

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
 Data File : BF088648.D
 Acq On : 3 Jul 2016 14:35
 Operator : UM/SJ
 Sample : H3837-14
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C1.2-04

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-BF063016.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	1.850	21	23	34	rVB	53339	73849	2.89%	0.301%
2	2.661	90	94	97	rVB	99897	162961	6.37%	0.664%
3	3.004	121	124	136	rBV	65710	125718	4.91%	0.512%
4	4.947	291	294	298	rBV	193104	256696	10.03%	1.046%
5	5.381	329	332	334	rBV	2030604	2367377	92.53%	9.647%
6	6.422	419	423	425	rBV	1926803	2496917	97.59%	10.175%
7	6.547	431	434	437	rBV	2134739	2149892	84.03%	8.760%
8	6.787	452	455	456	rBV	594553	671327	26.24%	2.736%
9	6.936	466	468	471	rVB	1681614	1718362	67.16%	7.002%
10	7.347	501	504	506	rBV	1630658	1641665	64.16%	6.690%
11	8.067	564	567	569	rBV	1067796	934333	36.52%	3.807%
12	9.142	658	661	664	rVB	2408858	2503386	97.84%	10.201%
13	9.542	693	696	698	rVB	250199	271073	10.59%	1.105%
14	9.816	717	720	722	rBB	1163077	1034852	40.45%	4.217%
15	10.605	786	789	791	rBV	1581569	1720704	67.25%	7.012%
16	10.731	799	800	804	rBV	30378	36997	1.45%	0.151%
17	11.176	837	839	841	rBV	74748	70208	2.74%	0.286%
18	11.291	847	849	852	rVB	997669	1038607	40.59%	4.232%
19	11.839	894	897	898	rBV	32074	34720	1.36%	0.141%
20	12.879	985	988	991	rBV	2635287	2558532	100.00%	10.426%
21	13.862	1070	1074	1077	rBV	64126	192849	7.54%	0.786%
22	13.919	1077	1079	1081	rVB	1165282	1034074	40.42%	4.214%
23	14.502	1126	1130	1143	rBV	34357	121853	4.76%	0.497%
24	15.017	1172	1175	1177	rBV	23395	25667	1.00%	0.105%
25	15.314	1198	1201	1204	rBV	691030	799756	31.26%	3.259%
26	15.771	1238	1241	1246	rVB	17060	30063	1.18%	0.123%
27	16.823	1330	1333	1338	rVB	111188	194089	7.59%	0.791%
28	16.971	1340	1346	1351	rVB	36248	84419	3.30%	0.344%
29	17.337	1375	1378	1389	rBV6	10013	51909	2.03%	0.212%
30	18.114	1441	1446	1456	rVB8	8952	46271	1.81%	0.189%
31	19.074	1524	1530	1536	rBV2	27483	91745	3.59%	0.374%

