

Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
 Data File : BF096335.D
 Acq On : 30 Jun 2017 14:16
 Operator : SJ/MA
 Sample : I3883-11 5X
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 G53-0-1.5

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-BF062717.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	3.775	281	287	291	rBV2	20743	31800	2.32%	0.249%
2	4.322	377	380	388	rBV2	12262	16831	1.23%	0.132%
3	4.951	484	487	495	rVB	175400	169842	12.41%	1.331%
4	5.375	555	559	563	rBV	690619	578102	42.25%	4.530%
5	6.392	728	732	741	rVB	893605	708072	51.75%	5.548%
6	6.534	753	756	760	rBV	786475	641132	46.86%	5.023%
7	6.769	793	796	800	rBV	1135819	1000704	73.14%	7.841%
8	6.834	805	807	810	rBV	15076	14555	1.06%	0.114%
9	6.928	819	823	826	rBV	626881	510521	37.31%	4.000%
10	7.322	886	890	894	rBV	452040	399709	29.22%	3.132%
11	7.745	958	962	967	rBV2	10829	14801	1.08%	0.116%
12	7.975	998	1001	1007	rVB	73935	70864	5.18%	0.555%
13	8.051	1010	1014	1018	rBV	1510446	1368144	100.00%	10.720%
14	8.492	1084	1089	1093	rBV	15309	18593	1.36%	0.146%
15	8.657	1113	1117	1120	rBV	35074	30202	2.21%	0.237%
16	8.763	1130	1135	1139	rVB4	13331	18080	1.32%	0.142%
17	8.869	1150	1153	1157	rBV3	10438	15604	1.14%	0.122%
18	9.086	1188	1190	1193	rVB2	19458	16824	1.23%	0.132%
19	9.128	1193	1197	1200	rBV	902088	688381	50.31%	5.394%
20	9.222	1209	1213	1216	rBV2	50977	47805	3.49%	0.375%
21	9.386	1236	1241	1246	rBV4	17751	25170	1.84%	0.197%
22	9.469	1249	1255	1257	rBV3	21440	27843	2.04%	0.218%
23	9.522	1261	1264	1266	rBV	121058	99872	7.30%	0.783%
24	9.751	1301	1303	1307	rVB	63847	52320	3.82%	0.410%
25	9.804	1307	1312	1316	rBV	1265177	1229292	89.85%	9.632%
26	9.839	1316	1318	1322	rVB	22538	18832	1.38%	0.148%
27	10.010	1344	1347	1350	rVB	41339	33619	2.46%	0.263%
28	10.051	1350	1354	1356	rBV3	15185	17462	1.28%	0.137%
29	10.251	1385	1388	1391	rVB	65765	54728	4.00%	0.429%
30	10.351	1402	1405	1407	rBV	18924	15000	1.10%	0.118%
31	10.469	1422	1425	1429	rVB	35198	38775	2.83%	0.304%
32	10.551	1436	1439	1442	rBV5	12523	14864	1.09%	0.116%
33	10.586	1442	1445	1448	rVV2	73171	67491	4.93%	0.529%
34	10.628	1449	1452	1459	rVB	100854	94356	6.90%	0.739%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063017\
 Data File : BF096335.D
 Acq On : 30 Jun 2017 14:16
 Operator : SJ/MA
 Sample : I3883-11 5X
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 G53-0-1.5

