

Data Path : U:\HPCHEM1\BNA F\DATA\BF101816\
 Data File : BF090629.D
 Acq On : 18 Oct 2016 15:51
 Operator : UM/SJ
 Sample : H5304-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-TP

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-BF101316.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	5.080	237	240	246	rBV	589061	822071	19.77%	1.401%
2	5.503	274	277	279	rBV	3222503	3241921	77.95%	5.526%
3	6.531	364	367	376	rBV	3307960	3619959	87.04%	6.171%
4	6.669	376	379	381	rBV	3592161	3777886	90.84%	6.440%
5	6.771	386	388	397	rVB5	30078	72082	1.73%	0.123%
6	6.897	397	399	410	rBV	1435172	1428667	34.35%	2.435%
7	7.057	410	413	415	rBV	2873507	2848994	68.50%	4.857%
8	7.457	446	448	451	rBV	1582584	1976688	47.53%	3.370%
9	7.549	454	456	464	rVB	66634	135945	3.27%	0.232%
10	7.926	484	489	491	rBV2	47591	81831	1.97%	0.139%
11	8.189	509	512	514	rBV	1988815	2017872	48.52%	3.440%
12	9.263	604	606	609	rBV	4104229	3682396	88.54%	6.277%
13	9.343	612	613	618	rVB3	29501	62302	1.50%	0.106%
14	9.606	634	636	639	rBV	25802	60988	1.47%	0.104%
15	9.663	639	641	643	rVV	383012	458465	11.02%	0.782%
16	9.800	651	653	655	rBV	259055	263428	6.33%	0.449%
17	9.857	655	658	662	rVV2	108949	228769	5.50%	0.390%
18	9.949	663	666	667	rVV	1744357	2035543	48.94%	3.470%
19	9.972	667	668	670	rVB	70805	72505	1.74%	0.124%
20	10.143	681	683	686	rBV3	54978	73267	1.76%	0.125%
21	10.372	702	703	708	rVB2	71642	98866	2.38%	0.169%
22	10.452	708	710	712	rBV2	35336	48199	1.16%	0.082%
23	10.486	712	713	717	rVB	45633	64008	1.54%	0.109%
24	10.600	720	723	726	rBV2	55854	95828	2.30%	0.163%
25	10.738	732	735	737	rBV2	1367332	1934023	46.50%	3.297%
26	10.852	743	745	751	rVB	167247	209903	5.05%	0.358%
27	11.046	759	762	763	rBV3	31815	43813	1.05%	0.075%
28	11.240	777	779	781	rBV	38732	46948	1.13%	0.080%
29	11.298	781	784	785	rBV2	86224	102704	2.47%	0.175%
30	11.332	785	787	790	rVB	59057	73196	1.76%	0.125%
31	11.435	793	796	800	rBV2	1587738	2658841	63.93%	4.532%
32	11.503	800	802	804	rVB	198475	212803	5.12%	0.363%
33	11.663	813	816	820	rBV3	58906	152664	3.67%	0.260%
34	11.732	820	822	823	rVV	53421	70377	1.69%	0.120%

Data Path : U:\HPCHEM1\BNA F\DATA\BF101816\
Data File : BF090629.D
Acq On : 18 Oct 2016 15:51
Operator : UM/SJ
Sample : H5304-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-TP

