

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
 Data File : BF087873.D
 Acq On : 10 Jun 2016 14:32
 Operator : UM/SJ
 Sample : H3426-06 2X
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-52

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-BF060716.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	1.747	13	14	23	rVB	188631	335951	4.84%	1.266%
2	1.872	23	25	94	rVB	2860813	6939825	100.00%	26.149%
3	4.970	293	296	301	rVB	71802	80364	1.16%	0.303%
4	5.393	331	333	336	rBV	1008214	967403	13.94%	3.645%
5	6.444	422	425	427	rBV	851398	1097456	15.81%	4.135%
6	6.570	434	436	439	rBV	1054524	1089770	15.70%	4.106%
7	6.810	455	457	459	rBV	985388	794021	11.44%	2.992%
8	6.970	468	471	473	rBV	792991	883964	12.74%	3.331%
9	7.370	504	506	509	rBV	737180	646720	9.32%	2.437%
10	8.102	567	570	572	rBV	1031771	1082387	15.60%	4.078%
11	9.176	661	664	666	rBV	1350097	1361542	19.62%	5.130%
12	9.565	696	698	700	rVB	122068	92243	1.33%	0.348%
13	9.850	720	723	724	rBV	1030928	1054195	15.19%	3.972%
14	10.628	789	791	793	rVB	810022	695246	10.02%	2.620%
15	11.325	850	852	853	rBV	1207111	1123187	16.18%	4.232%
16	11.393	856	858	860	rVB	159029	149597	2.16%	0.564%
17	11.816	893	895	897	rBV	47459	78525	1.13%	0.296%
18	11.851	897	898	900	rVB	112606	83077	1.20%	0.313%
19	11.931	903	905	909	rVB2	141776	191294	2.76%	0.721%
20	12.113	920	921	925	rVB2	54588	90336	1.30%	0.340%
21	12.525	955	957	960	rVB	629906	697817	10.06%	2.629%
22	12.674	967	970	974	rBV3	24142	69417	1.00%	0.262%
23	12.754	974	977	980	rBV	708503	782527	11.28%	2.949%
24	12.902	988	990	993	rVB	1202159	1059544	15.27%	3.992%
25	12.971	993	996	1000	rBV3	45570	98810	1.42%	0.372%
26	13.085	1000	1006	1008	rBV	98219	169166	2.44%	0.637%
27	13.154	1008	1012	1013	rBV	59259	96360	1.39%	0.363%
28	13.188	1013	1015	1016	rBV	74245	84325	1.22%	0.318%
29	13.691	1057	1059	1061	rBV2	68193	111649	1.61%	0.421%
30	13.794	1066	1068	1072	rVB3	47932	104540	1.51%	0.394%
31	13.942	1078	1081	1086	rBV3	770351	1542286	22.22%	5.811%
32	14.959	1167	1170	1174	rBV	282205	594515	8.57%	2.240%
