

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010617\
 Data File : BF092132.D
 Acq On : 6 Jan 2017 22:18
 Operator : UM/SJ
 Sample : I1045-06 5X
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RAP-SP4

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-BF122116.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	2.024	10	12	27	rVB	42699	224528	20.30%	1.772%
2	4.767	249	252	259	rVB	122639	199203	18.01%	1.573%
3	5.247	293	294	300	rBV	288756	447553	40.47%	3.533%
4	6.322	385	388	392	rBV	339507	401167	36.28%	3.167%
5	6.424	395	397	399	rBV	424055	436135	39.44%	3.443%
6	6.642	414	416	419	rBV	1095422	926680	83.80%	7.315%
7	6.802	427	430	432	rVB	332702	344615	31.16%	2.720%
8	7.213	463	466	468	rBV	228254	236432	21.38%	1.866%
9	7.453	482	487	489	rBV3	14521	23475	2.12%	0.185%
10	7.933	526	529	531	rBV	1296779	1105867	100.00%	8.730%
11	8.367	565	567	571	rVB	22548	28266	2.56%	0.223%
12	8.539	580	582	584	rBV2	21936	24592	2.22%	0.194%
13	8.962	617	619	621	rVB2	21446	21201	1.92%	0.167%
14	9.008	621	623	625	rVB	568119	436831	39.50%	3.448%
15	9.099	628	631	634	rBV	34259	45379	4.10%	0.358%
16	9.156	634	636	639	rVB3	9352	19112	1.73%	0.151%
17	9.270	644	646	648	rBV2	11406	19248	1.74%	0.152%
18	9.339	651	652	654	rBV2	19259	25342	2.29%	0.200%
19	9.408	657	658	660	rVB2	51526	61809	5.59%	0.488%
