

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071916\
 Data File : BF089113.D
 Acq On : 19 Jul 2016 12:44
 Operator : UM/SJ
 Sample : H4044-11
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 F9-B1(6-12)C

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-BF063016.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	41	rVB	852147	1502157	100.00%	11.788%
2	4.753	274	277	283	rVB	58355	85122	5.67%	0.668%
3	5.210	315	317	320	rBV	1123338	1091925	72.69%	8.568%
4	5.884	373	376	378	rBB	81743	110338	7.35%	0.866%
5	6.284	408	411	413	rBV	973582	1296827	86.33%	10.176%
6	6.387	418	420	423	rBV	960492	1190647	79.26%	9.343%
7	6.456	425	426	429	rBV	37841	43479	2.89%	0.341%
8	6.616	438	440	442	rBV	257978	290666	19.35%	2.281%
9	6.707	446	448	450	rBB	34023	28975	1.93%	0.227%
10	6.776	452	454	457	rVB	998615	862930	57.45%	6.771%
11	7.187	487	490	492	rBV	669828	681021	45.34%	5.344%
12	7.907	551	553	555	rBV	502492	413071	27.50%	3.241%
13	8.982	645	647	650	rBV	974136	1211477	80.65%	9.507%
14	9.382	680	682	684	rBV	284963	228931	15.24%	1.796%
15	9.656	703	706	708	rBB	486369	425354	28.32%	3.338%
16	10.102	744	745	747	rVB	20192	16031	1.07%	0.126%
17	10.445	772	775	777	rVB2	569926	707111	47.07%	5.549%
18	10.571	785	786	791	rBV	25080	30762	2.05%	0.241%
19	11.016	823	825	827	rBV	17360	18753	1.25%	0.147%
20	11.131	832	835	836	rBV	447728	396887	26.42%	3.114%
21	12.125	921	922	925	rBV2	47468	37813	2.52%	0.297%
22	12.331	938	940	942	rBV	32869	27606	1.84%	0.217%
23	12.548	957	959	961	rBV	36297	48857	3.25%	0.383%
24	12.708	971	973	976	rVB	812764	950017	63.24%	7.455%
