

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
 Data File : BF085895.D
 Acq On : 30 Mar 2016 19:25
 Operator : UM/SJ
 Sample : H2027-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GRID-16COMP

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-BF032416.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	4.973	233	235	249	rVB	100305	141443	5.29%	0.642%
2	5.396	269	272	282	rBV	2127009	2181459	81.65%	9.898%
3	6.436	361	363	366	rBV	1531660	2196067	82.20%	9.964%
4	6.561	372	374	377	rBV	1705998	2332869	87.32%	10.585%
5	6.801	393	395	397	rBV	453702	581420	21.76%	2.638%
6	6.950	406	408	411	rBV	1773029	1773912	66.40%	8.049%
7	7.362	442	444	447	rBV	1321042	1355803	50.75%	6.152%
8	7.476	451	454	459	rVB	28262	45964	1.72%	0.209%
9	8.082	505	507	510	rBV	878723	763235	28.57%	3.463%
10	9.167	599	602	604	rBV	2063982	2671663	100.00%	12.122%
11	9.556	634	636	638	rBV	491336	402218	15.05%	1.825%
12	9.773	651	655	657	rBV	70391	64815	2.43%	0.294%
13	9.842	658	661	663	rVB	667635	760024	28.45%	3.449%
14	10.002	672	675	679	rBV2	11715	29130	1.09%	0.132%
15	10.276	695	699	700	rBV2	60248	101365	3.79%	0.460%
16	10.493	715	718	721	rBV	30985	54892	2.05%	0.249%
17	10.630	727	730	732	rBV	1233369	1334993	49.97%	6.057%
18	10.745	738	740	744	rVB	97146	112670	4.22%	0.511%
19	11.190	777	779	780	rBV	59633	48568	1.82%	0.220%
20	11.316	788	790	793	rBV	610093	653884	24.47%	2.967%
21	11.373	793	795	799	rVB2	13455	26771	1.00%	0.121%
22	11.556	807	811	814	rBV	15483	29248	1.09%	0.133%
23	11.613	814	816	820	rVB	30736	29107	1.09%	0.132%
24	11.853	835	837	839	rBV	60247	72176	2.70%	0.327%
