

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
 Data File : BF096160.D
 Acq On : 23 Jun 2017 15:29
 Operator : SJ/MA
 Sample : I3776-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GHD-GW-01

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	1.540	7	9	47	rVB	980378	1945980	87.63%	10.547%
2	4.434	498	501	514	rBV	28428	79875	3.60%	0.433%
3	5.151	620	623	654	rBV	241464	780021	35.13%	4.227%
4	6.851	909	912	920	rBV	162641	374819	16.88%	2.031%
5	6.916	920	923	944	rVB	857648	1681040	75.70%	9.111%
6	7.257	978	981	995	rBV	233505	350197	15.77%	1.898%
7	7.492	1014	1021	1039	rBV	986291	1425077	64.17%	7.723%
8	8.181	1134	1138	1162	rBV	626848	1086856	48.94%	5.890%
9	8.610	1206	1211	1216	rBV	24441	37659	1.70%	0.204%
10	9.198	1308	1311	1319	rBV4	15565	32042	1.44%	0.174%
11	9.292	1323	1327	1339	rVV	331017	512240	23.07%	2.776%
12	9.410	1342	1347	1356	rVB3	20389	33932	1.53%	0.184%
13	10.098	1456	1464	1470	rBV3	65548	175140	7.89%	0.949%
14	10.151	1470	1473	1482	rVB	57587	100376	4.52%	0.544%
15	11.075	1624	1630	1640	rVB	1640209	2220646	100.00%	12.035%
16	11.669	1728	1731	1737	rVB3	18972	24611	1.11%	0.133%
17	11.774	1746	1749	1764	rVB	47880	86091	3.88%	0.467%
18	12.110	1802	1806	1813	rBV2	430765	571059	25.72%	3.095%
19	12.686	1899	1904	1910	rBV2	47469	69830	3.14%	0.378%
20	12.845	1926	1931	1936	rBV	57919	76218	3.43%	0.413%
21	13.327	2009	2013	2017	rBV2	18078	24867	1.12%	0.135%
22	13.410	2022	2027	2041	rBV	783971	1204493	54.24%	6.528%
23	13.657	2065	2069	2076	rBV	72810	105025	4.73%	0.569%
24	13.739	2079	2083	2085	rVV4	17500	26441	1.19%	0.143%
25	14.504	2209	2213	2226	rVB2	440349	606124	27.29%	3.285%
26	15.557	2382	2392	2403	rBV4	253693	509027	22.92%	2.759%
27	16.651	2573	2578	2580	rBV	90100	109178	4.92%	0.592%
28	16.745	2590	2594	2598	rVB	62592	72876	3.28%	0.395%
29	16.898	2614	2620	2624	rBV	1619829	2051981	92.40%	11.121%
30	17.021	2637	2641	2647	rBV	276530	366023	16.48%	1.984%
31	17.751	2762	2765	2768	rVB	24677	25085	1.13%	0.136%
32	17.933	2793	2796	2802	rVB4	18880	23303	1.05%	0.126%
33	18.156	2830	2834	2839	rBV4	75379	116339	5.24%	0.631%
34	18.245	2843	2849	2857	rBV2	492698	796821	35.88%	4.318%

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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	18.315	2858	2861	2866	rVB2	26437	37083	1.67%	0.201%
36	18.950	2966	2969	2977	rVB2	22326	31768	1.43%	0.172%
37	19.286	3021	3026	3030	rBV	52039	79109	3.56%	0.429%
38	19.321	3030	3032	3036	rVB3	21393	22228	1.00%	0.120%
39	19.680	3088	3093	3097	rBV2	19360	24893	1.12%	0.135%
40	19.921	3130	3134	3147	rBV	260850	401735	18.09%	2.177%
41	20.015	3147	3150	3155	rVB2	22100	27360	1.23%	0.148%
42	20.233	3183	3187	3194	rBV5	15623	30189	1.36%	0.164%
43	20.350	3203	3207	3210	rBV	22447	25841	1.16%	0.140%
44	20.709	3264	3268	3276	rVB5	17689	40233	1.81%	0.218%
45	21.115	3331	3337	3344	rBV5	14166	29666	1.34%	0.161%