25	13.325	1025	1027	1030	rVB	15073	15474	1.03%	0.121%
26	13.485	1037	1041	1043	rBV2	22953	32411	2.16%	0.254%
27	13.622	1051	1053	1056	rBV2	54961	67918	4.52%	0.533%
28	13.748	1061	1064	1069	rVV	364364	372203	24.78%	2.921%
29	14.262	1106	1109	1112	rBV3	15158	35163	2.34%	0.276%
30	14.548	1131	1134	1137	rBV3	17067	40386	2.69%	0.317%
31	14.742	1149	1151	1157	rBV	20395	54671	3.64%	0.429%
32	14.834	1157	1159	1160	rBV	16425	16890	1.12%	0.133%
33	14.994	1171	1173	1176	rVB	15195	18487	1.23%	0.145%
34	15.051	1176	1178	1180	rBV	19184	30584	2.04%	0.240%

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Smoothing : ON Filtering: 5
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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35	15.108	1180	1183	1185	rBV	226151	275832	18.36%	2.164%
36	15.520	1217	1219	1221	rBV	21352	36916	2.46%	0.290%
37	15.943	1254	1256	1258	rVB2	12208	18090	1.20%	0.142%
38	16.845	1332	1335	1340	rVB4	12962	31857	2.12%	0.250%

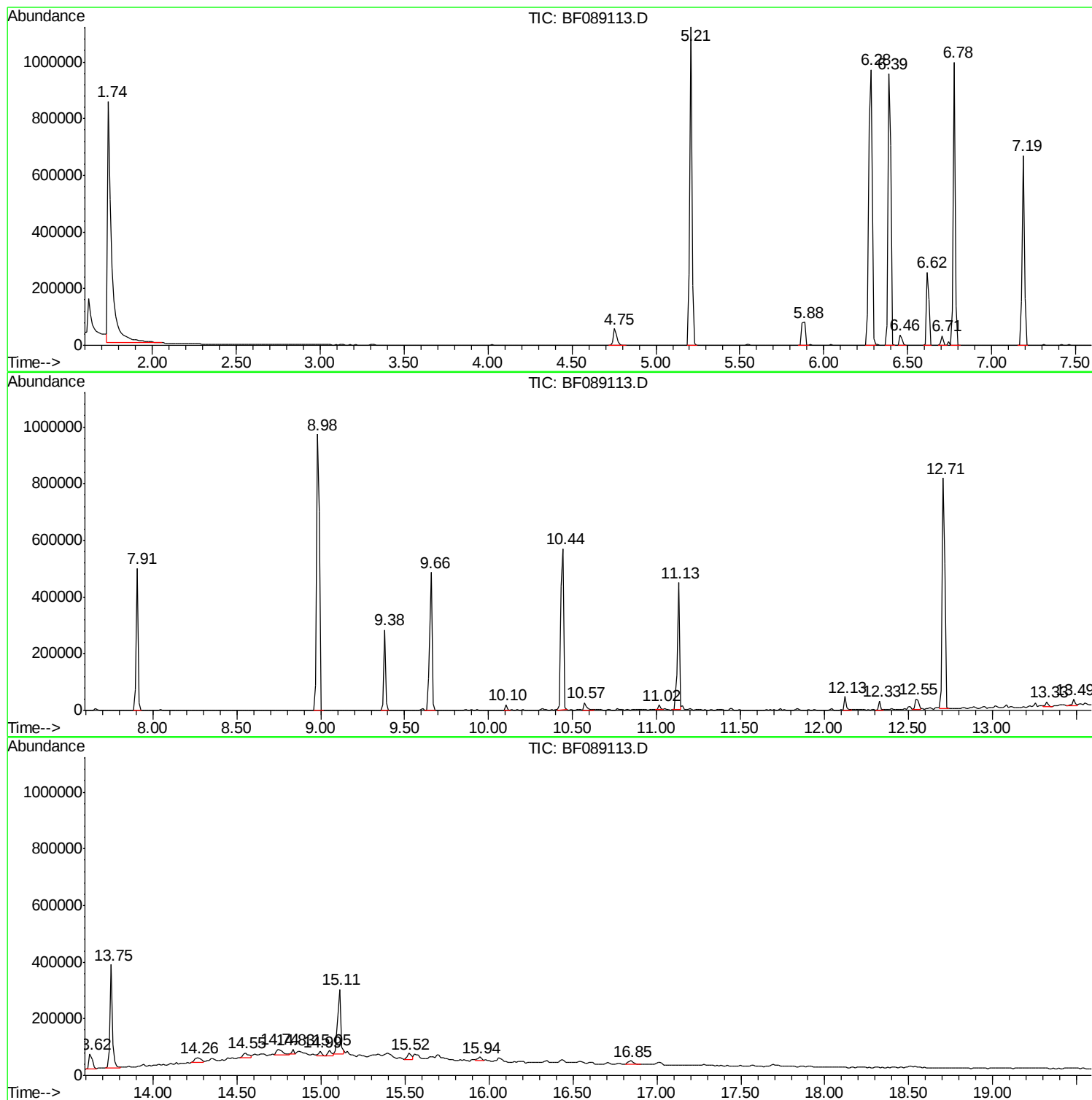
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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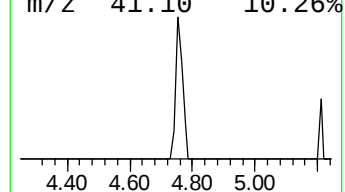
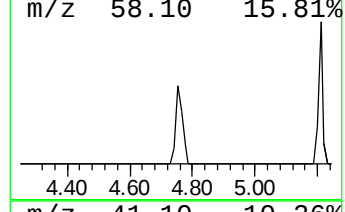
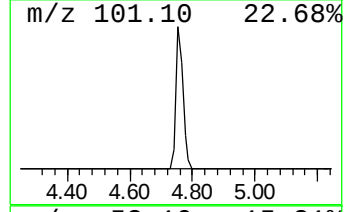
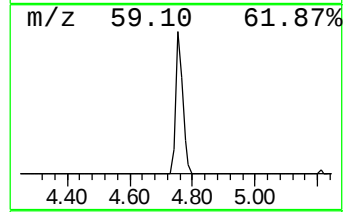
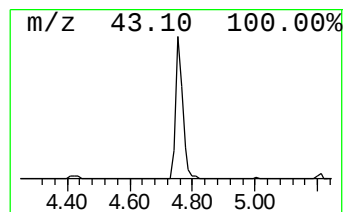
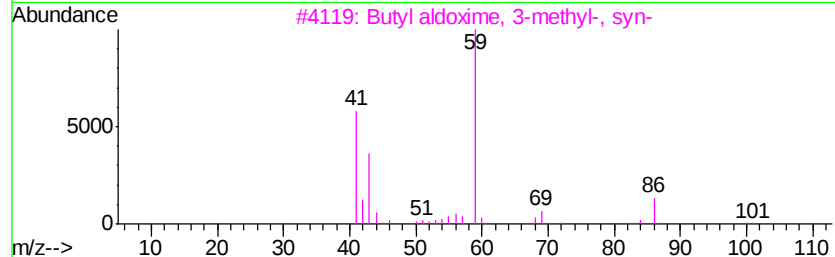
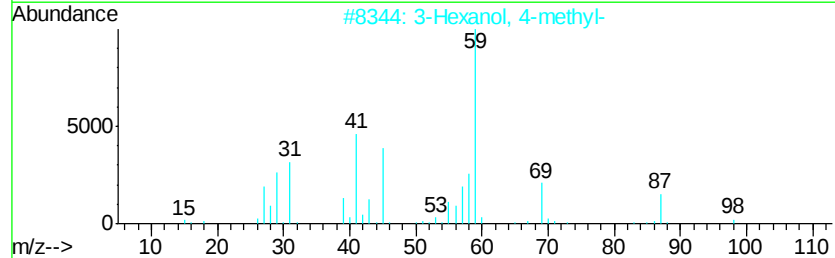
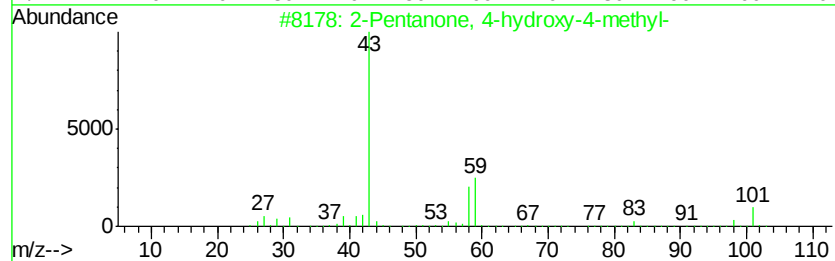
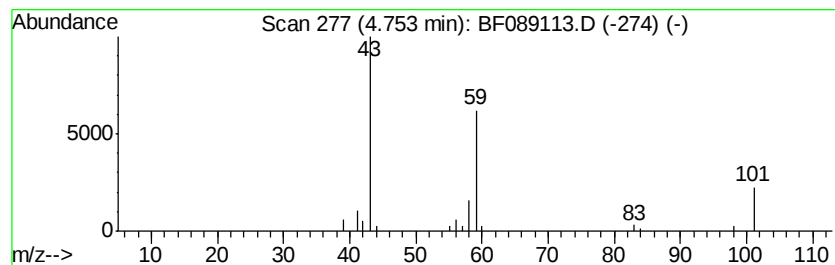
