

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX110918\
 Data File : VX005881.D
 Acq On : 10 Nov 2018 00:51
 Operator : JC/MD
 Sample : J5889-04
 Misc : 11.32g/5mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WALL-D

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\82X110718W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.696	65	89	90	rBV	15681	80812	14.07%	2.053%
2	2.800	266	270	276	rBV2	3185	6577	1.15%	0.167%
3	3.025	301	307	314	rBV2	2779	7217	1.26%	0.183%
4	5.507	702	714	728	rBV	63227	191352	33.31%	4.861%
5	5.659	728	739	752	rVV	125331	346649	60.35%	8.806%
6	6.067	795	806	821	rBV	75750	203616	35.45%	5.172%
7	6.860	925	936	952	rBV2	164439	417373	72.66%	10.602%
8	8.713	1233	1240	1251	rBV	372250	574401	100.00%	14.591%
9	10.116	1464	1470	1483	rBV	336495	479708	83.51%	12.186%
10	10.359	1505	1510	1513	rBV3	4320	7833	1.36%	0.199%
11	11.140	1632	1638	1649	rBV	310958	401618	69.92%	10.202%
12	12.079	1787	1792	1800	rVB	420038	509782	88.75%	12.950%
13	13.414	2000	2011	2015	rBV6	20098	76232	13.27%	1.936%
14	14.133	2124	2129	2137	rBV7	6034	18546	3.23%	0.471%
15	14.273	2146	2152	2161	rVB5	21700	61446	10.70%	1.561%
16	14.377	2164	2169	2176	rVB5	12285	27429	4.78%	0.697%
17	14.676	2214	2218	2219	rBV4	6089	8761	1.53%	0.223%
18	14.694	2219	2221	2226	rVB	17144	22358	3.89%	0.568%
19	14.785	2230	2236	2242	rBV2	17078	42477	7.40%	1.079%
20	14.840	2242	2245	2249	rVB	8468	10534	1.83%	0.268%
21	15.060	2272	2281	2289	rBV3	12821	37087	6.46%	0.942%
22	15.255	2305	2313	2315	rBV5	6020	13380	2.33%	0.340%
23	15.352	2320	2329	2333	rBV5	6666	19709	3.43%	0.501%
24	15.450	2340	2345	2347	rBV3	7491	12006	2.09%	0.305%
25	15.474	2347	2349	2355	rVV6	6270	13056	2.27%	0.332%
26	15.554	2355	2362	2369	rVB2	29600	62596	10.90%	1.590%
27	15.688	2380	2384	2387	rBV	20550	32427	5.65%	0.824%
28	15.724	2387	2390	2399	rVB3	20491	39462	6.87%	1.002%
29	15.919	2414	2422	2427	rBV2	9129	22463	3.91%	0.571%
30	16.072	2443	2447	2452	rBV2	8439	13475	2.35%	0.342%
