

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062222\
 Data File : VX029722.D
 Acq On : 23 Jun 2022 05:21
 Operator : JC/MD
 Sample : N3293-01
 Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 30873

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\82X061822W.M
 Title : SW846 8260

Signal : TIC: VX029722.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.953	297	306	324	rBV	21154	68986	4.82%	0.711%
2	5.391	694	706	721	rBV2	146921	442666	30.93%	4.561%
3	5.550	721	732	748	rVB	301457	871248	60.88%	8.978%
4	5.958	788	799	816	rBV	157817	442528	30.92%	4.560%
5	6.367	858	866	880	rBV4	5977	20458	1.43%	0.211%
6	6.763	921	931	949	rBV	448346	1088087	76.03%	11.212%
7	8.647	1232	1240	1253	rBV	880053	1431206	100.00%	14.747%
8	8.763	1253	1259	1272	rVB	5785	15416	1.08%	0.159%
9	10.055	1465	1471	1486	rVB	845046	1186722	82.92%	12.228%
10	11.085	1634	1640	1650	rBV	655609	875601	61.18%	9.022%
11	11.756	1746	1750	1758	rVB	9038	15417	1.08%	0.159%
12	12.024	1788	1794	1801	rBV	915777	1118102	78.12%	11.521%
13	13.841	2088	2092	2099	rVB6	9717	18218	1.27%	0.188%
14	13.932	2099	2107	2111	rBV9	10139	23943	1.67%	0.247%
15	14.487	2193	2198	2203	rBV8	7246	16994	1.19%	0.175%
16	14.579	2205	2213	2216	rBV9	6594	14854	1.04%	0.153%
17	14.640	2216	2223	2226	rBV	37951	67682	4.73%	0.697%
18	14.725	2233	2237	2240	rBV4	9686	15373	1.07%	0.158%
19	14.780	2243	2246	2255	rVB	35313	57584	4.02%	0.593%
20	15.182	2309	2312	2315	rBV4	8611	14617	1.02%	0.151%
21	15.377	2340	2344	2347	rBV2	34482	49786	3.48%	0.513%
22	15.481	2354	2361	2366	rBV	115370	185223	12.94%	1.909%
23	15.566	2370	2375	2378	rVV	41079	58228	4.07%	0.600%
24	15.615	2378	2383	2386	rVV	122037	187539	13.10%	1.932%
25	15.652	2386	2389	2396	rVB	111354	169136	11.82%	1.743%
26	15.737	2398	2403	2408	rBV6	13199	24429	1.71%	0.252%
27	15.841	2410	2420	2424	rBV	55377	148765	10.39%	1.533%
28	15.987	2440	2444	2454	rVB	35462	72670	5.08%	0.749%
29	16.091	2456	2461	2466	rVB	51977	82393	5.76%	0.849%
30	16.158	2468	2472	2474	rBV5	12376	18574	1.30%	0.191%
31	16.194	2474	2478	2485	rVB3	38201	65810	4.60%	0.678%
32	16.267	2485	2490	2491	rBV2	20288	28498	1.99%	0.294%
33	16.298	2493	2495	2499	rVB2	23516	27856	1.95%	0.287%
34	16.353	2499	2504	2509	rBV	74159	136634	9.55%	1.408%
35	16.475	2520	2524	2530	rVB5	29242	54229	3.79%	0.559%
36	16.560	2533	2538	2540	rVV2	44481	75775	5.29%	0.781%

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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\82X061822W.M
Title : SW846 8260

37	16.597	2540	2544	2549	rVV	124912	242348	16.93%	2.497%
38	16.658	2549	2554	2564	rVB2	126664	271171	18.95%	2.794%

