

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
 Data File : VX021572.D
 Acq On : 29 Mar 2021 13:18
 Operator : JC/MD
 Sample : M1785-13 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-2

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\82X032421W.M
 Title : SW846 8260

Signal : TIC: VX021572.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.464	733	744	757	rBV2	48952	139878	26.20%	3.443%
2	5.629	761	772	784	rBV	72597	200993	37.64%	4.947%
3	6.029	829	840	852	rBV	54676	141027	26.41%	3.471%
4	6.829	964	976	989	rBV	120463	287362	53.82%	7.072%
5	8.694	1285	1293	1311	rBV	262253	402047	75.29%	9.895%
6	10.094	1525	1531	1540	rBV	288691	384510	72.01%	9.463%
7	10.235	1549	1555	1560	rBV	20938	28666	5.37%	0.705%
8	10.341	1565	1573	1580	rBV	22113	33548	6.28%	0.826%
9	10.630	1615	1622	1629	rBV5	3319	7941	1.49%	0.195%
10	10.818	1644	1654	1659	rBV2	6501	10887	2.04%	0.268%
11	10.894	1661	1667	1676	rBV6	4887	9225	1.73%	0.227%
12	11.000	1680	1685	1695	rBV	72784	91182	17.08%	2.244%
13	11.118	1700	1705	1711	rVV	236689	311234	58.29%	7.660%
14	11.165	1711	1713	1718	rVB2	4370	5416	1.01%	0.133%
15	11.259	1726	1729	1733	rVB4	4479	5975	1.12%	0.147%
16	11.341	1738	1743	1752	rBV	121998	147130	27.55%	3.621%
17	11.436	1752	1759	1764	rVV	36574	59643	11.17%	1.468%
18	11.488	1764	1768	1777	rVB	14570	20471	3.83%	0.504%
19	11.653	1790	1796	1800	rBV5	4866	7414	1.39%	0.182%
20	11.753	1805	1813	1815	rVV	10768	15447	2.89%	0.380%
21	11.788	1815	1819	1830	rVB	455417	533981	100.00%	13.142%
22	11.900	1830	1838	1840	rBV	16486	22696	4.25%	0.559%
23	11.930	1840	1843	1848	rVB	30927	38018	7.12%	0.936%
24	12.006	1853	1856	1859	rVV	5532	6849	1.28%	0.169%
25	12.059	1859	1865	1871	rVV	303433	391034	73.23%	9.624%
26	12.124	1871	1876	1886	rVB	131020	159573	29.88%	3.927%
27	12.218	1886	1892	1897	rBV	15471	19273	3.61%	0.474%
28	12.283	1897	1903	1910	rBV	112247	143662	26.90%	3.536%
29	12.353	1910	1915	1923	rVB4	20884	43591	8.16%	1.073%
30	12.442	1926	1930	1937	rBV	15270	18765	3.51%	0.462%
31	12.571	1946	1952	1954	rBV	15977	22352	4.19%	0.550%
32	12.594	1954	1956	1960	rVV	15719	16046	3.00%	0.395%
33	12.653	1960	1966	1969	rVV	53380	68803	12.88%	1.693%
34	12.683	1969	1971	1976	rVV	18505	20349	3.81%	0.501%
35	12.742	1976	1981	1988	rVV2	47873	77037	14.43%	1.896%
36	12.883	2000	2005	2009	rVB2	13280	19025	3.56%	0.468%

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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\82X032421W.M
Title : SW846 8260

37	12.959	2009	2018	2022	rVV	27078	35057	6.57%	0.863%
38	13.000	2022	2025	2031	rVB	33901	39942	7.48%	0.983%
39	13.206	2057	2060	2071	rVB3	5355	8275	1.55%	0.204%
40	13.330	2076	2081	2087	rVB2	31973	45537	8.53%	1.121%
41	13.459	2099	2103	2111	rVB	6990	8651	1.62%	0.213%
42	13.818	2159	2164	2169	rVB	11275	14724	2.76%	0.362%