20	9.625	676	677	679	rBV	32253	28430	2.57%	0.224%
21	9.682	679	682	683	rVV	1061816	993031	89.80%	7.839%
22	9.705	683	684	689	rVB	24641	34933	3.16%	0.276%
23	9.888	694	700	701	rBV4	25872	44951	4.06%	0.355%
24	10.002	708	710	713	rVB4	10780	21529	1.95%	0.170%
25	10.082	715	717	719	rVV3	9839	18209	1.65%	0.144%
26	10.128	719	721	723	rVB	32469	29459	2.66%	0.233%
27	10.219	728	729	733	rVB2	21942	33942	3.07%	0.268%
28	10.322	736	738	739	rBV	39296	41407	3.74%	0.327%
29	10.470	748	751	753	rBV	173469	187791	16.98%	1.482%
30	10.596	760	762	766	rBV2	55601	88877	8.04%	0.702%
31	10.916	785	790	792	rBV5	11406	28373	2.57%	0.224%
32	11.042	799	801	802	rBV	44586	38601	3.49%	0.305%
33	11.076	802	804	806	rVB	34432	42364	3.83%	0.334%
34	11.156	809	811	812	rBV	1079828	897899	81.19%	7.088%

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35	11.179	812	813	815	rVV	124852	97838	8.85%	0.772%
36	11.225	815	817	819	rVB2	28176	45828	4.14%	0.362%
37	11.271	819	821	823	rBV2	8338	17500	1.58%	0.138%
38	11.396	829	832	833	rBV2	43920	55411	5.01%	0.437%
39	11.465	836	838	841	rBV2	39565	57519	5.20%	0.454%
40	11.568	845	847	850	rBV4	13252	17430	1.58%	0.138%
41	11.659	850	855	856	rBV3	38807	74811	6.76%	0.591%
42	11.762	863	864	869	rVB2	37448	76094	6.88%	0.601%
