

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
 Data File : BF098907.D
 Acq On : 28 Sep 2017 14:36
 Operator : SJ/JU
 Sample : I5428-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A-B-C-DRUM-COMP

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-BF092317.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	2.228	20	24	31	rVB	104883	146113	3.25%	0.424%
2	5.151	516	521	532	rVB	543599	771038	17.13%	2.236%
3	5.539	581	587	590	rBV	3582764	3949688	87.75%	11.454%
4	6.545	751	758	761	rBV	3413997	4001222	88.89%	11.604%
5	6.686	777	782	785	rBV	3850063	4049092	89.95%	11.743%
6	6.916	816	821	824	rBV	1129260	903589	20.07%	2.620%
7	7.075	843	848	851	rVB	3468022	3156522	70.12%	9.154%
8	7.481	911	917	920	rBV	2588675	2646560	58.80%	7.675%
9	8.198	1031	1039	1042	rBV	1464421	1222974	27.17%	3.547%
10	8.486	1081	1088	1091	rBV5	42629	61131	1.36%	0.177%
11	8.816	1141	1144	1147	rBV	72791	83414	1.85%	0.242%
12	9.075	1185	1188	1191	rBV2	93508	92740	2.06%	0.269%
13	9.192	1205	1208	1209	rBV	137213	120102	2.67%	0.348%
14	9.210	1209	1211	1216	rVV	257477	237253	5.27%	0.688%
15	9.274	1216	1222	1225	rBV	4300958	4501289	100.00%	13.054%
16	9.316	1225	1229	1231	rBV3	155236	191953	4.26%	0.557%
17	9.351	1231	1235	1238	rBV5	288622	459179	10.20%	1.332%
18	9.592	1273	1276	1277	rBV3	315241	332919	7.40%	0.965%
19	9.663	1285	1288	1292	rBV2	1445622	2118316	47.06%	6.143%
20	9.704	1292	1295	1296	rVV2	318945	312005	6.93%	0.905%
21	9.869	1321	1323	1326	rVB2	1258690	1216612	27.03%	3.528%
22	9.957	1336	1338	1342	rVB	1426892	1485648	33.00%	4.309%
23	14.092	2038	2041	2048	rVB	705402	744374	16.54%	2.159%
24	15.574	2289	2293	2301	rVB	599200	845022	18.77%	2.451%
25	16.027	2367	2370	2375	rVB	82637	122029	2.71%	0.354%
26	16.080	2376	2379	2388	rVB3	79373	166357	3.70%	0.482%
27	16.551	2455	2459	2465	rVB2	54399	98303	2.18%	0.285%
