

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
 Data File : BF095779.D
 Acq On : 8 Jun 2017 12:52
 Operator : SJ/MA
 Sample : I3469-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-2(0-2)20170603

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-BF060517.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	4.587	506	510	533	rBV2	68247	212517	8.26%	0.950%
2	5.269	621	626	646	rBV	1259998	2082386	80.95%	9.306%
3	6.933	903	909	919	rBV	1276545	2131180	82.85%	9.524%
4	7.028	919	925	941	rVB	1652557	2339693	90.96%	10.456%
5	7.369	979	983	997	rBB	283223	383100	14.89%	1.712%
6	7.604	1017	1023	1047	rVB	1240920	1684148	65.47%	7.526%
7	8.286	1133	1139	1163	rBV	887033	1351201	52.53%	6.038%
8	9.398	1323	1328	1340	rBV	417095	548956	21.34%	2.453%
9	11.186	1623	1632	1635	rBV	1839340	2572321	100.00%	11.496%
10	11.874	1743	1749	1756	rBV	226832	281721	10.95%	1.259%
11	12.221	1802	1808	1813	rBV2	493069	607800	23.63%	2.716%
12	12.268	1813	1816	1821	rVB2	23000	30419	1.18%	0.136%
13	13.080	1950	1954	1958	rBV	29092	36131	1.40%	0.161%
14	13.521	2023	2029	2036	rBV	1031956	1398135	54.35%	6.248%
15	13.851	2080	2085	2095	rBV	33921	53677	2.09%	0.240%
16	14.615	2210	2215	2219	rVV	468542	608522	23.66%	2.719%
17	14.651	2219	2221	2230	rVB	60184	77578	3.02%	0.347%
18	15.633	2383	2388	2397	rVB3	113468	146104	5.68%	0.653%
19	16.427	2518	2523	2530	rBV	206406	253518	9.86%	1.133%
20	16.733	2570	2575	2582	rBV	267121	314764	12.24%	1.407%
21	16.850	2590	2595	2600	rVB2	44233	52322	2.03%	0.234%
