

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110416\
 Data File : BF091034.D
 Acq On : 4 Nov 2016 21:35
 Operator : UM/SJ
 Sample : H5526-02
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-98-4.5-5.0

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-BF110316.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	1.778	7	8	35	rVB	3343658	7208870	100.00%	12.037%
2	2.133	36	39	55	rVB2	179723	426223	5.91%	0.712%
3	4.864	275	278	290	rBV	757705	1346197	18.67%	2.248%
4	5.310	313	317	319	rBV	3692751	5664939	78.58%	9.459%
5	6.362	405	409	411	rBV	4281276	5850118	81.15%	9.768%
6	6.476	416	419	421	rBV	5056030	5636295	78.19%	9.411%
7	6.705	436	439	441	rBV	950413	1048148	14.54%	1.750%
8	6.853	450	452	455	rBV	3332525	4419349	61.30%	7.379%
9	7.276	486	489	491	rBV	3268120	3866311	53.63%	6.456%
10	7.390	497	499	506	rVB	70158	135229	1.88%	0.226%
11	7.985	549	551	554	rBV	1318754	1378337	19.12%	2.301%
12	9.070	643	646	648	rBV	5698996	5541032	76.86%	9.252%
13	9.470	678	681	683	rBV	1393612	1312363	18.20%	2.191%
14	9.745	702	705	707	rBV	1254170	1453712	20.17%	2.427%
15	10.179	742	743	745	rVB	77571	79056	1.10%	0.132%
16	10.396	759	762	766	rBV	36491	74712	1.04%	0.125%
17	10.533	771	774	776	rBV	3095849	3235243	44.88%	5.402%
18	10.659	783	785	789	rBV	107598	178247	2.47%	0.298%