28	17.162	2558	2563	2572	rVB	59138	118271	2.63%	0.343%
29	17.680	2645	2651	2658	rVB8	41899	98199	2.18%	0.285%
30	17.880	2682	2685	2695	rVB4	39819	94918	2.11%	0.275%
31	18.744	2825	2832	2842	rVB4	48304	134864	3.00%	0.391%

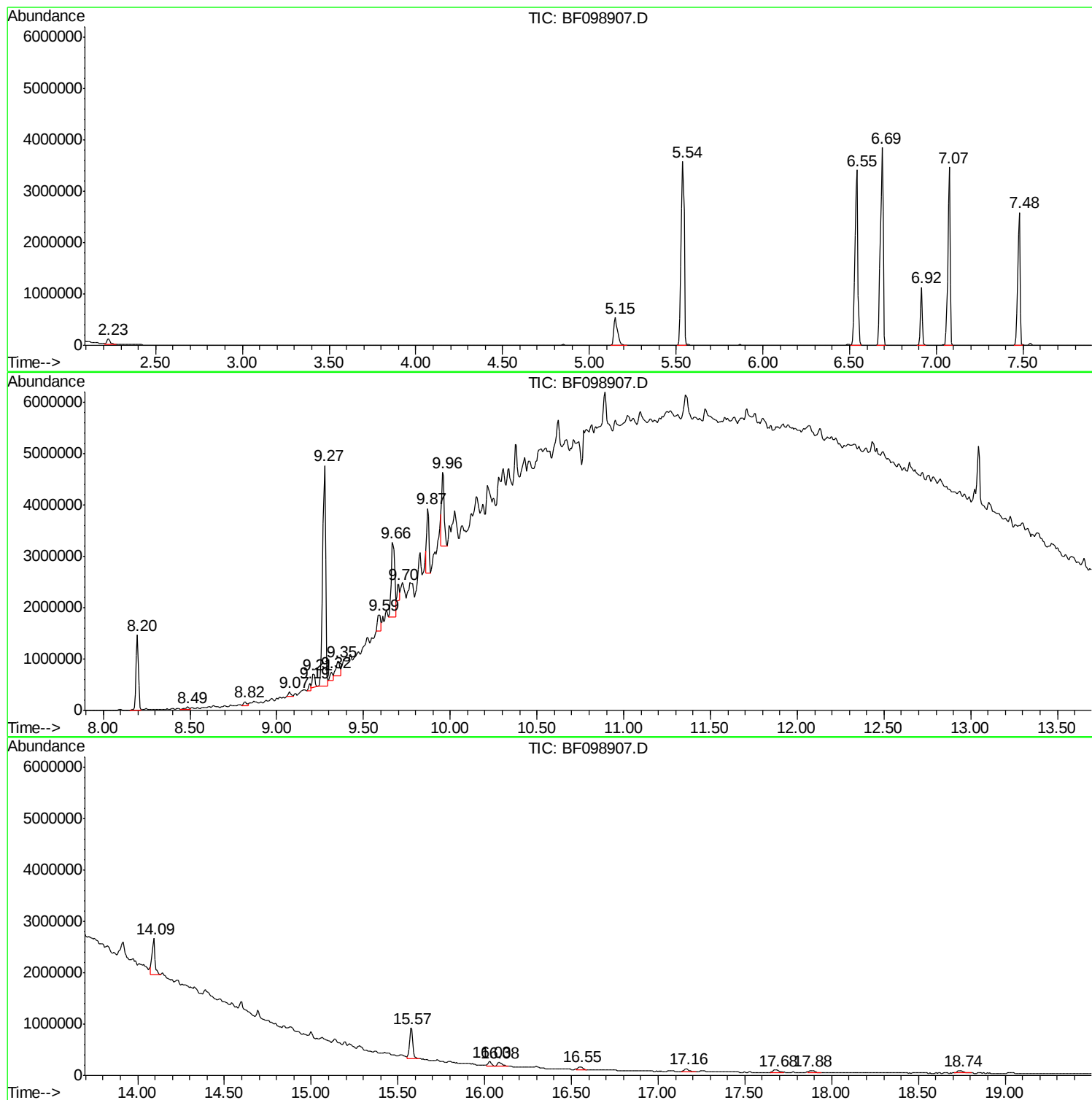
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ClientSampleId :
A-B-C-DRUM-COMP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.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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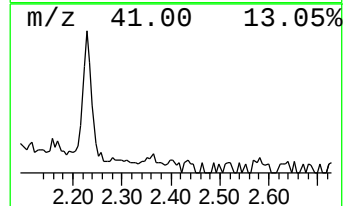
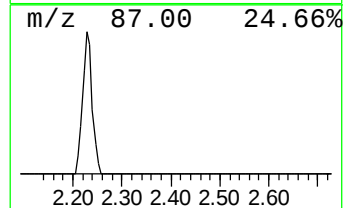
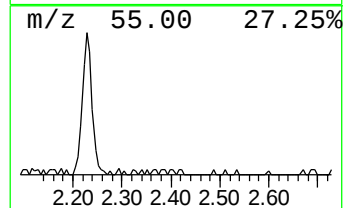
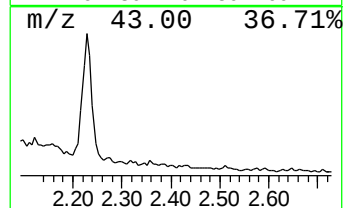
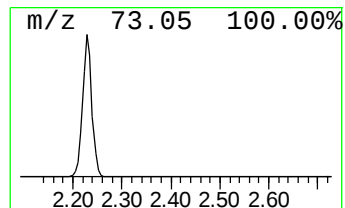
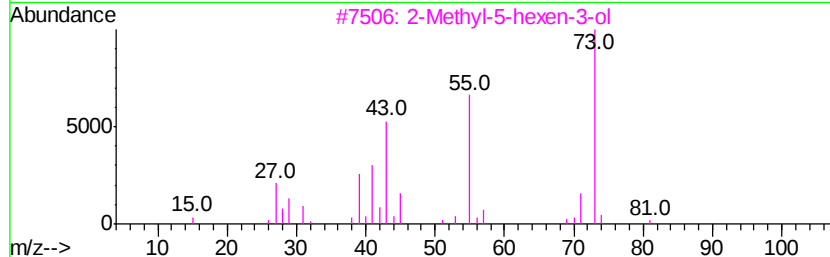
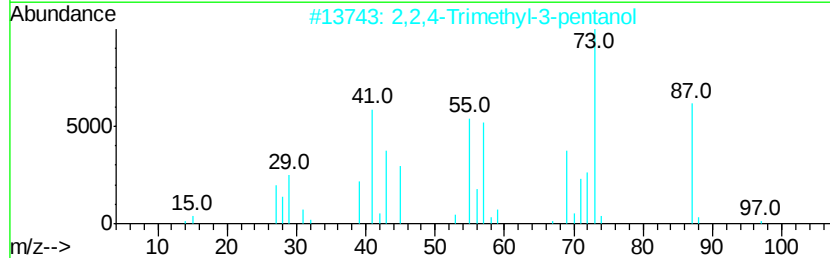
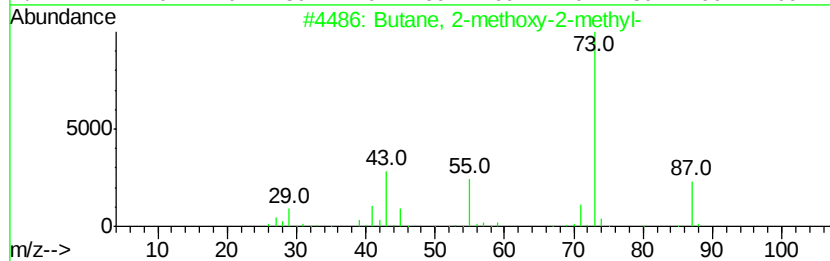
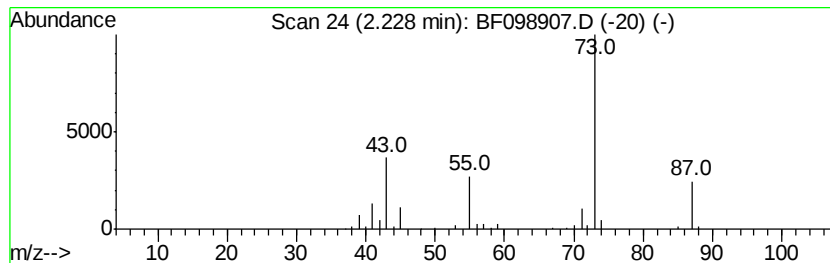
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	3.23 ng	146113	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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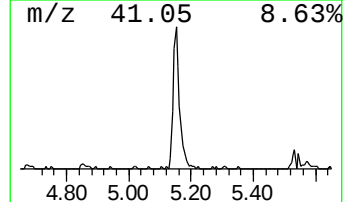
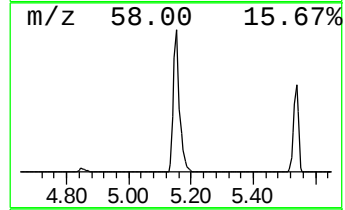
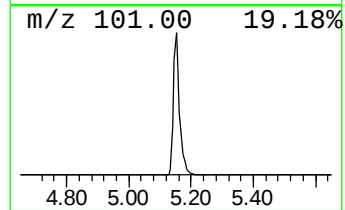
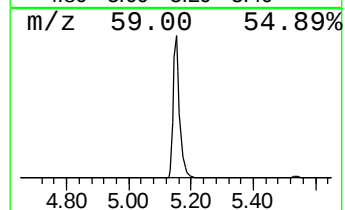
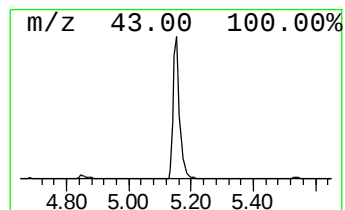
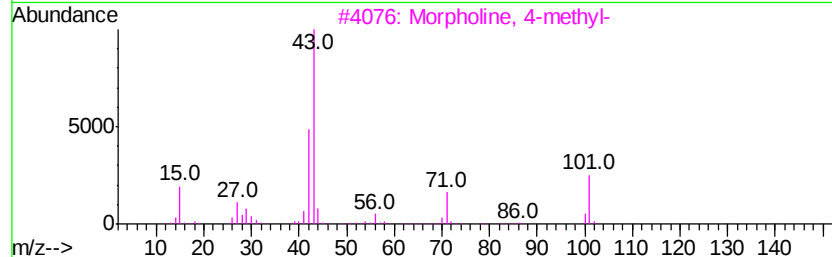
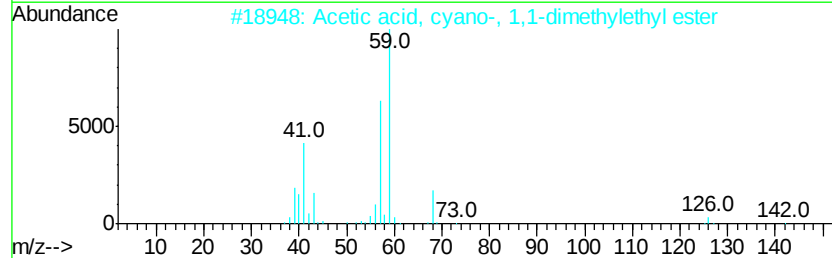
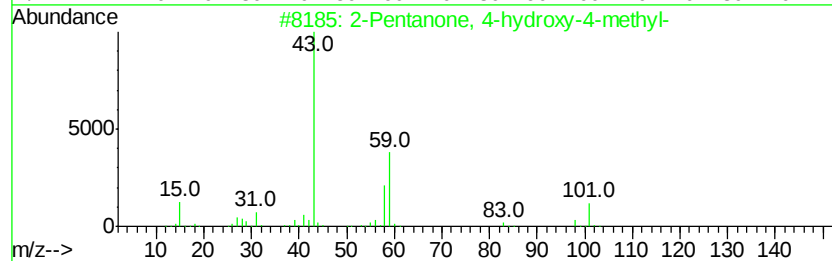
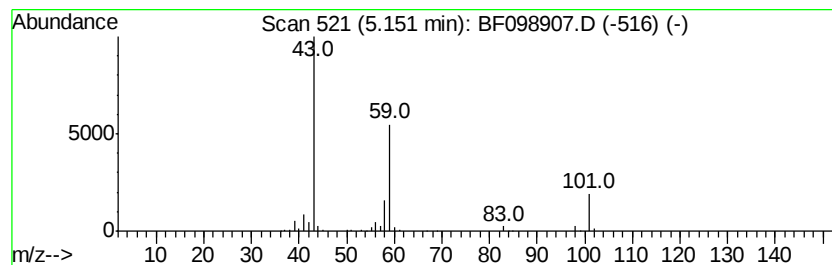
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	17.07 ng	771038	1,4-Dichlorobenzene-d4	6.92

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-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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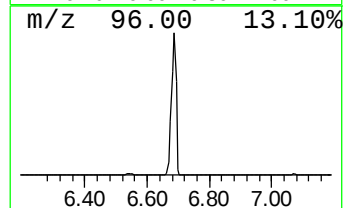
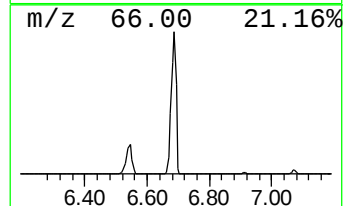
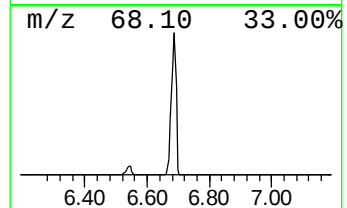
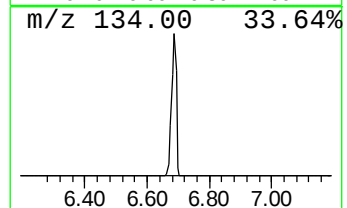
