

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
 Data File : VN067505.D
 Acq On : 25 Jun 2021 15:31
 Operator : JC/MD
 Sample : M2806-03 10X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-3R

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_N\methods\82N062421W.M
 Title : SW846 8260

Signal : TIC: VN067505.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	77	89	108	rBV4	41529	70780	2.84%	0.475%
2	8.024	2227	2250	2261	rBV	179880	433425	17.40%	2.910%
3	8.088	2261	2274	2298	rVB2	327801	749484	30.09%	5.032%
4	8.440	2382	2405	2432	rBV2	257535	587635	23.59%	3.945%
5	8.971	2584	2603	2631	rBV2	538236	1142635	45.87%	7.671%
6	10.443	3132	3152	3181	rBV	867293	1679662	67.43%	11.276%
7	11.746	3620	3638	3660	rBV	754485	1372148	55.08%	9.212%
8	11.846	3663	3675	3688	rVB2	76365	132217	5.31%	0.888%
9	11.956	3697	3716	3755	rVB2	187506	440452	17.68%	2.957%
10	12.283	3812	3838	3845	rBV5	29319	81390	3.27%	0.546%
11	12.457	3893	3903	3913	rBV5	31165	45943	1.84%	0.308%
12	12.581	3937	3949	3966	rVB	201325	352411	14.15%	2.366%
13	12.733	3991	4006	4024	rBV2	534154	931673	37.40%	6.255%
14	12.814	4024	4036	4048	rVB7	20845	37889	1.52%	0.254%
15	12.921	4059	4076	4090	rBV	292090	505287	20.28%	3.392%
16	12.986	4090	4100	4107	rBV	41706	68658	2.76%	0.461%
17	13.061	4119	4128	4143	rVB	95952	157484	6.32%	1.057%
18	13.297	4203	4216	4219	rBV6	22988	31108	1.25%	0.209%
19	13.372	4230	4244	4264	rVB	1501768	2491125	100.00%	16.724%
20	13.500	4275	4292	4304	rBV3	140158	299754	12.03%	2.012%
21	13.562	4304	4315	4326	rVB	45524	77392	3.11%	0.520%
22	13.677	4343	4358	4365	rBV	590201	1080896	43.39%	7.256%
23	13.774	4384	4394	4406	rVB3	43582	70191	2.82%	0.471%
24	13.841	4406	4419	4424	rBV2	120017	184624	7.41%	1.239%
25	13.879	4424	4433	4444	rVB2	212259	339175	13.62%	2.277%
26	14.005	4468	4480	4493	rVB3	61811	100735	4.04%	0.676%
27	14.131	4514	4527	4533	rBV3	85327	139699	5.61%	0.938%
28	14.219	4549	4560	4572	rVB	192896	298600	11.99%	2.005%
29	14.281	4572	4583	4589	rBV2	45586	70534	2.83%	0.474%
30	14.329	4590	4601	4613	rVB4	167981	295710	11.87%	1.985%
31	14.466	4638	4652	4662	rBV4	51692	85925	3.45%	0.577%
32	14.541	4662	4680	4687	rBV	61207	106983	4.29%	0.718%
33	14.581	4687	4695	4705	rVB2	79058	120055	4.82%	0.806%
34	14.812	4771	4781	4791	rBV6	17452	29804	1.20%	0.200%
35	14.922	4806	4822	4838	rBV4	93924	200263	8.04%	1.344%
36	15.086	4871	4883	4898	rVB4	34141	58143	2.33%	0.390%

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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-3R

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_N\methods\82N062421W.M
Title : SW846 8260

