

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
 Data File : BF089057.D
 Acq On : 16 Jul 2016 16:10
 Operator : UM/SJ
 Sample : H3989-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 Q7-B200(0-5)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	1.644	4	5	14	rVB	60801	123536	8.34%	0.754%
2	1.770	14	16	46	rVB	575726	1096218	73.99%	6.690%
3	2.787	104	105	115	rBV	6478	18014	1.22%	0.110%
4	4.810	279	282	287	rBV	101616	167501	11.31%	1.022%
5	5.256	319	321	324	rBV	1149591	1330243	89.79%	8.118%
6	6.319	411	414	417	rBV	1231123	1345493	90.82%	8.211%
7	6.433	422	424	427	rBB	1361850	1347671	90.97%	8.224%
8	6.662	442	444	446	rBB	462061	364357	24.59%	2.224%
9	6.822	455	458	460	rBB	1370706	1220852	82.41%	7.451%
10	7.233	491	494	496	rBV	944445	946230	63.87%	5.775%
11	7.953	554	557	559	rBV	393792	458620	30.96%	2.799%
12	9.028	648	651	654	rBV	1597127	1481482	100.00%	9.041%
13	9.428	683	686	688	rVB	373123	300628	20.29%	1.835%
14	9.702	707	710	712	rBV	552392	476351	32.15%	2.907%
15	10.148	748	749	751	rVB	22487	18016	1.22%	0.110%
16	10.239	753	757	761	rVV2	9276	17740	1.20%	0.108%
17	10.491	776	779	781	rBV	684592	706980	47.72%	4.315%
18	10.616	789	790	794	rVB	22737	38737	2.61%	0.236%
19	10.708	797	798	800	rVB2	14286	19094	1.29%	0.117%
20	10.742	800	801	803	rBV2	12227	16150	1.09%	0.099%
21	11.074	828	830	831	rBV2	22515	29193	1.97%	0.178%
22	11.176	837	839	843	rVB2	447202	536748	36.23%	3.276%