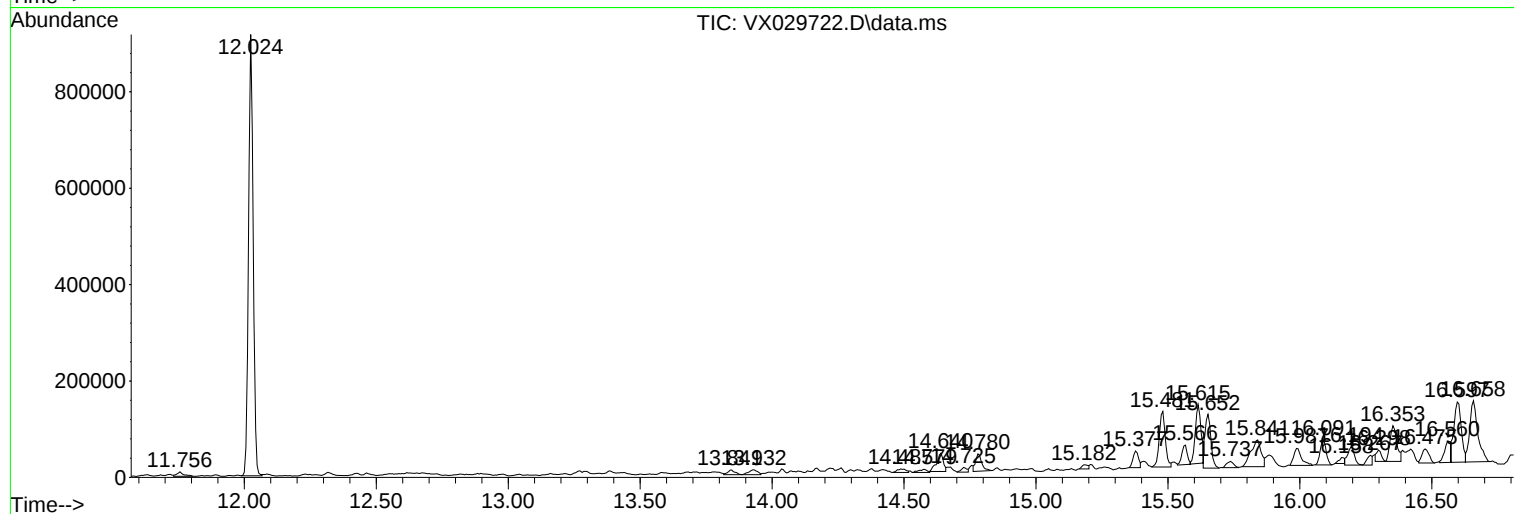
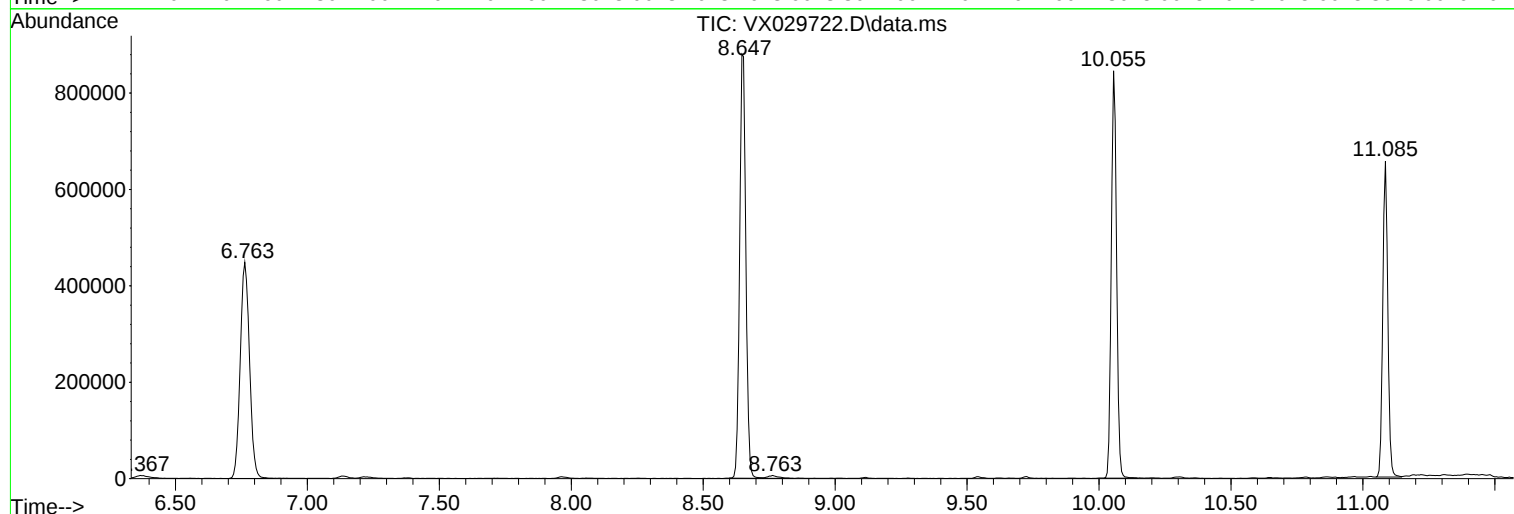
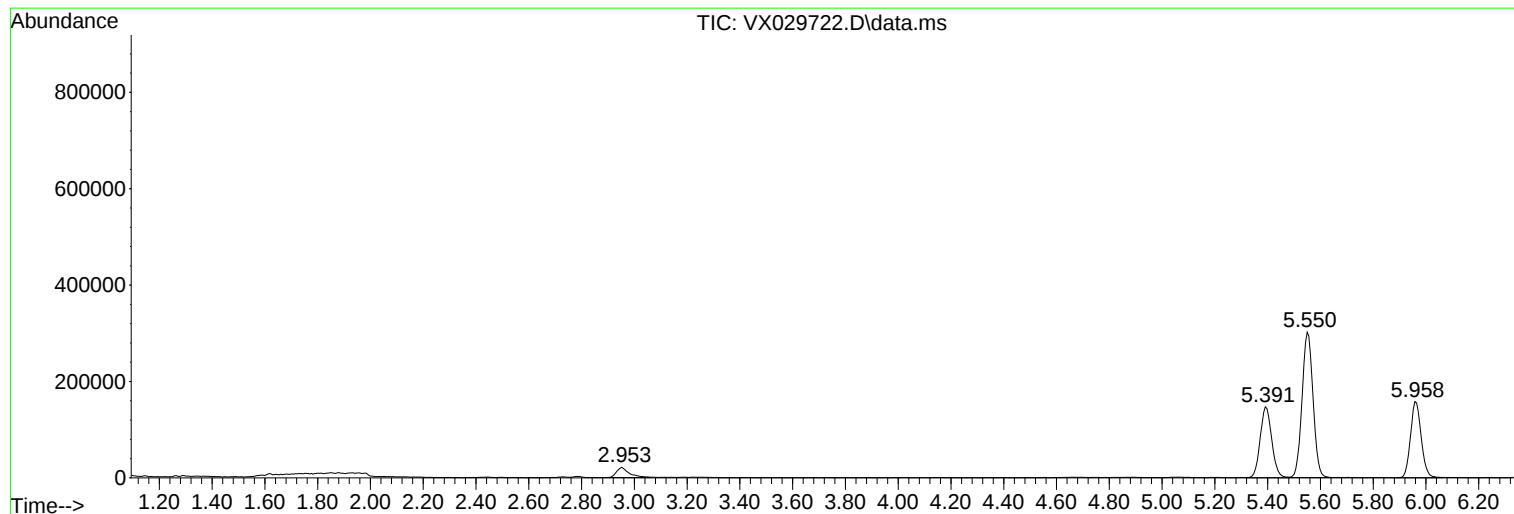
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



