

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092716\
 Data File : BF090267.D
 Acq On : 27 Sep 2016 22:16
 Operator : UM/SJ
 Sample : H4949-06
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-3-2-LOC-3(10-15)

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-BF092016.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	1.644	4	5	56	rVB	2590374	7210738	84.99%	13.957%
2	3.004	117	124	127	rBV	3648799	8484134	100.00%	16.422%
3	4.559	257	260	274	rBV	372626	720616	8.49%	1.395%
4	5.039	299	302	304	rBV	2727244	3131548	36.91%	6.061%
5	6.136	395	398	401	rBV	2463045	3119311	36.77%	6.038%
6	6.239	405	407	410	rVV	2515491	3392642	39.99%	6.567%
7	6.479	425	428	430	rBV	649450	788327	9.29%	1.526%
8	6.627	439	441	444	rBV	2104767	2540684	29.95%	4.918%
9	7.050	475	478	480	rBV	1969472	2004565	23.63%	3.880%
10	7.759	538	540	543	rBV	967700	1040834	12.27%	2.015%
11	8.845	632	635	637	rBV	3466444	3559305	41.95%	6.889%
12	9.245	667	670	672	rBV	1084616	1081590	12.75%	2.093%
13	9.496	690	692	694	rVV	1042613	1110395	13.09%	2.149%
14	9.965	731	733	734	rVB	95937	88807	1.05%	0.172%
15	10.285	758	761	764	rBV	1907364	1934459	22.80%	3.744%
16	10.434	770	774	778	rBV	106708	163096	1.92%	0.316%
17	10.971	818	821	825	rBV2	917796	1299196	15.31%	2.515%
18	11.496	865	867	869	rVV	98325	100239	1.18%	0.194%
19	11.576	872	874	878	rVB2	128808	229988	2.71%	0.445%
20	11.759	888	890	895	rVB2	63987	100456	1.18%	0.194%
21	12.011	909	912	914	rBV	93420	126822	1.49%	0.245%
22	12.091	918	919	923	rVB	86839	89432	1.05%	0.173%
23	12.171	923	926	928	rBV	675219	886002	10.44%	1.715%
24	12.388	942	945	947	rVV	1017025	991518	11.69%	1.919%
25	12.548	957	959	962	rVV	1857012	2029035	23.92%	3.927%
26	12.617	962	965	967	rVV2	63692	91756	1.08%	0.178%
27	12.719	969	974	976	rVB2	96511	194733	2.30%	0.377%
28	12.822	981	983	985	rBV	105297	120961	1.43%	0.234%
29	13.222	1015	1018	1022	rBV	62175	92977	1.10%	0.180%
30	13.325	1025	1027	1028	rBV	82452	96562	1.14%	0.187%
31	13.360	1028	1030	1035	rVV4	60100	183757	2.17%	0.356%
32	13.462	1038	1039	1045	rVB3	210369	299464	3.53%	0.580%
33	13.577	1046	1049	1056	rVV2	1005189	1713746	20.20%	3.317%
34	14.102	1092	1095	1099	rVB3	50296	120057	1.42%	0.232%

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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

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35	14.560	1133	1135	1140	rBV	432037	719890	8.49%	1.393%
36	14.800	1154	1156	1158	rBV	218366	223414	2.63%	0.432%
37	14.845	1158	1160	1162	rVV	332266	312333	3.68%	0.605%
38	14.903	1162	1165	1169	rVV	553782	745291	8.78%	1.443%
39	16.034	1261	1264	1268	rVB2	127718	203573	2.40%	0.394%
40	16.366	1290	1293	1300	rVB	98710	193038	2.28%	0.374%
41	18.240	1453	1457	1466	rVB7	24001	129171	1.52%	0.250%