19	11.105	822	824	825	rBV	77960	84236	1.17%	0.141%
20	11.219	832	834	836	rBV	1371344	1264019	17.53%	2.111%
21	12.431	938	940	942	rBV	378221	411973	5.71%	0.688%
22	12.659	957	960	961	rBV	248713	389501	5.40%	0.650%
23	12.694	961	963	968	rVB2	62477	106891	1.48%	0.178%
24	12.808	970	973	975	rBV	4556309	4061413	56.34%	6.781%
25	13.608	1040	1043	1046	rBV3	51056	159220	2.21%	0.266%
26	13.711	1050	1052	1054	rBV	340277	410349	5.69%	0.685%
27	13.848	1061	1064	1071	rBV2	1048169	1552865	21.54%	2.593%
28	14.282	1100	1102	1105	rBV2	24342	73698	1.02%	0.123%
29	14.522	1121	1123	1129	rVB	75045	120572	1.67%	0.201%
30	14.694	1136	1138	1143	rVB3	67623	104485	1.45%	0.174%
31	14.854	1149	1152	1157	rBV	308504	549774	7.63%	0.918%
32	15.128	1174	1176	1179	rVB	144180	184086	2.55%	0.307%
33	15.185	1179	1181	1183	rVB	164640	201113	2.79%	0.336%
34	15.242	1183	1186	1188	rBV	684601	862021	11.96%	1.439%

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ClientSampleId :
SB-98-4.5-5.0

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-BF110316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.711	1224	1227	1237	rVB3	67727	199568	2.77%	0.333%
36	16.545	1297	1300	1304	rBV2	88705	176064	2.44%	0.294%
37	16.934	1332	1334	1340	rVB	64370	124756	1.73%	0.208%

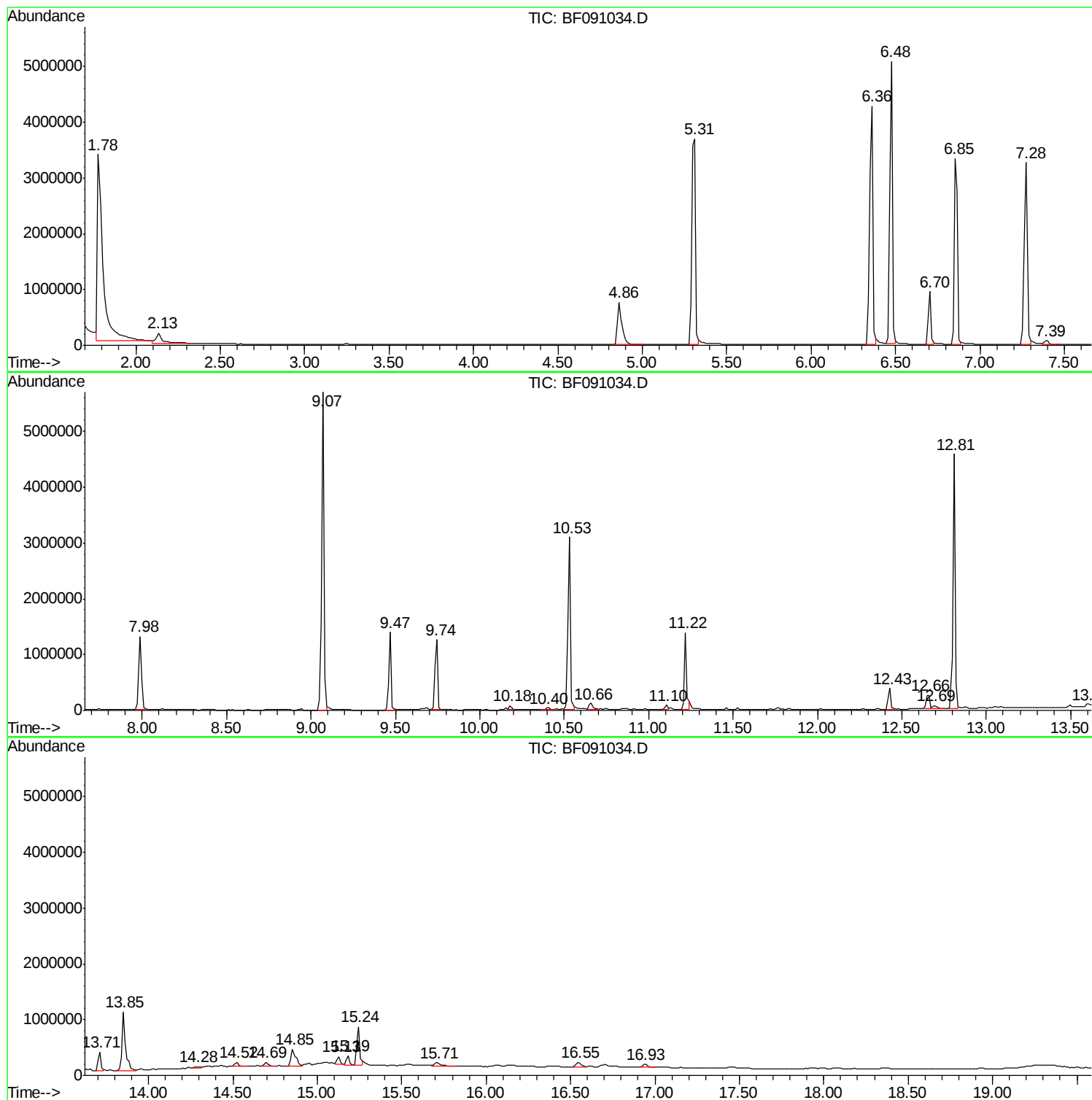
