

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
 Data File : BF085279.D
 Acq On : 9 Mar 2016 2:19
 Operator : UM/SJ
 Sample : H1703-02
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-38COMP(0.5-4.0)

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-BF030316.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.167	250	252	260	rVB	663610	1022410	22.95%	2.459%
2	5.567	284	287	290	rBV	2841502	3934836	88.32%	9.465%
3	6.584	373	376	378	rBV	3416776	3694598	82.93%	8.887%
4	6.722	386	388	391	rBV	2966360	4163849	93.46%	10.016%
5	6.962	406	409	411	rBV	1073179	1022320	22.95%	2.459%
6	7.122	420	423	425	rBV	2440968	3270800	73.42%	7.867%
7	7.522	455	458	460	rBV	2642482	2685076	60.27%	6.459%
8	8.242	518	521	524	rBV	1518043	1340240	30.08%	3.224%
9	9.316	612	615	618	rBV	3141028	4455212	100.00%	10.716%
10	9.682	646	647	648	rBV	42980	57185	1.28%	0.138%
11	9.716	648	650	651	rVB	609916	694807	15.60%	1.671%
12	9.933	666	669	671	rBV	81503	112778	2.53%	0.271%
13	10.002	672	675	677	rVB	1553077	1488624	33.41%	3.581%
14	10.425	709	712	714	rBV2	208857	211953	4.76%	0.510%
15	10.642	728	731	735	rBV	54174	109458	2.46%	0.263%
16	10.791	741	744	746	rBV	2584923	2845086	63.86%	6.843%
17	10.905	752	754	758	rBV	133423	229298	5.15%	0.552%
18	11.088	768	770	775	rBV3	21699	57367	1.29%	0.138%
19	11.351	790	793	794	rBV	70612	76145	1.71%	0.183%
20	11.488	802	805	807	rBV	1188605	1448293	32.51%	3.484%