43	11.876	872	874	877	rVB2	39942	47221	4.27%	0.373%
44	11.979	877	883	886	rBV5	37336	96667	8.74%	0.763%
45	12.025	886	887	888	rBV	14128	18227	1.65%	0.144%
46	12.082	891	892	895	rBV3	27072	52545	4.75%	0.415%
47	12.162	895	899	900	rBV4	20337	54698	4.95%	0.432%
48	12.208	901	903	904	rBV	52885	61577	5.57%	0.486%
49	12.265	906	908	909	rVB	54318	51236	4.63%	0.404%
50	12.299	909	911	912	rBV2	24173	35523	3.21%	0.280%
51	12.368	915	917	919	rVV	198229	207699	18.78%	1.640%
52	12.414	919	921	924	rBV3	22376	50011	4.52%	0.395%
53	12.585	934	936	938	rBV2	143953	213337	19.29%	1.684%
54	12.631	938	940	941	rVV2	45287	50108	4.53%	0.396%
55	12.745	948	950	952	rBV	281586	385963	34.90%	3.047%
56	12.916	963	965	967	rVB2	47953	56106	5.07%	0.443%
57	12.985	969	971	973	rVV2	82687	100426	9.08%	0.793%
58	13.328	1000	1001	1003	rBV	80580	101547	9.18%	0.802%
59	13.785	1039	1041	1045	rBV	928528	1096480	99.15%	8.656%
60	14.277	1082	1084	1085	rBV	149264	162245	14.67%	1.281%
61	14.574	1108	1110	1117	rBV3	259604	570948	51.63%	4.507%
62	15.157	1159	1161	1163	rVB	489522	697989	63.12%	5.510%
63	16.288	1257	1260	1262	rBV3	221507	557621	50.42%	4.402%

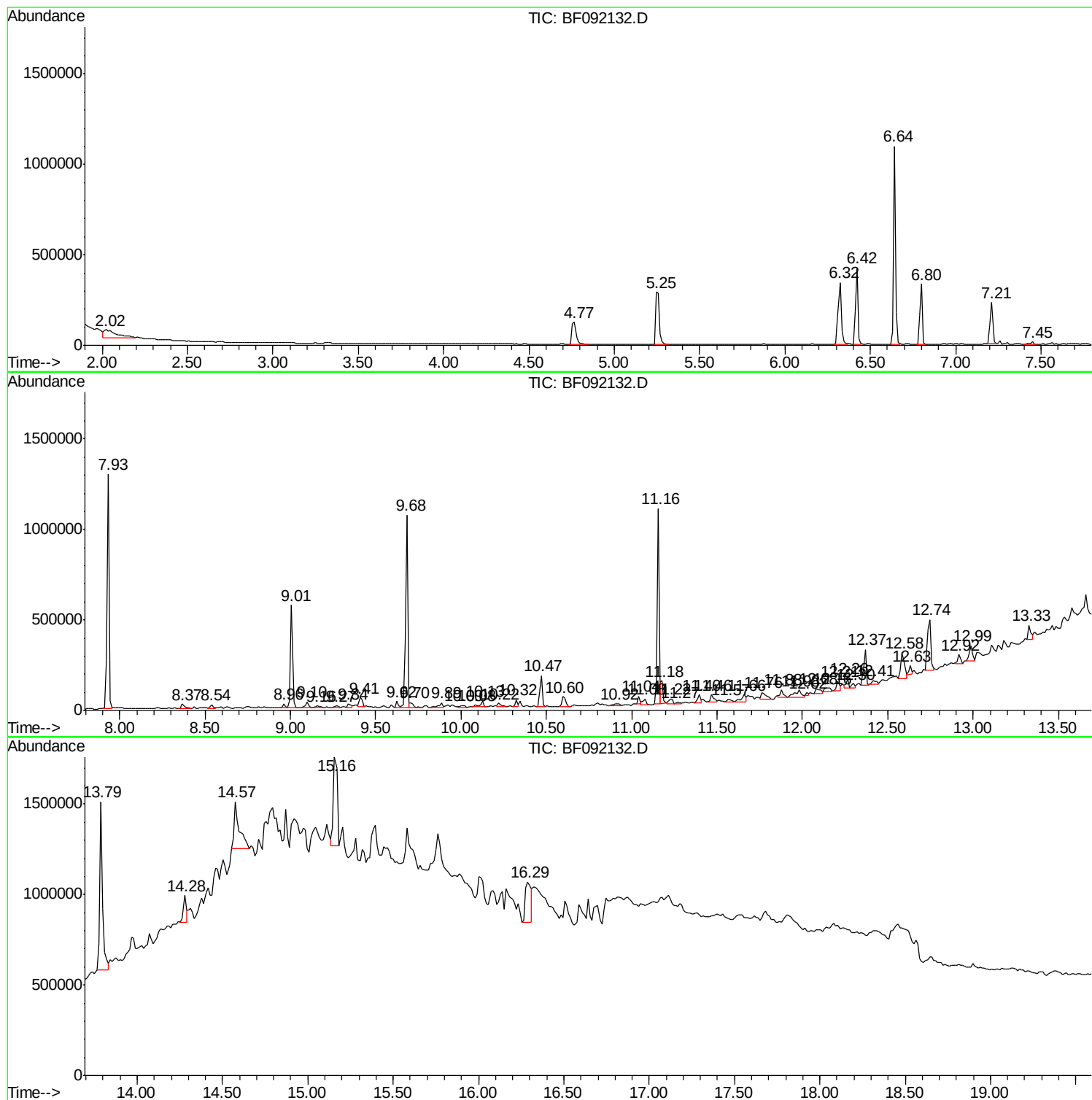
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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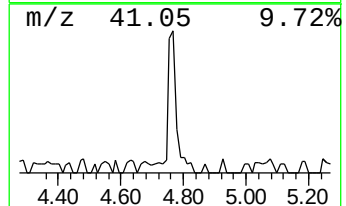
