

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
 Data File : BF091763.D
 Acq On : 19 Dec 2016 4:25
 Operator : UM/SJ
 Sample : H6011-01
 Misc :
 ALS Vial : 50 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-12

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-BF121716.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	4.933	246	249	253	rBV	542630	829018	9.72%	1.398%
2	5.367	284	287	289	rBV	3434693	3581722	42.01%	6.038%
3	6.407	375	378	380	rBV	2496220	2489001	29.19%	4.196%
4	6.533	386	389	392	rBV	4997191	5598525	65.66%	9.438%
5	6.761	407	409	411	rBV	1456634	1599074	18.75%	2.696%
6	6.921	420	423	426	rBV	5018994	5055952	59.30%	8.524%
7	7.333	456	459	462	rBV	4072718	4422439	51.87%	7.456%
8	7.550	475	478	485	rVB2	63470	121310	1.42%	0.205%
9	8.053	519	522	524	rBV	2497180	2325498	27.27%	3.920%
10	8.647	572	574	575	rVB	176341	140697	1.65%	0.237%
11	8.979	599	603	606	rBV3	80038	189989	2.23%	0.320%
12	9.139	613	617	619	rBV	5771670	8526337	100.00%	14.374%
13	9.527	647	651	653	rBV2	178014	249435	2.93%	0.421%
14	9.802	672	675	677	rBV	2552647	2423152	28.42%	4.085%
15	9.962	687	689	691	rBV3	95799	164260	1.93%	0.277%
16	10.328	718	721	726	rBV2	222003	280165	3.29%	0.472%
17	10.590	741	744	747	rBV2	3431450	5033682	59.04%	8.486%
