

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040416\
 Data File : BF086039.D
 Acq On : 4 Apr 2016 15:32
 Operator : UM/SJ
 Sample : H2055-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BH-3(5-10)

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-BF040216.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	4.967	249	252	262	rBV	53595	114472	2.99%	0.342%
2	5.367	284	287	289	rBV	2590688	3286570	85.79%	9.810%
3	6.407	375	378	386	rBV	2640139	3034708	79.22%	9.059%
4	6.533	386	389	391	rBV	3236913	3374572	88.09%	10.073%
5	6.762	407	409	415	rBV	812458	745930	19.47%	2.227%
6	6.922	420	423	425	rBV	1918882	2629821	68.65%	7.850%
7	7.333	456	459	461	rBV	2159802	2326319	60.73%	6.944%
8	8.042	519	521	524	rBV	892902	976192	25.48%	2.914%
9	9.128	613	616	618	rBV	3129659	3830729	100.00%	11.435%
10	9.516	648	650	653	rBV	411320	444379	11.60%	1.326%
11	9.733	665	669	671	rBV	72087	68053	1.78%	0.203%
12	9.802	672	675	677	rVV	846055	1089626	28.44%	3.253%
13	10.236	709	713	714	rBV	80920	102836	2.68%	0.307%
14	10.453	729	732	735	rBV	32956	62360	1.63%	0.186%
15	10.591	741	744	746	rBV	2489410	2537580	66.24%	7.575%
16	10.705	752	754	761	rVB	118897	145287	3.79%	0.434%
17	11.151	791	793	794	rBV	58491	49589	1.29%	0.148%
