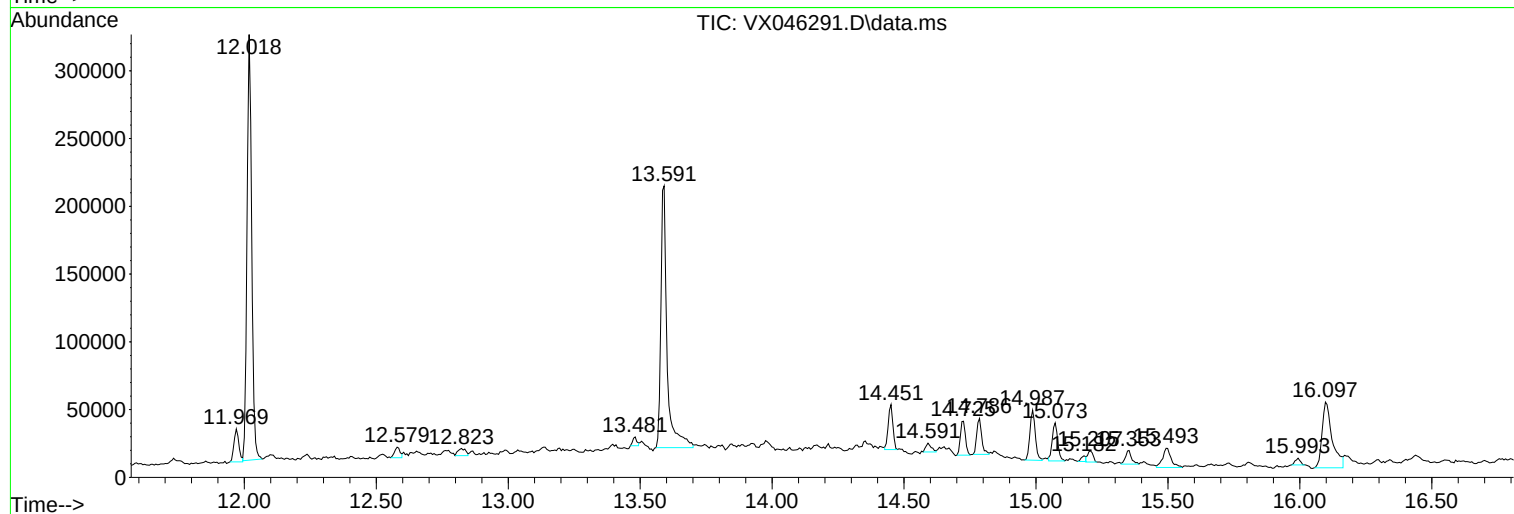
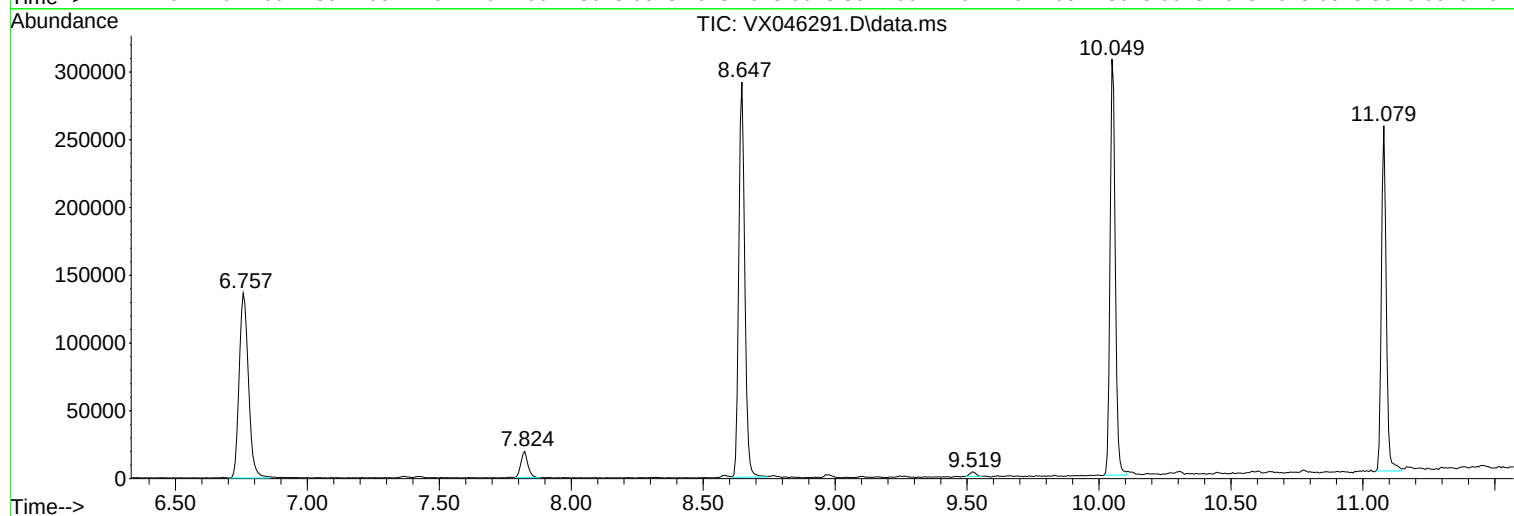
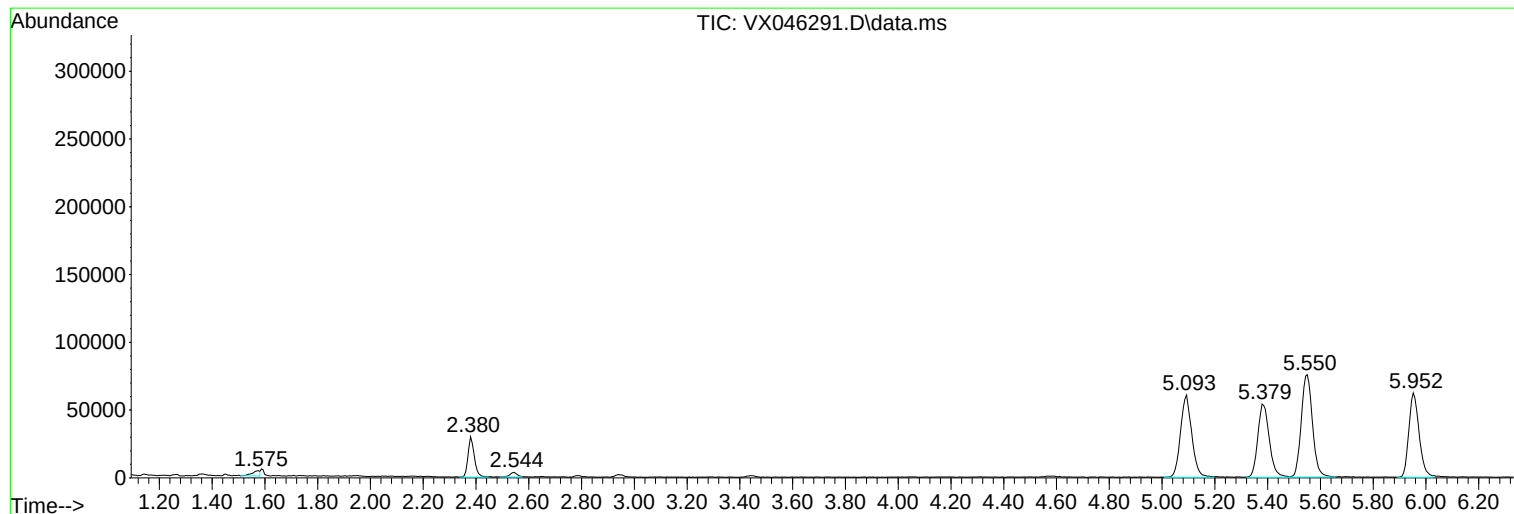
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ClientSampleId :
WATER-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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



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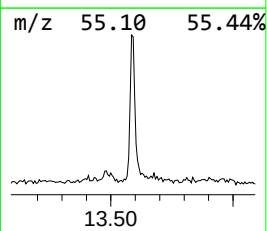
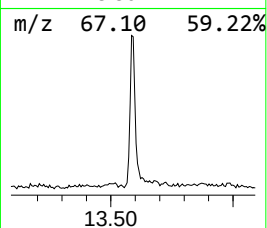
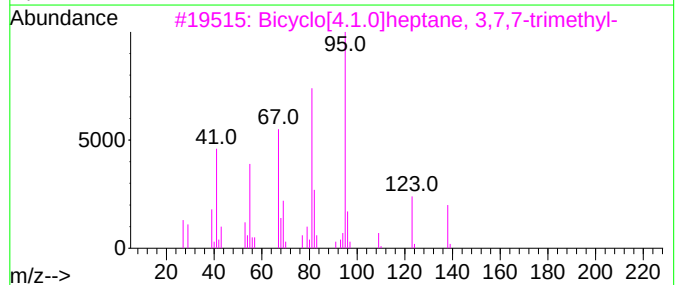
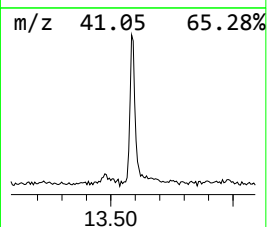
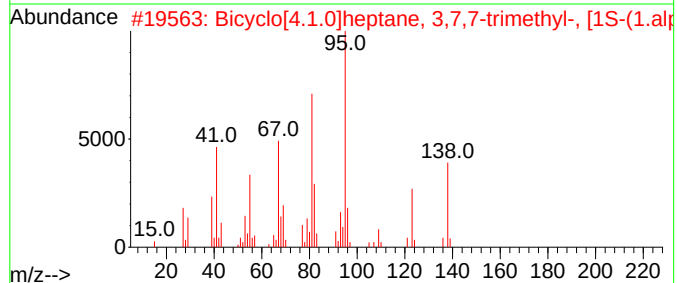
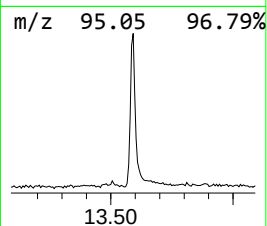
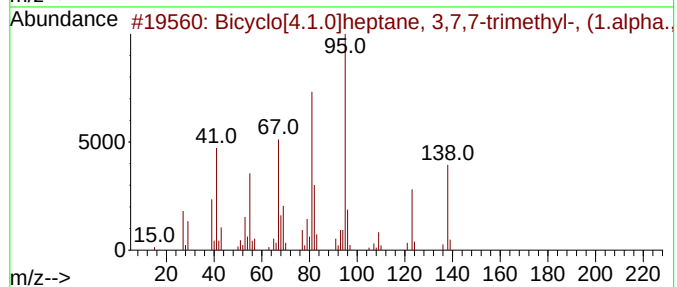
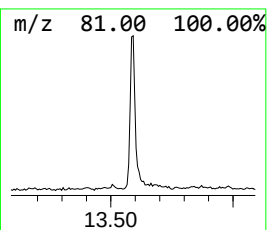
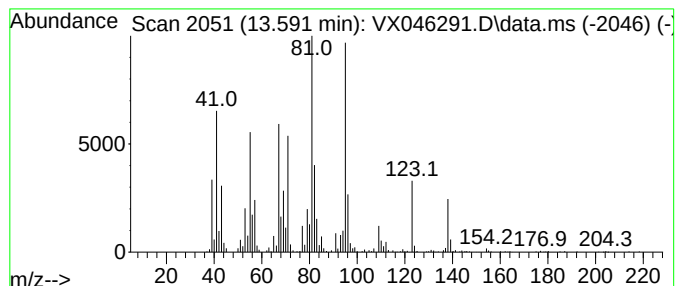
