

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080416\
 Data File : BF089611.D
 Acq On : 5 Aug 2016 4:08
 Operator : UM/SJ
 Sample : H4345-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PURGE-WATER

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-BF080416.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	5.347	326	329	344	rVB	31511	113808	1.29%	0.711%
2	7.096	480	482	499	rVB	201758	469615	5.32%	2.934%
3	7.439	510	512	526	rBV	119511	232302	2.63%	1.452%
4	7.679	531	533	554	rVB	288990	488191	5.53%	3.051%
5	8.353	589	592	602	rBV	143408	327933	3.71%	2.049%
6	9.188	616	665	667	rBV2	654676	8832893	100.00%	55.194%
7	9.405	676	684	687	rVV3	101106	413727	4.68%	2.585%
8	9.473	687	690	697	rVV	248343	420164	4.76%	2.625%
9	11.245	843	845	854	rVB	532001	726232	8.22%	4.538%
10	11.542	868	871	874	rBV	100296	133364	1.51%	0.833%
11	12.296	934	937	949	rVV	333924	538635	6.10%	3.366%
12	12.696	969	972	983	rBV	111195	293003	3.32%	1.831%
13	13.062	1002	1004	1010	rVV3	45649	170116	1.93%	1.063%
14	13.439	1036	1037	1046	rBV	78404	157361	1.78%	0.983%
15	13.576	1046	1049	1057	rVB2	317887	488124	5.53%	3.050%
16	13.782	1064	1067	1070	rBV	155946	279407	3.16%	1.746%
17	14.068	1090	1092	1103	rVB	43420	92550	1.05%	0.578%
18	14.685	1143	1146	1159	rVB	291682	421267	4.77%	2.632%
19	15.691	1232	1234	1242	rBV	92794	137715	1.56%	0.861%