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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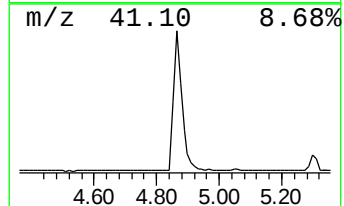
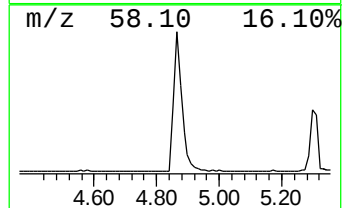
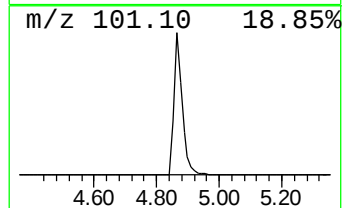
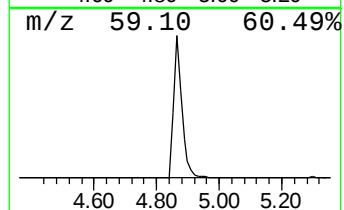
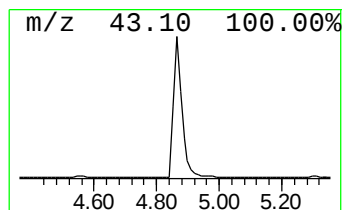
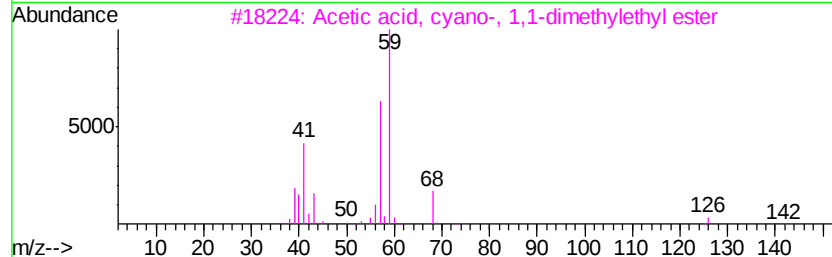
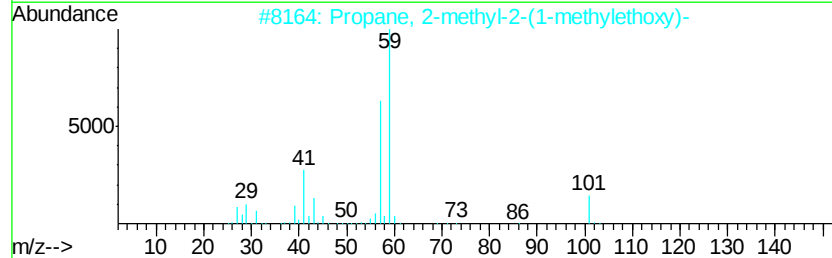
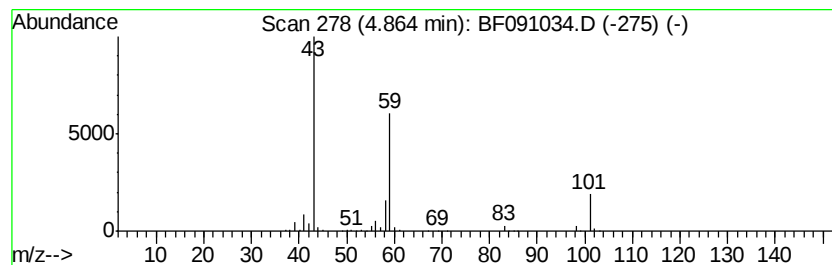
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	25.69 ng	1346200	1,4-Dichlorobenzene-d4	6.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O		017348-59-3	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2		001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2		000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO		000109-02-4	9



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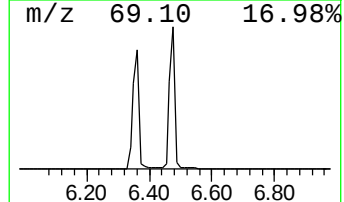
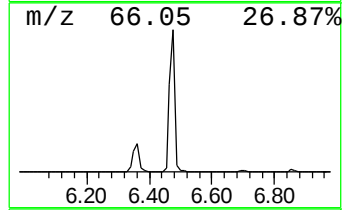
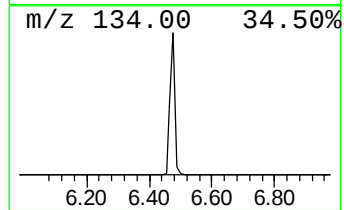
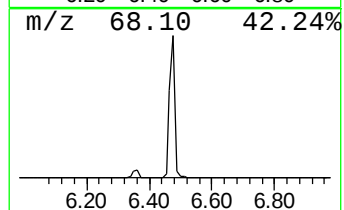
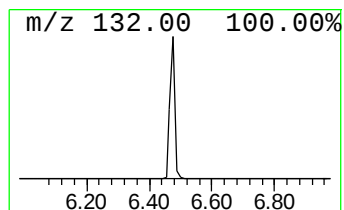
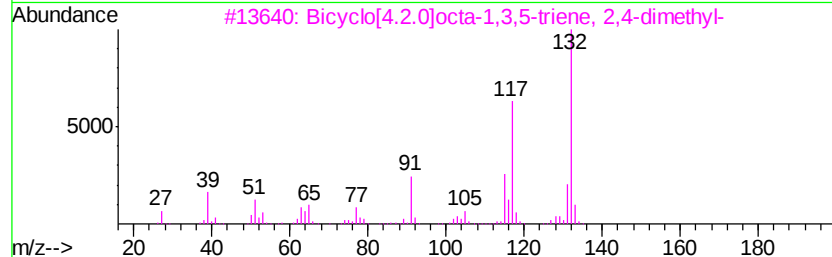
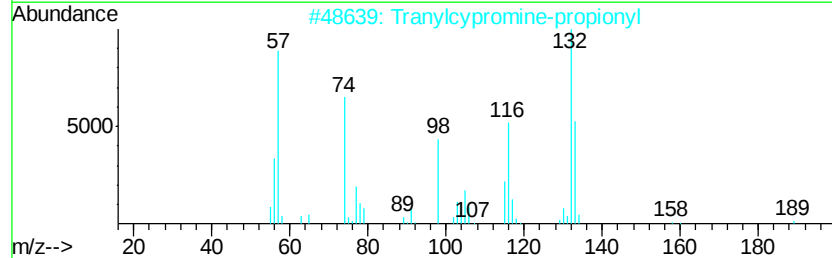
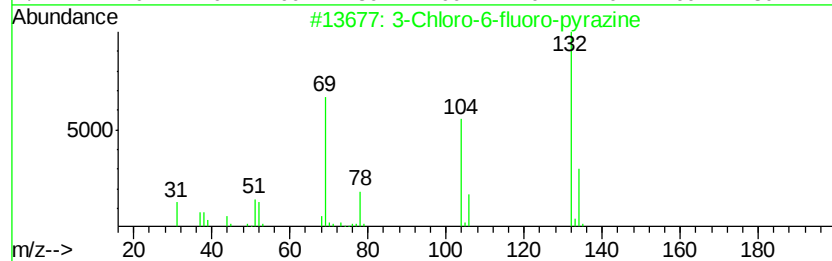
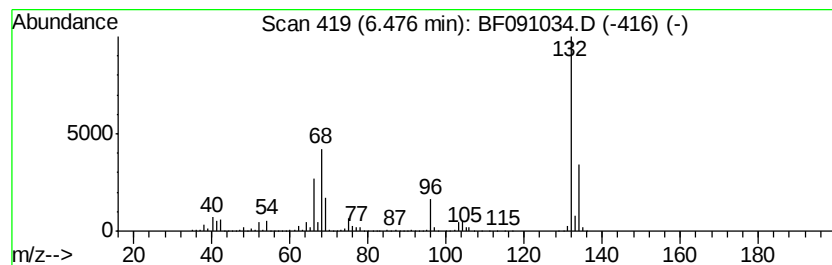