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 1 Bicyclo[4.1.0]heptane, 3,7,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.591	40.78 ug/l	316878	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	018968-23-5	93
2			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	002778-68-9	83
3			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	81
4			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001879-07-8	81
5			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-27-2	76



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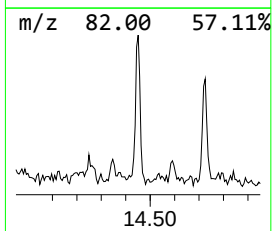
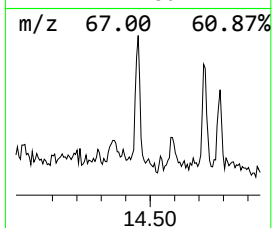
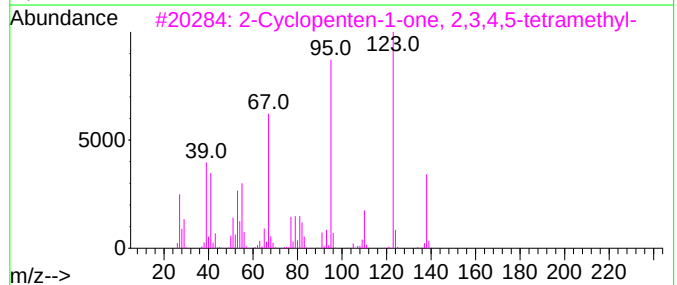
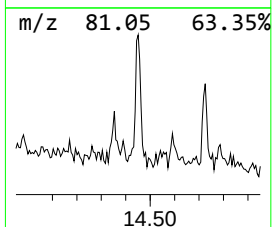
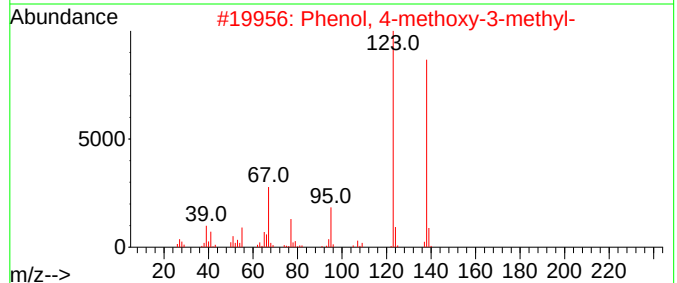
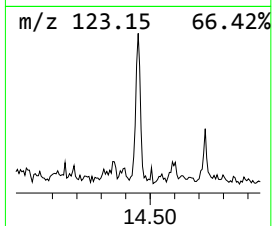
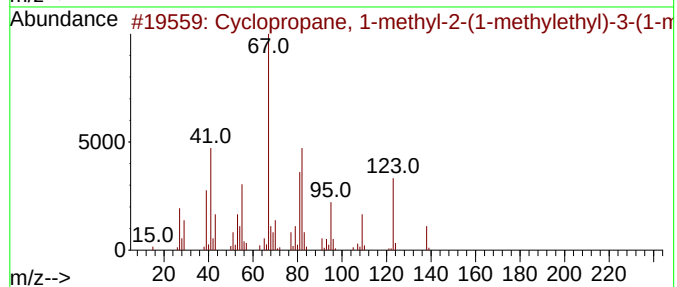
