

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022417\
 Data File : BF093177.D
 Acq On : 25 Feb 2017 7:56
 Operator : SJ/MA
 Sample : I1973-05
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 E2-Y5N-SW

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-BF013017.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	5.001	252	255	269	rVB	1339445	2180101	44.13%	5.286%
2	5.436	290	293	295	rBV	4284933	4940017	100.00%	11.977%
3	6.476	381	384	387	rBV	3536471	4894594	99.08%	11.867%
4	6.602	393	395	398	rVB	4152681	4376220	88.59%	10.610%
5	6.830	413	415	418	rBV	1070810	931225	18.85%	2.258%
6	6.990	426	429	431	rBV	3707872	3369375	68.21%	8.169%
7	7.402	462	465	468	rBV	2179893	3167097	64.11%	7.679%
8	8.122	526	528	533	rVB	1406772	1225912	24.82%	2.972%
9	9.208	620	623	625	rBV	3287150	4312431	87.30%	10.456%
10	9.596	655	657	661	rVB	351677	297407	6.02%	0.721%
11	9.882	679	682	684	rBV	997966	1175851	23.80%	2.851%
12	10.305	718	719	721	rVB	75444	67481	1.37%	0.164%
13	10.671	748	751	753	rBV	2093489	2120043	42.92%	5.140%
14	10.785	759	761	765	rVB	98752	145067	2.94%	0.352%
15	10.968	775	777	782	rBV4	20310	51294	1.04%	0.124%
16	11.231	797	800	801	rBV	104149	99777	2.02%	0.242%
17	11.368	809	812	814	rBV	653031	956682	19.37%	2.320%