31	16.169	2459	2463	2469	rVB4	4926	9111	1.59%	0.231%
32	16.352	2488	2493	2496	rBV4	5771	11857	2.06%	0.301%
33	16.444	2503	2508	2516	rVB	12978	24872	4.33%	0.632%
34	16.572	2525	2529	2533	rVB3	4427	7858	1.37%	0.200%

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35	16.694	2535	2549	2554	rBV	27288	78457	13.66%	1.993%
36	16.755	2554	2559	2564	rBV	22483	44079	7.67%	1.120%

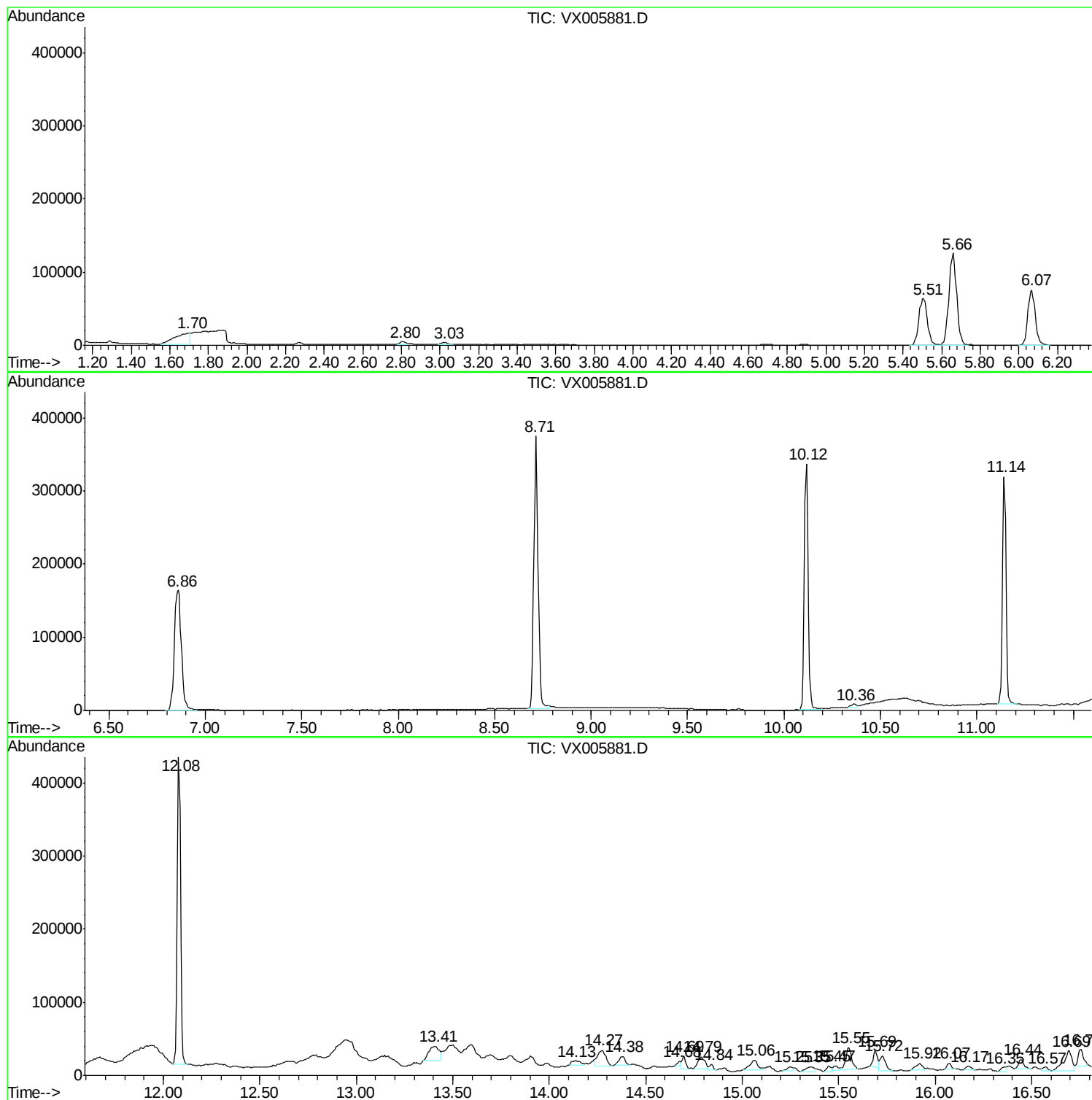
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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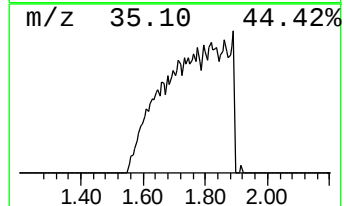
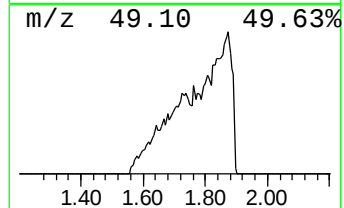
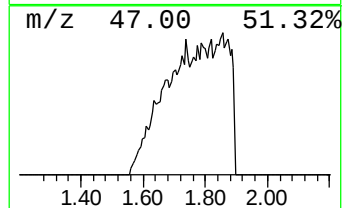
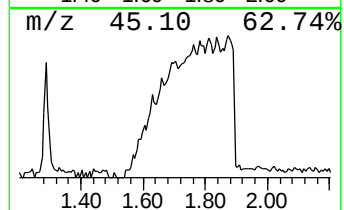
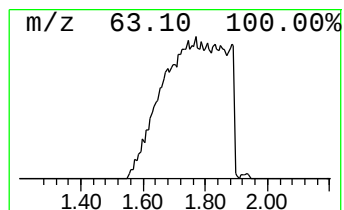
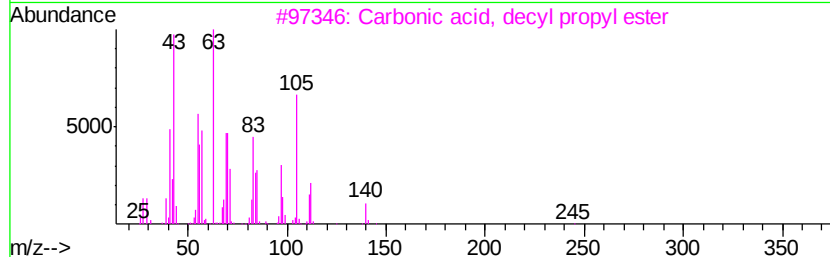
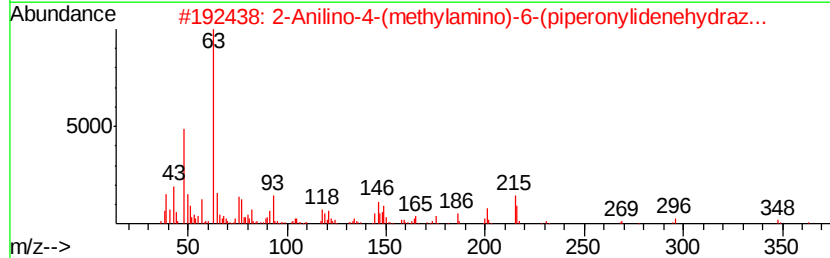
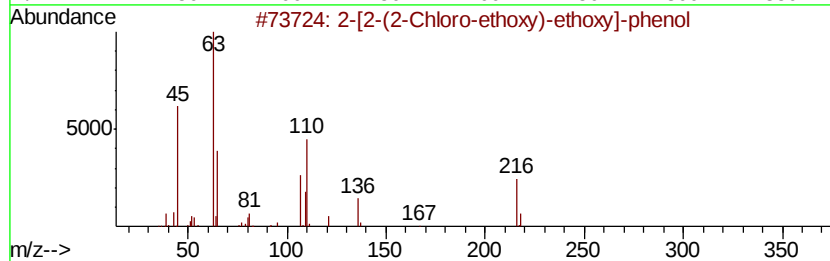
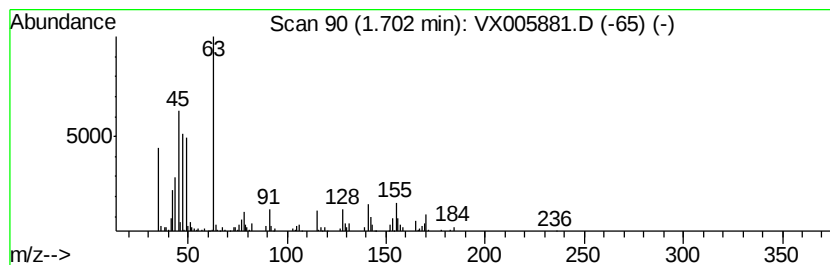
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Quant Title : SW846 8260