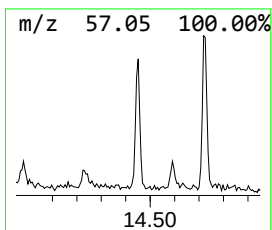
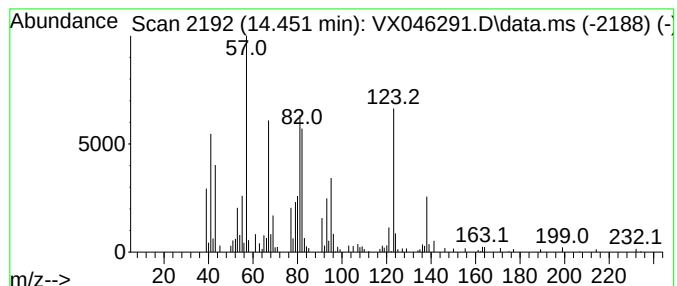
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclopropane, 1-methyl-2-(1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	5.25 ug/l	40775	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1-methyl-2-(1-meth...	138	C10H18	024524-52-5	64
2			Phenol, 4-methoxy-3-methyl-	138	C8H10O2	014786-82-4	49
3			2-Cyclopenten-1-one, 2,3,4,5-tet...	138	C9H14O	054458-61-6	41
4			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	38
5			2(1H)-Pyridinone, 1-ethyl-	123	C7H9NO	013337-79-6	38



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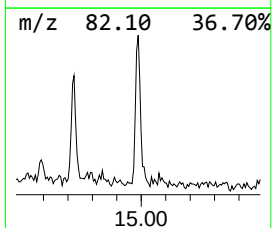
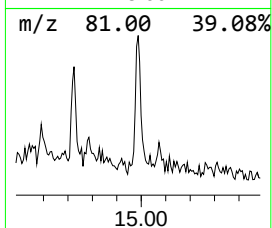
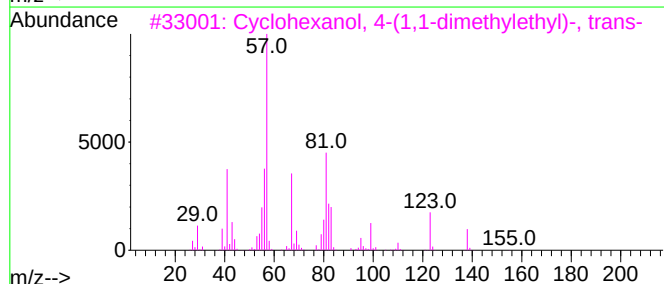
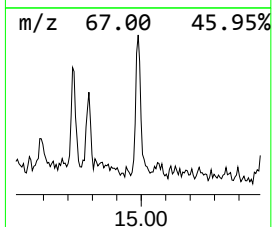