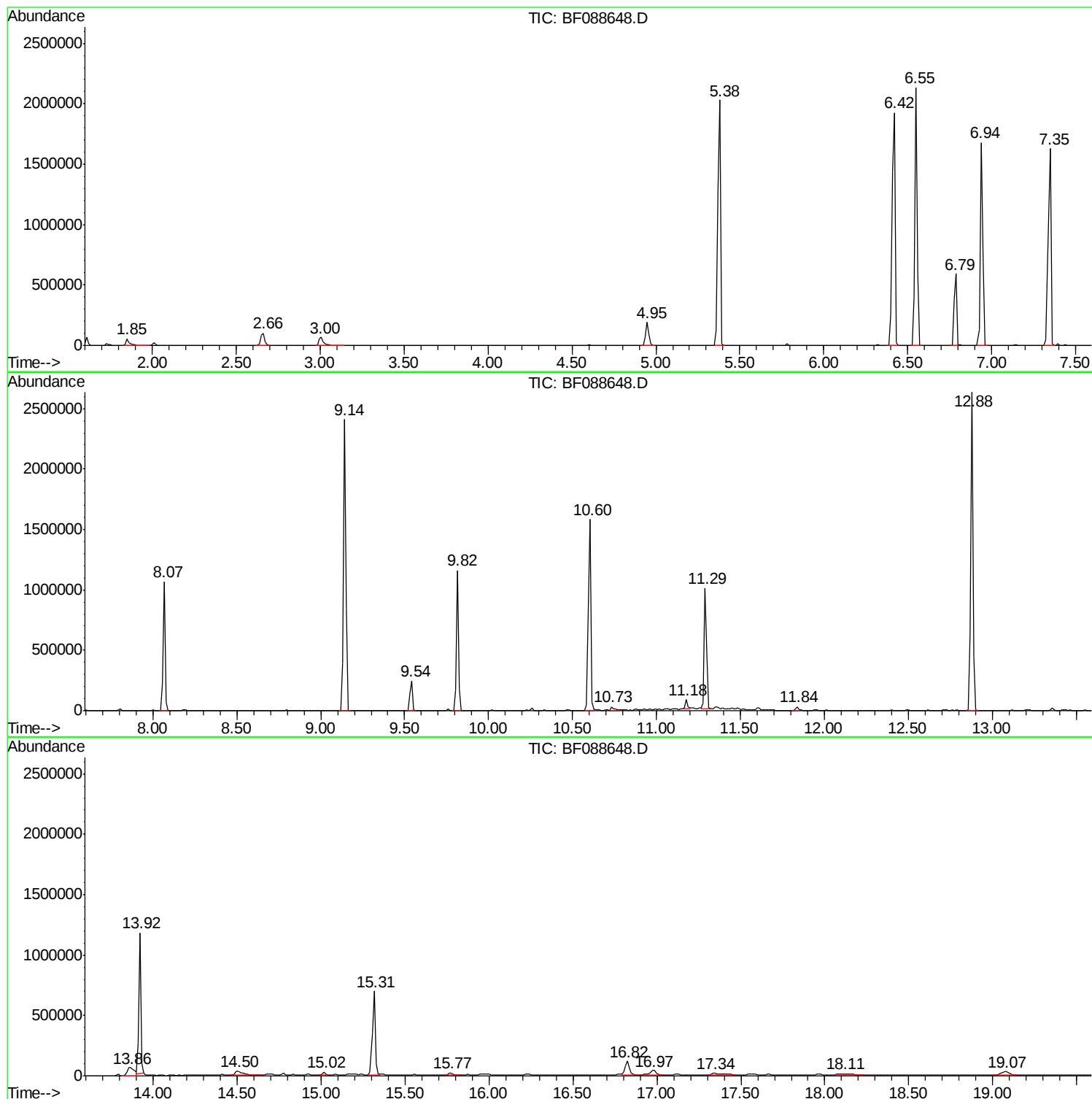
Sum of corrected areas: 24540871

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088648.D
Acq On : 3 Jul 2016 14:35
Operator : UM/SJ
Sample : H3837-14
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C1.2-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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\BF070316\
Data File : BF088648.D
Acq On : 3 Jul 2016 14:35
Operator : UM/SJ
Sample : H3837-14
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C1.2-04

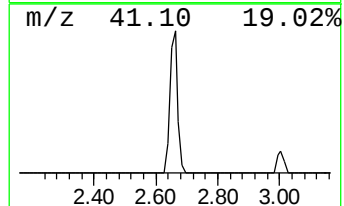
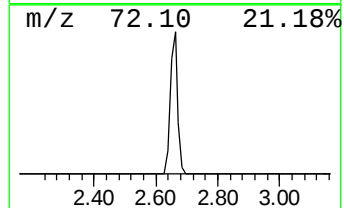
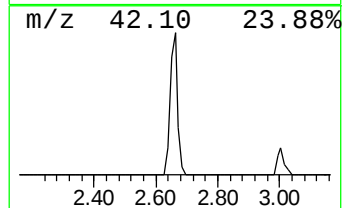
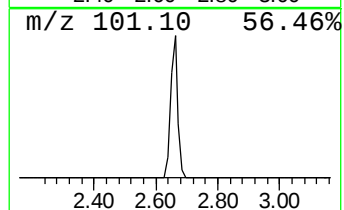
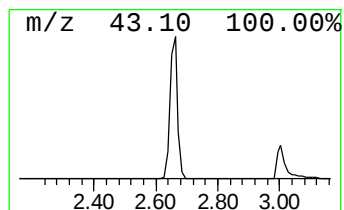
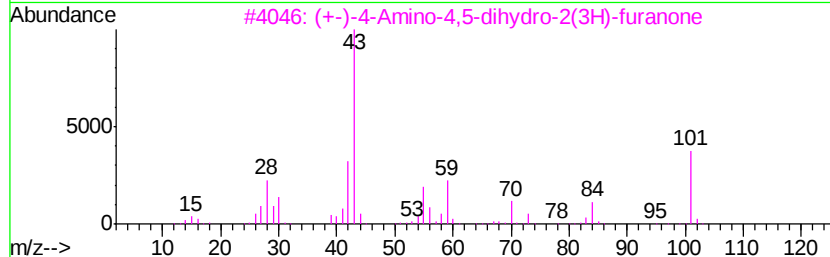
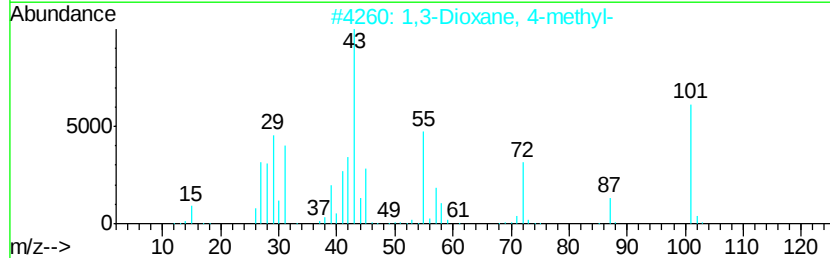
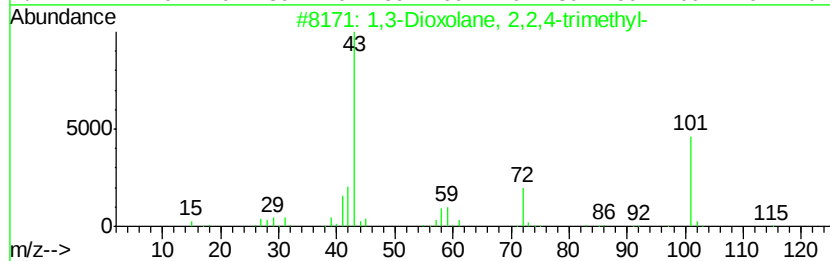
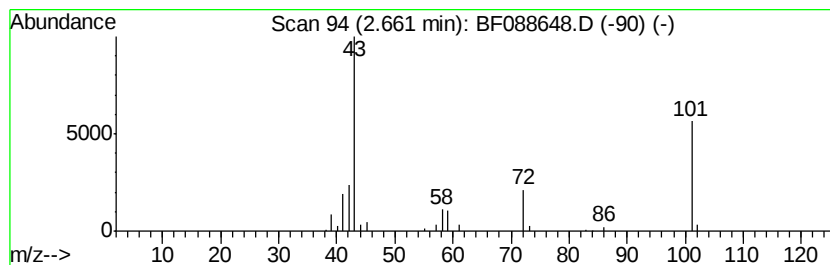
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.66	4.85 ng	162961	1,4-Dichlorobenzene-d4	6.79