21	11.545	807	810	813	rVB2	28994	59708	1.34%	0.144%
22	12.002	848	850	857	rVB2	243245	327288	7.35%	0.787%
23	12.254	871	872	875	rBV	44433	56351	1.26%	0.136%
24	12.722	908	913	917	rBV	817360	1186412	26.63%	2.854%
25	12.791	917	919	928	rVB	399576	482860	10.84%	1.161%
26	13.065	941	943	946	rBV	3259243	3748634	84.14%	9.017%
27	13.957	1019	1021	1028	rBV	102985	215881	4.85%	0.519%
28	14.117	1032	1035	1038	rVV	1137134	1120855	25.16%	2.696%
29	14.871	1099	1101	1105	rBV2	92507	129883	2.92%	0.312%
30	14.962	1107	1109	1112	rVB	50633	69670	1.56%	0.168%
31	15.580	1160	1163	1166	rBV	639806	815216	18.30%	1.961%
32	16.048	1199	1204	1208	rBV	29656	59269	1.33%	0.143%
33	16.551	1242	1248	1261	rVB2	49370	220748	4.95%	0.531%
34	17.146	1295	1300	1306	rBV	19323	57122	1.28%	0.137%

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ClientSampleId :
SB-38COMP(0.5-4.0)

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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.854	1358	1362	1367	rVB	16868	49333	1.11%	0.119%
36	18.700	1429	1436	1440	rBV3	20650	54074	1.21%	0.130%

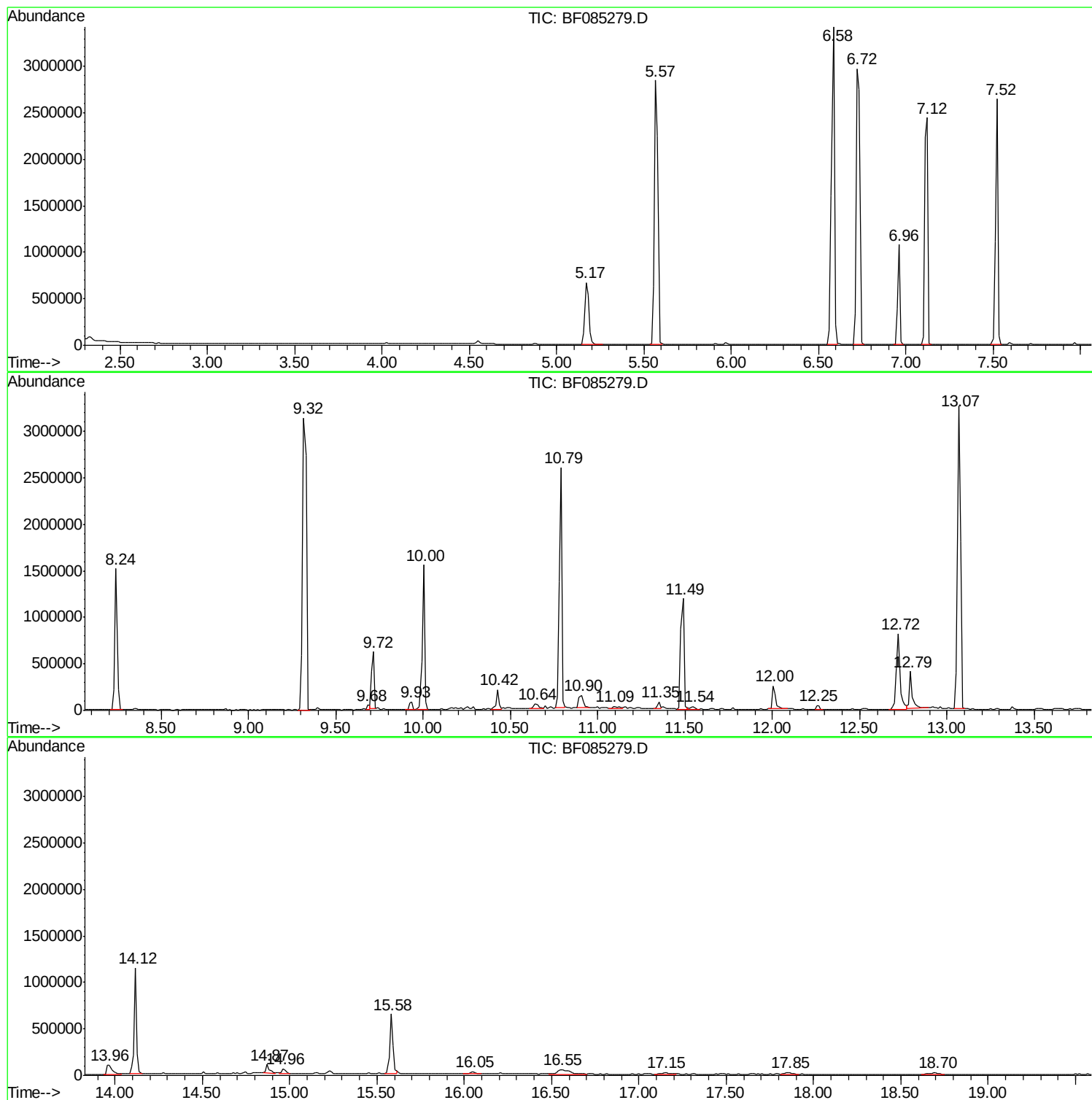
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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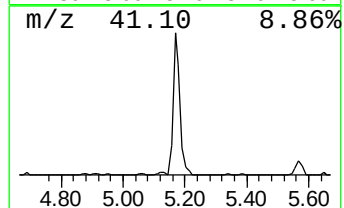
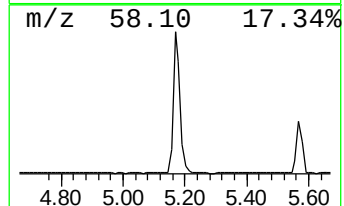
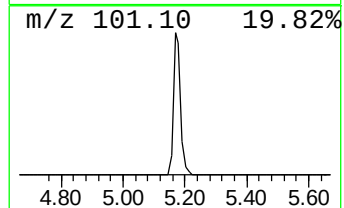
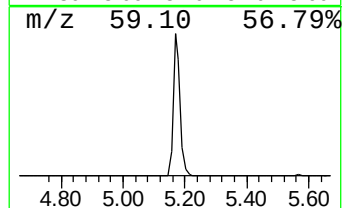
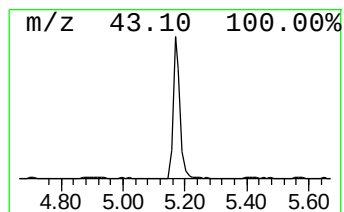
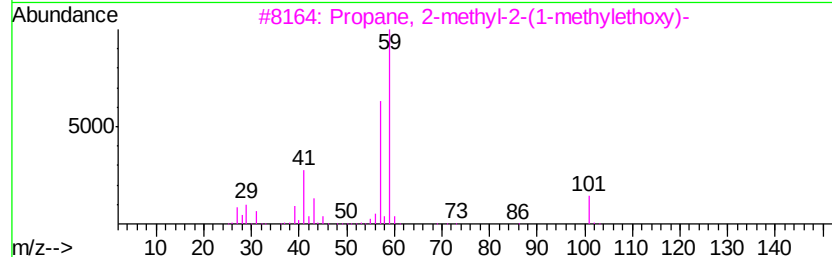