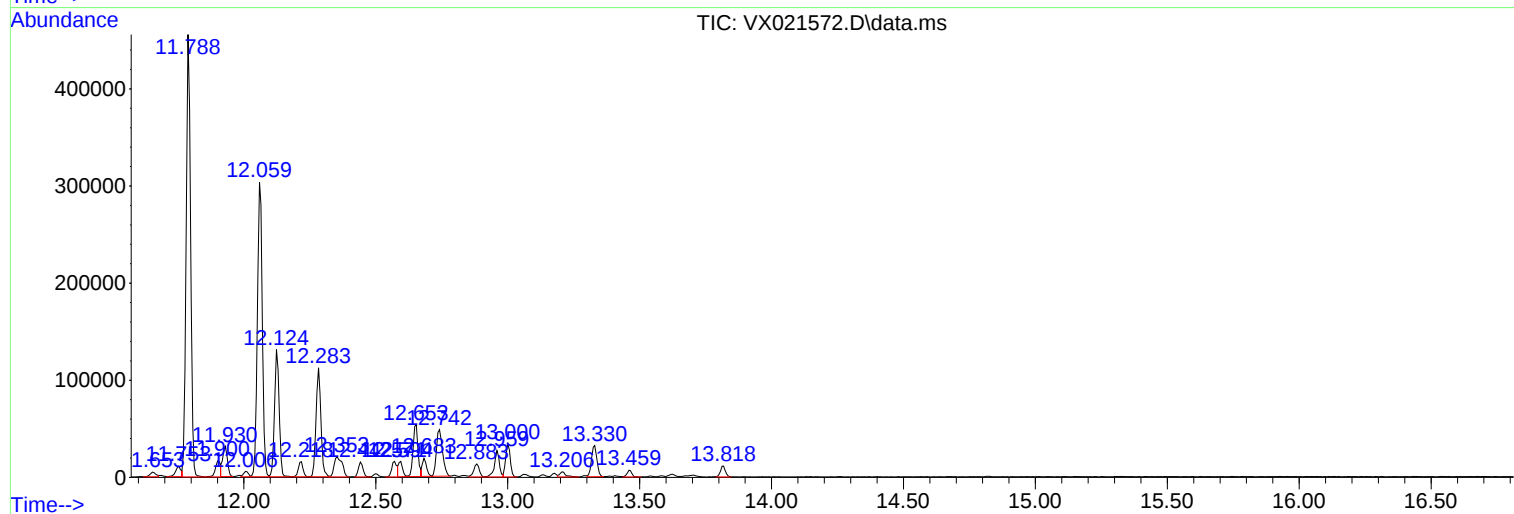
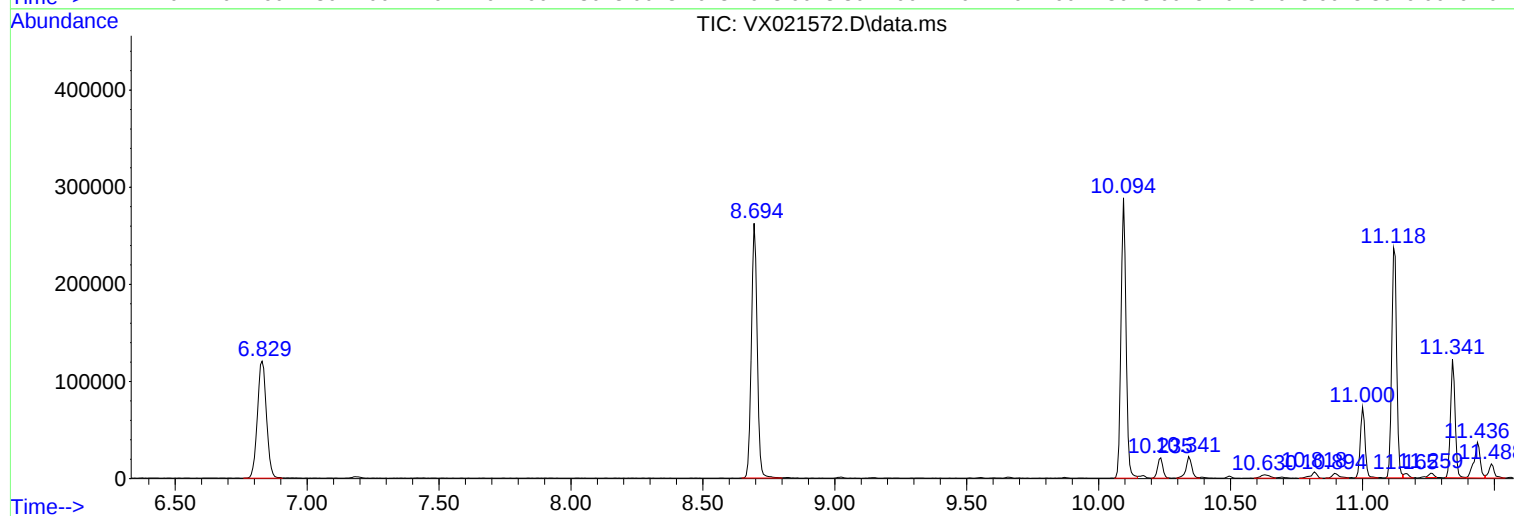
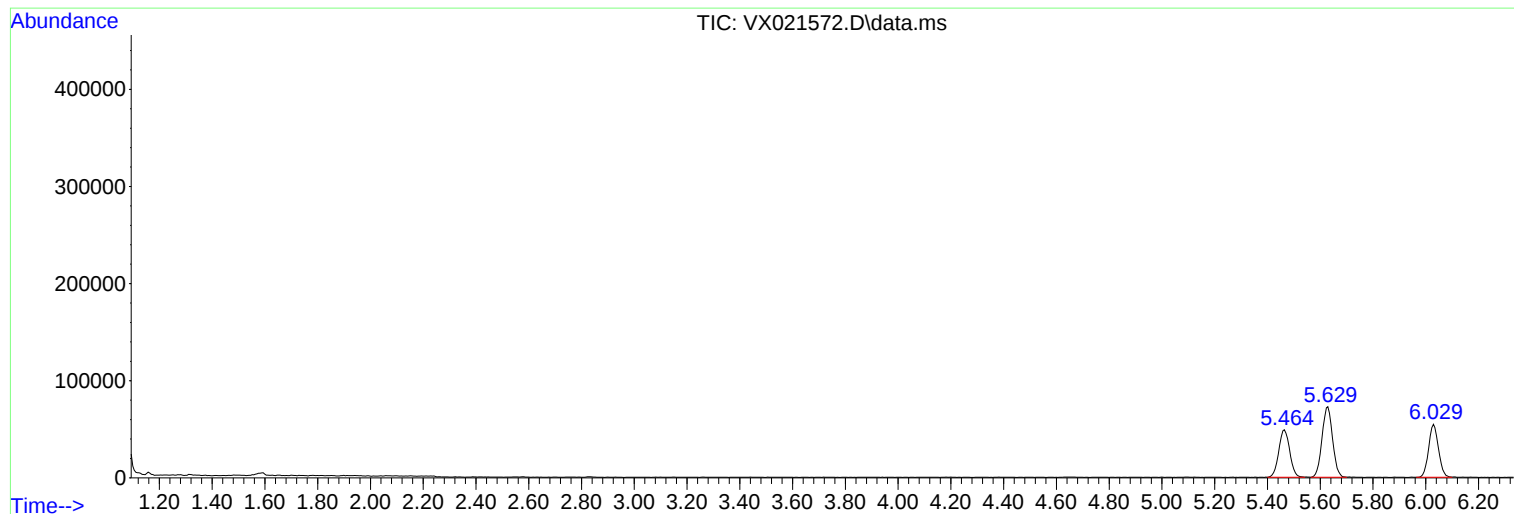
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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