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown6.48 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	107.55 ng	5636300	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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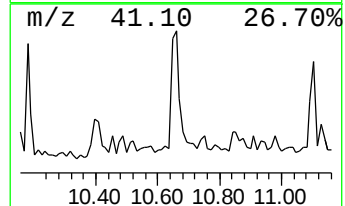
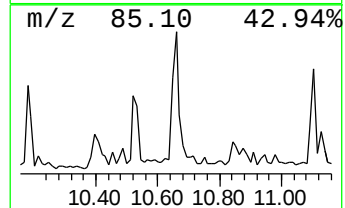
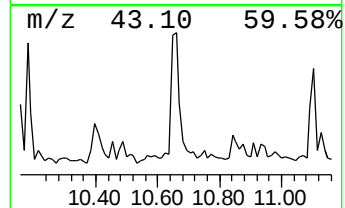
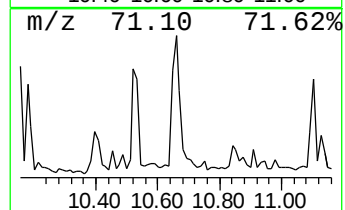
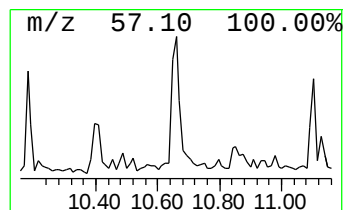
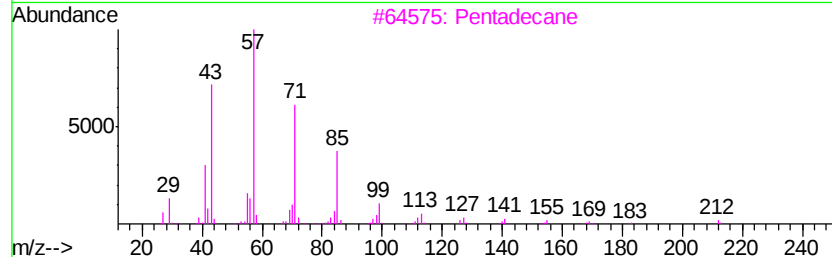
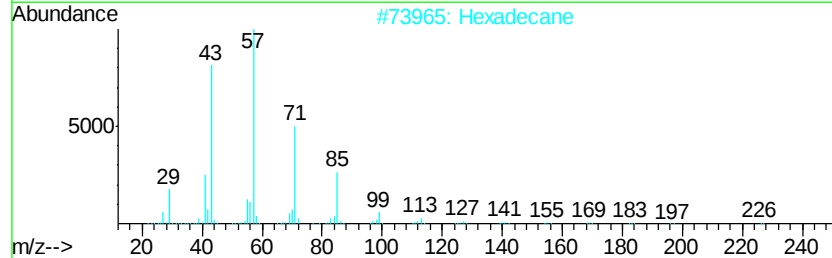
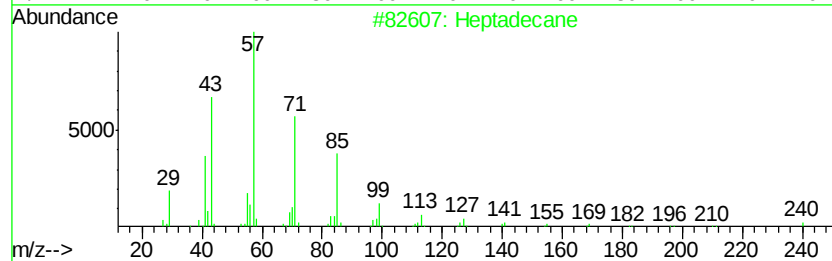
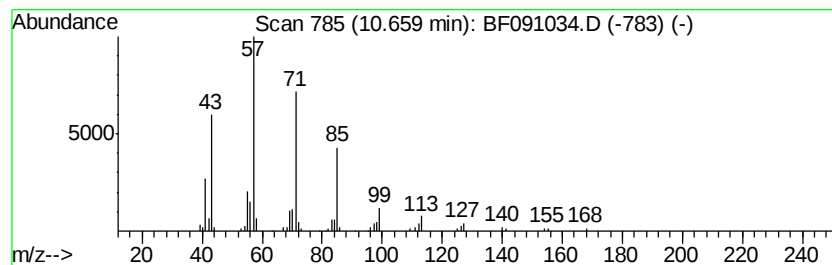
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.66	2.82 ng	178247	Phenanthrene-d10		11.22
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Tritetracontane	605	C43H88	007098-21-7	90
5	Heneicosane	296	C21H44	000629-94-7	90



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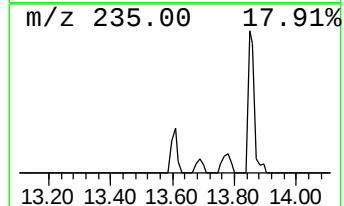
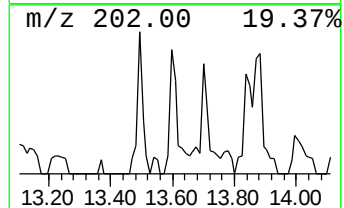
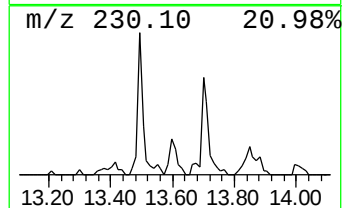
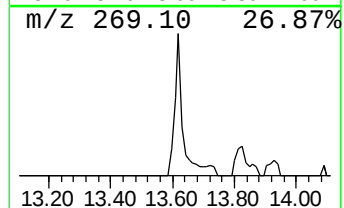
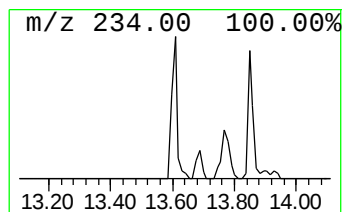
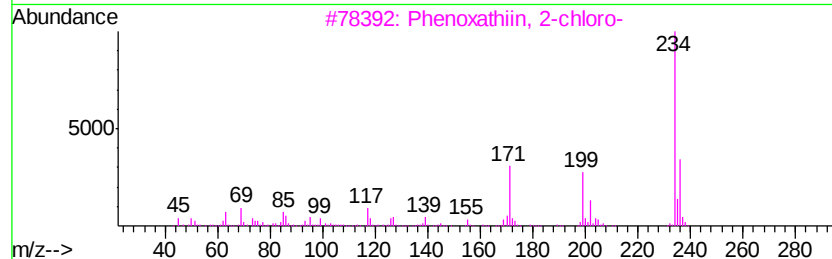
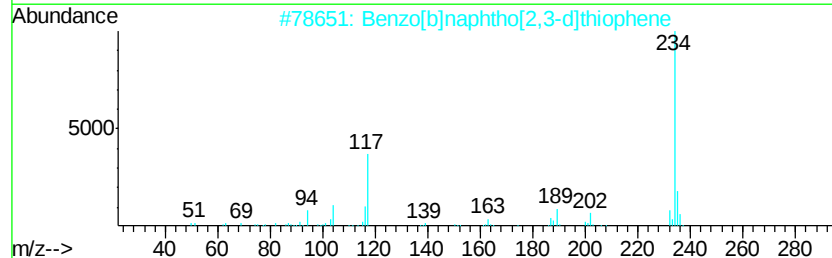
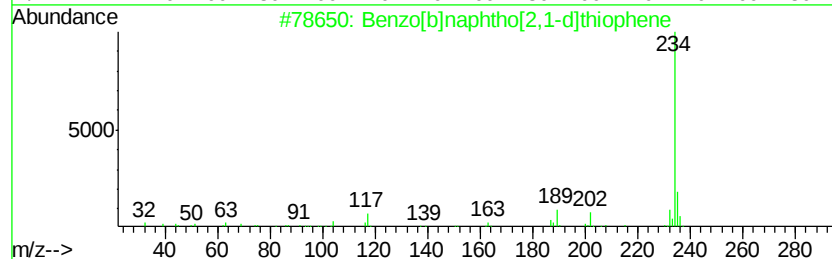
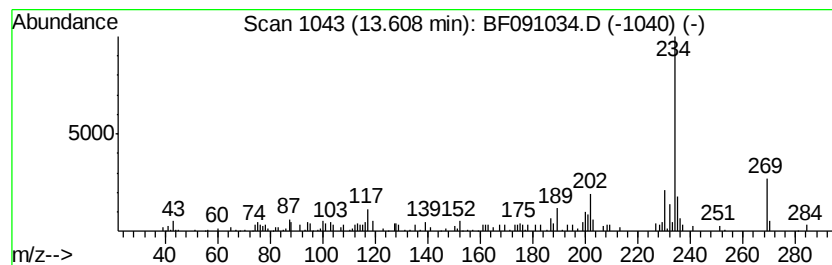
