

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
 Data File : BF085288.D
 Acq On : 9 Mar 2016 6:30
 Operator : UM/SJ
 Sample : H1712-04
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-44-COMP-0.5-2.0

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	249	252	260	rBV	812208	1270498	25.18%	2.936%
2	5.579	284	288	290	rBV	3214096	4908763	97.30%	11.343%
3	6.584	373	376	379	rBV	3102316	4778579	94.72%	11.043%
4	6.733	386	389	391	rBV	4422187	4932777	97.78%	11.399%
5	6.962	407	409	411	rBV	1104239	949608	18.82%	2.194%
6	7.122	420	423	425	rVB	3835636	3890540	77.12%	8.990%
7	7.522	455	458	461	rBV	2541511	2900767	57.50%	6.703%
8	7.602	462	465	468	rVB	79370	129409	2.57%	0.299%
9	8.242	519	521	524	rBV	1265777	1167508	23.14%	2.698%
10	9.328	613	616	618	rBV	4328597	5044752	100.00%	11.658%
11	9.716	647	650	651	rBV	864554	841186	16.67%	1.944%
12	9.933	666	669	671	rBV	103062	109038	2.16%	0.252%
13	10.002	673	675	677	rVB	1444275	1247205	24.72%	2.882%
14	10.425	711	712	714	rVB	162540	161854	3.21%	0.374%
15	10.642	728	731	735	rBV	56677	117090	2.32%	0.271%
16	10.791	741	744	746	rBV	2909017	2857252	56.64%	6.603%
17	10.905	752	754	759	rBV	160956	245667	4.87%	0.568%
18	11.099	768	771	775	rBV3	21287	61275	1.21%	0.142%
19	11.351	791	793	794	rBV	114934	104090	2.06%	0.241%
20	11.488	802	805	807	rBV	1196425	1161531	23.02%	2.684%
21	11.556	808	811	813	rVB3	29662	59185	1.17%	0.137%
22	12.002	848	850	857	rBV2	190031	251529	4.99%	0.581%
23	12.699	908	911	913	rBV	40766	77379	1.53%	0.179%
24	12.791	917	919	921	rBV	238452	258524	5.12%	0.597%
25	12.825	921	922	924	rVB	88384	67762	1.34%	0.157%
26	12.916	929	930	936	rVB	29303	94059	1.86%	0.217%
27	13.065	941	943	946	rBV	2663706	3192882	63.29%	7.378%
28	13.957	1019	1021	1027	rBV	100015	170595	3.38%	0.394%
29	14.117	1033	1035	1038	rVB	843732	810123	16.06%	1.872%
30	15.157	1124	1126	1130	rBV	22394	54127	1.07%	0.125%
31	15.591	1161	1164	1170	rBV	534370	883009	17.50%	2.040%
32	16.048	1201	1204	1207	rVB	40396	55942	1.11%	0.129%
33	16.300	1222	1226	1237	rVB5	45415	193591	3.84%	0.447%
34	16.563	1246	1249	1255	rBV2	38371	89305	1.77%	0.206%

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Instrument :
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ClientSampleId :
SB-44-COMP-0.5-2.0

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.145	1298	1300	1306	rVB2	26323	60231	1.19%	0.139%
36	17.854	1358	1362	1367	rVB2	29126	76703	1.52%	0.177%

