

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
 Data File : BF098576.D
 Acq On : 15 Sep 2017 18:39
 Operator : SJ/JU
 Sample : I5229-06
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 UT5400S16

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-BF091117.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	3.010	153	157	174	rBV2	17509	72660	2.25%	0.223%
2	4.828	462	466	479	rBV	233251	335130	10.39%	1.027%
3	5.257	535	539	560	rBV	3212295	3224155	100.00%	9.877%
4	6.298	711	716	732	rBV	3202688	3201617	99.30%	9.808%
5	6.416	732	736	739	rBV	3670241	3220825	99.90%	9.867%
6	6.639	771	774	782	rBV	949579	835692	25.92%	2.560%
7	6.798	797	801	804	rBV	2505122	2258496	70.05%	6.919%
8	7.210	866	871	884	rBV	1885276	2045972	63.46%	6.268%
9	7.927	988	993	999	rBV	1252682	1122553	34.82%	3.439%
10	9.004	1170	1176	1179	rBV	3089977	2838069	88.03%	8.694%
11	9.404	1239	1244	1247	rBV	463160	409951	12.71%	1.256%
12	9.492	1254	1259	1266	rVB2	31024	51099	1.58%	0.157%
13	9.680	1285	1291	1295	rBV	1344549	1257293	39.00%	3.852%
14	10.086	1354	1360	1362	rBV2	24333	37520	1.16%	0.115%
15	10.469	1420	1425	1436	rBV	2121556	2051182	63.62%	6.284%
16	10.586	1441	1445	1451	rVB	61303	61886	1.92%	0.190%
17	11.163	1538	1543	1546	rBV	1594183	1346364	41.76%	4.124%
18	11.698	1630	1634	1637	rBV	33860	36601	1.14%	0.112%
19	12.380	1744	1750	1755	rBV2	36656	62815	1.95%	0.192%
20	12.751	1808	1813	1816	rBV	3061094	3013567	93.47%	9.232%
21	13.304	1905	1907	1912	rVB3	34511	39133	1.21%	0.120%
22	13.645	1961	1965	1972	rBV	304241	363319	11.27%	1.113%
23	13.798	1987	1991	1995	rBV	1387076	1221864	37.90%	3.743%
24	13.962	2015	2019	2024	rBV6	27447	41435	1.29%	0.127%
25	14.274	2067	2072	2077	rBV2	108502	155653	4.83%	0.477%
26	14.545	2115	2118	2127	rBV2	144100	174054	5.40%	0.533%
27	14.627	2127	2132	2135	rVV	102389	110363	3.42%	0.338%
