

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082123\
 Data File : VX037143.D
 Acq On : 21 Aug 2023 20:07
 Operator : JC/MD
 Sample : 04014-04 10X
 Misc : 7.77g/5.0mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 NEVINS-SB06-Z84-85

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\82X081723W.M
 Title : SW846 8260

Signal : TIC: VX037143.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.038	804	812	828	rVB	1164295	3089054	6.65%	1.535%
2	6.763	921	931	943	rBV	259518	620572	1.34%	0.308%
3	8.647	1234	1240	1247	rBV	567213	886446	1.91%	0.441%
4	10.055	1466	1471	1476	rBV	549491	729494	1.57%	0.363%
5	10.195	1488	1494	1500	rBV	8457422	11317550	24.35%	5.624%
6	10.299	1504	1511	1518	rVV	4481181	6079125	13.08%	3.021%
7	10.640	1562	1567	1582	rVB	2708825	3496313	7.52%	1.737%
8	10.964	1614	1620	1628	rBV	961245	1222805	2.63%	0.608%
9	11.079	1634	1639	1650	rBV	518094	670208	1.44%	0.333%
10	11.305	1671	1676	1683	rBV	396596	467889	1.01%	0.233%
11	11.378	1683	1688	1690	rBV	4101198	5429429	11.68%	2.698%
12	11.451	1696	1700	1712	rVB	1028542	1290291	2.78%	0.641%
13	11.610	1721	1726	1734	rBV	1111068	1432762	3.08%	0.712%
14	11.750	1740	1749	1754	rBV	3821322	4951244	10.65%	2.460%
15	11.811	1754	1759	1764	rVB	609320	740750	1.59%	0.368%
16	11.969	1777	1785	1788	rBV	505591	657478	1.41%	0.327%
17	12.018	1788	1793	1799	rVV2	785584	1205475	2.59%	0.599%
18	12.085	1799	1804	1808	rVV	1467907	1783400	3.84%	0.886%
19	12.134	1808	1812	1816	rVB	610941	736461	1.58%	0.366%
20	12.244	1824	1830	1837	rBV	14460468	19235216	41.39%	9.559%
21	12.317	1837	1842	1847	rVV2	1512073	1925599	4.14%	0.957%
22	12.555	1878	1881	1885	rVB	483280	601340	1.29%	0.299%
23	12.610	1885	1890	1894	rBV	1712783	2098055	4.51%	1.043%
24	12.695	1900	1904	1910	rBV	534772	909587	1.96%	0.452%
25	12.750	1910	1913	1917	rVB	527458	606198	1.30%	0.301%
26	12.792	1917	1920	1924	rBV	413887	469749	1.01%	0.233%
27	12.963	1944	1948	1953	rBV	804675	964405	2.08%	0.479%
28	13.170	1977	1982	1986	rVB	1266137	1540118	3.31%	0.765%
29	13.286	1992	2001	2006	rBV2	1261835	1919996	4.13%	0.954%
30	13.341	2006	2010	2016	rVV	3916043	4569910	9.83%	2.271%
31	13.427	2018	2024	2029	rVV	5735757	7444938	16.02%	3.700%
32	13.500	2033	2036	2040	rVV	618172	771830	1.66%	0.384%
33	13.548	2040	2044	2048	rVV	465177	683307	1.47%	0.340%
34	13.792	2074	2084	2088	rBV	25902335	46471394	100.00%	23.094%
35	13.872	2091	2097	2101	rVV	1167945	1613938	3.47%	0.802%
36	14.097	2131	2134	2137	rVV	712827	878807	1.89%	0.437%

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Stop Thrs : 0

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	14.134	2137	2140	2145	rVV2	364038	643470	1.38%	0.320%
38	14.219	2149	2154	2157	rBV	827806	1140455	2.45%	0.567%
39	14.256	2157	2160	2164	rVB	406121	550902	1.19%	0.274%
40	14.317	2164	2170	2177	rBV	855705	1452087	3.12%	0.722%
41	14.524	2200	2204	2211	rVB2	426239	657702	1.42%	0.327%
42	14.597	2211	2216	2218	rVV	404509	504162	1.08%	0.251%
43	14.640	2218	2223	2233	rVV	13524876	17986978	38.71%	8.938%
44	14.786	2240	2247	2258	rVB	12677649	17665451	38.01%	8.779%
45	15.207	2308	2316	2321	rBV	1412850	1979456	4.26%	0.984%
46	15.371	2331	2343	2347	rBV	2467092	3829564	8.24%	1.903%
47	15.475	2354	2360	2365	rBV	2250936	3559224	7.66%	1.769%
48	15.615	2377	2383	2386	rBV	2607491	4055118	8.73%	2.015%
49	15.652	2386	2389	2395	rVB	1326662	1873638	4.03%	0.931%
50	15.835	2409	2419	2424	rBV	662890	1791120	3.85%	0.890%
51	15.987	2437	2444	2454	rVB	418647	755537	1.63%	0.375%
52	16.322	2491	2499	2508	rBV	1720204	3274636	7.05%	1.627%