22	16.933	2604	2609	2612	rBV2	21658	26802	1.04%	0.120%
23	16.998	2612	2620	2623	rVV	1662152	2194402	85.31%	9.807%
24	17.068	2623	2632	2640	rVB4	11935	28037	1.09%	0.125%
25	17.209	2652	2656	2660	rVB	25879	35713	1.39%	0.160%
26	17.297	2667	2671	2675	rVB	22624	26592	1.03%	0.119%
27	17.350	2675	2680	2684	rBV4	19500	40470	1.57%	0.181%
28	17.398	2685	2688	2693	rVB	23151	26354	1.02%	0.118%
29	17.780	2750	2753	2759	rVB3	33856	39046	1.52%	0.174%
30	17.845	2759	2764	2767	rBV	41237	45987	1.79%	0.206%
31	18.244	2827	2832	2833	rBV2	100417	113059	4.40%	0.505%
32	18.327	2841	2846	2850	rBV2	491110	628561	24.44%	2.809%
33	18.362	2850	2852	2858	rVB	80790	95928	3.73%	0.429%
34	18.456	2865	2868	2874	rVB	23254	26653	1.04%	0.119%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.662	2899	2903	2907	rBV	111367	129160	5.02%	0.577%
36	18.839	2928	2933	2937	rBV2	21868	30878	1.20%	0.138%
37	19.050	2964	2969	2974	rVB	123720	147230	5.72%	0.658%
38	19.415	3027	3031	3035	rBV	102981	116737	4.54%	0.522%
39	19.480	3039	3042	3048	rVB	29475	35286	1.37%	0.158%
40	19.597	3058	3062	3065	rBV	123181	166075	6.46%	0.742%
41	19.621	3065	3066	3072	rVB	49300	61188	2.38%	0.273%
42	19.709	3078	3081	3085	rVB	27913	28391	1.10%	0.127%
43	19.768	3087	3091	3095	rBV	75992	91553	3.56%	0.409%
44	19.886	3107	3111	3115	rBV	76360	79349	3.08%	0.355%
45	19.944	3118	3121	3126	rVV	123765	123798	4.81%	0.553%
46	19.997	3126	3130	3140	rVV	366116	468302	18.21%	2.093%
47	20.109	3146	3149	3155	rVB2	48461	61586	2.39%	0.275%