18	10.716	752	755	759	rVB4	149660	308209	3.61%	0.520%
19	11.288	802	805	807	rBV	2405693	2286801	26.82%	3.855%
20	11.825	850	852	856	rVB3	230539	336958	3.95%	0.568%
21	12.613	919	921	926	rVB	155308	212228	2.49%	0.358%
22	12.705	927	929	931	rVB	348848	316645	3.71%	0.534%
23	12.876	941	944	947	rBV	6302573	6874541	80.63%	11.590%
24	12.922	947	948	957	rVB5	44034	92394	1.08%	0.156%
25	13.402	988	990	992	rBV2	163940	173788	2.04%	0.293%
26	13.448	992	994	996	rVV	1898252	1812864	21.26%	3.056%
27	13.768	1020	1022	1032	rVB2	163989	305426	3.58%	0.515%
28	13.916	1032	1035	1038	rBV	1977208	1880381	22.05%	3.170%
29	15.322	1155	1158	1160	rVV	1083426	1427970	16.75%	2.407%
30	15.357	1160	1161	1170	rVB	73131	156972	1.84%	0.265%
31	16.225	1234	1237	1245	rVB	45835	101313	1.19%	0.171%

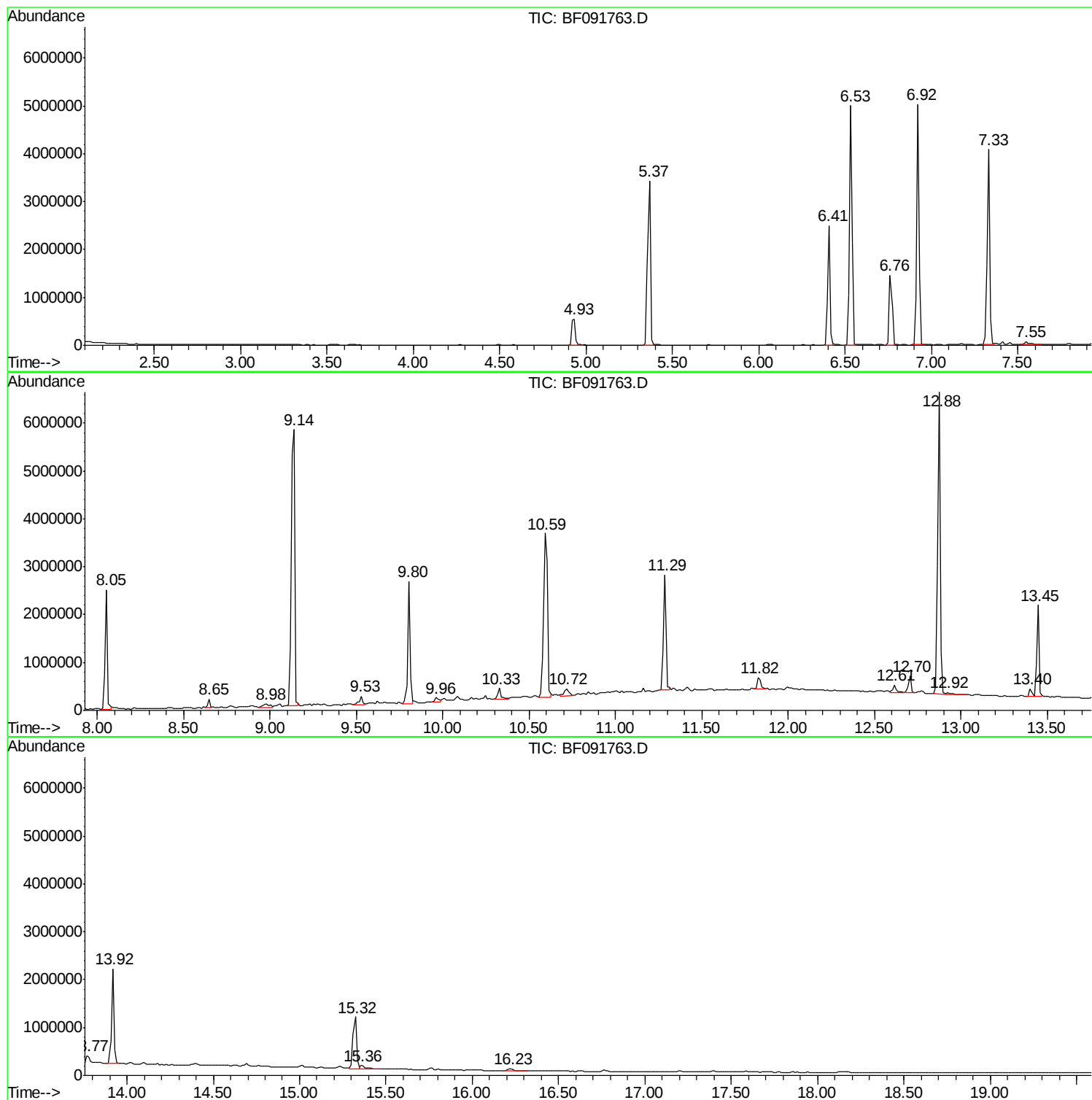
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Instrument :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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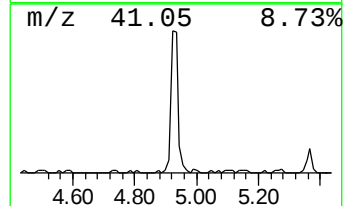
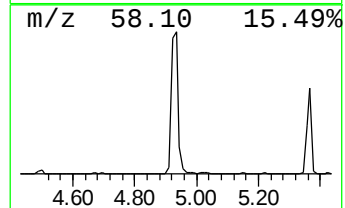
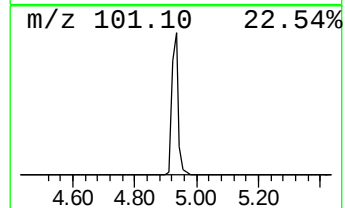
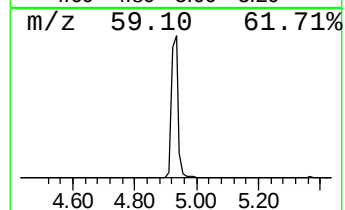
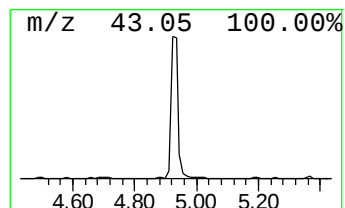
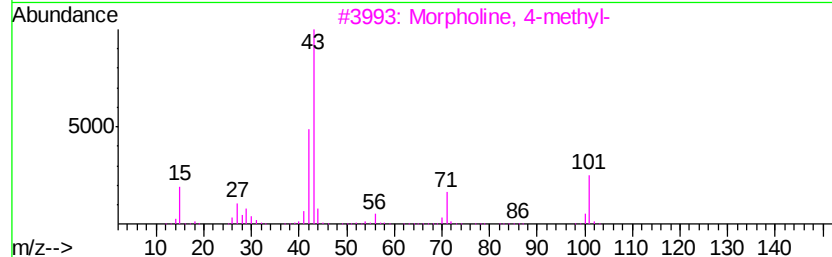
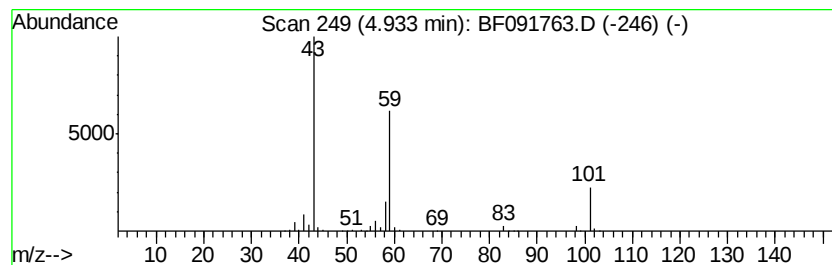
