

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
 Data File : BF090259.D
 Acq On : 27 Sep 2016 18:37
 Operator : UM/SJ
 Sample : H4933-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B1B-15-15.5-BGS

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-BF092016.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	1.644	4	5	57	rVB	2639956	7357089	100.00%	20.656%
2	4.547	256	259	269	rBV	331338	573182	7.79%	1.609%
3	5.027	298	301	304	rBV	2240168	2487664	33.81%	6.984%
4	6.124	394	397	400	rBV	1944890	2616445	35.56%	7.346%
5	6.239	404	407	409	rBV	2688104	2893752	39.33%	8.125%
6	6.467	425	427	430	rBV	895880	850955	11.57%	2.389%
7	6.627	438	441	443	rBV	2362285	2285405	31.06%	6.417%
8	7.039	474	477	480	rBV	1310049	1664081	22.62%	4.672%
9	7.759	538	540	542	rBV	1324697	1173089	15.95%	3.294%
10	8.845	632	635	637	rBV	2609297	3472004	47.19%	9.748%
11	9.233	667	669	672	rBV	796881	1111834	15.11%	3.122%
12	9.496	690	692	695	rVV	1555470	1330844	18.09%	3.737%
13	10.285	758	761	763	rBV	1558459	1871205	25.43%	5.254%
14	10.433	772	774	778	rBV	77588	130687	1.78%	0.367%
15	10.959	818	820	823	rBV	824428	1154884	15.70%	3.243%
16	11.222	841	843	848	rBV	83616	106579	1.45%	0.299%
17	11.531	868	870	880	rBV2	158826	202893	2.76%	0.570%
18	12.548	956	959	962	rBV	2377872	2394453	32.55%	6.723%
19	13.462	1037	1039	1044	rBV	144402	191896	2.61%	0.539%
20	13.577	1046	1049	1051	rBV	711672	876347	11.91%	2.460%
21	14.445	1122	1125	1127	rBV	114448	113224	1.54%	0.318%
22	14.891	1162	1164	1167	rBV	718228	758467	10.31%	2.130%

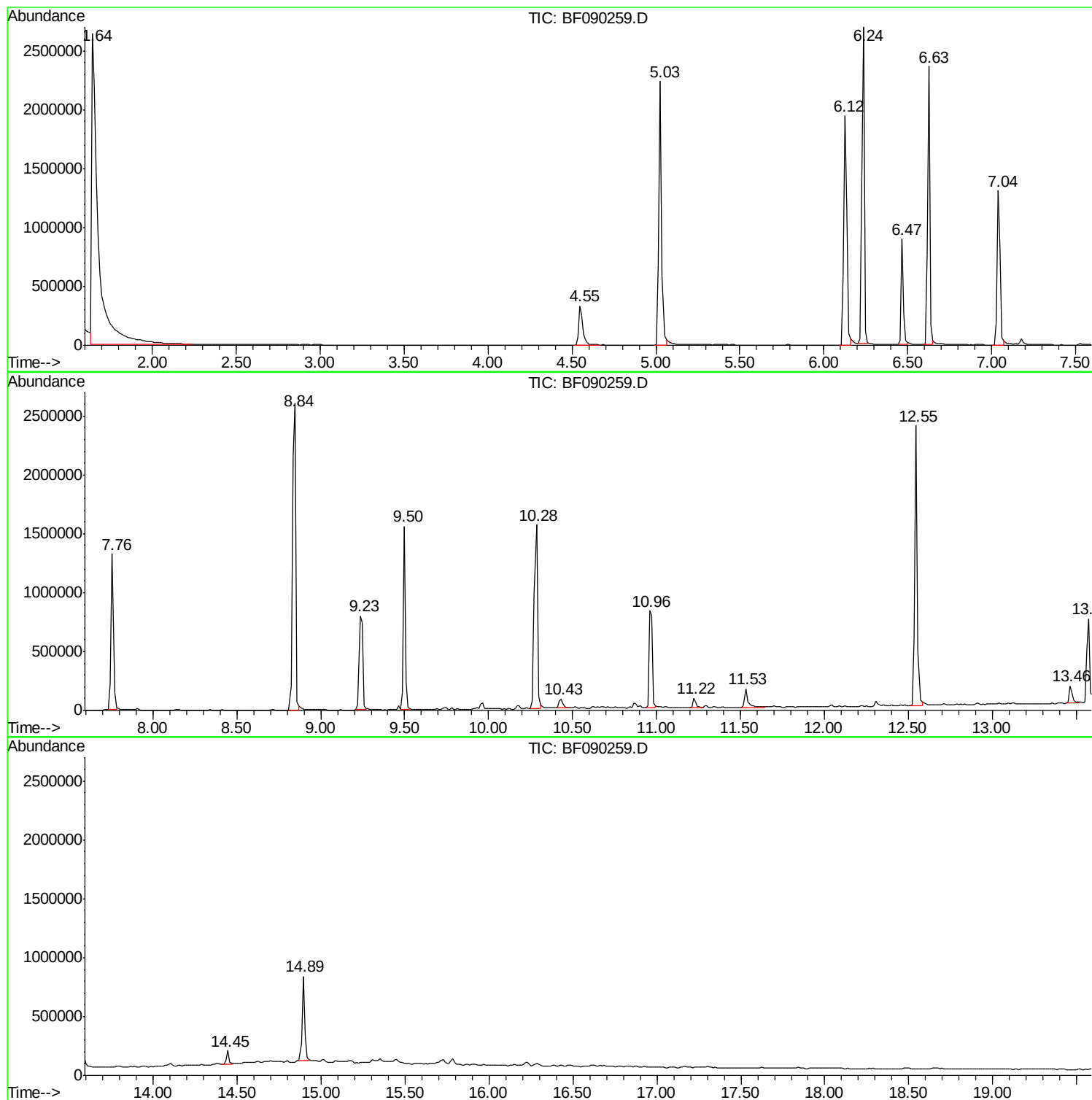
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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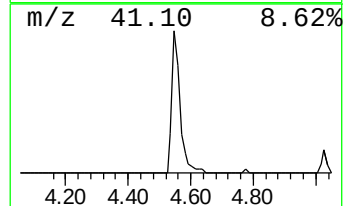
