

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
 Data File : BF099165.D
 Acq On : 6 Oct 2017 23:31
 Operator : SJ/JU
 Sample : I5516-02
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PZ-6

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-BF092317.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	2.163	8	13	22	rVB	521634	686375	19.08%	2.536%
2	5.087	506	510	524	rVB	211896	256598	7.13%	0.948%
3	5.481	573	577	581	rBV	1719667	1536116	42.71%	5.676%
4	6.487	744	748	755	rVB	1162134	978787	27.21%	3.616%
5	6.634	768	773	776	rBV	2837880	2676401	74.41%	9.889%
6	6.863	808	812	815	rBV	939262	761547	21.17%	2.814%
7	7.022	834	839	842	rVB	2583552	2469301	68.66%	9.123%
8	7.428	901	908	911	rBV	2013758	2044228	56.84%	7.553%
9	7.657	941	947	949	rBV	33247	43856	1.22%	0.162%
10	8.045	1007	1013	1016	rBV2	45799	70097	1.95%	0.259%
11	8.145	1025	1030	1033	rBV	1155990	1062404	29.54%	3.925%
12	8.322	1057	1060	1067	rVB5	28553	47787	1.33%	0.177%
13	8.516	1088	1093	1099	rBV4	48609	78486	2.18%	0.290%
14	8.675	1114	1120	1123	rBV2	39570	57490	1.60%	0.212%
15	8.851	1147	1150	1153	rBV3	41919	56874	1.58%	0.210%
16	8.963	1165	1169	1171	rBV3	39881	47809	1.33%	0.177%
17	8.986	1171	1173	1179	rVB2	72604	94446	2.63%	0.349%
18	9.128	1194	1197	1199	rBV2	42082	37024	1.03%	0.137%
