

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052816\
 Data File : BF087503.D
 Acq On : 29 May 2016 4:53
 Operator : UM/SJ
 Sample : H3272-03
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-6

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-BF052316.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	4.696	271	272	290	rBV	101145	321998	7.77%	1.006%
2	5.370	329	331	352	rBV	676858	1552214	37.46%	4.850%
3	5.633	352	354	363	rVB	29882	73115	1.76%	0.228%
4	5.976	382	384	393	rBV	19964	54515	1.32%	0.170%
5	6.982	470	472	474	rBV	81288	141379	3.41%	0.442%
6	7.027	474	476	482	rVV	434888	909161	21.94%	2.841%
7	7.119	482	484	489	rVV	2180328	3113759	75.14%	9.729%
8	7.199	489	491	498	rVB	87956	167520	4.04%	0.523%
9	7.473	513	515	521	rBV	457469	857287	20.69%	2.679%
10	7.564	521	523	526	rVV	110343	165174	3.99%	0.516%
11	7.622	526	528	531	rVV2	26165	41845	1.01%	0.131%
12	7.702	532	535	549	rVV	1801208	2640955	63.73%	8.252%
13	7.896	549	552	560	rVB2	107191	207595	5.01%	0.649%
14	8.387	588	595	607	rBV2	1714166	2897537	69.92%	9.054%
15	9.119	655	659	662	rBV3	65056	151541	3.66%	0.474%
16	9.165	662	663	669	rVB	271427	499021	12.04%	1.559%
17	9.496	690	692	700	rBV	726867	1085523	26.20%	3.392%
18	10.353	763	767	771	rVV	47026	98686	2.38%	0.308%
19	10.479	773	778	781	rVV4	13945	45328	1.09%	0.142%
20	10.593	785	788	792	rVV4	26106	80372	1.94%	0.251%
21	10.811	805	807	810	rVV	190965	332295	8.02%	1.038%
22	10.856	810	811	819	rVB3	57711	105668	2.55%	0.330%
23	11.279	844	848	854	rBV	3184166	4143955	100.00%	12.948%
24	11.976	907	909	919	rBV	109597	198038	4.78%	0.619%
25	12.319	937	939	942	rBV	792097	1136622	27.43%	3.551%
