

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
 Data File : VX027957.D
 Acq On : 04 Apr 2022 15:01
 Operator : JC/MD
 Sample : N2249-02 5X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-2

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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\82X032922W.M
 Title : SW846 8260

Signal : TIC: VX027957.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	21	26	42	rBV	33120	58323	6.34%	1.181%
2	1.752	103	109	116	rVB	23691	32566	3.54%	0.659%
3	1.953	138	142	152	rVB3	7946	13173	1.43%	0.267%
4	2.867	288	292	304	rVB4	9230	22651	2.46%	0.459%
5	4.312	518	529	541	rVB	16462	46860	5.10%	0.949%
6	5.391	694	706	715	rBV2	55826	161887	17.60%	3.277%
7	5.556	724	733	753	rVB	101750	290132	31.55%	5.873%
8	5.958	788	799	814	rBV2	64372	169616	18.44%	3.434%
9	6.763	922	931	942	rBV	147839	355837	38.69%	7.203%
10	8.653	1232	1241	1249	rBV	299595	468771	50.97%	9.489%
11	10.055	1465	1471	1481	rBV	303993	403729	43.90%	8.173%
12	10.195	1489	1494	1502	rVB	129271	162053	17.62%	3.280%
13	10.305	1505	1512	1530	rVB	666227	919669	100.00%	18.617%