37	15.507	5025	5040	5055	rVB2	14555	25708	1.03%	0.173%
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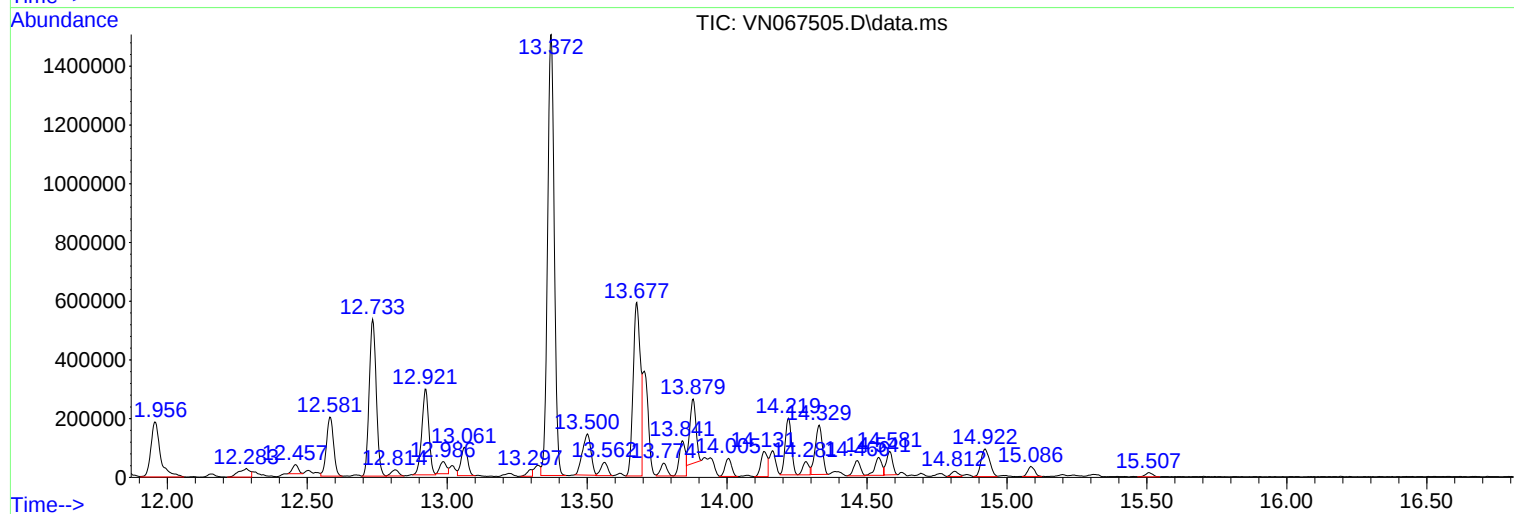
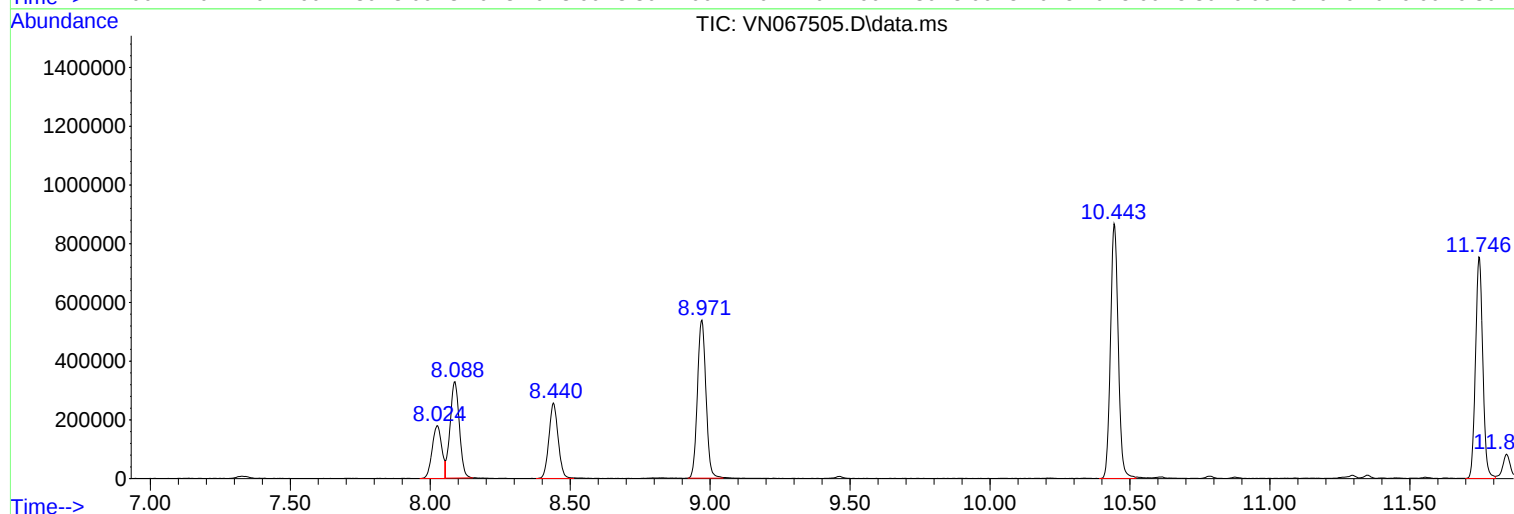
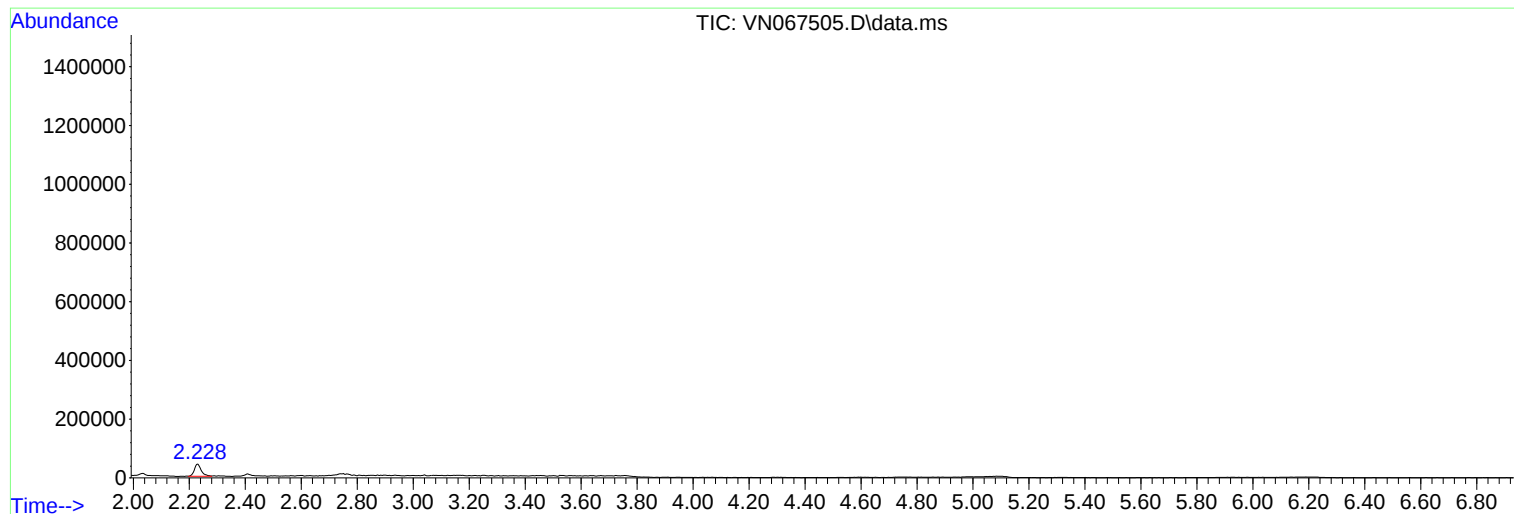
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_N
ClientSampleId :
MW-3R