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	10.37 ng	829018	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	72
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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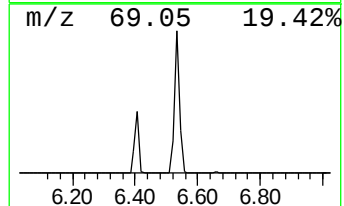
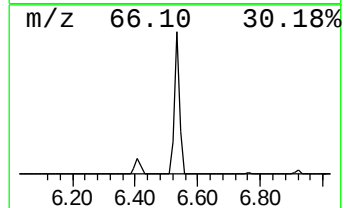
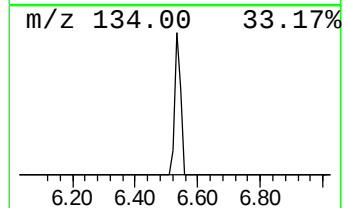
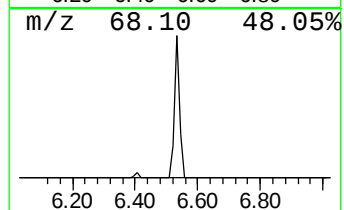
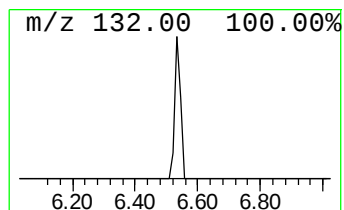
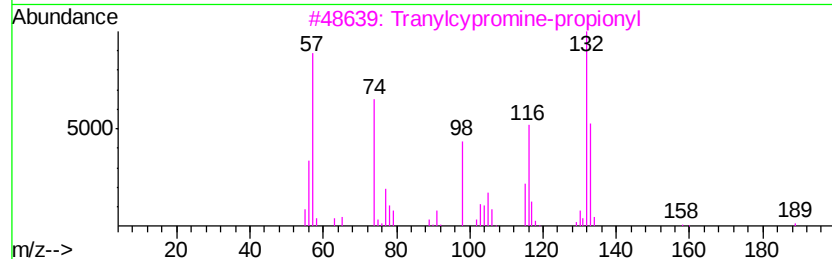
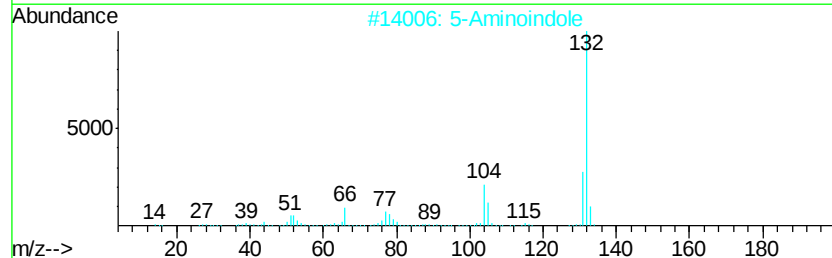
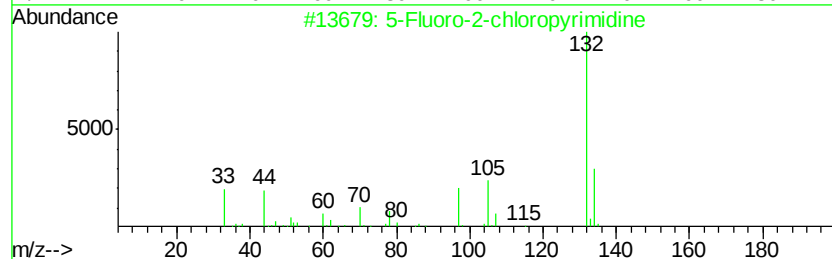
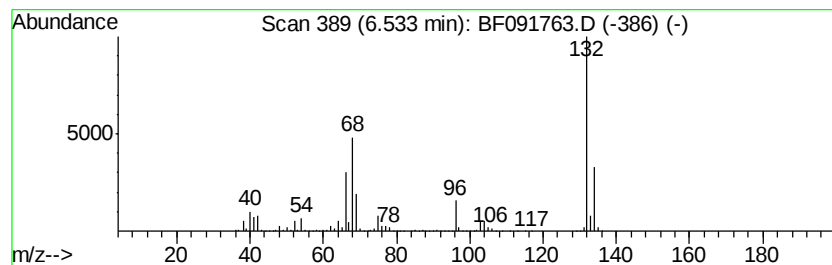
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Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	70.02 ng	5598530	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypramine-propionyl	189	C12H15NO	1000123-86-3	10
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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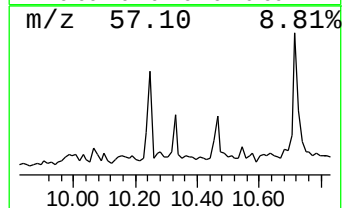
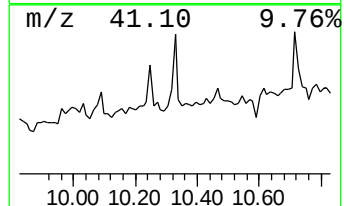
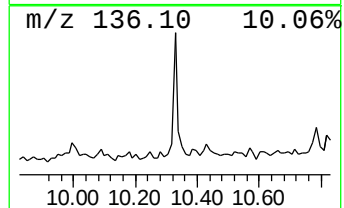
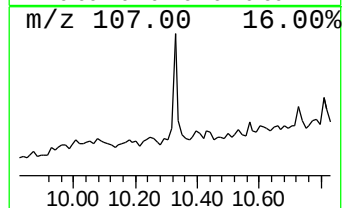
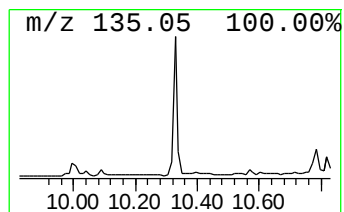
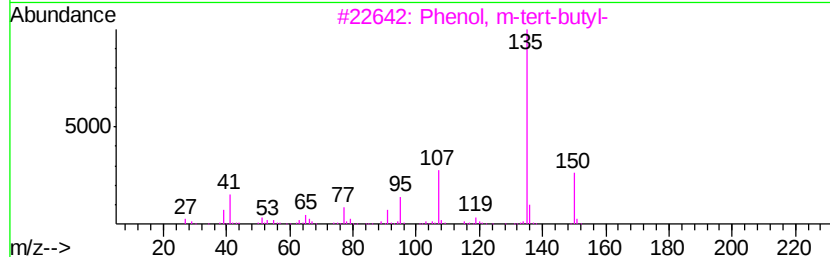
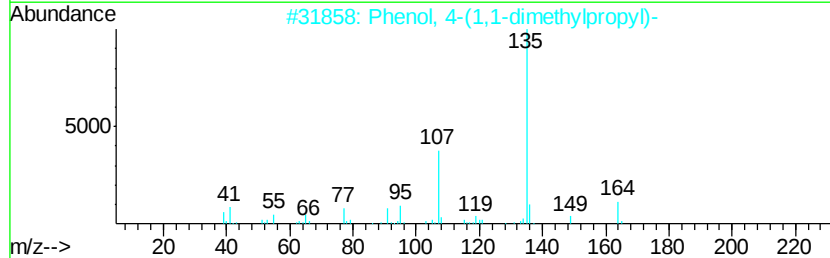
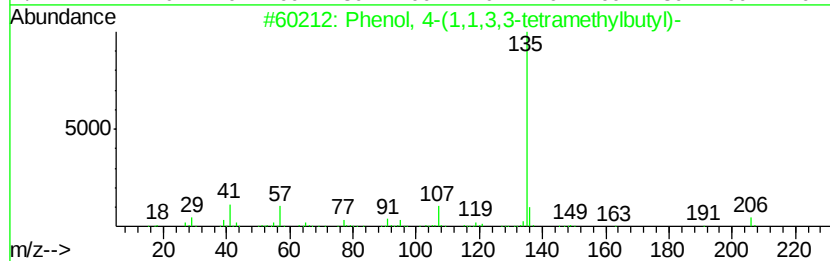
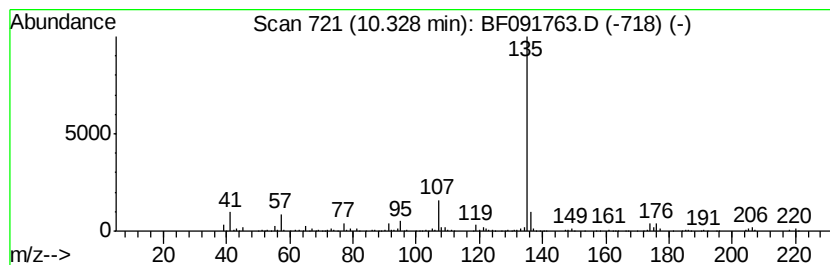