26	12.376	942	944	948	rVB	374223	510477	12.32%	1.595%
27	13.165	1010	1013	1014	rBV	42802	53746	1.30%	0.168%
28	13.622	1050	1053	1065	rVV	1870156	2711677	65.44%	8.473%
29	13.794	1065	1068	1070	rVV3	35307	62777	1.51%	0.196%
30	13.839	1070	1072	1078	rVV	251378	462027	11.15%	1.444%
31	13.931	1078	1080	1090	rVB	74235	156332	3.77%	0.488%
32	14.731	1147	1150	1160	rVB	711209	1131186	27.30%	3.534%
33	14.937	1166	1168	1176	rVB	79321	129707	3.13%	0.405%
34	15.714	1234	1236	1240	rVB3	32476	54225	1.31%	0.169%

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35	17.085	1353	1356	1359	rBV	3483637	4097946	98.89%	12.804%
36	18.377	1463	1469	1472	rBV2	39604	115888	2.80%	0.362%
37	18.434	1472	1474	1485	rVB	602032	895172	21.60%	2.797%
38	20.114	1618	1621	1632	rBV	323079	602157	14.53%	1.881%

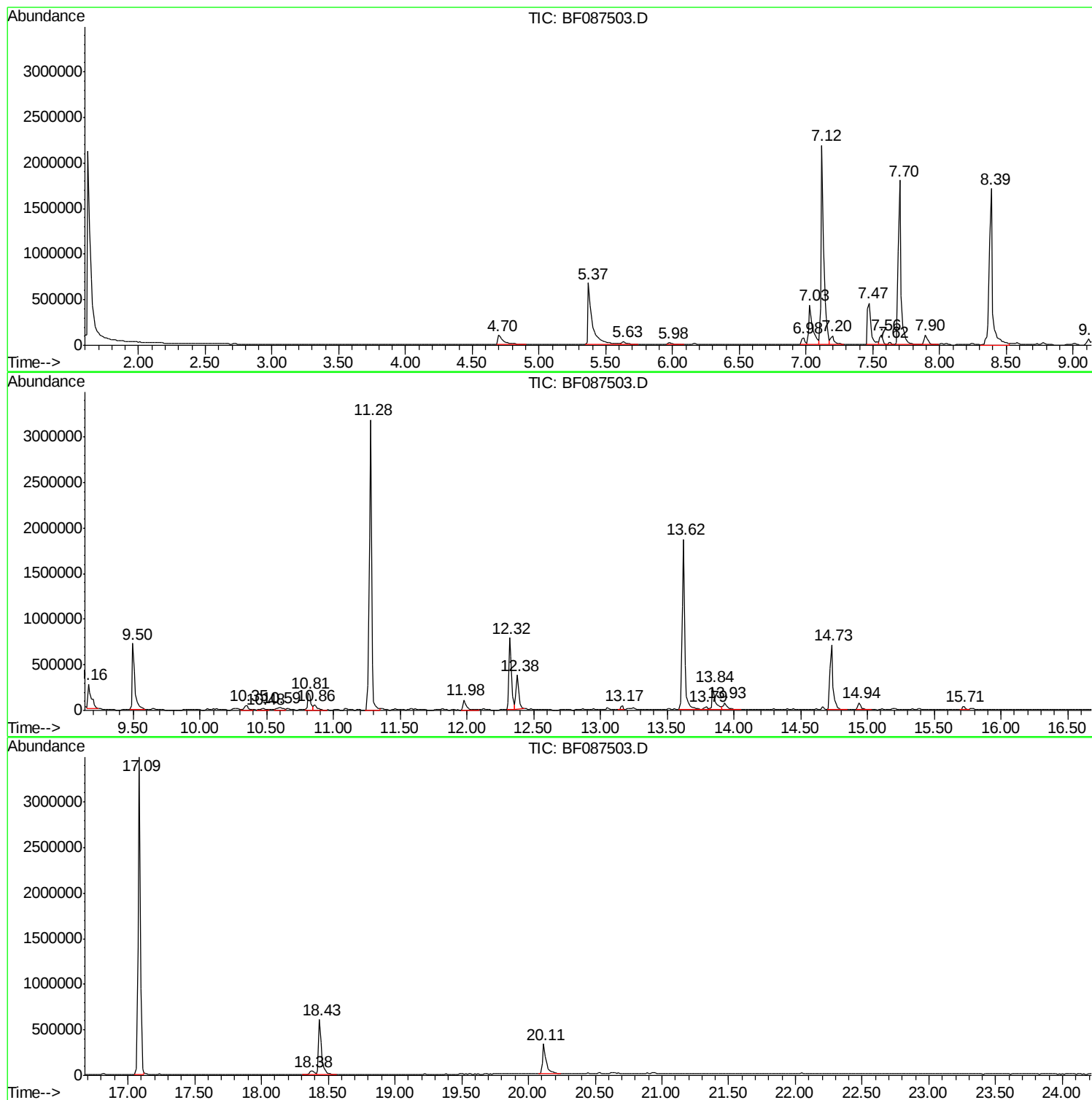
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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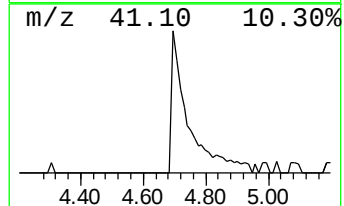
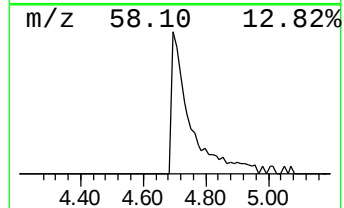
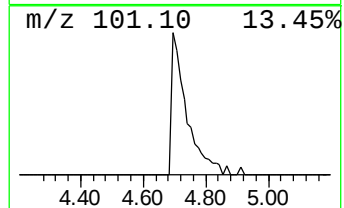
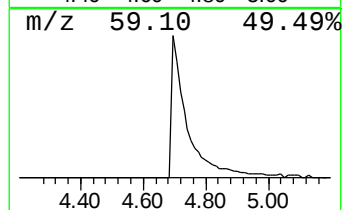
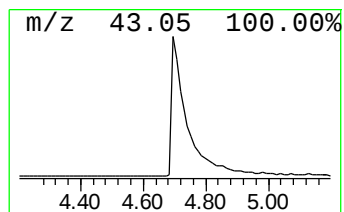
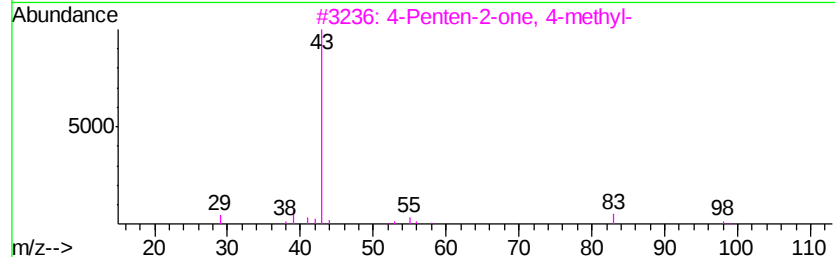
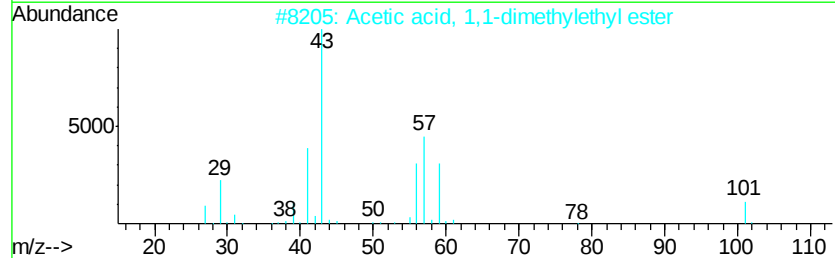
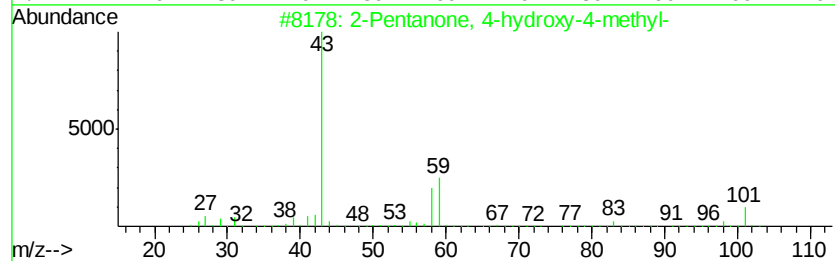
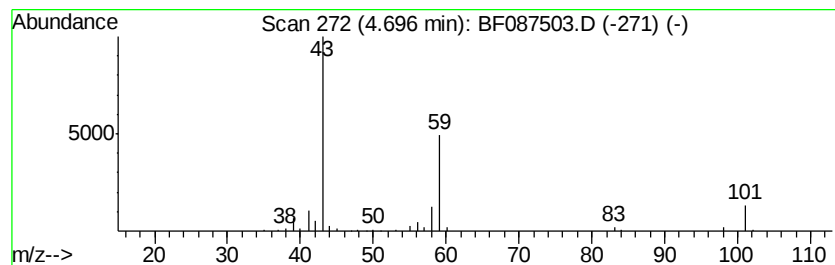
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	7.51 ng	321998	1,4-Dichlorobenzene-d4	7.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4			Diacetamide	101	C4H7NO2	000625-77-4	9
5			Butane	58	C4H10	000106-97-8	9



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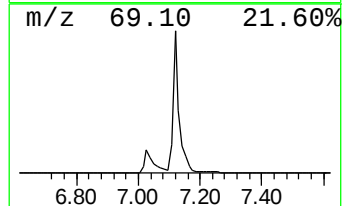
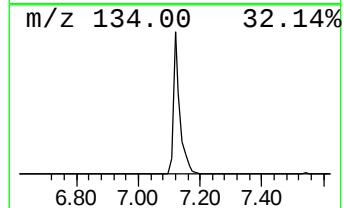
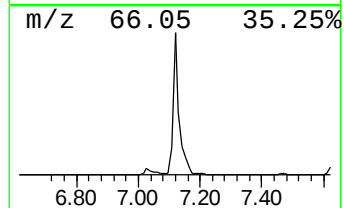