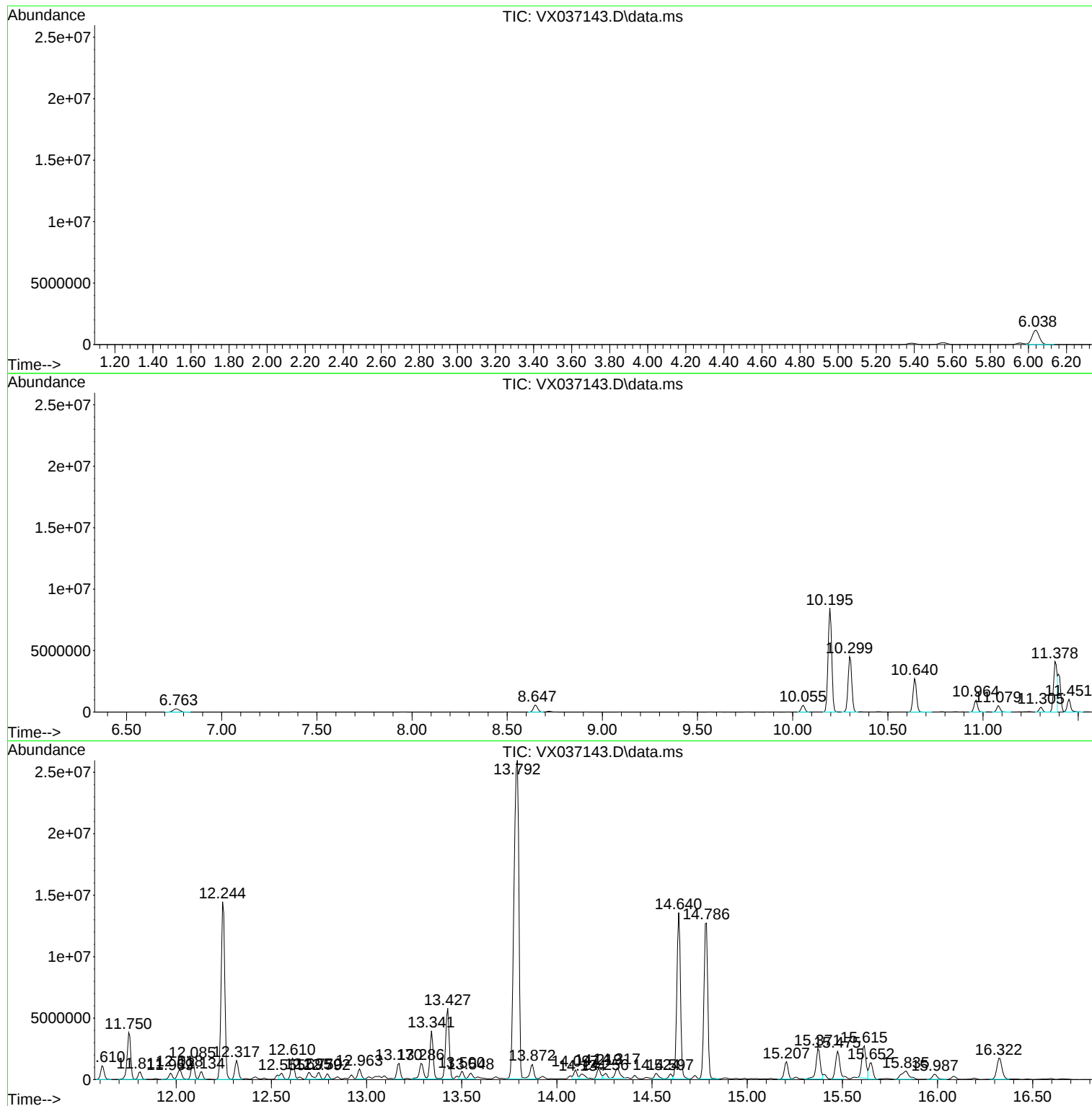
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ClientSampleId :
NEVINS-SB06-Z84-85