19	9.175	1202	1205	1208	rBV2	76733	65599	1.82%	0.242%
20	9.222	1208	1213	1216	rBV	3471287	3596680	100.00%	13.289%
21	9.316	1226	1229	1232	rBV3	48330	50297	1.40%	0.186%
22	9.380	1238	1240	1242	rBV2	34906	37292	1.04%	0.138%
23	9.410	1243	1245	1248	rVB3	39131	40659	1.13%	0.150%
24	9.463	1251	1254	1256	rBV	53069	44574	1.24%	0.165%
25	9.522	1259	1264	1267	rBV4	70937	118860	3.30%	0.439%
26	9.610	1277	1279	1283	rVB2	112258	95898	2.67%	0.354%
27	9.710	1291	1296	1300	rBV6	88057	152928	4.25%	0.565%
28	9.822	1309	1315	1319	rBV7	65584	137749	3.83%	0.509%
29	9.898	1324	1328	1332	rVV	1296230	1167834	32.47%	4.315%
30	9.945	1332	1336	1338	rVV4	54852	57440	1.60%	0.212%
31	10.151	1368	1371	1376	rBV4	69308	91571	2.55%	0.338%
32	10.198	1376	1379	1382	rVV3	44839	53915	1.50%	0.199%
33	10.239	1382	1386	1391	rVB4	91614	126124	3.51%	0.466%
34	10.316	1397	1399	1403	rVB4	62364	65048	1.81%	0.240%

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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	10.451	1419	1422	1425	rBV2	85319	86452	2.40%	0.319%
36	10.692	1458	1463	1466	rBV	1899592	1924433	53.51%	7.110%
37	10.792	1477	1480	1486	rVB	49958	54444	1.51%	0.201%
38	11.386	1577	1581	1584	rBV	1333074	1118872	31.11%	4.134%
39	11.904	1666	1669	1673	rBV	92155	95486	2.65%	0.353%
