

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092617\
 Data File : BF098834.D
 Acq On : 26 Sep 2017 16:08
 Operator : SJ/JU
 Sample : I5363-05 10X
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-3-C-COMP

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	2.169	11	14	22	rVB2	16181	25250	1.79%	0.184%
2	5.122	513	516	523	rBV	82019	81387	5.77%	0.592%
3	5.398	559	563	567	rVB	82917	71384	5.06%	0.519%
4	5.522	578	584	587	rBV	519517	492584	34.90%	3.583%
5	5.751	620	623	628	rVB	40233	36350	2.58%	0.264%
6	6.528	751	755	759	rBV	570411	509006	36.07%	3.703%
7	6.675	777	780	784	rVB	673959	530817	37.61%	3.861%
8	6.910	817	820	824	rVB	1045293	926177	65.63%	6.737%
9	7.069	843	847	850	rBV	478415	401620	28.46%	2.922%
10	7.469	911	915	918	rBV	393640	301737	21.38%	2.195%
11	8.192	1035	1038	1041	rBV	1380949	1297243	91.92%	9.437%
12	8.904	1156	1159	1162	rBV	53257	40840	2.89%	0.297%
13	9.004	1173	1176	1179	rBV	28912	23939	1.70%	0.174%
14	9.269	1217	1221	1224	rBV	722810	634332	44.95%	4.614%
15	9.345	1231	1234	1236	rBV2	15816	16435	1.16%	0.120%
16	9.527	1262	1265	1270	rBV2	16338	20137	1.43%	0.146%
17	9.604	1275	1278	1281	rVV	21073	20628	1.46%	0.150%
18	9.657	1285	1287	1291	rVB	79799	65922	4.67%	0.480%