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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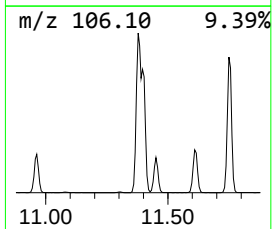
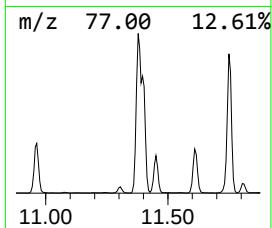
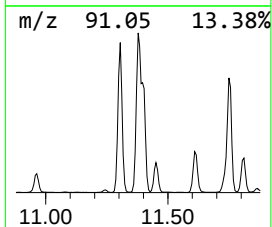
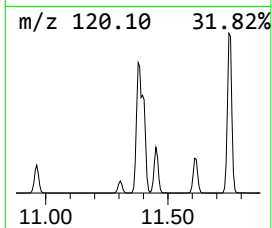
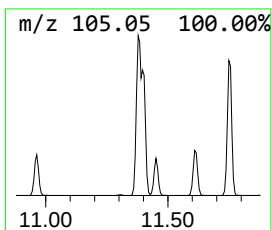
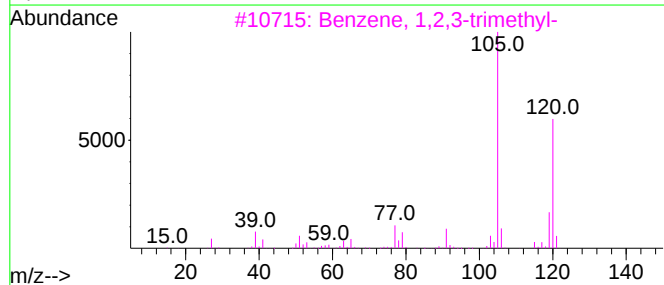
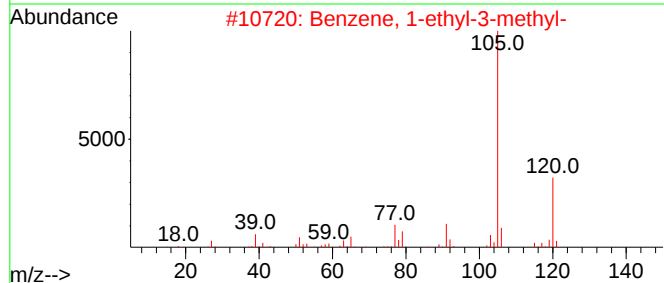
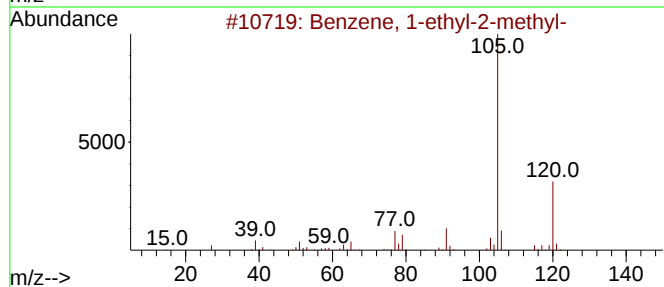
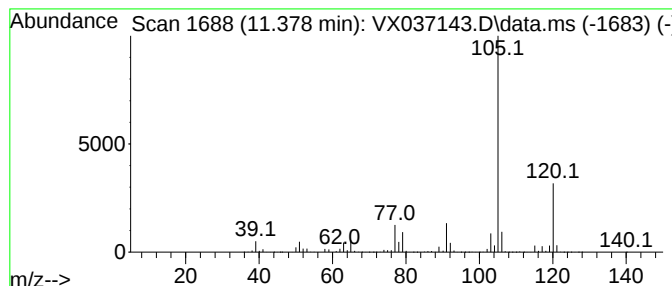
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	225.20 ug/l	5429430	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	95
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NEVINS-SB06-Z84-85