18	11.974	863	865	871	rVV4	41955	91293	1.85%	0.221%
19	12.099	875	876	880	rVB3	50290	61848	1.25%	0.150%
20	12.454	905	907	910	rVB2	34189	56133	1.14%	0.136%
21	12.579	915	918	920	rBV	208390	201154	4.07%	0.488%
22	12.808	934	938	941	rVB	181690	241628	4.89%	0.586%
23	12.945	948	950	953	rVB	1913776	2627988	53.20%	6.372%
24	13.025	954	957	960	rBV3	28063	54457	1.10%	0.132%
25	13.128	963	966	968	rVB	34970	72477	1.47%	0.176%
26	13.197	968	972	974	rBV2	34491	55627	1.13%	0.135%
27	13.642	1007	1011	1013	rBV3	26893	63994	1.30%	0.155%
28	13.848	1027	1029	1035	rVB3	116555	163347	3.31%	0.396%
29	14.008	1039	1043	1044	rBV2	695573	1071692	21.69%	2.598%
30	14.179	1055	1058	1060	rBV4	18819	55511	1.12%	0.135%
31	14.465	1081	1083	1086	rBV3	38873	83175	1.68%	0.202%
32	15.025	1129	1132	1136	rBV	139358	279452	5.66%	0.678%
33	15.311	1155	1157	1160	rBV	74347	95754	1.94%	0.232%
34	15.380	1160	1163	1165	rVV	104710	145876	2.95%	0.354%

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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-BF013017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.437	1165	1168	1176	rVB	591703	808879	16.37%	1.961%
36	15.860	1202	1205	1207	rBV	29841	54662	1.11%	0.133%
37	16.843	1288	1291	1294	rBV	34070	68907	1.39%	0.167%