23	11.256	843	846	848	rBV2	30290	44623	3.01%	0.272%
24	11.496	864	867	870	rVB2	21758	27793	1.88%	0.170%
25	11.679	881	883	884	rBV	31106	25649	1.73%	0.157%
26	11.702	884	885	888	rVV	32113	36156	2.44%	0.221%
27	11.759	888	890	891	rVB	52981	65256	4.40%	0.398%
28	11.782	891	892	897	rVB	34393	62436	4.21%	0.381%
29	11.896	897	902	906	rBV2	17923	26824	1.81%	0.164%
30	11.999	907	911	913	rVB2	20332	35082	2.37%	0.214%
31	12.228	929	931	932	rBV	22515	21935	1.48%	0.134%
32	12.308	937	938	941	rBV2	16076	20152	1.36%	0.123%
33	12.388	943	945	947	rBV	263581	276393	18.66%	1.687%
34	12.457	947	951	952	rBV3	28455	64334	4.34%	0.393%

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35	12.525	955	957	960	rBV4	31071	39412	2.66%	0.241%
36	12.605	962	964	966	rBV2	203766	278432	18.79%	1.699%
37	12.651	966	968	972	rVB3	26592	49951	3.37%	0.305%
38	12.765	976	978	980	rVB	1166804	1044783	70.52%	6.376%
39	12.834	980	984	985	rBV2	19390	22762	1.54%	0.139%
40	12.914	988	991	992	rBV2	24876	50053	3.38%	0.305%
41	12.948	992	994	996	rVB	26280	40667	2.75%	0.248%
42	13.005	997	999	1001	rVB2	26273	27435	1.85%	0.167%
43	13.039	1001	1002	1008	rBV2	28457	68744	4.64%	0.420%
44	13.131	1008	1010	1012	rVB	18357	19630	1.33%	0.120%
45	13.165	1012	1013	1014	rBV	26189	24900	1.68%	0.152%
46	13.199	1014	1016	1017	rBV	38076	46398	3.13%	0.283%
47	13.554	1045	1047	1048	rBV	28388	33448	2.26%	0.204%
48	13.679	1056	1058	1061	rVB2	54154	64410	4.35%	0.393%
