

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071216\
 Data File : BF088926.D
 Acq On : 12 Jul 2016 16:23
 Operator : UM/SJ
 Sample : H3889-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-1

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-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	2.135	44	48	54	rBV	24158	79403	3.37%	0.702%
2	5.278	320	323	325	rBV	1022158	1027710	43.58%	9.088%
3	6.239	405	407	410	rVB	145284	131732	5.59%	1.165%
4	6.341	413	416	419	rBV	923088	925252	39.24%	8.182%
5	6.467	425	427	430	rVB	1157984	1027791	43.59%	9.088%
6	6.707	445	448	449	rBV	253009	304784	12.93%	2.695%
7	6.799	453	456	458	rBV	1837296	2056630	87.22%	18.186%
8	6.856	458	461	464	rVV	1582621	2358078	100.00%	20.851%
9	7.267	494	497	499	rBV	731423	625805	26.54%	5.534%
10	7.907	550	553	554	rBV3	38424	68195	2.89%	0.603%
11	7.942	554	556	558	rBV2	305044	294977	12.51%	2.608%
12	7.987	558	560	563	rVV	498816	522364	22.15%	4.619%
13	8.044	563	565	566	rVV	92991	88894	3.77%	0.786%
14	8.284	585	586	588	rVB2	114411	128061	5.43%	1.132%
15	8.353	590	592	593	rVV	248416	216428	9.18%	1.914%
16	8.456	598	601	603	rBV2	247998	398645	16.91%	3.525%
17	8.536	603	608	613	rBV6	147200	537426	22.79%	4.752%
18	8.627	613	616	618	rBV3	134454	311766	13.22%	2.757%
19	8.685	618	621	622	rBV3	114915	204999	8.69%	1.813%

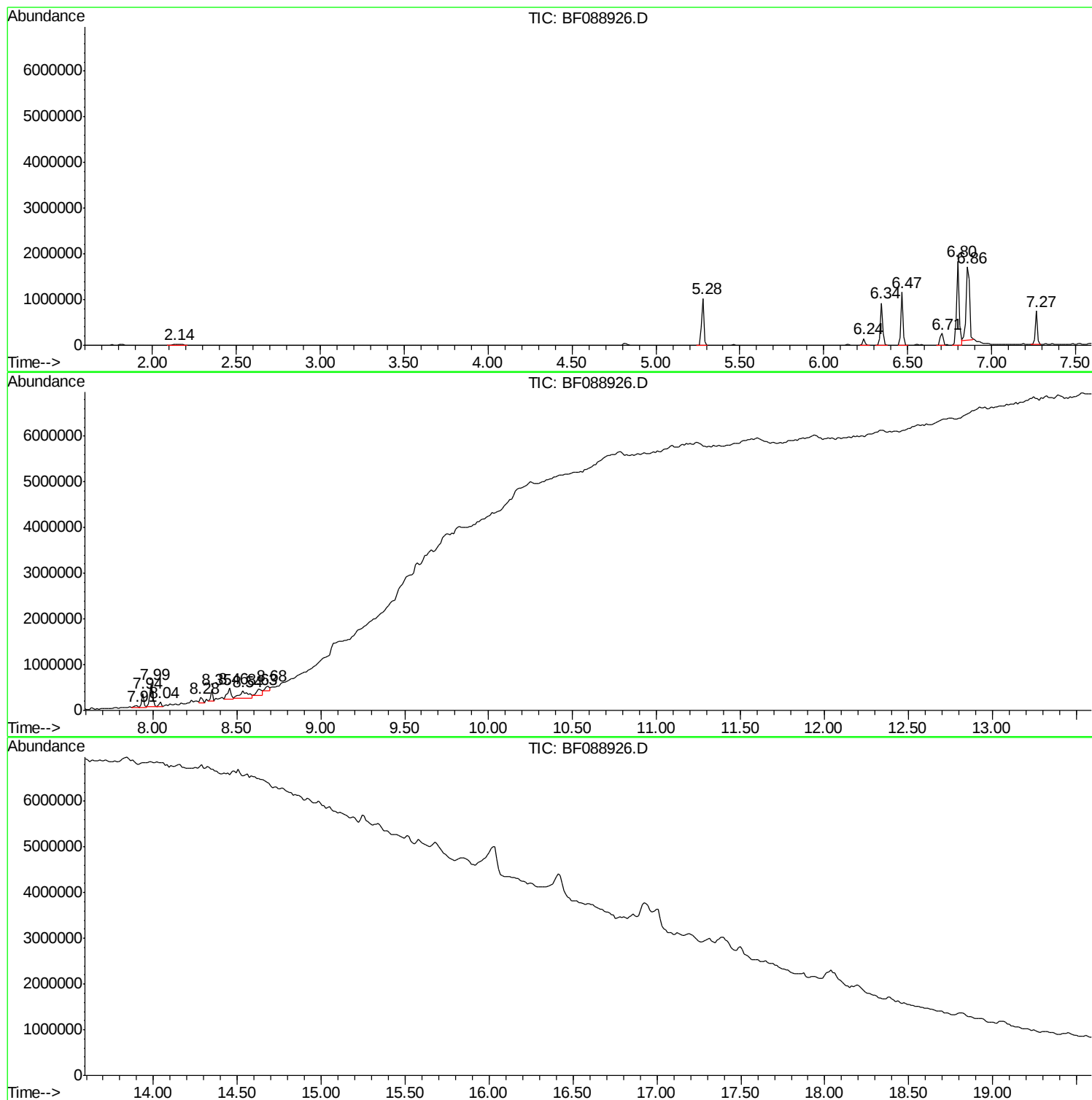
Sum of corrected areas: 11308940

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071216\
Data File : BF088926.D
Acq On : 12 Jul 2016 16:23
Operator : UM/SJ
Sample : H3889-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-1

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\BF071216\
Data File : BF088926.D
Acq On : 12 Jul 2016 16:23
Operator : UM/SJ
Sample : H3889-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-1

