

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051316\
 Data File : BF086988.D
 Acq On : 13 May 2016 23:48
 Operator : UM/SJ
 Sample : H2877-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-32

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-BF050916.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.735	12	13	70	rVB	4355344	9853965	100.00%	21.205%
2	4.741	275	276	283	rBV	58707	102472	1.04%	0.221%
3	5.199	314	316	332	rBV	1520711	2009559	20.39%	4.324%
4	6.273	407	410	417	rBV	1049420	1276838	12.96%	2.748%
5	6.387	417	420	422	rBV	2574022	3532413	35.85%	7.601%
6	6.604	437	439	442	rBV	711908	941185	9.55%	2.025%
7	6.764	450	453	456	rBV	3230008	3118440	31.65%	6.710%
8	7.187	487	490	492	rBV	3076175	3178457	32.26%	6.840%
9	7.896	550	552	555	rBV	1232885	1218951	12.37%	2.623%
10	8.982	644	647	649	rBV	4926709	5026854	51.01%	10.817%
11	9.382	680	682	684	rBV	110810	105092	1.07%	0.226%
12	9.645	703	705	708	rBV	1518171	1395982	14.17%	3.004%
13	10.090	735	744	746	rBV	110863	114664	1.16%	0.247%
14	10.433	771	774	777	rBV2	2818344	3205328	32.53%	6.897%
15	10.559	783	785	792	rVB	100724	129001	1.31%	0.278%
16	11.119	832	834	837	rBV	1262837	1347781	13.68%	2.900%
17	11.348	852	854	860	rVB	119319	191548	1.94%	0.412%
18	11.668	880	882	887	rBV2	80039	129243	1.31%	0.278%
19	12.456	948	951	953	rBV2	87797	115046	1.17%	0.248%
20	12.502	953	955	957	rVV	199102	323037	3.28%	0.695%
21	12.548	957	959	961	rVB	452956	472296	4.79%	1.016%
22	12.616	961	965	968	rVB2	122651	194771	1.98%	0.419%
23	12.708	970	973	976	rBV	3597617	4747856	48.18%	10.217%
24	13.245	1018	1020	1022	rBV	405469	356970	3.62%	0.768%