49	13.805	1066	1069	1073	rBV2	451893	661236	44.63%	4.035%
50	14.800	1154	1156	1160	rBV	114788	208440	14.07%	1.272%
51	15.062	1177	1179	1182	rVB	75754	101771	6.87%	0.621%
52	15.120	1182	1184	1187	rVV	79360	116284	7.85%	0.710%
53	15.177	1187	1189	1198	rVB	207083	328556	22.18%	2.005%
54	16.171	1274	1276	1284	rVB2	44235	89313	6.03%	0.545%
55	16.846	1332	1335	1340	rBV	31317	78206	5.28%	0.477%
56	17.028	1349	1351	1352	rBV2	25811	30115	2.03%	0.184%
57	17.086	1355	1356	1357	rVB	46560	31940	2.16%	0.195%
58	18.286	1459	1461	1462	rVB2	37286	27897	1.88%	0.170%
59	18.503	1479	1480	1482	rBV2	17853	19539	1.32%	0.119%
60	18.823	1506	1508	1511	rVB4	37548	60638	4.09%	0.370%
61	18.937	1516	1518	1520	rVB3	41900	54691	3.69%	0.334%

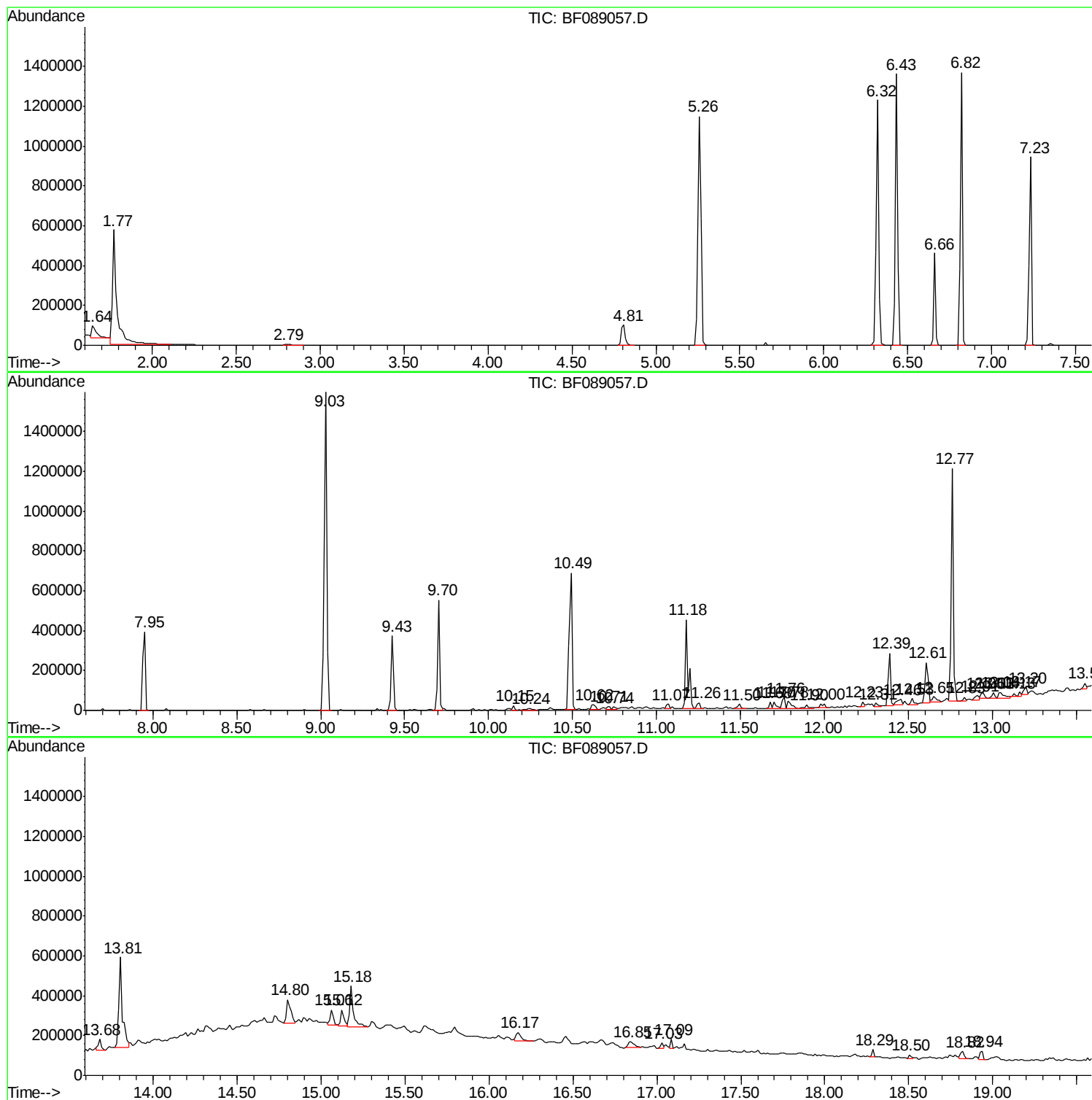
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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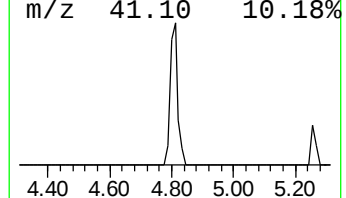
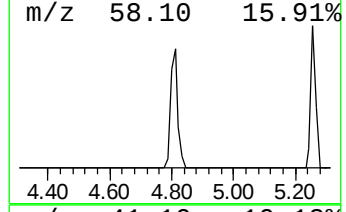
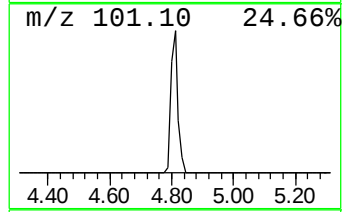
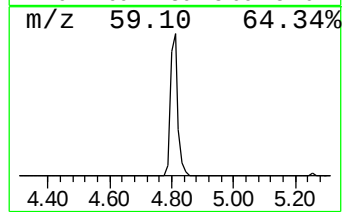
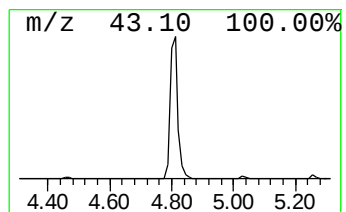
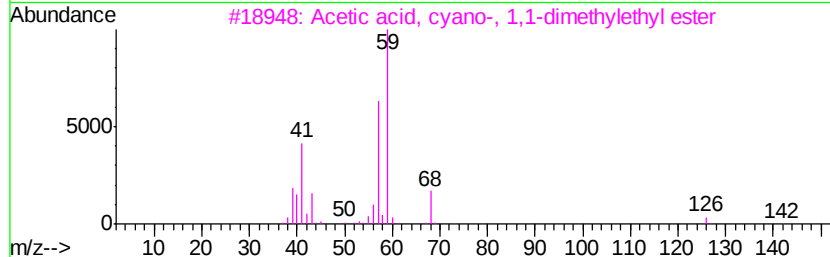
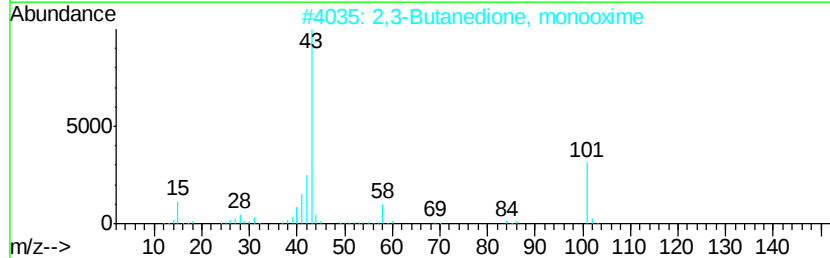
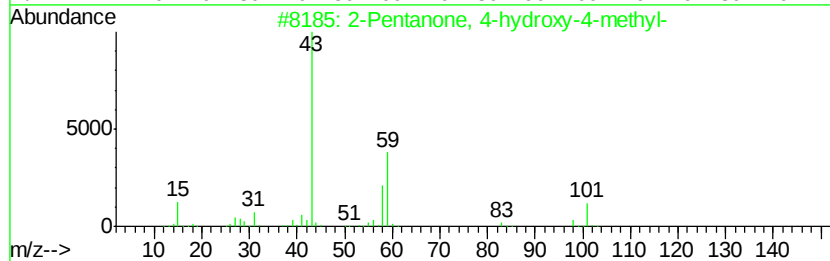
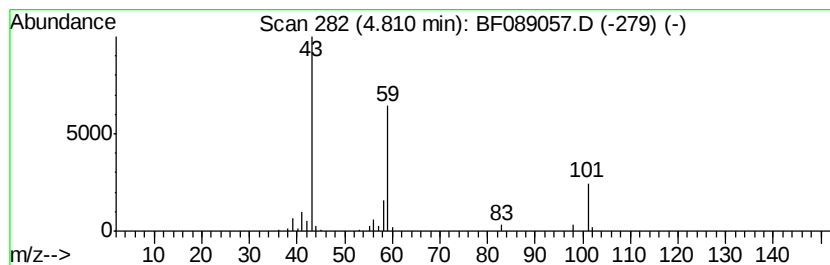
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	9.19 ng	167501	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Acetone	58	C3H6O	000067-64-1	10