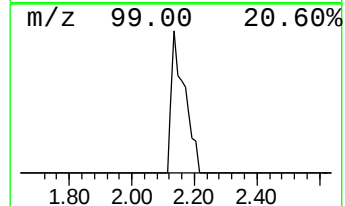
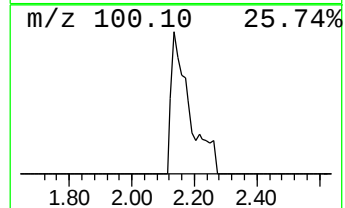
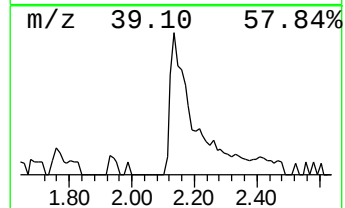
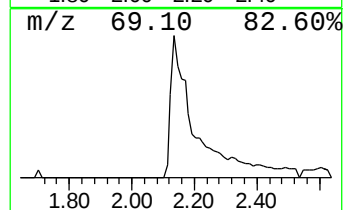
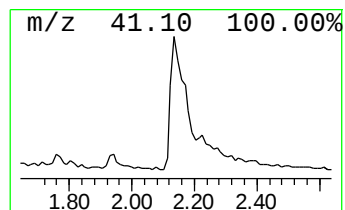
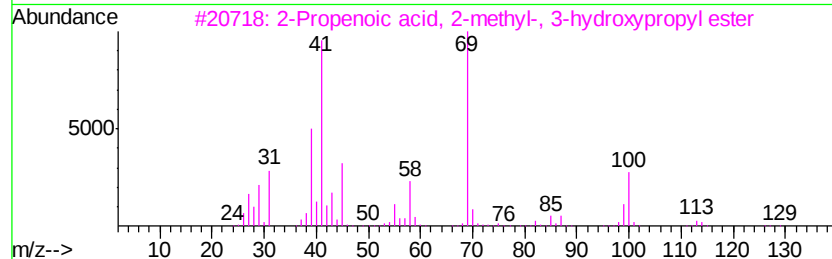
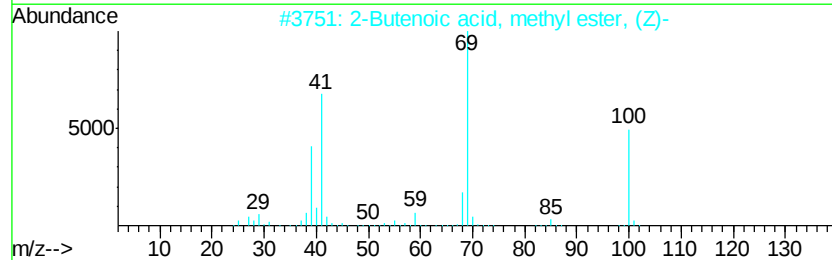
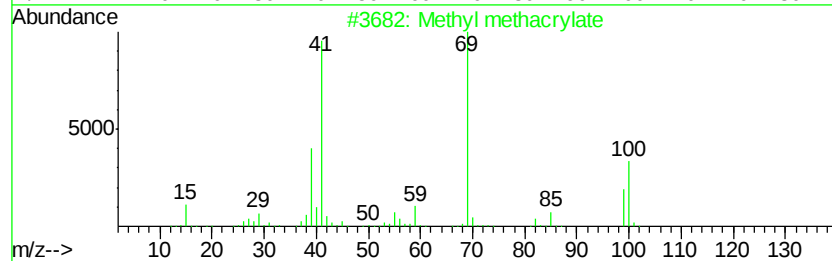
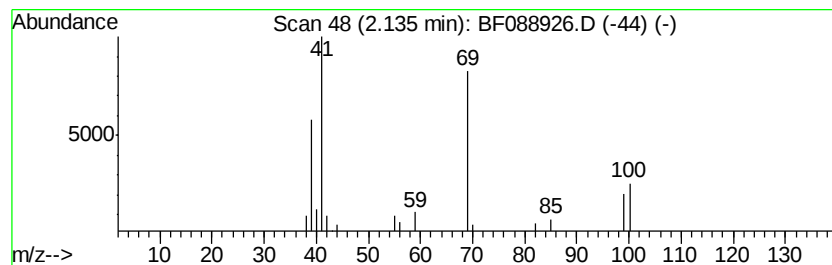
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Methyl methacrylate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	5.21 ng	79403	1,4-Dichlorobenzene-d4	6.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methyl methacrylate	100	C5H8O2	000080-62-6	91
2		2-Butenoic acid, methyl ester, (Z)-	100	C5H8O2	004358-59-2	72
3		2-Propenoic acid, 2-methyl-, 3-h...	144	C7H12O3	002761-09-3	72
4		2-Butenoic acid, ethyl ester, (Z)-	114	C6H10O2	006776-19-8	45
5		Cyclopropanecarboxylic acid, met...	100	C5H8O2	002868-37-3	40



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071216\
Data File : BF088926.D
Acq On : 12 Jul 2016 16:23
Operator : UM/SJ
Sample : H3889-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-1