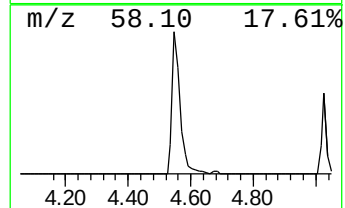
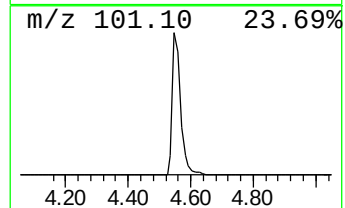
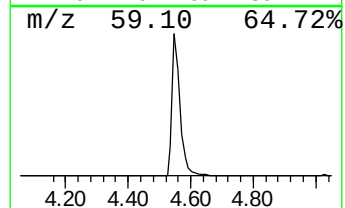
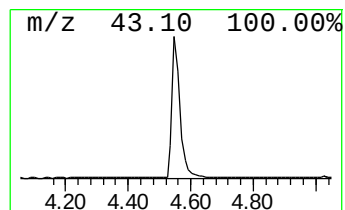
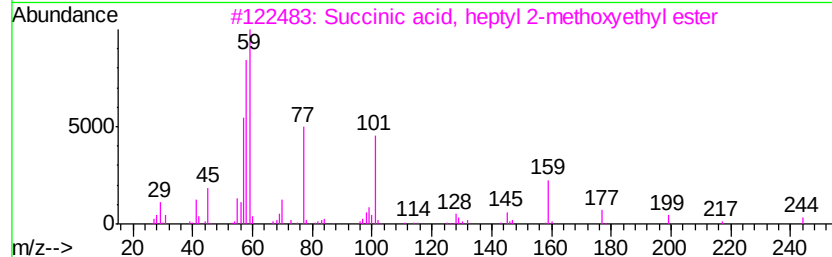
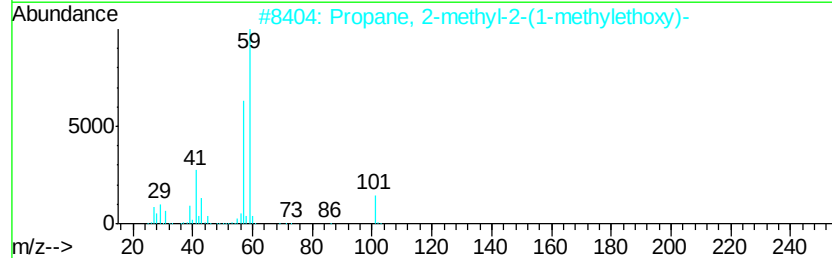
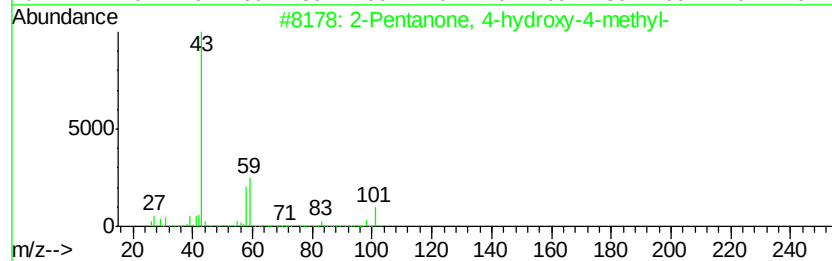
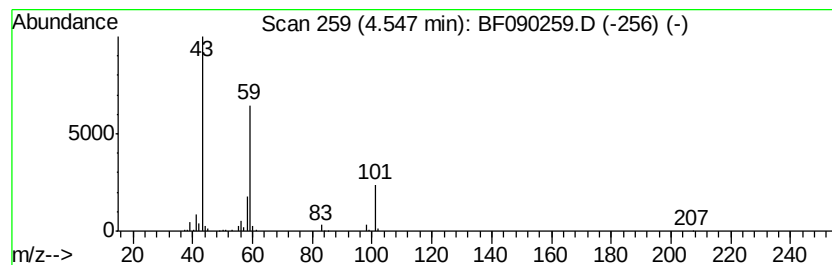
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	13.47 ng	573182	1,4-Dichlorobenzene-d4	6.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	53
3		Succinic acid, heptyl 2-methoxyethyl ester	274	C14H26O5	1000325-80-7	28
4		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17



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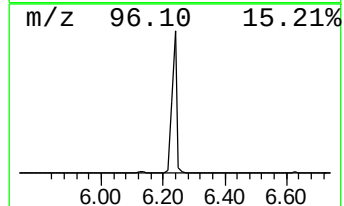
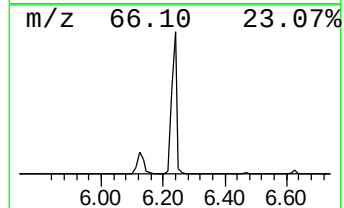
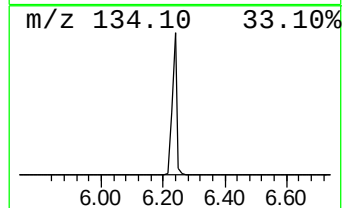