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2		1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	56
3		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	9
4		2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	9
5		2-Butanone	72	C4H8O	000078-93-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088648.D
Acq On : 3 Jul 2016 14:35
Operator : UM/SJ
Sample : H3837-14
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C1.2-04

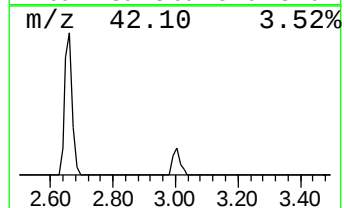
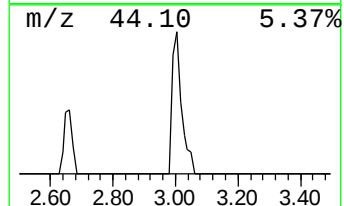
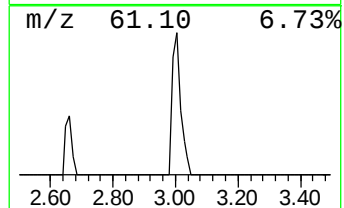
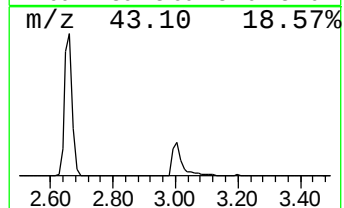
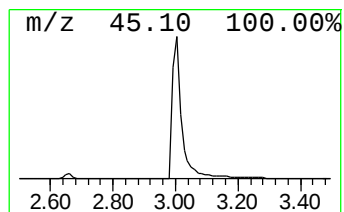
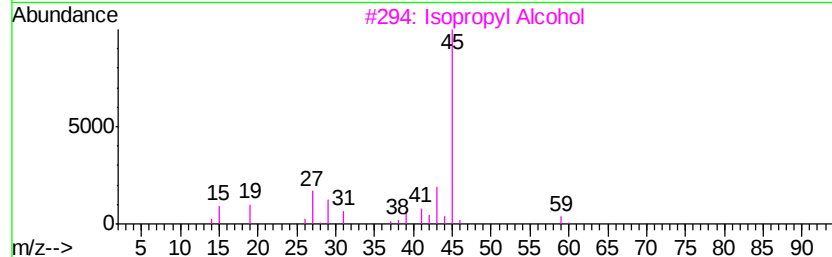
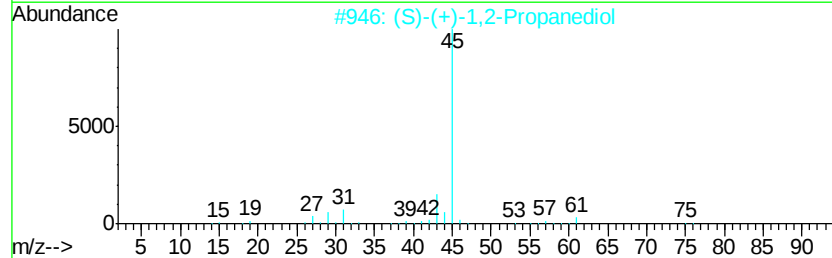
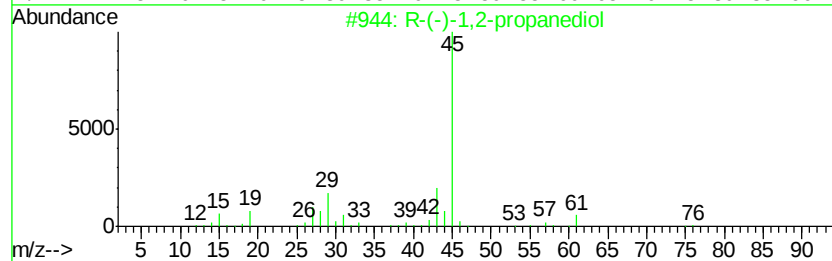
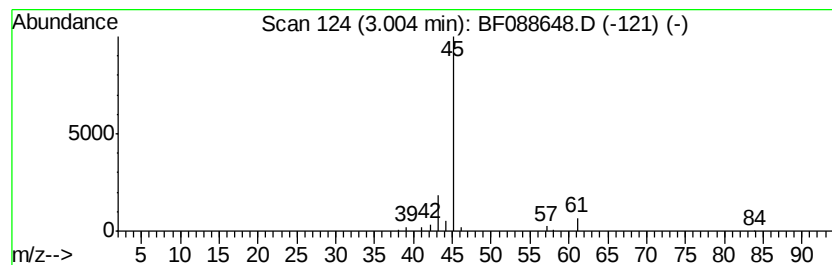
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 R-(-)-1,2-propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	3.75 ng	125718	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4		Propylene Glycol	76	C3H8O2	000057-55-6	9
5		Formamide	45	CH3NO	000075-12-7	5



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088648.D
Acq On : 3 Jul 2016 14:35
Operator : UM/SJ
Sample : H3837-14
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C1.2-04