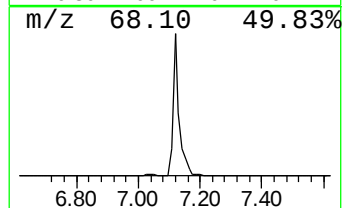
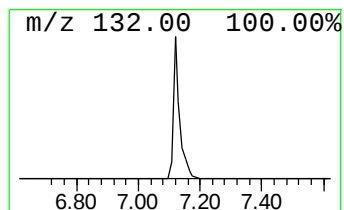
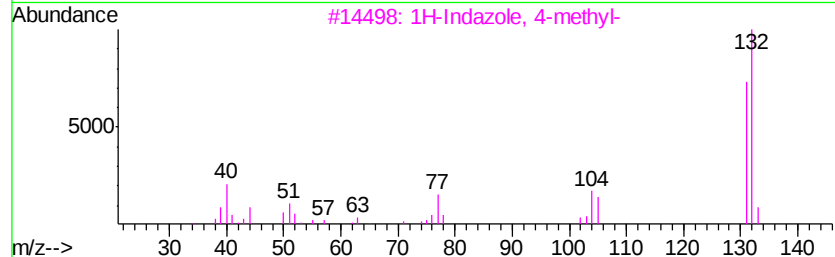
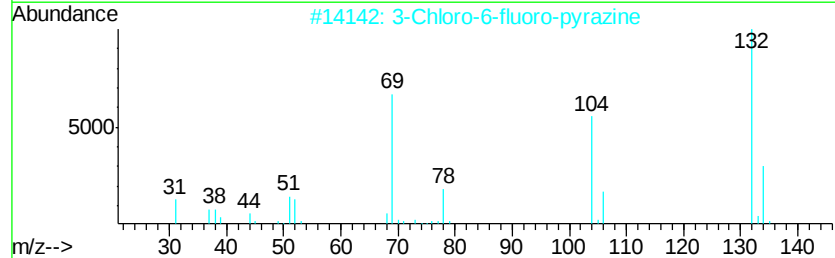
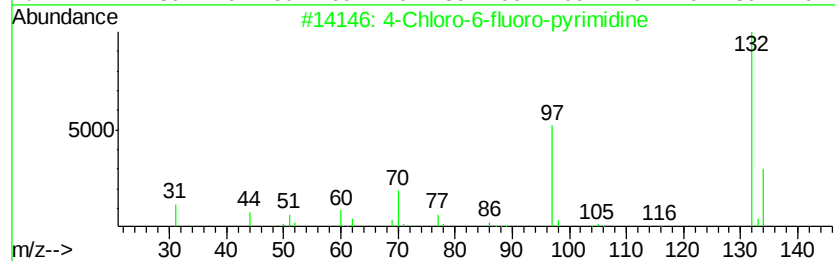
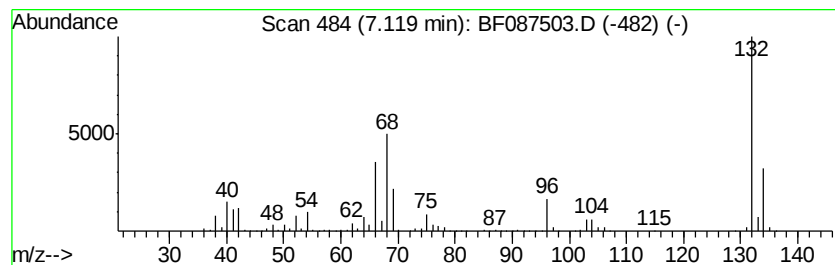
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Peak Number 2 unknown7.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	72.64 ng	3113760	1,4-Dichlorobenzene-d4	7.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Indazole, 4-methyl-	132	C8H8N2	1000316-00-9	25
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22



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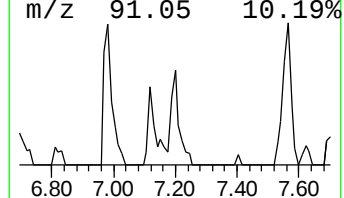
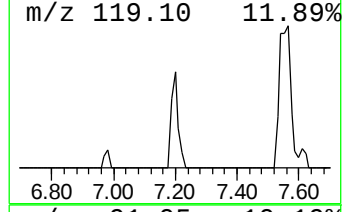
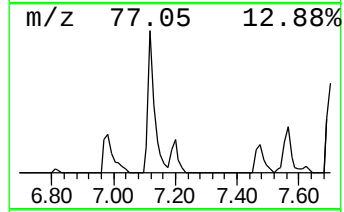
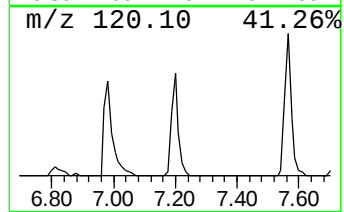
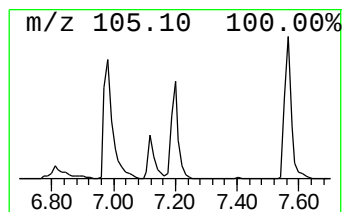
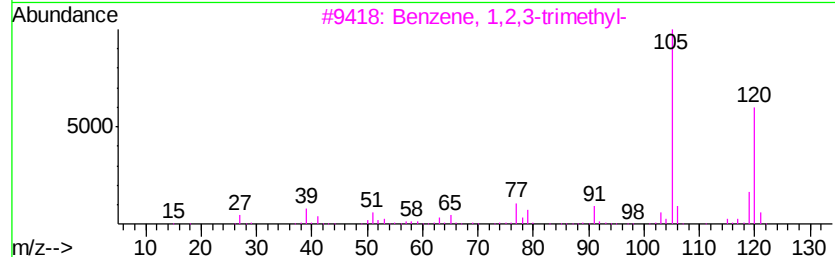
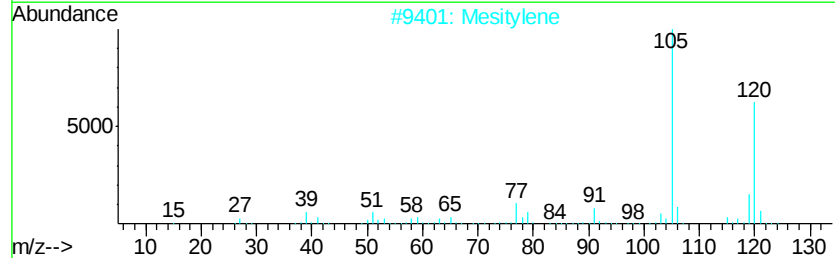
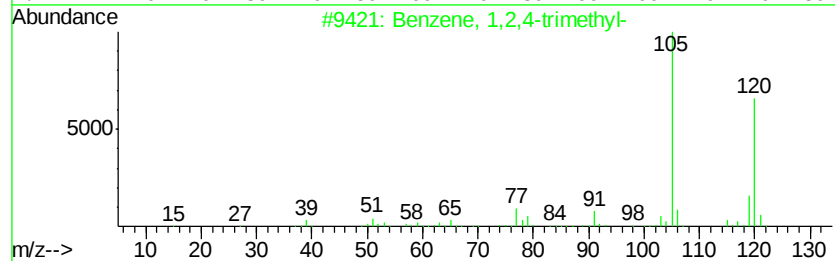
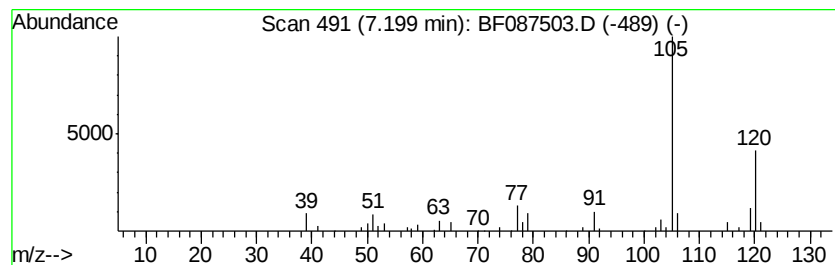
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Peak Number 3 Benzene, 1,2,4-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	3.91 ng	167520	1,4-Dichlorobenzene-d4	7.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
2		Mesitylene	120	C9H12	000108-67-8	94
3		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
4		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
5		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



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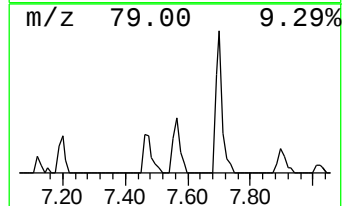
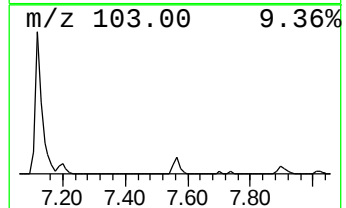
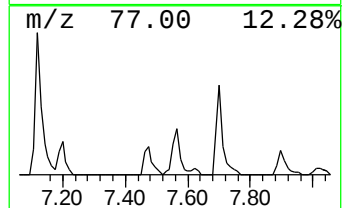
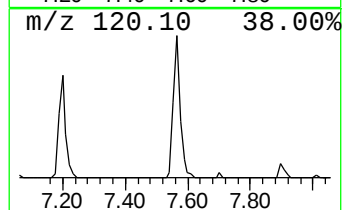