48	20.450	3203	3207	3210	rBV2	34153	50588	1.97%	0.226%
49	20.815	3266	3269	3280	rVB7	19647	49251	1.91%	0.220%
50	21.174	3325	3330	3338	rVB	59129	107018	4.16%	0.478%
51	21.503	3381	3386	3394	rBV	51290	101749	3.96%	0.455%
52	21.715	3417	3422	3426	rBV2	15876	34779	1.35%	0.155%

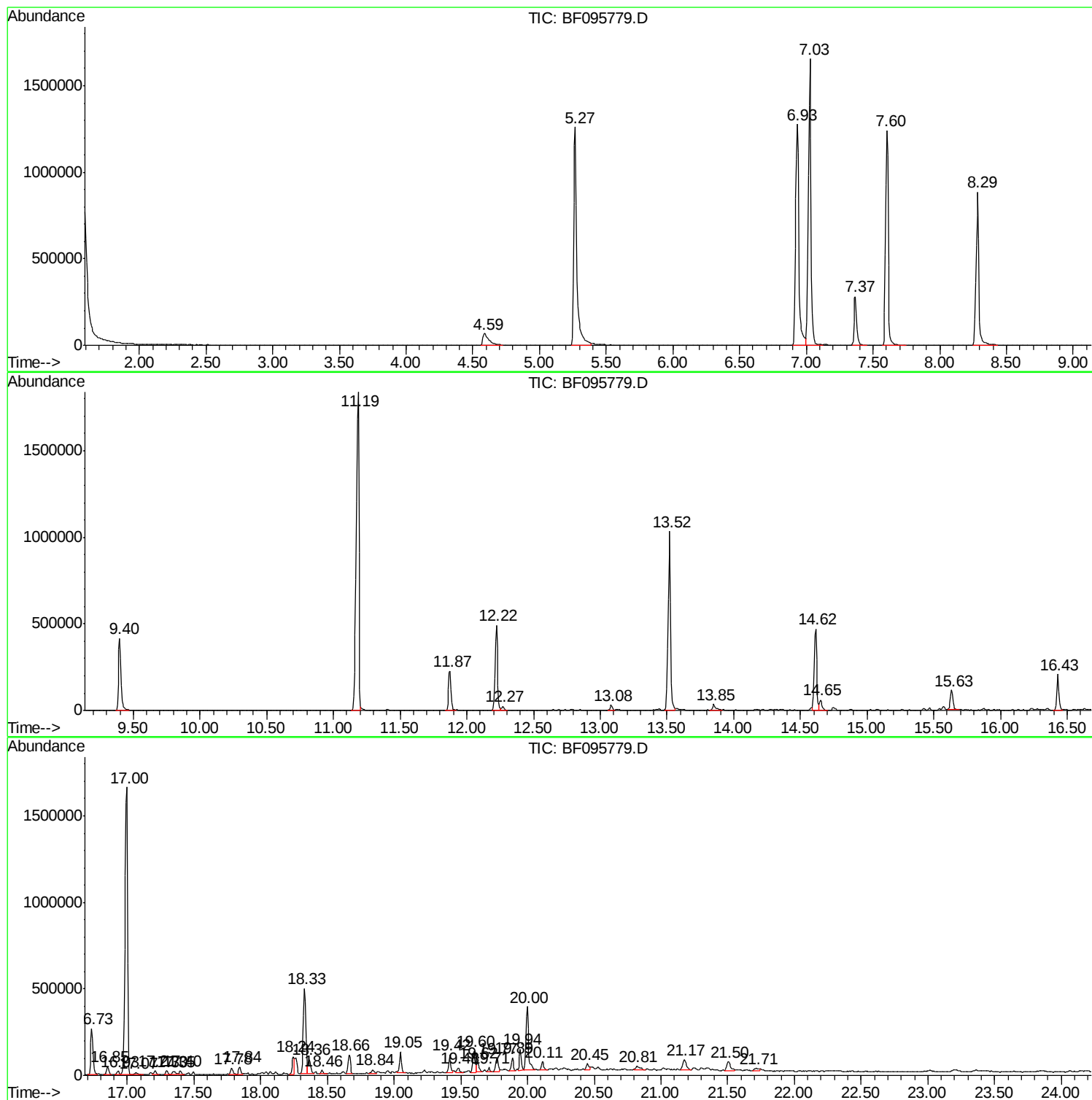
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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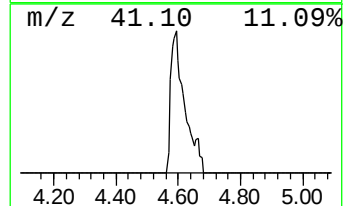
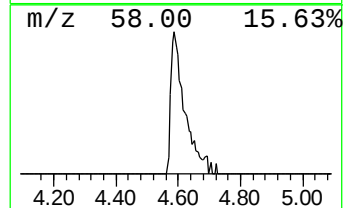
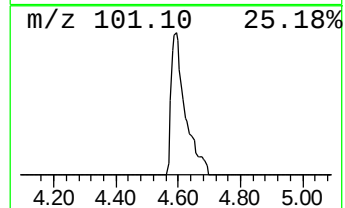
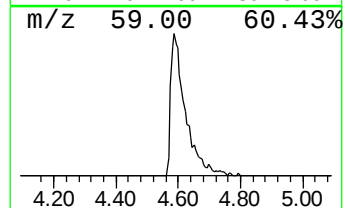
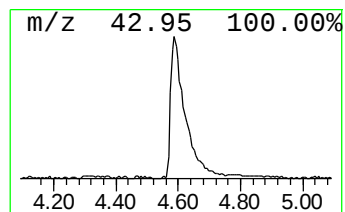
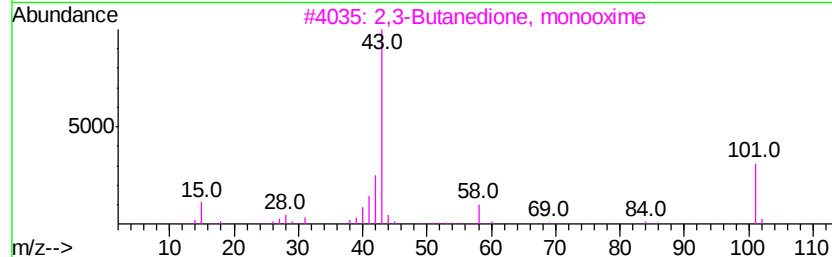
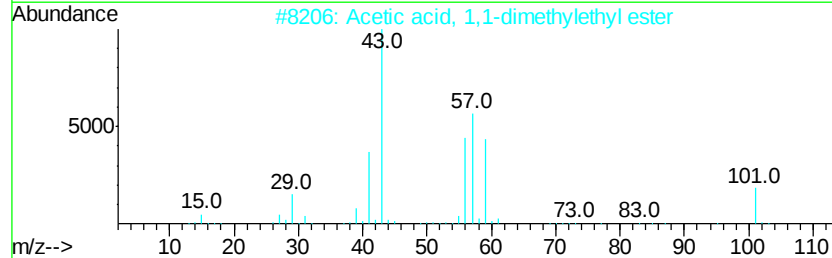
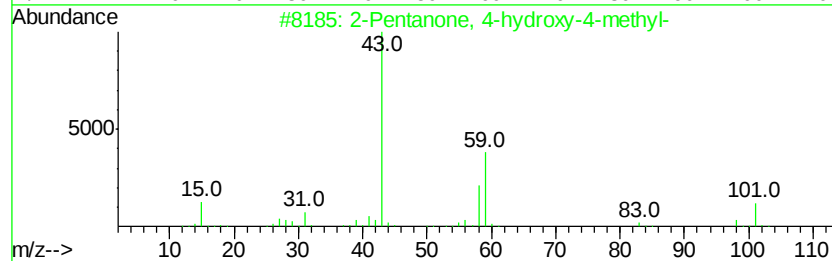
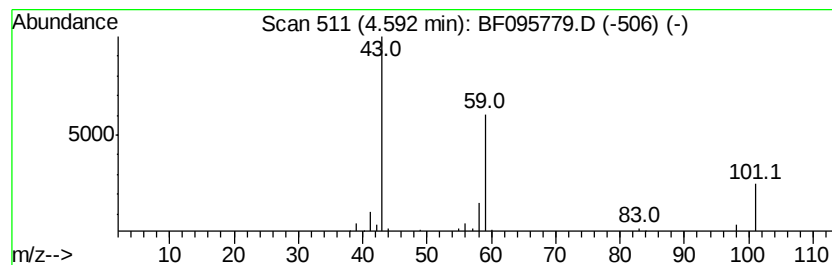
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown4.59 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.59	11.09 ng	212517	1,4-Dichlorobenzene-d4	7.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	9



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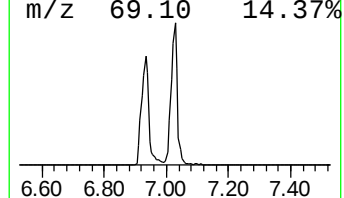
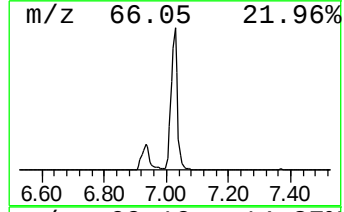
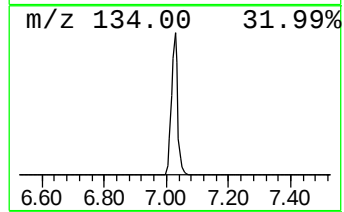
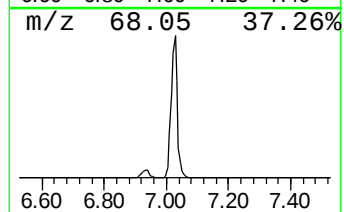
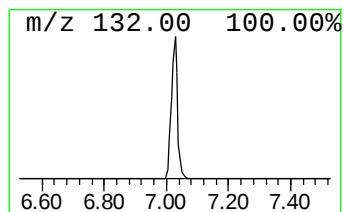
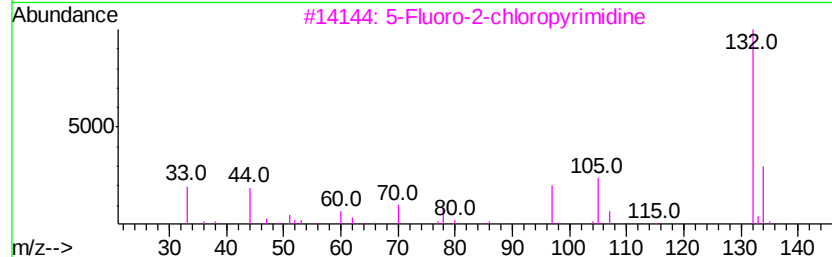
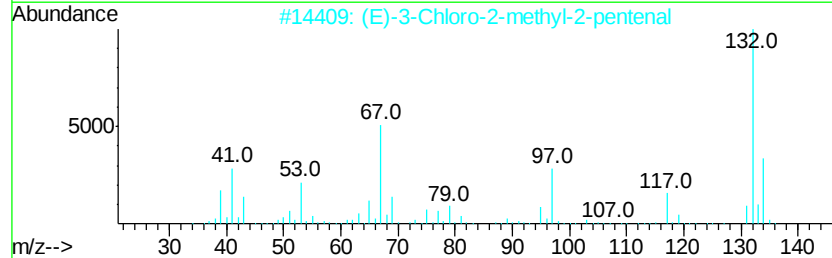
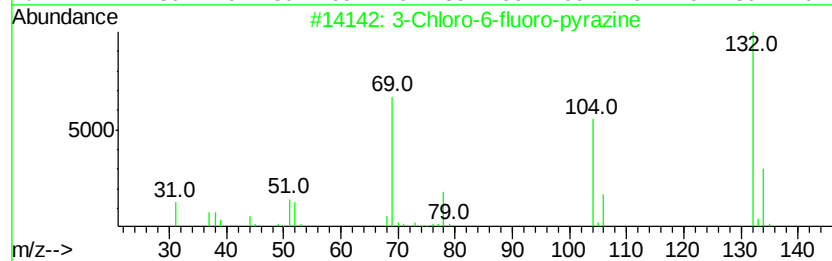
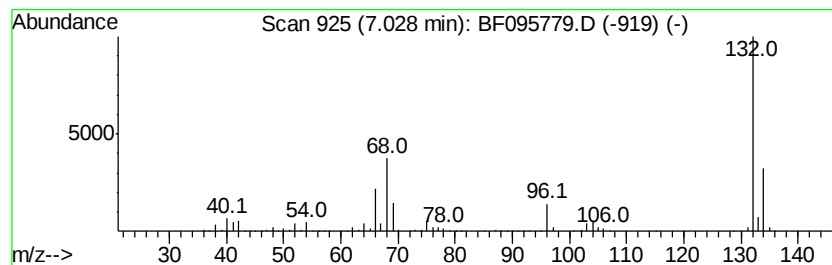
