

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
 Data File : BF098581.D
 Acq On : 15 Sep 2017 21:01
 Operator : SJ/JU
 Sample : I5229-09
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 UT5400S19

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	2.993	151	154	166	rBV	28397	88620	2.17%	0.235%
2	3.552	243	249	255	rBV2	25062	43978	1.08%	0.116%
3	4.834	463	467	481	rBV	241924	401623	9.84%	1.064%
4	5.257	535	539	553	rBV	3963139	4022189	98.51%	10.653%
5	6.304	711	717	732	rBV	3400375	4082989	100.00%	10.814%
6	6.416	732	736	739	rBV	4198586	4039069	98.92%	10.698%
7	6.640	771	774	781	rBV	998199	872953	21.38%	2.312%
8	6.798	797	801	804	rBV	3143302	2791634	68.37%	7.394%
9	7.216	866	872	875	rBV	2529123	2514748	61.59%	6.660%
10	7.928	988	993	1005	rBV	1276564	1190207	29.15%	3.152%
11	9.004	1170	1176	1179	rBV	3826530	3638072	89.10%	9.636%
12	9.404	1239	1244	1247	rBV	619145	524177	12.84%	1.388%
13	9.681	1285	1291	1297	rVB	1285764	1293321	31.68%	3.425%
14	10.116	1362	1365	1368	rVB	55869	48424	1.19%	0.128%
15	10.475	1420	1426	1429	rBV	2341586	2452793	60.07%	6.496%
16	10.586	1440	1445	1453	rBV	79053	79225	1.94%	0.210%
17	11.163	1539	1543	1546	rBV	1579977	1344712	32.93%	3.562%
18	12.374	1743	1749	1756	rVB4	26399	49210	1.21%	0.130%
19	12.751	1807	1813	1816	rBV	3970668	3814644	93.43%	10.103%
20	13.639	1961	1964	1972	rBV	334696	404508	9.91%	1.071%
21	13.798	1987	1991	1995	rBV	1307465	1181083	28.93%	3.128%
22	14.274	2066	2072	2078	rBV	146793	211063	5.17%	0.559%
23	14.545	2115	2118	2126	rBV	399647	389046	9.53%	1.030%
24	14.698	2140	2144	2148	rVB	104051	109021	2.67%	0.289%
25	14.868	2169	2173	2175	rBV	151148	159410	3.90%	0.422%
26	14.892	2175	2177	2183	rVB	115341	140905	3.45%	0.373%
27	15.198	2224	2229	2239	rVB	719314	873089	21.38%	2.312%
28	15.398	2259	2263	2267	rBV3	51536	65429	1.60%	0.173%
29	15.604	2293	2298	2303	rBV	108058	157179	3.85%	0.416%
30	15.657	2303	2307	2312	rVV2	43493	70128	1.72%	0.186%
31	15.974	2357	2361	2369	rVB9	47104	87033	2.13%	0.231%
32	16.051	2369	2374	2378	rBV3	26995	49230	1.21%	0.130%
33	16.310	2414	2418	2425	rBV6	33806	66590	1.63%	0.176%
34	16.521	2448	2454	2459	rBV9	22358	43087	1.06%	0.114%

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Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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35	16.580	2459	2464	2470	rVB5	27587	56026	1.37%	0.148%
36	16.657	2474	2477	2485	rVB8	23874	51727	1.27%	0.137%
37	17.021	2533	2539	2548	rVB7	66822	167041	4.09%	0.442%
38	18.321	2754	2760	2769	rVB6	73134	182321	4.47%	0.483%