20	17.040	1350	1352	1359	rBV	277163	425384	4.82%	2.658%
21	17.200	1363	1366	1368	rBV	252240	331648	3.75%	2.072%
22	18.377	1467	1469	1474	rVV	179104	298820	3.38%	1.867%
23	20.046	1613	1615	1622	rVB	134645	211086	2.39%	1.319%

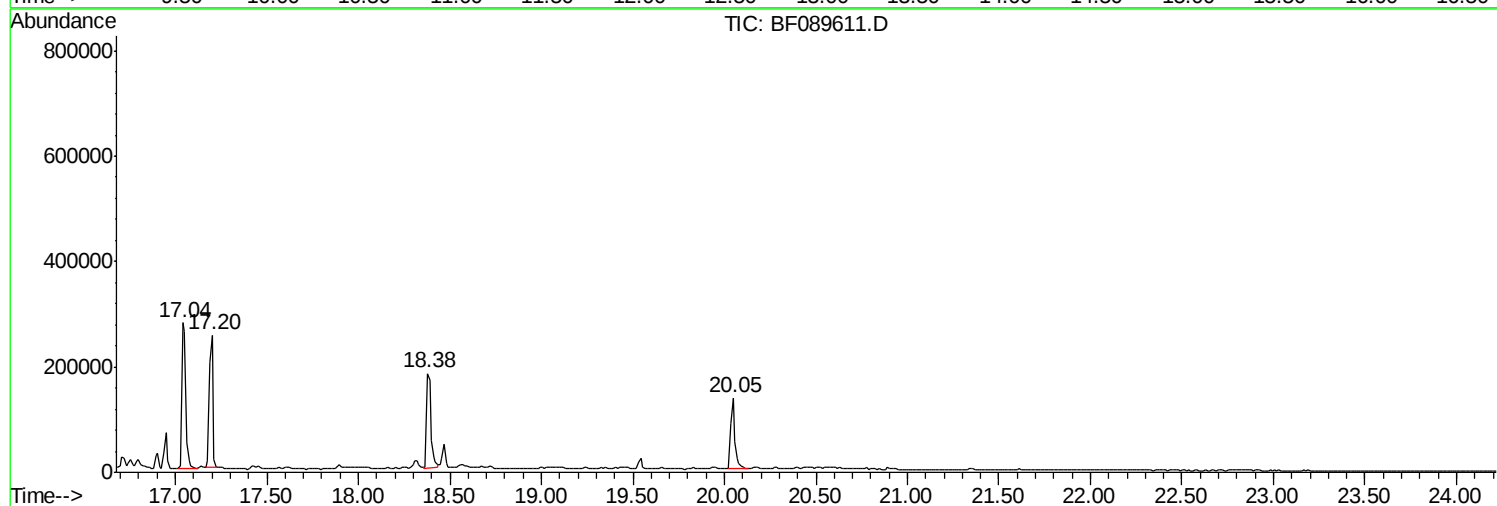
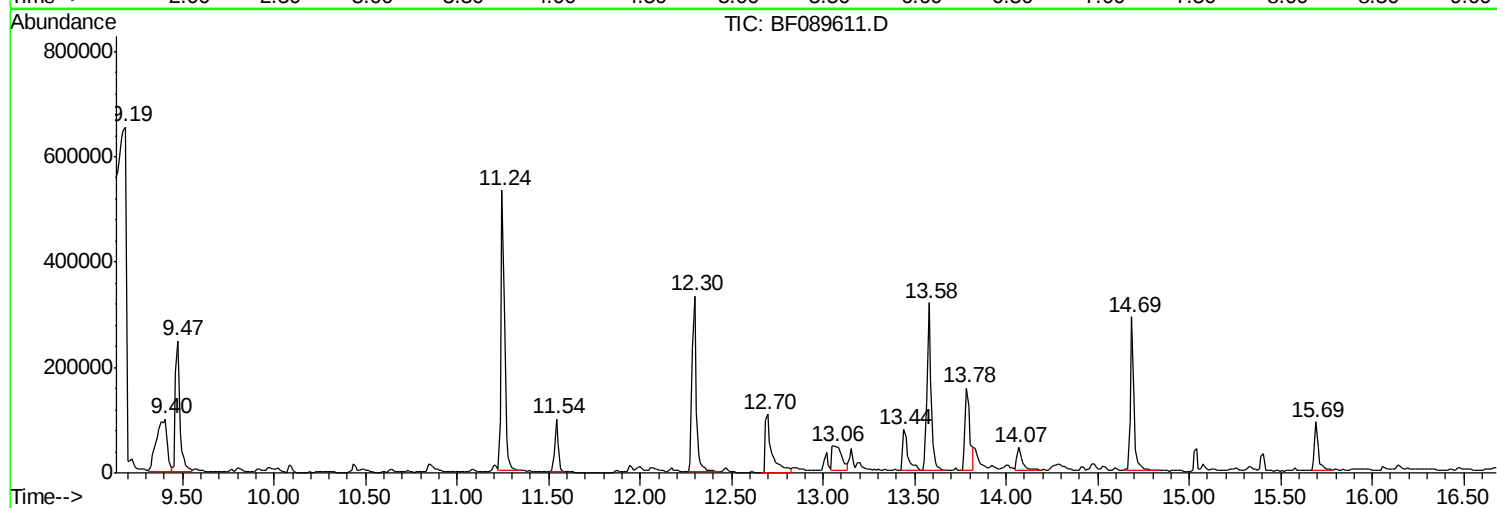
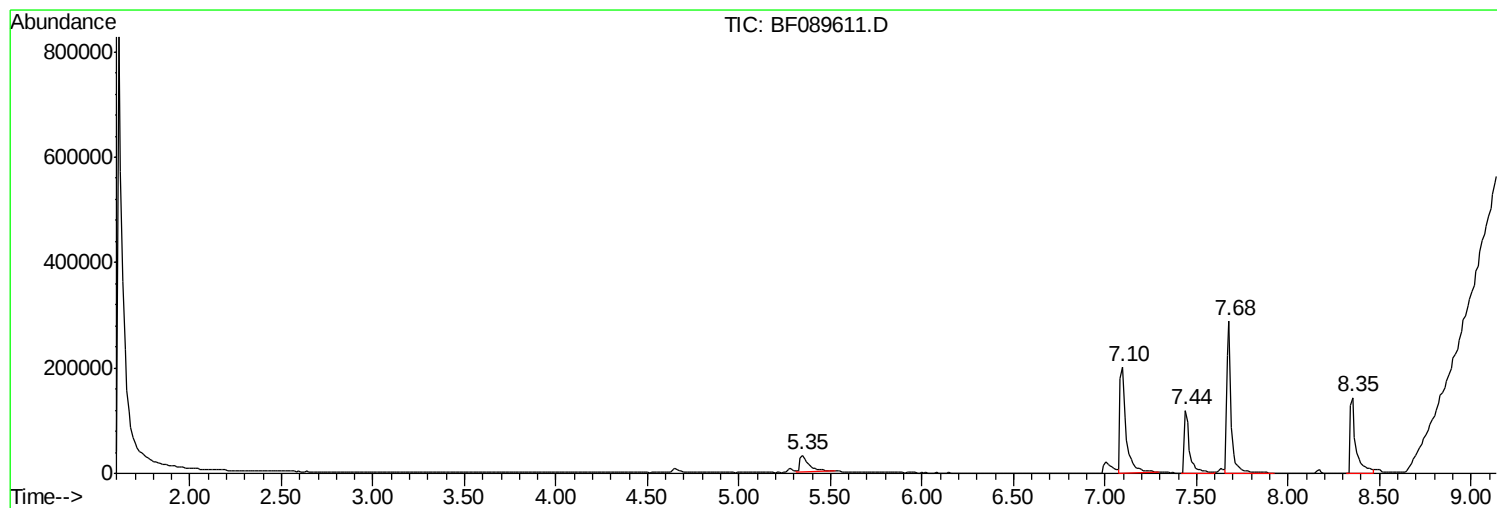
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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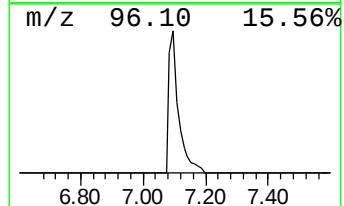
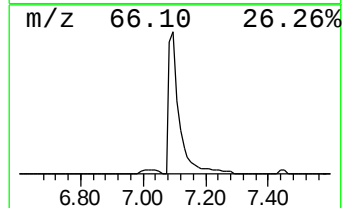
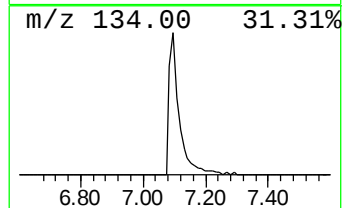
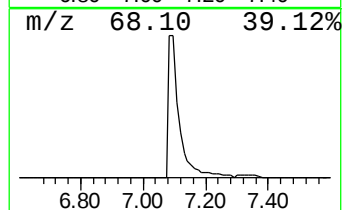
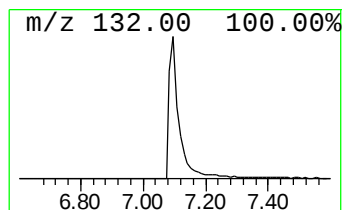
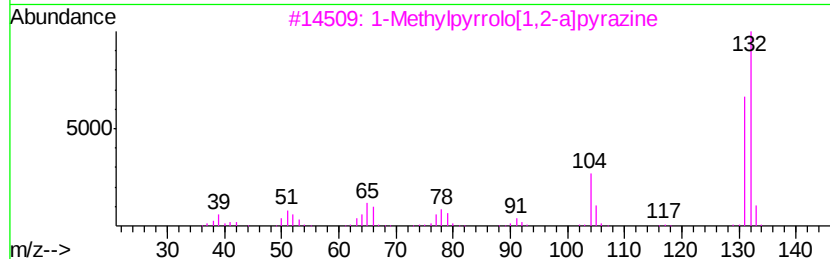
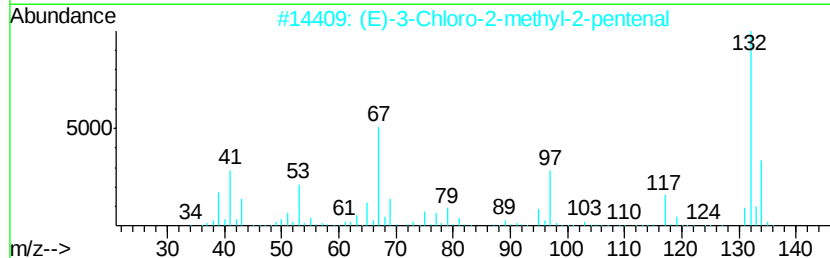
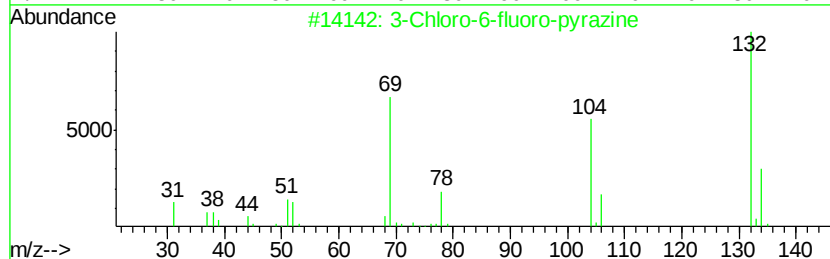
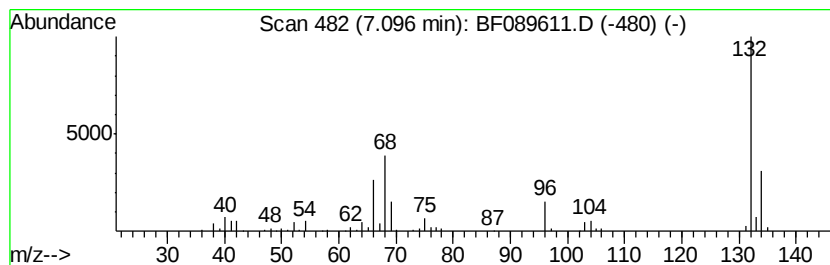
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.10 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.10	40.43 ng	469615	1,4-Dichlorobenzene-d4	7.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9



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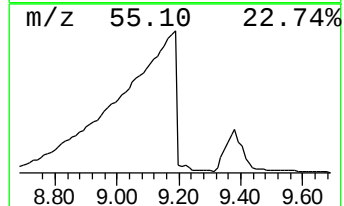
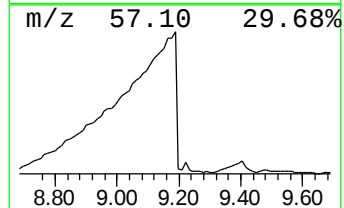
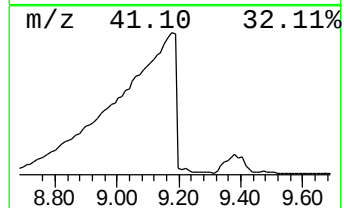
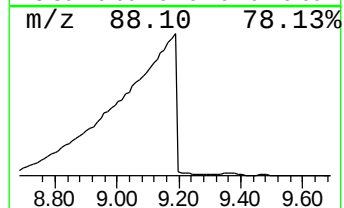
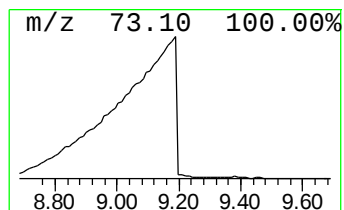
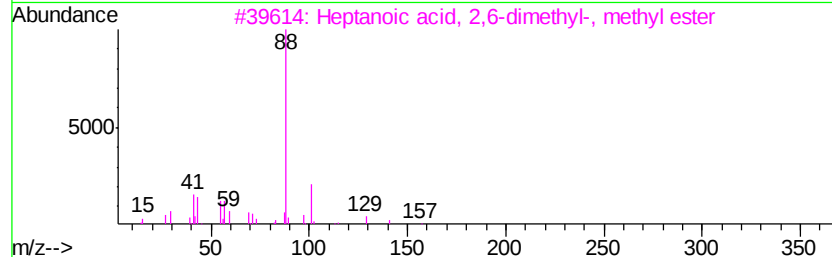
