

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040717\
 Data File : BF094275.D
 Acq On : 7 Apr 2017 16:14
 Operator : SJ/MA
 Sample : I2572-04
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT-2891

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	27	43	48	rBV3	58549	255048	4.89%	0.514%
2	2.522	106	108	110	rVB	89307	63439	1.22%	0.128%
3	3.993	354	358	372	rVB	478856	729610	13.98%	1.470%
4	4.387	419	425	429	rBV	3917807	4778918	91.56%	9.629%
5	4.992	523	528	535	rBV2	42488	74763	1.43%	0.151%
6	5.463	601	608	612	rVB2	3734653	5219345	100.00%	10.517%
7	5.598	624	631	634	rBV	4071983	5009219	95.97%	10.094%
8	5.845	669	673	677	rBV	1107124	1017383	19.49%	2.050%
9	6.028	698	704	707	rBV	3384419	3809115	72.98%	7.675%
10	6.498	776	784	787	rBV	2733913	3300031	63.23%	6.650%
11	7.051	874	878	886	rVB2	45999	56301	1.08%	0.113%
12	7.345	923	928	932	rBV	1450992	1380496	26.45%	2.782%
13	7.504	947	955	958	rBV	2887132	3674283	70.40%	7.404%
14	7.722	987	992	996	rVB	211856	187533	3.59%	0.378%
15	8.675	1147	1154	1157	rVB	4268580	4860863	93.13%	9.795%
16	9.163	1233	1237	1241	rBV	530334	520432	9.97%	1.049%
17	9.486	1285	1292	1295	rBV	1520088	1514745	29.02%	3.052%
18	9.516	1295	1297	1301	rVB	276885	238679	4.57%	0.481%
19	10.080	1389	1393	1397	rBV	67588	64831	1.24%	0.131%
20	10.380	1442	1444	1449	rVB	76492	67646	1.30%	0.136%
21	10.463	1451	1458	1461	rBV	2617433	3039709	58.24%	6.125%
22	10.663	1488	1492	1494	rBV	91937	93143	1.78%	0.188%
23	11.216	1582	1586	1590	rVB2	77064	81956	1.57%	0.165%
24	11.304	1597	1601	1604	rBV	1282362	1366740	26.19%	2.754%
25	11.333	1604	1606	1609	rVB	248021	208578	4.00%	0.420%
26	11.886	1693	1700	1704	rBV	134689	162477	3.11%	0.327%
27	11.927	1704	1707	1710	rVV	56868	61498	1.18%	0.124%