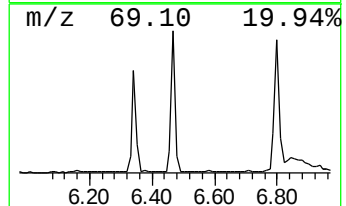
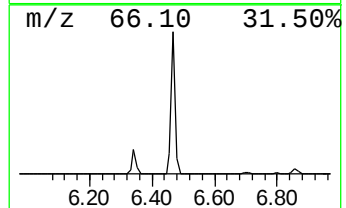
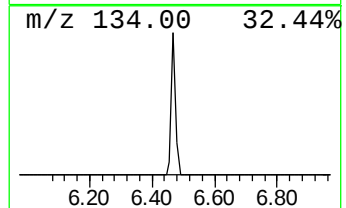
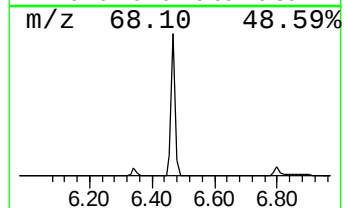
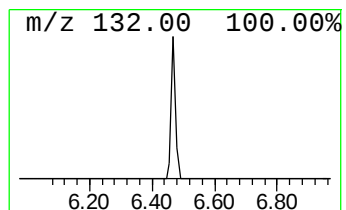
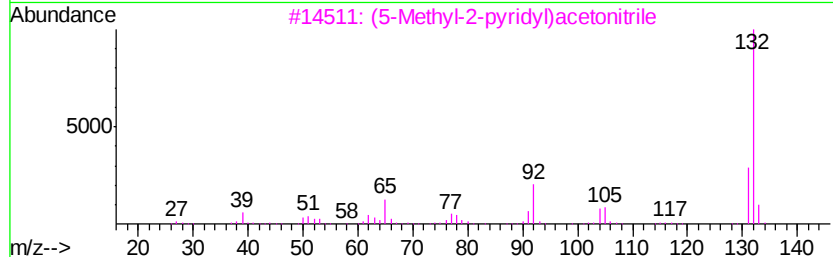
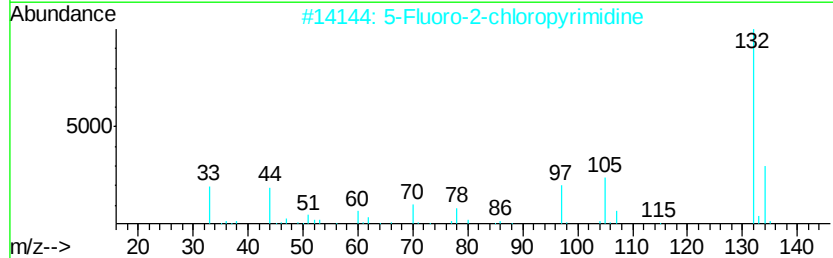
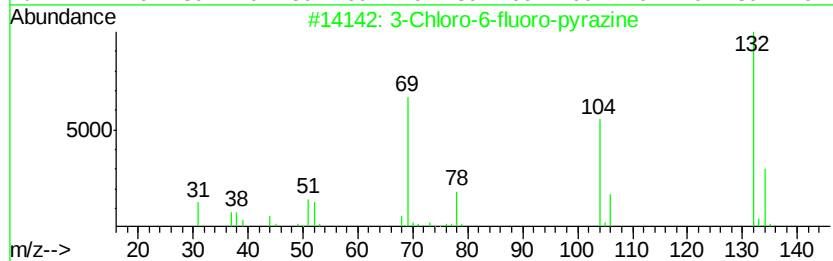
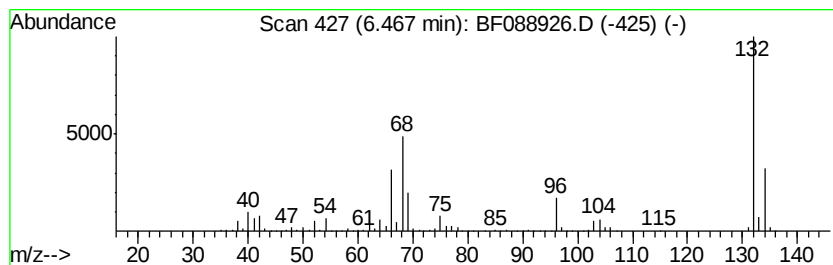
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.47 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	67.44 ng	1027790	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088926.D
Acq On : 12 Jul 2016 16:23
Operator : UM/SJ
Sample : H3889-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
SS-1

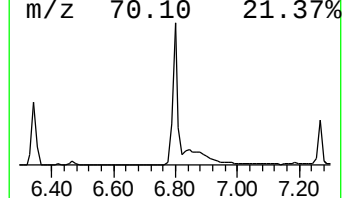
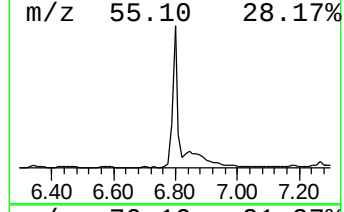
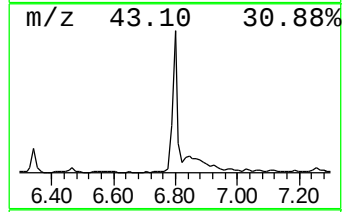
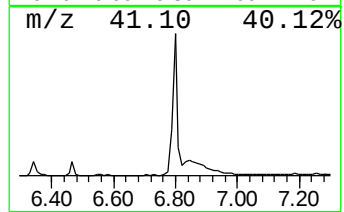
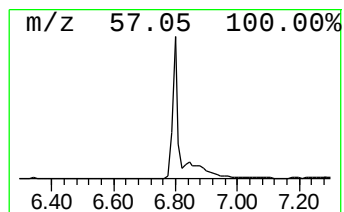
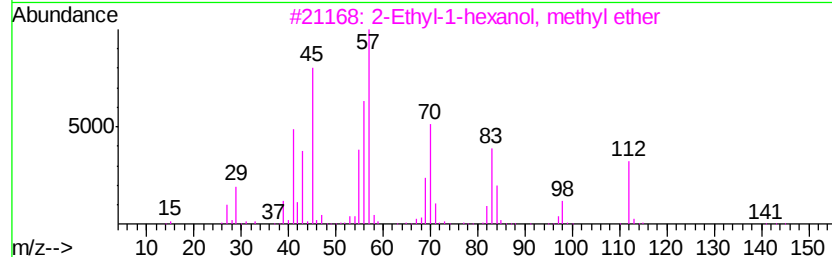
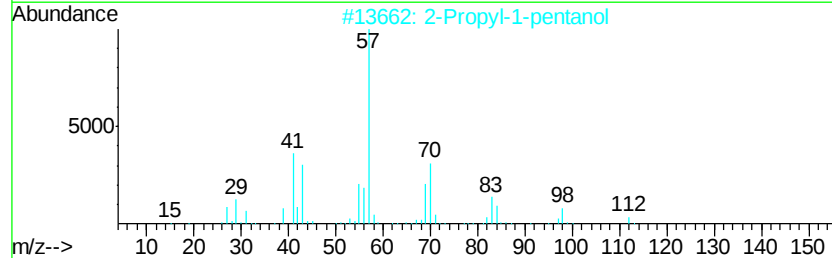
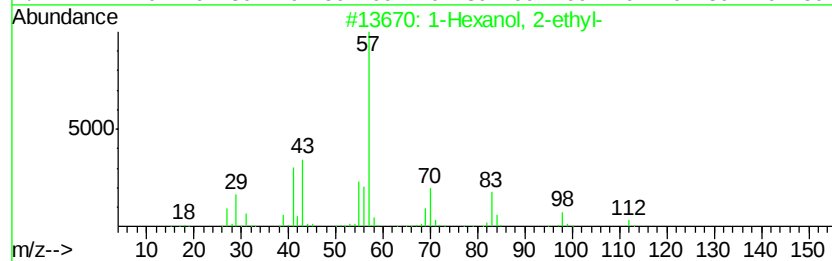
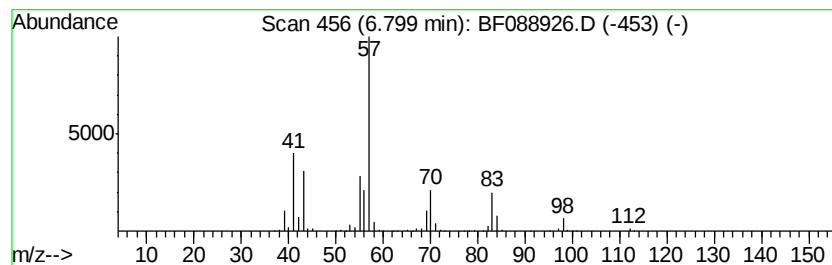
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.80	134.96 ng	2056630	1,4-Dichlorobenzene-d4	6.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78	
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50	
3	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50	
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	45	
5	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	43	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071216\
Data File : BF088926.D
Acq On : 12 Jul 2016 16:23
Operator : UM/SJ
Sample : H3889-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-1