25	12.631	903	905	908	rBV2	24860	37514	1.40%	0.170%
26	12.905	926	929	931	rBV	2131506	1866139	69.85%	8.467%
27	13.134	947	949	951	rBV	23504	30831	1.15%	0.140%
28	13.808	1001	1008	1013	rBV2	95588	321048	12.02%	1.457%
29	13.956	1018	1021	1023	rBV	622199	627289	23.48%	2.846%
30	14.425	1054	1062	1069	rBV8	31862	196016	7.34%	0.889%
31	14.699	1084	1086	1091	rBV4	31535	78952	2.96%	0.358%
32	14.791	1092	1094	1098	rVB	70556	80926	3.03%	0.367%
33	15.031	1113	1115	1121	rVB4	16649	35529	1.33%	0.161%
34	15.374	1142	1145	1150	rVB	471416	618460	23.15%	2.806%

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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 >
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35	15.797	1180	1182	1186	rVB	18759	36291	1.36%	0.165%
36	16.254	1220	1222	1231	rVB	32899	100448	3.76%	0.456%
37	16.802	1268	1270	1274	rVB3	21152	41901	1.57%	0.190%
38	19.351	1486	1493	1504	rBV4	33533	203930	7.63%	0.925%

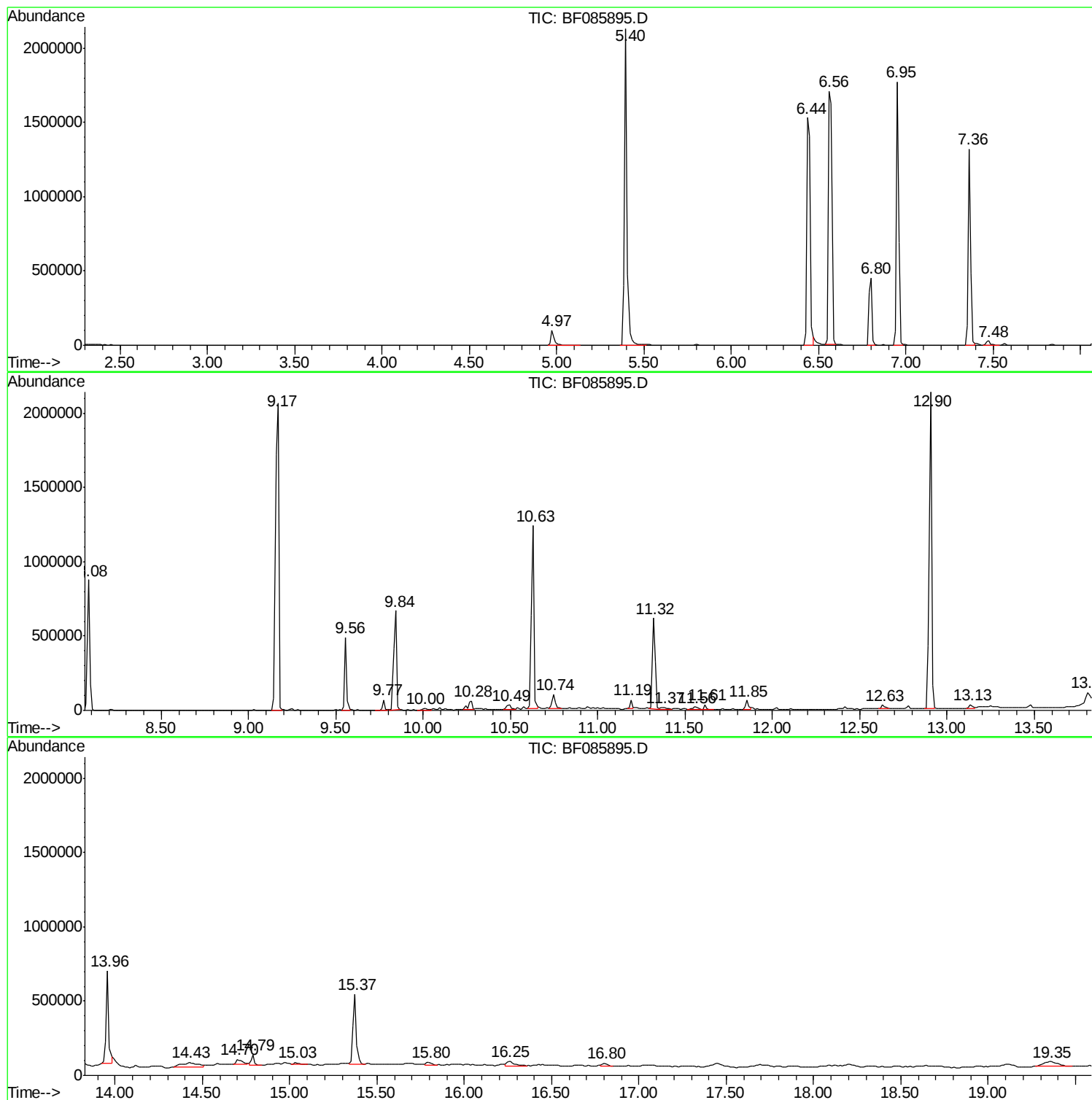
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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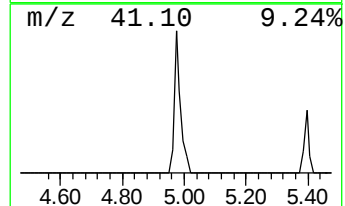
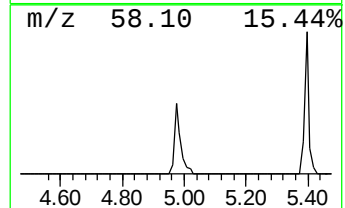
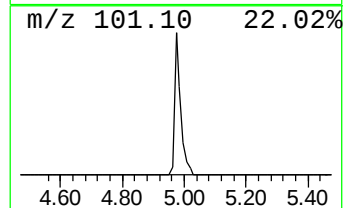
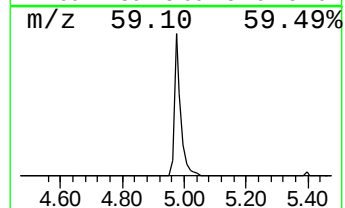
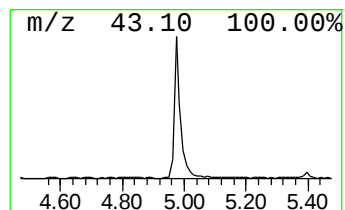
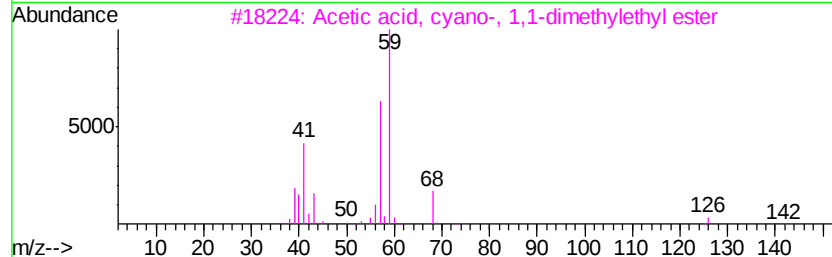
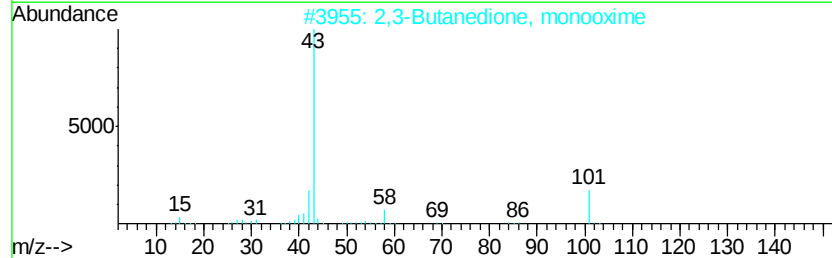
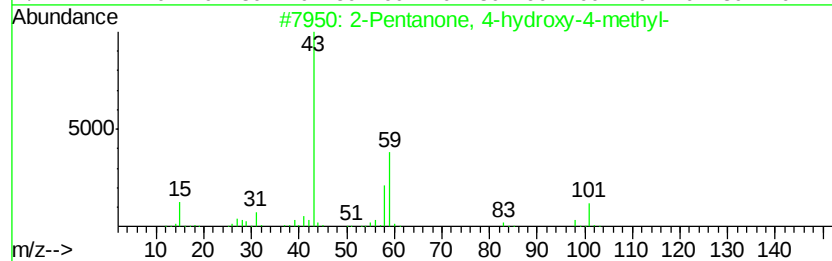
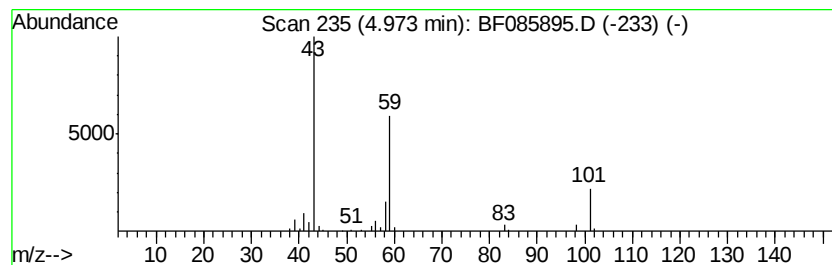
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	4.87 ng	141443	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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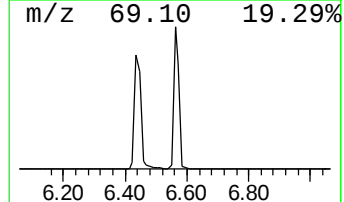