40	12.686	1800	1802	1809	rBV3	45044	53477	1.49%	0.198%
41	12.974	1845	1851	1854	rBV	3053019	3261630	90.68%	12.051%
42	13.557	1947	1950	1953	rVB	150895	121738	3.38%	0.450%
43	14.021	2025	2029	2033	rBV	807544	747749	20.79%	2.763%
44	15.498	2275	2280	2288	rVB	471790	609942	16.96%	2.254%
45	16.433	2432	2439	2445	rVB3	21864	42573	1.18%	0.157%
46	17.721	2654	2658	2670	rVB6	14549	40505	1.13%	0.150%

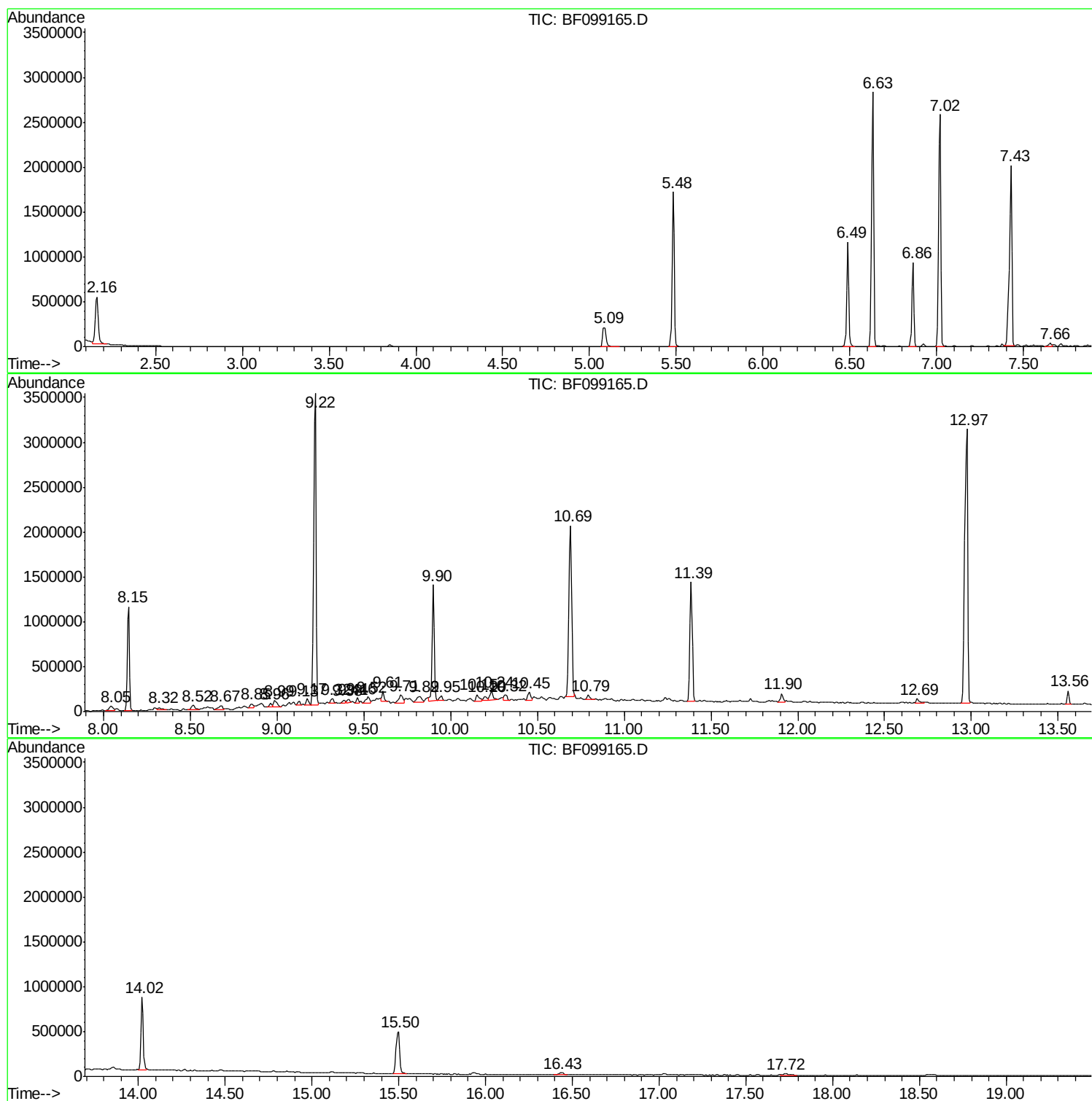
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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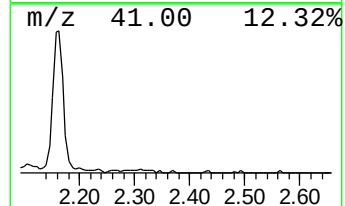
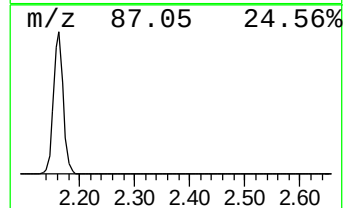
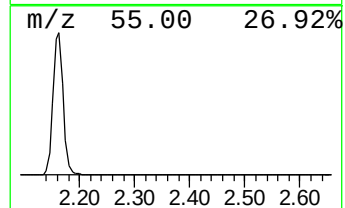
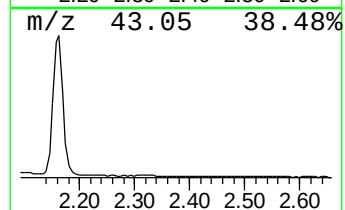
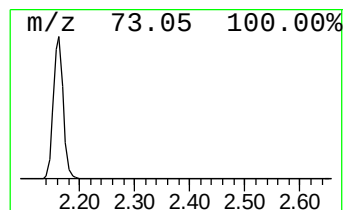
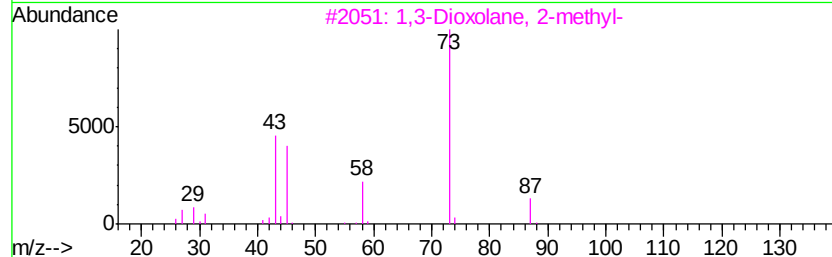
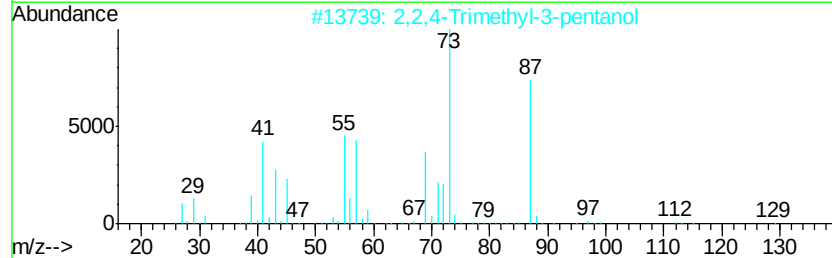
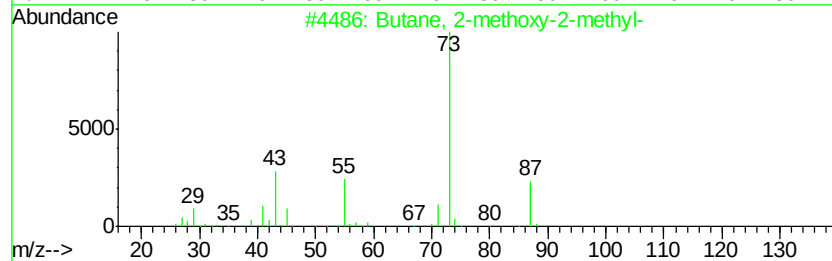
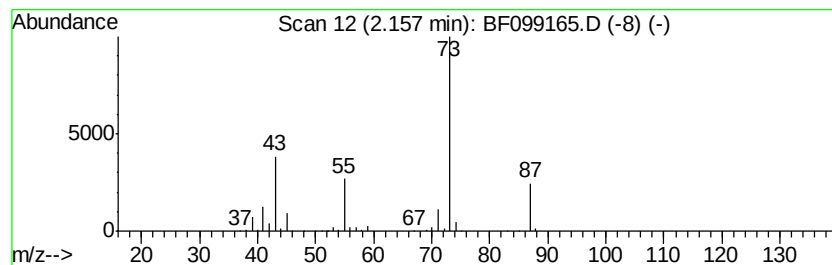
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	18.03 ng	686375	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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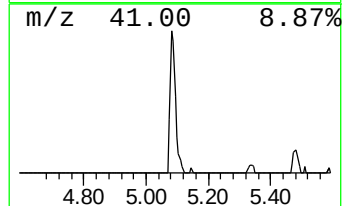
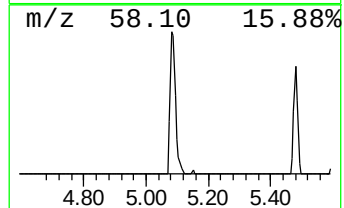
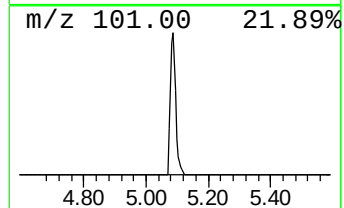
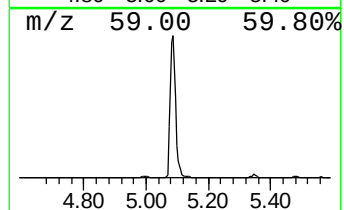
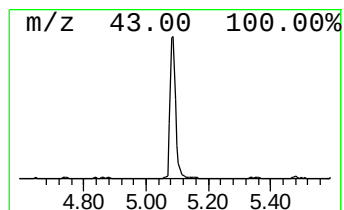