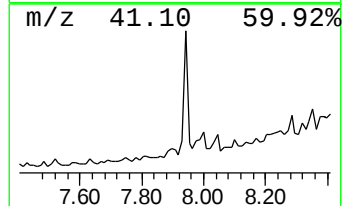
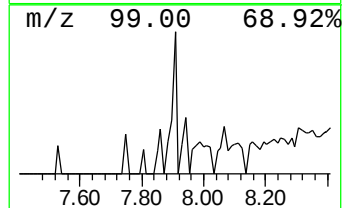
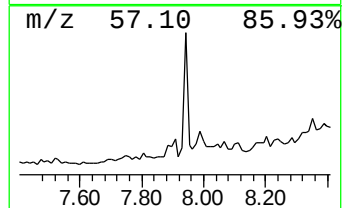
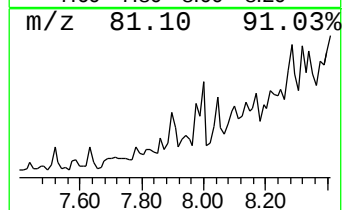
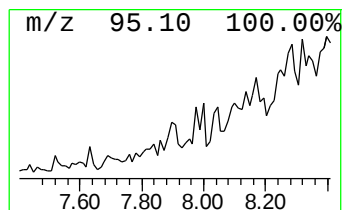
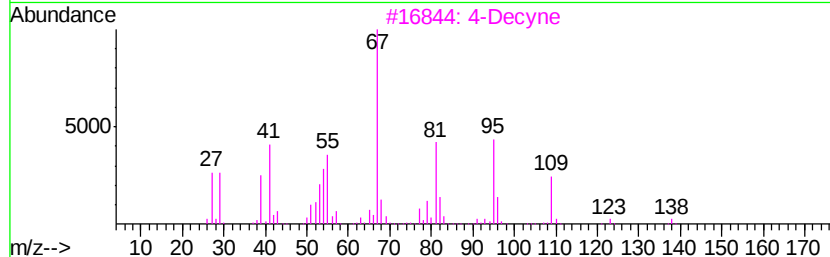
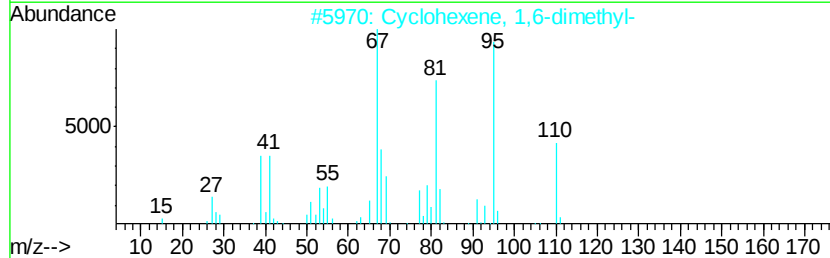
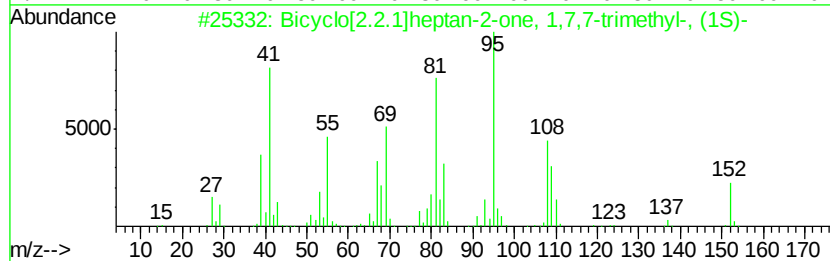
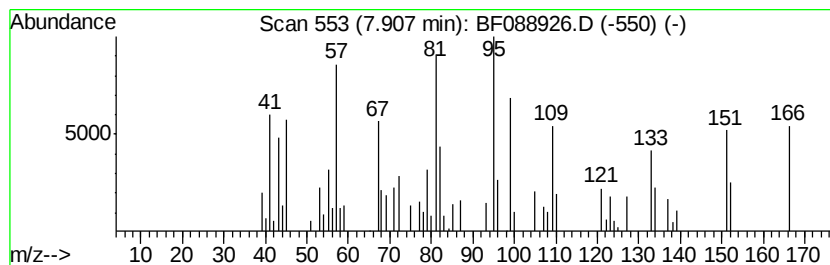
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown7.91 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.91	2.61 ng	68195	Naphthalene-d8	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	43
2		Cyclohexene, 1,6-dimethyl-	110	C8H14	001759-64-4	42
3		4-Decyne	138	C10H18	002384-86-3	38
4		3-Dodecyne	166	C12H22	006790-27-8	30
5		Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071216\
Data File : BF088926.D
Acq On : 12 Jul 2016 16:23
Operator : UM/SJ
Sample : H3889-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-1

