

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100117\
 Data File : BF098987.D
 Acq On : 1 Oct 2017 12:57
 Operator : SJ/JU
 Sample : I5457-08
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TW-1_092617

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

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	2.216	17	22	36	rVB	326196	450321	10.52%	1.628%
2	5.128	513	517	526	rVB	239908	265491	6.20%	0.960%
3	5.522	580	584	587	rBV	1918721	1659562	38.77%	5.998%
4	6.522	750	754	757	rBV	1316419	1041372	24.33%	3.764%
5	6.669	775	779	783	rBV	2725794	2767616	64.65%	10.003%
6	6.904	815	819	822	rBV	872615	779549	18.21%	2.817%
7	7.057	841	845	849	rVB	2800569	2727492	63.71%	9.858%
8	7.463	909	914	917	rBV	2005564	2263683	52.88%	8.181%
9	8.186	1032	1037	1040	rBV	1099765	1037177	24.23%	3.749%
10	9.263	1214	1220	1223	rBV	3963863	4281007	100.00%	15.472%
11	9.363	1234	1237	1242	rVB3	47600	53152	1.24%	0.192%
12	9.651	1282	1286	1289	rBV	64268	54969	1.28%	0.199%
13	9.939	1330	1335	1339	rBV2	1280240	1148788	26.83%	4.152%
14	10.133	1364	1368	1375	rBV	95812	92177	2.15%	0.333%
15	10.316	1395	1399	1401	rBV	54191	44735	1.04%	0.162%
16	10.733	1464	1470	1473	rBV	2158251	2057379	48.06%	7.436%
17	10.810	1480	1483	1485	rBV2	44548	47921	1.12%	0.173%
18	10.833	1485	1487	1494	rVB	46476	46744	1.09%	0.169%
19	10.969	1507	1510	1513	rBV	129690	99295	2.32%	0.359%
20	11.427	1584	1588	1592	rBV	1322967	1116825	26.09%	4.036%
21	11.639	1620	1624	1630	rBV2	50804	58912	1.38%	0.213%
22	12.457	1760	1763	1769	rBV	248924	253157	5.91%	0.915%
23	12.686	1799	1802	1807	rVB	227139	174410	4.07%	0.630%
24	13.016	1853	1858	1861	rBV	3506878	3487551	81.47%	12.605%
25	13.210	1888	1891	1893	rBV	44852	45544	1.06%	0.165%
26	13.451	1929	1932	1935	rBV	90528	74853	1.75%	0.271%
27	13.898	2004	2008	2012	rBV	50939	58729	1.37%	0.212%
28	14.033	2028	2031	2033	rBV	79865	64306	1.50%	0.232%
29	14.068	2033	2037	2041	rVB	934237	802456	18.74%	2.900%
30	15.557	2285	2290	2296	rVB	496180	613458	14.33%	2.217%