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-BF101316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.938	837	840	841	rBV	107065	152865	3.68%	0.261%
36	11.961	841	842	844	rVV	251726	246327	5.92%	0.420%
37	12.006	844	846	848	rVV2	59184	107661	2.59%	0.184%
38	12.041	848	849	854	rVB	212789	375337	9.02%	0.640%
39	12.258	863	868	871	rBV2	95683	256124	6.16%	0.437%
40	12.486	886	888	889	rBV	141431	163316	3.93%	0.278%
41	12.521	889	891	893	rVV	99574	136793	3.29%	0.233%
42	12.566	893	895	899	rVB2	176363	207399	4.99%	0.354%
43	12.646	900	902	905	rBV	2488552	2279066	54.80%	3.885%
44	12.738	909	910	912	rBV	133724	163450	3.93%	0.279%
45	12.875	918	922	925	rBV	2433135	2604579	62.63%	4.440%
46	13.024	932	935	937	rBV	2249945	2606956	62.68%	4.444%
47	13.092	939	941	943	rBV2	121587	184419	4.43%	0.314%
48	13.252	953	955	958	rBV4	93850	172451	4.15%	0.294%
49	13.309	958	960	964	rBV	198342	267502	6.43%	0.456%
50	13.401	966	968	969	rVB	101513	92869	2.23%	0.158%
51	13.435	969	971	973	rBV	91260	127753	3.07%	0.218%
52	13.709	993	995	998	rBV	214157	278743	6.70%	0.475%
53	13.824	1003	1005	1006	rBV	155582	231690	5.57%	0.395%
54	13.926	1012	1014	1019	rVB	244303	366353	8.81%	0.625%
55	14.075	1024	1027	1034	rVV2	2009704	4158878	100.00%	7.089%
56	14.464	1059	1061	1063	rBV	174703	218215	5.25%	0.372%
57	15.127	1116	1119	1123	rBV	1281739	2936221	70.60%	5.005%
58	15.424	1142	1145	1148	rVB	719693	1136178	27.32%	1.937%
59	15.481	1148	1150	1153	rVV	1062659	1642389	39.49%	2.800%
60	15.549	1153	1156	1166	rVB2	1209609	2882378	69.31%	4.913%
61	17.001	1280	1283	1288	rVB2	428571	949284	22.83%	1.618%
62	17.435	1318	1321	1330	rVB	407529	943618	22.69%	1.609%