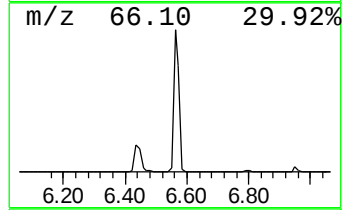
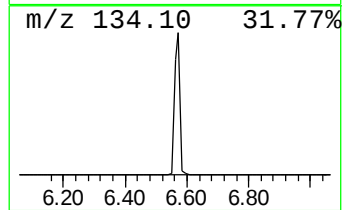
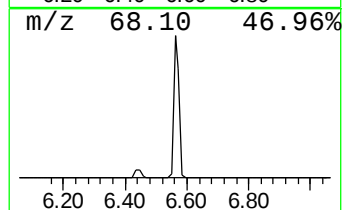
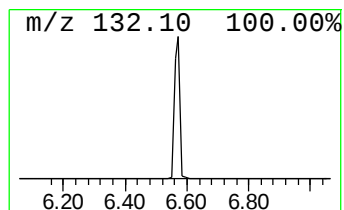
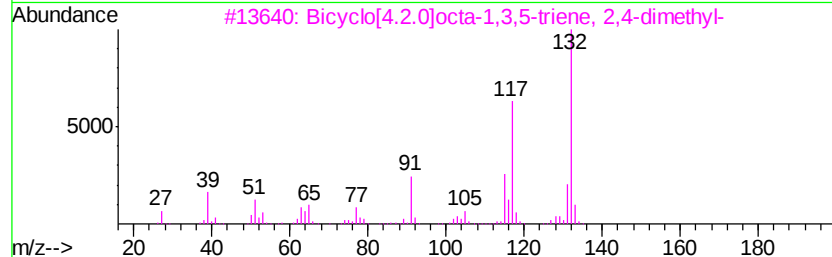
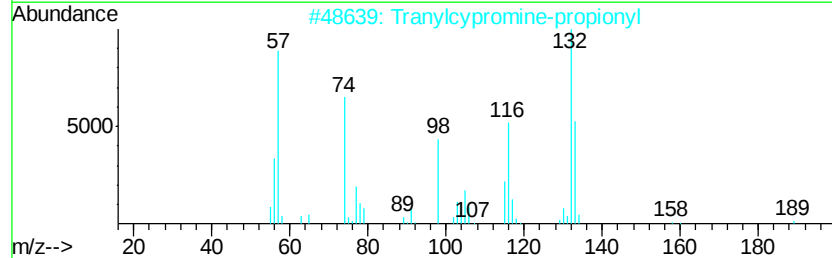
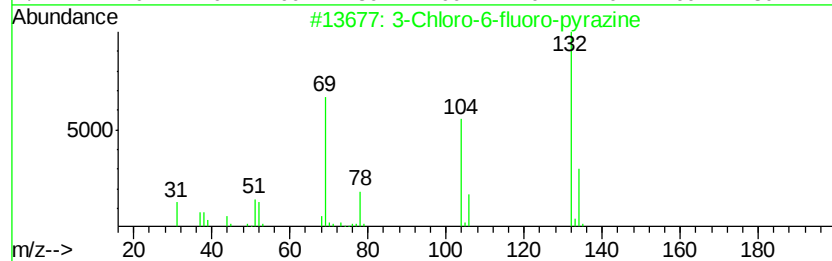
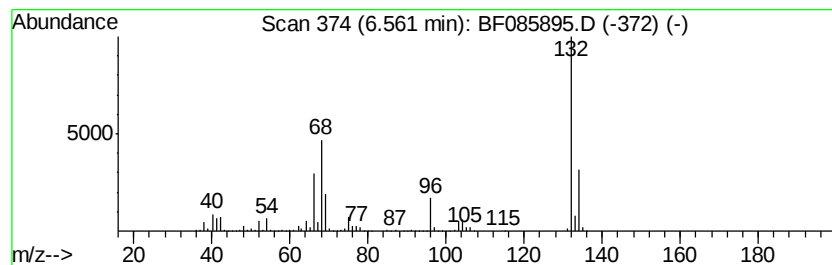
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	80.25 ng	2332870	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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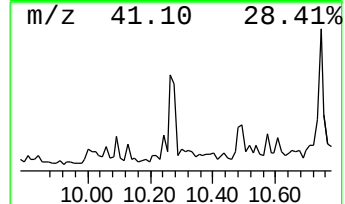
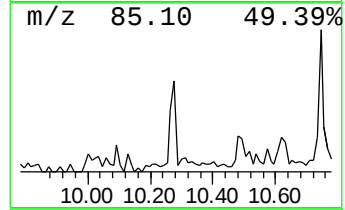
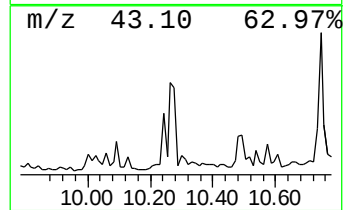
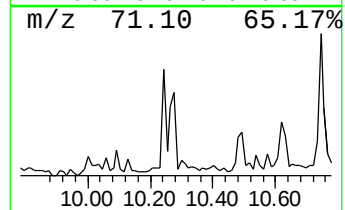
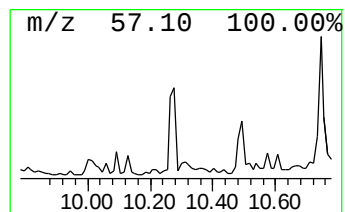
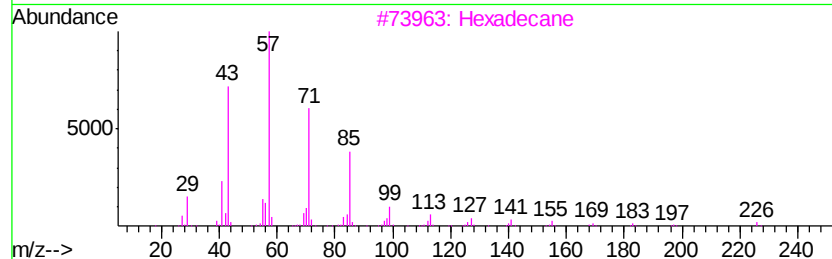
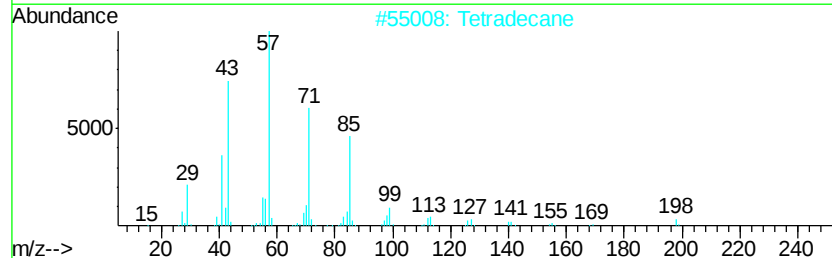
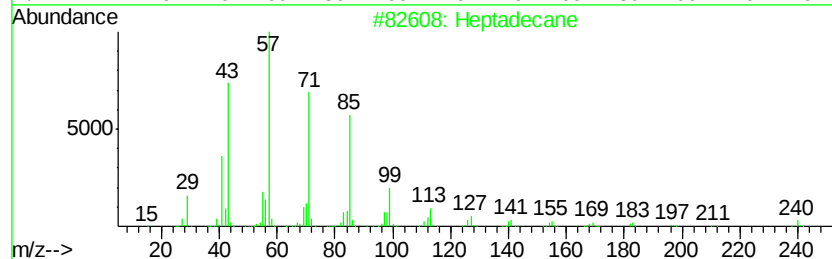
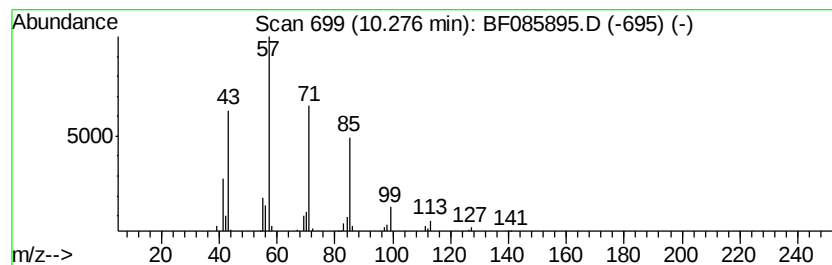
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.28	2.67 ng	101365	Acenaphthene-d10	9.84
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	91
2	Tetradecane	198 C14H30	000629-59-4	91
3	Hexadecane	226 C16H34	000544-76-3	90
4	Octadecane	254 C18H38	000593-45-3	90
5	Pentadecane	212 C15H32	000629-62-9	90



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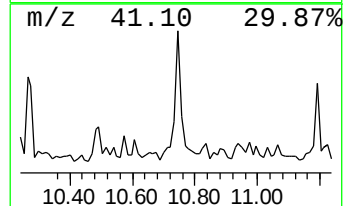
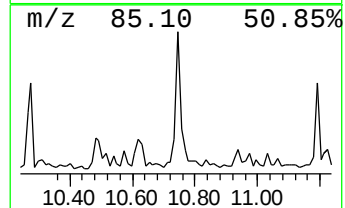
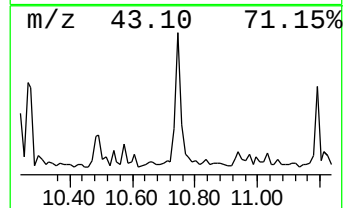
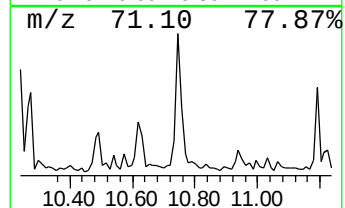
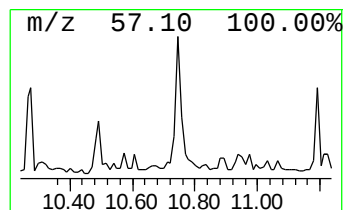
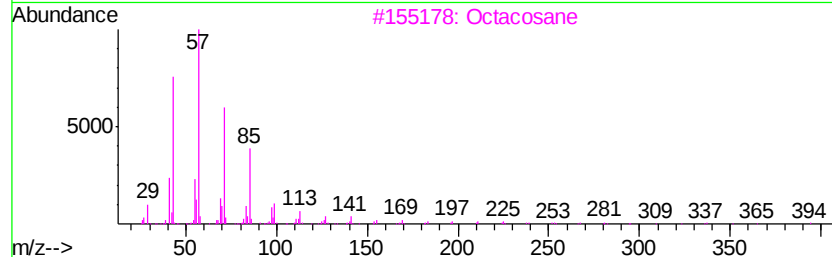
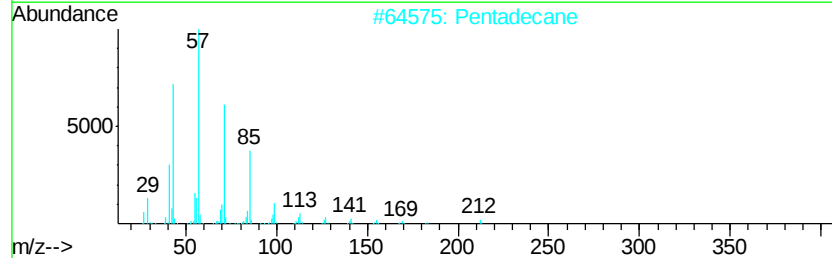