28	11.963	1710	1713	1717	rVB	60642	59350	1.14%	0.120%
29	12.057	1727	1729	1733	rBV	68582	66727	1.28%	0.134%
30	12.610	1819	1823	1826	rBV	64531	68220	1.31%	0.137%
31	12.798	1851	1855	1858	rVB	260074	259883	4.98%	0.524%
32	13.068	1894	1901	1905	rBV	261019	310611	5.95%	0.626%
33	13.210	1921	1925	1932	rBV	217846	263447	5.05%	0.531%
34	13.292	1932	1939	1942	rVV	3238021	3771836	72.27%	7.600%

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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:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.380	2120	2124	2131	rBV	206023	258039	4.94%	0.520%
36	14.451	2132	2136	2145	rVB2	135482	191799	3.67%	0.386%
37	14.557	2148	2154	2157	rBV	988631	1083274	20.75%	2.183%
38	14.586	2157	2159	2162	rVB	89402	73340	1.41%	0.148%
39	15.427	2299	2302	2308	rVB	149036	174049	3.33%	0.351%
40	15.780	2359	2362	2365	rBV	74329	105046	2.01%	0.212%
41	16.121	2418	2420	2426	rVV	69043	87880	1.68%	0.177%
42	16.186	2426	2431	2442	rVB	737231	891154	17.07%	1.796%
43	16.403	2465	2468	2477	rVB	86234	126505	2.42%	0.255%

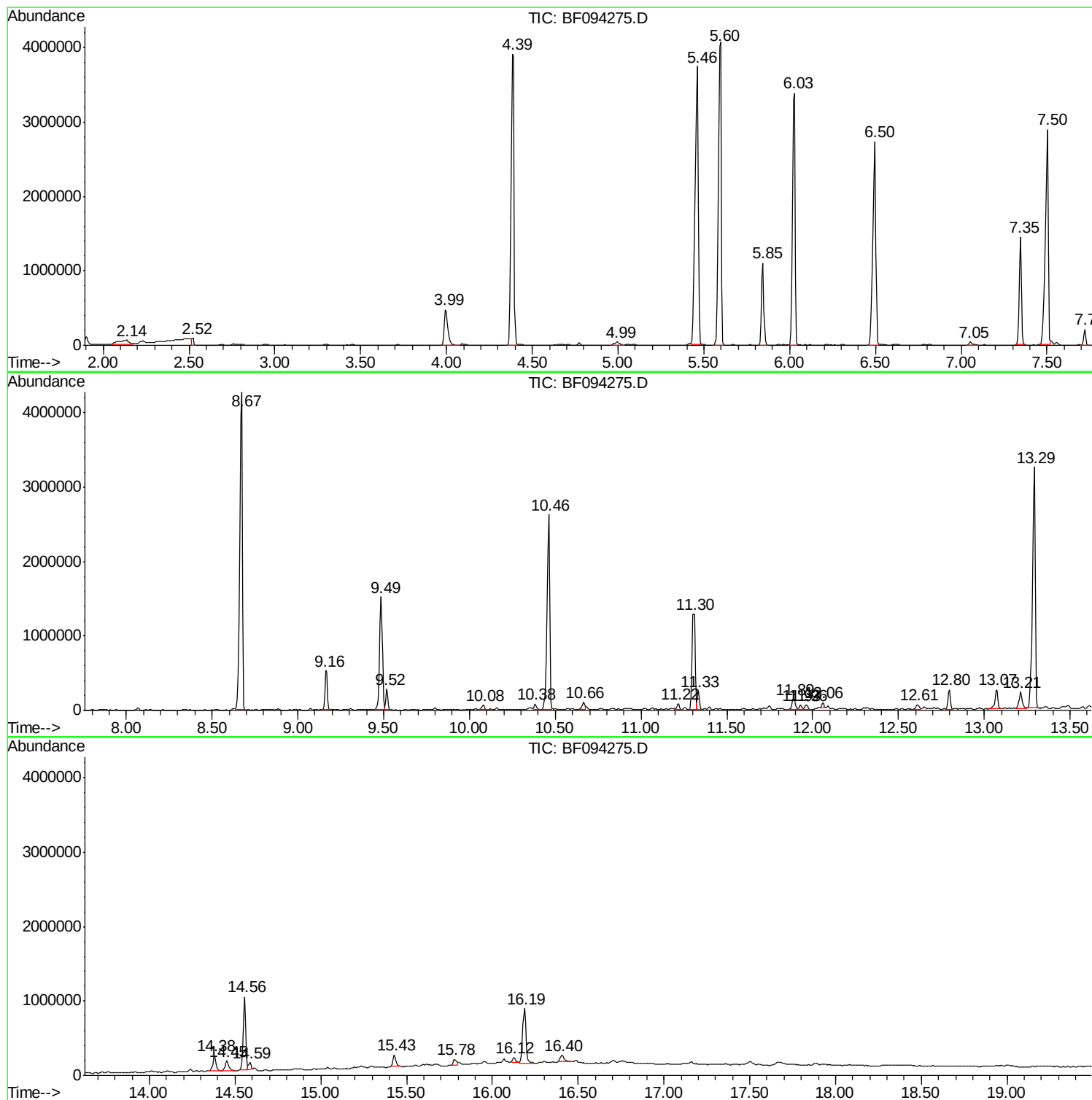
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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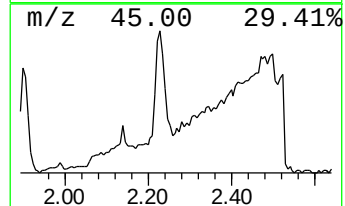
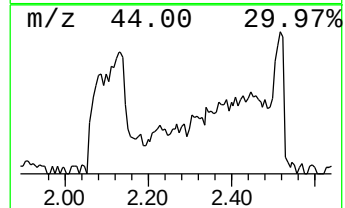
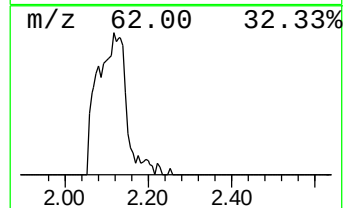
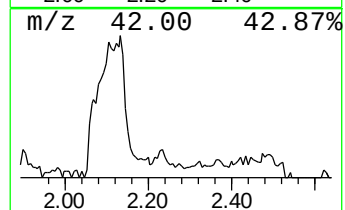
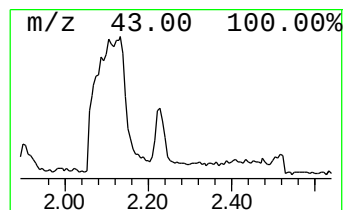
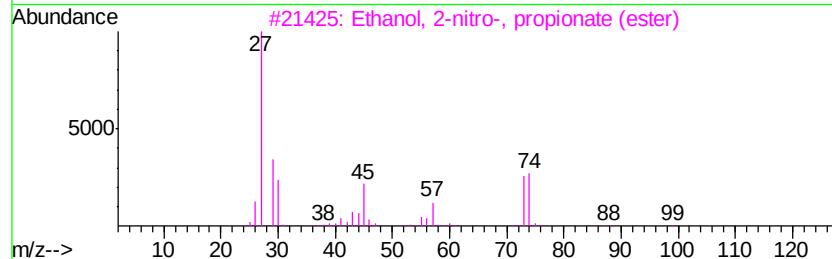
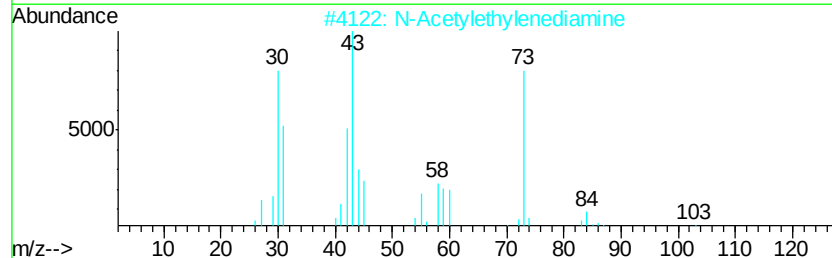
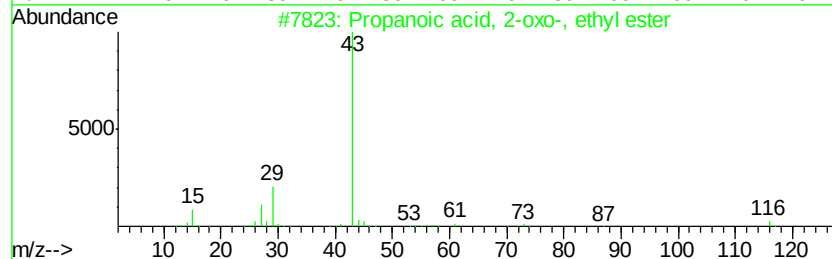
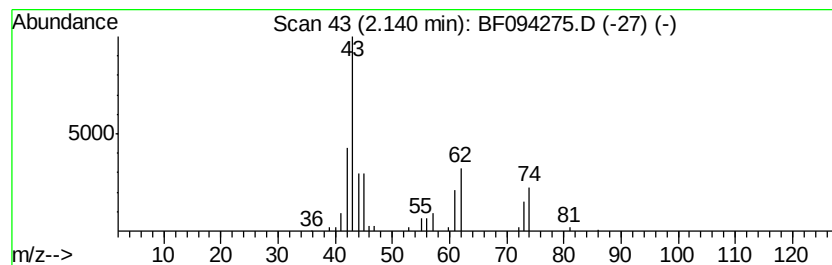
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown2.14 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	5.01 ng	255048	1,4-Dichlorobenzene-d4	5.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-oxo-, ethyl ester	116	C5H8O3	000617-35-6	9