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Operator : JC/MD
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Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30873

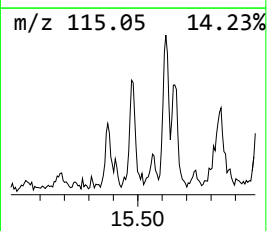
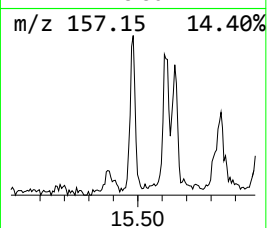
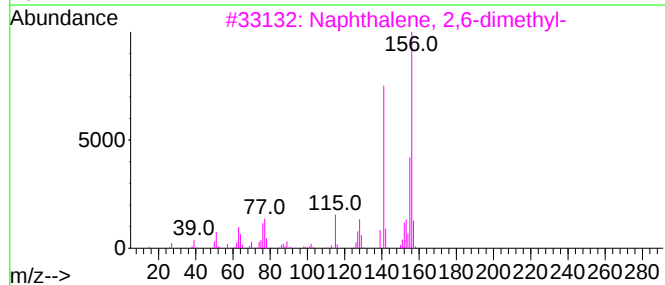
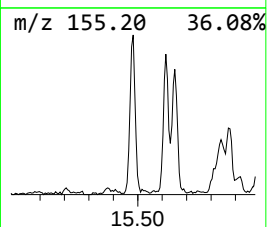
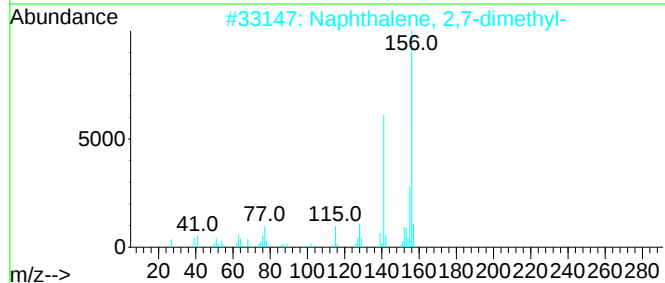
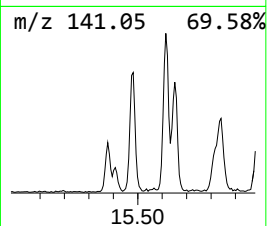
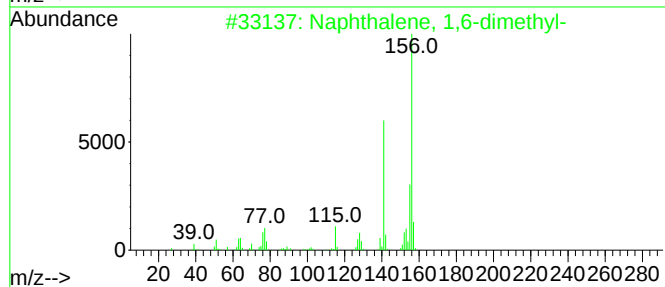
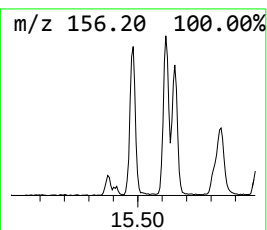
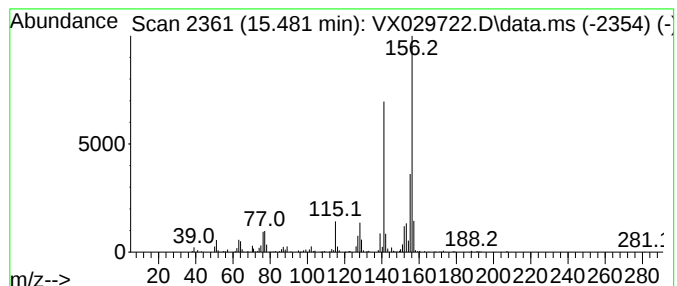
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	8.28 ug/l	185223	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
4			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97