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Instrument :
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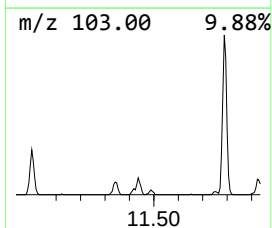
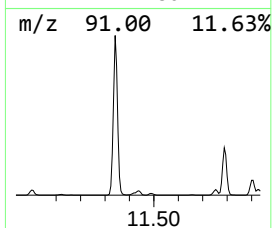
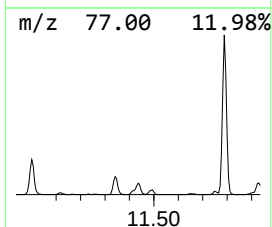
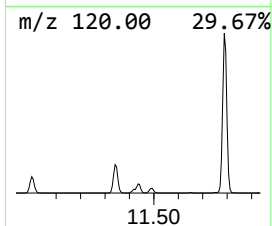
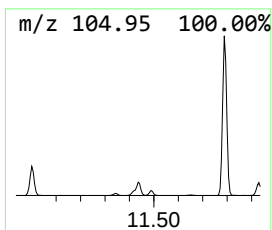
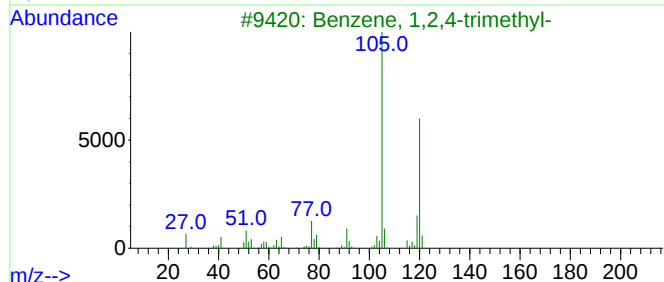
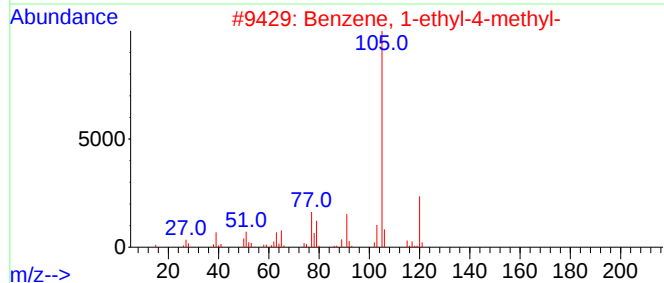
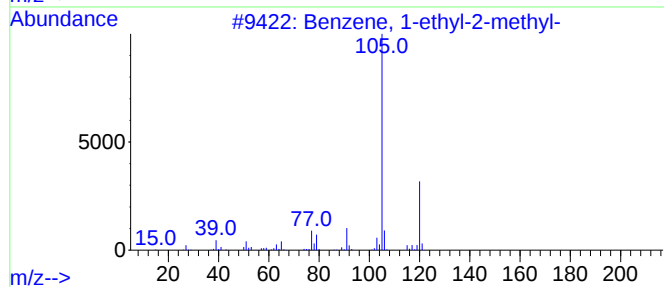
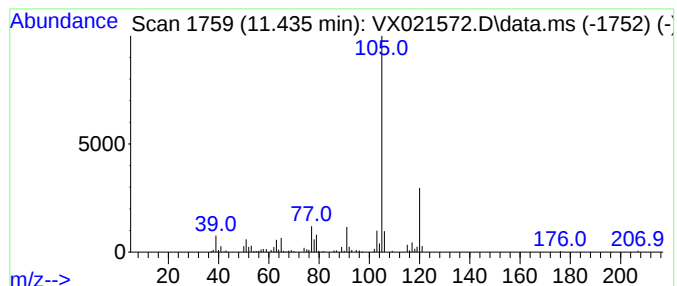
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.435	7.63 ug/l	59643	1,4-Dichlorobenzene-d4	12.065