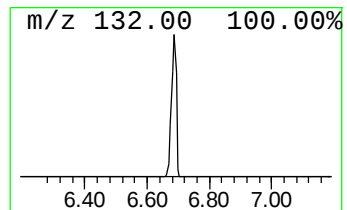
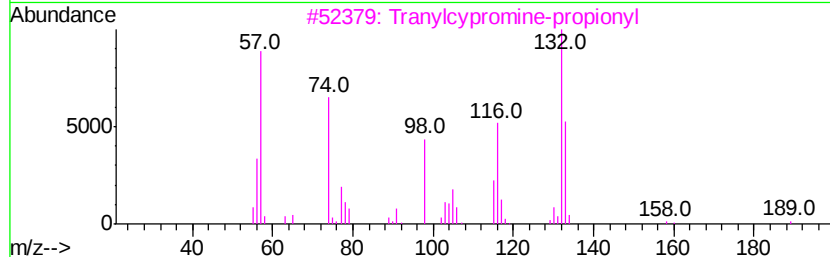
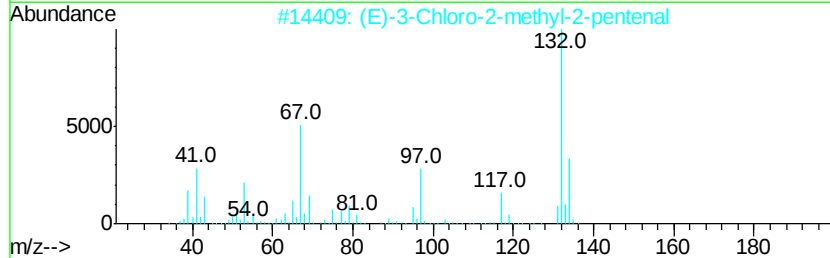
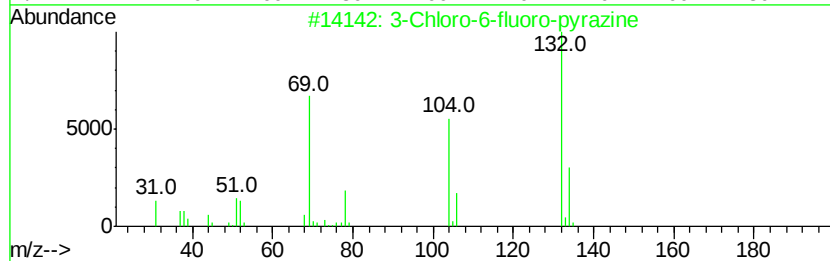
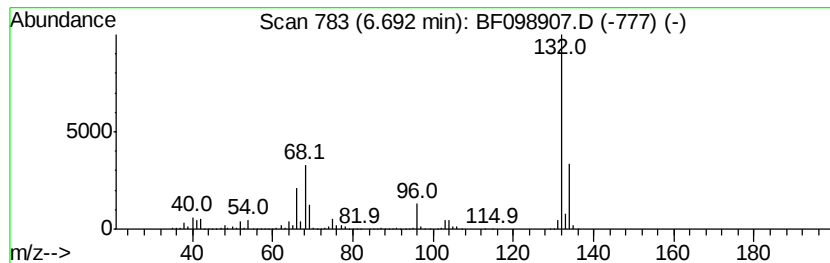
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	89.62 ng	4049090	1,4-Dichlorobenzene-d4	6.92

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	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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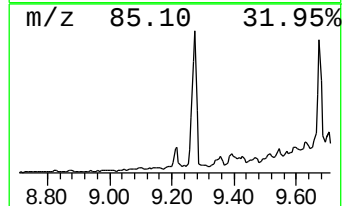
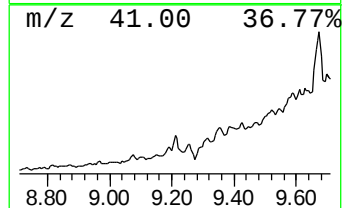
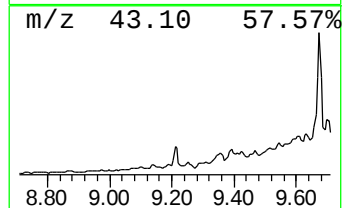
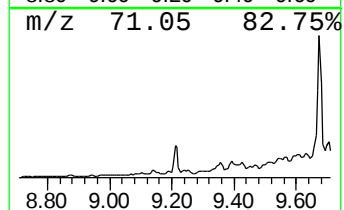
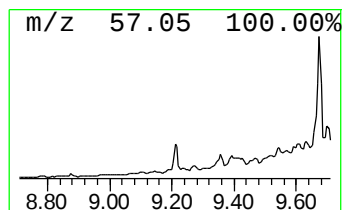
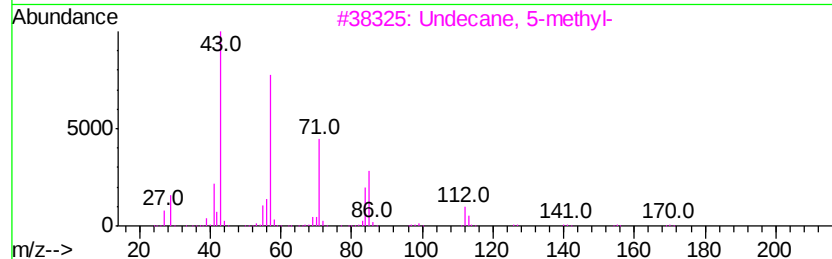
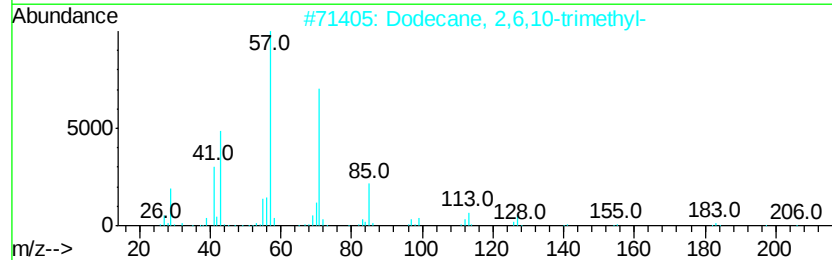
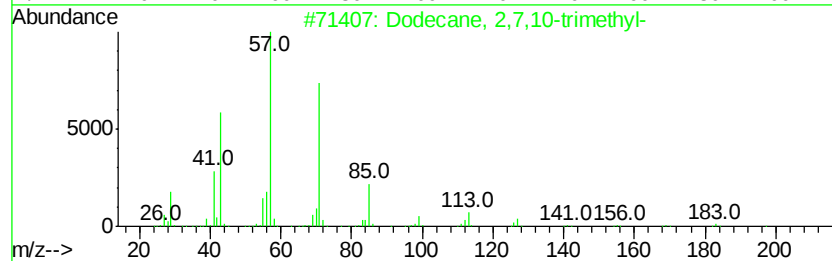
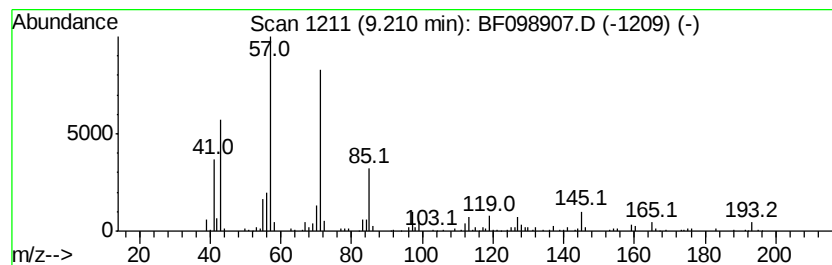
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Dodecane, 2,7,10-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.21	3.19 ng	237253	Acenaphthene-d10	9.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
2		Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64
3		Undecane, 5-methyl-	170	C12H26	001632-70-8	59
4		Oxalic acid, isobutyl neopentyl ...	216	C11H20O4	1000309-72-6	53
5		Oxalic acid, butyl neopentyl ester	216	C11H20O4	1000309-72-8	50



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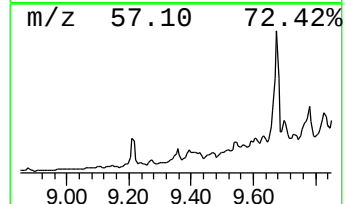
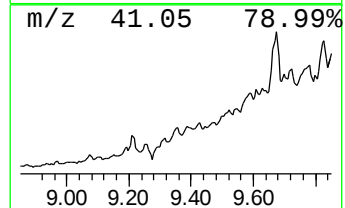
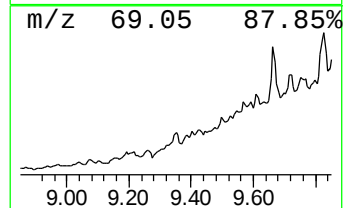
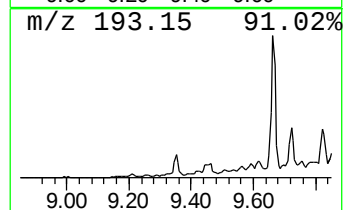
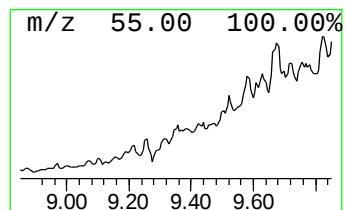
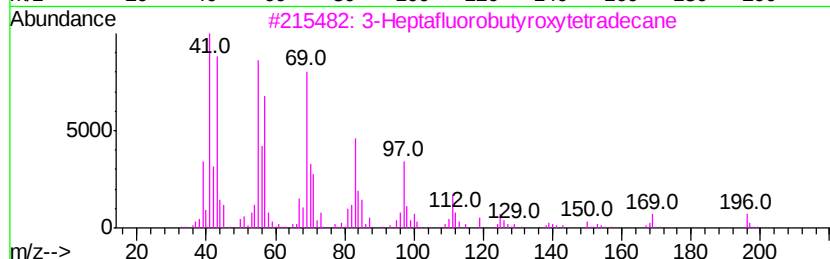
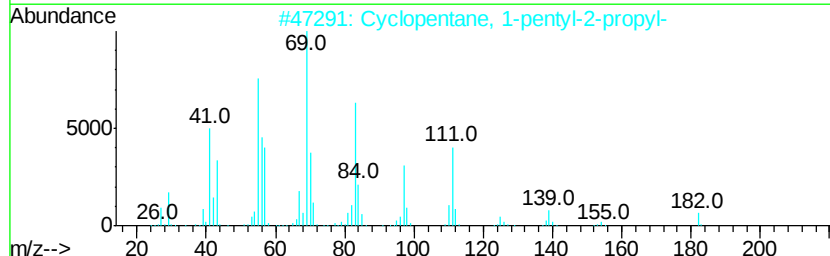
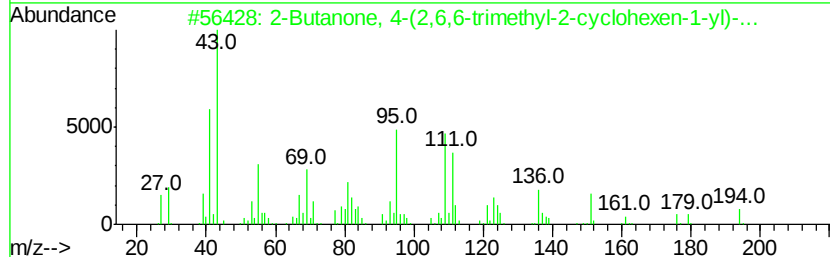
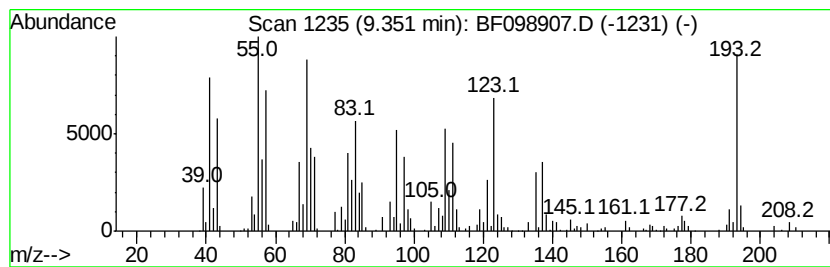