14	10.647	1562	1568	1575	rBV	42933	56201	6.11%	1.138%
15	10.964	1615	1620	1625	rVB	9801	12211	1.33%	0.247%
16	11.085	1634	1640	1654	rVB	265738	343675	37.37%	6.957%
17	11.305	1671	1676	1683	rVB	16606	20430	2.22%	0.414%
18	11.384	1683	1689	1696	rBV	98306	184110	20.02%	3.727%
19	11.451	1696	1700	1708	rVB	62903	77409	8.42%	1.567%
20	11.616	1722	1727	1733	rVB	82799	100110	10.89%	2.027%
21	11.756	1744	1750	1757	rBV	278029	340960	37.07%	6.902%
22	12.024	1789	1794	1800	rBV	294032	354719	38.57%	7.181%
23	12.091	1800	1805	1810	rVV	92335	114852	12.49%	2.325%
24	12.244	1823	1830	1838	rBV	70147	89828	9.77%	1.818%
25	12.317	1838	1842	1847	rBV	7264	9696	1.05%	0.196%
26	12.616	1885	1891	1894	rBV	8096	9590	1.04%	0.194%
27	12.701	1901	1905	1912	rVB2	8387	10618	1.15%	0.215%
28	12.963	1945	1948	1953	rVB	8624	9816	1.07%	0.199%
29	13.292	1997	2002	2007	rVB2	14693	19674	2.14%	0.398%
30	13.780	2076	2082	2090	rVB	62895	80842	8.79%	1.636%

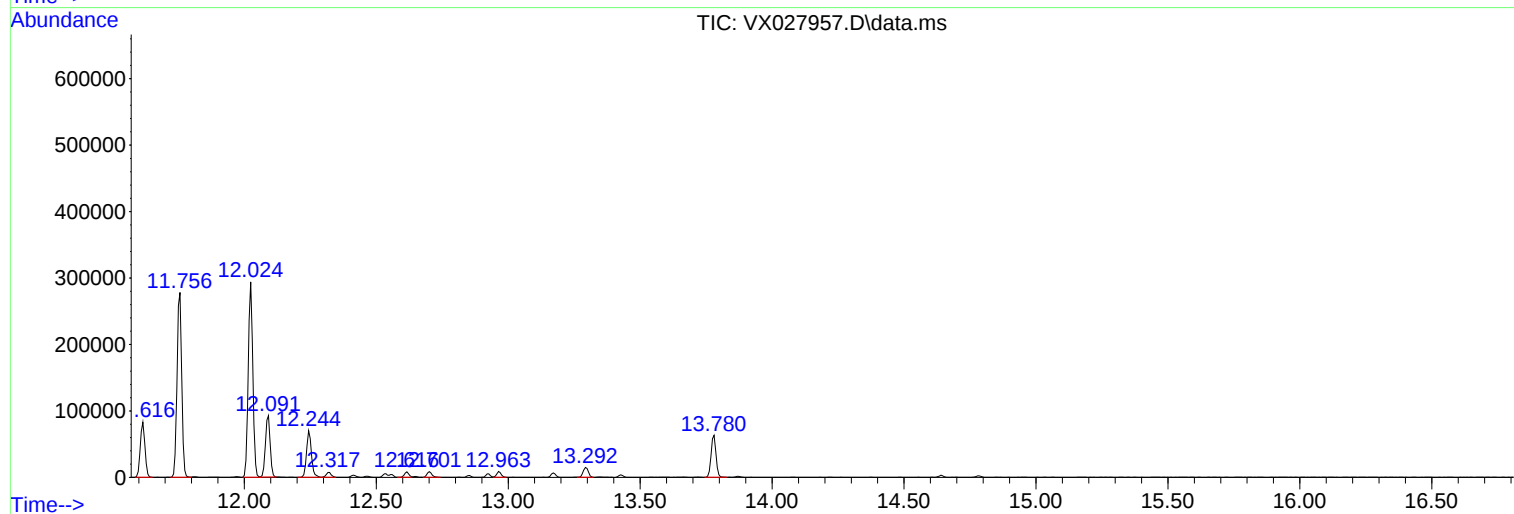
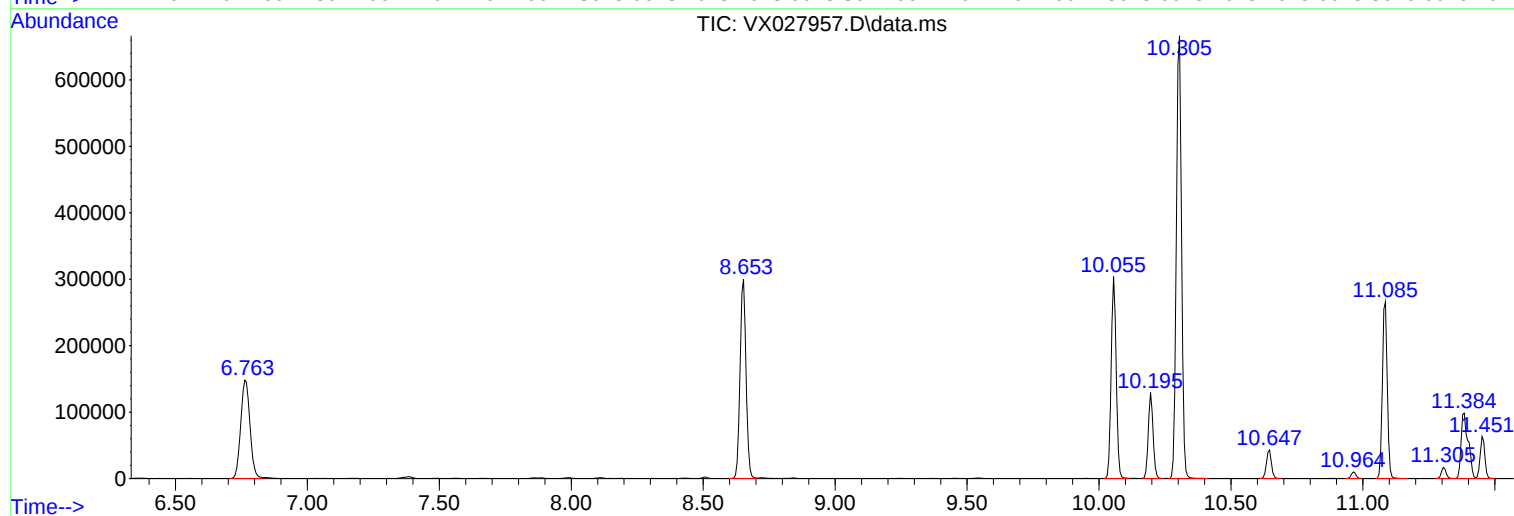
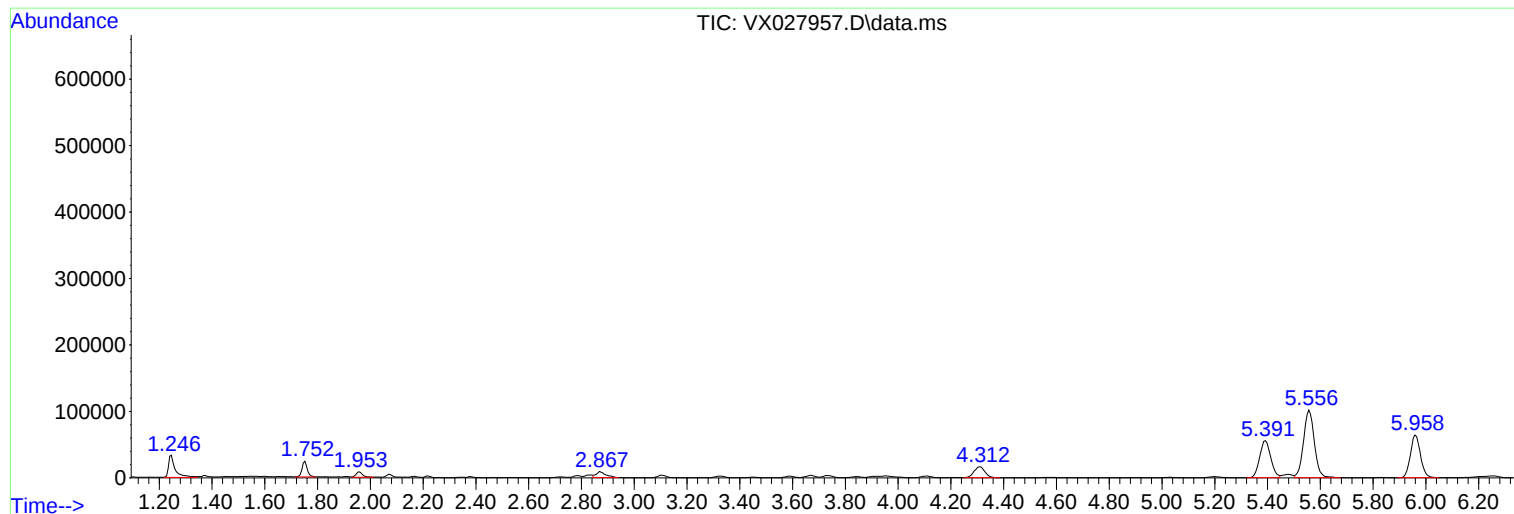
