

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
 Data File : VN082276.D
 Acq On : 22 May 2024 06:21
 Operator : JC\MD
 Sample : P2494-16 40X
 Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 51 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 16

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\82N051524W.M
 Title : SW846 8260

Signal : TIC: VN082276.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.824	141	148	154	rVB3	10705	23201	1.09%	0.151%
2	8.171	1046	1057	1061	rBV	155838	375881	17.65%	2.449%
3	8.224	1061	1066	1080	rVB	279007	639524	30.02%	4.166%
4	8.582	1117	1127	1140	rBV2	201914	612708	28.77%	3.992%
5	9.100	1207	1215	1225	rBV	426450	877626	41.20%	5.718%
6	10.565	1456	1464	1471	rBV	657784	1251170	58.74%	8.151%
7	10.629	1471	1475	1487	rVV	229226	418918	19.67%	2.729%
8	11.865	1677	1685	1695	rBV	616796	1117399	52.46%	7.280%
9	11.965	1696	1702	1708	rVV	42408	74186	3.48%	0.483%
10	12.070	1712	1720	1731	rVB	224784	423471	19.88%	2.759%
11	12.400	1763	1776	1784	rBV	152955	277399	13.02%	1.807%
12	12.588	1799	1808	1809	rBV6	15010	29094	1.37%	0.190%
13	12.629	1812	1815	1823	rVB6	11145	30670	1.44%	0.200%
14	12.847	1846	1852	1863	rVB	488204	870059	40.85%	5.668%
15	13.035	1877	1884	1889	rVB2	14354	26468	1.24%	0.172%
16	13.100	1889	1895	1899	rBV	55680	103801	4.87%	0.676%
17	13.170	1902	1907	1914	rVB3	89397	166710	7.83%	1.086%
18	13.335	1919	1935	1942	rBV4	64439	243451	11.43%	1.586%
19	13.482	1954	1960	1967	rBV	167084	271853	12.76%	1.771%
20	13.670	1972	1992	2006	rBV4	128989	681841	32.01%	4.442%
21	13.794	2006	2013	2022	rVB2	607351	1124131	52.78%	7.324%
22	14.012	2035	2050	2059	rBV6	195084	712028	33.43%	4.639%
23	14.106	2060	2066	2075	rVV6	102898	269991	12.68%	1.759%
24	14.247	2086	2090	2092	rBV3	14657	23321	1.09%	0.152%
25	14.270	2092	2094	2100	rVV2	19504	27488	1.29%	0.179%
26	14.329	2100	2104	2109	rVB	23983	33661	1.58%	0.219%
27	14.447	2118	2124	2126	rBV8	18830	36694	1.72%	0.239%
28	14.488	2127	2131	2132	rVV3	23301	36870	1.73%	0.240%
29	14.570	2136	2145	2152	rVV5	54767	185094	8.69%	1.206%
30	14.635	2152	2156	2157	rVV4	24823	40137	1.88%	0.261%
31	14.659	2157	2160	2163	rVV3	34304	58406	2.74%	0.381%
32	14.688	2163	2165	2170	rVV	33367	48409	2.27%	0.315%
33	14.794	2176	2183	2186	rBV7	14088	34661	1.63%	0.226%
34	14.847	2187	2192	2202	rVB5	32121	93130	4.37%	0.607%
35	14.958	2204	2211	2217	rVB3	57842	104554	4.91%	0.681%
36	15.041	2218	2225	2245	rBV9	47608	239140	11.23%	1.558%

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Integrator: RTE

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Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

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Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

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37	15.206	2245	2253	2260	rBV10	17341	41228	1.94%	0.269%
38	15.317	2267	2272	2280	rVB10	18162	45284	2.13%	0.295%
39	15.435	2286	2292	2297	rBV10	16637	37419	1.76%	0.244%
40	15.517	2301	2306	2308	rBV6	12490	23102	1.08%	0.151%
41	15.641	2314	2327	2339	rBV	1058549	2130010	100.00%	13.877%
42	15.747	2339	2345	2351	rVV3	34354	77682	3.65%	0.506%
43	15.829	2355	2359	2371	rVB3	44953	98339	4.62%	0.641%
44	15.947	2371	2379	2386	rBV3	17328	54863	2.58%	0.357%
45	16.023	2386	2392	2395	rBV6	13243	26359	1.24%	0.172%
46	16.253	2421	2431	2439	rBV8	23848	80625	3.79%	0.525%
47	16.494	2464	2472	2477	rBV8	14789	41715	1.96%	0.272%
48	16.717	2504	2510	2513	rBV5	15905	30518	1.43%	0.199%
49	16.782	2513	2521	2522	rBV	692570	1079014	50.66%	7.030%