25	13.291	1022	1024	1025	rVV	117034	108838	1.10%	0.234%
26	13.496	1041	1042	1050	rVB	131997	218987	2.22%	0.471%
27	13.622	1050	1053	1062	rBV	303737	490039	4.97%	1.055%
28	13.748	1062	1064	1067	rBV	1316656	1263329	12.82%	2.719%
29	13.931	1078	1080	1084	rBV	161911	159912	1.62%	0.344%
30	14.239	1104	1107	1109	rBV	113950	126728	1.29%	0.273%
31	14.525	1130	1132	1135	rBV	105877	120452	1.22%	0.259%
32	15.108	1180	1183	1185	rBV	785789	895036	9.08%	1.926%

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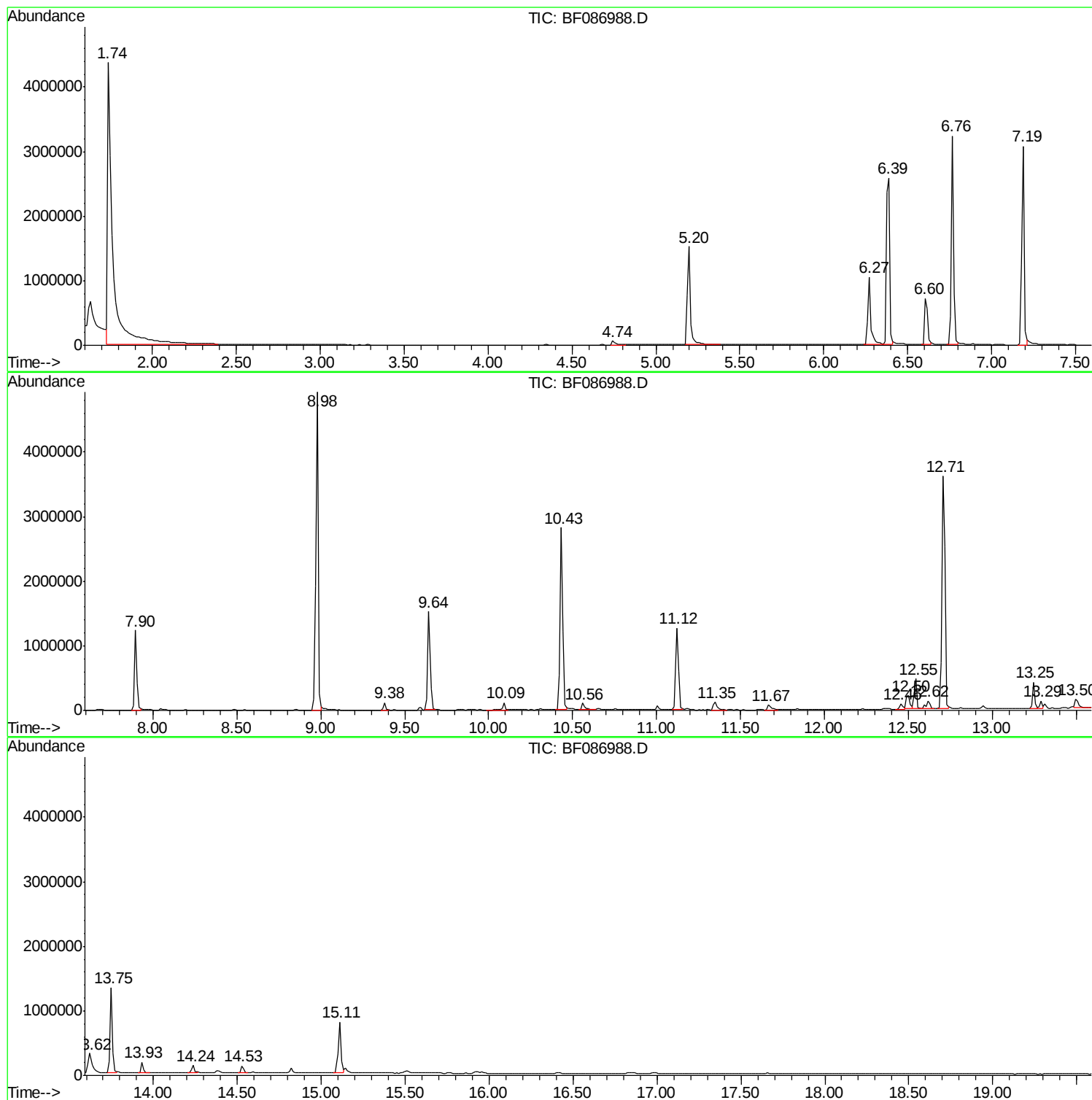
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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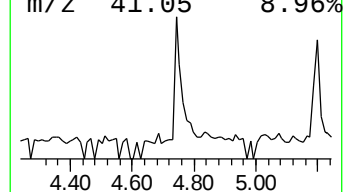
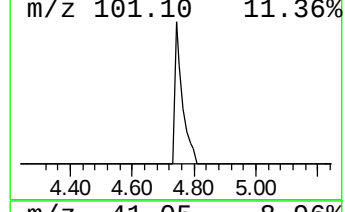
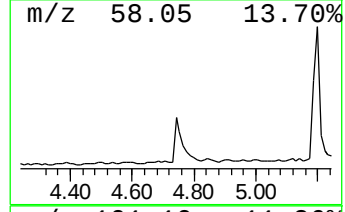
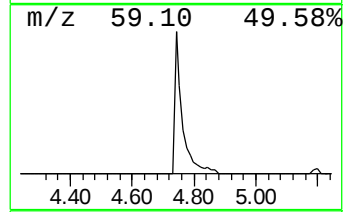
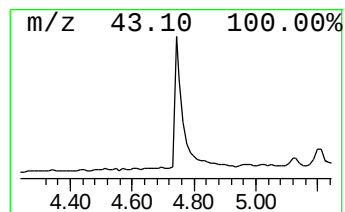
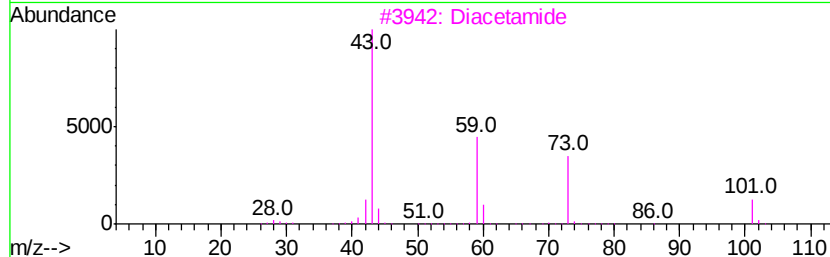
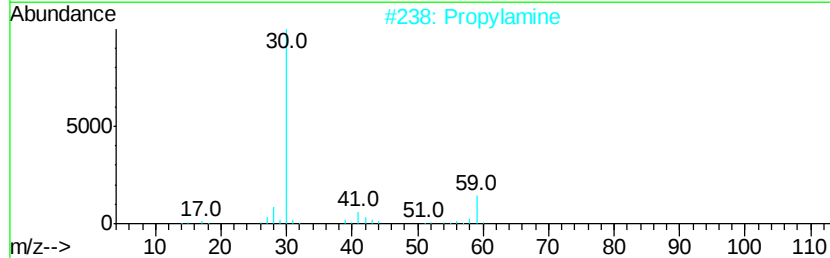
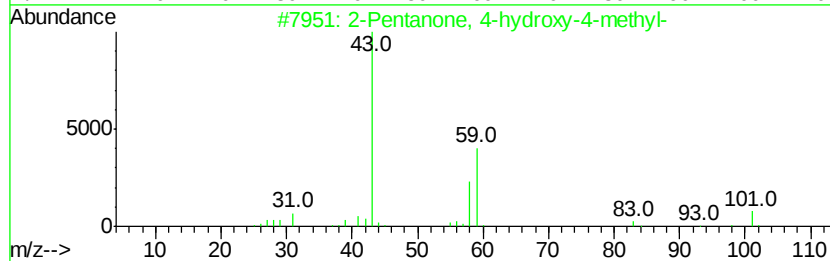
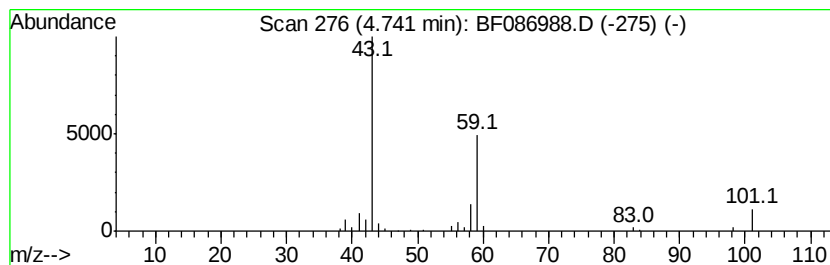
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	2.18 ng	102472	1,4-Dichlorobenzene-d4	6.62

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propylamine	59	C3H9N	000107-10-8	9
3			Diacetamide	101	C4H7NO2	000625-77-4	9
4			1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	9
5			2-Pentanone, 5-(acetyloxy)-	144	C7H12O3	005185-97-7	9



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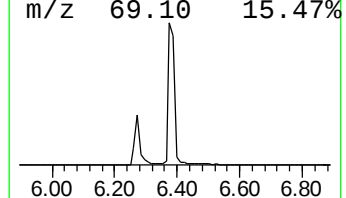
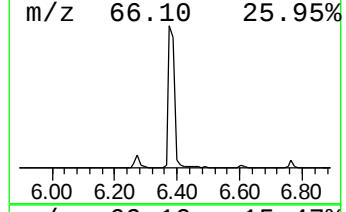
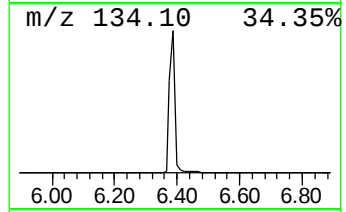
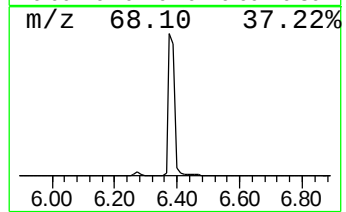
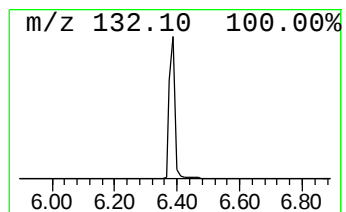