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-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	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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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

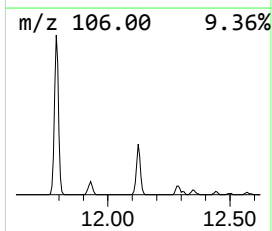
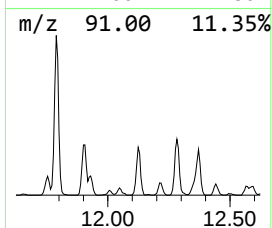
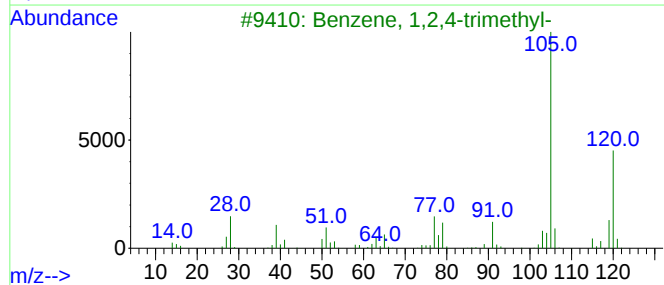
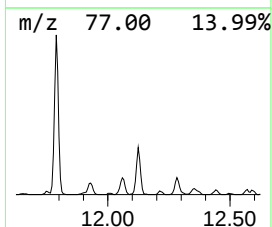
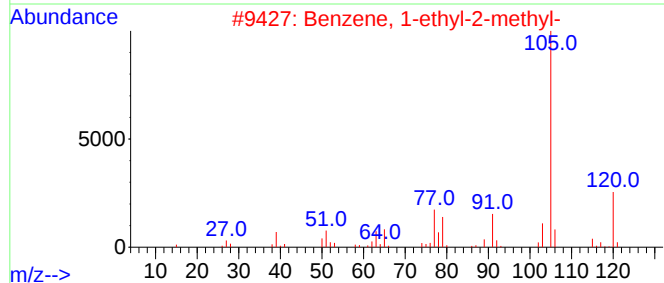
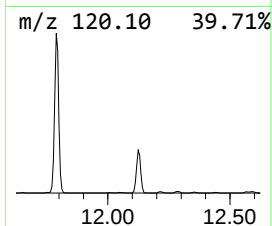
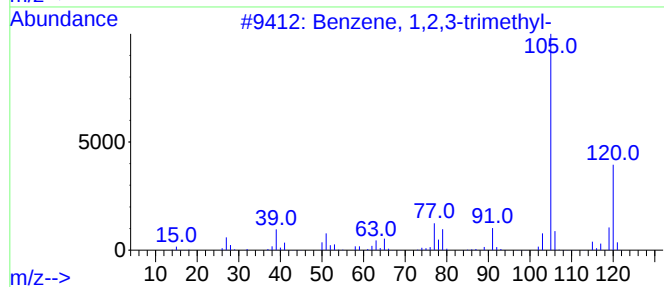
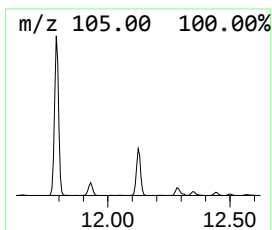
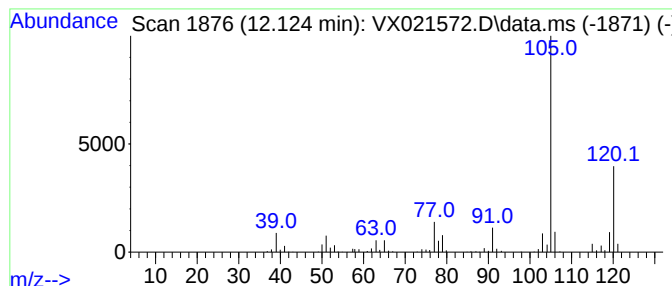
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.124	20.40 ug/l	159573	1,4-Dichlorobenzene-d4	12.065

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
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			Mesitylene	120	C9H12	000108-67-8	91