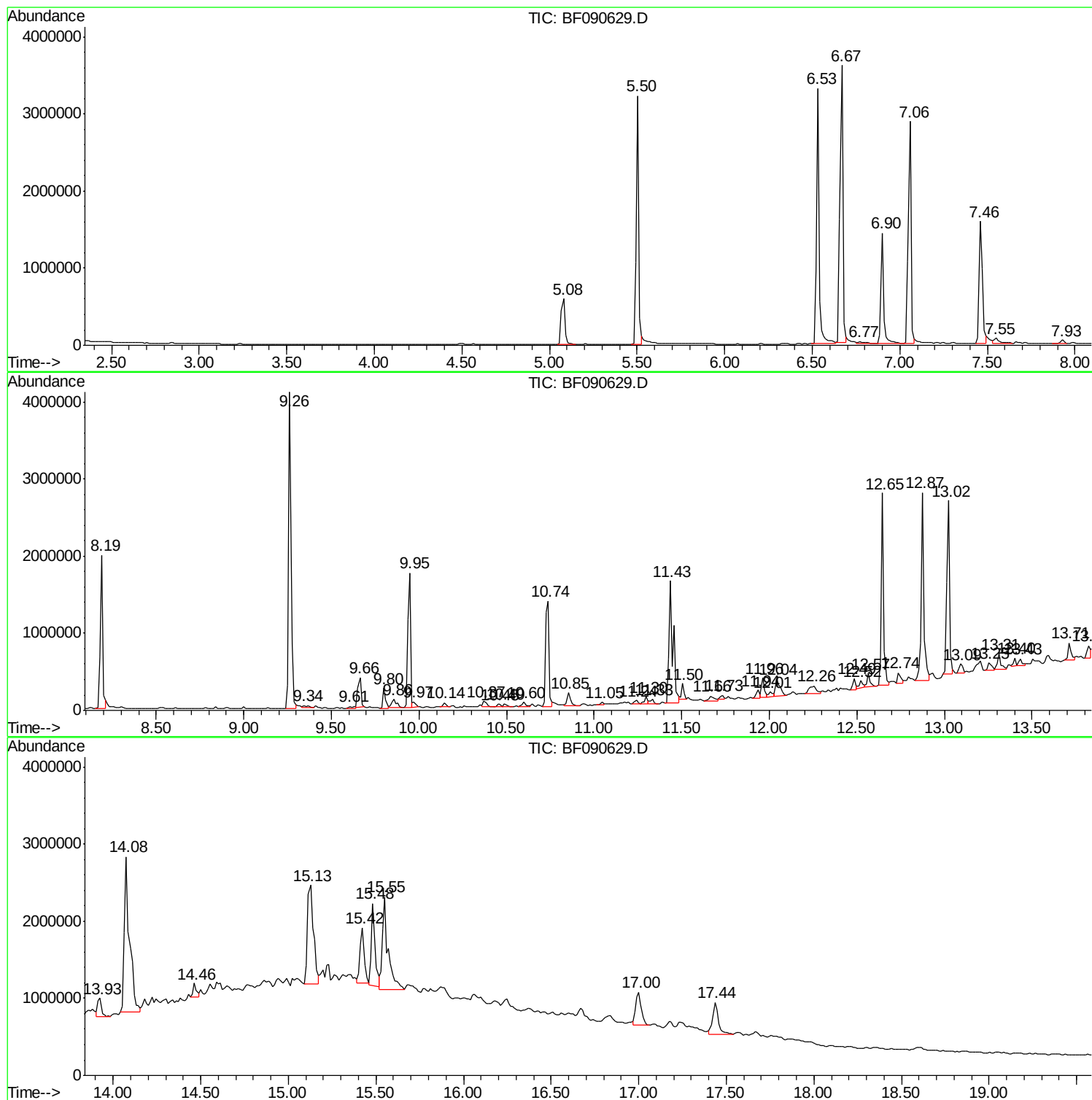
Sum of corrected areas: 58662566

Data Path : U:\HPCHEM1\BNA F\DATA\BF101816\
Data File : BF090629.D
Acq On : 18 Oct 2016 15:51
Operator : UM/SJ
Sample : H5304-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-TP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : U:\HPCHEM1\BNA_F\DATA\BF101816\
Data File : BF090629.D
Acq On : 18 Oct 2016 15:51
Operator : UM/SJ
Sample : H5304-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

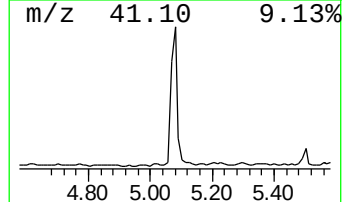
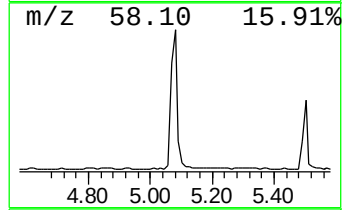
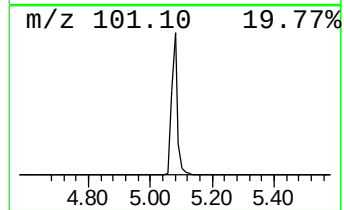
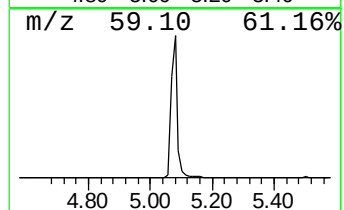