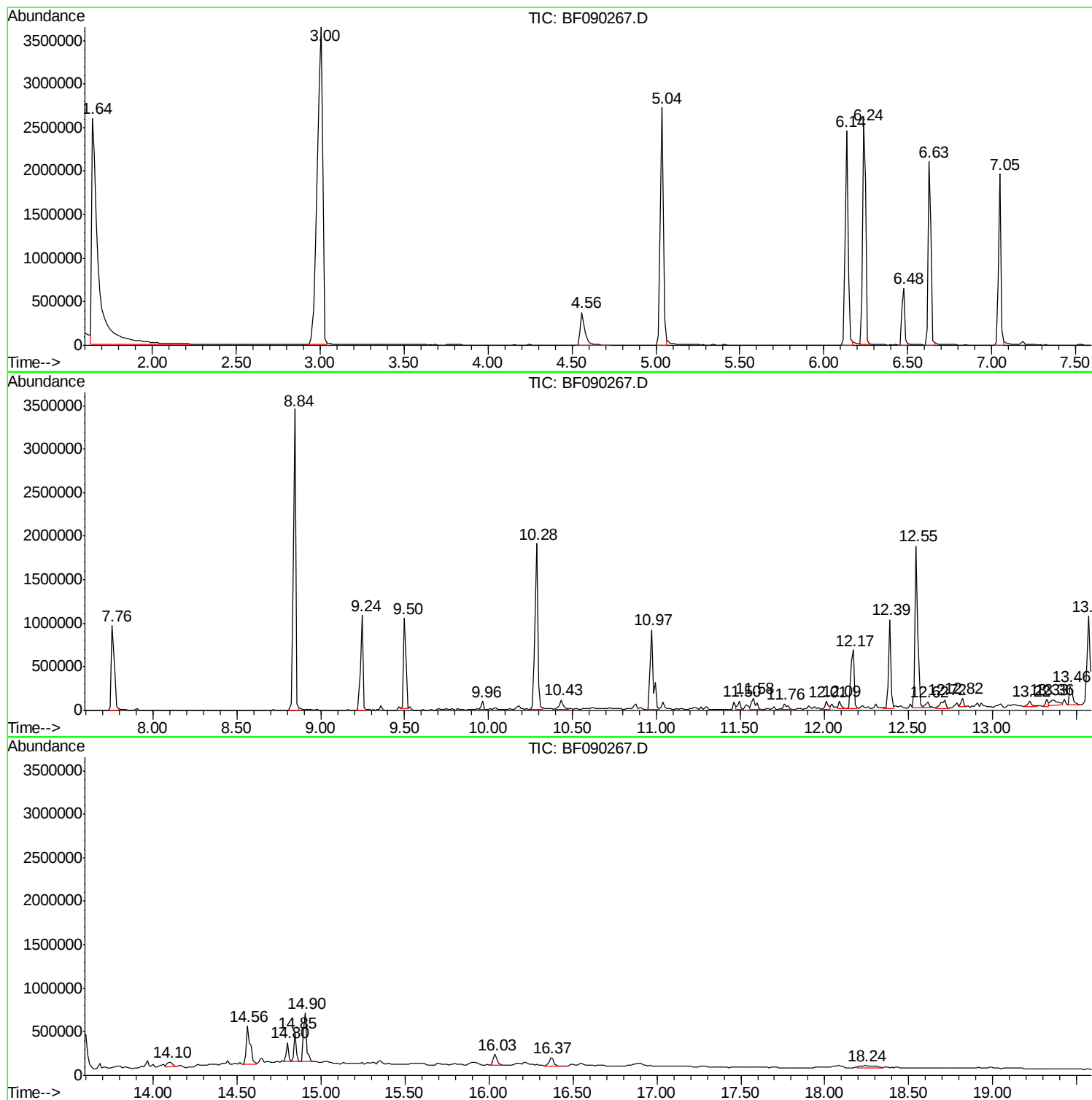
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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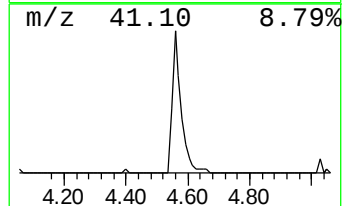
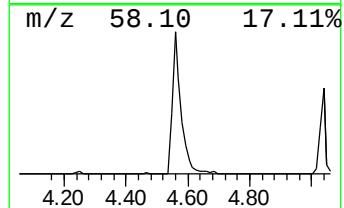
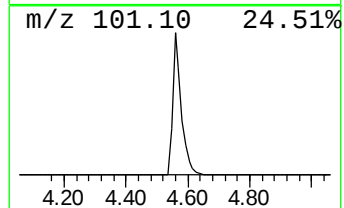
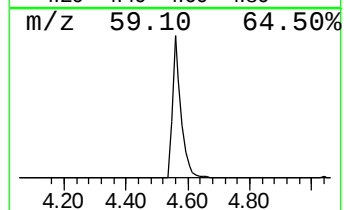
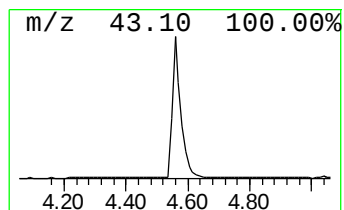
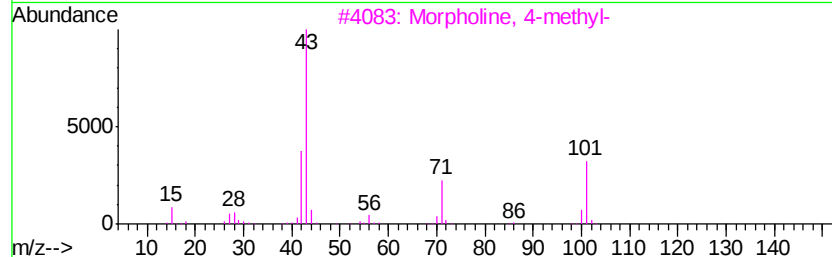
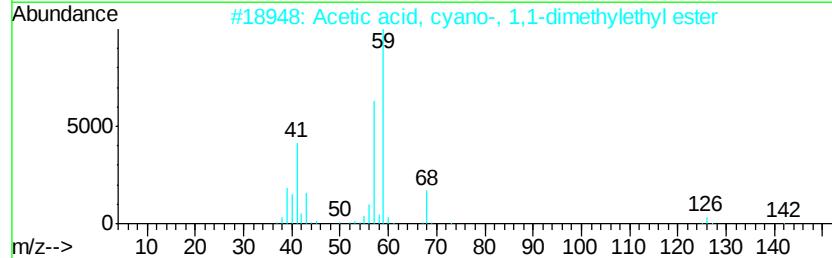
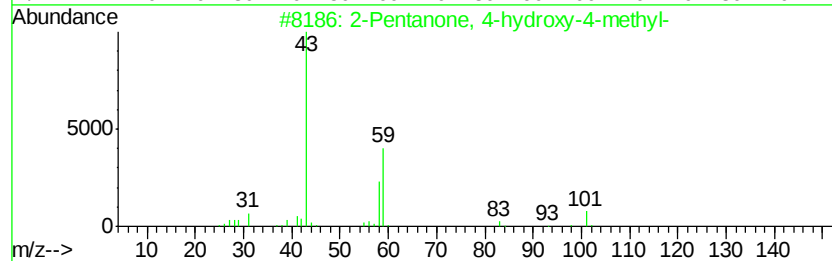
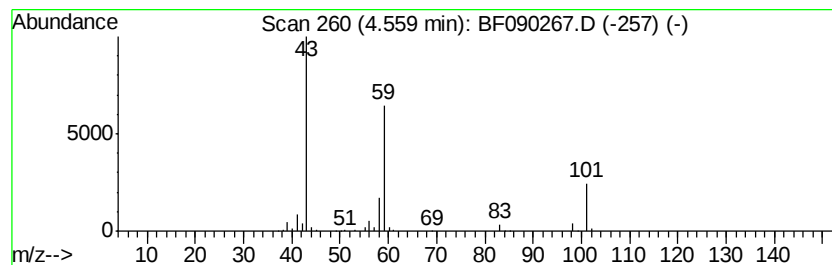
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	18.28 ng	720616	1,4-Dichlorobenzene-d4	6.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Acetone	58	C3H6O	000067-64-1	9