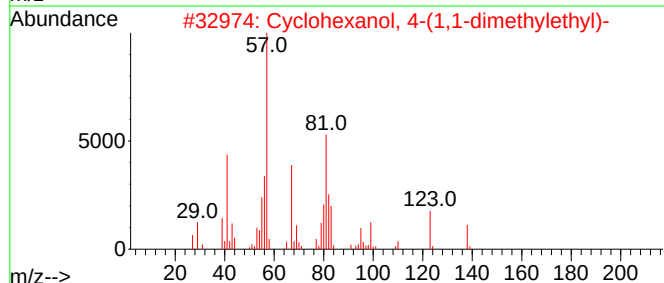
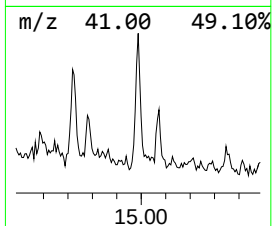
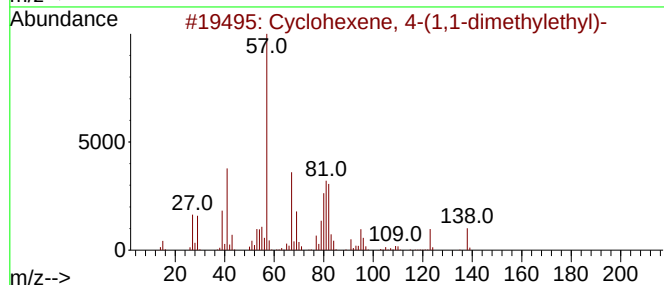
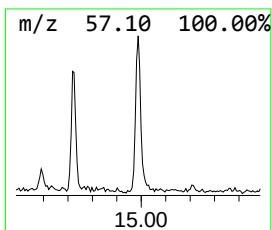
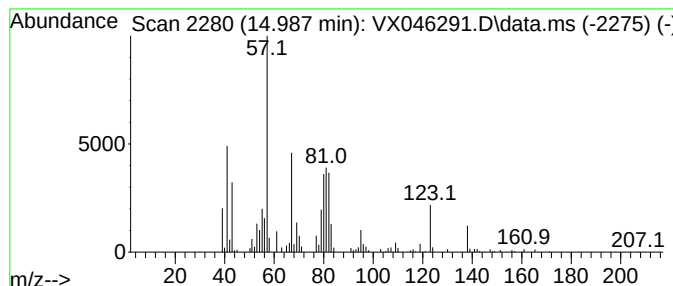
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Quant Title : SW846 8260

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

Peak Number 3 Cyclohexene, 4-(1,1-dimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.987	6.73 ug/l	52317	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 4-(1,1-dimethylethyl)-	138	C10H18	002228-98-0	87
2			Cyclohexanol, 4-(1,1-dimethylethyl)-	156	C10H20O	000098-52-2	72
3			Cyclohexanol, 4-(1,1-dimethylethyl)-	156	C10H20O	021862-63-5	59
4			Cyclohexanol, 2-(1,1-dimethylethyl)-	156	C10H20O	007214-18-8	58
5			Cyclohexanol, 2-(1,1-dimethylethyl)-	156	C10H20O	013491-79-7	50