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

Peak Number 1 unknown1.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.70	11.66 ug/l	80812	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-[2-(2-Chloro-ethoxy)-ethoxy]-p...	216	C10H13ClO3	1000317-46-1	28
2		2-Anilino-4-(methylamino)-6-(pip...	363	C18H17N7O2	1000225-97-3	23
3		Carbonic acid, decyl propyl ester	244	C14H28O3	1000314-53-7	12
4		1-Bromo-1-chloroethane	142	C2H4BrCl	000593-96-4	9
5		Carmustine	213	C5H9Cl2N3O2	000154-93-8	9



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Instrument :
MSVOA_X
ClientSampled :
WALL-D

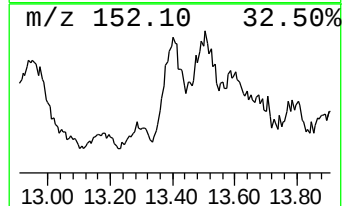
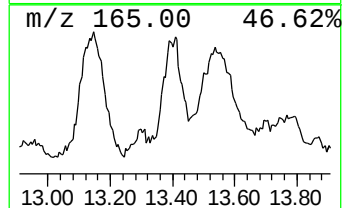
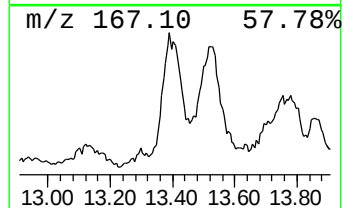
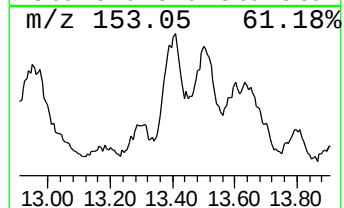
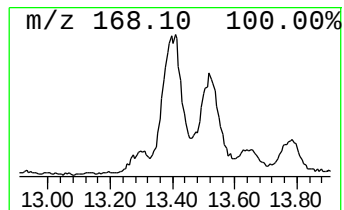
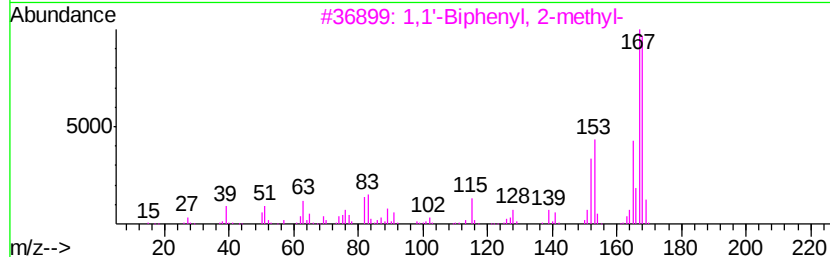
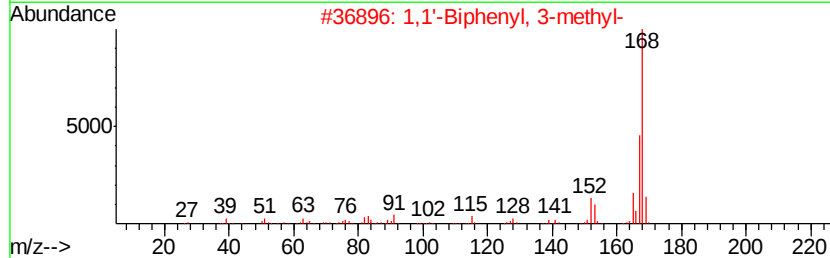
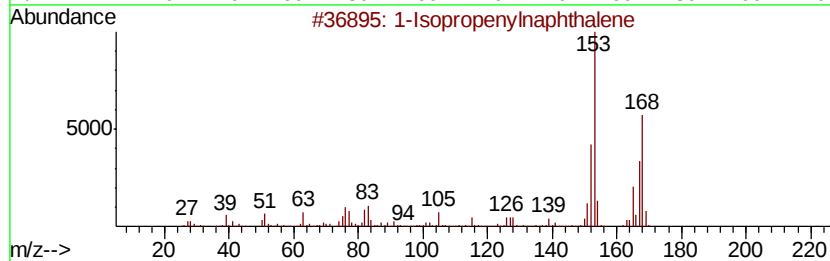