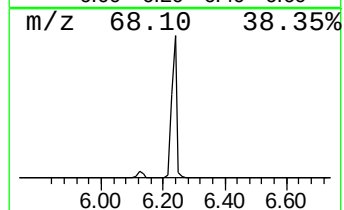
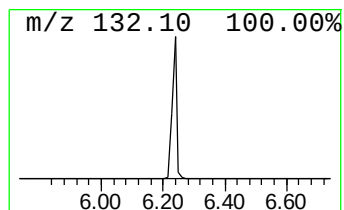
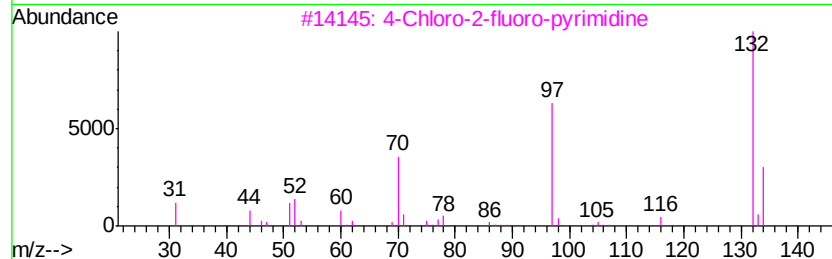
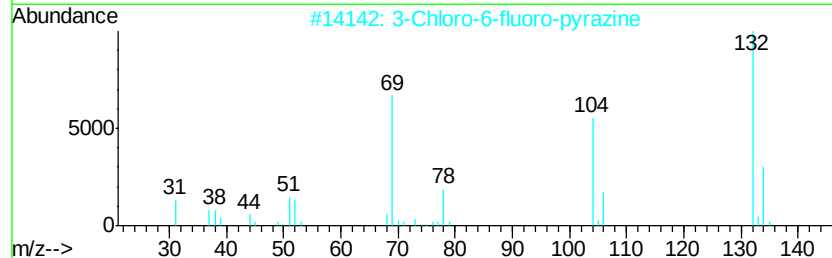
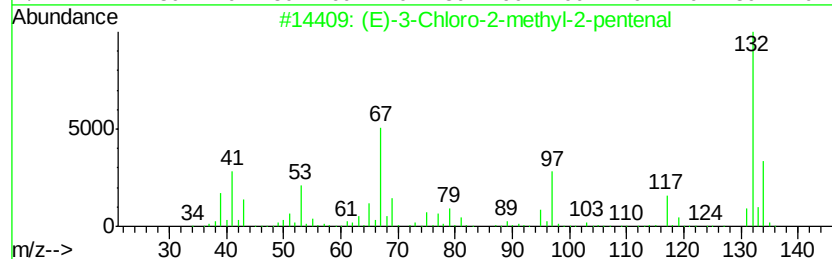
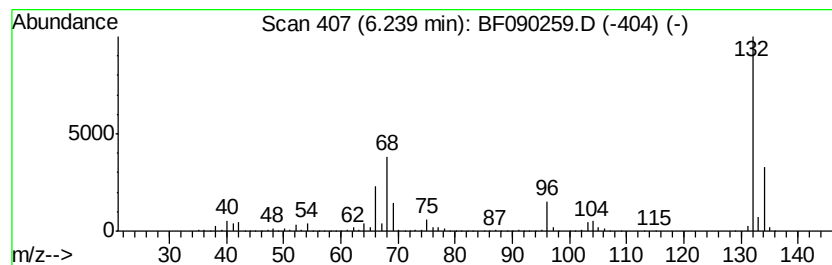
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Peak Number 3 unknown6.24 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	68.01 ng	2893750	1,4-Dichlorobenzene-d4	6.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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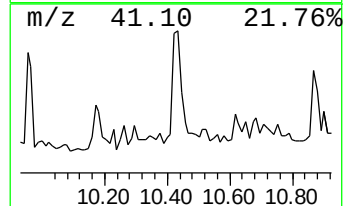
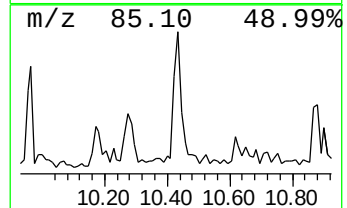
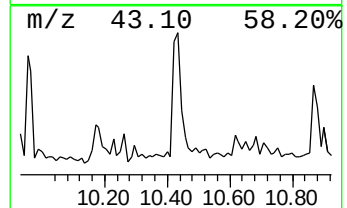
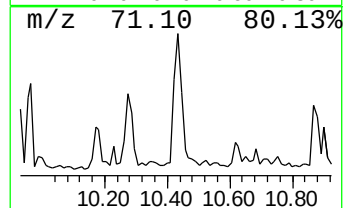
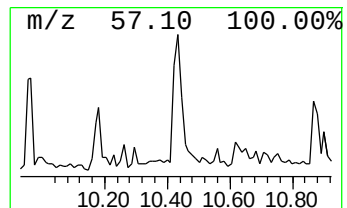
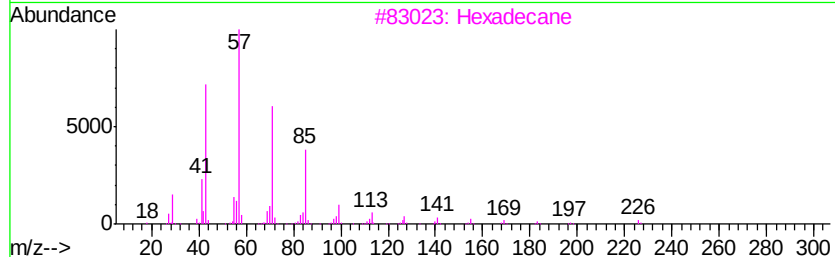
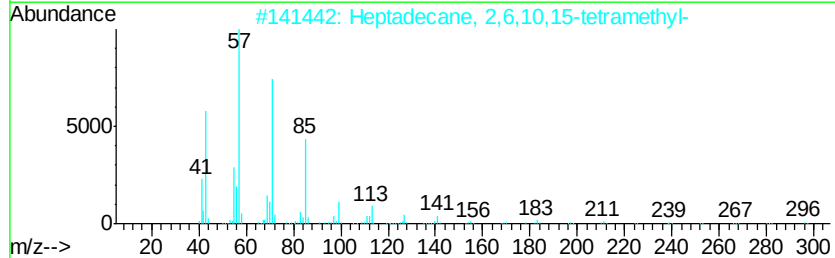