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Instrument :
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ClientSampleId :
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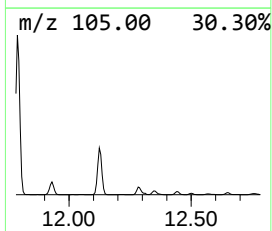
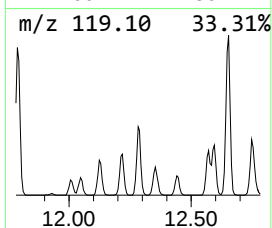
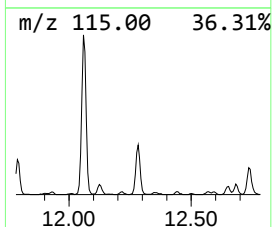
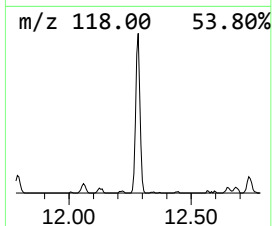
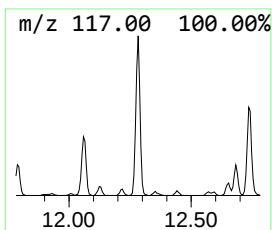
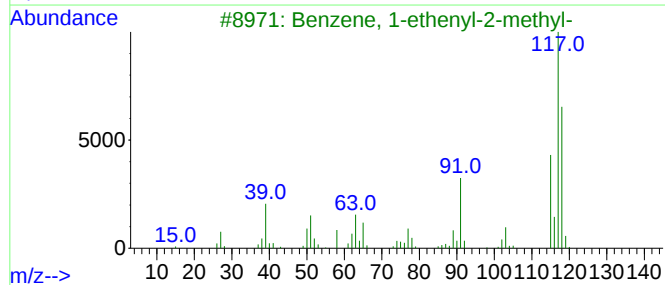
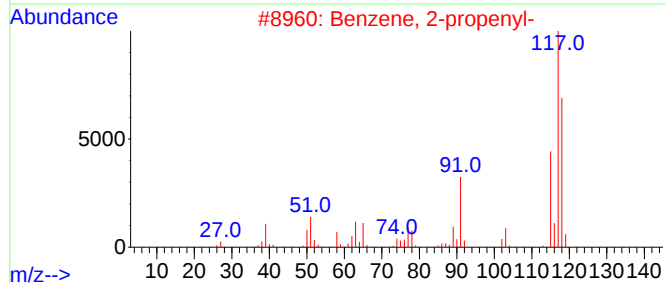
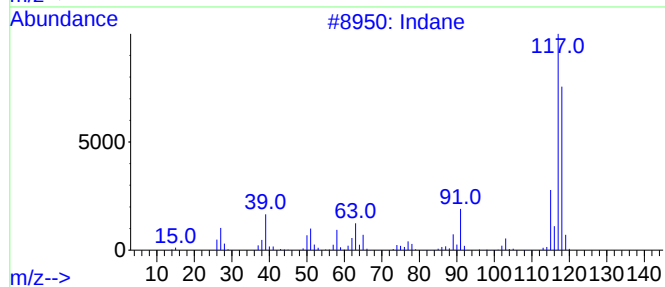
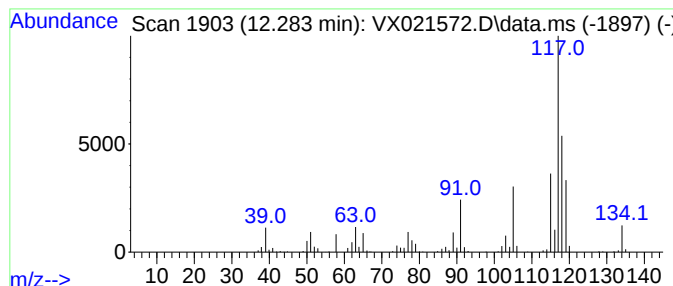
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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

Peak Number 3 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.283	18.37 ug/l	143662	1,4-Dichlorobenzene-d4	12.065

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	86
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	86
4			7-Methylenecycloocta-1,3,5-triene	118	C9H10	002570-13-0	64
5			Deltacyclene	118	C9H10	007785-10-6	64