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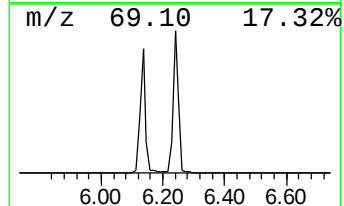
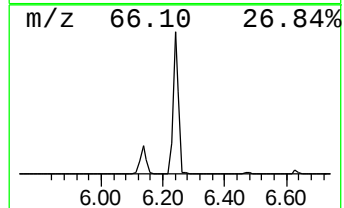
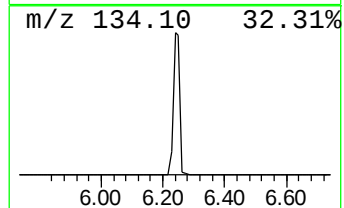
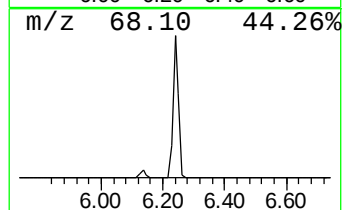
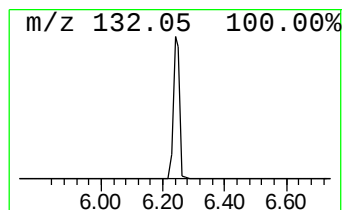
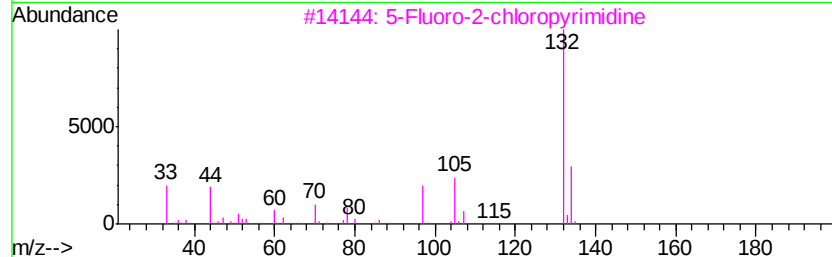
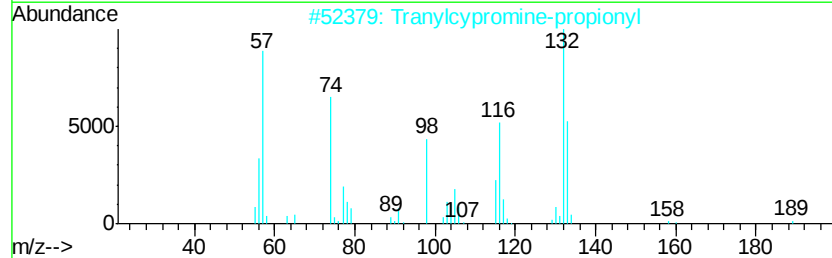
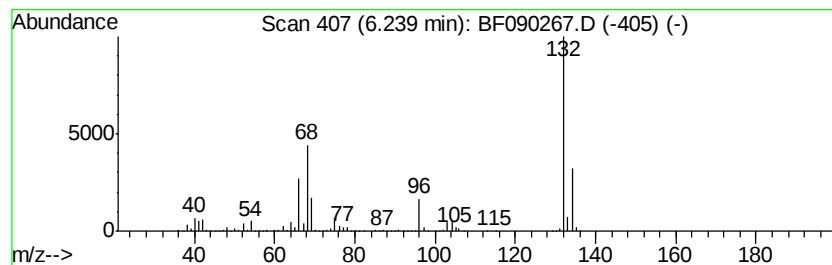
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown6.24 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	86.07 ng	3392640	1,4-Dichlorobenzene-d4	6.48

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16		
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10		
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9		
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9		
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9		