28	14.698	2140	2144	2147	rBV2	46255	47904	1.49%	0.147%
29	14.868	2169	2173	2176	rBV	376739	395434	12.26%	1.211%
30	14.898	2176	2178	2182	rVB4	46777	53525	1.66%	0.164%
31	15.198	2224	2229	2236	rBV	812356	978858	30.36%	2.999%
32	15.398	2258	2263	2266	rBV	84327	107801	3.34%	0.330%
33	15.603	2294	2298	2302	rBV	73820	98982	3.07%	0.303%
34	15.656	2302	2307	2312	rVV	49971	84497	2.62%	0.259%

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

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
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35	16.315	2413	2419	2426	rBV2	105057	192532	5.97%	0.590%
36	17.021	2533	2539	2551	rBV7	117137	319232	9.90%	0.978%
37	17.509	2618	2622	2629	rVB9	48055	90786	2.82%	0.278%
38	17.727	2653	2659	2666	rBV8	80843	203510	6.31%	0.623%
39	17.862	2677	2682	2691	rBV7	80459	199955	6.20%	0.613%
40	18.327	2753	2761	2770	rVB7	54171	184197	5.71%	0.564%
41	19.209	2904	2911	2920	rVB7	35145	96664	3.00%	0.296%

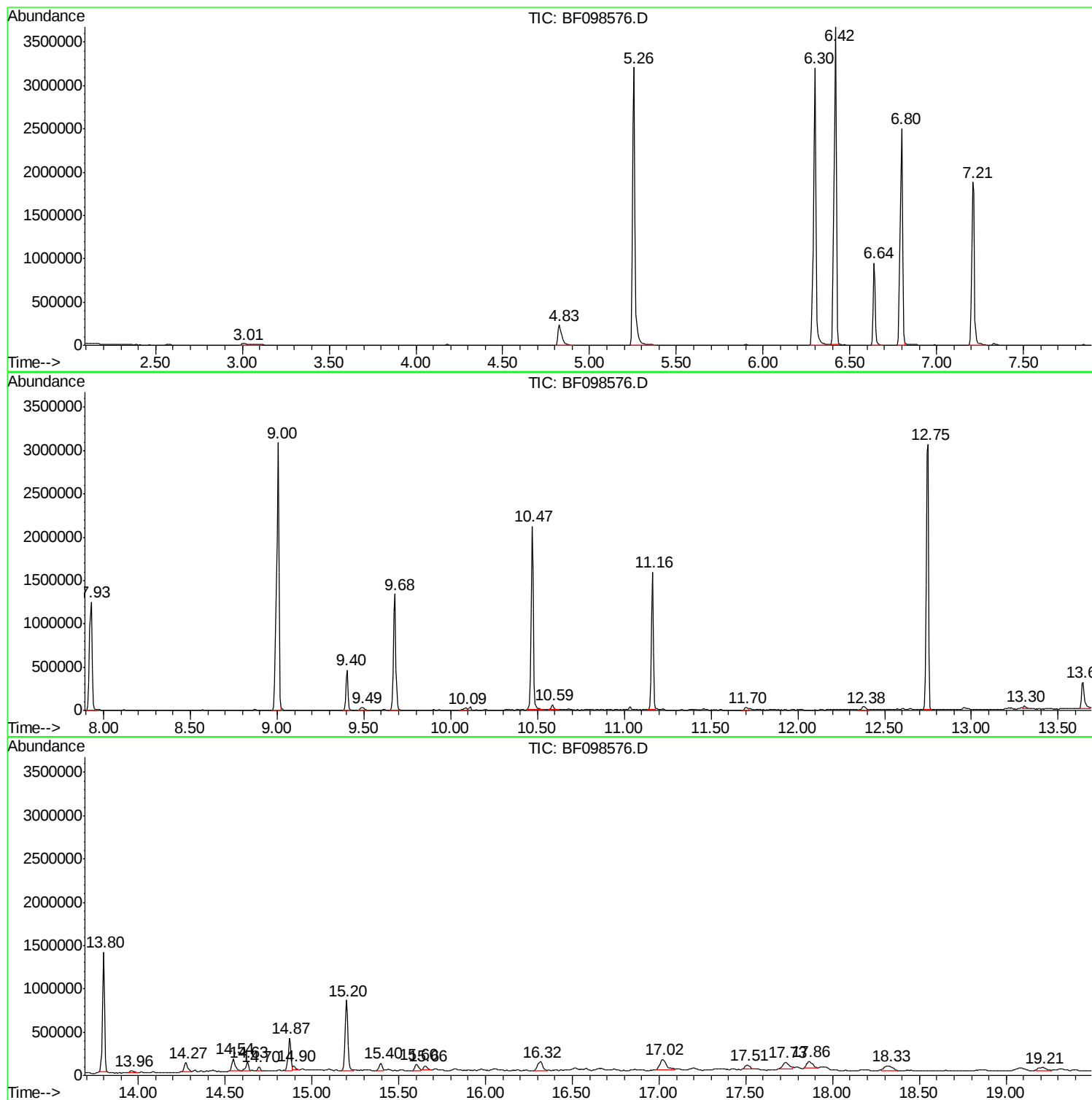
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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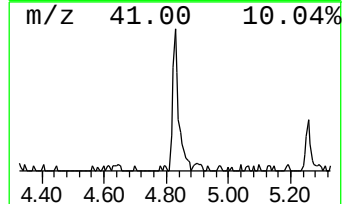
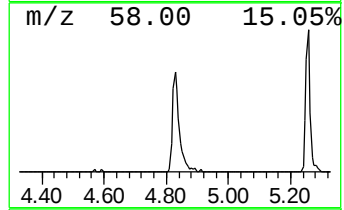
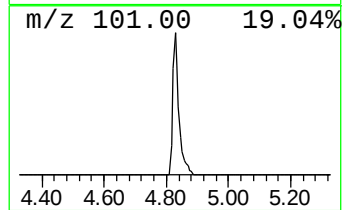
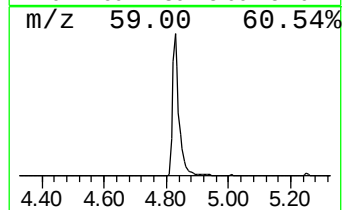
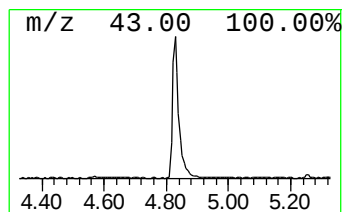
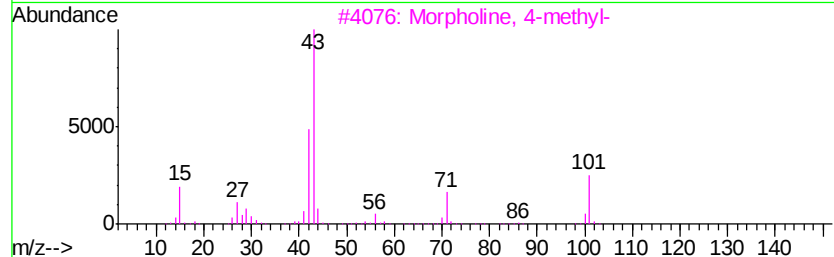
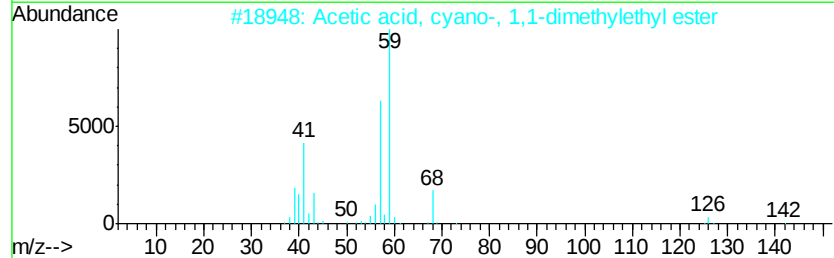
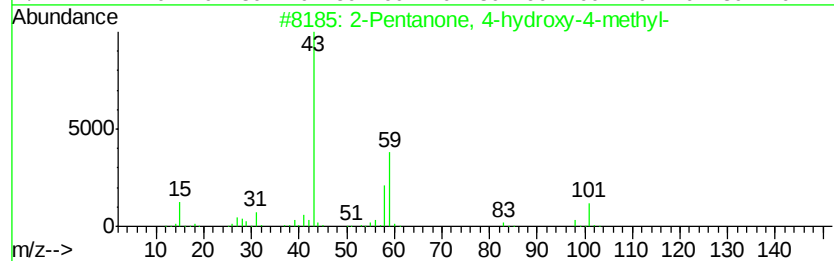
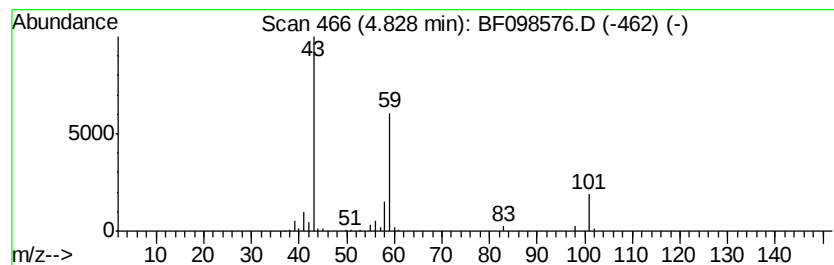
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	8.02 ng	335130	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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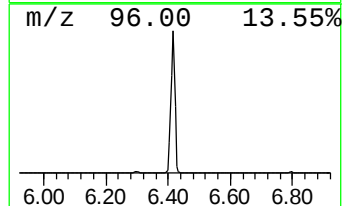
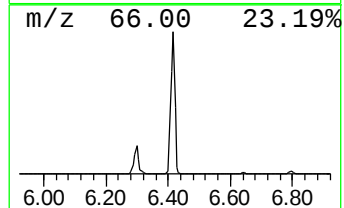
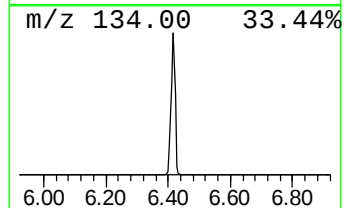
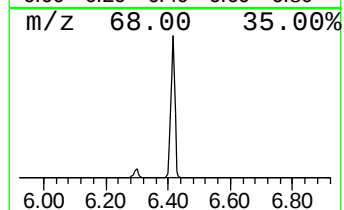