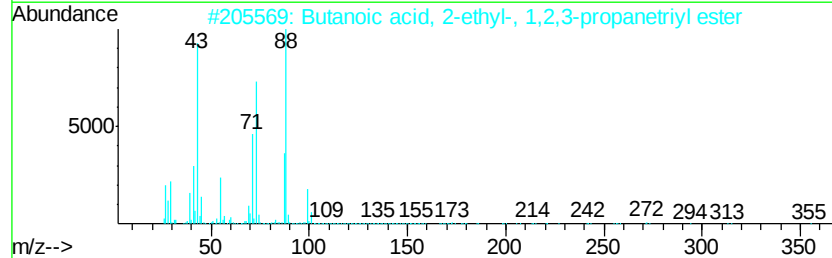
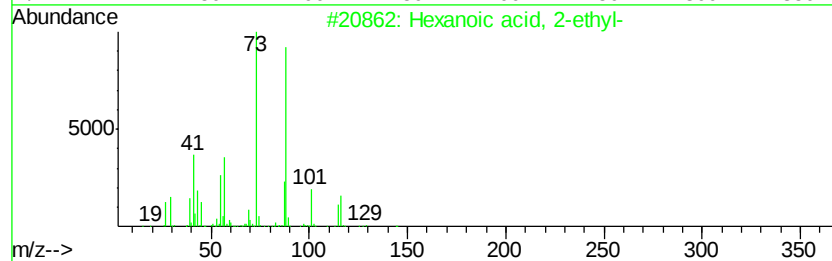
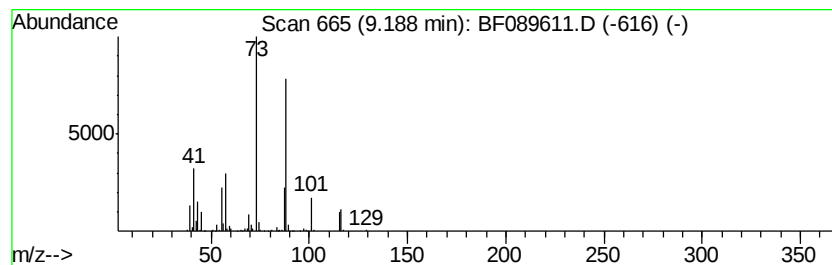
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Peak Number 3 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.19	420.45 ng	8832890	Naphthalene-d8	9.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
3		Heptanoic acid, 2,6-dimethyl-, m...	172	C10H20O2	033315-72-9	40
4		Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40
5		1,4-Dioxane	88	C4H8O2	000123-91-1	37



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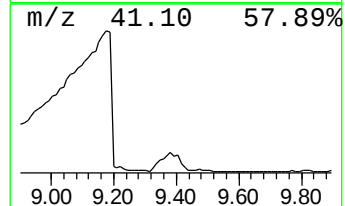
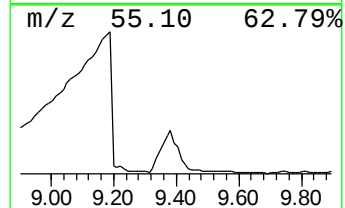
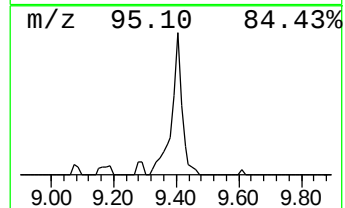
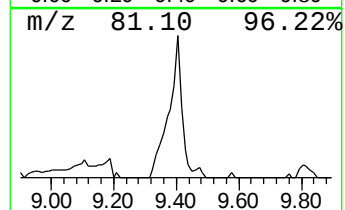
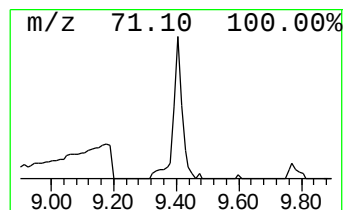
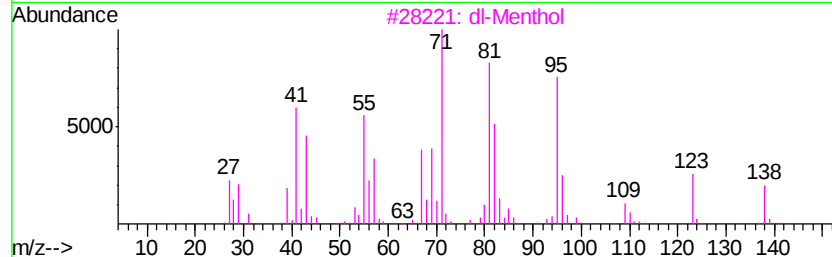
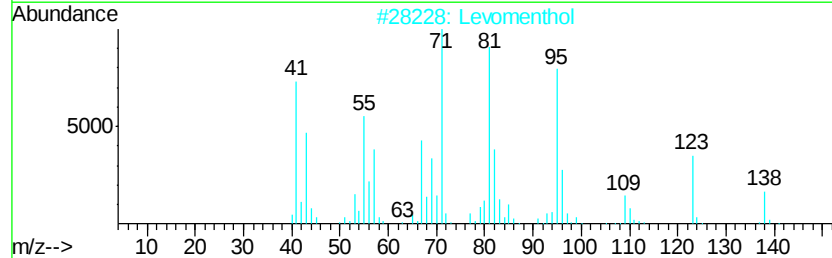
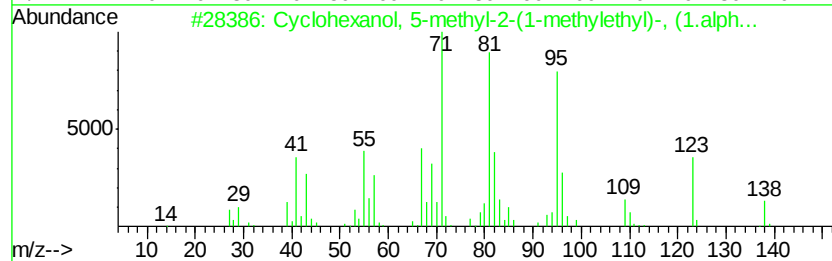
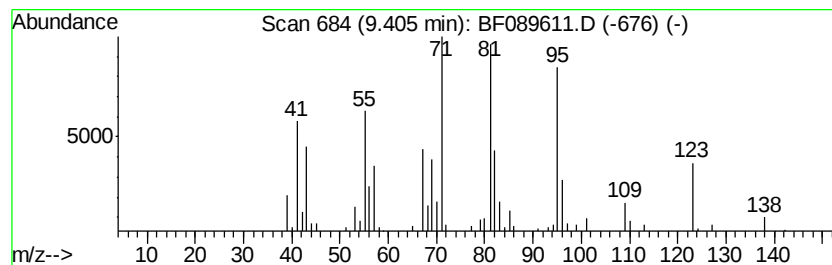
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Peak Number 4 Cyclohexanol, 5-methyl-2-(1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.40	19.69 ng	413727	Napthalene-d8	9.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	91
2		Levomenthol	156	C10H20O	002216-51-5	91
3		dl-Menthol	156	C10H20O	000089-78-1	90
4		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	90