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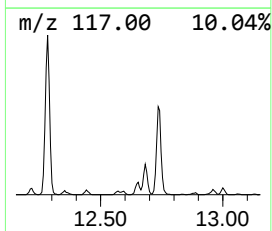
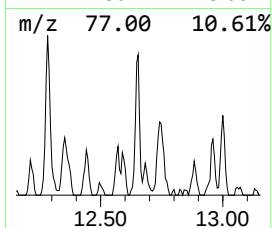
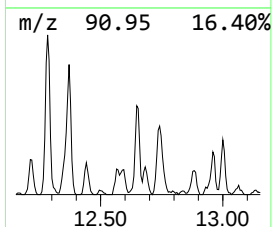
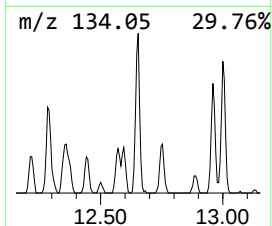
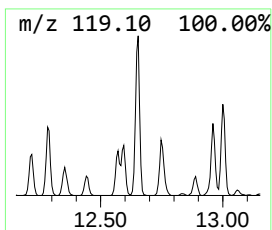
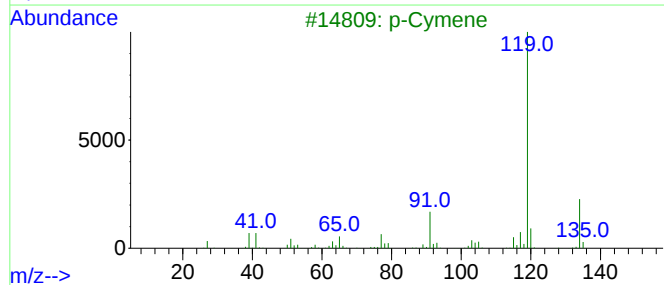
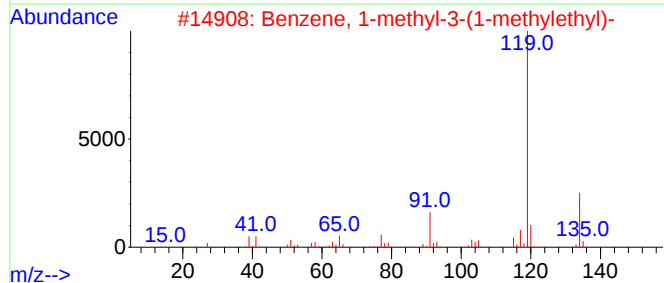
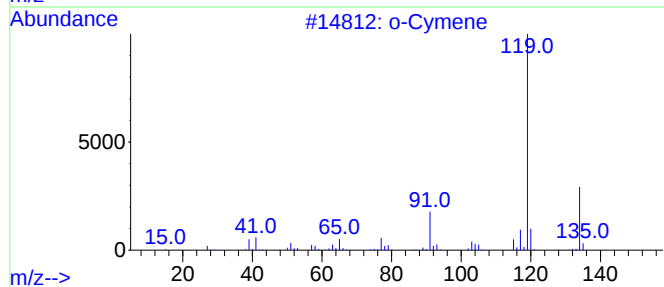
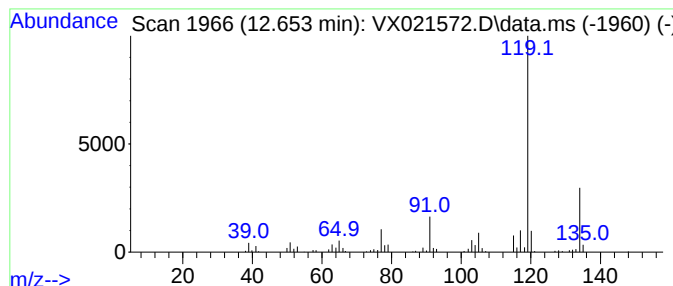
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Quant Title : SW846 8260

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

Peak Number 4 o-Cymene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.653	8.80 ug/l	68803	1,4-Dichlorobenzene-d4	12.065

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	97
2			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	97
3			p-Cymene	134	C10H14	000099-87-6	97
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95



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ClientSampleId :
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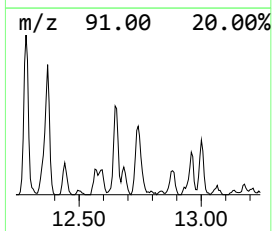
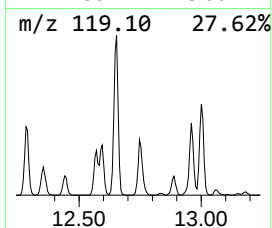
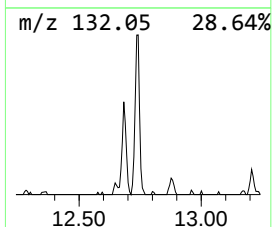
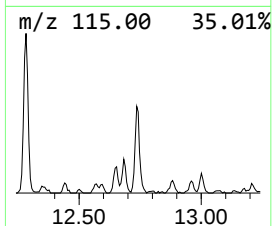
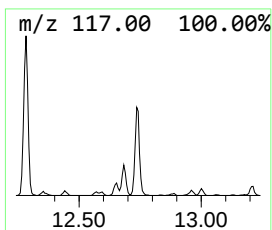
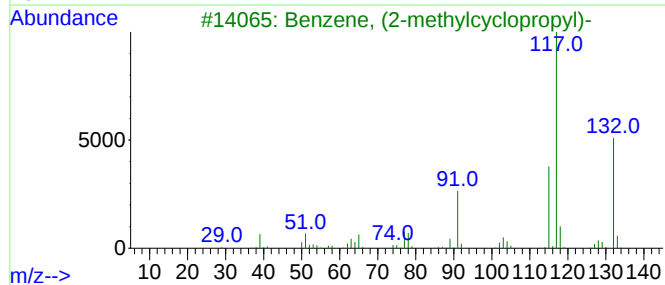
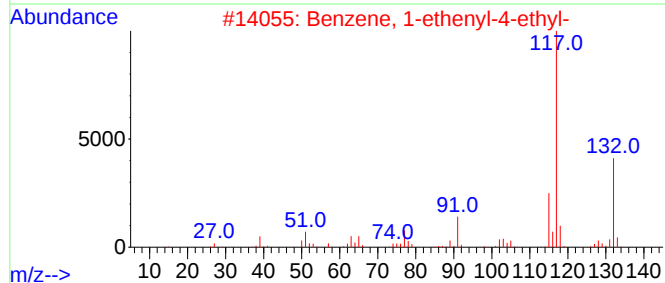
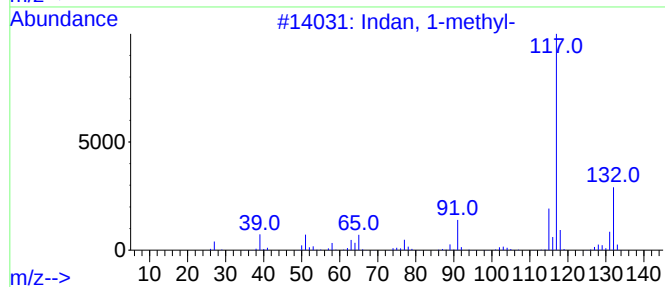
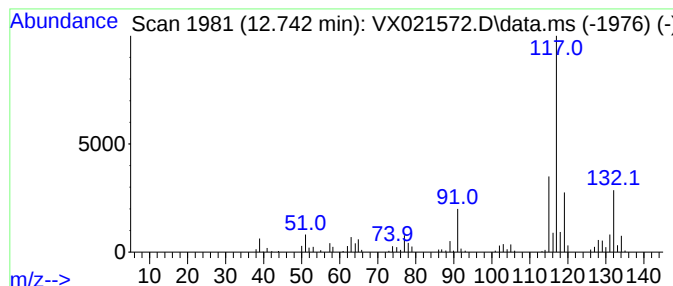
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Quant Title : SW846 8260