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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



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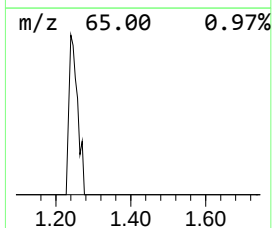
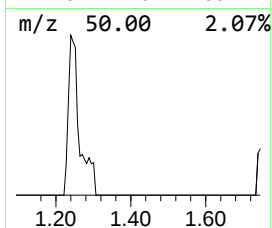
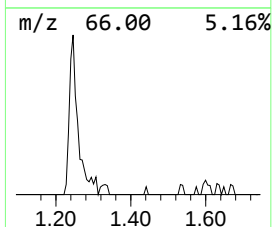
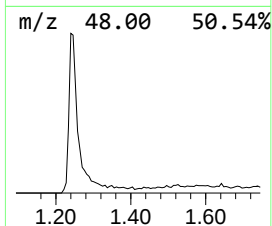
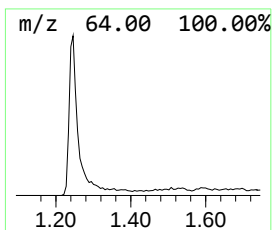
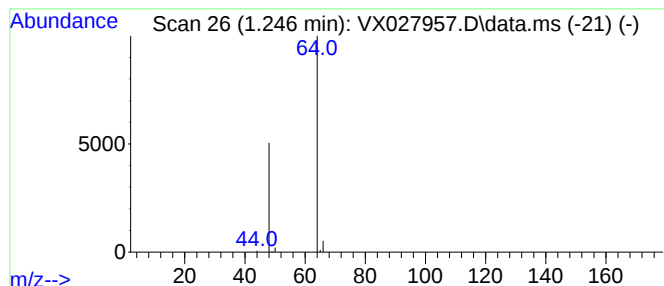
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Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	10.05 ug/l	58323	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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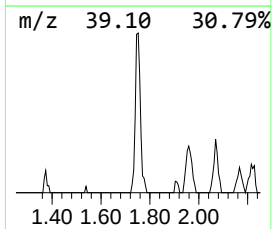
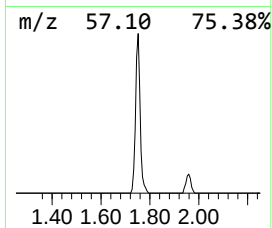
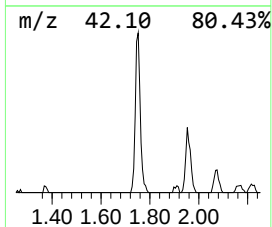
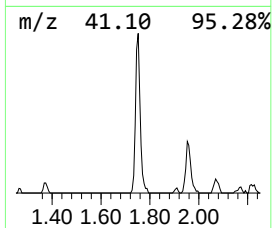
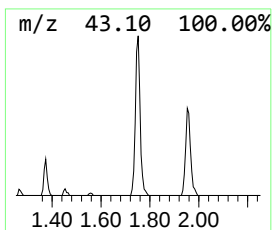
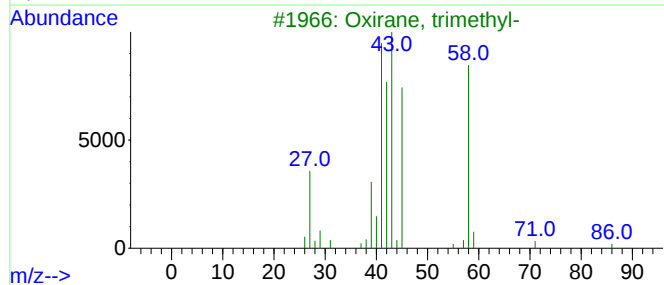
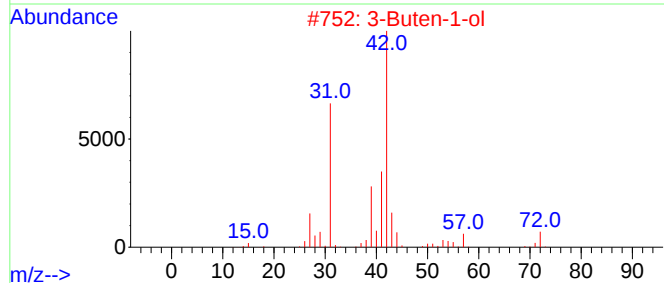
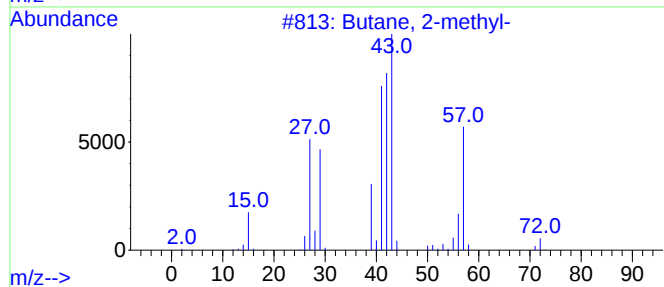
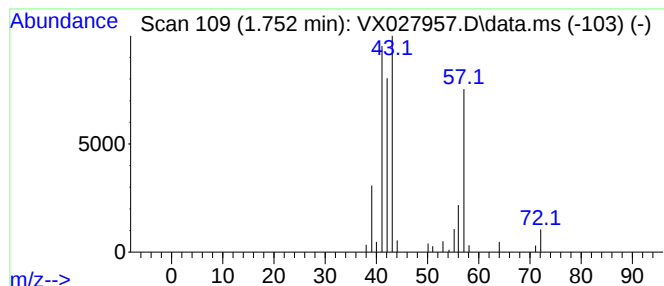
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	5.61 ug/l	32566	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	87