38	17.003	1301	1305	1308	rBV3	39999	84342	1.71%	0.204%
39	17.117	1312	1315	1323	rVB	203173	428068	8.67%	1.038%
40	17.265	1325	1328	1333	rBV	29325	68321	1.38%	0.166%

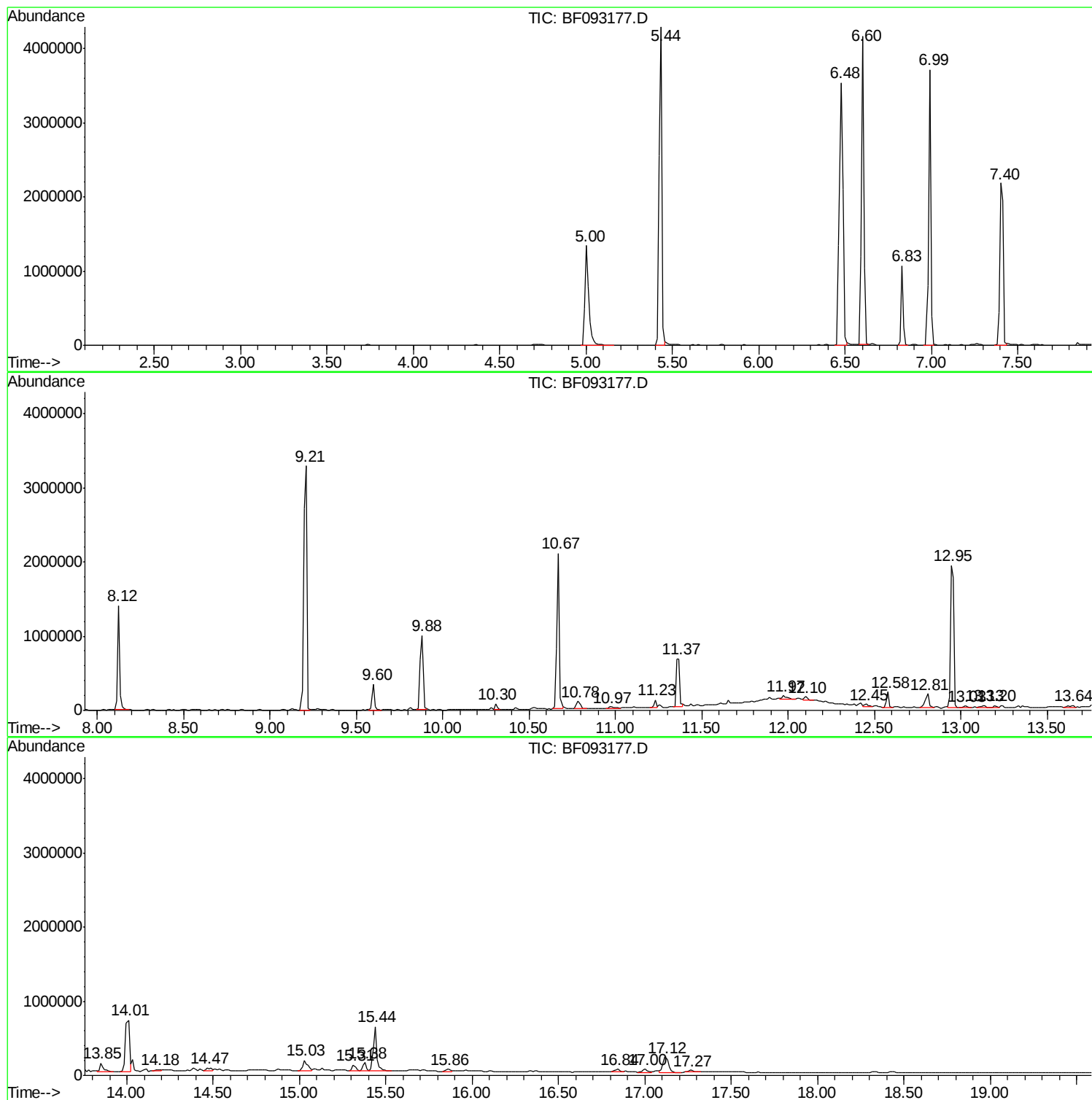
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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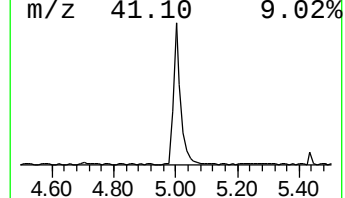
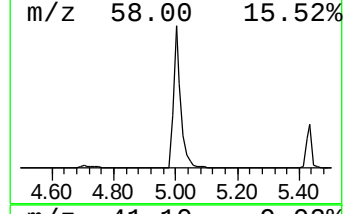
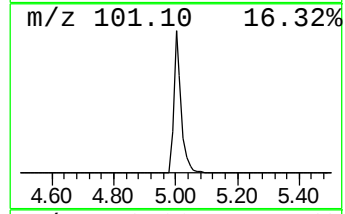
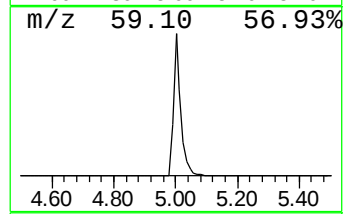
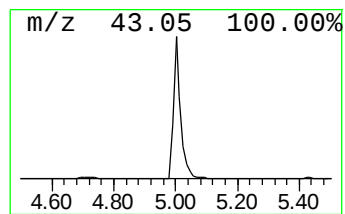
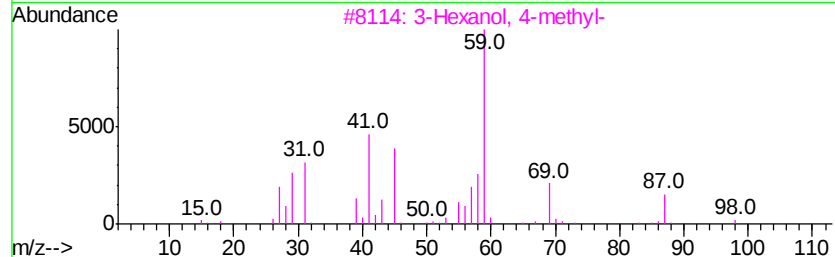
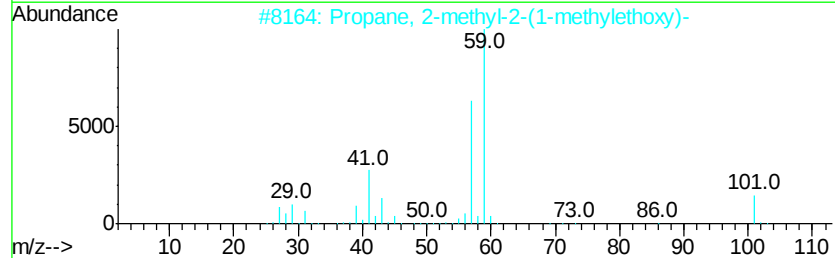
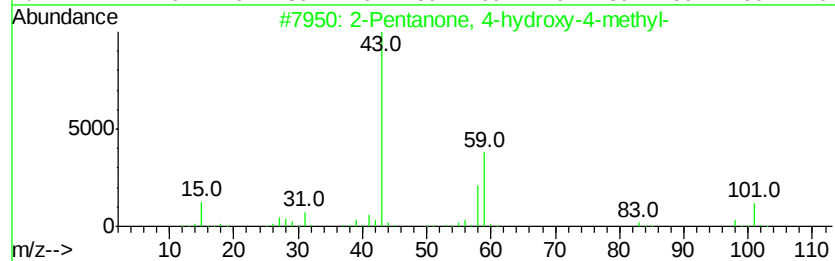
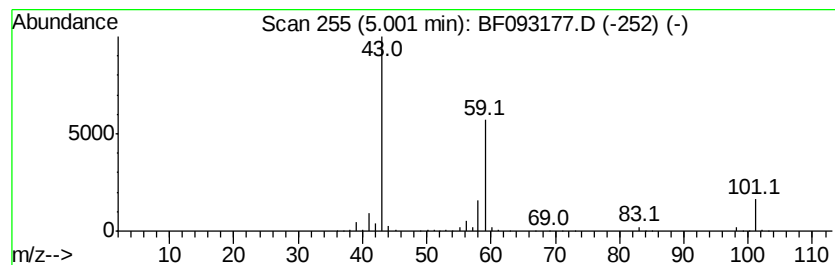
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	46.82 ng	2180100	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23



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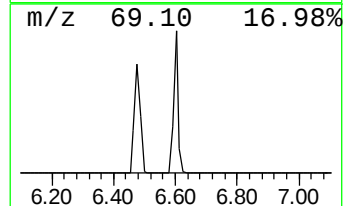
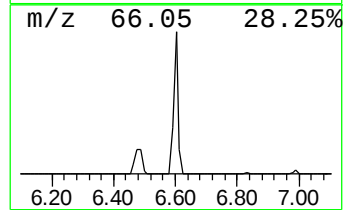
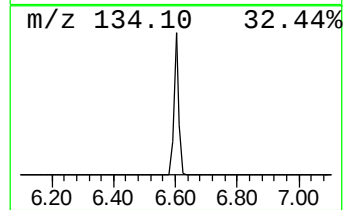
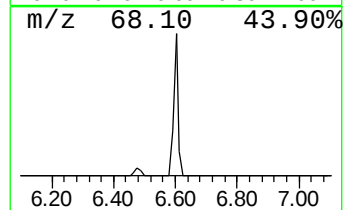
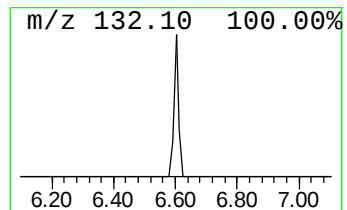
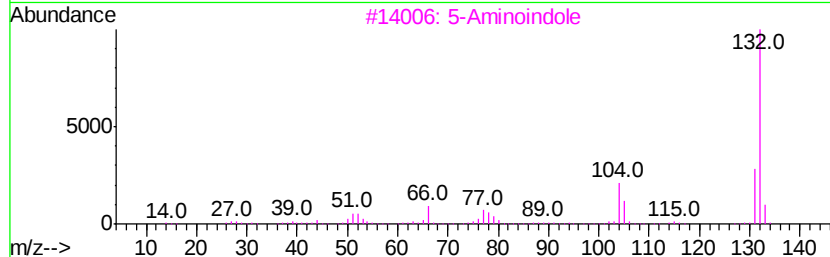
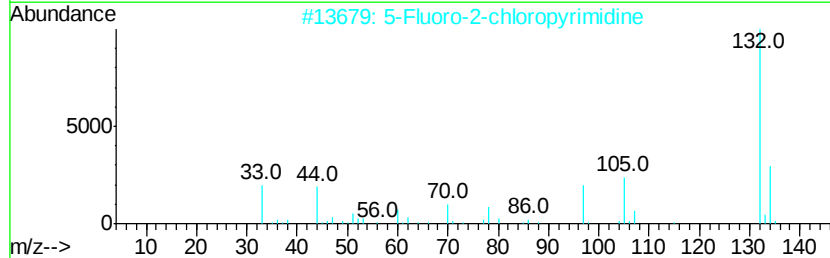
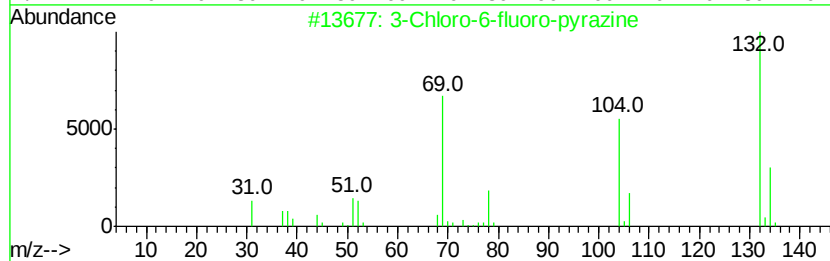