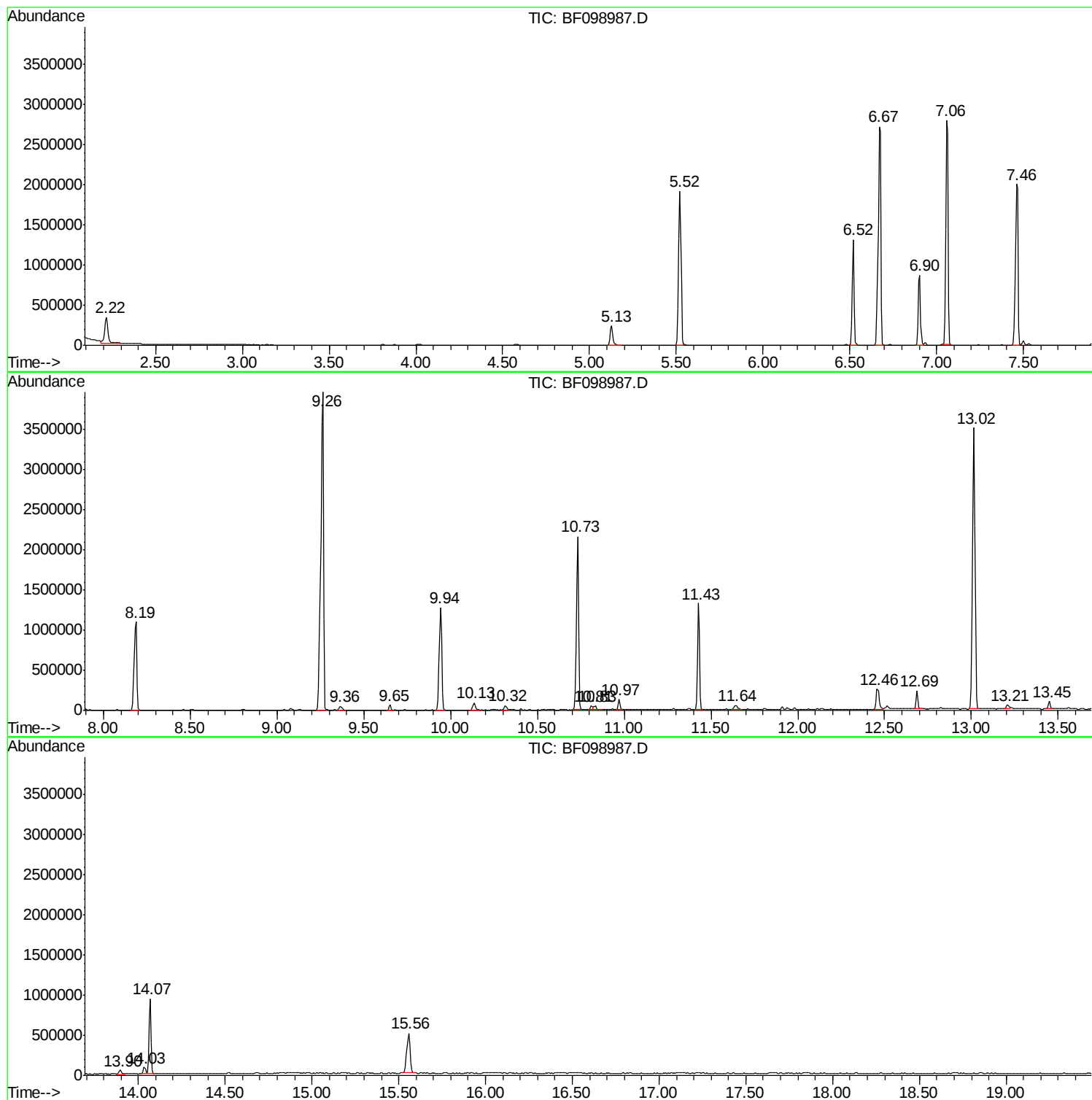
Sum of corrected areas: 27668631

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100117\
Data File : BF098987.D
Acq On : 1 Oct 2017 12:57
Operator : SJ/JU
Sample : I5457-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-1_092617

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\BF100117\
Data File : BF098987.D
Acq On : 1 Oct 2017 12:57
Operator : SJ/JU
Sample : I5457-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-1_092617