33	15.051	1176	1178	1181	rVB2	56257	86322	1.24%	0.325%
34	15.234	1192	1194	1197	rVB	149639	222461	3.21%	0.838%

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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

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35	15.302	1197	1200	1202	rBV	211538	332028	4.78%	1.251%
36	15.360	1202	1205	1211	rVB	660460	930640	13.41%	3.507%
37	16.022	1261	1263	1268	rVB2	59986	130672	1.88%	0.492%
38	16.708	1320	1323	1328	rVB2	106702	197144	2.84%	0.743%
39	17.120	1356	1359	1364	rVB	71443	168124	2.42%	0.633%
40	19.188	1536	1540	1548	rVB3	60775	223660	3.22%	0.843%

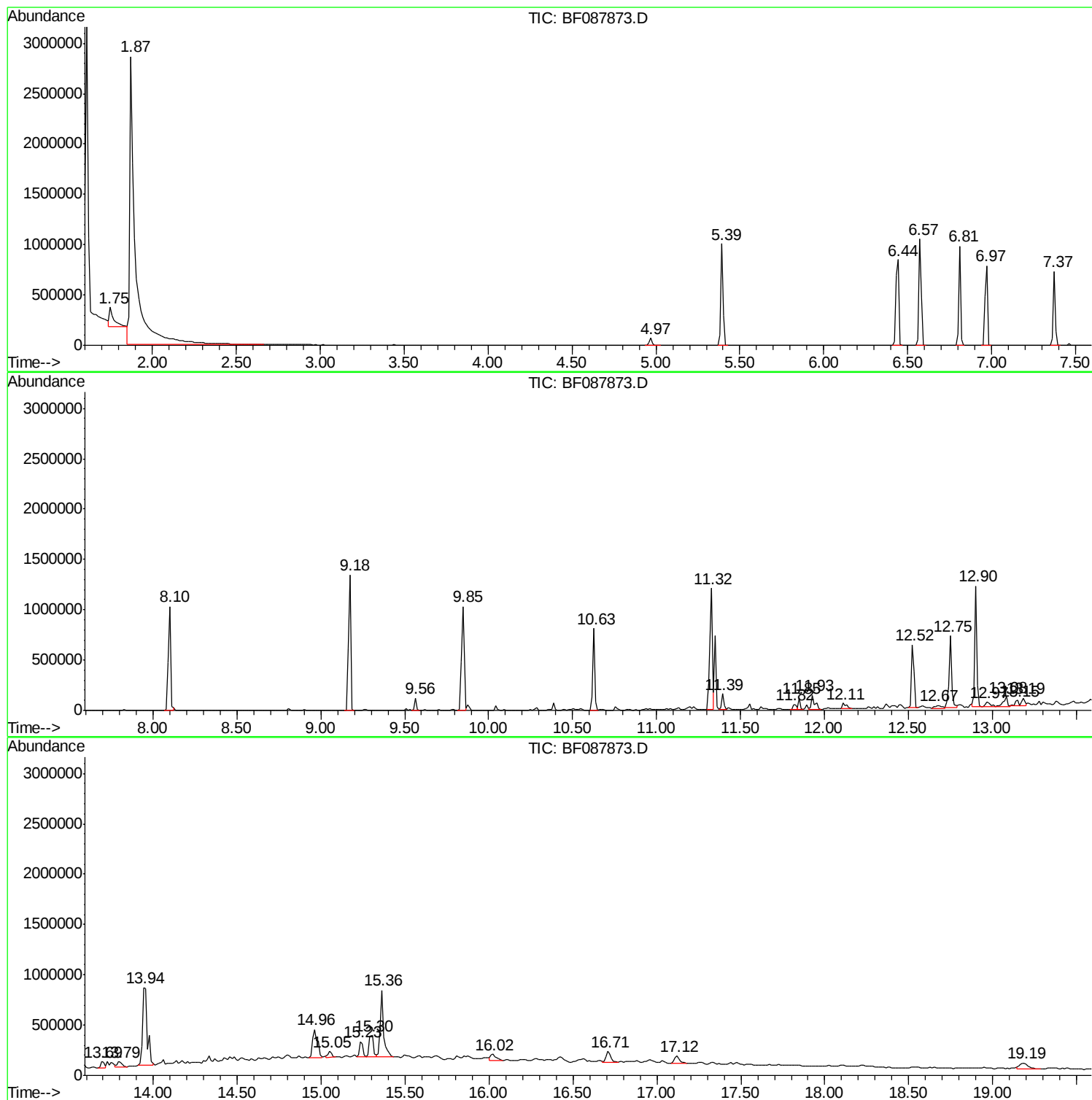
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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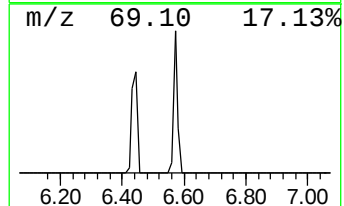
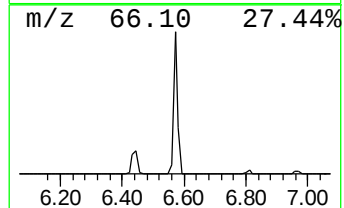
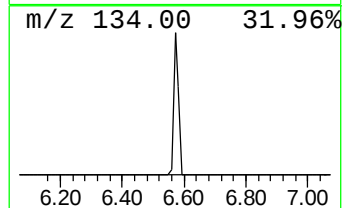
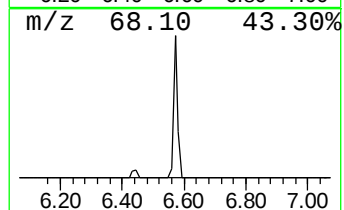
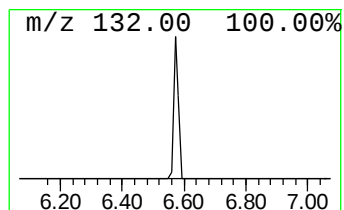
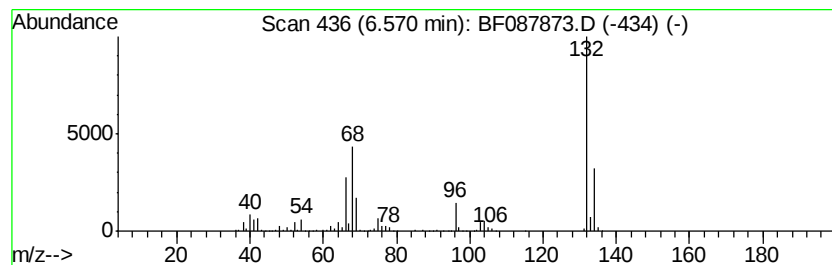