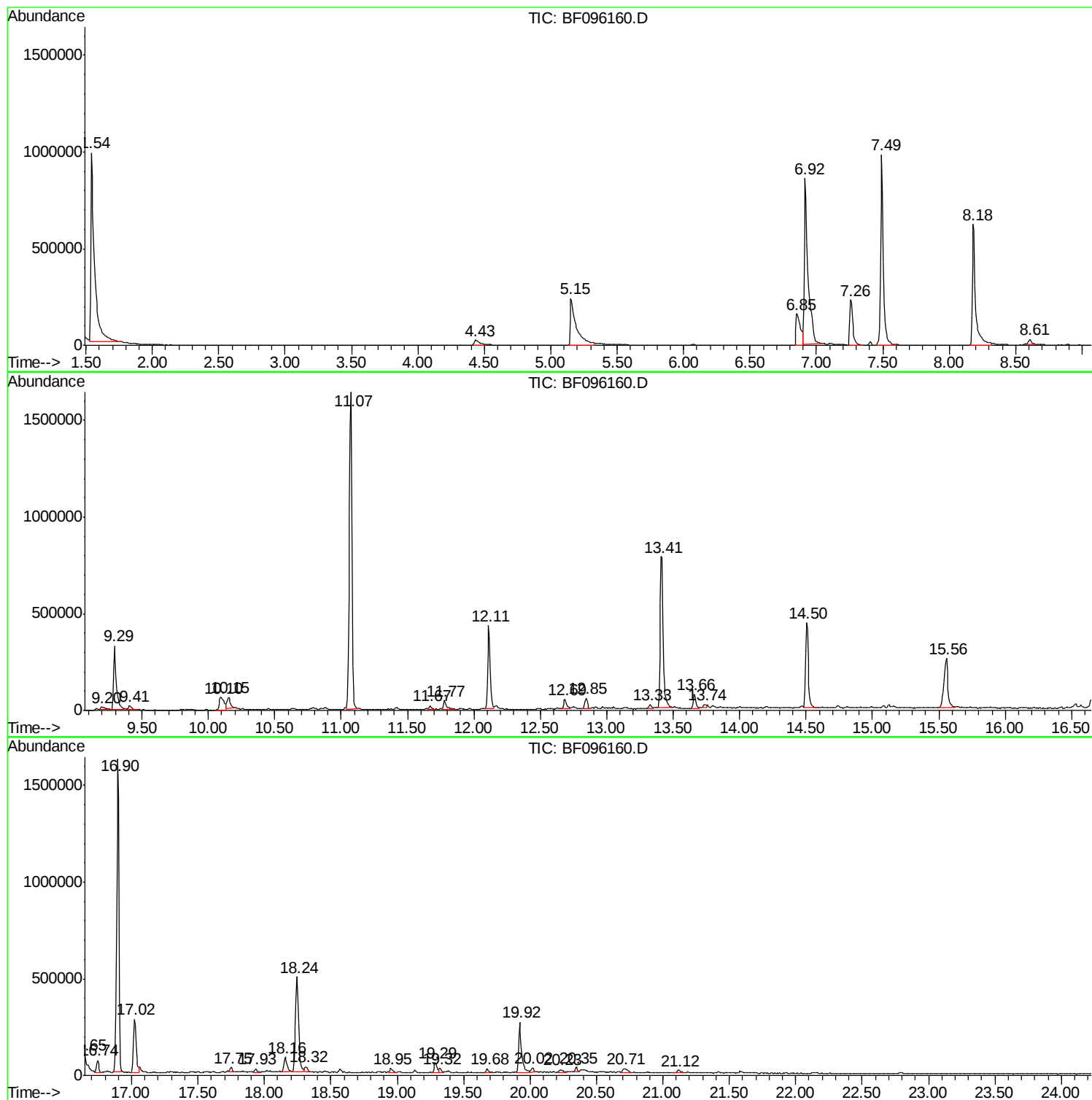
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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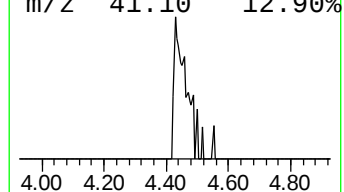
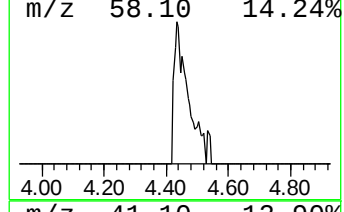
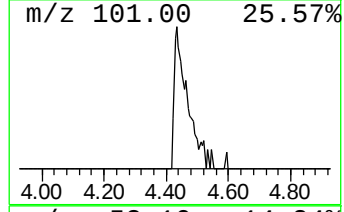
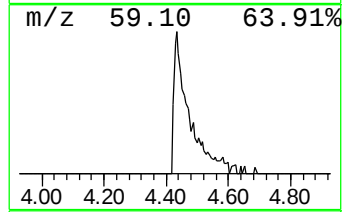
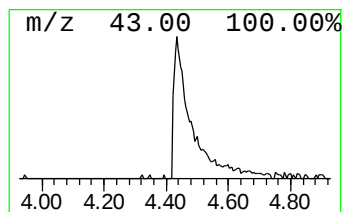
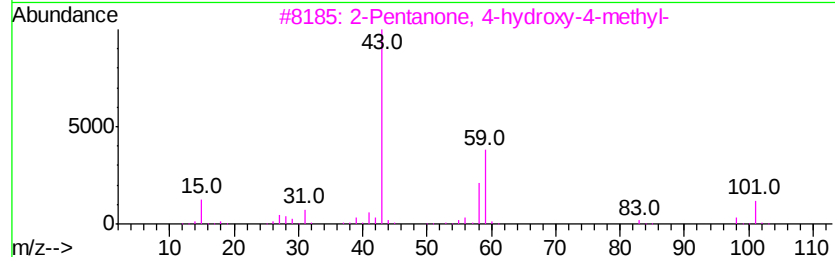
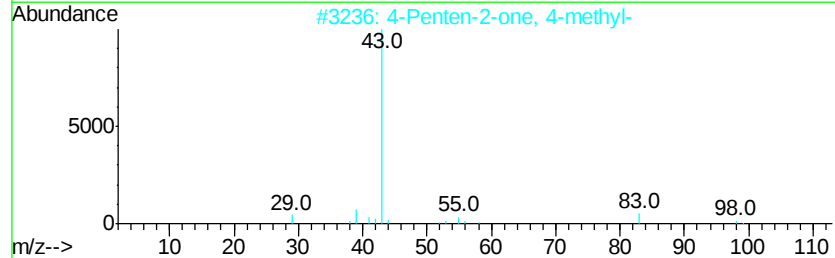
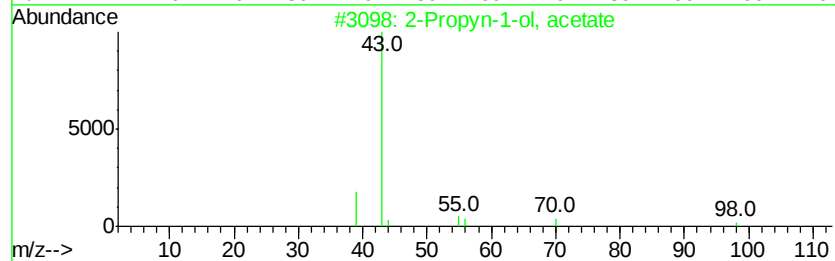
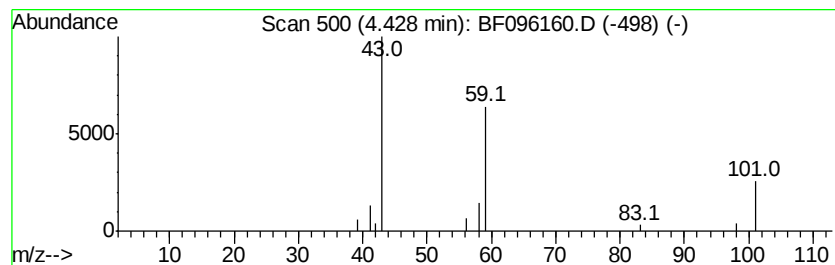
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown4.43 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.43	4.56 ng	79875	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
2		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
3		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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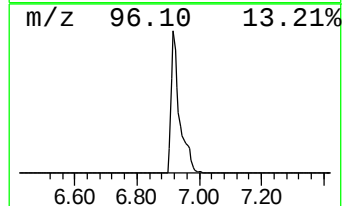
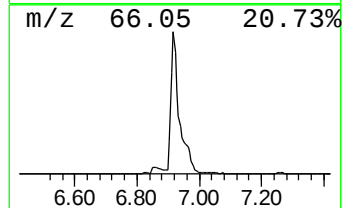
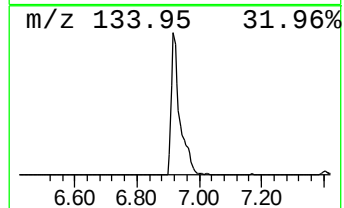
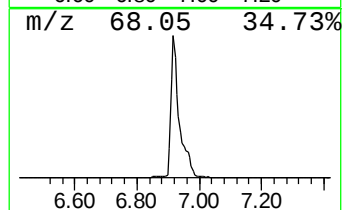
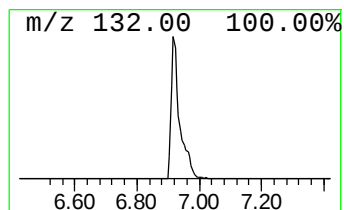
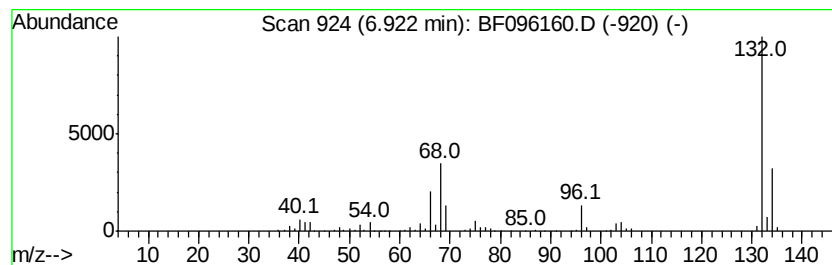
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.92 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.92	96.01 ng	1681040	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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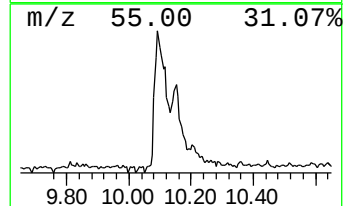
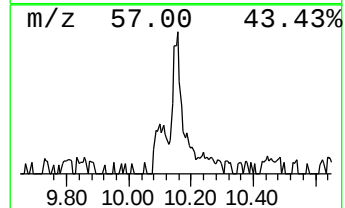
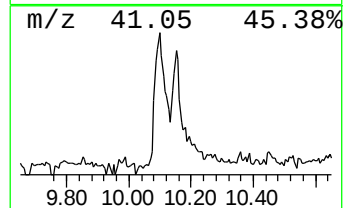
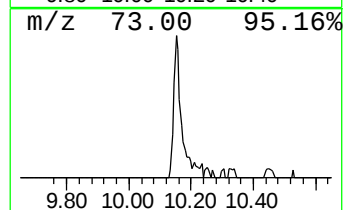
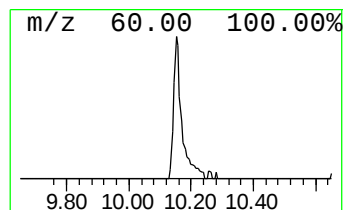
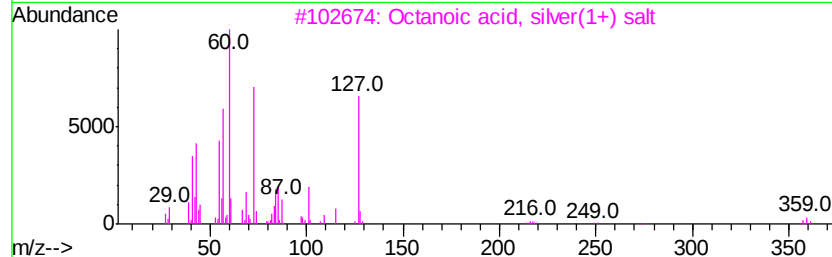
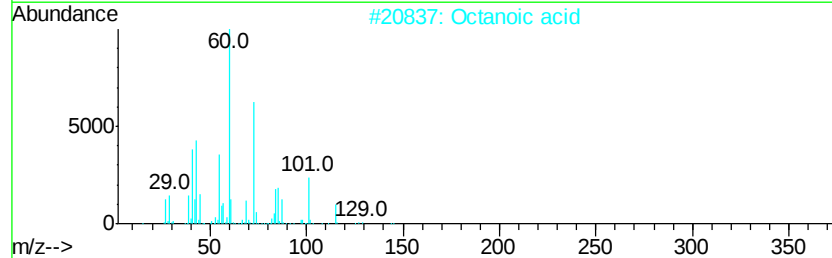
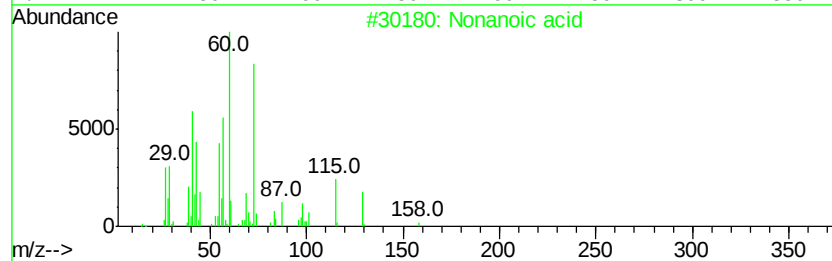
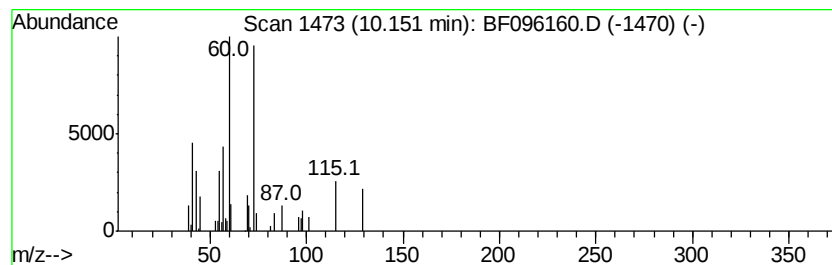
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Nonanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.15	3.92 ng	100376	Naphthalene-d8	9.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanoic acid	158	C9H18O2	000112-05-0	78
2		Octanoic acid	144	C8H16O2	000124-07-2	50
3		Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	40
4		Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	38
5		Hexanoic acid	116	C6H12O2	000142-62-1	38