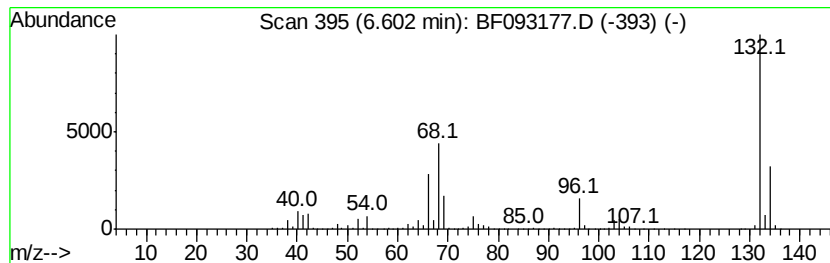
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	93.99 ng	4376220	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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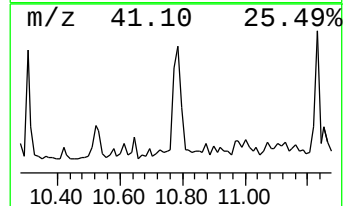
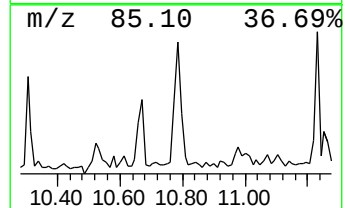
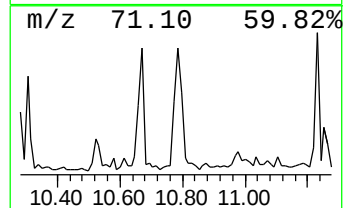
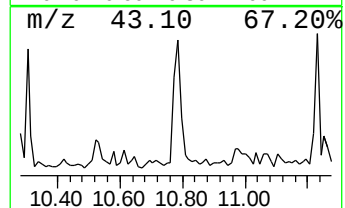
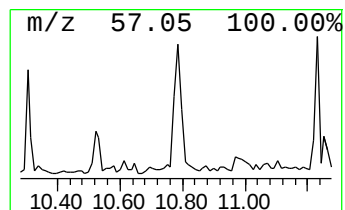
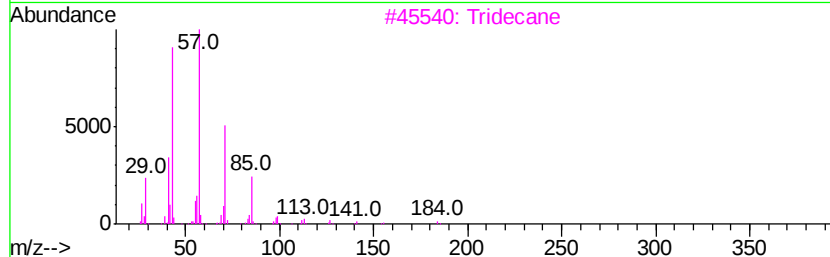
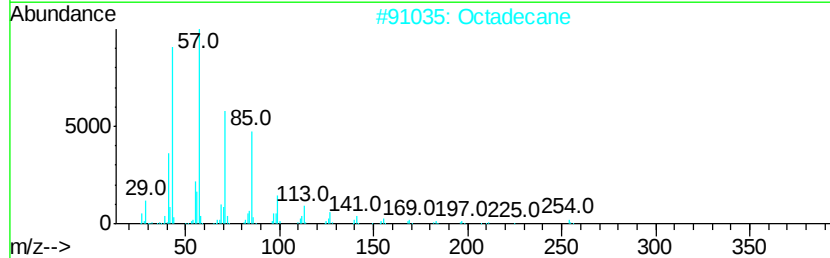
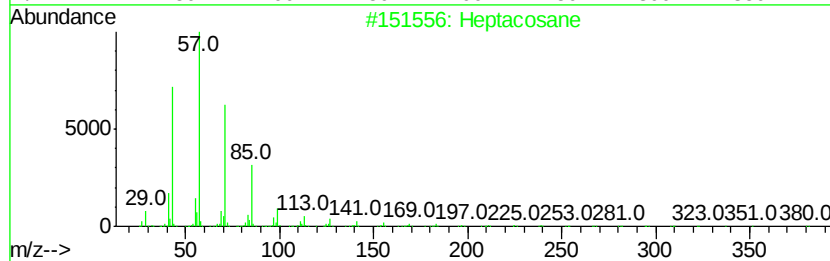
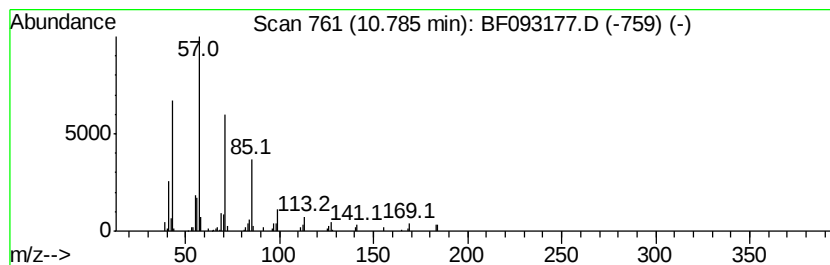
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.78	3.03 ng	145067	Phenanthrene-d10	11.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Octadecane		254	C18H38	000593-45-3	91
3	Tridecane		184	C13H28	000629-50-5	90
4	Heptadecane		240	C17H36	000629-78-7	90
5	Tetracosane		338	C24H50	000646-31-1	87



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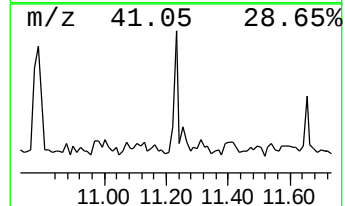
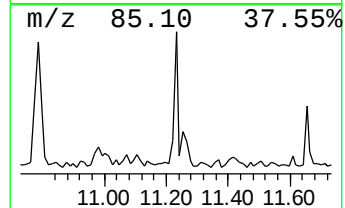
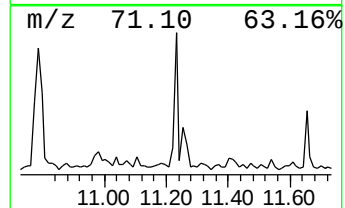
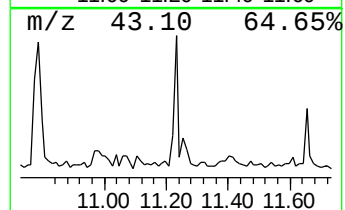
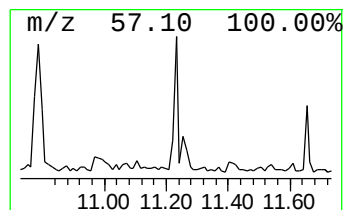
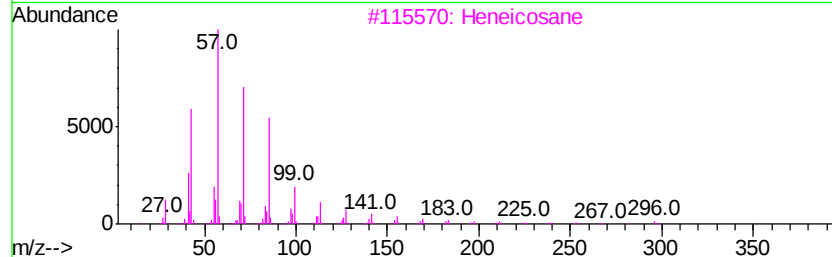
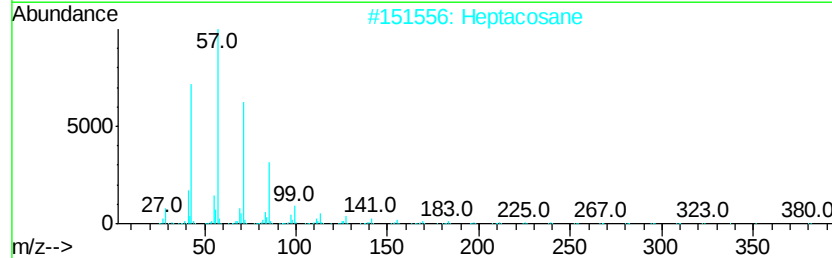