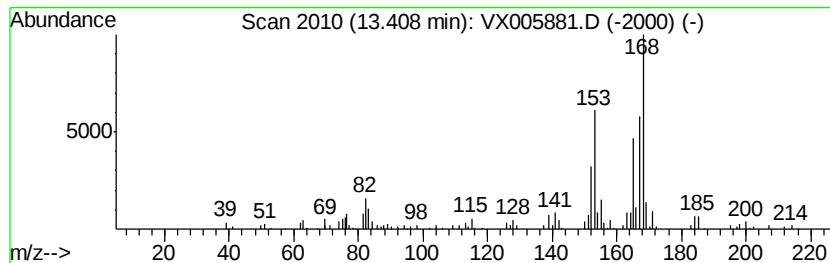
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Isopropenylnaphthalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.41	7.48 ug/l	76232	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Isopropenylnaphthalene	168	C13H12	001855-47-6	62
2		1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	60
3		1,1'-Biphenyl, 2-methyl-	168	C13H12	000643-58-3	50
4		Naphthalene, 1-(2-propenyl)-	168	C13H12	002489-86-3	46
5		1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	46



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ALS Vial : 32 Sample Multiplier: 1

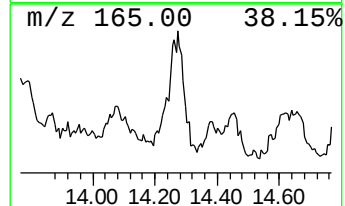
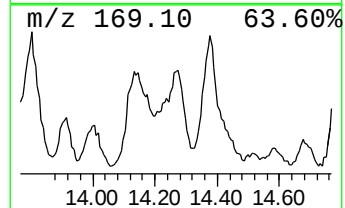
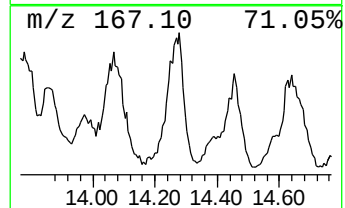
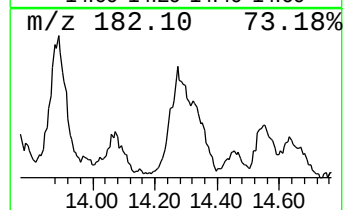
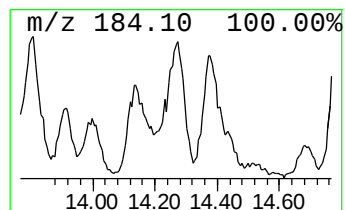
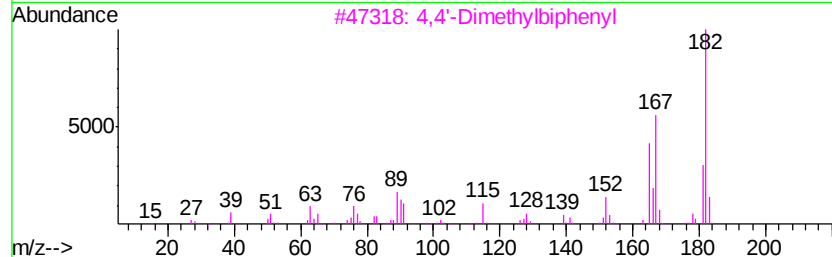
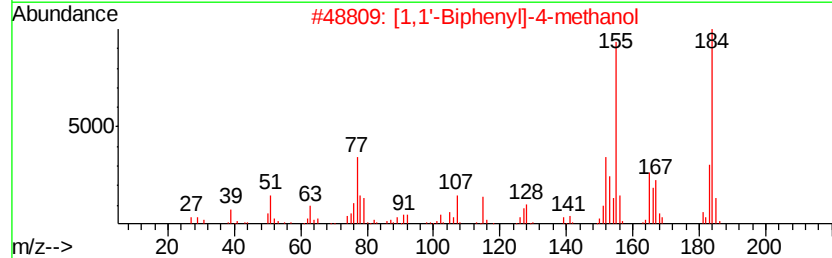
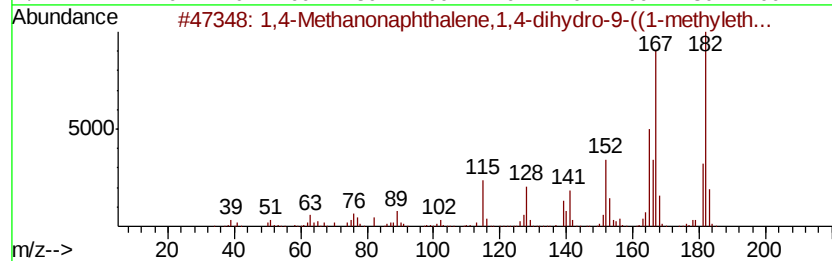
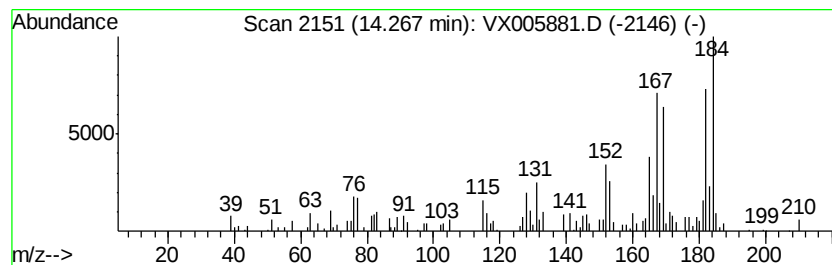