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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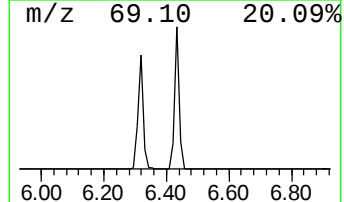
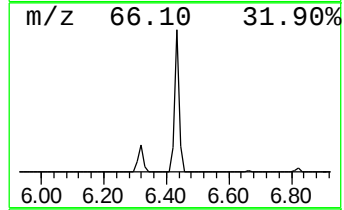
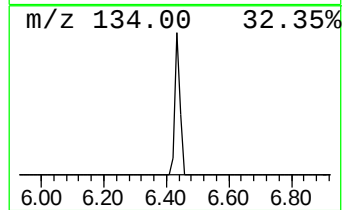
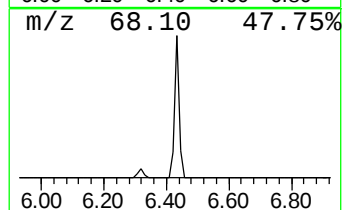
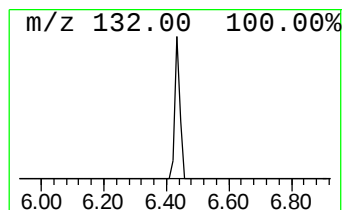
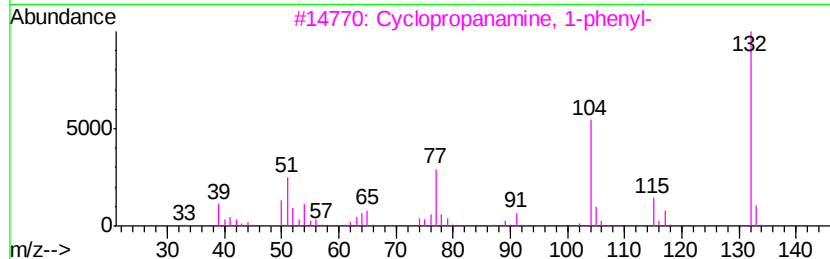
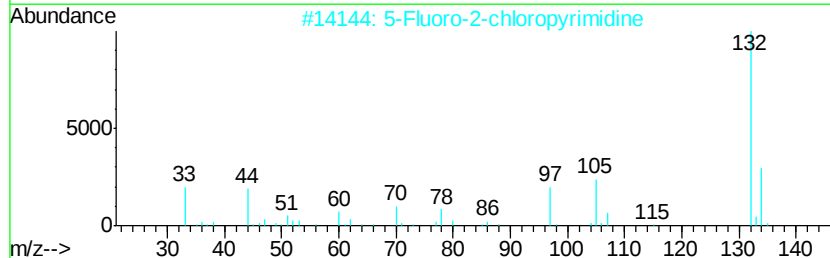
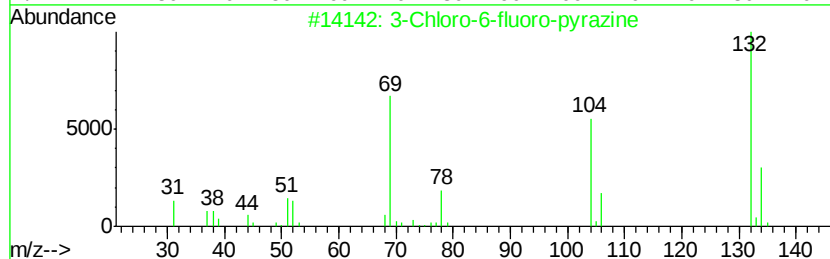
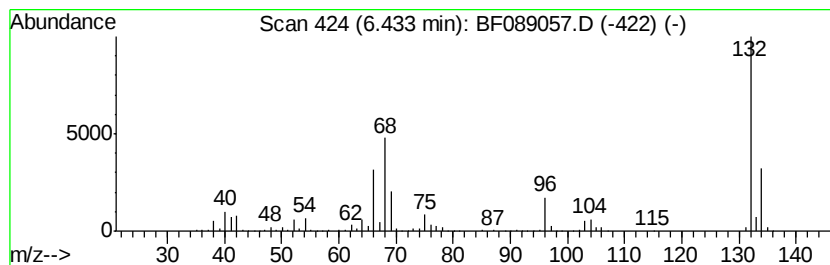
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.43 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	73.98 ng	1347670	1,4-Dichlorobenzene-d4	6.66

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		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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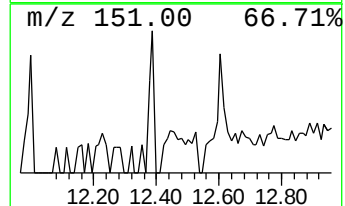
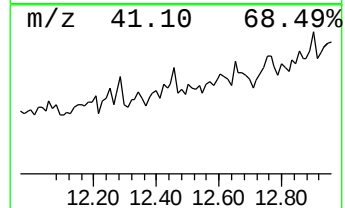
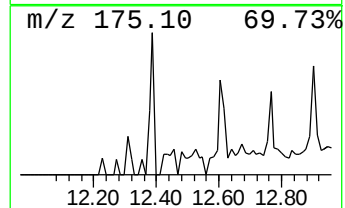
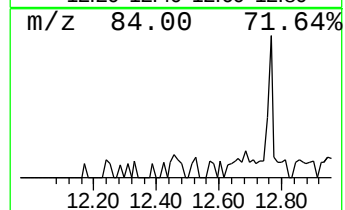
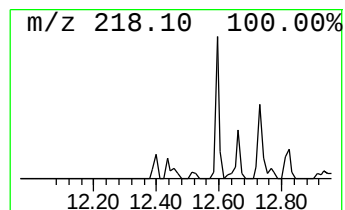
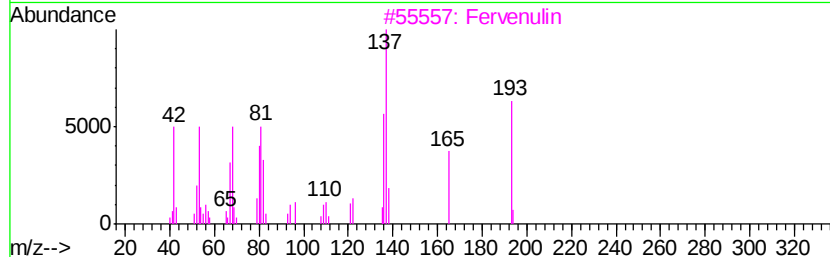
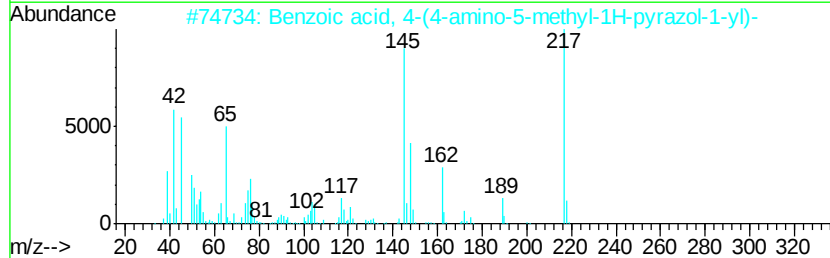
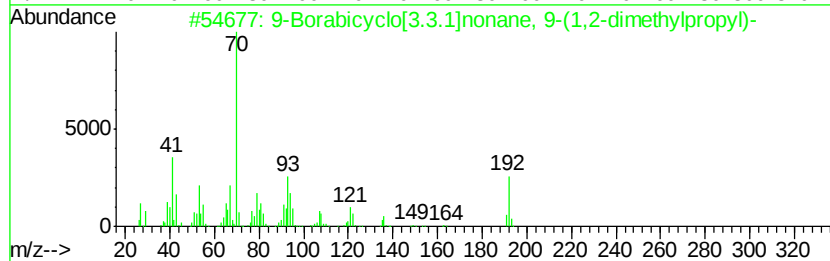
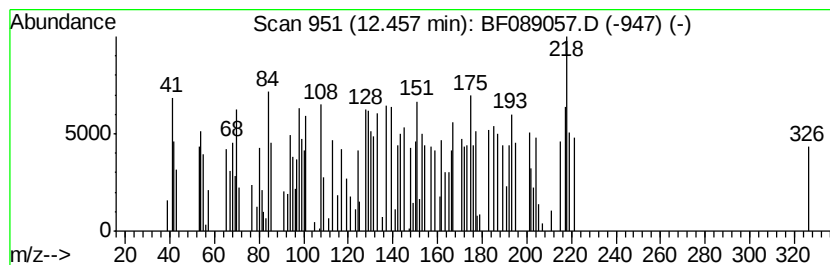
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 unknown12.46 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	2.40 ng	64334	Phenanthrene-d10	11.18

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Borabicyclo[3.3.1]nonane, 9-(1...	192	C13H25B	063942-78-9	14		