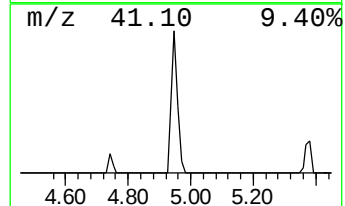
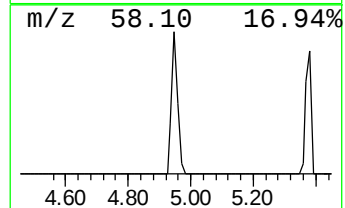
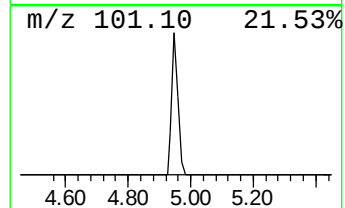
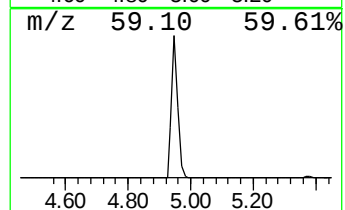
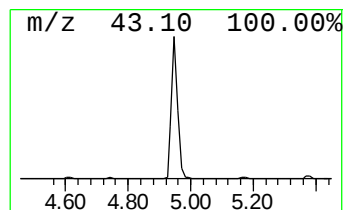
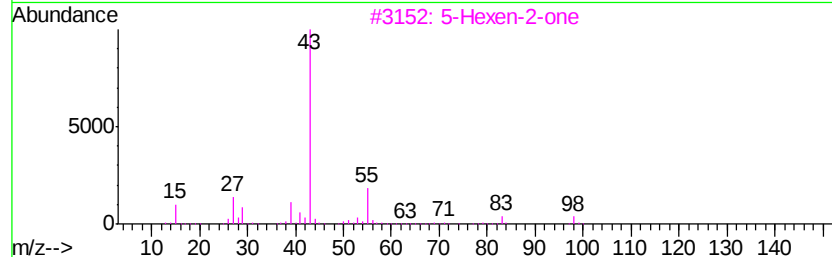
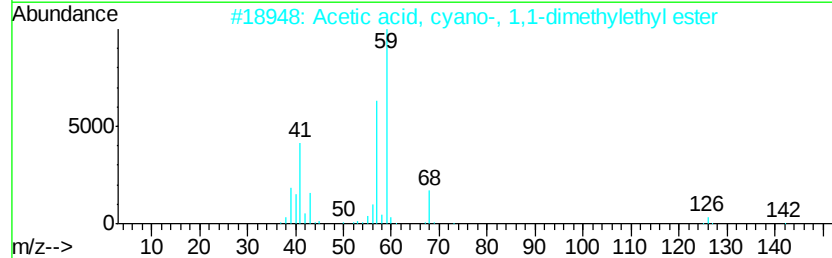
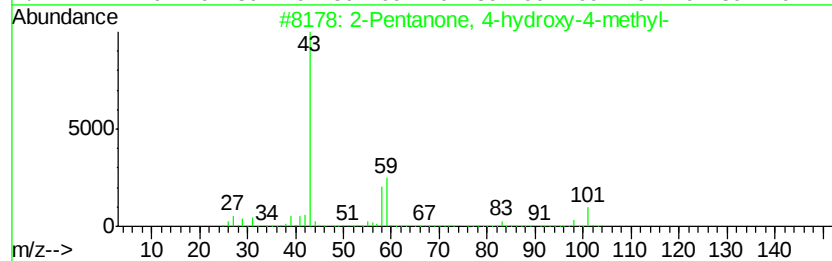
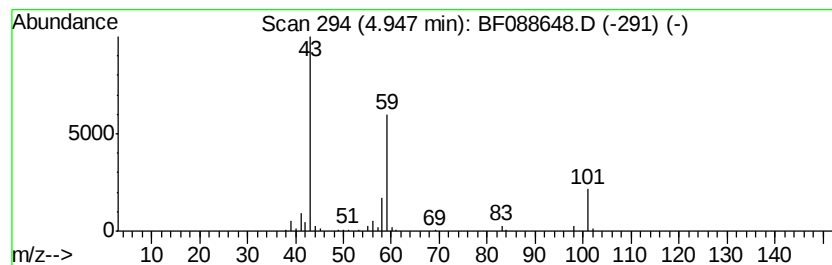
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	7.65 ng	256696	1,4-Dichlorobenzene-d4	6.79

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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088648.D
Acq On : 3 Jul 2016 14:35
Operator : UM/SJ
Sample : H3837-14
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C1.2-04