19	9.810	1310	1313	1317	rVV	35410	30387	2.15%	0.221%
20	9.869	1319	1323	1326	rVB2	16983	21395	1.52%	0.156%
21	9.951	1333	1337	1340	rBV	1705195	1411231	100.00%	10.266%
22	9.980	1340	1342	1345	rVB	55114	45050	3.19%	0.328%
23	10.151	1367	1371	1375	rVB	50581	46062	3.26%	0.335%
24	10.369	1407	1408	1411	rVB	23486	17848	1.26%	0.130%
25	10.492	1427	1429	1437	rBV2	30028	32957	2.34%	0.240%
26	10.586	1443	1445	1451	rVB3	14652	21427	1.52%	0.156%
27	10.733	1467	1470	1475	rBV	416639	333423	23.63%	2.425%
28	10.857	1486	1491	1496	rVB2	47903	66995	4.75%	0.487%
29	11.210	1546	1551	1553	rVB	50932	52769	3.74%	0.384%
30	11.239	1553	1556	1559	rVB	24284	21976	1.56%	0.160%
31	11.292	1562	1565	1567	rVV2	39657	35093	2.49%	0.255%
32	11.321	1567	1570	1576	rVB3	24361	36137	2.56%	0.263%
33	11.439	1586	1590	1592	rBV	1569565	1328316	94.12%	9.663%
34	11.463	1592	1594	1597	rVV	208437	165277	11.71%	1.202%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092617\
 Data File : BF098834.D
 Acq On : 26 Sep 2017 16:08
 Operator : SJ/JU
 Sample : I5363-05 10X
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-3-C-COMP

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

35	11.510	1600	1602	1605	rVV	65014	49687	3.52%	0.361%