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Peak Number 5 Phenol, 4-(1,1,3,3-tetramet... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	2.31 ng	280165	Acenaphthene-d10	9.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	72		
2	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	64		
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	64		
4	4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	64		
5	Silane, trimethylphenyl-	150	C9H14Si	000768-32-1	59		



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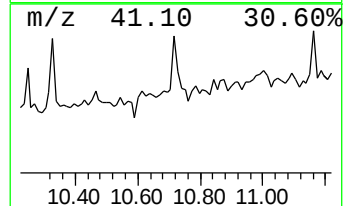
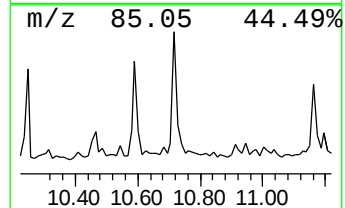
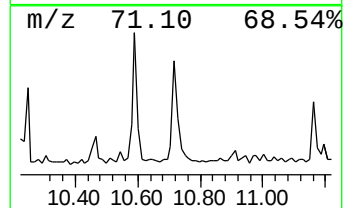
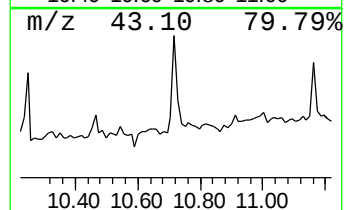
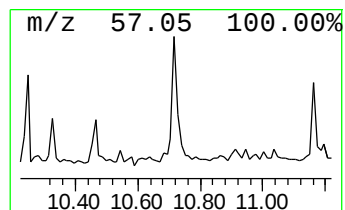
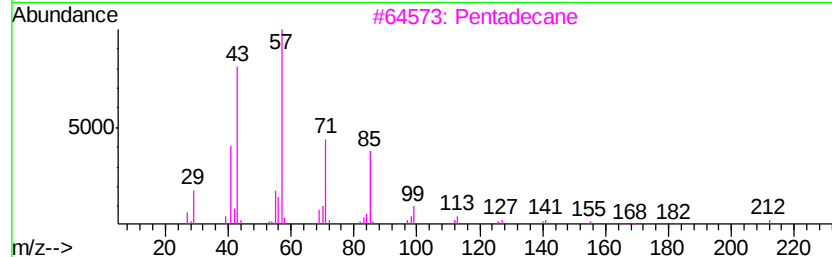
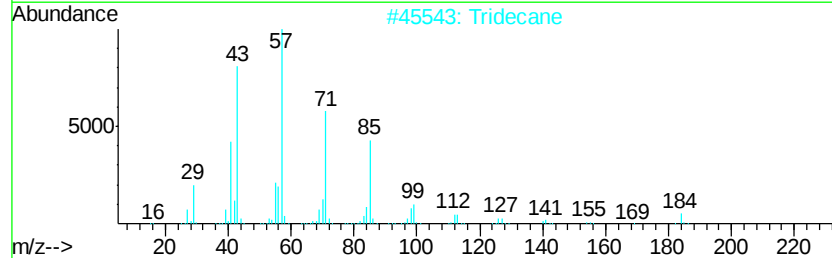
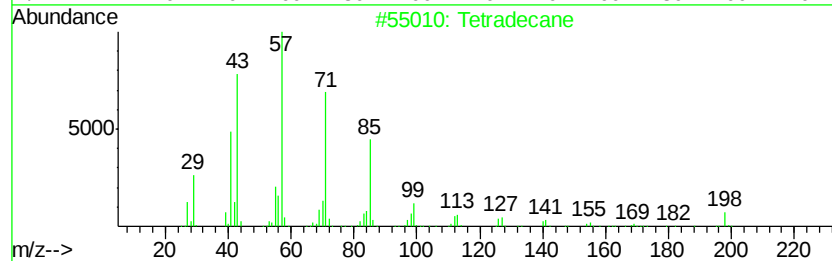
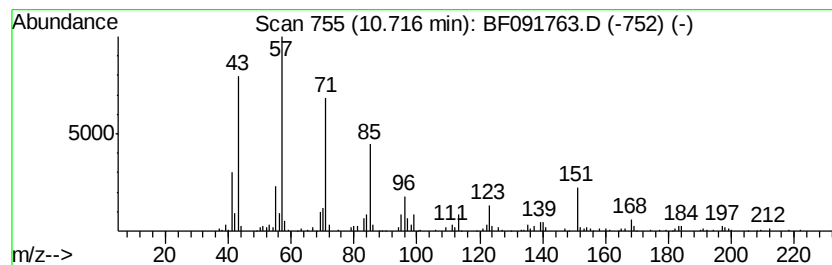
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Peak Number 6 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.72	2.70 ng	308209	Phenanthrene-d10	11.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	58
2	Tridecane	184	C13H28	000629-50-5	58
3	Pentadecane	212	C15H32	000629-62-9	58
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	52