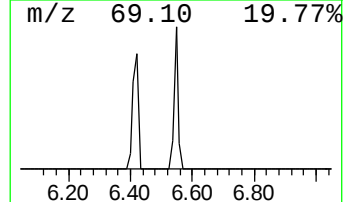
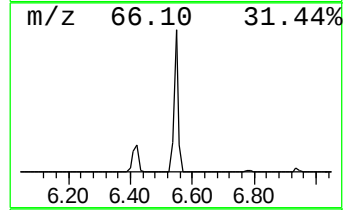
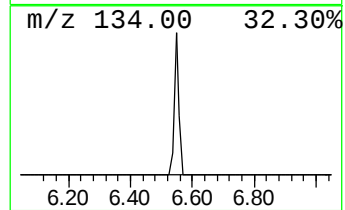
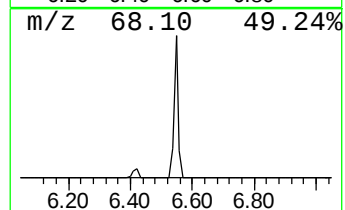
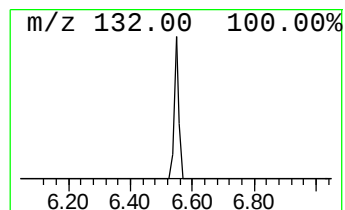
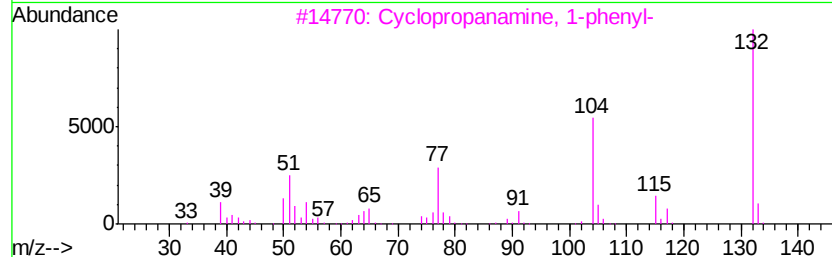
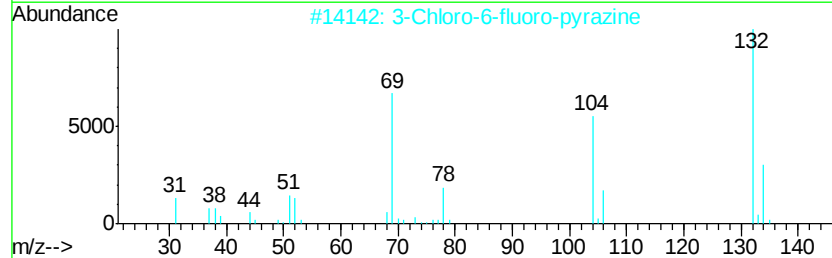
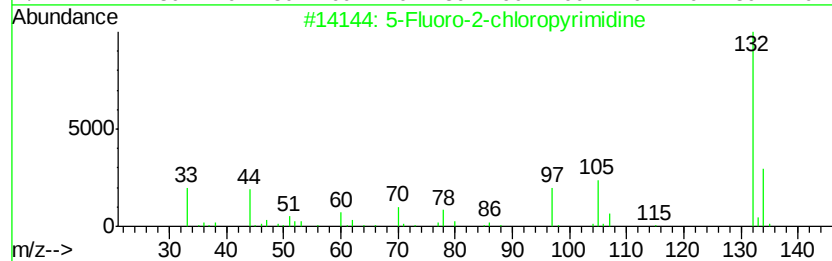
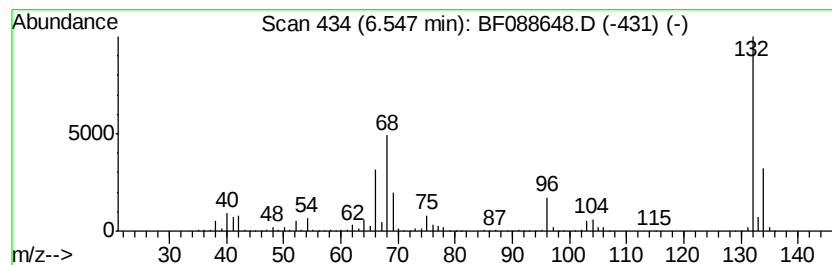
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	64.05 ng	2149890	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088648.D
Acq On : 3 Jul 2016 14:35
Operator : UM/SJ
Sample : H3837-14
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C1.2-04

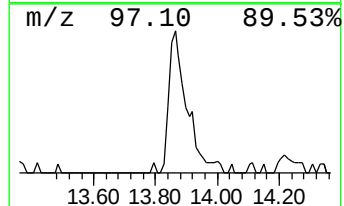
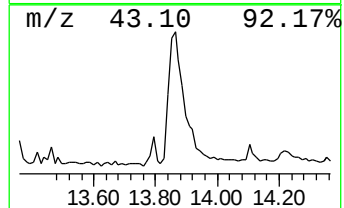
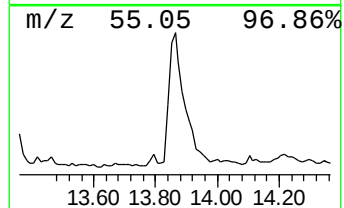
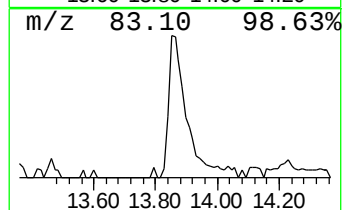
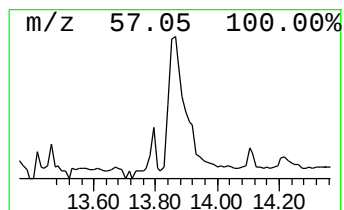
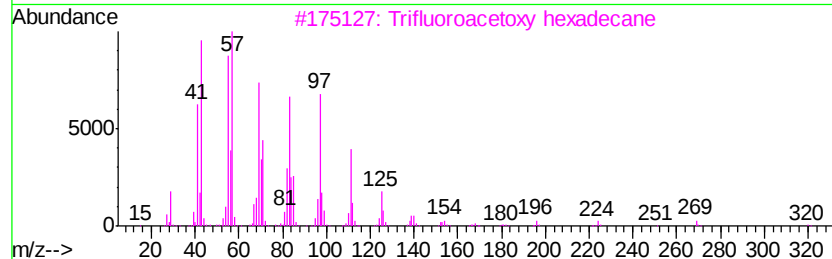
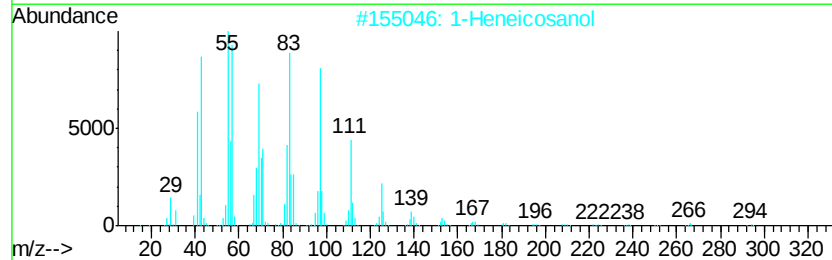
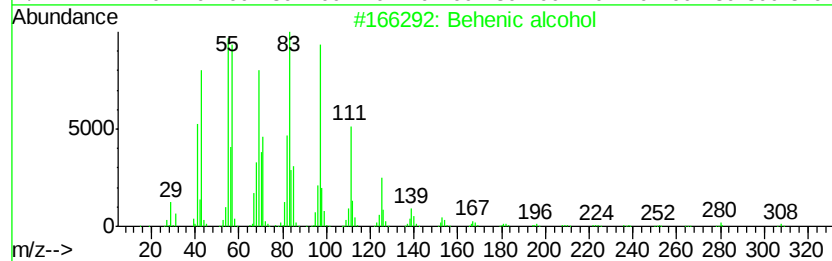
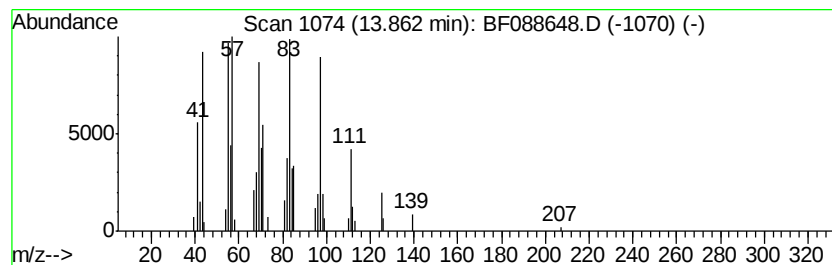
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Behenic alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	3.73 ng	192849	Chrysene-d12	13.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	93
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088648.D
Acq On : 3 Jul 2016 14:35
Operator : UM/SJ
Sample : H3837-14
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C1.2-04

