

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061917\
 Data File : BF096016.D
 Acq On : 19 Jun 2017 20:34
 Operator : SJ/MA
 Sample : I3698-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-007

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	1.557	10	12	37	rBV	1141961	1996264	99.79%	11.066%
2	4.504	510	513	529	rBV2	47234	149019	7.45%	0.826%
3	5.192	627	630	660	rBV	761927	1632377	81.60%	9.049%
4	6.875	912	916	927	rBV	961312	1534527	76.71%	8.507%
5	6.963	927	931	952	rVB	1165626	2000418	100.00%	11.089%
6	7.304	985	989	1009	rVB	294432	431256	21.56%	2.391%
7	7.539	1024	1029	1045	rBV	973548	1363077	68.14%	7.556%
8	8.222	1141	1145	1188	rBV	621364	1056445	52.81%	5.856%
9	9.339	1330	1335	1360	rBV	377678	600328	30.01%	3.328%
10	11.116	1631	1637	1650	rBV	1576408	1990430	99.50%	11.034%
11	11.816	1752	1756	1768	rBV	165463	227391	11.37%	1.261%
12	12.151	1809	1813	1820	rBV2	460555	625125	31.25%	3.465%
13	13.016	1952	1960	1964	rBB	20328	26301	1.31%	0.146%
14	13.451	2030	2034	2058	rBV	647326	984587	49.22%	5.458%
15	13.780	2086	2090	2098	rBV	20414	31169	1.56%	0.173%
16	14.551	2217	2221	2237	rVB2	350364	541947	27.09%	3.004%
17	15.574	2390	2395	2410	rBV	86767	121443	6.07%	0.673%
18	16.680	2579	2583	2586	rBV2	31660	40286	2.01%	0.223%
19	16.927	2620	2625	2636	rVB2	1146176	1329556	66.46%	7.370%
20	18.186	2833	2839	2849	rBV2	67337	111460	5.57%	0.618%
21	18.280	2851	2855	2865	rBV	265926	376448	18.82%	2.087%
22	18.992	2971	2976	2981	rBV4	13338	22240	1.11%	0.123%
23	19.415	3044	3048	3054	rBV	37355	40532	2.03%	0.225%
24	19.944	3135	3138	3151	rBV	257901	390803	19.54%	2.166%