5	Dodecane	170	C12H26	000112-40-3	52



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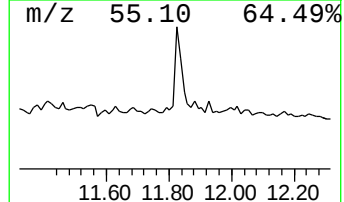
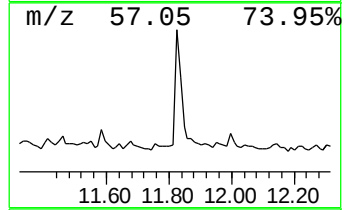
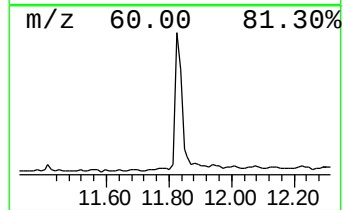
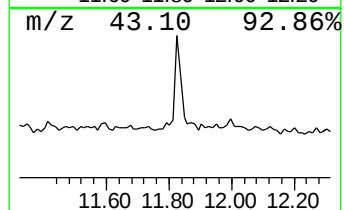
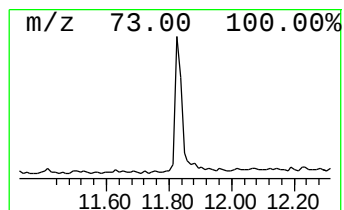
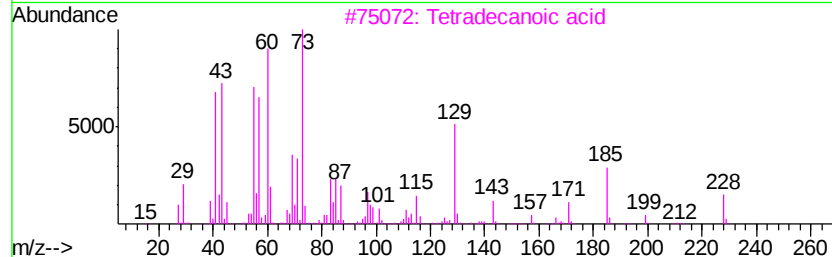
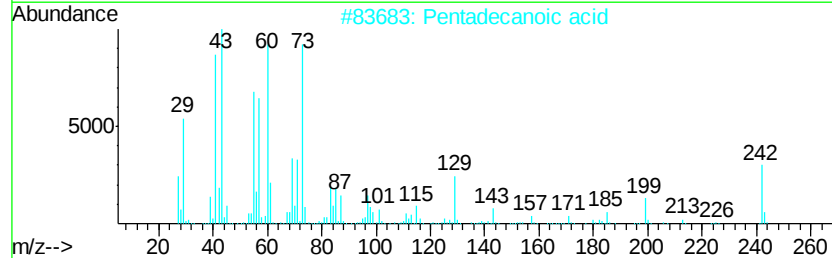
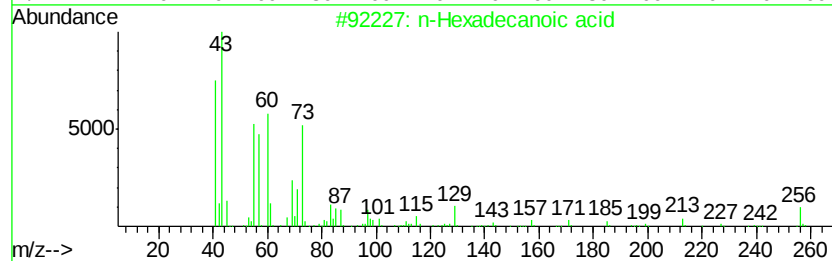
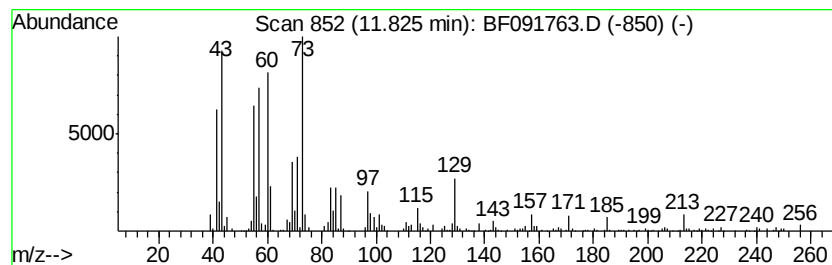
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Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.82	2.95 ng	336958	Phenanthrene-d10		11.29
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Dodecane, 1,2-dibromo-	326	C12H24Br2	055334-42-4	30



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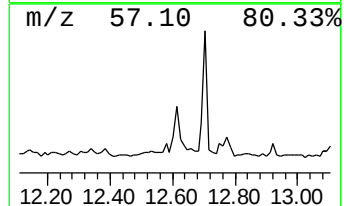
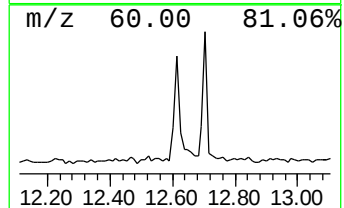
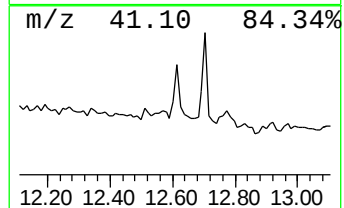
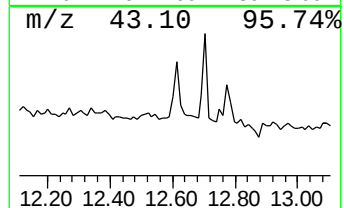
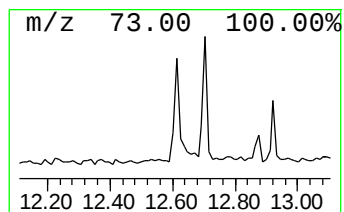
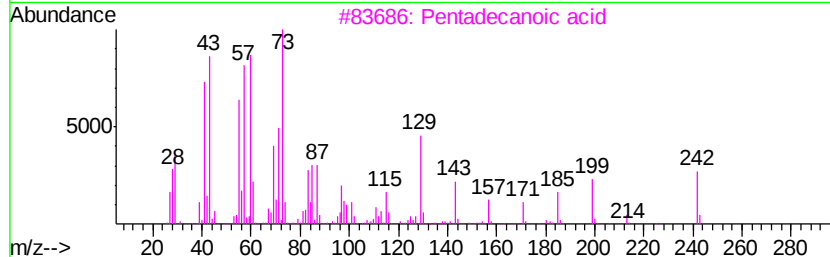
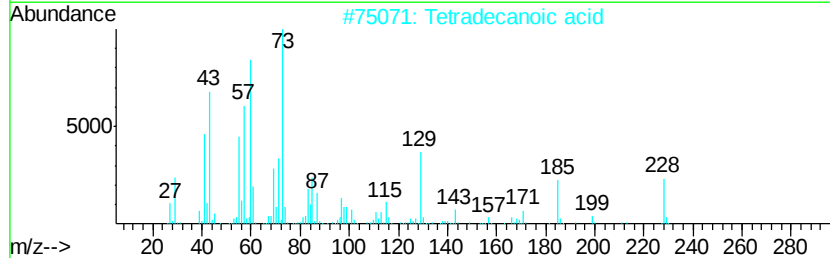
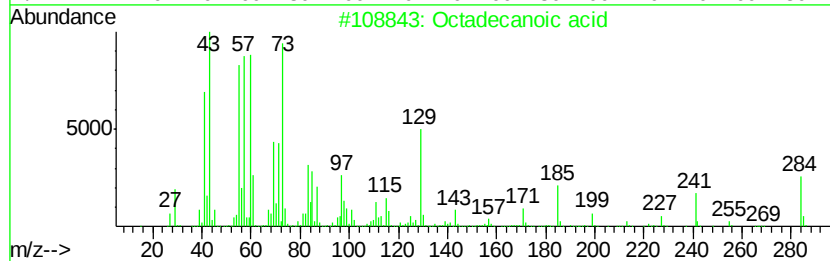
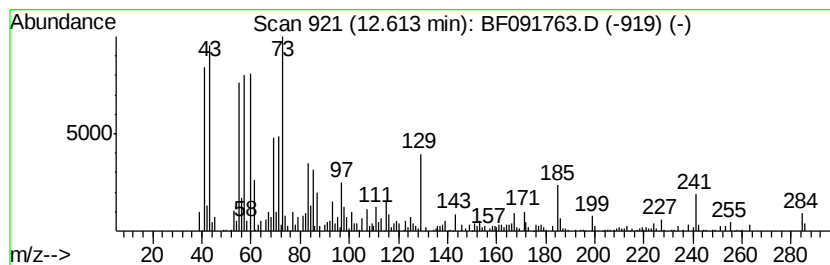
Instrument :
BNA_F
ClientSampleId :
MW-12

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121716.M