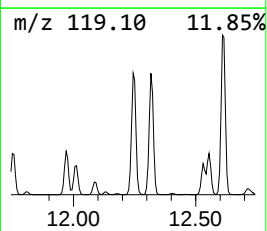
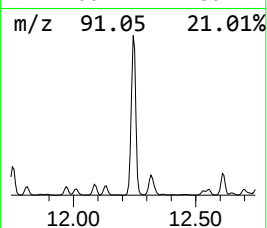
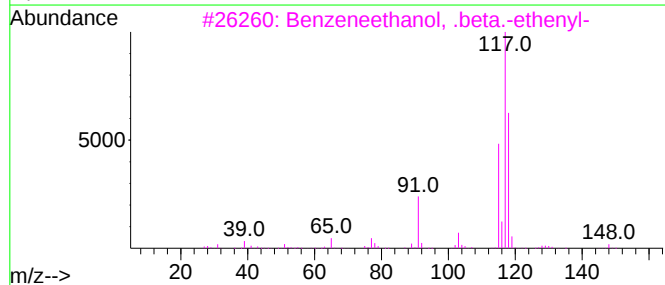
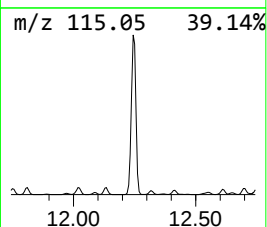
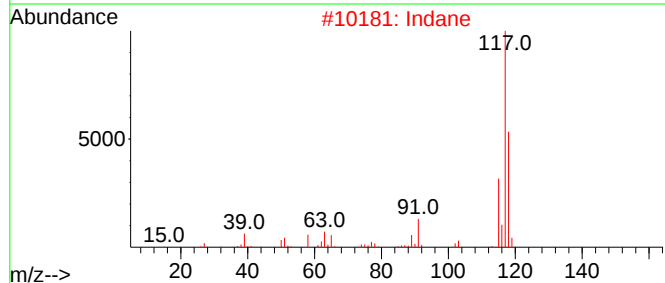
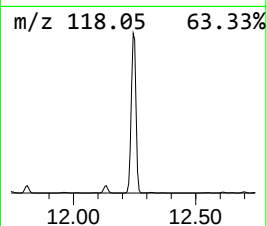
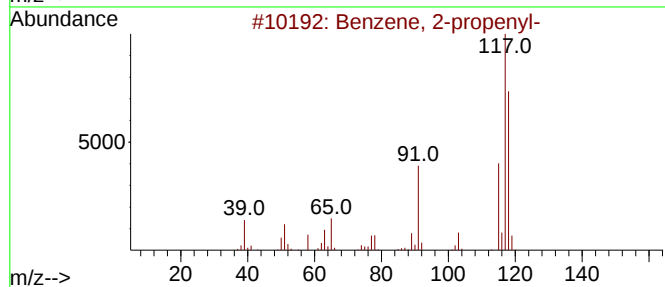
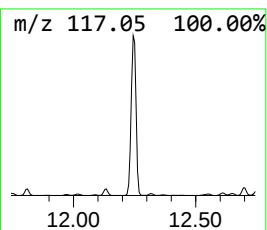
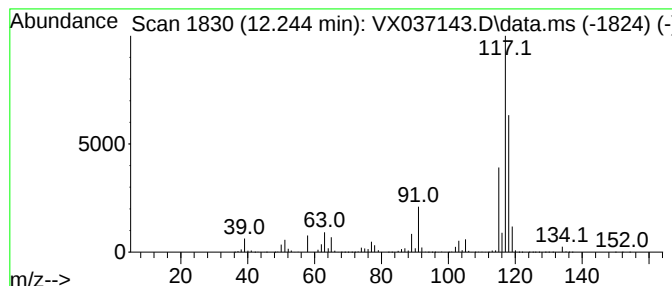
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 2-propenyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	797.83 ug/l	19235200	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
2			Indane	118	C9H10	000496-11-7	76
3			Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	72
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	62



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Misc : 7.77g/5.0mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NEVINS-SB06-Z84-85

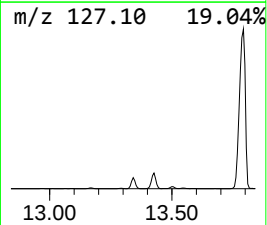
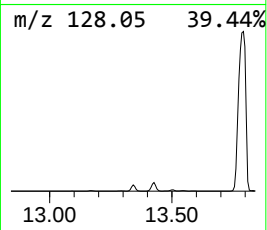
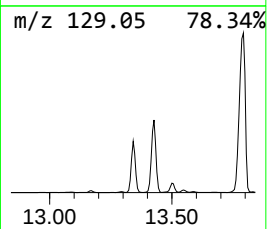
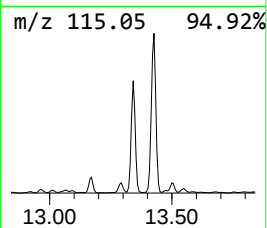
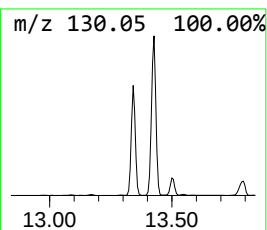
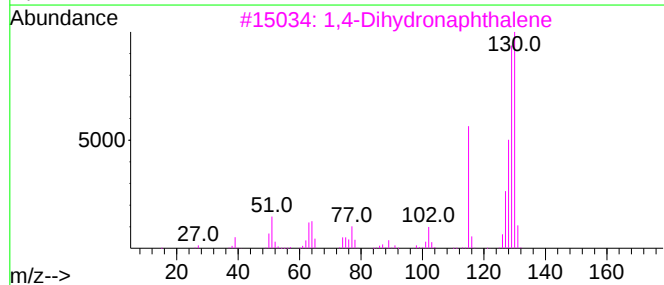
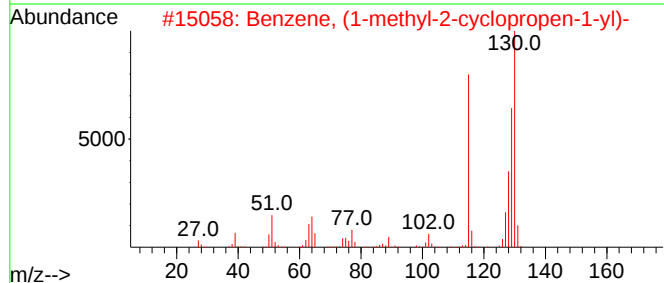
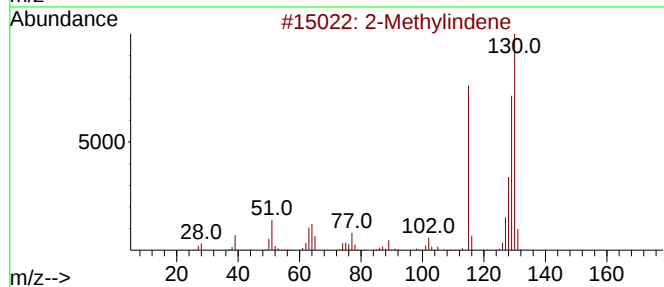
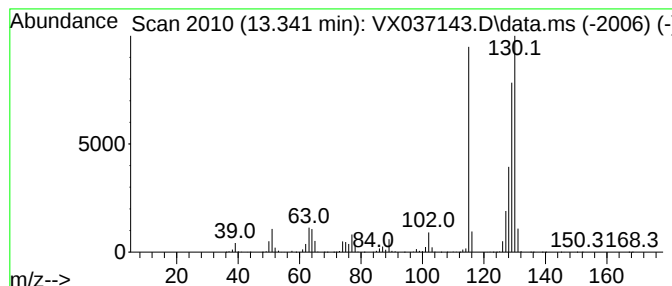
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 3 2-Methylindene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	189.55 ug/l	4569910	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Methylindene	130	C10H10	002177-47-1	95
2		Benzene, (1-methyl-2-cyclopropen-1-yl)-	130	C10H10	065051-83-4	95
3		1,4-Dihydronaphthalene	130	C10H10	000612-17-9	95
4		1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
5		Cycloprop[a]indene, 1,1a,6,6a-tetrahydro-	130	C10H10	015677-15-3	93