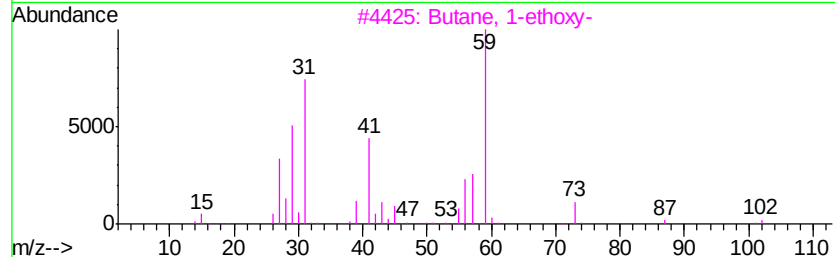
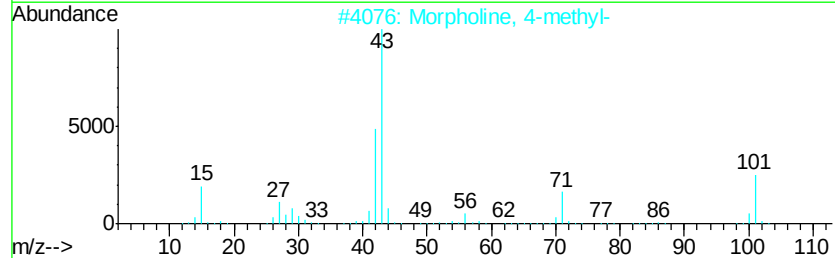
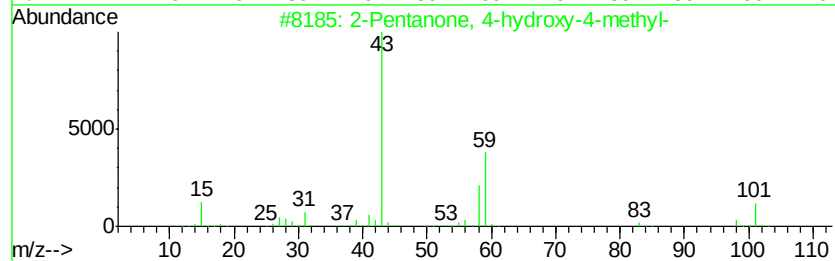
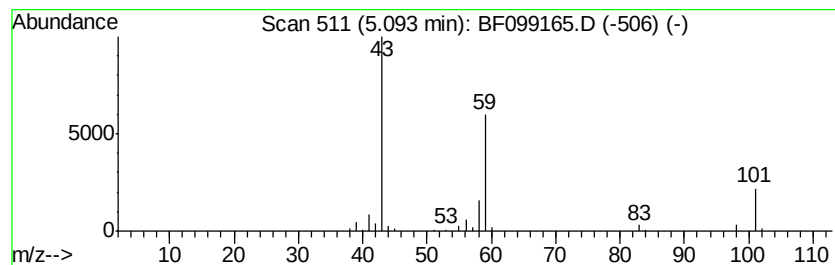
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	6.74 ng	256598	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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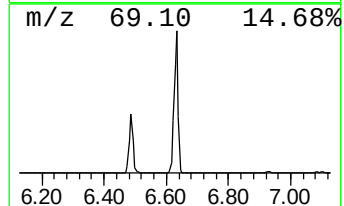
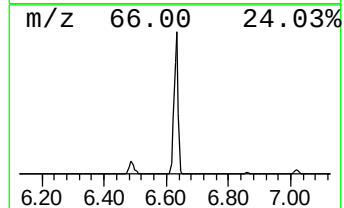
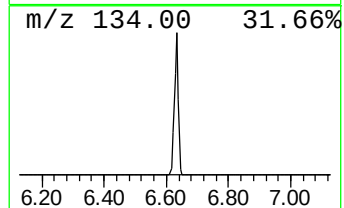
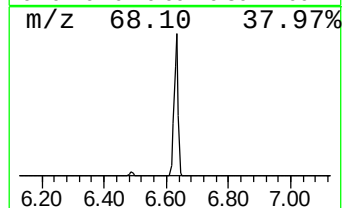
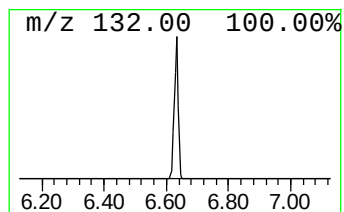
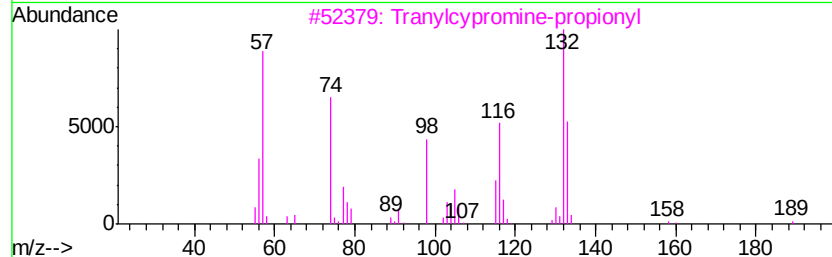
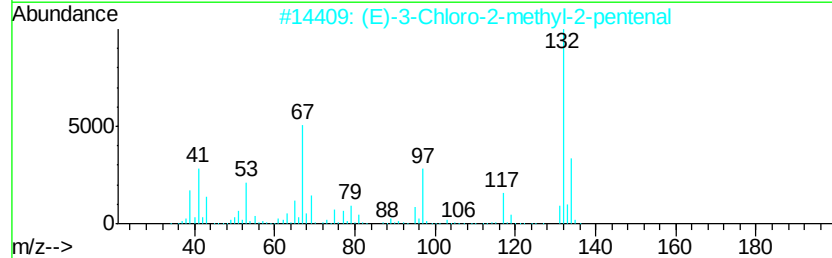
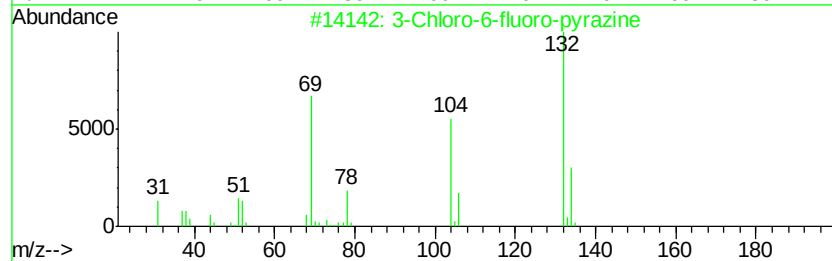
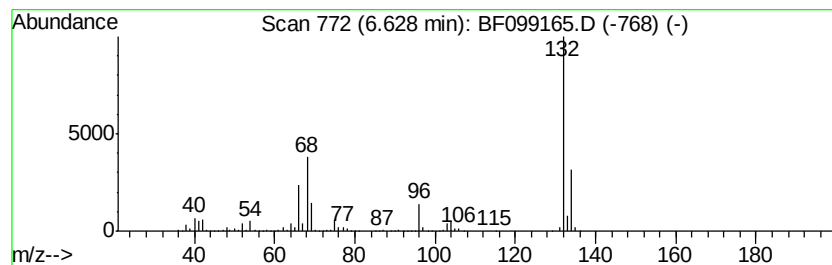
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	70.29 ng	2676400	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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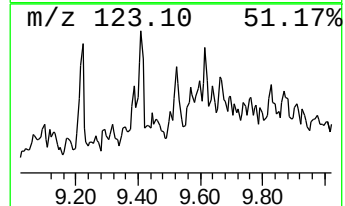
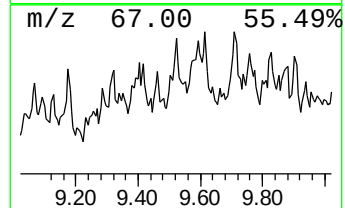
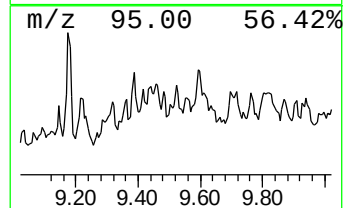
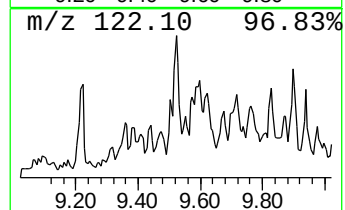
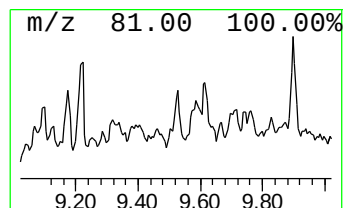
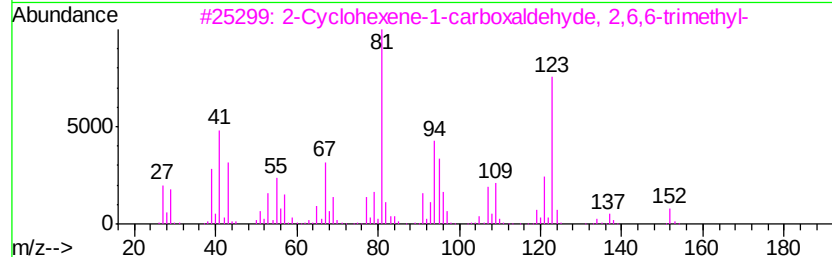
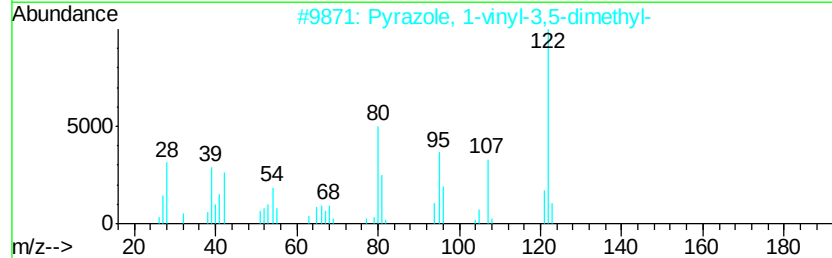
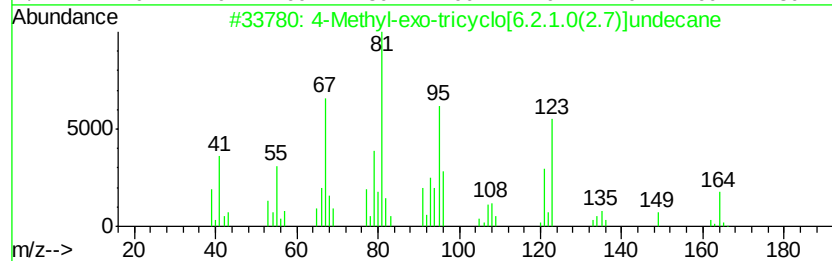
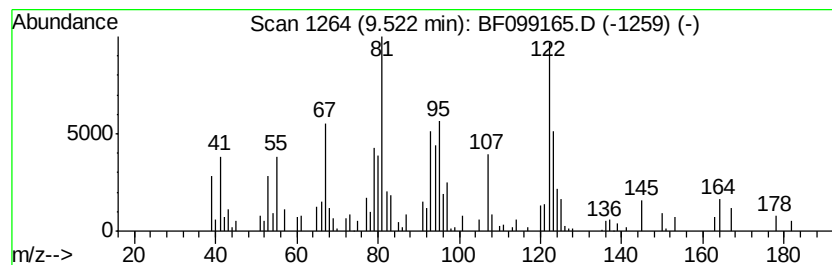