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 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.61	2.26 ng	212228	Chrysene-d12	13.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Heptadecane	240	C17H36	000629-78-7	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121816\
Data File : BF091763.D
Acq On : 19 Dec 2016 4:25
Operator : UM/SJ
Sample : H6011-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

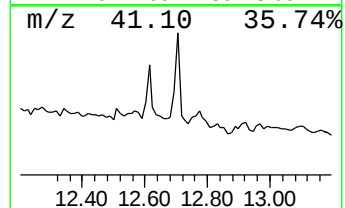
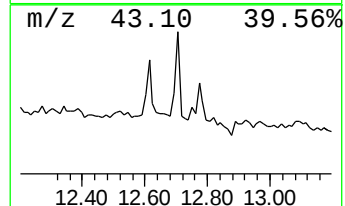
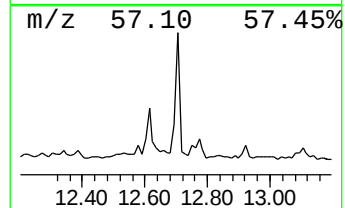
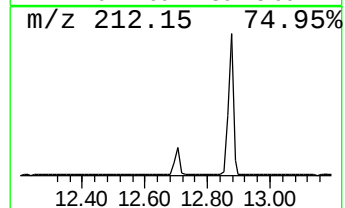
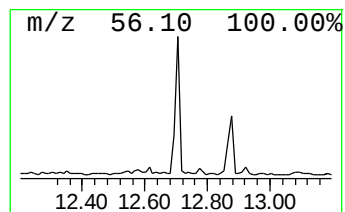
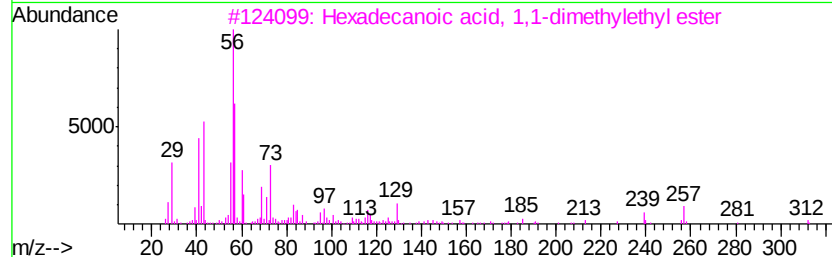
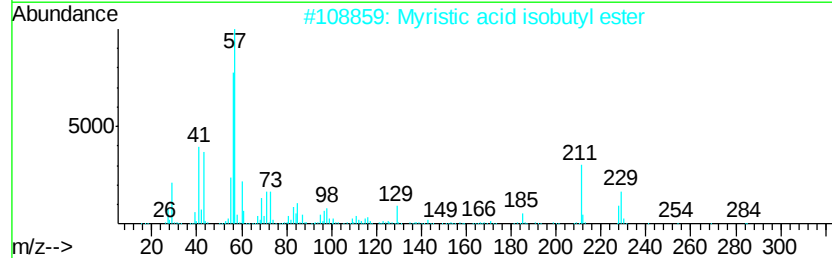
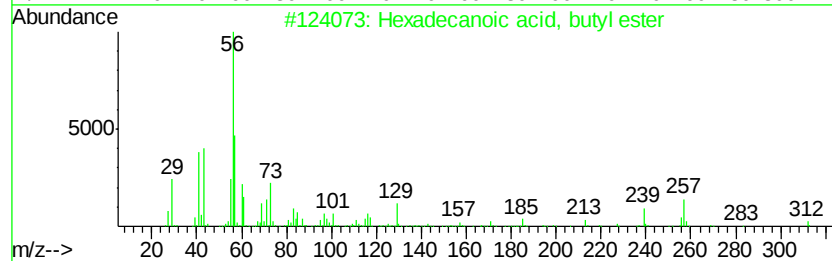
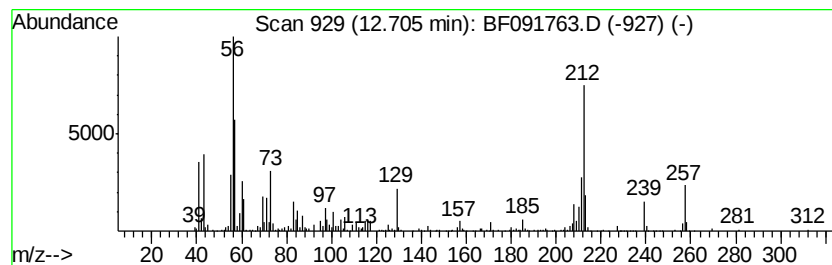
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.70	3.37 ng	316645	Chrysene-d12	13.92		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	70
2		Myristic acid isobutyl ester	284	C18H36O2	025263-97-2	43
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	41
4		Nipecotic acid	129	C6H11NO2	000498-95-3	27
5		Acridin-9-amine, 1,2,3,4-tetrahy...	212	C14H16N2	005778-78-9	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091763.D
Acq On : 19 Dec 2016 4:25
Operator : UM/SJ