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,4-Methanonaphthalene,1,4-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.27	6.03 ug/l	61446	1,4-Dichlorobenzene-d4	12.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Methanonaphthalene,1,4-dihyd...	182	C14H14	007350-72-3	89
2	[1,1'-Biphenyl]-4-methanol	184	C13H12O	003597-91-9	60
3	4,4'-Dimethylbiphenyl	182	C14H14	000613-33-2	55
4	Tricyclo[4.4.1.0(2,5)]undeca-1(1...	182	C14H14	055836-29-8	50
5	7-Phenylbicyclo[3.2.1]octa-2,6-d...	182	C14H14	1000201-01-7	46



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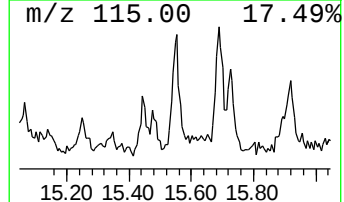
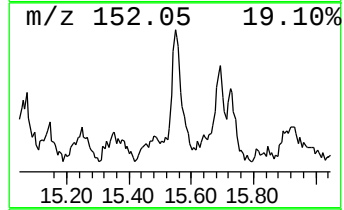
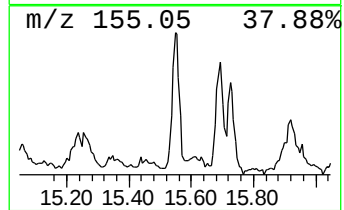
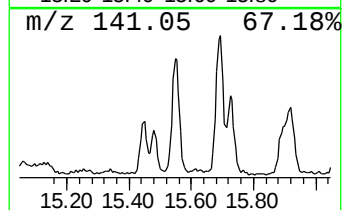
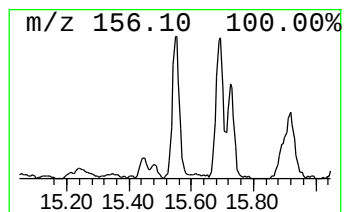
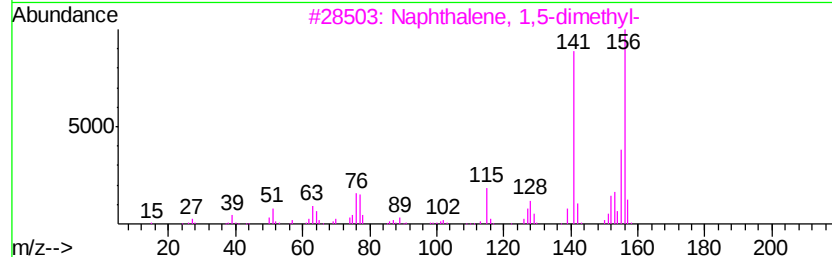
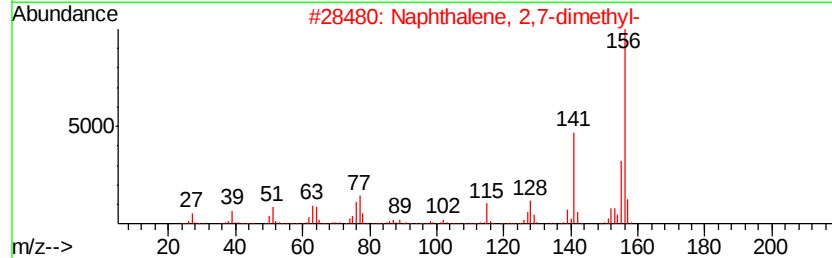
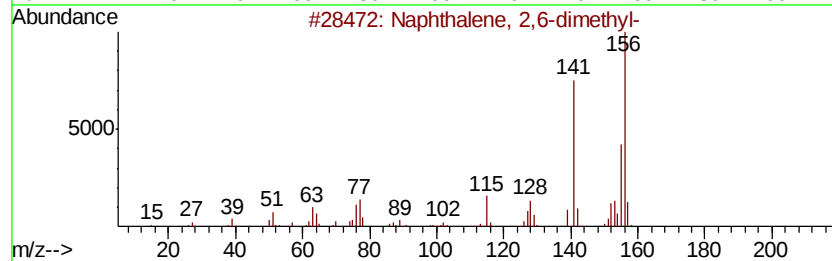
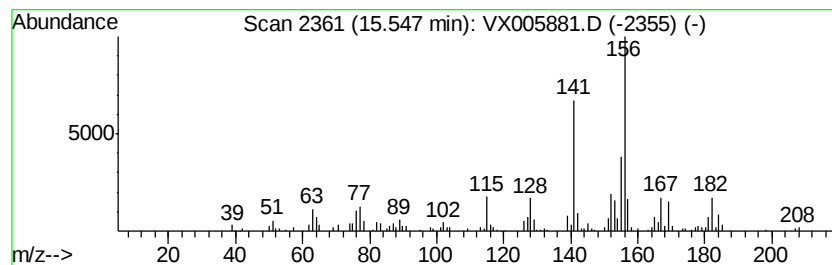