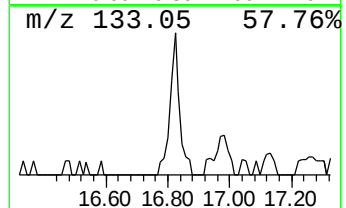
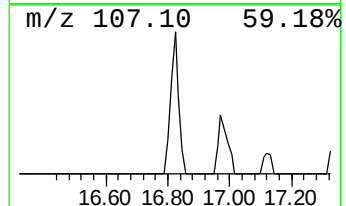
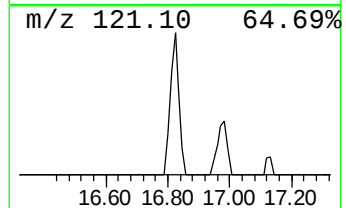
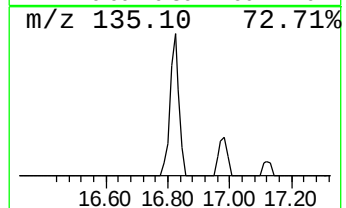
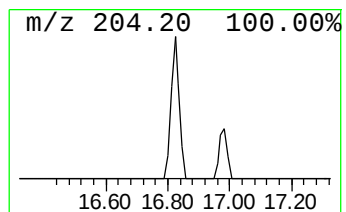
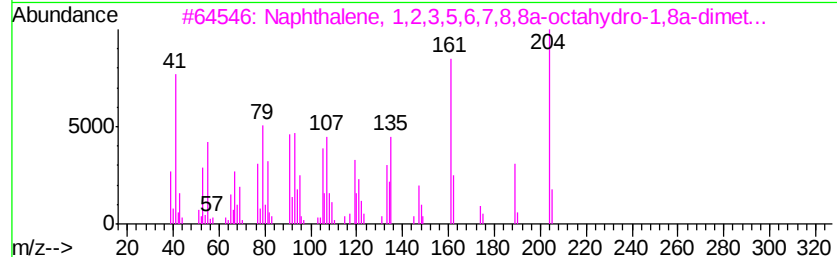
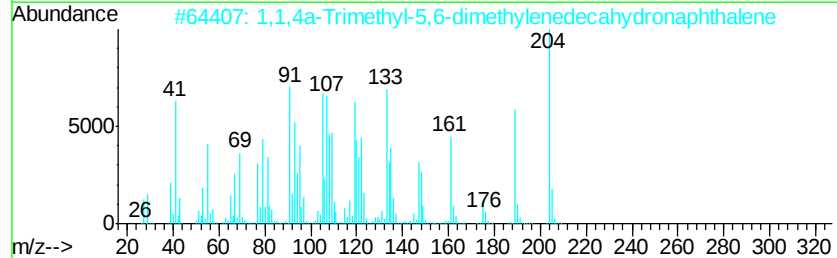
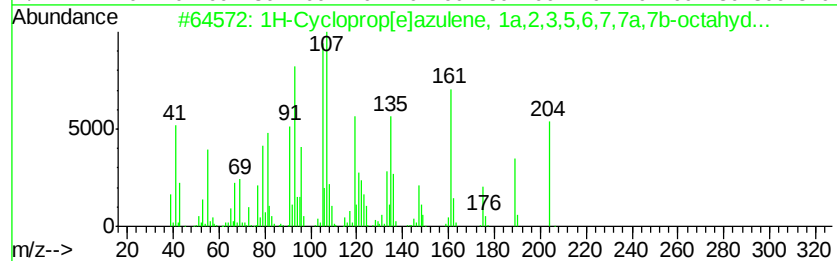
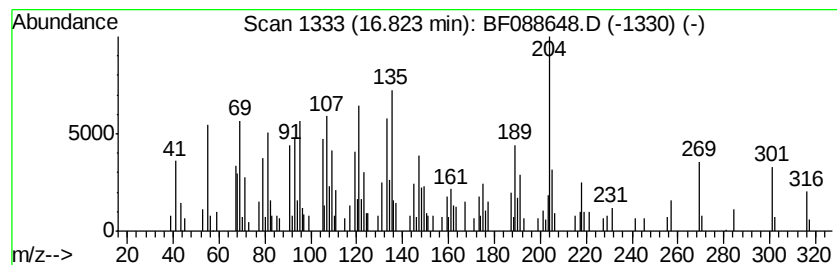
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1H-Cycloprop[e]azulene, 1a,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.82	4.85 ng	194089	Perylene-d12	15.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Cycloprop[elazulene, 1a,2,3,5...	204	C15H24	021747-46-6	78
2		1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	64
3		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	62
4		1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	58
5		Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	52