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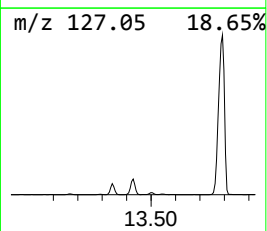
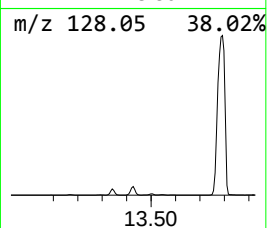
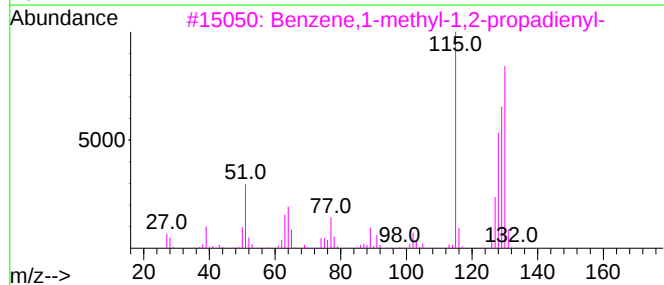
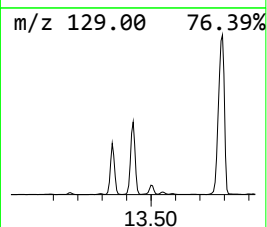
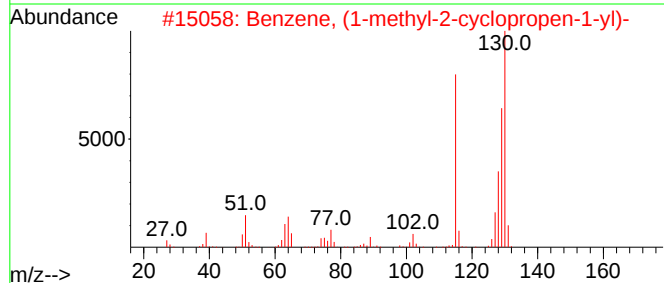
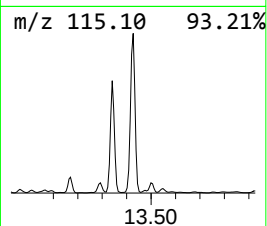
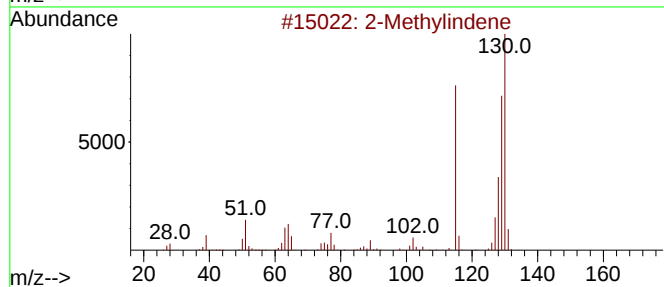
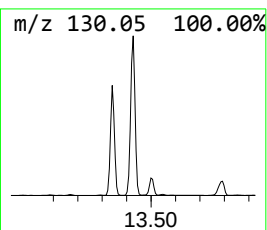
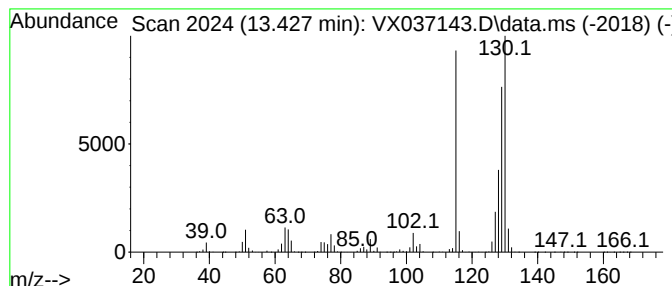
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, (1-methyl-2-cyclop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.427	308.80 ug/l	7444940	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindene			130	C10H10	002177-47-1	95
2	Benzene, (1-methyl-2-cyclopropen...			130	C10H10	065051-83-4	95
3	Benzene,1-methyl-1,2-propadienyl-			130	C10H10	022433-39-2	94
4	1H-Indene, 1-methyl-			130	C10H10	000767-59-9	94
5	Cycloprop[a]indene, 1,1a,6,6a-te...			130	C10H10	015677-15-3	94