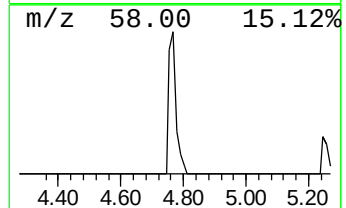
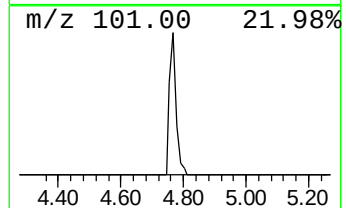
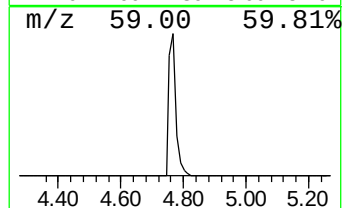
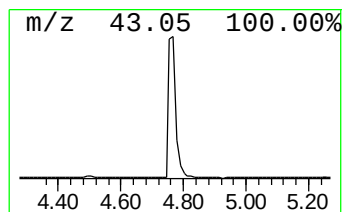
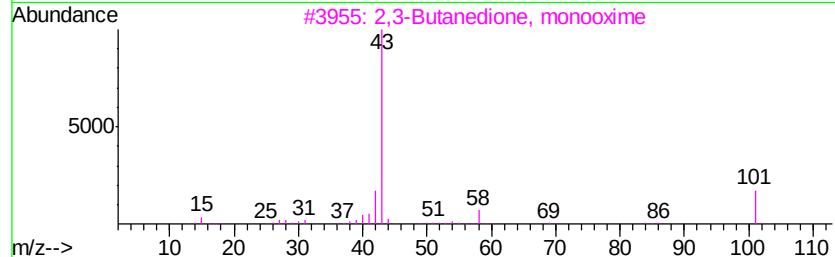
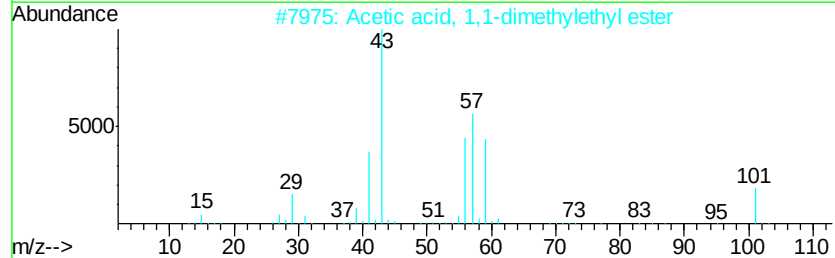
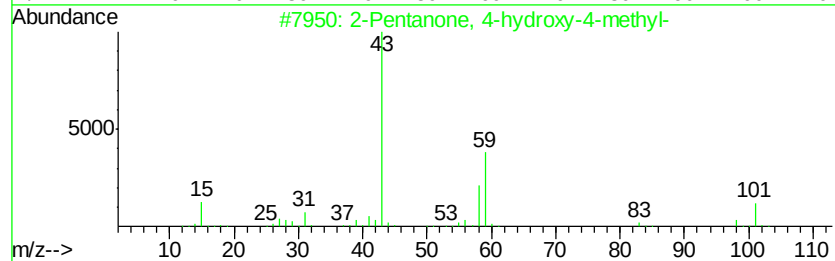
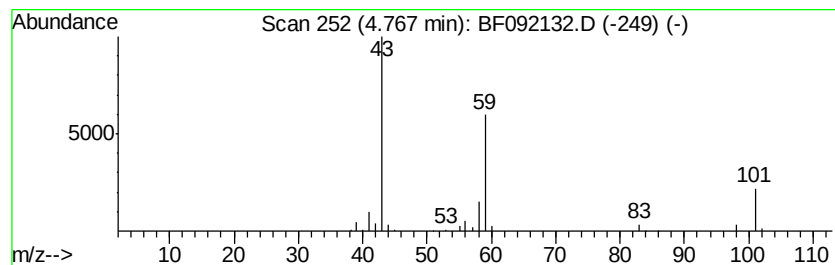
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.77	4.30 ng	199203	1,4-Dichlorobenzene-d4	6.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
5			3-Hexanol	102	C6H14O	000623-37-0	25



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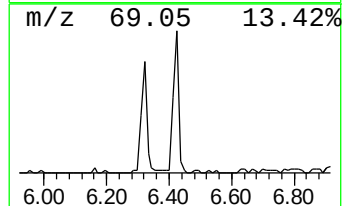
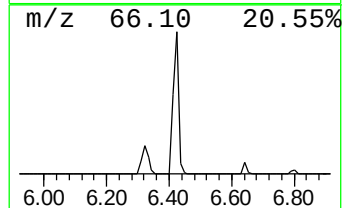
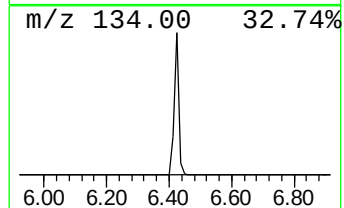
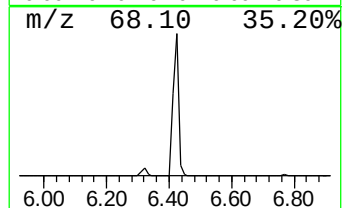
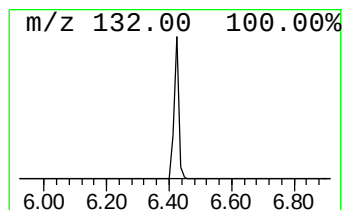
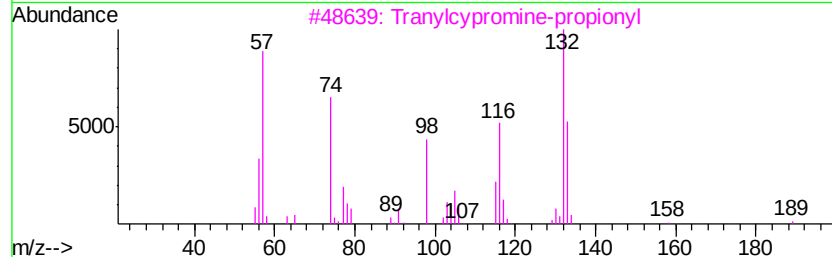
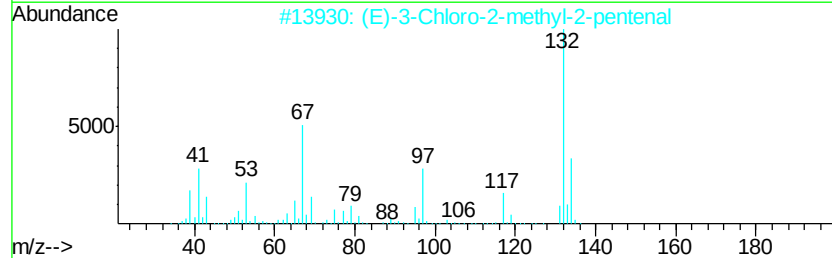
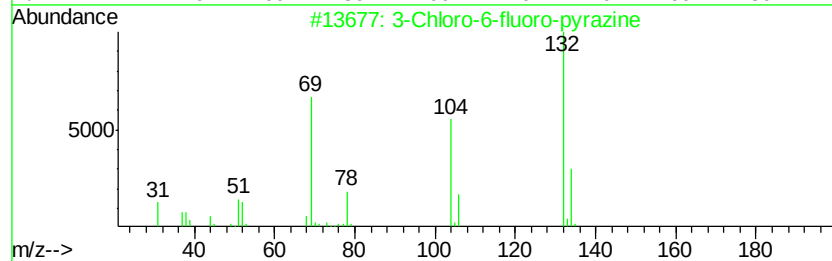
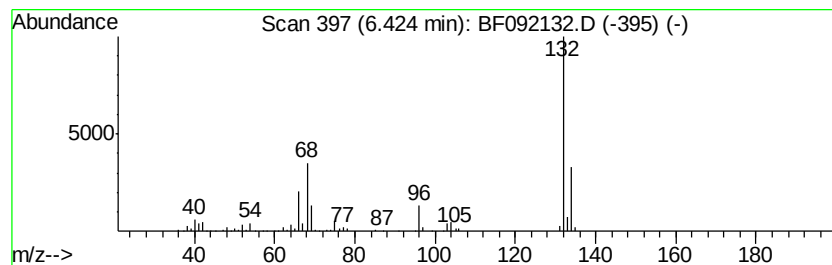
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.42 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	9.41 ng	436135	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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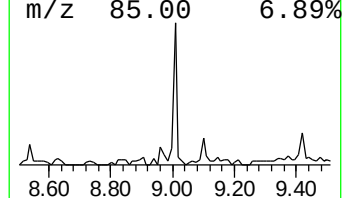
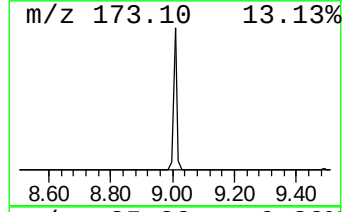
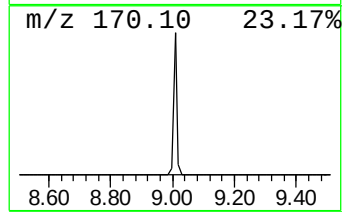