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.03 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	122.15 ng	2339690	1,4-Dichlorobenzene-d4	7.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		Xenon	132	Xe	007440-63-3	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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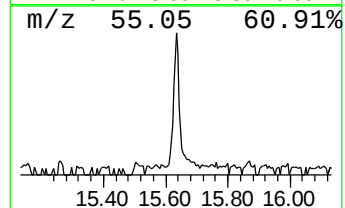
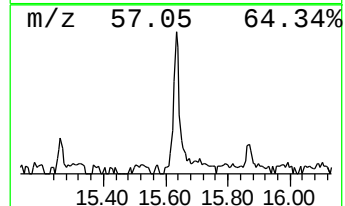
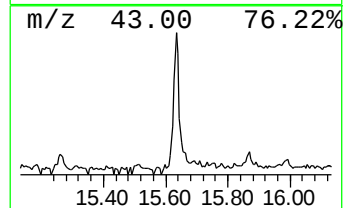
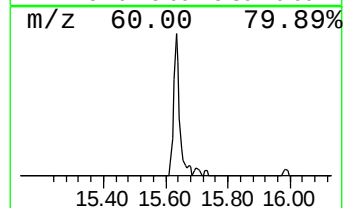
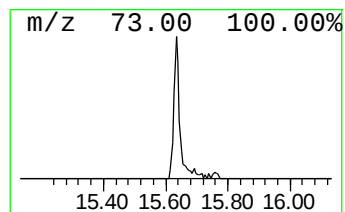
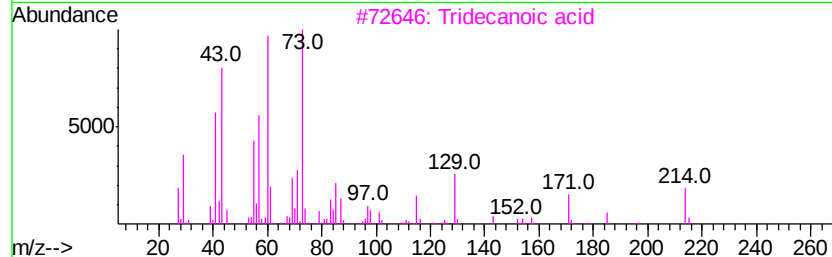
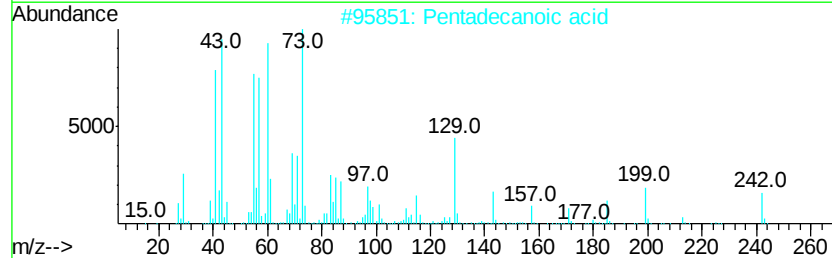
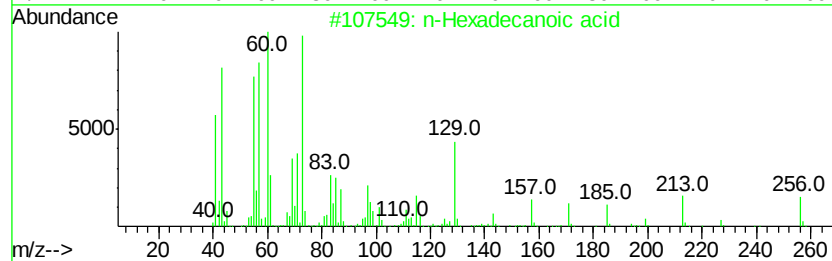
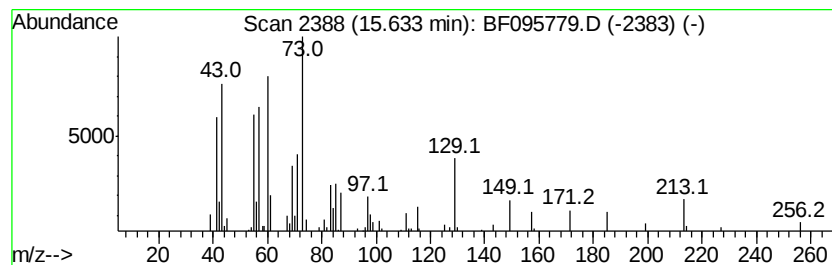
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	4.80 ng	146104	Phenanthrene-d10	14.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
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	86
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25



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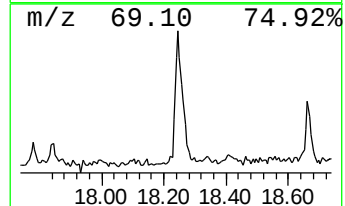
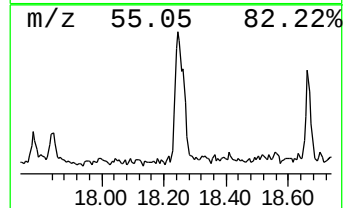
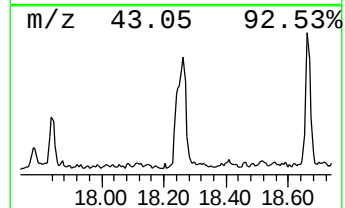
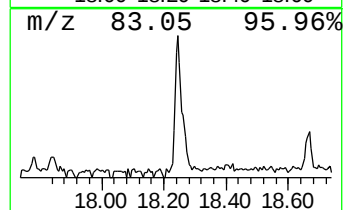
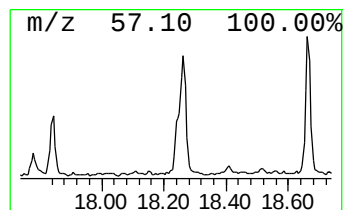
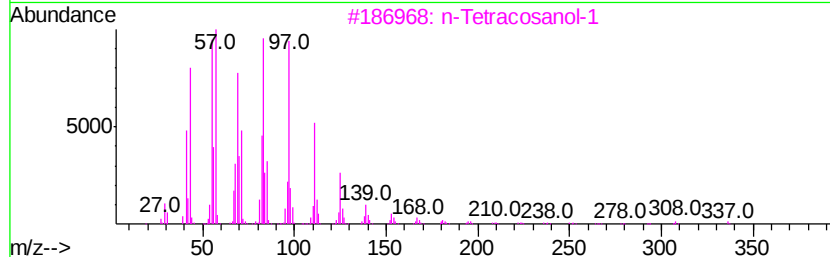
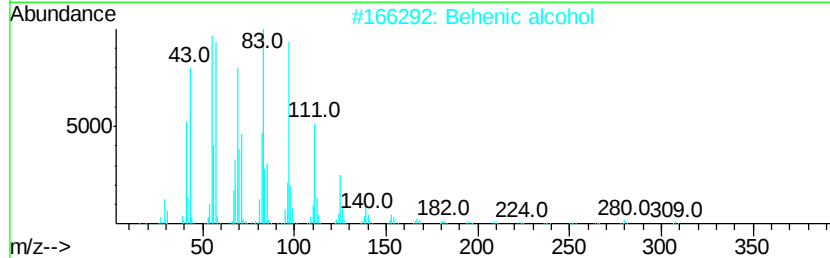
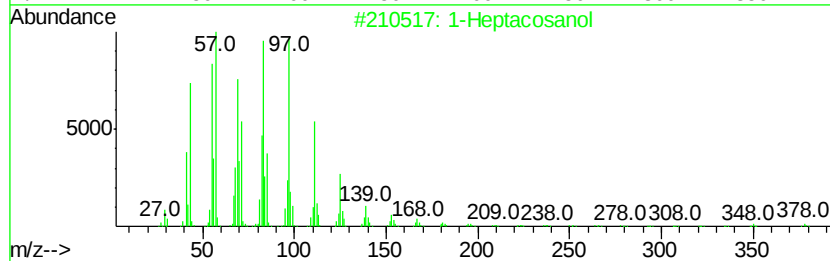
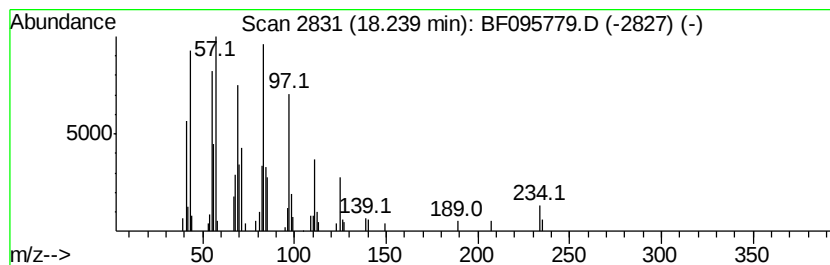
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heptacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.24	3.60 ng	113059	Chrysene-d12	18.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	94