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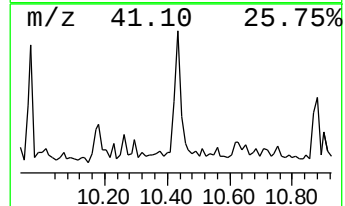
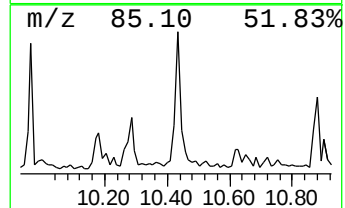
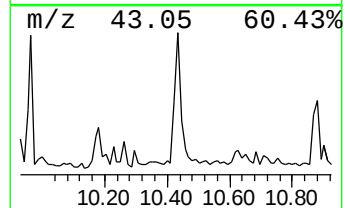
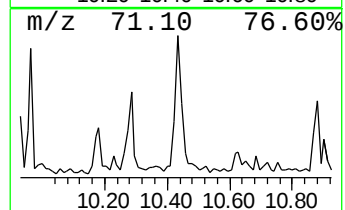
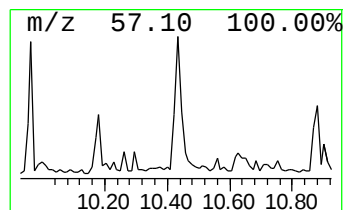
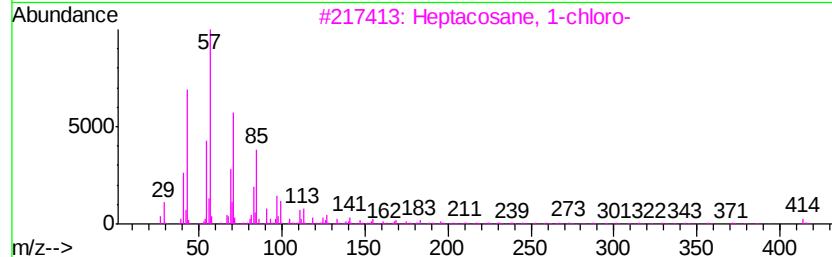
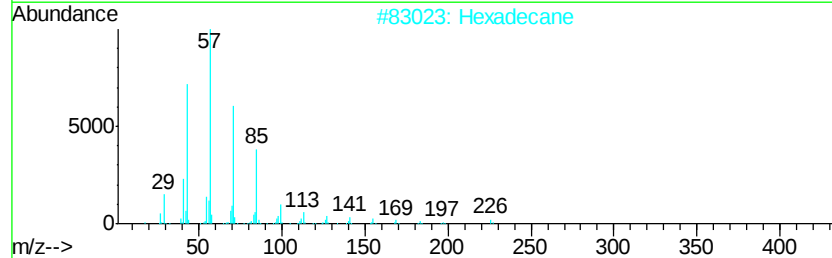
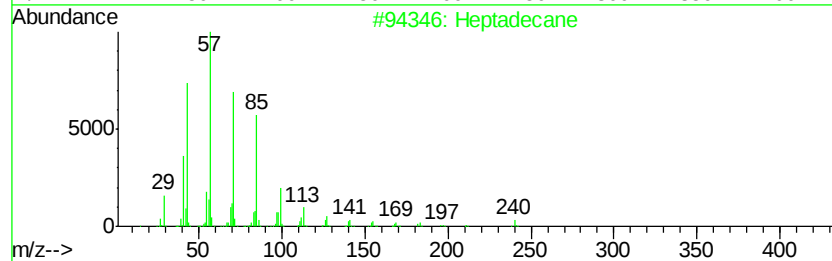
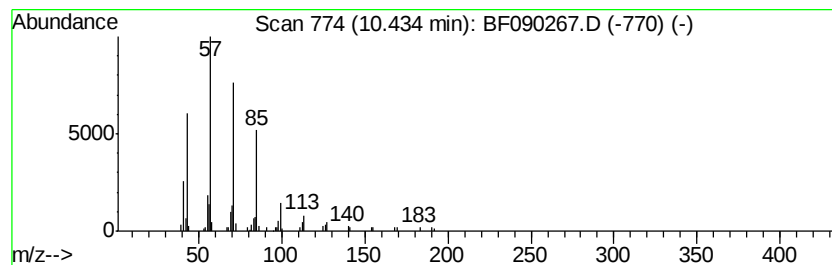
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.43	2.51 ng	163096	Phenanthrene-d10		10.97
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	90
4	Tritetracontane	605	C43H88	007098-21-7	90
5	Heneicosane	296	C21H44	000629-94-7	90



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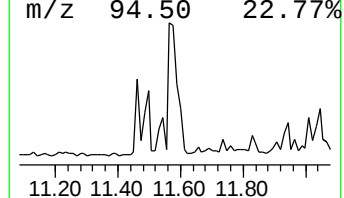
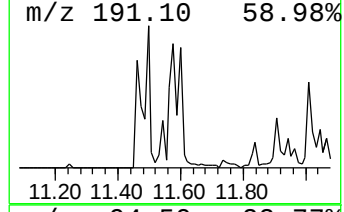
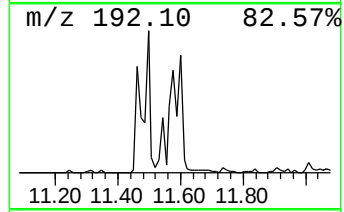
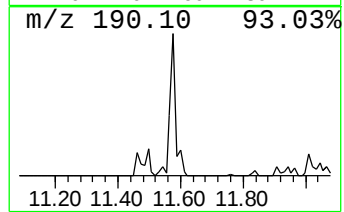
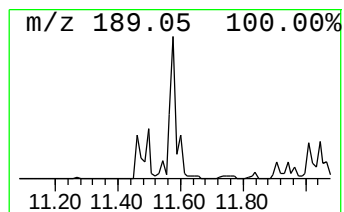
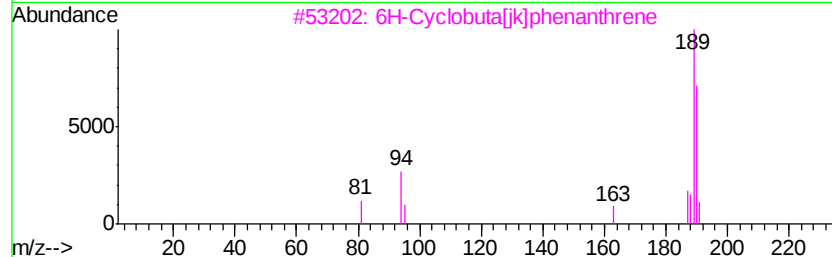
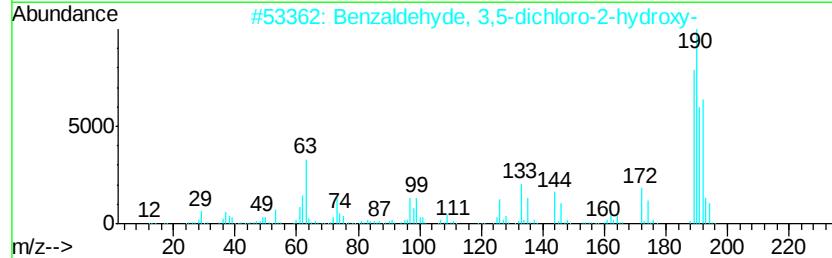
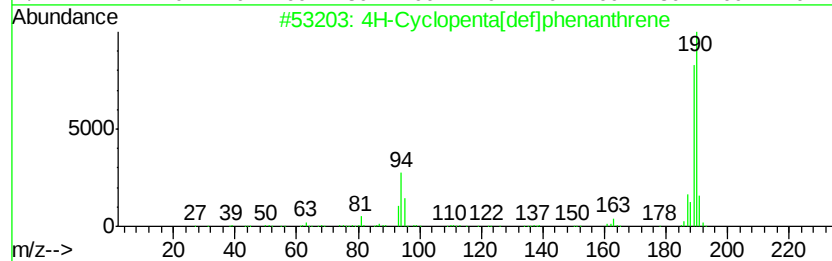
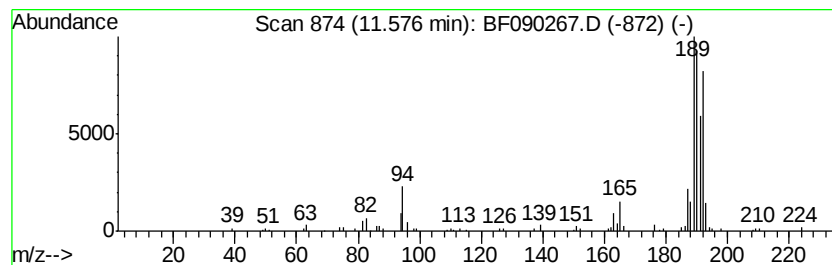
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.58	3.54 ng	229988	Phenanthrene-d10	10.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	90
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	72
3	6H-Cyclobuta[ik]phenanthrene	190	C15H10	083469-43-6	49
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	42
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	38