36	11.645	1622	1625	1626	rBV	20759	19850	1.41%	0.144%
37	11.663	1626	1628	1633	rVB	32265	32899	2.33%	0.239%
38	11.816	1651	1654	1656	rBV	33167	27242	1.93%	0.198%
39	11.951	1672	1677	1678	rBV2	46912	64483	4.57%	0.469%
40	12.051	1691	1694	1696	rBV2	39630	48379	3.43%	0.352%
41	12.233	1722	1725	1727	rBV	65009	51448	3.65%	0.374%
42	12.257	1727	1729	1732	rVB3	21168	19213	1.36%	0.140%
43	12.380	1748	1750	1752	rVB	39408	28185	2.00%	0.205%
44	12.486	1766	1768	1770	rBV2	28405	20512	1.45%	0.149%
45	12.515	1771	1773	1776	rBV3	21818	25496	1.81%	0.185%
46	12.568	1780	1782	1785	rBV2	26587	27743	1.97%	0.202%
47	12.651	1792	1796	1799	rBV	282701	230627	16.34%	1.678%
48	12.692	1800	1803	1805	rBV4	26128	27528	1.95%	0.200%
49	12.880	1832	1835	1841	rVB	226775	215795	15.29%	1.570%
50	13.015	1855	1858	1863	rVB	603111	535186	37.92%	3.893%
51	13.157	1879	1882	1884	rBV	57244	55138	3.91%	0.401%
52	13.710	1974	1976	1979	rVB2	63926	53500	3.79%	0.389%
53	13.874	2002	2004	2007	rBV	84338	87133	6.17%	0.634%
54	14.074	2034	2038	2041	rBV	1026530	1010930	71.63%	7.354%
55	14.104	2041	2043	2048	rVB	145558	129833	9.20%	0.944%
56	14.204	2058	2060	2063	rBV	142804	136967	9.71%	0.996%