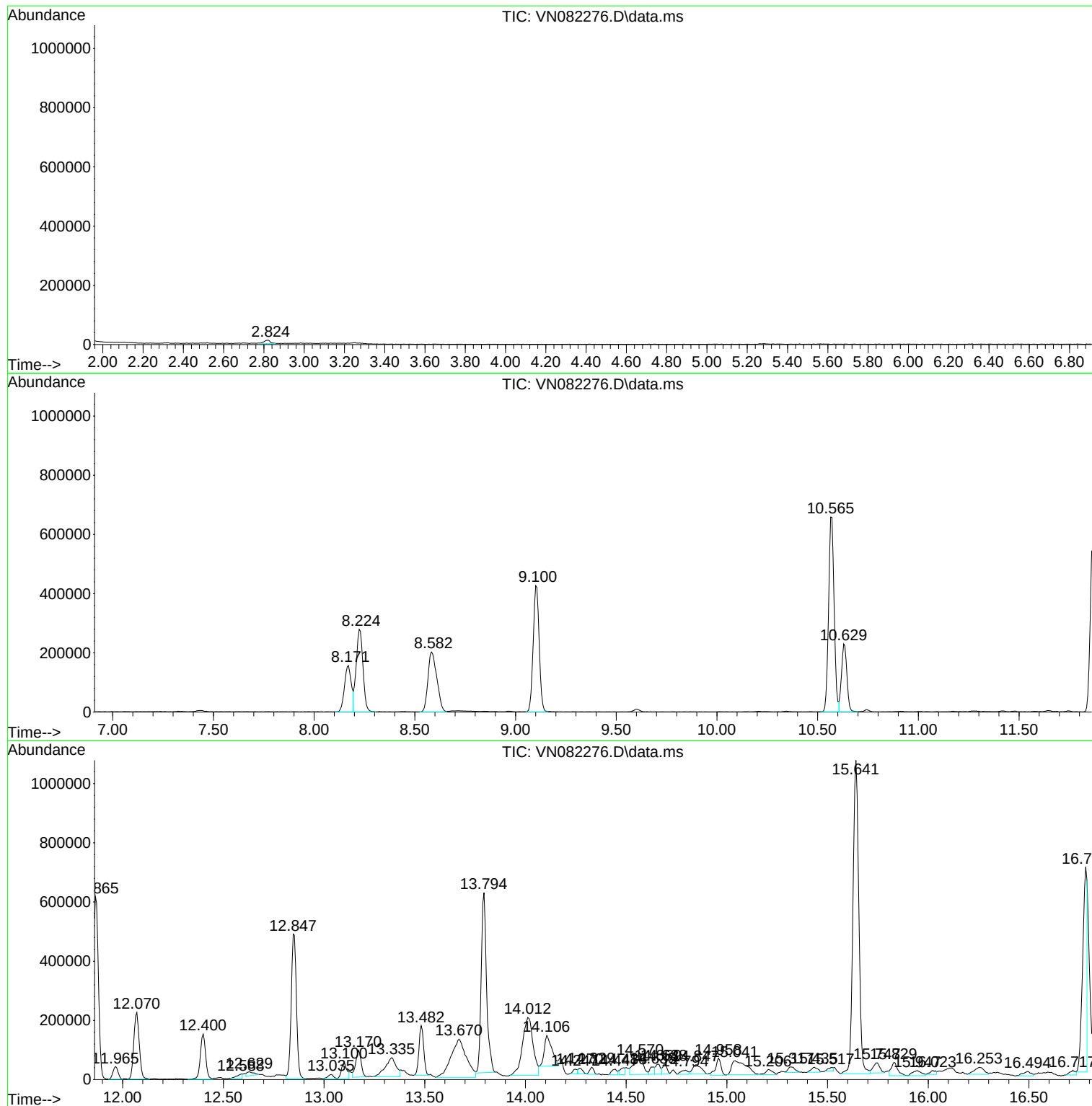
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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



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ALS Vial : 51 Sample Multiplier: 1