25	20.415	3215	3218	3224	rVV4	26073	46527	2.33%	0.258%
26	21.462	3389	3396	3406	rBV6	45993	122056	6.10%	0.677%
27	21.821	3451	3457	3458	rBV5	15952	23058	1.15%	0.128%
28	22.091	3497	3503	3511	rVB10	11021	30050	1.50%	0.167%
29	22.186	3512	3519	3526	rBV5	23504	51211	2.56%	0.284%
30	22.733	3606	3612	3620	rBV8	18848	51378	2.57%	0.285%
31	22.862	3627	3634	3646	rVB6	34559	91575	4.58%	0.508%

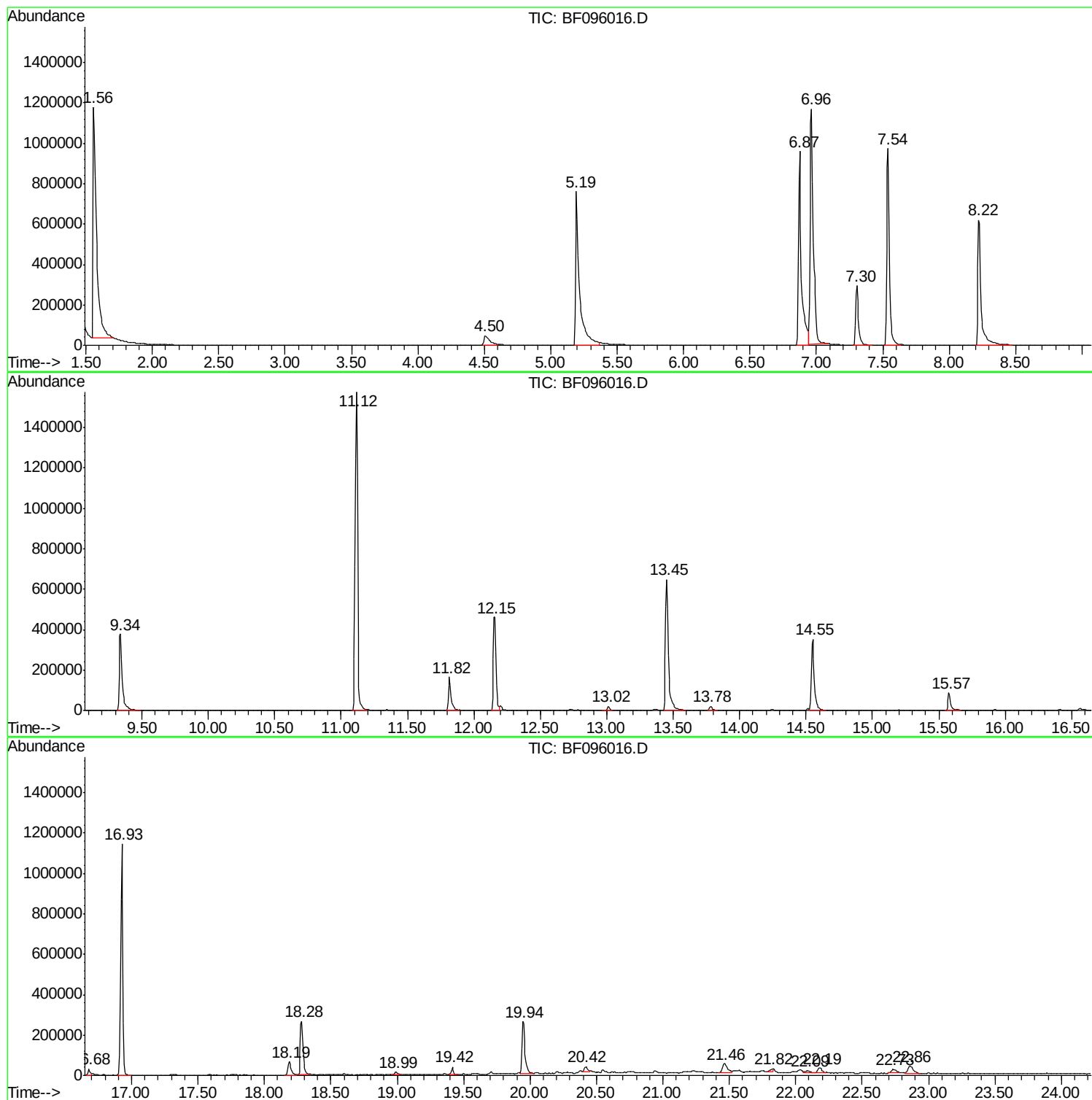
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Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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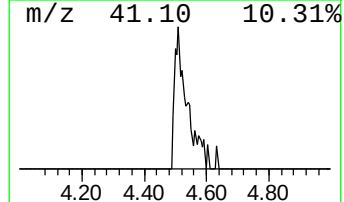
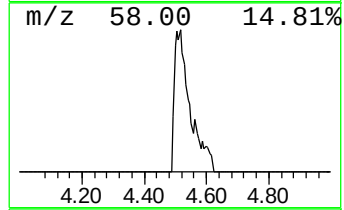
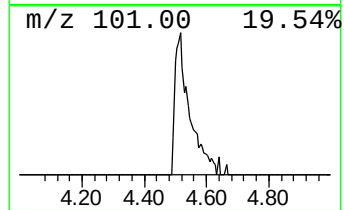
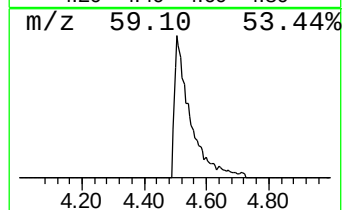
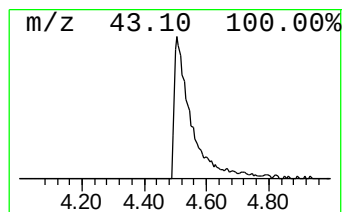
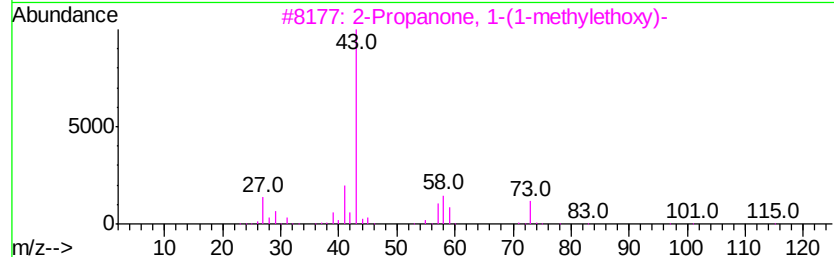
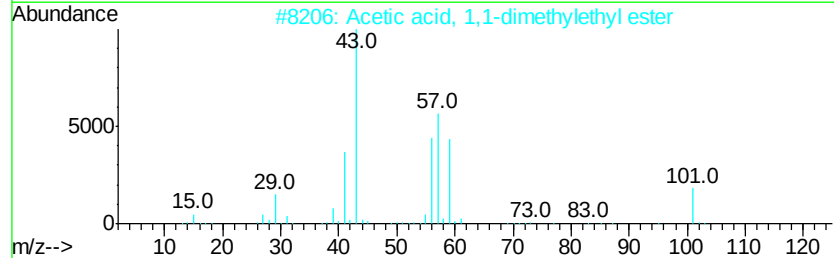
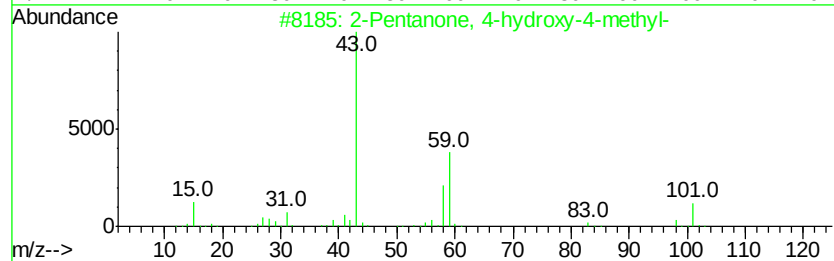
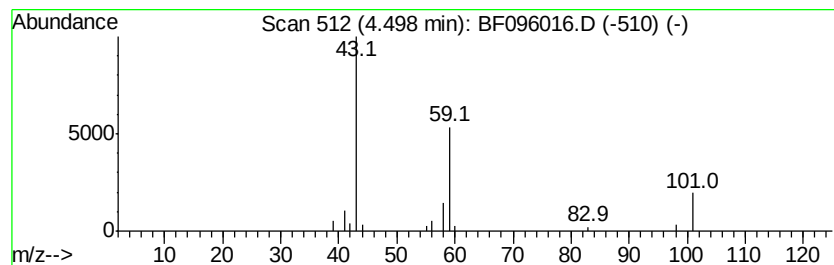
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.50	6.91 ng	149019	1,4-Dichlorobenzene-d4	7.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
4			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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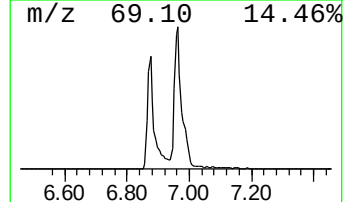
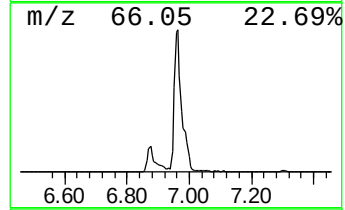
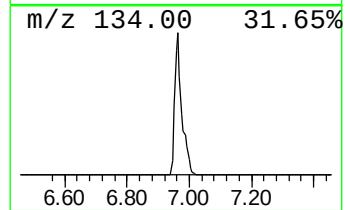
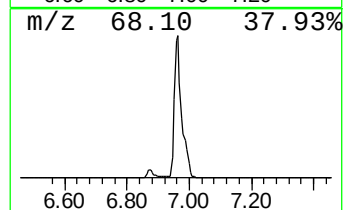
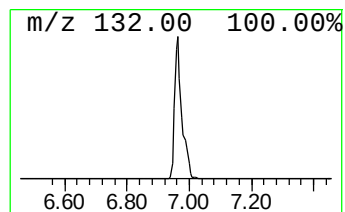
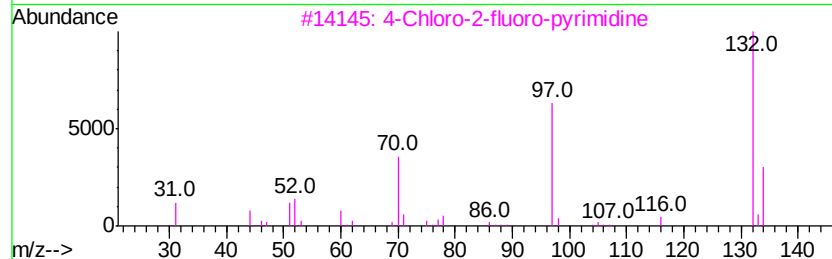
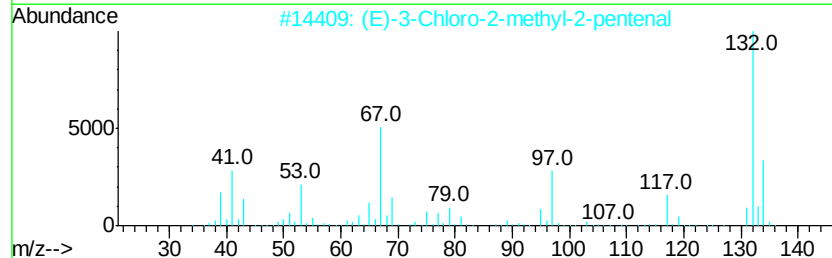
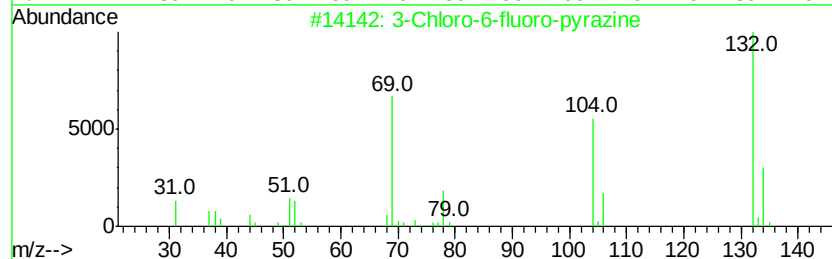
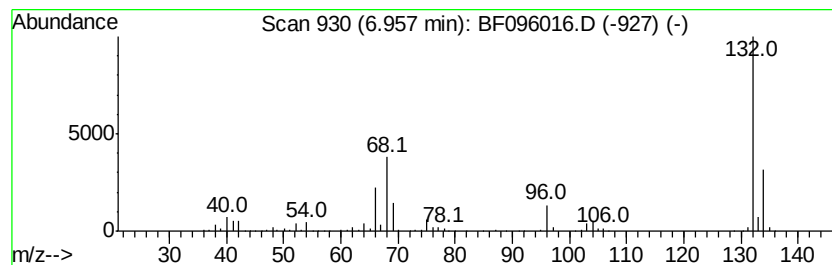