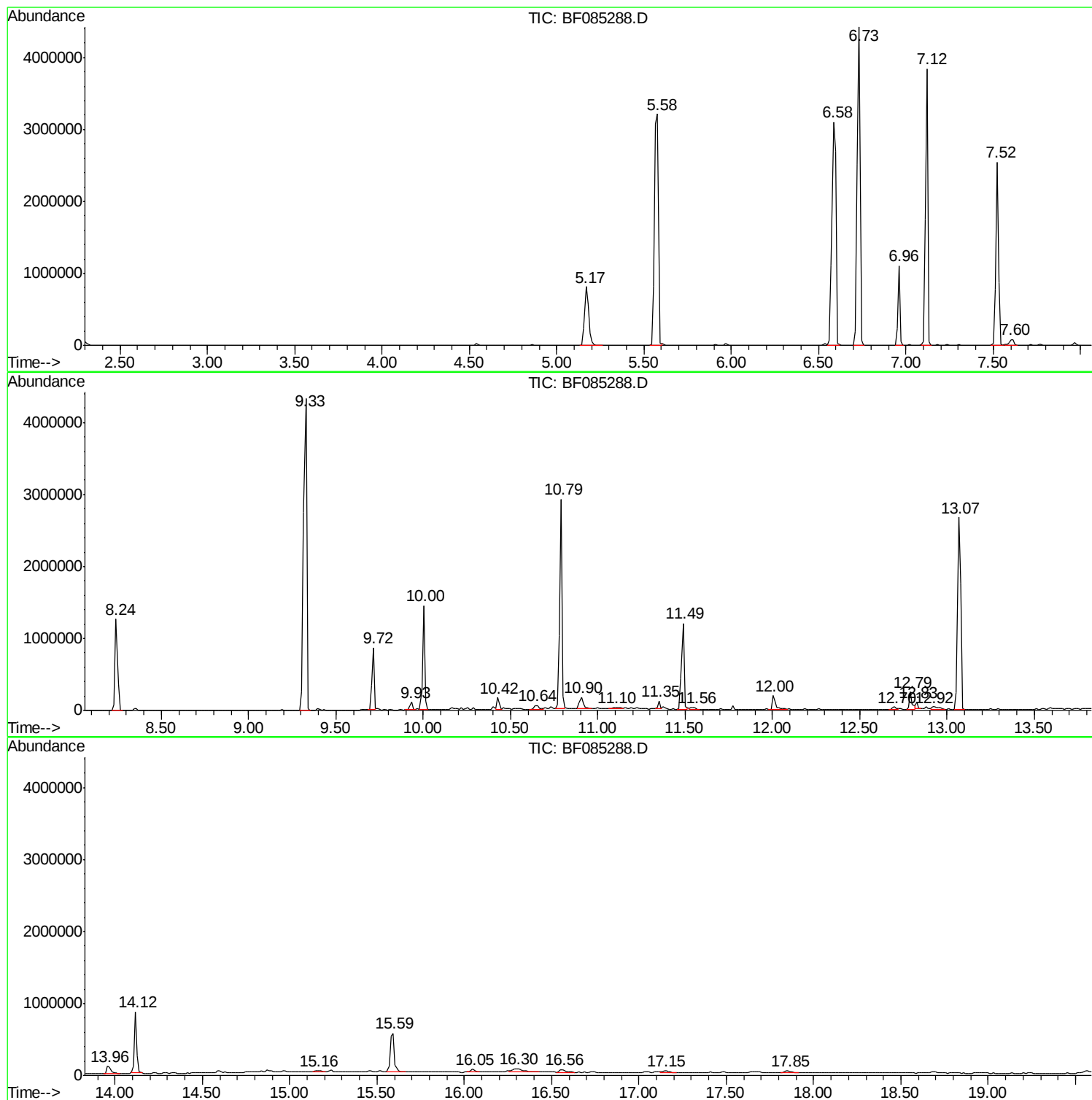
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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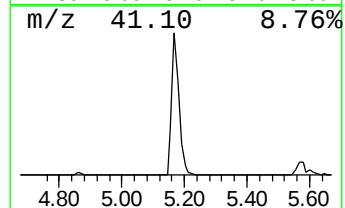
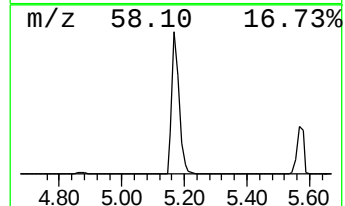
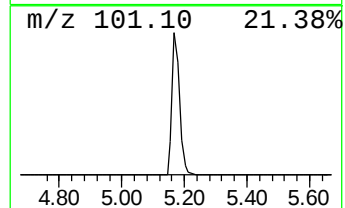
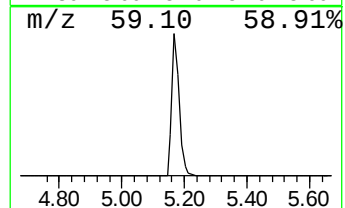
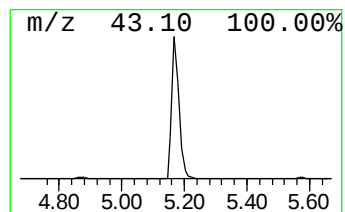
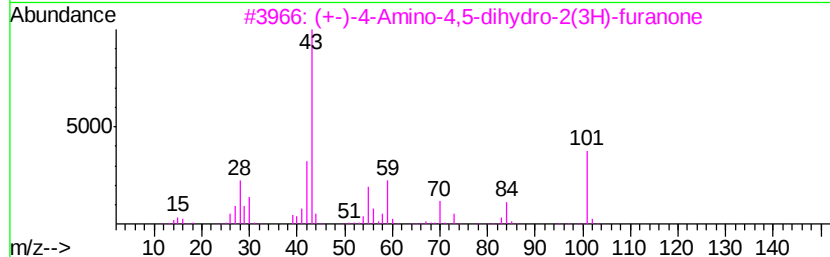
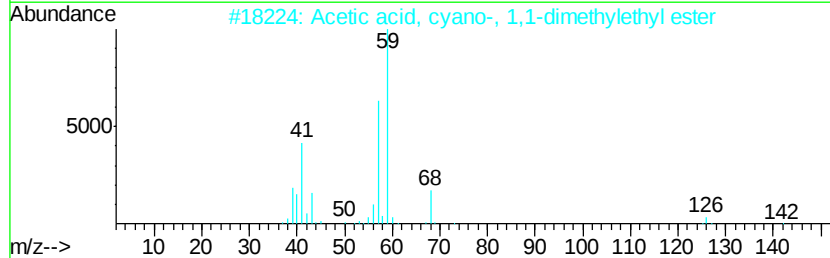
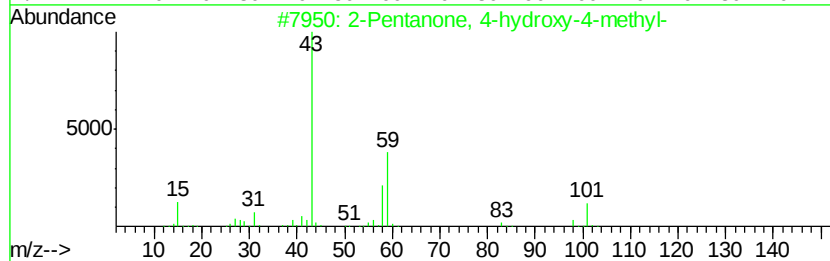
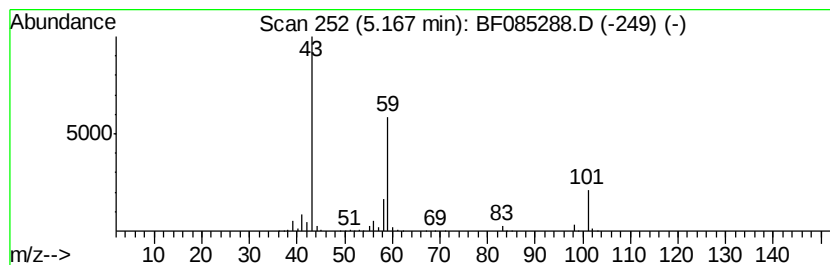
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	26.76 ng	1270500	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
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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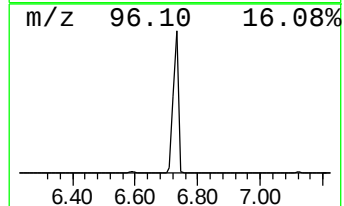
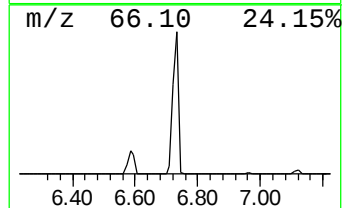
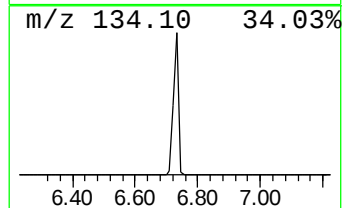
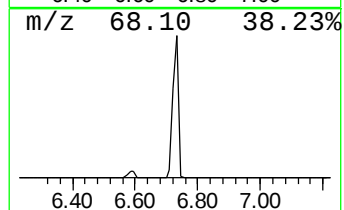
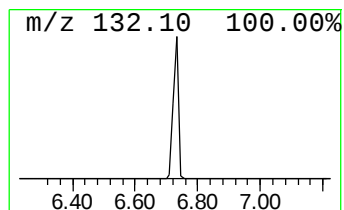
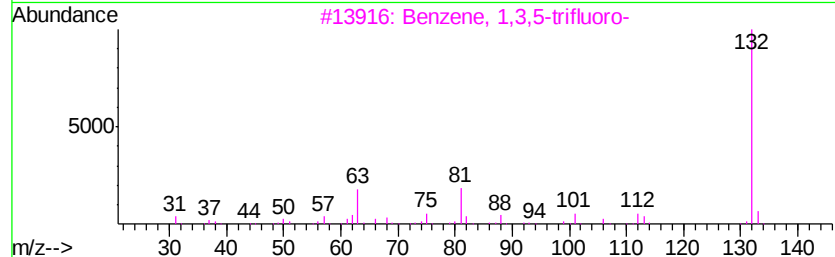
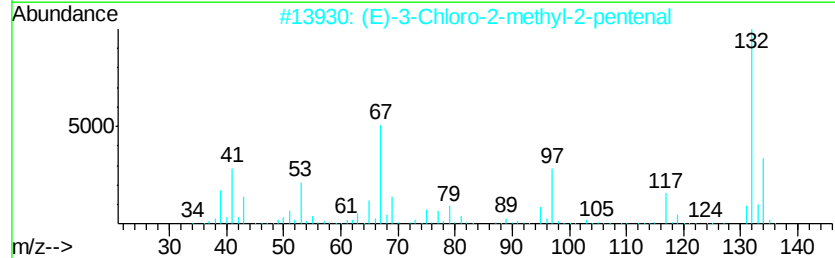
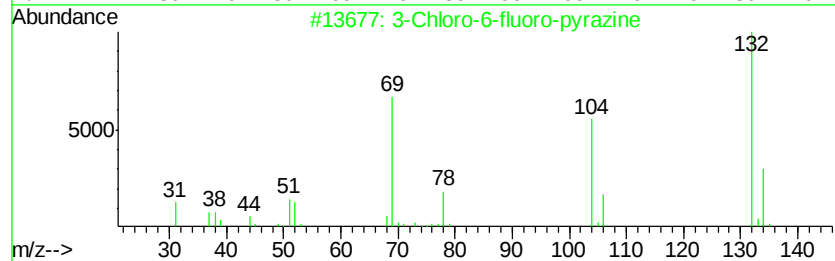
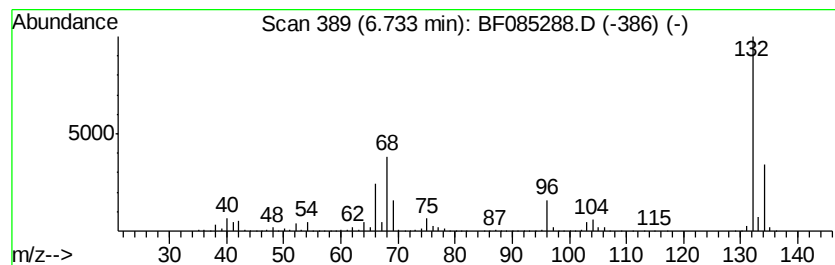
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	103.89 ng	4932780	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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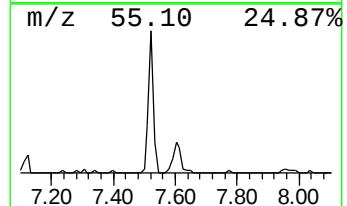
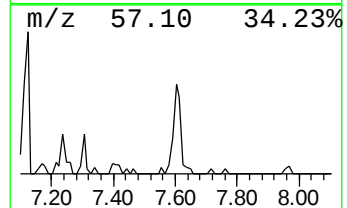
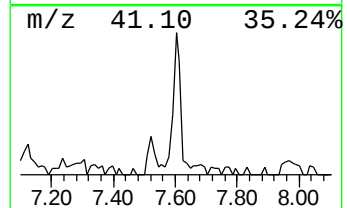
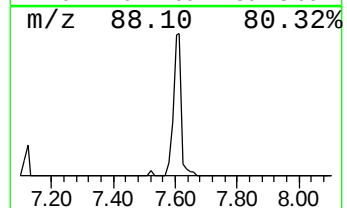
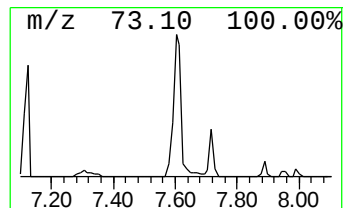
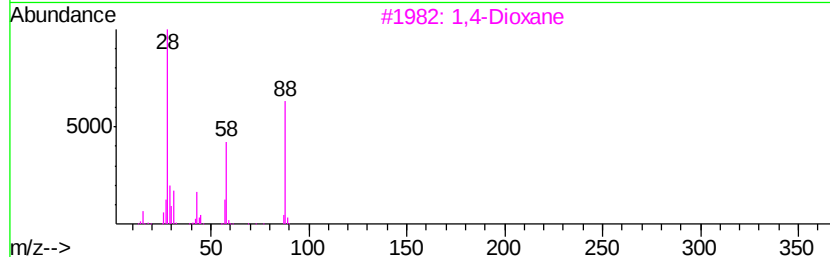
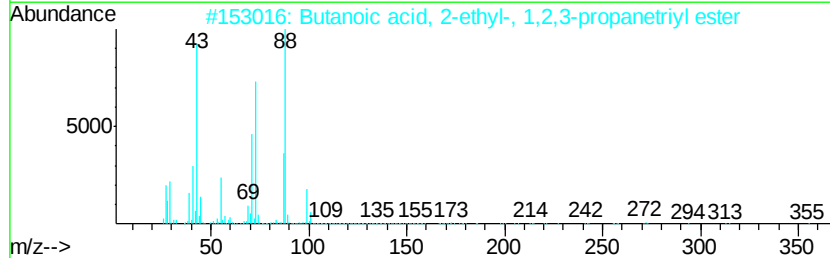
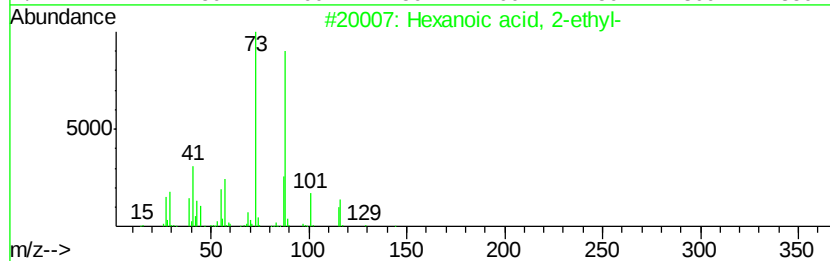
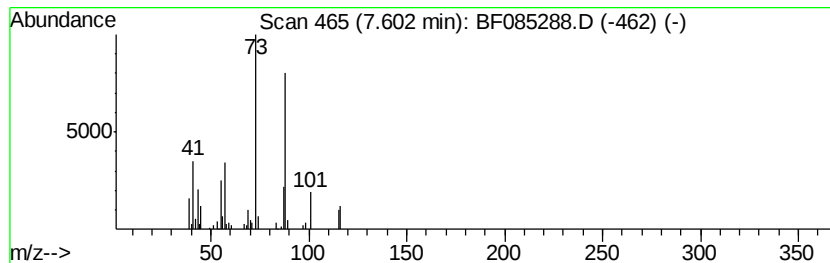
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	2.22 ng	129409	Naphthalene-d8	8.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	59
3		1,4-Dioxane	88	C4H8O2	000123-91-1	43
4		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	40
5		Hexanamide, 6-(heptyloxy)-	229	C13H27NO2	055191-08-7	40