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Peak Number 6 unknown9.35 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.35	6.18 ng	459179	Acenaphthene-d10	9.96	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 4-(2,6,6-trimethyl-2...	194	C13H22O	039721-65-8	30
2	Cyclopentane, 1-pentyl-2-propyl-	182	C13H26	062199-51-3	25
3	3-Heptafluorobutvroxvtetradecane	410	C18H29F7O2	1000245-49-8	18
4	1-Anthracenamine	193	C14H11N	000610-49-1	18
5	2-Heptafluorobutyroxypentadecane	424	C19H31F7O2	1000245-50-0	18



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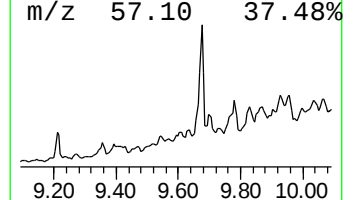
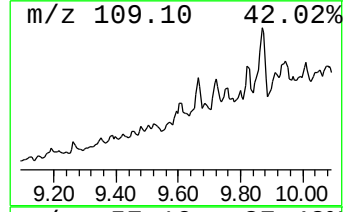
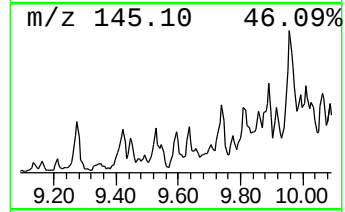
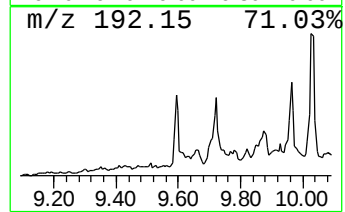
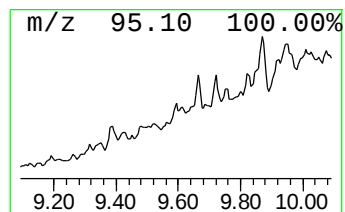
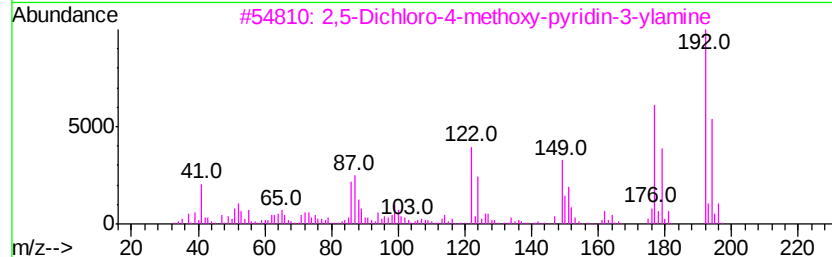
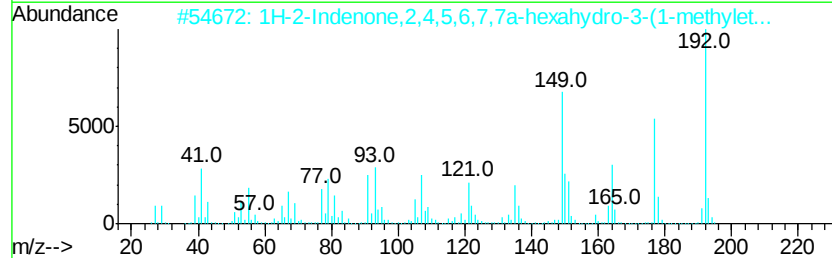
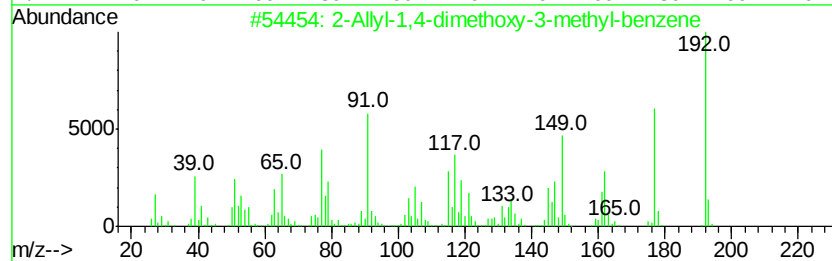
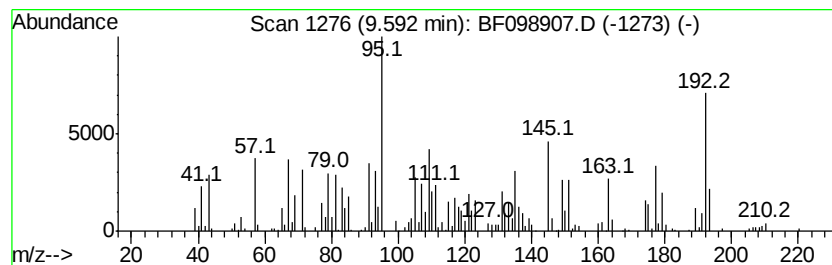
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown9.59 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.59	4.48 ng	332919	Acenaphthene-d10	9.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Allyl-1,4-dimethoxy-3-methyl-b...	192	C12H16O2	1000187-53-7	20
2		1H-2-Indenone,2,4,5,6,7,7a-hexah...	192	C13H20O	1000196-69-5	15
3		2,5-Dichloro-4-methoxy-pyridin-3...	192	C6H6Cl2N2O	1000300-22-4	14
4		2-Furoic acid, but-3-yn-2-yl ester	164	C9H8O3	1000299-23-2	11
5		Acetic acid, 7-oxobicyclo[2.2.1]...	182	C10H14O3	1000187-21-9	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098907.D
Acq On : 28 Sep 2017 14:36
Operator : SJ/JU
Sample : I5428-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
A-B-C-DRUM-COMP

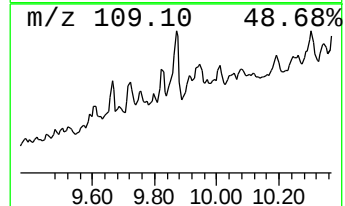
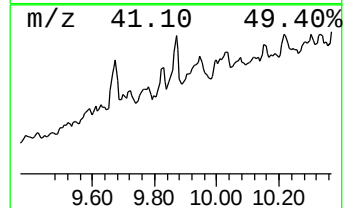
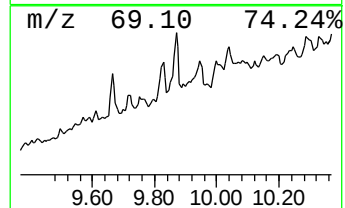
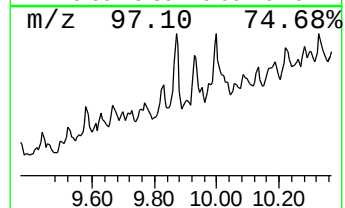
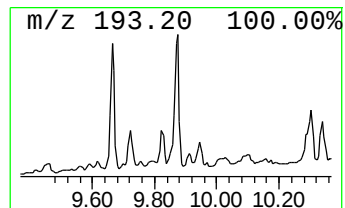
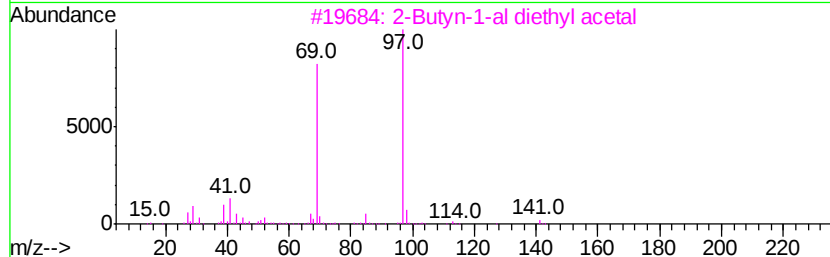