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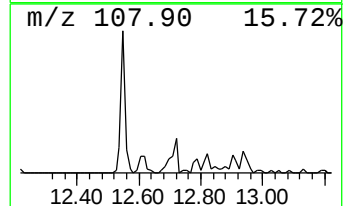
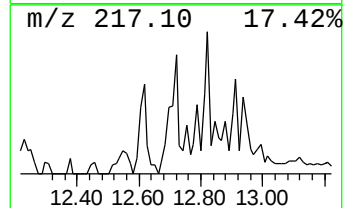
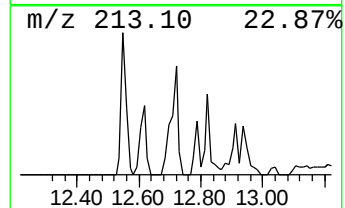
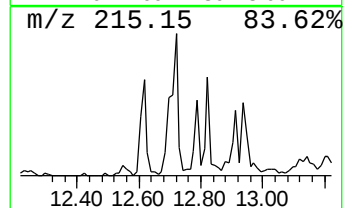
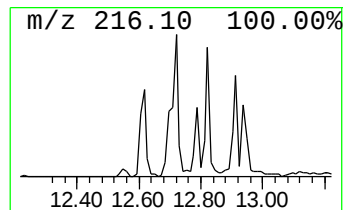
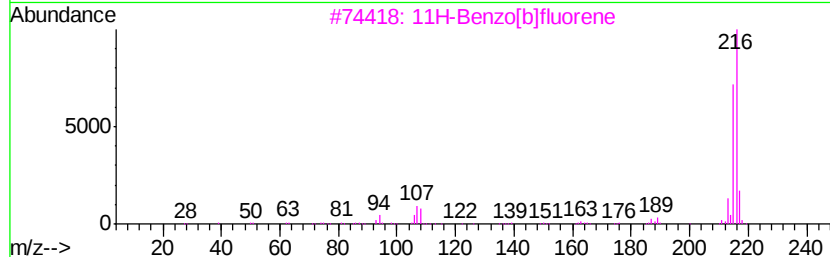
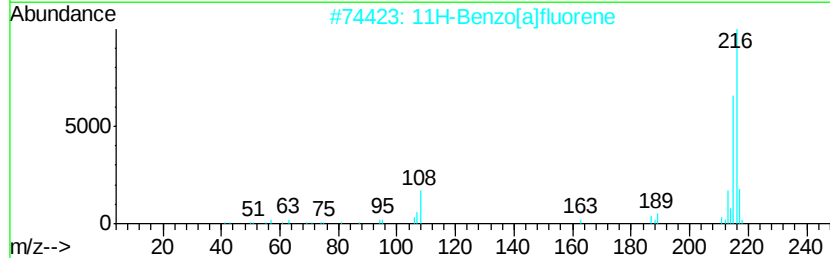
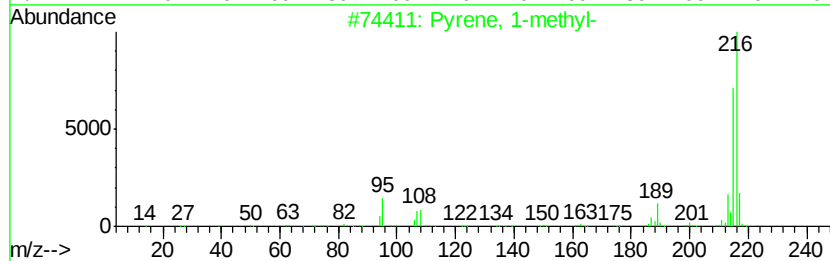
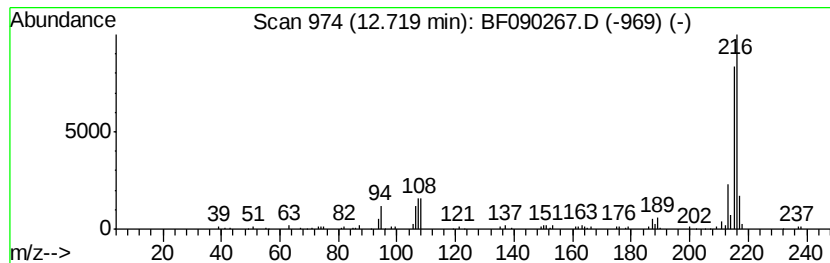
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Pyrene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	2.27 ng	194733	Chrysene-d12	13.58
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Pyrene, 1-methyl-	216 C17H12	002381-21-7 97
2		11H-Benzo[a]fluorene	216 C17H12	000238-84-6 95
3		11H-Benzo[b]fluorene	216 C17H12	000243-17-4 94
4		Pyrene, 2-methyl-	216 C17H12	003442-78-2 91
5		Fluoranthene, 2-methyl-	216 C17H12	033543-31-6 89