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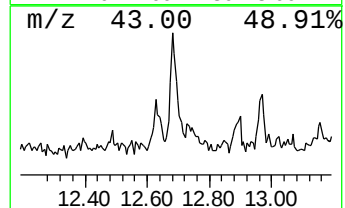
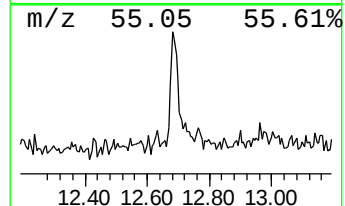
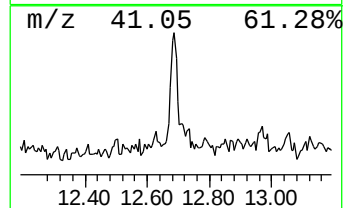
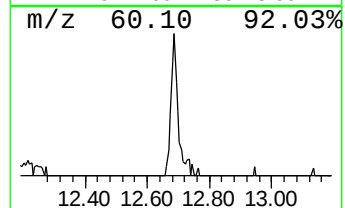
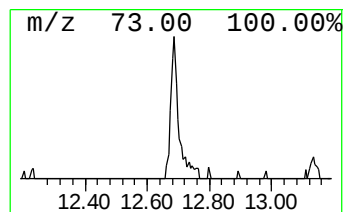
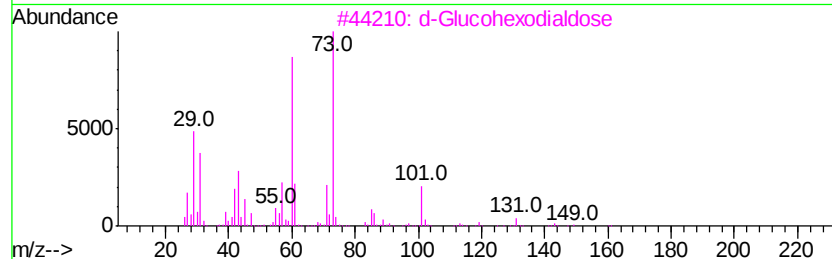
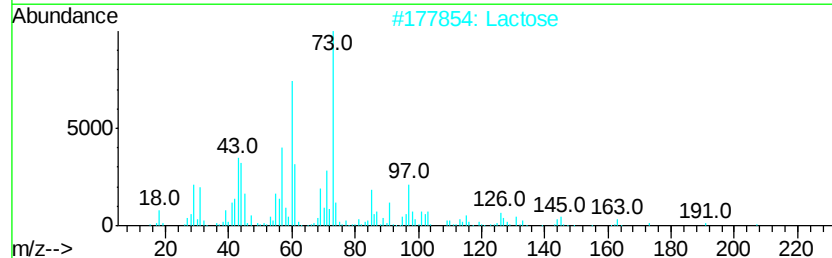
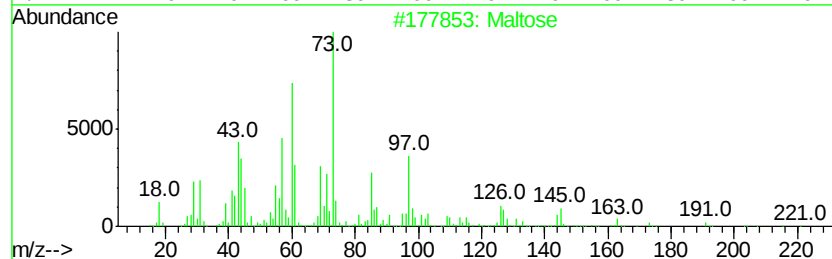
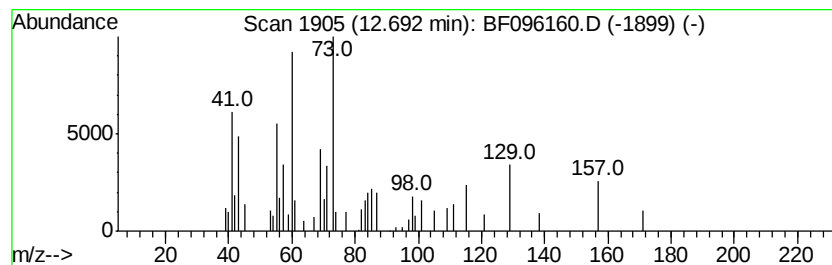
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown12.69 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	2.45 ng	69830	Acenaphthene-d10	12.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Maltose	342	C12H22O11	000069-79-4	47
2		Lactose	342	C12H22O11	000063-42-3	38
3		d-Glucohexodialdose	178	C6H10O6	1000149-19-1	38
4		Octanoic acid	144	C8H16O2	000124-07-2	38
5		.alpha.-d-Riboside, 1-O-dodecyl-	318	C17H34O5	1000154-76-8	37