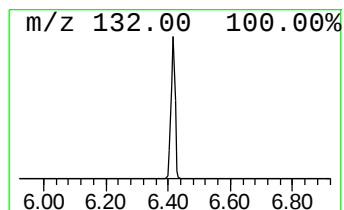
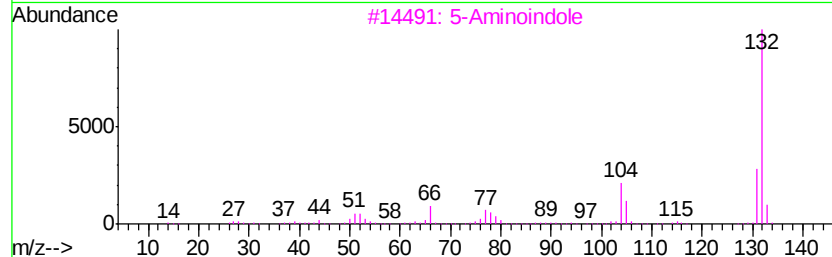
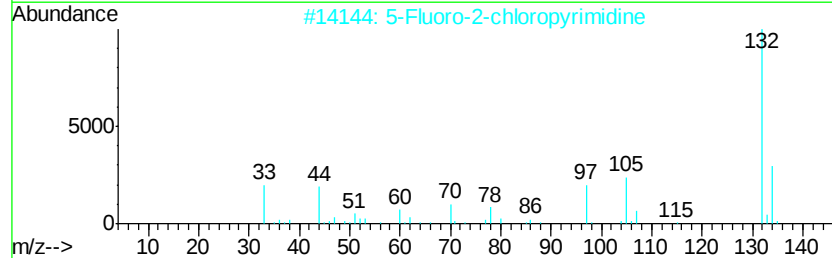
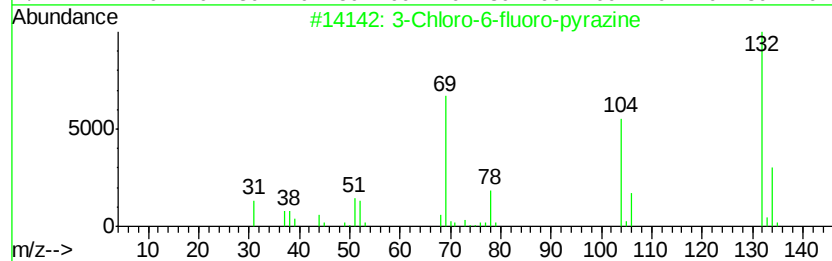
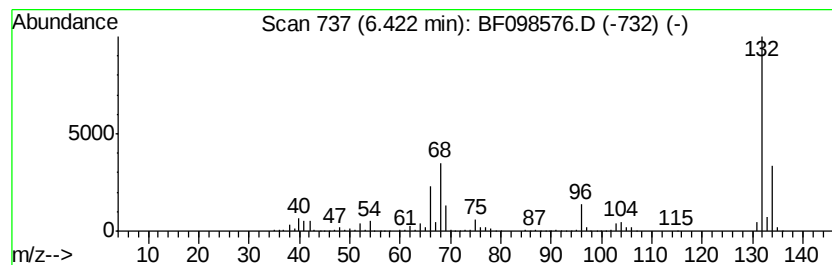
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	77.08 ng	3220830	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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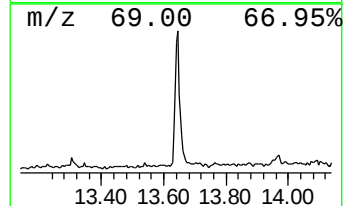
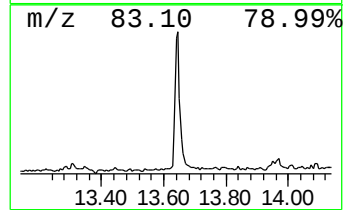
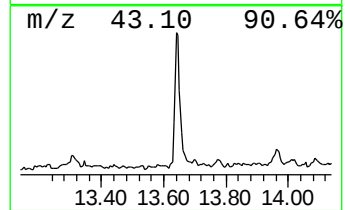
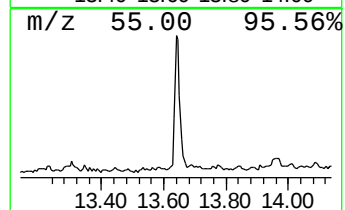
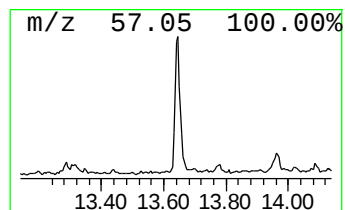
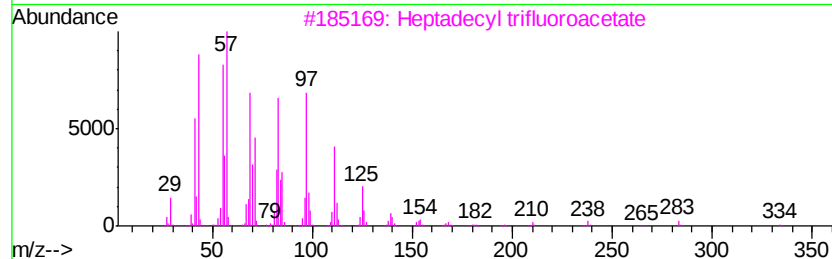
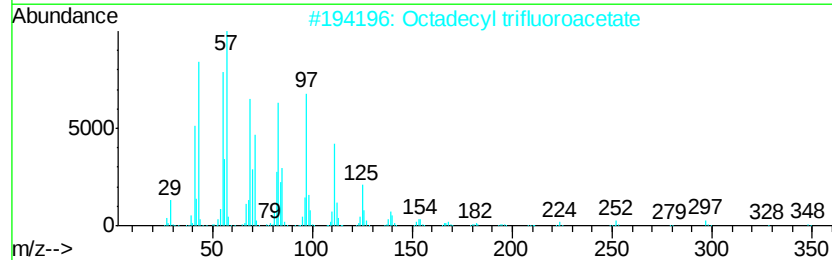
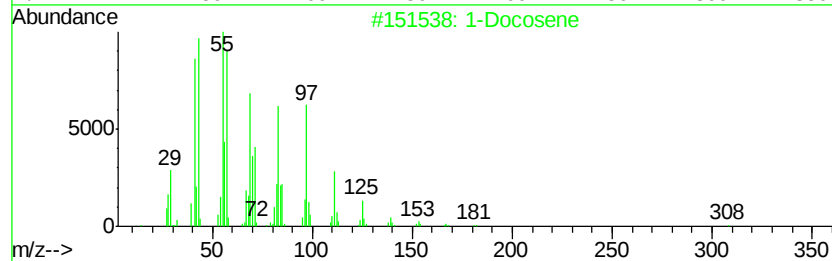
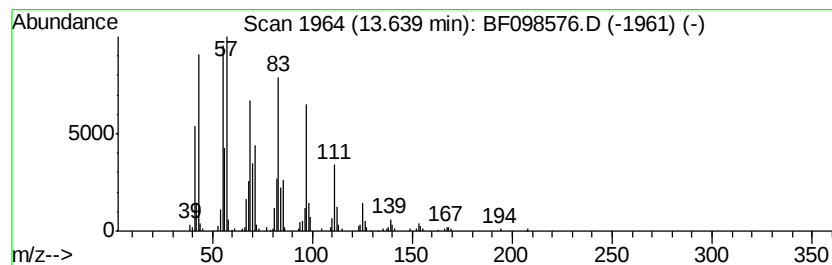
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	5.95 ng	363319	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	94
2		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



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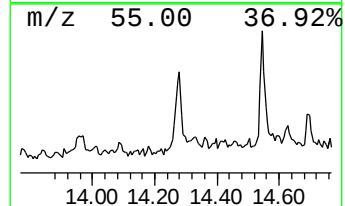
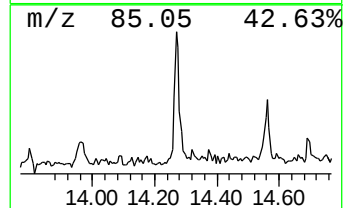
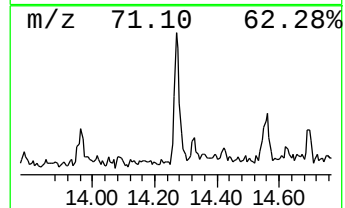
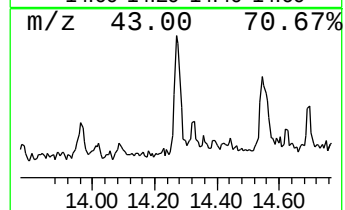
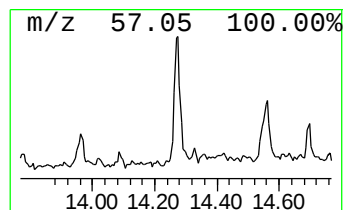
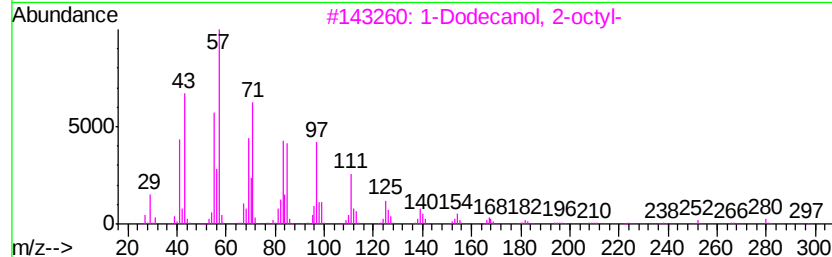
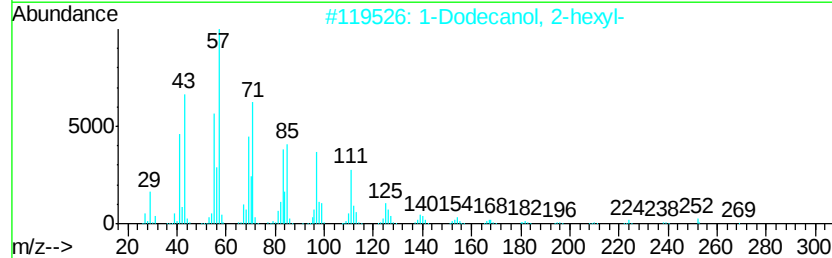
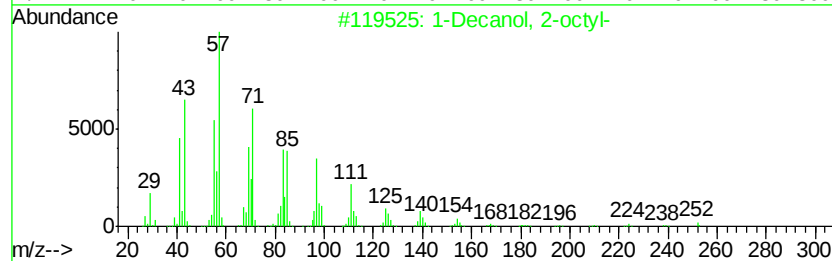
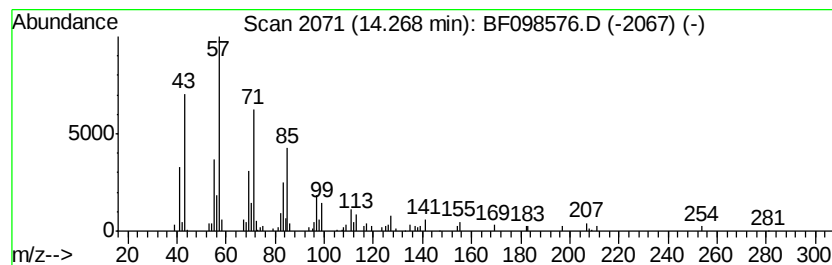
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Decanol, 2-octyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.27	2.55 ng	155653	Chrysene-d12	13.80
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Decanol, 2-octyl-	270 C18H38O	045235-48-1	91
2	1-Dodecanol, 2-hexyl-	270 C18H38O	110225-00-8	91
3	1-Dodecanol, 2-octyl-	298 C20H42O	005333-42-6	91
4	Ethanol, 2-(tetradecyloxy)-	258 C16H34O2	002136-70-1	74
5	1-Decanol, 2-hexyl-	242 C16H34O	002425-77-6	74