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Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30873

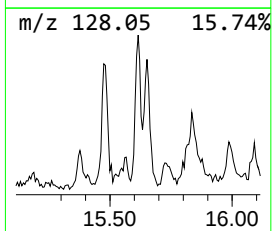
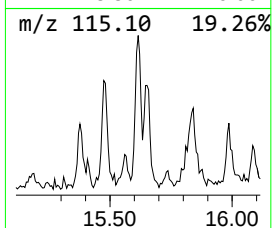
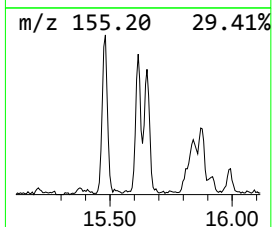
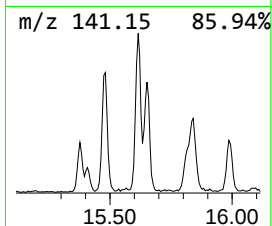
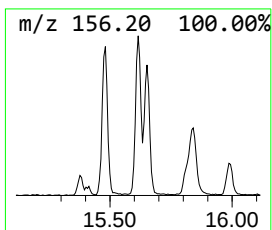
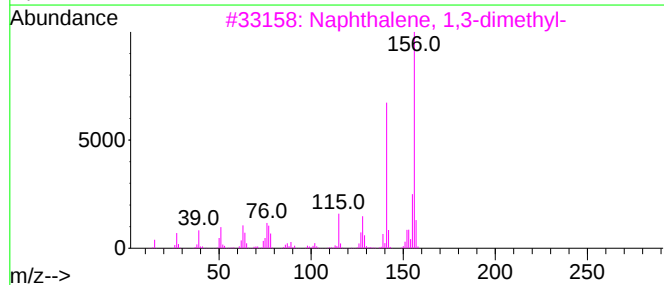
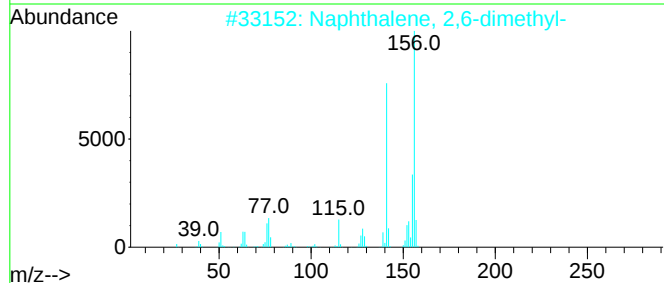
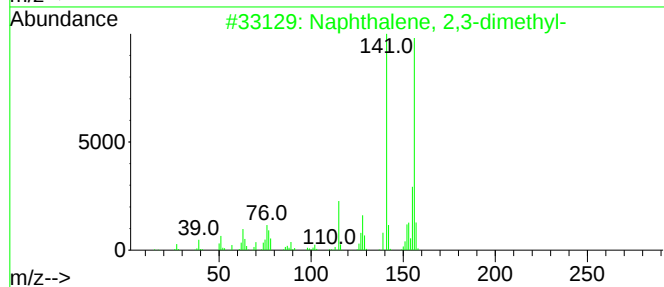
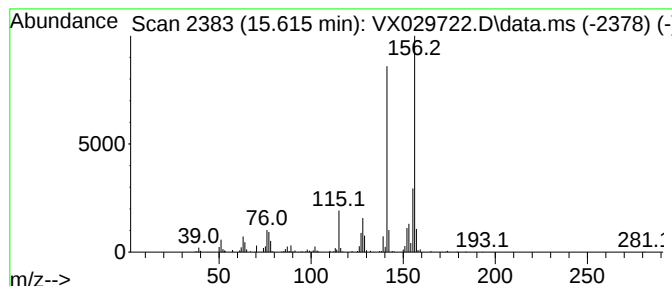
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	8.39 ug/l	187539	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, 2,6-dimethyl-	156	C12H12	000581-42-0	97
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96



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Data File : VX029722.D
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Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30873