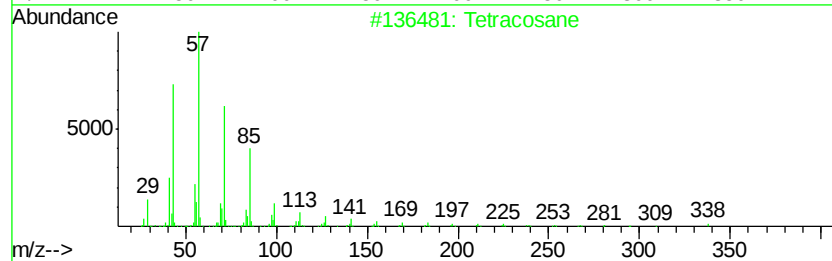
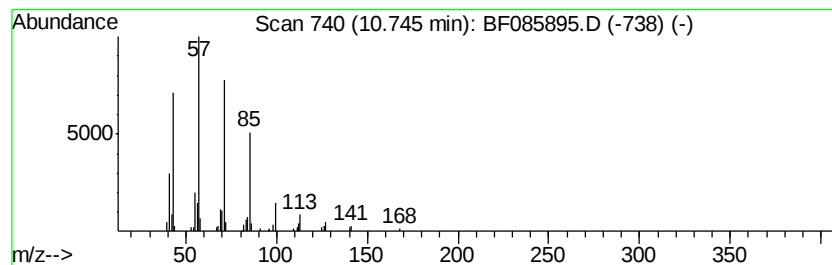
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.74	3.45 ng	112670	Phenanthrene-d10		11.32
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Pentadecane	212	C15H32	000629-62-9	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Heptadecane	240	C17H36	000629-78-7	90
5	Octadecane	254	C18H38	000593-45-3	90



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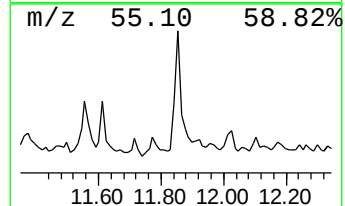
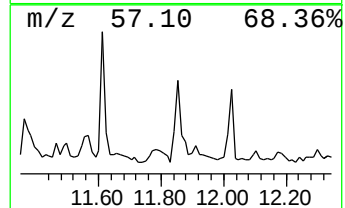
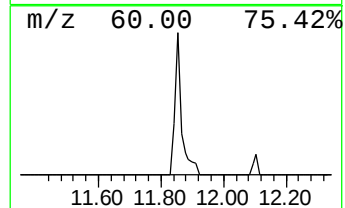
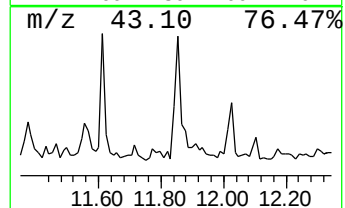
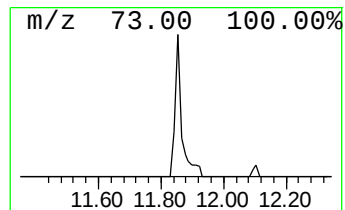
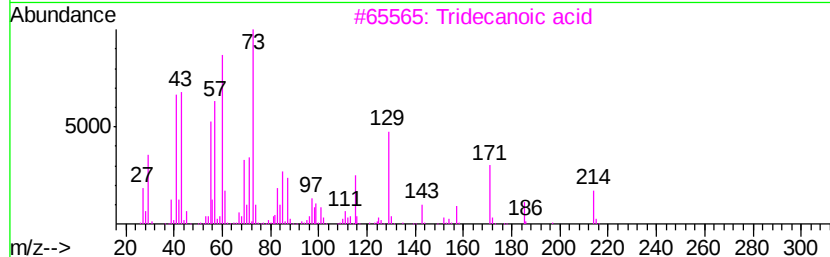
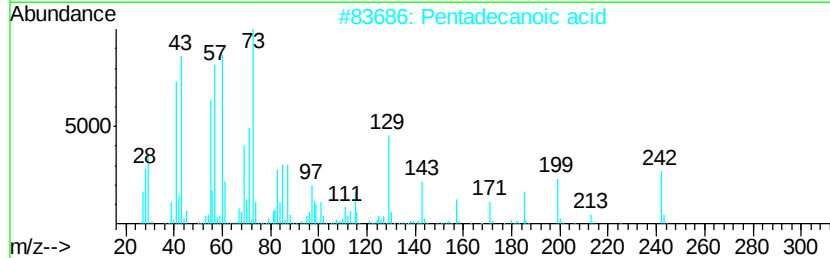
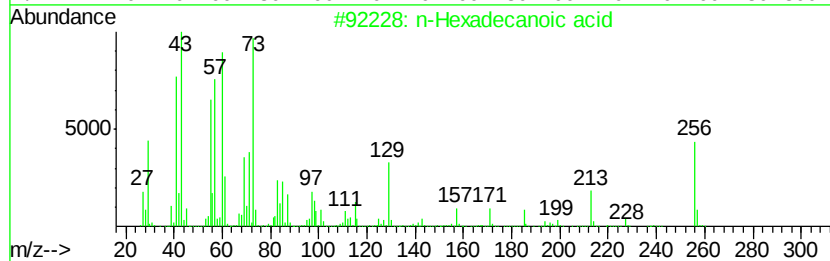
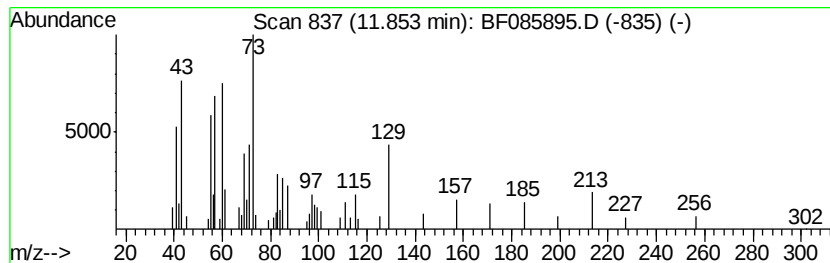
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.85	2.21 ng	72176	Phenanthrene-d10	11.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	59



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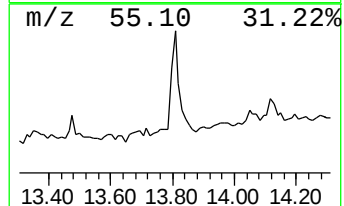
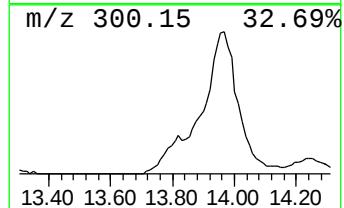
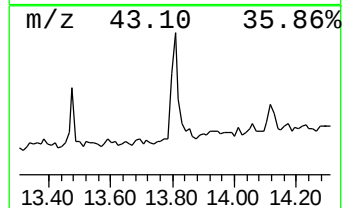
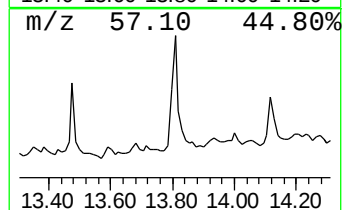
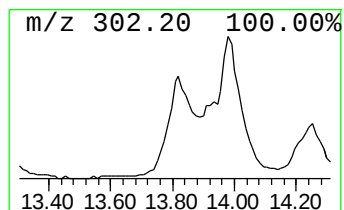
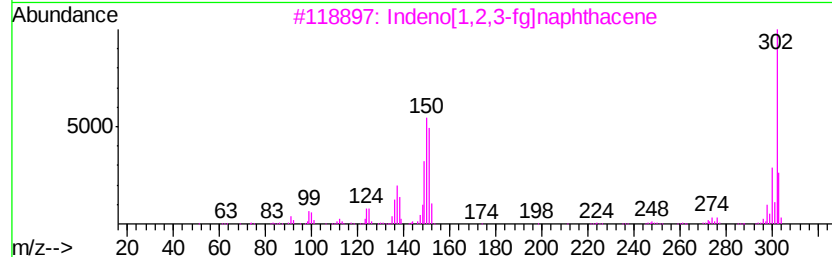
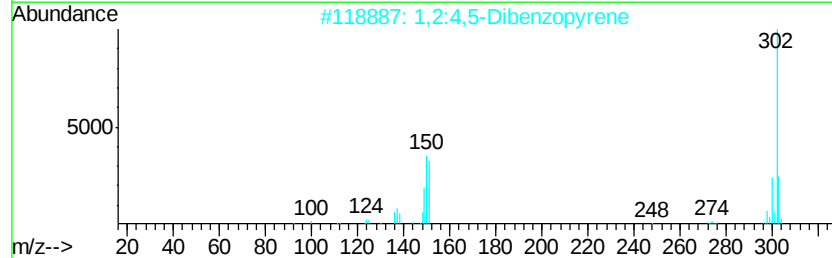
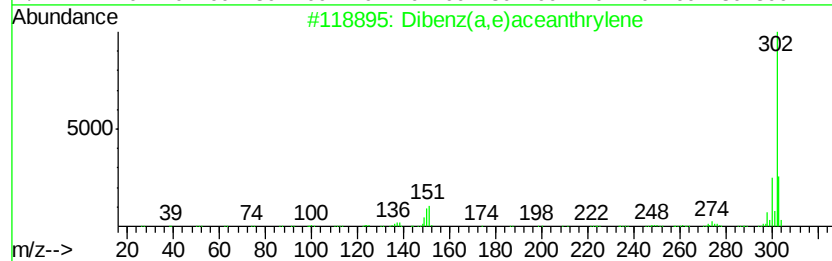
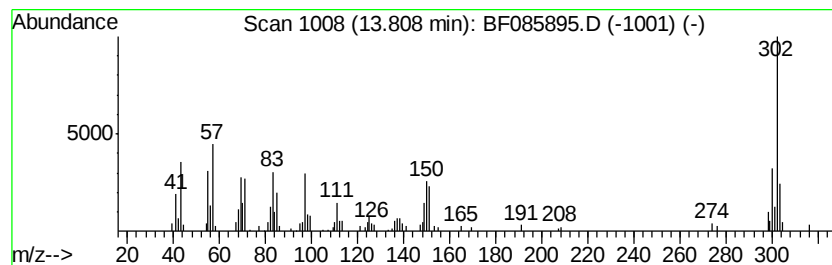
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dibenz(a,e)aceanthrylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	10.24 ng	321048	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenz(a,e)aceanthrylene	302	C24H14	005385-75-1	94