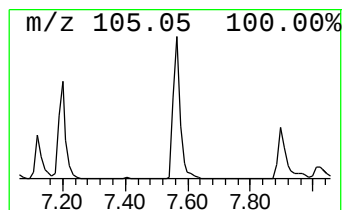
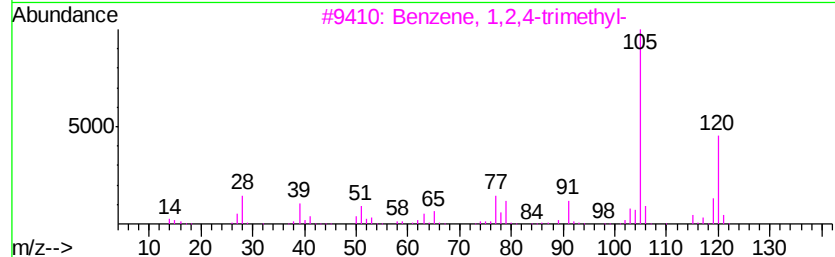
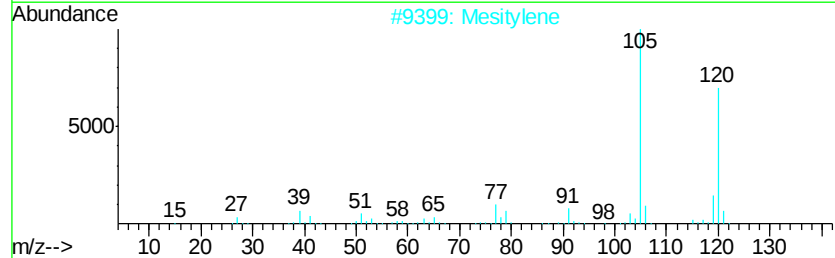
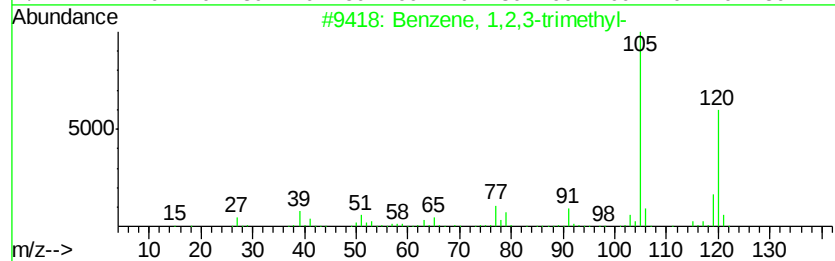
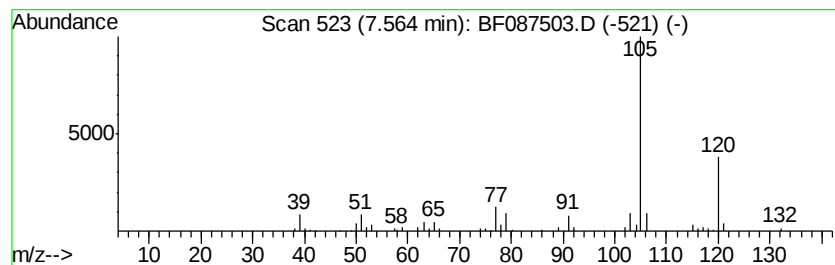
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	3.85 ng	165174	1,4-Dichlorobenzene-d4	7.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
2		Mesitylene	120	C9H12	000108-67-8	91
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
4		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



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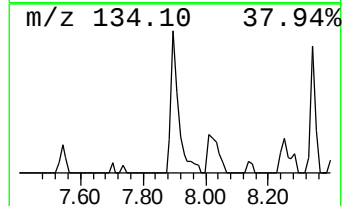
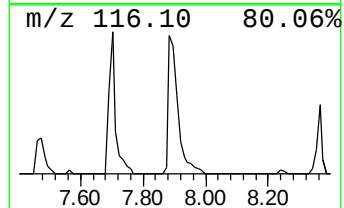
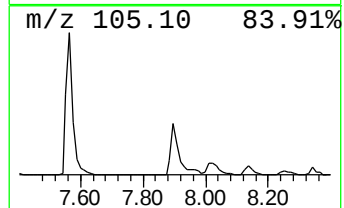
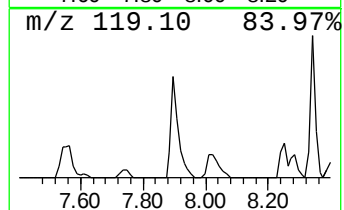
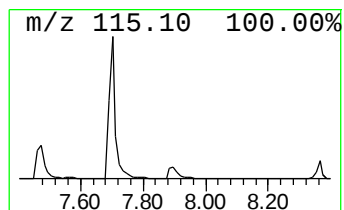
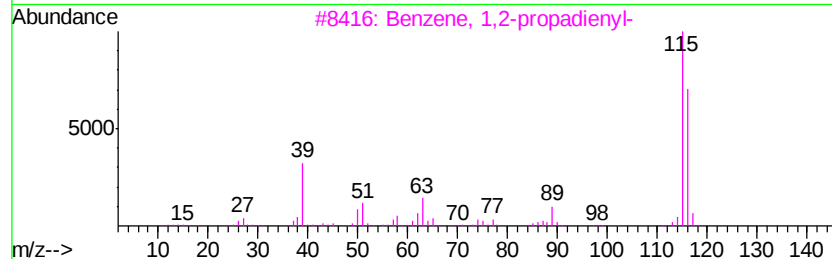
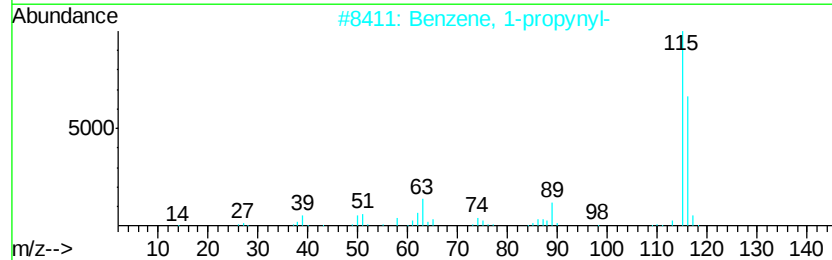
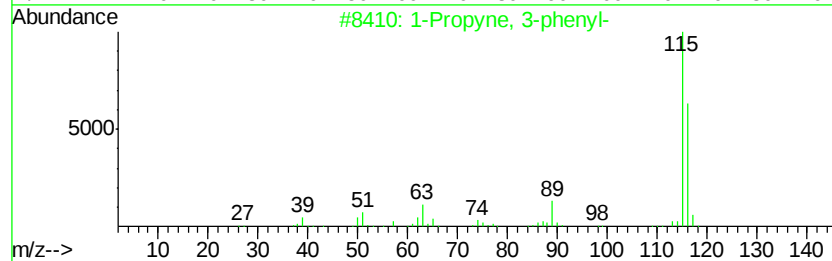
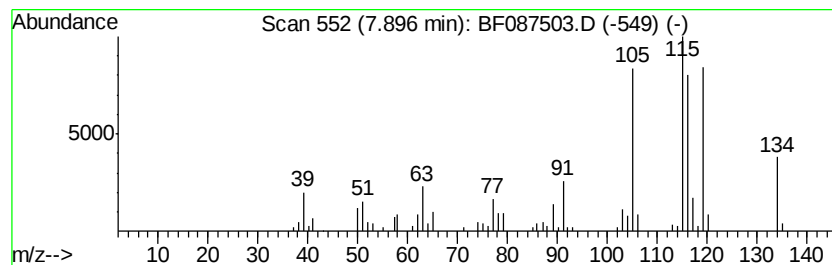
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Peak Number 6 1-Propyne, 3-phenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.90	4.84 ng	207595	1,4-Dichlorobenzene-d4	7.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	55
2		Benzene, 1-propynyl-	116	C9H8	000673-32-5	55
3		Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	55
4		3-Methylphenylacetylene	116	C9H8	000766-82-5	55
5		Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052816\
Data File : BF087503.D
Acq On : 29 May 2016 4:53
Operator : UM/SJ
Sample : H3272-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

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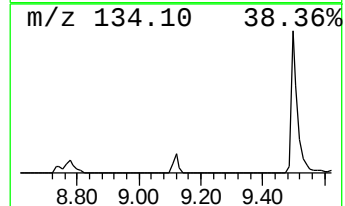
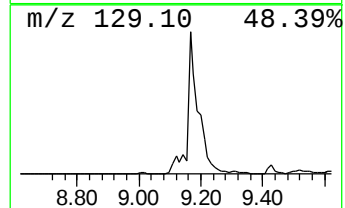