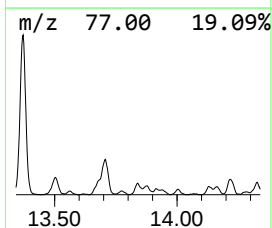
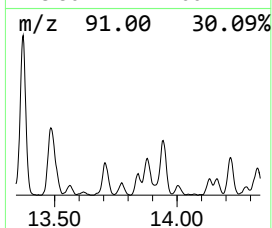
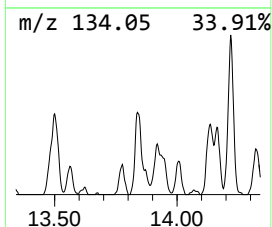
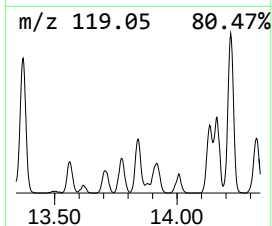
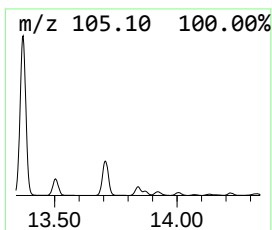
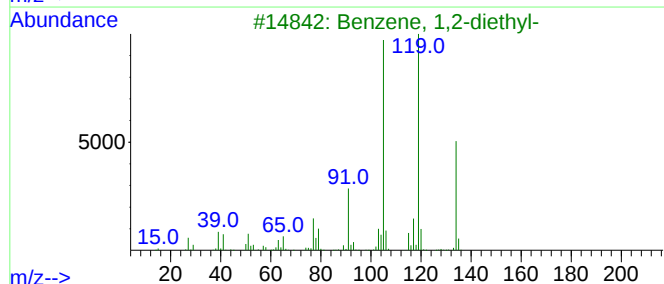
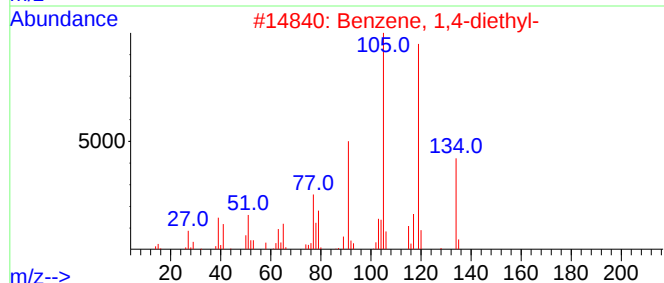
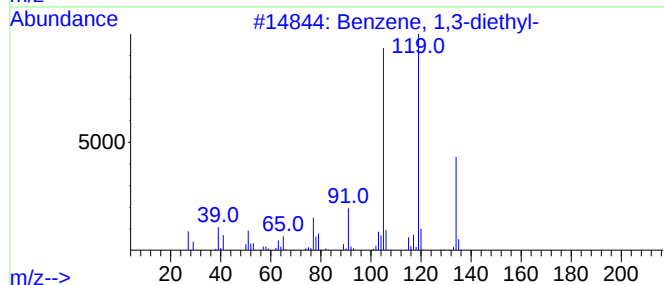
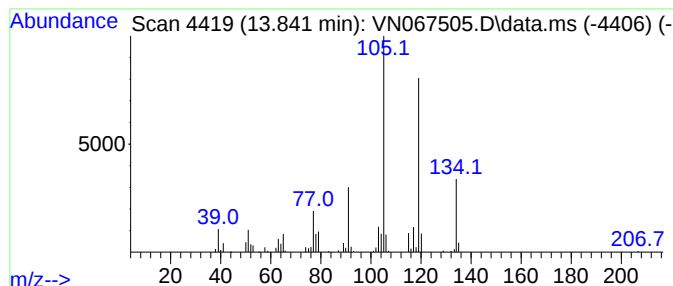
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1,3-diethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.841	8.54 ug/l	184624	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	97
2			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	96
3			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
4			o-Cymene	134	C10H14	000527-84-4	93
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	87