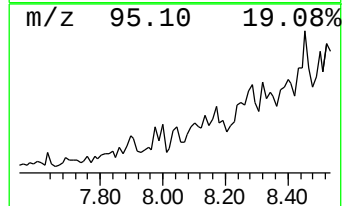
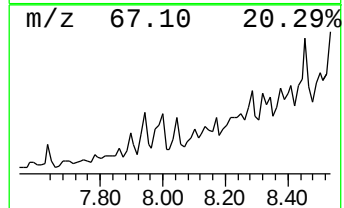
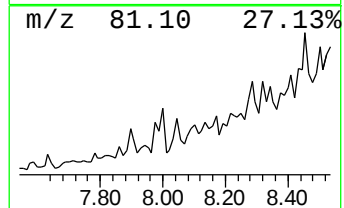
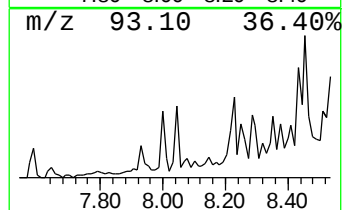
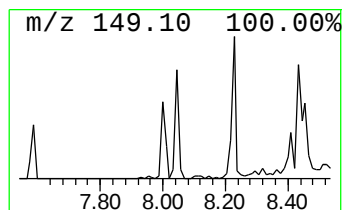
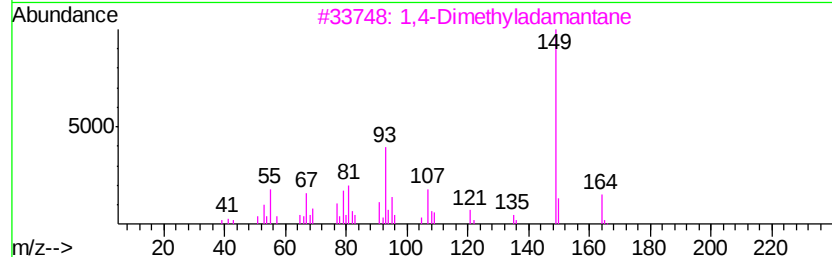
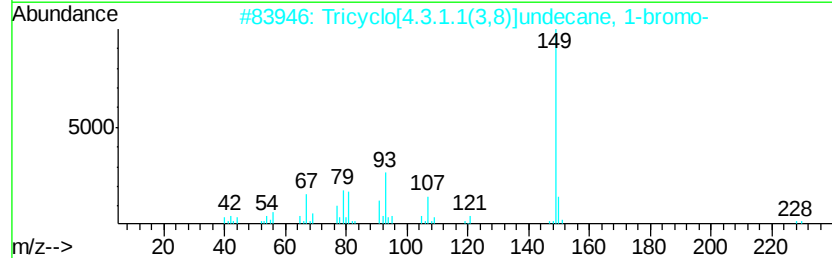
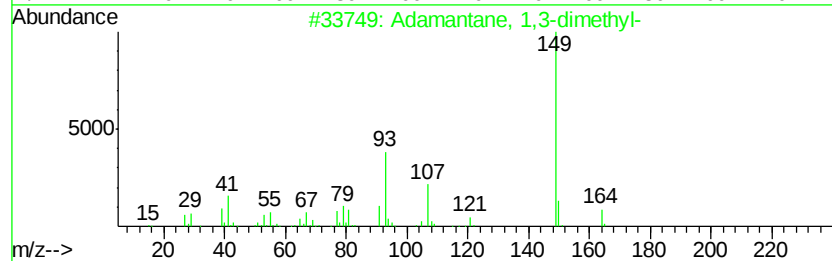
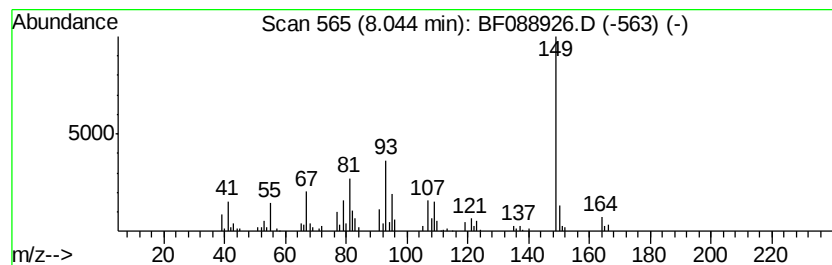
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Adamantane, 1,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.04	3.40 ng	88894	Naphthalene-d8	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	70
2		Tricyclo[4.3.1.1(3,8)]undecane, ...	228	C11H17Br	021898-96-4	64
3		1,4-Dimethyladamantane	164	C12H20	024145-88-8	60
4		1H-S-Triazolo[1,5-a]pyridin-4-yl...	149	C7H7N3O	013980-64-8	47
5		Pyridine, pentamethyl-	149	C10H15N	003748-83-2	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071216\
Data File : BF088926.D
Acq On : 12 Jul 2016 16:23
Operator : UM/SJ
Sample : H3889-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-1