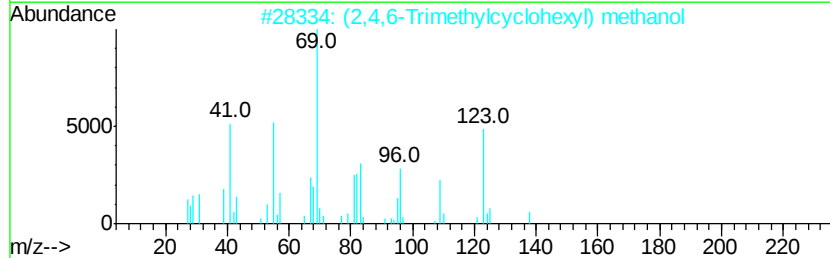
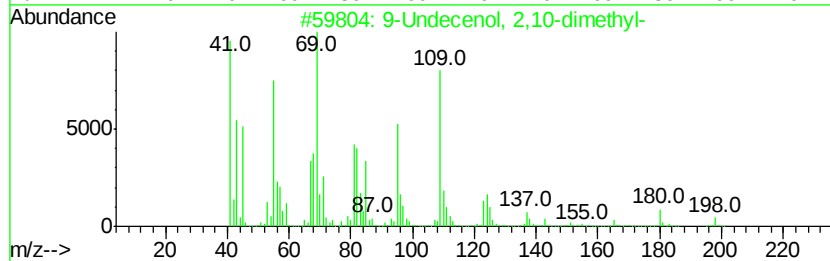
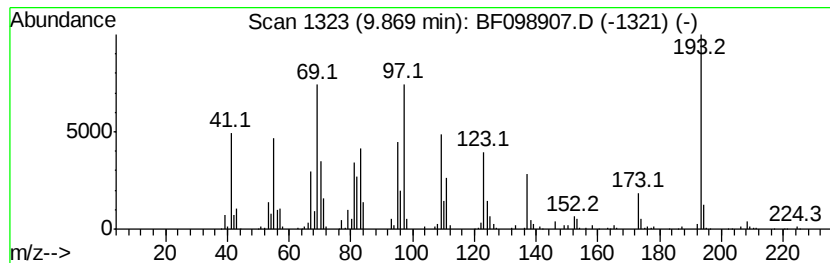
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown9.87 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.87	16.38 ng	1216610	Acenaphthene-d10	9.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Undecenol, 2,10-dimethyl-	198	C13H26O	1000131-86-0	27
2		(2,4,6-Trimethylcyclohexyl) meth...	156	C10H20O	013702-56-2	22
3		2-Butyn-1-ol diethyl acetal	142	C8H14O2	002806-97-5	22
4		7-Ethyl-2-undecen-6-one	196	C13H24O	1000374-14-9	22
5		1-Heptyne, 3-ethoxy-3,4-dimethyl-	168	C11H20O	054411-04-0	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098907.D
Acq On : 28 Sep 2017 14:36
Operator : SJ/JU
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Misc :
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ClientSampleId :
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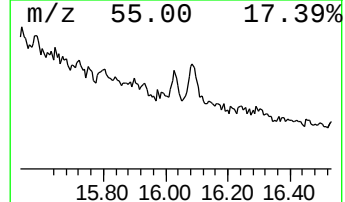
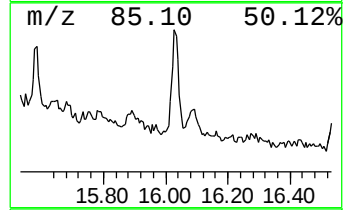
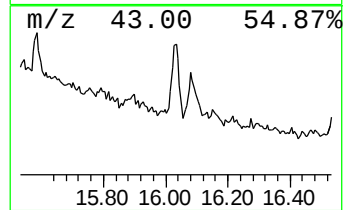
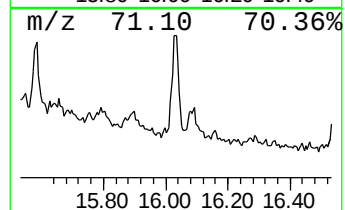
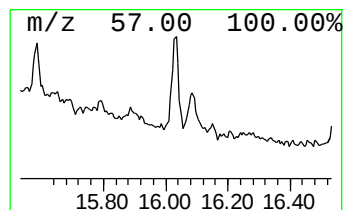
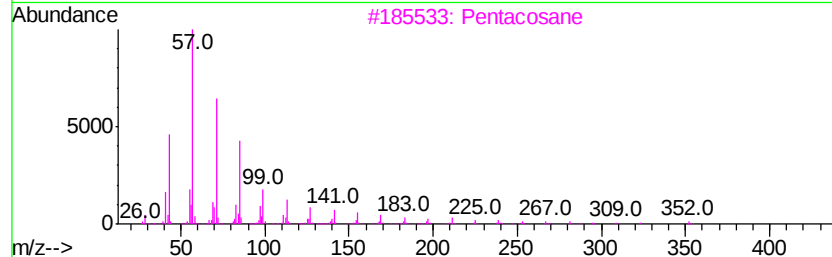
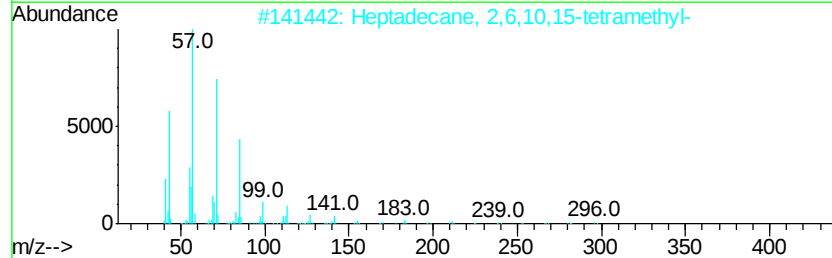
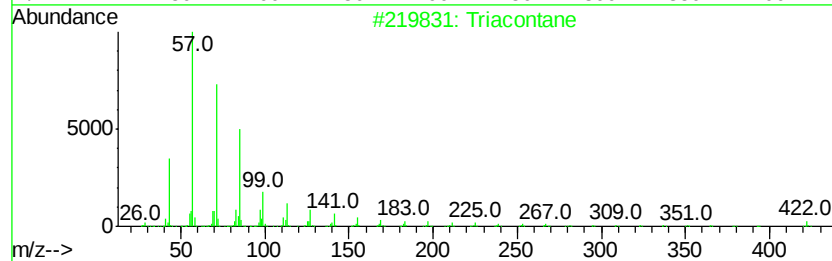
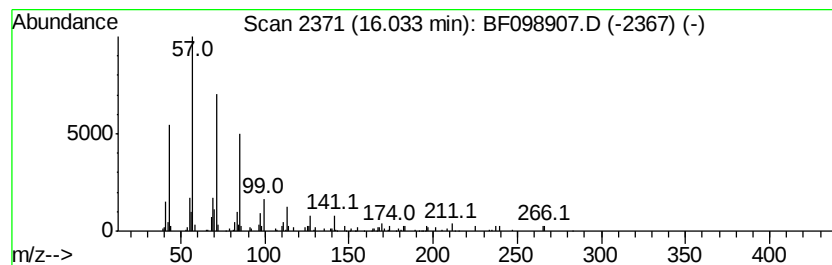
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	2.89 ng	122029	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	90
2		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
3		Pentacosane	352	C25H52	000629-99-2	86
4		Tetratriacontane	479	C34H70	014167-59-0	83
5		Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098907.D
Acq On : 28 Sep 2017 14:36
Operator : SJ/JU
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ClientSampleId :
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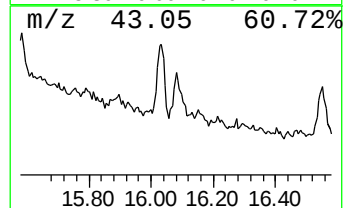