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3R

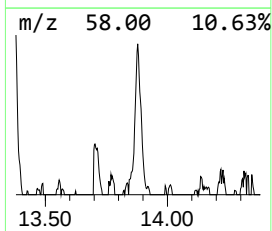
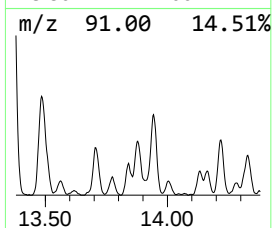
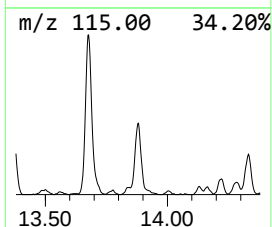
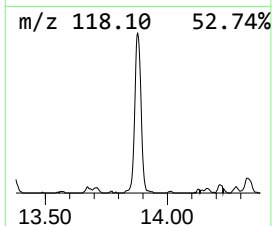
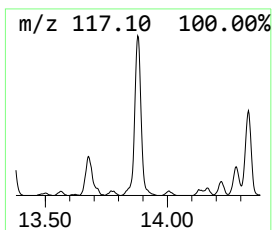
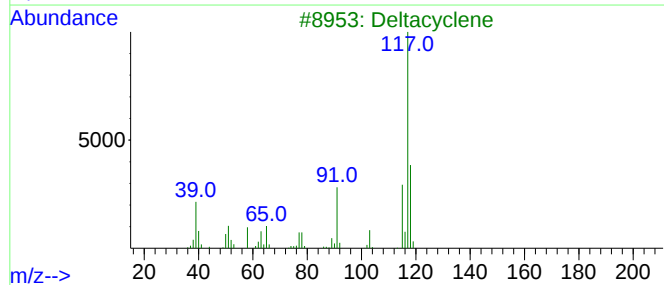
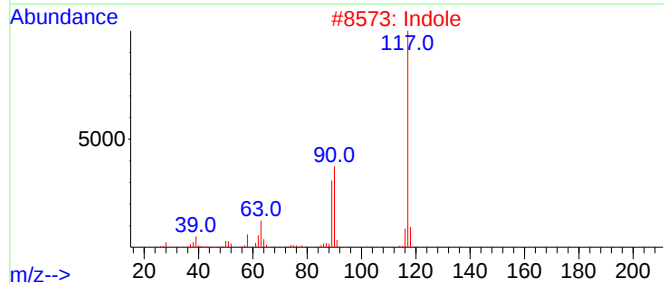
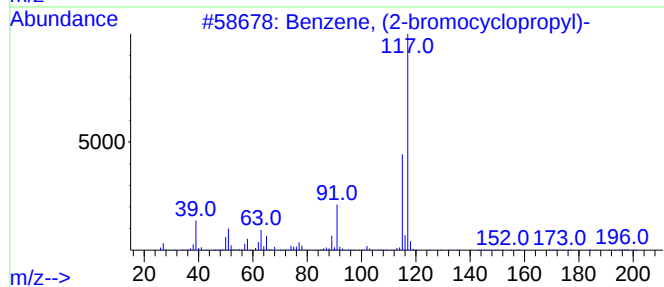
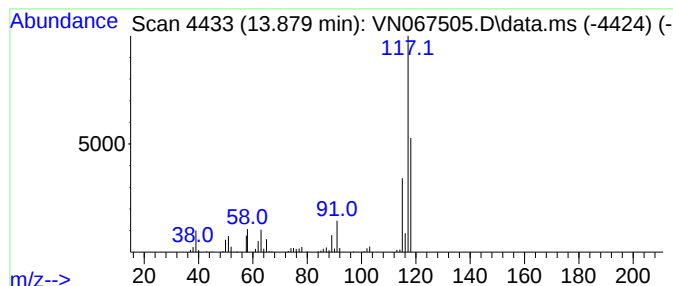
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, (2-bromocyclopropyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.879	15.69 ug/l	339175	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	53
2			Indole	117	C8H7N	000120-72-9	49
3			Deltacyclene	118	C9H10	007785-10-6	45
4			1,3-Methanopentalene, 1,2,3,5-te...	118	C9H10	128600-88-4	45
5			Benzyl nitrile	117	C8H7N	000140-29-4	43