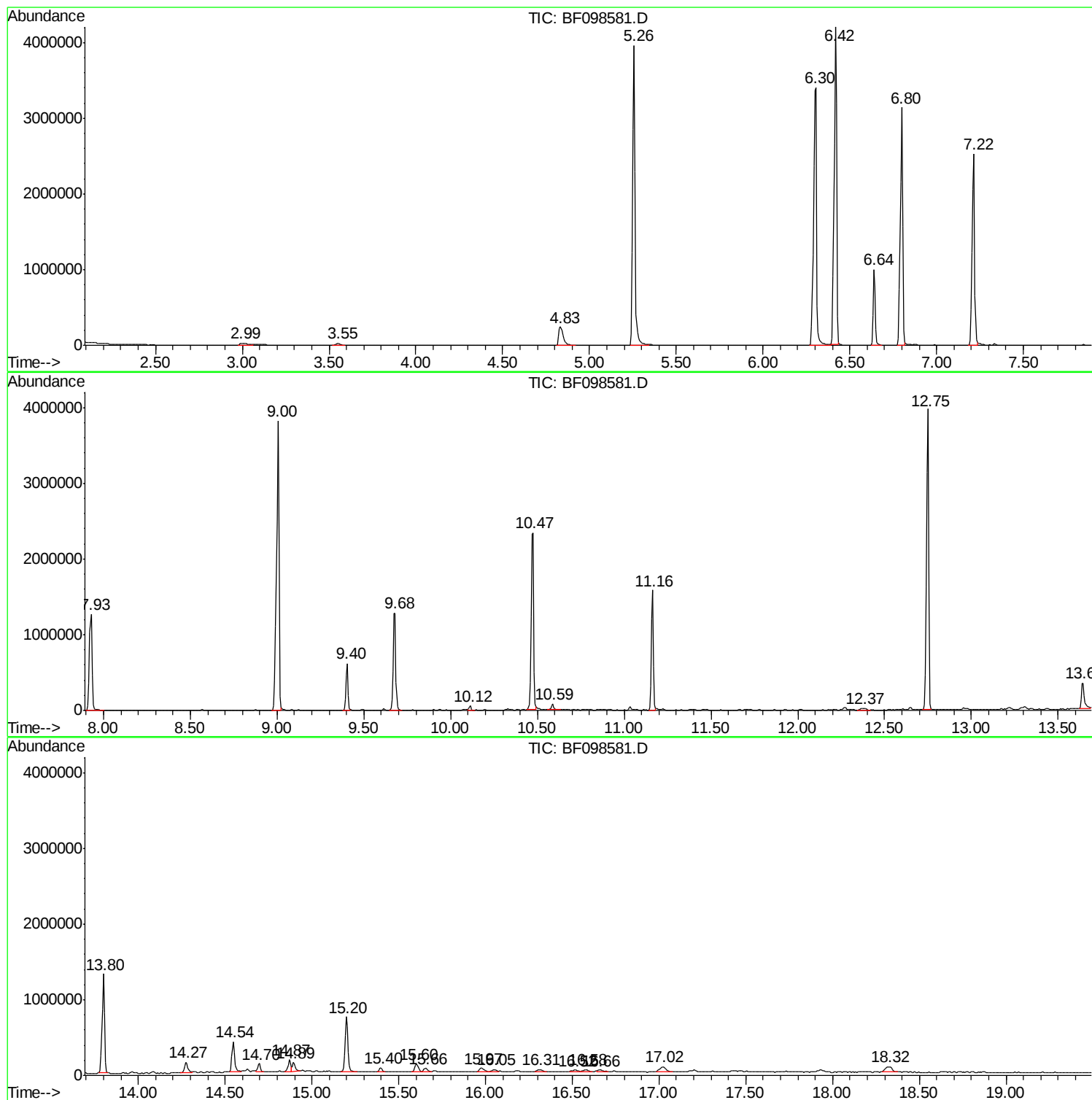
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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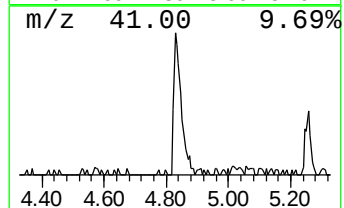
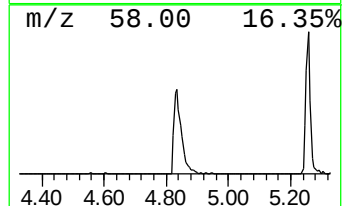
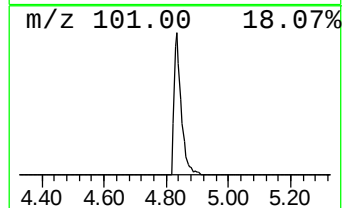
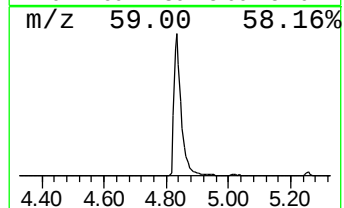
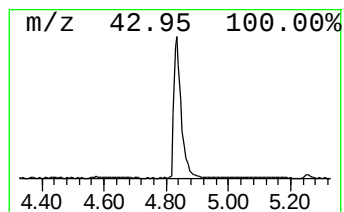
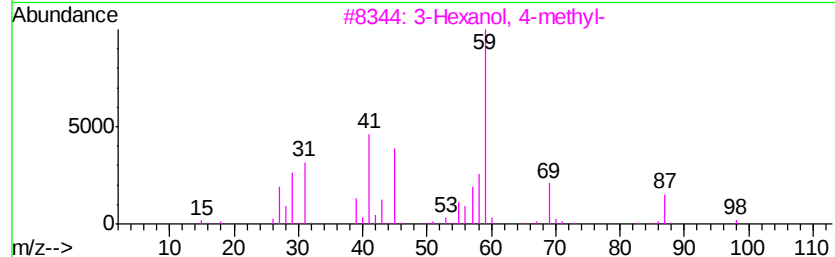
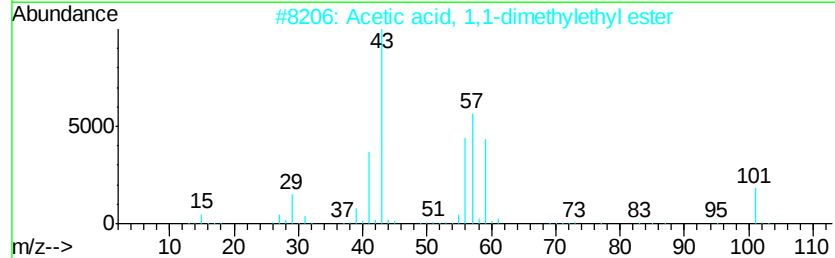
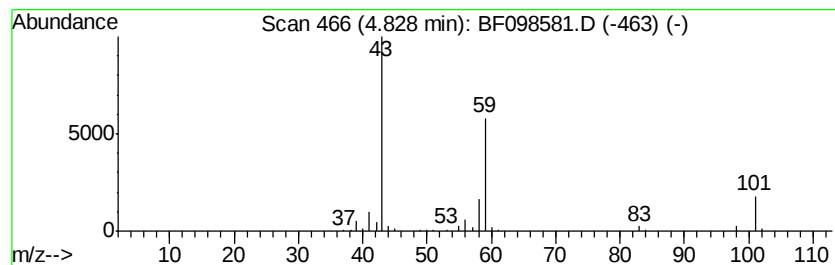
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	9.20 ng	401623	1,4-Dichlorobenzene-d4	6.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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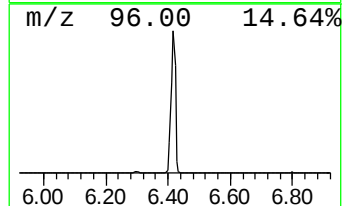
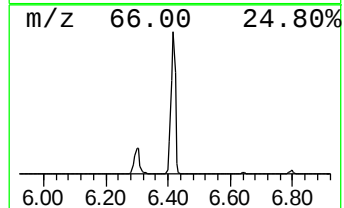
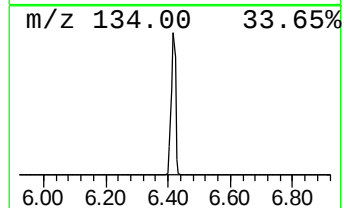
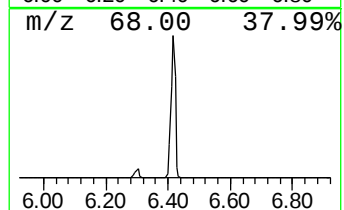
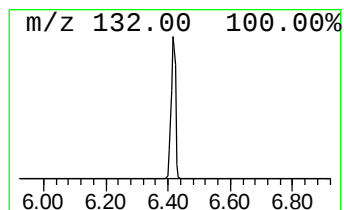
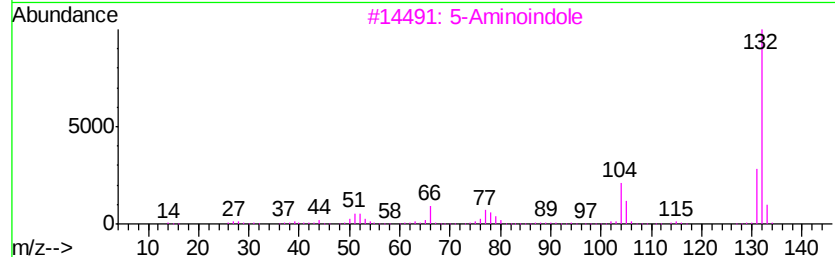
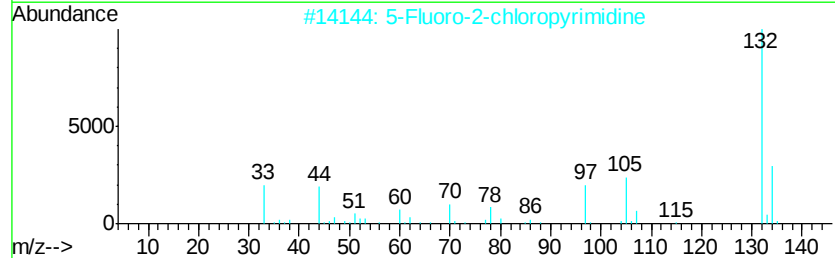
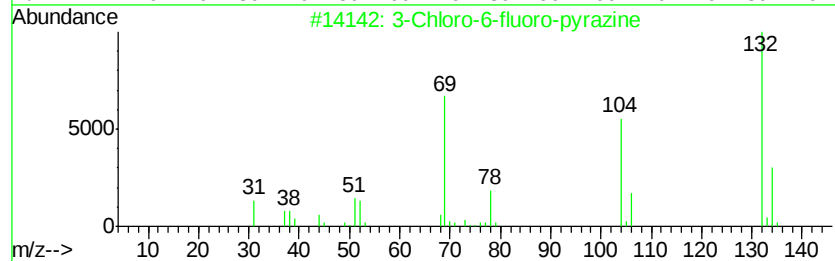
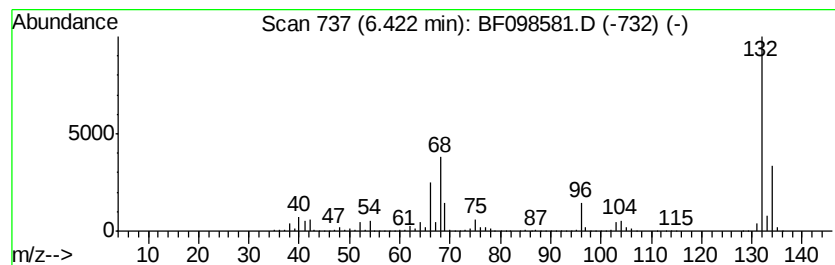
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	92.54 ng	4039070	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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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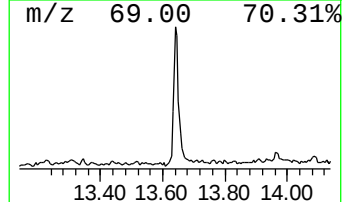
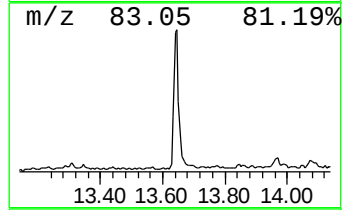
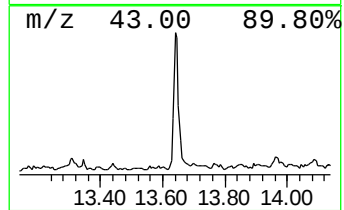
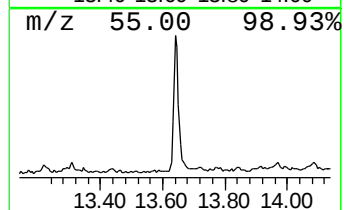
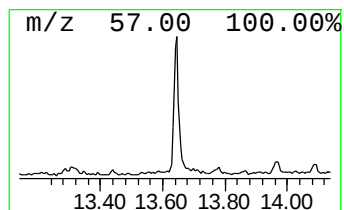
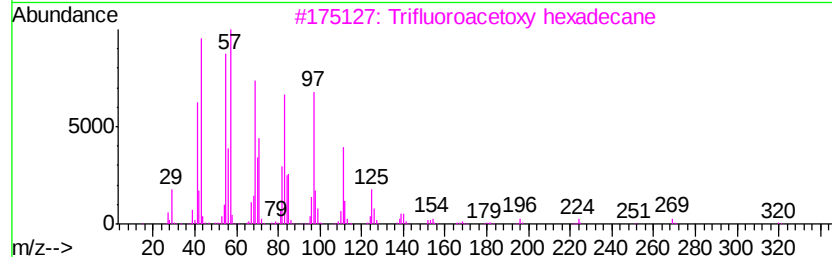
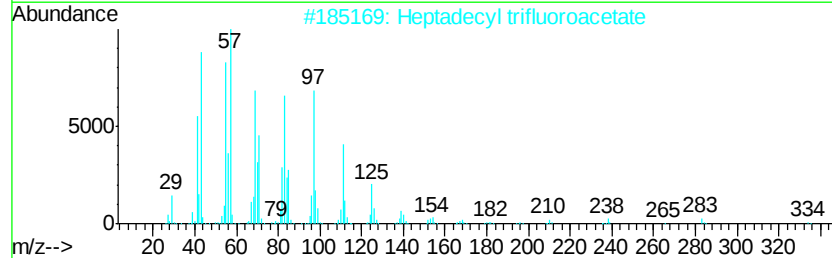
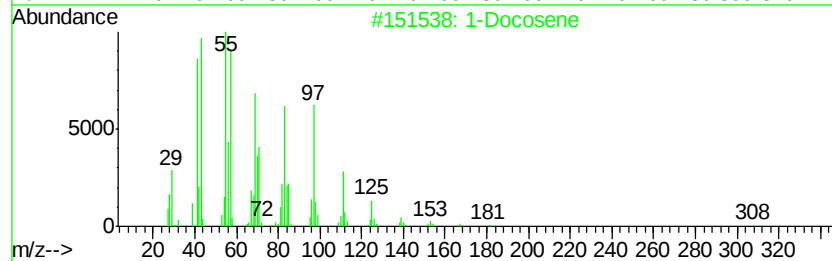
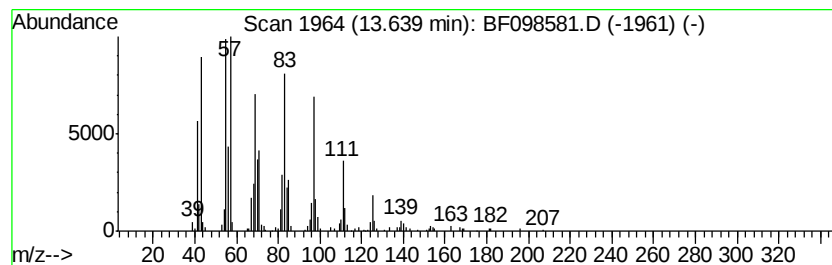
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	6.85 ng	404508	Chrysene-d12	13.80