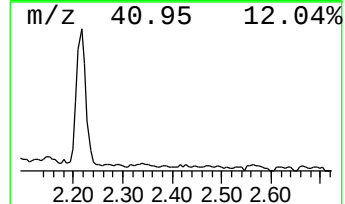
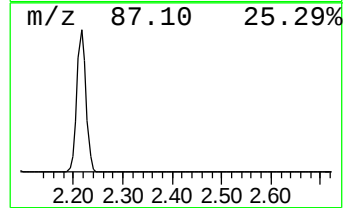
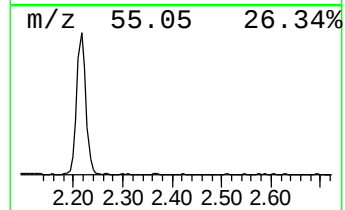
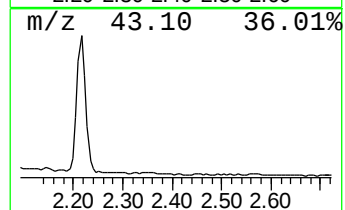
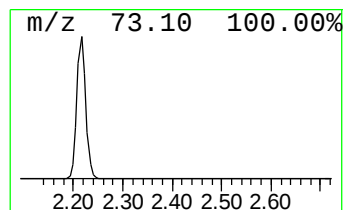
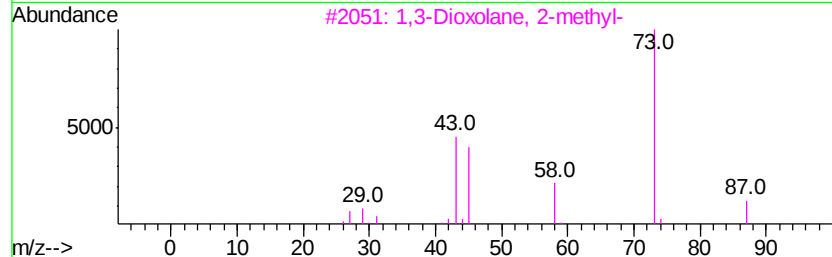
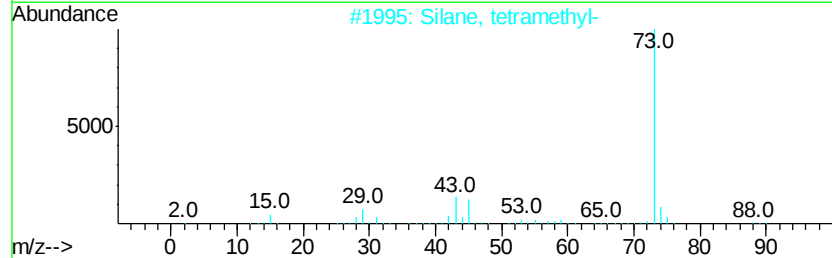
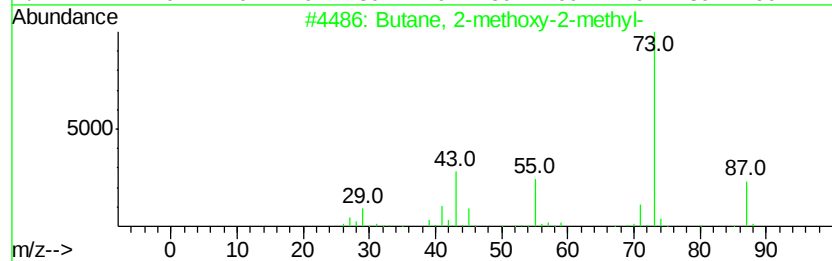
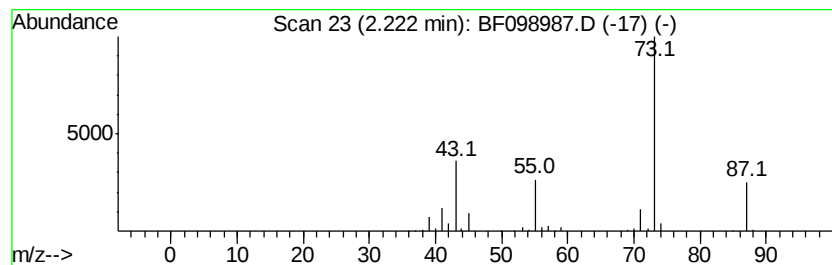
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.22	11.55 ng	450321	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100117\
Data File : BF098987.D
Acq On : 1 Oct 2017 12:57
Operator : SJ/JU
Sample : I5457-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-1_092617