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
Data File : BF090267.D
Acq On : 27 Sep 2016 22:16
Operator : UM/SJ
Sample : H4949-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

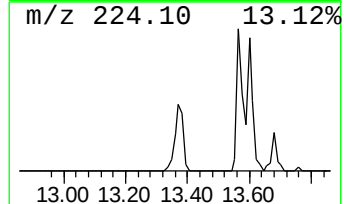
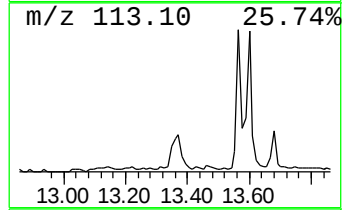
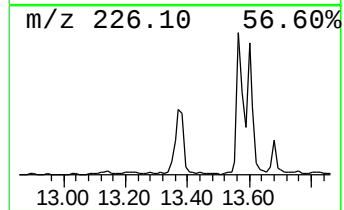
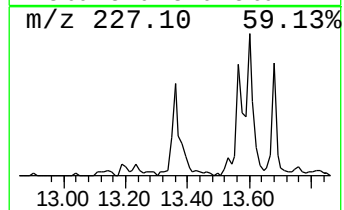
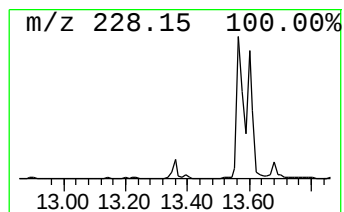
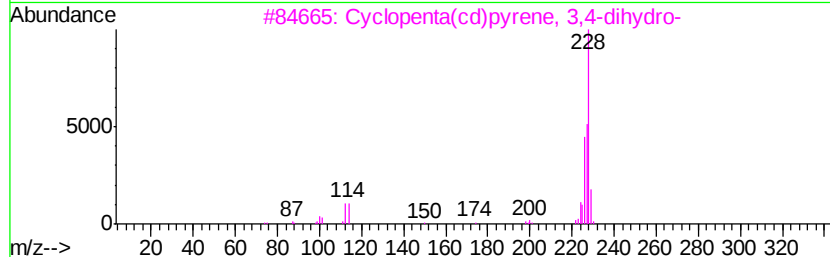
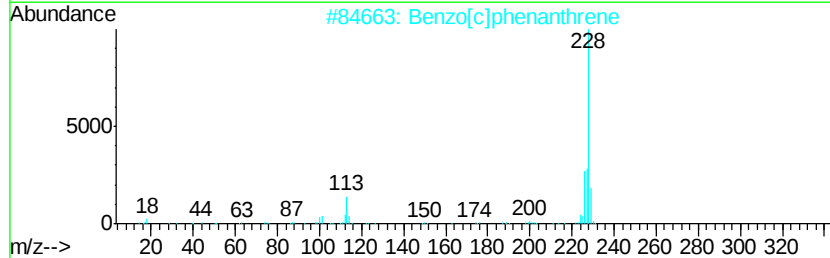
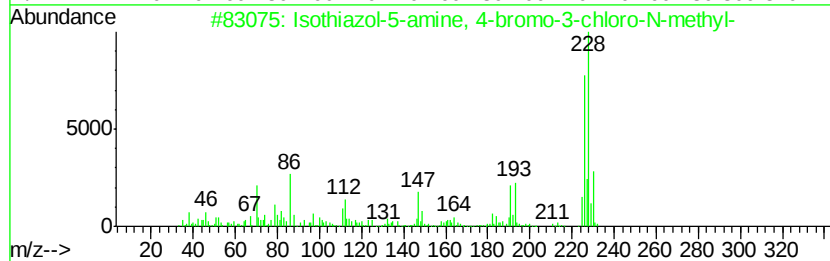
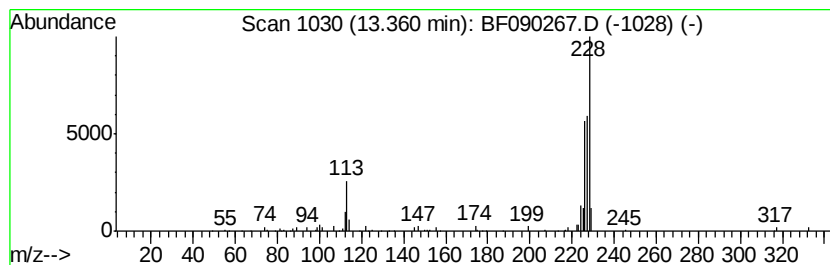
Instrument :
BNA_F
ClientSampleId :
S-3-2-LOC-3(10-15)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Isothiazol-5-amine, 4-bromo... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.36	2.14 ng	183757	Chrysene-d12	13.58	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isothiazol-5-amine, 4-bromo-3-ch...	226	C4H4BrClN2S	1000272-59-9	58
2	Benzo[c]phenanthrene	228	C18H12	000195-19-7	53
3	Cvclopenta(cd)pvrene, 3,4-dihydro-	228	C18H12	025732-74-5	47
4	1,2,3-Triazole, 4-triethylqermvl...	257	C9H17GeN3O	184588-50-9	33
5	Thiazolo[4,5-f]quinoline, 2,7,9-...	228	C13H12N2S	038463-39-7	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092716\
Data File : BF090267.D
Acq On : 27 Sep 2016 22:16
Operator : UM/SJ
Sample : H4949-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-3-2-LOC-3(10-15)