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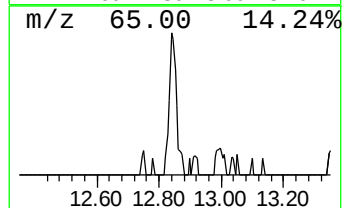
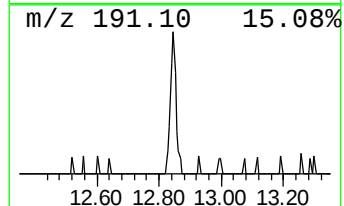
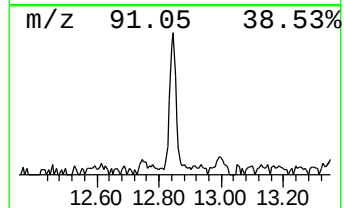
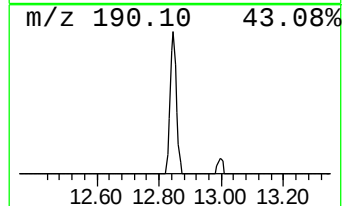
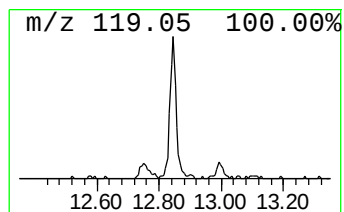
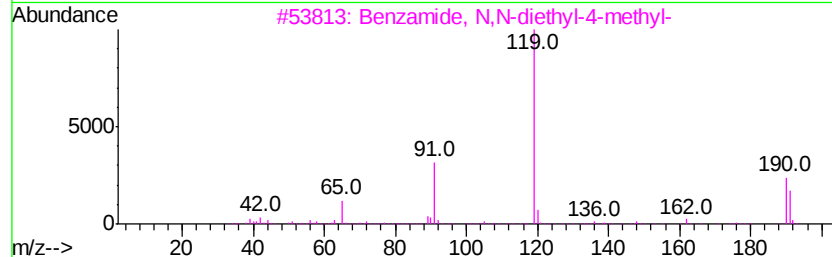
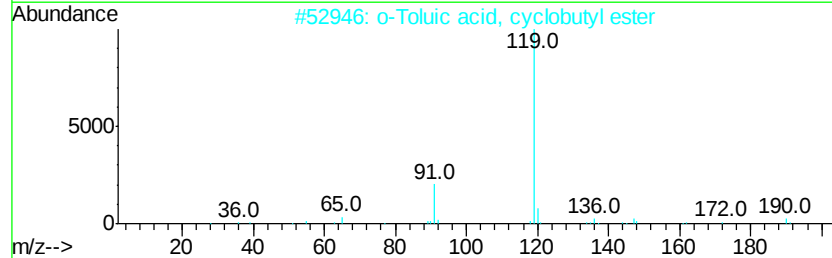
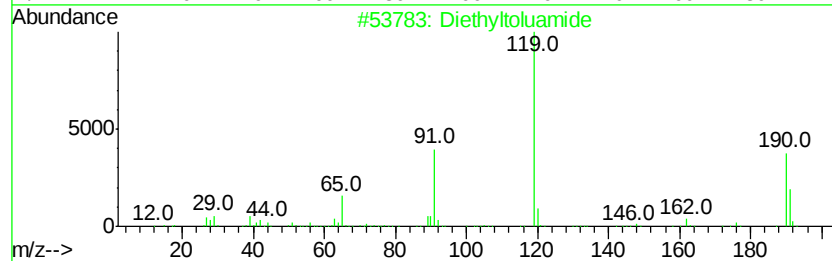
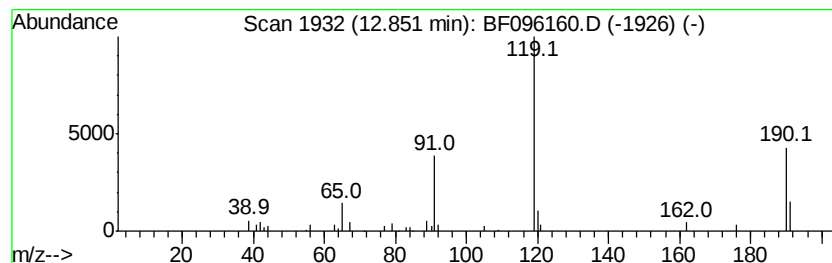
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 8 Diethyltoluamide Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	2.67 ng	76218	Acenaphthene-d10	12.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethyltoluamide	191	C12H17NO	000134-62-3	94
2		o-Toluic acid, cyclobutyl ester	190	C12H14O2	1000292-22-3	80
3		Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	80
4		4-Oxo-4-(para-tolyl)-butyric acid	192	C11H12O3	004619-20-9	64
5		(+)-di-O-4-Toluoyl-D-tartaric acid	386	C20H18O8	032634-68-7	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062317\
Data File : BF096160.D
Acq On : 23 Jun 2017 15:29
Operator : SJ/MA
Sample : I3776-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
GHD-GW-01