2		1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	93
3		Indeno[1,2,3-fg]naphthacene	302	C24H14	000203-11-2	92
4		3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	64
5		3,4:9,10-Dibenzopyrene	302	C24H14	000189-55-9	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085895.D
Acq On : 30 Mar 2016 19:25
Operator : UM/SJ
Sample : H2027-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

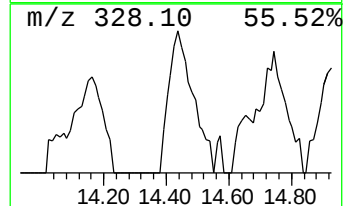
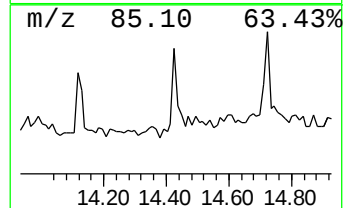
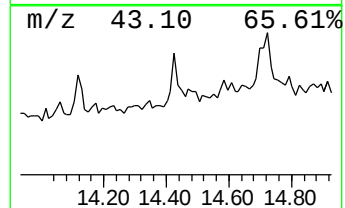
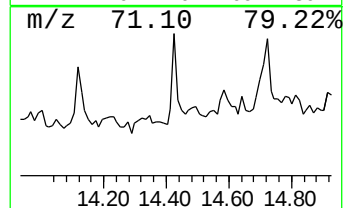
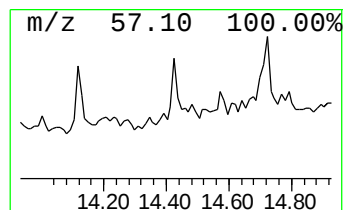
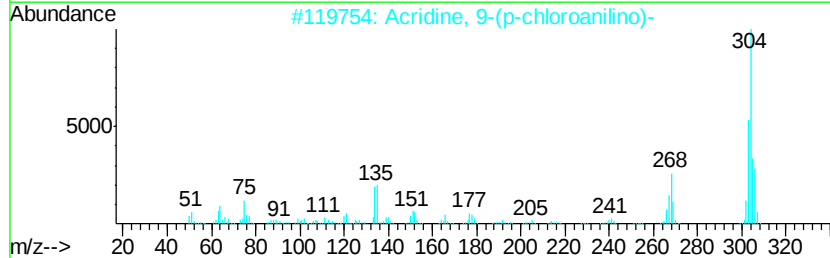
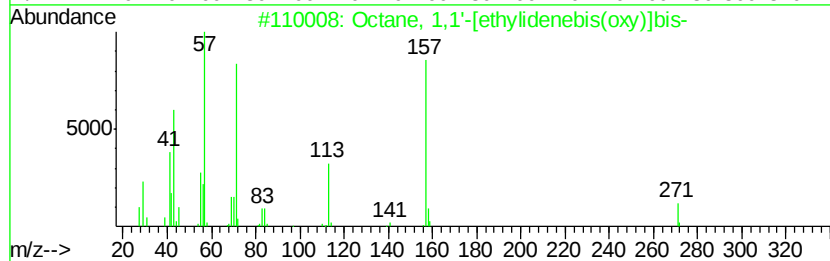
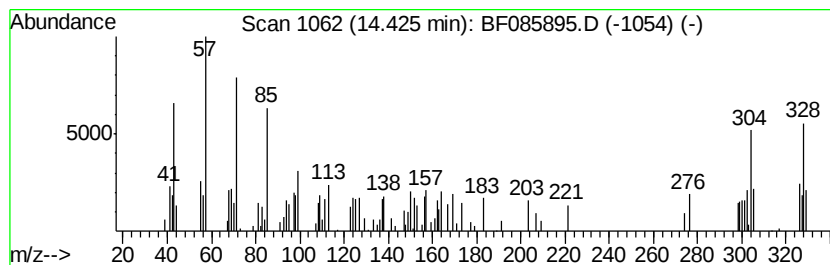
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.43 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.43	6.25 ng	196016	Chrysene-d12	13.96	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 1,1'-[ethylidenebis(oxy)]...	286	C18H38O2	093941-00-5	22
2	Acridine, 9-(p-chloroanilino)-	304	C19H13ClN2	061462-75-7	9
3	6H-[1,3]Dioxolo[5,6]benzofuro[3,...	328	C18H16O6	002694-70-4	9
4	(1H)Benzimidazole, 5-fluoro-2-(3...	328	C18H18F2N4	174468-71-4	9
5	4H-1-Benzopyran-4-one, 3-(2,4-di...	328	C18H16O6	054443-60-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
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Acq On : 30 Mar 2016 19:25
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Sample : H2027-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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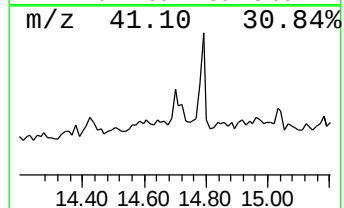