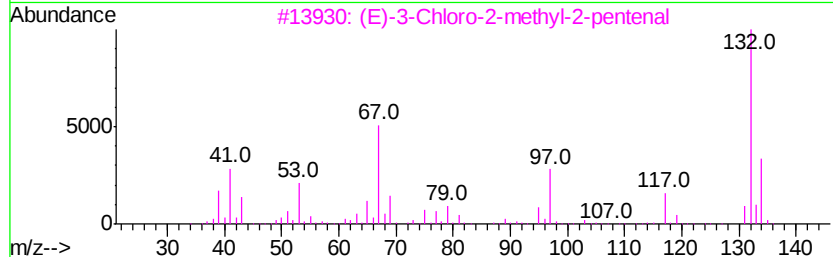
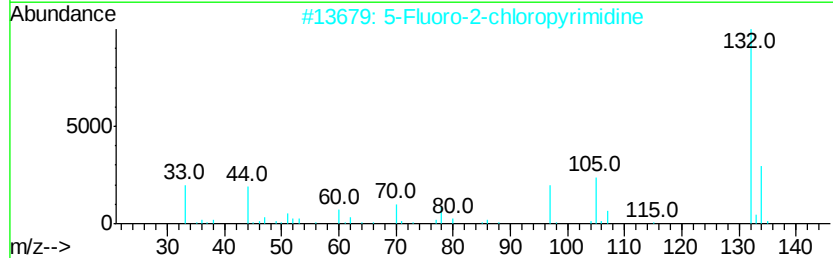
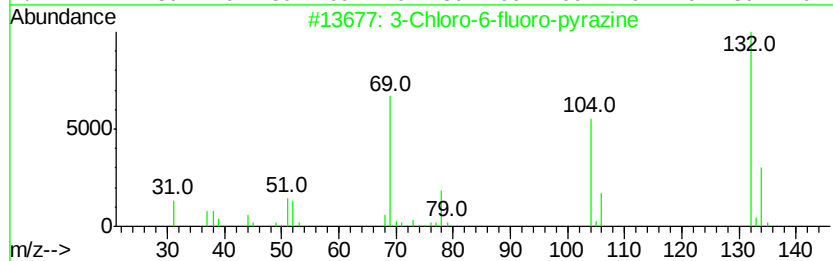
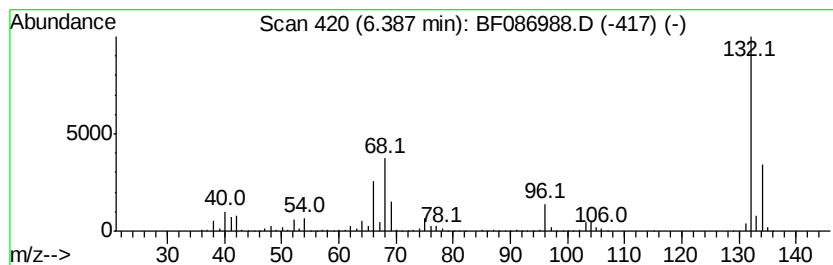
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Peak Number 3 unknown6.39 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	75.06 ng	3532410	1,4-Dichlorobenzene-d4	6.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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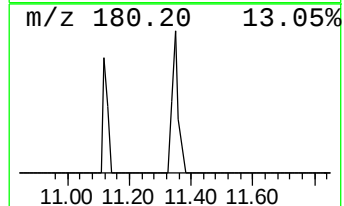
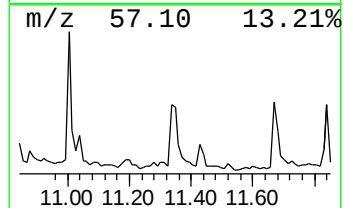
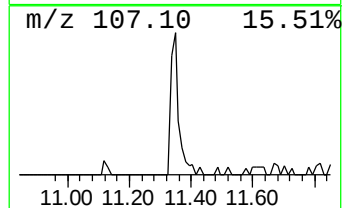
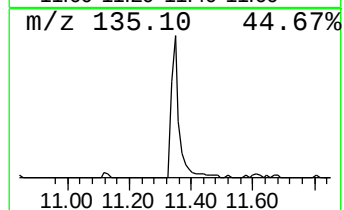
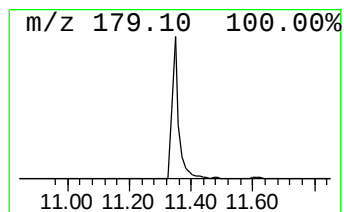
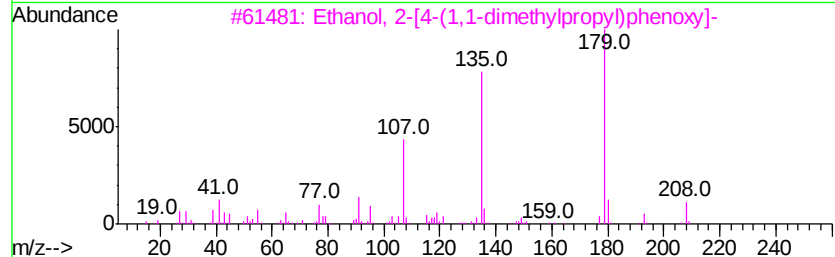
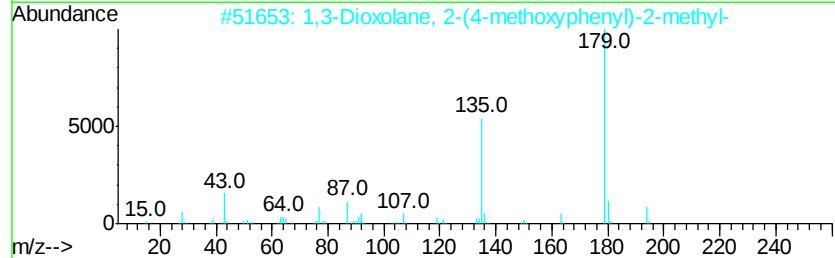
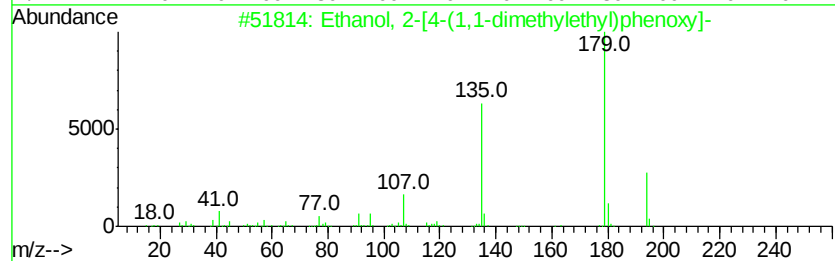
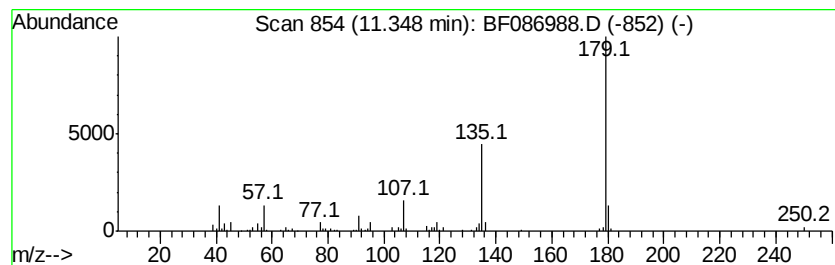
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Peak Number 5 Ethanol, 2-[4-(1,1-dimethyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.35	2.84 ng	191548	Phenanthrene-d10	11.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-[4-(1,1-dimethylethyl)...	194	C12H18O2	000713-46-2	80
2		1,3-Dioxolane, 2-(4-methoxypheny...	194	C11H14O3	036881-00-2	72
3		Ethanol, 2-[4-(1,1-dimethylpropyl...	208	C13H20O2	006382-07-6	64
4		Acetic acid, [2-[2-propenylamin...	235	C12H13NO4	000119-45-9	37
5		2-Cyclopenten-1-one, 3-(1-hepten...	250	C15H26OSi	1000159-28-7	37



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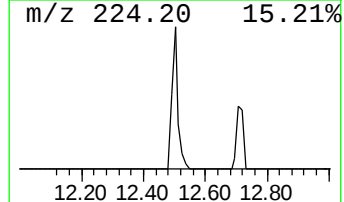
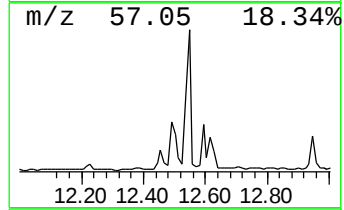
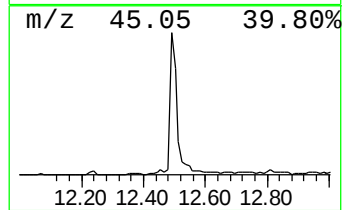
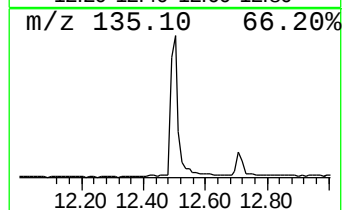
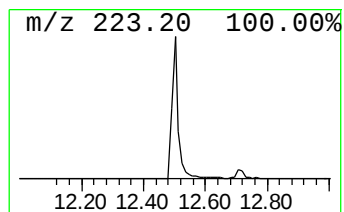