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



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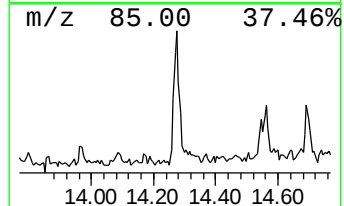
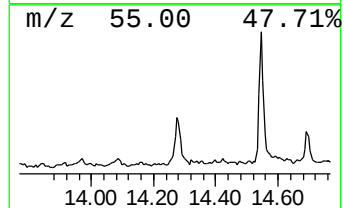
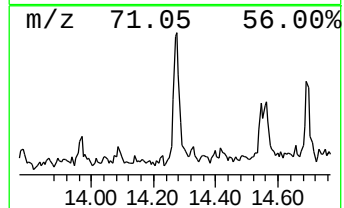
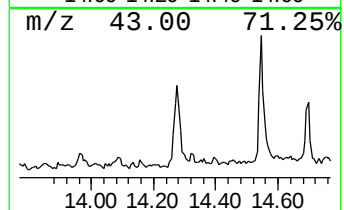
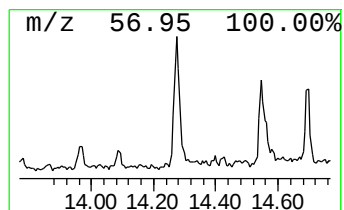
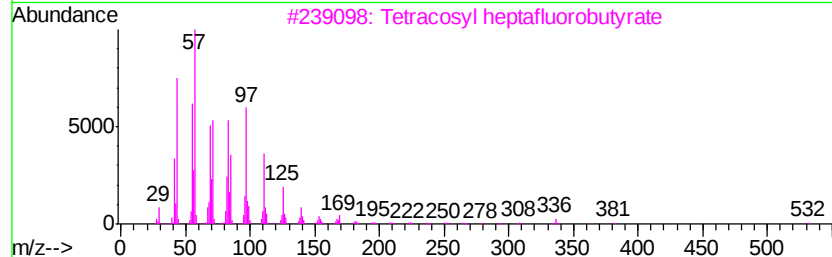
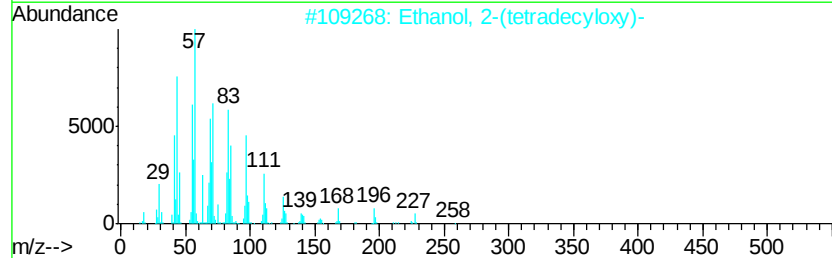
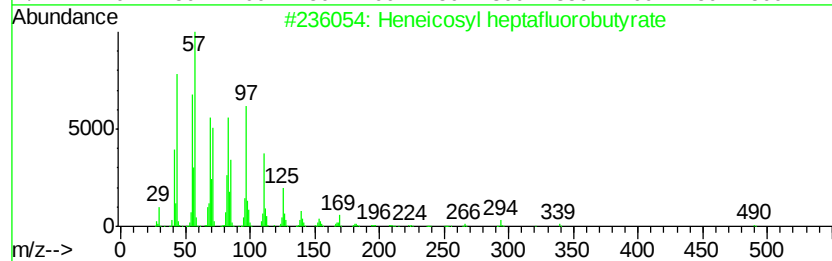
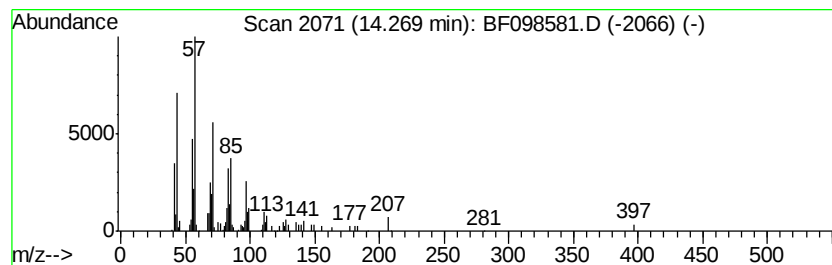
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heneicosyl heptafluorobutyrate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.27	3.57 ng	211063	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3		Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91