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3R

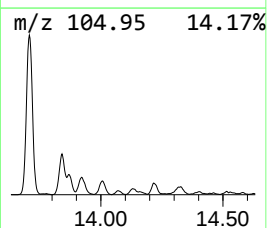
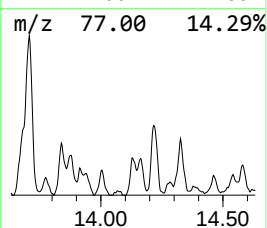
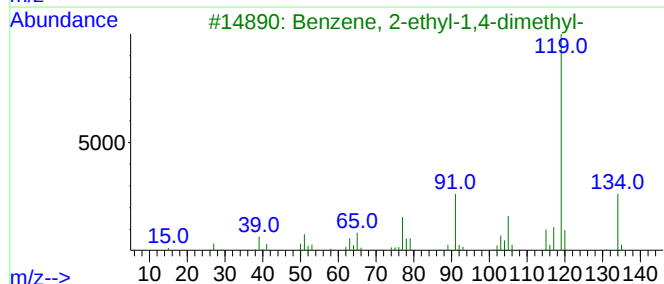
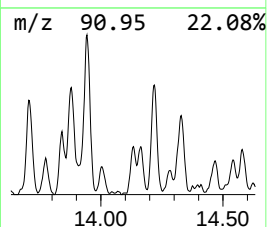
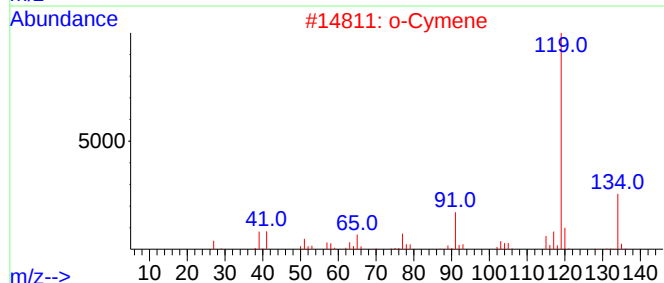
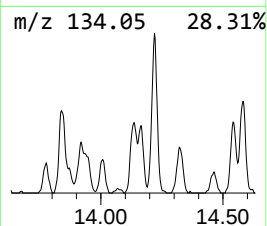
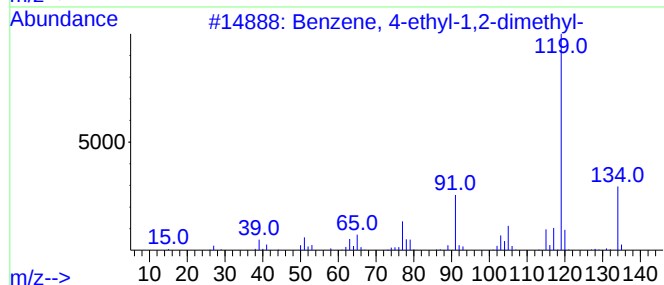
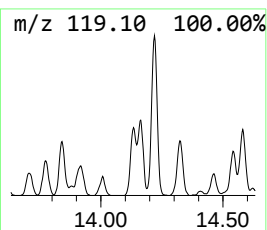
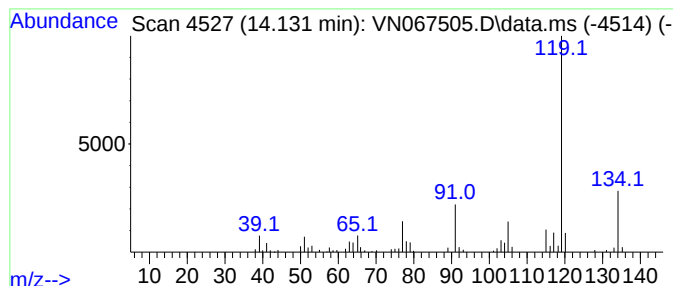
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.131	6.46 ug/l	139699	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
2			o-Cymene	134	C10H14	000527-84-4	94
3			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
4			p-Cymene	134	C10H14	000099-87-6	93
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93



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Instrument :
MSVOA_N
ClientSampleId :
MW-3R