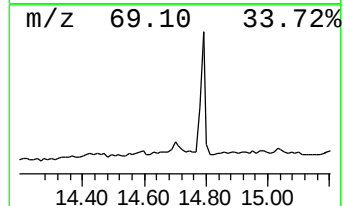
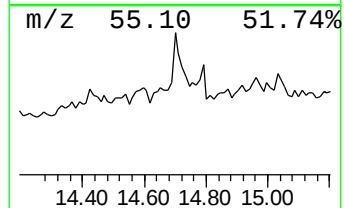
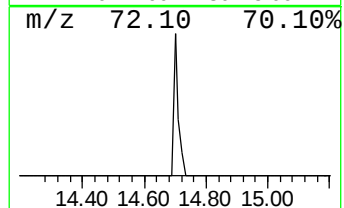
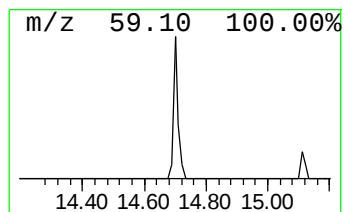
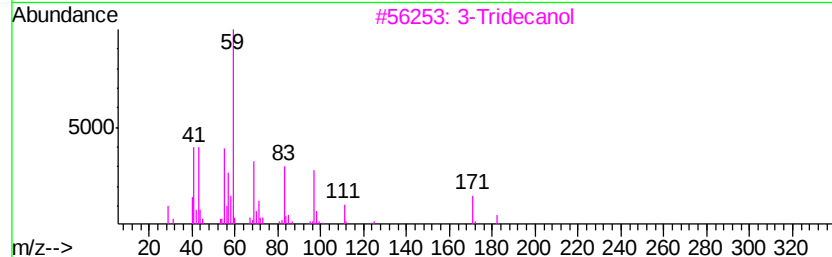
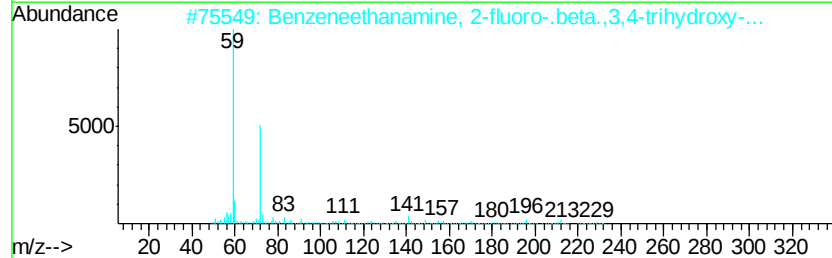
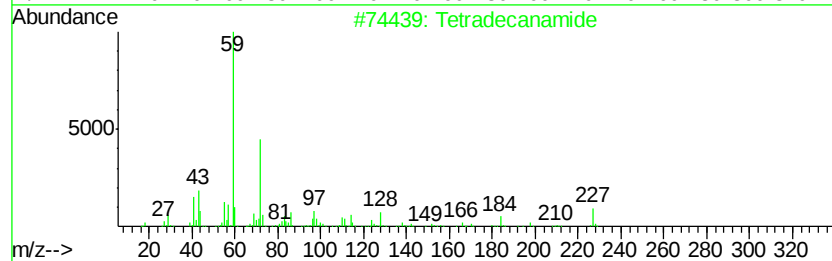
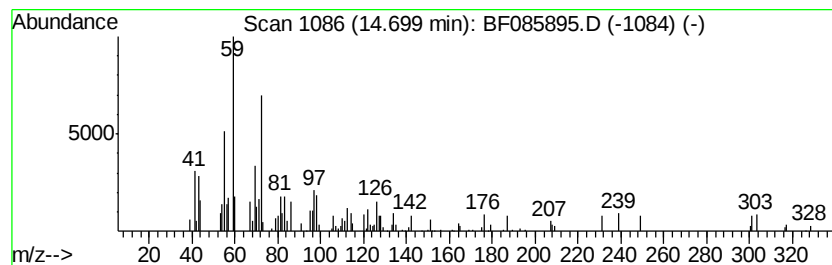
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.70 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	2.55 ng	78952	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecanamide	227	C14H29NO	000638-58-4	47
2		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	47
3		3-Tridecanol	200	C13H28O	010289-68-6	38
4		Dodecanamide	199	C12H25NO	001120-16-7	37
5		4.beta.H,5.alpha.H-Eudesman-11-ol	224	C15H28O	031756-53-3	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085895.D
Acq On : 30 Mar 2016 19:25
Operator : UM/SJ
Sample : H2027-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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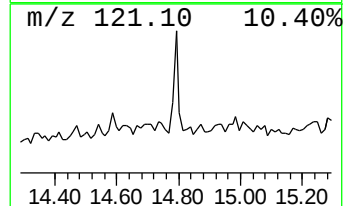
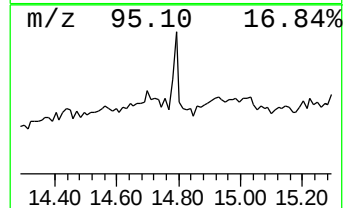
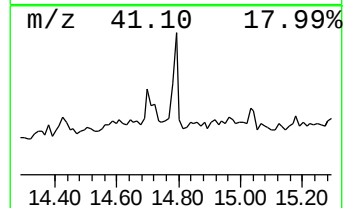
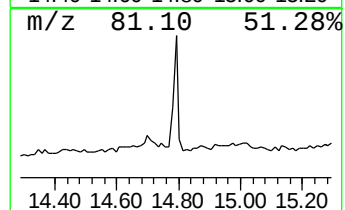
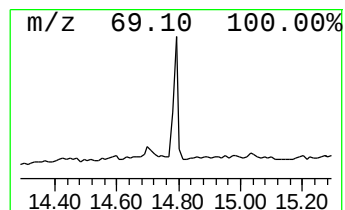
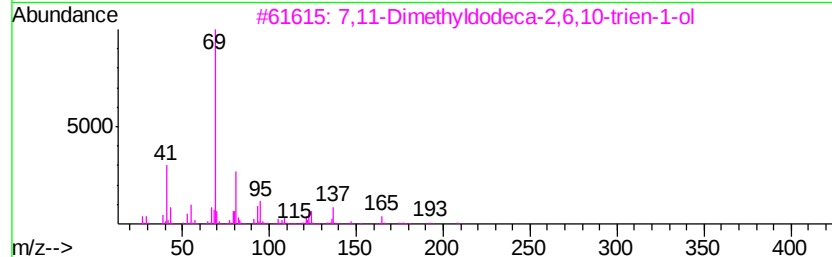
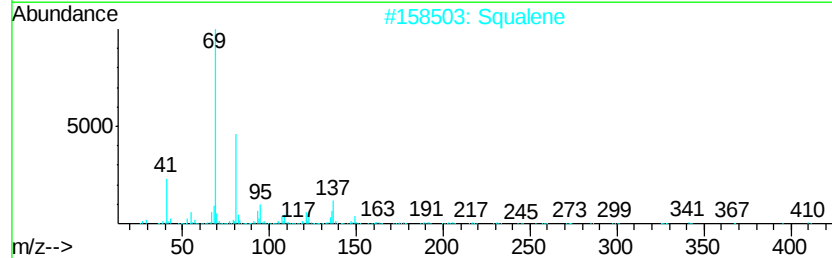
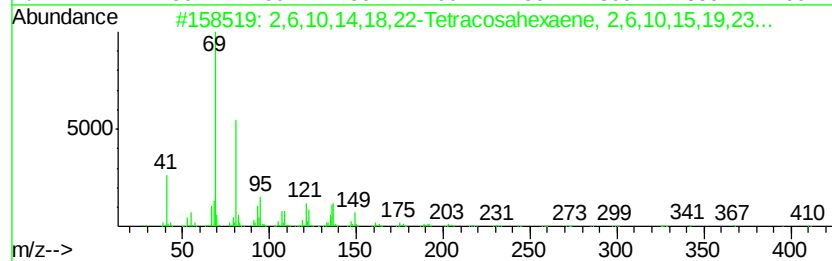
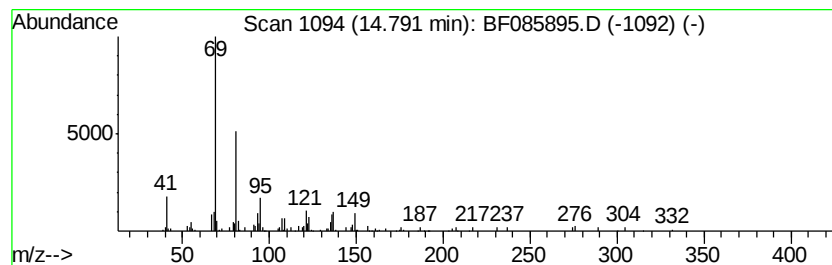
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2,6,10,14,18,22-Tetracosahexaene... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.62 ng	80926	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	86	