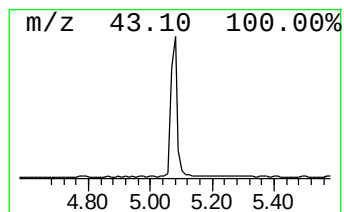
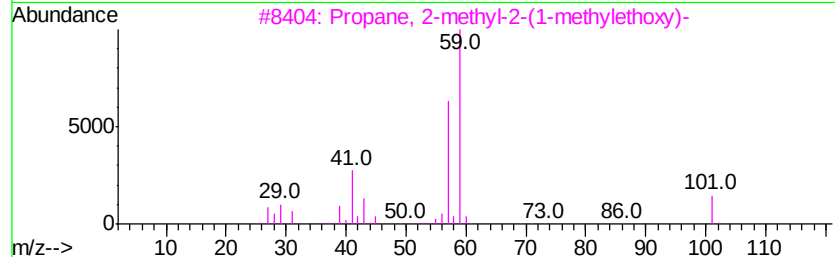
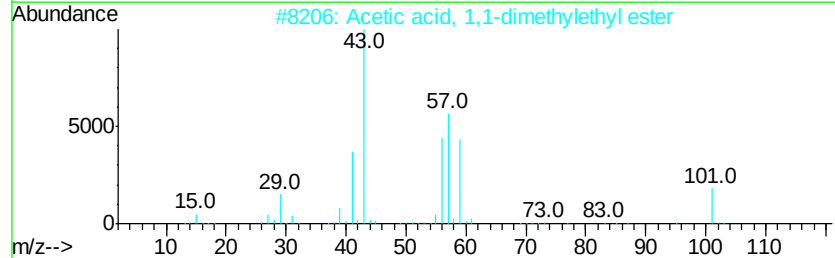
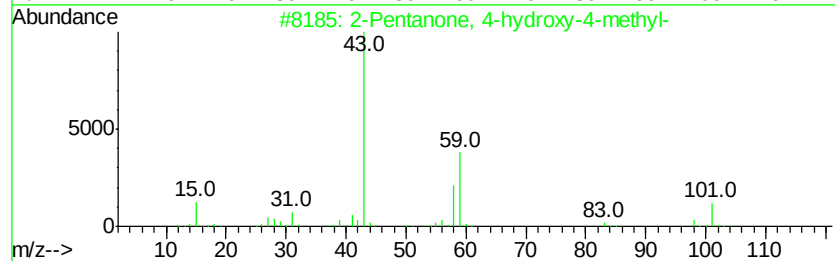
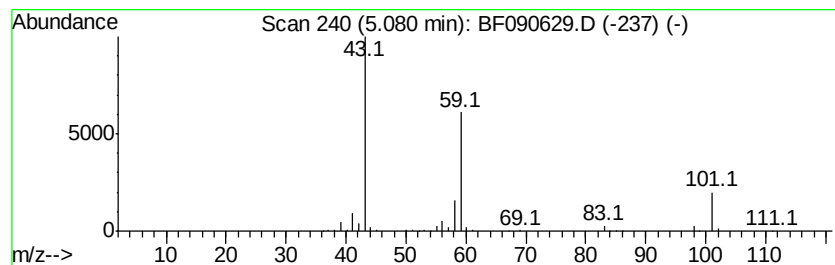
Instrument :
BNA_F
ClientSampleId :
COMP-TP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.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.	
5.08	11.51 ng	822071	1,4-Dichlorobenzene-d4	6.90	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : U:\HPCHEM1\BNA F\DATA\BF101816\
Data File : BF090629.D
Acq On : 18 Oct 2016 15:51
Operator : UM/SJ
Sample : H5304-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-TP