2	Benzoic acid, 4-(4-amino-5-methy...	217	C11H11N3O2	1000351-42-4	14		
3	Fervenulin	193	C7H7N5O2	000483-57-8	11		
4	Pyrazole-3-carboxaldehyde, 4-nit...	156	C4H4N4O3	1000267-55-1	11		
5	9-Borabicyclo[3.3.1]nonane, 9-me...	168	C9H17BS	1000154-59-5	11		



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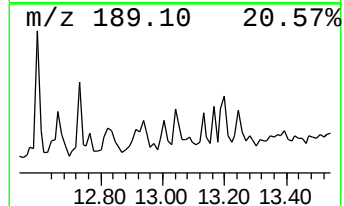
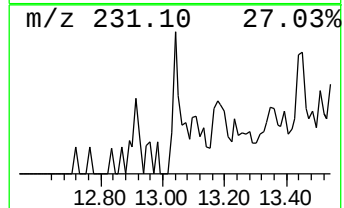
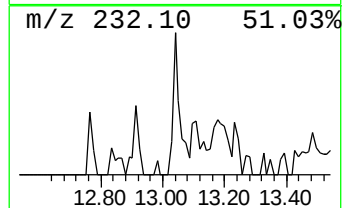
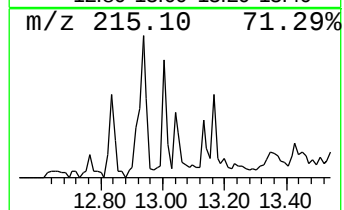
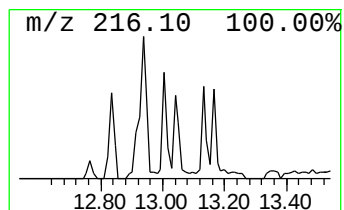
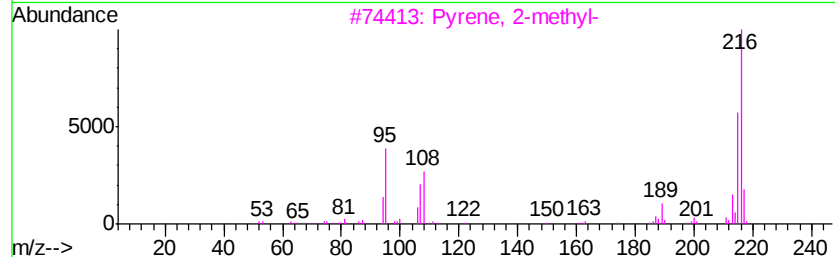
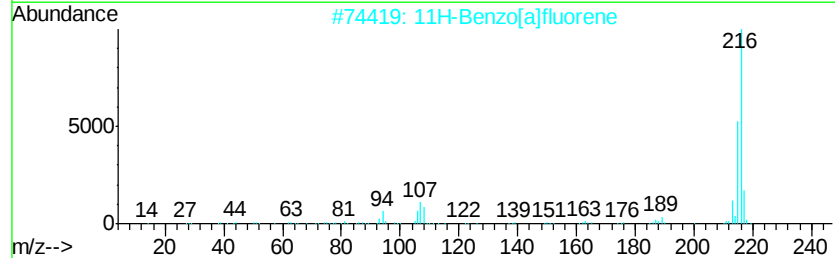
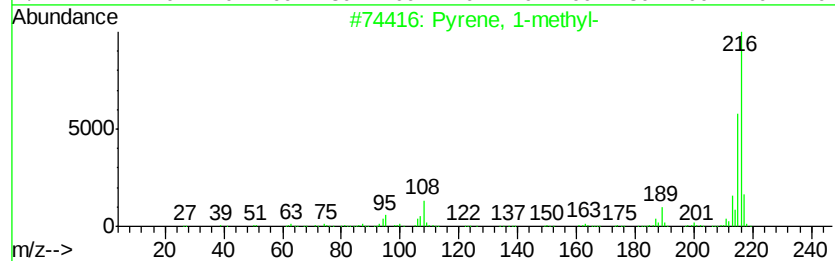
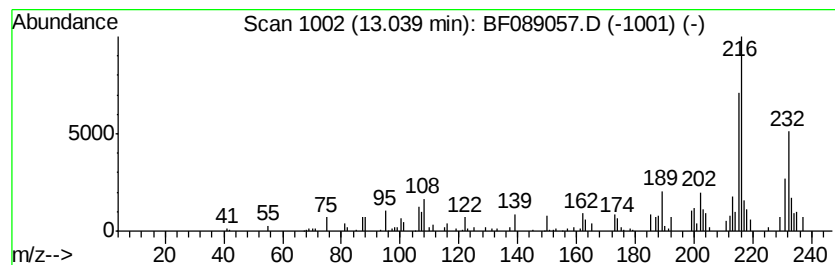
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Peak Number 7 Pyrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.04	2.08 ng	68744	Chrysene-d12	13.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	55
3	Pyrene, 2-methyl-	216	C17H12	003442-78-2	55
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	55
5	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	50



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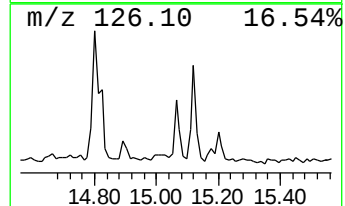
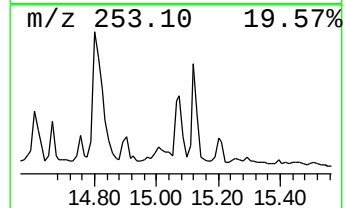
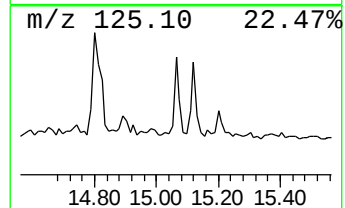
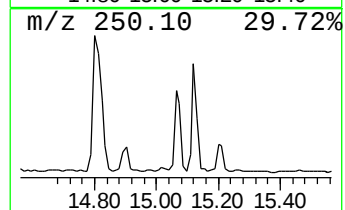
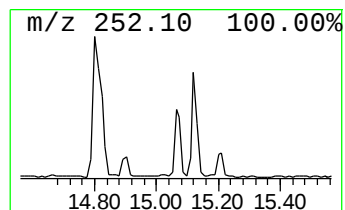
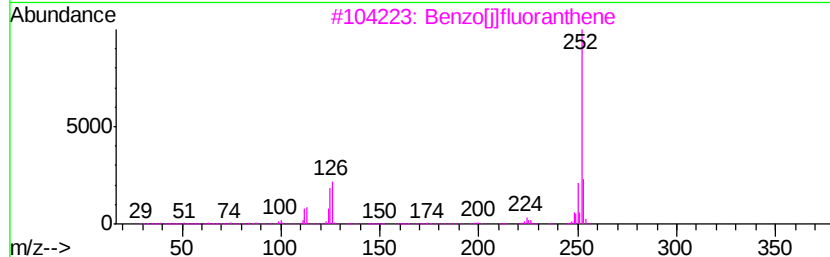
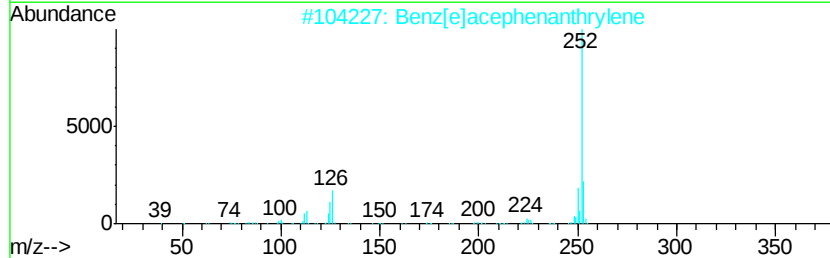
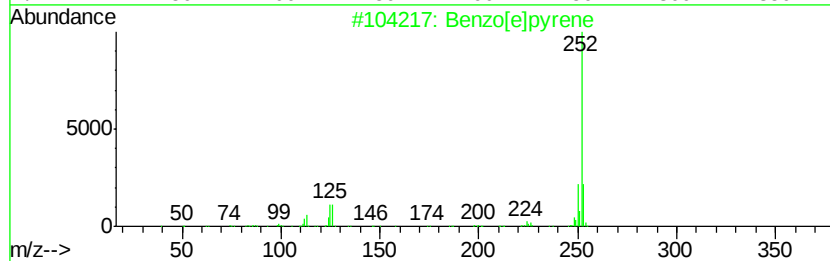