2			3-Buten-1-ol	72	C4H8O	000627-27-0	43
3			Oxirane, trimethyl-	86	C5H10O	005076-19-7	33
4			1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	33
5			Pentane	72	C5H12	000109-66-0	28



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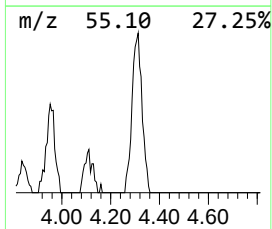
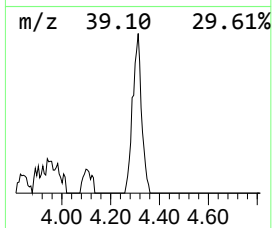
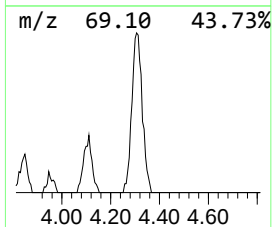
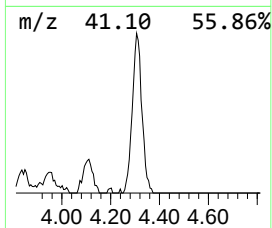
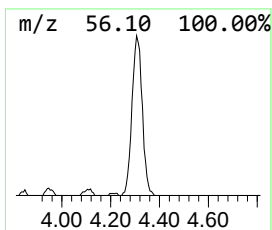
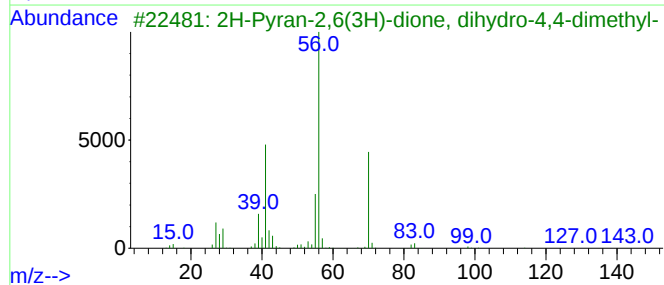
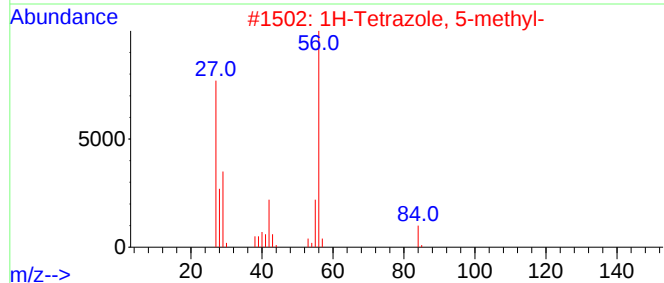
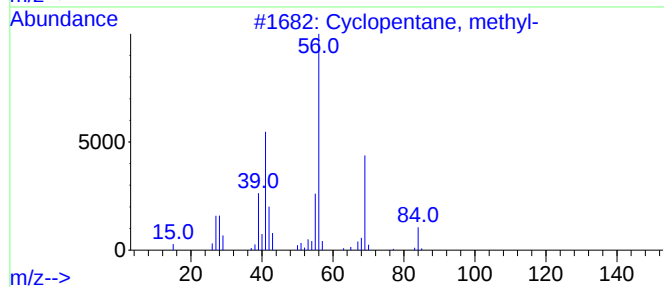
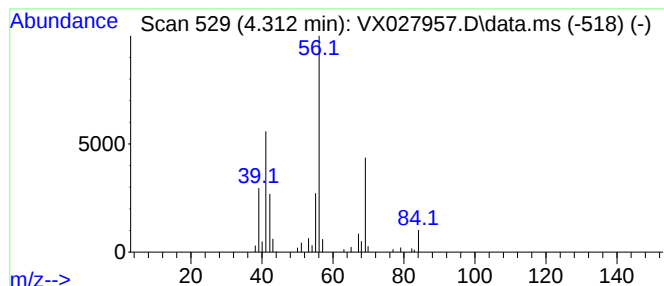
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Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	8.08 ug/l	46860	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3			2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	53
4			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	38



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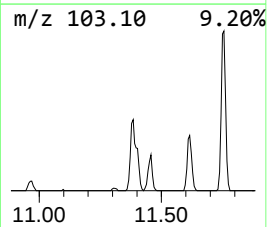