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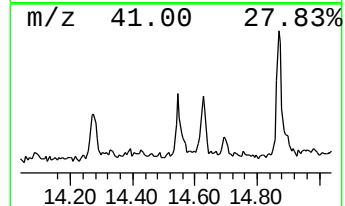
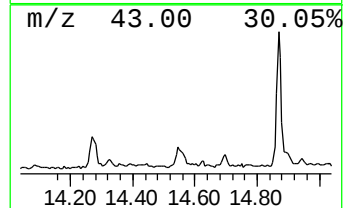
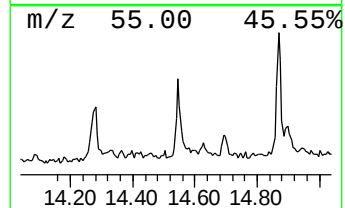
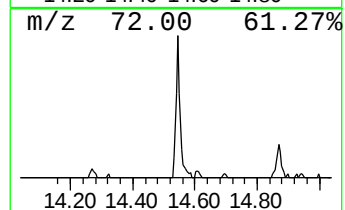
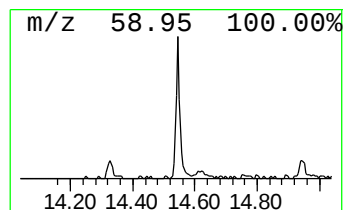
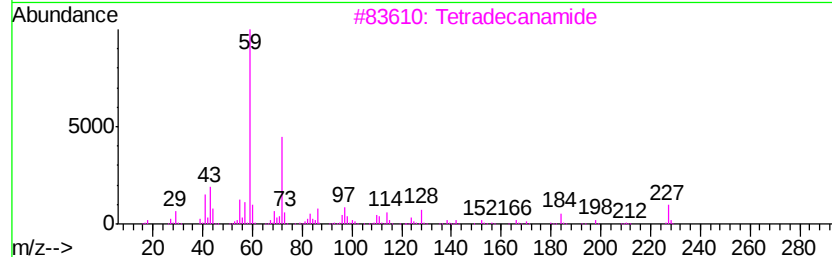
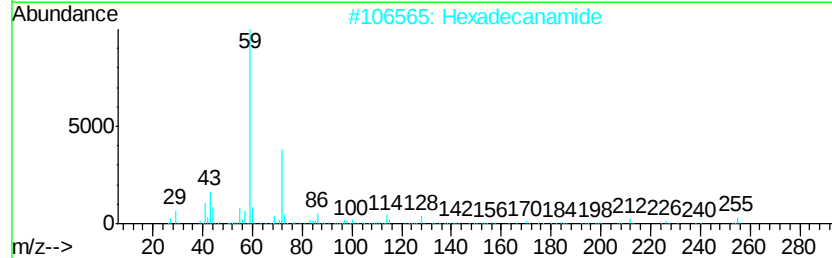
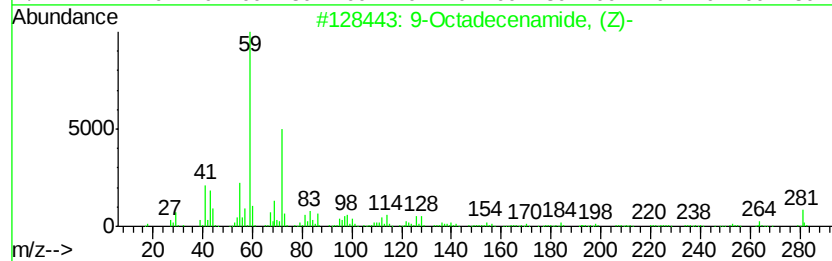
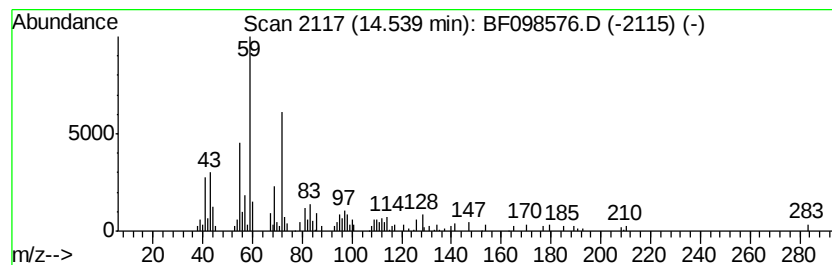
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	3.56 ng	174054	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2		Hexadecanamide	255	C16H33NO	000629-54-9	72
3		Tetradecanamide	227	C14H29NO	000638-58-4	72
4		Cyclohexanecarboxamide	127	C7H13NO	001122-56-1	27
5		3,4-Dihydroxy-.alpha.-(isopropyl...	211	C11H17NO3	007683-59-2	15



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Operator : SJ/JU
Sample : I5229-06
Misc :
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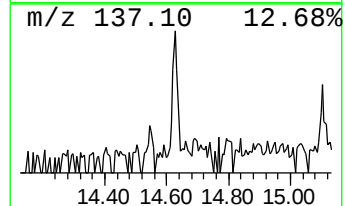
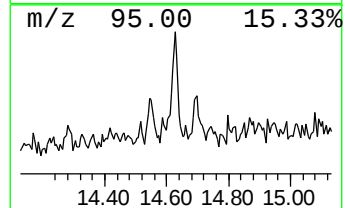
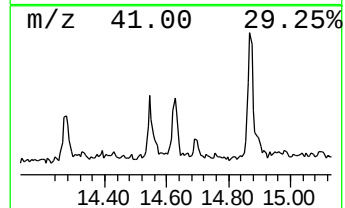
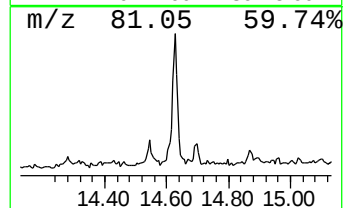
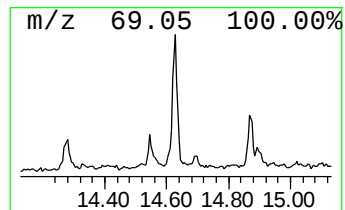
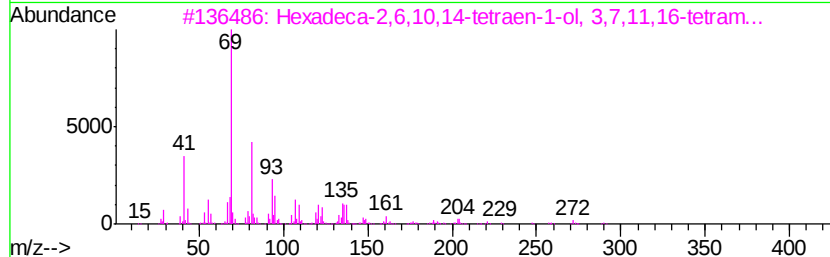
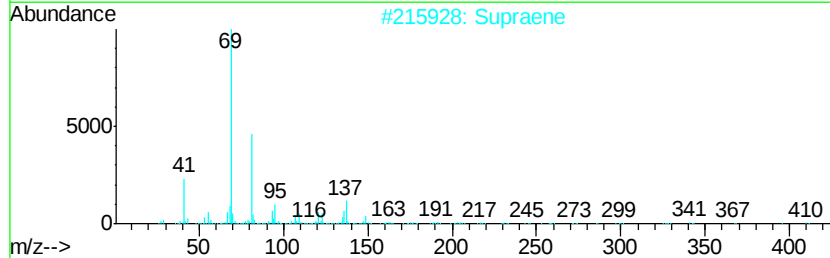
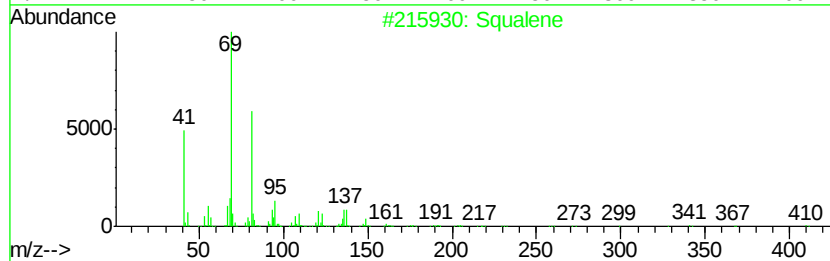
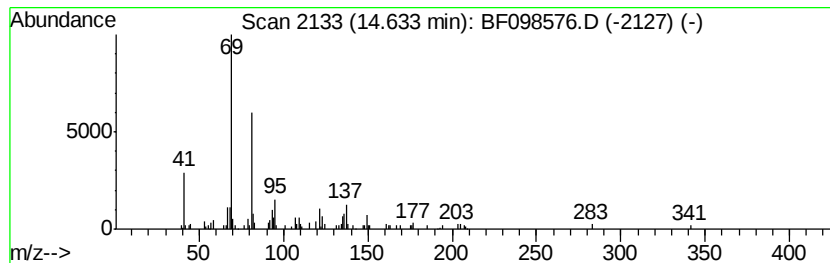
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	2.25 ng	110363	Perylene-d12	15.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	000111-02-4	91
2	Supraene	410 C30H50	007683-64-9	91
3	Hexadeca-2,6,10,14-tetraen-1-ol,...	290 C20H34O	007614-21-3	78
4	7,11-Dimethyldodeca-2,6,10-trien...	208 C14H24	125529-10-4	74
5	4,8,12-Tetradecatrienal, 5,9,13-...	248 C17H28O	066408-55-7	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
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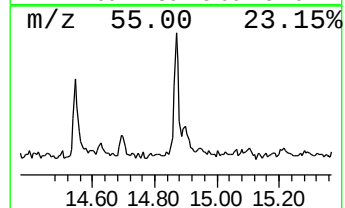