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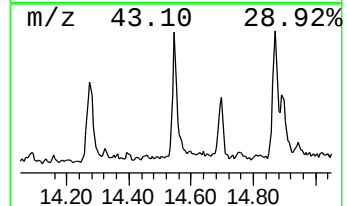
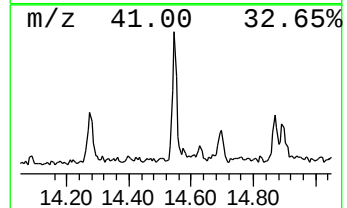
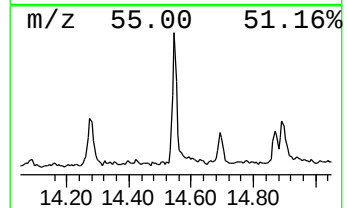
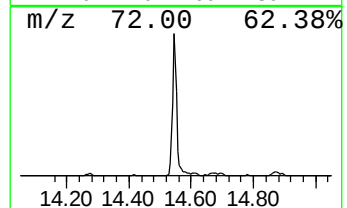
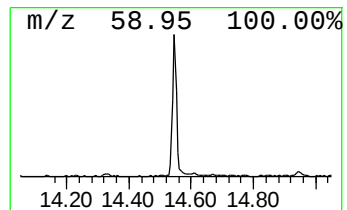
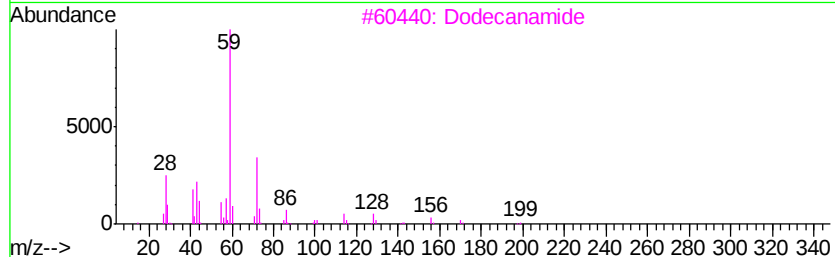
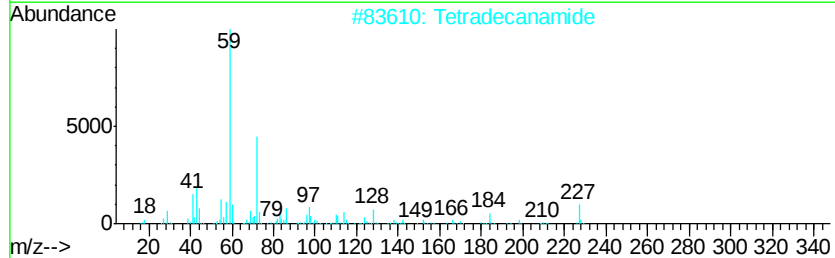
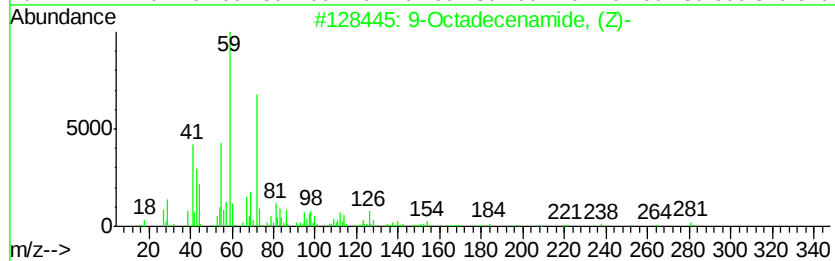
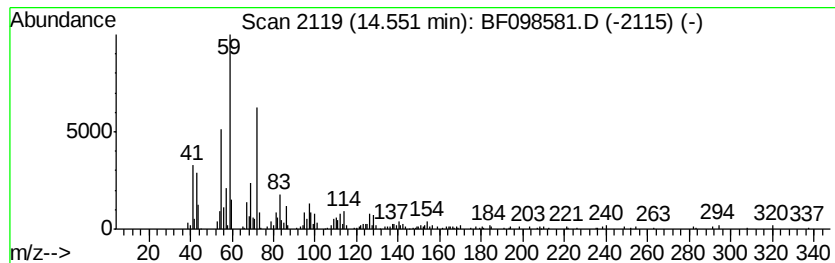
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Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	8.91 ng	389046	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		Tetradecanamide	227	C14H29NO	000638-58-4	78
3		Dodecanamide	199	C12H25NO	001120-16-7	70
4		Octadecanamide	283	C18H37NO	000124-26-5	53
5		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50