Sample : H6011-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-12

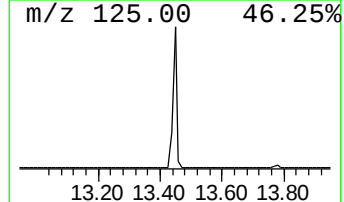
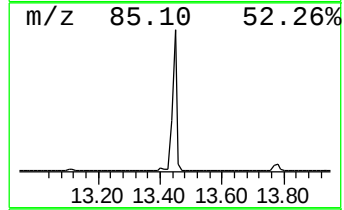
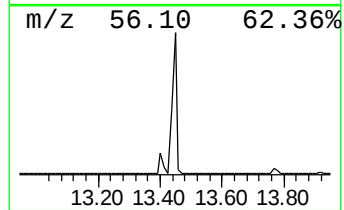
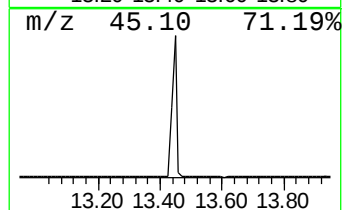
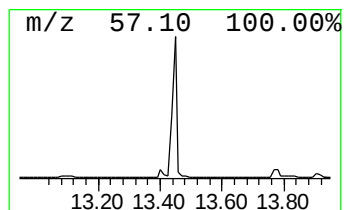
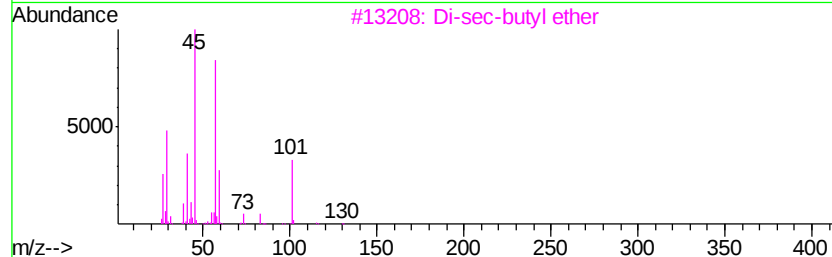
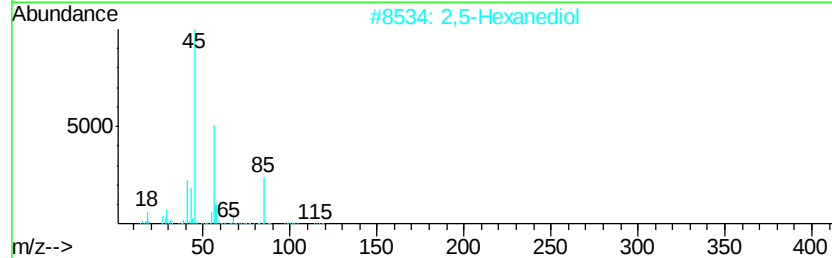
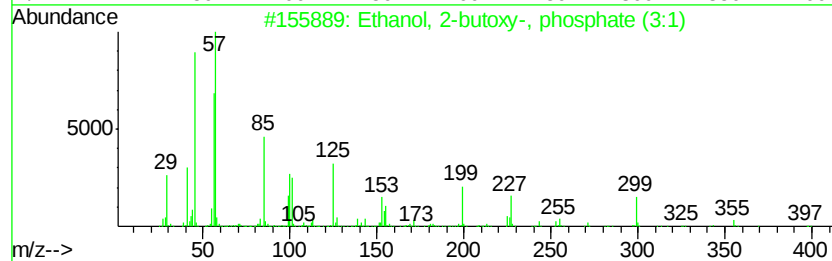
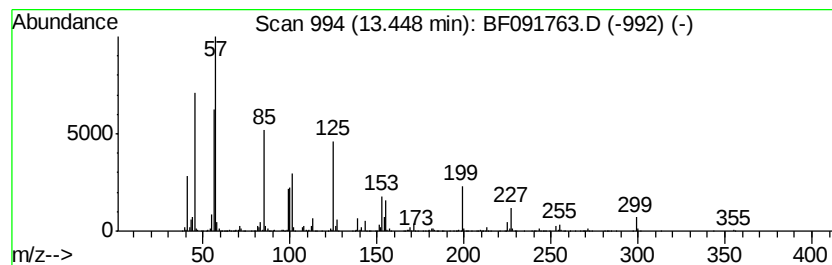
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Ethanol, 2-butoxy-, phospho... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	19.28 ng	1812860	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	80
2		2,5-Hexanediol	118	C6H14O2	002935-44-6	35
3		Di-sec-butyl ether	130	C8H18O	006863-58-7	10
4		Butane, 1,1'-[ethylidenebis(oxy)...]	174	C10H22O2	000871-22-7	10
5		Furan, tetrahydro-2,5-dimethyl-,...	100	C6H12O	002144-41-4	10



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Data File : BF091763.D
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Sample : H6011-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-12

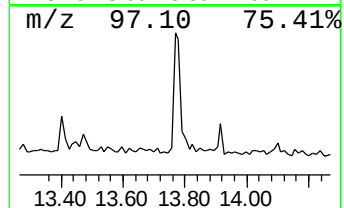
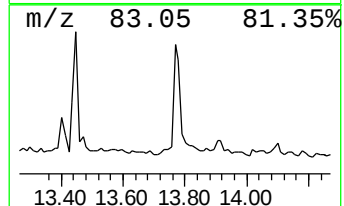
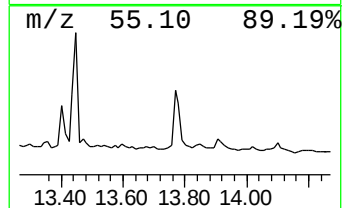
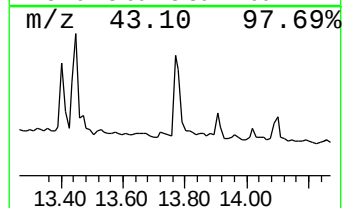
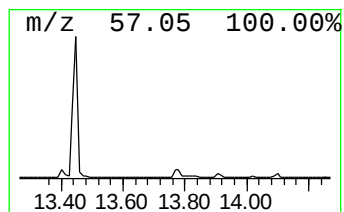