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Peak Number 4 Naphthalene, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.55	6.14 ug/l	62596	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
2		Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3		Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96
4		Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5		Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	93



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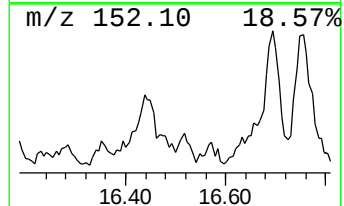
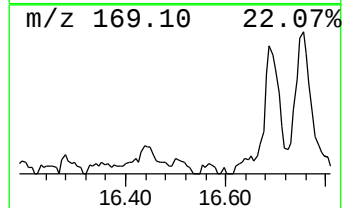
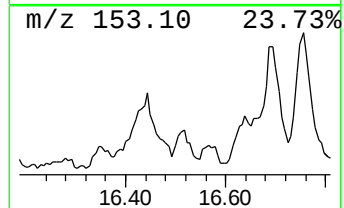
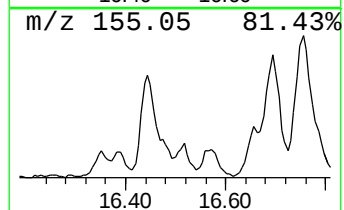
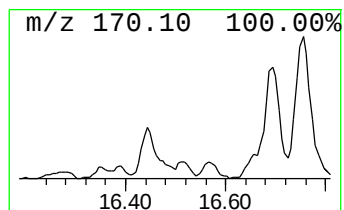
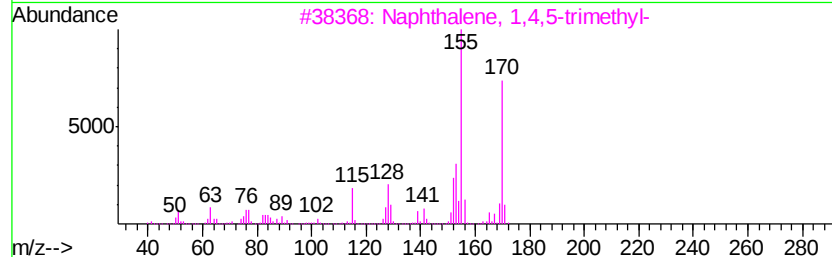
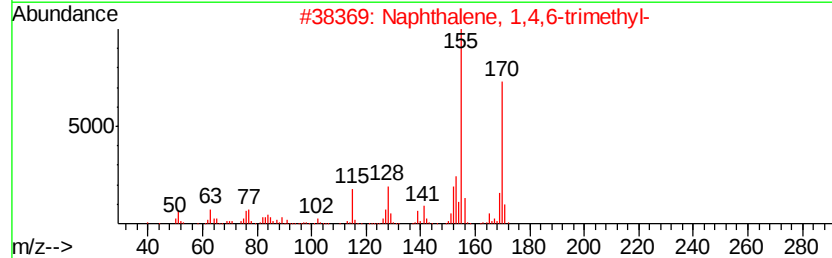
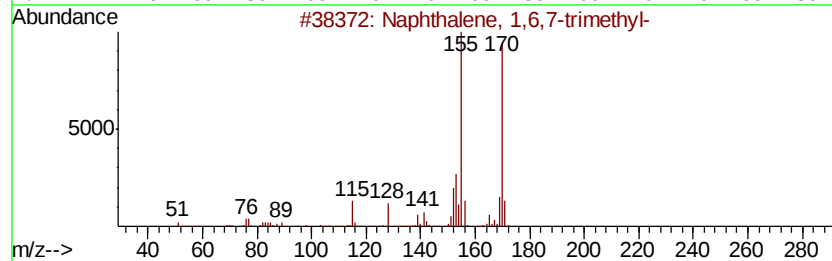
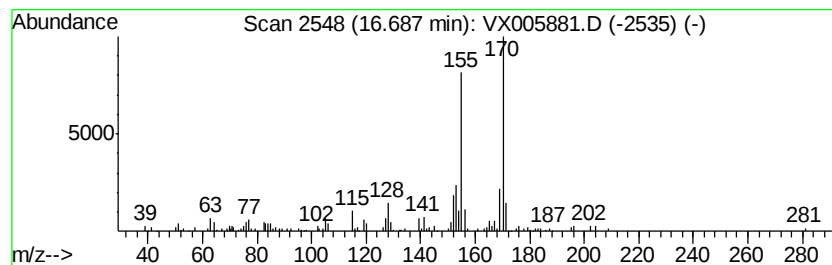
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Peak Number 5 Naphthalene, 1,6,7-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	7.70 ug/l	78457	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	96
2		Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	96
3		Naphthalene, 1,4,5-trimethyl-	170	C13H14	002131-41-1	95
4		Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	94
5		4,6,8-Trimethylazulene	170	C13H14	000941-81-1	93



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX110918\
Data File : VX005881.D
Acq On : 10 Nov 2018 00:51
Operator : JC/MD
Sample : J5889-04
Misc : 11.32g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WALL-D

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.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
unknown1.70	1.70	11.7	ug/l	80812	1	5.66	346649	50.0
1-Isopropenyl naph...	13.41	7.5	ug/l	76232	4	12.08	509782	50.0
1,4-Methanonaphth...	14.27	6.0	ug/l	61446	4	12.08	509782	50.0
Naphthalene, 2,6-...	15.55	6.1	ug/l	62596	4	12.08	509782	50.0
Naphthalene, 1,6,...	16.69	7.7	ug/l	78457	4	12.08	509782	50.0