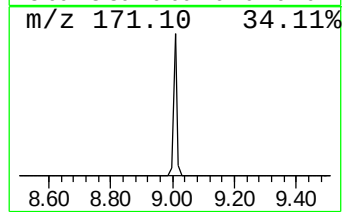
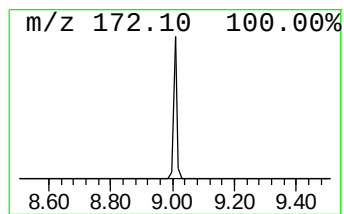
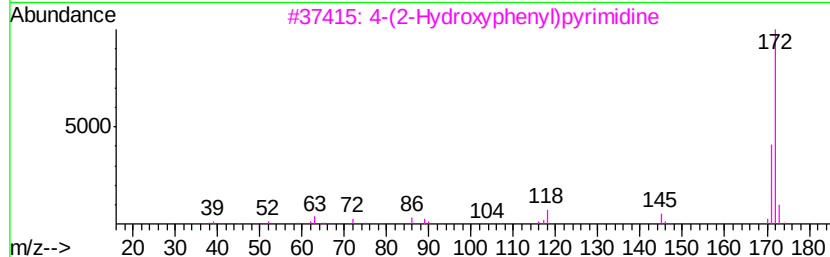
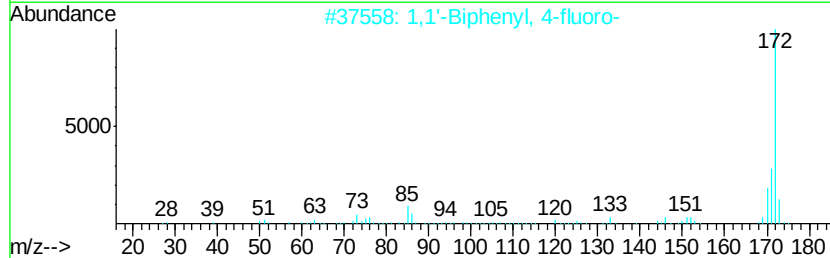
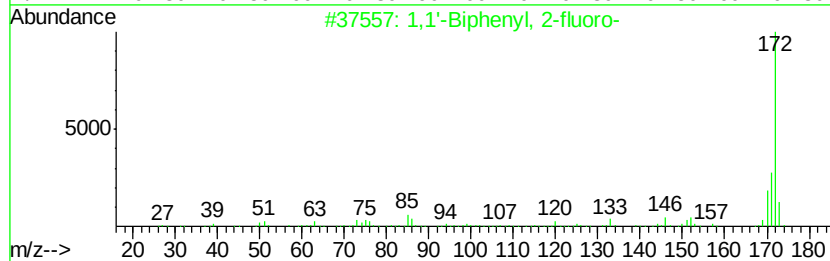
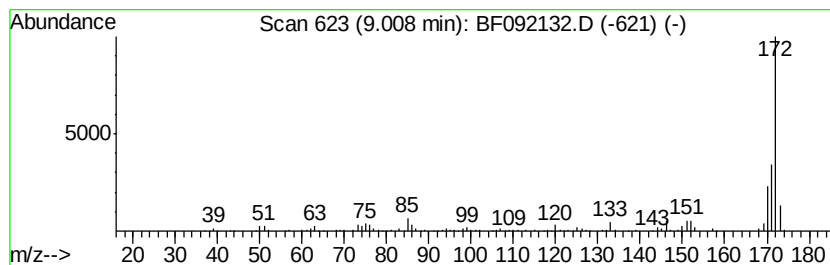
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,1'-Biphenyl, 2-fluoro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.01	8.80 ng	436831	Acenaphthene-d10	9.68	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2-fluoro-	172	C12H9F	000321-60-8	96
2	1,1'-Biphenyl, 4-fluoro-	172	C12H9F	000324-74-3	93
3	4-(2-Hydroxyphenyl)pyrimidine	172	C10H8N2O	068535-55-7	59
4	5-Hydroxy-2-phenylpyrimidine	172	C10H8N2O	066739-85-3	49
5	4-Pyrimidinol, 5-phenyl-	172	C10H8N2O	022433-69-8	42



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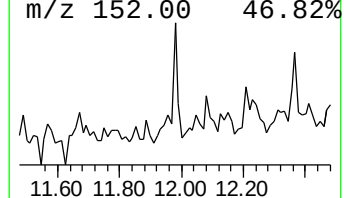
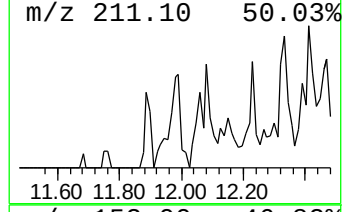
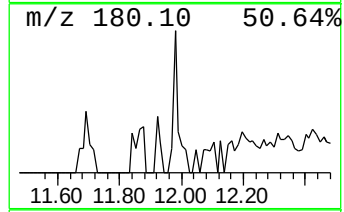
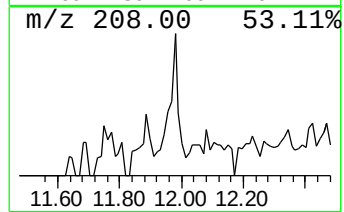
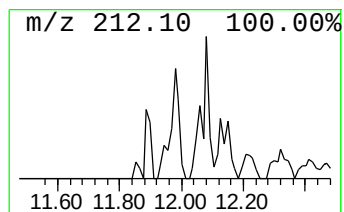
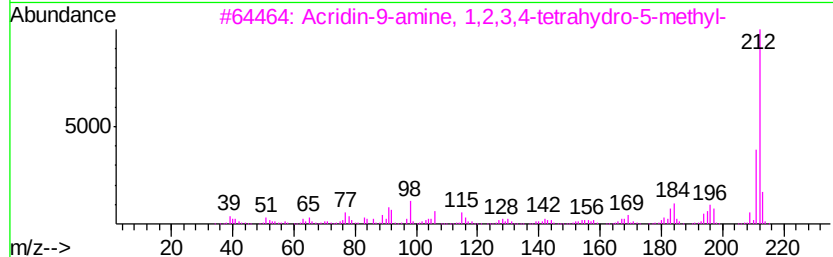
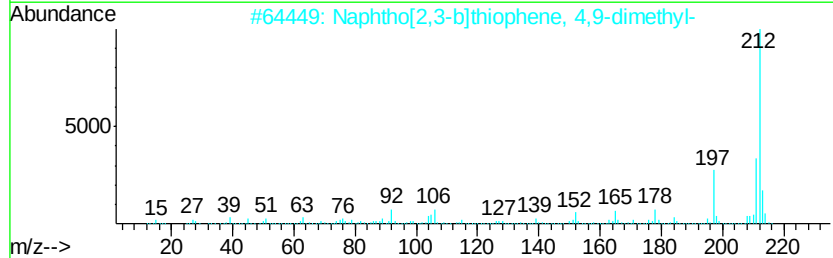
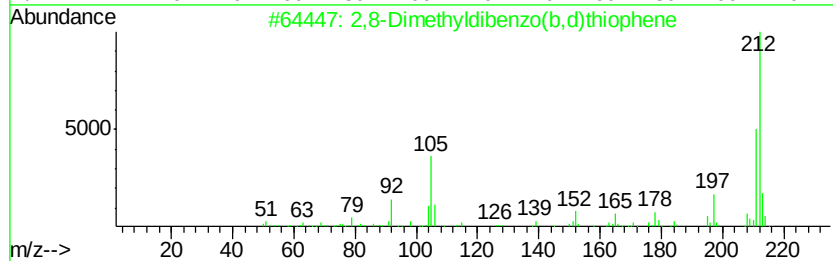
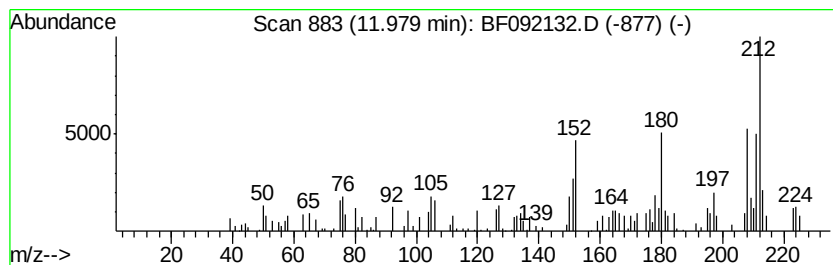