Instrument :
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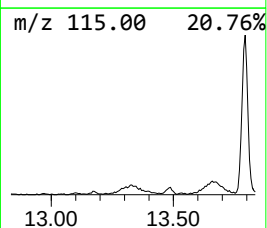
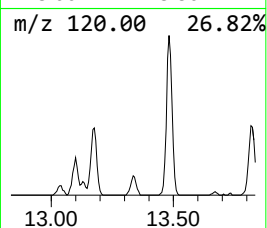
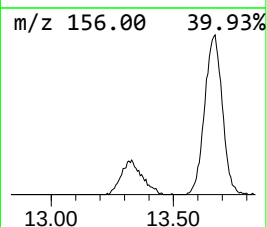
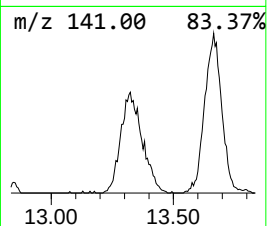
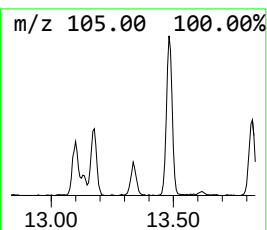
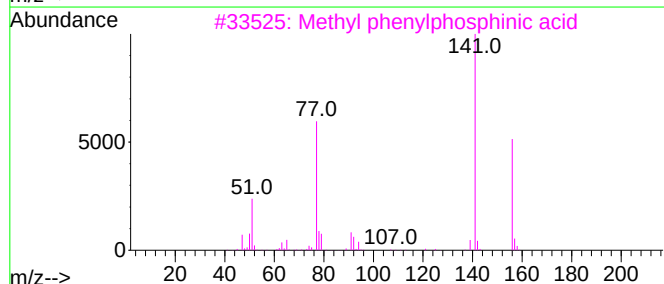
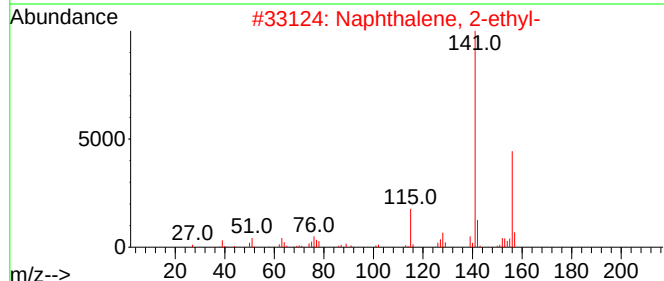
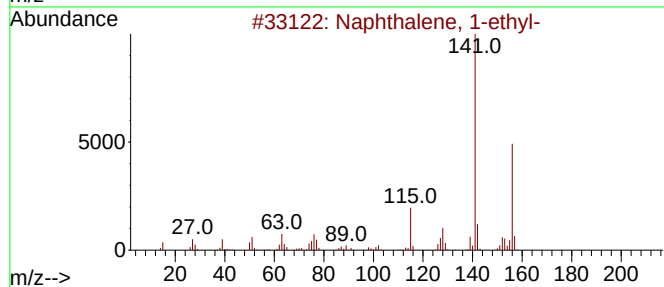
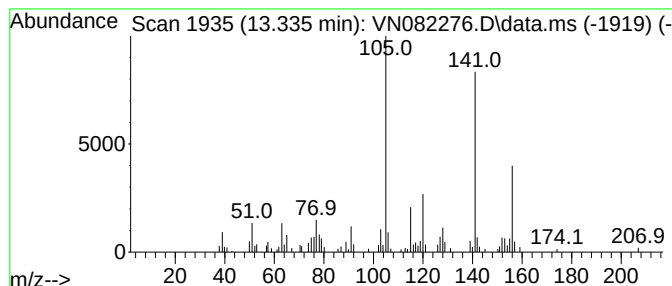
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 1 Naphthalene, 1-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	10.83 ug/l	243451	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	64
2			Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	62
3			Methyl phenylphosphinic acid	156	C7H9O2P	004271-13-0	46
4			1,4-Dimethylazulene	156	C12H12	001127-69-1	42
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	25