5		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	86



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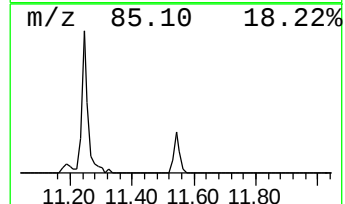
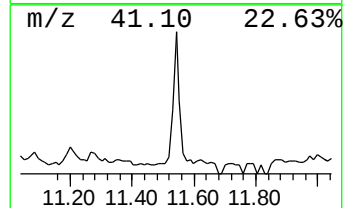
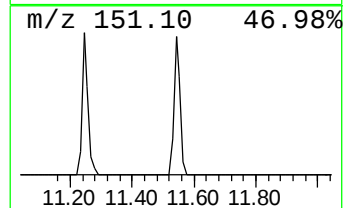
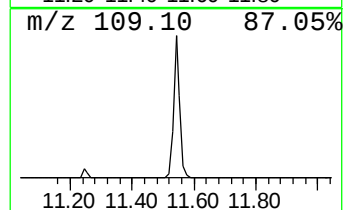
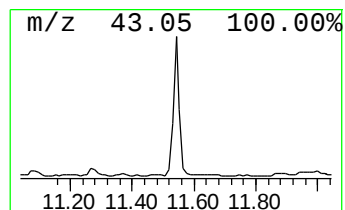
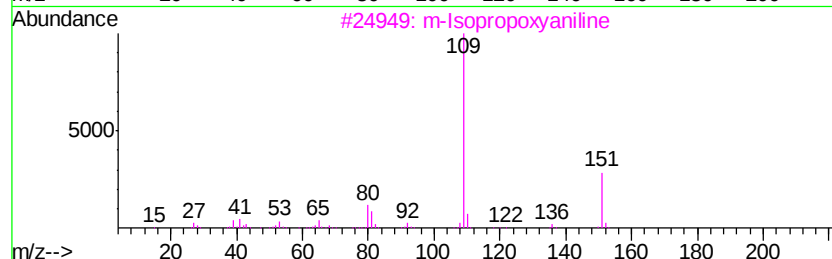
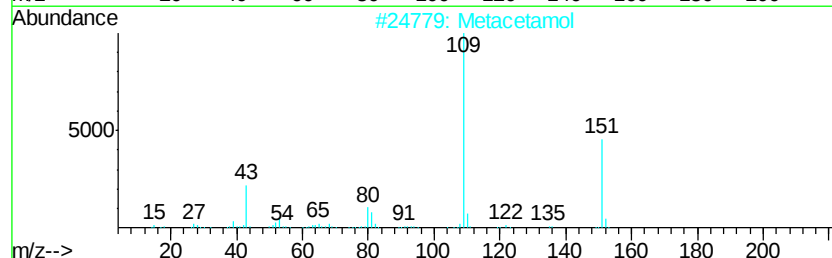
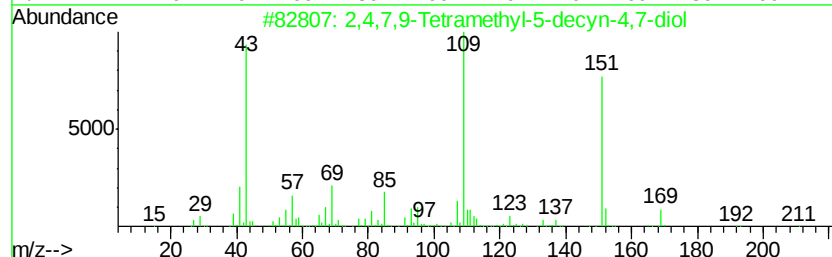
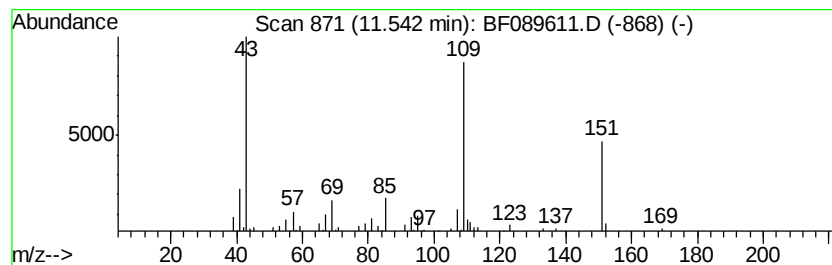
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Peak Number 5 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	4.95 ng	133364	Acenaphthene-d10	12.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2		Metacetamol	151	C8H9NO2	000621-42-1	58
3		m-Isopropoxvaniline	151	C9H13NO	041406-00-2	58
4		Pvridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
5		Acetaminophen	151	C8H9NO2	000103-90-2	53



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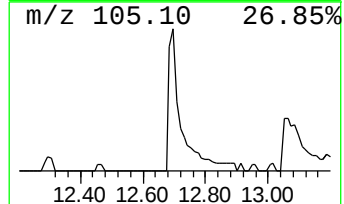
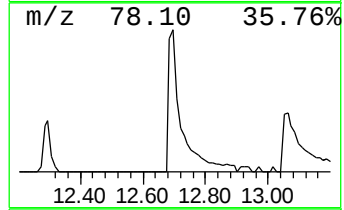
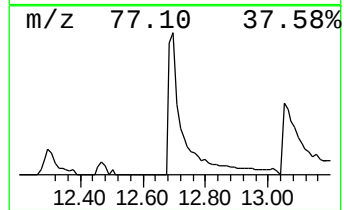
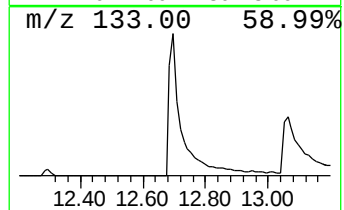
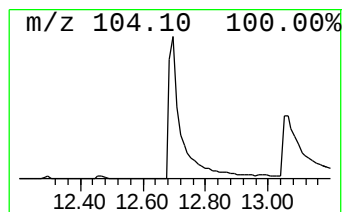
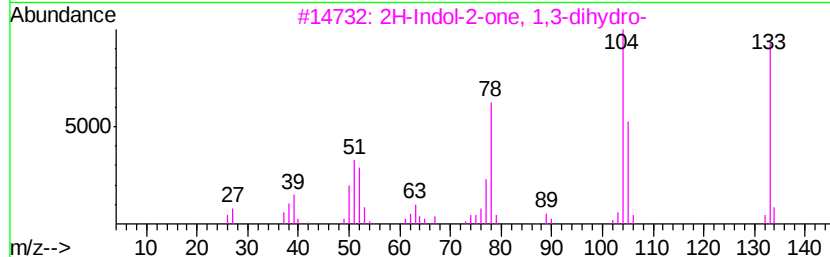
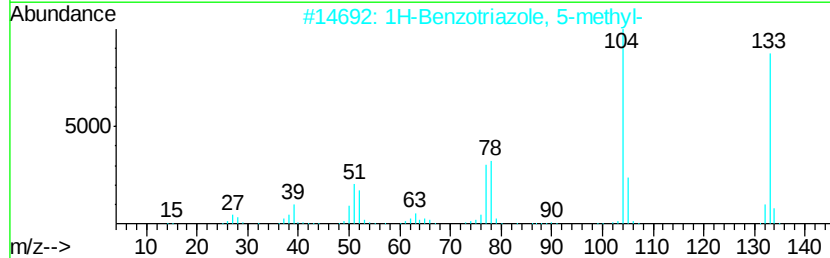
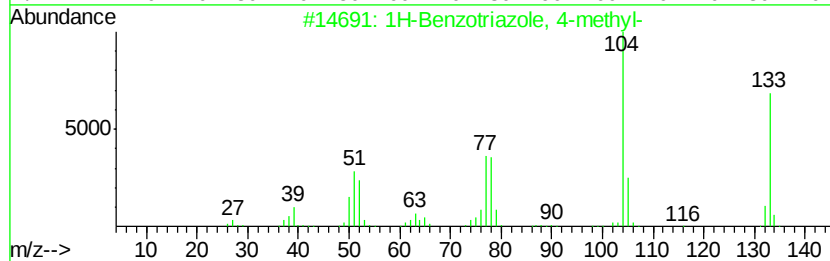
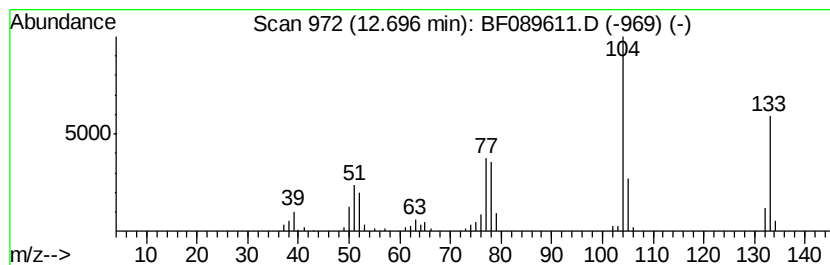