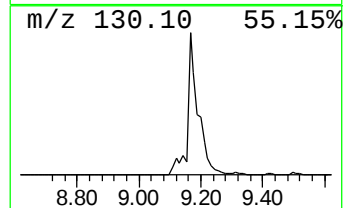
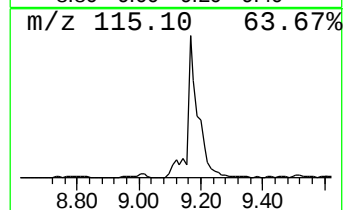
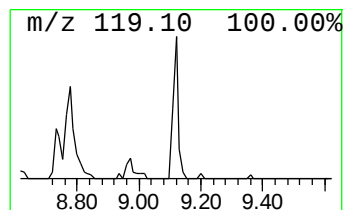
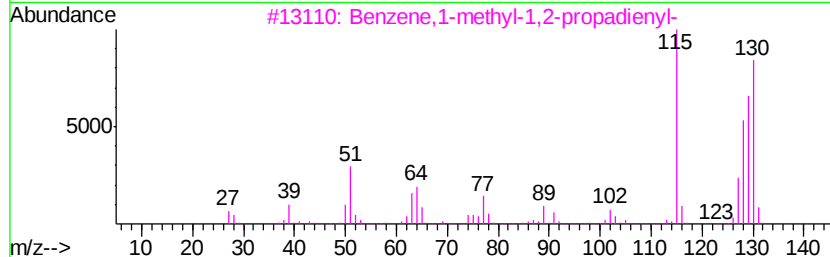
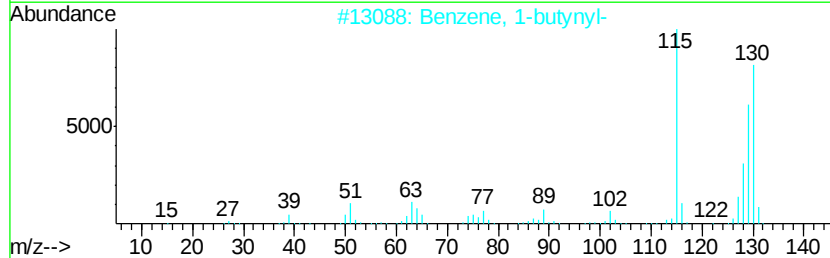
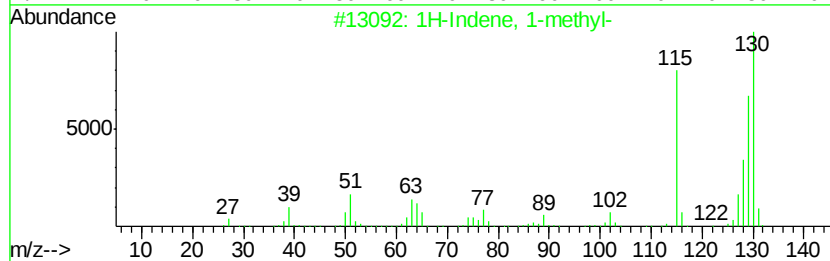
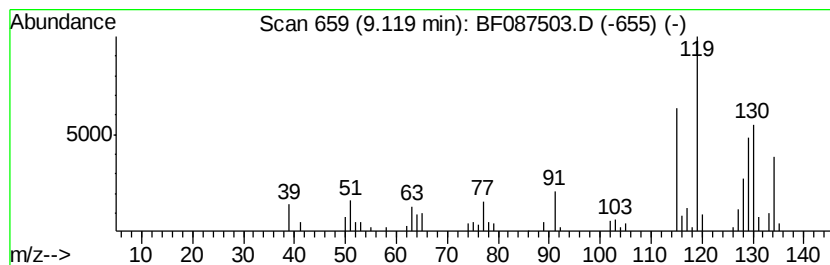
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1H-Indene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.12	2.79 ng	151541	Naphthalene-d8	9.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	83
2	Benzene, 1-butynyl-	130	C10H10	000622-76-4	83
3	Benzene, 1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	81
4	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	80
5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052816\
Data File : BF087503.D
Acq On : 29 May 2016 4:53
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Sample : H3272-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

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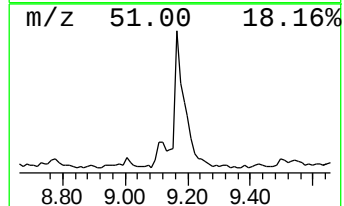
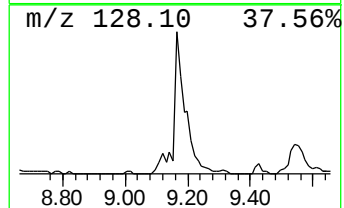
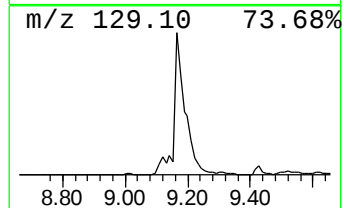
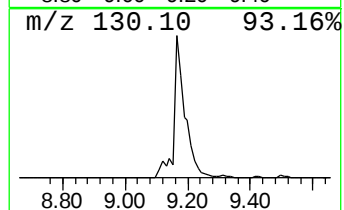
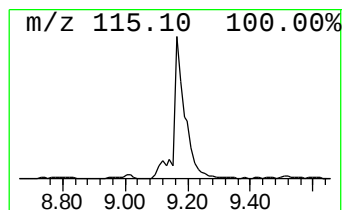
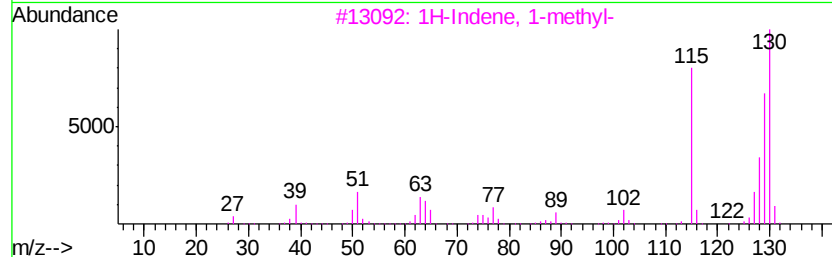
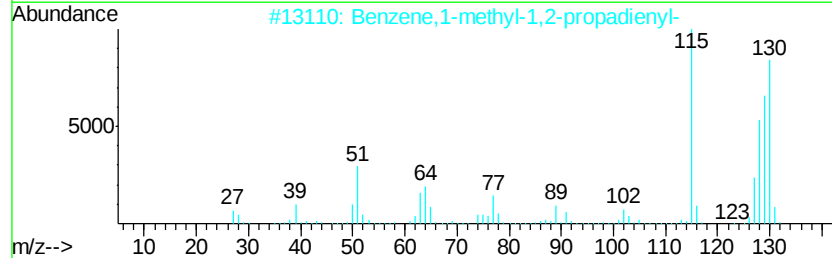
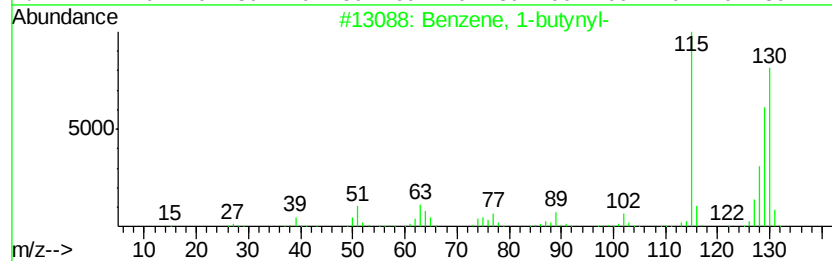
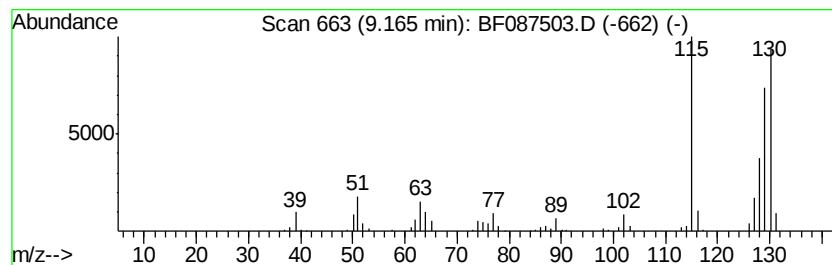
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzene, 1-butynyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.16	9.19 ng	499021	Naphthalene-d8	9.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-butynyl-	130	C10H10	000622-76-4	97
2		Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	96