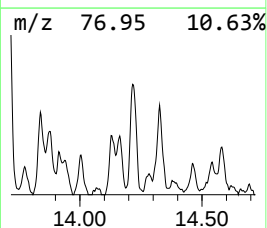
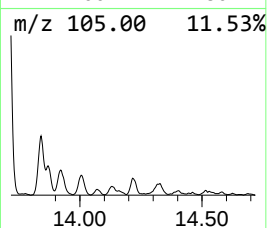
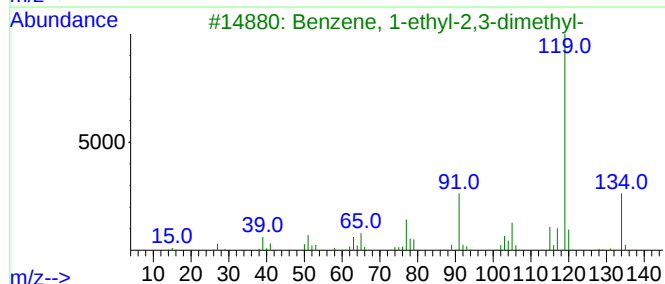
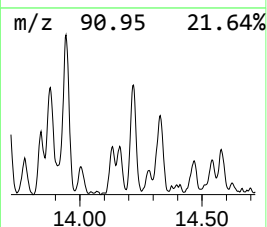
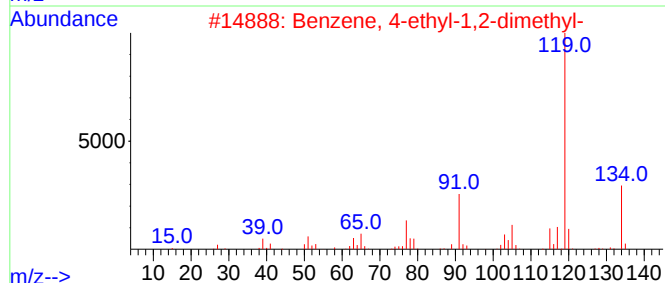
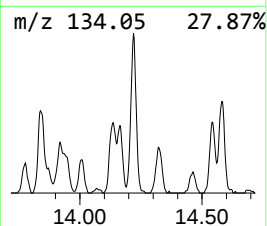
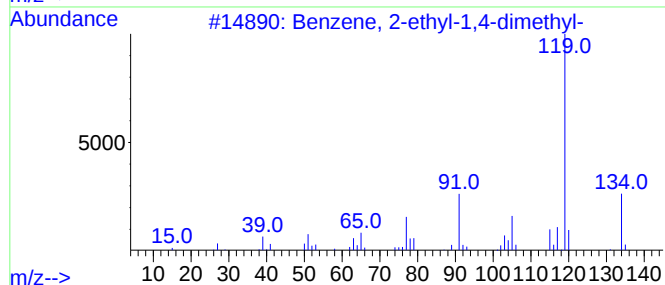
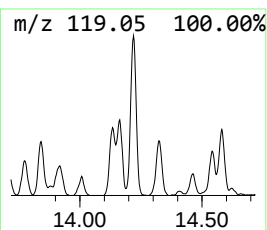
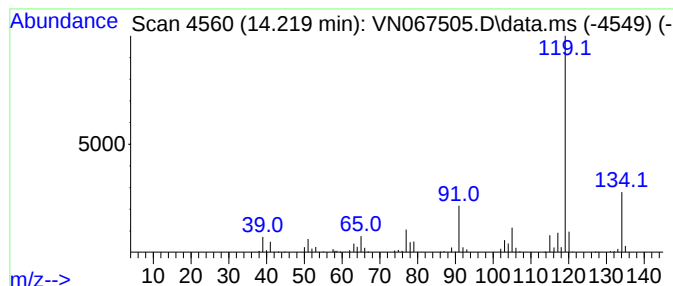
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.219	13.81 ug/l	298600	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
4			o-Cymene	134	C10H14	000527-84-4	95
5			p-Cymene	134	C10H14	000099-87-6	95



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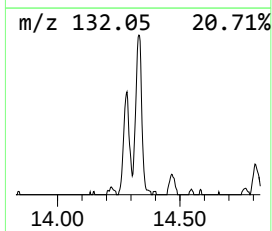
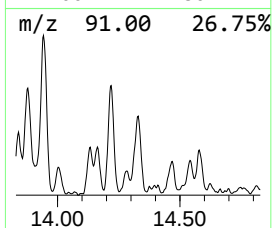
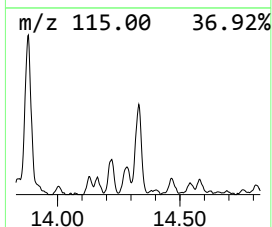
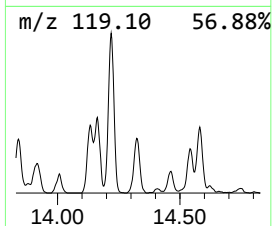
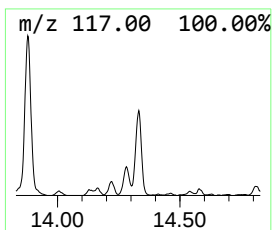
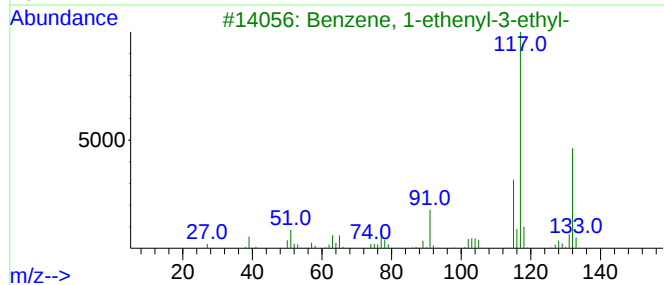
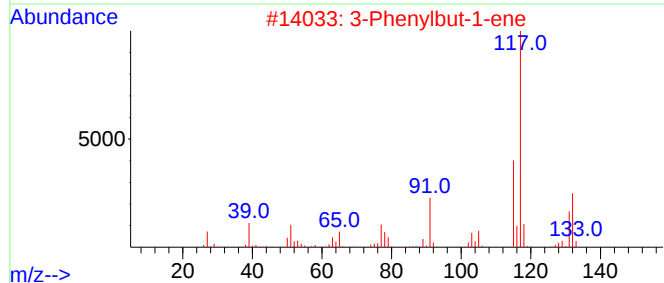
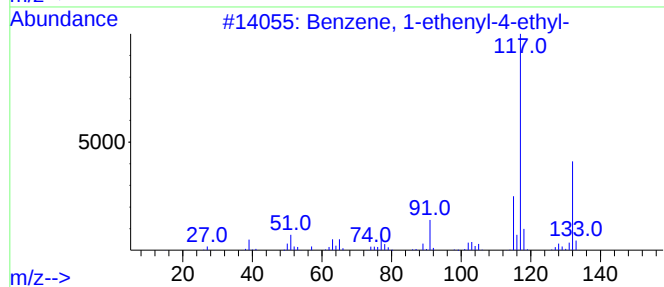
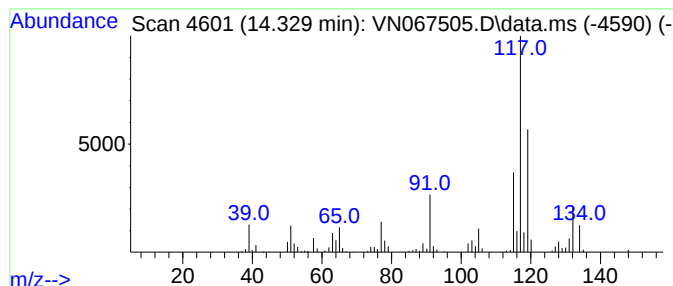
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	13.68 ug/l	295710	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	70
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	64
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	62
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	62
5			Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067505.D
Acq On : 25 Jun 2021 15:31
Operator : JC/MD
Sample : M2806-03 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3R