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

Peak Number 5 Indan, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.742	9.85 ug/l	77037	1,4-Dichlorobenzene-d4	12.065

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	81
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	76
3			Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	76
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	74
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021572.D
Acq On : 29 Mar 2021 13:18
Operator : JC/MD
Sample : M1785-13 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

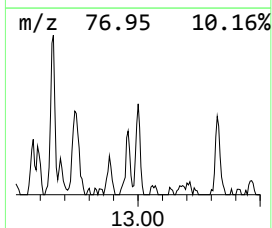
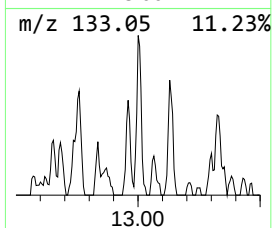
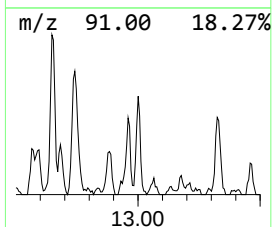
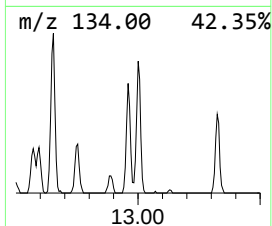
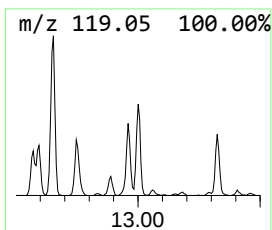
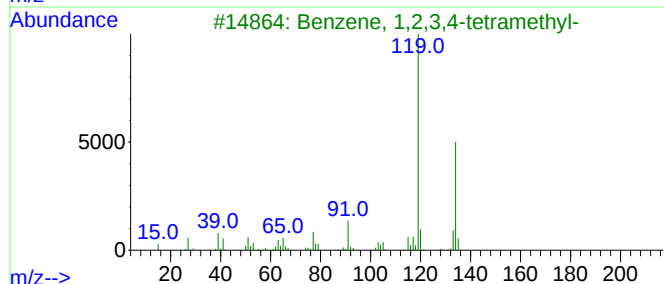
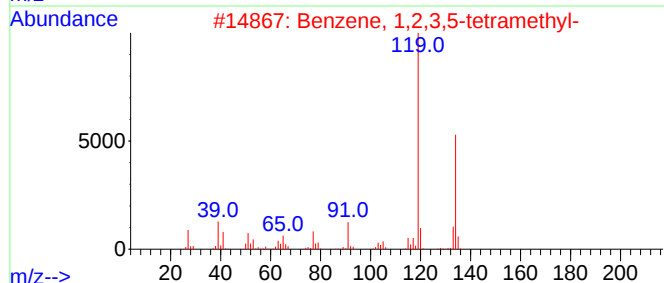
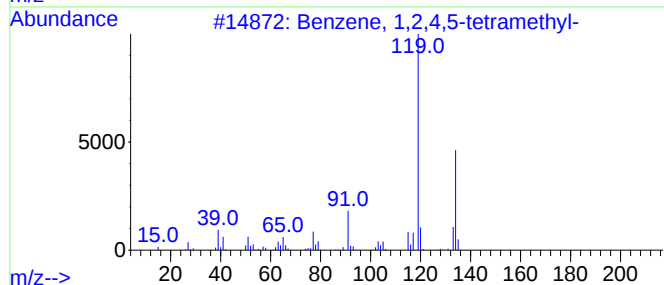
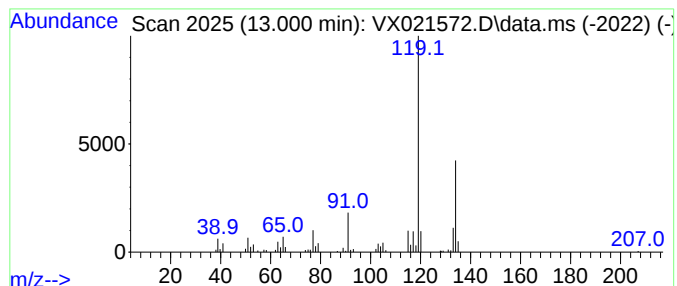
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.000	5.11 ug/l	39942	1,4-Dichlorobenzene-d4	12.065