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Peak Number 6 1H-Benzotriazole, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.70	10.88 ng	293003	Acenaphthene-d10	12.30	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	98
2	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	95
3	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	76
4	1H-Indol-5-ol	133	C8H7NO	001953-54-4	76
5	Benzene, 1-azido-2-methyl-	133	C7H7N3	031656-92-5	74



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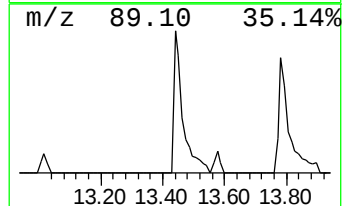
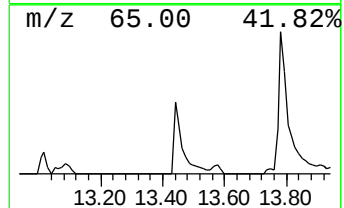
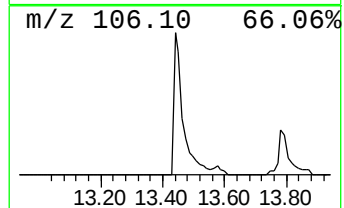
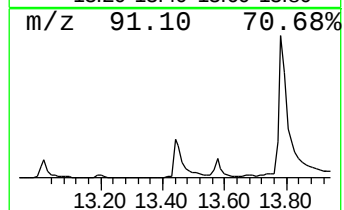
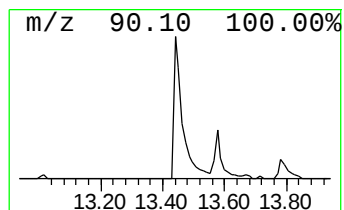
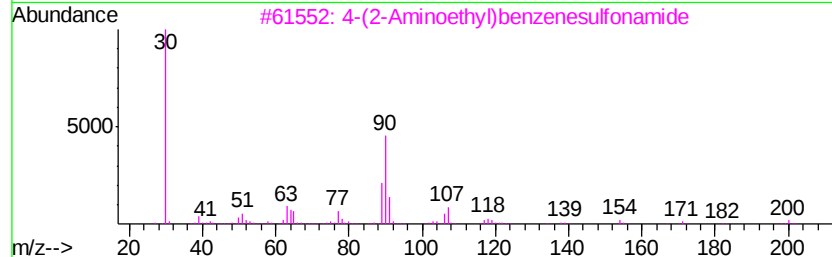
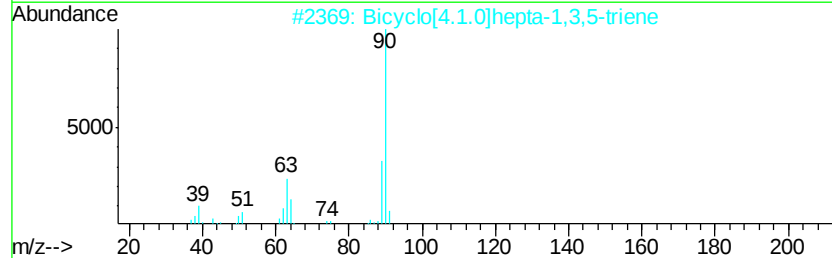
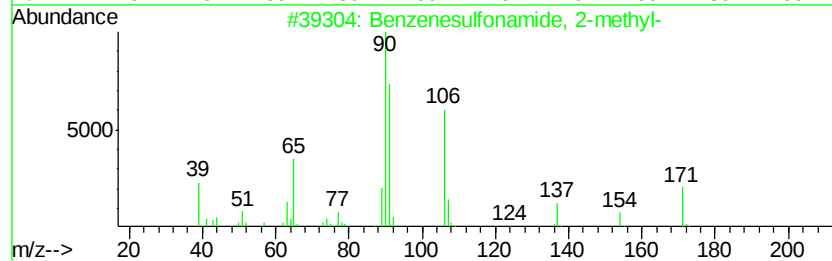
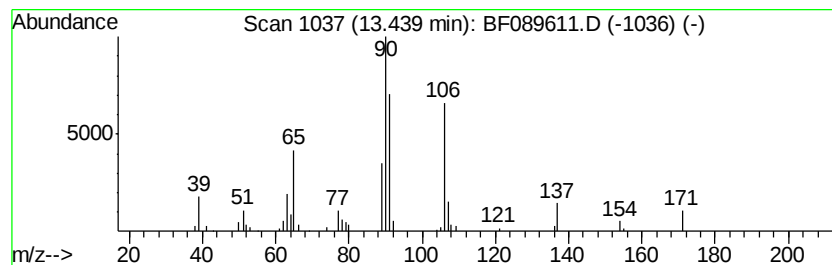
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzenesulfonamide, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	5.84 ng	157361	Acenaphthene-d10	12.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	95
2		Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	47
3		4-(2-Aminoethyl)benzenesulfonamide	200	C8H12N2O2S	035303-76-5	33
4		Gluconic acid	196	C6H12O7	000526-95-4	23
5		Benzene, 1-methyl-4-nitro-	137	C7H7NO2	000099-99-0	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080416\