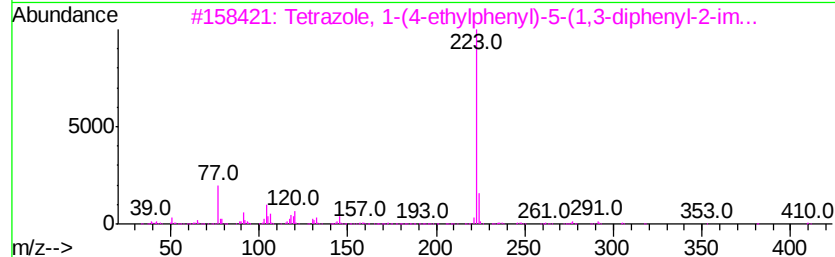
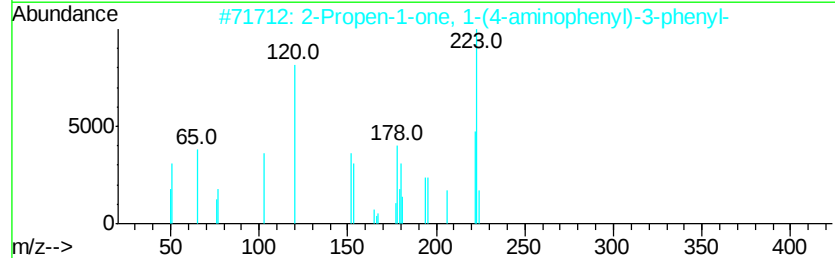
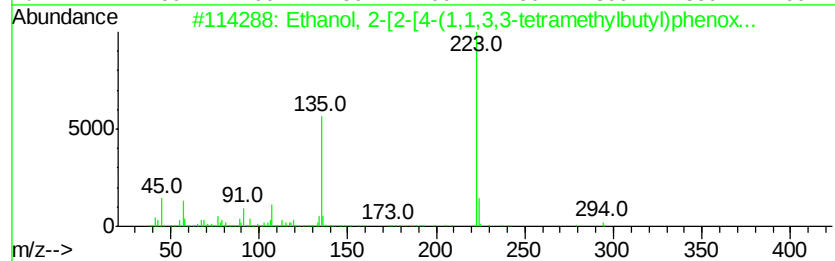
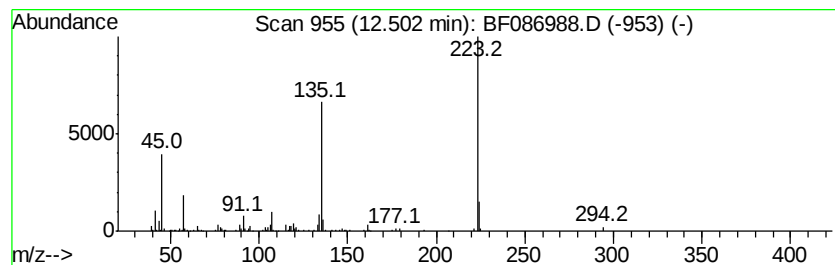
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Peak Number 6 Ethanol, 2-[2-[4-(1,1,3,3-t... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	5.11 ng	323037	Chrysene-d12	13.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	94
2		2-Propen-1-one, 1-(4-aminophenyl...	223	C15H13NO	002403-30-7	43
3		Tetrazole, 1-(4-ethylphenyl)-5-(...	410	C25H26N6	125038-06-4	35
4		Benzenamine, N,N-dimethyl-4-(2-p...	223	C16H17N	001145-73-9	35
5		9-Acridinecarboxylic acid	223	C14H9NO2	005336-90-3	25



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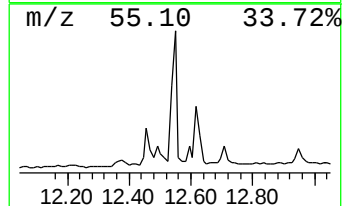
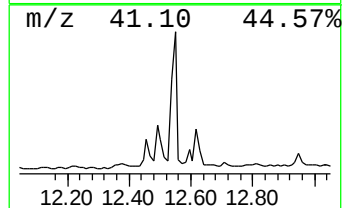
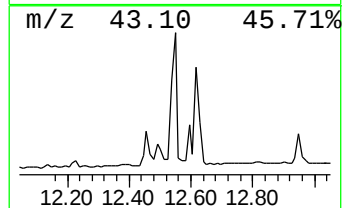
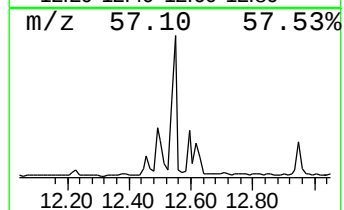
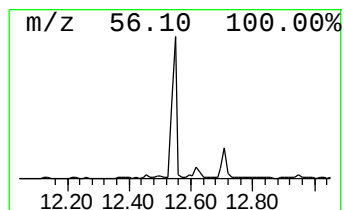
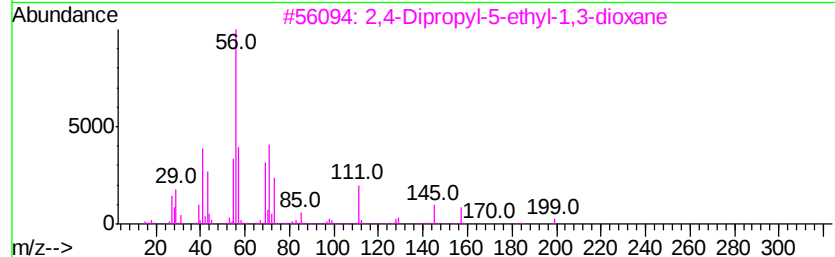
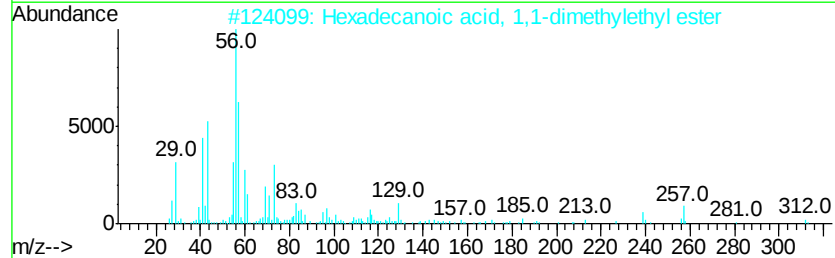
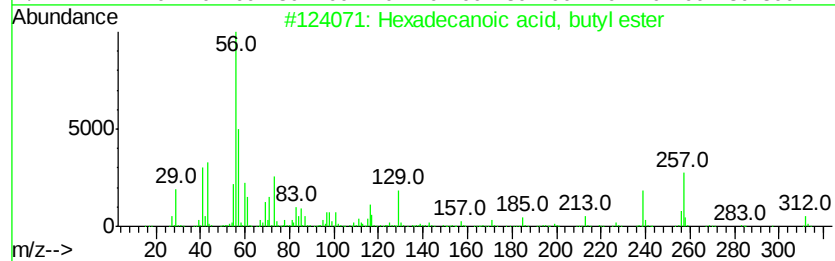
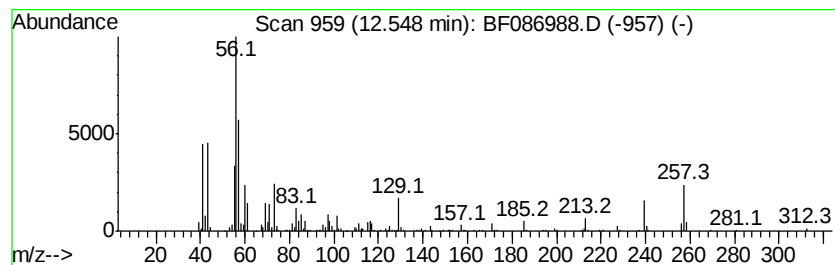
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	7.48 ng	472296	Chrysene-d12	13.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	41
3		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	37
4		2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	35
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051316\
Data File : BF086988.D
Acq On : 13 May 2016 23:48
Operator : UM/SJ
Sample : H2877-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-32

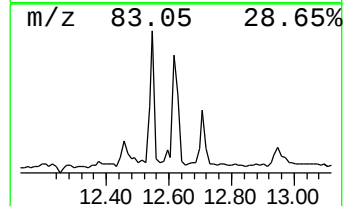
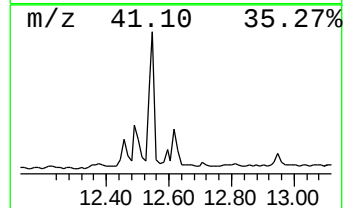