18	11.276	802	804	807	rBV	1142715	1160370	30.29%	3.464%
19	11.813	849	851	859	rBV2	275794	318951	8.33%	0.952%
20	12.591	917	919	925	rBV	59949	106825	2.79%	0.319%
21	12.682	925	927	930	rVB	179957	204793	5.35%	0.611%
22	12.865	940	943	946	rBV	3570205	3521902	91.94%	10.513%
23	13.345	979	985	987	rBV	167369	176319	4.60%	0.526%
24	13.391	987	989	991	rVV	164433	138628	3.62%	0.414%
25	13.757	1019	1021	1030	rBV	277849	453146	11.83%	1.353%
26	13.917	1032	1035	1037	rBV	1131181	1138104	29.71%	3.397%
27	14.077	1047	1049	1057	rBV	25445	39551	1.03%	0.118%
28	14.385	1073	1076	1082	rBV2	22500	71566	1.87%	0.214%
29	14.740	1105	1107	1110	rBV	348940	358678	9.36%	1.071%
30	15.322	1155	1158	1167	rVB	589093	954519	24.92%	2.849%
31	15.722	1190	1193	1196	rBV	23952	38338	1.00%	0.114%

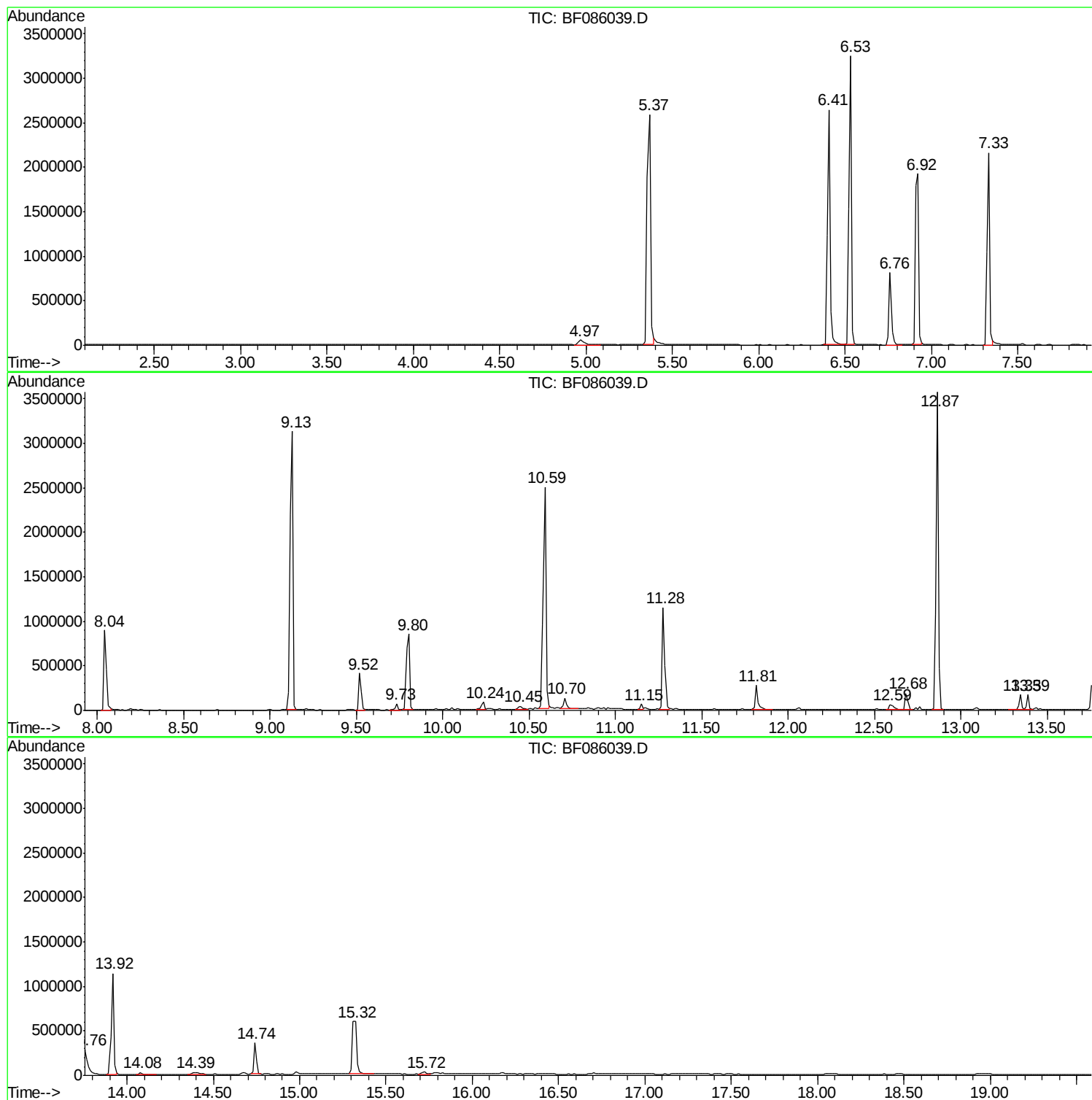
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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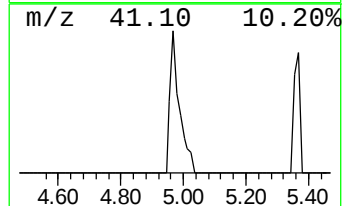
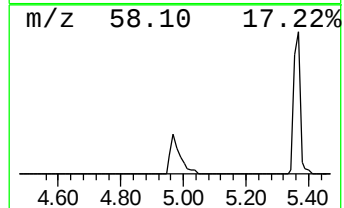
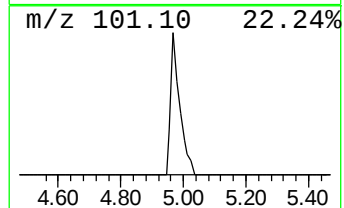
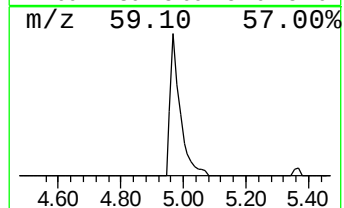
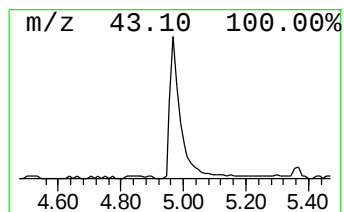
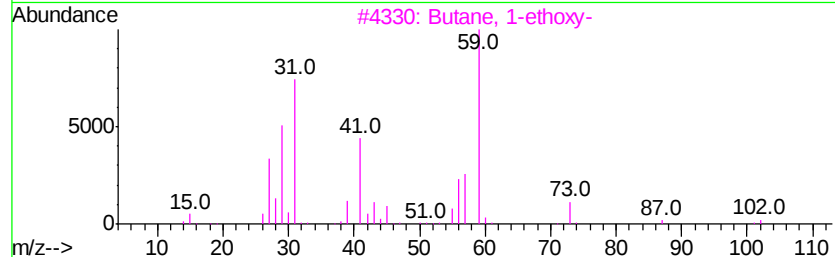
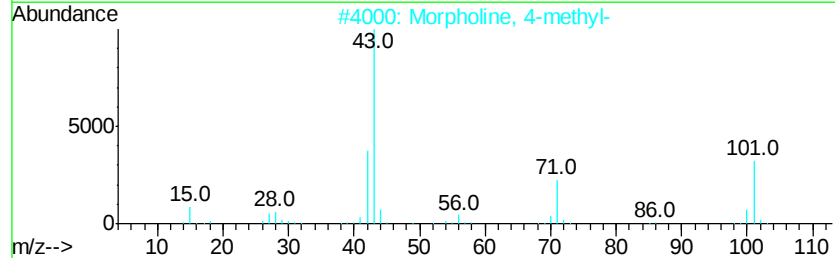
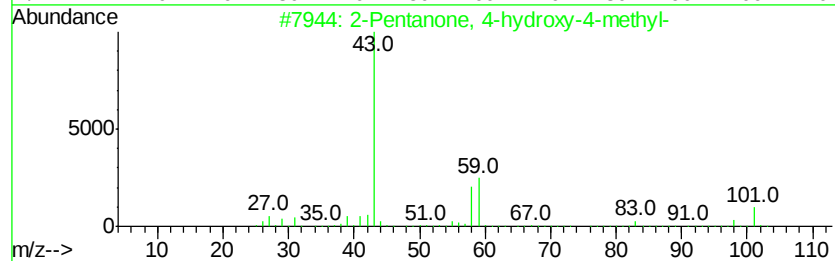