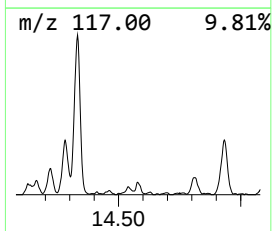
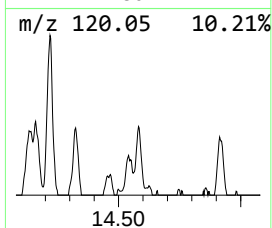
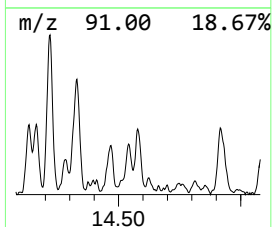
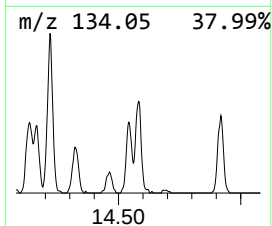
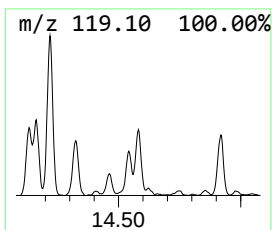
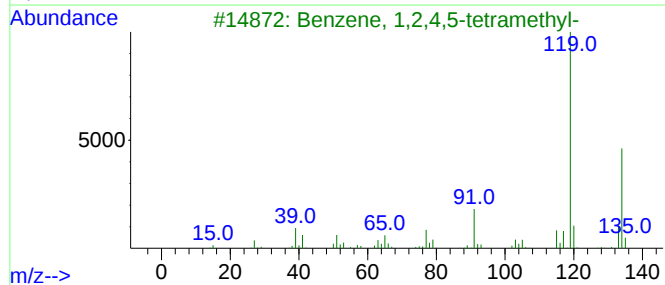
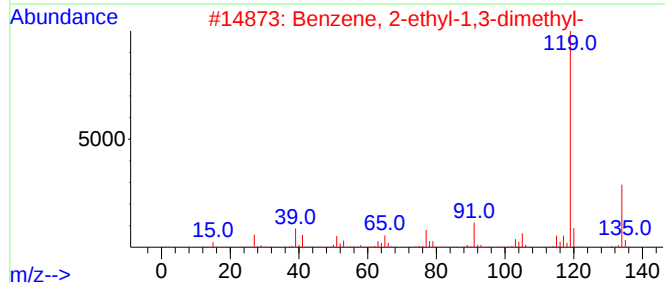
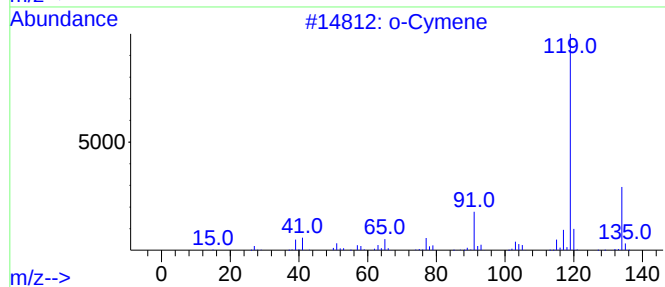
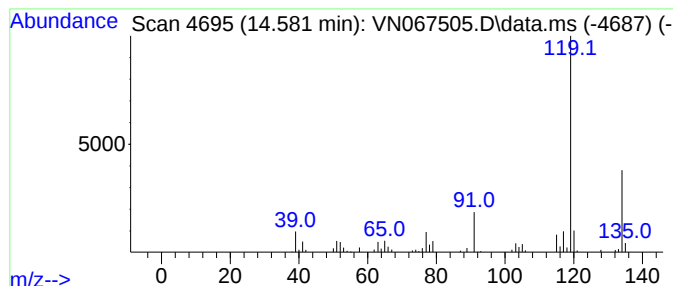
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Quant Title : SW846 8260