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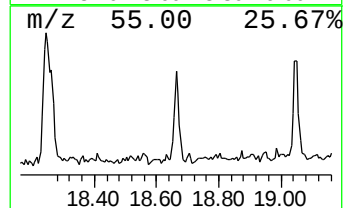
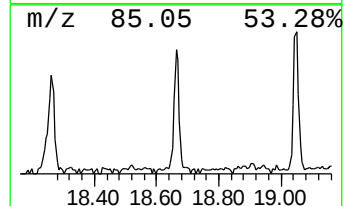
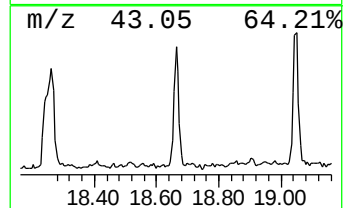
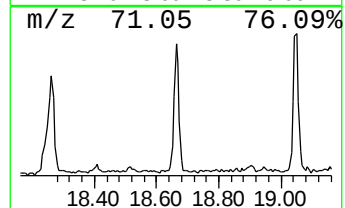
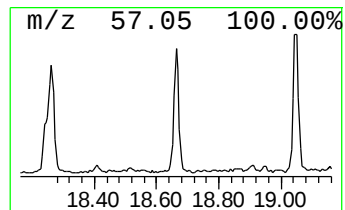
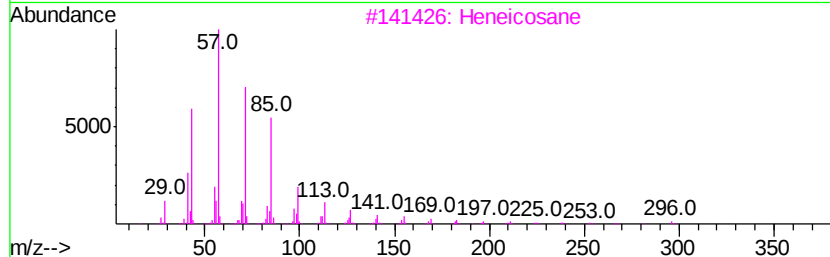
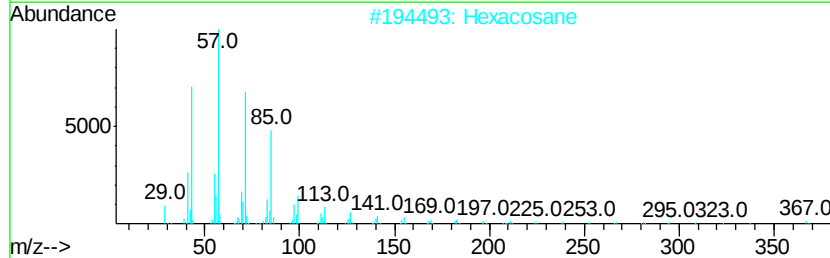
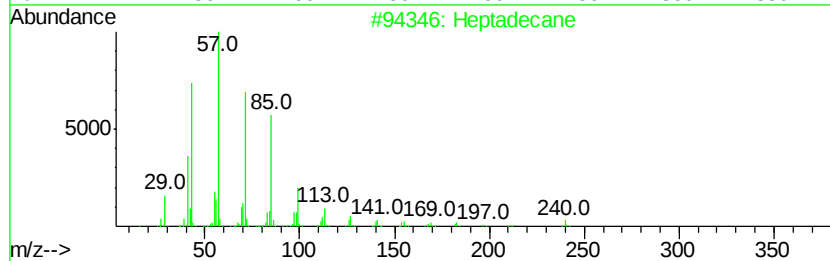
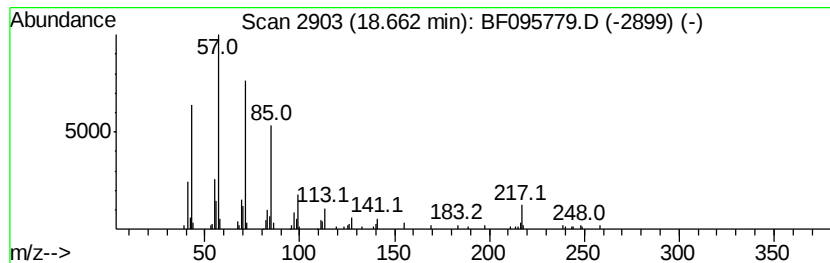
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ClientSampleId :
SB-2(0-2)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.66	4.11 ng	129160	Chrysene-d12	18.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	96
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Docosane	310	C22H46	000629-97-0	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
Data File : BF095779.D
Acq On : 8 Jun 2017 12:52
Operator : SJ/MA
Sample : I3469-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2(0-2)20170603

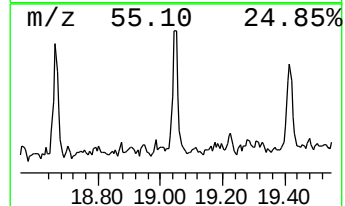
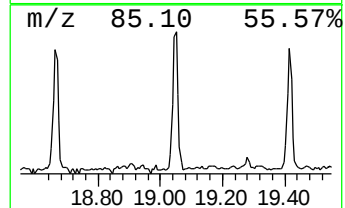
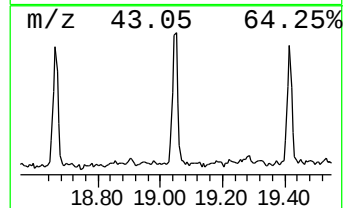
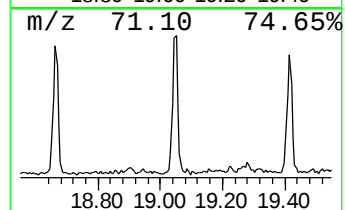
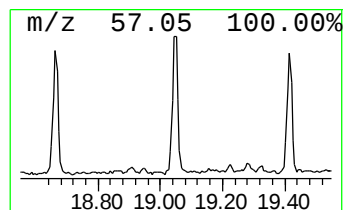
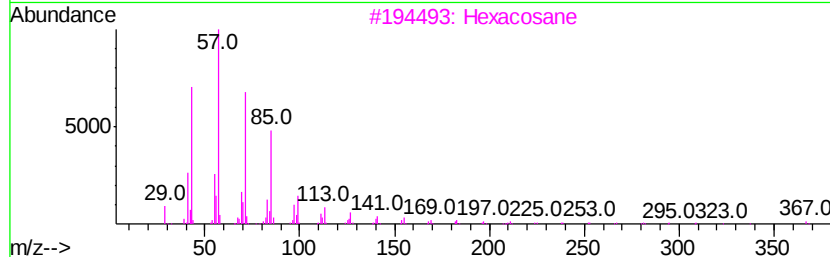
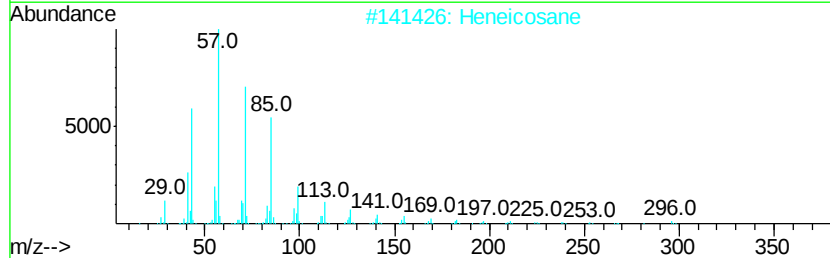
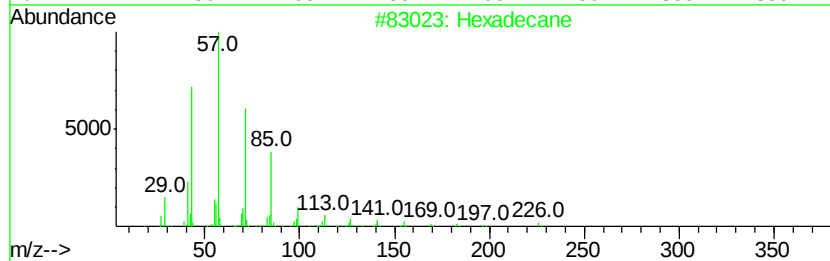
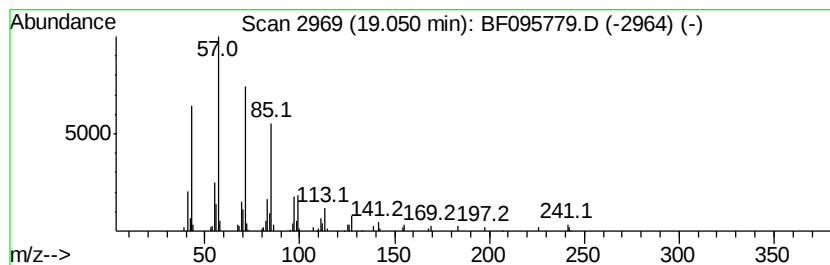
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.05	4.68 ng	147230	Chrysene-d12	18.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	95