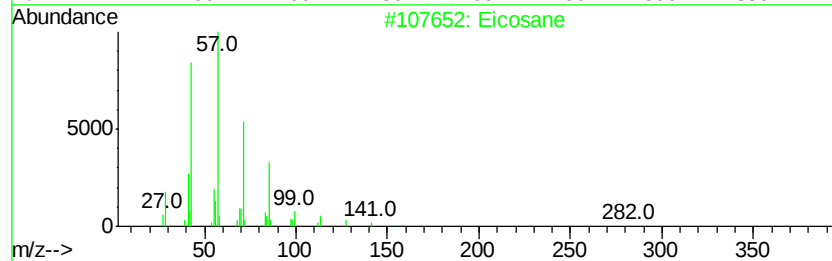
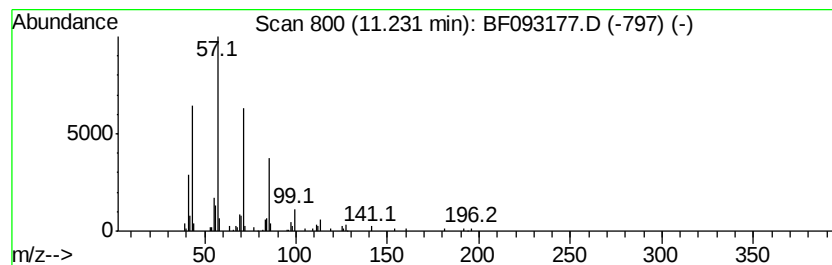
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.23	2.09 ng	99777	Phenanthrene-d10		11.37	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Heptacosane		380	C27H56	000593-49-7	87
3	Heneicosane		296	C21H44	000629-94-7	86
4	Hexadecane		226	C16H34	000544-76-3	86
5	Dodecane, 2-methyl-6-propyl-		226	C16H34	055045-08-4	80



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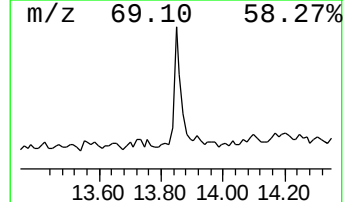
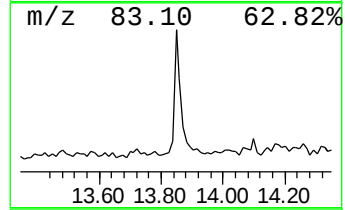
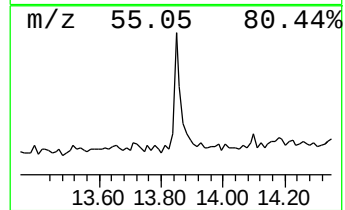
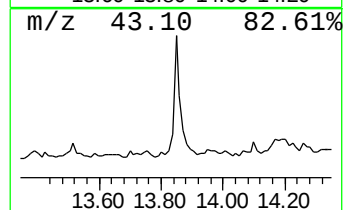
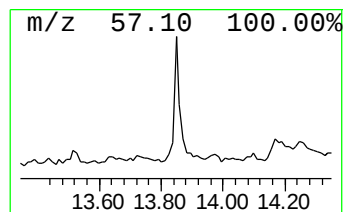
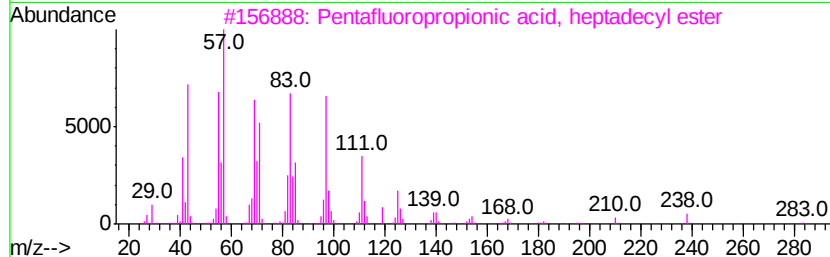
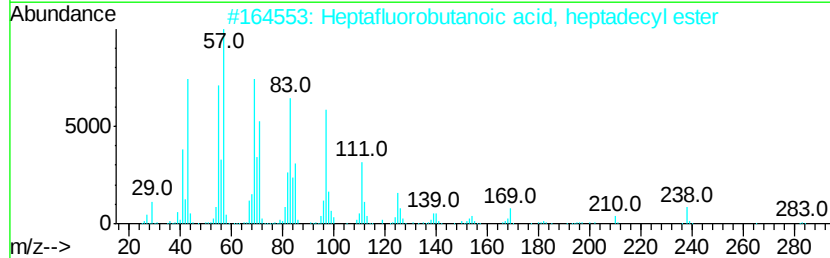
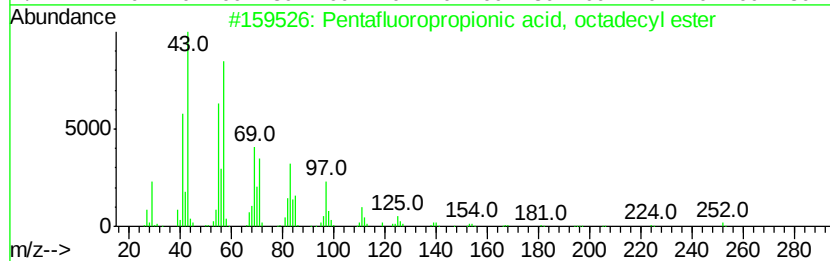
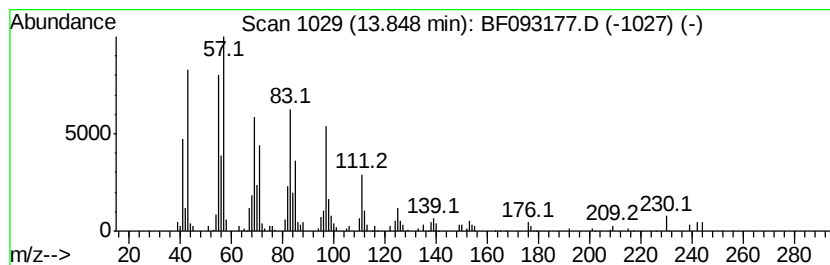
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	3.05 ng	163347	Chrysene-d12	14.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, octadecyl...	416	C21H37F5O2	1000280-07-7	90
2		Heptafluorobutanoic acid, heptadecyl...	452	C21H35F7O2	1000282-97-3	87
3		Pentafluoropropionic acid, heptadecyl...	402	C20H35F5O2	1000283-04-2	87
4		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	80
5		1-Octadecanol	270	C18H38O	000112-92-5	76