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-BF062717.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.722	1465	1468	1469	rBV	92213	74608	5.45%	0.585%
36	11.039	1519	1522	1528	rVB7	27067	47585	3.48%	0.373%
37	11.086	1528	1530	1535	rVB5	12883	14683	1.07%	0.115%
38	11.139	1537	1539	1541	rVV2	15341	18121	1.32%	0.142%
39	11.169	1541	1544	1546	rVV2	63408	64317	4.70%	0.504%
40	11.198	1547	1549	1553	rVB2	41263	40994	3.00%	0.321%
41	11.286	1560	1564	1566	rBV	1142806	955679	69.85%	7.488%
42	11.310	1566	1568	1571	rVV	169890	133562	9.76%	1.047%
43	11.357	1572	1576	1579	rVB2	58405	62010	4.53%	0.486%
44	11.592	1613	1616	1619	rBV2	42724	38546	2.82%	0.302%
45	11.792	1647	1650	1652	rBV3	23608	24242	1.77%	0.190%
46	11.816	1652	1654	1658	rVB2	57538	45647	3.34%	0.358%
47	11.863	1659	1662	1663	rBV3	17458	15498	1.13%	0.121%
48	11.898	1664	1668	1670	rVV4	50564	57044	4.17%	0.447%
49	11.922	1670	1672	1674	rVB3	29254	20376	1.49%	0.160%
50	11.998	1683	1685	1687	rBV	29914	24449	1.79%	0.192%
51	12.080	1697	1699	1701	rBV	27865	23065	1.69%	0.181%
52	12.263	1728	1730	1732	rBV2	23312	24806	1.81%	0.194%
53	12.339	1740	1743	1745	rBV	42473	39764	2.91%	0.312%
54	12.363	1745	1747	1749	rVV3	17113	19899	1.45%	0.156%
55	12.392	1749	1752	1754	rVB2	42849	40359	2.95%	0.316%
56	12.498	1767	1770	1772	rBV	262756	239064	17.47%	1.873%
57	12.721	1803	1808	1812	rBV	253389	274978	20.10%	2.155%
58	12.845	1826	1829	1830	rBV3	30588	31780	2.32%	0.249%
59	12.869	1830	1833	1836	rVV	579666	493794	36.09%	3.869%
60	13.116	1873	1875	1878	rVB	67951	53208	3.89%	0.417%
61	13.351	1913	1915	1921	rVB	112937	118941	8.69%	0.932%
62	13.457	1931	1933	1936	rBV3	54477	47114	3.44%	0.369%
63	13.921	2007	2012	2014	rBV	901821	959686	70.15%	7.519%
64	13.945	2014	2016	2018	rVB	93109	74434	5.44%	0.583%
65	15.345	2251	2254	2259	rVB2	431302	534241	39.05%	4.186%