57	14.245	2064	2067	2070	rVV	233364	190777	13.52%	1.388%
58	14.274	2070	2072	2074	rVV	71313	59466	4.21%	0.433%
59	14.298	2074	2076	2079	rVB	79811	60405	4.28%	0.439%
60	15.127	2214	2217	2220	rBV	115803	159828	11.33%	1.163%
61	15.568	2287	2292	2305	rVB	735817	1037642	73.53%	7.548%
62	17.121	2553	2556	2562	rVB2	116878	178770	12.67%	1.300%

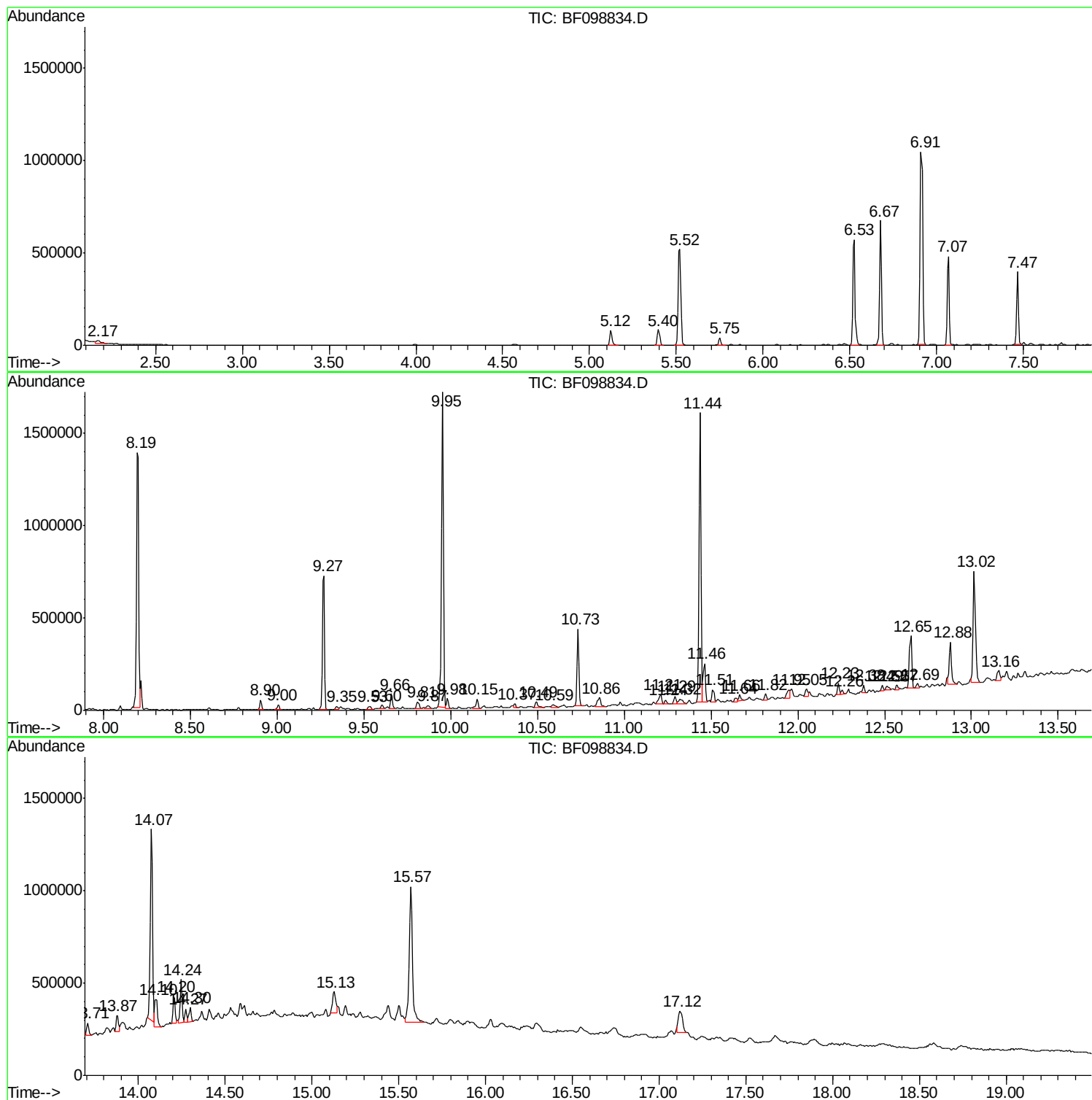
Sum of corrected areas: 13746793

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092617\
Data File : BF098834.D
Acq On : 26 Sep 2017 16:08
Operator : SJ/JU
Sample : I5363-05 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3-C-COMP

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092617\
Data File : BF098834.D
Acq On : 26 Sep 2017 16:08
Operator : SJ/JU
Sample : I5363-05 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3-C-COMP

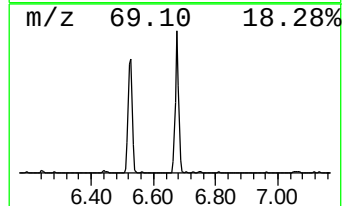
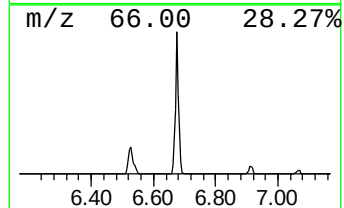
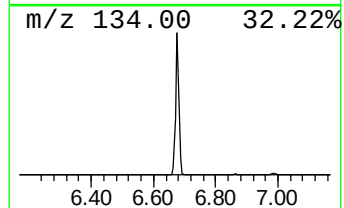
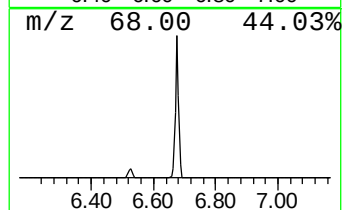
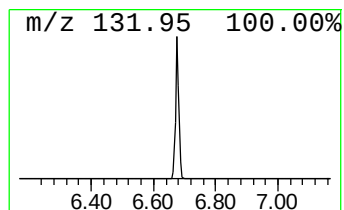
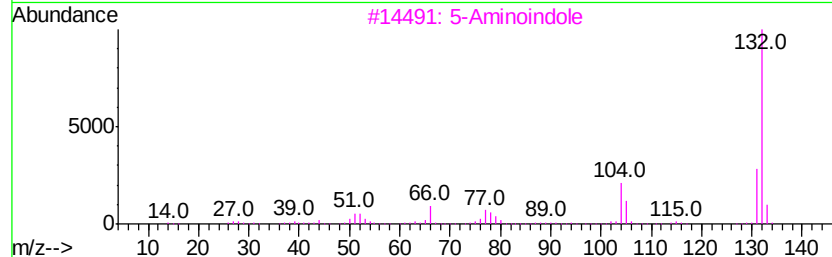
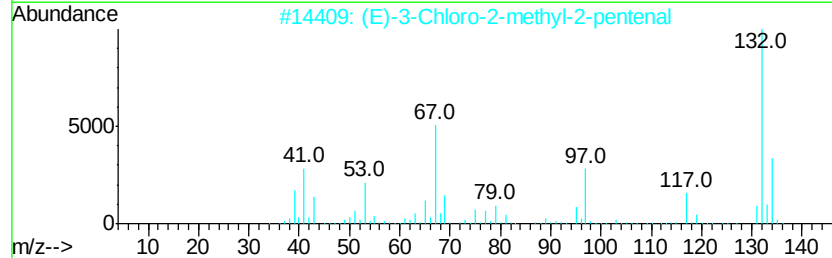
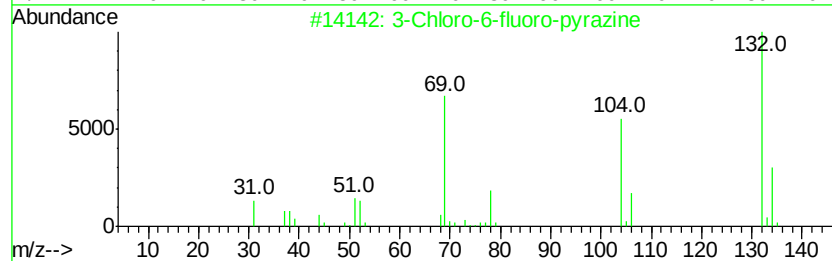
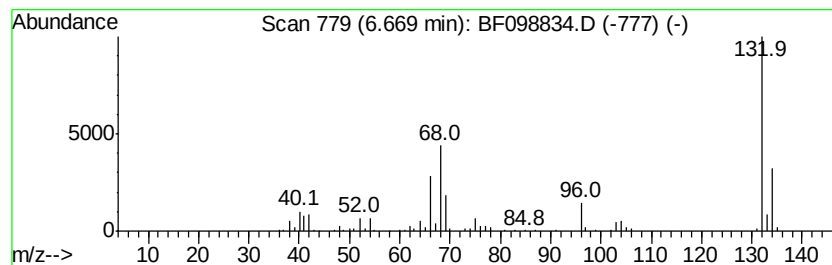