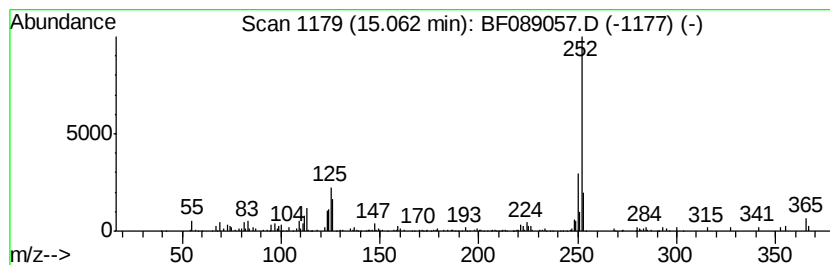
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	6.20 ng	101771	Perylene-d12	15.18

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	96
2		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	95
3		Benzo[i]fluoranthene	252	C20H12	000205-82-3	94
4		Perylene	252	C20H12	000198-55-0	93
5		Benzo[a]pyrene	252	C20H12	000050-32-8	89



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089057.D
Acq On : 16 Jul 2016 16:10
Operator : UM/SJ
Sample : H3989-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q7-B200(0-5)C

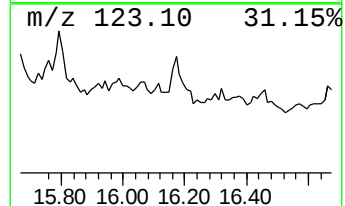
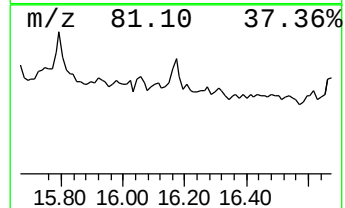
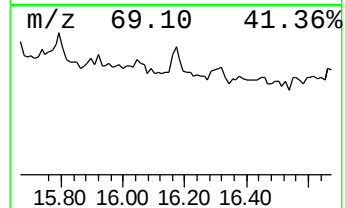
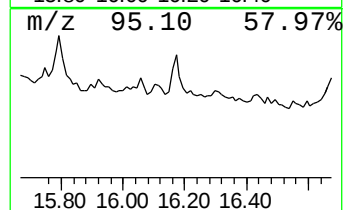
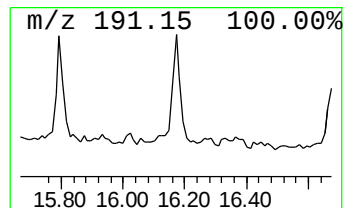
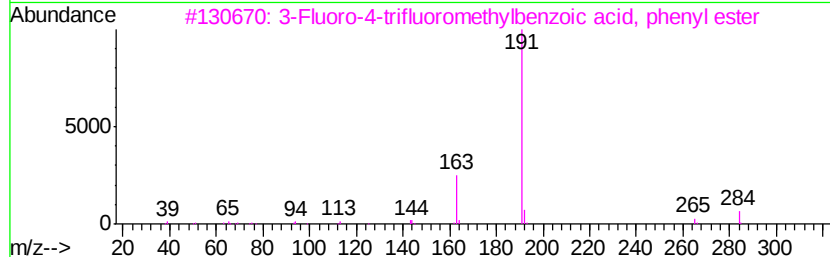
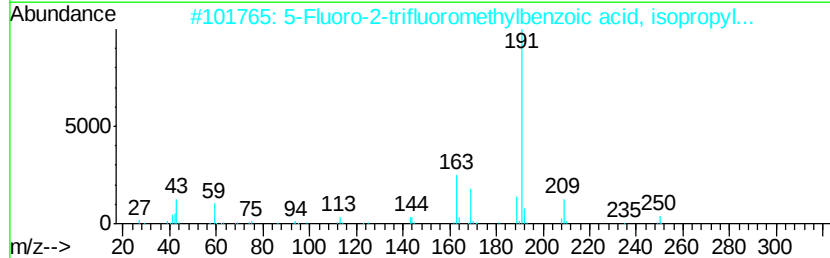
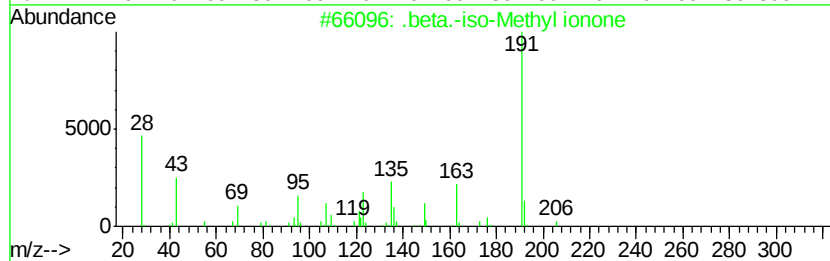
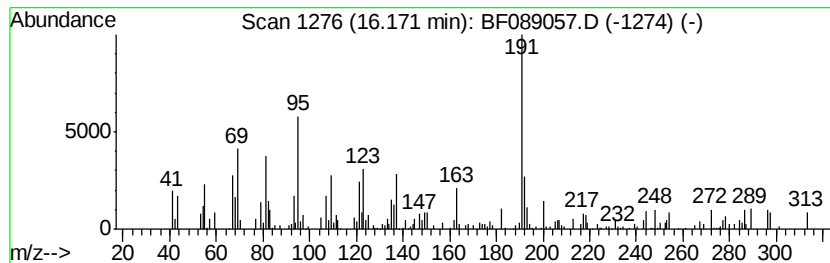
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 .beta.-iso-Methyl ionone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	5.44 ng	89313	Perylene-d12	15.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	58
2		5-Fluoro-2-trifluoromethylbenzoi...	250	C11H10F4O2	1000357-62-3	41
3		3-Fluoro-4-trifluoromethylbenzoi...	284	C14H8F4O2	1000357-93-7	38
4		2'-Fluoro-6'-(trifluoromethyl)-a...	206	C9H6F4O	174013-29-7	35
5		5-Fluoro-2-trifluoromethylbenzoi...	284	C14H8F4O2	1000357-62-7	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071616\