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022417\
Data File : BF093177.D
Acq On : 25 Feb 2017 7:56
Operator : SJ/MA
Sample : I1973-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-Y5N-SW

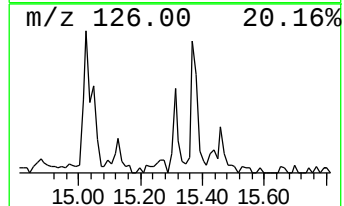
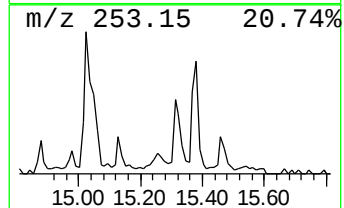
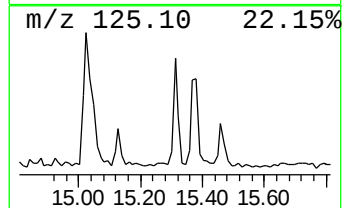
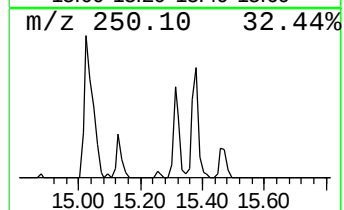
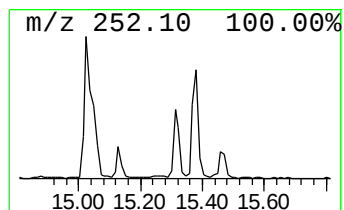
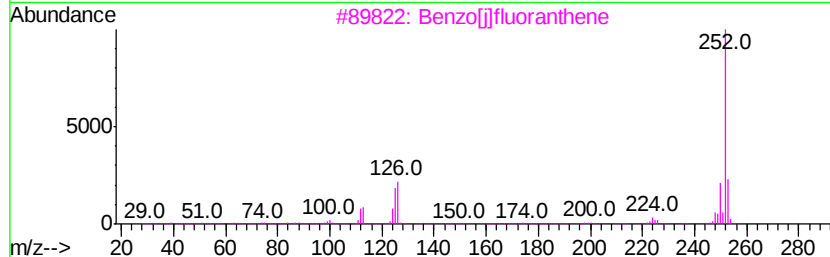
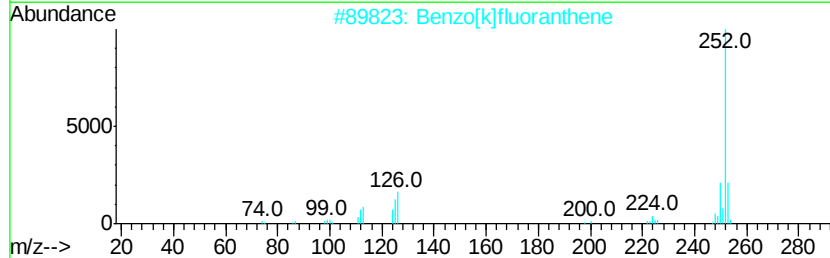
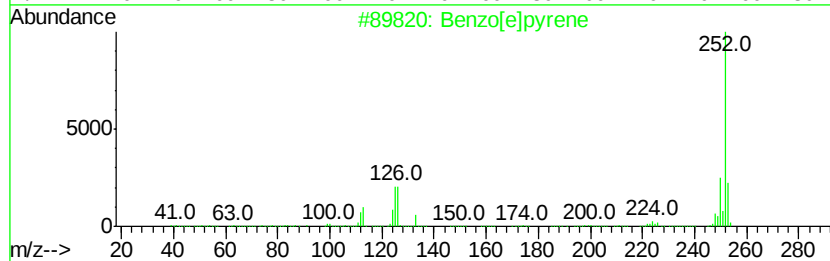
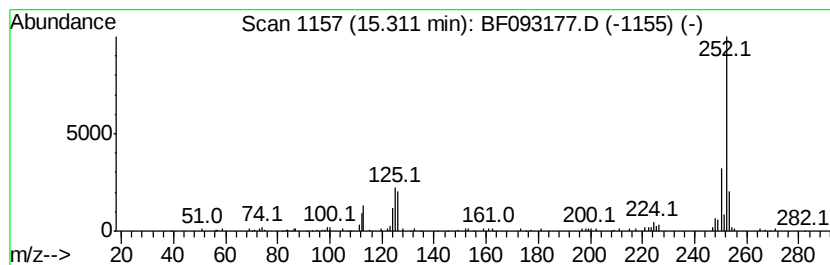
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	2.37 ng	95754	Perylene-d12	15.44

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	98
3		Benzo[i]fluoranthene	252	C20H12	000205-82-3	98
4		Perylene	252	C20H12	000198-55-0	98
5		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	98



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022417\
Data File : BF093177.D
Acq On : 25 Feb 2017 7:56
Operator : SJ/MA
Sample : I1973-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-Y5N-SW

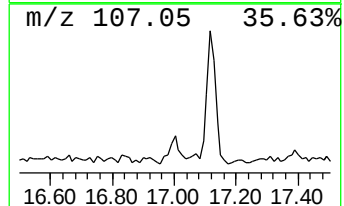
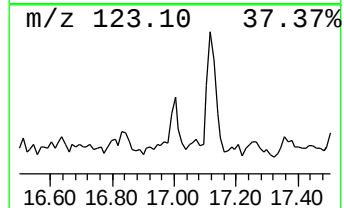
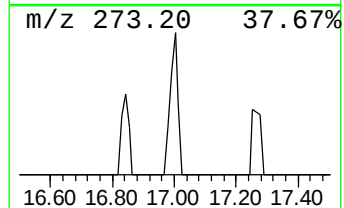