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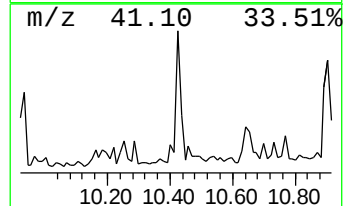
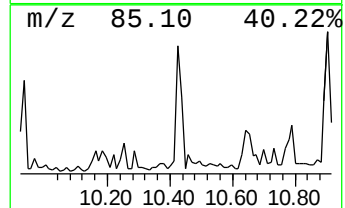
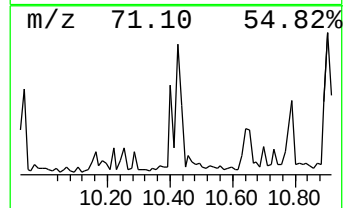
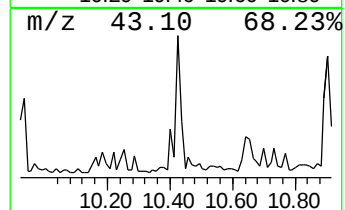
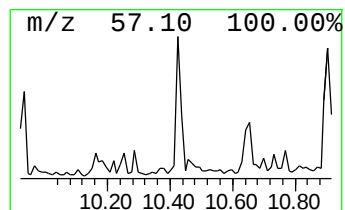
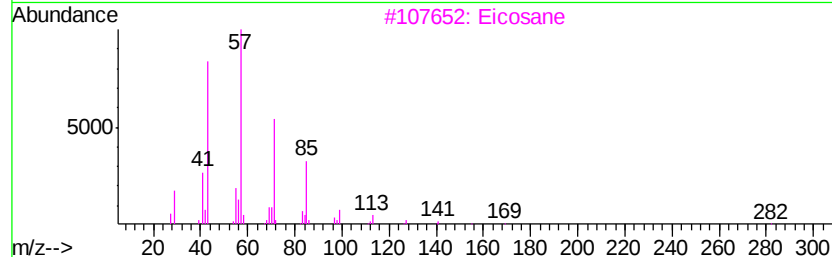
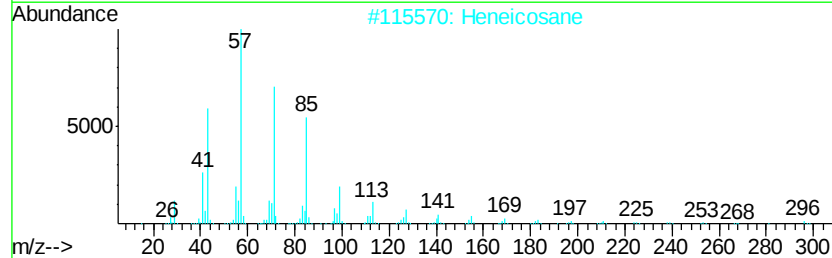
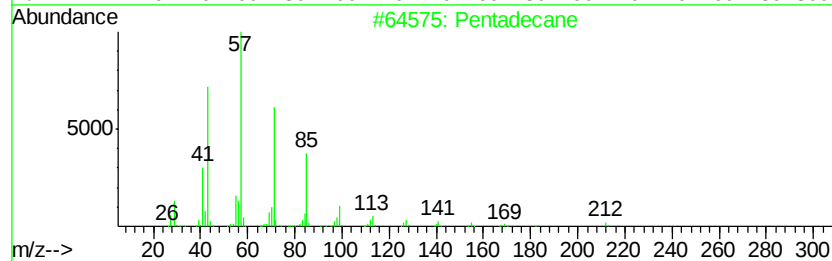
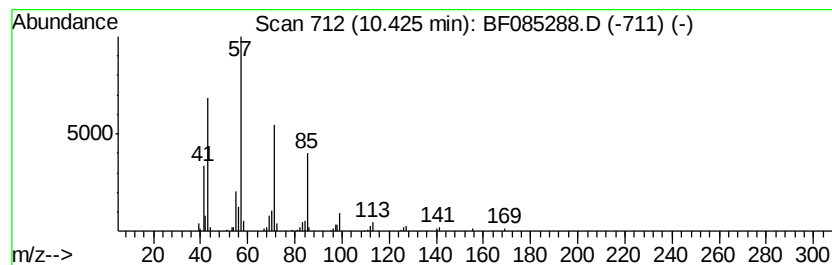
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.42	2.60 ng	161854	Acenaphthene-d10	10.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentadecane	212 C15H32	000629-62-9	86
2	Heneicosane	296 C21H44	000629-94-7	83
3	Eicosane	282 C20H42	000112-95-8	83
4	Heptadecane	240 C17H36	000629-78-7	83
5	Tetradecane	198 C14H30	000629-59-4	80