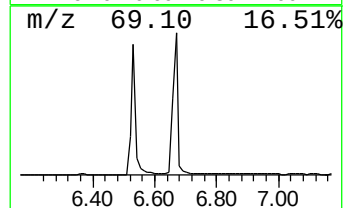
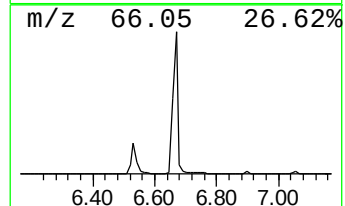
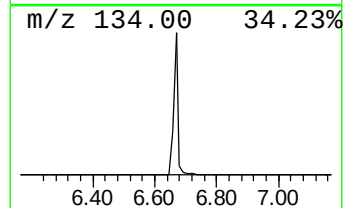
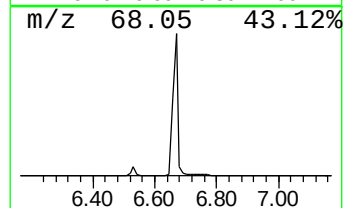
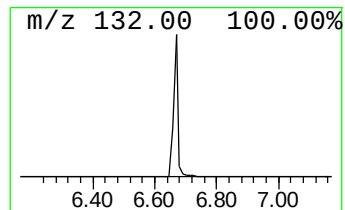
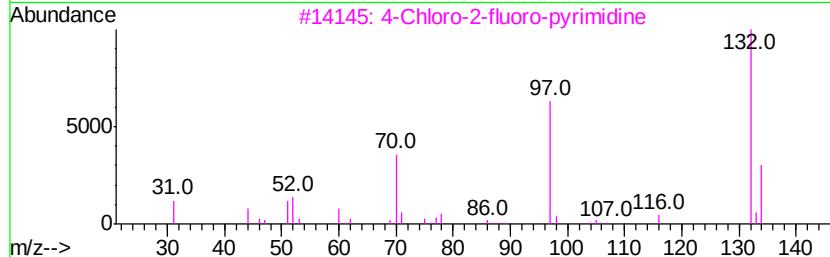
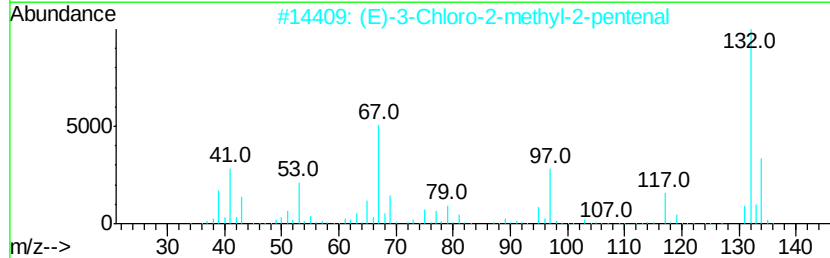
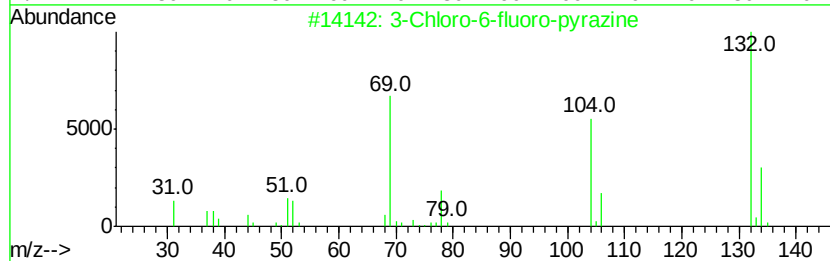
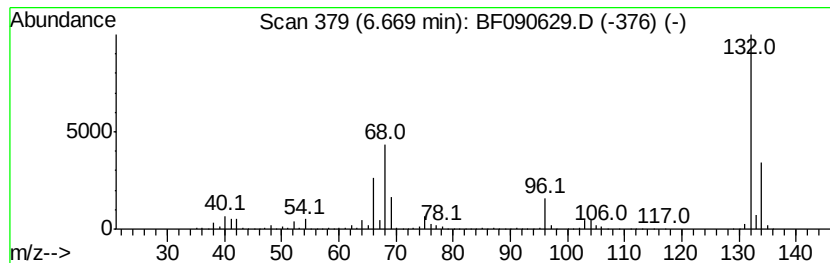
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	52.89 ng	3777890	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	9
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