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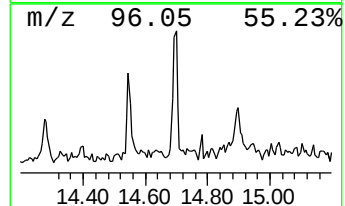
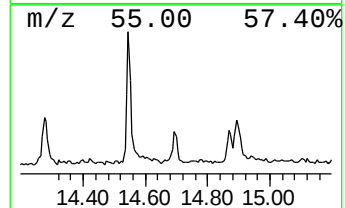
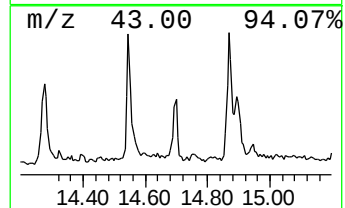
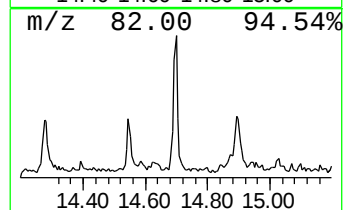
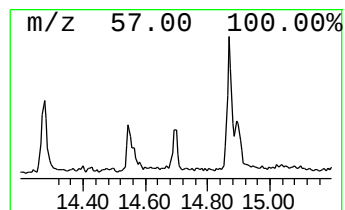
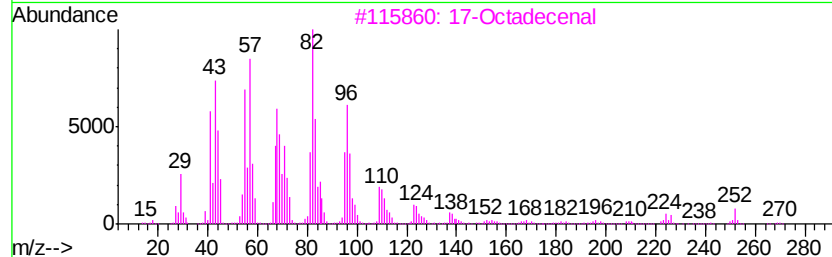
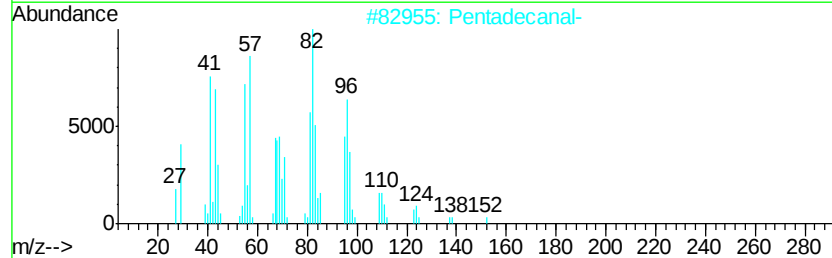
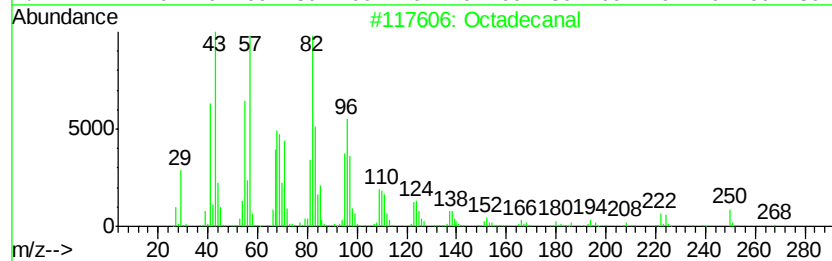
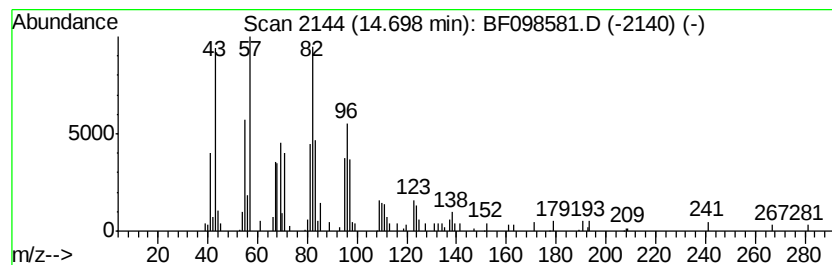
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanal Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	2.50 ng	109021	Perylene-d12	15.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecanal	268 C18H36O	000638-66-4	91
2	Pentadecanal-	226 C15H30O	002765-11-9	90
3	17-Octadecenal	266 C18H34O	056554-86-0	86
4	Heptadecanal	254 C17H34O	1000376-70-0	83
5	Hexadecanal	240 C16H32O	000629-80-1	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098581.D
Acq On : 15 Sep 2017 21:01
Operator : SJ/JU
Sample : I5229-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UT5400S19

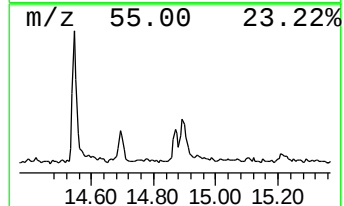
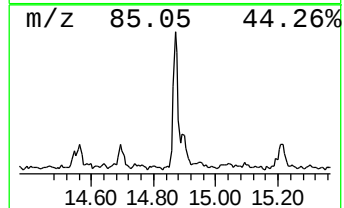
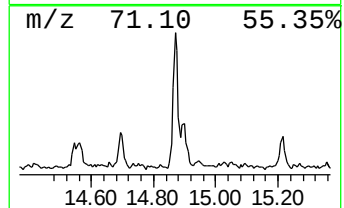
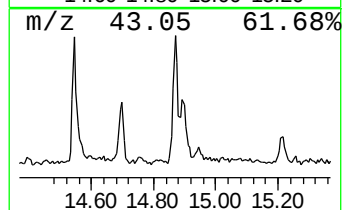
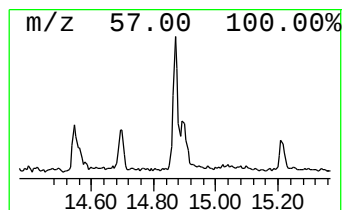
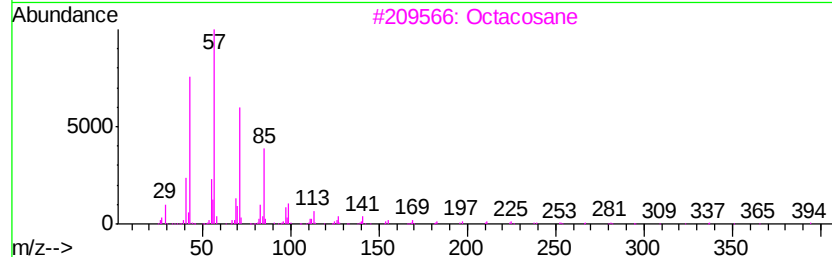
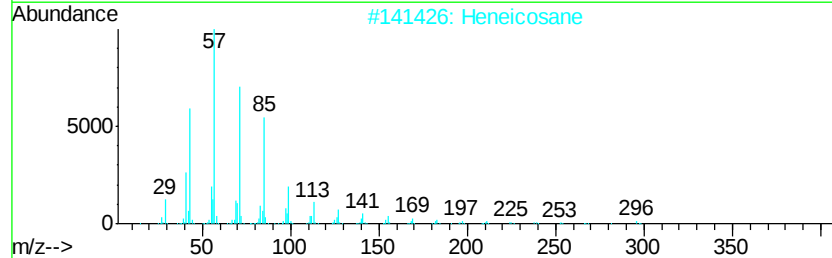
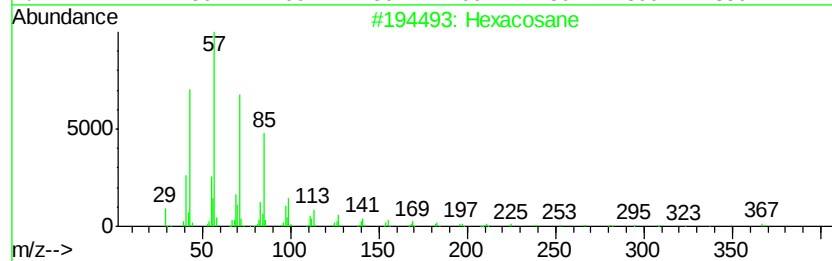
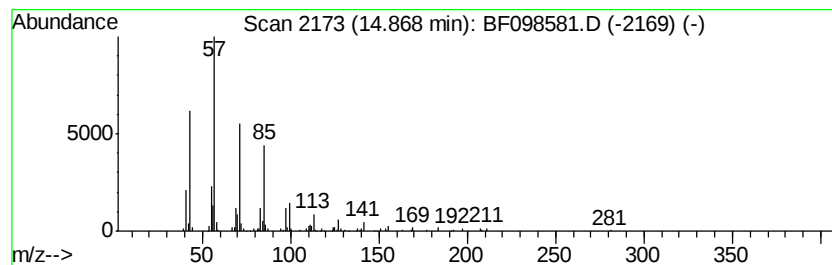
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	3.65 ng	159410	Perylene-d12	15.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Octacosane		394	C28H58	000630-02-4	90
4	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	90
5	Pentadecane		212	C15H32	000629-62-9	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
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Acq On : 15 Sep 2017 21:01
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ALS Vial : 10 Sample Multiplier: 1