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown11.98 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	2.15 ng	96667	Phenanthrene-d10	11.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,8-Dimethyldibenzo(b,d)thiophene	212	C14H12S	001207-15-4	49
2		Naphtho[2,3-b]thiophene, 4,9-dim...	212	C14H12S	016587-34-1	45
3		Acridin-9-amine, 1,2,3,4-tetrahy...	212	C14H16N2	005778-78-9	43
4		2-Phenyl-2,3-dihydrobenzo[b]thio...	212	C14H12S	054493-00-4	41
5		9,10-Anthracenedione	208	C14H8O2	000084-65-1	38



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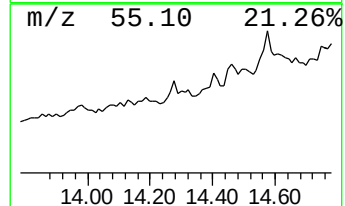
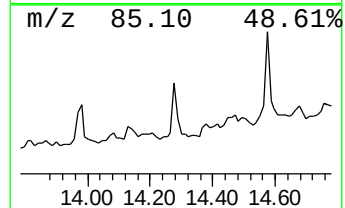
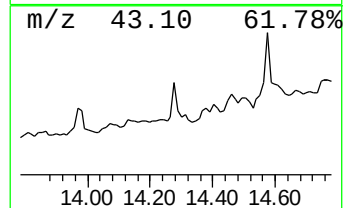
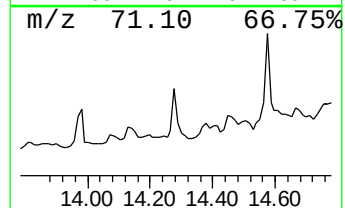
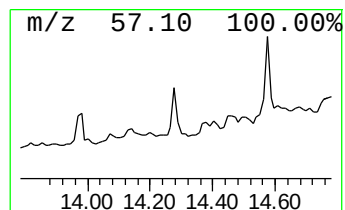
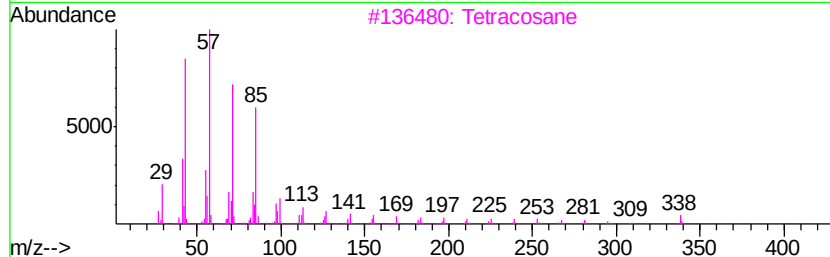
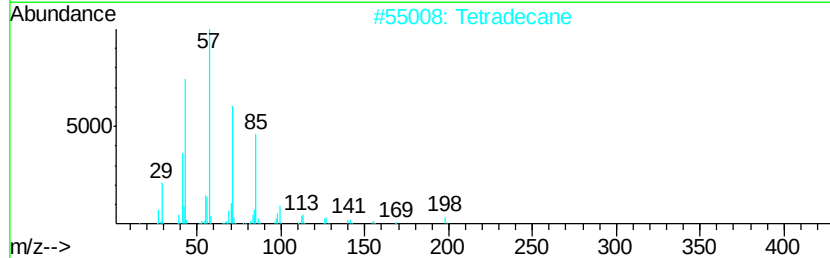
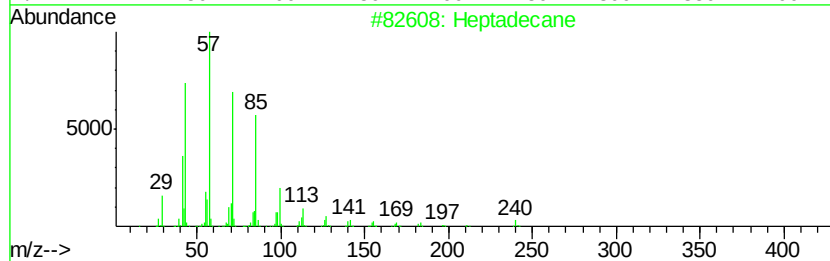
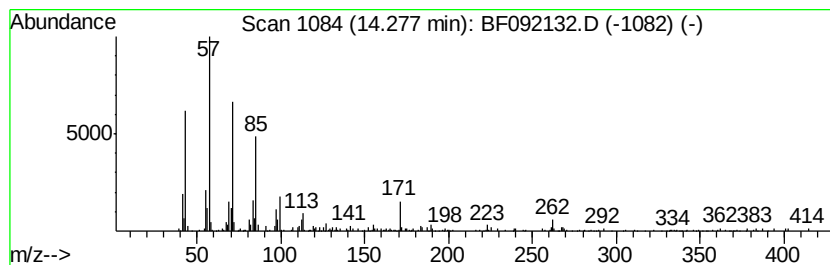
Instrument :
BNA_F
ClientSampleId :
RAP-SP4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.28	2.96 ng	162245	Chrysene-d12	13.79
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	95
2	Tetradecane	198 C14H30	000629-59-4	93
3	Tetracosane	338 C24H50	000646-31-1	93
4	Octacosane	394 C28H58	000630-02-4	83
5	Nonadecane	268 C19H40	000629-92-5	76



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010617\
Data File : BF092132.D
Acq On : 6 Jan 2017 22:18