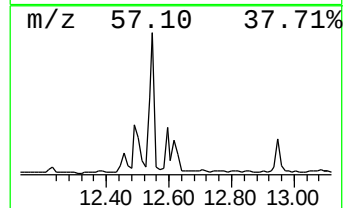
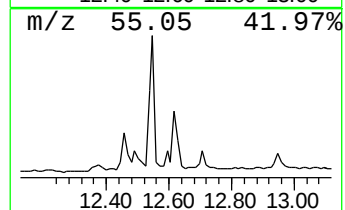
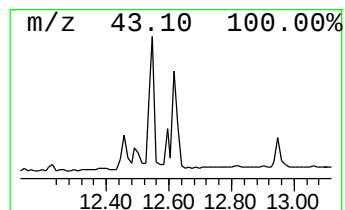
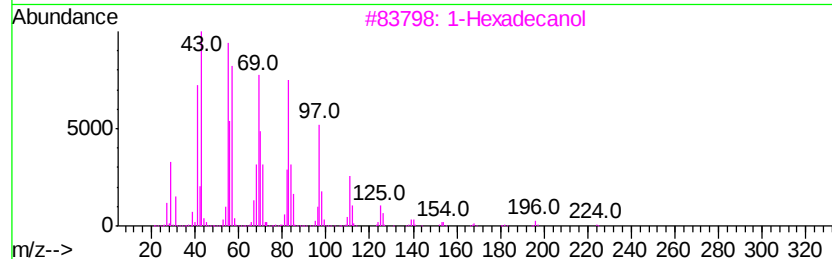
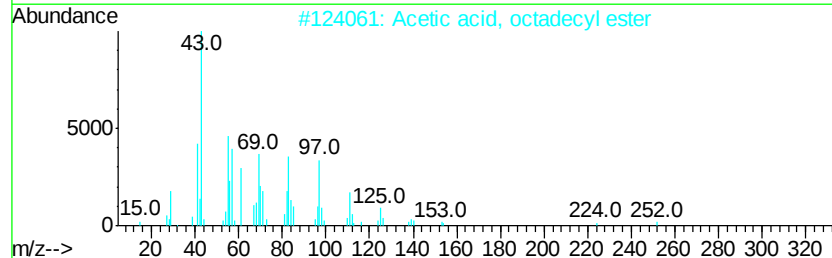
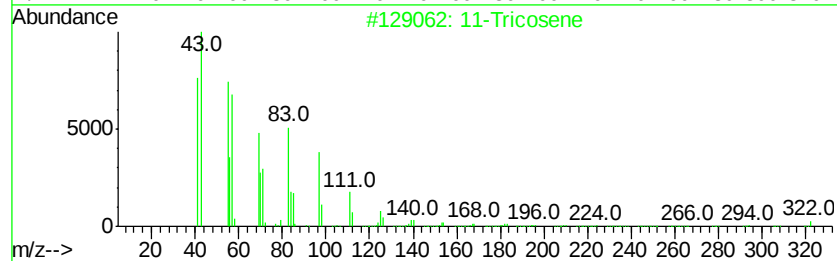
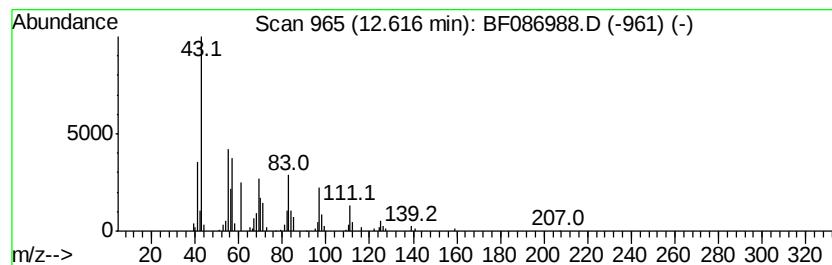
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 11-Tricosene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	3.08 ng	194771	Chrysene-d12	13.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Tricosene		322	C23H46	052078-56-5	74
2	Acetic acid, octadecyl ester		312	C20H40O2	000822-23-1	72
3	1-Hexadecanol		242	C16H34O	036653-82-4	68
4	Trichloroacetic acid, pentadecyl...		372	C17H31Cl3O2	074339-53-0	62
5	Trifluoroacetic acid, n-heptadec...		324	C17H31F3O2	1000216-79-2	52



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051316\
Data File : BF086988.D
Acq On : 13 May 2016 23:48
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Sample : H2877-03
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Instrument :
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ClientSampleId :
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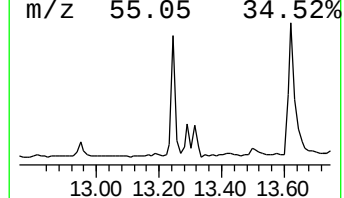
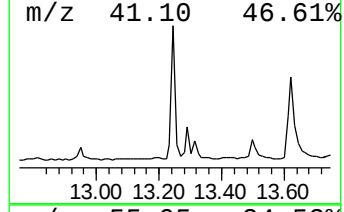
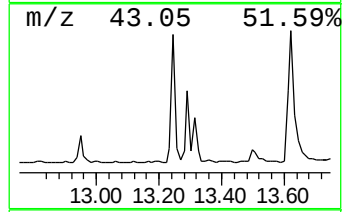
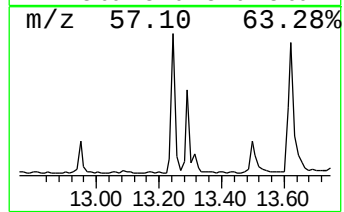
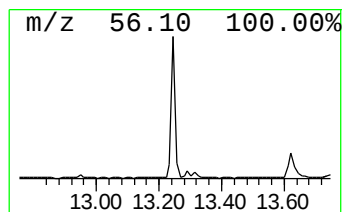
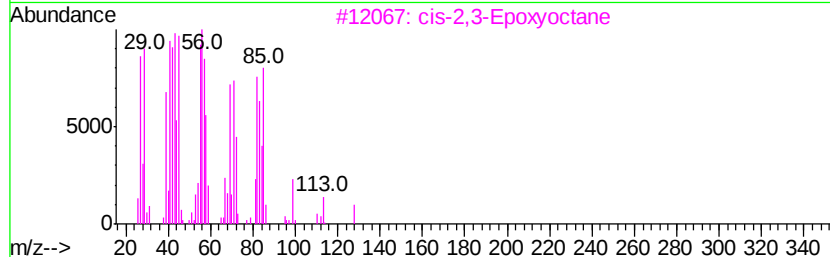
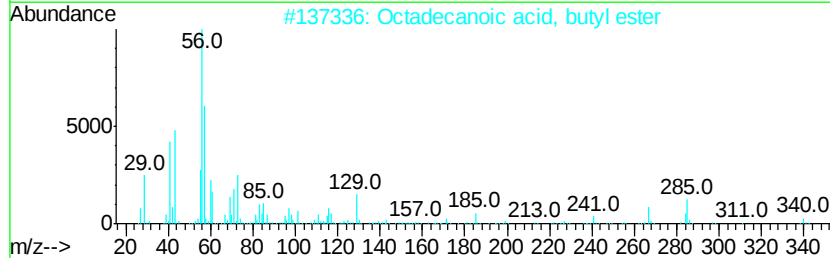
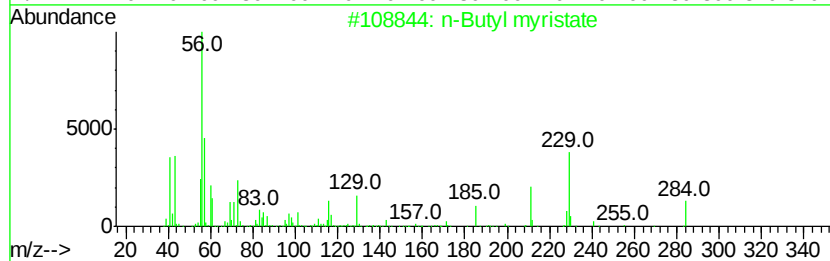
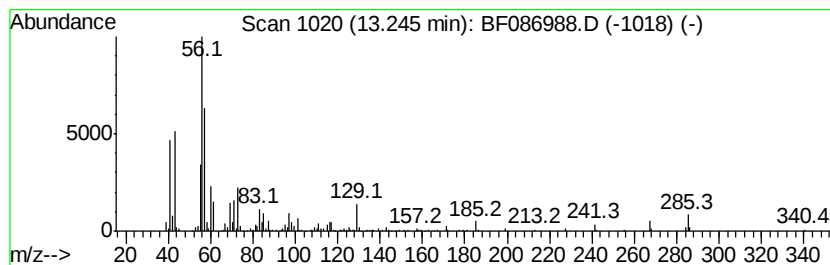