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Peak Number 3 unknown6.96 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.96	92.77 ng	2000420	1,4-Dichlorobenzene-d4	7.30

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		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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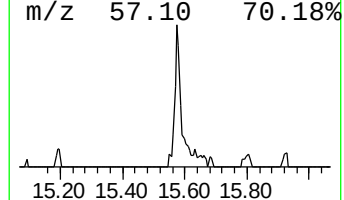
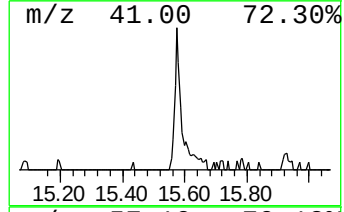
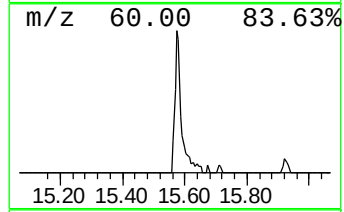
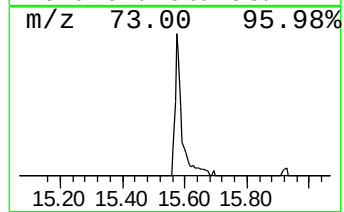
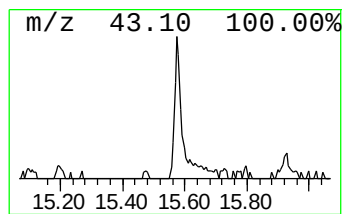
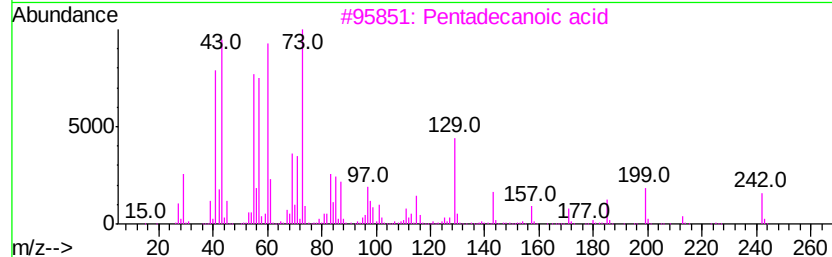
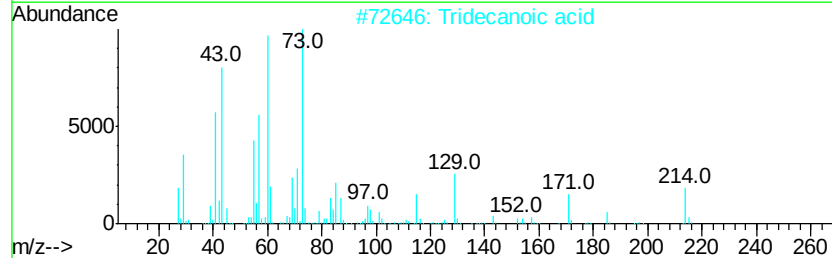
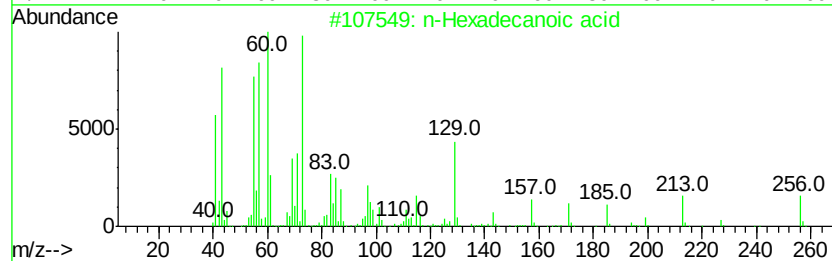
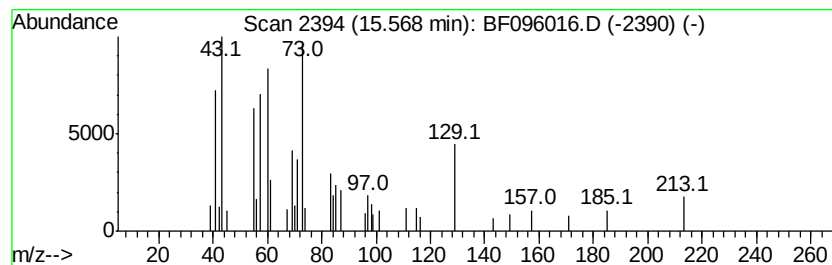
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	4.48 ng	121443	Phenanthrene-d10	14.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5		Dodecanoic acid	200	C12H24O2	000143-07-7	64



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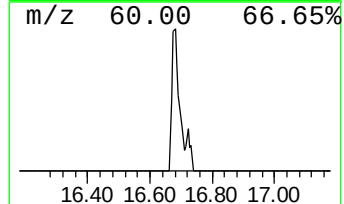
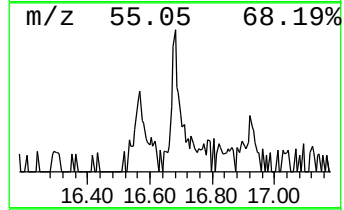
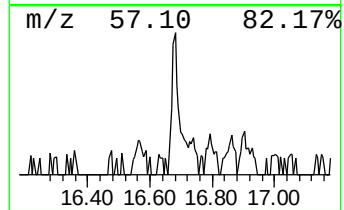
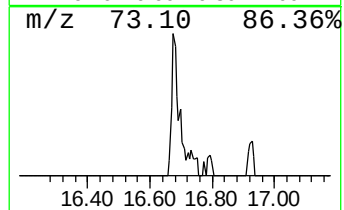
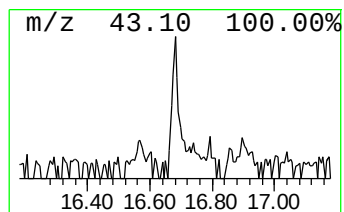
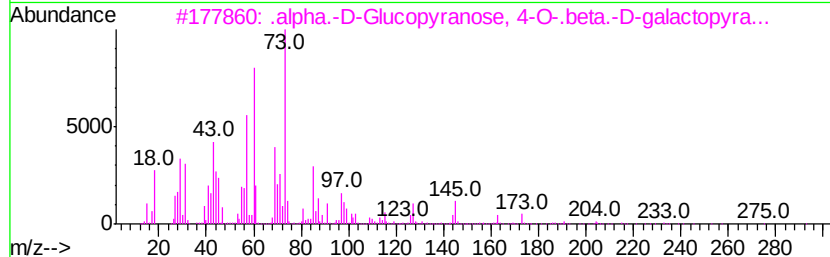
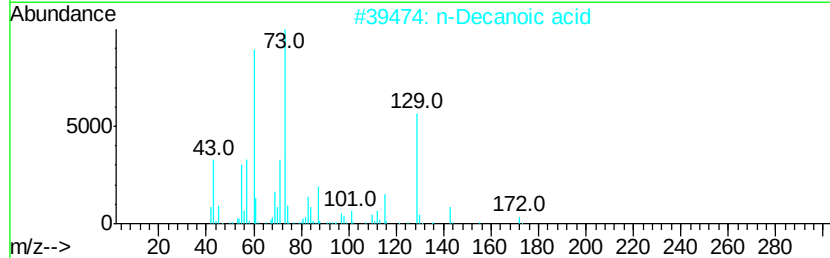
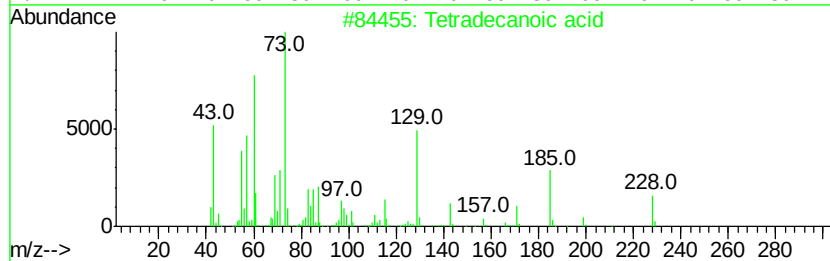
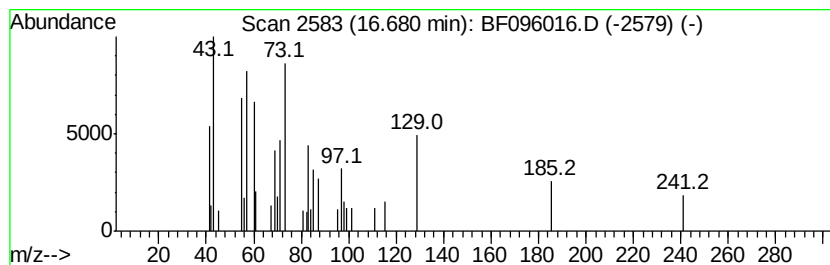
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Peak Number 6 Tetradecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.68	2.14 ng	40286	Chrysene-d12	18.28	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
2	n-Decanoic acid	172	C10H20O2	000334-48-5	43