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Heptadecane	240	C17H36	000629-78-7	91
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095779.D
Acq On : 8 Jun 2017 12:52
Operator : SJ/MA
Sample : I3469-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2(0-2)20170603

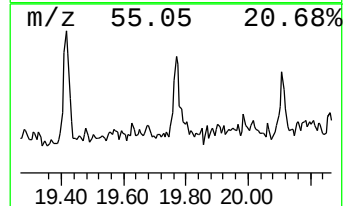
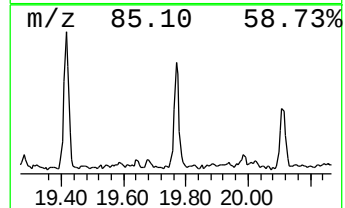
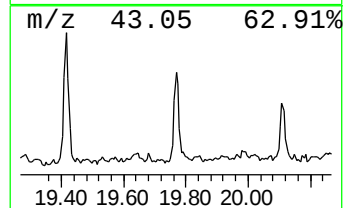
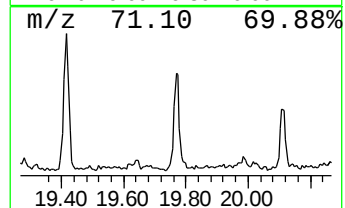
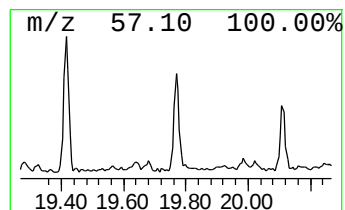
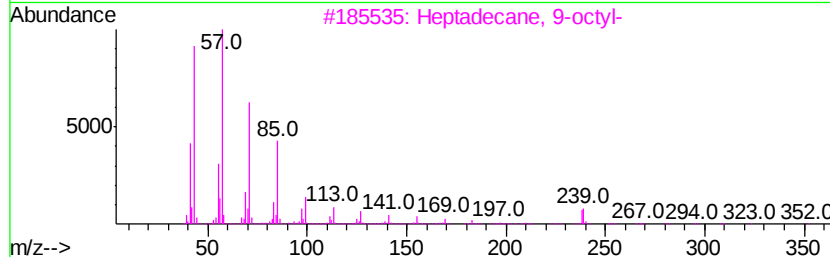
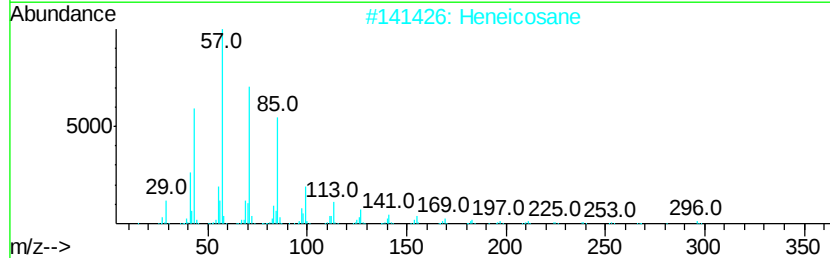
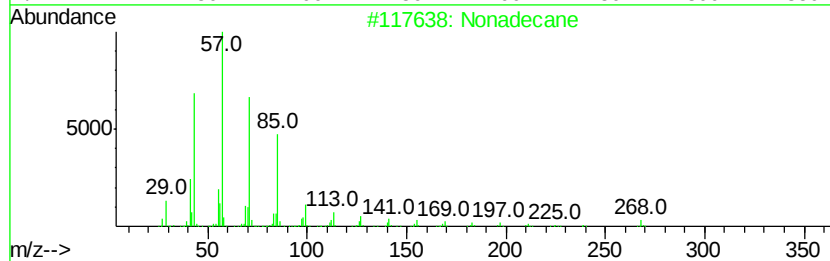
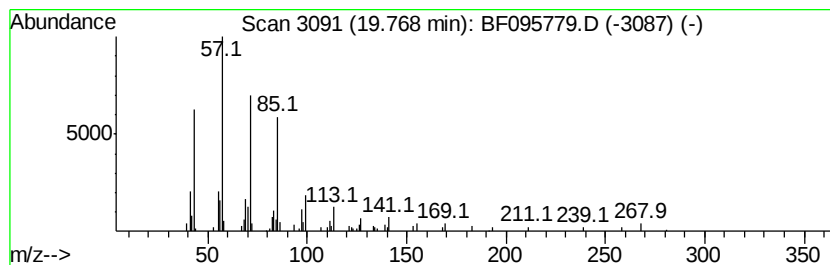
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.77	3.91 ng	91553	Perylene-d12	20.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	95
2		Heneicosane	296	C21H44	000629-94-7	90
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4		Hexacosane	366	C26H54	000630-01-3	90
5		2-methyloctacosane	408	C29H60	1000376-72-8	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
Data File : BF095779.D
Acq On : 8 Jun 2017 12:52
Operator : SJ/MA
Sample : I3469-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-2(0-2)20170603

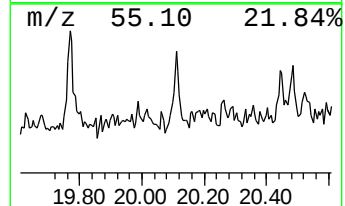
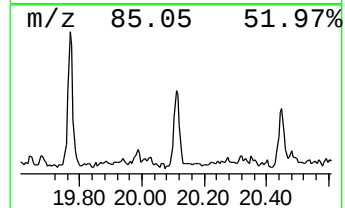
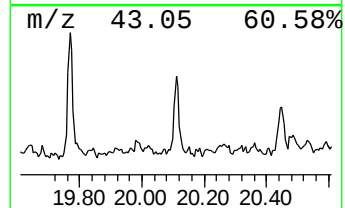
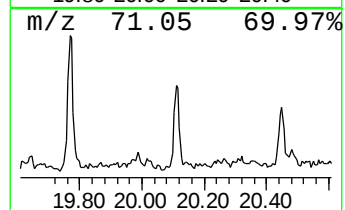
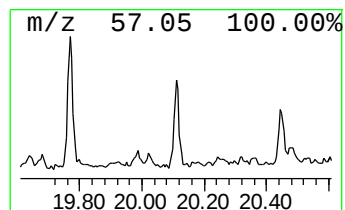
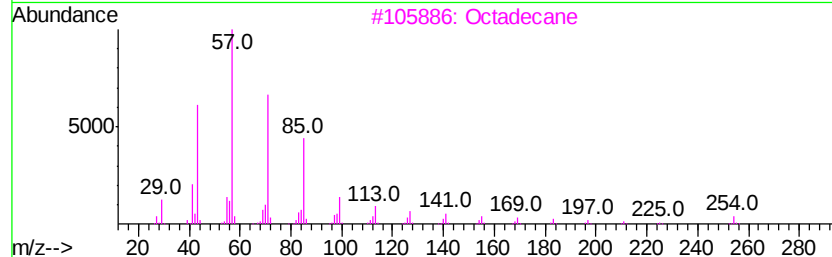
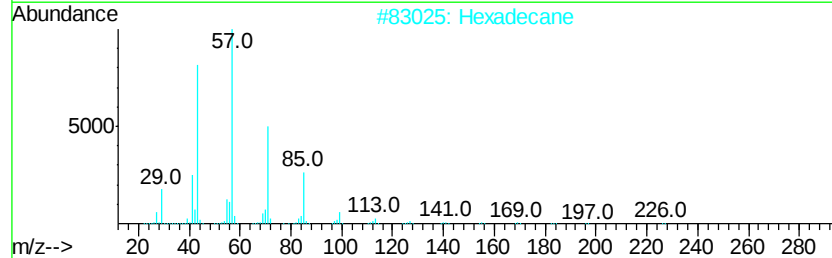