2		N-Acetyethylenediamine	102	C4H10N2O	001001-53-2	9
3		Ethanol, 2-nitro-, propionate (e...	147	C5H9NO4	005390-28-3	9
4		Acetic acid, anhydride with form...	88	C3H4O3	002258-42-6	9
5		1,4-Butanediol	90	C4H10O2	000110-63-4	9



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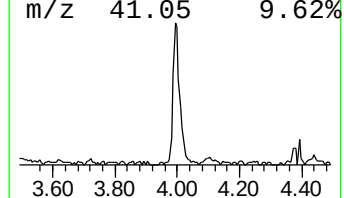
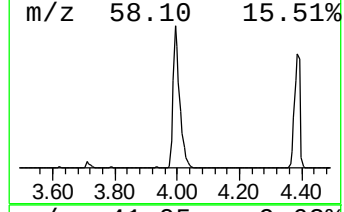
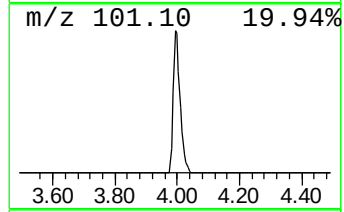
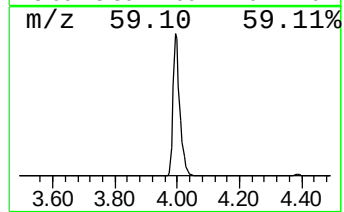
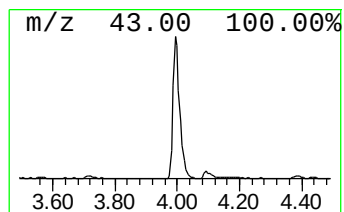
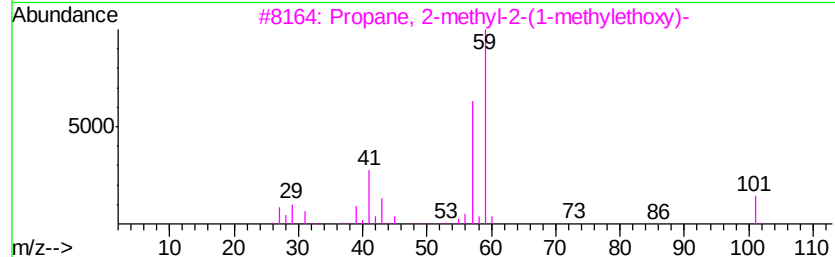
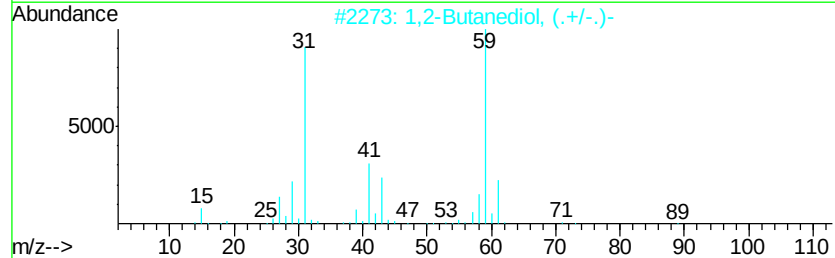
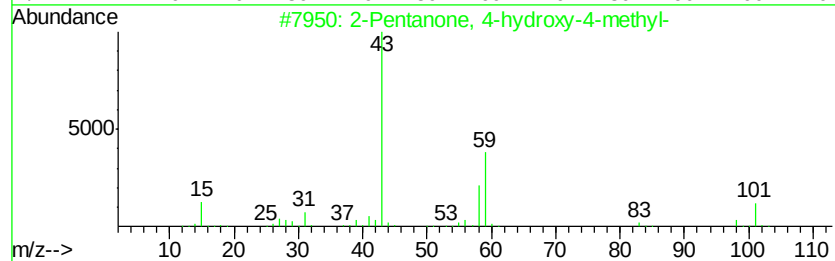
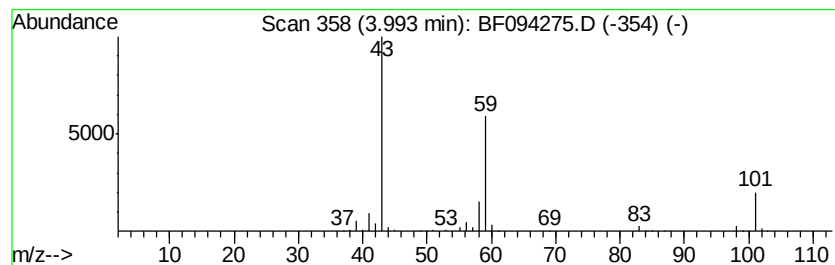
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown3.99 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.99	14.34 ng	729610	1,4-Dichlorobenzene-d4	5.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		1,2-Butanediol, (.+/-.)-	90	C4H10O2	026171-83-5	25
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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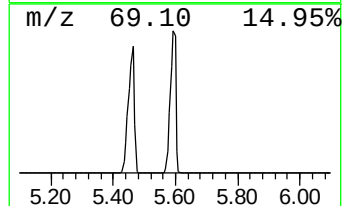
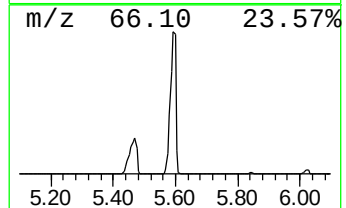
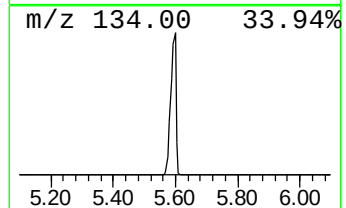
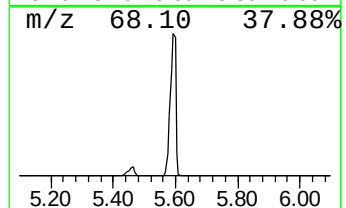
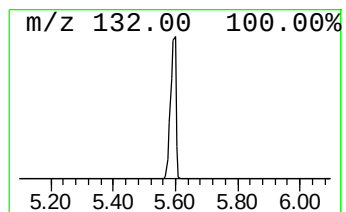
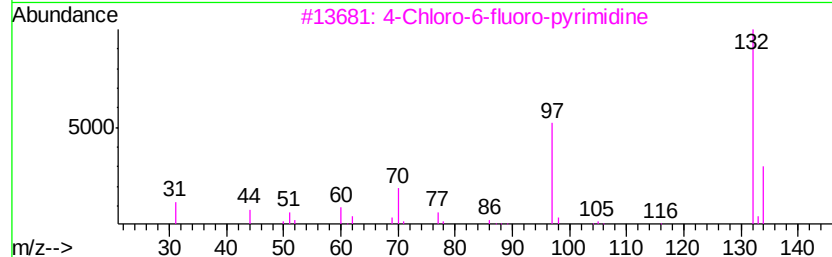
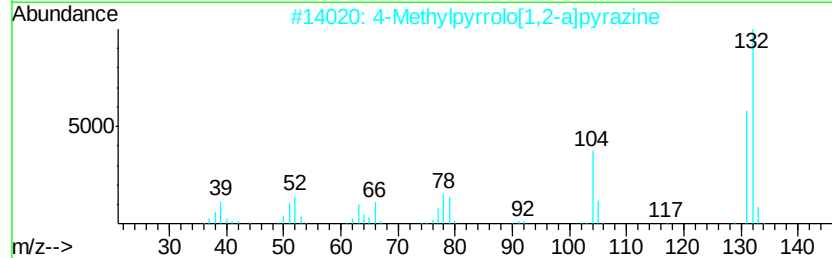
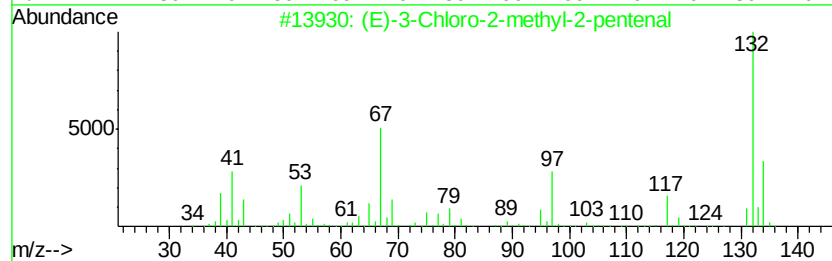
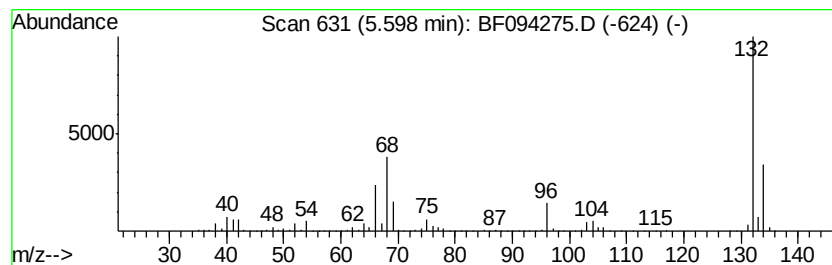
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown5.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	98.47 ng	5009220	1,4-Dichlorobenzene-d4	5.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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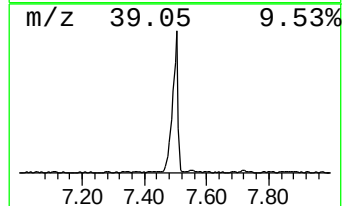