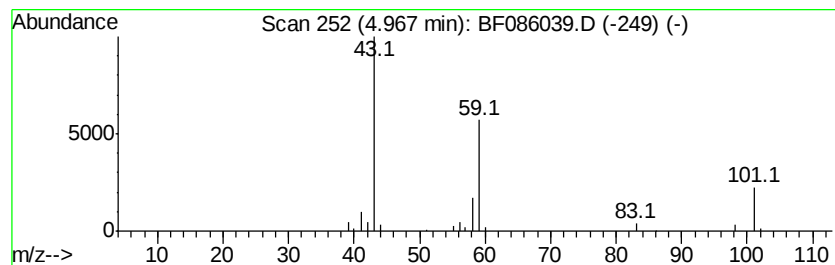
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	3.07 ng	114472	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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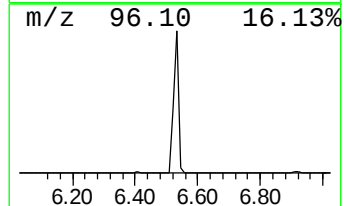
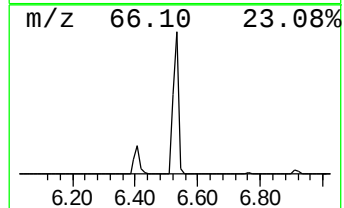
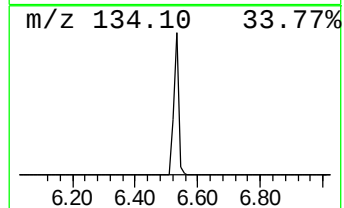
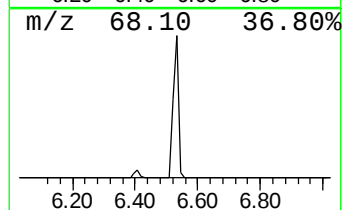
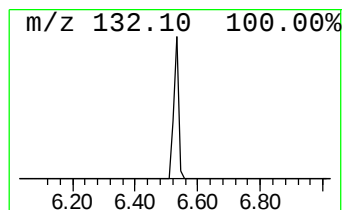
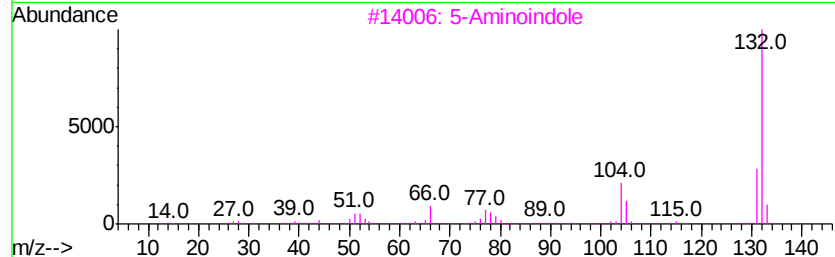
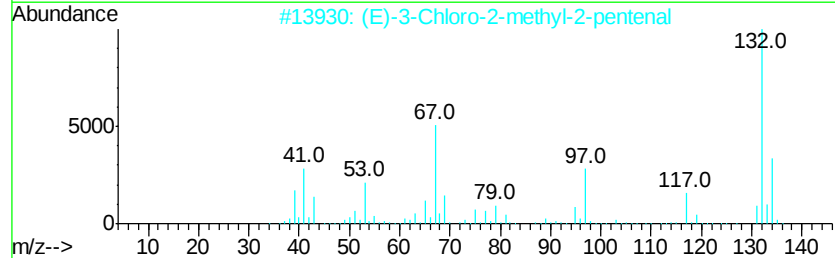
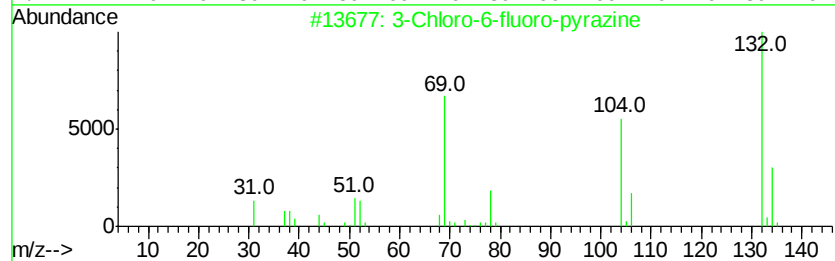
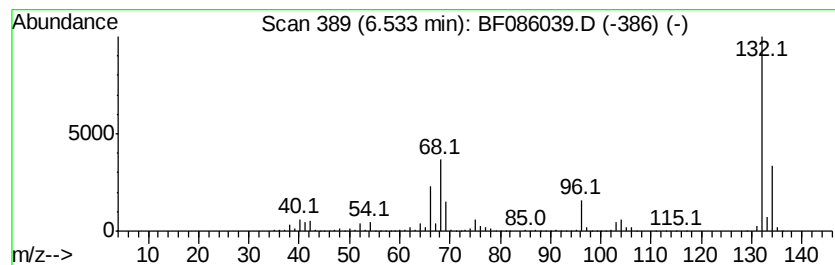
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Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	90.48 ng	3374570	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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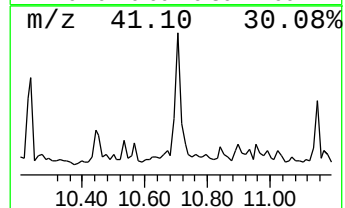
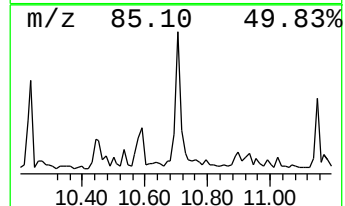
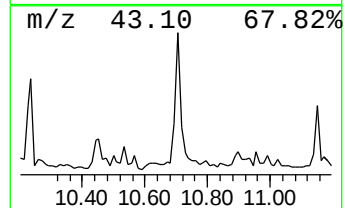
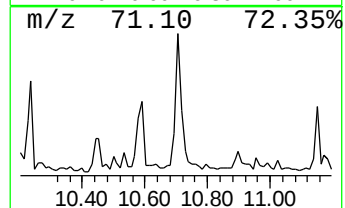
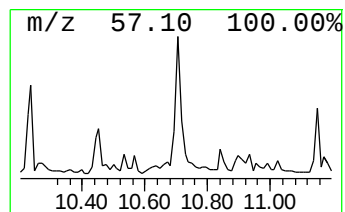
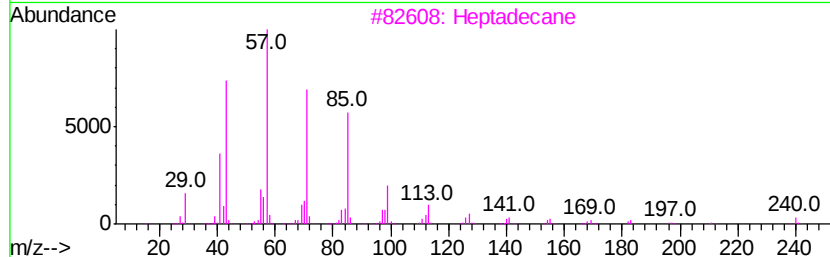
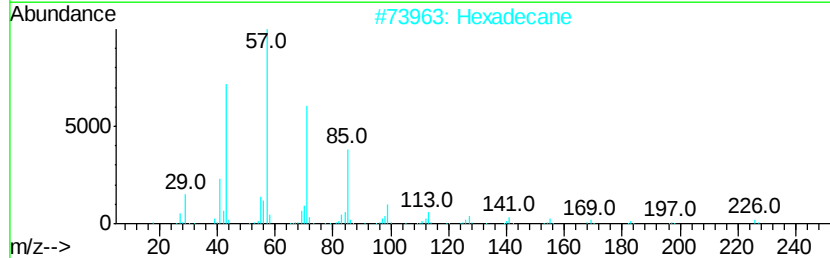
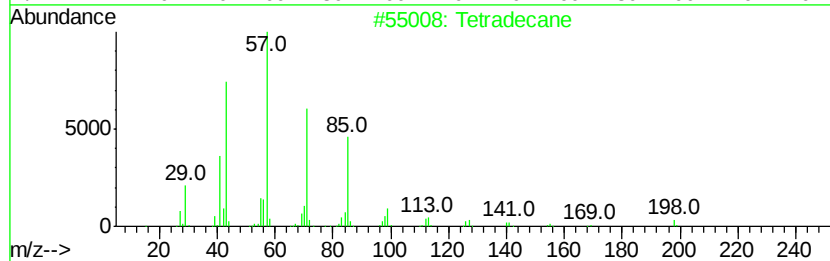
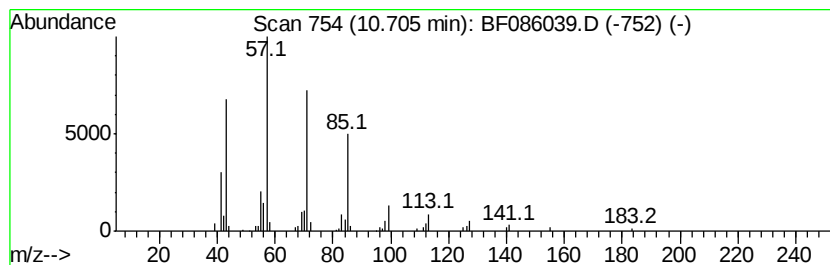