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 n-Butyl myristate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.25	5.65 ng	356970	Chrysene-d12	13.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Butyl myristate	284	C18H36O2	000110-36-1	86	
2	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	53	
3	cis-2,3-Epoxyoctane	128	C8H16O	023024-54-6	46	
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43	
5	4-Propylcyclohexylamine	141	C9H19N	102653-37-2	43	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051316\
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Acq On : 13 May 2016 23:48
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Sample : H2877-03
Misc :
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ClientSampleId :
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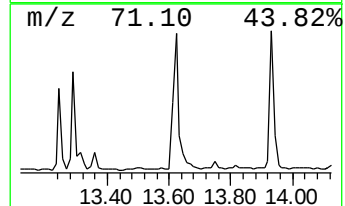
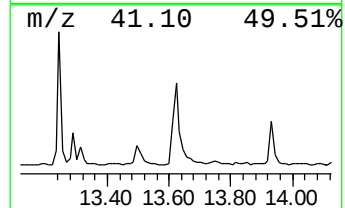
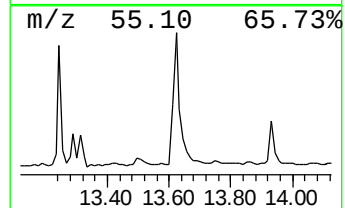
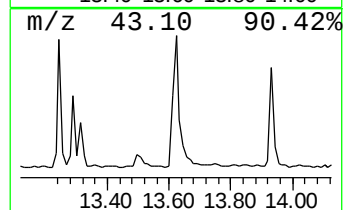
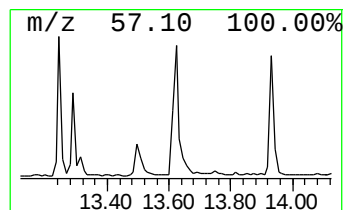
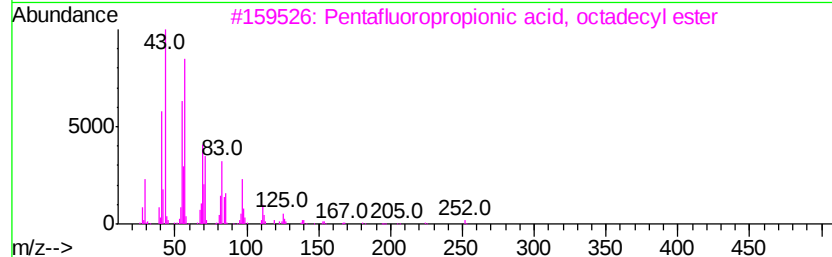
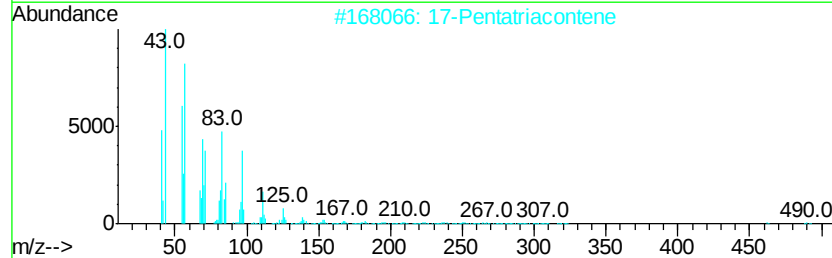
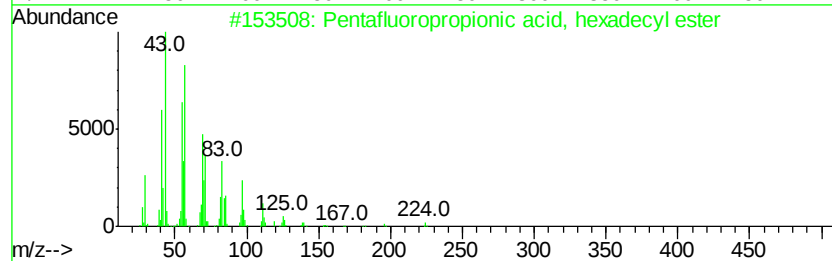
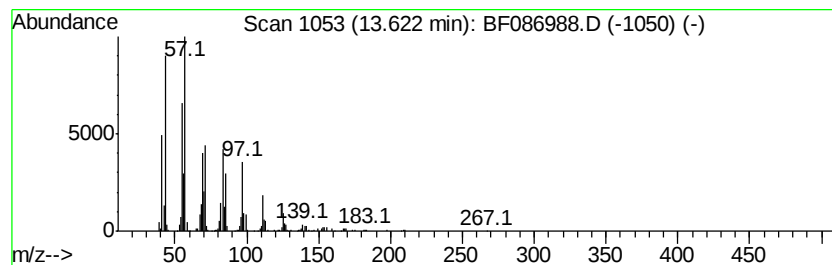
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.62	7.76 ng	490039	Chrysene-d12	13.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
2			17-Pentatriacontene	491	C35H70	006971-40-0	91
3			Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91
4			Oxirane, [(dodecyl)oxymethyl]-	242	C15H30O2	002461-18-9	91
5			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051316\
Data File : BF086988.D
Acq On : 13 May 2016 23:48
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Sample : H2877-03
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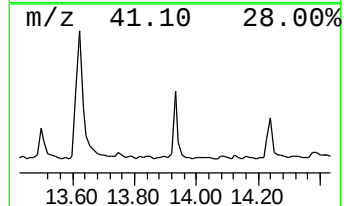