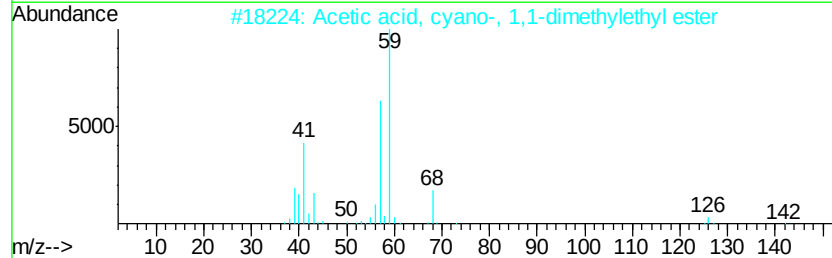
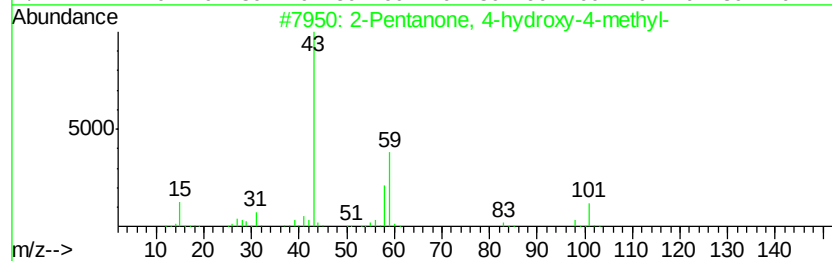
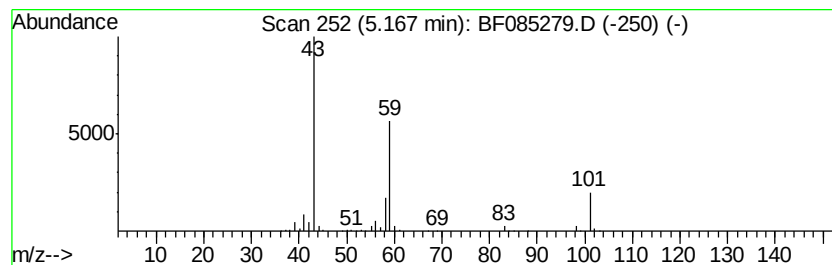
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	20.00 ng	1022410	1,4-Dichlorobenzene-d4	6.96

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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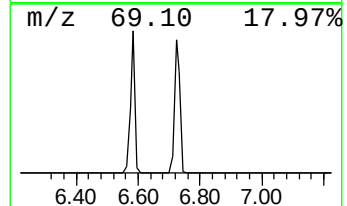
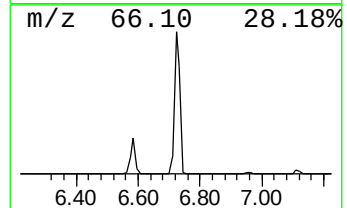
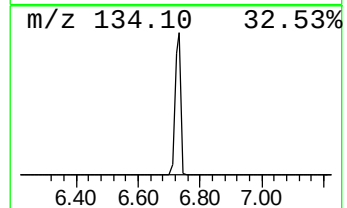
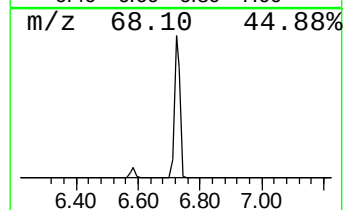
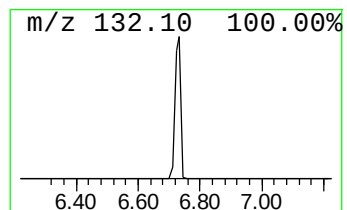
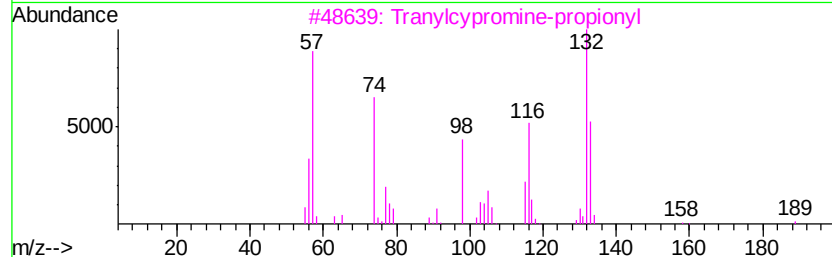
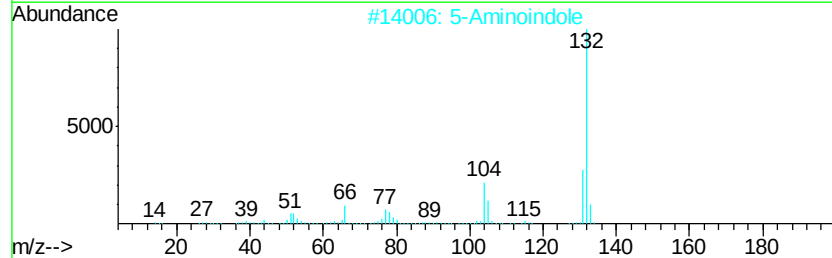
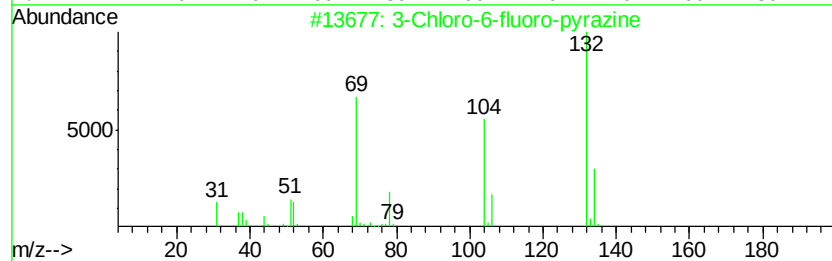
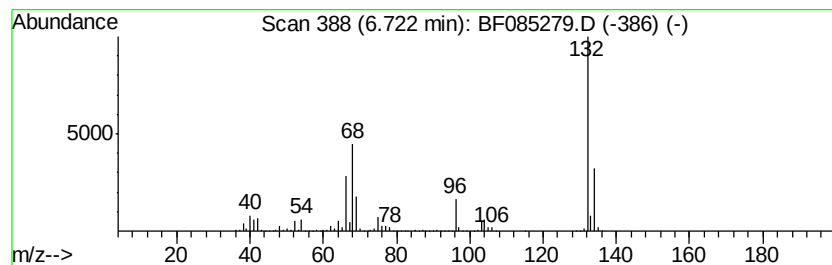
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	81.46 ng	4163850	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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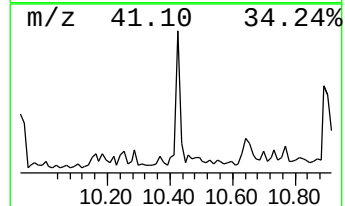
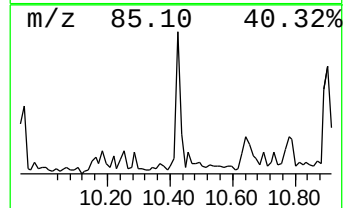
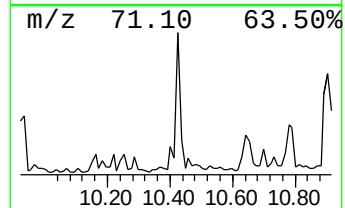
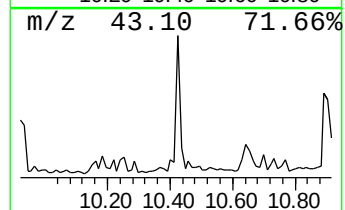
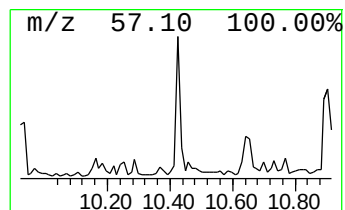
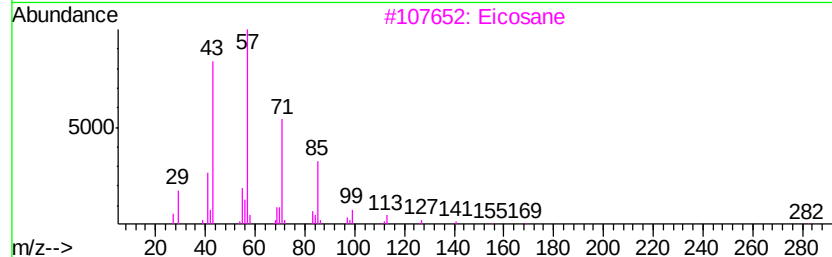
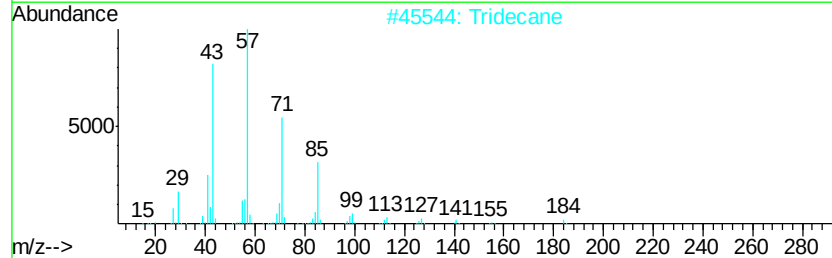
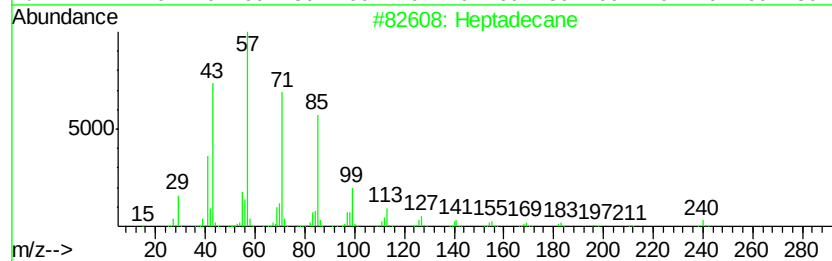
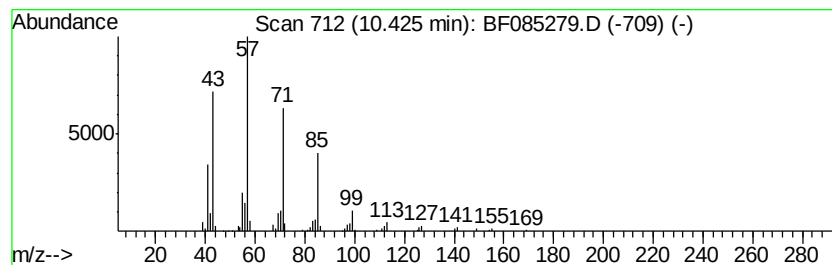
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.42	2.85 ng	211953	Acenaphthene-d10		10.00
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Tridecane	184	C13H28	000629-50-5	90