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Peak Number 4 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.50 ng	145287	Phenanthrene-d10	11.28
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tetradecane	198 C14H30	000629-59-4 91
2		Hexadecane	226 C16H34	000544-76-3 91
3		Heptadecane	240 C17H36	000629-78-7 90
4		Octadecane	254 C18H38	000593-45-3 90
5		2-Bromo dodecane	248 C12H25Br	013187-99-0 90



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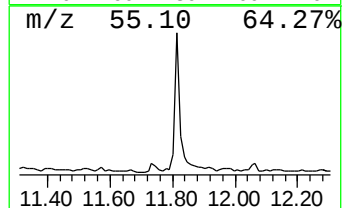
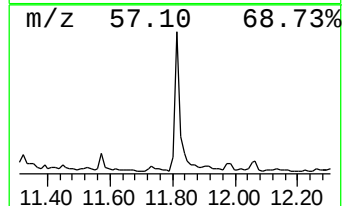
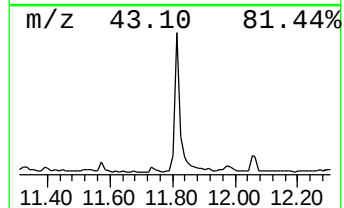
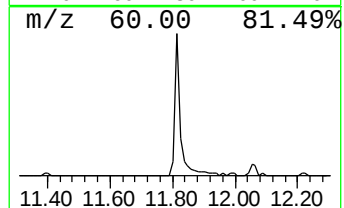
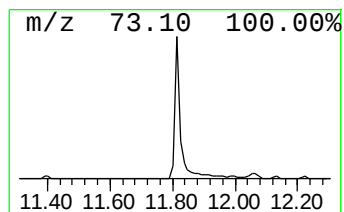
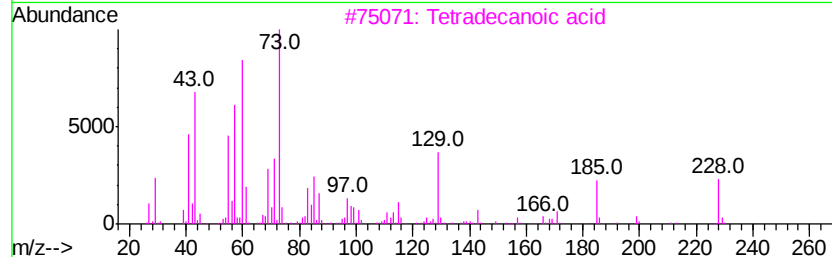
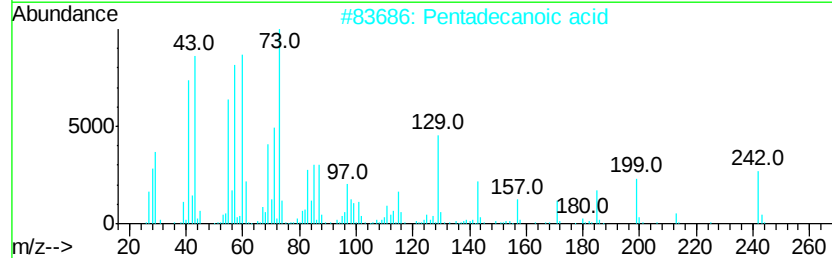
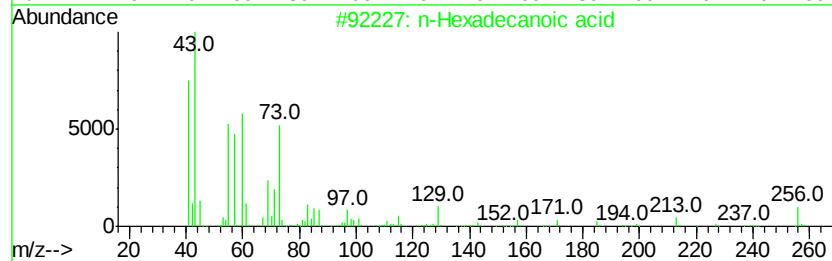
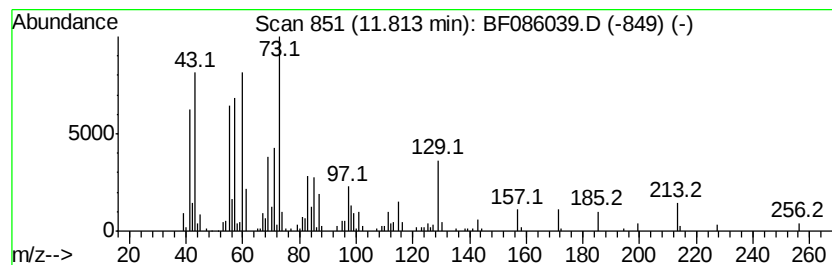
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	5.50 ng	318951	Phenanthrene-d10	11.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		Tridecanoic acid	214	C13H26O2	000638-53-9	74
5		Tridecane	184	C13H28	000629-50-5	11



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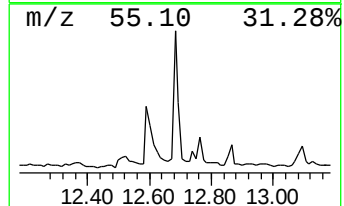
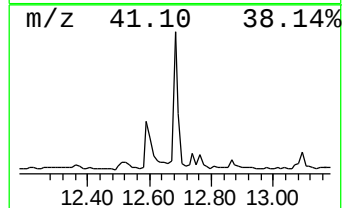
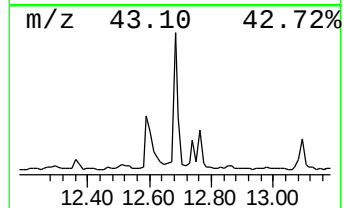
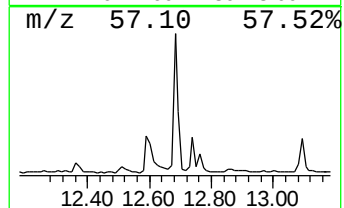