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown9.52 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.52	2.04 ng	118860	Acenaphthene-d10	9.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Methyl-exo-tricyclo[6.2.1.0(2....	164	C12H20	1000215-29-8	46
2		Pyrazole, 1-vinyl-3,5-dimethyl-	122	C7H10N2	015967-75-6	38
3		2-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	000432-24-6	38
4		3-Amino-5-cyclopropylpyrazole	123	C6H9N3	1000342-82-6	30
5		1,2-Benzenediamine, N-methyl-	122	C7H10N2	004760-34-3	27



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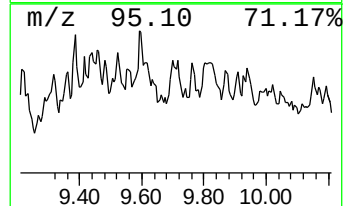
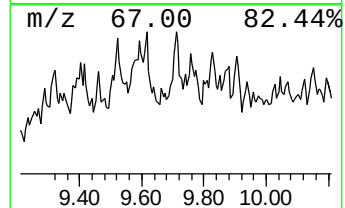
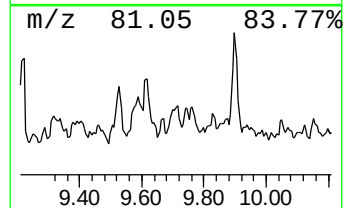
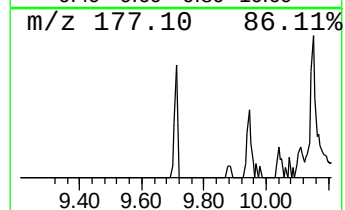
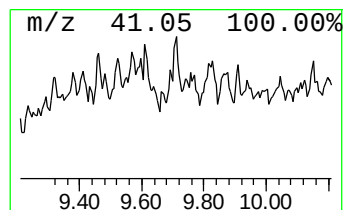
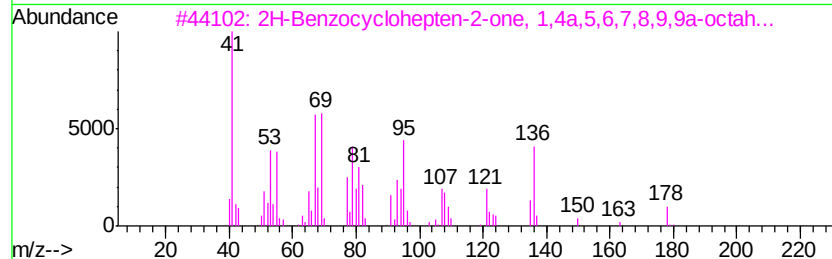
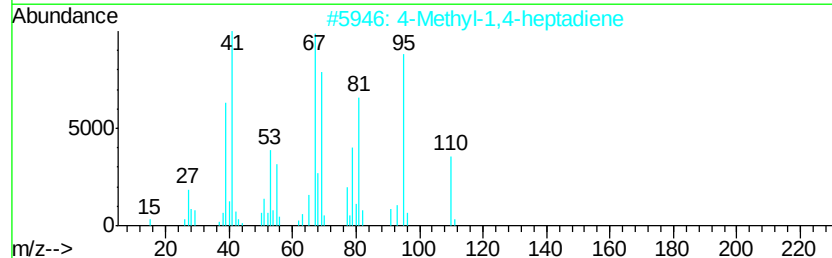
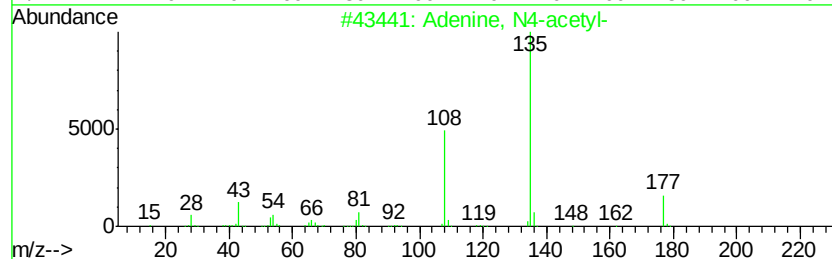
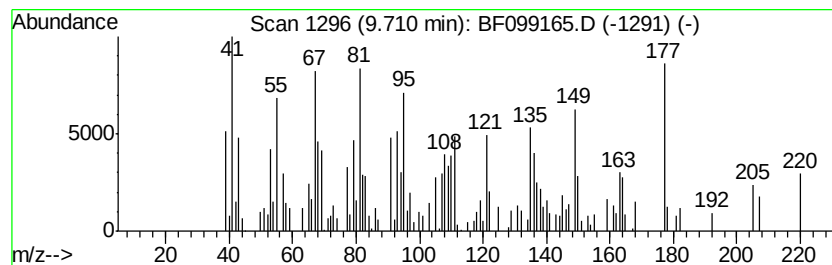
Instrument :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown9.71 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
9.71	2.62 ng	152928	Acenaphthene-d10	9.90		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adenine, N4-acetyl-	177	C7H7N5O	1000374-31-9	49	
2	4-Methyl-1,4-heptadiene	110	C8H14	013857-55-1	46	