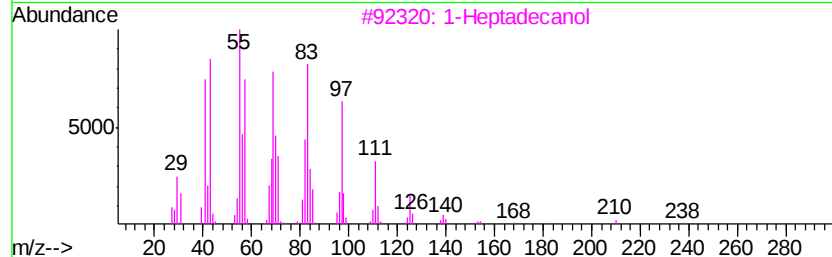
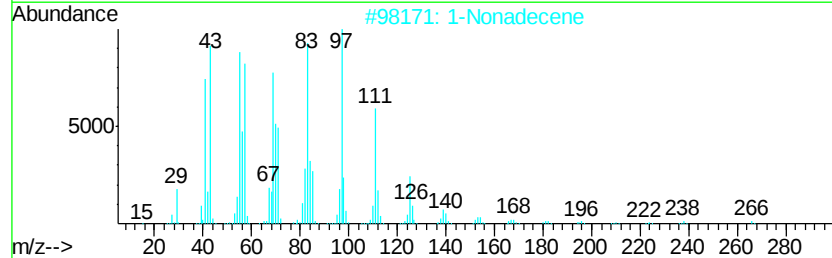
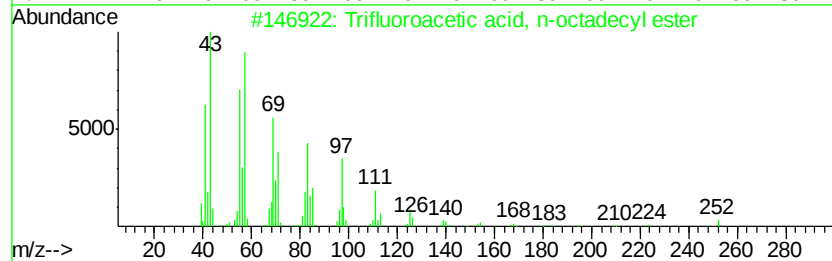
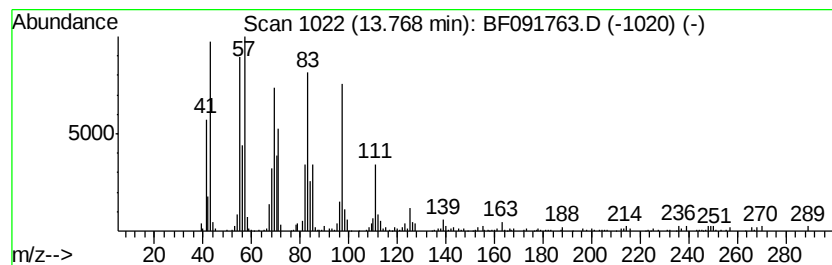
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Trifluoroacetic acid, n-oct... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	3.25 ng	305426	Chrysene-d12	13.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	91
2			1-Nonadecene	266	C19H38	018435-45-5	87
3			1-Heptadecanol	256	C17H36O	001454-85-9	81
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81
5			1-Hexadecanol	242	C16H34O	036653-82-4	74



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Operator : UM/SJ
Sample : H6011-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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...	4.93	10.4	ng	829018	1	6.76	1599070	20.0
unknown6.53	6.53	70.0	ng	5598530	1	6.76	1599070	20.0
Phenol, 4-(1,1,3,...	10.33	2.3	ng	280165	3	9.80	2423150	20.0
Tetradecane	10.72	2.7	ng	308209	4	11.29	2286800	20.0
n-Hexadecanoic acid	11.82	3.0	ng	336958	4	11.29	2286800	20.0
Octadecanoic acid	12.61	2.3	ng	212228	5	13.92	1880380	20.0
Hexadecanoic acid...	12.70	3.4	ng	316645	5	13.92	1880380	20.0
Ethanol, 2-butoxy...	13.45	19.3	ng	1812860	5	13.92	1880380	20.0
Trifluoroacetic a...	13.77	3.3	ng	305426	5	13.92	1880380	20.0