3		1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
4		Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93
5		2-Methylindene	130	C10H10	002177-47-1	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052816\
Data File : BF087503.D
Acq On : 29 May 2016 4:53
Operator : UM/SJ
Sample : H3272-03
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ClientSampleId :
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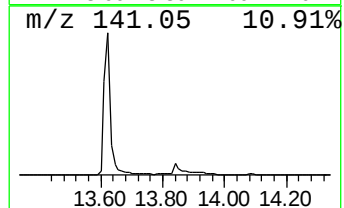
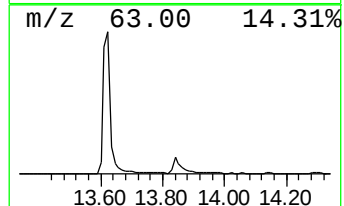
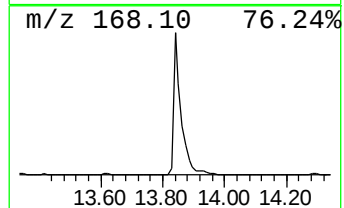
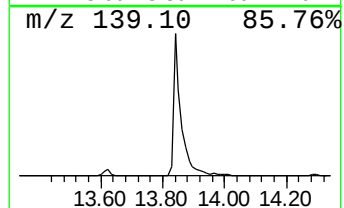
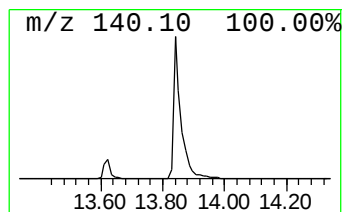
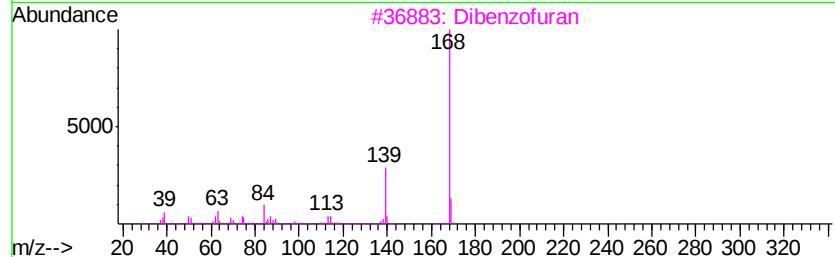
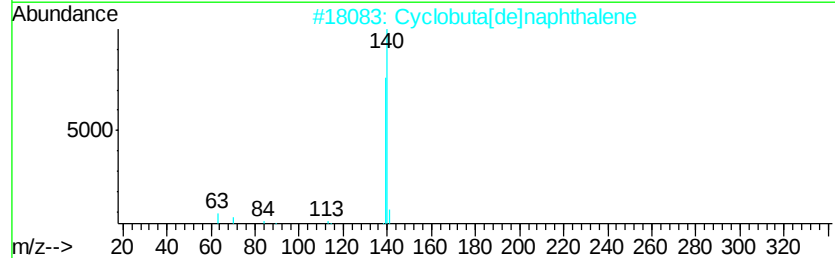
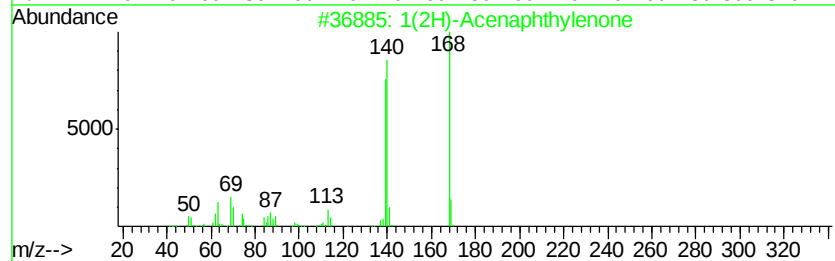
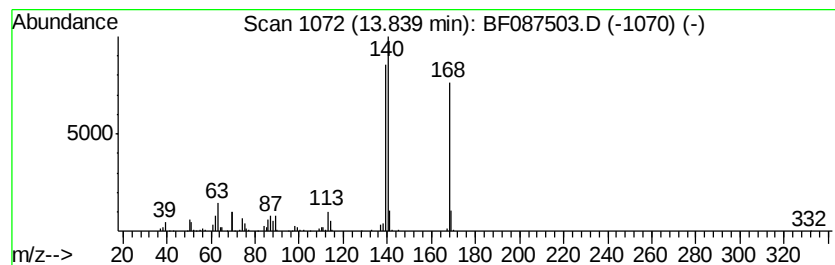
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1(2H)-Acenaphthylenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	8.17 ng	462027	Phenanthrene-d10	14.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1(2H)-Acenaphthylenone	168	C12H8O	002235-15-6	93
2		Cyclobuta[de]naphthalene	140	C11H8	024973-91-9	58
3		Dibenzofuran	168	C12H8O	000132-64-9	50
4		Benzene, 1,3,5-trimethoxy-	168	C9H12O3	000621-23-8	47
5		4H-Pyran-4-one, 2-ethyl-3-hydroxy-	140	C7H8O3	004940-11-8	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052816\
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Acq On : 29 May 2016 4:53
Operator : UM/SJ
Sample : H3272-03
Misc :
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ClientSampleId :
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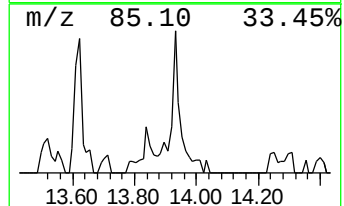
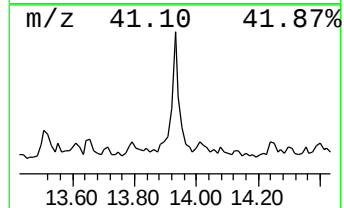