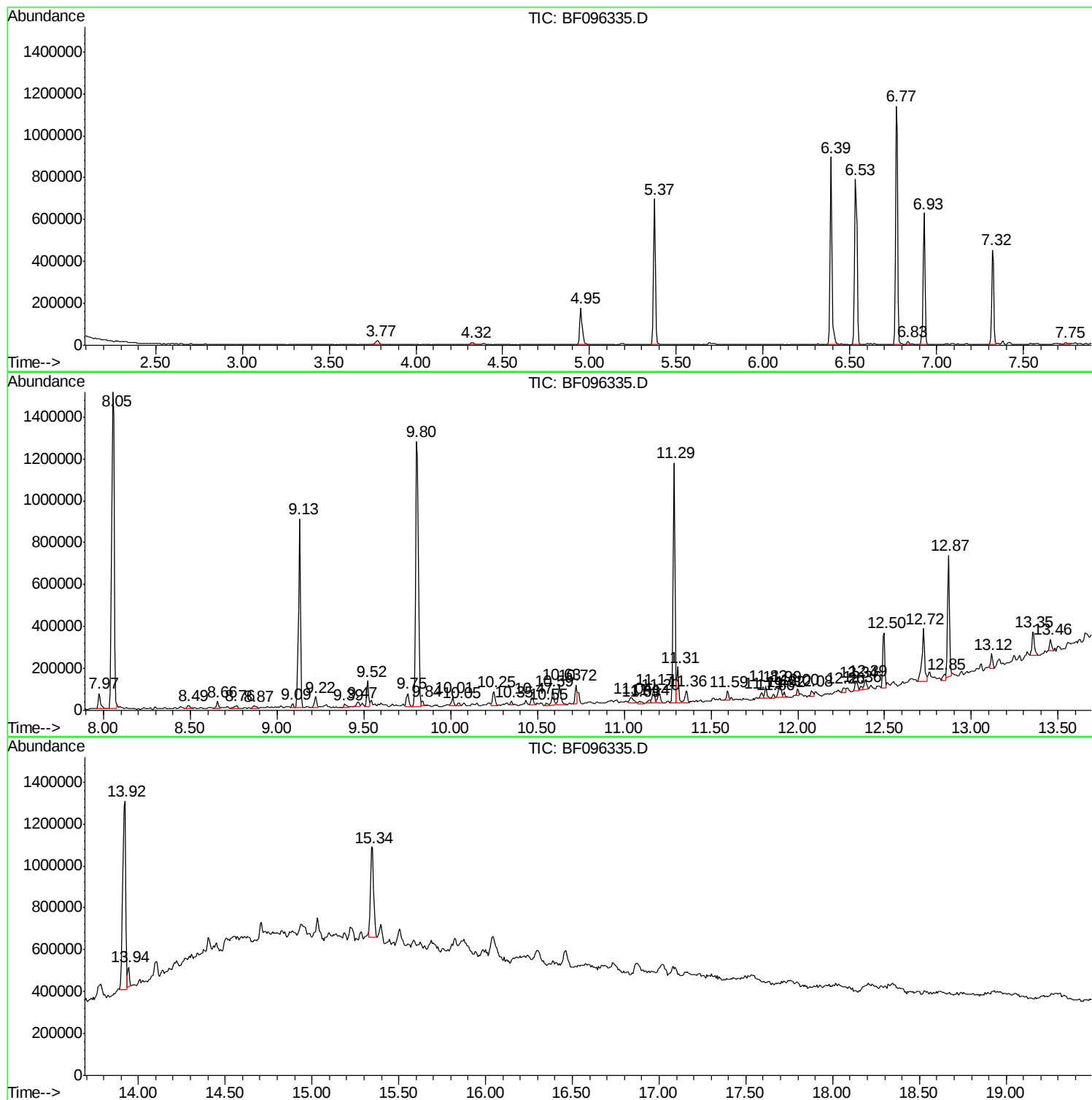
Sum of corrected areas: 12762684

Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
Data File : BF096335.D
Acq On : 30 Jun 2017 14:16
Operator : SJ/MA
Sample : I3883-11 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G53-0-1.5

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF062717.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\BF063017\
Data File : BF096335.D
Acq On : 30 Jun 2017 14:16
Operator : SJ/MA
Sample : I3883-11 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G53-0-1.5

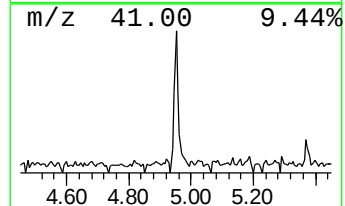
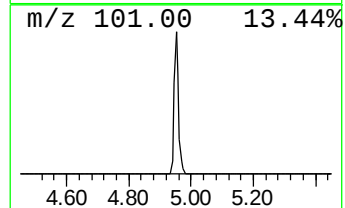
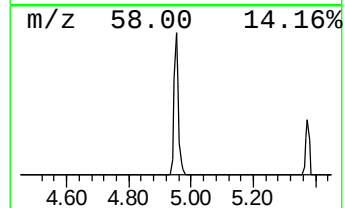
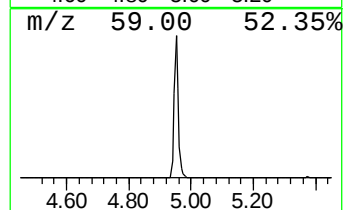
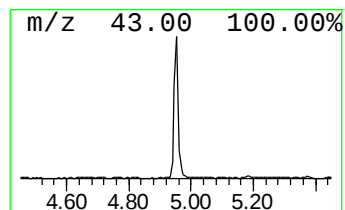
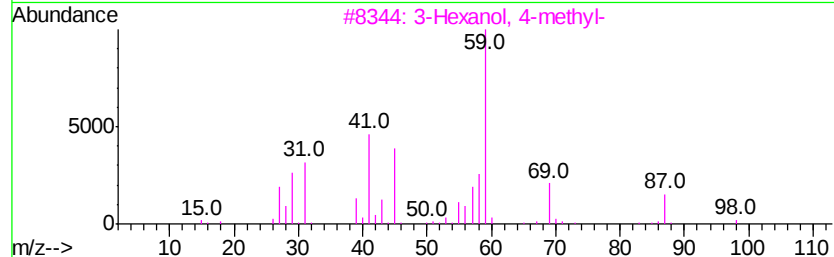
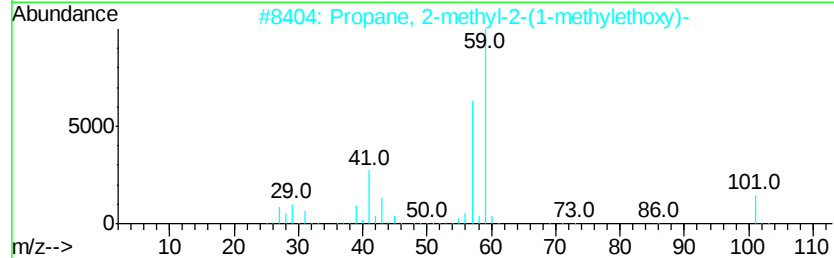
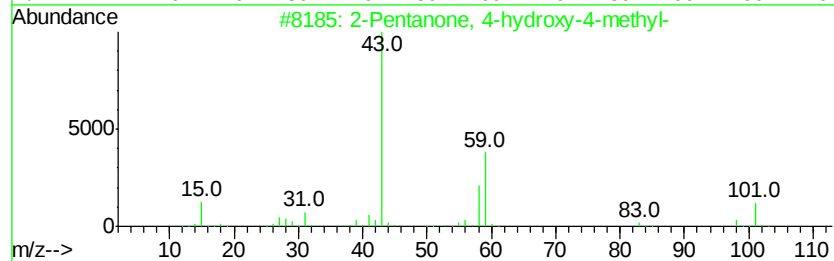
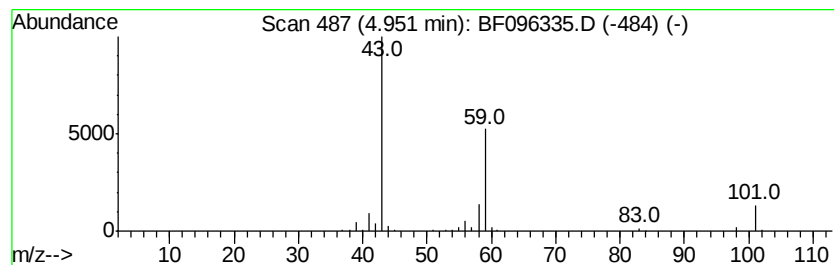
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
4.95	3.39 ng	169842	1,4-Dichlorobenzene-d4	6.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
Data File : BF096335.D
Acq On : 30 Jun 2017 14:16
Operator : SJ/MA
Sample : I3883-11 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G53-0-1.5