Data File : BF089057.D
Acq On : 16 Jul 2016 16:10
Operator : UM/SJ
Sample : H3989-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q7-B200(0-5)C

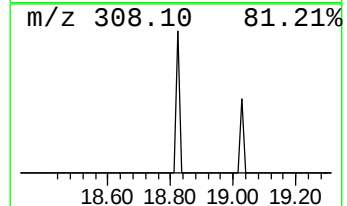
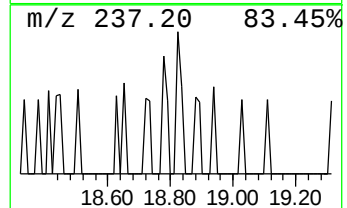
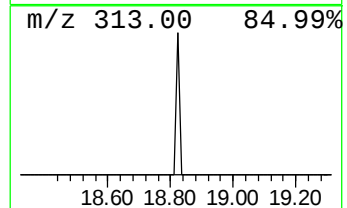
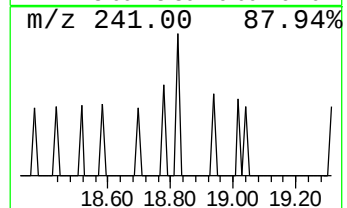
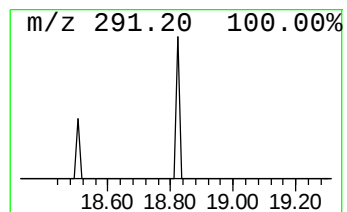
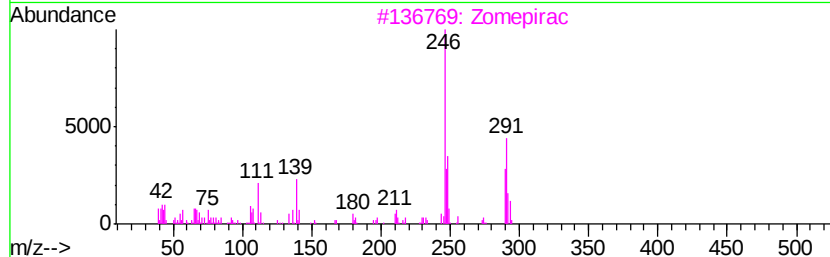
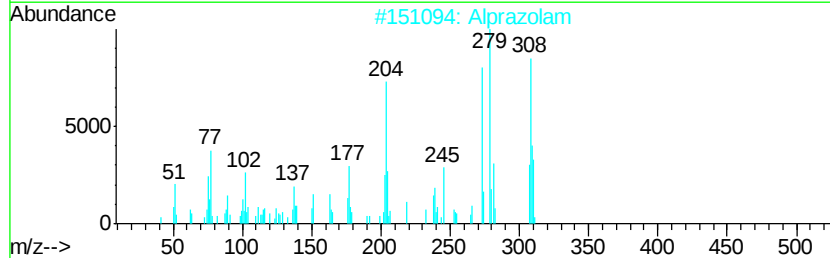
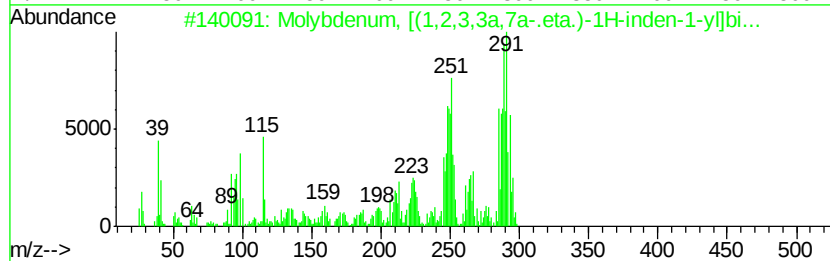
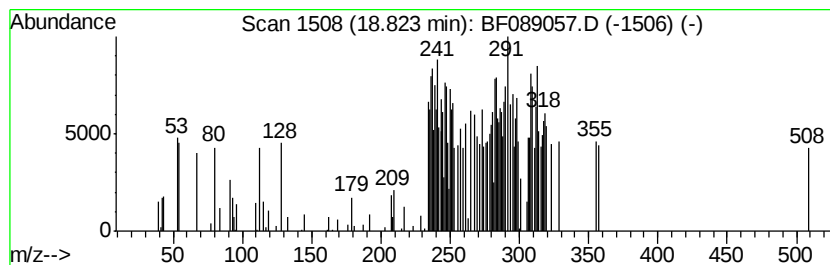
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown18.82 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.82	3.69 ng	60638	Perylene-d12	15.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Molybdenum, [(1,2,3,3a,7a-.eta.)...	295	C15H17Mo	125312-24-5	11
2		Alprazolam	308	C17H13ClN4	028981-97-7	11
3		Zomepirac	291	C15H14ClN3	033369-31-2	10
4		Pirimiphos methyl	305	C11H20N3O3PS	029232-93-7	10
5		2-Oxo-4,6-di(2-methoxyphenyl)-1,...	308	C18H16N2O3	1000070-57-0	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089057.D
Acq On : 16 Jul 2016 16:10
Operator : UM/SJ
Sample : H3989-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q7-B200(0-5)C

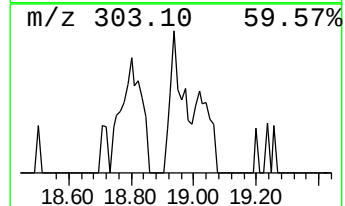
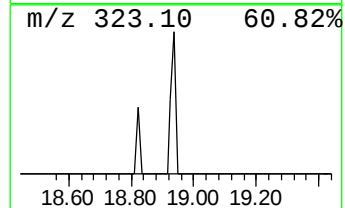
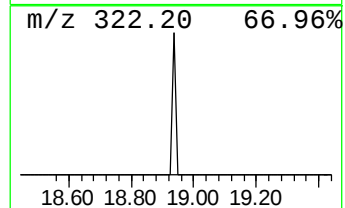
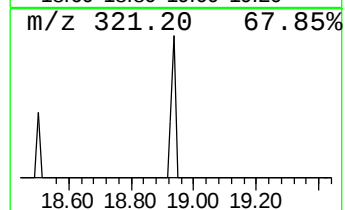
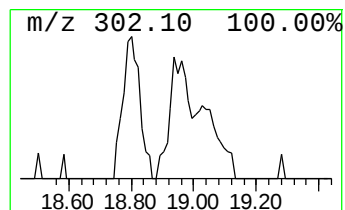