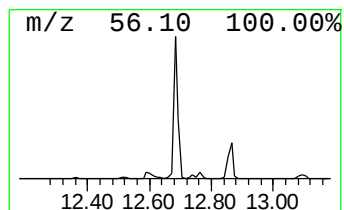
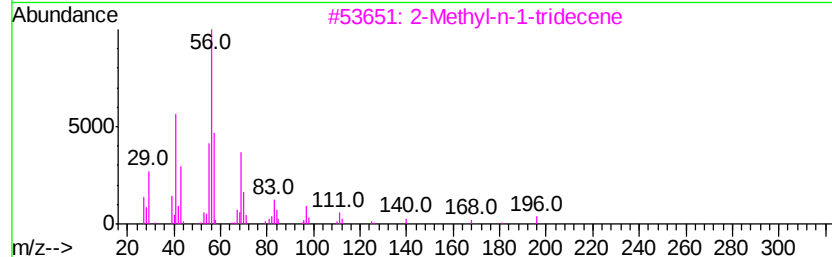
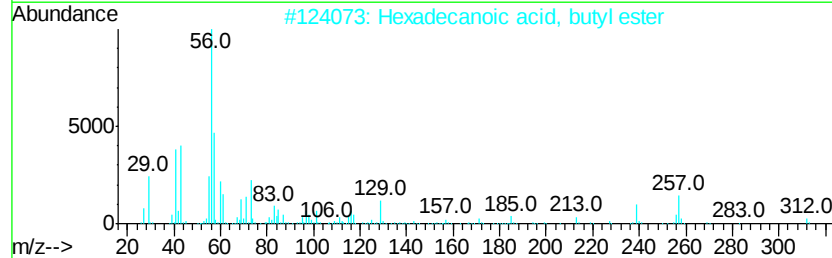
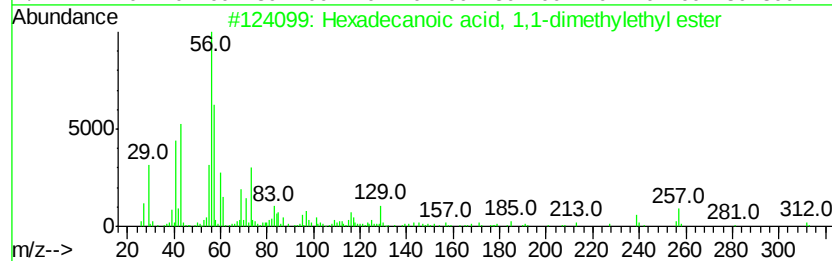
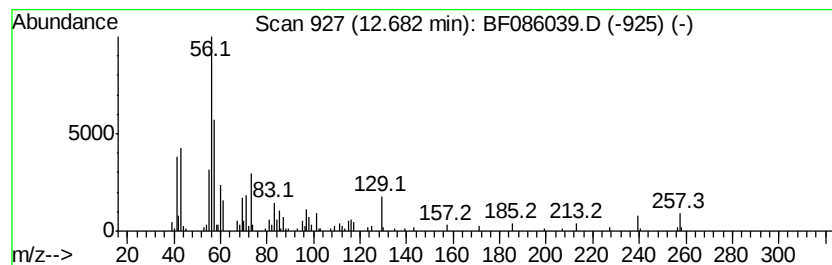
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Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	3.60 ng	204793	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
3		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	38
4		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	38
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38



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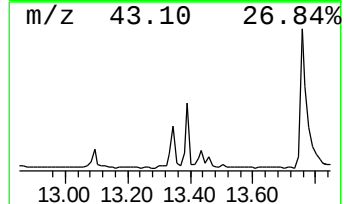
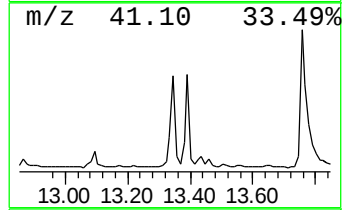
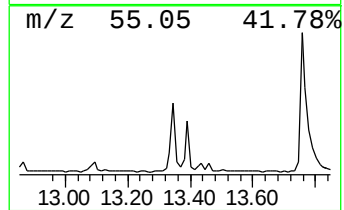
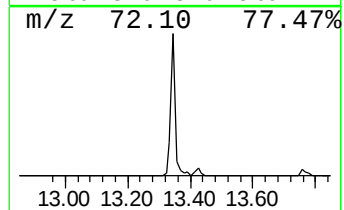
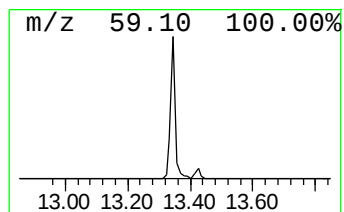
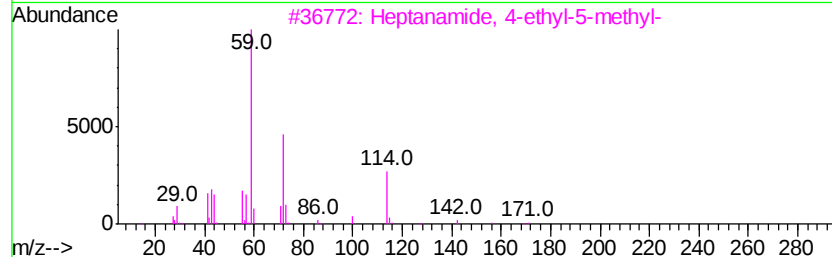
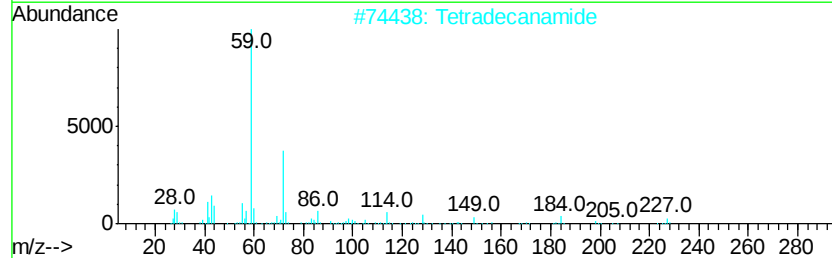
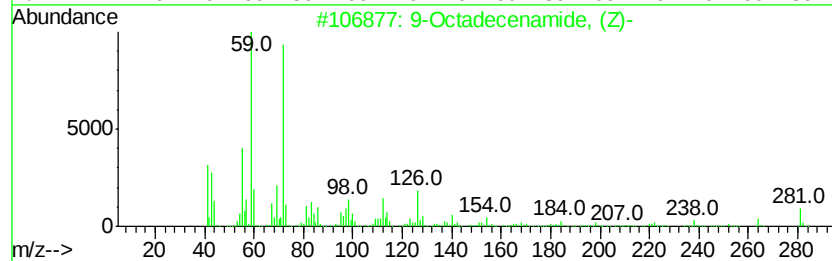
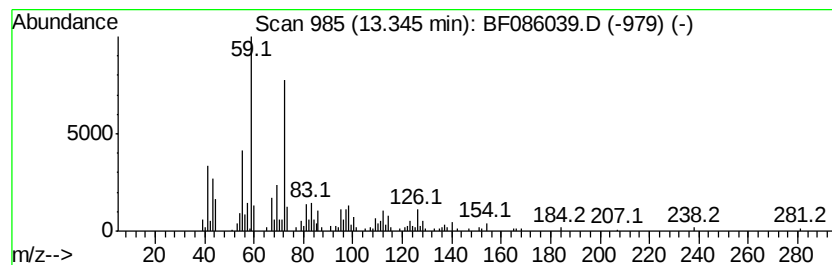
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ClientSampleId :
BH-3(5-10)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.35	3.10 ng	176319	Chrysene-d12	13.92		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86	
2	Tetradecanamide	227	C14H29NO	000638-58-4	59	