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.75	5.86 ng	85122	1,4-Dichlorobenzene-d4	6.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4		Acetone	58	C3H6O	000067-64-1	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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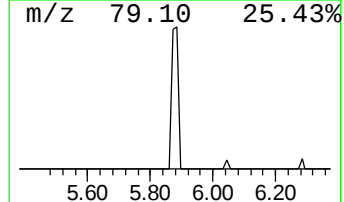
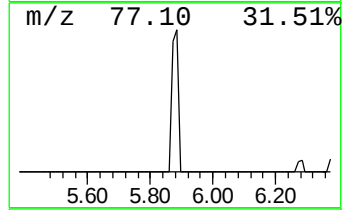
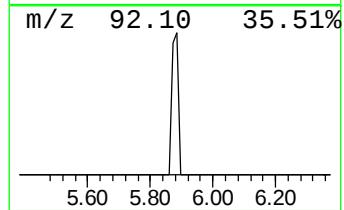
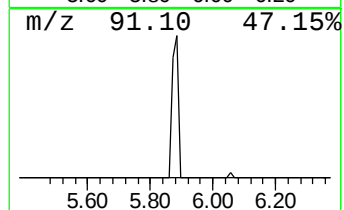
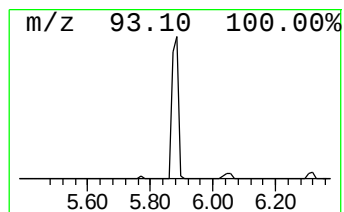
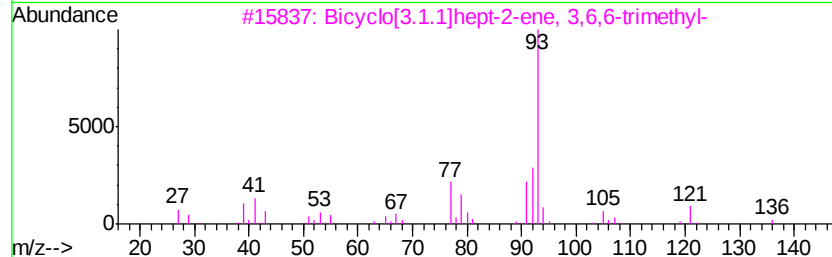
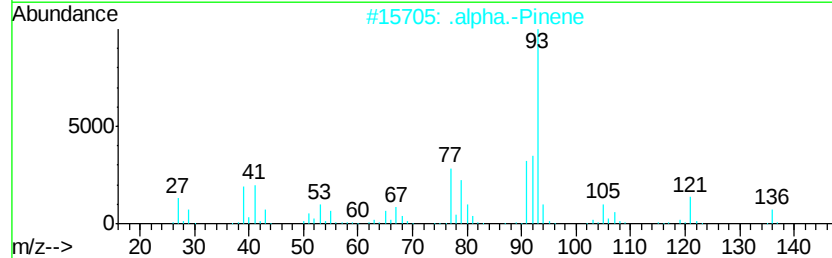
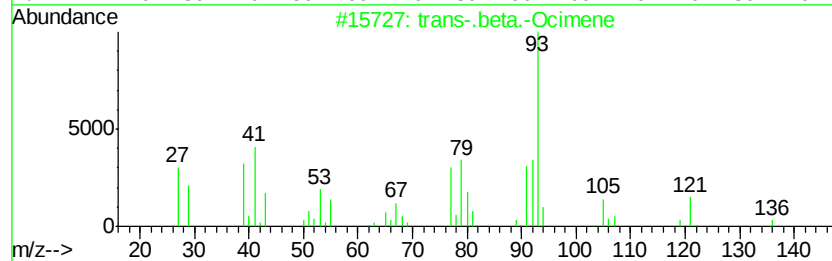
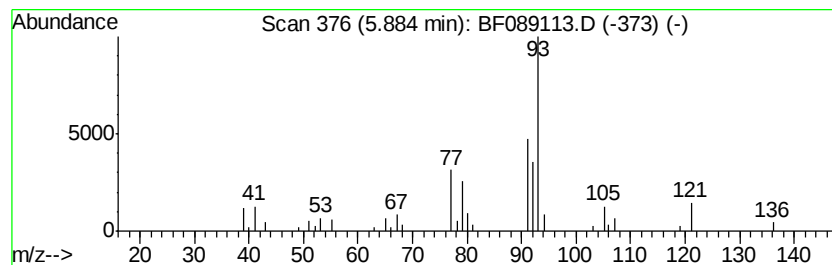
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Peak Number 3 trans-.beta.-Ocimene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.88	7.59 ng	110338	1,4-Dichlorobenzene-d4	6.62

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-.beta.-Ocimene	136	C10H16	003779-61-1	94
2			.alpha.-Pinene	136	C10H16	000080-56-8	91
3			Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91
4			1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	91
5			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91



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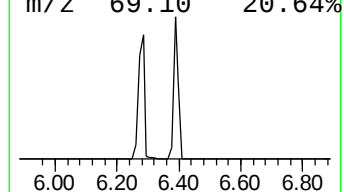
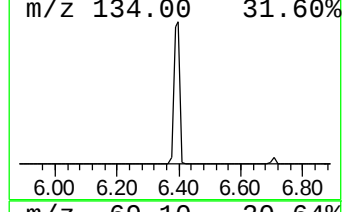
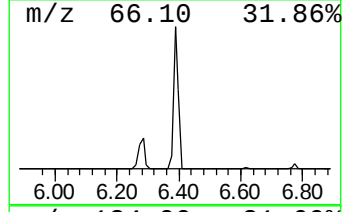
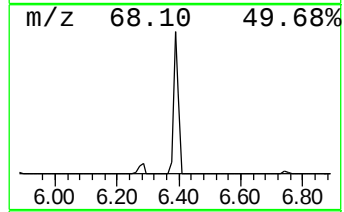
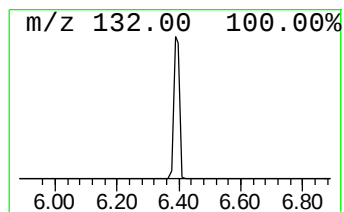
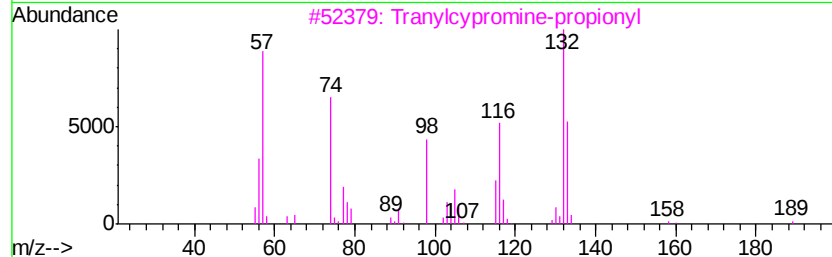
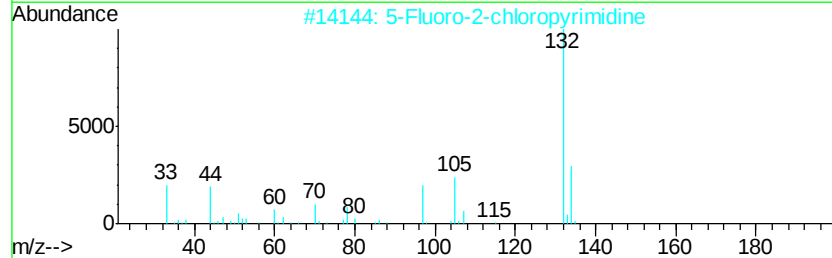
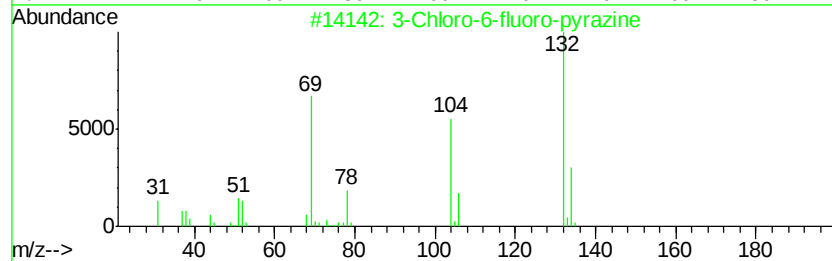
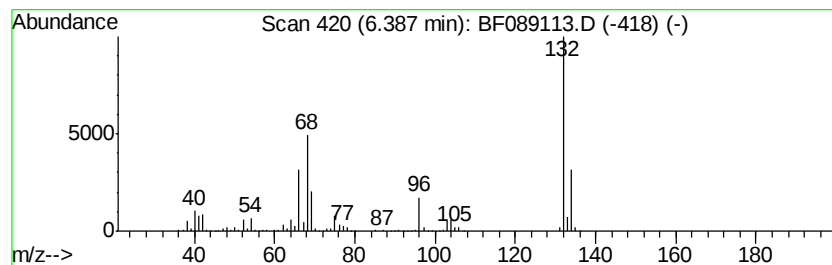