3	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	35
4	Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	30
5	Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	30



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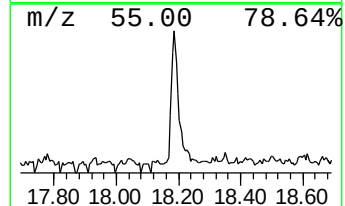
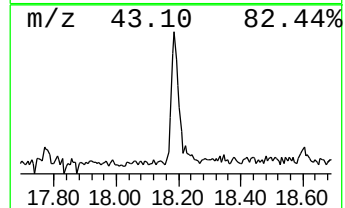
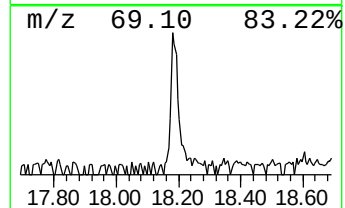
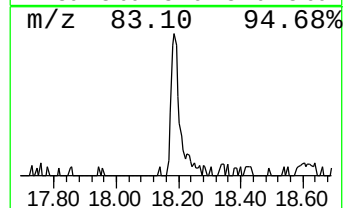
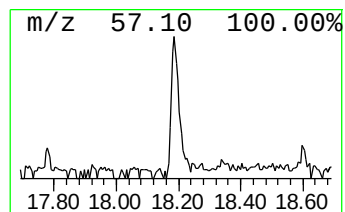
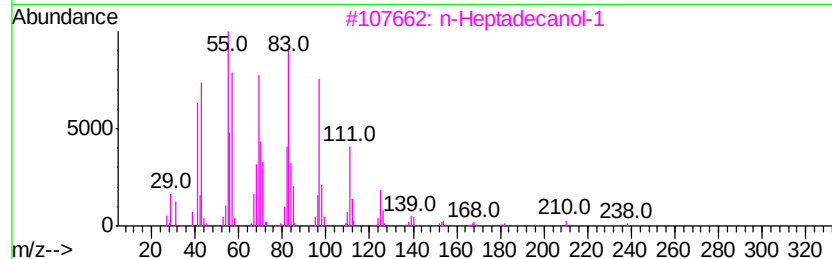
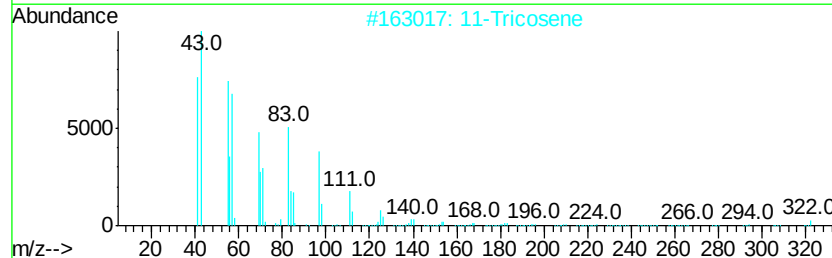
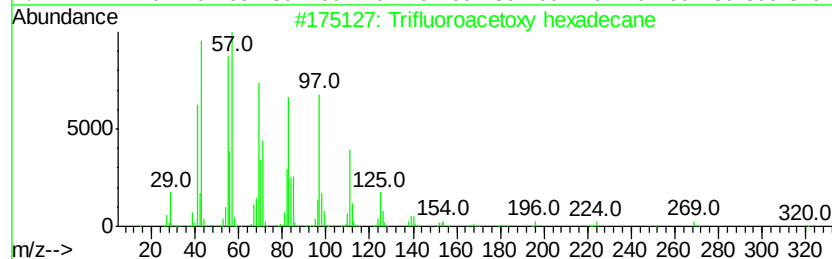
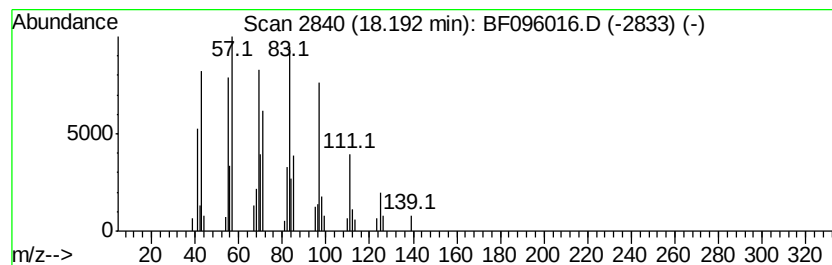
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.19	5.92 ng	111460	Chrysene-d12	18.28	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2	11-Tricosene	322	C23H46	052078-56-5	91
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	90
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	90
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	83



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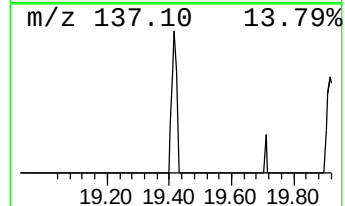
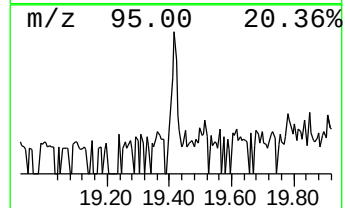
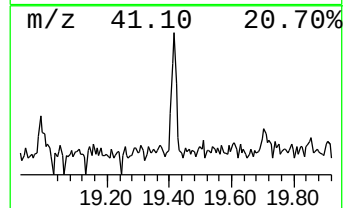
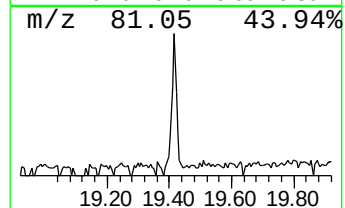
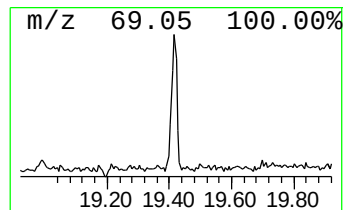
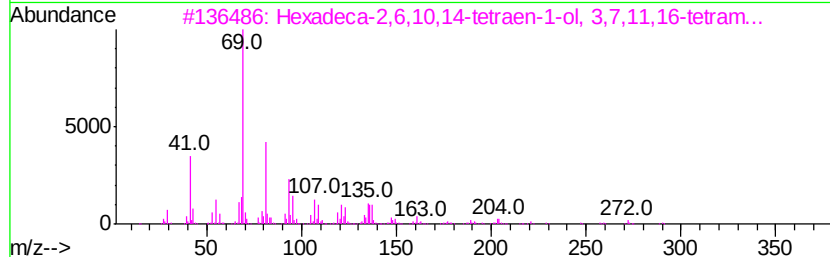
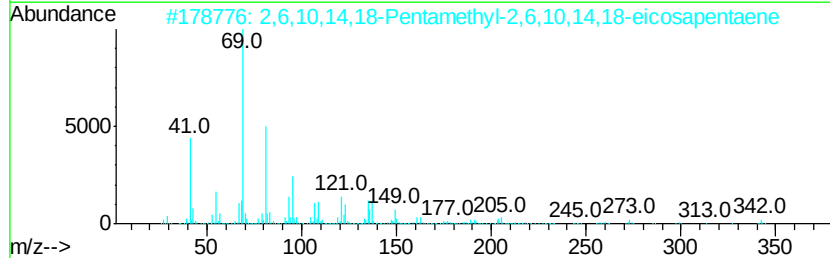
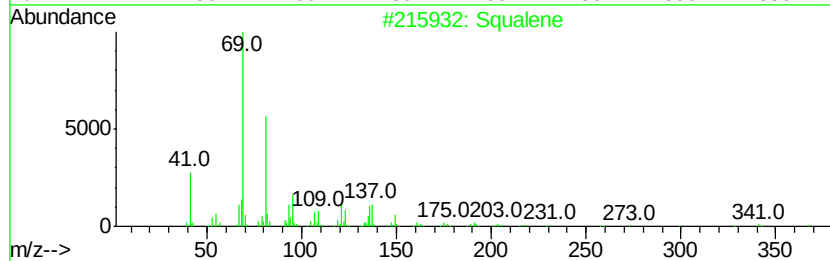
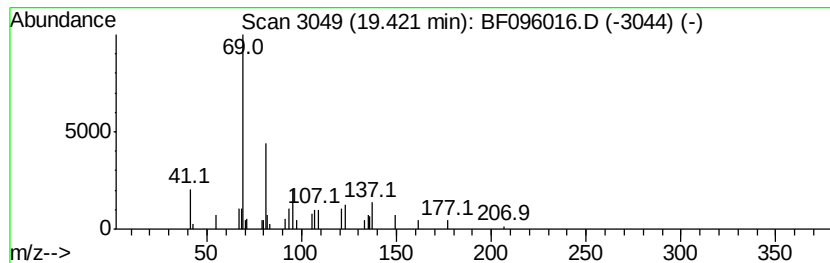
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.42	2.07 ng	40532	Perylene-d12	19.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	83
3	Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	80