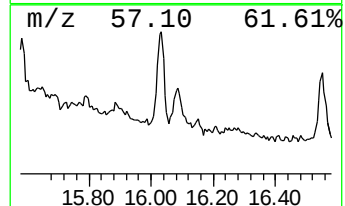
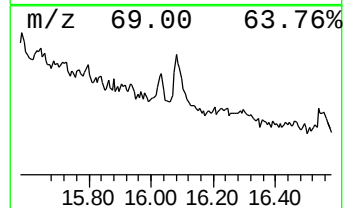
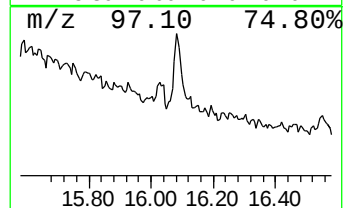
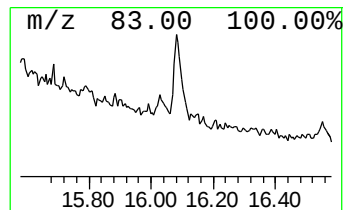
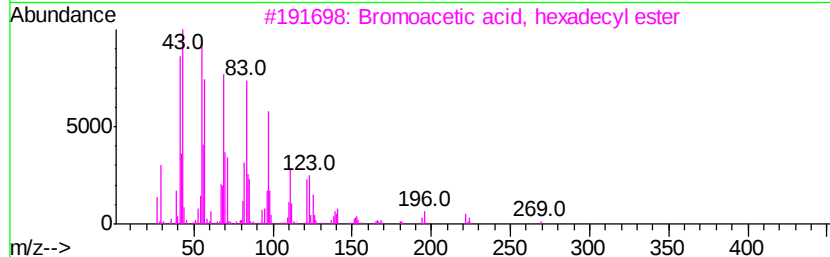
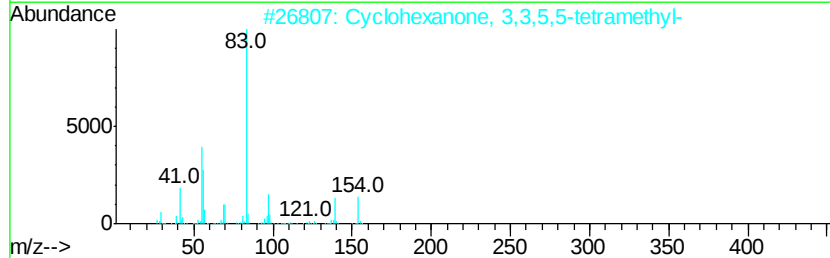
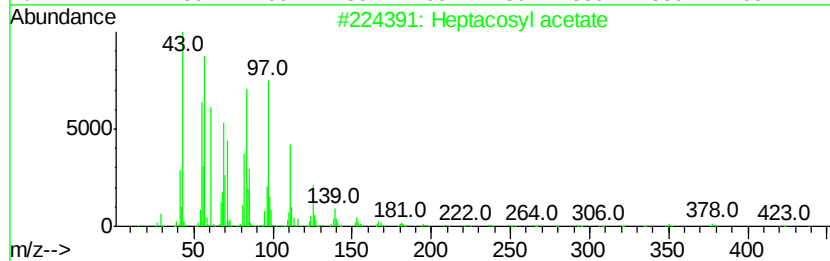
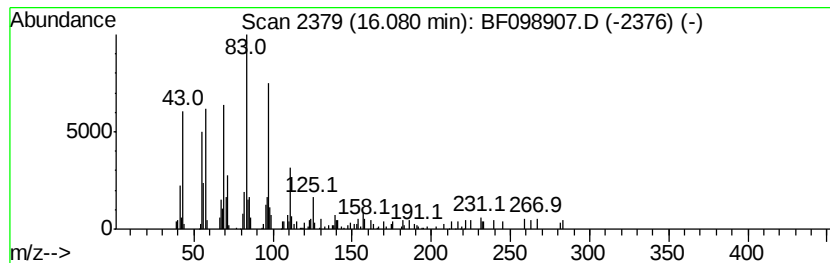
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown16.08 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	3.94 ng	166357	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosyl acetate	438	C29H58O2	1000351-78-2	38
2		Cyclohexanone, 3,3,5,5-tetramethyl-	154	C10H18O	014376-79-5	30
3		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	30
4		Cyclohexane, 1-methyl-2-propyl-	140	C10H20	004291-79-6	30
5		Cyclopentane, 1,1'-ethylidenebis-	166	C12H22	004413-21-2	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098907.D
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Operator : SJ/JU
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A-B-C-DRUM-COMP

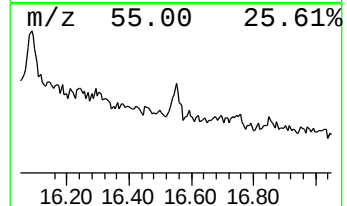
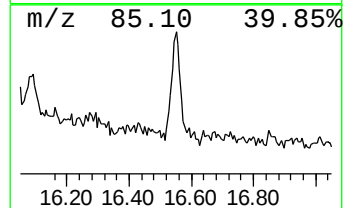
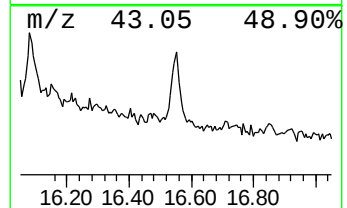
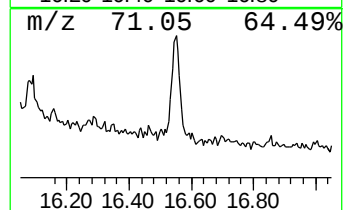
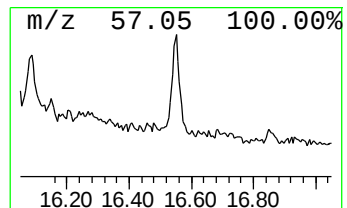
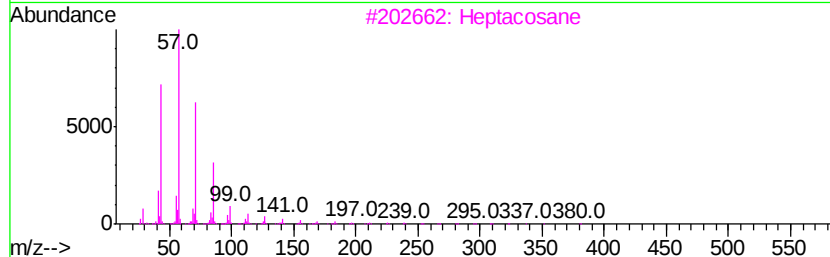
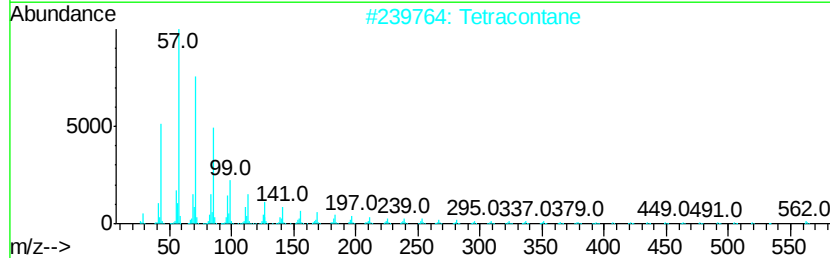
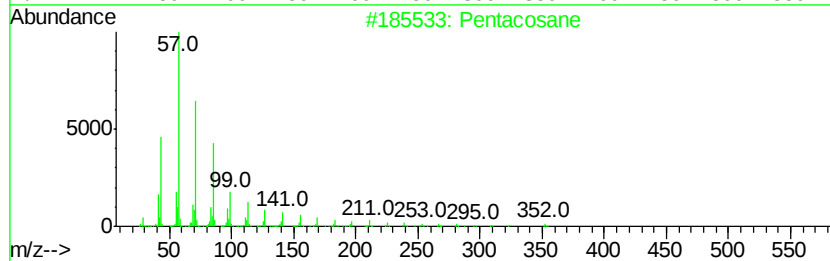
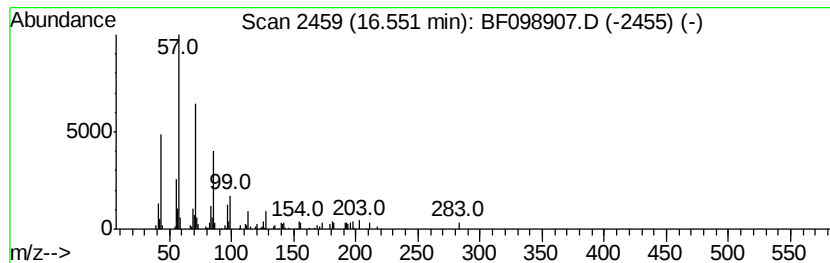
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	2.33 ng	98303	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	86
2		Tetracontane	563	C40H82	004181-95-7	78
3		Heptacosane	380	C27H56	000593-49-7	72
4		Octadecane	254	C18H38	000593-45-3	72
5		Hexacosane	366	C26H54	000630-01-3	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098907.D
Acq On : 28 Sep 2017 14:36
Operator : SJ/JU
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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A-B-C-DRUM-COMP