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Peak Number 4 unknown6.39 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	81.93 ng	1190650	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	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10



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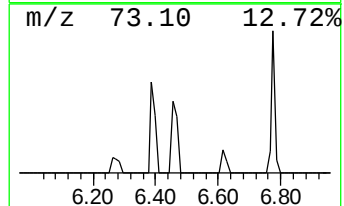
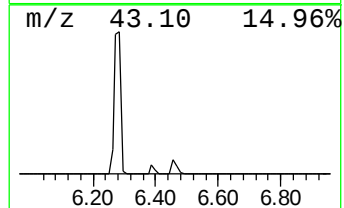
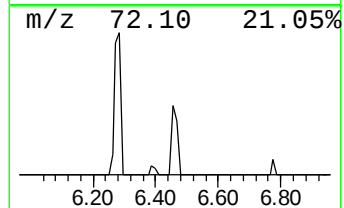
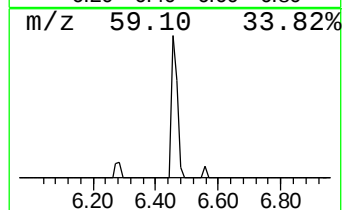
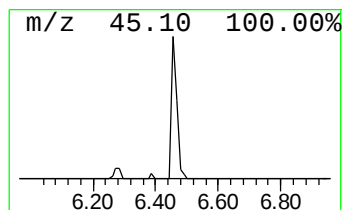
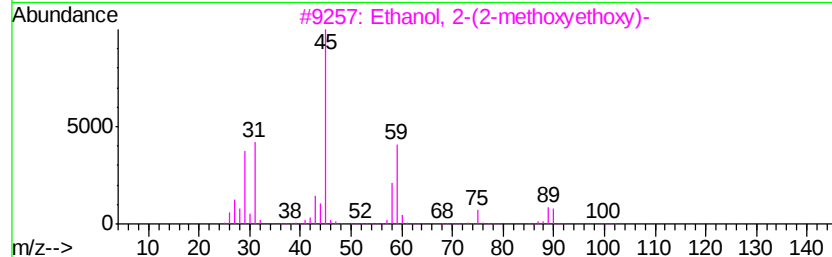
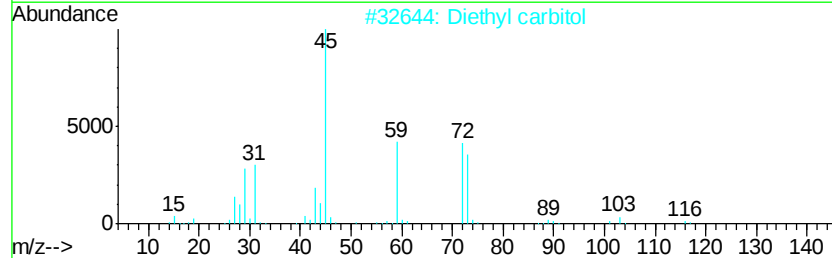
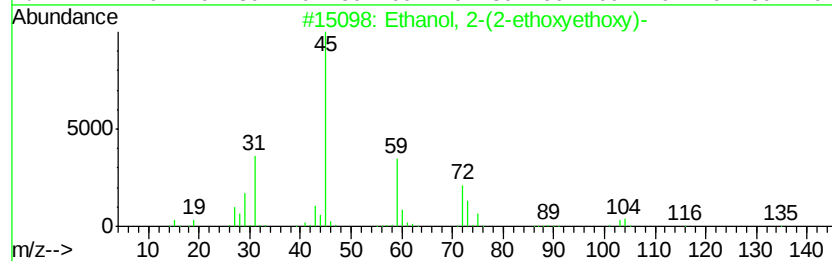
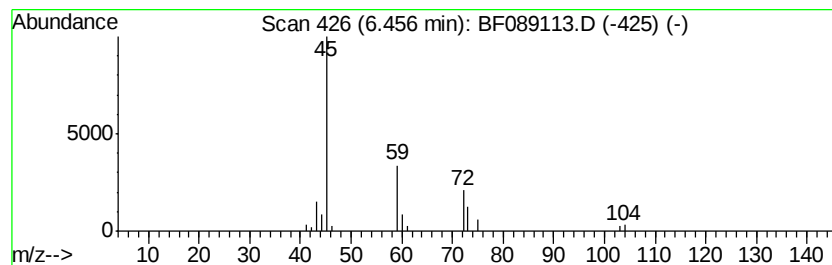
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Peak Number 5 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	2.99 ng	43479	1,4-Dichlorobenzene-d4	6.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2		Diethyl carbitol	162	C8H18O3	000112-36-7	78
3		Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	38
4		2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
5		Ethyl ether	74	C4H10O	000060-29-7	36



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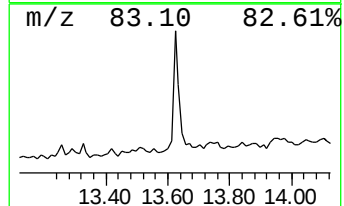
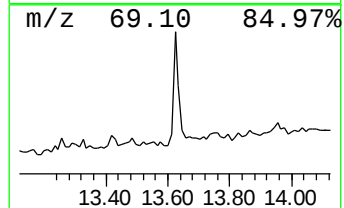
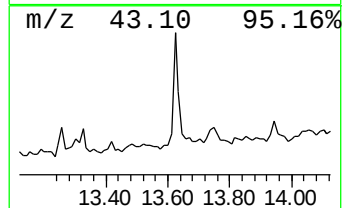
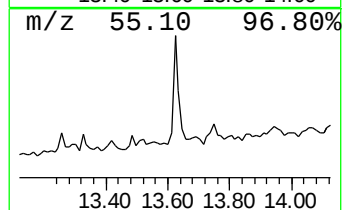
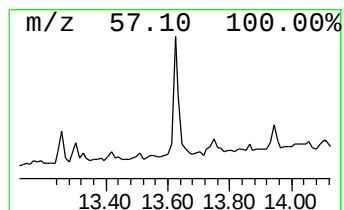
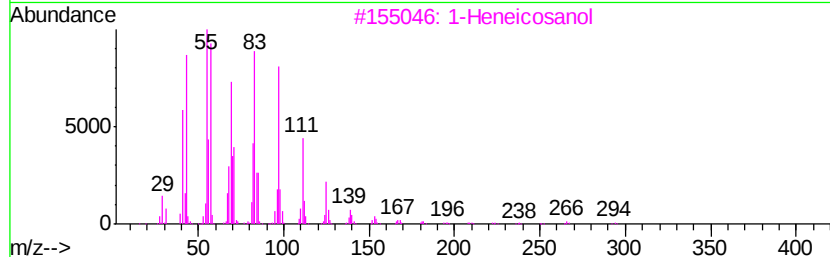
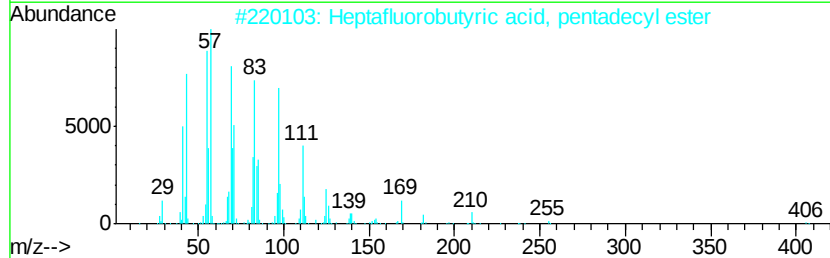
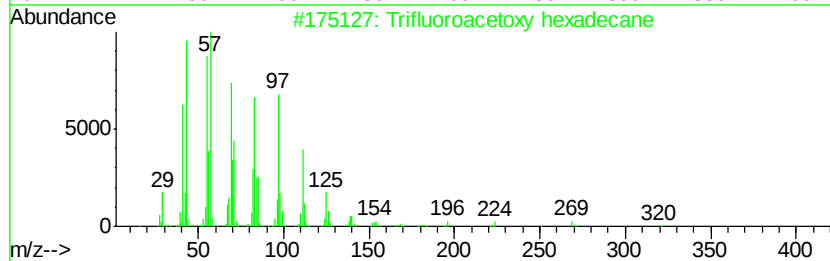
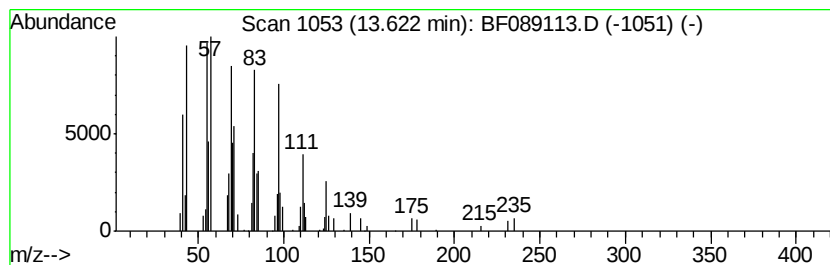
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Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.62	3.65 ng	67918	Chrysene-d12	13.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