Data File : BF089611.D
Acq On : 5 Aug 2016 4:08
Operator : UM/SJ
Sample : H4345-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PURGE-WATER

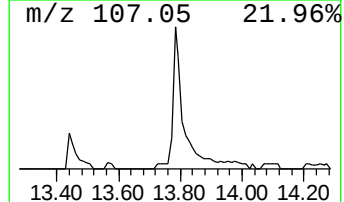
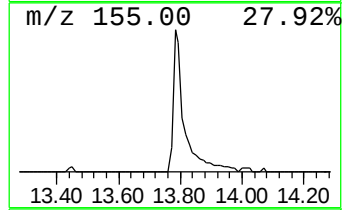
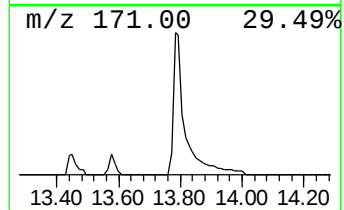
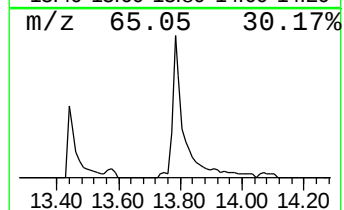
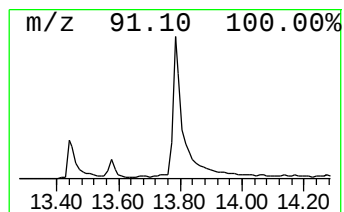
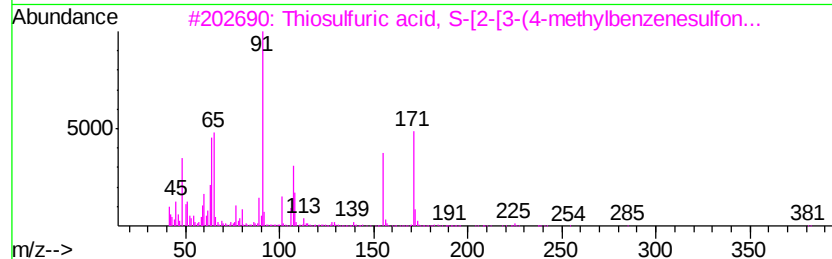
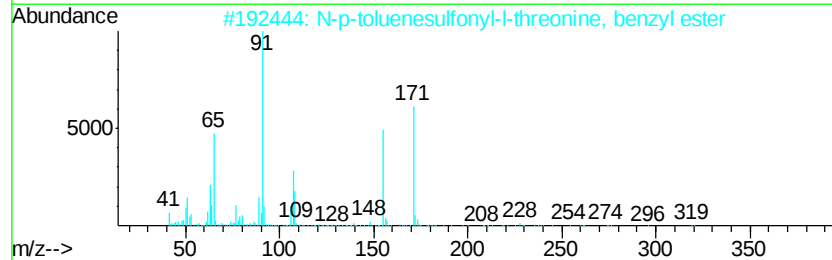
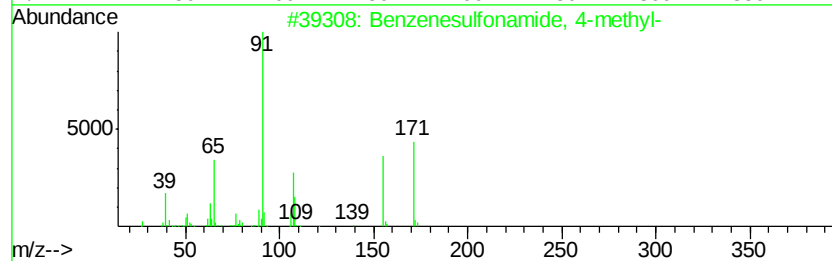
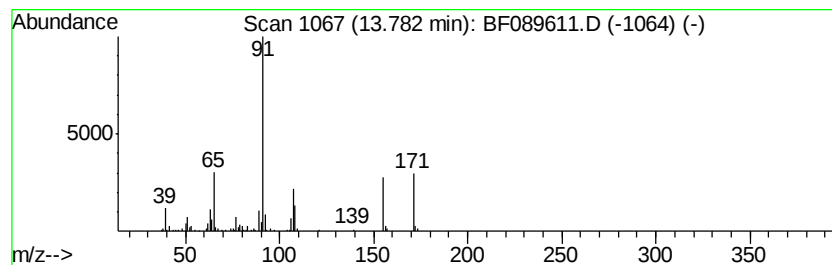
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzenesulfonamide, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	13.27 ng	279407	Phenanthrene-d10	14.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	98
2		N-p-toluenesulfonyl-L-threonine,...	363	C18H21NO5S	1000130-34-4	83
3		Thiosulfuric acid, S-[2-[3-(4-me...	381	C12H19N3O5S3	1000255-60-3	80
4		O-p-toluenesulfonyl-L-N-acetylser...	315	C13H17NO6S	1000126-44-8	72
5		2,2-Dimethyl-1,3-propanediol bis...	412	C19H24O6S2	022308-12-9	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080416\
Data File : BF089611.D
Acq On : 5 Aug 2016 4:08
Operator : UM/SJ
Sample : H4345-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PURGE-WATER

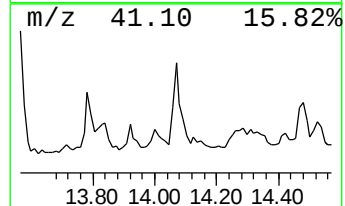
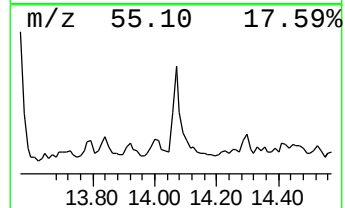
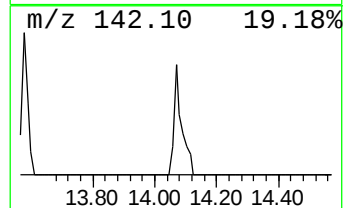