Data Path : U:\HPCHEM1\BNA F\DATA\BF101816\
Data File : BF090629.D
Acq On : 18 Oct 2016 15:51
Operator : UM/SJ
Sample : H5304-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-TP

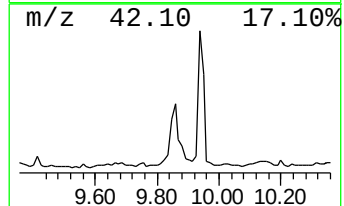
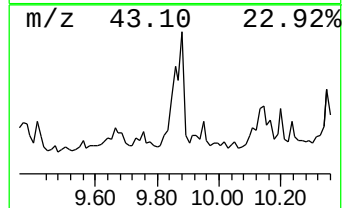
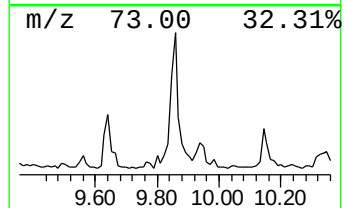
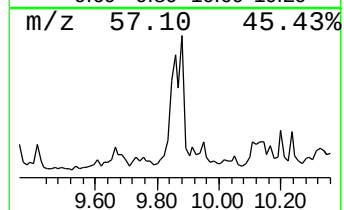
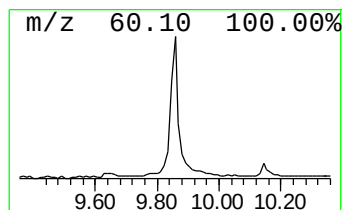
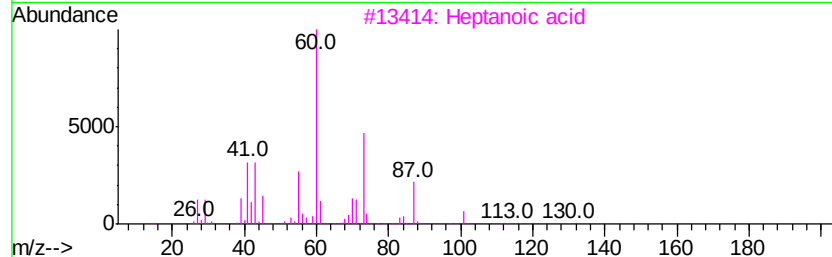
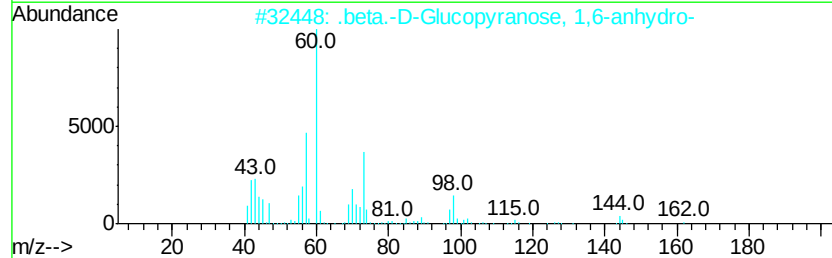
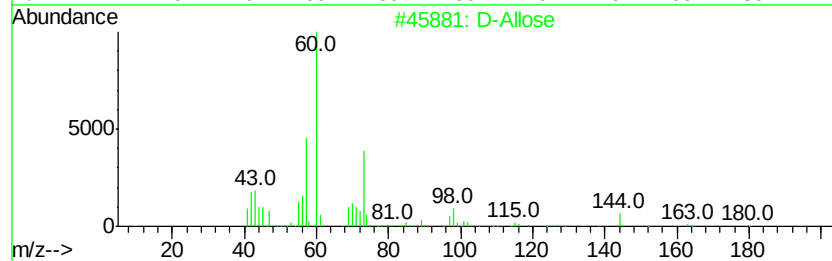
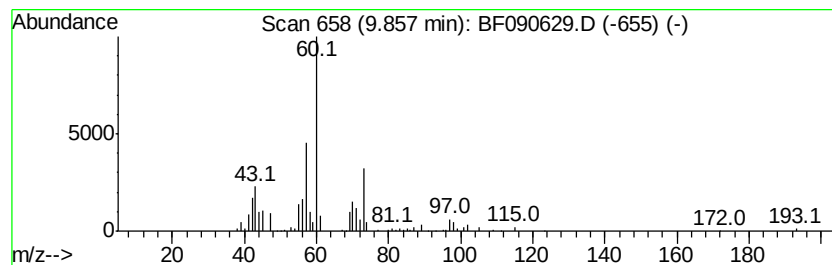
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 D-Allose Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.86	2.25 ng	228769	Acenaphthene-d10	9.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	D-Allose	180	C6H12O6	002595-97-3	90
2		.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	86
3		Heptanoic acid	130	C7H14O2	000111-14-8	59
4		Hexanoic acid	116	C6H12O2	000142-62-1	50
5		Butanoic acid	88	C4H8O2	000107-92-6	50



Data Path : U:\HPCHEM1\BNA_F\DATA\BF101816\
Data File : BF090629.D
Acq On : 18 Oct 2016 15:51
Operator : UM/SJ
Sample : H5304-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-TP