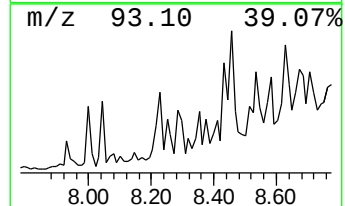
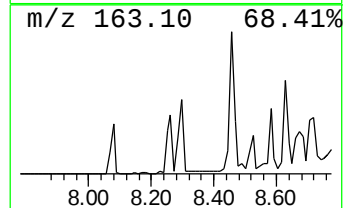
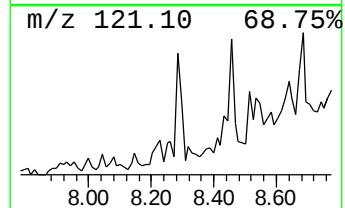
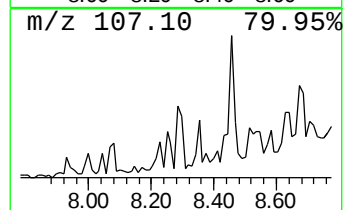
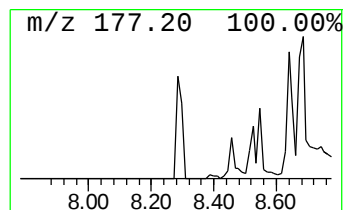
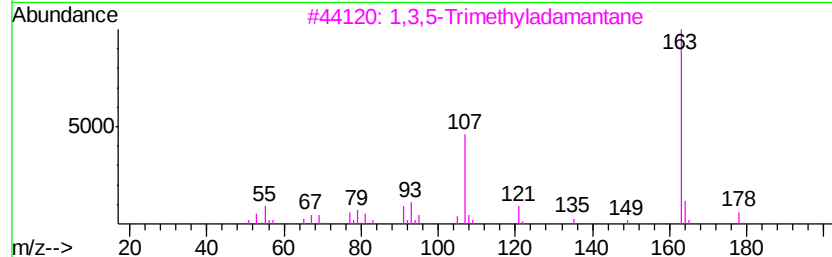
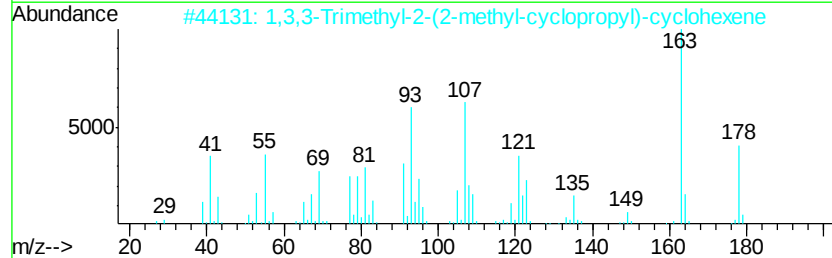
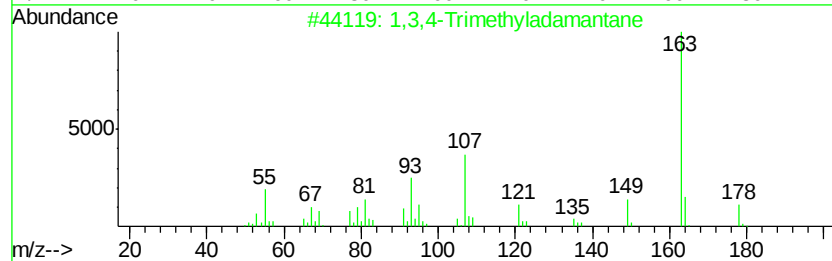
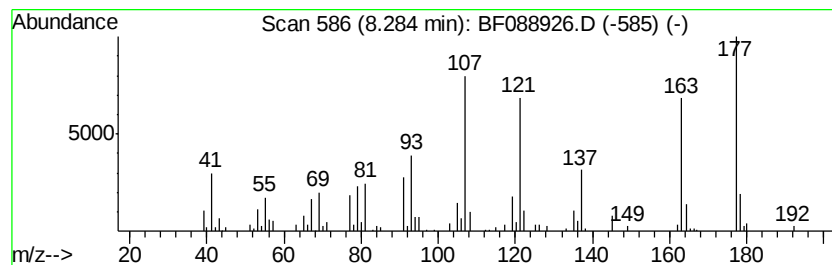
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown8.28 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.28	4.90 ng	128061	Naphthalene-d8	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,4-Trimethyladamantane	178	C13H22	1000214-98-3	45
2		1,3,3-Trimethyl-2-(2-methyl-cycl...	178	C13H22	285129-06-8	38
3		1,3,5-Trimethyladamantane	178	C13H22	000707-35-7	35
4		l-Tyrophanamide	180	C9H12N2O2	1000131-25-3	30
5		Tricyclo[3.1.0.0(2,4)]hexane, 3,...	164	C12H20	1000150-21-2	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088926.D
Acq On : 12 Jul 2016 16:23
Operator : UM/SJ
Sample : H3889-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-1

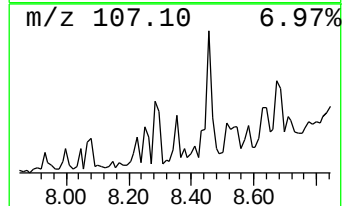
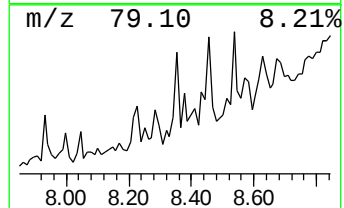
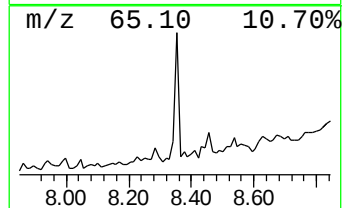
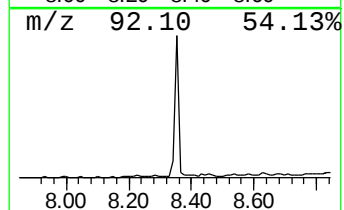
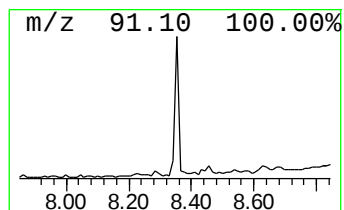
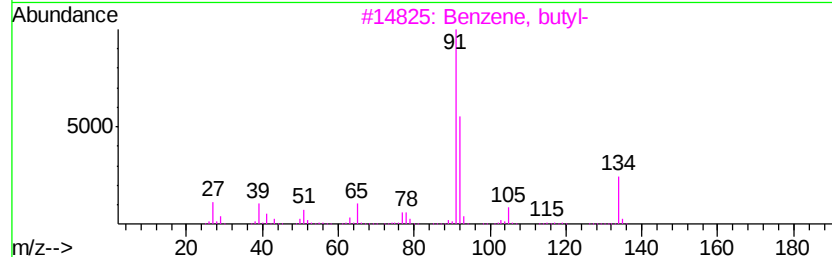
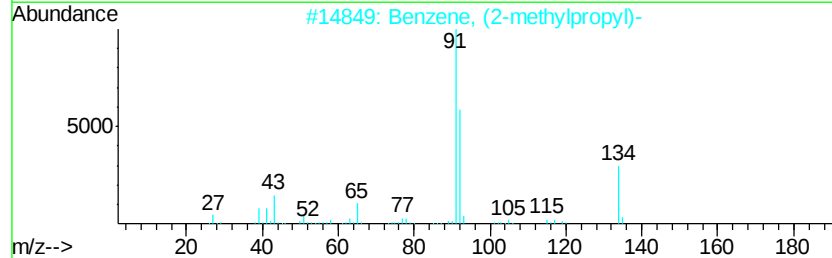
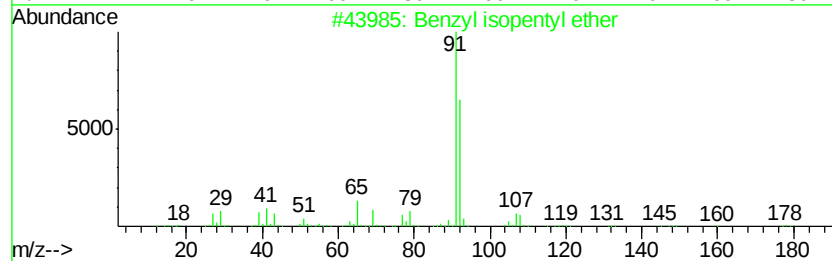
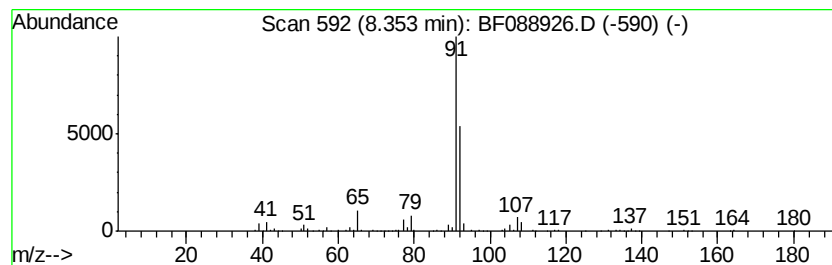
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzyl isopentyl ether Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.35	8.29 ng	216428	Napthalene-d8	7.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzyl isopentyl ether	178	C12H18O	000122-73-6	72
2		Benzene, (2-methylpropyl)-	134	C10H14	000538-93-2	64
3		Benzene, butyl-	134	C10H14	000104-51-8	64
4		Benzene, (butoxymethyl)-	164	C11H16O	000588-67-0	64
5		Toluene	92	C7H8	000108-88-3	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088926.D
Acq On : 12 Jul 2016 16:23
Operator : UM/SJ
Sample : H3889-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-1