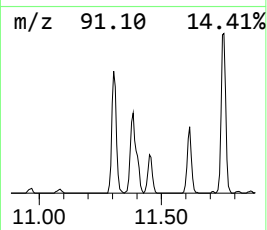
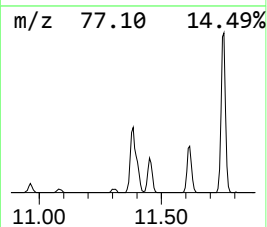
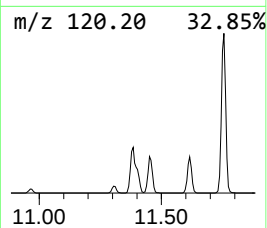
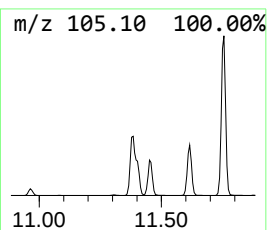
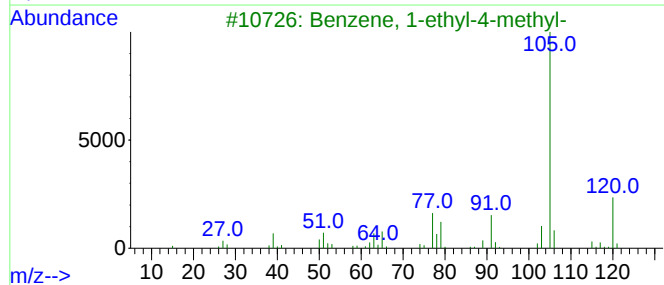
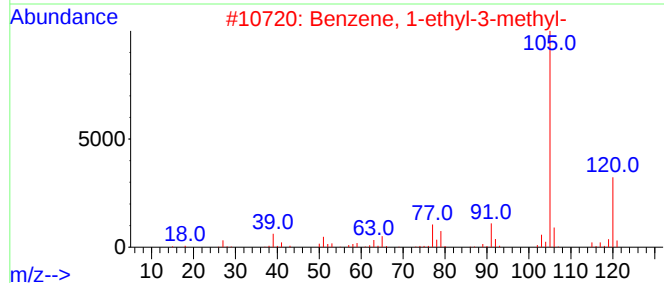
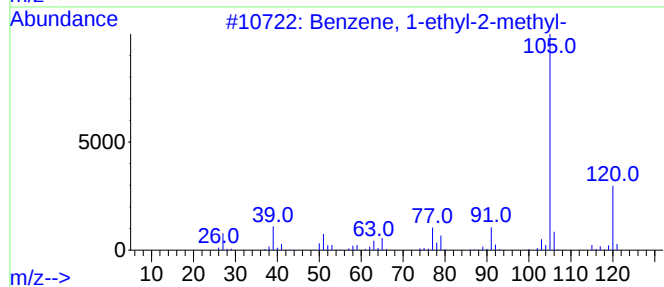
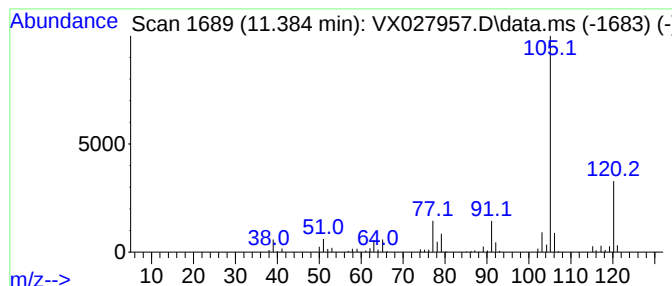
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	25.95 ug/l	184110	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	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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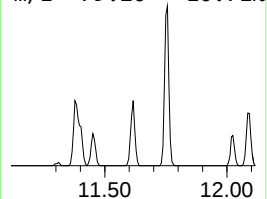
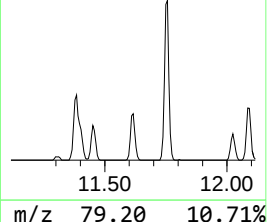
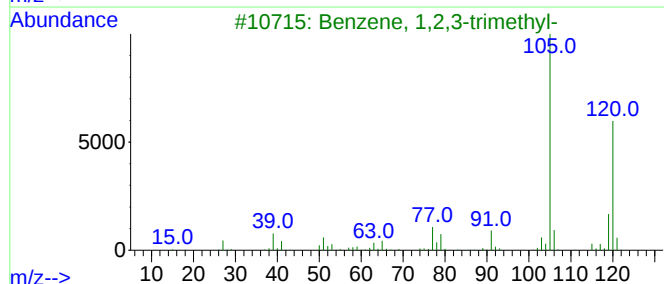
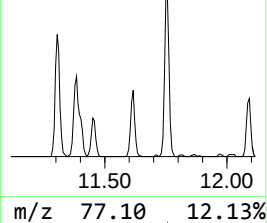
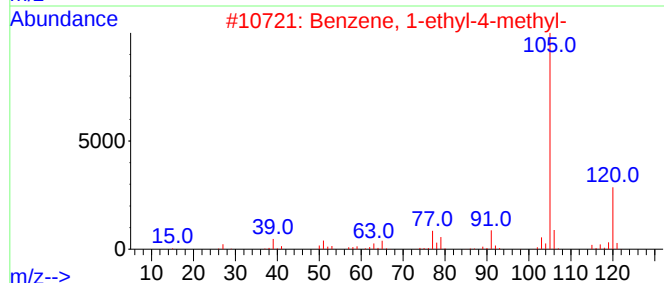
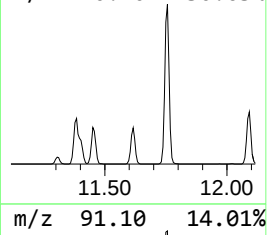
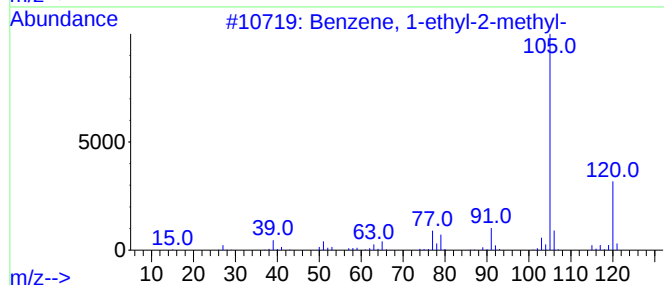
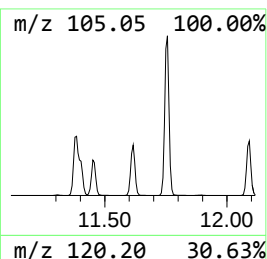
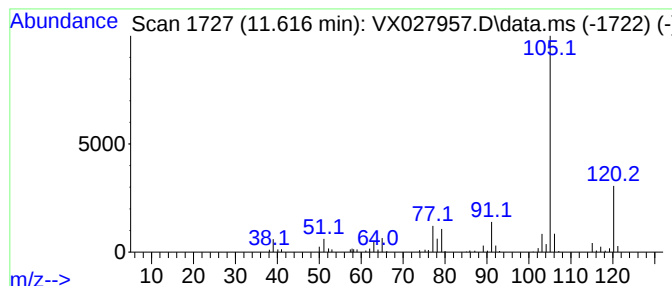
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	14.11 ug/l	100110	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	91