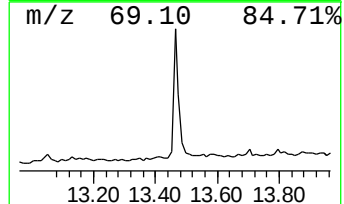
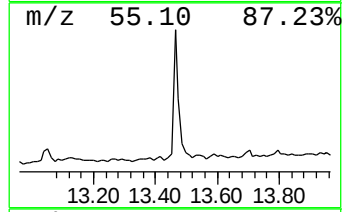
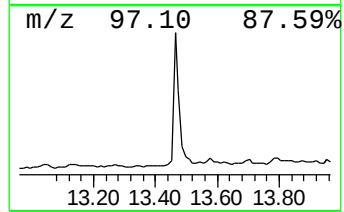
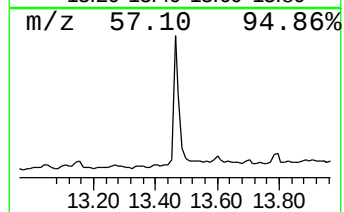
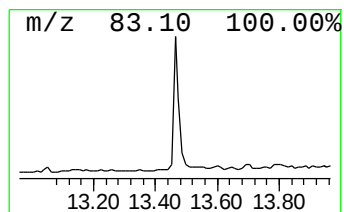
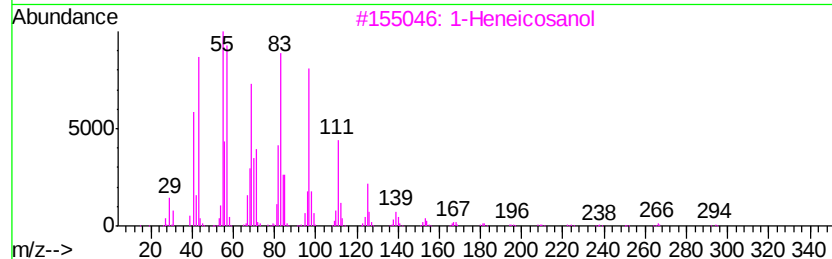
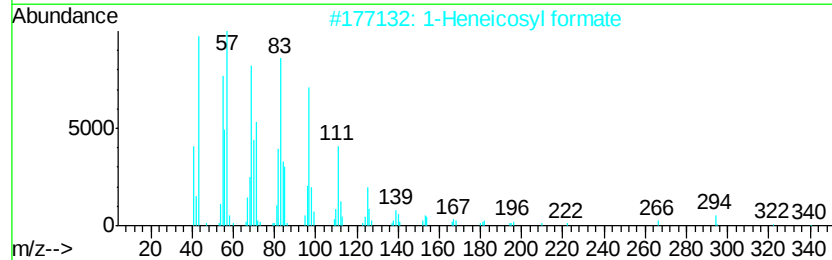
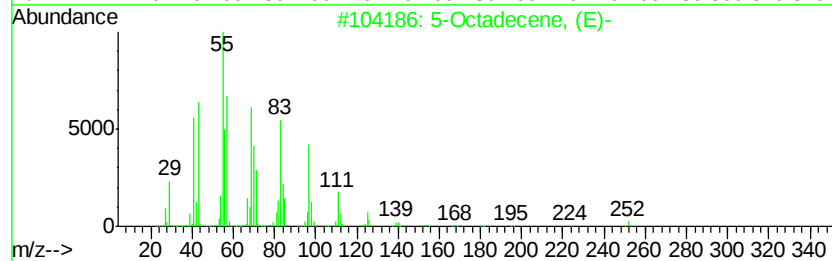
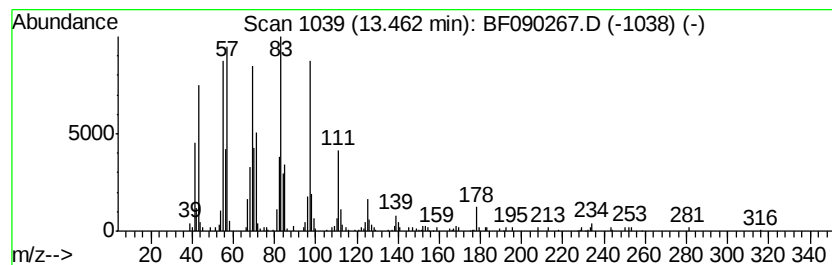
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 5-Octadecene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	3.49 ng	299464	Chrysene-d12	13.58

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Octadecene, (E)-	252	C18H36	007206-21-5	96
2			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5			1-Nonadecene	266	C19H38	018435-45-5	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092716\
Data File : BF090267.D
Acq On : 27 Sep 2016 22:16
Operator : UM/SJ
Sample : H4949-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-3-2-LOC-3(10-15)