3	2H-Benzocyclohepten-2-one, 1,4a,...	178	C12H18O	017429-26-4	41	
4	2-Cyclohexen-1-one, 4-ethyl-4-me...	138	C9H14O	017429-32-2	38	
5	Bicyclo[2.2.1]heptane, 2-methoxy...	168	C11H20O	004443-51-0	35	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099165.D
Acq On : 6 Oct 2017 23:31
Operator : SJ/JU
Sample : I5516-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-6

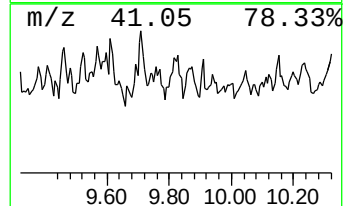
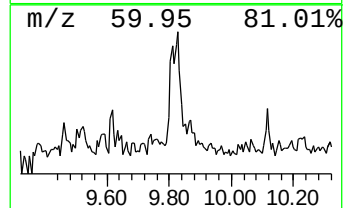
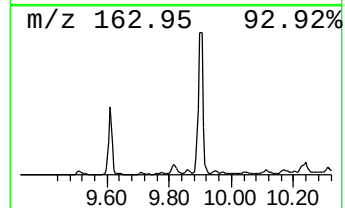
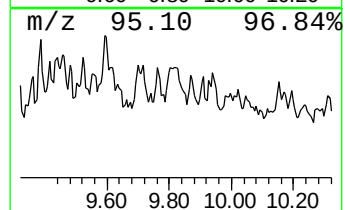
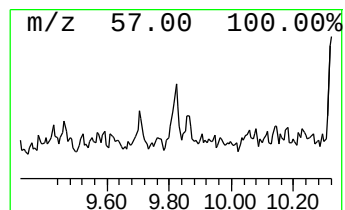
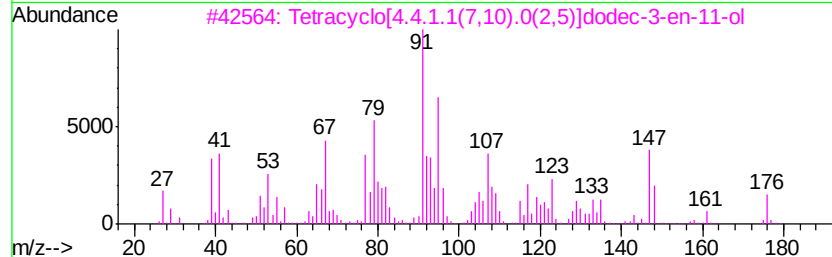
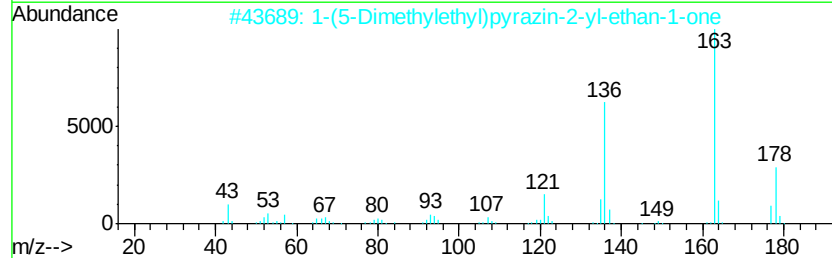
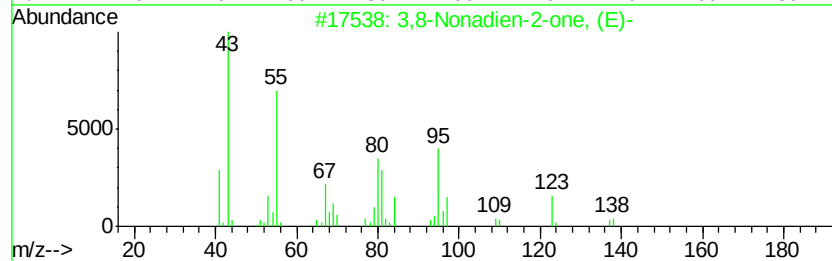
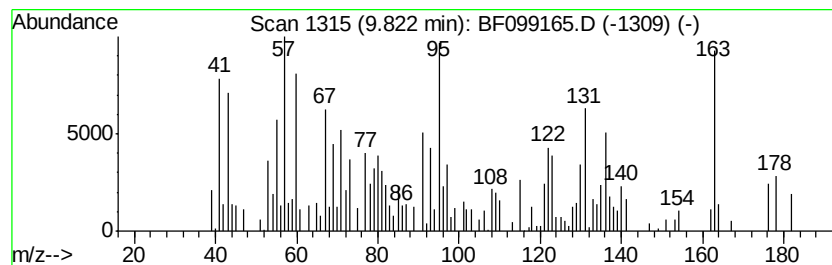
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown9.82 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.82	2.36 ng	137749	Acenaphthene-d10	9.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,8-Nonadien-2-one, (E)-			138	C9H14O	055282-90-1	25
2	1-(5-Dimethylethyl)pyrazin-2-yl-...			178	C10H14N2O	182306-61-2	20
3	Tetracyclo[4.4.1.1(7,10).0(2,5)]...			176	C12H16O	1000184-98-8	18
4	2-Methyl-2-phenylthiophane			178	C11H14S	014856-67-8	11
5	1,3,3-Trimethyl-2-(2-methyl-cycl...			178	C13H22	285129-06-8	11