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021572.D
Acq On : 29 Mar 2021 13:18
Operator : JC/MD
Sample : M1785-13 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

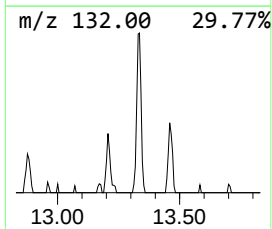
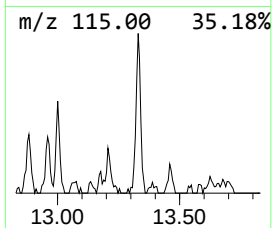
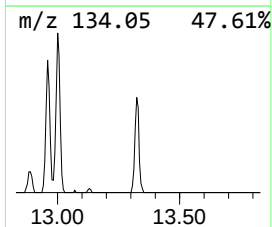
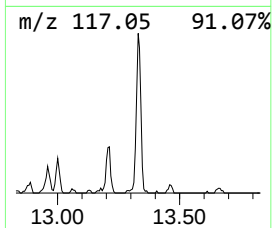
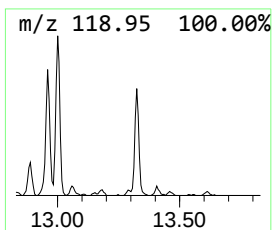
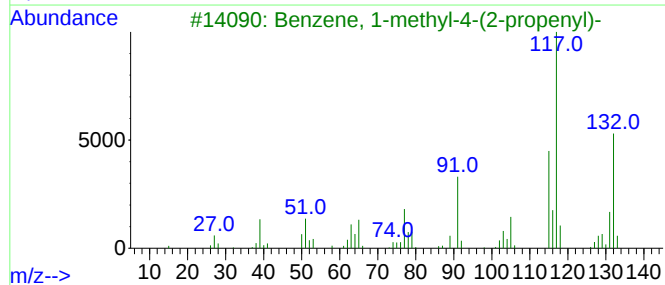
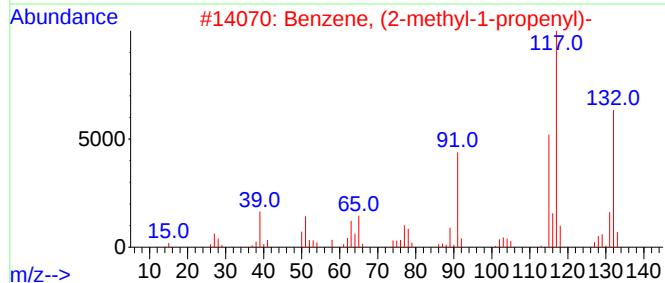
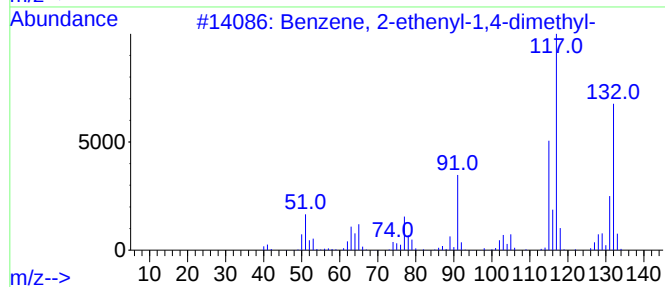
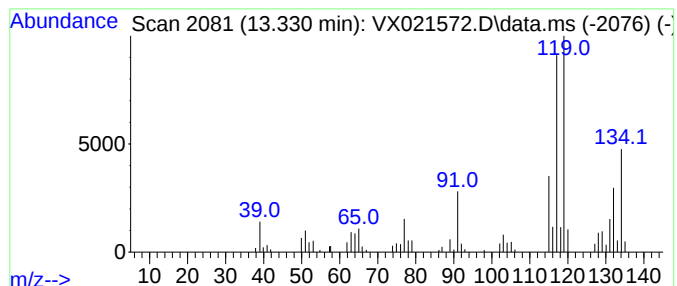
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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

Peak Number 7 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.330	5.82 ug/l	45537	1,4-Dichlorobenzene-d4	12.065

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	87
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	86
3			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	64
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	64
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021572.D
Acq On : 29 Mar 2021 13:18
Operator : JC/MD
Sample : M1785-13 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
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
Benzene, 1-ethy...	11.435	7.6	ug/l	59643	4	12.065	391034	50.0
Benzene, 1,2,3-...	12.124	20.4	ug/l	159573	4	12.065	391034	50.0
Indane	12.283	18.4	ug/l	143662	4	12.065	391034	50.0
o-Cymene	12.653	8.8	ug/l	68803	4	12.065	391034	50.0
Indan, 1-methyl-	12.742	9.8	ug/l	77037	4	12.065	391034	50.0
Benzene, 1,2,4,...	13.000	5.1	ug/l	39942	4	12.065	391034	50.0
Benzene, 2-ethe...	13.330	5.8	ug/l	45537	4	12.065	391034	50.0