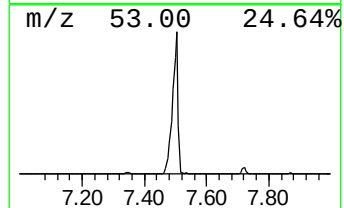
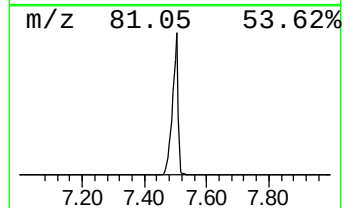
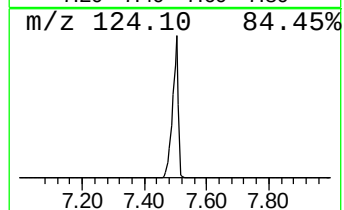
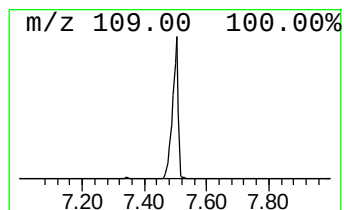
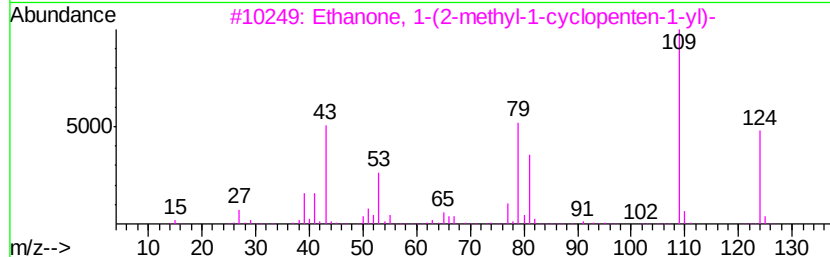
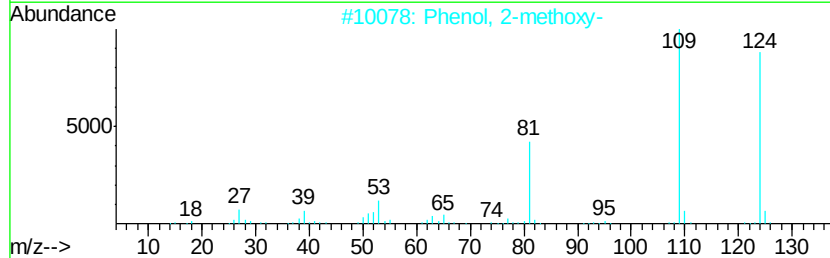
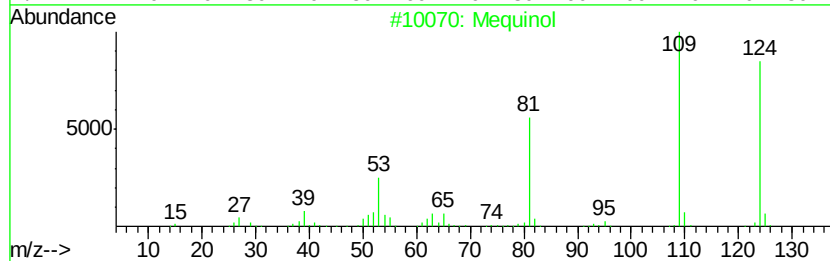
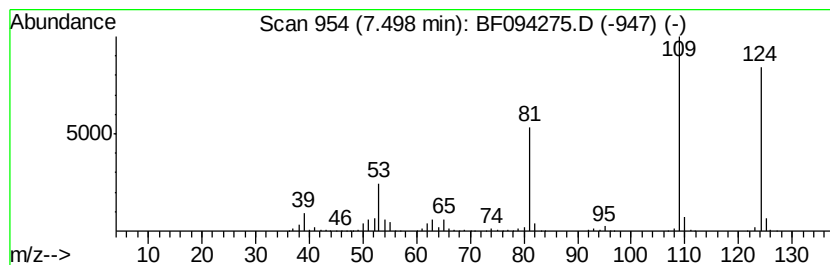
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Mequinol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.50	53.23 ng	3674280	Napthalene-d8	7.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Mequinol	124 C7H8O2	000150-76-5 97
2		Phenol, 2-methoxy-	124 C7H8O2	000090-05-1 94
3		Ethanone, 1-(2-methyl-1-cyclopent...	124 C8H12O	003168-90-9 91
4		2-Acetyl-5-methylfuran	124 C7H8O2	001193-79-9 80
5		2-Cyclopenten-1-one, 3,4,5-trime...	124 C8H12O	055683-21-1 78



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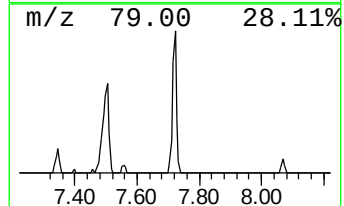
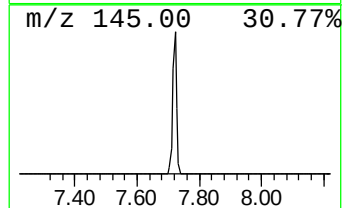
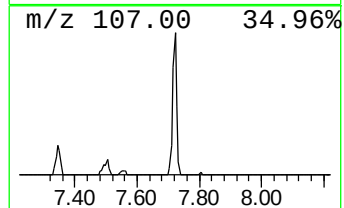
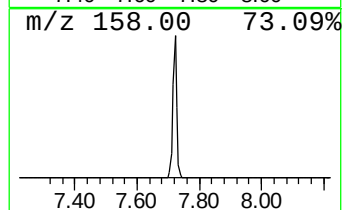
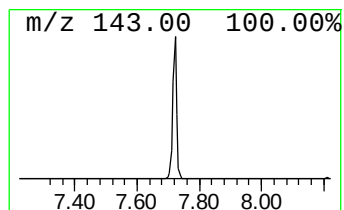
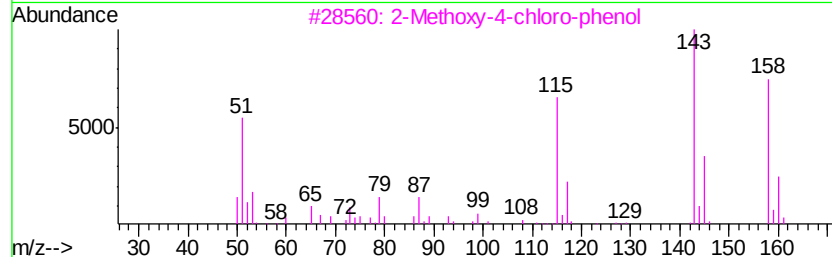
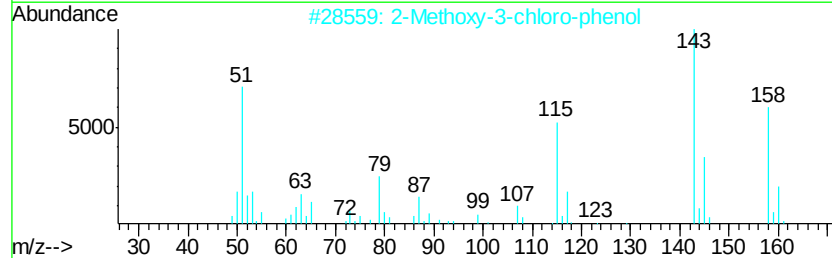
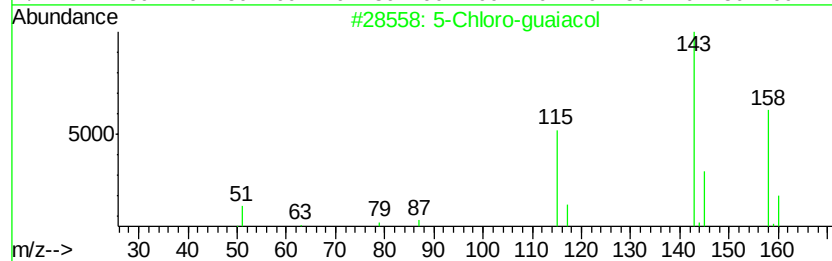
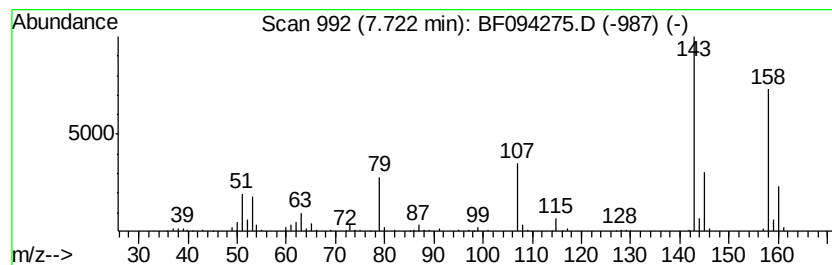
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 5-Chloro-guaiacol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.72	2.72 ng	187533	Napthalene-d8	7.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Chloro-quaiacol	158	C7H7ClO2	003743-23-5	81
2		2-Methoxy-3-chloro-phenol	158	C7H7ClO2	077102-92-2	80
3		2-Methoxy-4-chloro-phenol	158	C7H7ClO2	016766-30-6	58
4		4-Chloro-3-methylpyridine 1-oxide	143	C6H6ClNO	001073-34-3	43