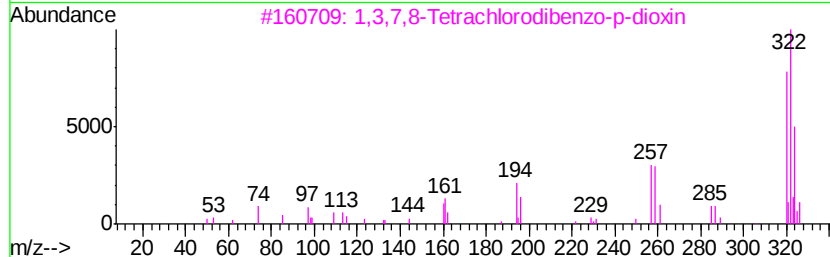
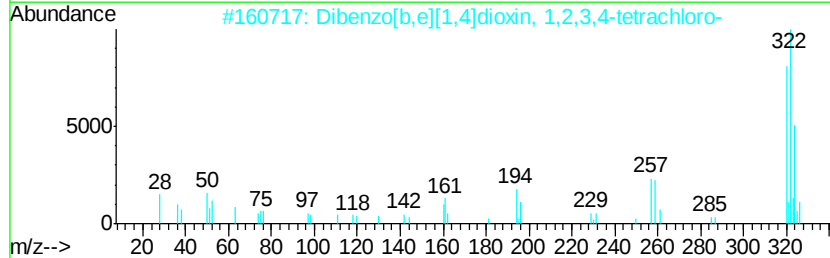
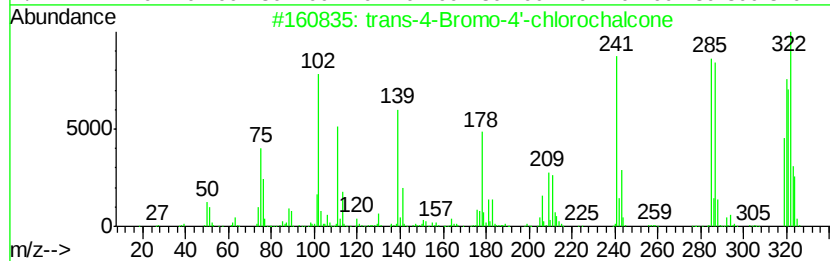
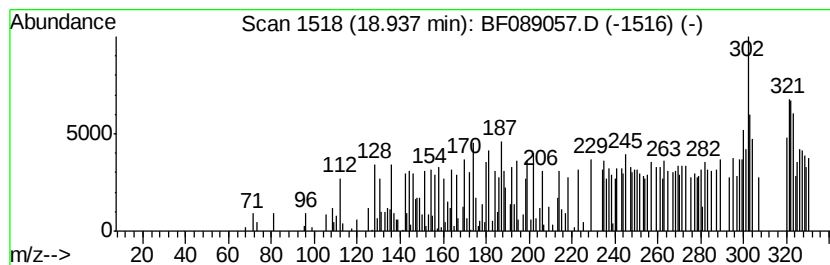
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 trans-4-Bromo-4'-chlorochal... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.94	3.33 ng	54691	Perylene-d12	15.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	trans-4-Bromo-4'-chlorochalcone	320	C15H10BrClO	019672-61-8	64
2		Dibenzo[b,e][1,4]dioxin, 1,2,3,4...	320	C12H4Cl4O2	030746-58-8	25
3		1,3,7,8-Tetrachlorodibenzo-p-dioxin	320	C12H4Cl4O2	050585-46-1	15
4		Imidazole, 2,5-dibromo-4-phenyl-	300	C9H6Br2N2	1000124-11-5	14
5		5H-Indano[1,2-c]pyridazin-5-one,...	302	C18H10N2O3	329720-51-6	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071616\
Data File : BF089057.D
Acq On : 16 Jul 2016 16:10
Operator : UM/SJ
Sample : H3989-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q7-B200(0-5)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...	4.81	9.2	ng	167501	1	6.66	364357	20.0
unknown6.43	6.43	74.0	ng	1347670	1	6.66	364357	20.0
unknown12.46	12.46	2.4	ng	64334	4	11.18	536748	20.0
Pyrene, 1-methyl-	13.04	2.1	ng	68744	5	13.81	661236	20.0
Benzo[e]pyrene	15.06	6.2	ng	101771	6	15.18	328556	20.0
.beta.-iso-Methyl...	16.17	5.4	ng	89313	6	15.18	328556	20.0
unknown18.82	18.82	3.7	ng	60638	6	15.18	328556	20.0
trans-4-Bromo-4'-...	18.94	3.3	ng	54691	6	15.18	328556	20.0