3	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	53	
4	1,1,2-Trimethyl-1-silacyclobutane	114	C6H14Si	030681-90-4	43	
5	Dodecanamide	199	C12H25NO	001120-16-7	38	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040416\
Data File : BF086039.D
Acq On : 4 Apr 2016 15:32
Operator : UM/SJ
Sample : H2055-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

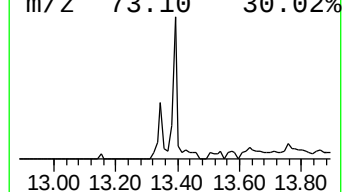
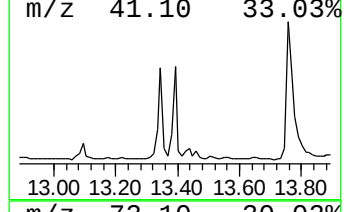
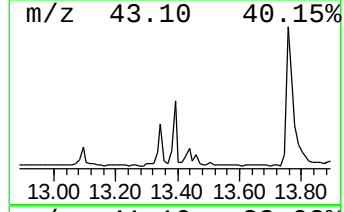
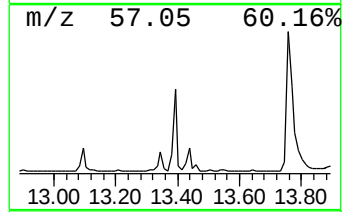
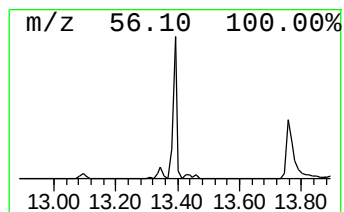
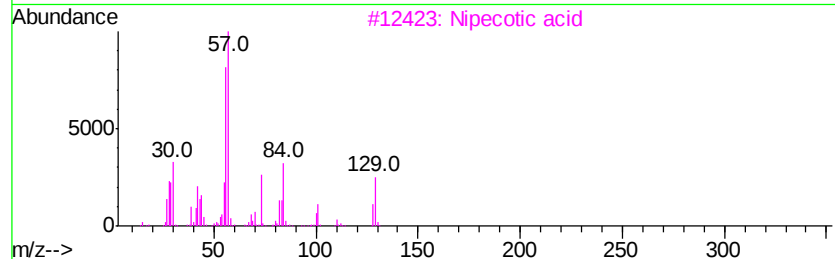
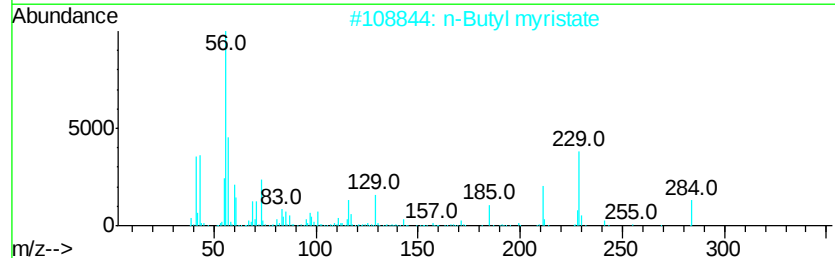
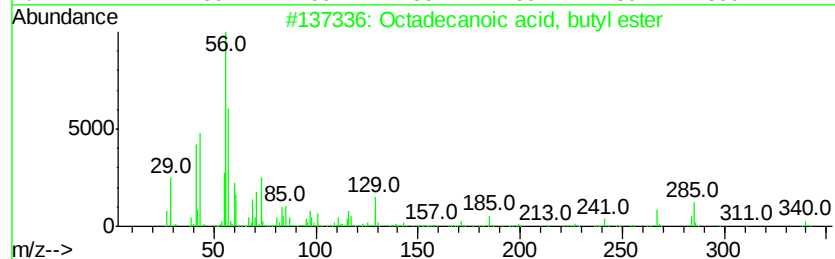
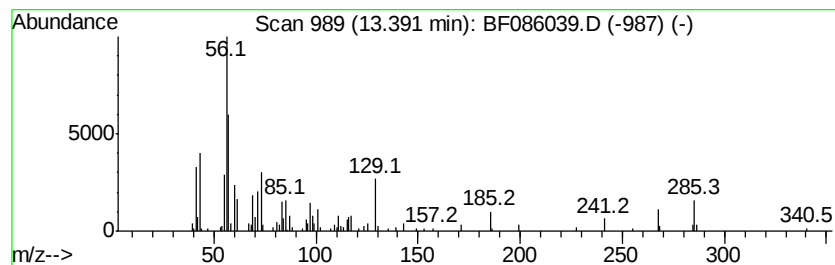
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ClientSampleId :
BH-3(5-10)

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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 Octadecanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.39	2.44 ng	138628	Chrysene-d12	13.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	96
2	n-Butyl myristate	284	C18H36O2	000110-36-1	64
3	Nipecotic acid	129	C6H11NO2	000498-95-3	50
4	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	43