3	Eicosane	282	C20H42	000112-95-8	83
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
5	Tetradecane	198	C14H30	000629-59-4	80



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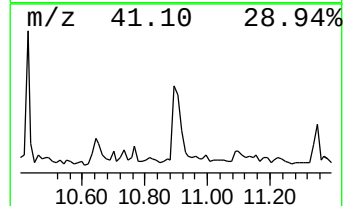
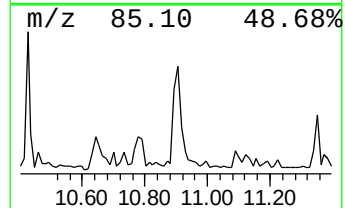
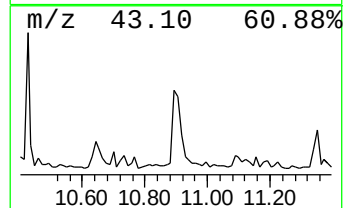
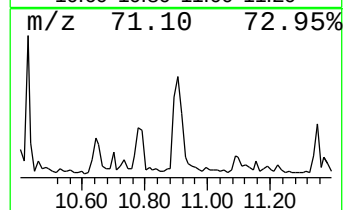
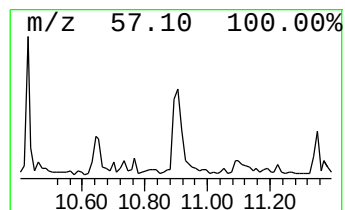
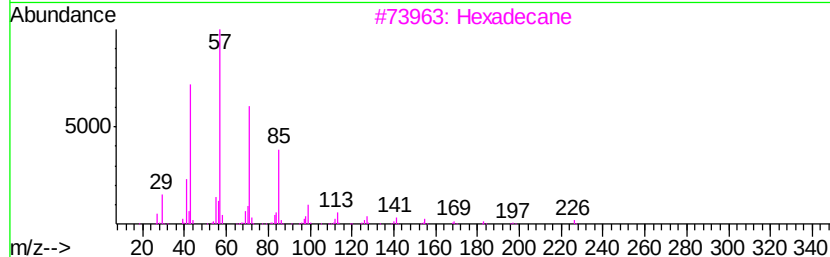
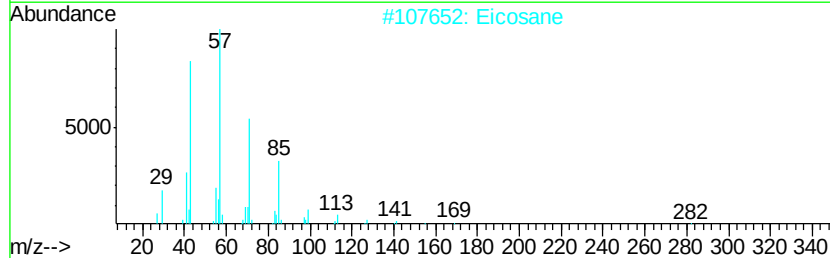
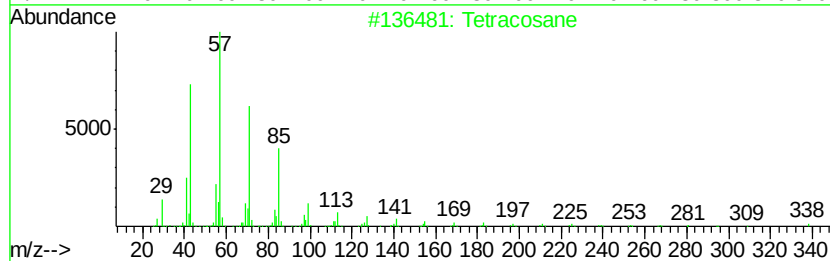
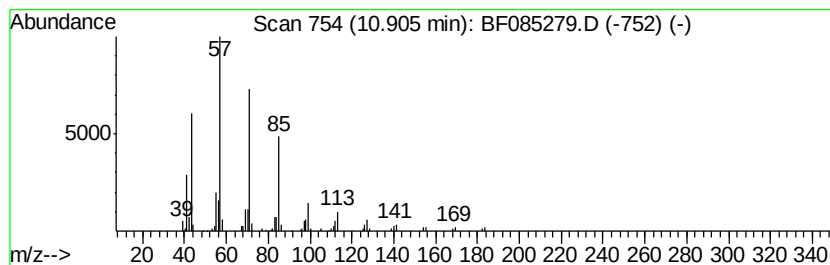
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	3.17 ng	229298	Phenanthrene-d10	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	91
2		Eicosane	282	C20H42	000112-95-8	91
3		Hexadecane	226	C16H34	000544-76-3	91
4		Heptadecane	240	C17H36	000629-78-7	91
5		Pentadecane	212	C15H32	000629-62-9	91



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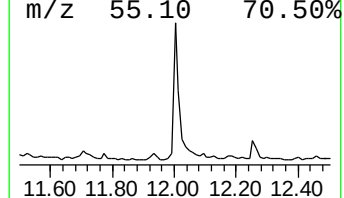
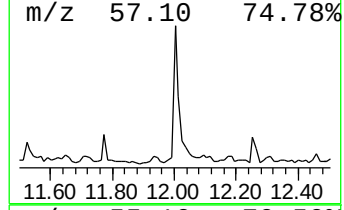
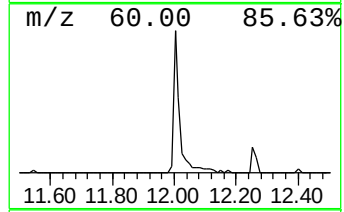
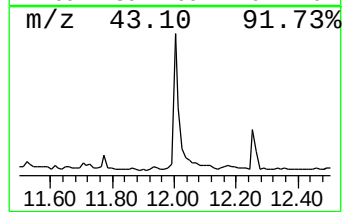
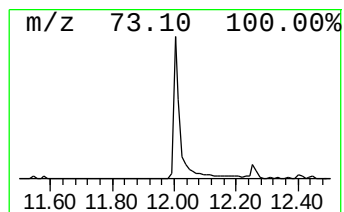
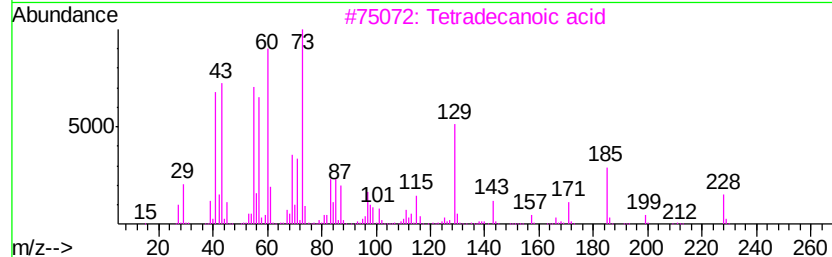
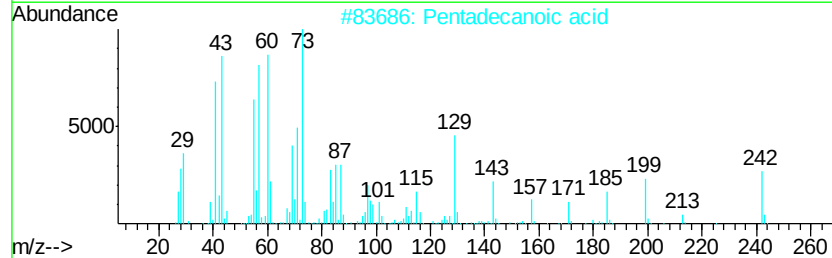
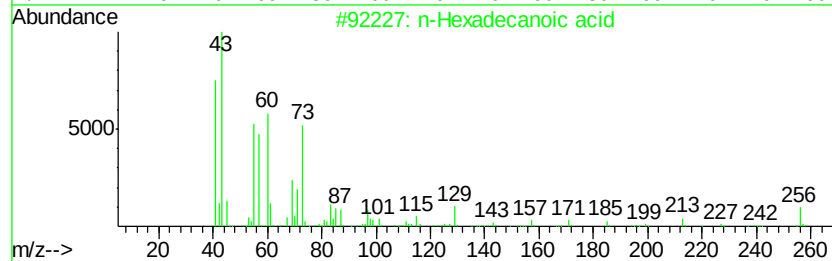
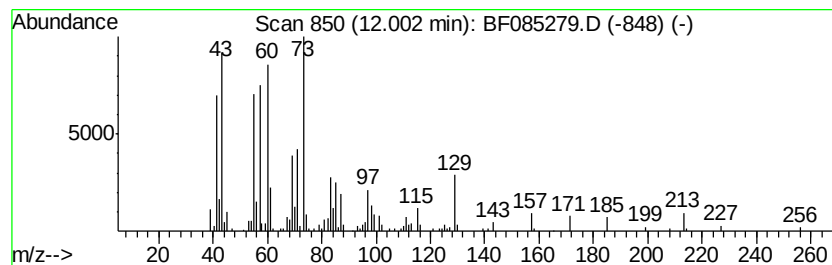
Instrument :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.00	4.52 ng	327288	Phenanthrene-d10	11.49	