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	24.66 ng	1089770	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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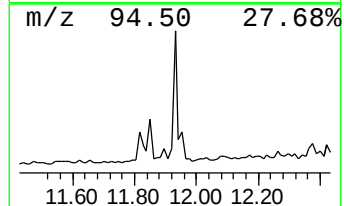
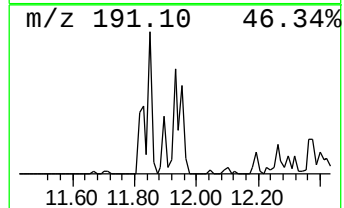
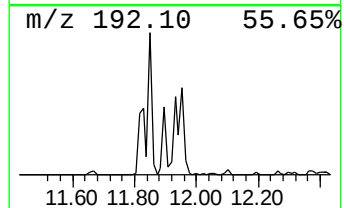
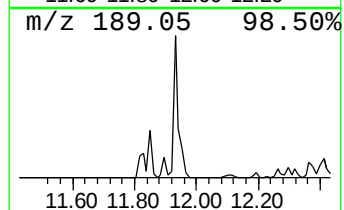
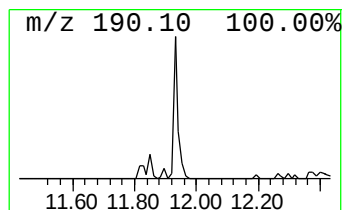
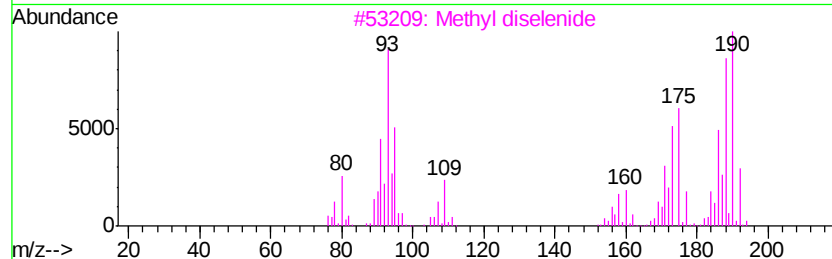
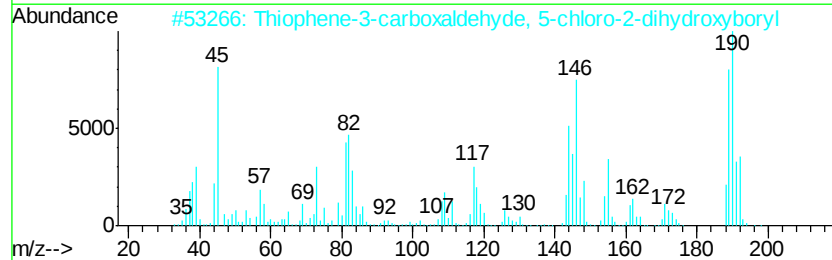
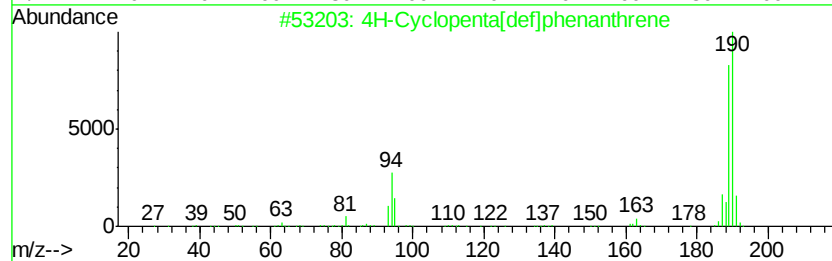
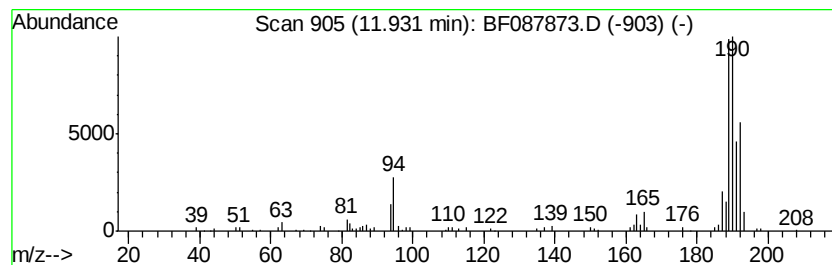
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	3.41 ng	191294	Phenanthrene-d10	11.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2		Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	47
3		Methyl diselenide	190	C2H6Se2	007101-31-7	38
4		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	25
5		Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	18



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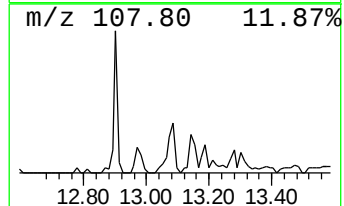
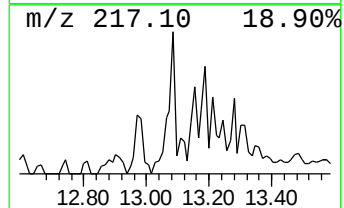