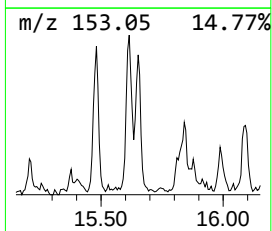
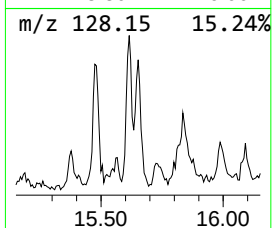
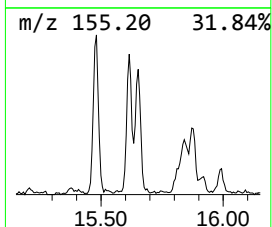
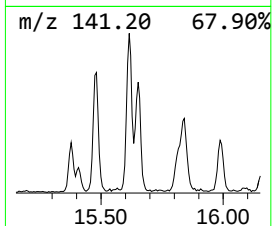
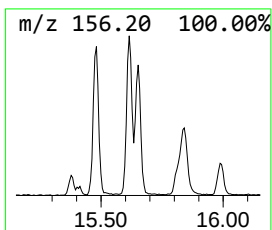
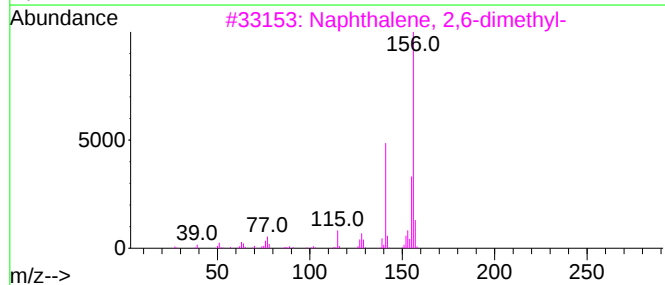
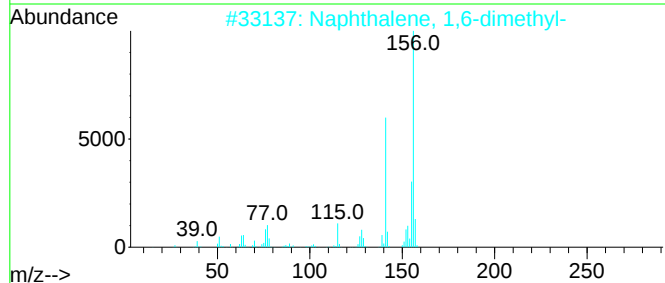
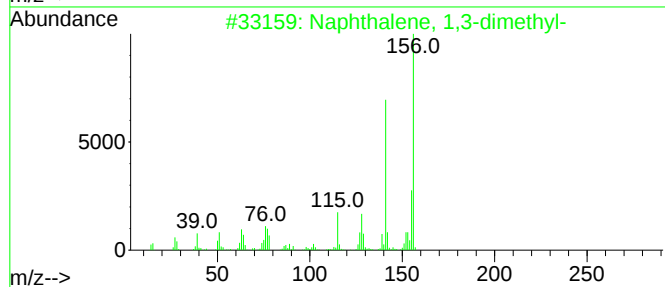
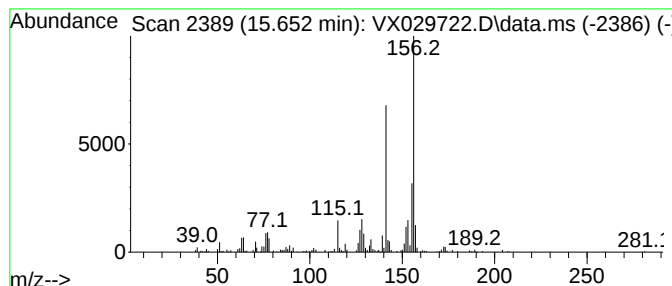
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 1,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.652	7.56 ug/l	169136	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	94
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	94
3			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	93
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	93
5			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	93



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Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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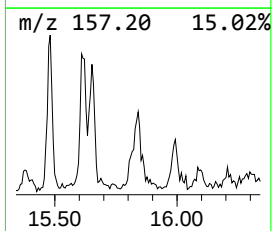
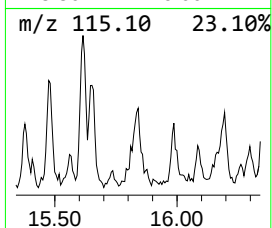
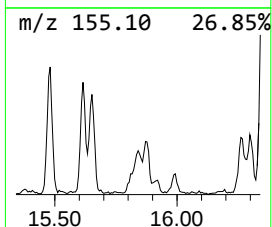
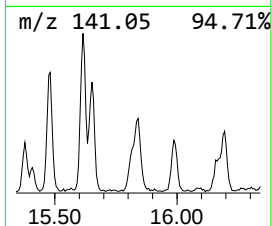
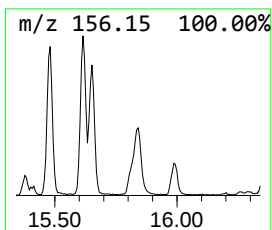
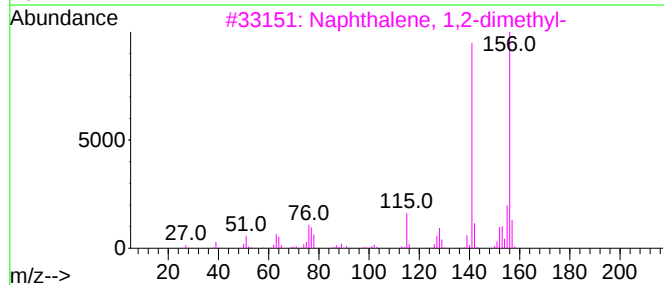
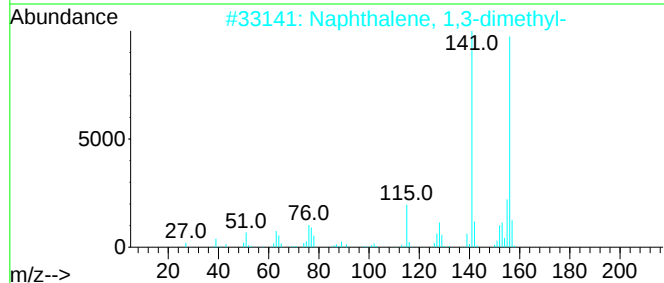
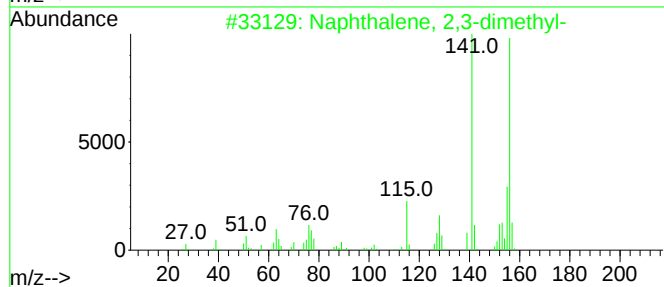
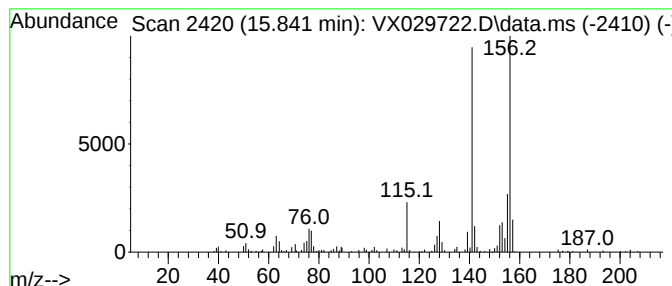
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, 1,2-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.841	6.65 ug/l	148765	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, 1,3-dimethyl-	156	C12H12	000575-41-7	97
3			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
5			Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	96