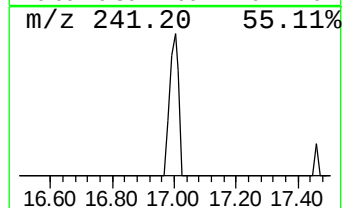
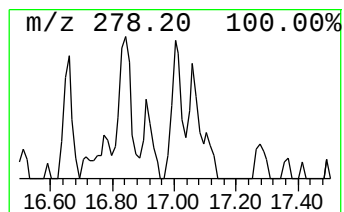
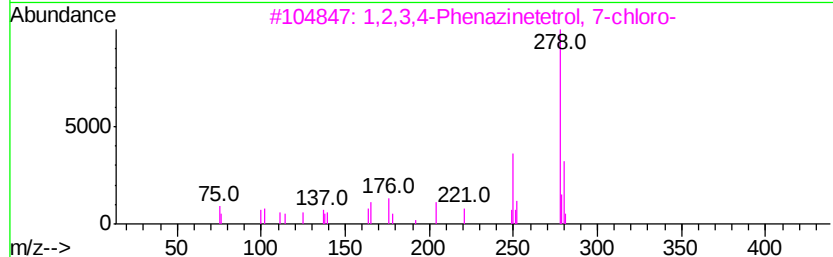
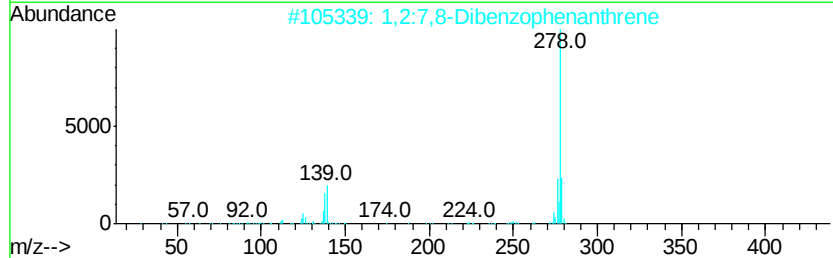
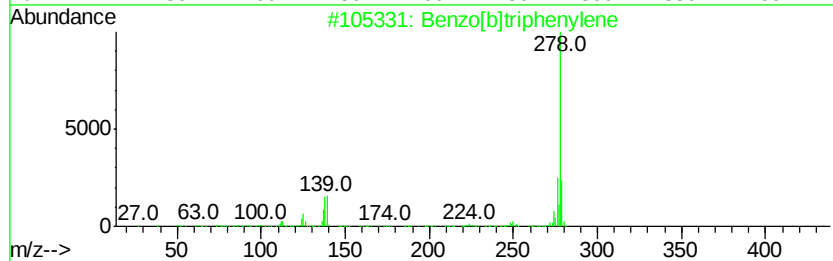
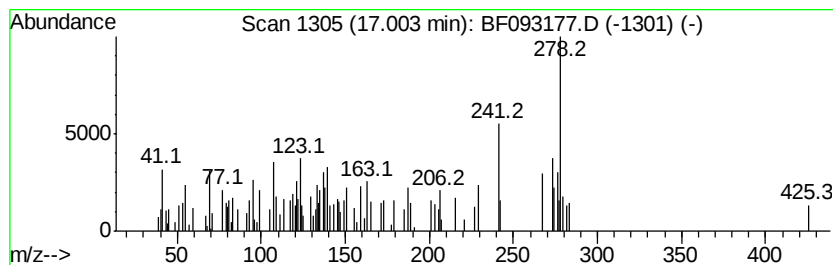
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown17.00 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.00	2.09 ng	84342	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[b]triphenylene	278	C22H14	000215-58-7	27
2		1,2:7,8-Dibenzophenanthrene	278	C22H14	000213-46-7	27
3		1,2,3,4-Phenazinetetrol, 7-chloro-	278	C12H7ClN2O4	023774-10-9	22
4		Cyclohexanone, (2,4-dinitrophenyl...)	278	C12H14N4O4	001589-62-4	22
5		Naphthalene, 2,6-dimethoxy-1,5-d...	278	C12H10N2O6	025314-97-0	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022417\
Data File : BF093177.D
Acq On : 25 Feb 2017 7:56
Operator : SJ/MA
Sample : I1973-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
E2-Y5N-SW

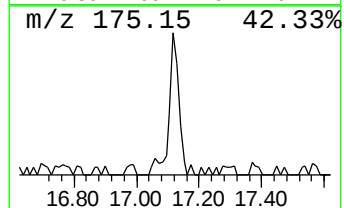
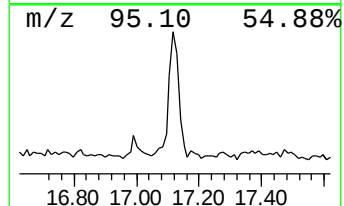
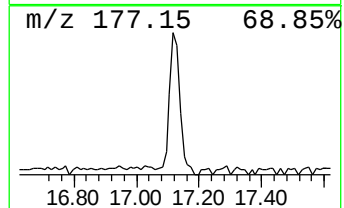
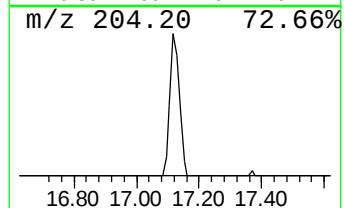
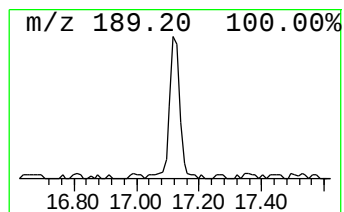
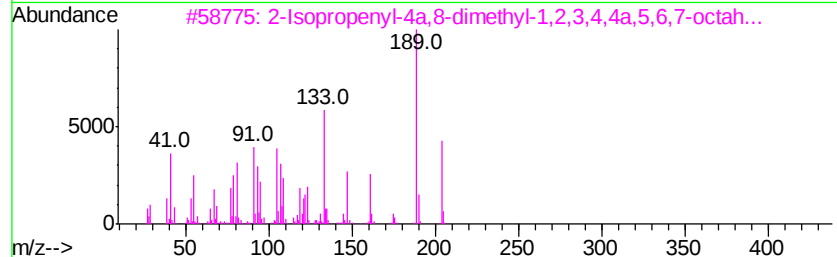
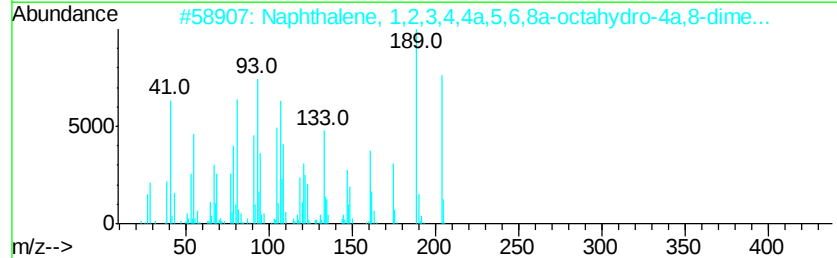
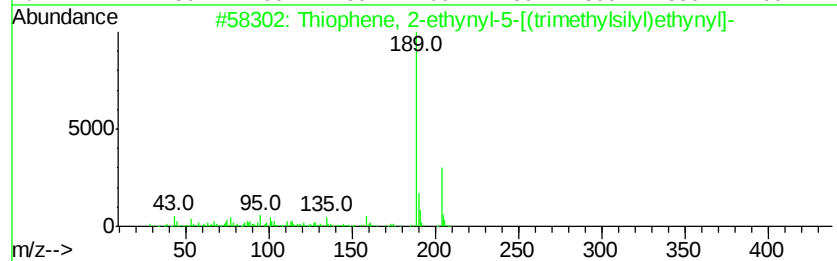