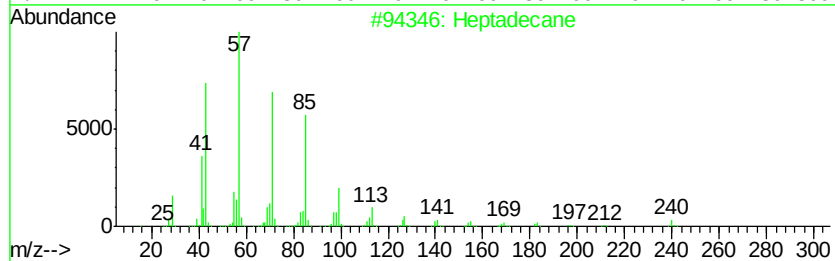
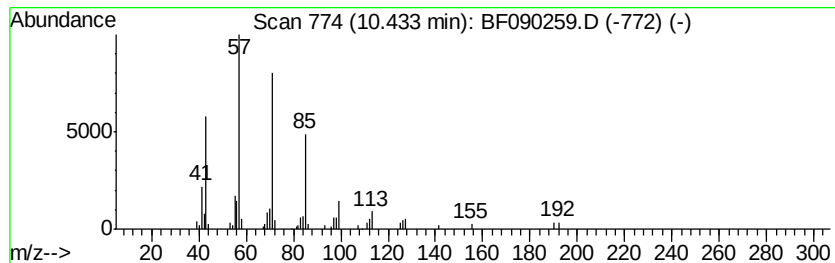
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Peak Number 5 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.43	2.26 ng	130687	Phenanthrene-d10	10.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Octacosane	394	C28H58	000630-02-4	86
5	Hexacosane	366	C26H54	000630-01-3	86



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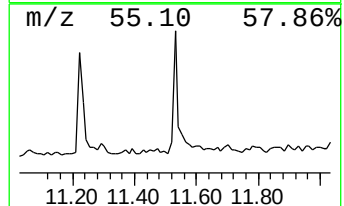
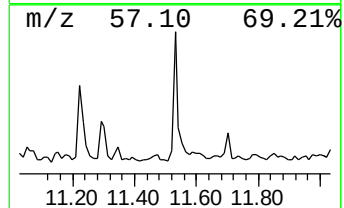
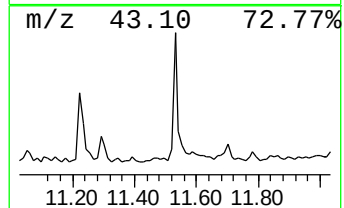
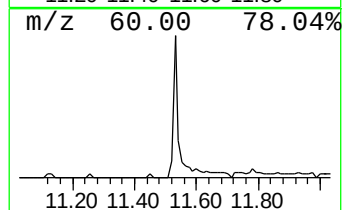
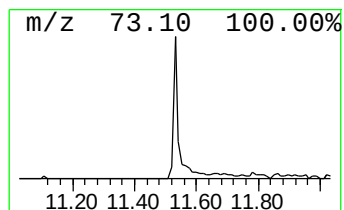
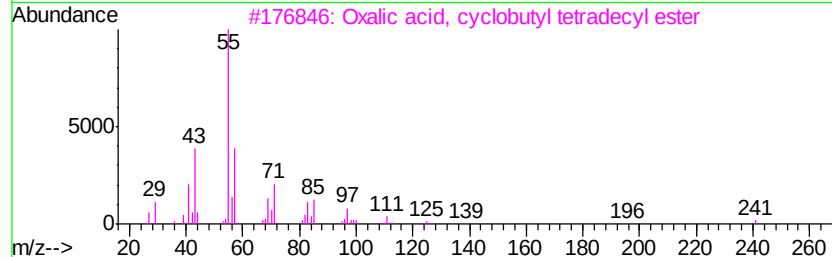
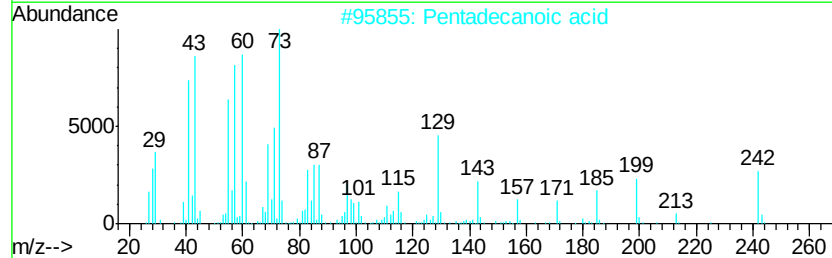
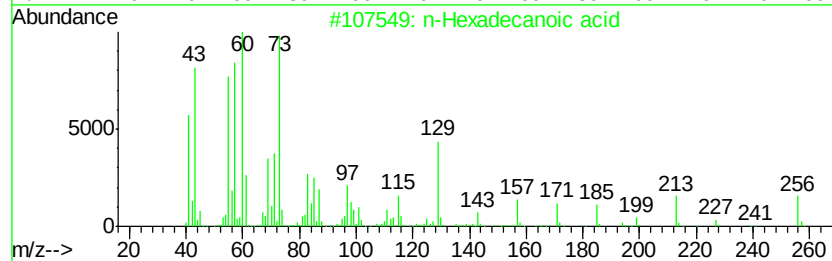
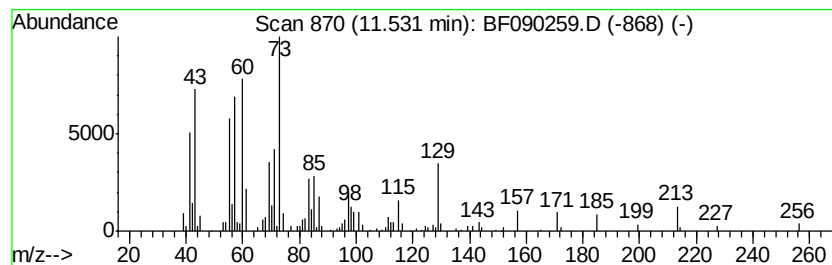