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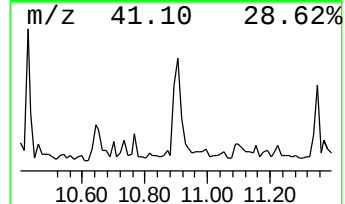
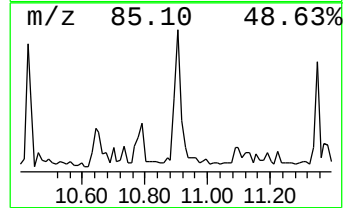
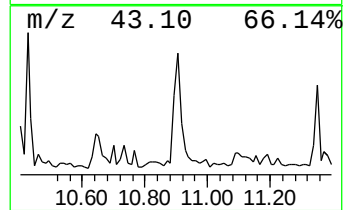
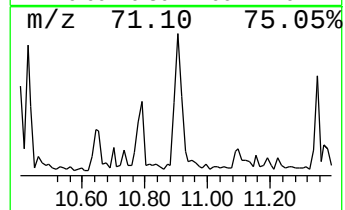
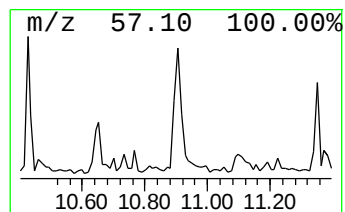
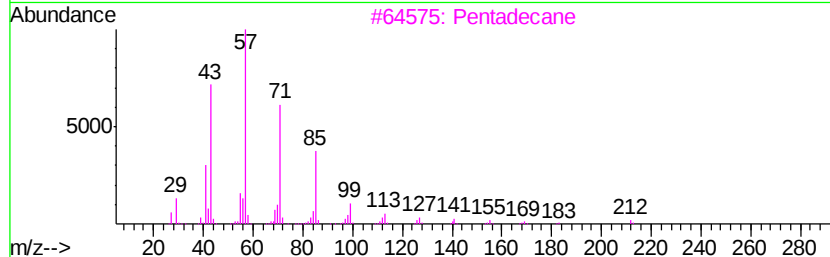
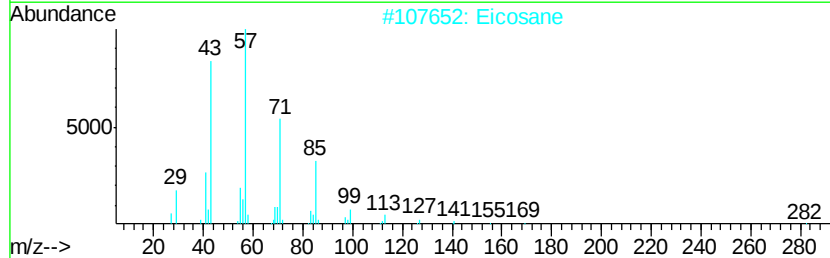
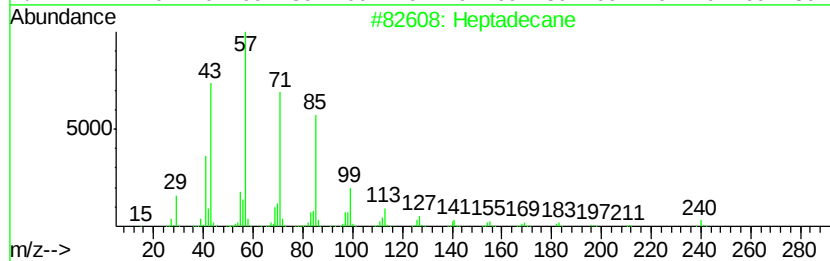
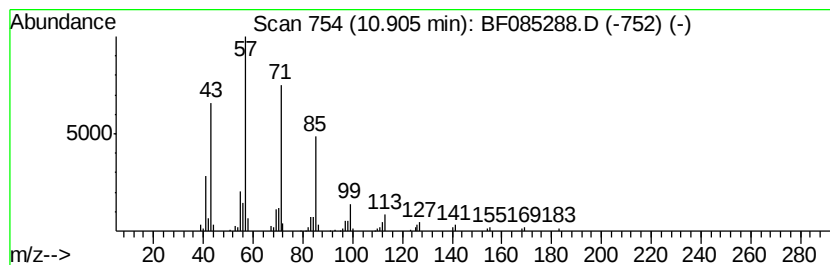
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	4.23 ng	245667	Phenanthrene-d10	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	91
2	Eicosane		282	C20H42	000112-95-8	91
3	Pentadecane		212	C15H32	000629-62-9	91
4	Tetradecane		198	C14H30	000629-59-4	91
5	Hexadecane		226	C16H34	000544-76-3	91