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzo[b]naphtho[2,1-d]thiop... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.61	2.05 ng	159220	Chrysene-d12	13.85		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[b]naphtho[2,1-d]thiophene	234	C16H10S	000239-35-0	64
2		Benzo[b]naphtho[2,3-d]thiophene	234	C16H10S	000243-46-9	60
3		Phenoxathiin, 2-chloro-	234	C12H7ClOS	010230-34-9	47
4		Quinoxalino[2,3-b]quinoxaline, 5...	234	C14H10N4	000531-46-4	46
5		Benzo[b]naphtho[1,2-d]thiophene	234	C16H10S	000205-43-6	43



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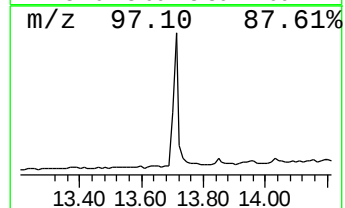
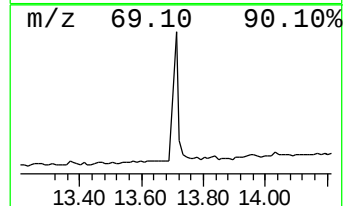
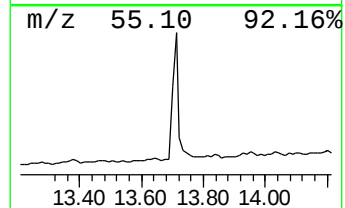
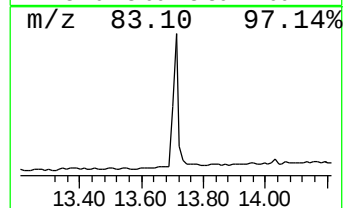
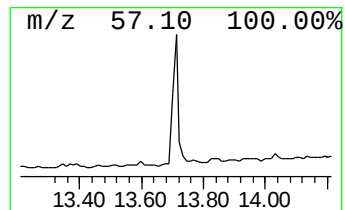
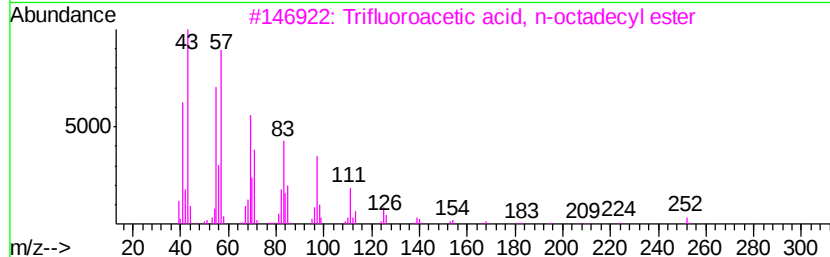
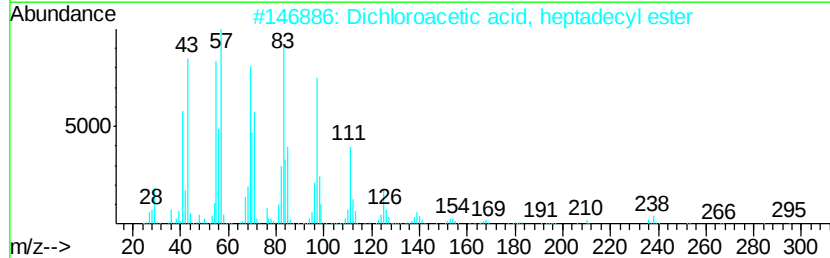
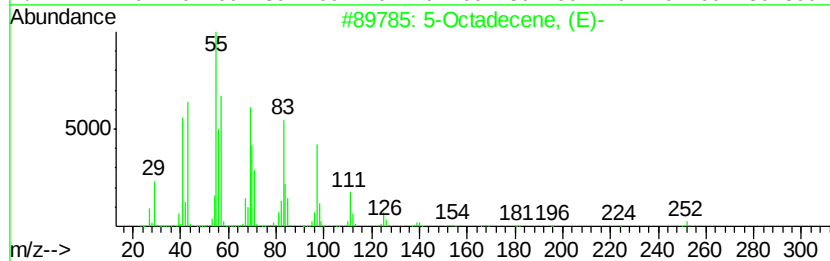
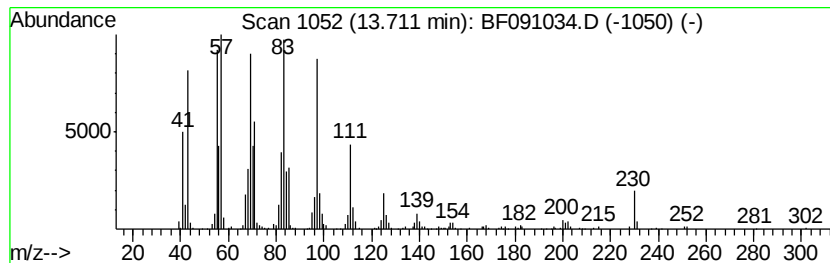
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 5-Octadecene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.71	5.29 ng	410349	Chrysene-d12	13.85		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-		252	C18H36	007206-21-5	93
2	Dichloroacetic acid, heptadecyl ...		366	C19H36Cl2O2	1000282-98-2	93
3	Trifluoroacetic acid, n-octadecy...		366	C20H37F3O2	079392-43-1	91
4	Trifluoroacetic acid, n-heptadec...		324	C17H31F3O2	1000216-79-2	91