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.53	3.51 ng	202893	Phenanthrene-d10	10.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Oxalic acid, cyclobutyl tetradec...	340	C20H36O4	1000309-70-9	18
4		Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	18
5		Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	18



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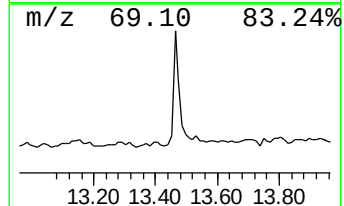
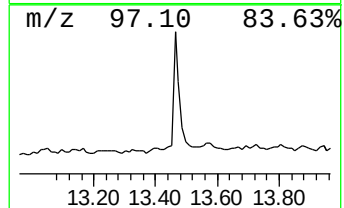
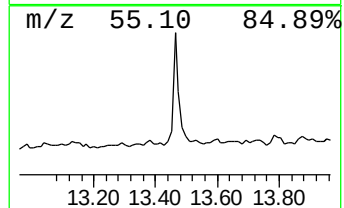
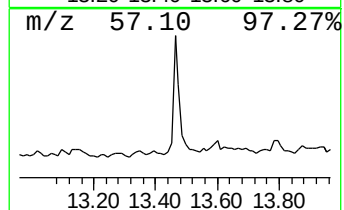
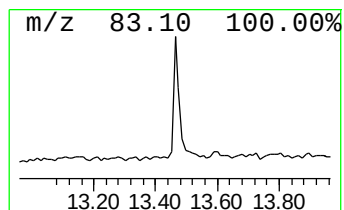
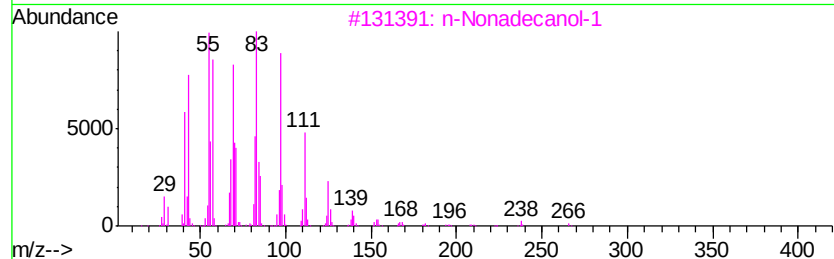
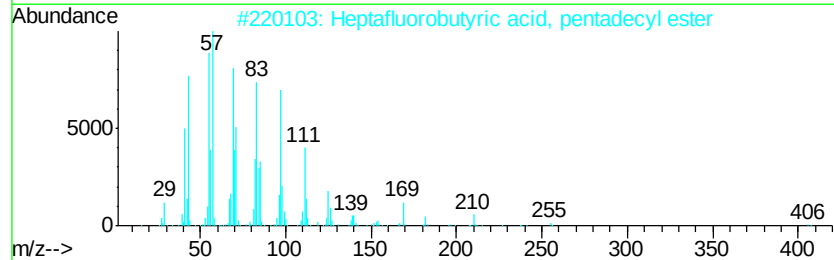
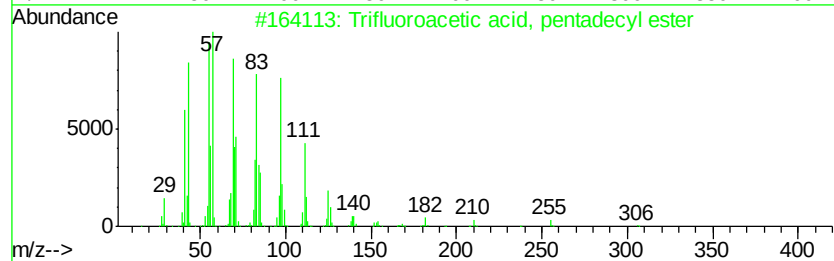
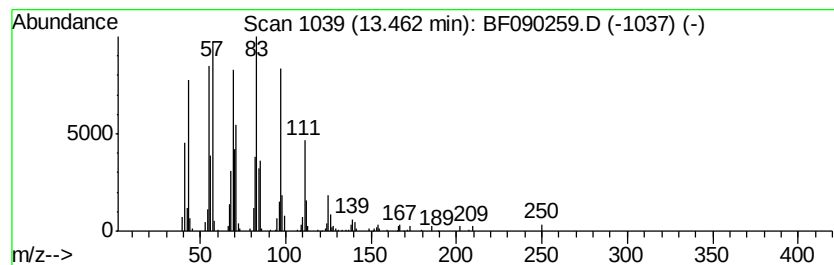
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Peak Number 7 Trifluoroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	4.38 ng	191896	Chrysene-d12	13.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93