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088648.D
Acq On : 3 Jul 2016 14:35
Operator : UM/SJ
Sample : H3837-14
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C1.2-04

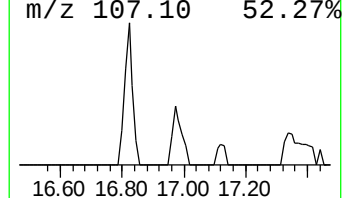
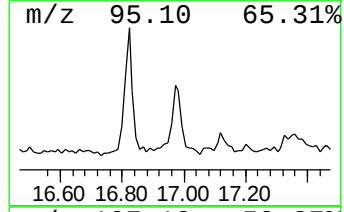
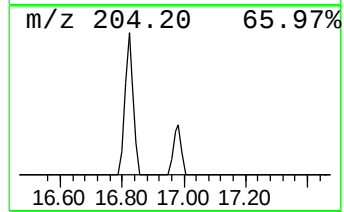
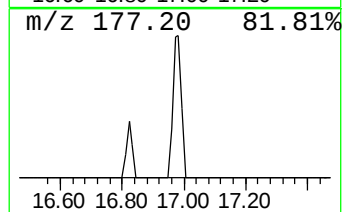
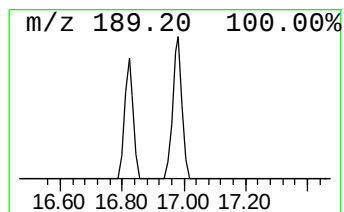
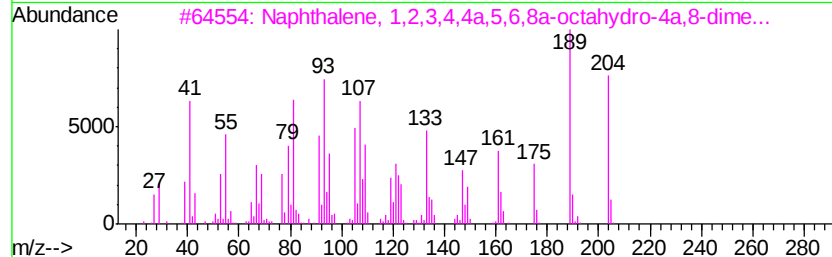
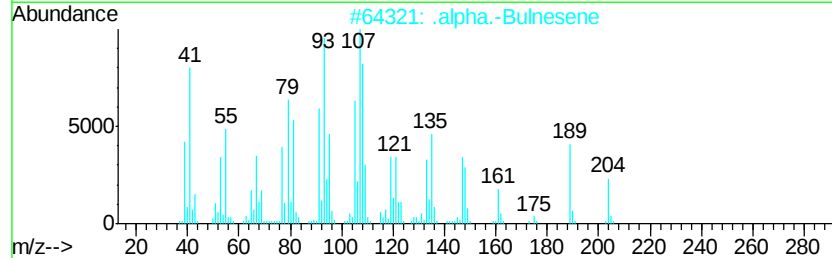
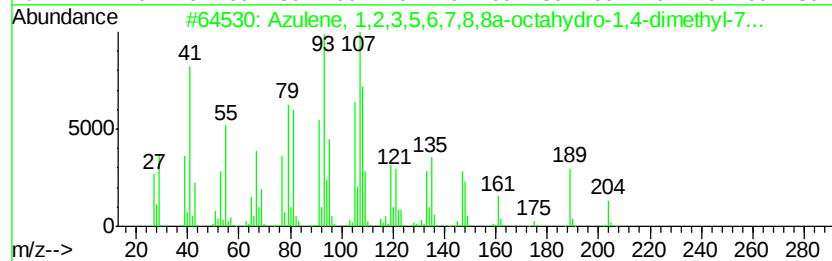
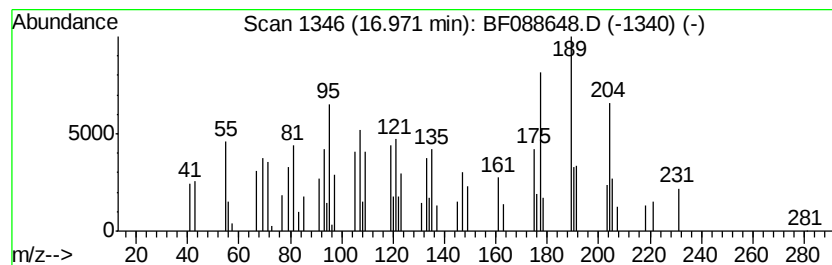
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Azulene, 1,2,3,5,6,7,8,8a-o... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.97	2.11 ng	84419	Perylene-d12	15.31

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	50
2			.alpha.-Bulnesene	204	C15H24	1000374-19-9	50
3			Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	45
4			.beta.-Humulene	204	C15H24	000116-04-1	38
5			5.beta.,7.beta.H,10.alpha.-Eudes...	222	C15H26O	025826-85-1	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088648.D
Acq On : 3 Jul 2016 14:35
Operator : UM/SJ
Sample : H3837-14
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C1.2-04