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ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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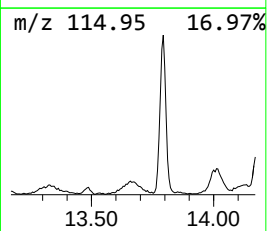
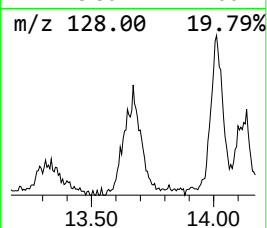
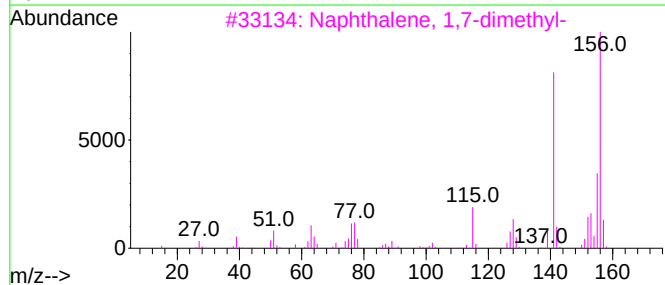
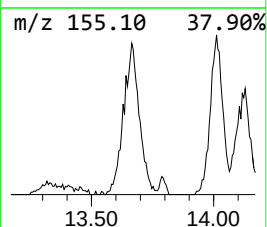
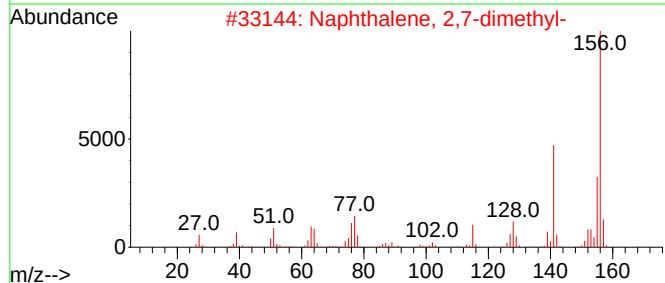
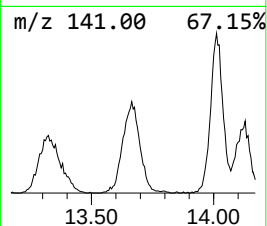
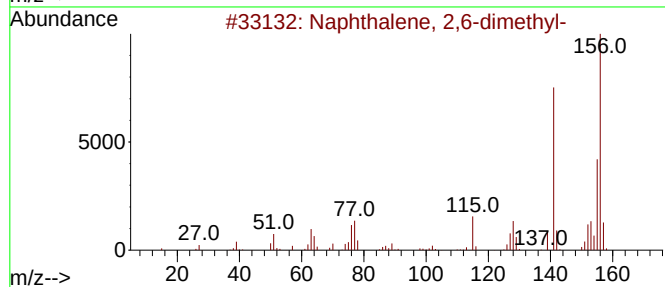
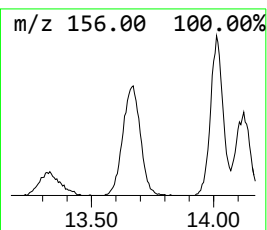
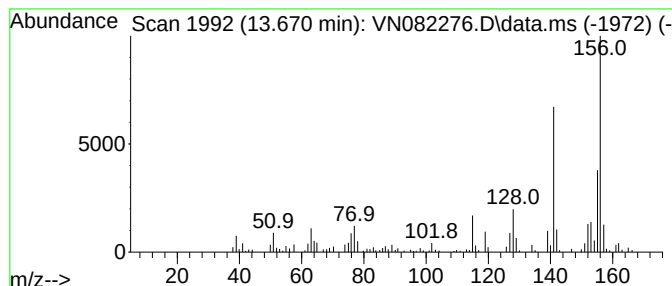
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 2 Naphthalene, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.670	30.33 ug/l	681841	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	95



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Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_N
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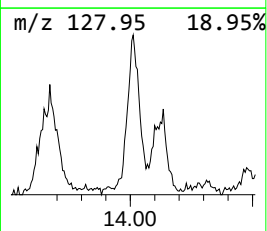
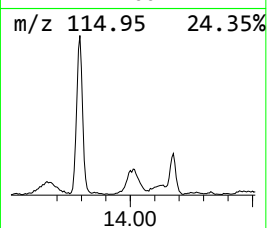
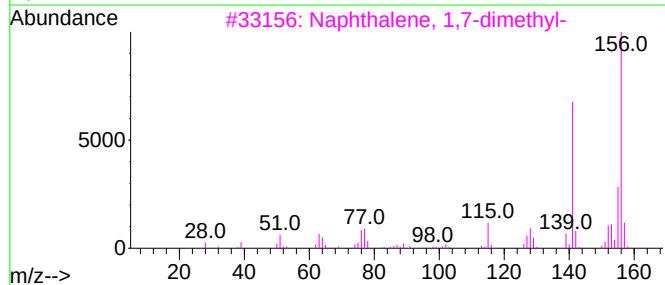
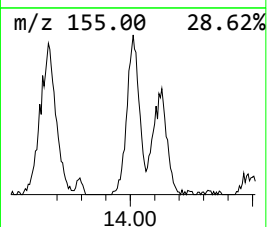
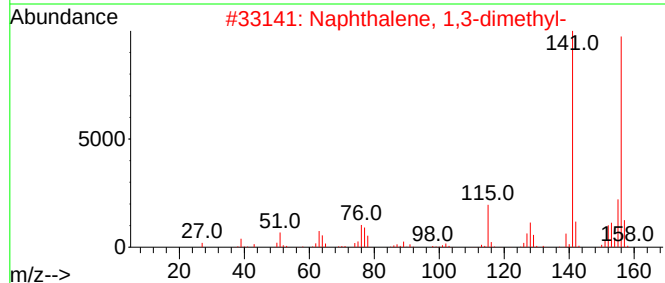
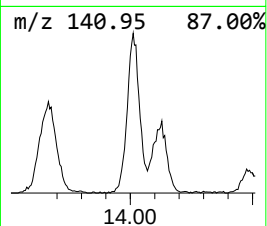
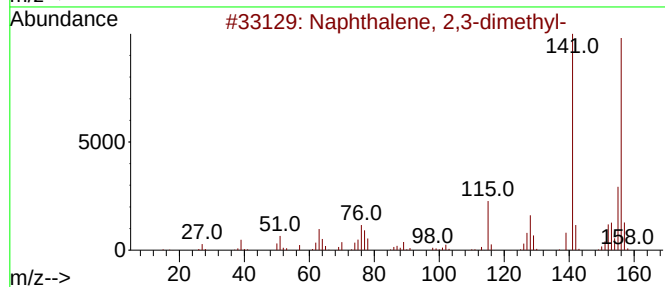
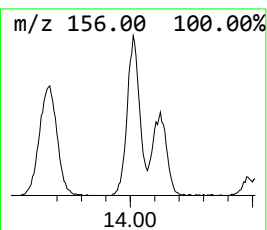
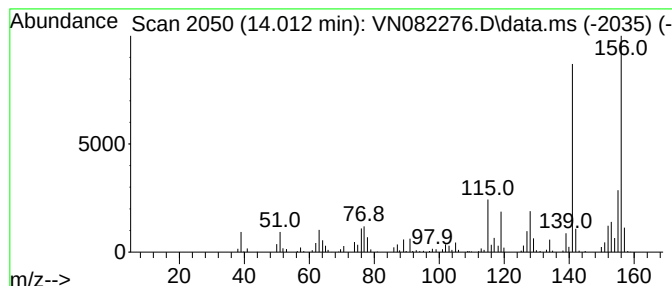
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.012	31.67 ug/l	712028	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5			Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	96