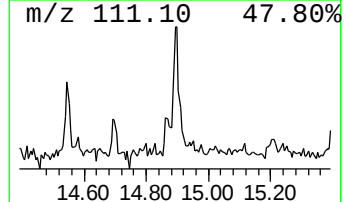
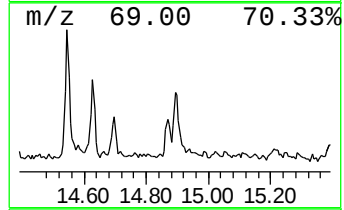
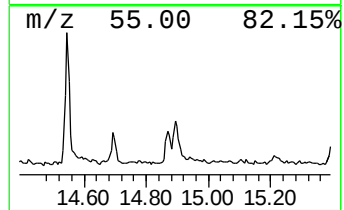
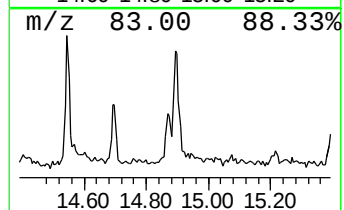
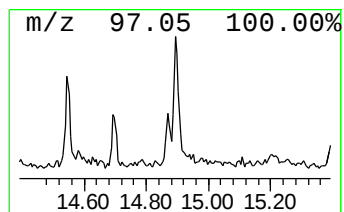
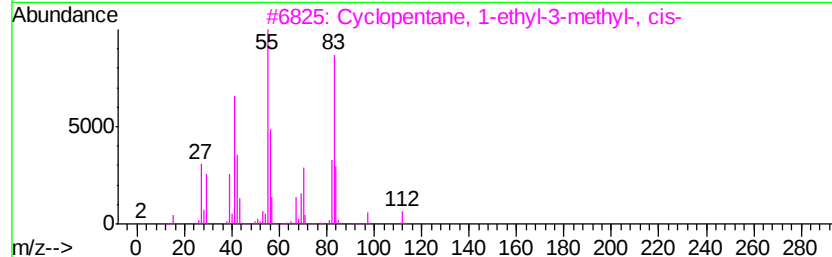
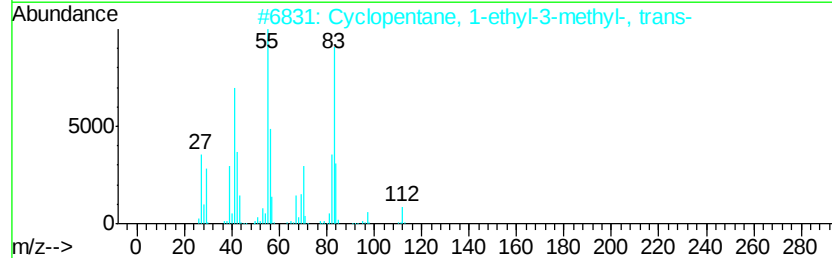
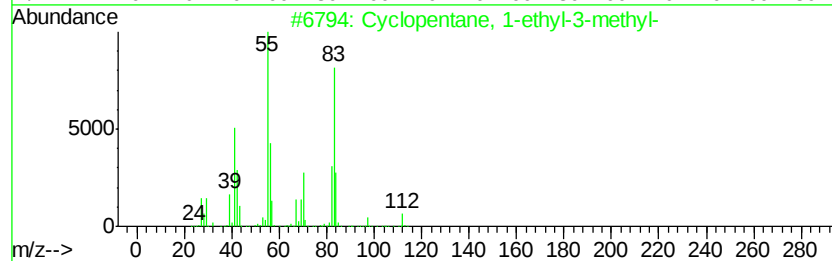
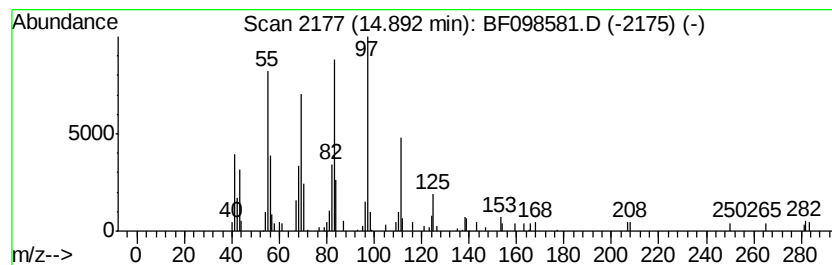
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclopentane, 1-ethyl-3-met... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.89	3.23 ng	140905	Perylene-d12	15.20		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, 1-ethyl-3-methyl-	112	C8H16	003726-47-4	50
2		Cyclopentane, 1-ethyl-3-methyl-,...	112	C8H16	002613-65-2	50
3		Cyclopentane, 1-ethyl-3-methyl-,...	112	C8H16	002613-66-3	45
4		Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	38
5		1H-Pyrazole, 4,5-dihydro-3,5,5-t...	112	C6H12N2	003975-85-7	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098581.D
Acq On : 15 Sep 2017 21:01
Operator : SJ/JU
Sample : I5229-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