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Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 42 Sample Multiplier: 1

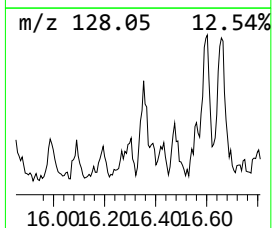
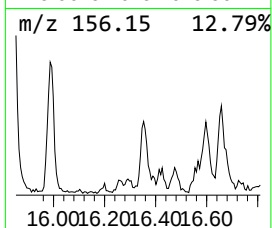
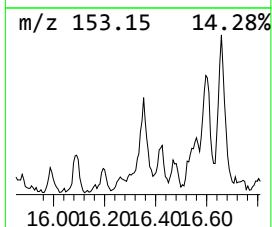
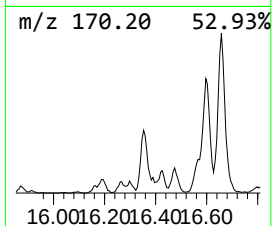
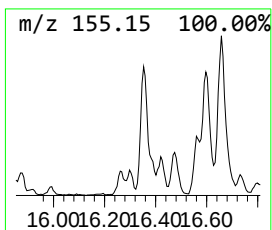
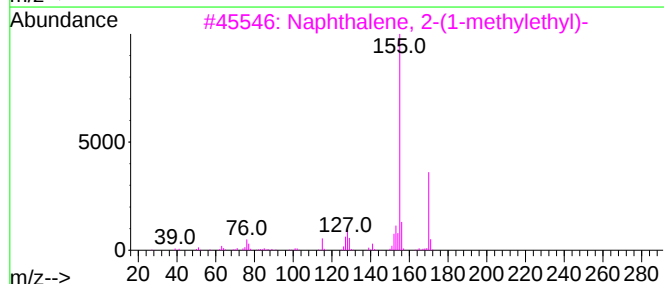
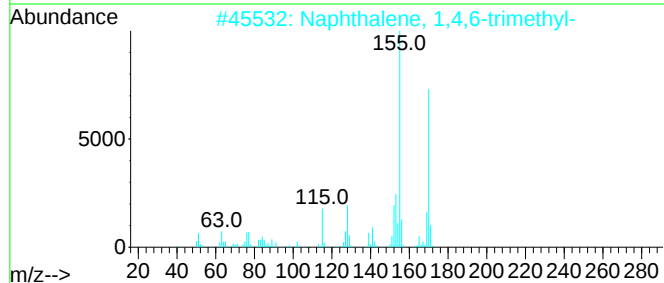
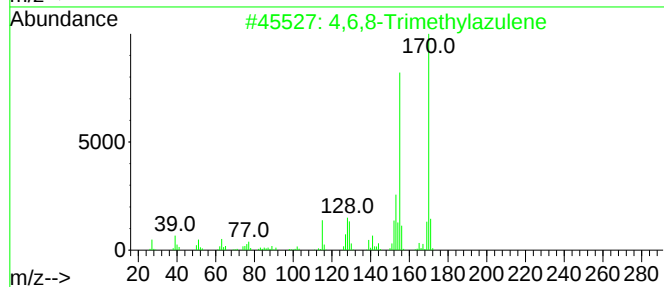
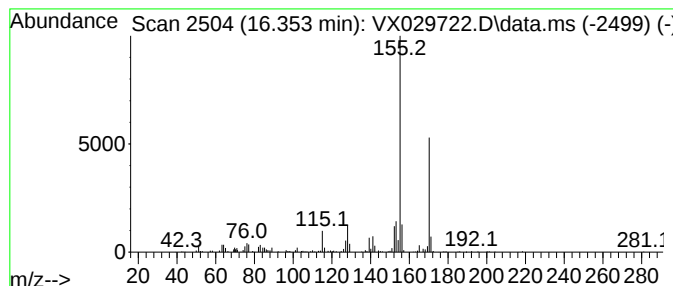
Instrument :
MSVOA_X
ClientSampleId :
30873