2	Squalene	410	C30H50	007683-64-9	74	
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64	
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	59	
5	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	56	



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Acq On : 30 Mar 2016 19:25
Operator : UM/SJ
Sample : H2027-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

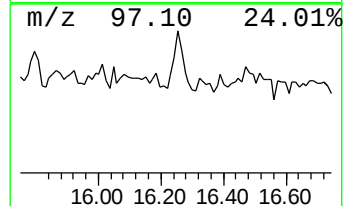
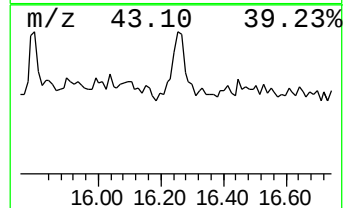
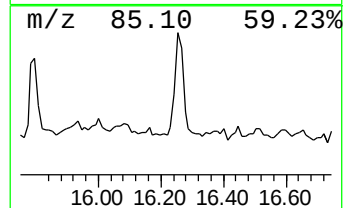
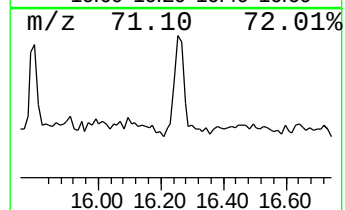
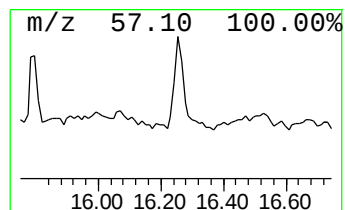
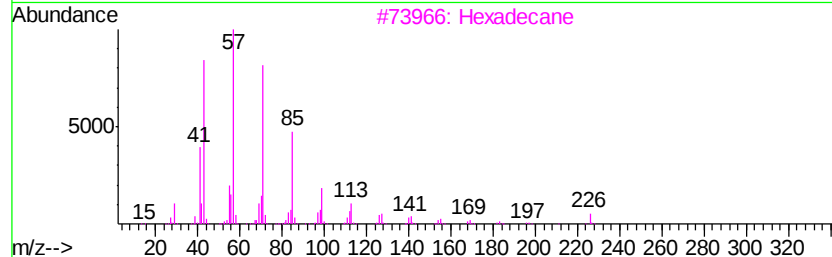
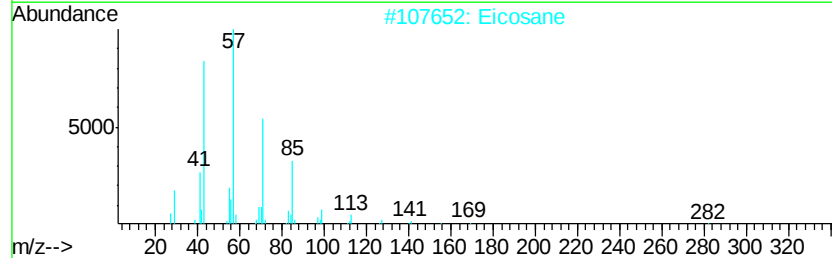
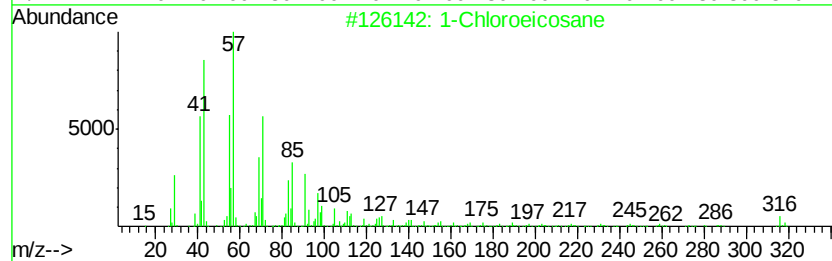
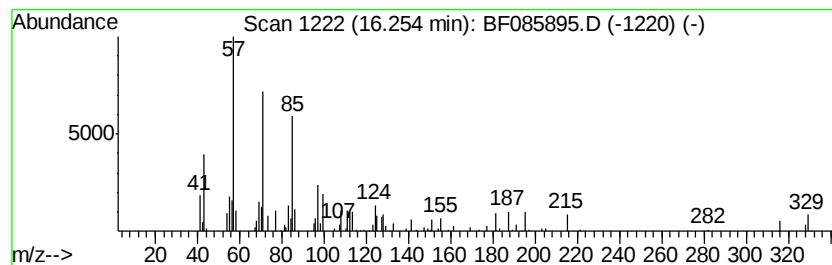
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Chloroeicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.25	3.25 ng	100448	Perylene-d12		15.37
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Chloroeicosane	316	C20H41Cl	042217-02-7	64
2	Eicosane	282	C20H42	000112-95-8	60
3	Hexadecane	226	C16H34	000544-76-3	52
4	Tetracosane	338	C24H50	000646-31-1	49
5	Tetratetracontane	619	C44H90	007098-22-8	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
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ALS Vial : 19 Sample Multiplier: 1

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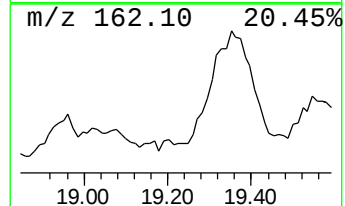
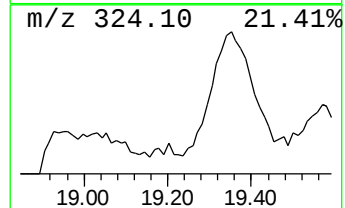
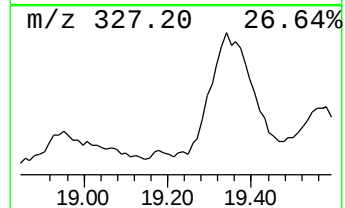
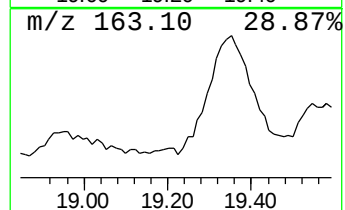
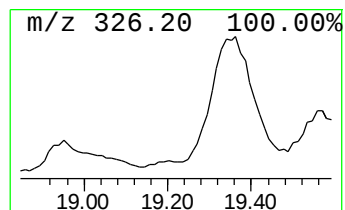
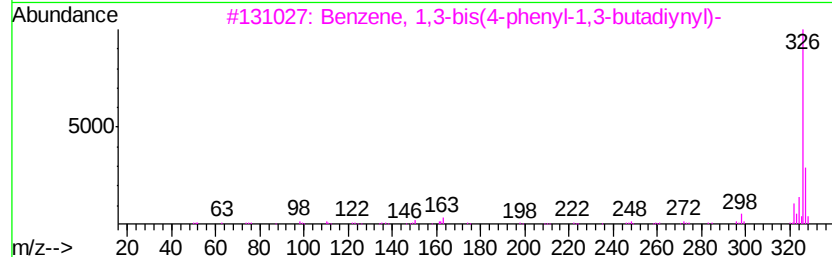