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ClientSampleId :
SB-44-COMP-0.5-2.0

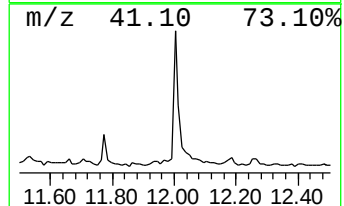
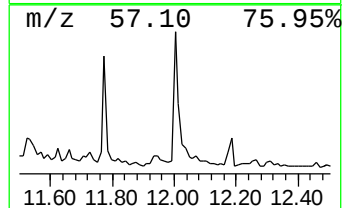
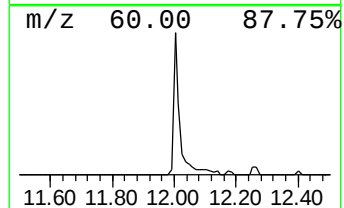
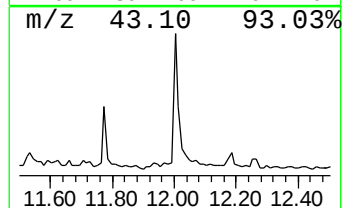
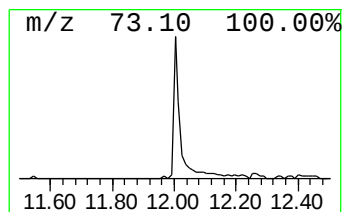
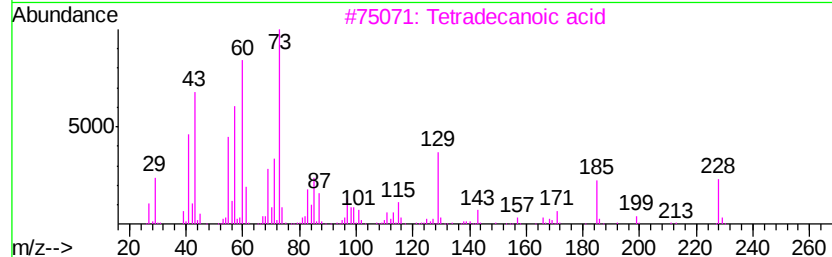
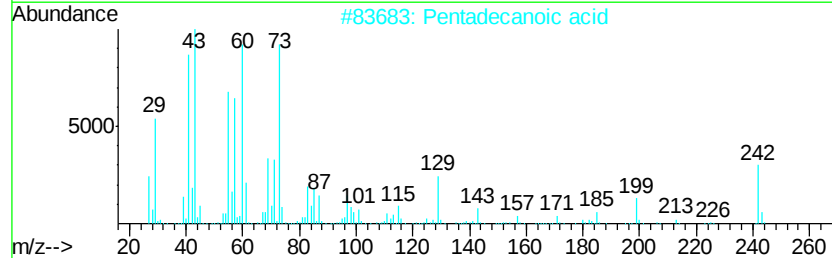
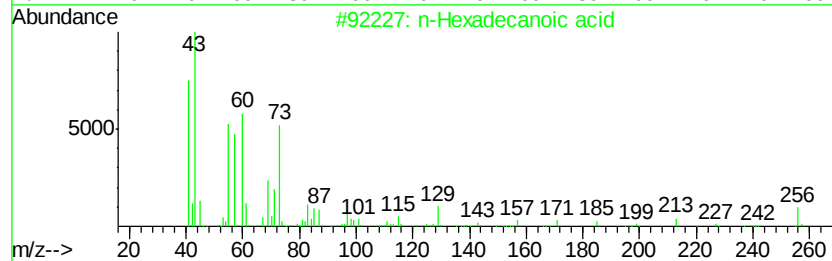
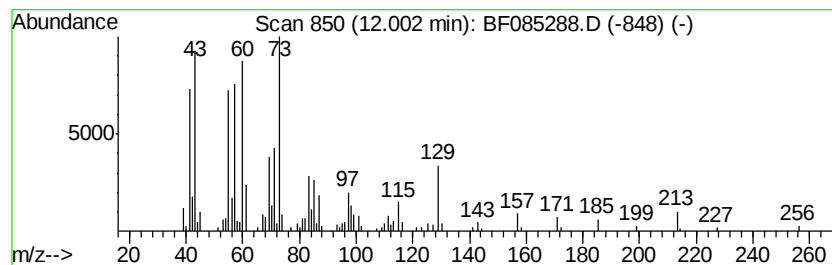
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	4.33 ng	251529	Phenanthrene-d10	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Tridecanoic acid	214	C13H26O2	000638-53-9	64
5		Amyl Nitrite	117	C5H11NO2	000110-46-3	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085288.D
Acq On : 9 Mar 2016 6:30
Operator : UM/SJ
Sample : H1712-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