5	Bromoacetic acid, octadecyl ester		390	C20H39BrO2	018992-03-5	91



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Data File : BF091034.D
Acq On : 4 Nov 2016 21:35
Operator : UM/SJ
Sample : H5526-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

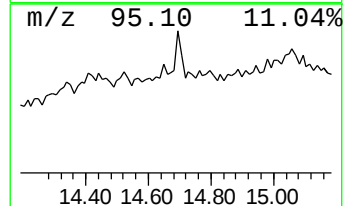
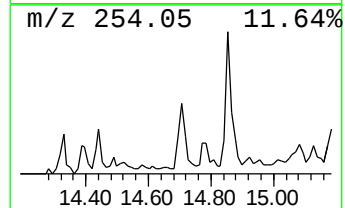
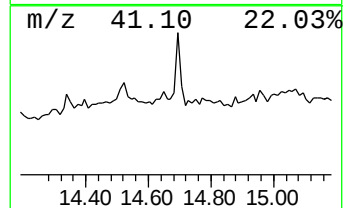
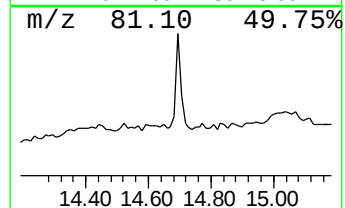
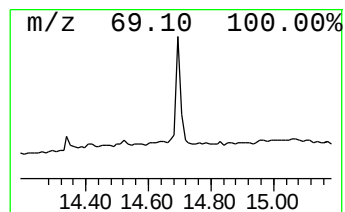
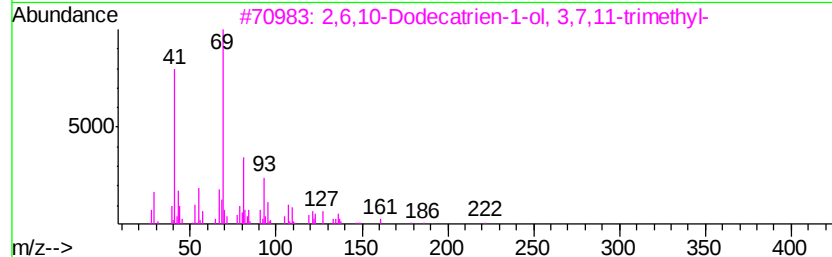
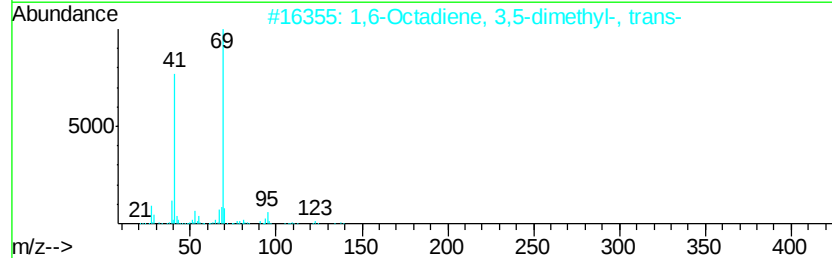
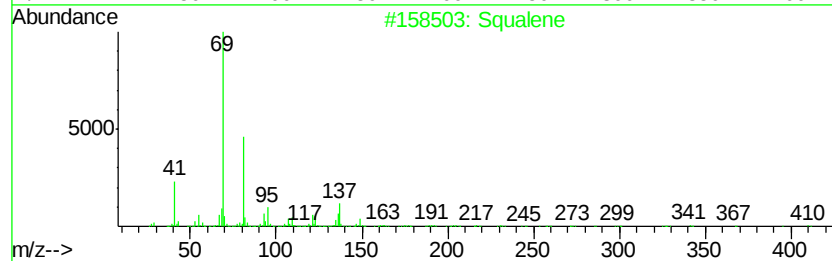
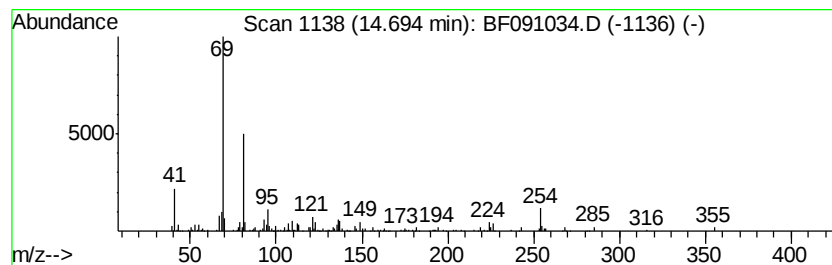
Instrument :
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ClientSampleId :
SB-98-4.5-5.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	2.42 ng	104485	Perylene-d12	15.24
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene		410 C30H50	007683-64-9 76
2	1,6-Octadiene, 3,5-dimethyl-, tr...		138 C10H18	074630-87-8 53
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...		222 C15H26O	004602-84-0 53
4	2,6-Octadiene, 4-methyl-		124 C9H16	074498-94-5 50
5	1,5-Heptadiene, 2,6-dimethyl-		124 C9H16	006709-39-3 47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110416\
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Acq On : 4 Nov 2016 21:35