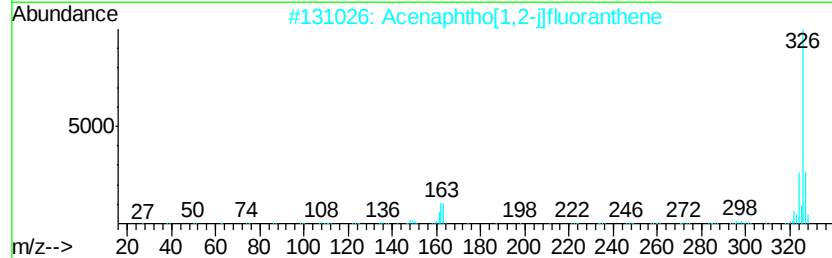
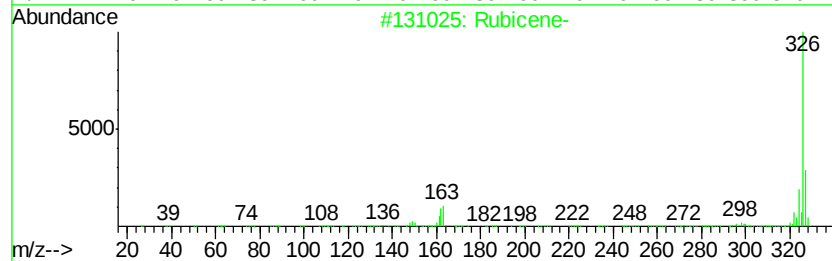
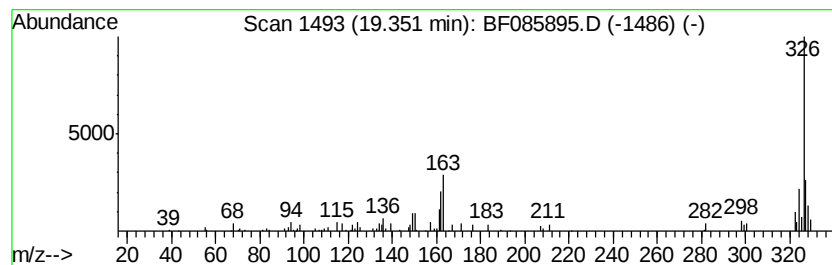
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Rubicene- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.35	6.59 ng	203930	Perylene-d12	15.37

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Rubicene-	326	C26H14	000197-61-5	76
2			Acenaphtho[1,2-j]fluoranthene	326	C26H14	000193-21-5	50
3			Benzene, 1,3-bis(4-phenyl-1,3-bu...	326	C26H14	037902-13-9	49
4			2-(4-Biphenyl)imidazo[2,1-b]be...	326	C21H14N2S	038956-29-5	47
5			6,7-Dimethyl-2-(3-methyl-thiophe...	326	C17H14N2OS2	1000297-09-9	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
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Operator : UM/SJ
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Misc :
ALS Vial : 19 Sample Multiplier: 1

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ClientSampleId :
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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...	4.97	4.9	ng	141443	1	6.80	581420	20.0
unknown6.56	6.56	80.3	ng	2332870	1	6.80	581420	20.0
Heptadecane	10.28	2.7	ng	101365	3	9.84	760024	20.0
Tetracosane	10.74	3.5	ng	112670	4	11.32	653884	20.0
n-Hexadecanoic acid	11.85	2.2	ng	72176	4	11.32	653884	20.0
Dibenz(a,e)aceant...	13.81	10.2	ng	321048	5	13.96	627289	20.0
unknown14.43	14.43	6.3	ng	196016	5	13.96	627289	20.0
unknown14.70	14.70	2.5	ng	78952	6	15.37	618460	20.0
2,6,10,14,18,22-T...	14.79	2.6	ng	80926	6	15.37	618460	20.0
1-Chloroeicosane	16.25	3.3	ng	100448	6	15.37	618460	20.0
Rubcene-	19.35	6.6	ng	203930	6	15.37	618460	20.0