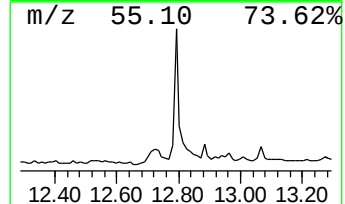
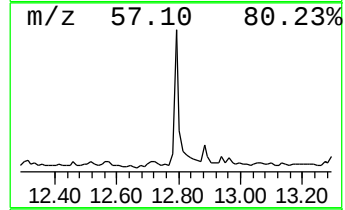
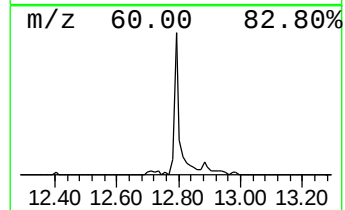
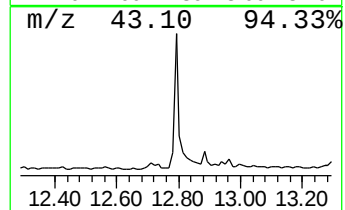
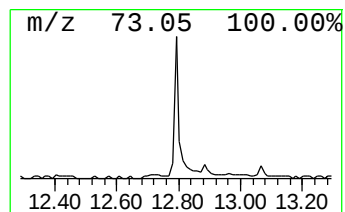
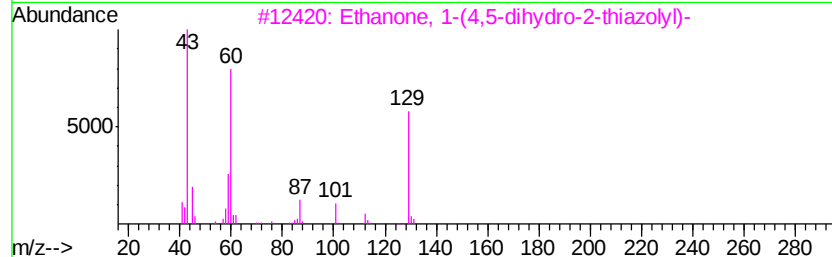
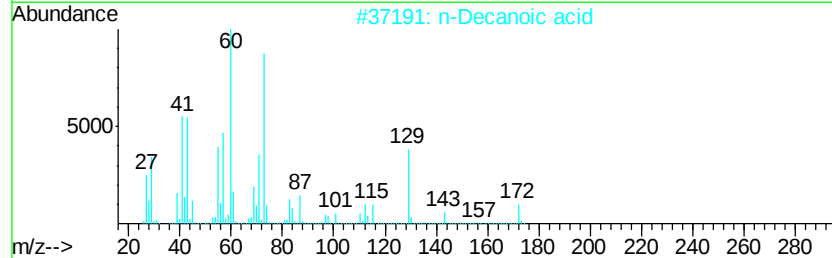
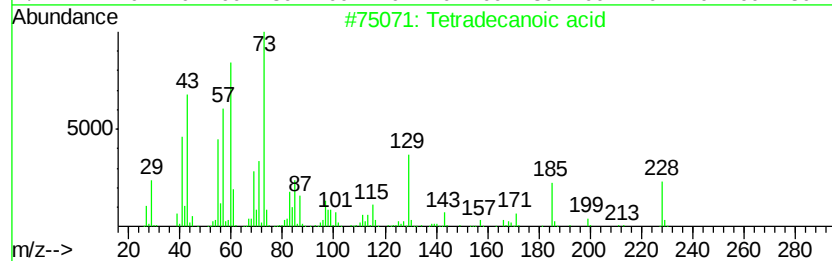
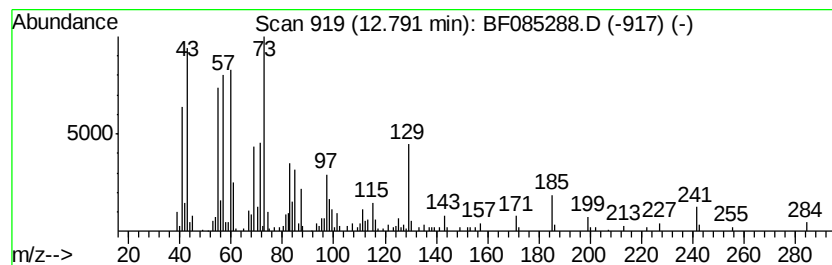
Instrument :
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ClientSampleId :
SB-44-COMP-0.5-2.0

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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 8 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.79	4.45 ng	258524	Phenanthrene-d10	11.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
2	n-Decanoic acid	172	C10H20O2	000334-48-5	68
3	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	43
4	Undecanoic acid	186	C11H22O2	000112-37-8	43
5	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085288.D
Acq On : 9 Mar 2016 6:30
Operator : UM/SJ
Sample : H1712-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-44-COMP-0.5-2.0