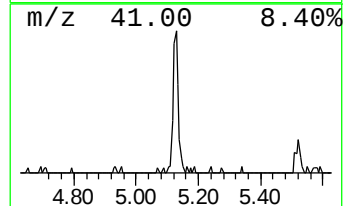
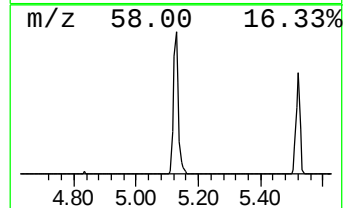
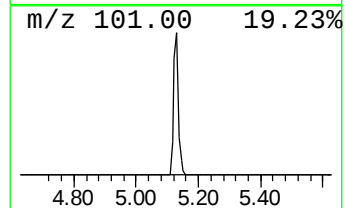
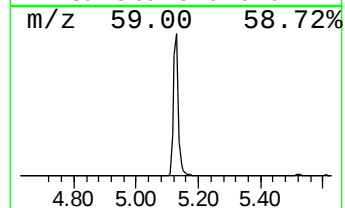
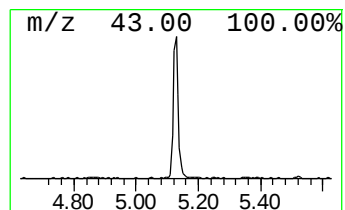
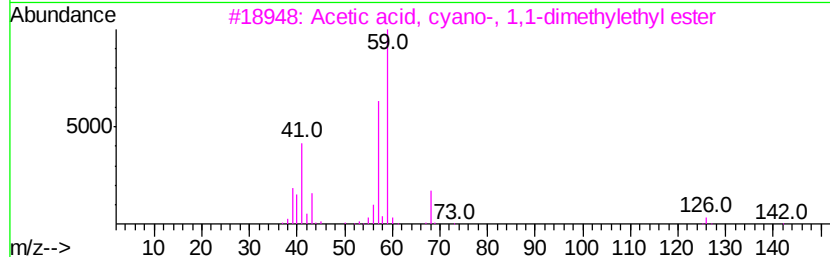
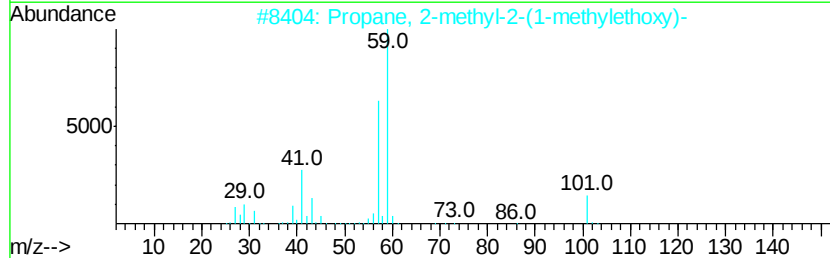
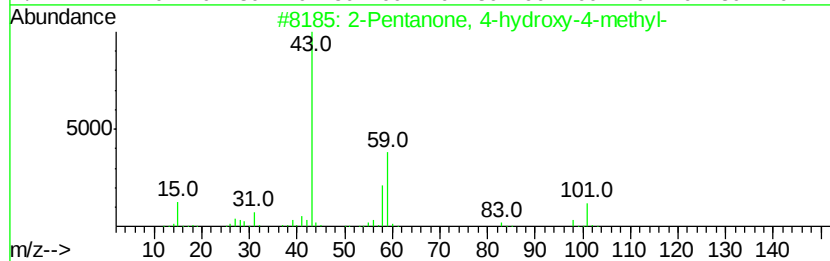
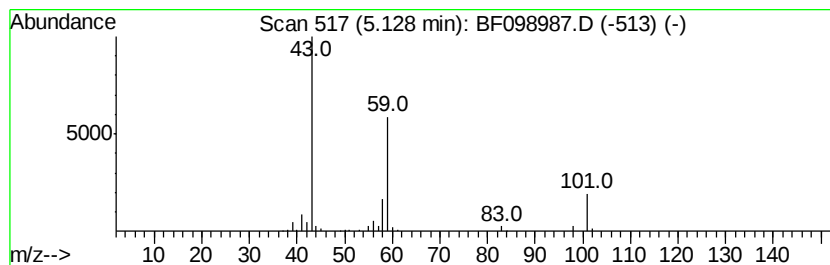
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	6.81 ng	265491	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
3		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100117\
Data File : BF098987.D
Acq On : 1 Oct 2017 12:57
Operator : SJ/JU
Sample : I5457-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-1_092617