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	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Hexadecane	226	C16H34	000544-76-3	11



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SB-38COMP(0.5-4.0)

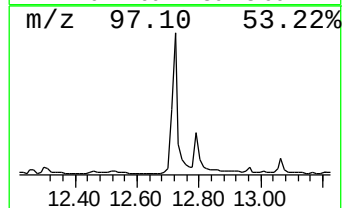
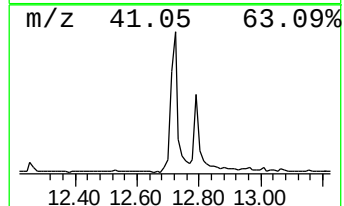
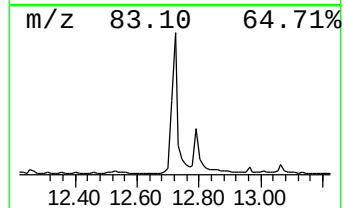
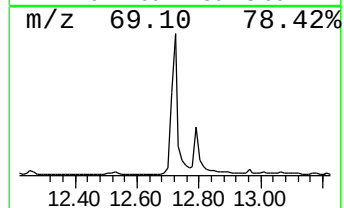
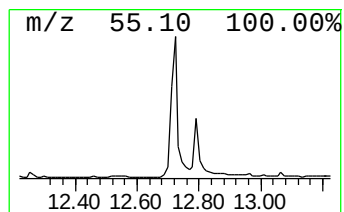
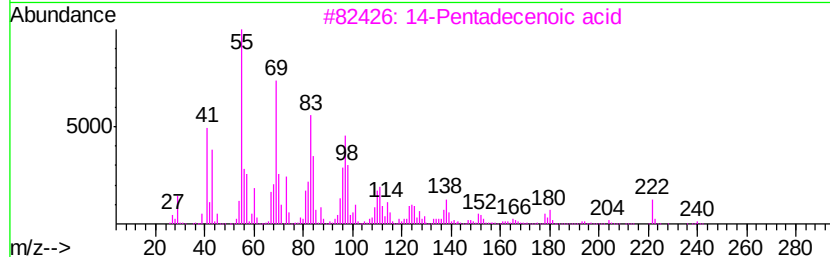
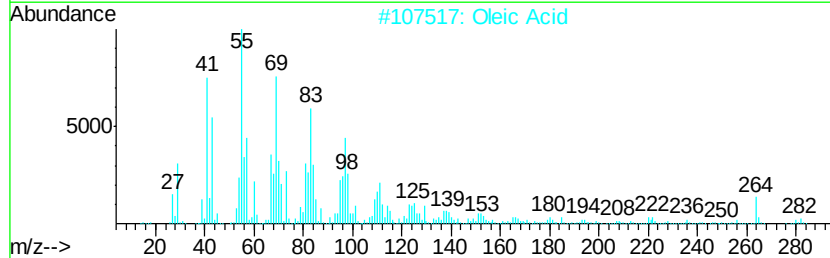
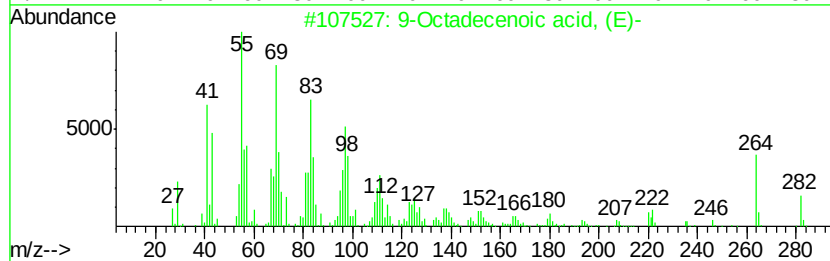
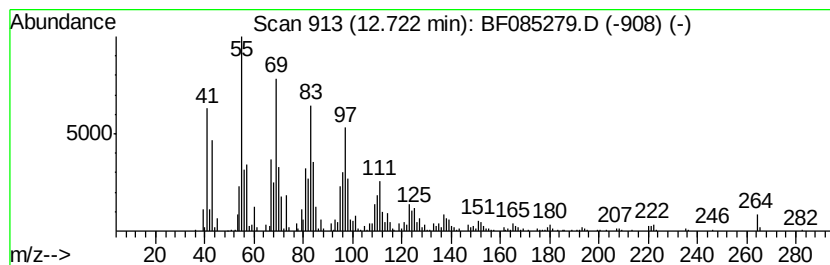
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenoic acid, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	16.38 ng	1186410	Phenanthrene-d10	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	93
2		Oleic Acid	282	C18H34O2	000112-80-1	90
3		14-Pentadecenoic acid	240	C15H28O2	017351-34-7	83
4		6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	64
5		Cyclododecanemethanol	198	C13H26O	001892-12-2	62



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085279.D
Acq On : 9 Mar 2016 2:19
Operator : UM/SJ
Sample : H1703-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-38COMP(0.5-4.0)

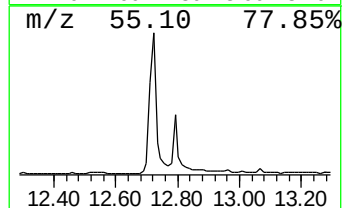
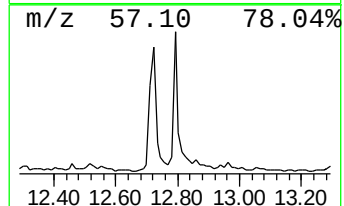
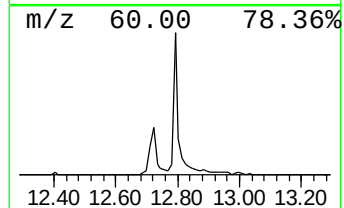
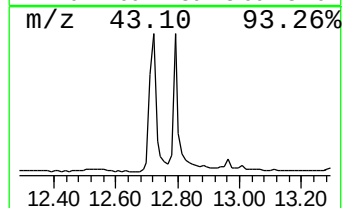
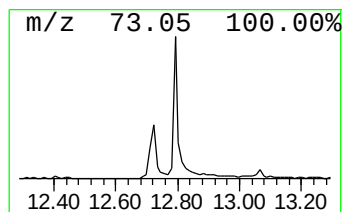
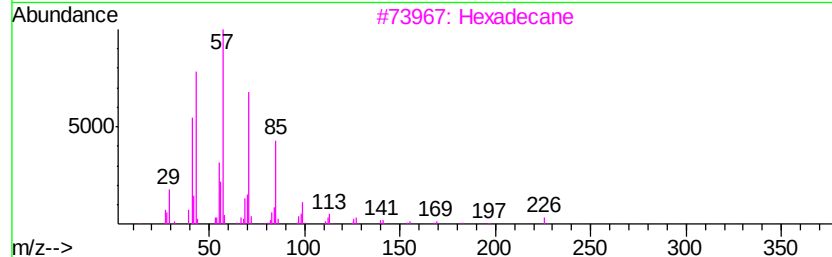