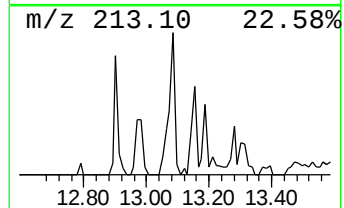
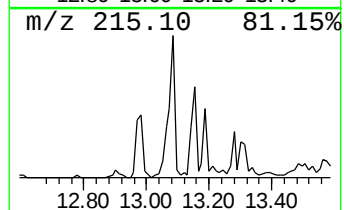
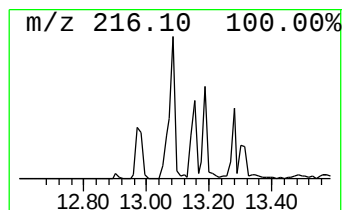
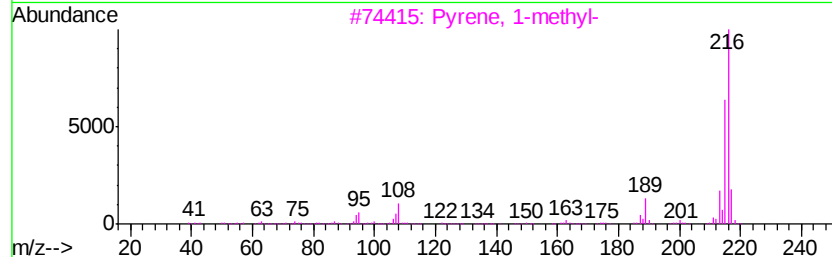
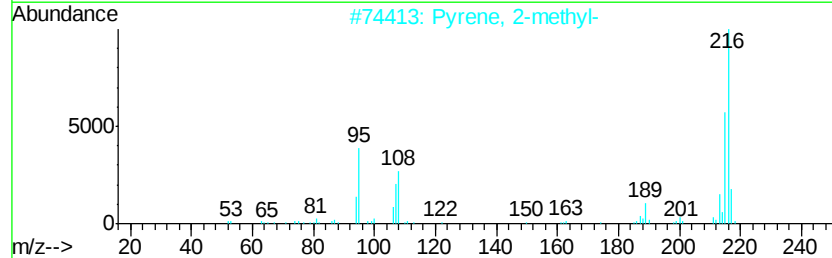
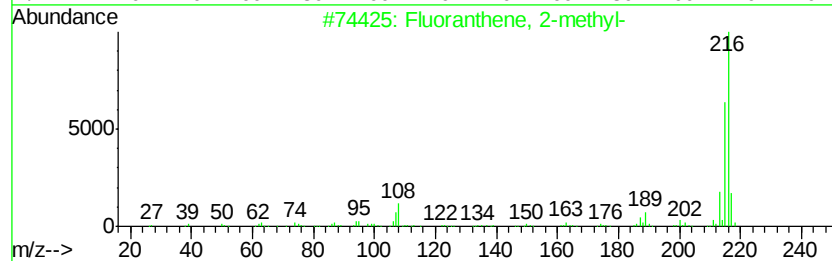
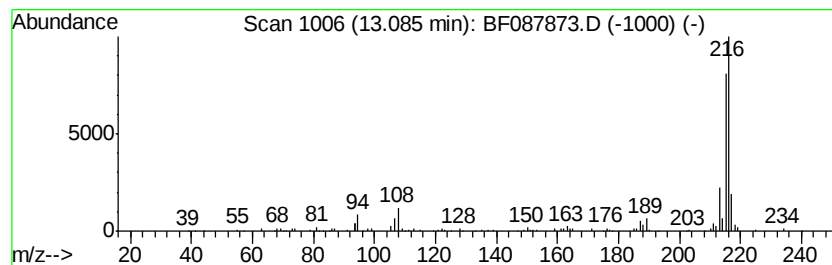
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Fluoranthene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.09	2.19 ng	169166	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
2		Pyrene, 2-methyl-	216	C17H12	003442-78-2	91
3		Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
4		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
5		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87



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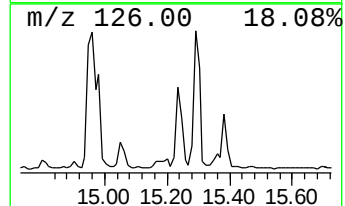
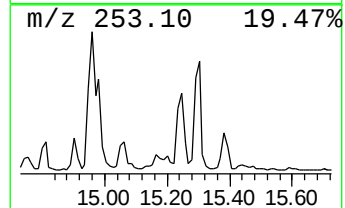
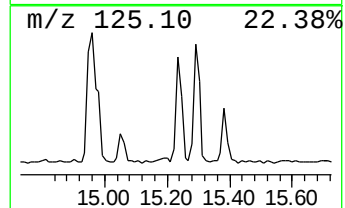
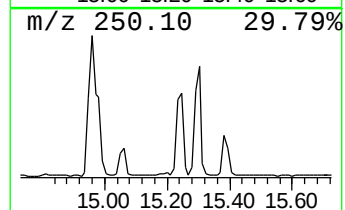
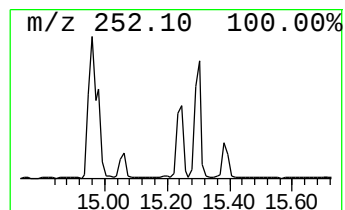
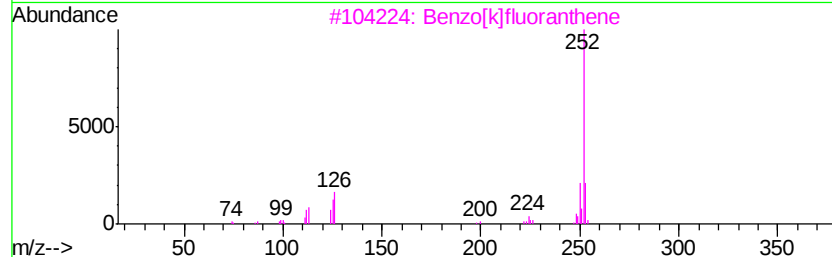
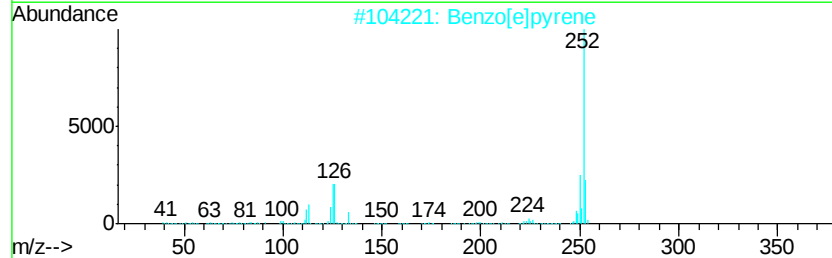