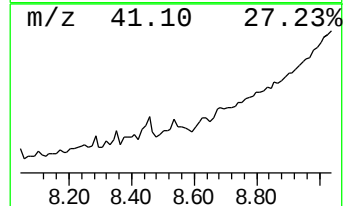
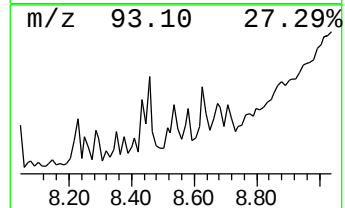
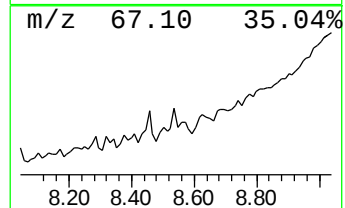
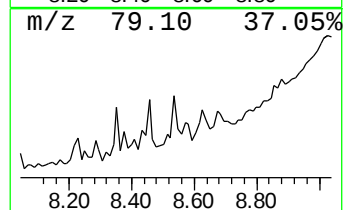
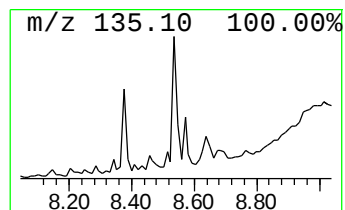
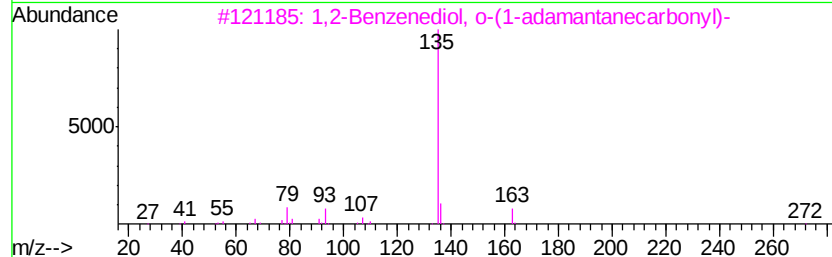
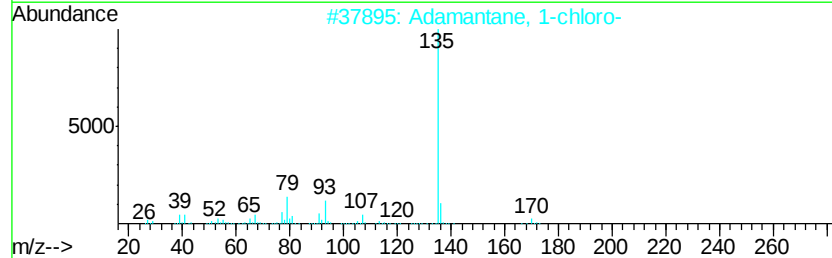
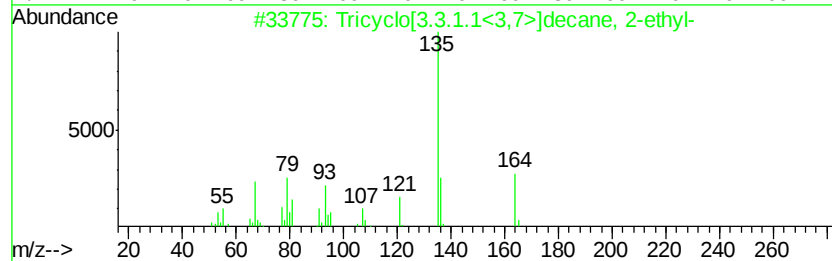
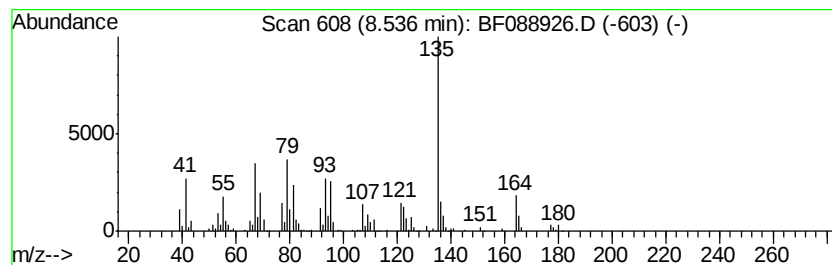
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tricyclo[3.3.1.1<3,7>]decan... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.54	20.58 ng	537426	Naphthalene-d8	7.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tricyclo[3.3.1.1<3,7>]decane, 2-...	164	C12H20	014451-87-7	72
2		Adamantane, 1-chloro-	170	C10H15Cl	000935-56-8	59
3		1,2-Benzenediol, o-(1-adamantane...	272	C17H20O3	1000325-99-6	58
4		Phosphonic dichloride, 1-adamantyl-	252	C10H15Cl2OP	1000294-15-7	53
5		N-(2-Ethyl-3-hydroxy-6-methyl-4-...	314	C19H26N2O2	1000260-99-4	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071216\
Data File : BF088926.D
Acq On : 12 Jul 2016 16:23
Operator : UM/SJ
Sample : H3889-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-1