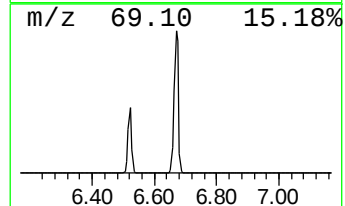
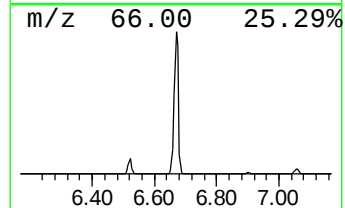
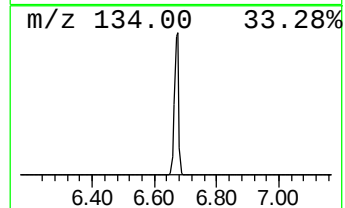
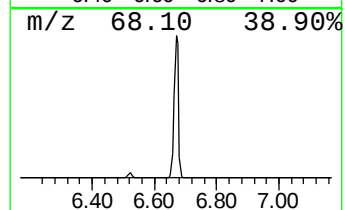
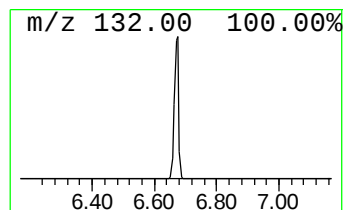
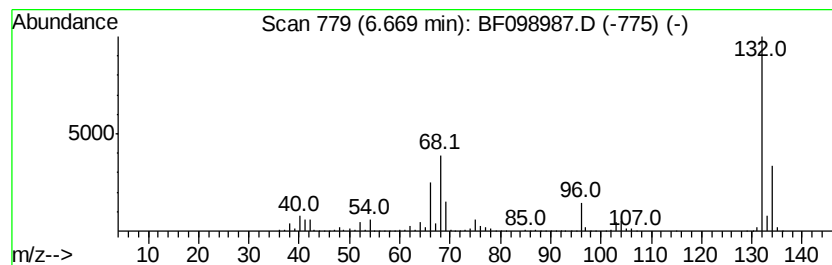
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	71.01 ng	2767620	1,4-Dichlorobenzene-d4	6.90

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100117\
Data File : BF098987.D
Acq On : 1 Oct 2017 12:57
Operator : SJ/JU
Sample : I5457-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