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 5 4,6,8-Trimethylazulene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.353	6.11 ug/l	136634	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,6,8-Trimethylazulene	170	C13H14	000941-81-1	90
2	Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	89
3	Naphthalene, 2-(1-methylethyl)-	170	C13H14	002027-17-0	87
4	3-(2-Methyl-propenyl)-1H-indene	170	C13H14	1000187-78-5	87
5	Naphthalene, 1,4,5-trimethyl-	170	C13H14	002131-41-1	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062222\
Data File : VX029722.D
Acq On : 23 Jun 2022 05:21
Operator : JC/MD
Sample : N3293-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30873

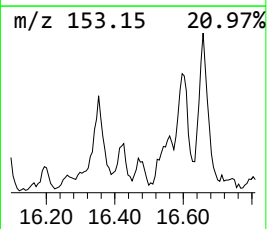
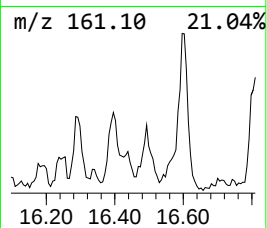
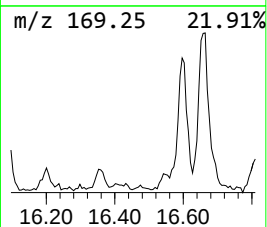
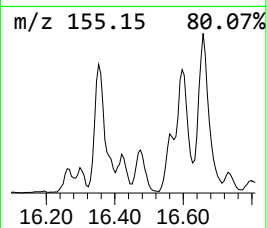
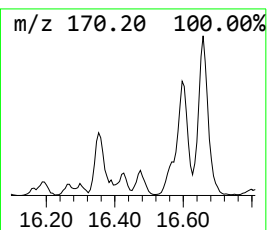
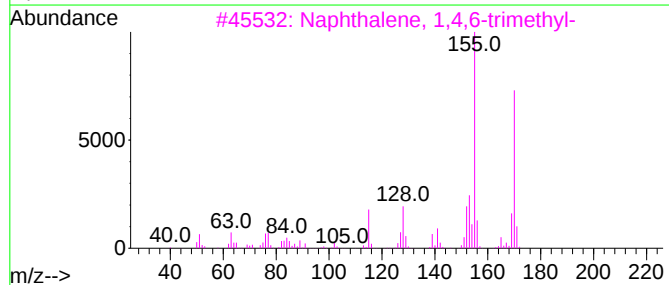
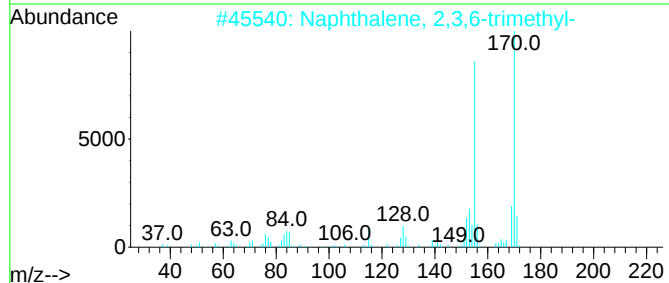
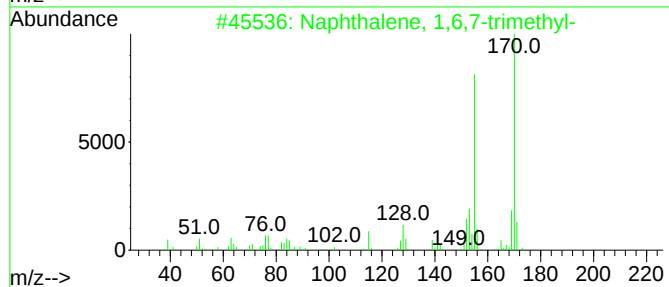
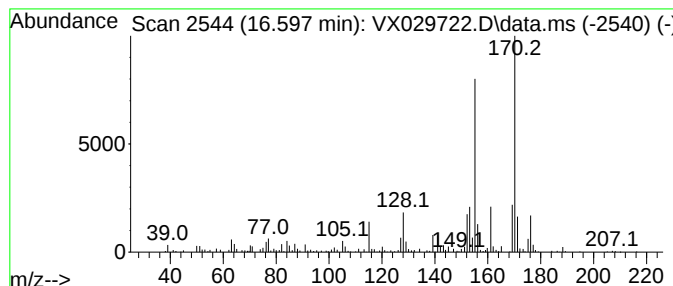
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1,6,7-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.597	10.84 ug/l	242348	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	93
2			Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	91
3			Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	91
4			4,6,8-Trimethylazulene	170	C13H14	000941-81-1	89
5			1-(2,2-Dimethylcyclopropyl)-2-ph...	170	C13H14	1000294-91-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062222\
Data File : VX029722.D
Acq On : 23 Jun 2022 05:21
Operator : JC/MD
Sample : N3293-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30873