Operator : UM/SJ
Sample : I1045-06 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RAP-SP4

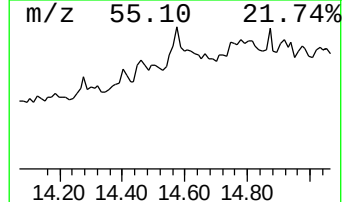
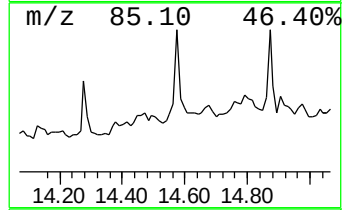
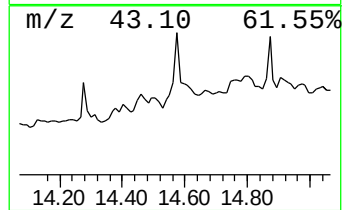
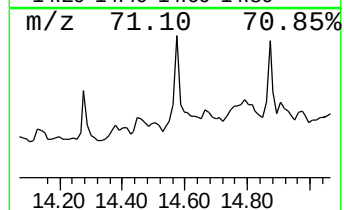
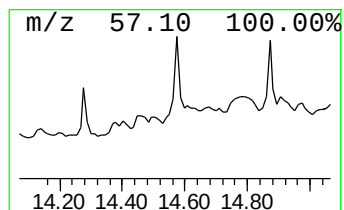
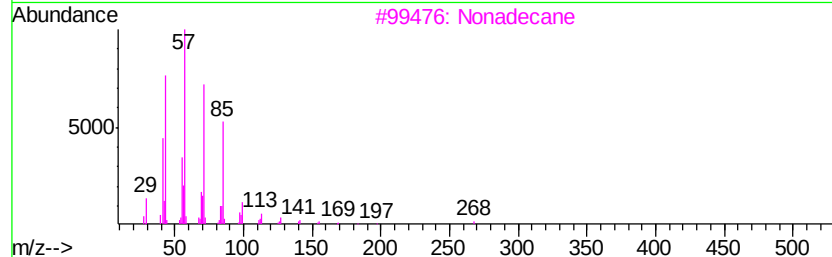
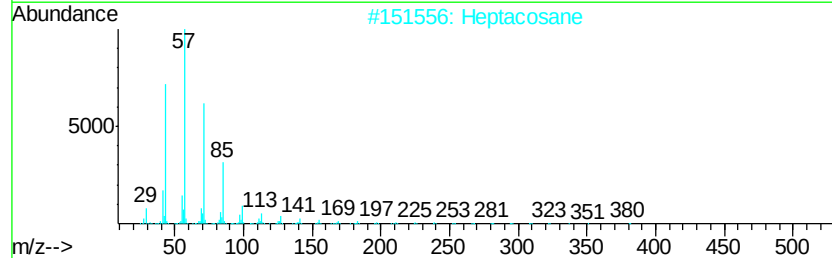
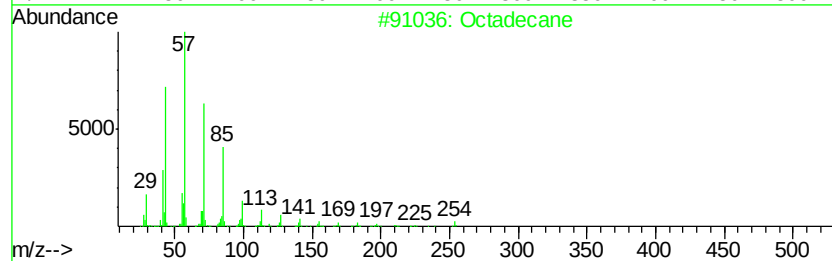
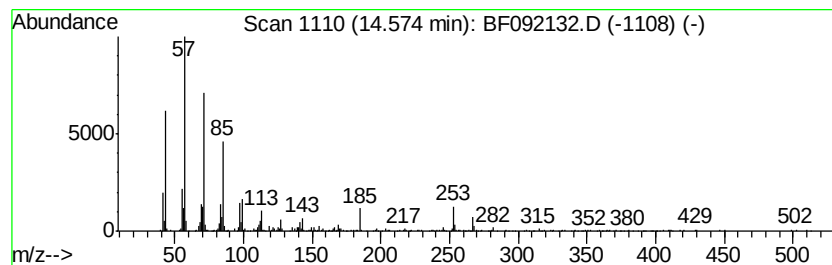
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	16.36 ng	570948	Perylene-d12	15.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	96
2		Heptacosane	380	C27H56	000593-49-7	95
3		Nonadecane	268	C19H40	000629-92-5	93
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	93
5		Eicosane	282	C20H42	000112-95-8	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010617\
Data File : BF092132.D
Acq On : 6 Jan 2017 22:18
Operator : UM/SJ
Sample : I1045-06 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RAP-SP4

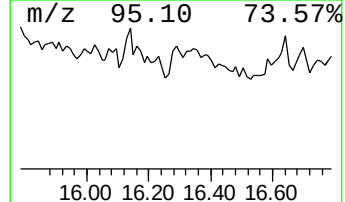
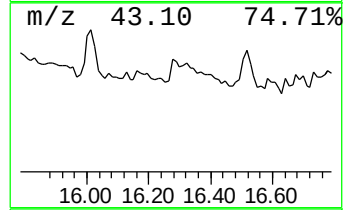
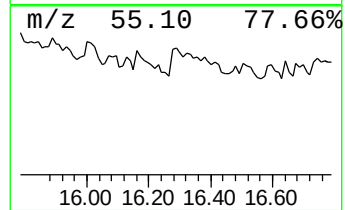
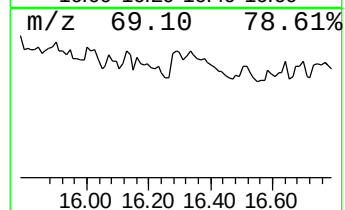
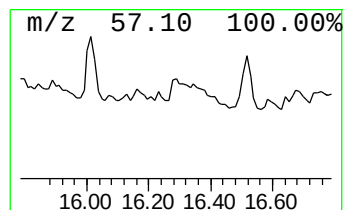
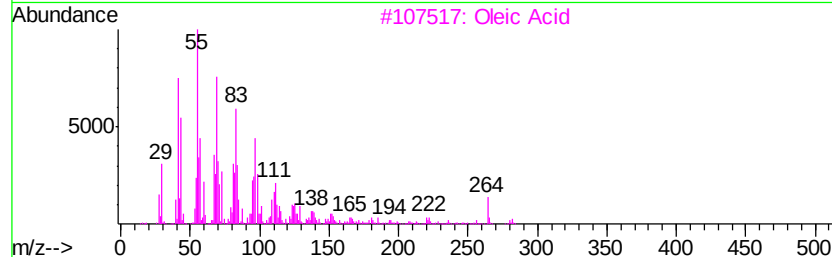
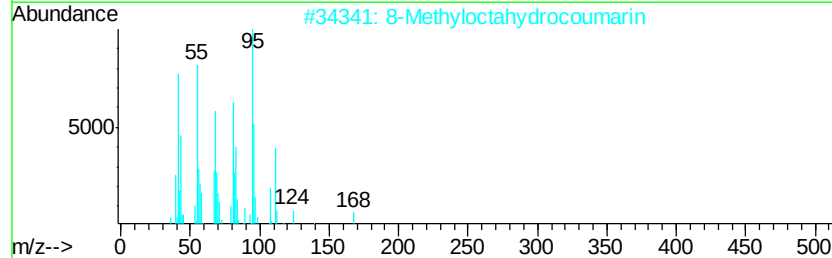
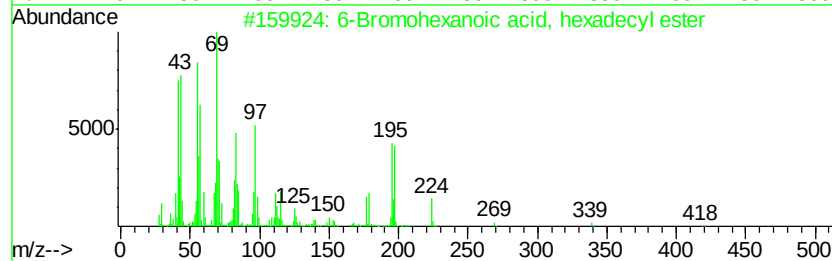