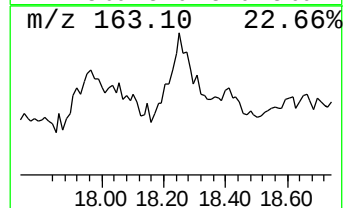
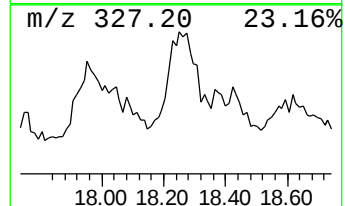
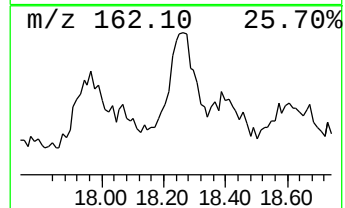
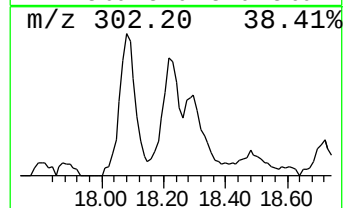
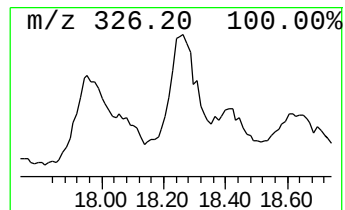
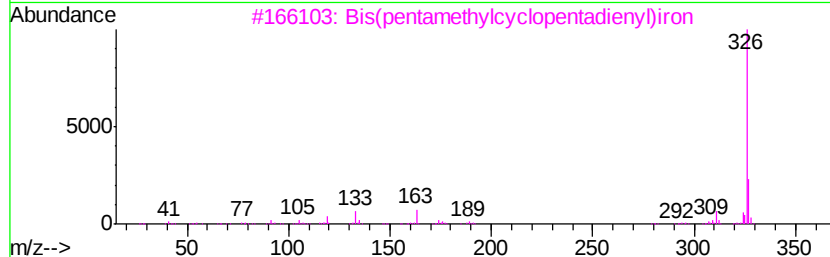
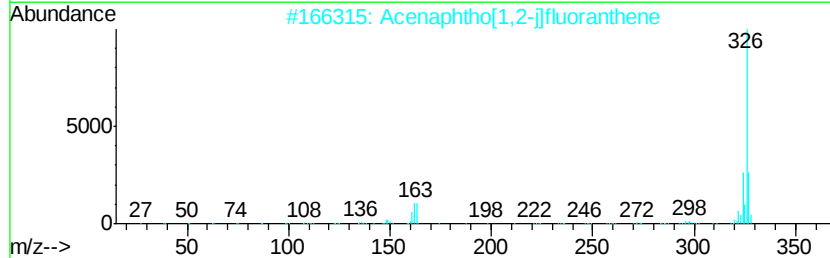
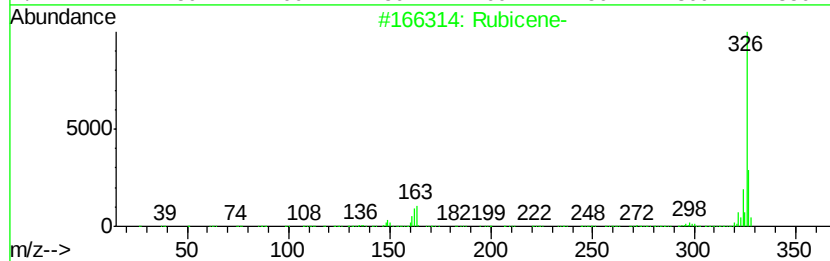
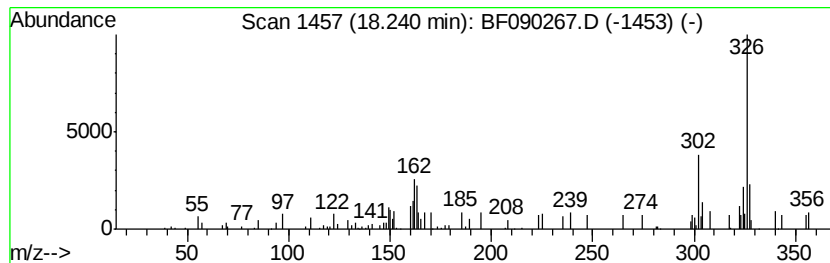
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Rubicene- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.24	3.47 ng	129171	Perylene-d12	14.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Rubicene-	326	C26H14	000197-61-5	55
2		Acenaphtho[1,2-ij]fluoranthene	326	C26H14	000193-21-5	55
3		Bis(pentamethylcyclopentadienyl)...	326	C20H30Fe	012126-50-0	38
4		5,7-Dimethoxy-3-(3,4-methylenedi...	326	C18H14O6	022044-59-3	35
5		Triphenylphosphonium cyclopentad...	326	C23H19P	029473-30-1	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092716\
Data File : BF090267.D
Acq On : 27 Sep 2016 22:16
Operator : UM/SJ
Sample : H4949-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-3-2-LOC-3(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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
2-Pentanone, 4-hy...	4.56	18.3	ng	720616	1	6.48	788327	20.0
unknown6.24	6.24	86.1	ng	3392640	1	6.48	788327	20.0
Heptadecane	10.43	2.5	ng	163096	4	10.97	1299200	20.0
4H-Cyclopenta[def...	11.58	3.5	ng	229988	4	10.97	1299200	20.0
Pyrene, 1-methyl-	12.72	2.3	ng	194733	5	13.58	1713750	20.0
Isothiazol-5-amin...	13.36	2.1	ng	183757	5	13.58	1713750	20.0
5-Octadecene, (E)-	13.46	3.5	ng	299464	5	13.58	1713750	20.0
Rubcene-	18.24	3.5	ng	129171	6	14.90	745291	20.0