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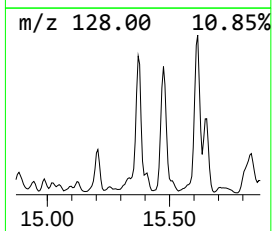
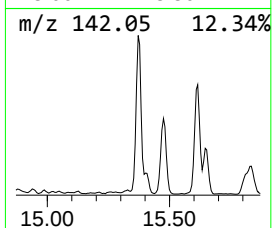
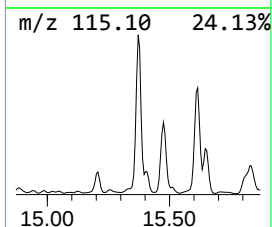
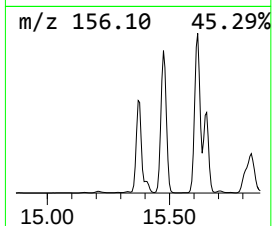
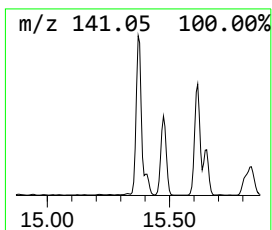
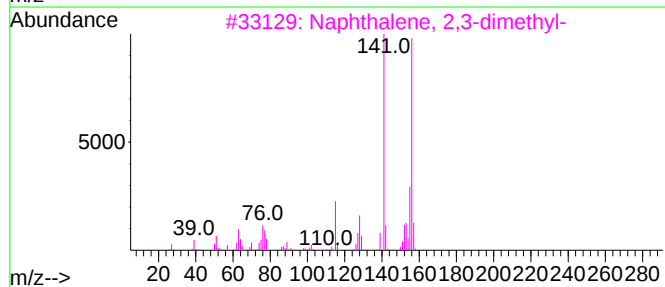
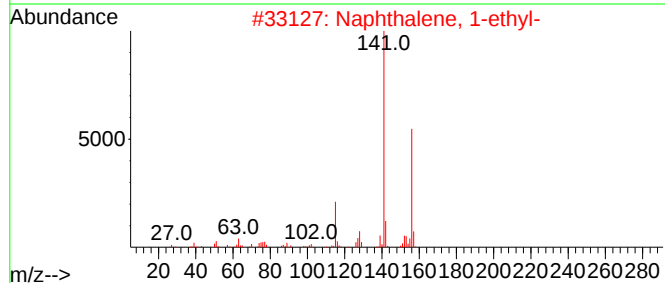
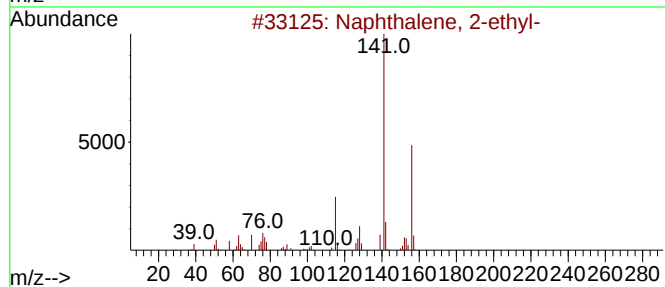
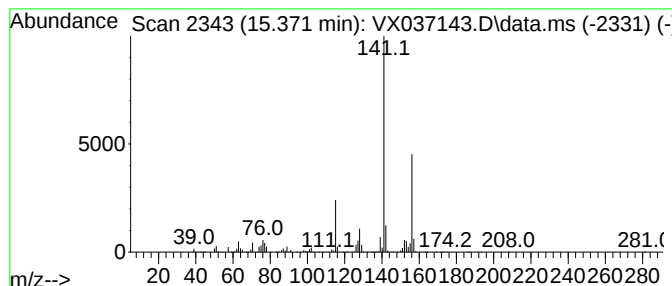
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.371	158.84 ug/l	3829560	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	96
2			Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	96
3			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	58
4			5-Acetyl-2-amino-4-methylthiazole	156	C6H8N2OS	030748-47-1	53
5			7-Methyl-trans-8-thiabicyclo[4.3...	156	C9H16S	060133-10-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082123\
Data File : VX037143.D
Acq On : 21 Aug 2023 20:07
Operator : JC/MD
Sample : 04014-04 10X
Misc : 7.77g/5.0mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB06-Z84-85