5		Phenol, 3-amino-2-chloro-	143	C6H6ClNO	056962-01-7	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040717\
Data File : BF094275.D
Acq On : 7 Apr 2017 16:14
Operator : SJ/MA
Sample : I2572-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

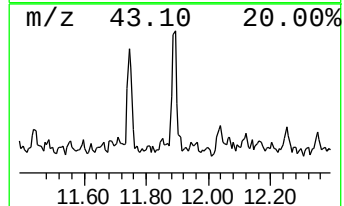
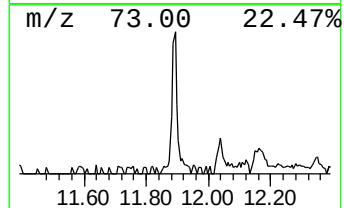
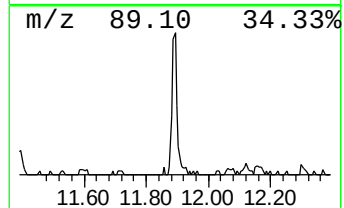
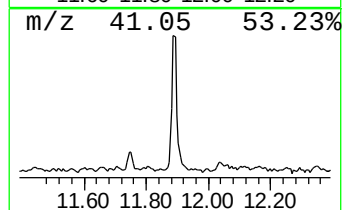
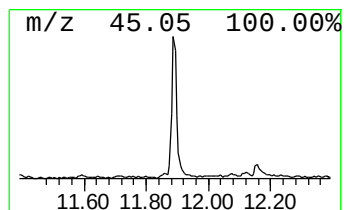
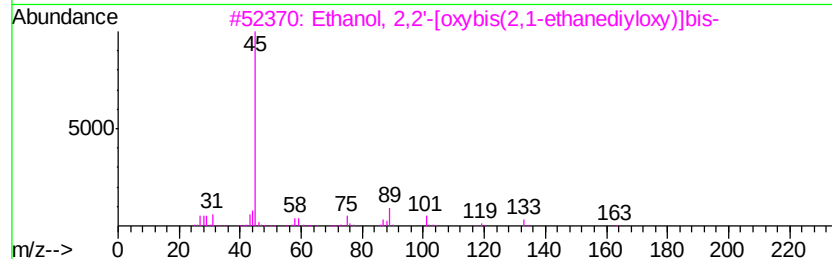
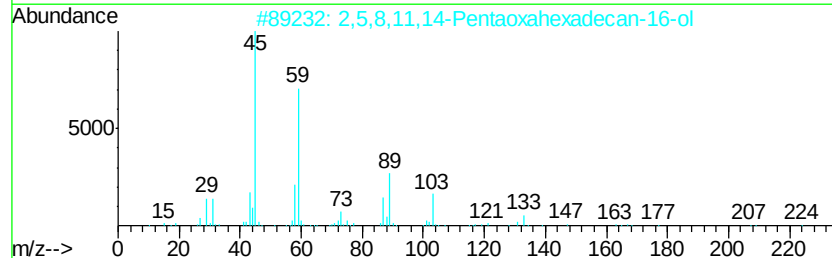
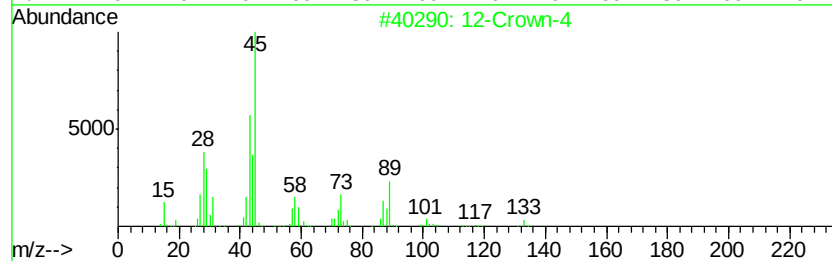
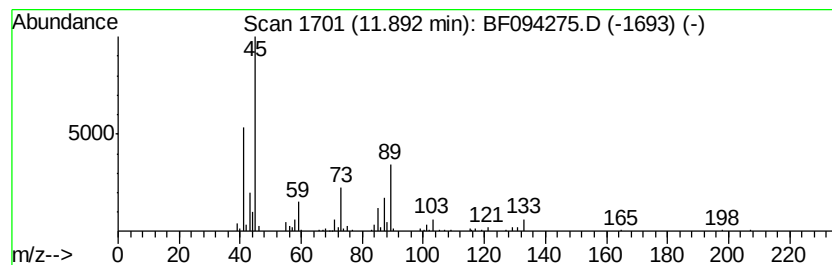
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 12-Crown-4 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.89	2.38 ng	162477	Phenanthrene-d10	11.31	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	12-Crown-4	176	C8H16O4	000294-93-9	72
2	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	64
3	Ethanol, 2,2'-[oxybis(2,1-ethane...	194	C8H18O5	000112-60-7	59
4	15-Crown-5	220	C10H20O5	033100-27-5	56
5	Pentaethylene glycol	238	C10H22O6	004792-15-8	56



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040717\
Data File : BF094275.D
Acq On : 7 Apr 2017 16:14
Operator : SJ/MA
Sample : I2572-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-2891

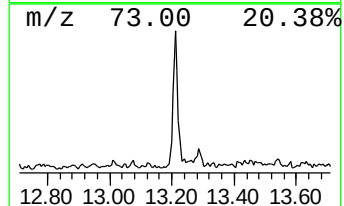
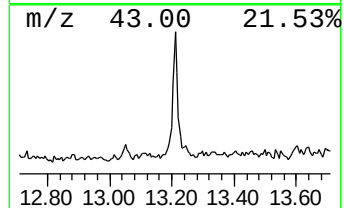
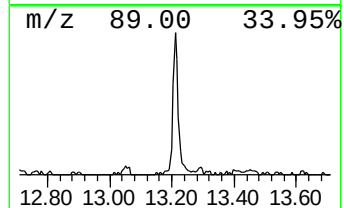
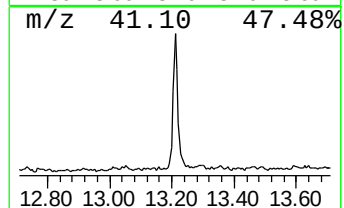
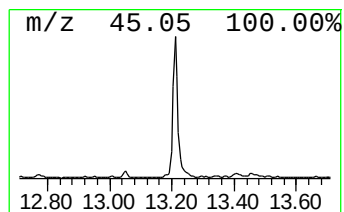
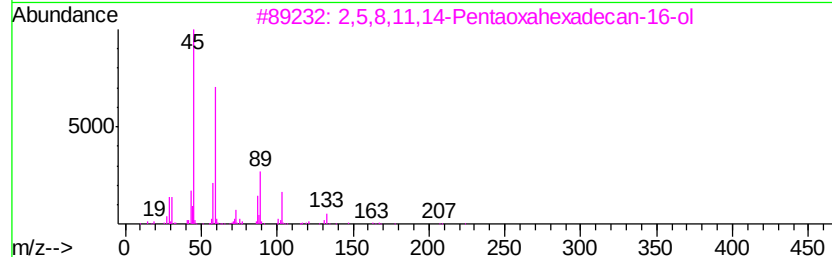
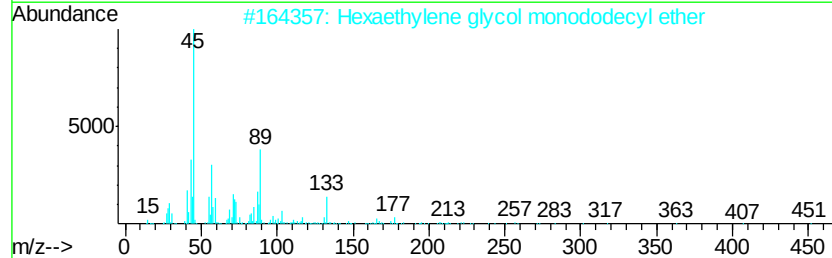
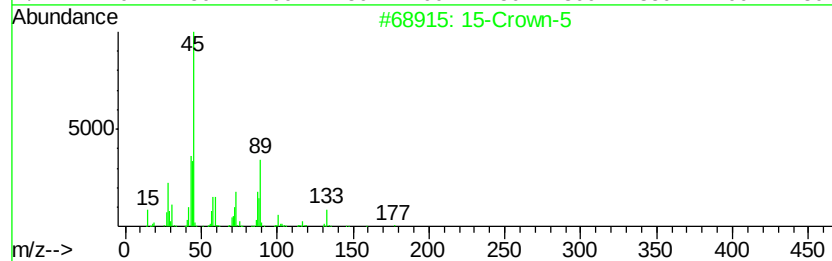
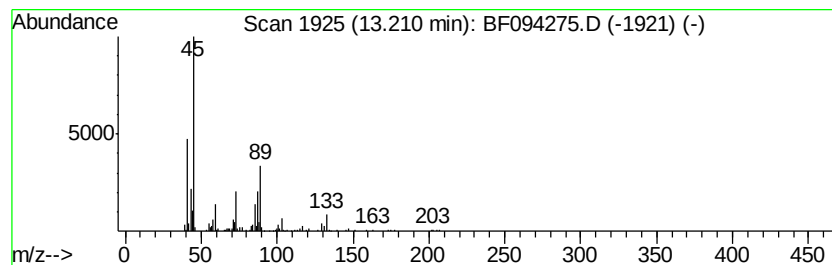