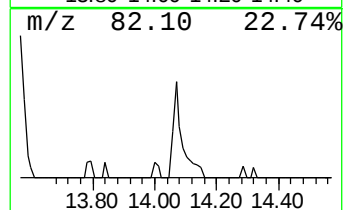
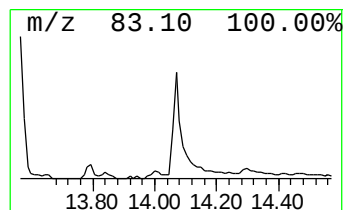
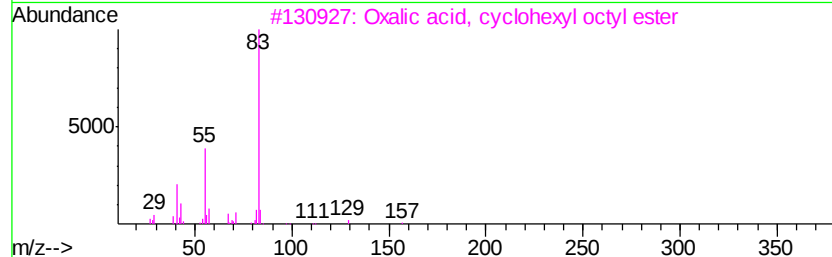
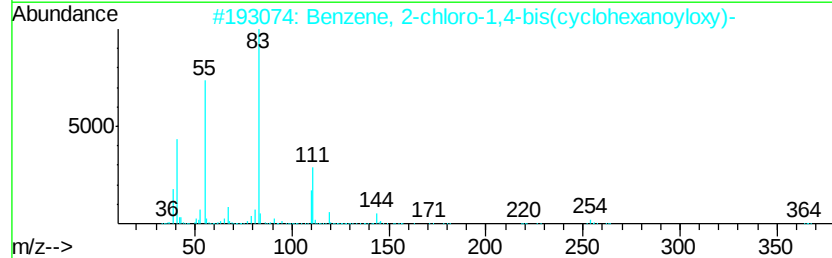
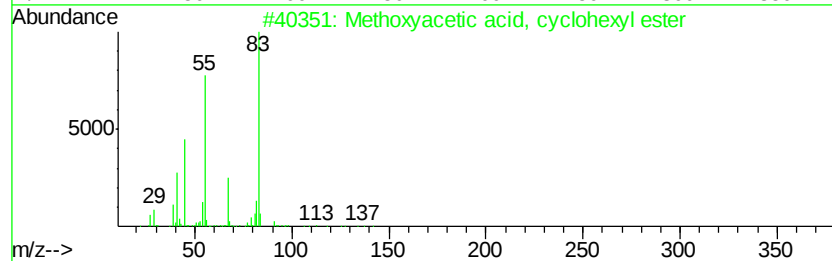
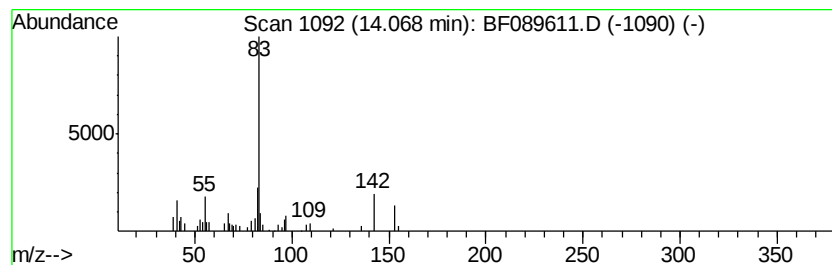
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Methoxyacetic acid, cyclohe... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.07	4.39 ng	92550	Phenanthrene-d10	14.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methoxvacetic acid, cvclohexvl e...	172	C9H16O3	1000282-69-4	50
2		Benzene, 2-chloro-1,4-bis(cvclohex...	364	C20H25ClO4	294874-04-7	47
3		Oxalic acid, cvclohexvl octvl ester	284	C16H28O4	1000309-31-0	47
4		Oxalic acid, cvclohexvl undecvl ...	326	C19H34O4	1000309-31-3	47
5		2-Pentene, 5-bromo-2,3-dimethyl-	176	C7H13Br	056312-52-8	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080416\
Data File : BF089611.D
Acq On : 5 Aug 2016 4:08
Operator : UM/SJ
Sample : H4345-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

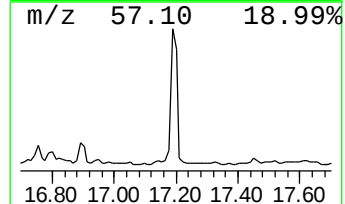
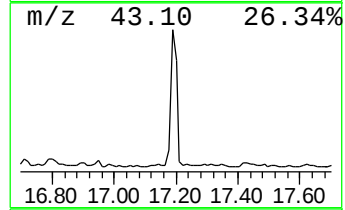
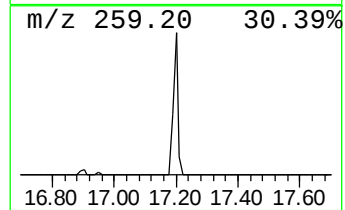
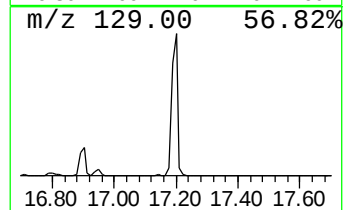
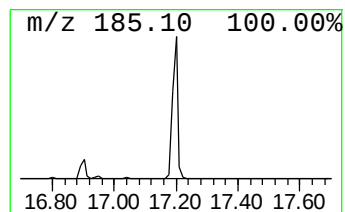
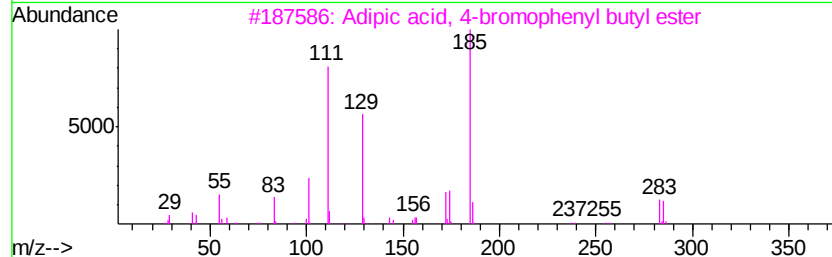
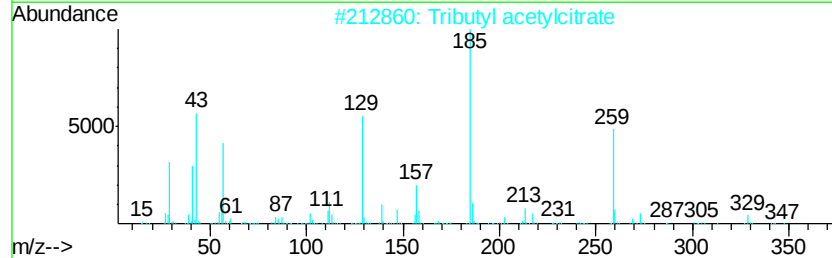
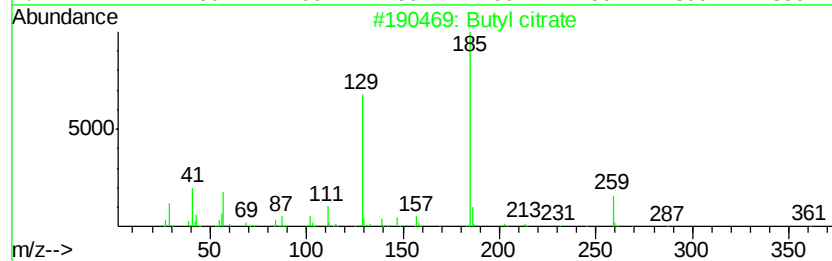