3		1-Heneicosanol	312	C21H44O	015594-90-8	95
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
5		Behenic alcohol	326	C22H46O	000661-19-8	94



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071916\
Data File : BF089113.D
Acq On : 19 Jul 2016 12:44
Operator : UM/SJ
Sample : H4044-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

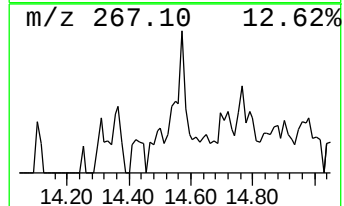
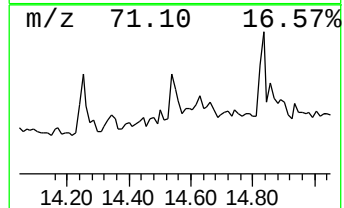
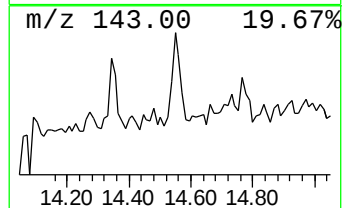
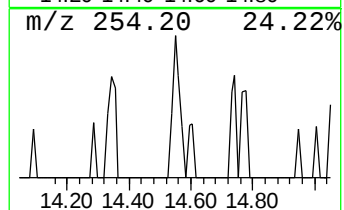
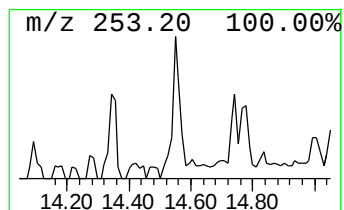
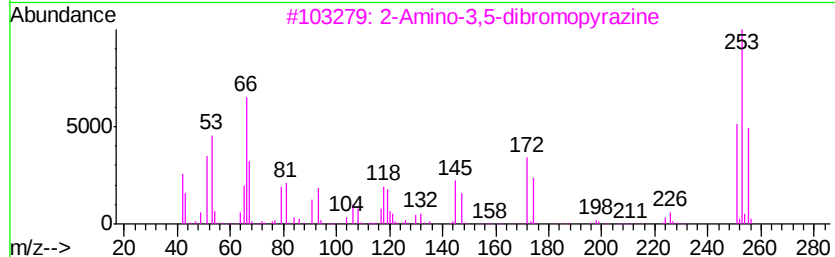
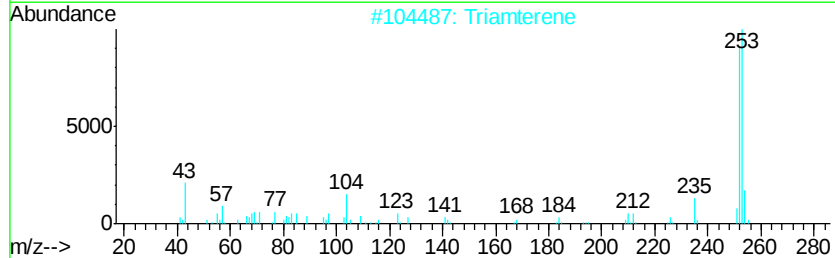
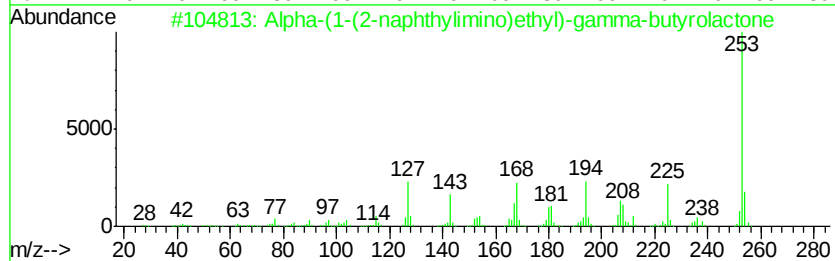
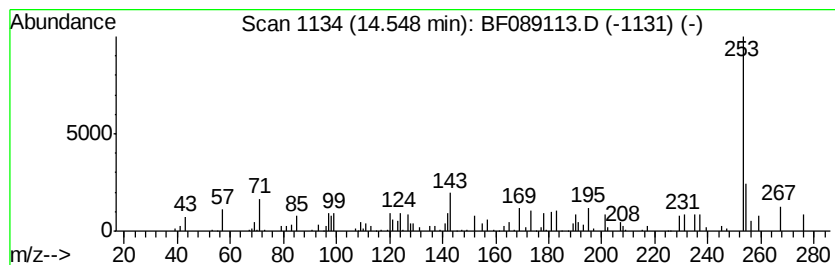
Instrument :
BNA_F
ClientSampleId :
F9-B1(6-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.55 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.55	2.93 ng	40386	Perylene-d12	15.11		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Alpha-(1-(2-naphthylimino)ethyl)...	253	C16H15N02	1000240-01-3	45	
2	Triamterene	253	C12H11N7	000396-01-0	43	
3	2-Amino-3,5-dibromopyrazine	251	C4H3Br2N3	024241-18-7	38	
4	3-Chloro-11H-pyrido[3',2'-4,5]py...	253	C14H8ClN3	1000212-59-4	38	
5	6H-Indolo[2,3-b]quinoxaline, 9-c...	253	C14H8ClN3	1000304-55-7	37	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071916\
Data File : BF089113.D
Acq On : 19 Jul 2016 12:44
Operator : UM/SJ
Sample : H4044-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