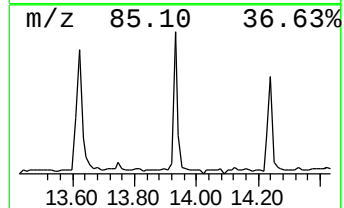
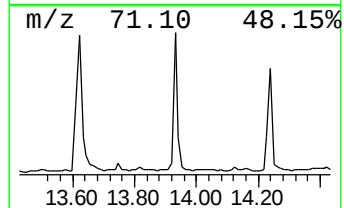
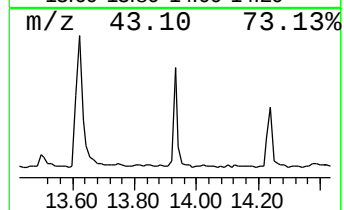
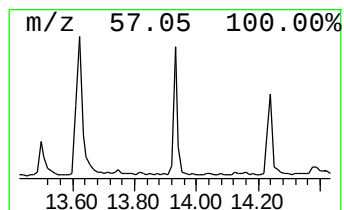
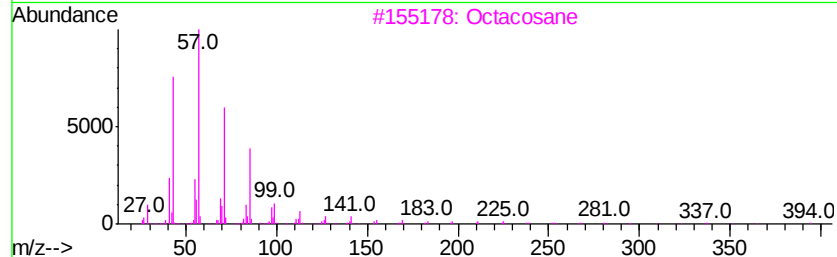
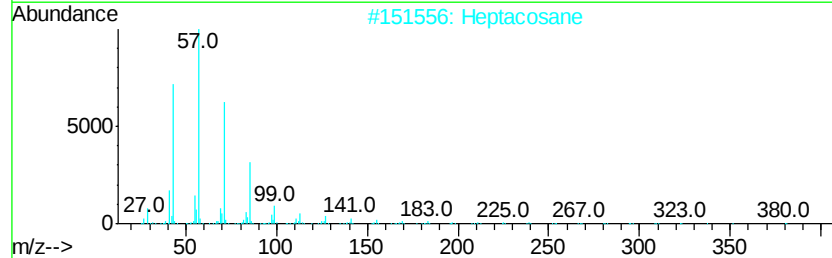
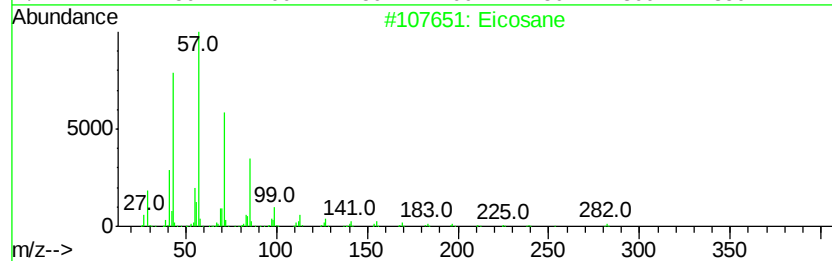
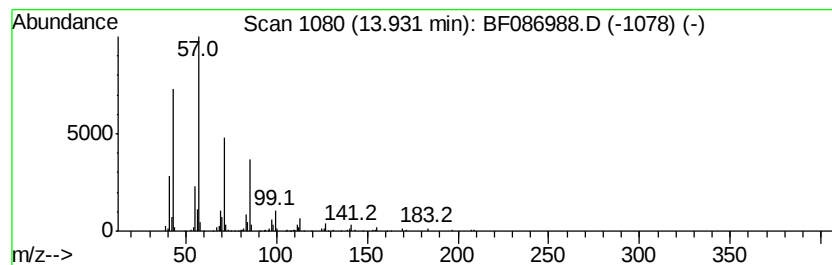
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	2.53 ng	159912	Chrysene-d12	13.75
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane		282 C20H42	000112-95-8 91
2	Heptacosane		380 C27H56	000593-49-7 91
3	Octacosane		394 C28H58	000630-02-4 91
4	Heneicosane		296 C21H44	000629-94-7 90
5	Pentacosane		352 C25H52	000629-99-2 90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051316\
Data File : BF086988.D
Acq On : 13 May 2016 23:48
Operator : UM/SJ
Sample : H2877-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

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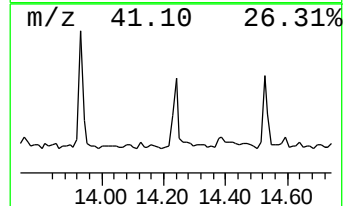
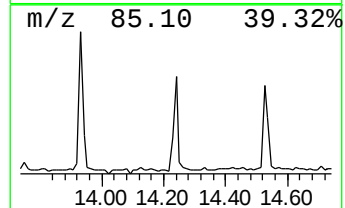
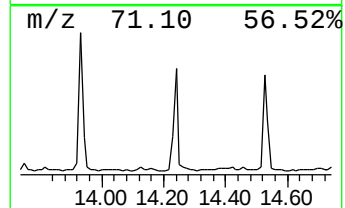
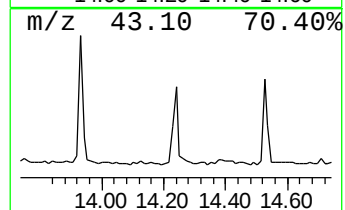
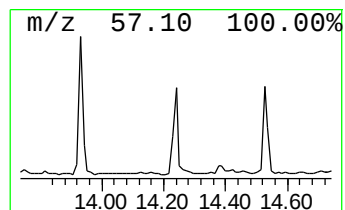
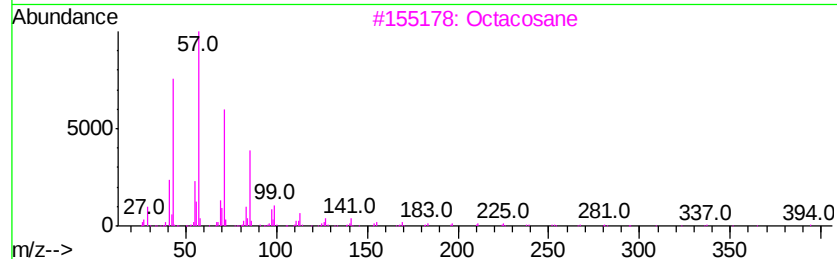
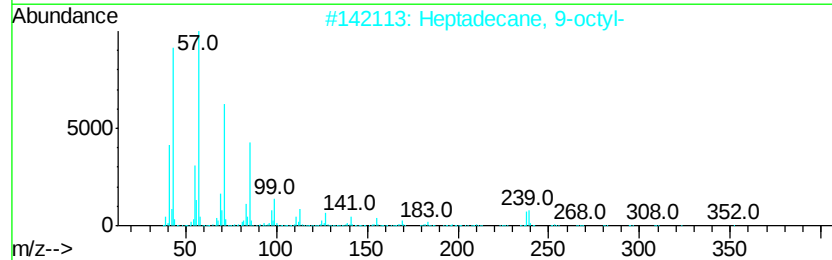
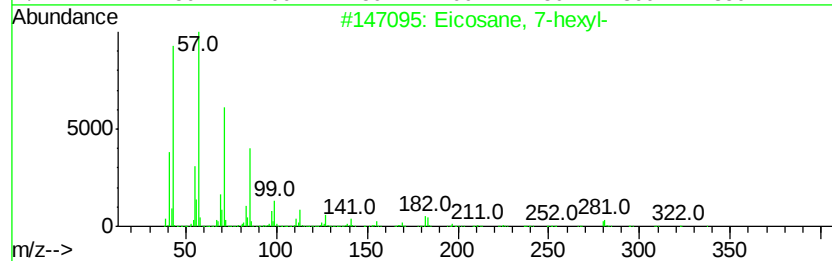
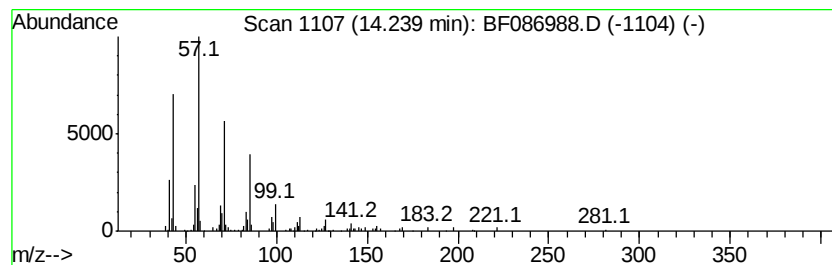
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Eicosane, 7-hexyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.24	2.01 ng	126728	Chrysene-d12	13.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Heptacosane	380	C27H56	000593-49-7	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051316\