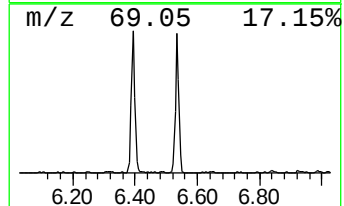
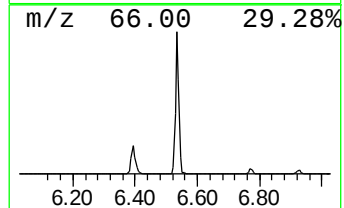
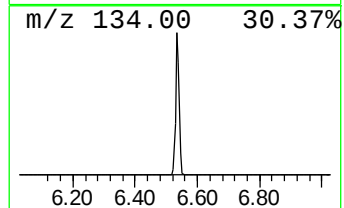
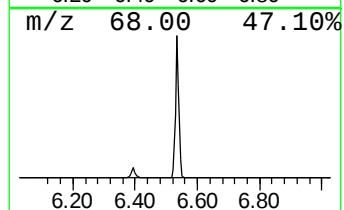
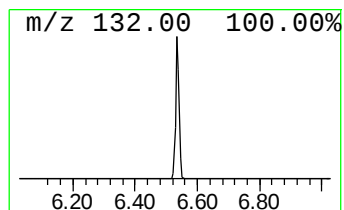
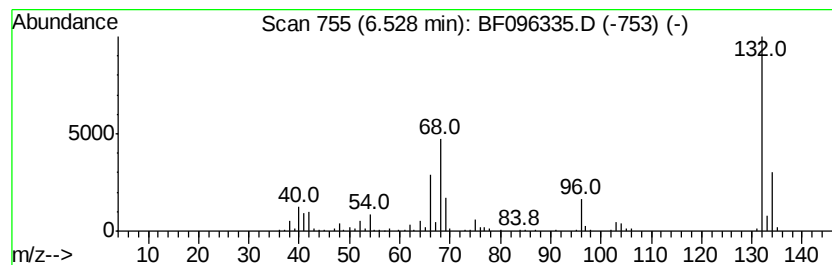
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	12.81 ng	641132	1,4-Dichlorobenzene-d4	6.77

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	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
Data File : BF096335.D
Acq On : 30 Jun 2017 14:16
Operator : SJ/MA
Sample : I3883-11 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G53-0-1.5