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WATER-COMP

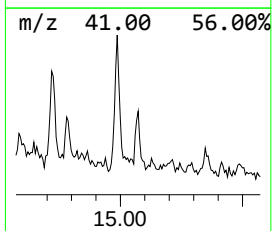
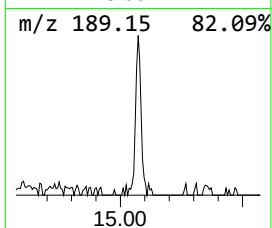
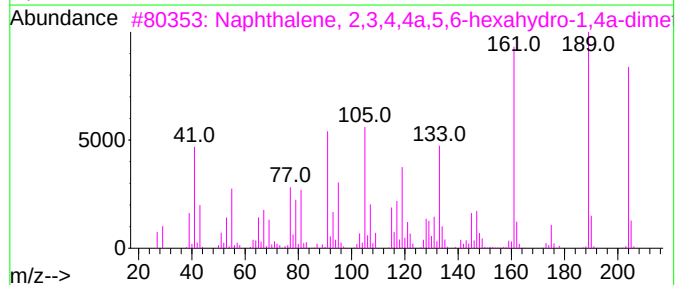
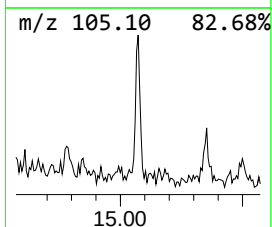
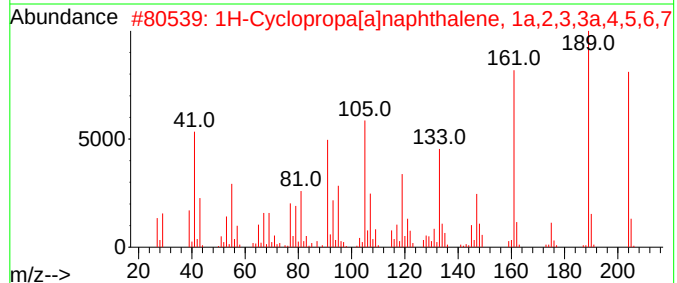
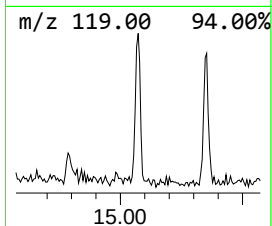
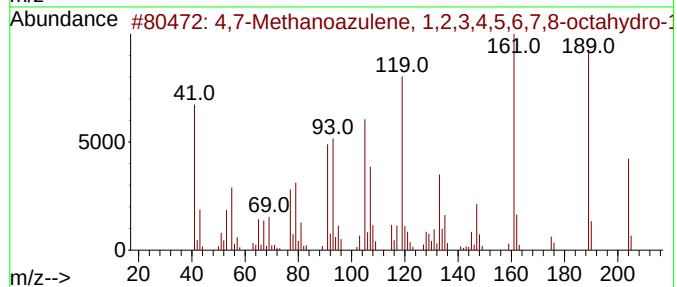
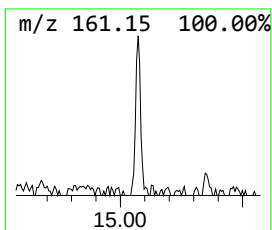
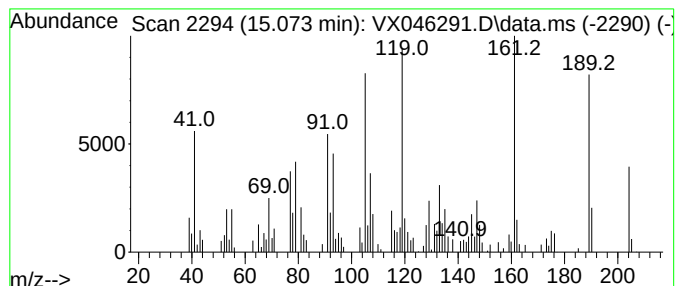
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Peak Number 4 4,7-Methanoazulene, 1,2,3,4... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.073	5.14 ug/l	39905	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,7-Methanoazulene, 1,2,3,4,5,6,...	204	C15H24	000514-51-2	98
2			1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	92