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

Peak Number 6 o-Cymene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.581	5.55 ug/l	120055	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	94
2			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	93
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91
5			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067505.D
Acq On : 25 Jun 2021 15:31
Operator : JC/MD
Sample : M2806-03 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3R

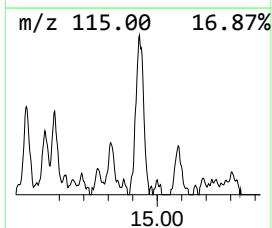
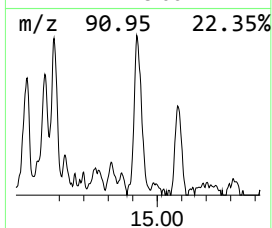
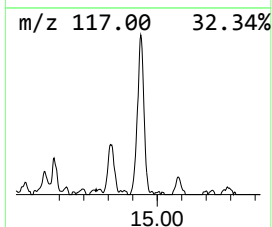
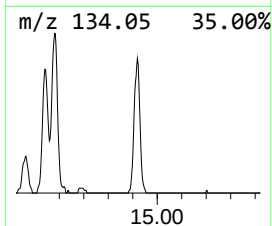
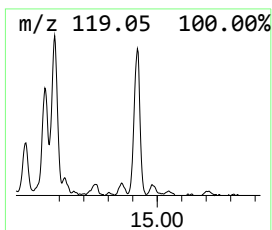
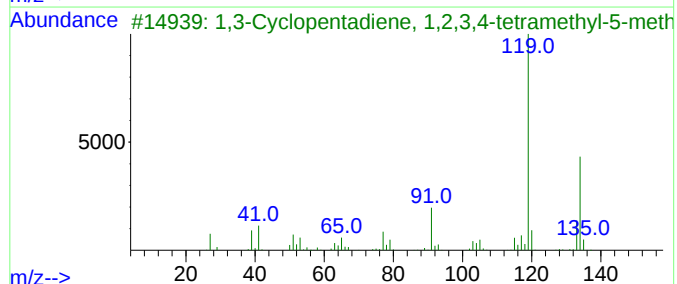
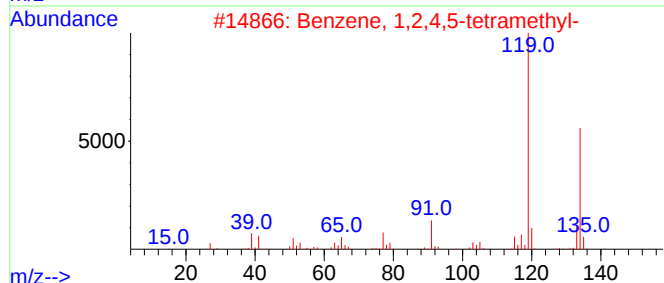
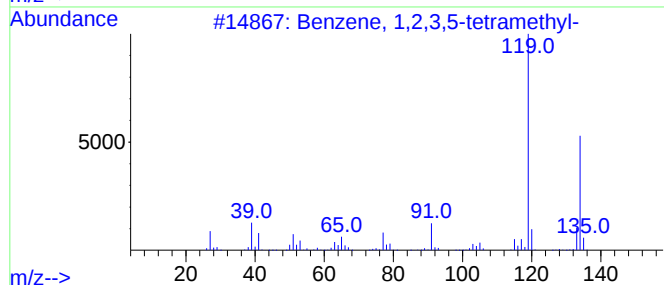
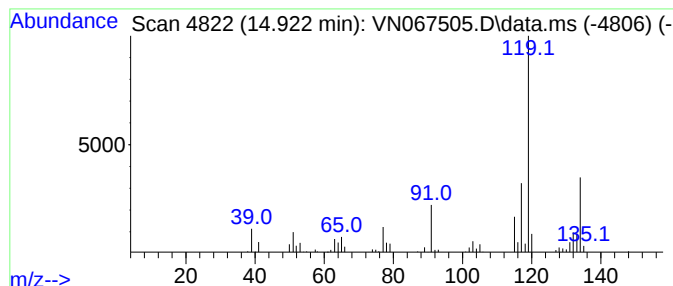
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.922	9.26 ug/l	200263	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	81
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	81
3			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	74
4			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	74
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067505.D
Acq On : 25 Jun 2021 15:31
Operator : JC/MD
Sample : M2806-03 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.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, 1,3-di...	13.841	8.5	ug/l	184624	4	13.675	1080900	50.0
Benzene, (2-bro...	13.879	15.7	ug/l	339175	4	13.675	1080900	50.0
Benzene, 4-ethy...	14.131	6.5	ug/l	139699	4	13.675	1080900	50.0
Benzene, 2-ethy...	14.219	13.8	ug/l	298600	4	13.675	1080900	50.0
Benzene, 1-ethe...	14.329	13.7	ug/l	295710	4	13.675	1080900	50.0
o-Cymene	14.581	5.5	ug/l	120055	4	13.675	1080900	50.0
Benzene, 1,2,3,...	14.922	9.3	ug/l	200263	4	13.675	1080900	50.0