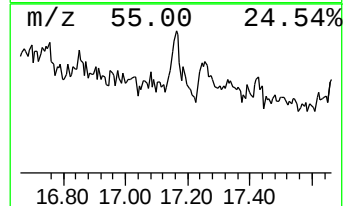
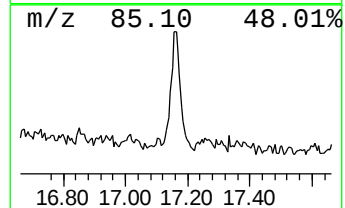
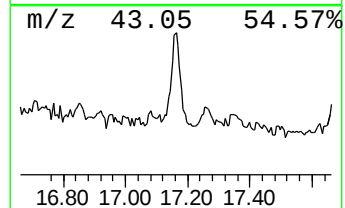
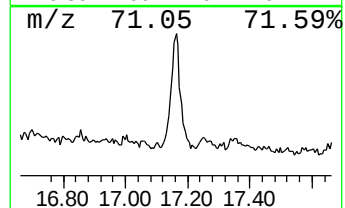
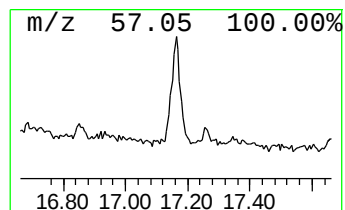
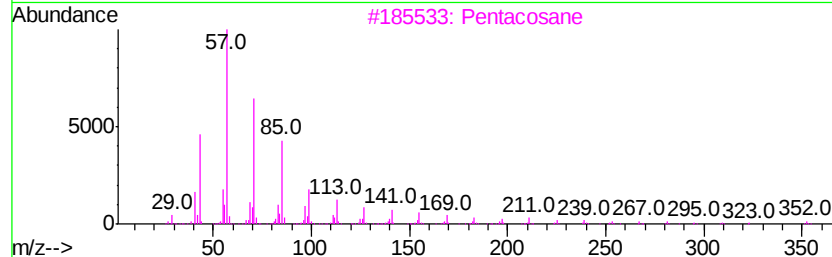
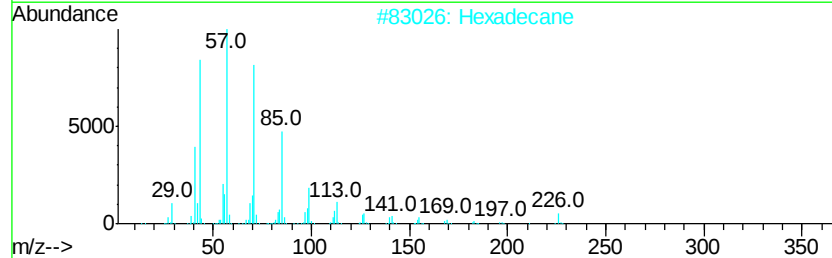
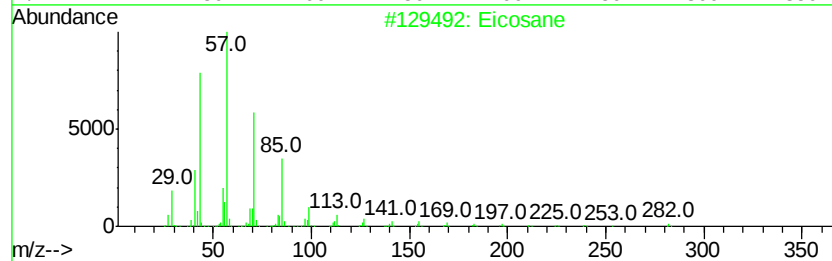
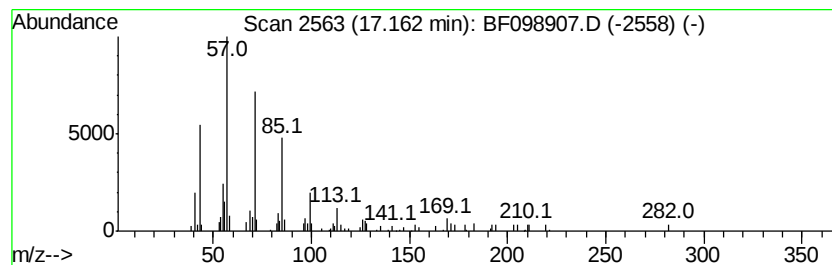
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.16	2.80 ng	118271	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	81
2		Hexadecane	226	C16H34	000544-76-3	80
3		Pentacosane	352	C25H52	000629-99-2	80
4		Eicosane, 10-methyl-	296	C21H44	054833-23-7	64
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
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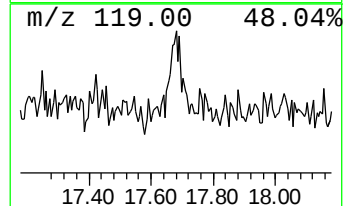
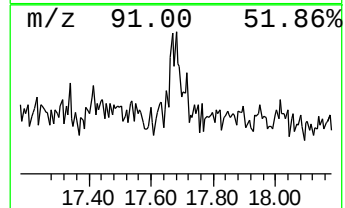
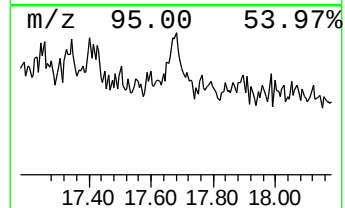
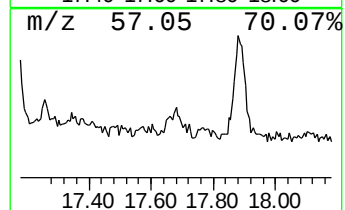
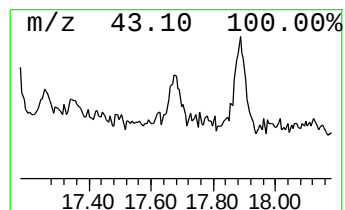
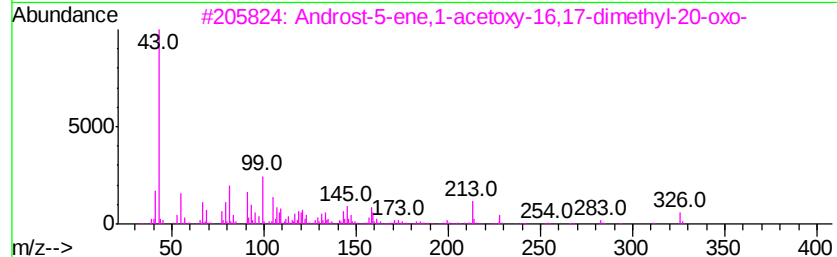
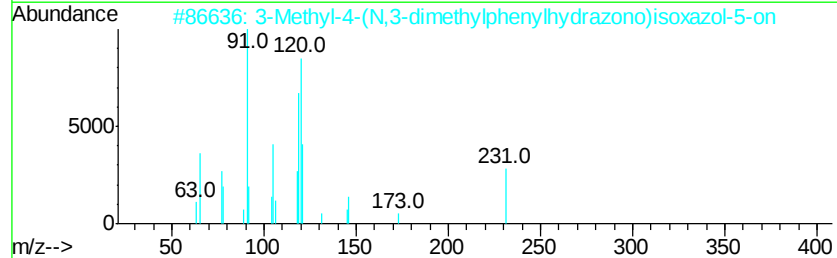
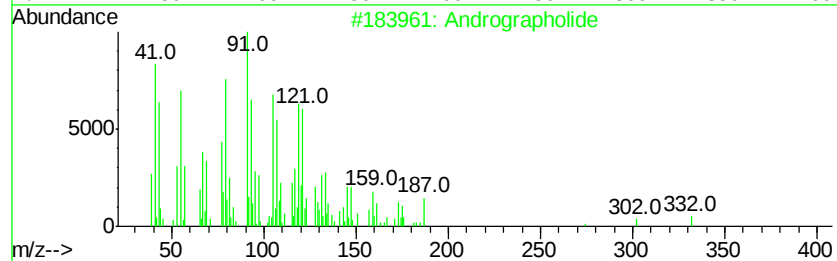
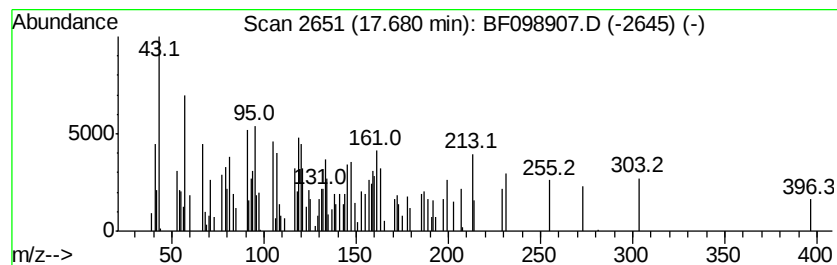
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.68 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.68	2.32 ng	98199	Perylene-d12	15.57
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Andrographolide	350	C20H30O5	005508-58-7 12
2	3-Methyl-4-(N,3-dimethylphenylhydrazono)isoxazol-5-one	231	C12H13N3O2	098664-22-3 10
3	Androst-5-ene,1-acetoxv-16,17-dimethyl-20-oxo-	386	C25H38O3	294866-91-4 10
4	Lanceol, cis	220	C15H24O	010067-28-4 10
5	Ethyl 2-acetamido-2-benzyloxy-3,4-dihydro-2H-pyran-6-carboxylate	319	C14H16F3N04	1000224-80-9 9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098907.D
Acq On : 28 Sep 2017 14:36
Operator : SJ/JU