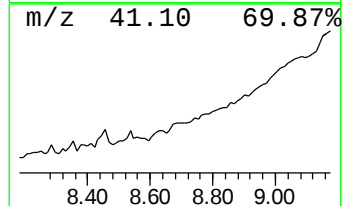
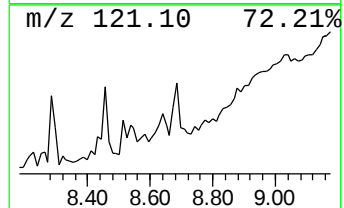
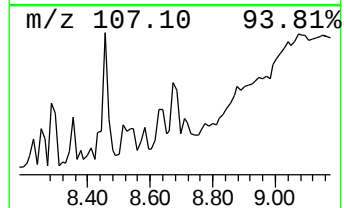
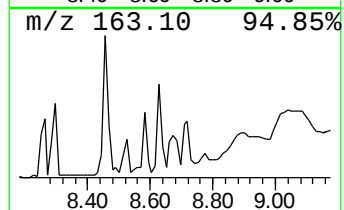
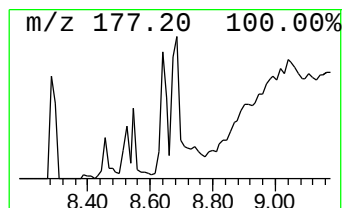
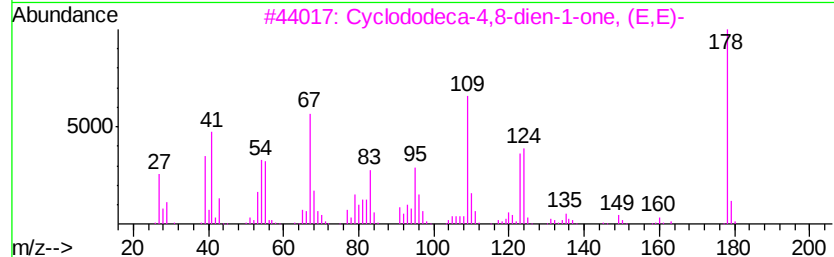
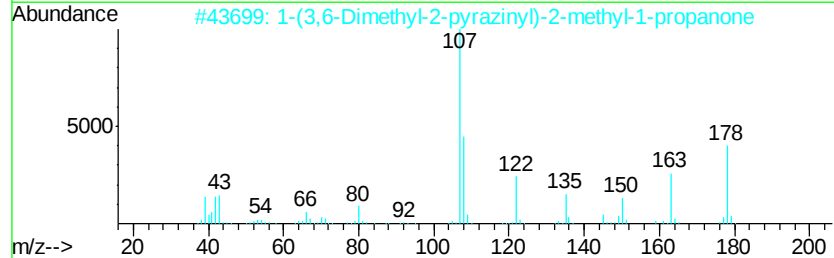
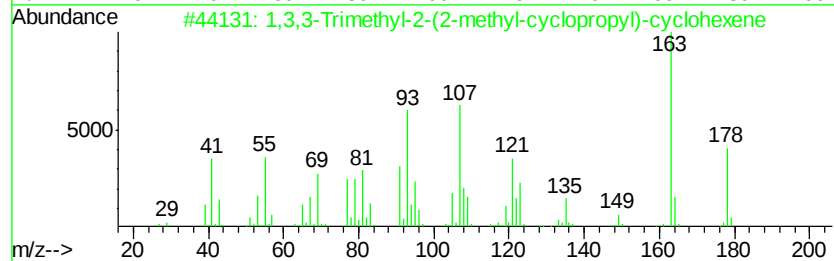
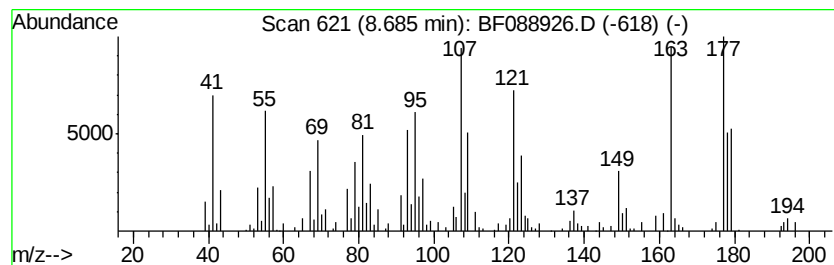
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown8.68 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.68	7.85 ng	204999	Napthalene-d8	7.99

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,3-Trimethyl-2-(2-methyl-cycl...	178	C13H22	285129-06-8	38
2			1-(3,6-Dimethyl-2-pyrazinyl)-2-m...	178	C10H14N2O	145984-66-3	22
3			Cyclododeca-4,8-dien-1-one, (E,E)-	178	C12H18O	1000163-28-2	14
4			1,3,3-Trimethylcyclohex-1-ene-4-...	168	C10H16O2	013746-43-5	14
5			[1,3,4]Oxadiazole, 2-amino-5-(4-...	179	C8H6FN3O	1000316-48-2	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071216\
Data File : BF088926.D
Acq On : 12 Jul 2016 16:23
Operator : UM/SJ
Sample : H3889-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-1

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
Methyl methacrylate	2.14	5.2	ng	79403	1	6.71	304784	20.0
unknown6.47	6.47	67.4	ng	1027790	1	6.71	304784	20.0
1-Hexanol, 2-ethyl-	6.80	135.0	ng	2056630	1	6.71	304784	20.0
unknown7.91	7.91	2.6	ng	68195	2	7.99	522364	20.0
Adamantane, 1,3-d...	8.04	3.4	ng	88894	2	7.99	522364	20.0
unknown8.28	8.28	4.9	ng	128061	2	7.99	522364	20.0
Benzyl isopentyl ...	8.35	8.3	ng	216428	2	7.99	522364	20.0
Tricyclo[3.3.1.1<...	8.54	20.6	ng	537426	2	7.99	522364	20.0
unknown8.68	8.68	7.8	ng	204999	2	7.99	522364	20.0