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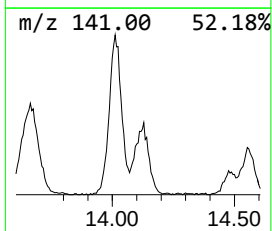
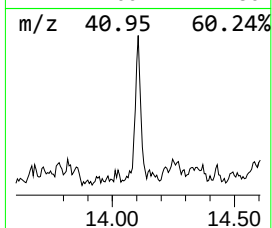
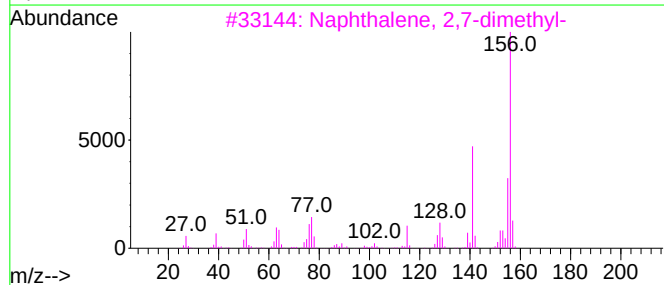
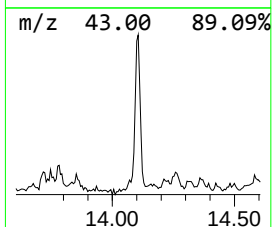
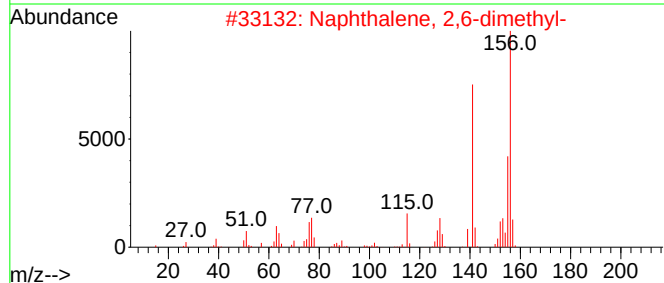
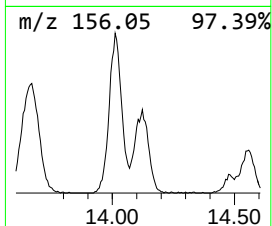
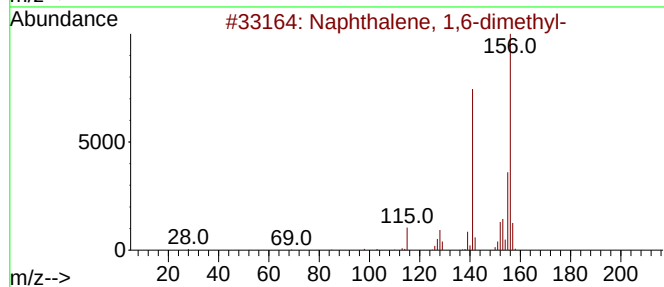
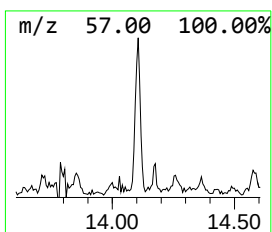
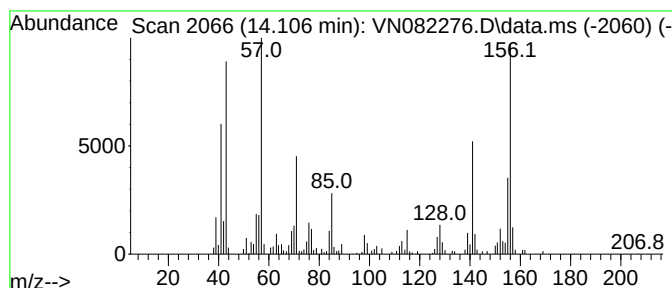
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, 1,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.106	12.01 ug/l	269991	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	94
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	93
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	93
4			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	91
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	70