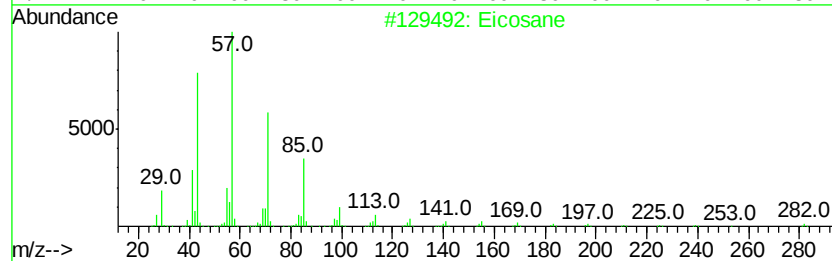
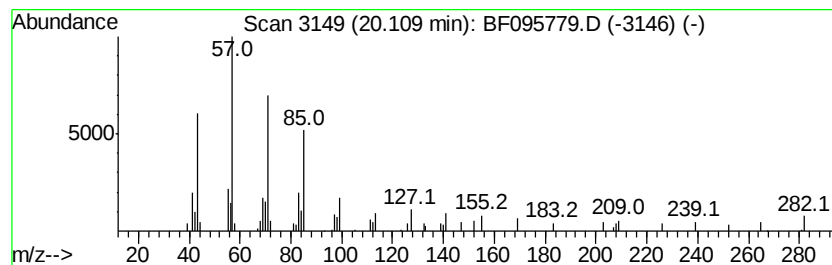
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.11	2.63 ng	61586	Perylene-d12	20.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	97
2		Hexadecane	226	C16H34	000544-76-3	94
3		Octadecane	254	C18H38	000593-45-3	83
4		Hexacosane	366	C26H54	000630-01-3	83
5		Heneicosane	296	C21H44	000629-94-7	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095779.D
Acq On : 8 Jun 2017 12:52
Operator : SJ/MA
Sample : I3469-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2(0-2)20170603

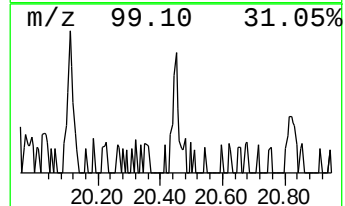
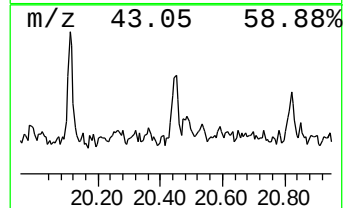
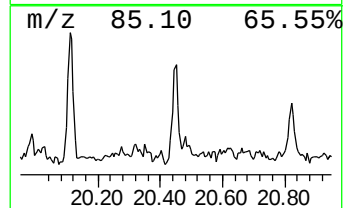
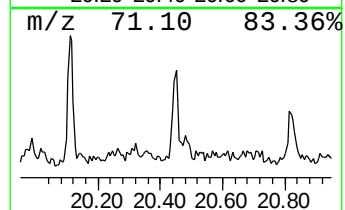
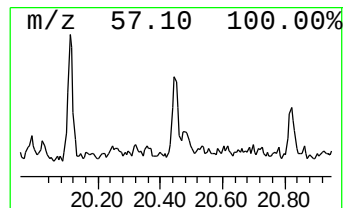
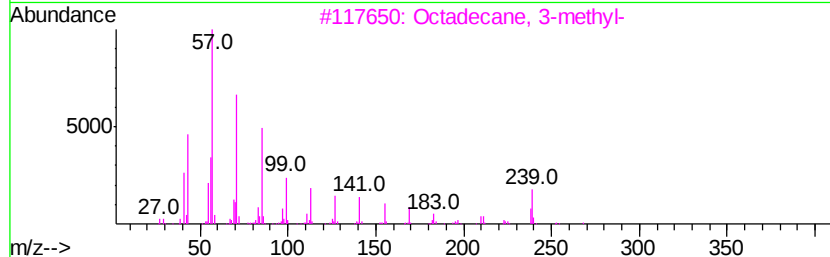
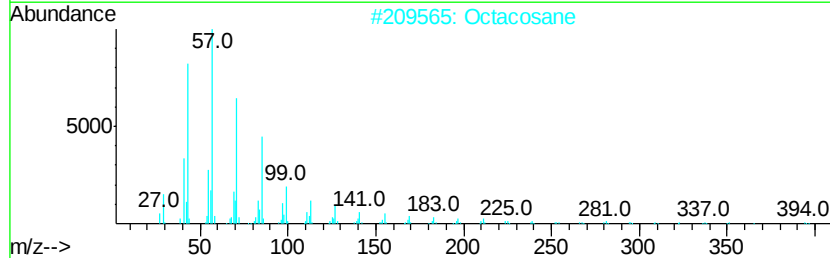
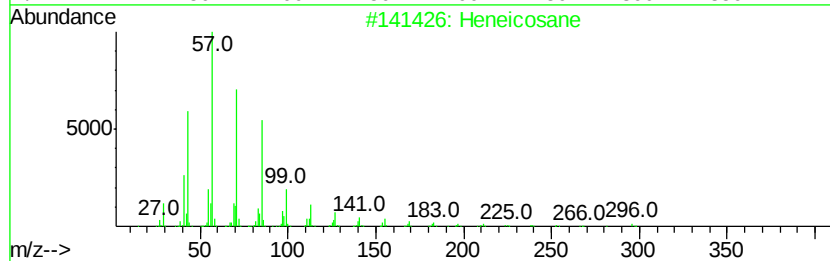
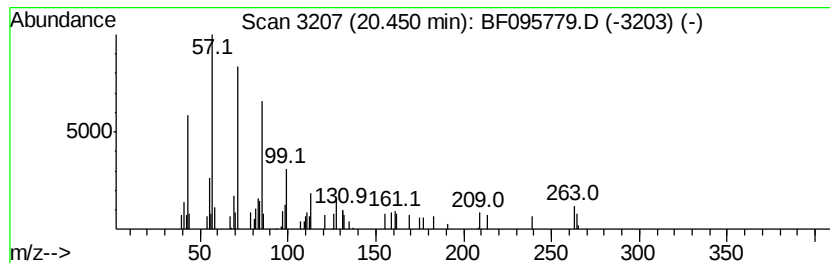
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.45	2.16 ng	50588	Perylene-d12	20.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	72
2			Octacosane	394	C28H58	000630-02-4	64
3			Octadecane, 3-methyl-	268	C19H40	006561-44-0	59
4			Heptadecane	240	C17H36	000629-78-7	59
5			Tetracosane	338	C24H50	000646-31-1	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
Data File : BF095779.D
Acq On : 8 Jun 2017 12:52
Operator : SJ/MA
Sample : I3469-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-2(0-2)20170603