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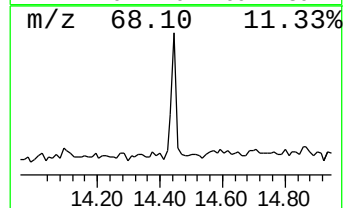
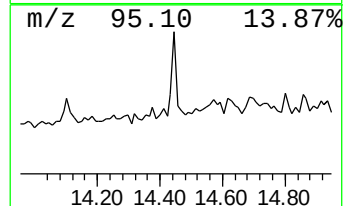
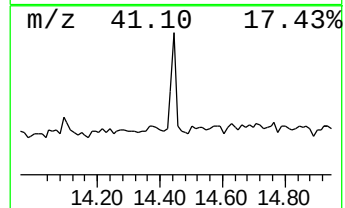
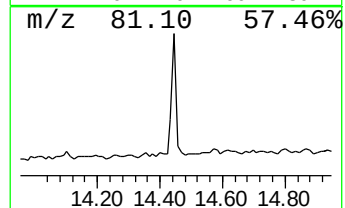
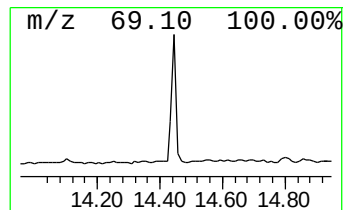
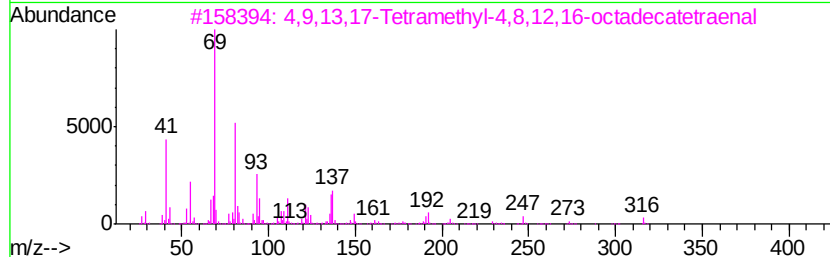
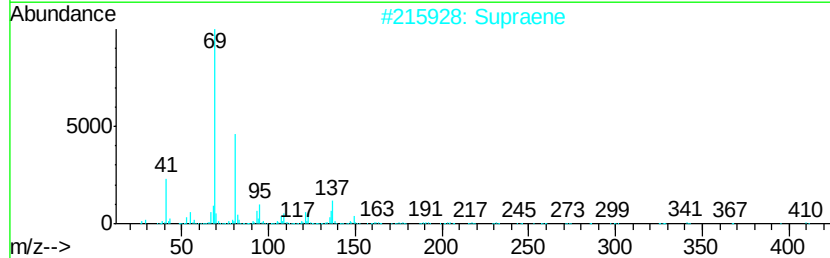
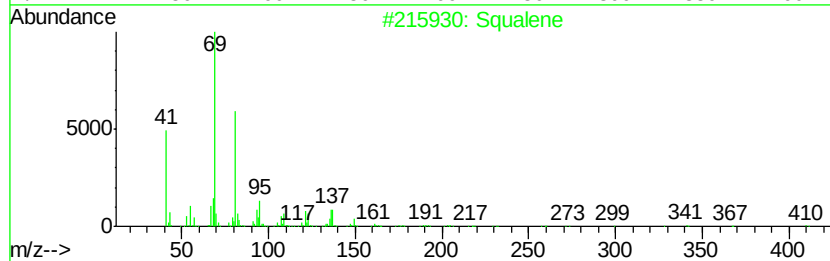
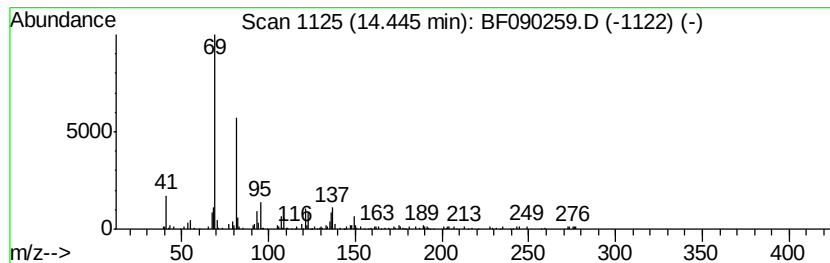
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BNA_F
ClientSampleId :
B1B-15-15.5-BGS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.99 ng	113224	Perylene-d12	14.89
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	000111-02-4	87
2	Supraene	410 C30H50	007683-64-9	83
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316 C22H36O	056882-09-8	72
4	1,5,9-Undecatriene, 2,6,10-trime...	192 C14H24	062951-96-6	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208 C14H24O	125529-10-4	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092716\
Data File : BF090259.D
Acq On : 27 Sep 2016 18:37
Operator : UM/SJ
Sample : H4933-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B1B-15-15.5-BGS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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...	4.55	13.5	ng	573182	1	6.47	850955	20.0
unknown6.24	6.24	68.0	ng	2893750	1	6.47	850955	20.0
Heptadecane	10.43	2.3	ng	130687	4	10.97	1154880	20.0
n-Hexadecanoic acid	11.53	3.5	ng	202893	4	10.97	1154880	20.0
Trifluoroacetic a...	13.46	4.4	ng	191896	5	13.58	876347	20.0
Squalene	14.45	3.0	ng	113224	6	14.89	758467	20.0