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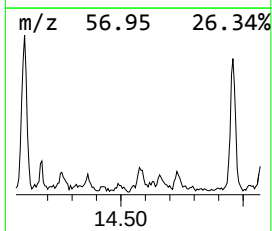
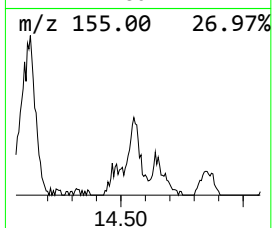
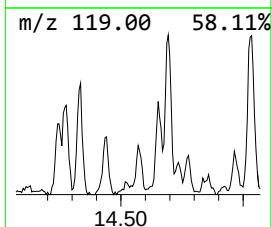
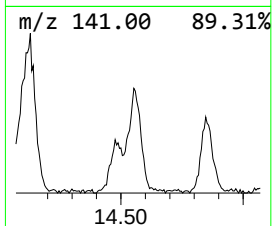
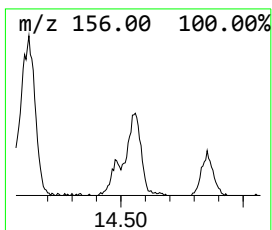
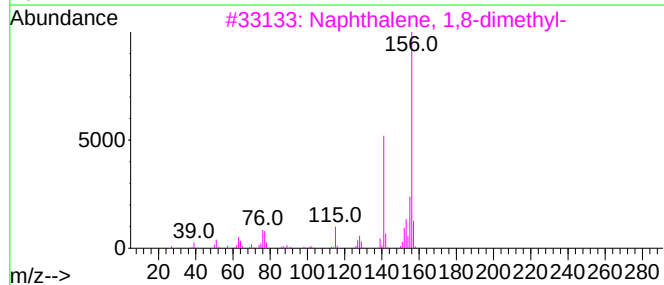
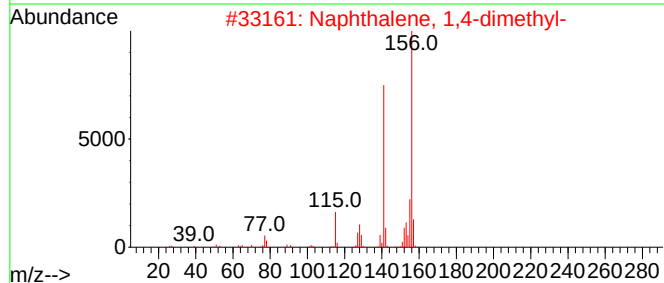
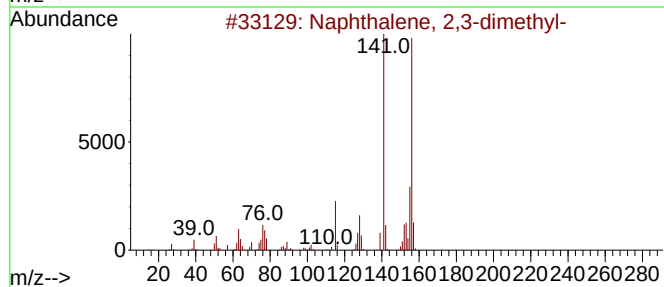
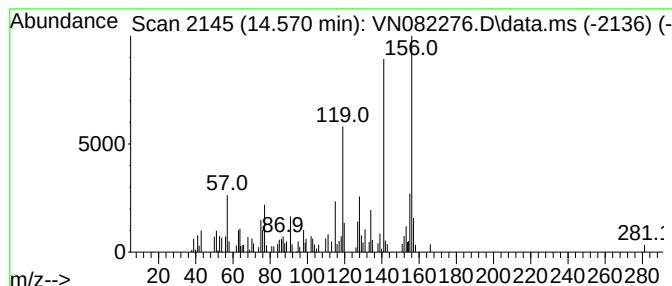
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Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 1,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.570	8.23 ug/l	185094	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	86
2			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	86
3			Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	70
4			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	70
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082276.D
Acq On : 22 May 2024 06:21
Operator : JC\MD
Sample : P2494-16 40X
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
16