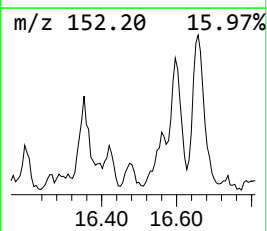
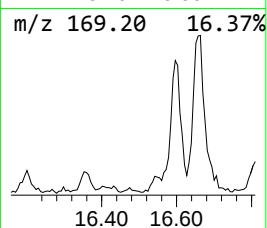
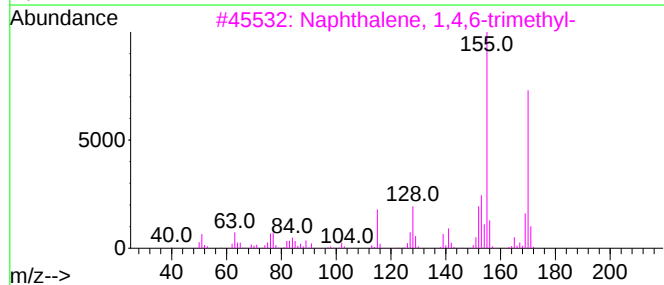
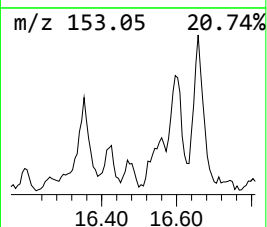
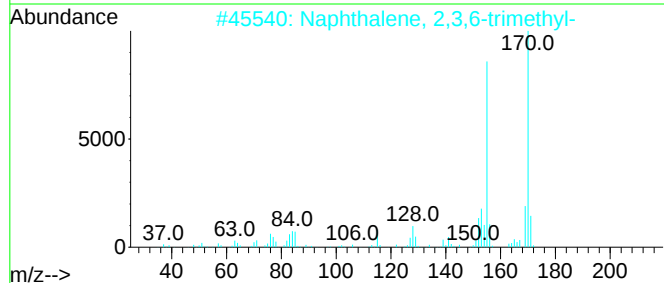
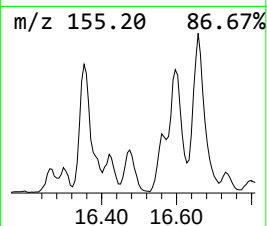
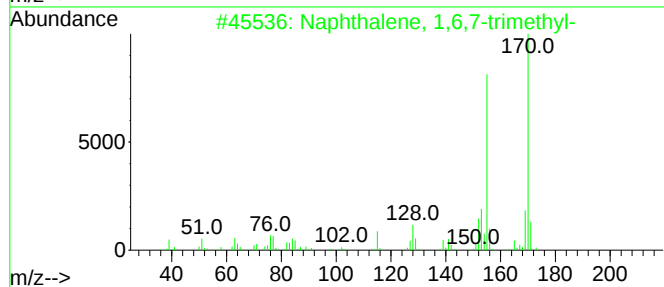
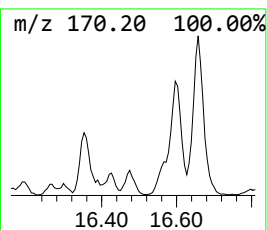
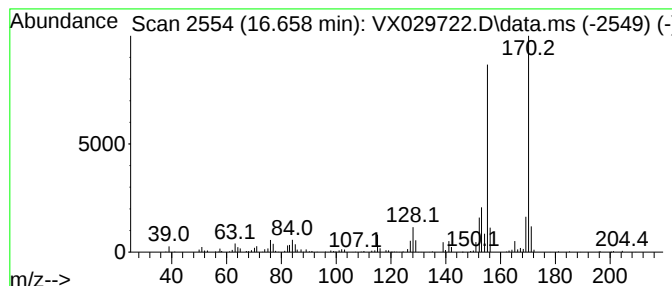
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 2,3,6-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.658	12.13 ug/l	271171	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	98
2			Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	97
3			Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	96
4			4,6,8-Trimethylazulene	170	C13H14	000941-81-1	94
5			Naphthalene, 1,4,5-trimethyl-	170	C13H14	002131-41-1	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062222\
Data File : VX029722.D
Acq On : 23 Jun 2022 05:21
Operator : JC/MD
Sample : N3293-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30873

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.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,...	15.481	8.3	ug/l	185223	4	12.024	1118100	50.0
Naphthalene, 2,...	15.615	8.4	ug/l	187539	4	12.024	1118100	50.0
Naphthalene, 1,...	15.652	7.6	ug/l	169136	4	12.024	1118100	50.0
Naphthalene, 1,...	15.841	6.7	ug/l	148765	4	12.024	1118100	50.0
4,6,8-Trimethyl...	16.353	6.1	ug/l	136634	4	12.024	1118100	50.0
Naphthalene, 1,...	16.597	10.8	ug/l	242348	4	12.024	1118100	50.0
Naphthalene, 2,...	16.658	12.1	ug/l	271171	4	12.024	1118100	50.0