F9-B1(6-12)C

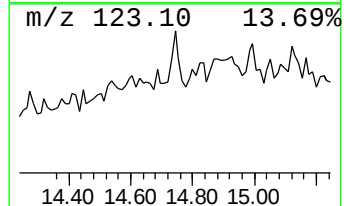
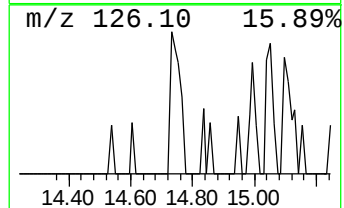
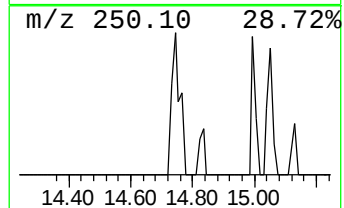
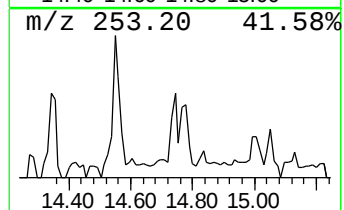
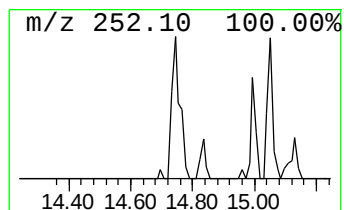
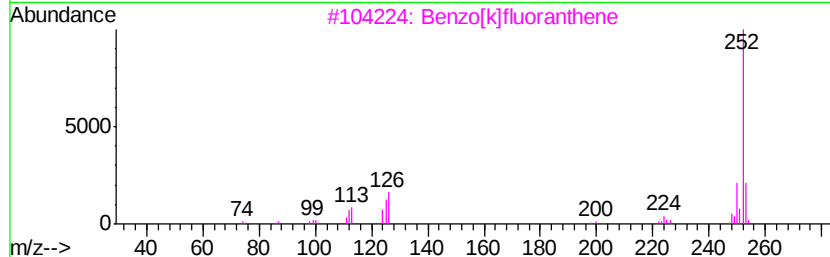
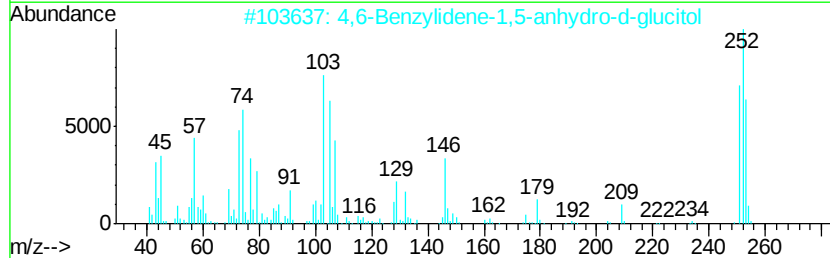
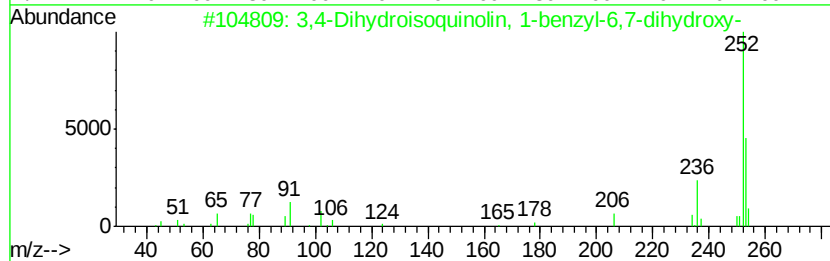
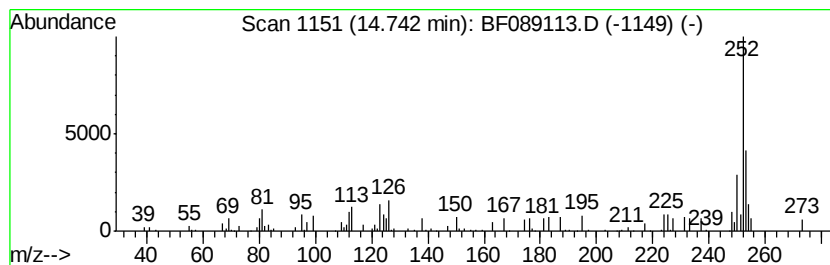
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 3,4-Dihydroisoquinolin, 1-b... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	3.96 ng	54671	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,4-Dihydroisoquinolin, 1-benzyl...	253	C16H15N02	017578-74-4	59
2		4,6-Benzylidene-1,5-anhydro-d-gl...	252	C13H16O5	1000128-98-6	58
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	53
4		Benzo[e]pyrene	252	C20H12	000192-97-2	52
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071916\
Data File : BF089113.D
Acq On : 19 Jul 2016 12:44
Operator : UM/SJ
Sample : H4044-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

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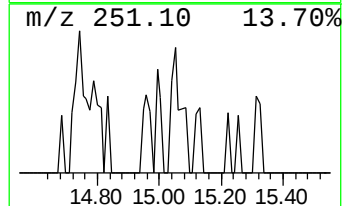
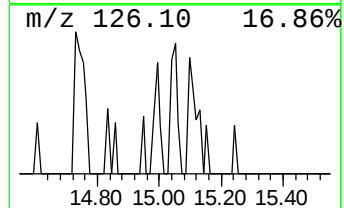
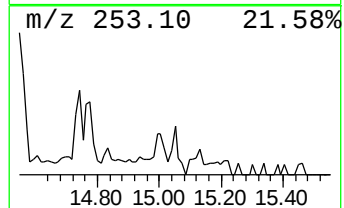
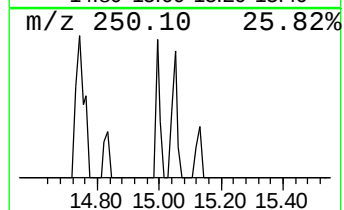
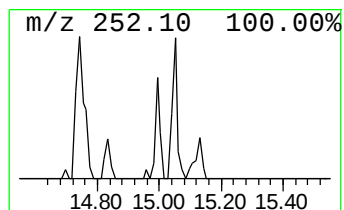
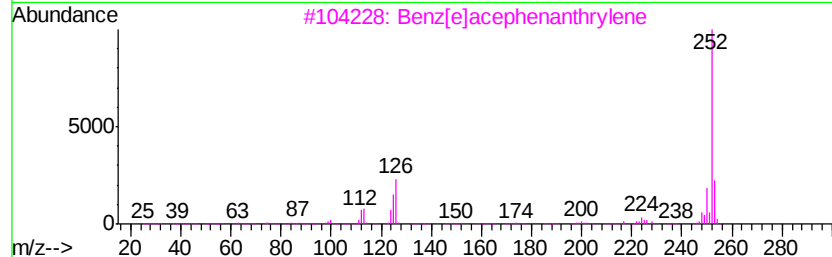
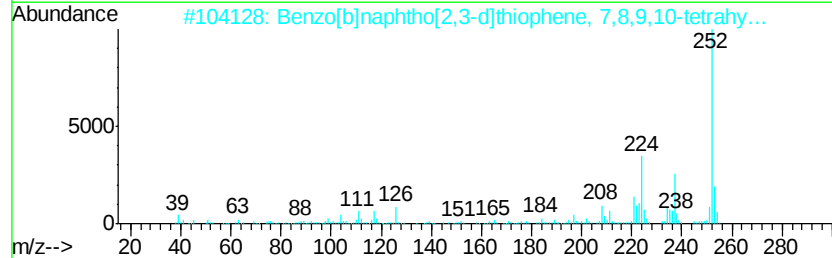
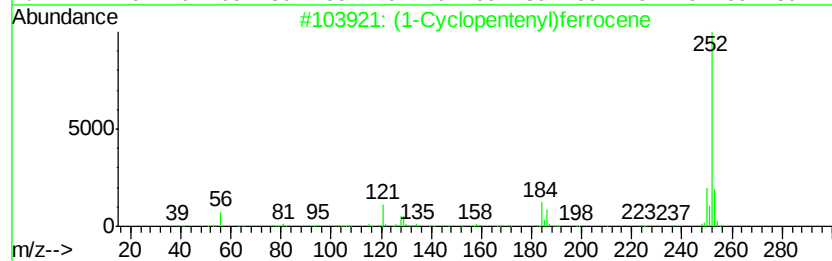
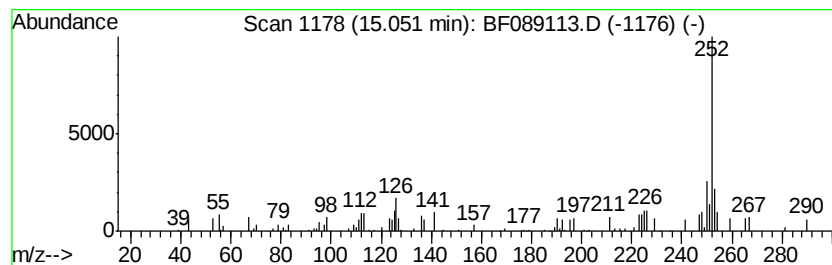
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 (1-Cyclopentenyl)ferrocene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.05	2.22 ng	30584	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	59