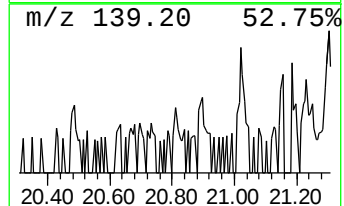
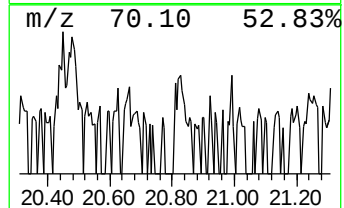
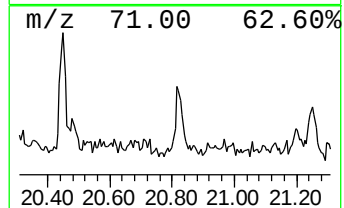
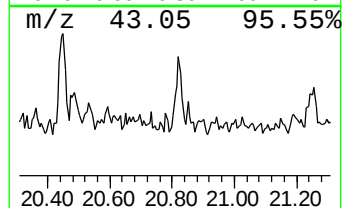
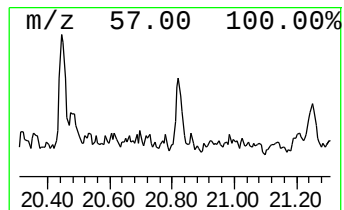
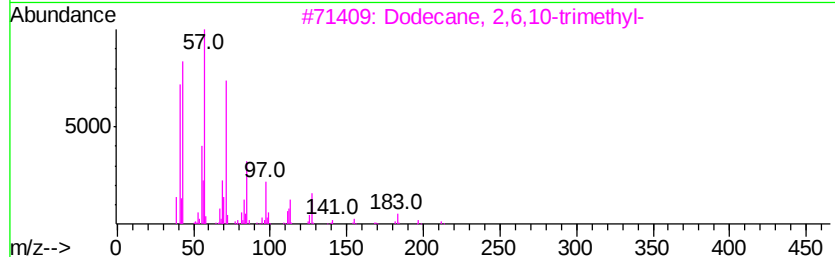
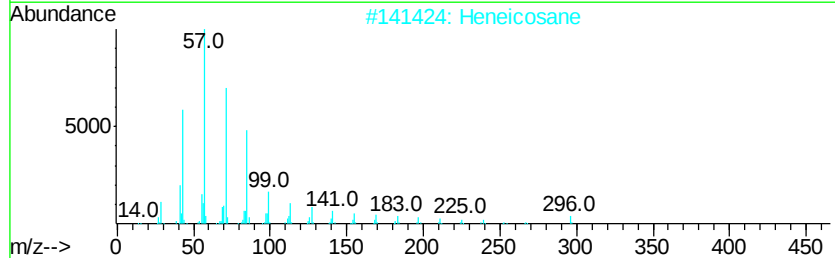
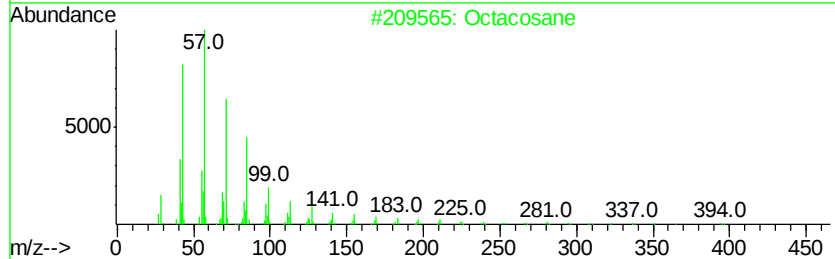
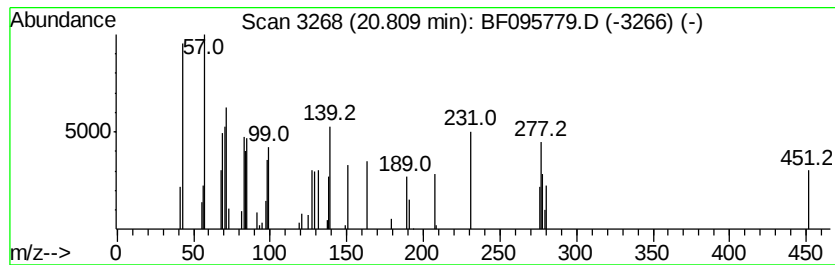
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Octacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.81	2.10 ng	49251	Perylene-d12	20.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	50
2			Heneicosane	296	C21H44	000629-94-7	47
3			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	47
4			Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	47
5			Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095779.D
Acq On : 8 Jun 2017 12:52
Operator : SJ/MA
Sample : I3469-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-2(0-2)20170603

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
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unknown7.03	7.03	122.2	ng	2339690	1	7.37	383100	20.0
n-Hexadecanoic acid	15.63	4.8	ng	146104	4	14.62	608522	20.0
1-Heptacosanol	18.24	3.6	ng	113059	5	18.33	628561	20.0
Heptadecane	18.66	4.1	ng	129160	5	18.33	628561	20.0
Hexadecane	19.05	4.7	ng	147230	5	18.33	628561	20.0
Nonadecane	19.77	3.9	ng	91553	6	20.00	468302	20.0
Eicosane	20.11	2.6	ng	61586	6	20.00	468302	20.0
Heneicosane	20.45	2.2	ng	50588	6	20.00	468302	20.0
Octacosane	20.81	2.1	ng	49251	6	20.00	468302	20.0