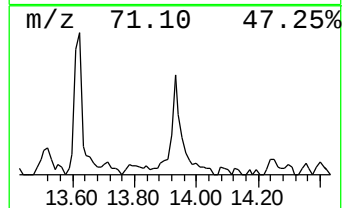
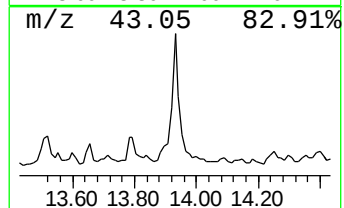
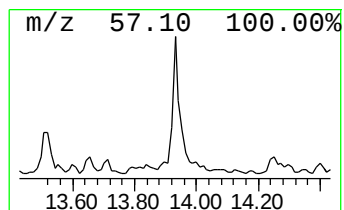
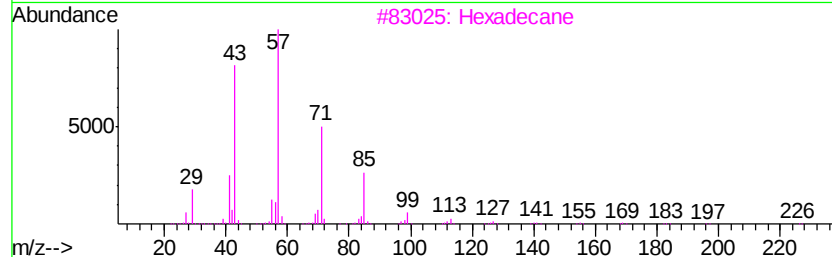
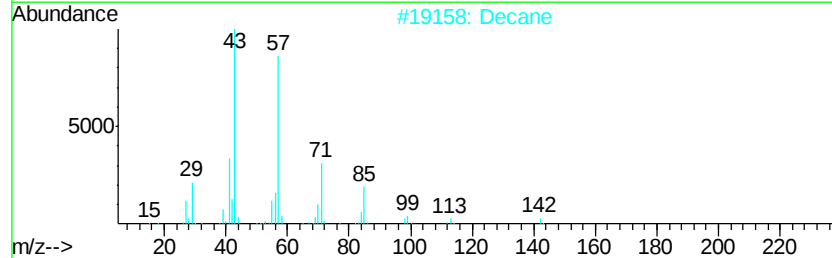
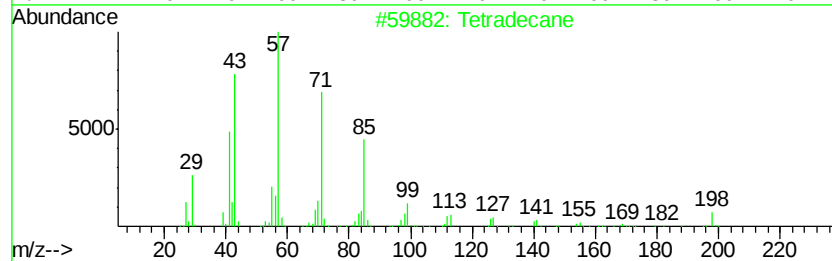
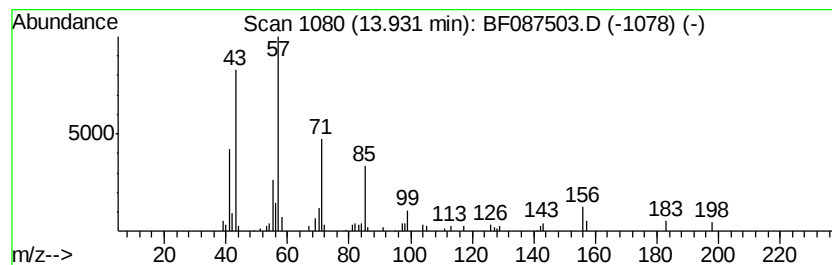
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	2.76 ng	156332	Phenanthrene-d10	14.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	81
2			Decane	142	C10H22	000124-18-5	76
3			Hexadecane	226	C16H34	000544-76-3	68
4			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	59
5			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052816\
Data File : BF087503.D
Acq On : 29 May 2016 4:53
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ClientSampleId :
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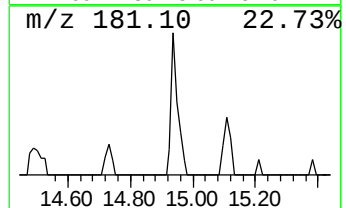
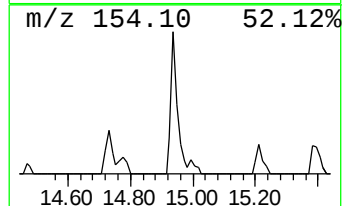
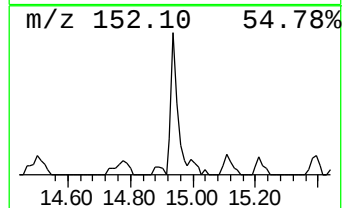
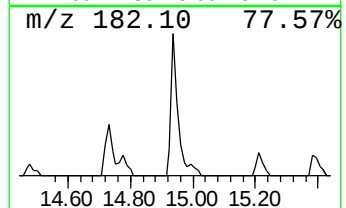
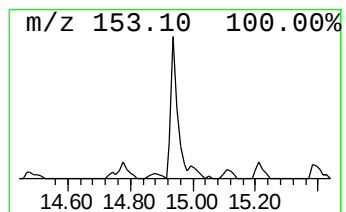
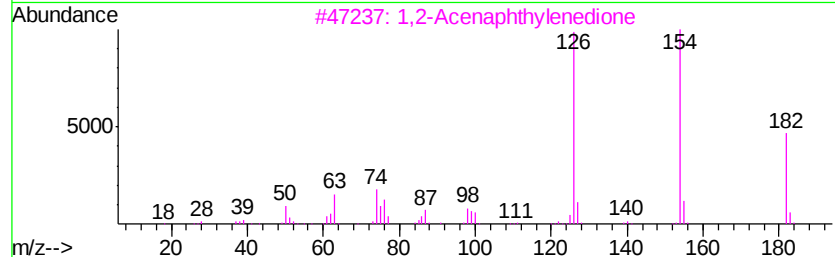
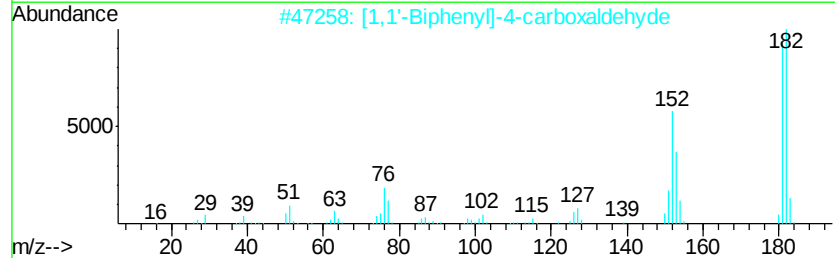
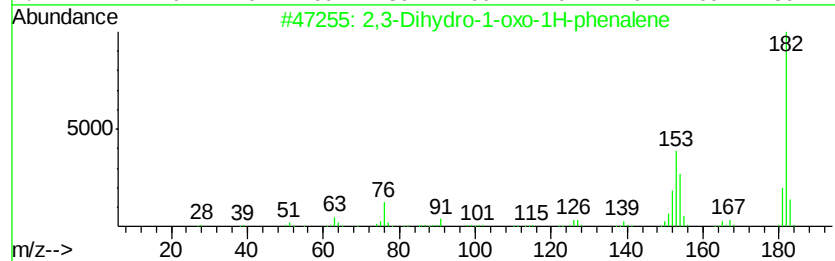
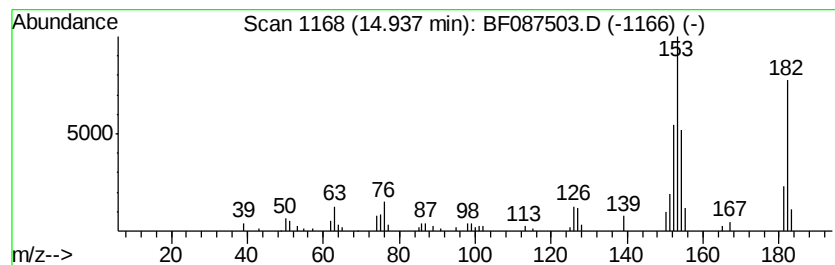
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2,3-Dihydro-1-oxo-1H-phenalene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	2.29 ng	129707	Phenanthrene-d10	14.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,3-Dihydro-1-oxo-1H-phenalene	182	C13H10O	000518-85-4	94
2		[1,1'-Biphenyl]-4-carboxaldehyde	182	C13H10O	003218-36-8	49
3		1,2-Acenaphthylenedione	182	C12H6O2	000082-86-0	38
4		3-Aminocarbazole	182	C12H10N2	006377-12-4	27