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Sample : H5526-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-98-4.5-5.0

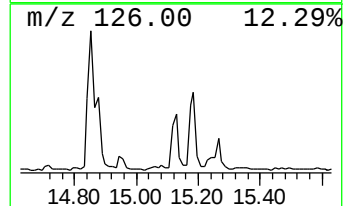
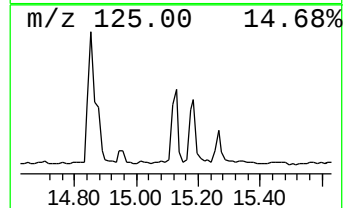
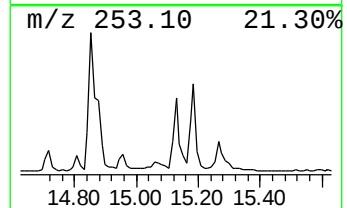
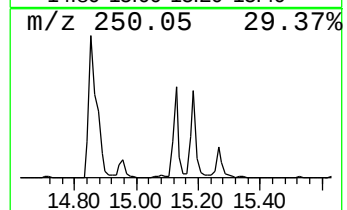
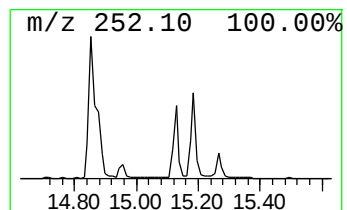
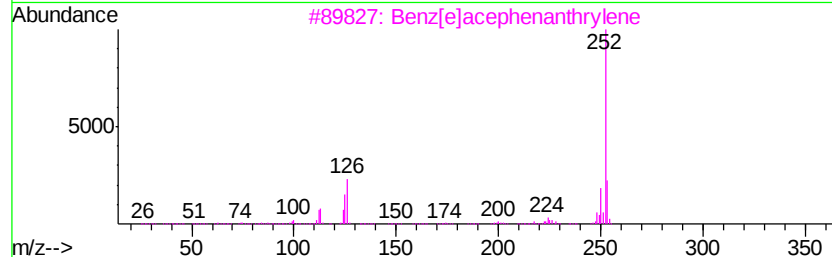
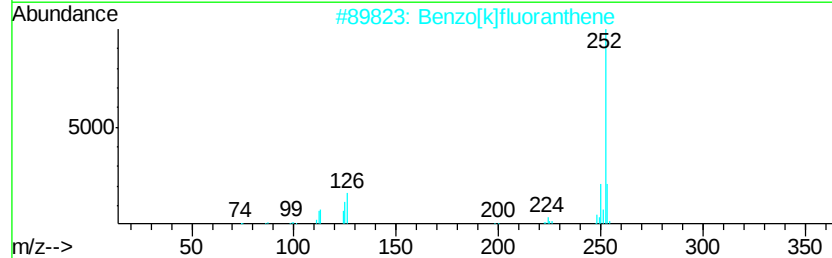
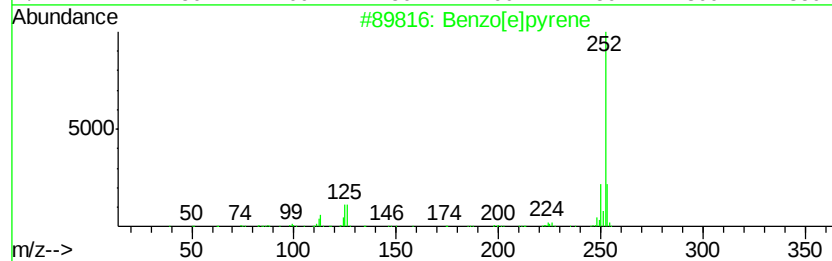
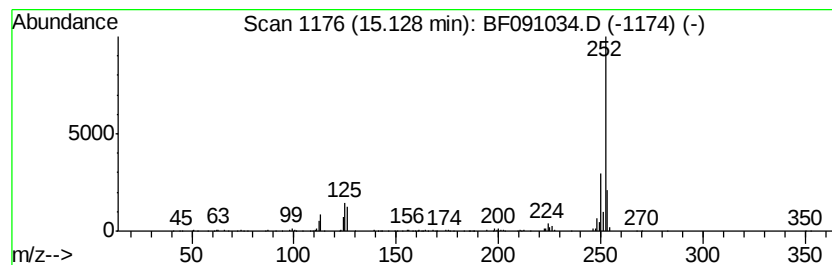
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	4.27 ng	184086	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2		Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
3		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
4		Benzo[a]pyrene	252	C20H12	000050-32-8	91
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	90



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Acq On : 4 Nov 2016 21:35
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Sample : H5526-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

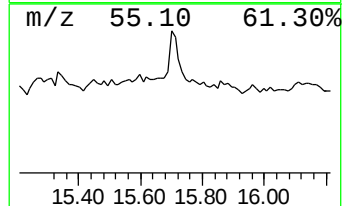
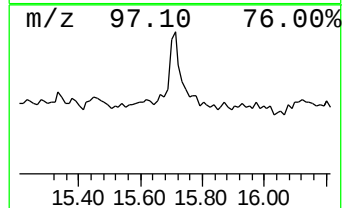
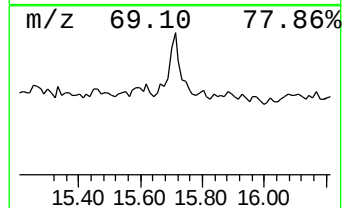
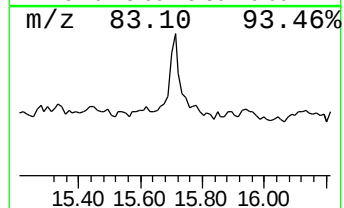
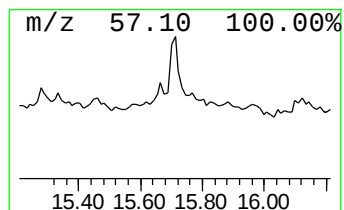
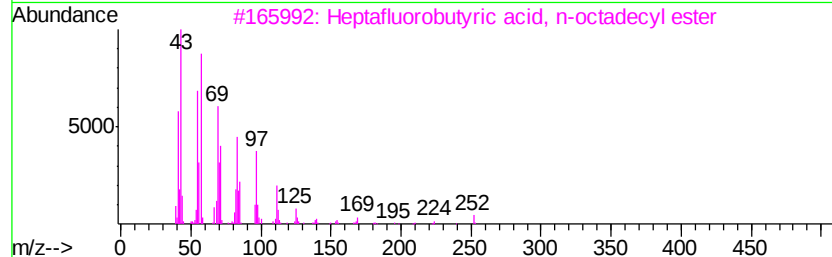
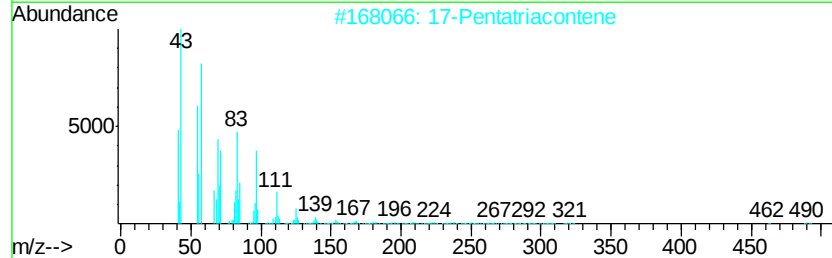