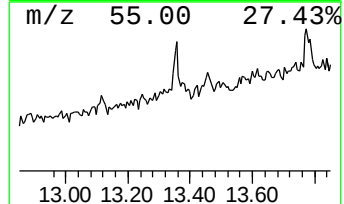
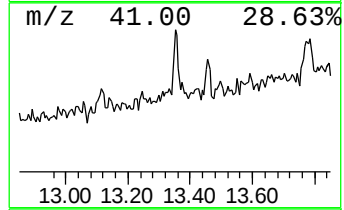
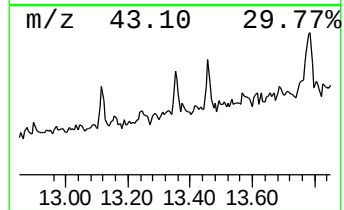
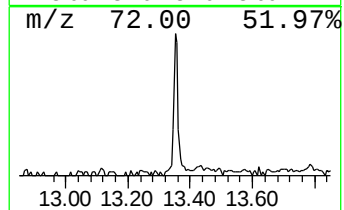
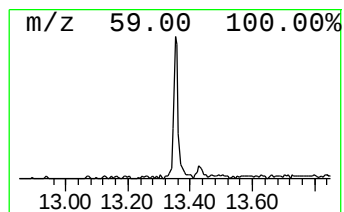
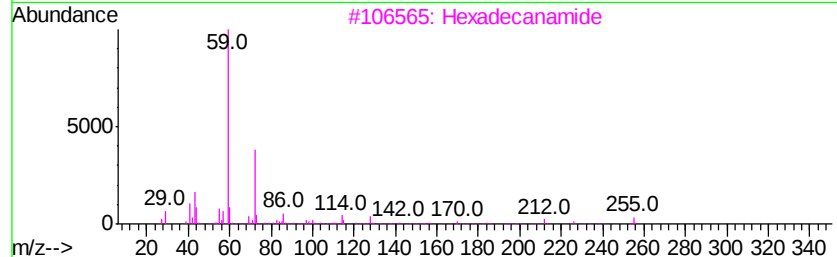
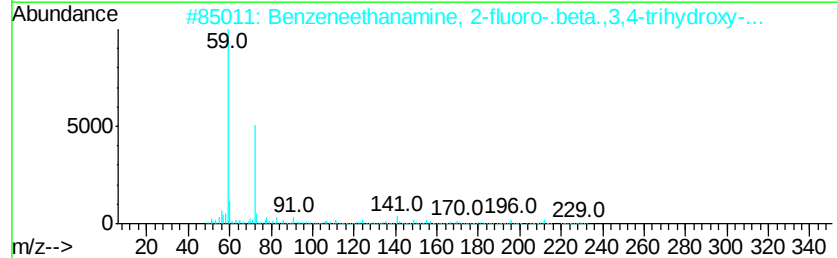
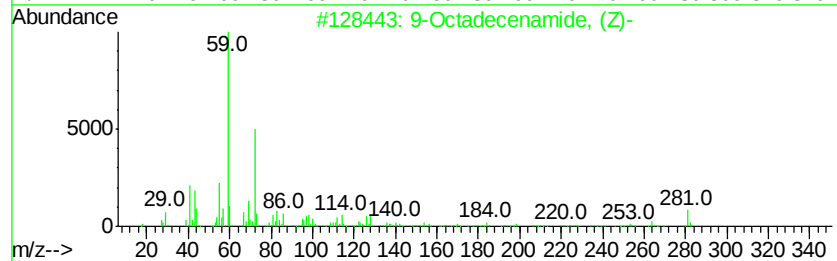
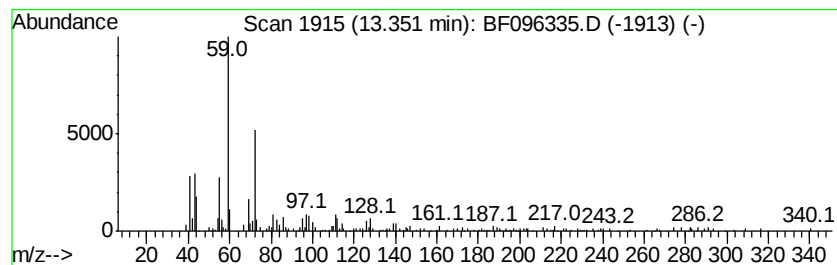
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	2.48 ng	118941	Chrysene-d12	13.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
2		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	80
3		Hexadecanamide	255	C16H33NO	000629-54-9	78
4		Tetradecanamide	227	C14H29NO	000638-58-4	72
5		Octanamide	143	C8H17NO	000629-01-6	45



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063017\
Data File : BF096335.D
Acq On : 30 Jun 2017 14:16
Operator : SJ/MA
Sample : I3883-11 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G53-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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...	4.95	3.4	ng	169842	1	6.77	1000700	20.0
unknown6.53	6.53	12.8	ng	641132	1	6.77	1000700	20.0
9-Octadecenamide, ...	13.35	2.5	ng	118941	5	13.92	959686	20.0