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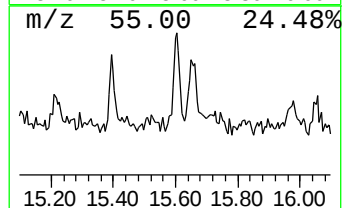
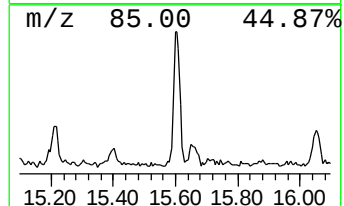
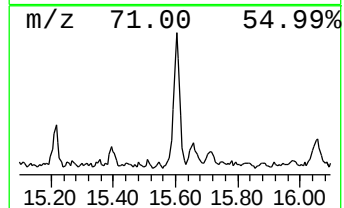
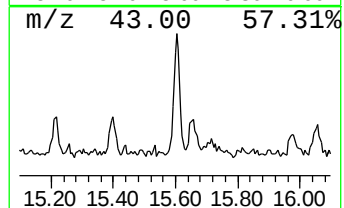
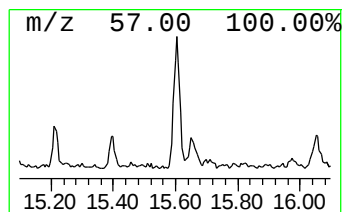
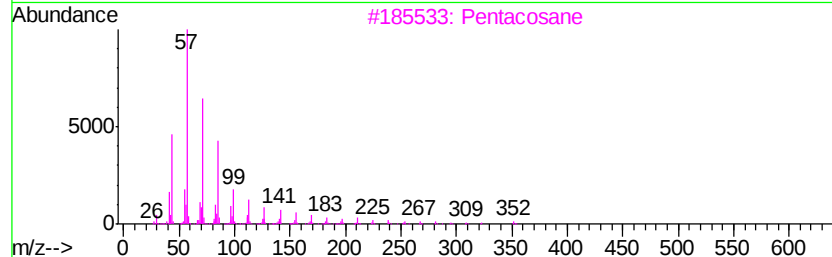
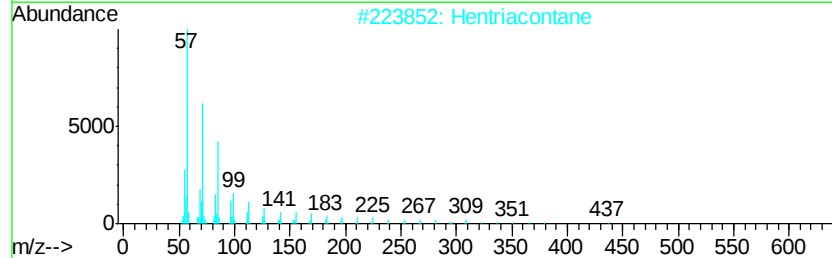
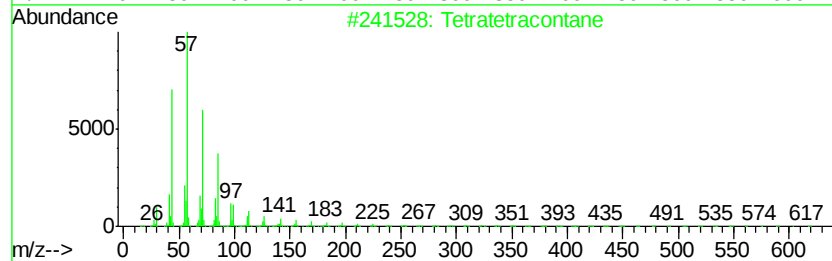
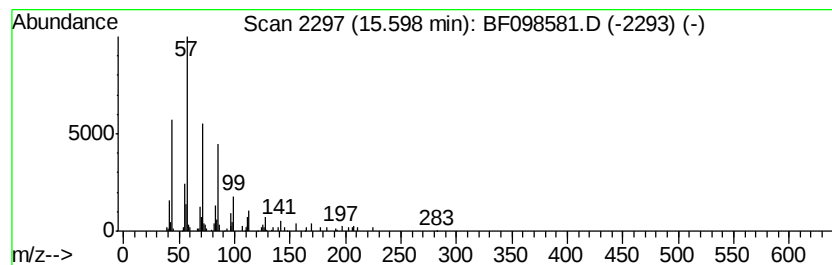
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetratetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	3.60 ng	157179	Perylene-d12	15.20

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Hentriacontane	437	C31H64	000630-04-6	91
3			Pentacosane	352	C25H52	000629-99-2	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098581.D
Acq On : 15 Sep 2017 21:01
Operator : SJ/JU
Sample : I5229-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

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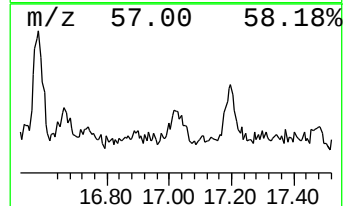
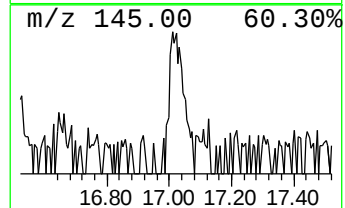
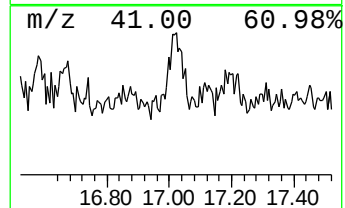
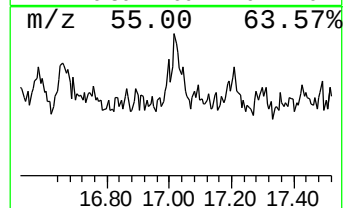
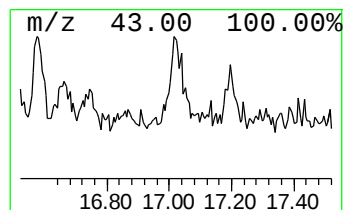
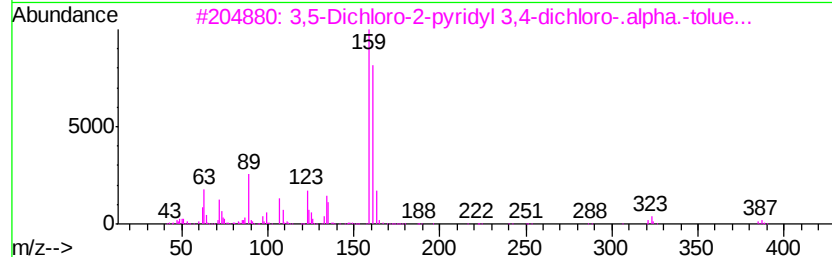
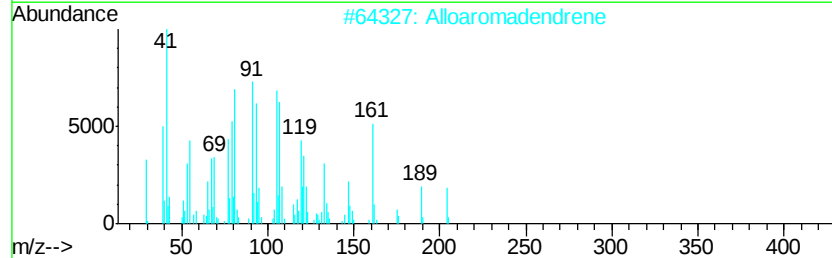
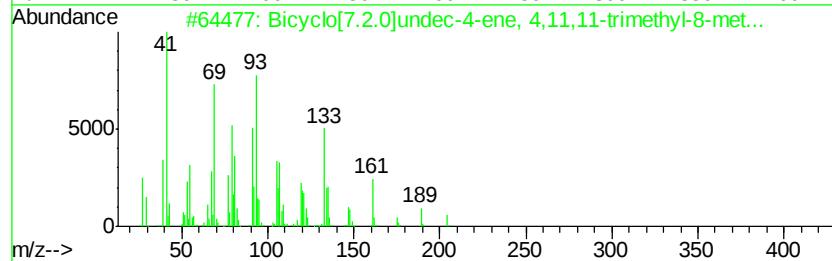
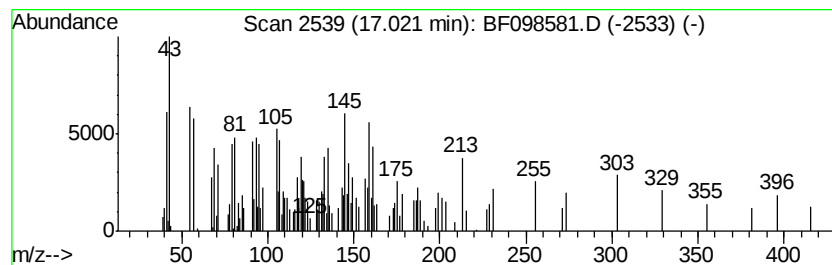
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.02 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.02	3.83 ng	167041	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	38
2		Alloaromadendrene	204	C15H24	025246-27-9	25
3		3,5-Dichloro-2-pyridyl 3,4-dichl...	385	C12H7Cl4N03S	058236-55-8	14
4		1H-1,3-Benzimidazole, 2-(2-pyrro...	187	C11H13N3	1000338-11-7	11
5		2,4-Dichlorobenzyl alcohol, 2-me...	246	C12H16Cl2O	1000378-10-8	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098581.D
Acq On : 15 Sep 2017 21:01
Operator : SJ/JU
Sample : I5229-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