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	11.46 ng	530817	1,4-Dichlorobenzene-d4	6.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092617\
Data File : BF098834.D
Acq On : 26 Sep 2017 16:08
Operator : SJ/JU
Sample : I5363-05 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3-C-COMP

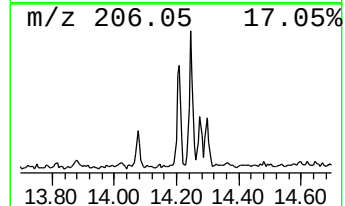
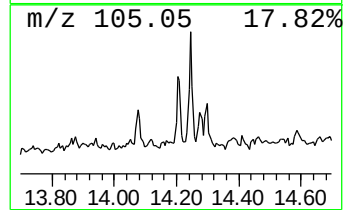
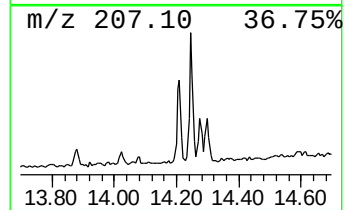
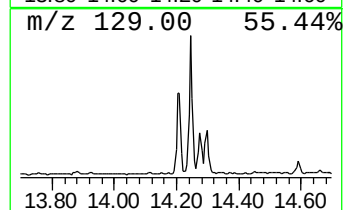
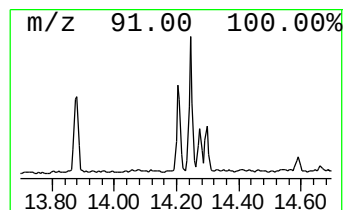
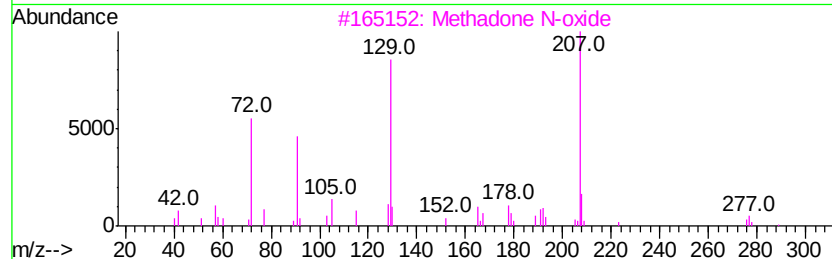
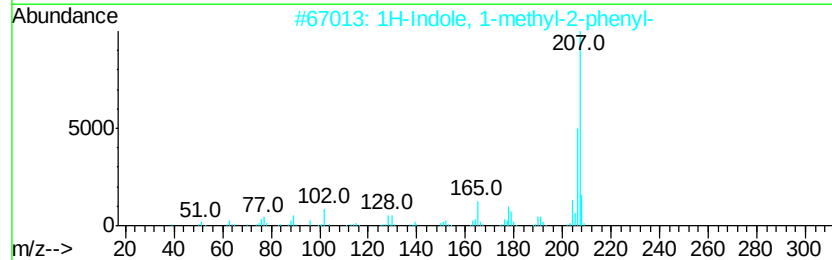
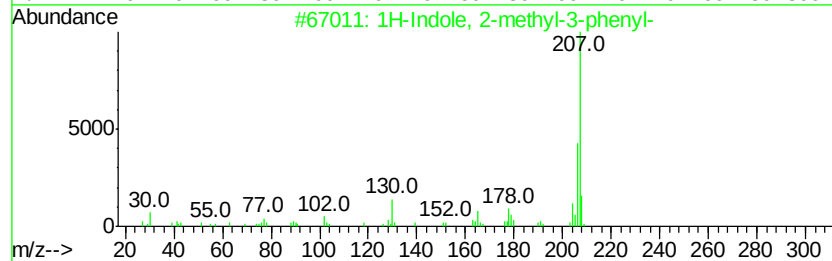
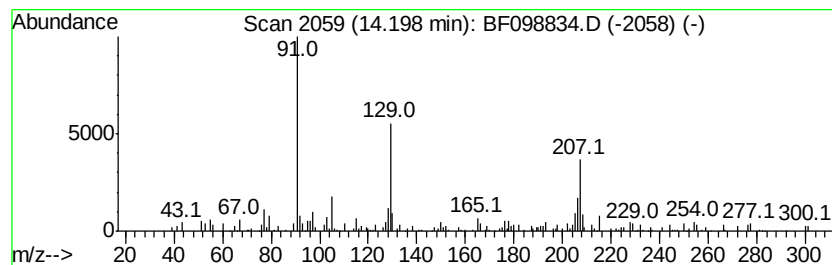
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown14.20 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	2.71 ng	136967	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	41
2		1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	41
3		Methadone N-oxide	325	C21H27NO2	1000120-80-7	40
4		5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	38
5		3-Methyl-2-phenylindole	207	C15H13N	010257-92-8	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092617\
Data File : BF098834.D
Acq On : 26 Sep 2017 16:08
Operator : SJ/JU