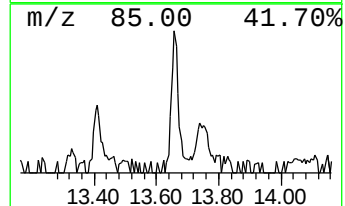
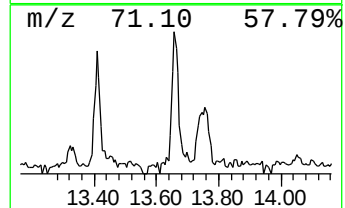
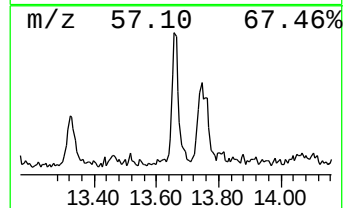
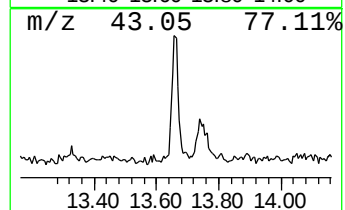
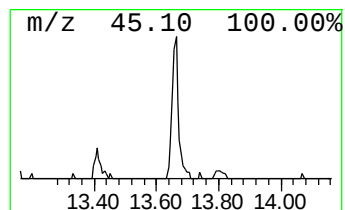
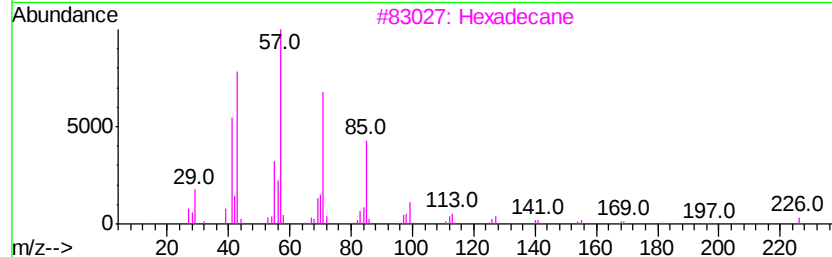
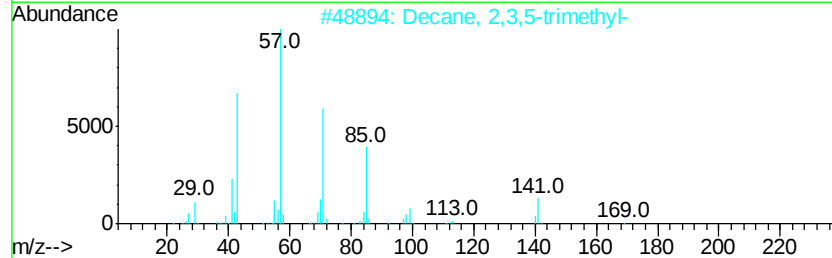
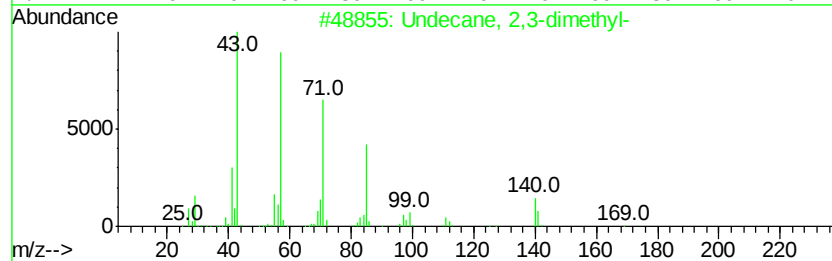
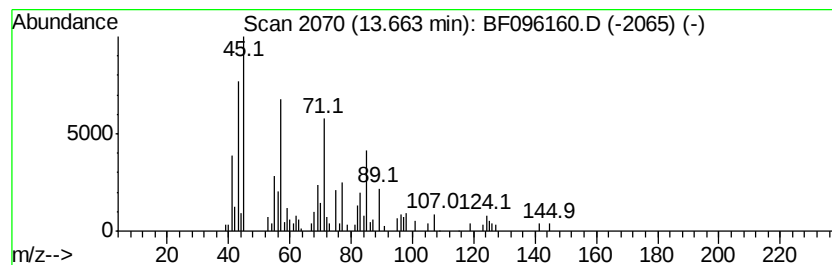
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.66 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	3.47 ng	105025	Phenanthrene-d10	14.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	27
2		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	27
3		Hexadecane	226	C16H34	000544-76-3	27
4		Octane, 4-methyl-	128	C9H20	002216-34-4	25
5		Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
Data File : BF096160.D
Acq On : 23 Jun 2017 15:29
Operator : SJ/MA
Sample : I3776-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHD-GW-01

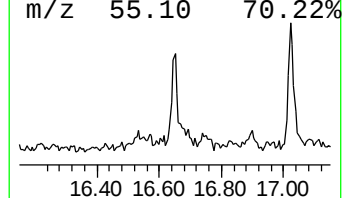
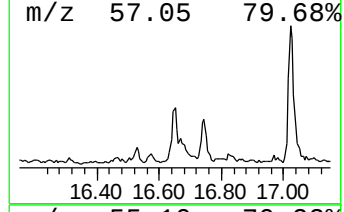
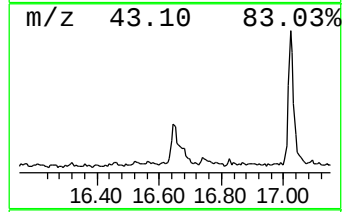
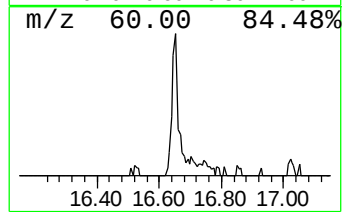
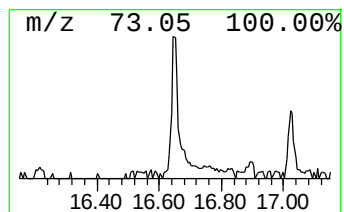
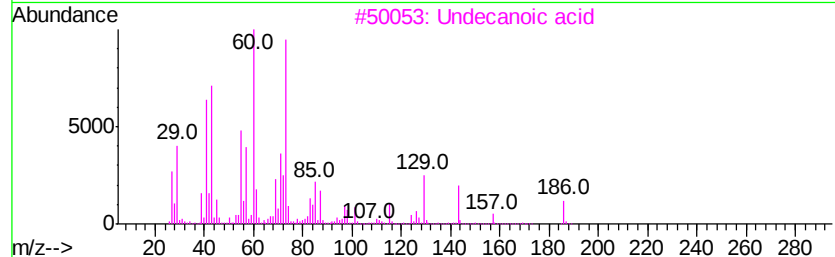
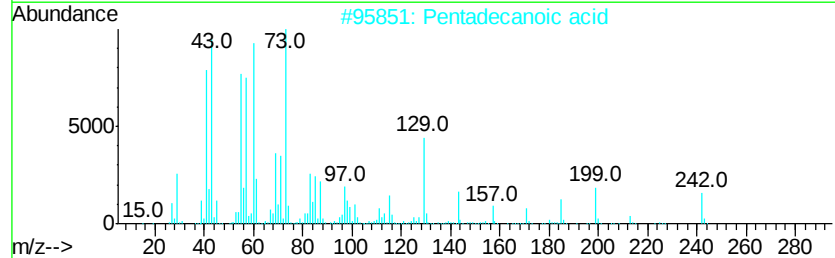
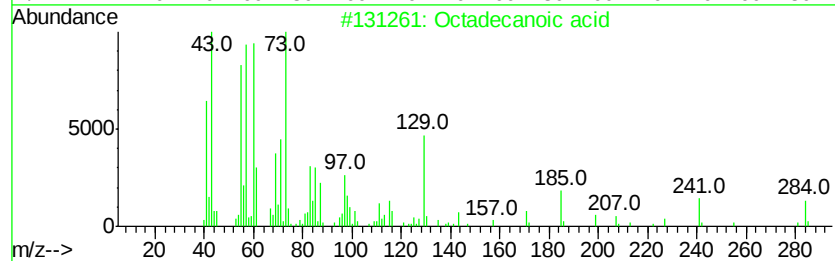
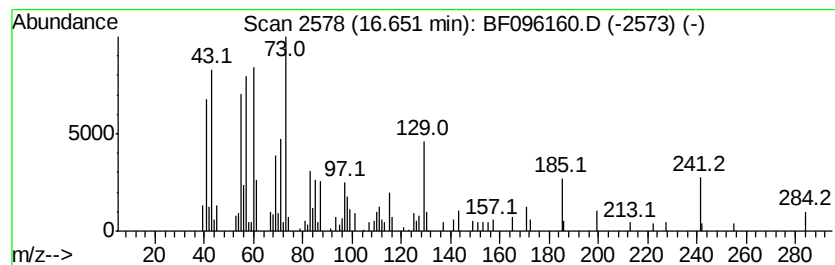
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.65	2.74 ng	109178	Chrysene-d12	18.24