2		Benzo[b]naphtho[2,3-d]thiophene, ...	252	C17H16S	024964-06-5	58
3		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	53
4		4,5-Diphenyl-2-imidazoethiol	252	C15H12N2S	002349-58-8	52
5		Benzo[a]pyrene	252	C20H12	000050-32-8	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071916\
Data File : BF089113.D
Acq On : 19 Jul 2016 12:44
Operator : UM/SJ
Sample : H4044-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
F9-B1(6-12)C

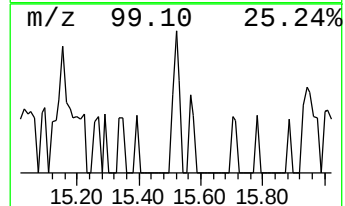
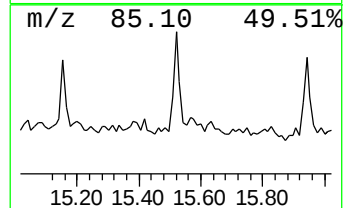
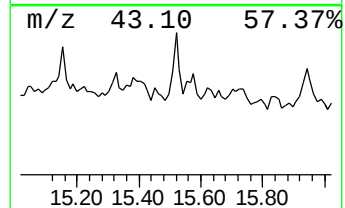
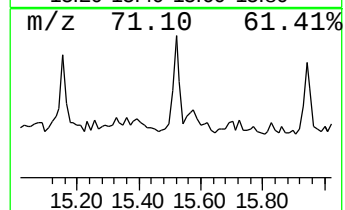
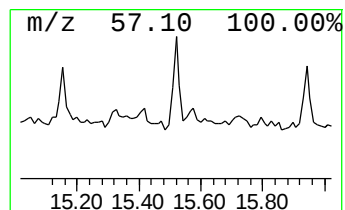
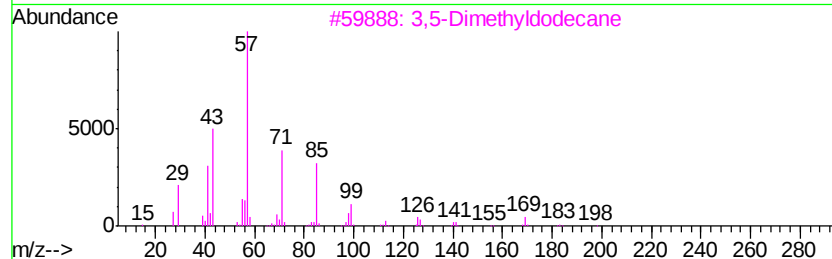
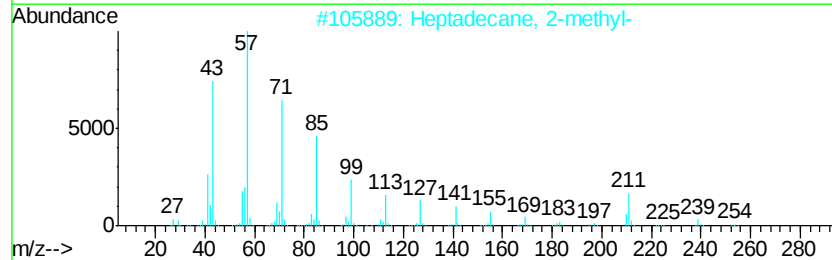
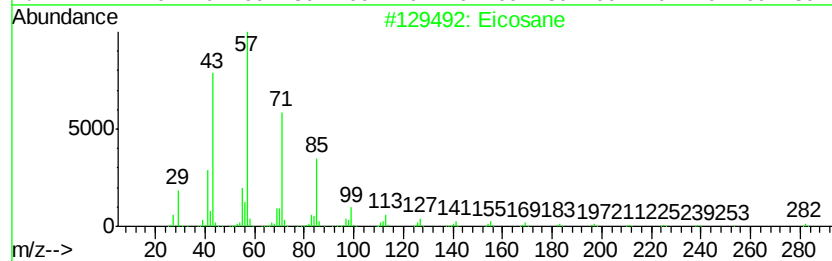
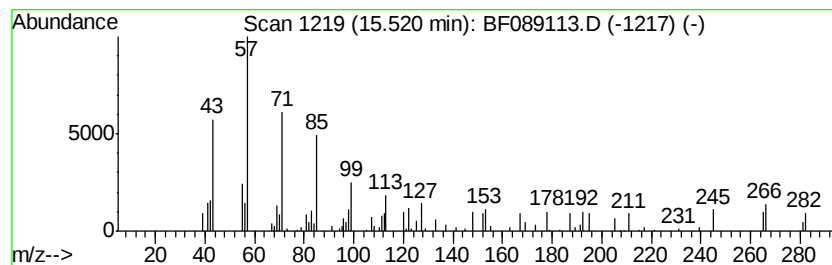
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown15.52 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.52	2.68 ng	36916	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	49
2		Heptadecane, 2-methyl-	254	C18H38	001560-89-0	47
3		3,5-Dimethyldodecane	198	C14H30	107770-99-0	47
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	43
5		Undecane, 2-methyl-	170	C12H26	007045-71-8	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071916\
Data File : BF089113.D
Acq On : 19 Jul 2016 12:44
Operator : UM/SJ
Sample : H4044-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
F9-B1(6-12)C

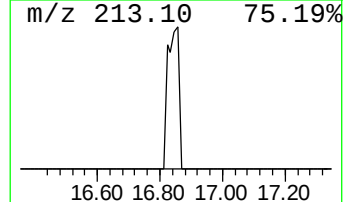
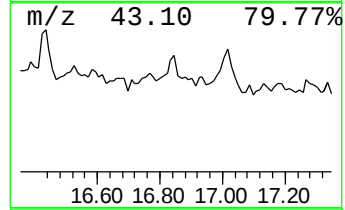