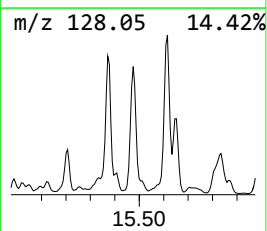
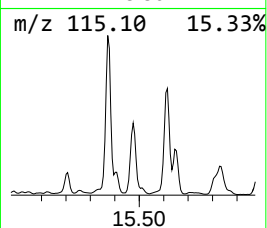
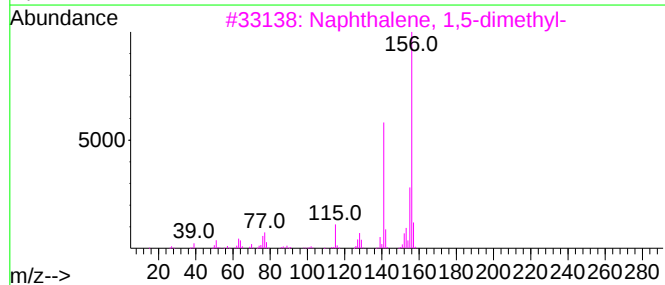
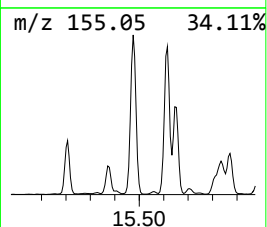
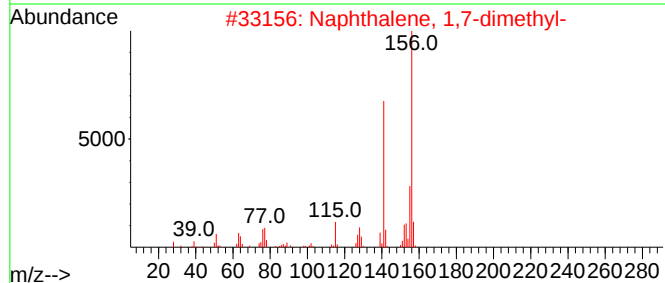
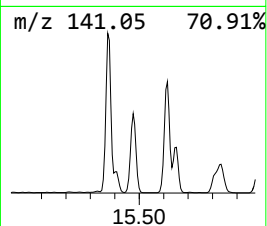
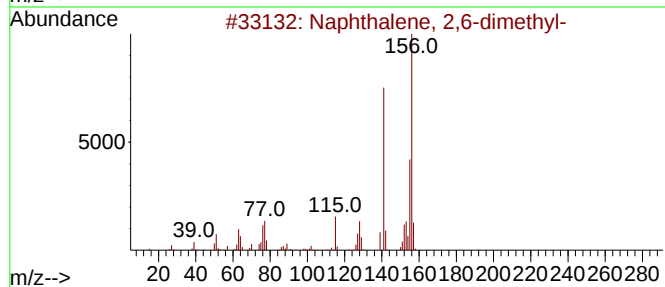
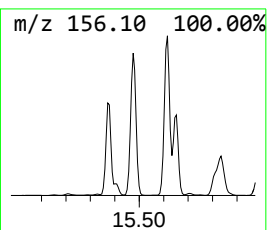
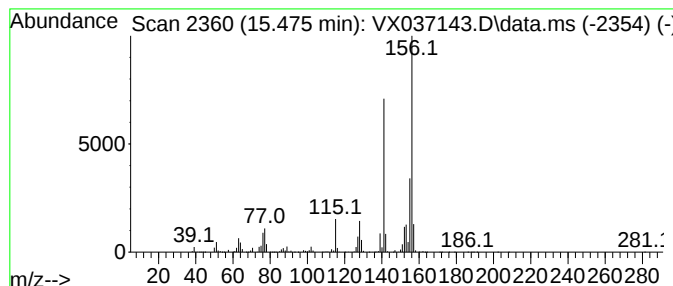
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 2,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	147.63 ug/l	3559220	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
2			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082123\
Data File : VX037143.D
Acq On : 21 Aug 2023 20:07
Operator : JC/MD
Sample : 04014-04 10X
Misc : 7.77g/5.0mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB06-Z84-85