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3			Undecanoic acid	186	C11H22O2	000112-37-8	74
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Tridecanoic acid	214	C13H26O2	000638-53-9	72



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Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\  
Data File : BF096160.D  
Acq On    : 23 Jun 2017  15:29  
Operator  : SJ/MA  
Sample    : I3776-01  
Misc      :  
ALS Vial  : 5      Sample Multiplier: 1
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Instrument :
BNA_F
ClientSampleId :
GHD-GW-01

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

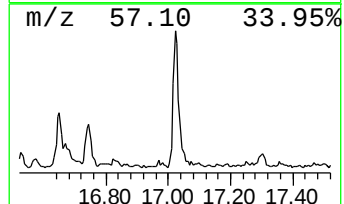
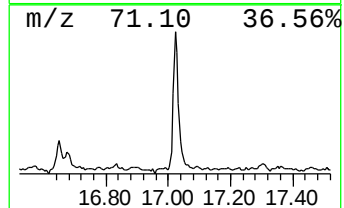
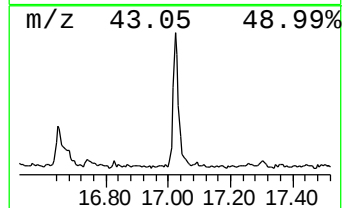
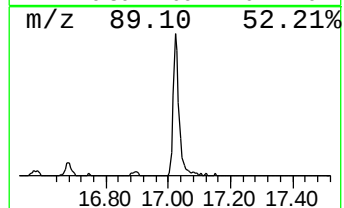
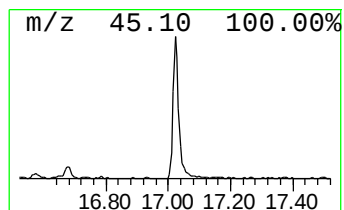
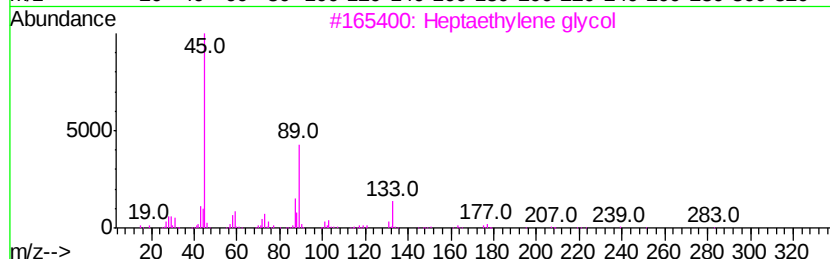
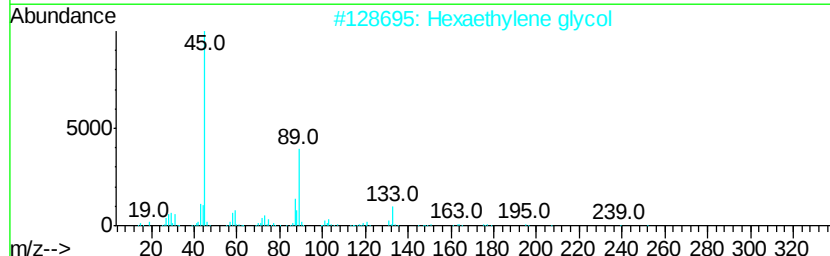
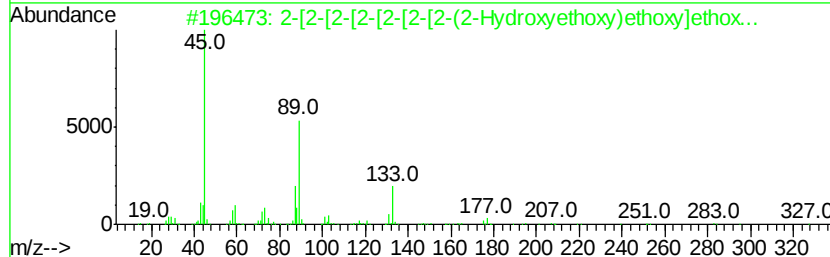
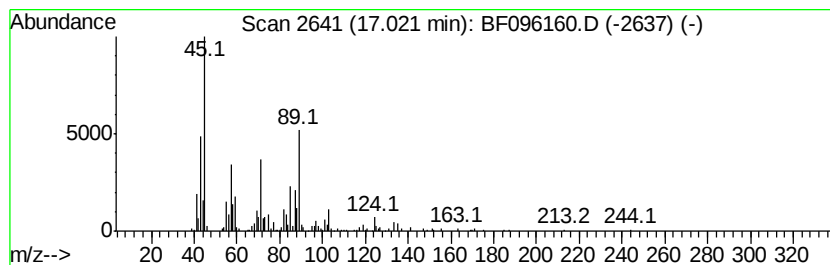
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TIC Integration Parameters: LSCINT.P

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Peak Number 12  2-[2-[2-[2-[2-[2-(2-Hydr...  Concentration Rank 5

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R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.02	9.19 ng	366023	Chrysene-d12	18.24		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-(2-Hydroxvet...	370	C16H3409	005117-19-1	64	
2	Hexaethylene glycol	282	C12H2607	002615-15-8	64	
3	Heptaethylene glycol	326	C14H3008	005617-32-3	64	
4	Pentaethylene glycol	238	C10H2206	004792-15-8	64	
5	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46012	1000352-13-2	64	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062317\
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Acq On : 23 Jun 2017 15:29
Operator : SJ/MA
Sample : I3776-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