Sample : I5428-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-B-C-DRUM-COMP

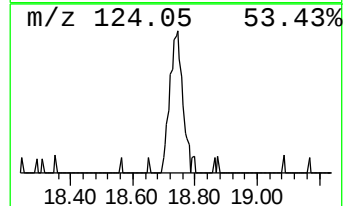
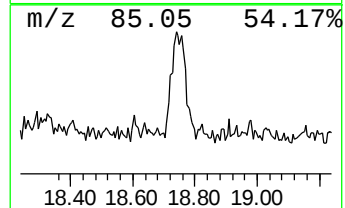
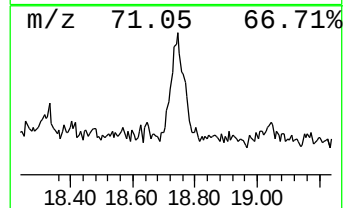
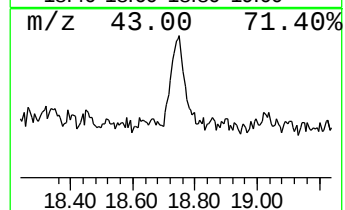
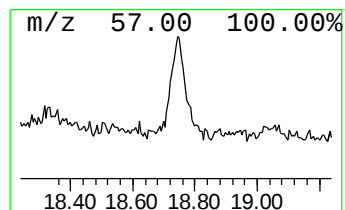
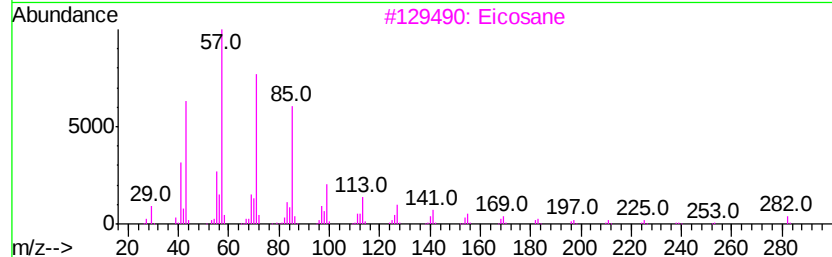
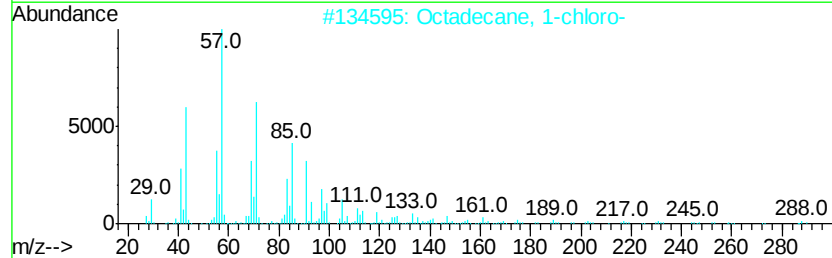
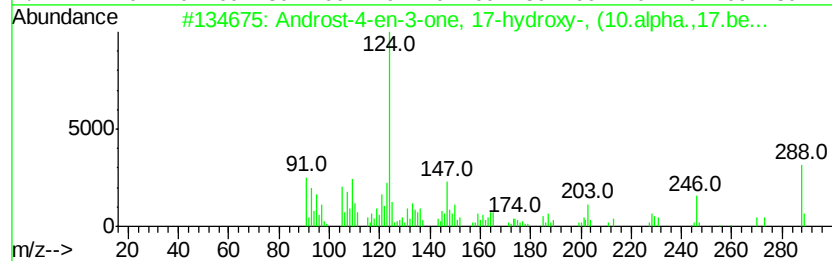
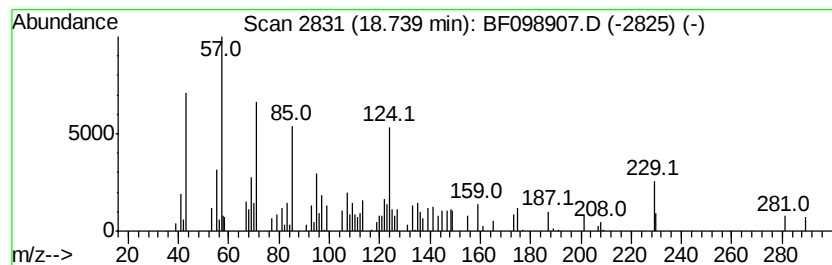
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown18.74 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.74	3.19 ng	134864	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Androst-4-en-3-one, 17-hydroxy-, ...	288	C19H28O2	000604-39-7	42
2		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	41
3		Eicosane	282	C20H42	000112-95-8	27
4		Hexatriacontane	507	C36H74	000630-06-8	27
5		Butanamide, N-[[5-(4-chloropheny...	279	C12H14ClN5O	1000320-12-4	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
 Data File : BF098907.D
 Acq On : 28 Sep 2017 14:36
 Operator : SJ/JU
 Sample : I5428-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A-B-C-DRUM-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.23	3.2	ng	146113	1	6.92	903589	20.0
2-Pentanone, 4-hy...	5.15	17.1	ng	771038	1	6.92	903589	20.0
unknown6.69	6.69	89.6	ng	4049090	1	6.92	903589	20.0
Dodecane, 2,7,10-...	9.21	3.2	ng	237253	3	9.96	1485650	20.0
unknown9.35	9.35	6.2	ng	459179	3	9.96	1485650	20.0
unknown9.59	9.59	4.5	ng	332919	3	9.96	1485650	20.0
unknown9.87	9.87	16.4	ng	1216610	3	9.96	1485650	20.0
triacontane	16.03	2.9	ng	122029	6	15.57	845022	20.0
unknown16.08	16.08	3.9	ng	166357	6	15.57	845022	20.0
Pentacosane	16.55	2.3	ng	98303	6	15.57	845022	20.0
Eicosane	17.16	2.8	ng	118271	6	15.57	845022	20.0
unknown17.68	17.68	2.3	ng	98199	6	15.57	845022	20.0
unknown18.74	18.74	3.2	ng	134864	6	15.57	845022	20.0