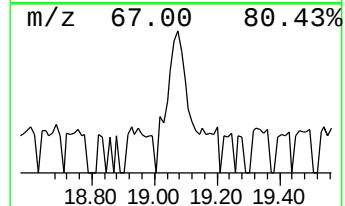
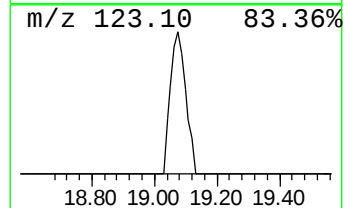
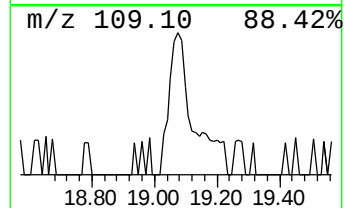
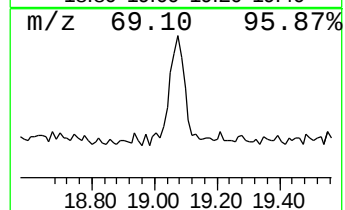
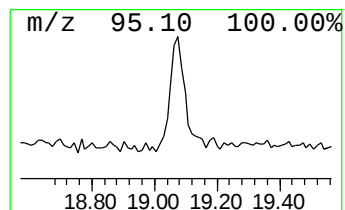
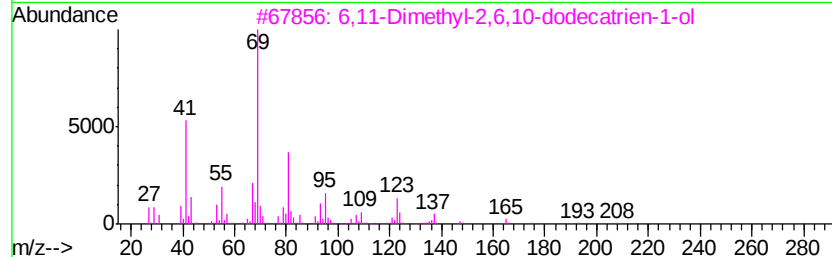
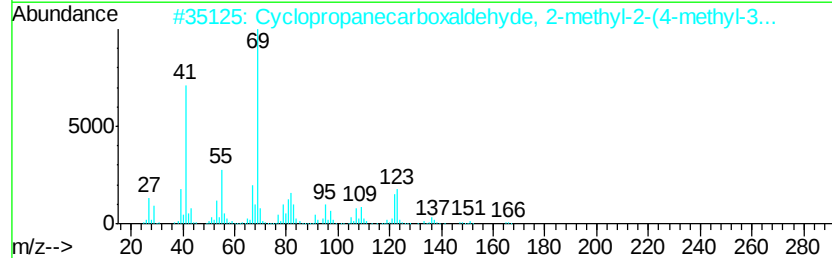
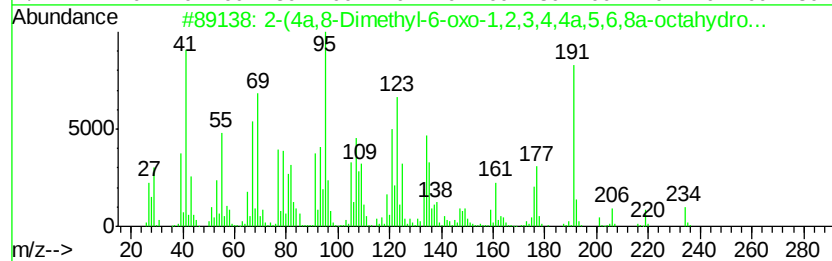
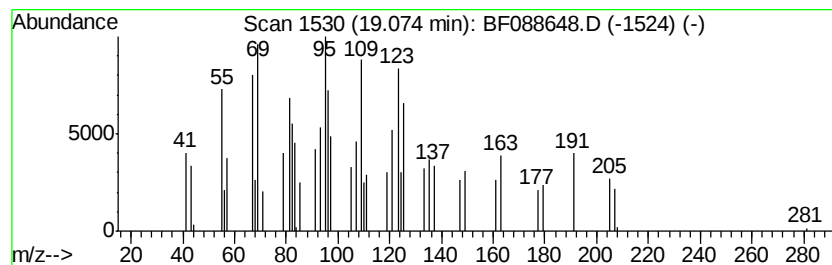
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown19.07 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.07	2.29 ng	91745	Perylene-d12	15.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-(4a,8-Dimethyl-6-oxo-1,2,3,4,4...	234	C15H22O2	1000190-21-8	38
2		Cyclopropanecarboxaldehyde, 2-me...	166	C11H18O	097231-35-1	35
3		6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	27
4		2-Methylbicyclo[3.2.1]octane	124	C9H16	1000215-28-0	22
5		2-(Fench-2-yl)fenchane	274	C20H34	1000105-83-1	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088648.D
Acq On : 3 Jul 2016 14:35
Operator : UM/SJ
Sample : H3837-14
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C1.2-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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
1,3-Dioxolane, 2,...	2.66	4.8	ng	162961	1	6.79	671327	20.0
R-(-)-1,2-propane...	3.00	3.8	ng	125718	1	6.79	671327	20.0
2-Pentanone, 4-hy...	4.95	7.7	ng	256696	1	6.79	671327	20.0
unknown6.55	6.55	64.0	ng	2149890	1	6.79	671327	20.0
Behenic alcohol	13.86	3.7	ng	192849	5	13.92	1034070	20.0
1H-Cycloprop[e]az...	16.82	4.8	ng	194089	6	15.31	799756	20.0
Azulene, 1,2,3,5,...	16.97	2.1	ng	84419	6	15.31	799756	20.0
unknown19.07	19.07	2.3	ng	91745	6	15.31	799756	20.0