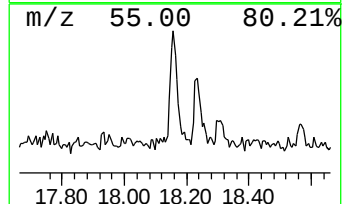
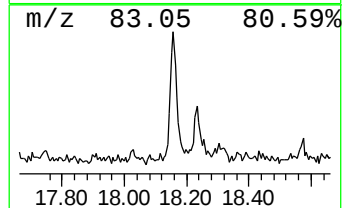
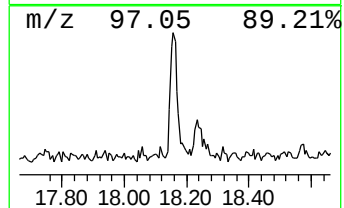
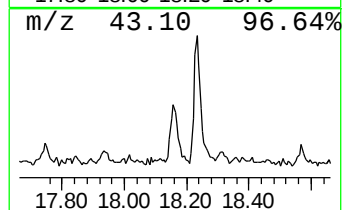
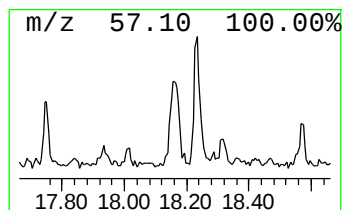
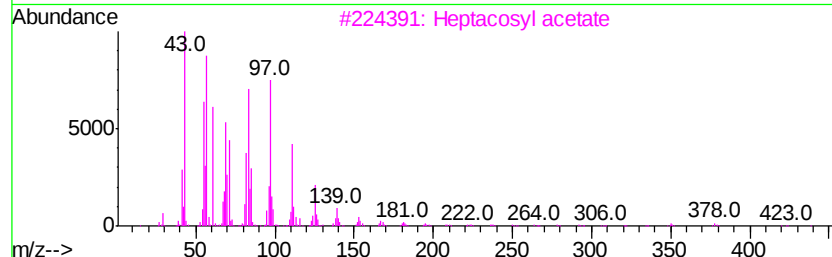
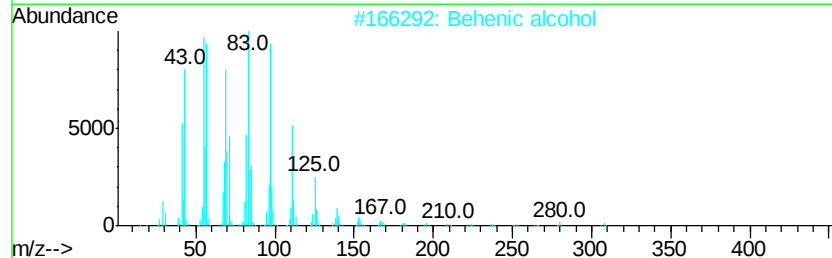
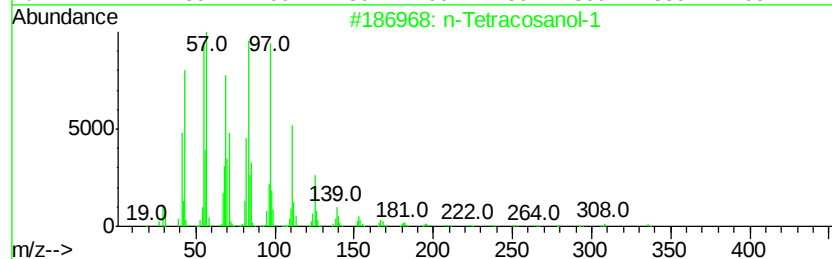
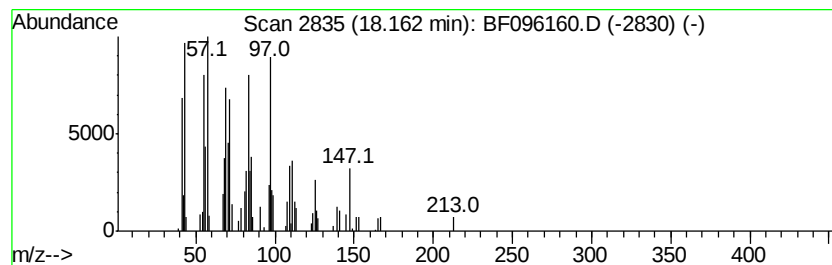
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 n-Tetracosanol-1 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.16	2.92 ng	116339	Chrysene-d12		18.24
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	Heptacosyl acetate	438	C29H58O2	1000351-78-2	90
4	1-Heptacosanol	396	C27H56O	002004-39-9	90
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	81



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
Data File : BF096160.D
Acq On : 23 Jun 2017 15:29
Operator : SJ/MA
Sample : I3776-01
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Instrument :
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ClientSampleId :
GHD-GW-01

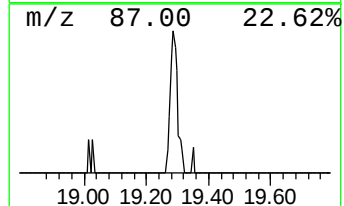
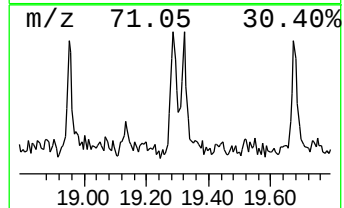
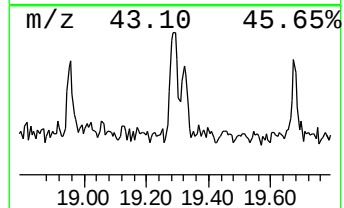
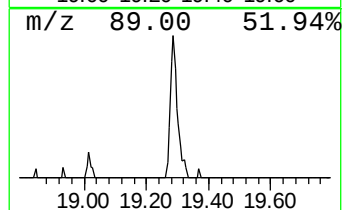
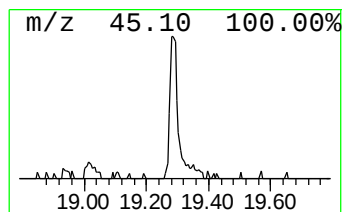
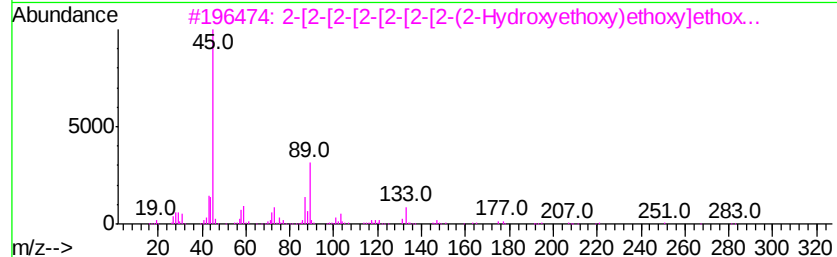
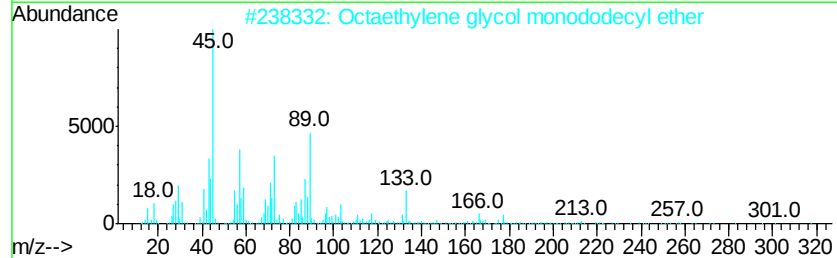
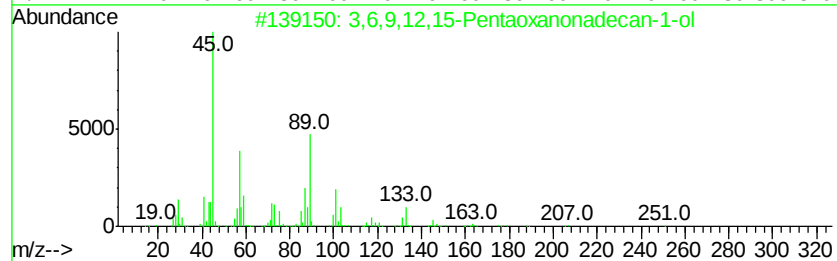
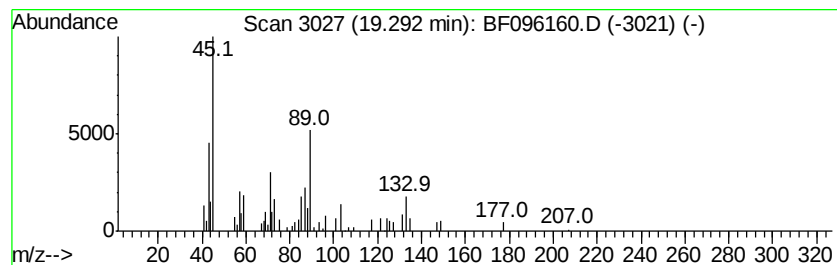
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 3,6,9,12,15-Pentaoxanonadec... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.29	3.94 ng	79109	Perylene-d12	19.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	90		
2	Octaethylene glycol monododecyl ...	538	C28H58O9	003055-98-9	87		
3	2-[2-[2-[2-[2-[2-(2-Hydroxyvet...	370	C16H34O9	005117-19-1	80		
4	Heptaethylene glycol	326	C14H30O8	005617-32-3	72		
5	Hexaethylene glycol	282	C12H26O7	002615-15-8	72		