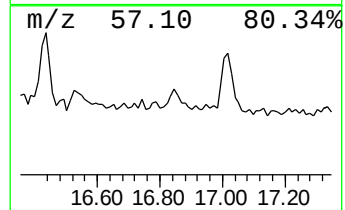
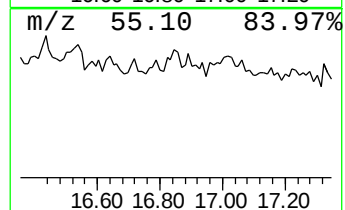
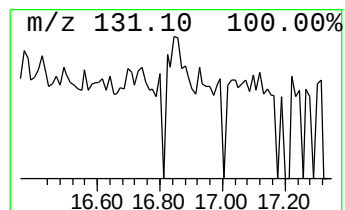
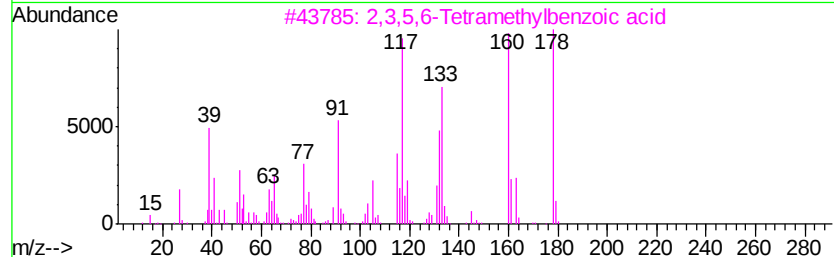
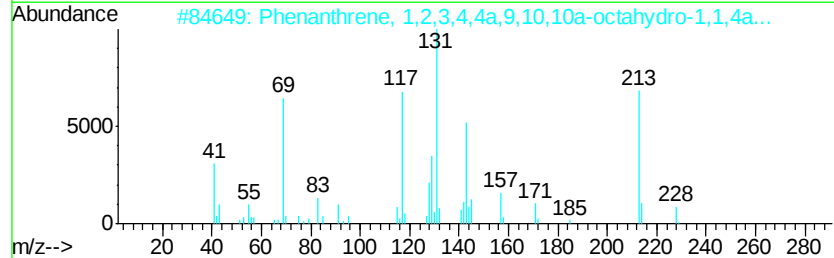
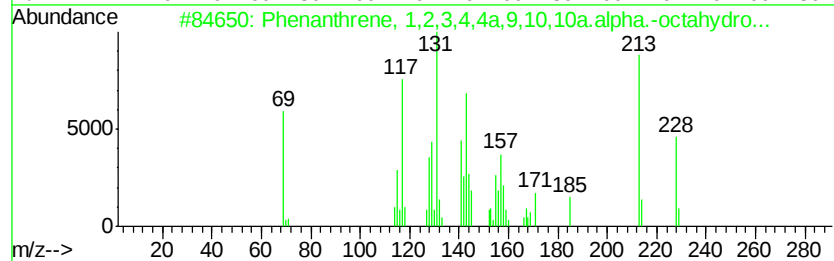
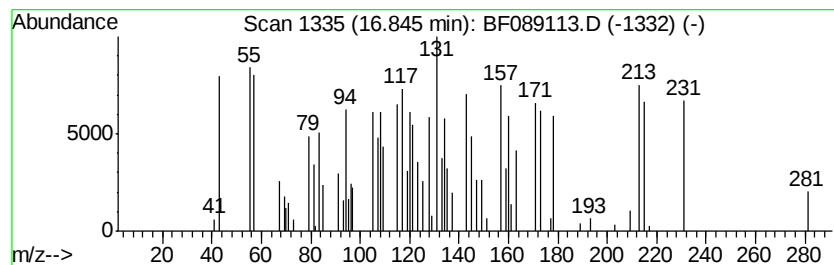
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown16.85 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.85	2.31 ng	31857	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenanthrene, 1,2,3,4,4a,9,10,10...	228	C17H24	000471-79-4	17
2		Phenanthrene, 1,2,3,4,4a,9,10,10...	228	C17H24	055090-42-1	17
3		2,3,5,6-Tetramethylbenzoic acid	178	C11H14O2	002604-45-7	11
4		Butanoic acid, 4-(1,1-dimethylet...	218	C11H22O4	106058-97-3	10
5		3-Bromophenyl isothiocyanate	213	C7H4BrNS	002131-59-1	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071916\
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
F9-B1(6-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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...	4.75	5.9	ng	85122	1	6.62	290666	20.0
trans-.beta.-Ocimene	5.88	7.6	ng	110338	1	6.62	290666	20.0
unknown6.39	6.39	81.9	ng	1190650	1	6.62	290666	20.0
Ethanol, 2-(2-eth...	6.46	3.0	ng	43479	1	6.62	290666	20.0
Trifluoroacetoxy ...	13.62	3.6	ng	67918	5	13.75	372203	20.0
unknown14.55	14.55	2.9	ng	40386	6	15.11	275832	20.0
3,4-Dihydroisoqui...	14.74	4.0	ng	54671	6	15.11	275832	20.0
(1-Cyclopentenyl)...	15.05	2.2	ng	30584	6	15.11	275832	20.0
unknown15.52	15.52	2.7	ng	36916	6	15.11	275832	20.0
unknown16.85	16.85	2.3	ng	31857	6	15.11	275832	20.0