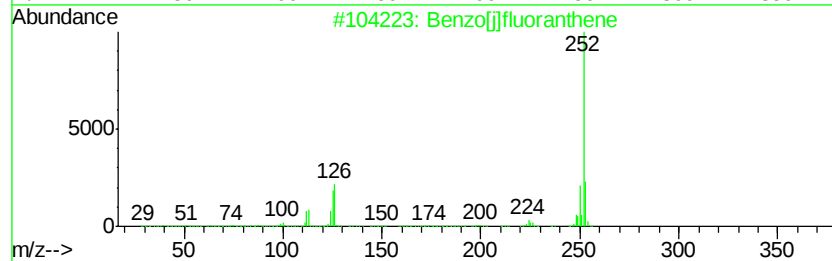
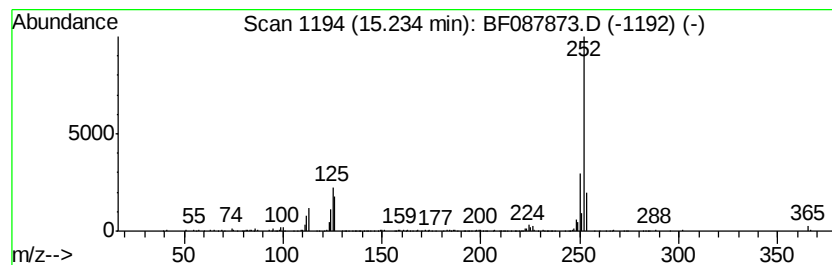
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzo[j]fluoranthene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	4.78 ng	222461	Perylene-d12	15.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[i]fluoranthene	252	C20H12	000205-82-3	98
2		Benzo[e]pyrene	252	C20H12	000192-97-2	98
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
4		Perylene	252	C20H12	000198-55-0	97
5		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96



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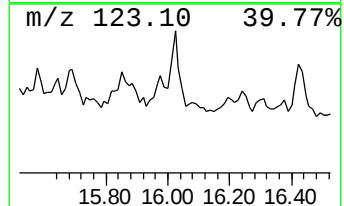
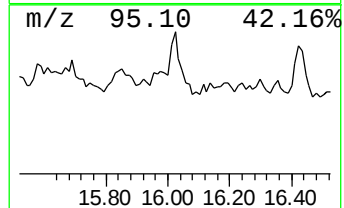
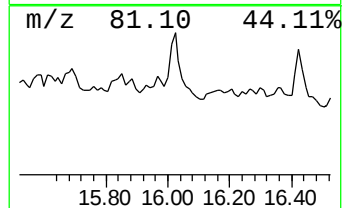
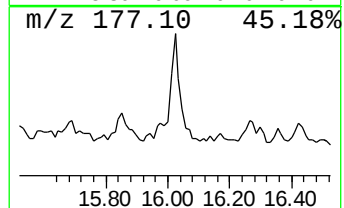
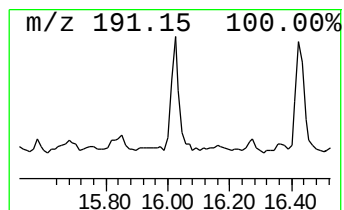
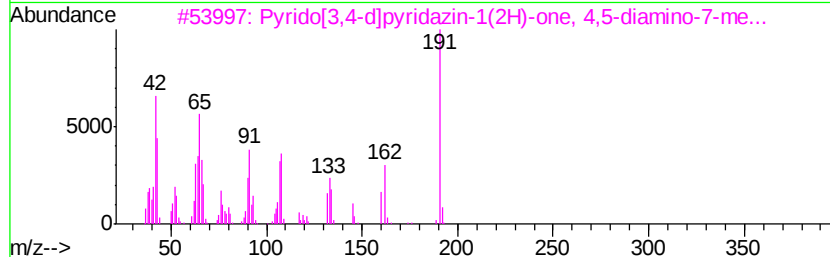
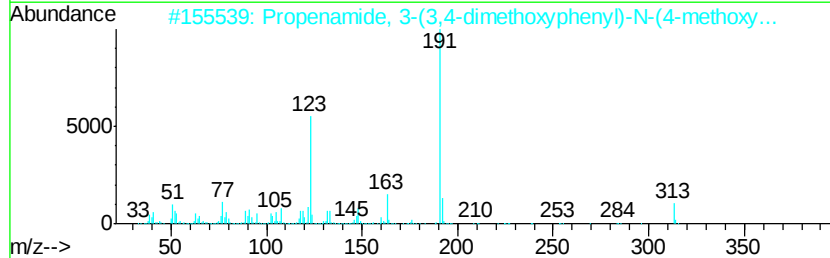
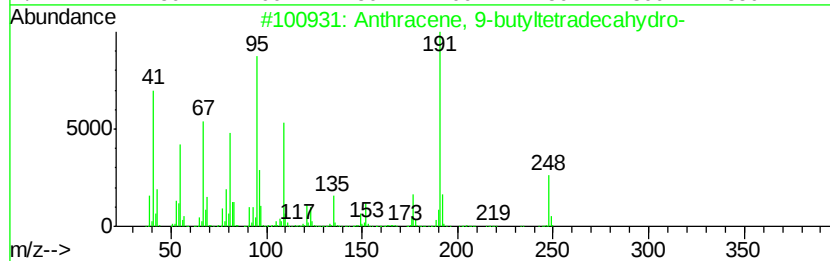
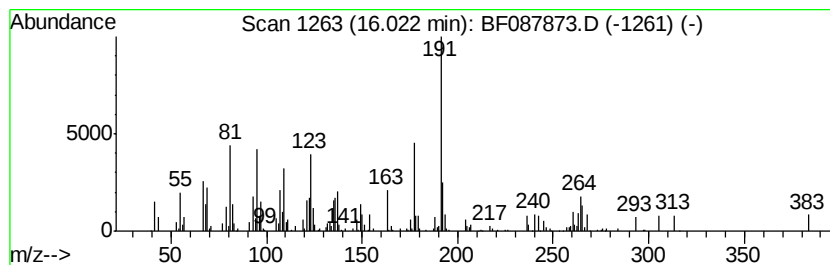
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TIC Library : C:\Database\NIST11.L