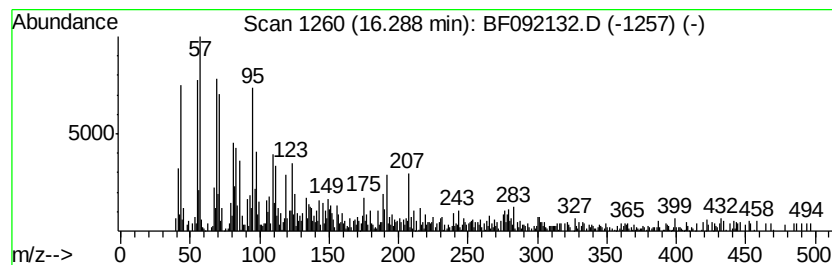
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 6-Bromohexanoic acid, hexad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.29	15.98 ng	557621	Perylene-d12	15.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6-Bromohexanoic acid, hexadecyl ...	418	C22H43BrO2	1000281-92-0	66
2		8-Methyloctahydrocoumarin	168	C10H16O2	021197-56-8	48
3		Oleic Acid	282	C18H34O2	000112-80-1	41
4		5-Nitrothiophene-2-carboxylic ac...	299	C14H21NO4S	1000253-41-7	41
5		Spirobicyclo[2.2.1]heptane-2,2'-...	236	C14H20O3	1000155-15-2	41



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010617\
Data File : BF092132.D
Acq On : 6 Jan 2017 22:18
Operator : UM/SJ
Sample : I1045-06 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RAP-SP4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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
2-Pentanone, 4-hy...	4.77	4.3	ng	199203	1	6.64	926680	20.0
unknown6.42	6.42	9.4	ng	436135	1	6.64	926680	20.0
1,1'-Biphenyl, 2-...	9.01	8.8	ng	436831	3	9.68	993031	20.0
unknown11.98	11.98	2.1	ng	96667	4	11.16	897899	20.0
Heptadecane	14.28	3.0	ng	162245	5	13.79	1096480	20.0
Octadecane	14.57	16.4	ng	570948	6	15.16	697989	20.0
6-Bromohexanoic a...	16.29	16.0	ng	557621	6	15.16	697989	20.0