Sample : I5363-05 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3-C-COMP

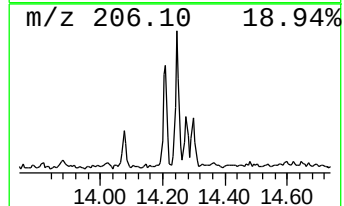
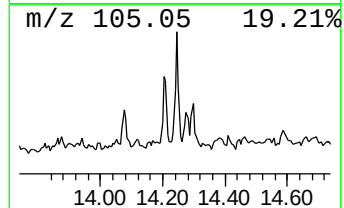
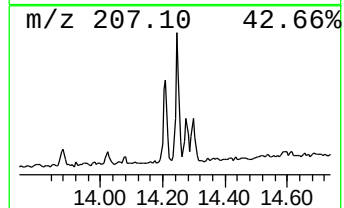
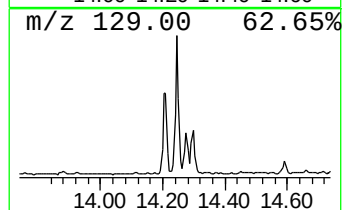
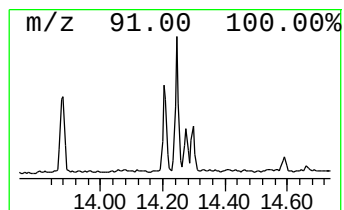
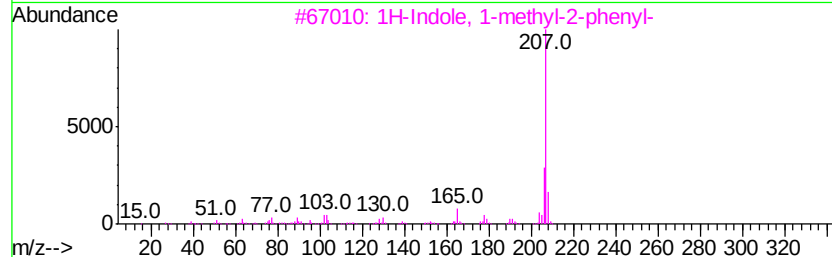
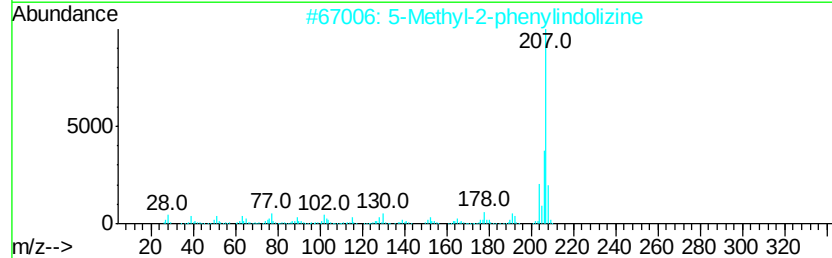
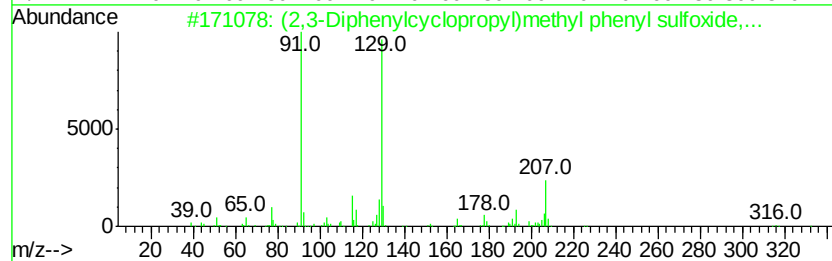
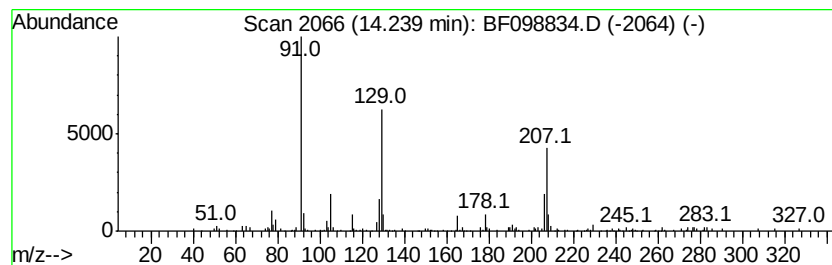
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown14.24 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.24	3.77 ng	190777	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	46
2		5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	43
3		1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	42
4		1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	38
5		1-benzylindole	207	C15H13N	1000334-31-3	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092617\
Data File : BF098834.D
Acq On : 26 Sep 2017 16:08
Operator : SJ/JU
Sample : I5363-05 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3-C-COMP

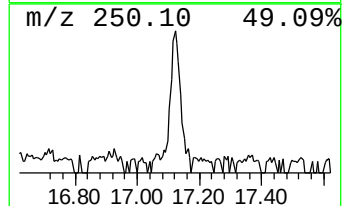
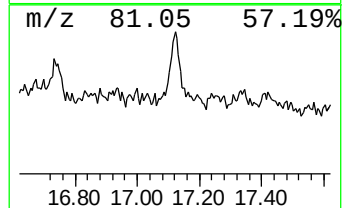
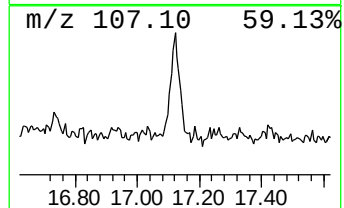
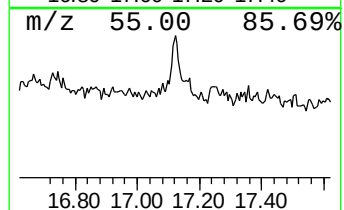