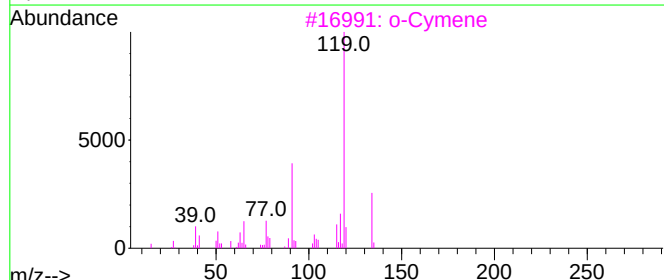
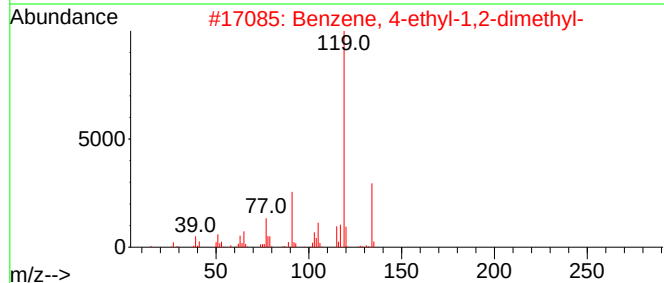
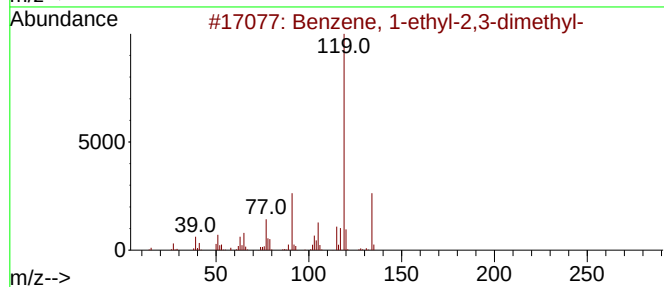
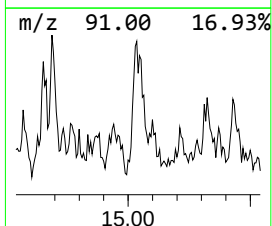
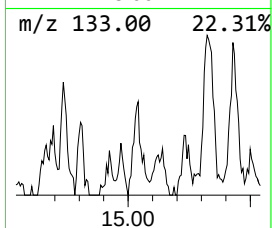
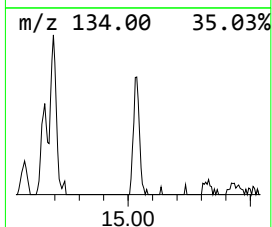
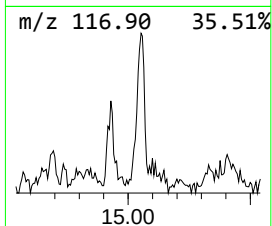
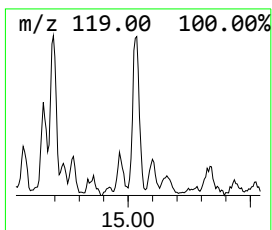
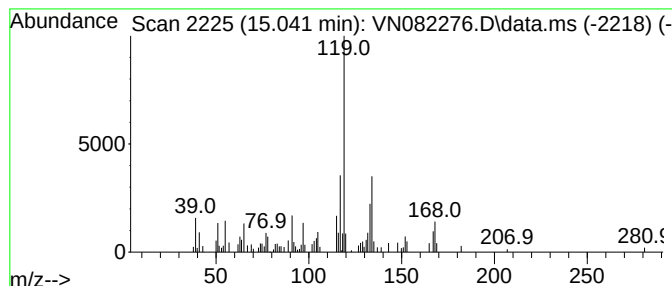
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.041	10.64 ug/l	239140	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	55
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	55
3			o-Cymene	134	C10H14	000527-84-4	53
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	49
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082276.D
Acq On : 22 May 2024 06:21
Operator : JC\MD
Sample : P2494-16 40X
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
16