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 15-Crown-5 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	4.86 ng	263447	Chrysene-d12	14.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	15-Crown-5	220	C10H20O5	033100-27-5	72
2		Hexaethylene glycol monododecyl ...	450	C24H50O7	003055-96-7	64
3		2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	59
4		12-Crown-4	176	C8H16O4	000294-93-9	56
5		Ethanol, 2,2'-[oxybis(2,1-ethane...	194	C8H18O5	000112-60-7	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040717\
Data File : BF094275.D
Acq On : 7 Apr 2017 16:14
Operator : SJ/MA
Sample : I2572-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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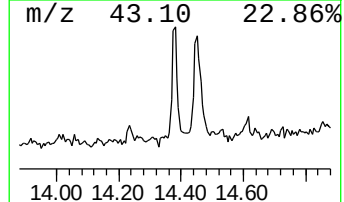
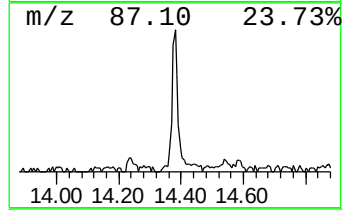
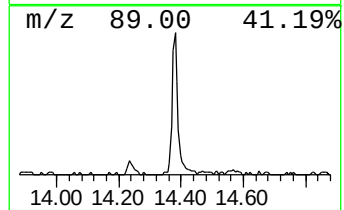
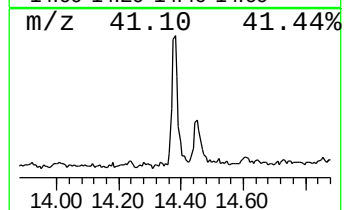
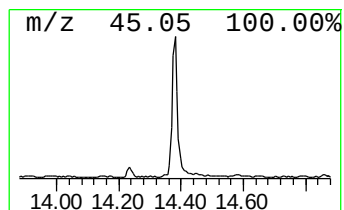
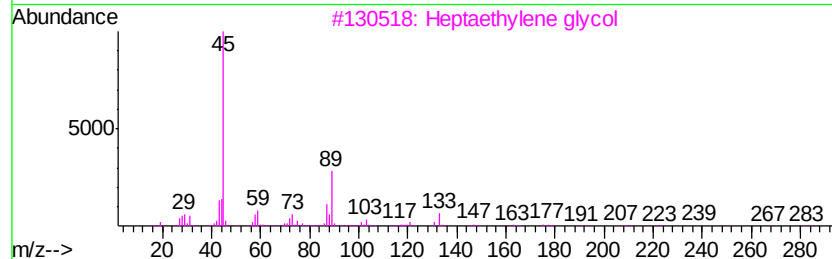
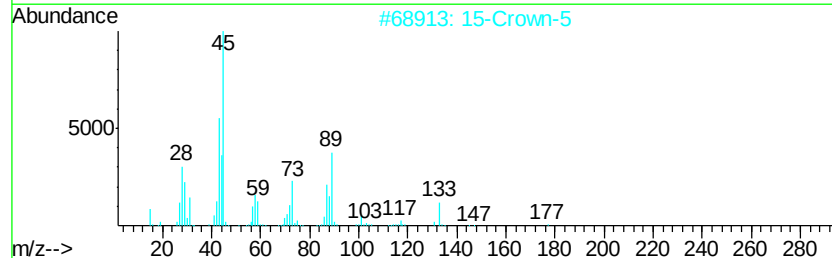
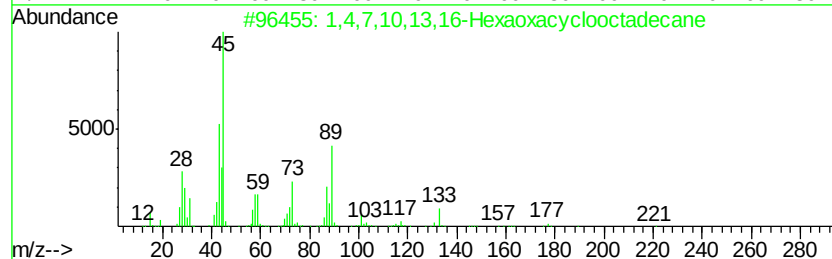
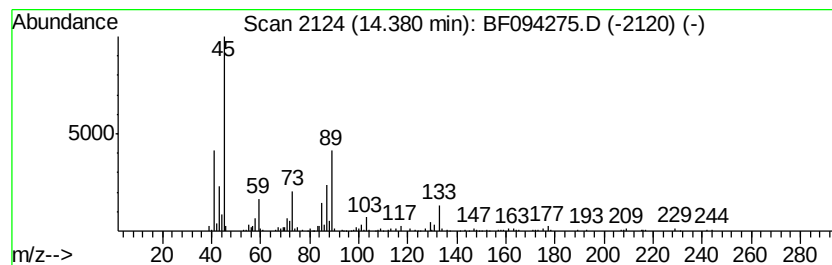
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1,4,7,10,13,16-Hexaoxacyclo... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.38	4.76 ng	258039	Chrysene-d12	14.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	78
2		15-Crown-5	220	C10H20O5	033100-27-5	78
3		Heptaethylene glycol	326	C14H30O8	005617-32-3	72
4		Hexaethylene glycol monododecyl ...	450	C24H50O7	003055-96-7	72
5		Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040717\
Data File : BF094275.D
Acq On : 7 Apr 2017 16:14
Operator : SJ/MA
Sample : I2572-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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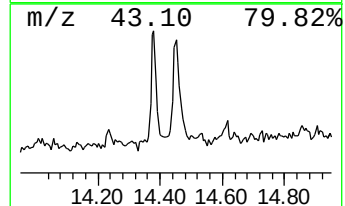
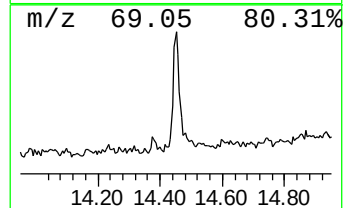
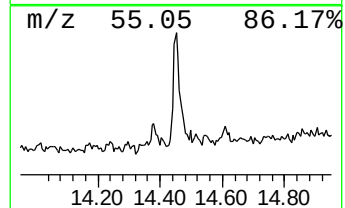