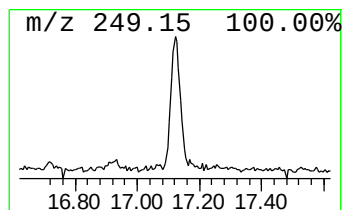
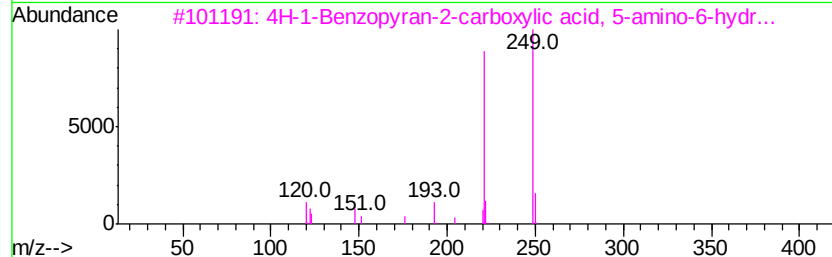
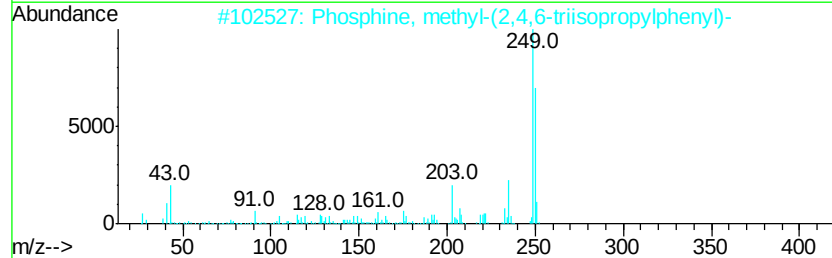
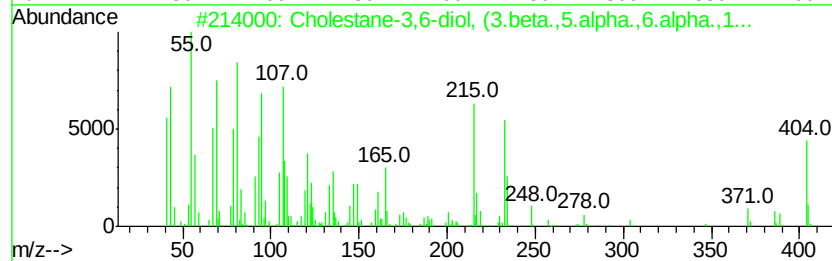
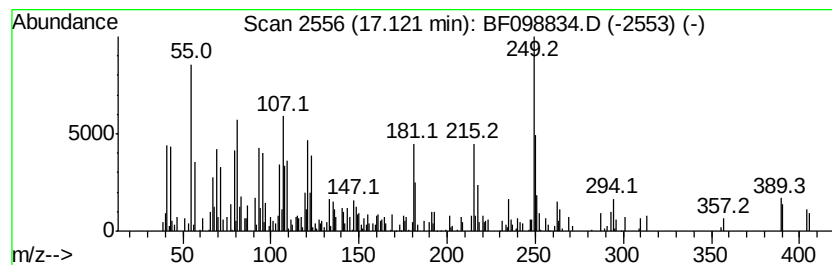
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown17.12 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.12	3.45 ng	178770	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cholestane-3,6-diol, (3.beta.,5....	404	C27H48O2	041083-77-6	35
2		Phosphine, methyl-(2,4,6-triisop...	250	C16H27P	158748-69-7	25
3		4H-1-Benzopyran-2-carboxylic aci...	249	C12H11NO5	032142-43-1	25
4		1-Ethanone, 1-{2-[(3,3-dimethyl-...	292	C16H24N2OS	077109-20-7	22
5		Benzene, 1-nitro-2-hydroxy-4-(p-...	249	C12H8FN04	189214-56-0	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092617\
Data File : BF098834.D
Acq On : 26 Sep 2017 16:08
Operator : SJ/JU
Sample : I5363-05 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3-C-COMP

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.67	6.67	11.5	ng	530817	1	6.91	926177	20.0
unknown14.20	14.20	2.7	ng	136967	5	14.07	1010930	20.0
unknown14.24	14.24	3.8	ng	190777	5	14.07	1010930	20.0
unknown17.12	17.12	3.5	ng	178770	6	15.57	1037640	20.0