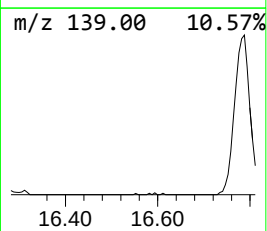
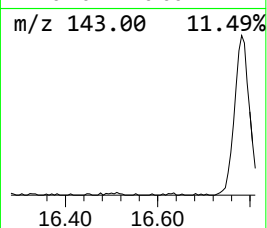
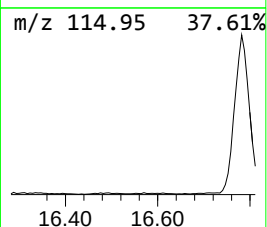
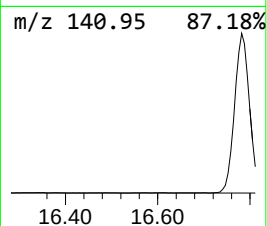
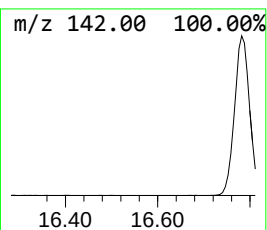
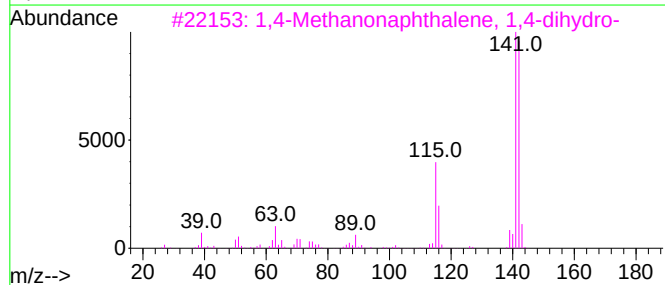
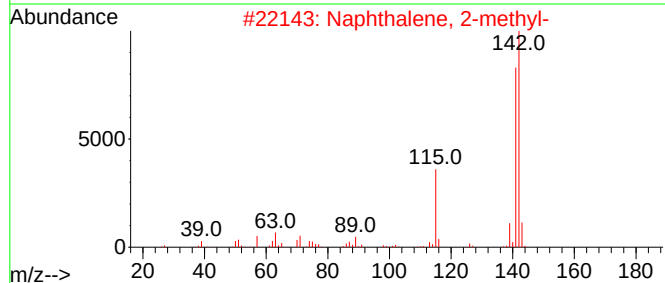
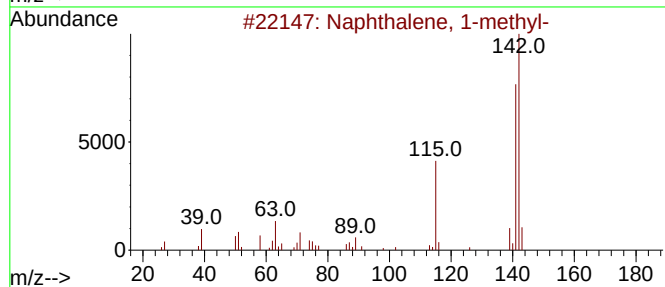
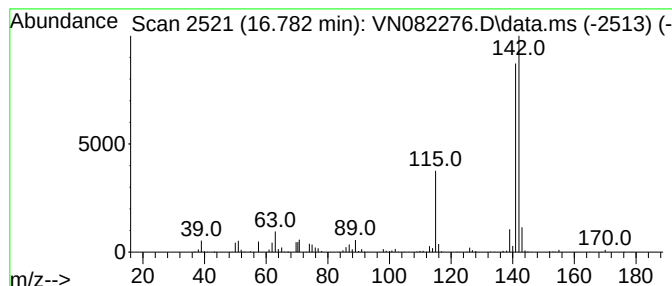
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.782	47.99 ug/l	1079010	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082276.D
Acq On : 22 May 2024 06:21
Operator : JC\MD
Sample : P2494-16 40X
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
16

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.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
Naphthalene, 1-...	13.335	10.8	ug/l	243451	4	13.794	1124130	50.0
Naphthalene, 2,...	13.670	30.3	ug/l	681841	4	13.794	1124130	50.0
Naphthalene, 2,...	14.012	31.7	ug/l	712028	4	13.794	1124130	50.0
Naphthalene, 1,...	14.106	12.0	ug/l	269991	4	13.794	1124130	50.0
Naphthalene, 1,...	14.570	8.2	ug/l	185094	4	13.794	1124130	50.0
Benzene, 1-ethy...	15.041	10.6	ug/l	239140	4	13.794	1124130	50.0
Naphthalene, 1-...	16.782	48.0	ug/l	1079010	4	13.794	1124130	50.0