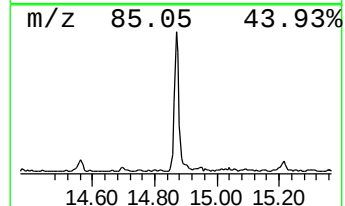
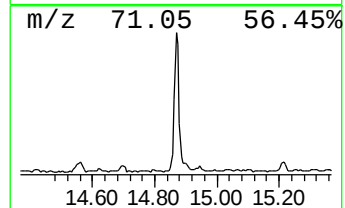
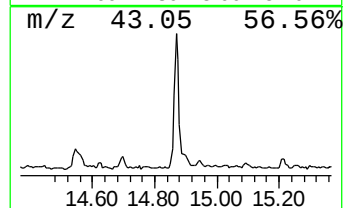
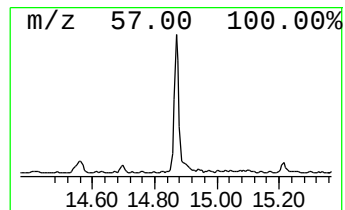
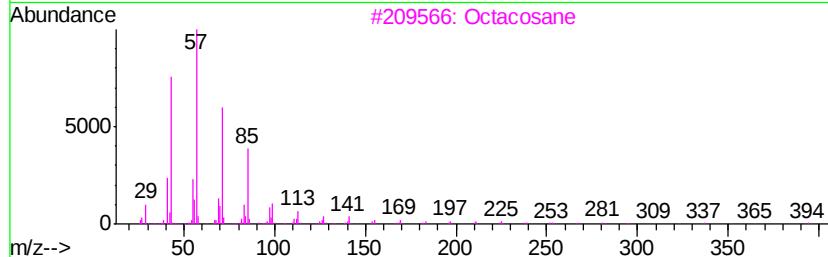
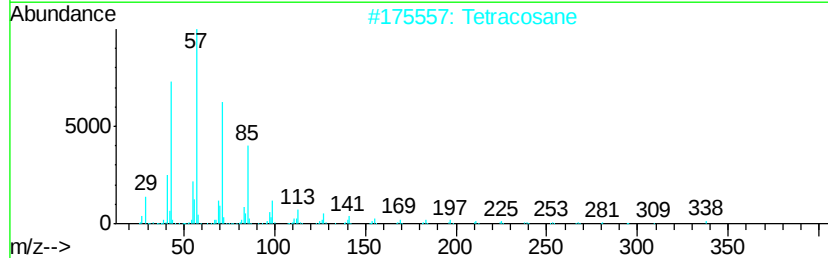
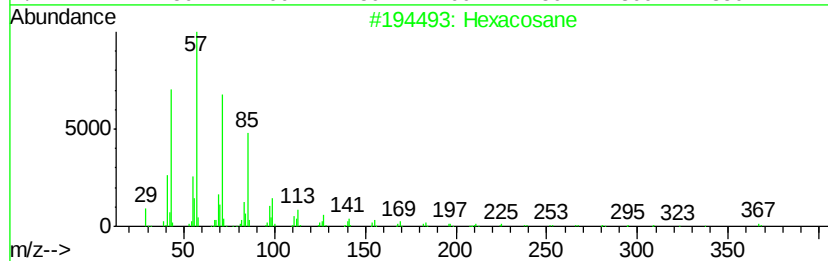
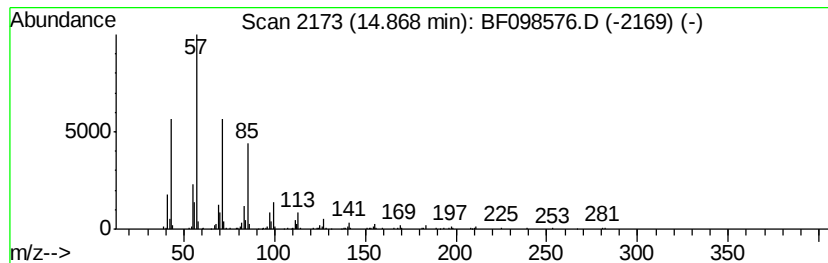
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	8.08 ng	395434	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Nonadecane	268	C19H40	000629-92-5	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
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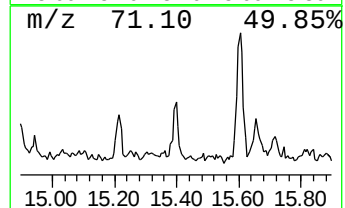
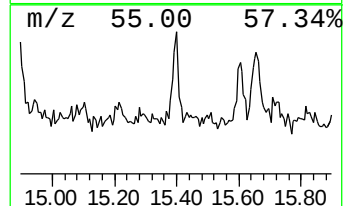
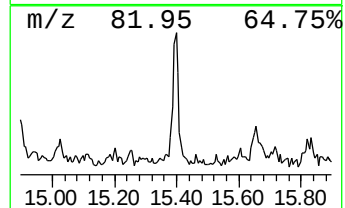
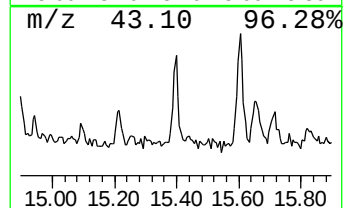
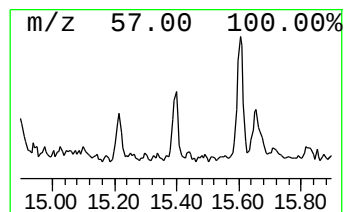
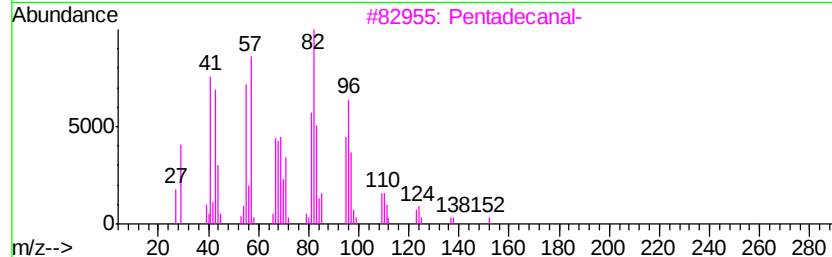
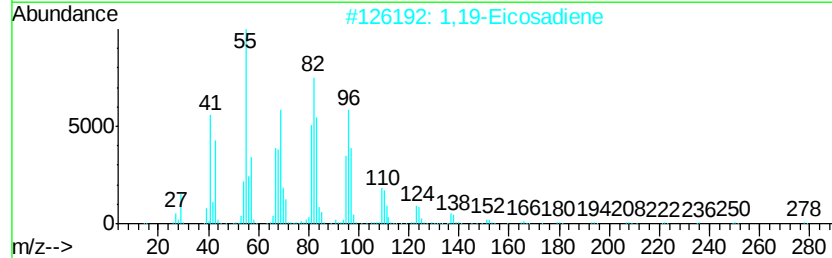
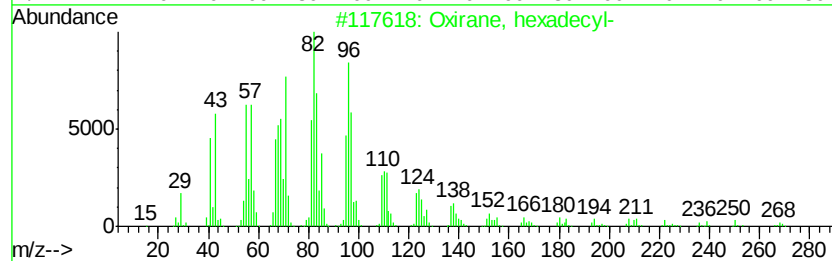
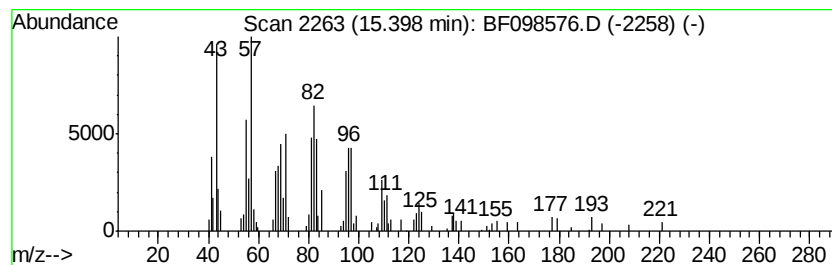
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Oxirane, hexadecyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.40	2.20 ng	107801	Perylene-d12	15.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Oxirane, hexadecyl-	268 C18H36O	007390-81-0 91
2		1,19-Eicosadiene	278 C20H38	014811-95-1 58
3		Pentadecanal-	226 C15H30O	002765-11-9 50
4		1,16-Hexadecanediol	258 C16H34O2	007735-42-4 49
5		17-Pentatriacontene	491 C35H70	006971-40-0 46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
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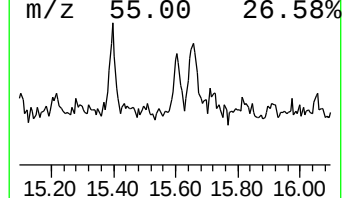
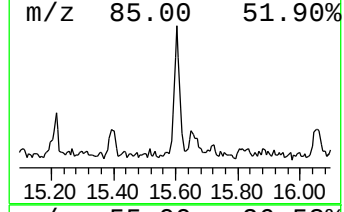
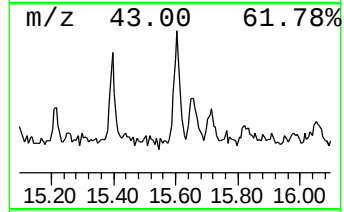
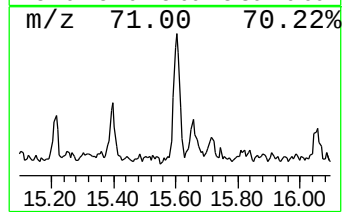
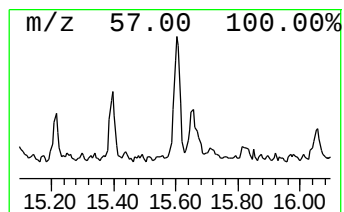
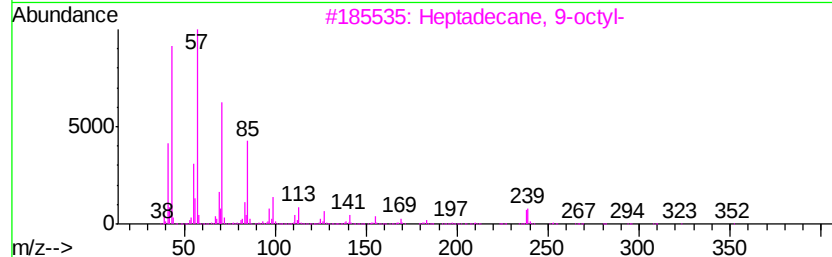
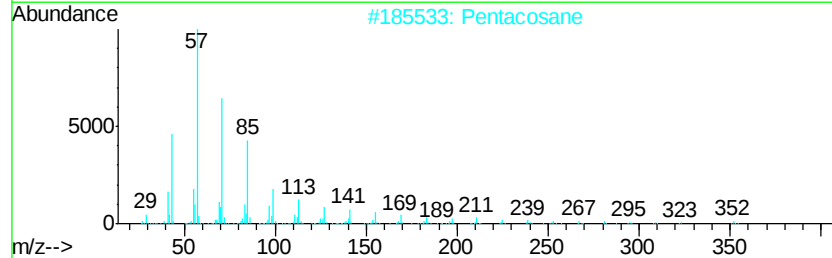