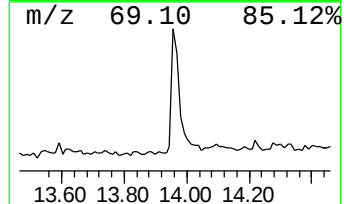
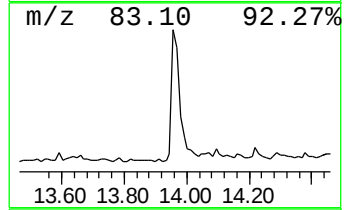
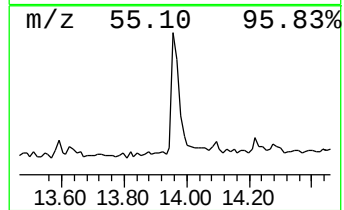
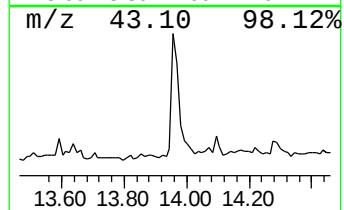
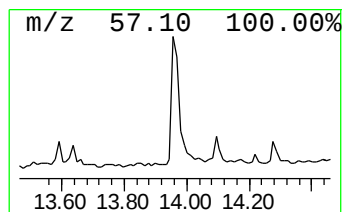
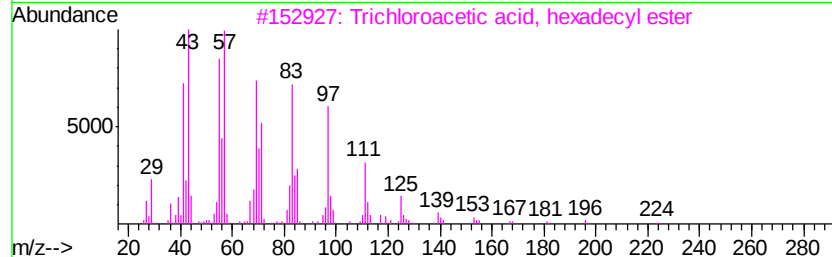
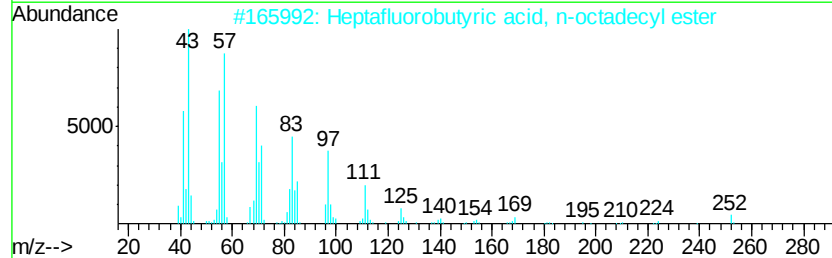
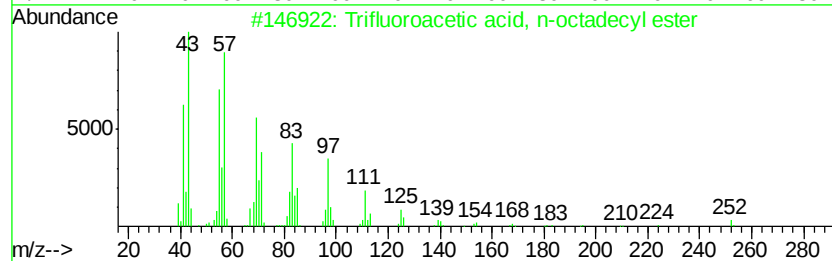
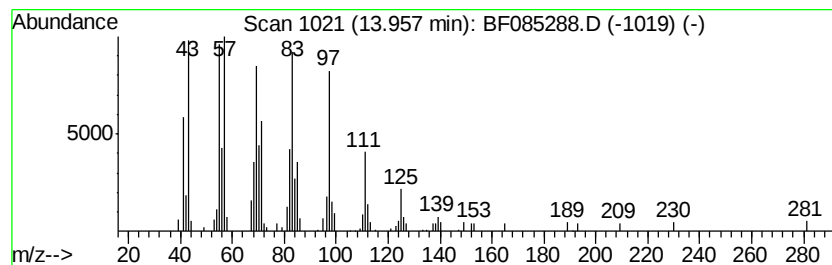
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Trifluoroacetic acid, n-oct... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	4.21 ng	170595	Chrysene-d12	14.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
2			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	90
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
4			1-Nonadecene	266	C19H38	018435-45-5	90
5			1-Octadecanol	270	C18H38O	000112-92-5	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085288.D
Acq On : 9 Mar 2016 6:30
Operator : UM/SJ
Sample : H1712-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

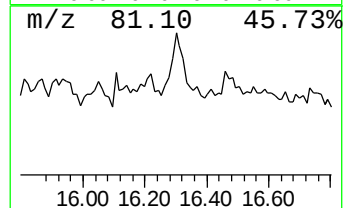
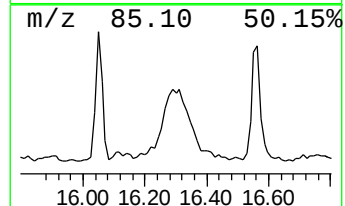
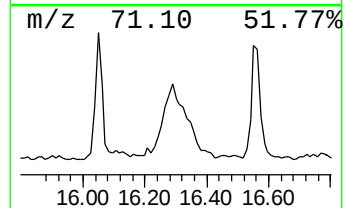
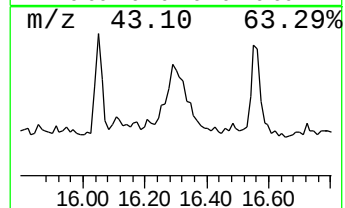
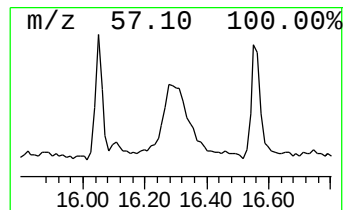
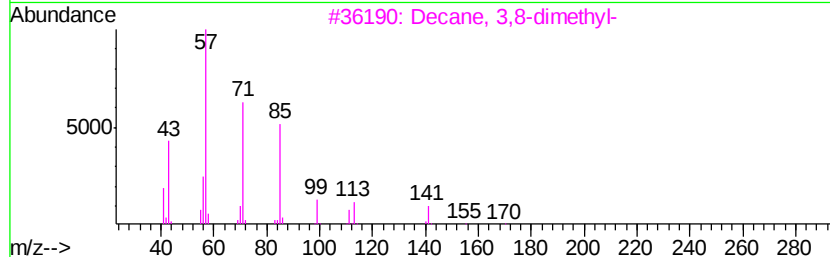
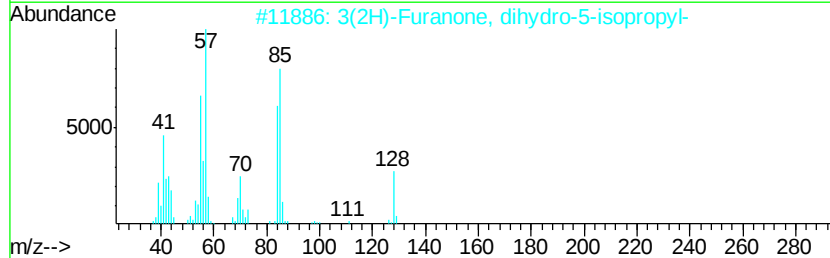
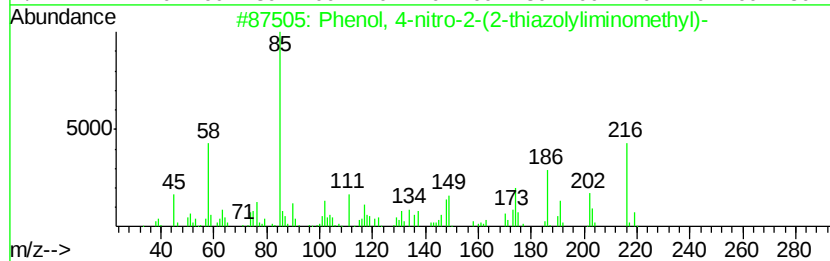
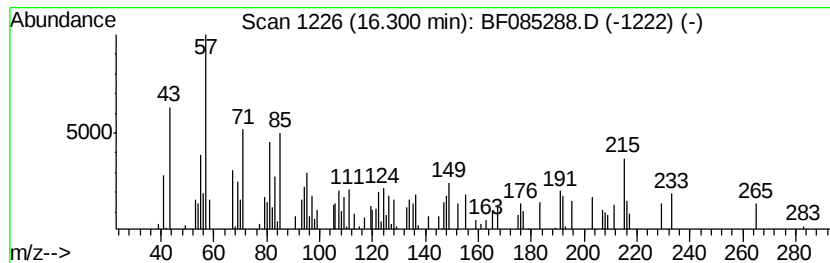
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.30 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.30	4.38 ng	193591	Perylene-d12	15.59	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-nitro-2-(2-thiazolylim...	249	C10H7N3O3S	078096-09-0	22
2	3(2H)-Furanone, dihydro-5-isopro...	128	C7H12O2	034004-69-8	11
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	10
4	Tridecane, 7-propyl-	226	C16H34	055045-09-5	10
5	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085288.D
Acq On : 9 Mar 2016 6:30
Operator : UM/SJ
Sample : H1712-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-44-COMP-0.5-2.0