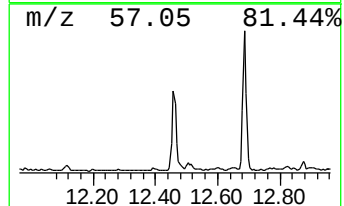
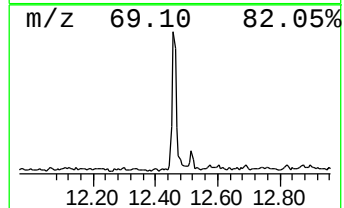
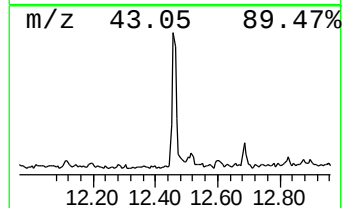
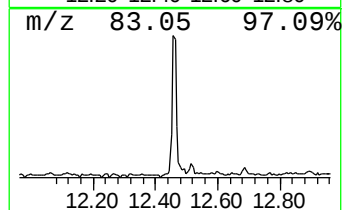
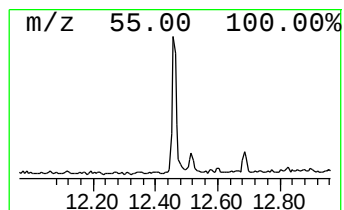
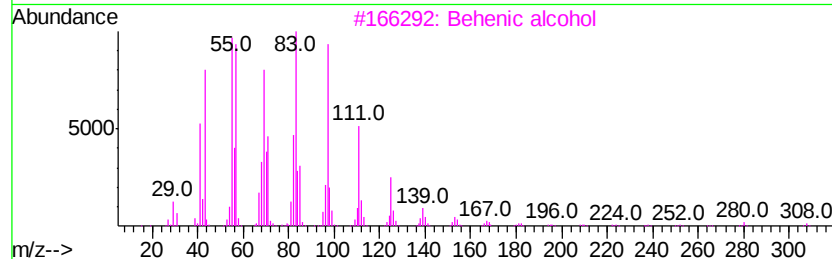
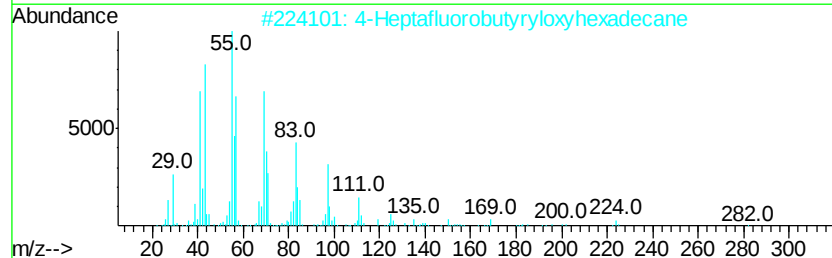
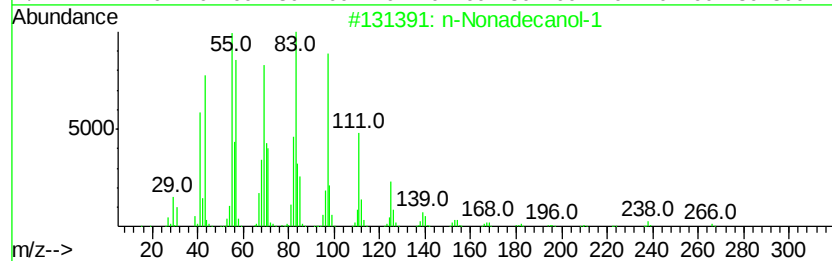
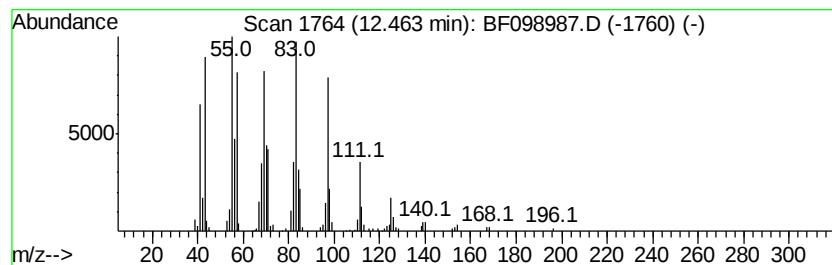
Instrument :
BNA_F
ClientSampleId :
TW-1_092617

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 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.46	4.53 ng	253157	Phenanthrene-d10	11.43	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	91
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
5	1-Hexadecanol	242	C16H34O	036653-82-4	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100117\
Data File : BF098987.D
Acq On : 1 Oct 2017 12:57
Operator : SJ/JU
Sample : I5457-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