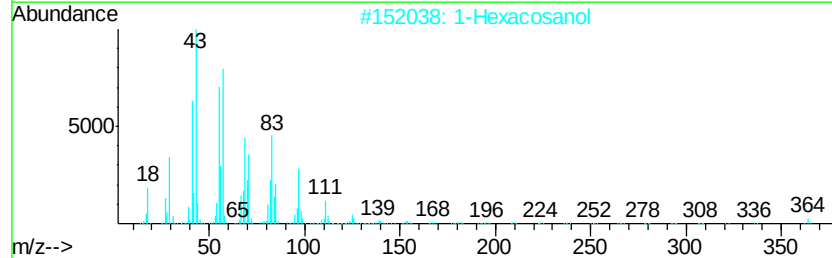
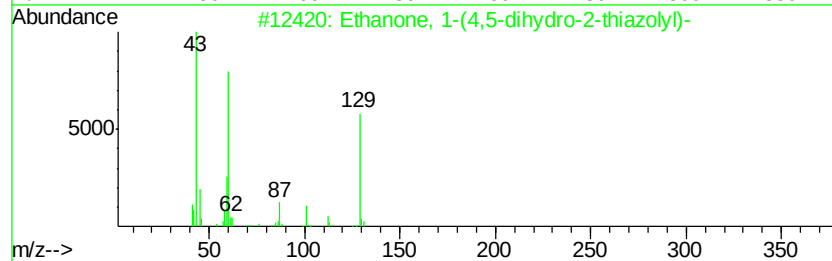
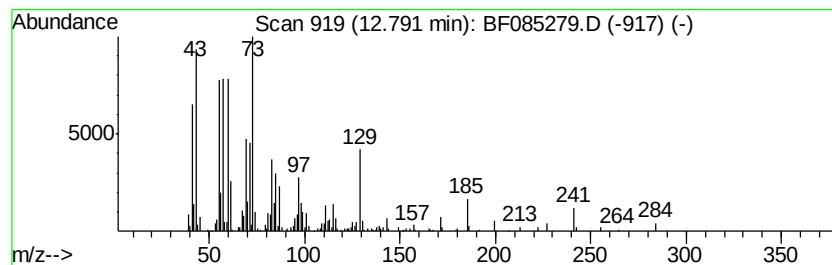
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown12.79 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	6.67 ng	482860	Phenanthrene-d10	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38
2		1-Hexacosanol	382	C26H54O	000506-52-5	18
3		Hexadecane	226	C16H34	000544-76-3	11
4		1-Tetracosanol	354	C24H50O	000506-51-4	11
5		Dodecane	170	C12H26	000112-40-3	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085279.D
Acq On : 9 Mar 2016 2:19
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Misc :
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Instrument :
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ClientSampleId :
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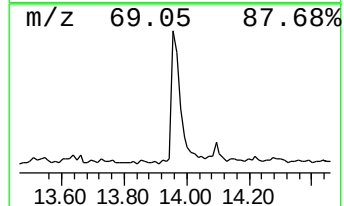
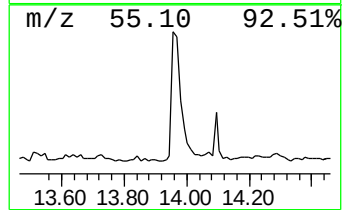
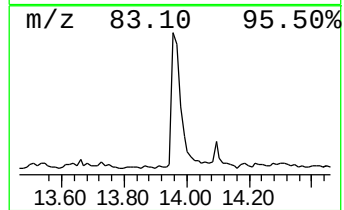
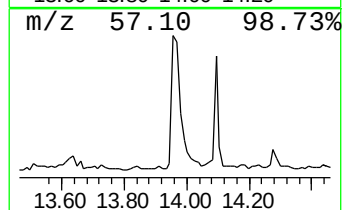
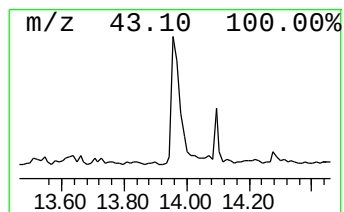
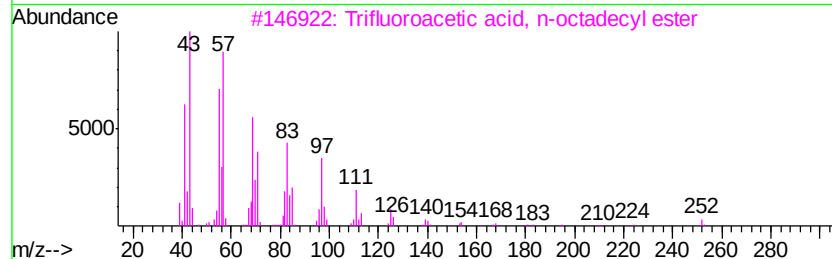
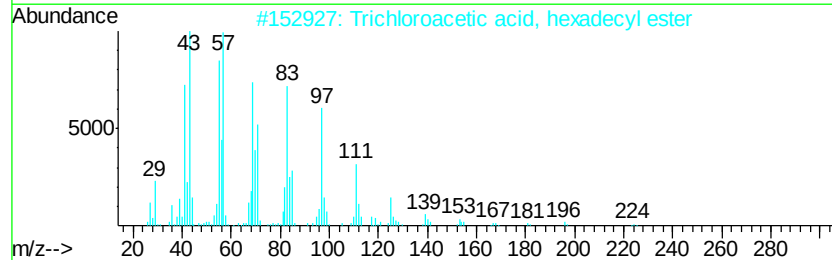
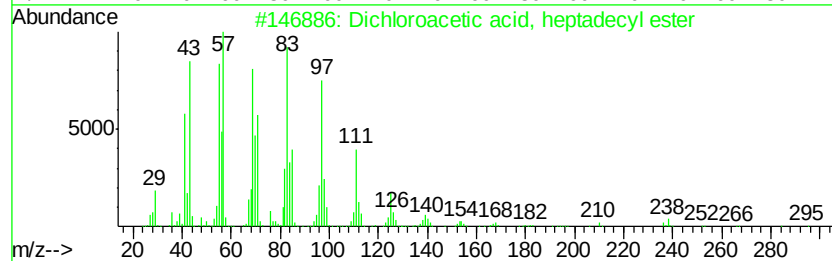
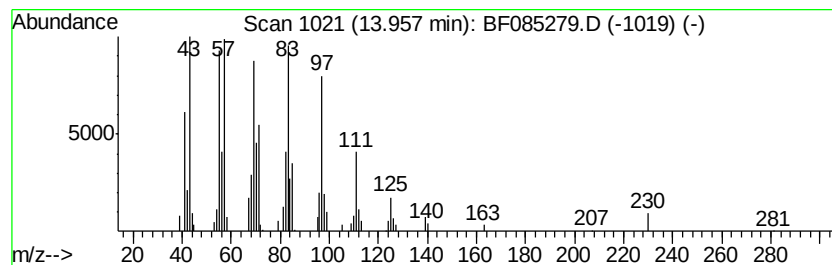
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Dichloroacetic acid, heptad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	3.85 ng	215881	Chrysene-d12	14.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