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Sample : I5516-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-6

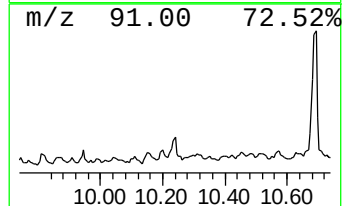
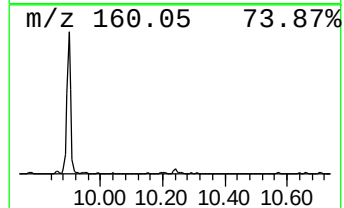
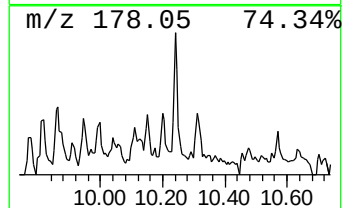
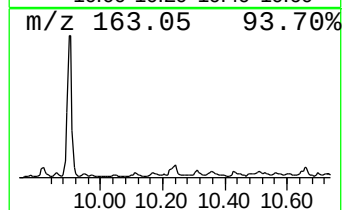
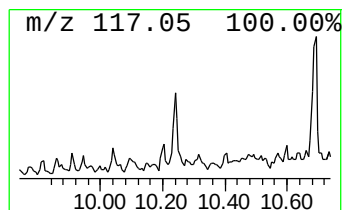
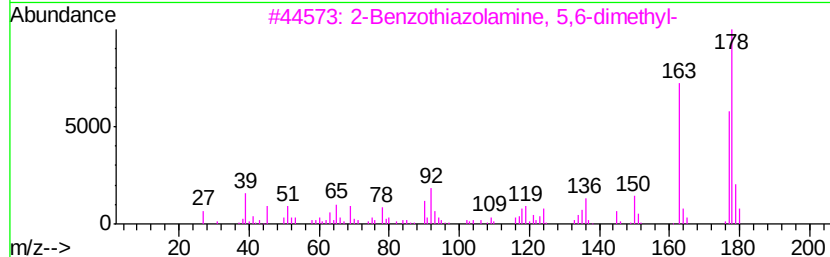
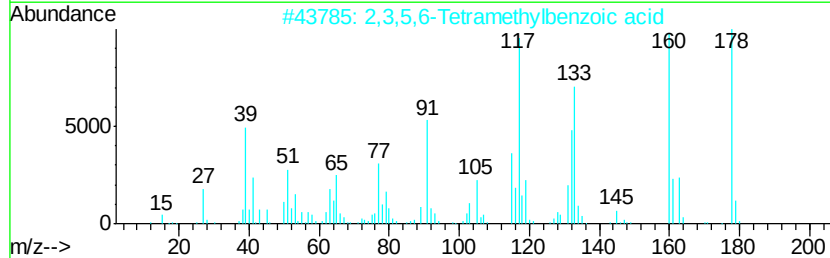
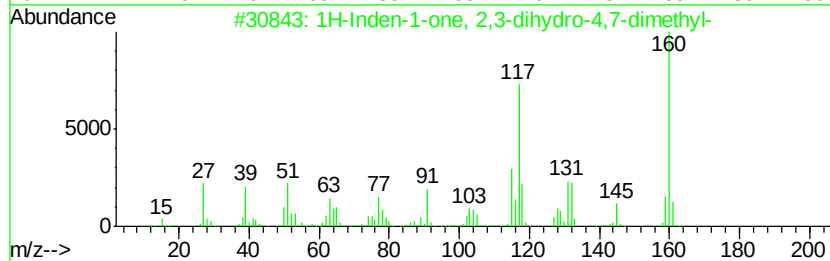
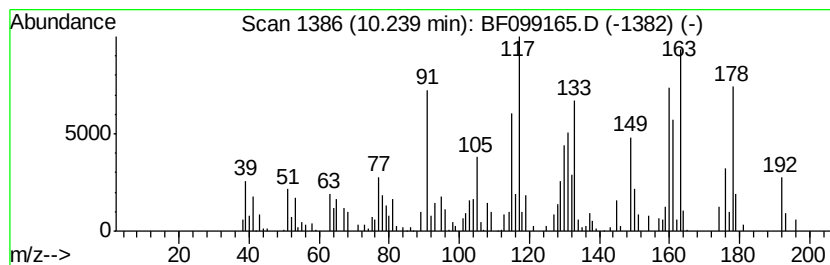
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown10.24 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.24	2.16 ng	126124	Acenaphthene-d10	9.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Inden-1-one, 2,3-dihydro-4,7-...	160	C11H12O	005037-60-5	47
2		2,3,5,6-Tetramethylbenzoic acid	178	C11H14O2	002604-45-7	43
3		2-Benzothiazolamine, 5,6-dimethyl-	178	C9H10N2S	029927-08-0	35
4		Thiophene, 2-(methylseleno)-	178	C5H6SSe	020892-42-6	25
5		Naphthalene, 6-ethyl-1,2,3,4-tet...	160	C12H16	022531-20-0	18



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Sample : I5516-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

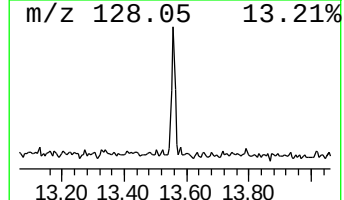
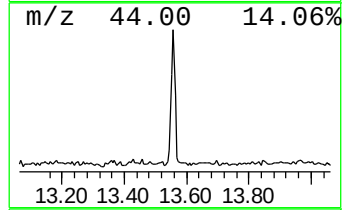
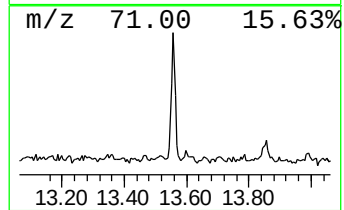
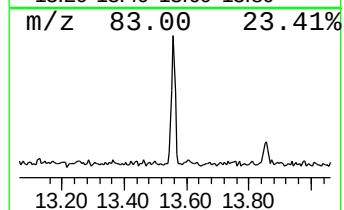