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Peak Number 8 unknown16.02 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	2.81 ng	130672	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 9-butyltetradecahydro-	248	C18H32	055133-89-6	38
2		Propenamide, 3-(3,4-dimethoxyphe...	313	C18H19N04	339165-72-9	38
3		Pvrido[3,4-d]pvridazin-1(2H)-one...	191	C8H9N5O	1000263-69-7	35
4		2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	32
5		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	27



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SS-52

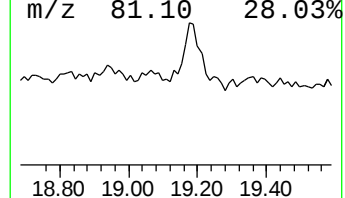
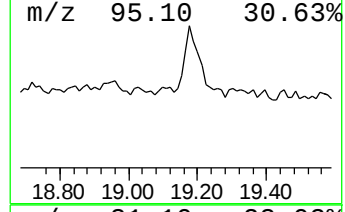
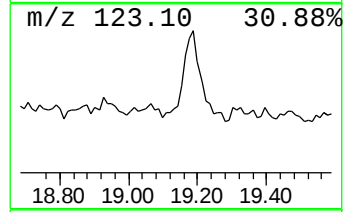
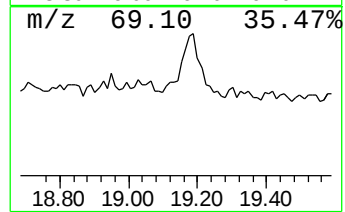
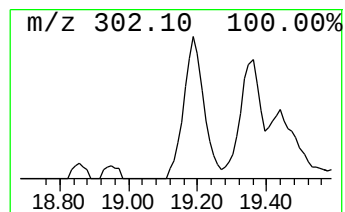
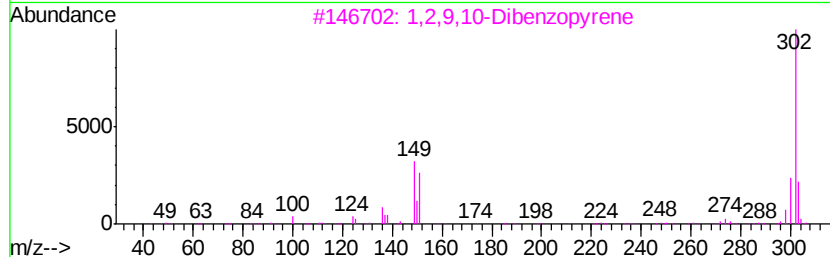
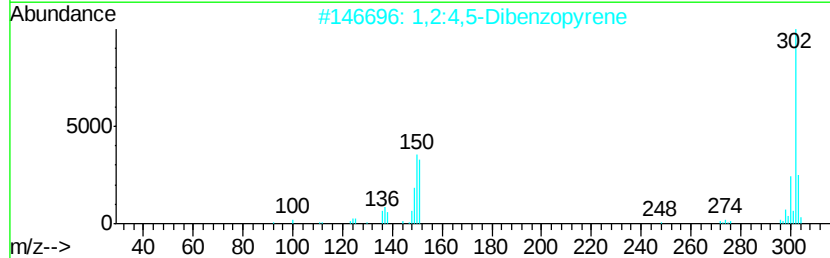
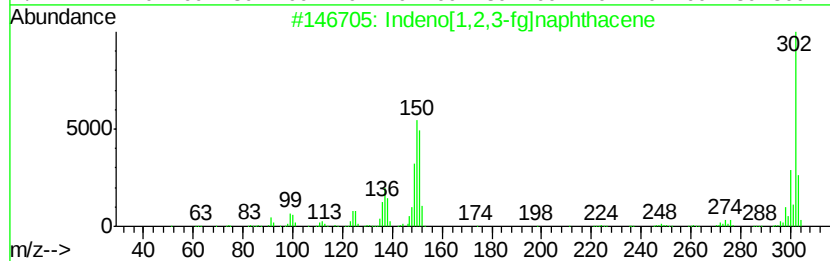
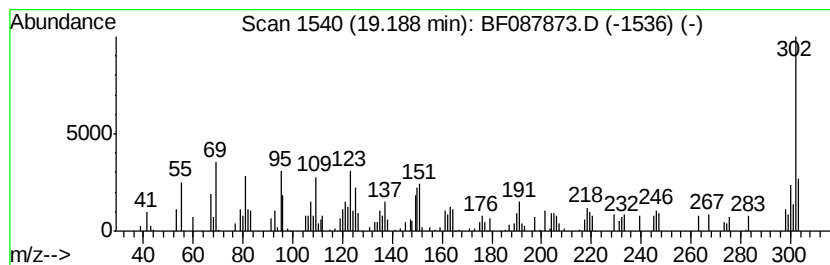
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Indeno[1,2,3-fg]naphthacene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.19	4.81 ng	223660	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indeno[1,2,3-fg]naphthacene	302	C24H14	000203-11-2	64
2		1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	52
3		1,2,9,10-Dibenzopyrene	302	C24H14	000191-30-0	49
4		2H-1-Benzopyran-2-one, 7-(3-meth...	302	C19H14N2O2	006025-18-9	45
5		[1,3]Benzimidazo[2,1-a]phthalazi...	302	C19H18N4	1000319-80-2	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061016\
Data File : BF087873.D
Acq On : 10 Jun 2016 14:32
Operator : UM/SJ
Sample : H3426-06 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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
unknown6.57	6.57	24.7	ng	1089770	1	6.97	883964	20.0
4H-Cyclopenta[def...	11.93	3.4	ng	191294	4	11.32	1123190	20.0
Fluoranthene, 2-m...	13.09	2.2	ng	169166	5	13.95	1542290	20.0
Benzo[j]fluoranthene	15.23	4.8	ng	222461	6	15.36	930640	20.0
unknown16.02	16.02	2.8	ng	130672	6	15.36	930640	20.0
Indeno[1,2,3-fg]n...	19.19	4.8	ng	223660	6	15.36	930640	20.0