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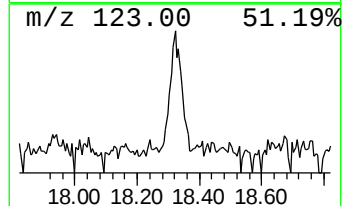
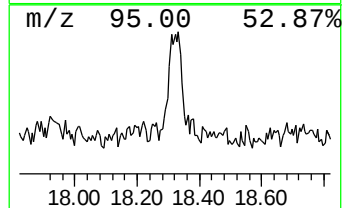
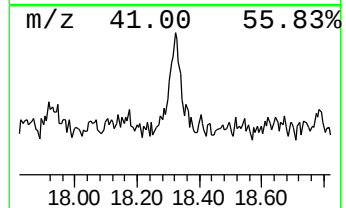
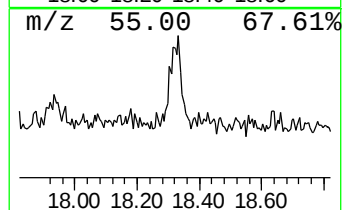
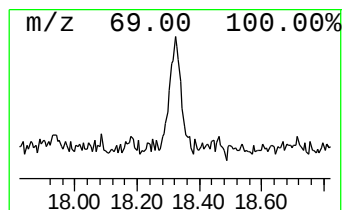
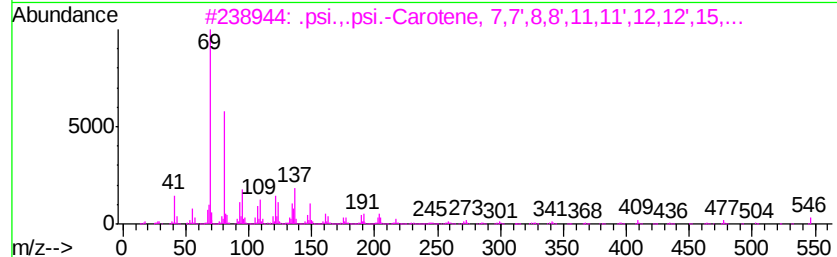
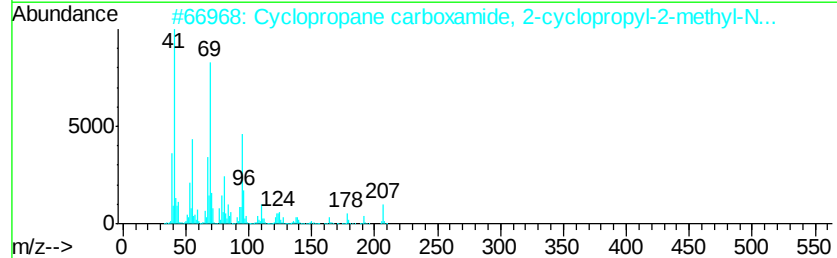
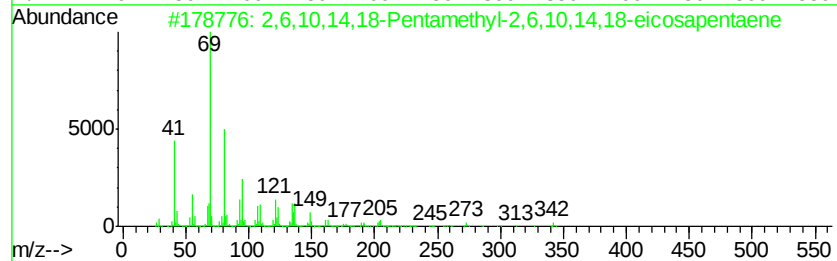
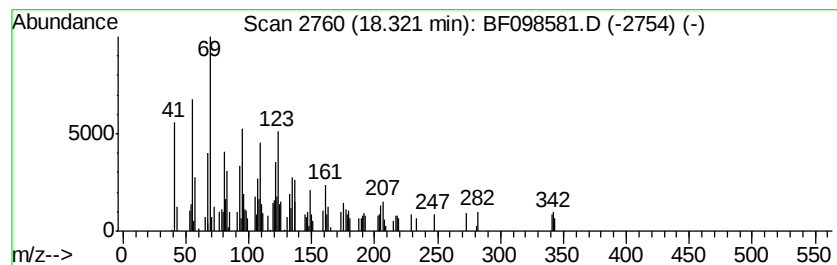
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2,6,10,14,18-Pentamethyl-2,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	4.18 ng	182321	Perylene-d12	15.20

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	62		
2	Cyclopropane carboxamide, 2-cycl...	207	C13H21NO	331416-19-4	42		
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	38		
4	5-Acetoxymethyl-2,6,10-trimethyl...	282	C17H30O3	1000144-12-3	38		
5	Carbamic acid, N-phenyl-, 1,5-di...	273	C17H23NO2	118723-77-6	35		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098581.D
Acq On : 15 Sep 2017 21:01
Operator : SJ/JU
Sample : I5229-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.83	9.2 ng		401623	1	6.64	872953	20.0
unknown6.42	6.42	92.5 ng		4039070	1	6.64	872953	20.0
1-Docosene	13.64	6.8 ng		404508	5	13.80	1181080	20.0
Heneicosyl heptaf...	14.27	3.6 ng		211063	5	13.80	1181080	20.0
9-Octadecenamide,...	14.55	8.9 ng		389046	6	15.20	873089	20.0
Octadecanal	14.70	2.5 ng		109021	6	15.20	873089	20.0
Hexacosane	14.87	3.6 ng		159410	6	15.20	873089	20.0
Cyclopentane, 1-e...	14.89	3.2 ng		140905	6	15.20	873089	20.0
Tetratetracontane	15.60	3.6 ng		157179	6	15.20	873089	20.0
unknown17.02	17.02	3.8 ng		167041	6	15.20	873089	20.0
2,6,10,14,18-Pent...	18.32	4.2 ng		182321	6	15.20	873089	20.0