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040416\
Data File : BF086039.D
Acq On : 4 Apr 2016 15:32
Operator : UM/SJ
Sample : H2055-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

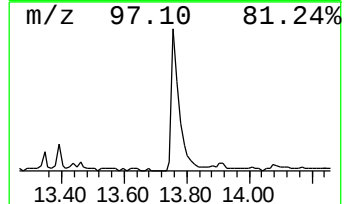
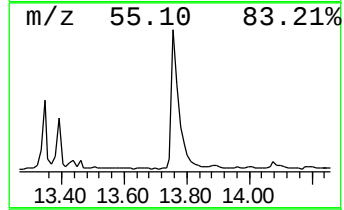
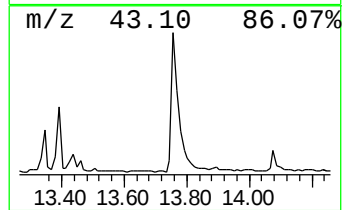
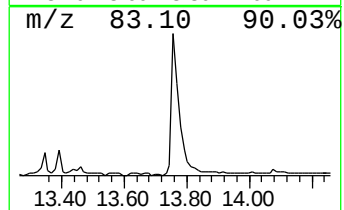
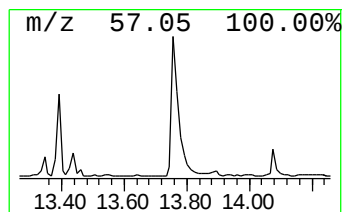
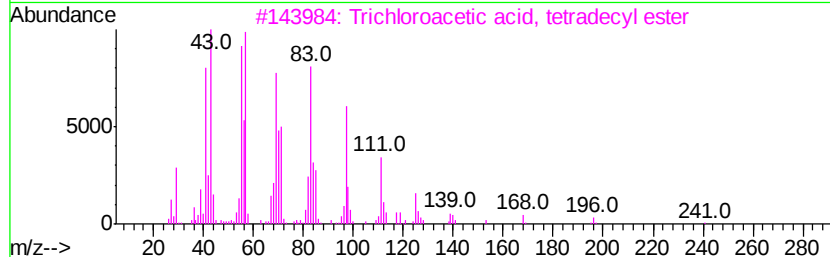
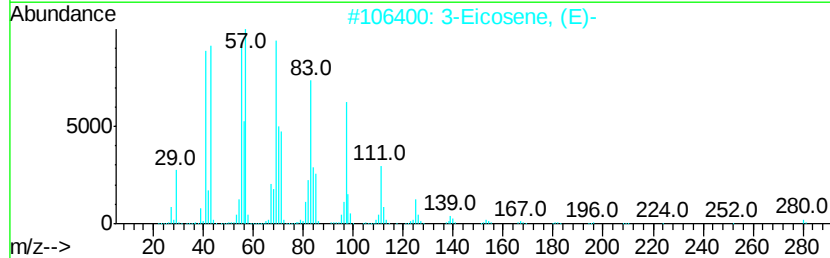
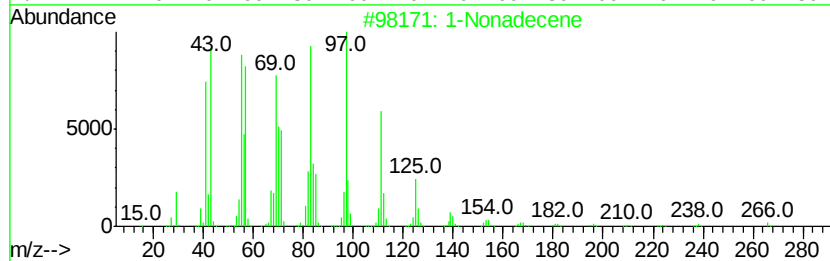
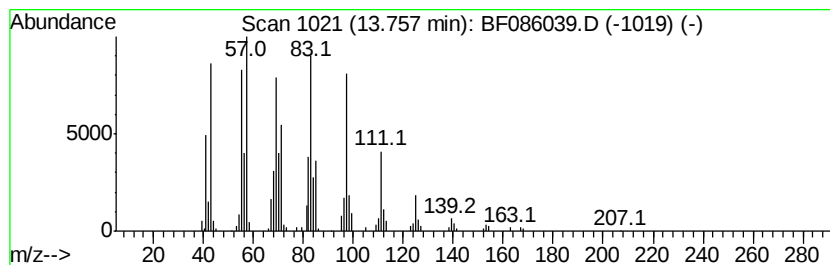
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	7.96 ng	453146	Chrysene-d12	13.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Nonadecene	266 C19H38	018435-45-5	91
2	3-Eicosene, (E)-	280 C20H40	074685-33-9	91
3	Trichloroacetic acid, tetradecyl...	358 C16H29Cl3O2	074339-52-9	91
4	1-Hexacosanol	382 C26H54O	000506-52-5	90
5	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040416\
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Sample : H2055-03
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BH-3(5-10)

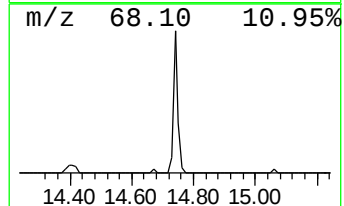
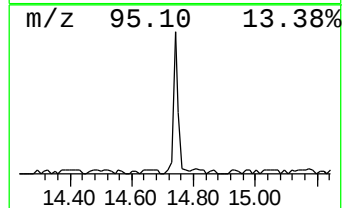
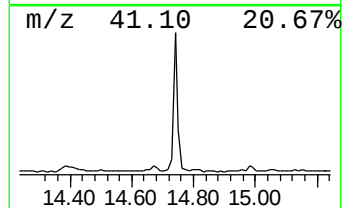
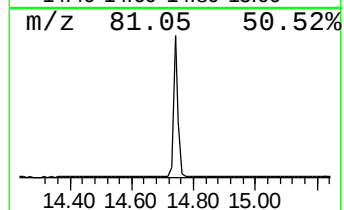