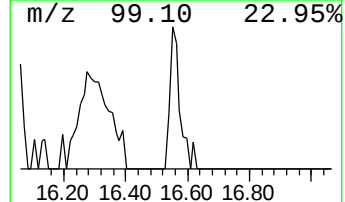
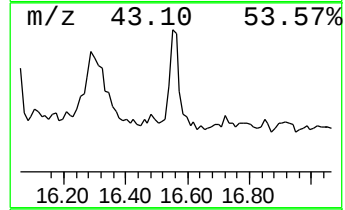
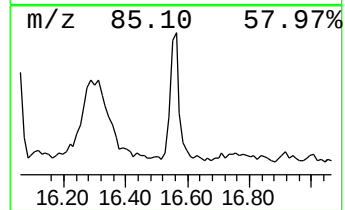
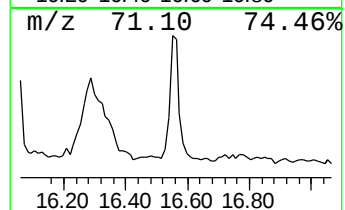
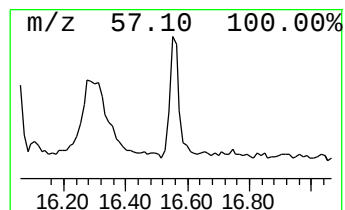
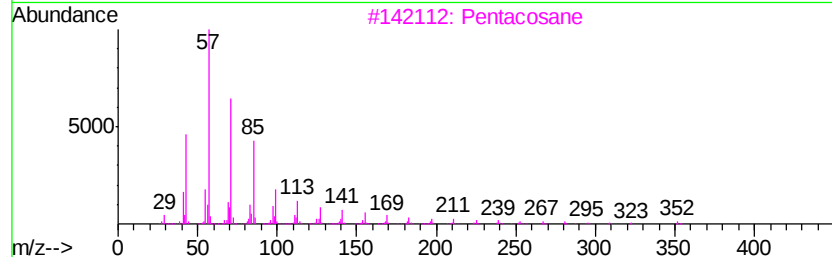
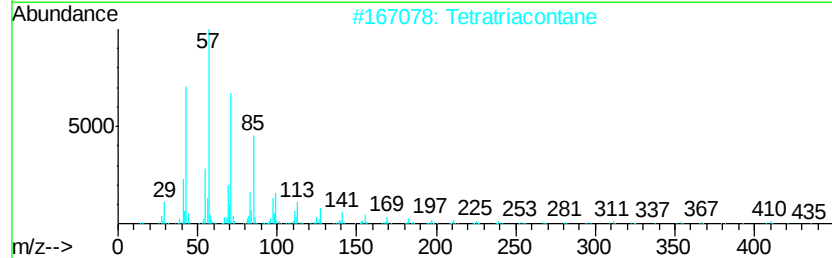
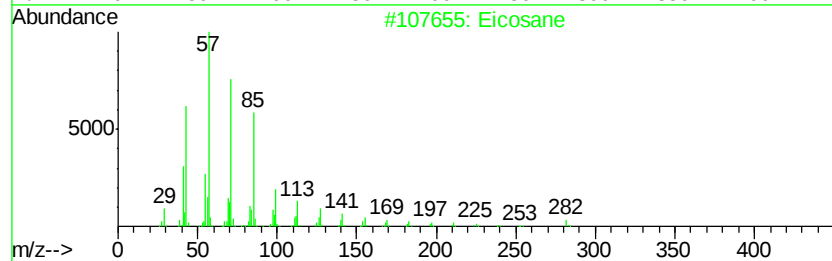
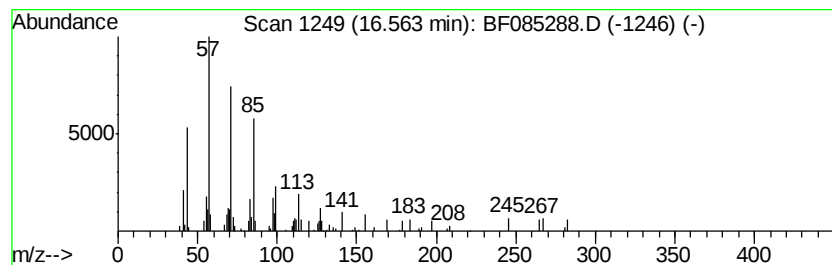
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.56	2.02 ng	89305	Perylene-d12	15.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	96
2		Tetratriacontane	479	C34H70	014167-59-0	90
3		Pentacosane	352	C25H52	000629-99-2	87
4		Octacosane	394	C28H58	000630-02-4	87
5		Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085288.D
Acq On : 9 Mar 2016 6:30
Operator : UM/SJ
Sample : H1712-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-44-COMP-0.5-2.0

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	26.8	ng	1270500	1	6.96	949608	20.0
unknown6.73	6.73	103.9	ng	4932780	1	6.96	949608	20.0
Hexanoic acid, 2-...	7.60	2.2	ng	129409	2	8.24	1167510	20.0
Pentadecane	10.42	2.6	ng	161854	3	10.00	1247210	20.0
Heptadecane	10.90	4.2	ng	245667	4	11.49	1161530	20.0
n-Hexadecanoic acid	12.00	4.3	ng	251529	4	11.49	1161530	20.0
Tetradecanoic acid	12.79	4.5	ng	258524	4	11.49	1161530	20.0
Trifluoroacetic a...	13.96	4.2	ng	170595	5	14.12	810123	20.0
unknown16.30	16.30	4.4	ng	193591	6	15.59	883009	20.0
Eicosane	16.56	2.0	ng	89305	6	15.59	883009	20.0