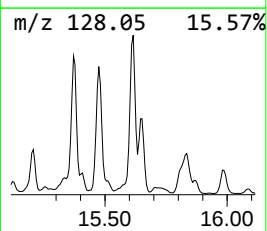
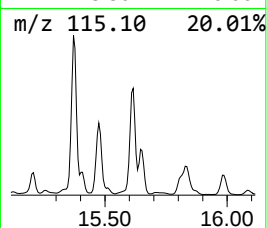
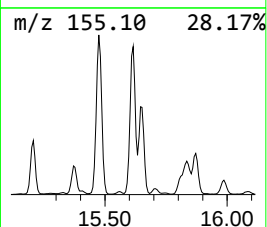
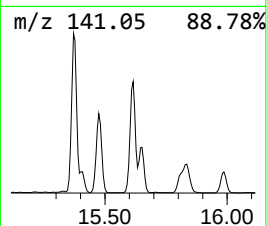
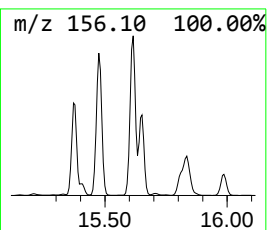
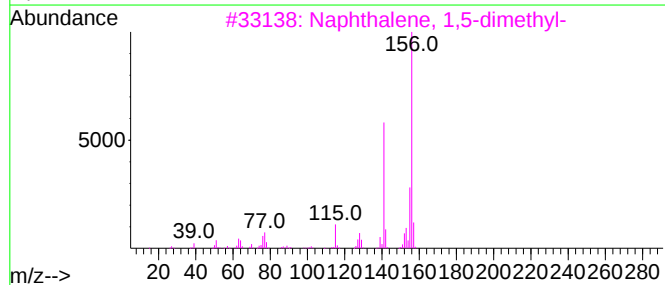
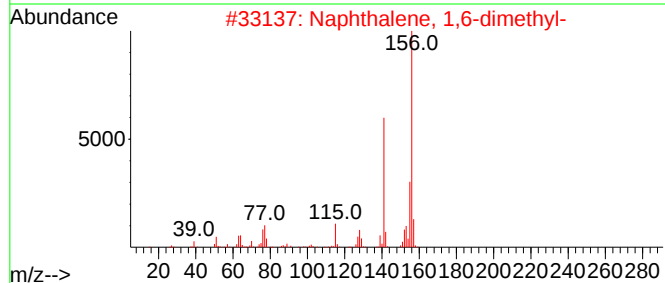
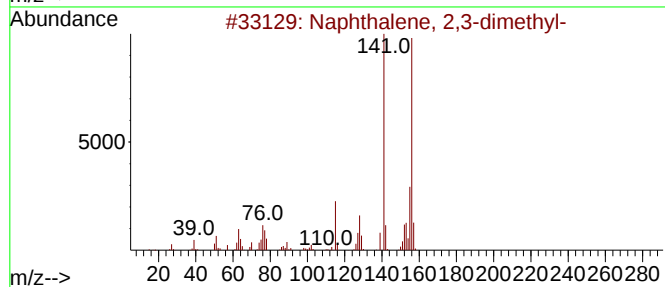
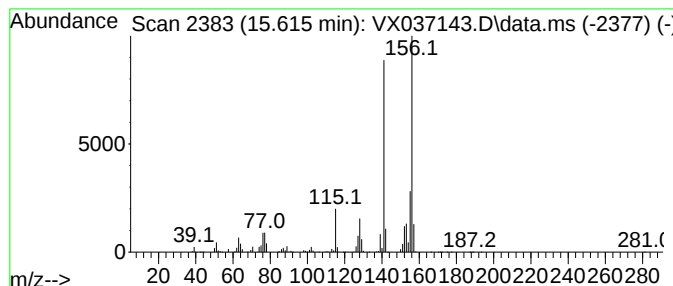
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	168.20 ug/l	4055120	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082123\
Data File : VX037143.D
Acq On : 21 Aug 2023 20:07
Operator : JC/MD
Sample : 04014-04 10X
Misc : 7.77g/5.0mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB06-Z84-85

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.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
Benzene, 1-ethy...	11.378	225.2	ug/l	5429430	4	12.024	1205480	50.0
Benzene, 2-prop...	12.244	797.8	ug/l	19235200	4	12.024	1205480	50.0
2-Methylindene	13.341	189.6	ug/l	4569910	4	12.024	1205480	50.0
Benzene, (1-met...	13.427	308.8	ug/l	7444940	4	12.024	1205480	50.0
Naphthalene, 2-...	15.371	158.8	ug/l	3829560	4	12.024	1205480	50.0
Naphthalene, 2,...	15.475	147.6	ug/l	3559220	4	12.024	1205480	50.0
Naphthalene, 2,...	15.615	168.2	ug/l	4055120	4	12.024	1205480	50.0