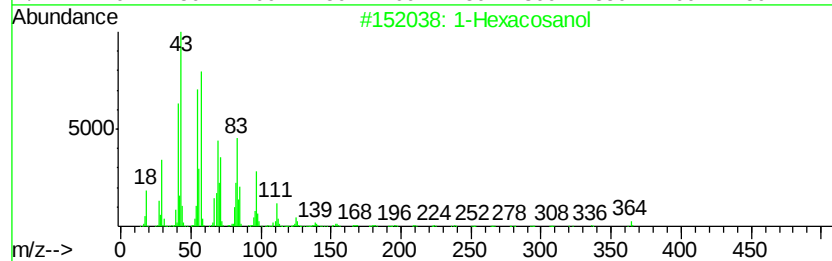
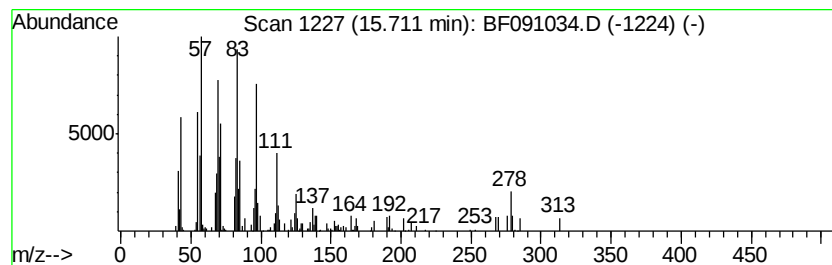
Instrument :
BNA_F
ClientSampleId :
SB-98-4.5-5.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Hexacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.71	4.63 ng	199568	Perylene-d12	15.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol	382	C26H54O	000506-52-5	87
2	17-Pentatriacontene	491	C35H70	006971-40-0	76
3	Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	74
4	Heptafluorobutanoic acid, heptadecyl ester	452	C21H35F7O2	1000282-97-3	70
5	2- Chloropropionic acid, octadecyl ester	360	C21H41ClO2	088104-31-8	70



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Sample : H5526-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-98-4.5-5.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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...	4.86	25.7	ng	1346200	1	6.70	1048150	20.0
unknown6.48	6.48	107.6	ng	5636300	1	6.70	1048150	20.0
Heptadecane	10.66	2.8	ng	178247	4	11.22	1264020	20.0
Benzo[b]naphtho[2...	13.61	2.0	ng	159220	5	13.85	1552870	20.0
5-Octadecene, (E)-	13.71	5.3	ng	410349	5	13.85	1552870	20.0
Squalene	14.69	2.4	ng	104485	6	15.24	862021	20.0
Benzo[e]pyrene	15.13	4.3	ng	184086	6	15.24	862021	20.0
1-Hexacosanol	15.71	4.6	ng	199568	6	15.24	862021	20.0