4	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72
5	Supraene	410	C30H50	007683-64-9	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061917\
Data File : BF096016.D
Acq On : 19 Jun 2017 20:34
Operator : SJ/MA
Sample : I3698-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-007

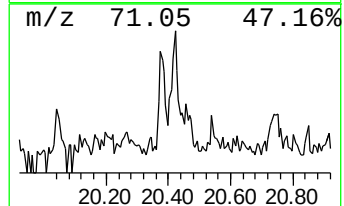
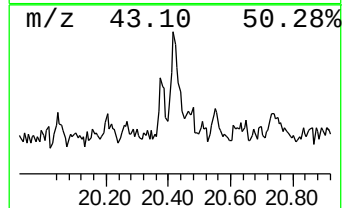
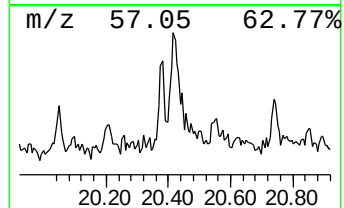
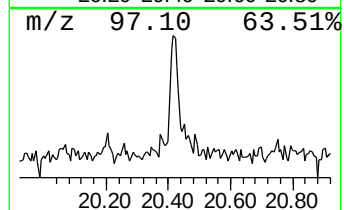
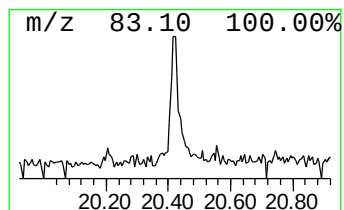
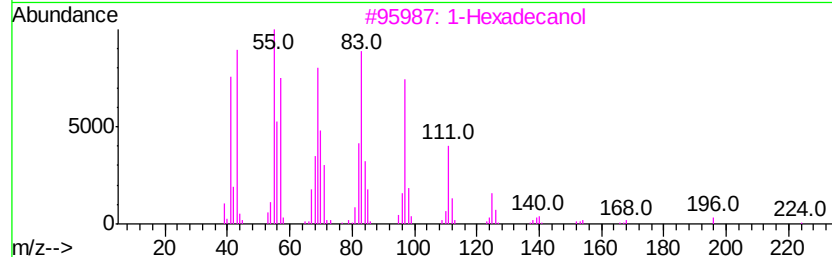
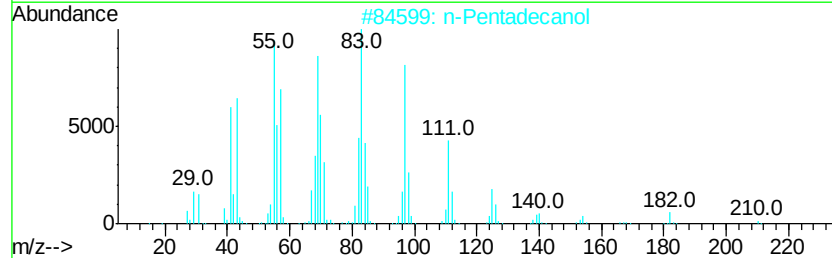
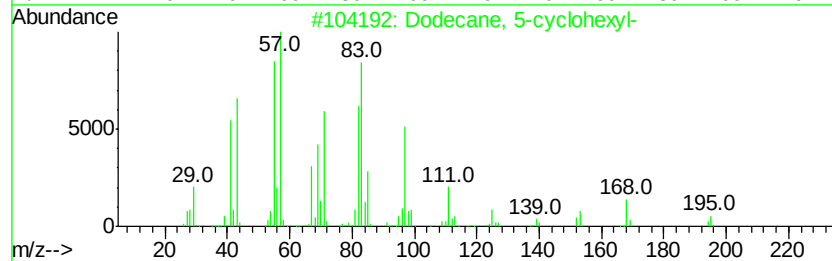
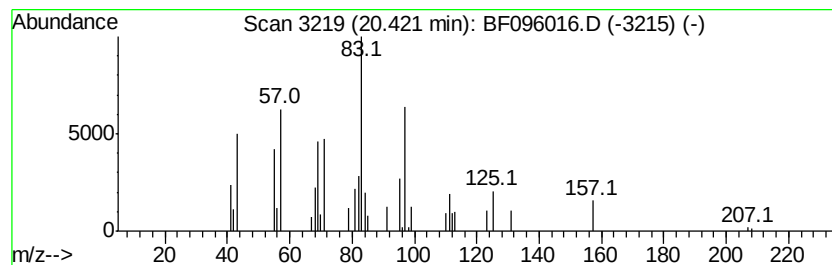
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Dodecane, 5-cyclohexyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.42	2.38 ng	46527	Perylene-d12	19.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 5-cyclohexyl-	252	C18H36	013151-85-4	50
2		n-Pentadecanol	228	C15H32O	000629-76-5	43
3		1-Hexadecanol	242	C16H34O	036653-82-4	43
4		5-Tetradecanol acetate	256	C16H32O2	051354-25-7	43
5		3-Heptene, 2,2,3,5,5,6,6-heptame...	196	C14H28	054845-26-0	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061917\
Data File : BF096016.D
Acq On : 19 Jun 2017 20:34
Operator : SJ/MA
Sample : I3698-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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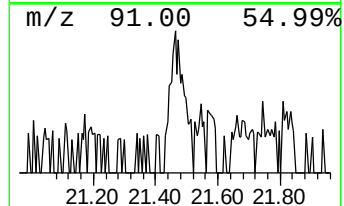
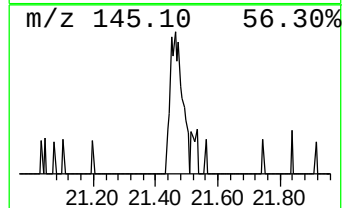
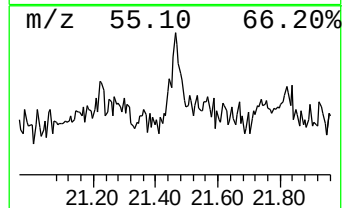
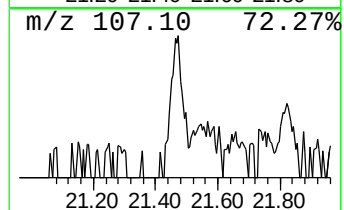
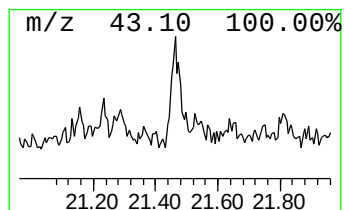
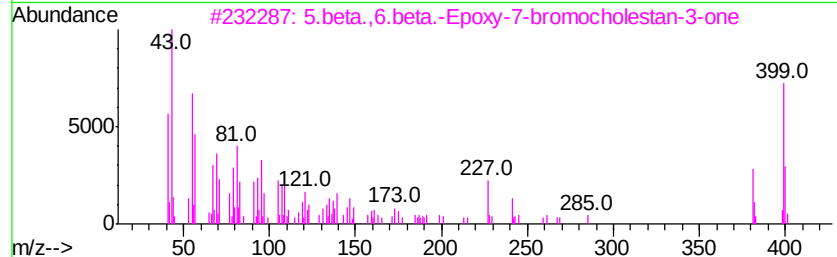