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Acq On : 13 May 2016 23:48
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ClientSampleId :
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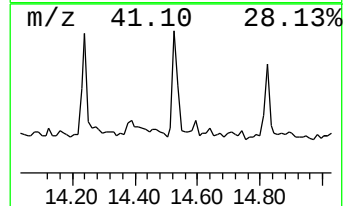
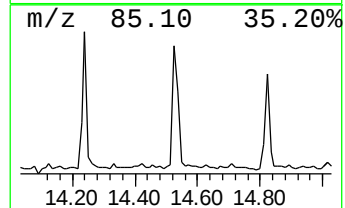
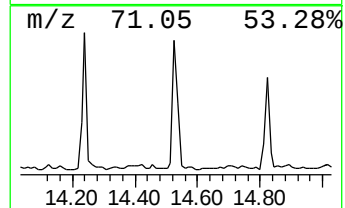
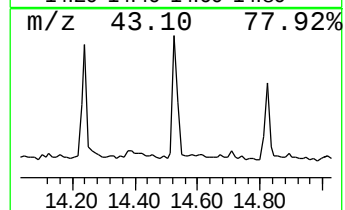
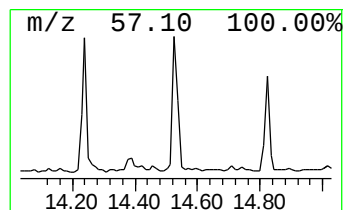
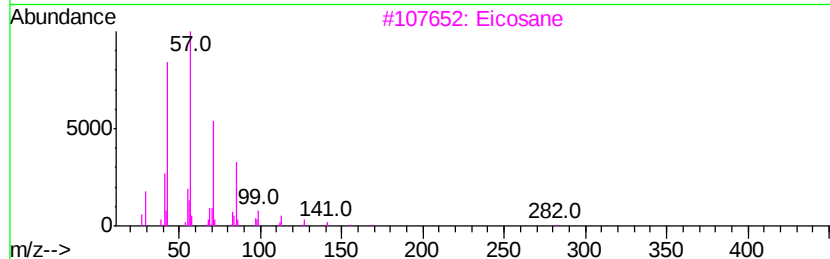
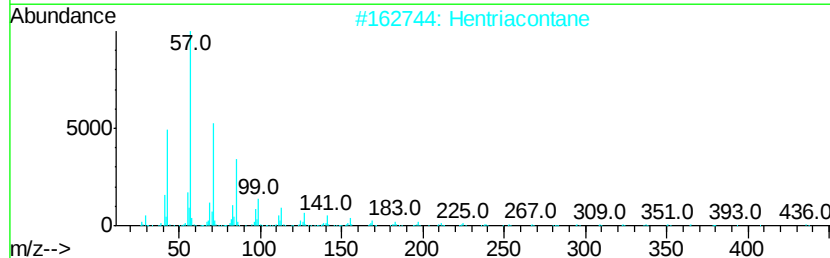
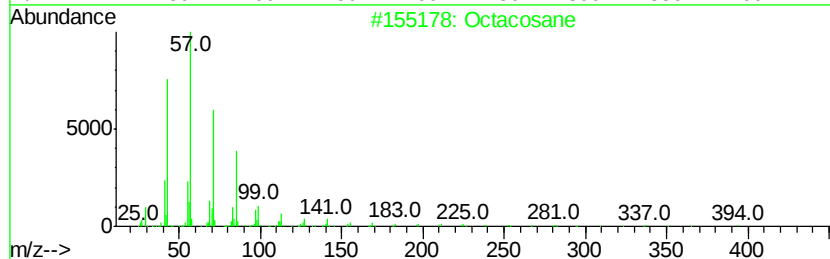
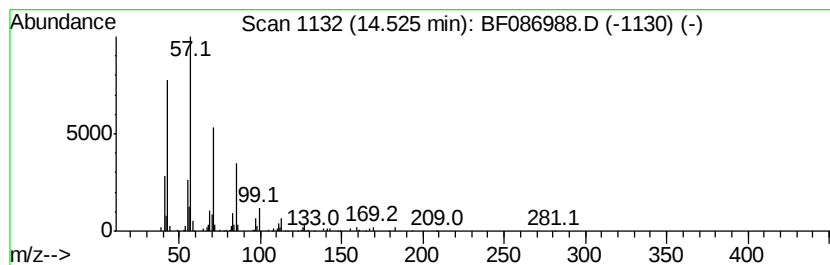
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	2.69 ng	120452	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		Hentriacontane	437	C31H64	000630-04-6	90
3		Eicosane	282	C20H42	000112-95-8	87
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
5		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051316\
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 ALS Vial : 14 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.39	6.39	75.1	ng	3532410	1	6.62	941185	20.0
Ethanol, 2-[4-(1,...	11.35	2.8	ng	191548	4	11.12	1347780	20.0
Ethanol, 2-[2-[4-...	12.50	5.1	ng	323037	5	13.75	1263330	20.0
Hexadecanoic acid...	12.55	7.5	ng	472296	5	13.75	1263330	20.0
11-Tricosene	12.62	3.1	ng	194771	5	13.75	1263330	20.0
n-Butyl myristate	13.25	5.7	ng	356970	5	13.75	1263330	20.0
unknown13.50	13.50	3.5	ng	218987	5	13.75	1263330	20.0
Pentafluoropropio...	13.62	7.8	ng	490039	5	13.75	1263330	20.0
Eicosane	13.93	2.5	ng	159912	5	13.75	1263330	20.0
Eicosane, 7-hexyl-	14.24	2.0	ng	126728	5	13.75	1263330	20.0
Octacosane	14.53	2.7	ng	120452	6	15.11	895036	20.0