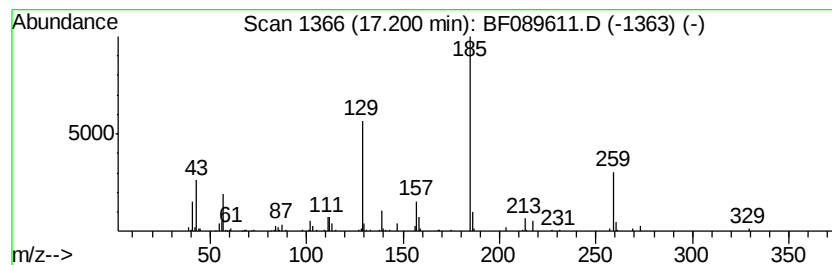
Instrument :
BNA_F
ClientSampleId :
PURGE-WATER

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Butyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.20	22.20 ng	331648	Chrysene-d12	18.39
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Butyl citrate	360 C18H32O7	000077-94-1 72
2		Tributyl acetylcitrate	402 C20H34O8	000077-90-7 64
3		Adipic acid, 4-bromophenyl butyl...	356 C16H21BrO4	1000324-37-9 53
4		[1,1'-Biphenyl]-4-ol, 3-amino-	185 C12H11NO	001134-36-7 43
5		Dibutyl adipate	258 C14H26O4	000105-99-7 42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080416\
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Operator : UM/SJ
Sample : H4345-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PURGE-WATER

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.10	7.10	40.4	ng	469615	1	7.44	232302	20.0
Hexanoic acid, 2-...	9.19	420.4	ng	8832890	2	9.47	420164	20.0
Cyclohexanol, 5-m...	9.40	19.7	ng	413727	2	9.47	420164	20.0
2,4,7,9-Tetrameth...	11.54	5.0	ng	133364	3	12.30	538635	20.0
1H-Benzotriazole,...	12.70	10.9	ng	293003	3	12.30	538635	20.0
Benzenesulfonamid...	13.44	5.8	ng	157361	3	12.30	538635	20.0
Benzenesulfonamid...	13.78	13.3	ng	279407	4	14.69	421267	20.0
Methoxyacetic aci...	14.07	4.4	ng	92550	4	14.69	421267	20.0
Butyl citrate	17.20	22.2	ng	331648	5	18.39	298820	20.0