5		4-Picoline, 2-(ethylthio)-	153	C8H11NS	019006-78-1	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052816\
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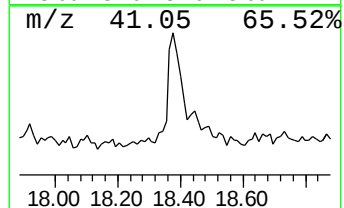
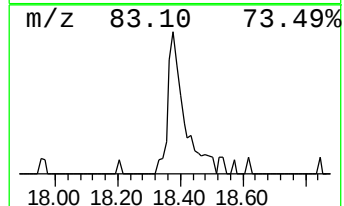
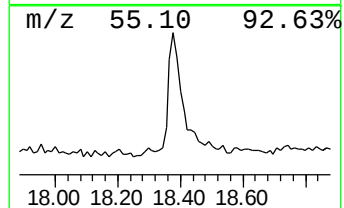
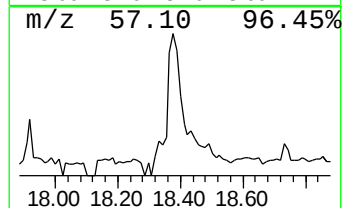
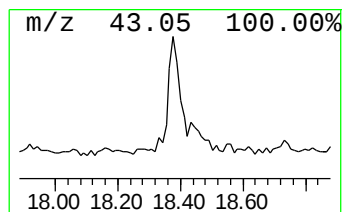
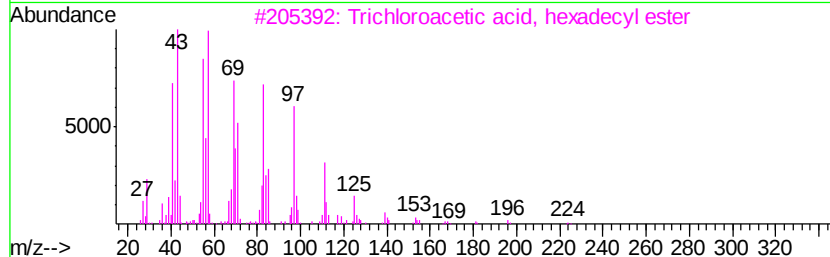
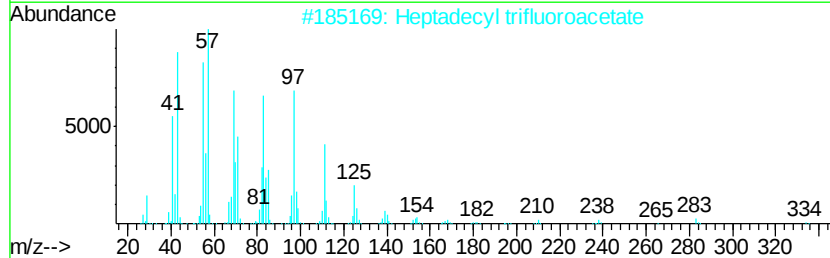
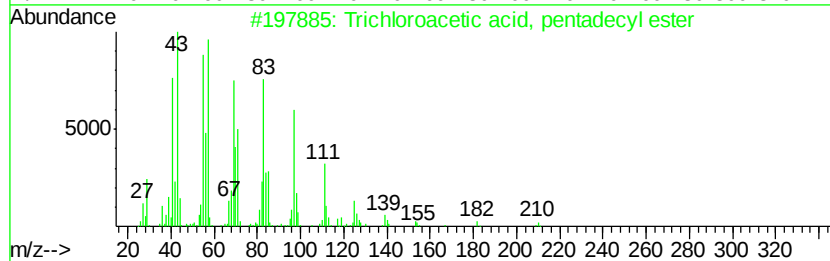
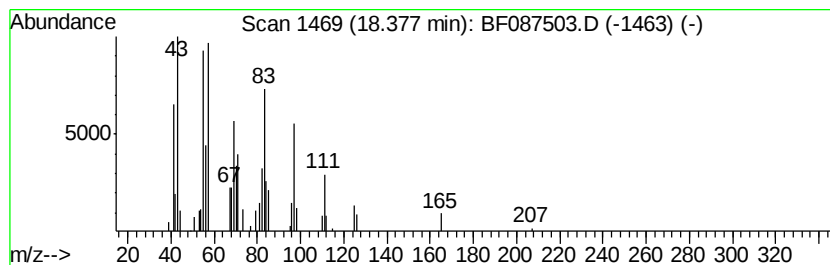
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Trichloroacetic acid, penta... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.38	2.59 ng	115888	Chrysene-d12	18.43

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4			1-Eicosanol	298	C20H42O	000629-96-9	91
5			1-Docosene	308	C22H44	001599-67-3	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052816\
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
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TIC Library : C:\Database\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.70	7.5	ng	321998	1	7.47	857287	20.0
unknown7.12	7.12	72.6	ng	3113760	1	7.47	857287	20.0
Benzene, 1,2,4-tr...	7.20	3.9	ng	167520	1	7.47	857287	20.0
Benzene, 1,2,3-tr...	7.56	3.9	ng	165174	1	7.47	857287	20.0
1-Propyne, 3-phenyl-	7.90	4.8	ng	207595	1	7.47	857287	20.0
1H-Indene, 1-methyl-	9.12	2.8	ng	151541	2	9.50	1085520	20.0
Benzene, 1-butynyl-	9.16	9.2	ng	499021	2	9.50	1085520	20.0
1(2H)-Acenaphthyl...	13.84	8.2	ng	462027	4	14.73	1131190	20.0
Tetradecane	13.93	2.8	ng	156332	4	14.73	1131190	20.0
2,3-Dihydro-1-oxo...	14.94	2.3	ng	129707	4	14.73	1131190	20.0
Trichloroacetic a...	18.38	2.6	ng	115888	5	18.43	895172	20.0