3		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
4		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
5		Cyclohexadecane	224	C16H32	000295-65-8	91



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Operator : UM/SJ
Sample : H1703-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-38COMP(0.5-4.0)

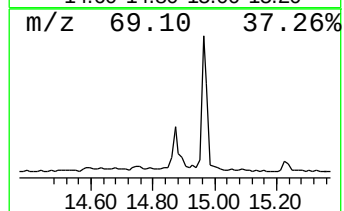
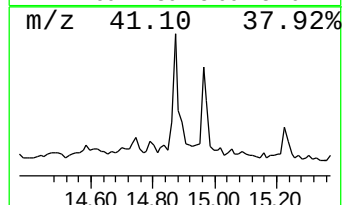
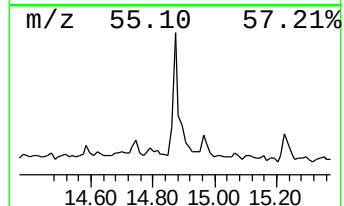
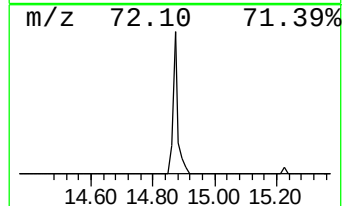
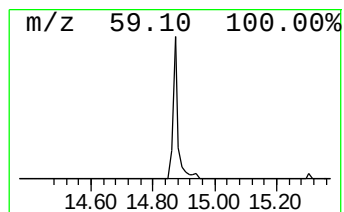
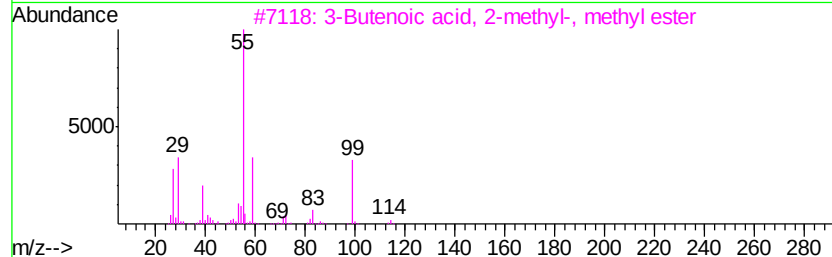
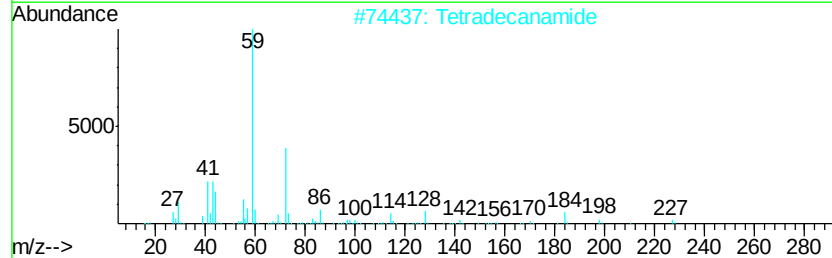
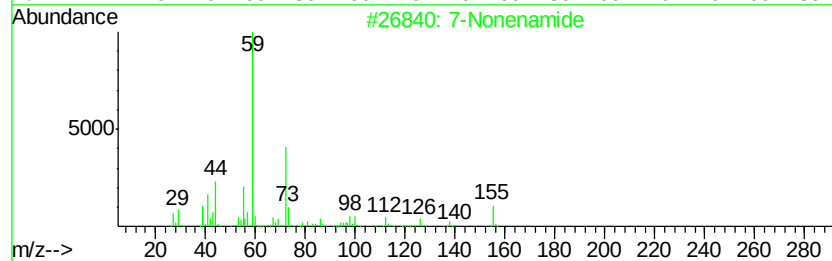
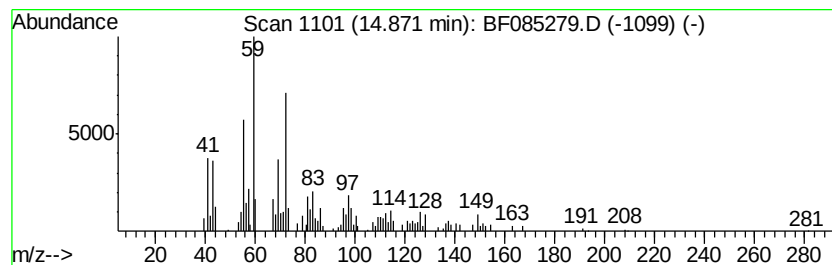
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 7-Nonenamide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	3.19 ng	129883	Perylene-d12	15.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Nonenamide	155	C9H17NO	090949-53-4	53
2		Tetradecanamide	227	C14H29NO	000638-58-4	53
3		3-Butenoic acid, 2-methyl-, meth...	114	C6H10O2	051747-33-2	47
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	43
5		2-Methyl-2-decanol	172	C11H24O	003396-02-9	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
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Misc :
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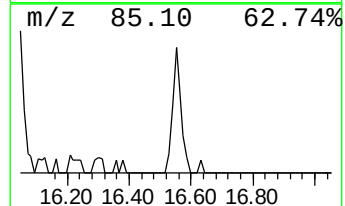
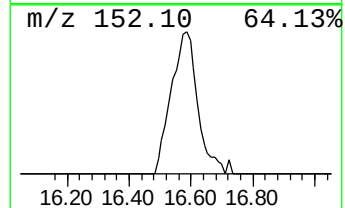