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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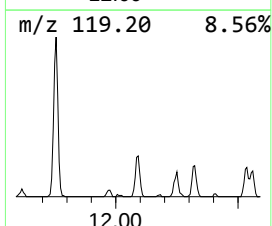
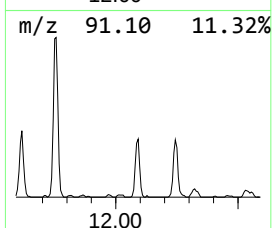
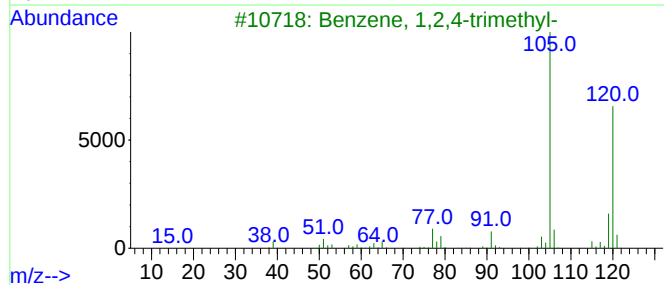
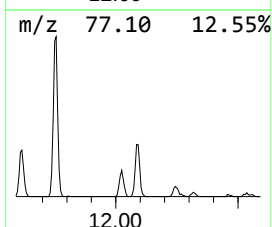
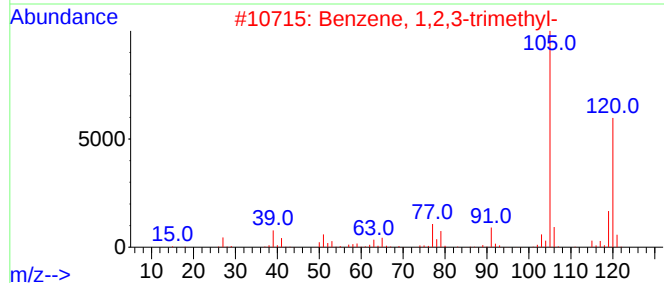
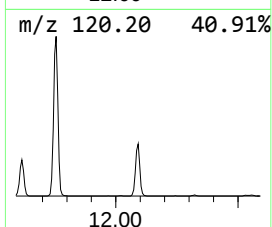
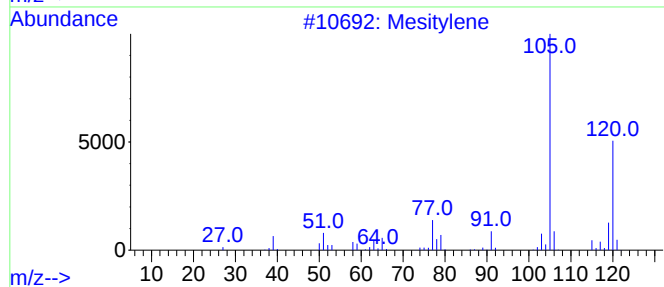
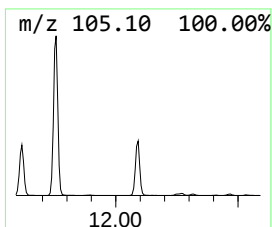
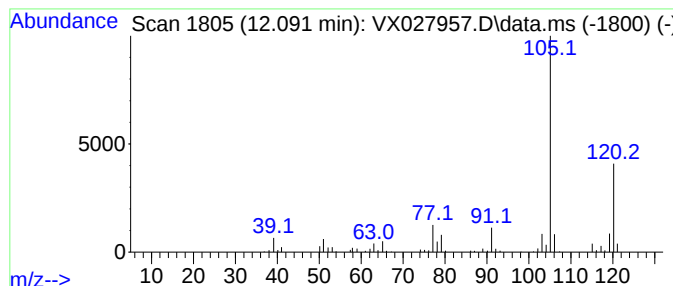
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Quant Title : SW846 8260

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

Peak Number 6 Mesitylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	16.19 ug/l	114852	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, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027957.D
Acq On : 04 Apr 2022 15:01
Operator : JC/MD
Sample : N2249-02 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

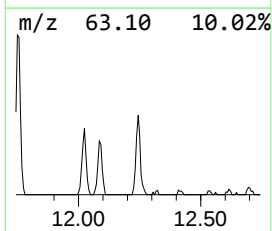
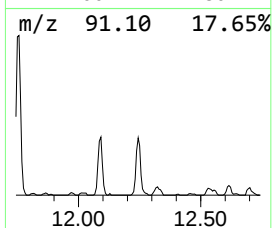
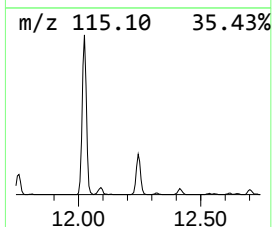
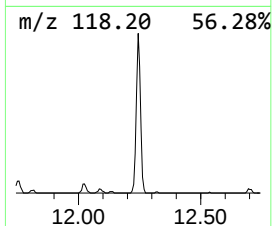