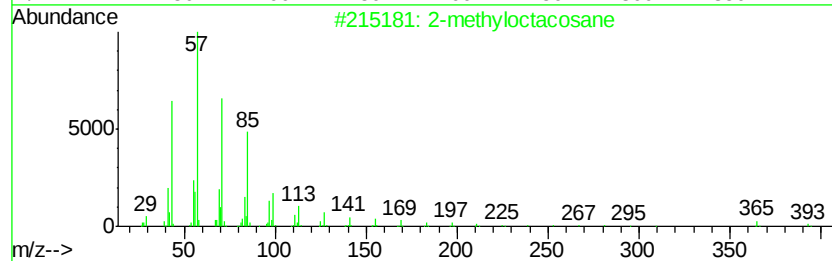
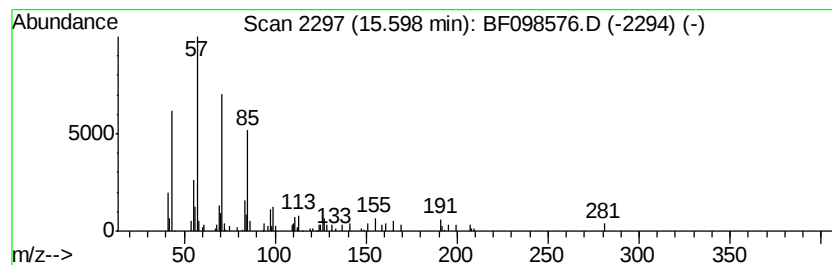
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-methyloctacosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	2.02 ng	98982	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	90
2		Pentacosane	352	C25H52	000629-99-2	90
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4		Octadecane	254	C18H38	000593-45-3	86
5		Heptadecane	240	C17H36	000629-78-7	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
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Acq On : 15 Sep 2017 18:39
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Misc :
ALS Vial : 5 Sample Multiplier: 1

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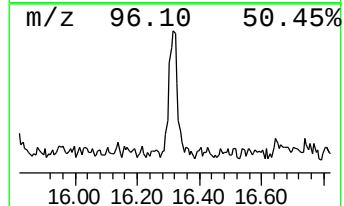
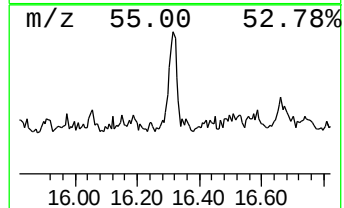
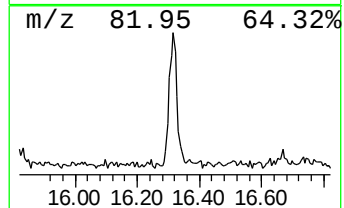
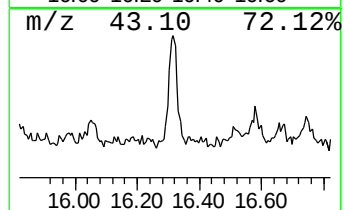
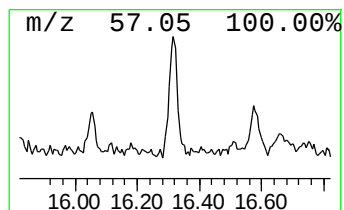
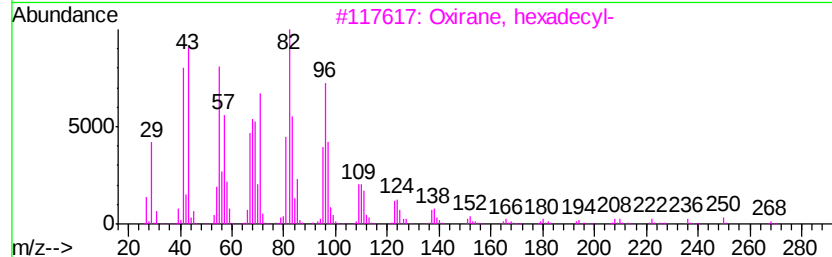
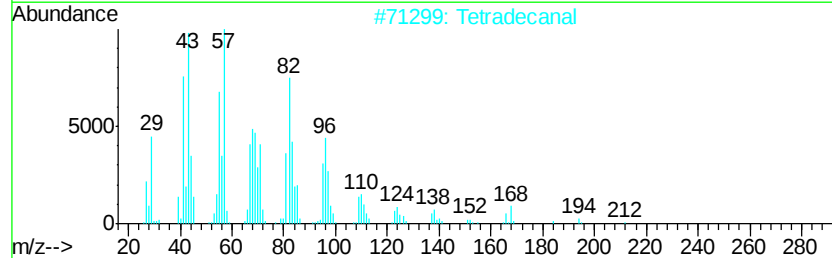
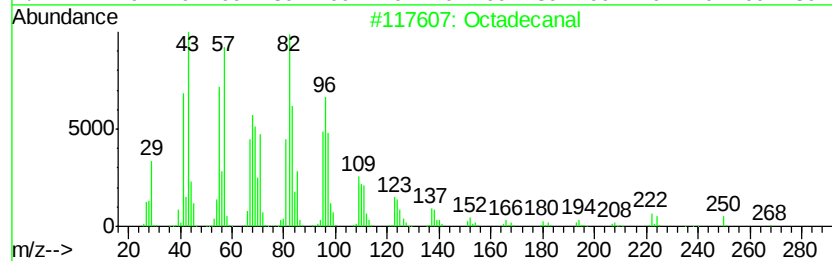
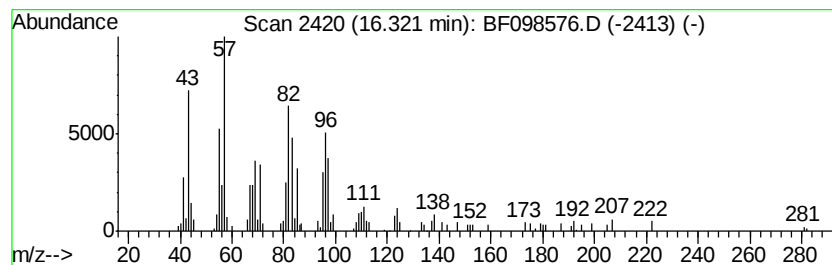
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	3.93 ng	192532	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanal	268	C18H36O	000638-66-4	81
2		Tetradecanal	212	C14H28O	000124-25-4	78
3		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	74
4		(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	52
5		1,15-Pentadecanediol	244	C15H32O2	014722-40-8	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
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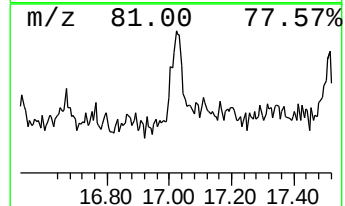
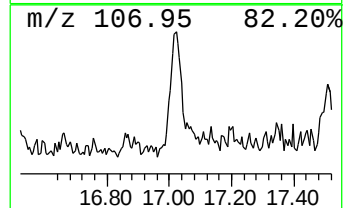
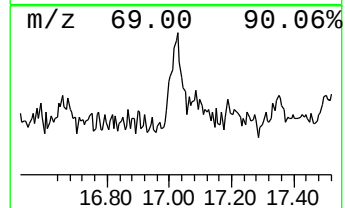
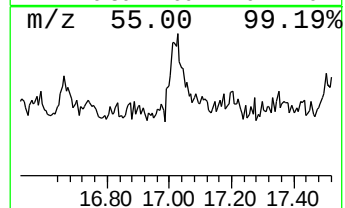
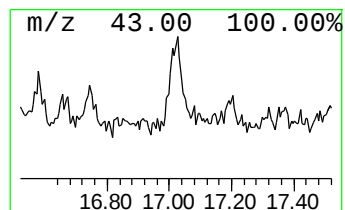
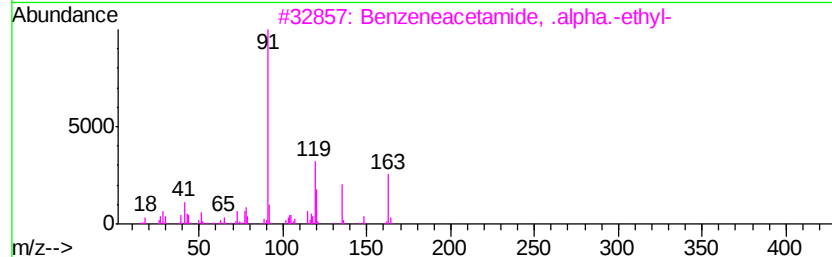