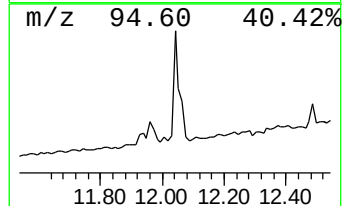
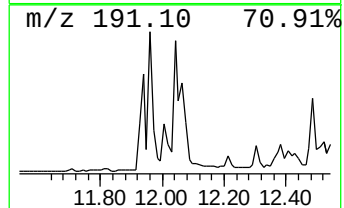
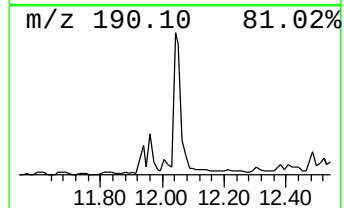
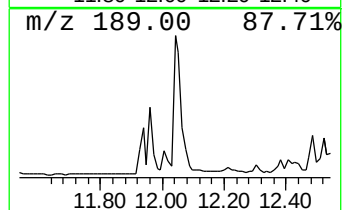
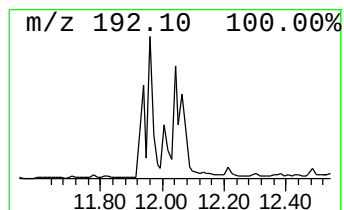
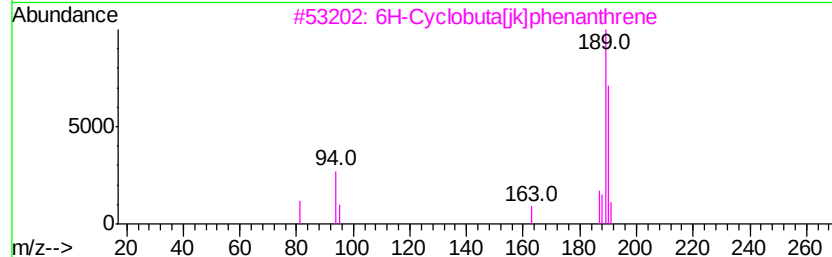
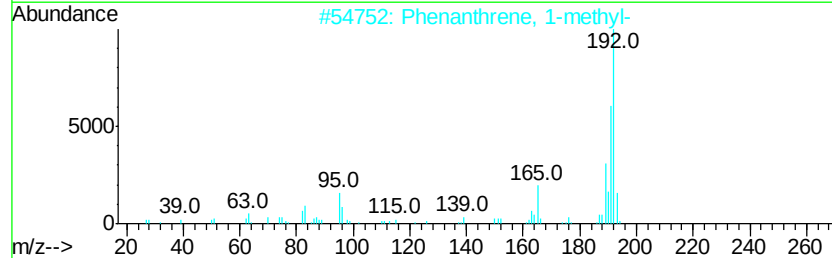
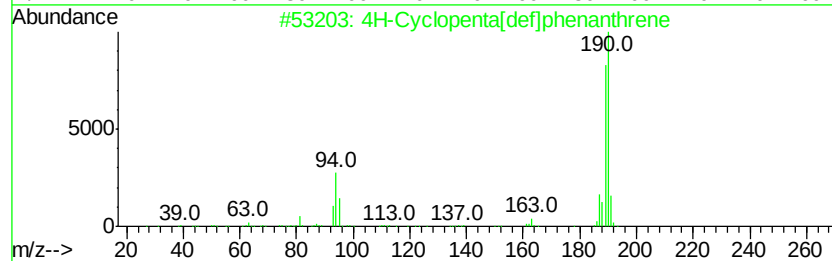
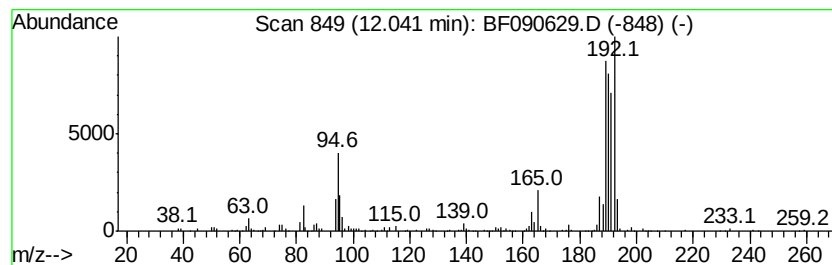
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	2.82 ng	375337	Phenanthrene-d10	11.43

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
2		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	56
3		6H-Cyclobuta[ik]phenanthrene	190	C15H10	083469-43-6	46
4		Naphtho[1,2-b]norborene	192	C15H12	1000210-14-8	42
5		Anthracene, 2-methyl-	192	C15H12	000613-12-7	42



Data Path : U:\HPCHEM1\BNA_F\DATA\BF101816\
Data File : BF090629.D
Acq On : 18 Oct 2016 15:51
Operator : UM/SJ
Sample : H5304-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-TP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.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...	5.08	11.5	ng	822071	1	6.90	1428670	20.0
unknown6.67	6.67	52.9	ng	3777890	1	6.90	1428670	20.0
D-Allose	9.86	2.3	ng	228769	3	9.95	2035540	20.0
4H-Cyclopenta[def...	12.04	2.8	ng	375337	4	11.43	2658840	20.0