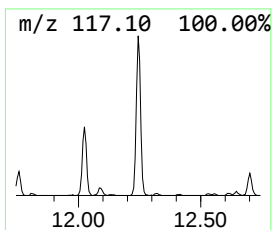
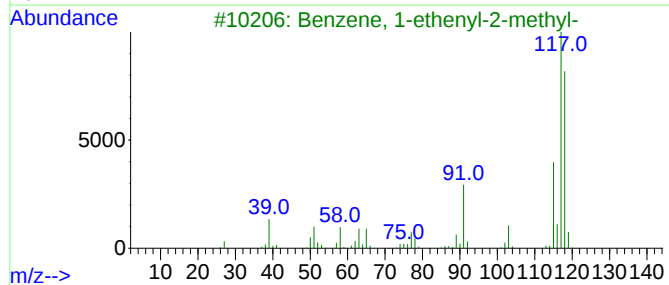
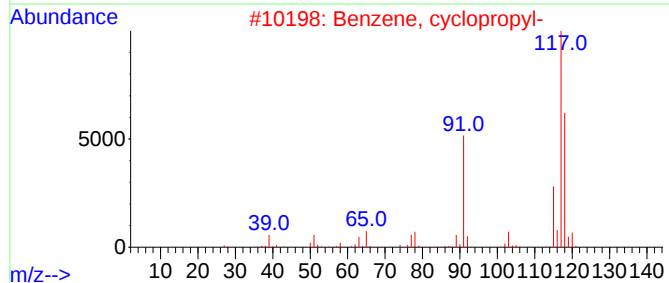
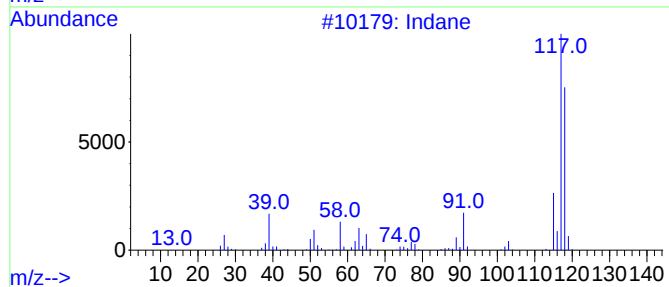
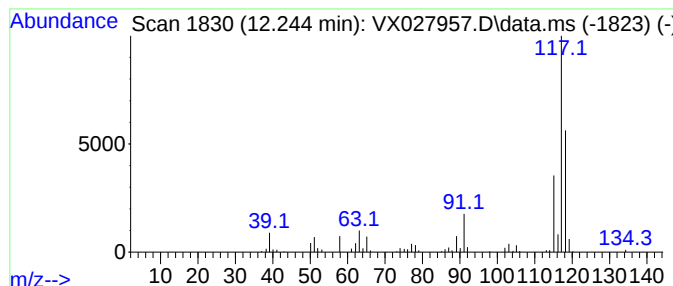
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Quant Title : SW846 8260

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

Peak Number 7 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	12.66 ug/l	89828	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	78
4			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	74
5			Deltacyclene	118	C9H10	007785-10-6	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VO040422\
Data File : VX027957.D
Acq On : 04 Apr 2022 15:01
Operator : JC/MD
Sample : N2249-02 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

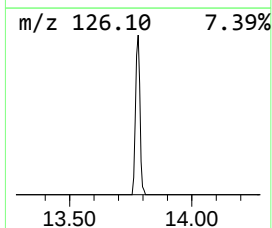
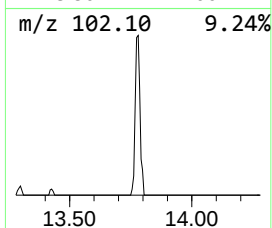
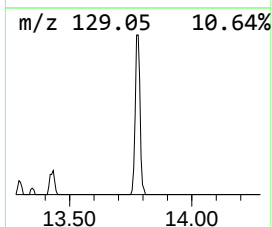
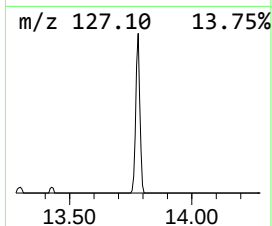
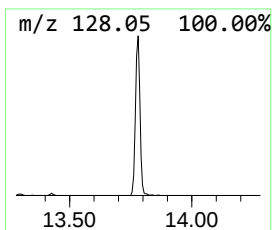
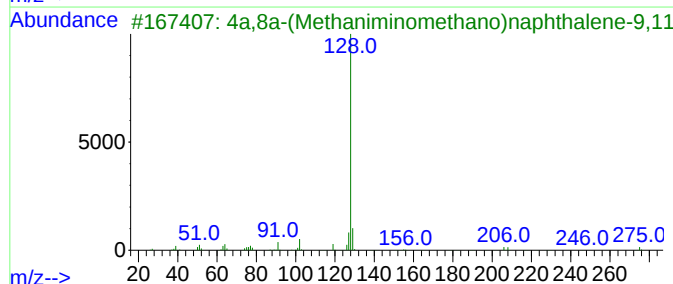
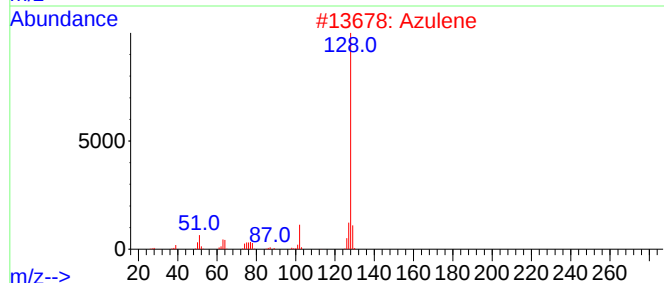