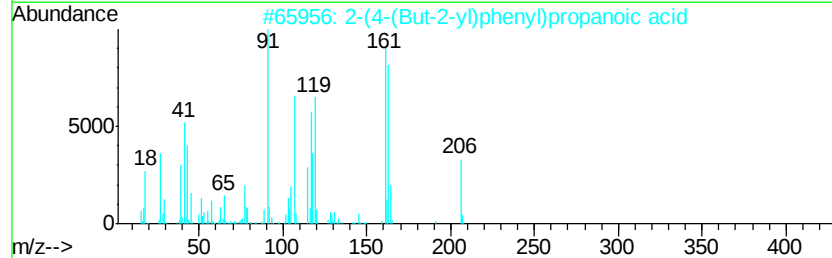
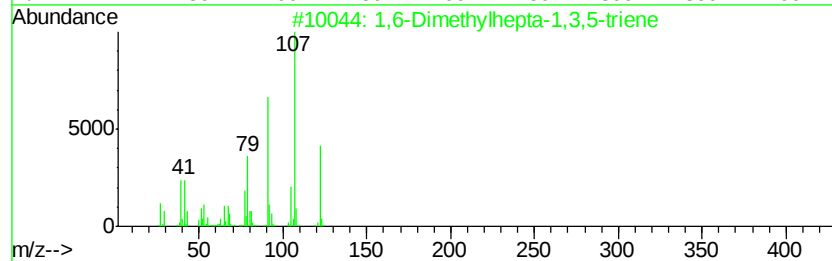
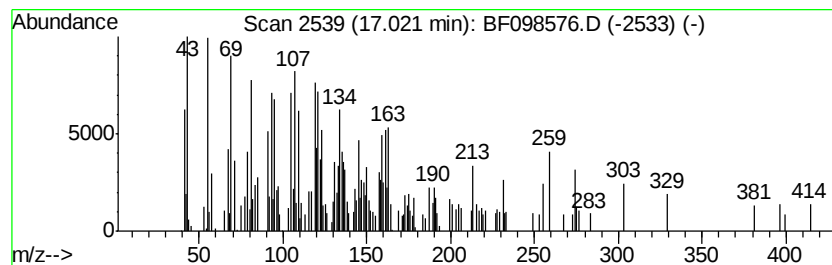
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.02	6.52 ng	319232	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,6-Dimethylhepta-1,3,5-triene	122	C9H14	1000196-61-0	25
2		2-(4-(But-2-yl)phenyl)propanoic ...	206	C13H18O2	064451-76-9	25
3		Benzeneacetamide, .alpha.-ethyl-	163	C10H13NO	000090-26-6	18
4		(-)-Neoclovene-(I), dihydro-	206	C15H26	1000152-82-1	18
5		1,1,3a-Trimethyl-1a,3a,5,6-tetra...	176	C12H16O	091531-54-3	15



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
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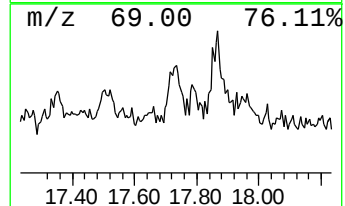
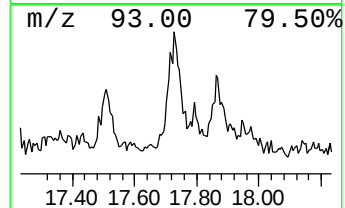
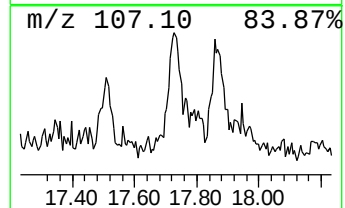
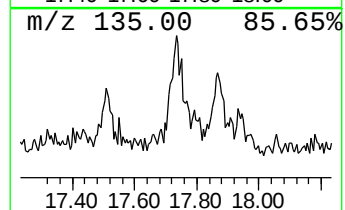
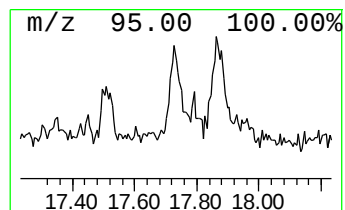
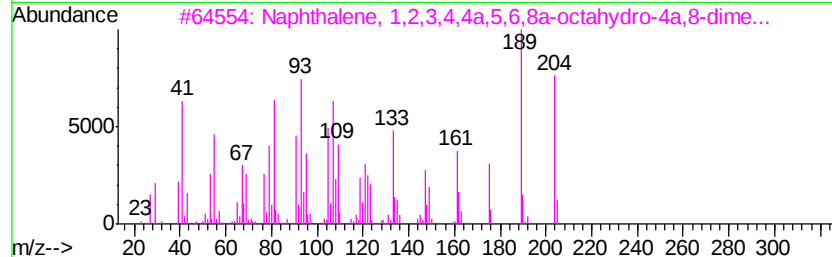
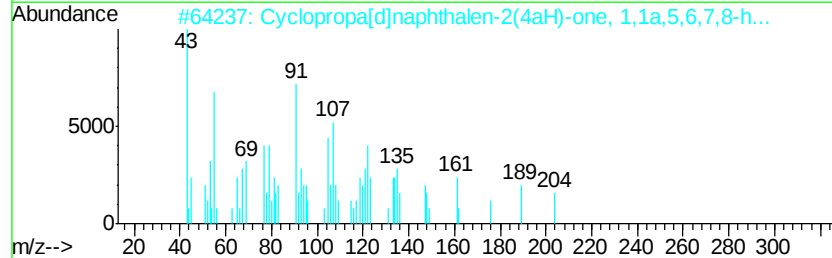
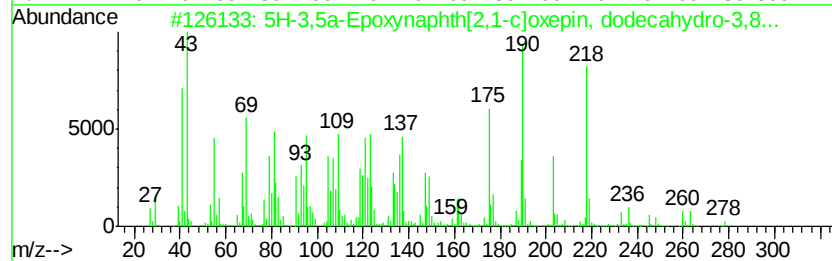
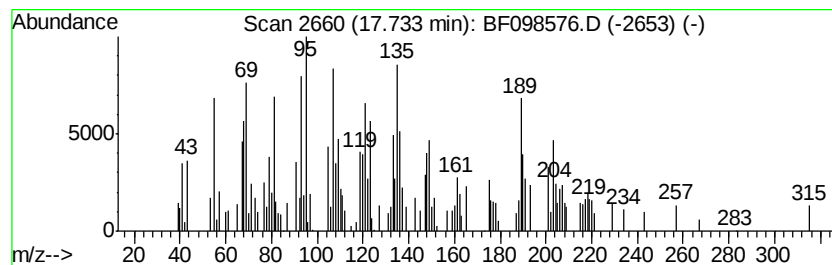
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.73 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.73	4.16 ng	203510	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5H-3,5a-Epoxy naphth[2,1-c]oxepin...	278	C18H30O2	001153-34-0	43
2		Cyclopropa[d]naphthalen-2(4aH)-o...	204	C14H20O	004677-90-1	35
3		Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	35
4		Guaia-9,11-diene	204	C15H24	1000374-19-8	25
5		1-Cycloheptene, 1,4-dimethyl-3-(...	204	C15H24	1000159-38-6	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098576.D
Acq On : 15 Sep 2017 18:39
Operator : SJ/JU
Sample : I5229-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UT5400S16

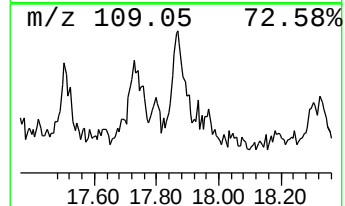
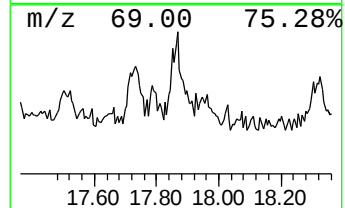
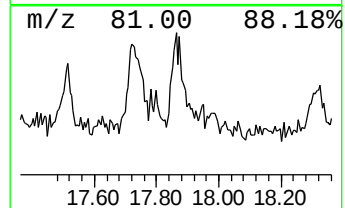