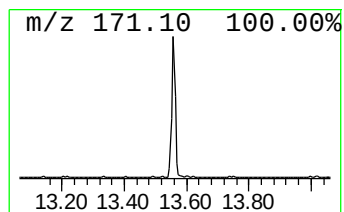
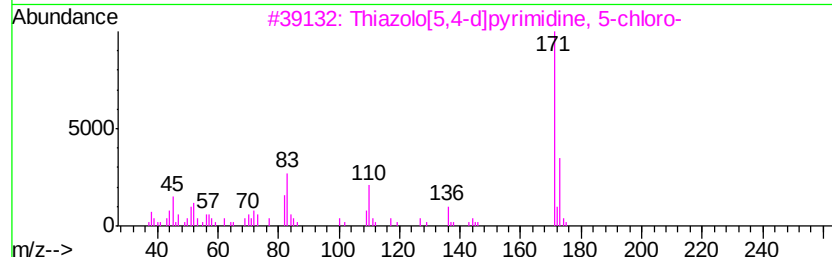
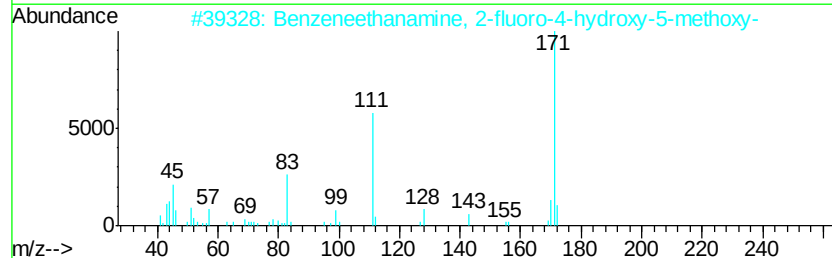
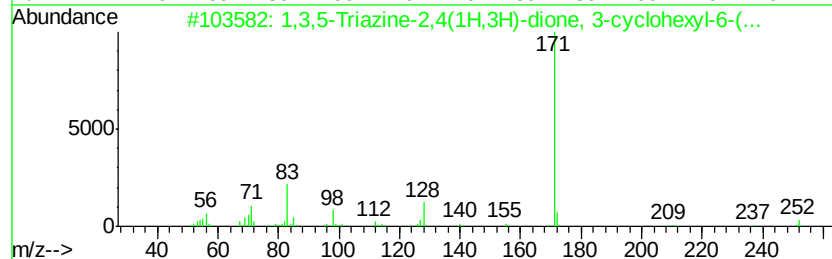
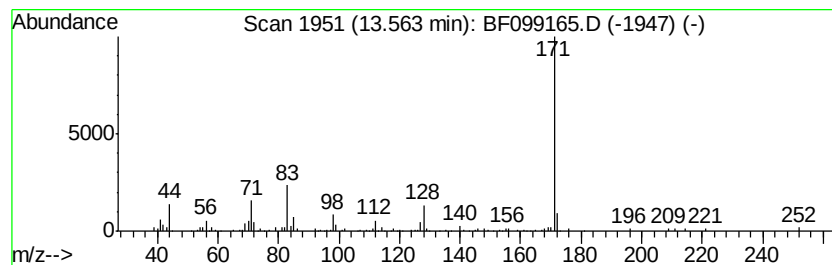
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.56	3.26 ng	121738	Chrysene-d12	14.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4(1H,3H)-dione,...	252	C12H20N4O2	051235-04-2	97
2	Benzeneethanamine, 2-fluoro-4-hy...	171	C8H10FN02	1000116-43-3	64
3	Thiazolo[5,4-d]pyrimidine, 5-chl...	171	C5H2ClN3S	013316-08-0	59
4	1,3,5-Triazaspiro[4.4]nonane-2-...	171	C7H13N3S	1000277-58-6	50
5	2,6-Difluorophenyl isocyanate	171	C7H3F2NS	065295-69-4	47



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Instrument :
BNA_F
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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
Butane, 2-methoxy...	2.16	18.0	ng	686375	1	6.86	761547	20.0
2-Pentanone, 4-hy...	5.09	6.7	ng	256598	1	6.86	761547	20.0
unknown6.63	6.63	70.3	ng	2676400	1	6.86	761547	20.0
unknown9.52	9.52	2.0	ng	118860	3	9.90	1167830	20.0
unknown9.71	9.71	2.6	ng	152928	3	9.90	1167830	20.0
unknown9.82	9.82	2.4	ng	137749	3	9.90	1167830	20.0
unknown10.24	10.24	2.2	ng	126124	3	9.90	1167830	20.0
1,3,5-Triazine-2,...	13.56	3.3	ng	121738	5	14.02	747749	20.0