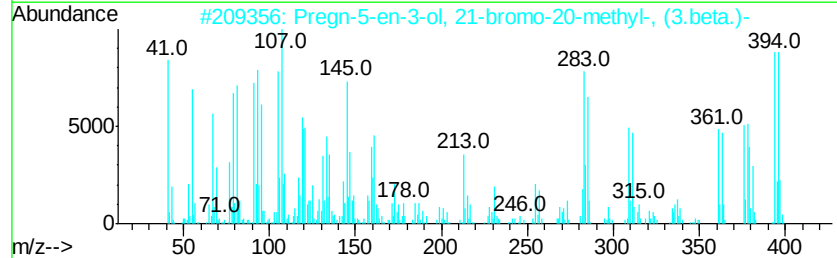
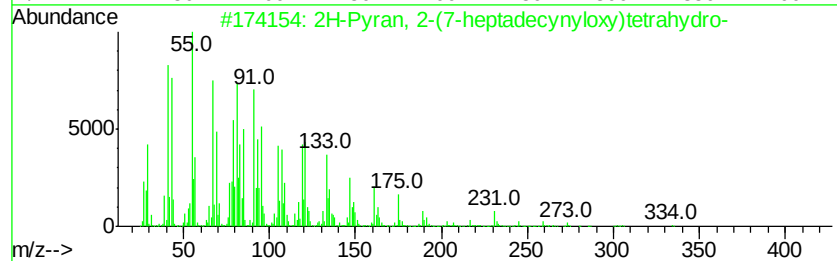
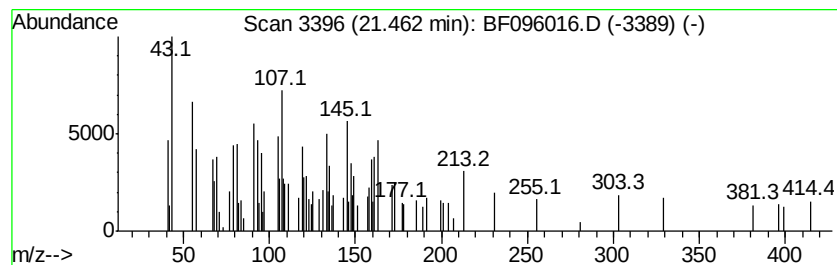
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown21.46 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.46	6.25 ng	122056	Perylene-d12	19.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-Pyran, 2-(7-heptadecynvloxv)t...	336	C22H40O2	056599-50-9	38
2		Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	35
3		5.beta.,6.beta.-Epoxy-7-bromocho...	478	C27H43BrO2	104825-82-3	14
4		1H-Cyclopropfelazulen-4-ol, deca...	222	C15H26O	000552-02-3	12
5		1,9-Dioxa-5-thianonane, 3,7-bis(...	574	C34H48B2O4S	1000162-27-0	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061917\
Data File : BF096016.D
Acq On : 19 Jun 2017 20:34
Operator : SJ/MA
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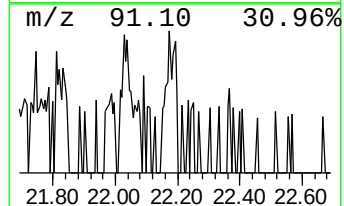
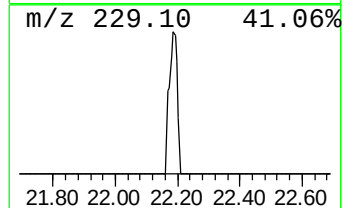
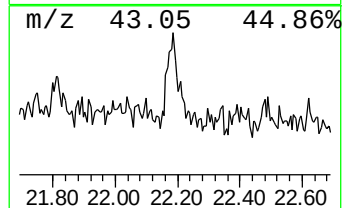
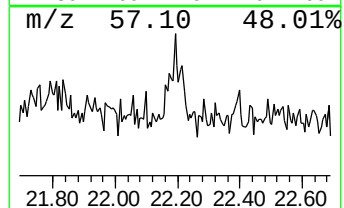
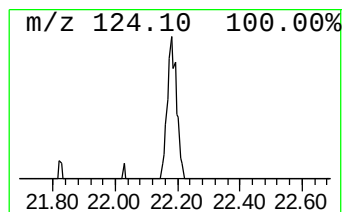
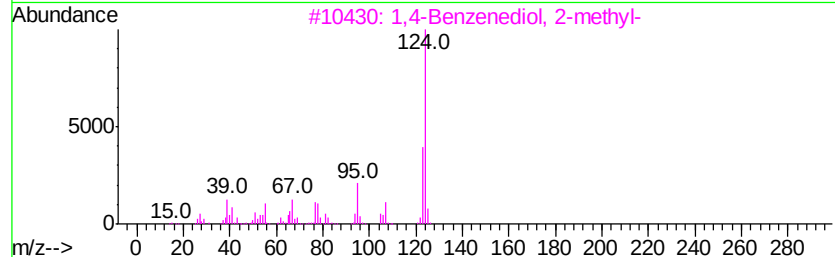
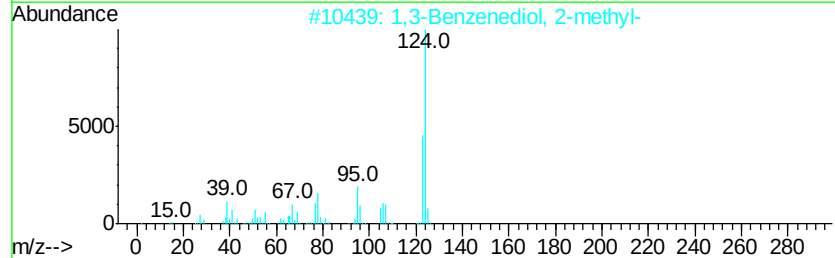
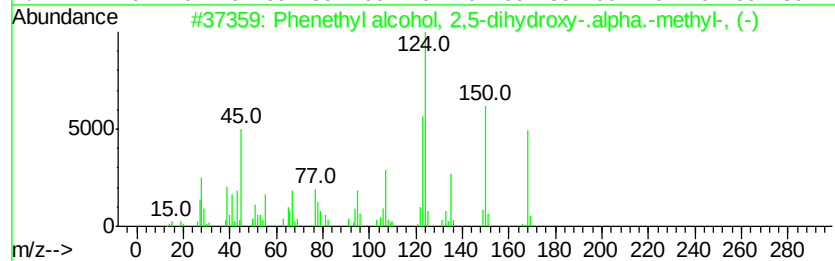
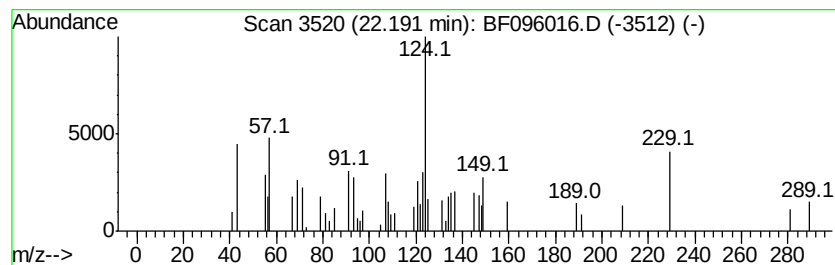
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown22.19 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.19	2.62 ng	51211	Perylene-d12	19.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenethyl alcohol, 2,5-dihydroxy...	168	C9H12O3	014293-26-6	38
2		1,3-Benzenediol, 2-methyl-	124	C7H8O2	000608-25-3	27
3		1,4-Benzenediol, 2-methyl-	124	C7H8O2	000095-71-6	27