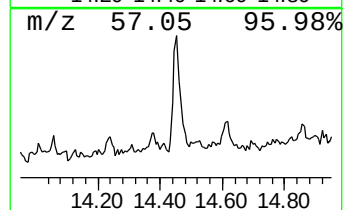
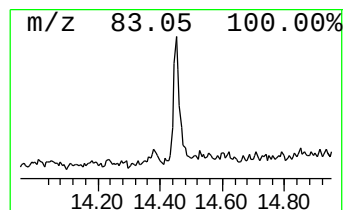
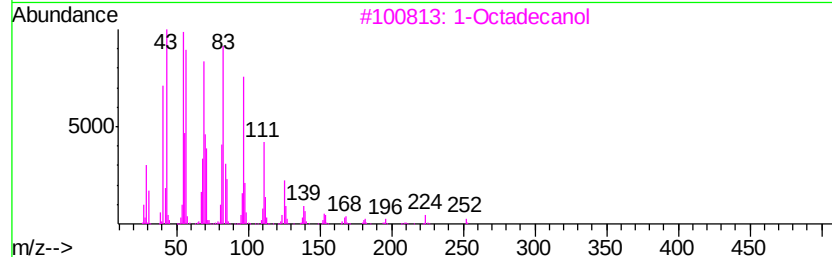
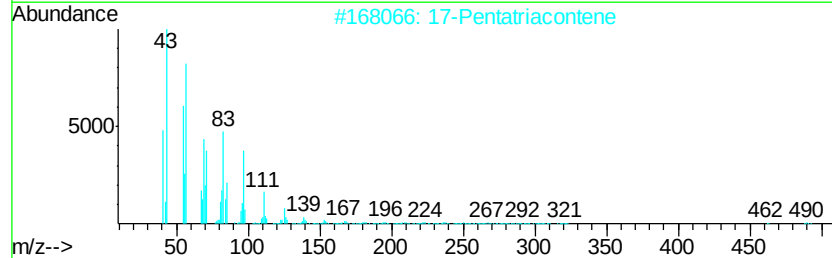
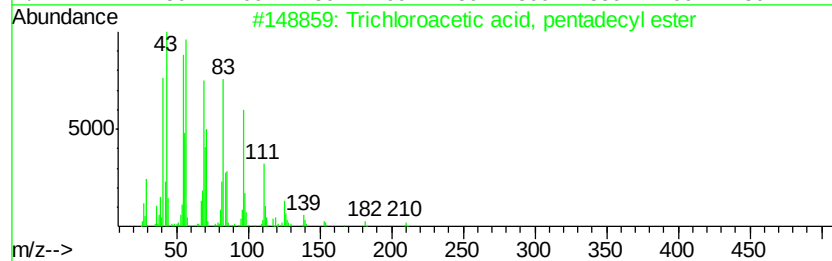
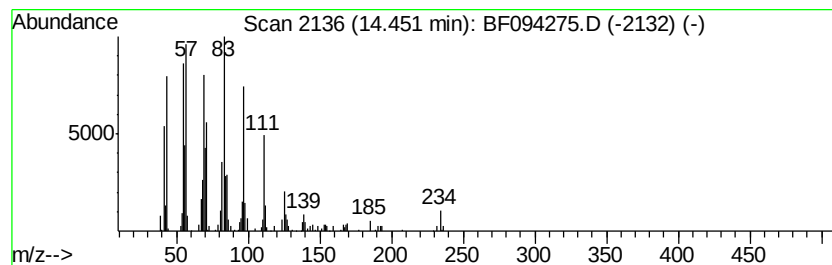
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Trichloroacetic acid, penta... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	3.54 ng	191799	Chrysene-d12	14.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
2			17-Pentatriacontene	491	C35H70	006971-40-0	80
3			1-Octadecanol	270	C18H38O	000112-92-5	76
4			3-Eicosene, (E)-	280	C20H40	074685-33-9	74
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040717\
Data File : BF094275.D
Acq On : 7 Apr 2017 16:14
Operator : SJ/MA
Sample : I2572-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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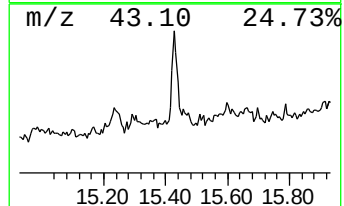
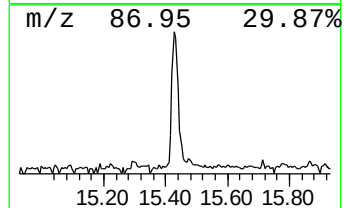
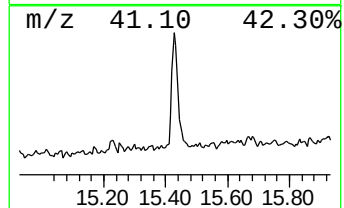
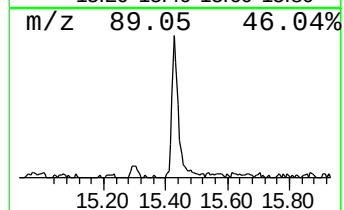
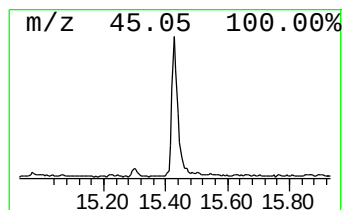
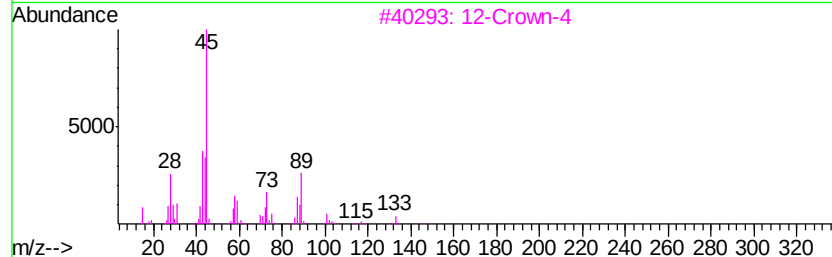
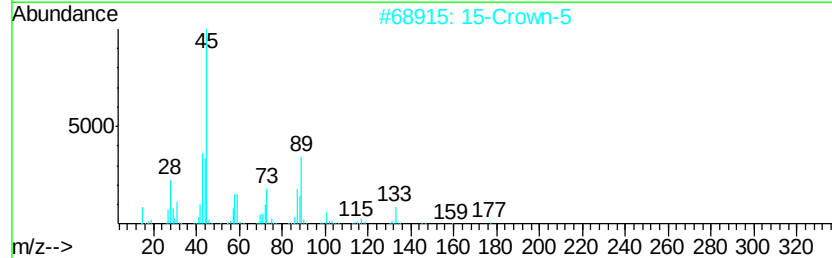
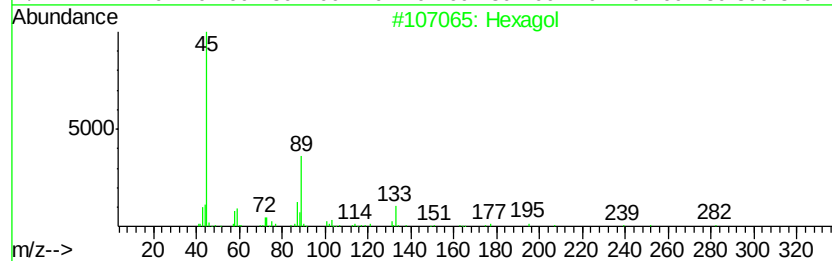
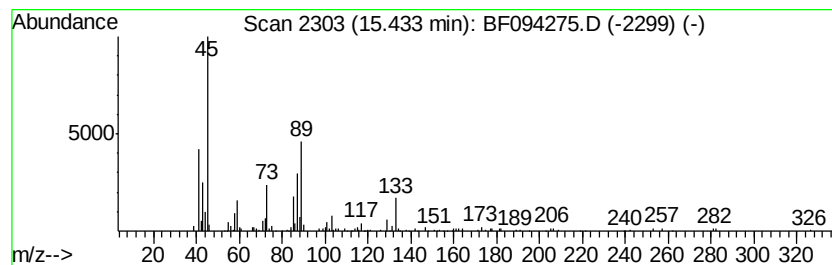
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Hexagol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.43	3.91 ng	174049	Perylene-d12	16.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexagol	282	C12H26O7	002615-15-8	81
2		15-Crown-5	220	C10H20O5	033100-27-5	78
3		12-Crown-4	176	C8H16O4	000294-93-9	64
4		Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	50
5		Cyclohexyl-15-crown-5	274	C14H26O5	017454-48-7	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040717\