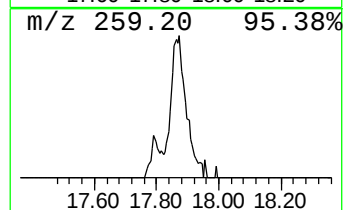
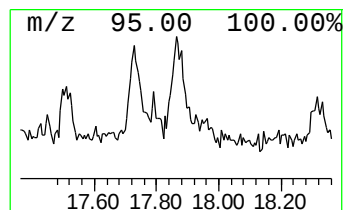
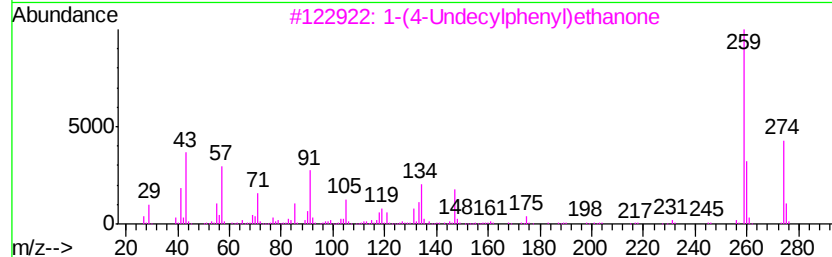
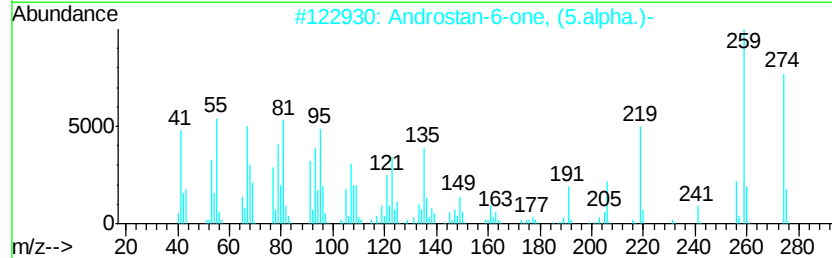
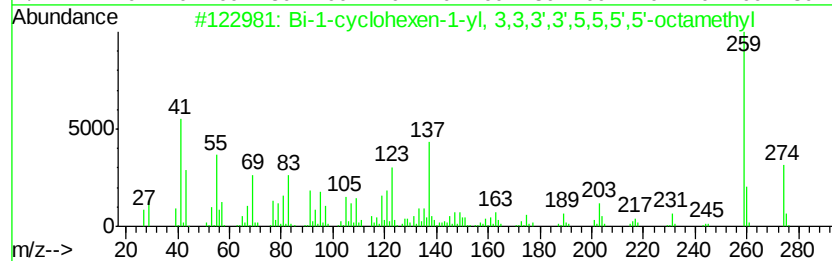
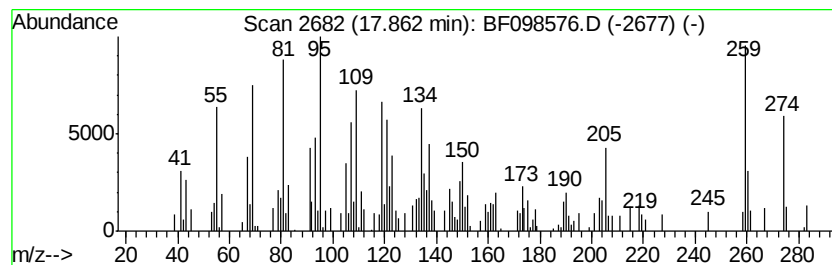
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown17.86 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.86	4.09 ng	199955	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bi-1-cyclohexen-1-yl, 3,3,3',3',...	274	C20H34	076993-52-7	35
2		Androstan-6-one, (5.alpha.)-	274	C19H30O	003676-06-0	30
3		1-(4-Undecylphenyl)ethanone	274	C19H30O	1000185-92-4	25
4		2-(3,7-Dimethyl-octa-2,6-dienyl)...	274	C18H26O2	107697-34-7	25
5		cis-p-Mentha-2,8-dien-1-ol	152	C10H16O	003886-78-0	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
 Data File : BF098576.D
 Acq On : 15 Sep 2017 18:39
 Operator : SJ/JU
 Sample : I5229-06
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 UT5400S16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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...	4.83	8.0	ng	335130	1	6.64	835692	20.0
unknown6.42	6.42	77.1	ng	3220830	1	6.64	835692	20.0
1-Docosene	13.64	6.0	ng	363319	5	13.80	1221860	20.0
1-Decanol, 2-octyl-	14.27	2.5	ng	155653	5	13.80	1221860	20.0
9-Octadecenamide,...	14.54	3.6	ng	174054	6	15.20	978858	20.0
Squalene	14.63	2.3	ng	110363	6	15.20	978858	20.0
Hexacosane	14.87	8.1	ng	395434	6	15.20	978858	20.0
Oxirane, hexadecyl-	15.40	2.2	ng	107801	6	15.20	978858	20.0
2-methyloctacosane	15.60	2.0	ng	98982	6	15.20	978858	20.0
Octadecanal	16.32	3.9	ng	192532	6	15.20	978858	20.0
unknown17.02	17.02	6.5	ng	319232	6	15.20	978858	20.0
unknown17.73	17.73	4.2	ng	203510	6	15.20	978858	20.0
unknown17.86	17.86	4.1	ng	199955	6	15.20	978858	20.0
unknown18.33	18.33	3.8	ng	184197	6	15.20	978858	20.0