4		2,4-Diaminophenol	124	C6H8N2O	000095-86-3	22
5		1,4-Benzenediol, 2-[8-hydroxy-3-...	278	C16H22O4	077828-64-9	16



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061917\
Data File : BF096016.D
Acq On : 19 Jun 2017 20:34
Operator : SJ/MA
Sample : I3698-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-007

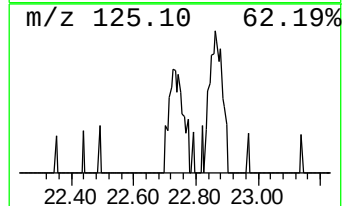
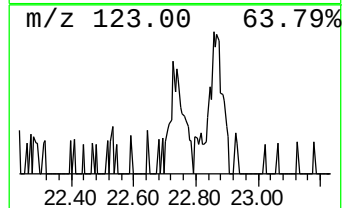
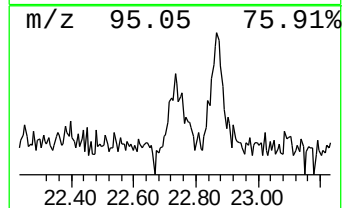
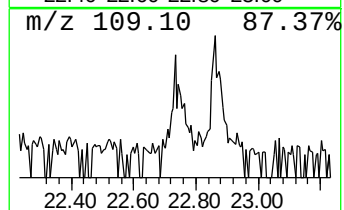
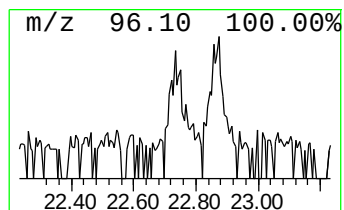
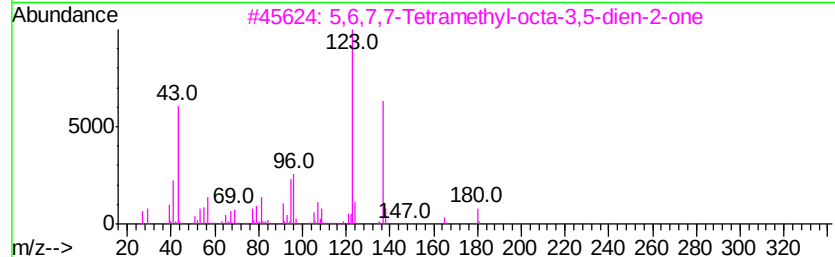
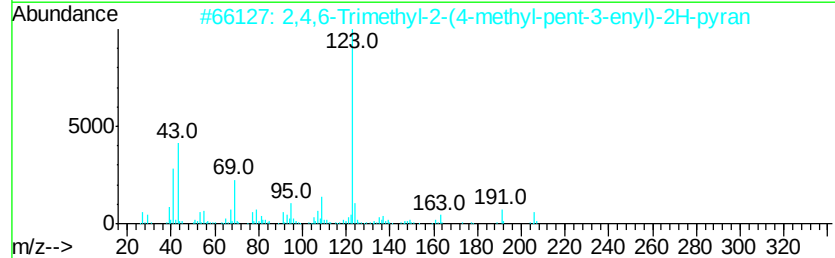
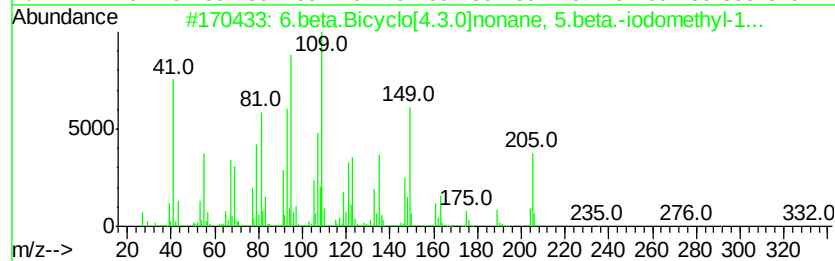
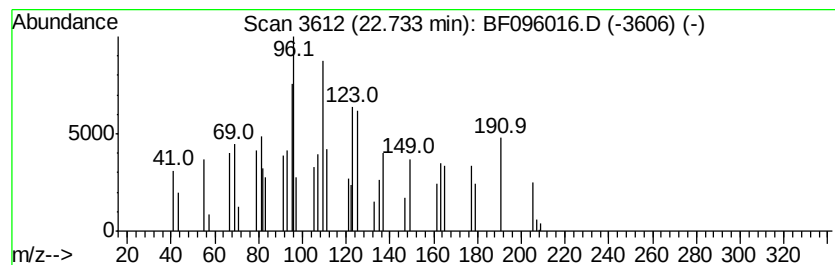
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown22.73 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.73	2.63 ng	51378	Perylene-d12	19.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6.beta.Bicvclo[4.3.0]nonane, 5.b...	332	C15H25I	1000195-85-9	38
2		2,4,6-Trimethyl-2-(4-methyl-pent...	206	C14H22O	1000193-58-6	32
3		5,6,7,7-Tetramethyl-octa-3,5-die...	180	C12H20O	1000190-70-9	32
4		1,4-Methanoazulene-9-methanol, d...	222	C15H26O	001139-17-9	27
5		Methoxy(methyl)chlorosilane	110	C2H7ClOSi	018151-27-4	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061917\
Data File : BF096016.D
Acq On : 19 Jun 2017 20:34
Operator : SJ/MA
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Misc :
ALS Vial : 19 Sample Multiplier: 1

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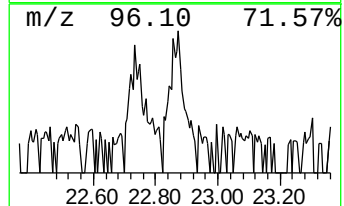
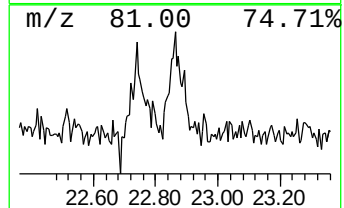
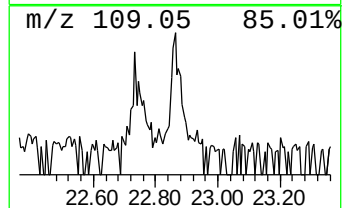