3			Naphthalene, 2,3,4,4a,5,6-hexahy...	204	C15H24	000473-14-3	91
4			.gamma.-Muurolene	204	C15H24	030021-74-0	86
5			Cyclohexene, 6-ethenyl-6-methyl-...	204	C15H24	005951-67-7	86



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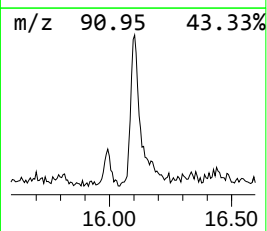
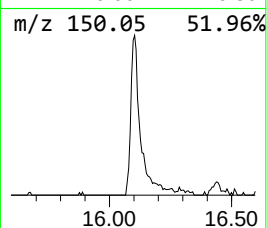
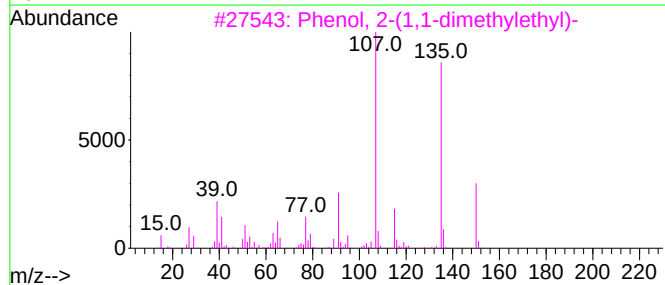
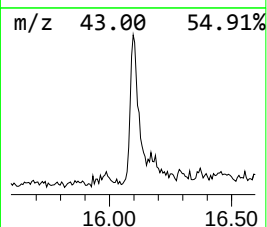
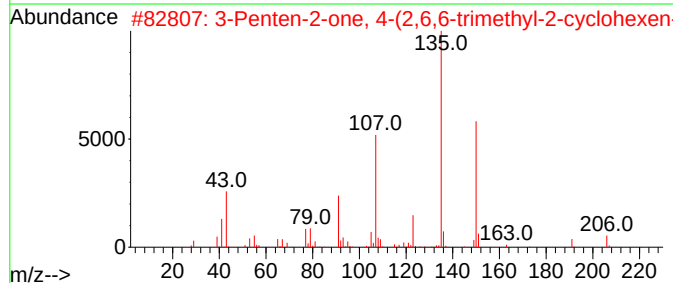
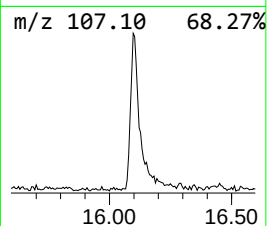
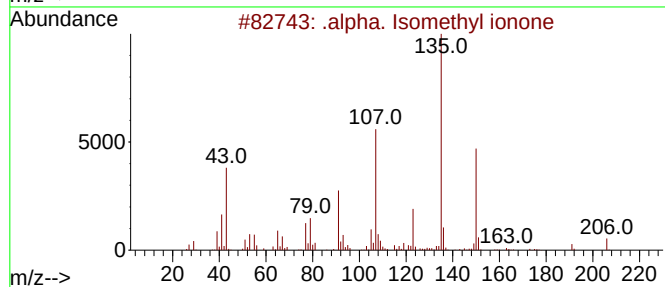
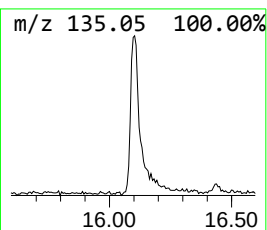
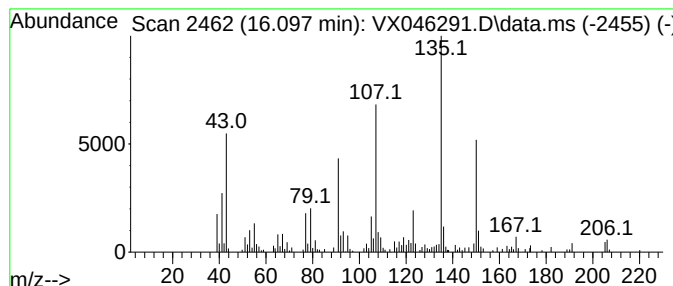
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Peak Number 5 .alpha. Isomethyl ionone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.097	16.77 ug/l	130309	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha. Isomethyl ionone	206	C14H22O	000127-51-5	98
2			3-Penten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-	206	C14H22O	114933-28-7	90
3			Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	74
4			Ethanone, 1-(6,6-dimethylbicyclo[2.2.2]oct-2-yl)-	150	C10H14O	024555-40-6	62
5			3-Methyl-4-isopropylphenol	150	C10H14O	003228-02-2	62



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WATER-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Bicyclo[4.1.0]h...	13.591	40.8	ug/l	316878	4	12.018	388537	50.0
Cyclopropane, 1...	14.451	5.3	ug/l	40775	4	12.018	388537	50.0
Cyclohexene, 4-...	14.987	6.7	ug/l	52317	4	12.018	388537	50.0
4,7-Methanoazul...	15.073	5.1	ug/l	39905	4	12.018	388537	50.0
.alpha. Isometh...	16.097	16.8	ug/l	130309	4	12.018	388537	50.0