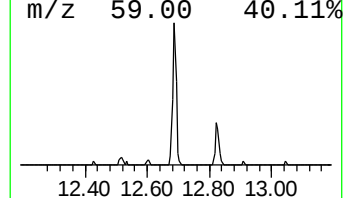
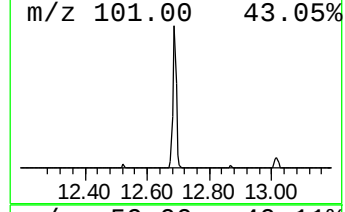
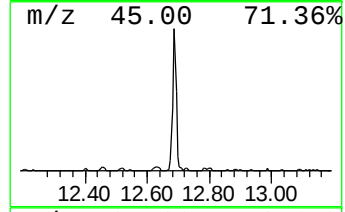
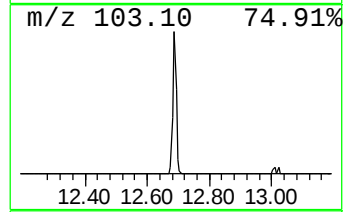
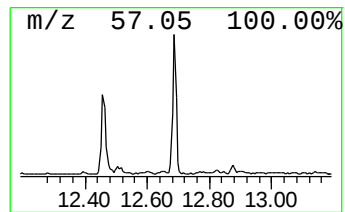
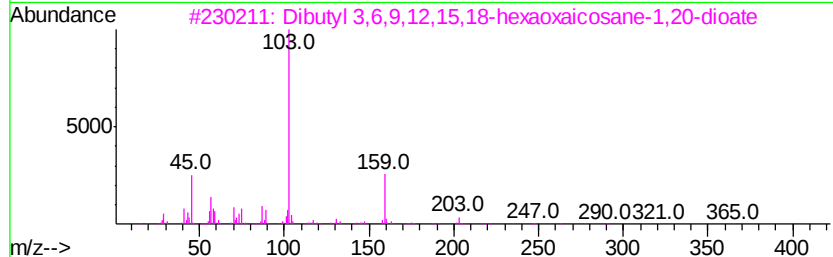
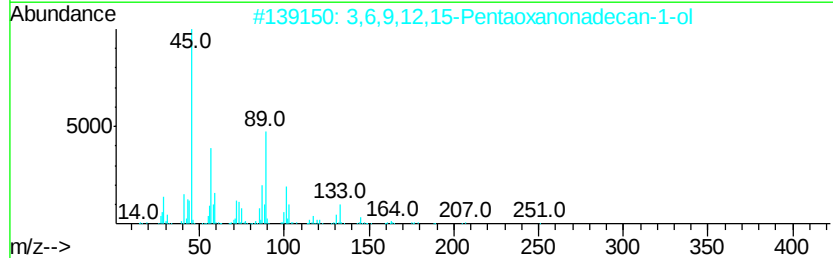
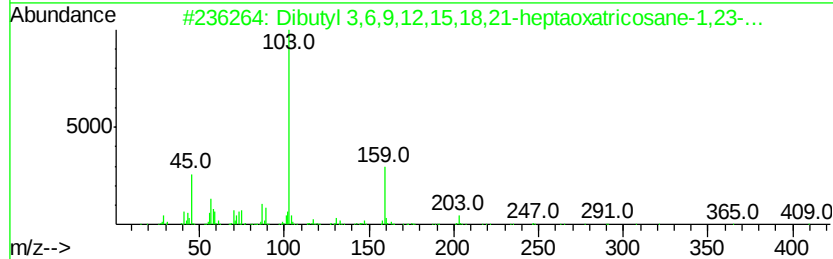
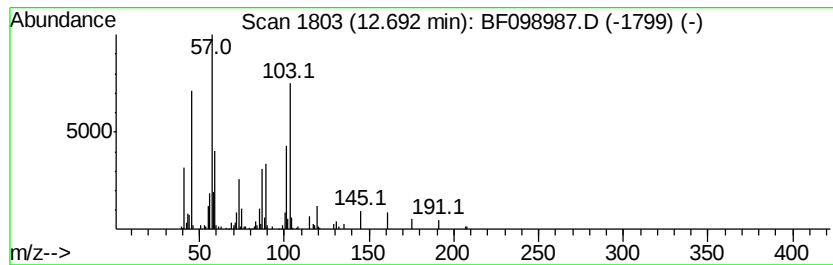
Instrument :
BNA_F
ClientSampleId :
TW-1_092617

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 unknown12.69 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.69	3.12 ng	174410	Phenanthrene-d10	11.43	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibutyl 3,6,9,12,15,18,21-heptao...	510	C24H46O11	1000366-79-9	38
2	3,6,9,12,15-Pentaoxonadecan-1-ol	294	C14H30O6	001786-94-3	35
3	Dibutyl 3,6,9,12,15,18-hexaoxaic...	466	C22H42O10	1000366-80-0	35
4	Orthoformic acid, tri-sec-butyl ...	232	C13H28O3	016754-48-6	27
5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100117\
Data File : BF098987.D
Acq On : 1 Oct 2017 12:57
Operator : SJ/JU
Sample : I5457-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-1_092617

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
Butane, 2-methoxy...	2.22	11.6	ng	450321	1	6.90	779549	20.0
2-Pentanone, 4-hy...	5.13	6.8	ng	265491	1	6.90	779549	20.0
unknown6.67	6.67	71.0	ng	2767620	1	6.90	779549	20.0
n-Nonadecanol-1	12.46	4.5	ng	253157	4	11.43	1116830	20.0
unknown12.69	12.69	3.1	ng	174410	4	11.43	1116830	20.0