Data File : BF094275.D
Acq On : 7 Apr 2017 16:14
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Sample : I2572-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

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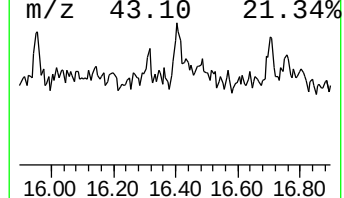
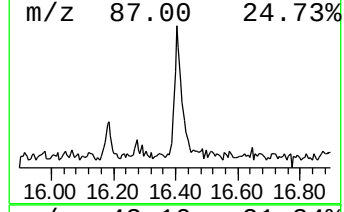
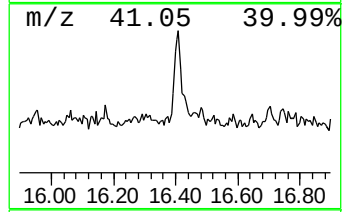
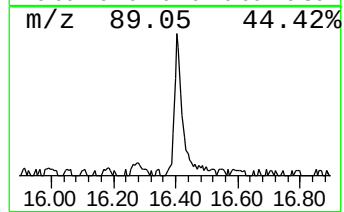
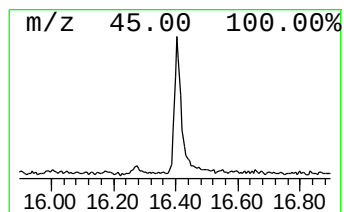
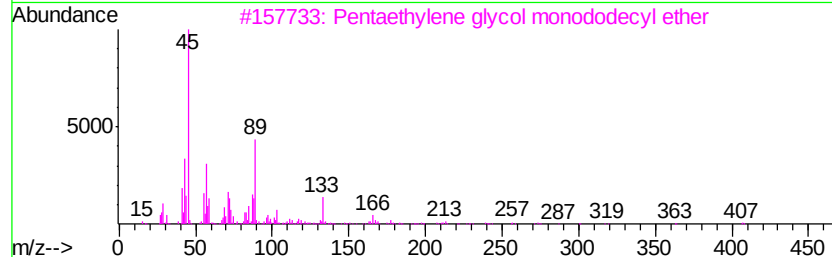
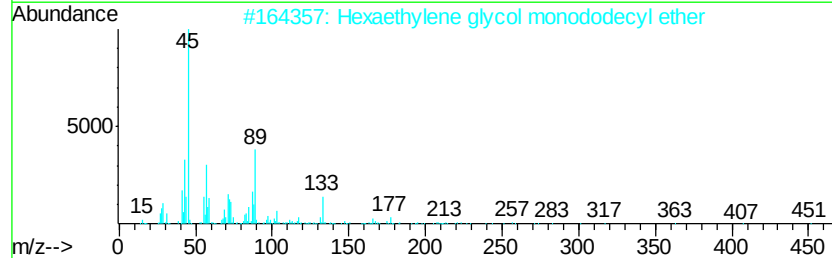
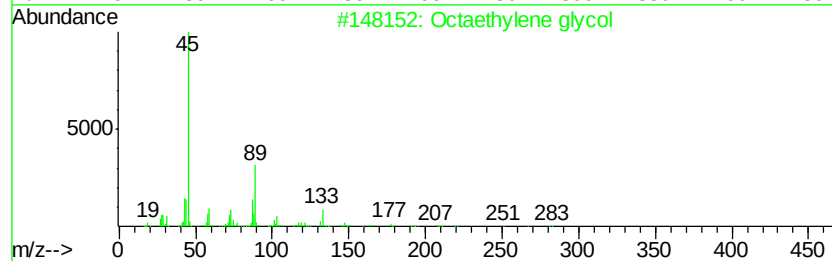
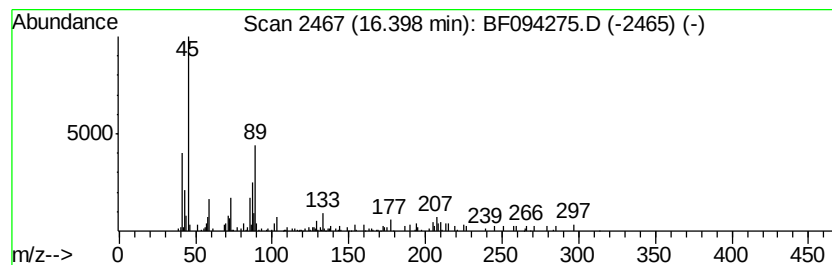
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Octaethylene glycol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	2.84 ng	126505	Perylene-d12	16.19

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octaethylene glycol	370	C16H34O9	1000289-34-2	72
2			Hexaethylene glycol monododecyl ...	450	C24H50O7	003055-96-7	64
3			Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	56
4			15-Crown-5	220	C10H20O5	033100-27-5	56
5			1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040717\
 Data File : BF094275.D
 Acq On : 7 Apr 2017 16:14
 Operator : SJ/MA
 Sample : I2572-04
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown5.60	5.60	98.5	ng	5009220	1	5.85	1017380	20.0
Mequinol	7.50	53.2	ng	3674280	2	7.35	1380500	20.0
5-Chloro-guaiacol	7.72	2.7	ng	187533	2	7.35	1380500	20.0
12-Crown-4	11.89	2.4	ng	162477	4	11.31	1366740	20.0
15-Crown-5	13.21	4.9	ng	263447	5	14.56	1083270	20.0
1,4,7,10,13,16-He...	14.38	4.8	ng	258039	5	14.56	1083270	20.0
Trichloroacetic a...	14.45	3.5	ng	191799	5	14.56	1083270	20.0
Hexagol	15.43	3.9	ng	174049	6	16.19	891154	20.0
Octaethylene glycol	16.40	2.8	ng	126505	6	16.19	891154	20.0