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
Data File : BF096160.D
Acq On : 23 Jun 2017 15:29
Operator : SJ/MA
Sample : I3776-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
GHD-GW-01

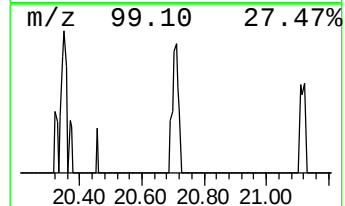
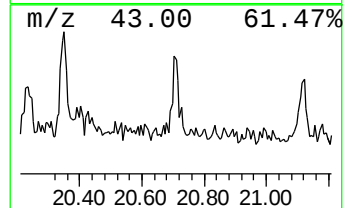
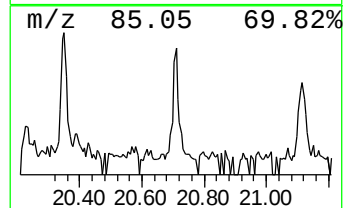
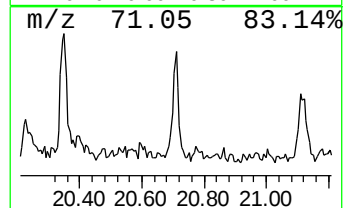
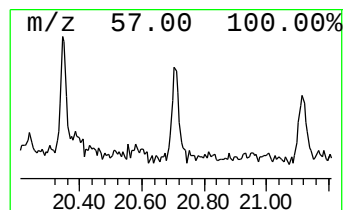
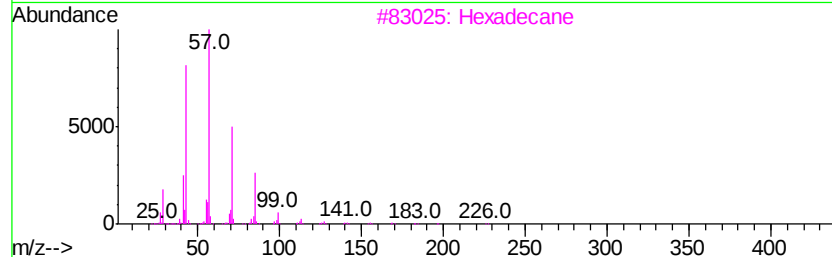
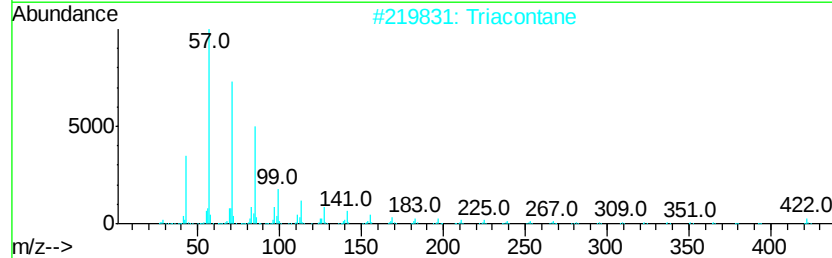
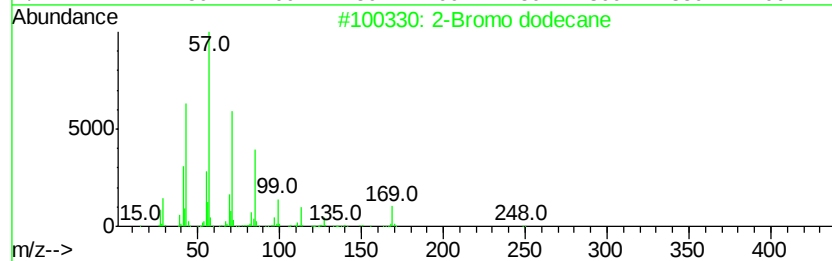
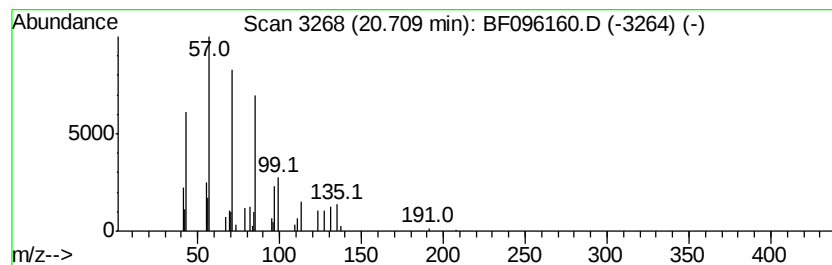
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 2-Bromo dodecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.71	2.00 ng	40233	Perylene-d12	19.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Bromo dodecane	248	C12H25Br	013187-99-0	64
2		triacontane	422	C30H62	000638-68-6	64
3		Hexadecane	226	C16H34	000544-76-3	64
4		Eicosane, 10-methyl-	296	C21H44	054833-23-7	59
5		Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062317\
Data File : BF096160.D
Acq On : 23 Jun 2017 15:29
Operator : SJ/MA
Sample : I3776-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHD-GW-01

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.92	6.92	96.0 ng		1681040	1	7.26	350197	20.0
Nonanoic acid	10.15	3.9 ng		100376	2	9.29	512240	20.0
unknown12.69	12.69	2.5 ng		69830	3	12.11	571059	20.0
Diethyltoluamide	12.85	2.7 ng		76218	3	12.11	571059	20.0
unknown13.66	13.66	3.5 ng		105025	4	14.50	606124	20.0
Octadecanoic acid	16.65	2.7 ng		109178	5	18.24	796821	20.0
2-[2-[2-[2-[2-...	17.02	9.2 ng		366023	5	18.24	796821	20.0
n-Tetracosanol-1	18.16	2.9 ng		116339	5	18.24	796821	20.0
3,6,9,12,15-Penta...	19.29	3.9 ng		79109	6	19.92	401735	20.0
2-Bromo dodecane	20.71	2.0 ng		40233	6	19.92	401735	20.0