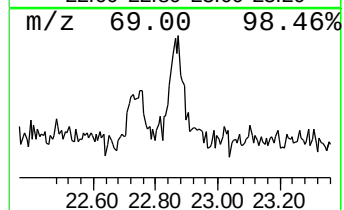
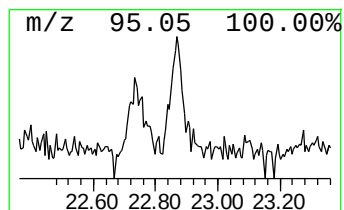
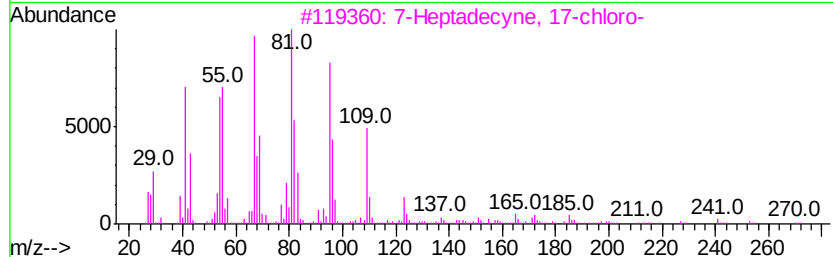
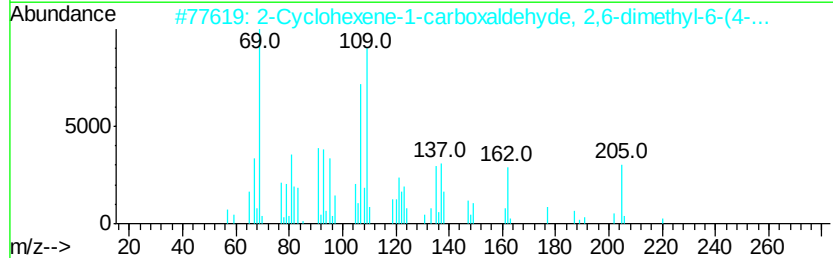
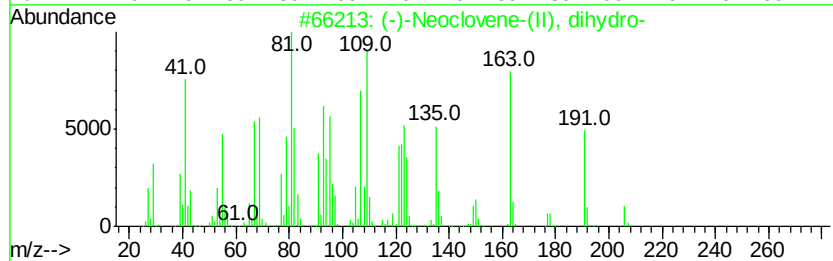
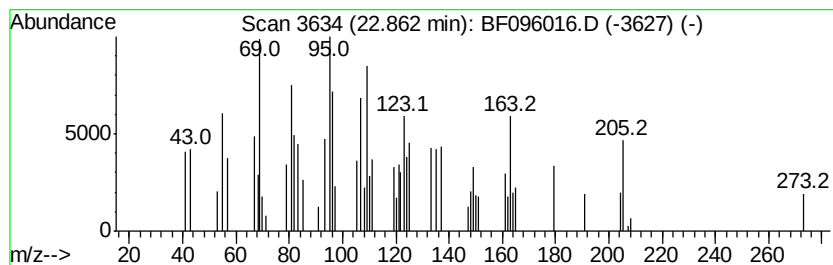
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 (-)-Neoclovene-(II), dihydro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.86	4.69 ng	91575	Perylene-d12	19.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(-)-Neoclovene-(II), dihydro-	206	C15H26	1000152-83-6	38
2			2-Cyclohexene-1-carboxaldehyde, ...	220	C15H24O	056772-07-7	27
3			7-Heptadecyne, 17-chloro-	270	C17H31Cl	056554-75-7	27
4			(4R*,5R*,9S*)-5,9-Dimethylspiro[...]	166	C11H18O	063088-19-7	27
5			Naphthalene, decahydro-1,6-dimet...	208	C15H28	029788-41-8	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061917\
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Acq On : 19 Jun 2017 20:34
Operator : SJ/MA
Sample : I3698-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.50	6.9	ng	149019	1	7.30	431256	20.0
unknown6.96	6.96	92.8	ng	2000420	1	7.30	431256	20.0
n-Hexadecanoic acid	15.57	4.5	ng	121443	4	14.55	541947	20.0
Tetradecanoic acid	16.68	2.1	ng	40286	5	18.28	376448	20.0
Trifluoroacetoxy ...	18.19	5.9	ng	111460	5	18.28	376448	20.0
Squalene	19.42	2.1	ng	40532	6	19.95	390803	20.0
Dodecane, 5-cyclo...	20.42	2.4	ng	46527	6	19.95	390803	20.0
unknown21.46	21.46	6.3	ng	122056	6	19.95	390803	20.0
unknown22.19	22.19	2.6	ng	51211	6	19.95	390803	20.0
unknown22.73	22.73	2.6	ng	51378	6	19.95	390803	20.0
(-)-Neoclovene-(I...	22.86	4.7	ng	91575	6	19.95	390803	20.0