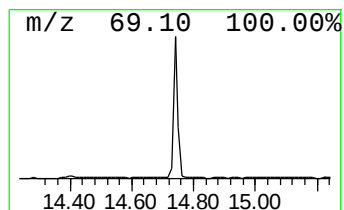
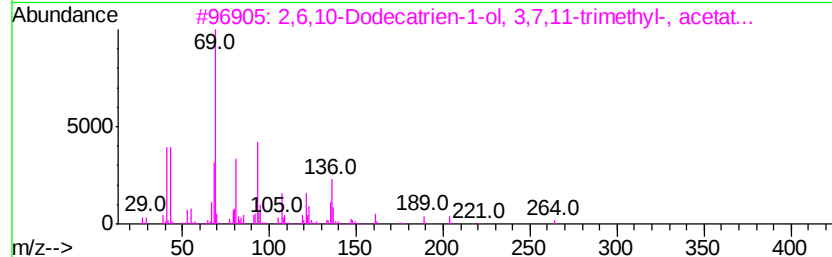
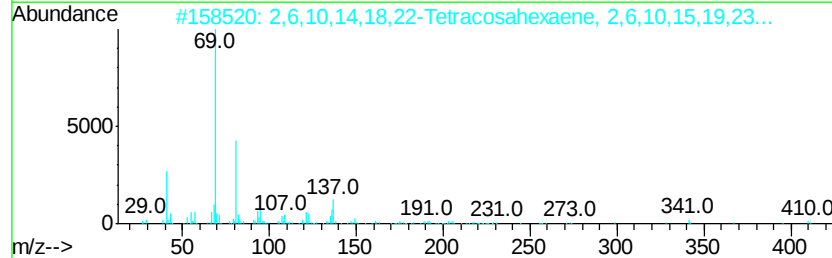
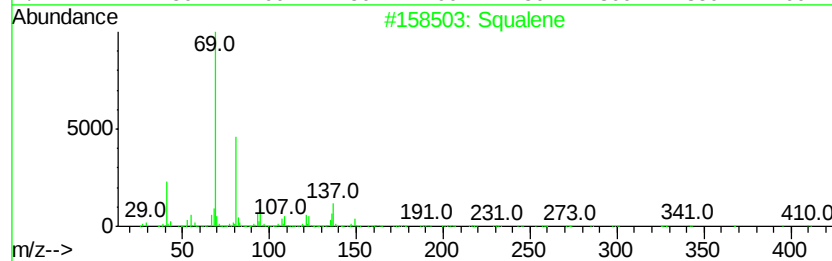
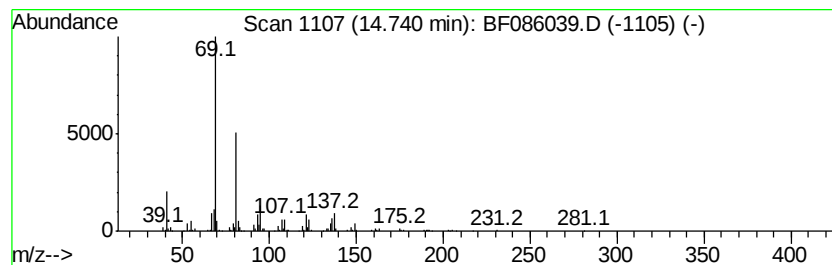
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	7.52 ng	358678	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	72
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5		2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	53



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Acq On : 4 Apr 2016 15:32
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Sample : H2055-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.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
2-Pentanone, 4-hy...	4.97	3.1 ng		114472	1	6.76	745930	20.0
unknown6.53	6.53	90.5 ng		3374570	1	6.76	745930	20.0
Tetradecane	10.70	2.5 ng		145287	4	11.28	1160370	20.0
n-Hexadecanoic acid	11.81	5.5 ng		318951	4	11.28	1160370	20.0
Hexadecanoic acid...	12.68	3.6 ng		204793	5	13.92	1138100	20.0
9-Octadecenamide,...	13.35	3.1 ng		176319	5	13.92	1138100	20.0
Octadecanoic acid...	13.39	2.4 ng		138628	5	13.92	1138100	20.0
1-Nonadecene	13.76	8.0 ng		453146	5	13.92	1138100	20.0
Squalene	14.74	7.5 ng		358678	6	15.32	954519	20.0