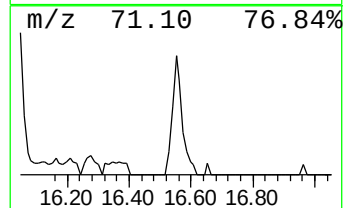
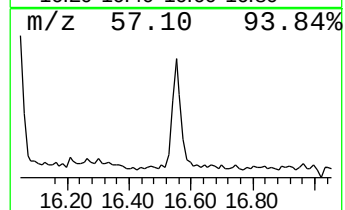
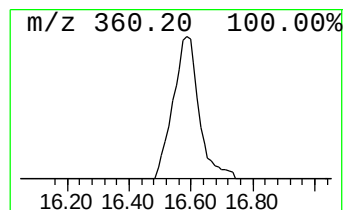
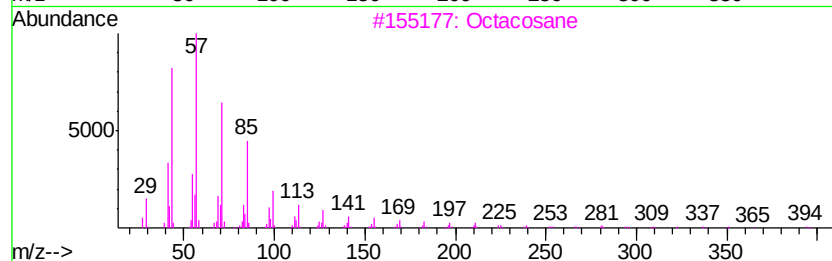
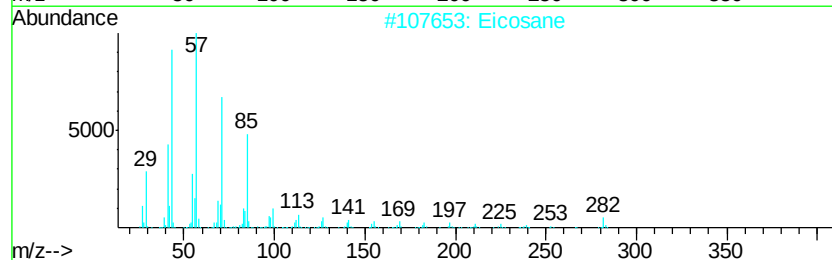
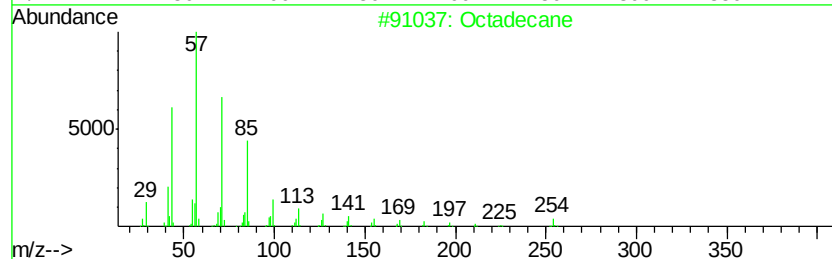
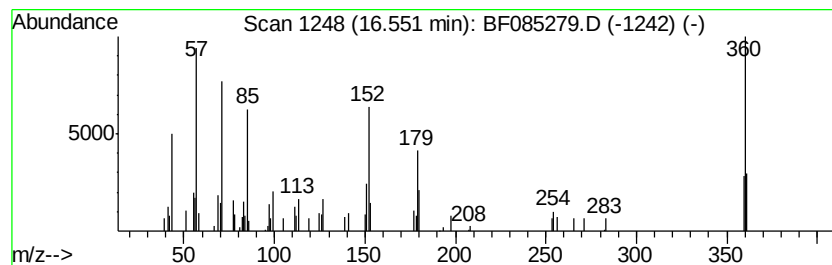
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.55 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	5.42 ng	220748	Perylene-d12	15.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	47
2		Eicosane	282	C20H42	000112-95-8	35
3		Octacosane	394	C28H58	000630-02-4	20
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	18
5		Docosane	310	C22H46	000629-97-0	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085279.D
Acq On : 9 Mar 2016 2:19
Operator : UM/SJ
Sample : H1703-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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
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unknown6.72	6.72	81.5	ng	4163850	1	6.96	1022320	20.0
Heptadecane	10.42	2.9	ng	211953	3	10.00	1488620	20.0
Tetracosane	10.90	3.2	ng	229298	4	11.49	1448290	20.0
n-Hexadecanoic acid	12.00	4.5	ng	327288	4	11.49	1448290	20.0
9-Octadecenoic ac...	12.72	16.4	ng	1186410	4	11.49	1448290	20.0
unknown12.79	12.79	6.7	ng	482860	4	11.49	1448290	20.0
Dichloroacetic ac...	13.96	3.9	ng	215881	5	14.12	1120860	20.0
7-Nonenamide	14.87	3.2	ng	129883	6	15.58	815216	20.0
unknown16.55	16.55	5.4	ng	220748	6	15.58	815216	20.0