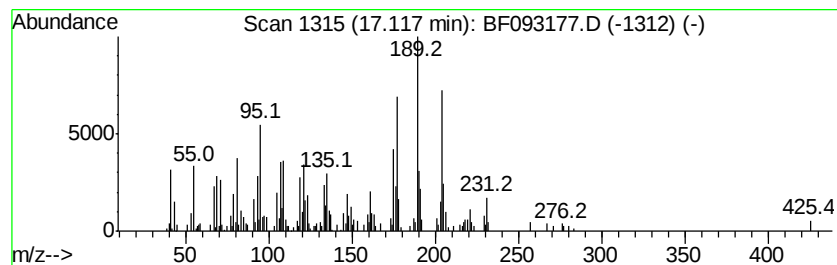
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.12 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.12	10.58 ng	428068	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiophene, 2-ethynyl-5-[(trimeth...	204	C11H12SSi	182323-29-1	49
2		Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	47
3		2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000192-43-5	43
4		1H-Cyclopropa[fa]naphthalene, 1a,...	204	C15H24	1000147-32-8	43
5		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022417\
Data File : BF093177.D
Acq On : 25 Feb 2017 7:56
Operator : SJ/MA
Sample : I1973-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-Y5N-SW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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...	5.00	46.8	ng	2180100	1	6.83	931225	20.0
unknown6.60	6.60	94.0	ng	4376220	1	6.83	931225	20.0
Heptacosane	10.78	3.0	ng	145067	4	11.37	956682	20.0
Eicosane	11.23	2.1	ng	99777	4	11.37	956682	20.0
Pentafluoropropio...	13.85	3.0	ng	163347	5	14.01	1071690	20.0
Benzo[e]pyrene	15.31	2.4	ng	95754	6	15.44	808879	20.0
unknown17.00	17.00	2.1	ng	84342	6	15.44	808879	20.0
unknown17.12	17.12	10.6	ng	428068	6	15.44	808879	20.0