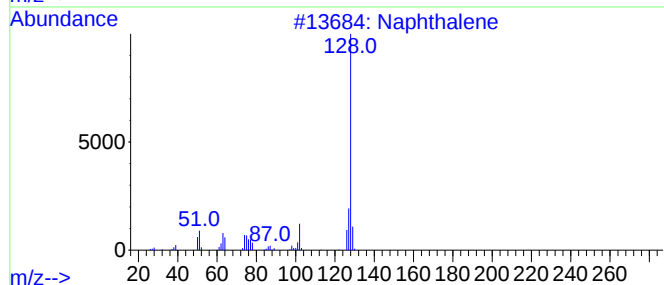
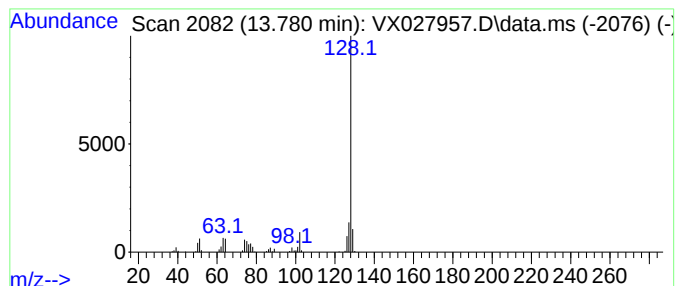
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	11.40 ug/l	80842	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	97
2			Azulene	128	C10H8	000275-51-4	91
3			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	74
4			4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	64
5			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027957.D
Acq On : 04 Apr 2022 15:01
Operator : JC/MD
Sample : N2249-02 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.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
Sulfur dioxide	1.246	10.1	ug/l	58323	1	5.556	290132	50.0
Butane, 2-methyl-	1.752	5.6	ug/l	32566	1	5.556	290132	50.0
Cyclopentane, m...	4.312	8.1	ug/l	46860	1	5.556	290132	50.0
Benzene, 1-ethy...	11.384	26.0	ug/l	184110	4	12.024	354719	50.0
Benzene, 1-ethy...	11.616	14.1	ug/l	100110	4	12.024	354719	50.0
Mesitylene	12.091	16.2	ug/l	114852	4	12.024	354719	50.0
Indane	12.244	12.7	ug/l	89828	4	12.024	354719	50.0
Naphthalene	13.780	11.4	ug/l	80842	4	12.024	354719	50.0