

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
 Data File : BF081321.D
 Acq On : 2 Sep 2015 00:13
 Operator : UM/IZ
 Sample : G3479-07
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COFF-3-4(0-2)

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-BF090115.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	4.456	246	251	263	rVB	612379	1269143	58.81%	7.276%
2	4.936	291	293	296	rBV	1290860	1841075	85.31%	10.555%
3	6.056	388	391	393	rBV	1815067	2157988	100.00%	12.372%
4	6.159	397	400	402	rBV	1348952	1852744	85.86%	10.622%
5	6.387	418	420	422	rVB	411644	352384	16.33%	2.020%
6	6.547	431	434	436	rBV	1054656	1321257	61.23%	7.575%
7	6.959	468	470	473	rBV	876063	1198246	55.53%	6.870%
8	7.679	530	533	535	rBV	441906	461457	21.38%	2.646%
9	8.765	624	628	630	rBV	1357198	1888632	87.52%	10.828%
10	9.165	660	663	665	rBV	364665	351218	16.28%	2.014%
11	9.416	682	685	687	rVB	569116	492948	22.84%	2.826%
12	9.862	721	724	725	rBV2	52635	63858	2.96%	0.366%
13	10.194	751	753	756	rBV2	855455	1041349	48.26%	5.970%
14	10.354	765	767	770	rBV	21507	27879	1.29%	0.160%
15	10.788	804	805	807	rBV	15637	23062	1.07%	0.132%
16	10.879	811	813	816	rBV	569066	484948	22.47%	2.780%
17	11.451	861	863	867	rBV2	48244	57074	2.64%	0.327%
18	12.468	949	952	954	rBV	1742617	1600233	74.15%	9.175%
19	13.394	1031	1033	1039	rBV	82341	184195	8.54%	1.056%
20	13.485	1039	1041	1044	rVV	454313	405877	18.81%	2.327%
21	14.800	1154	1156	1158	rBV	337110	330148	15.30%	1.893%
22	15.280	1193	1198	1204	rBV3	10947	36153	1.68%	0.207%

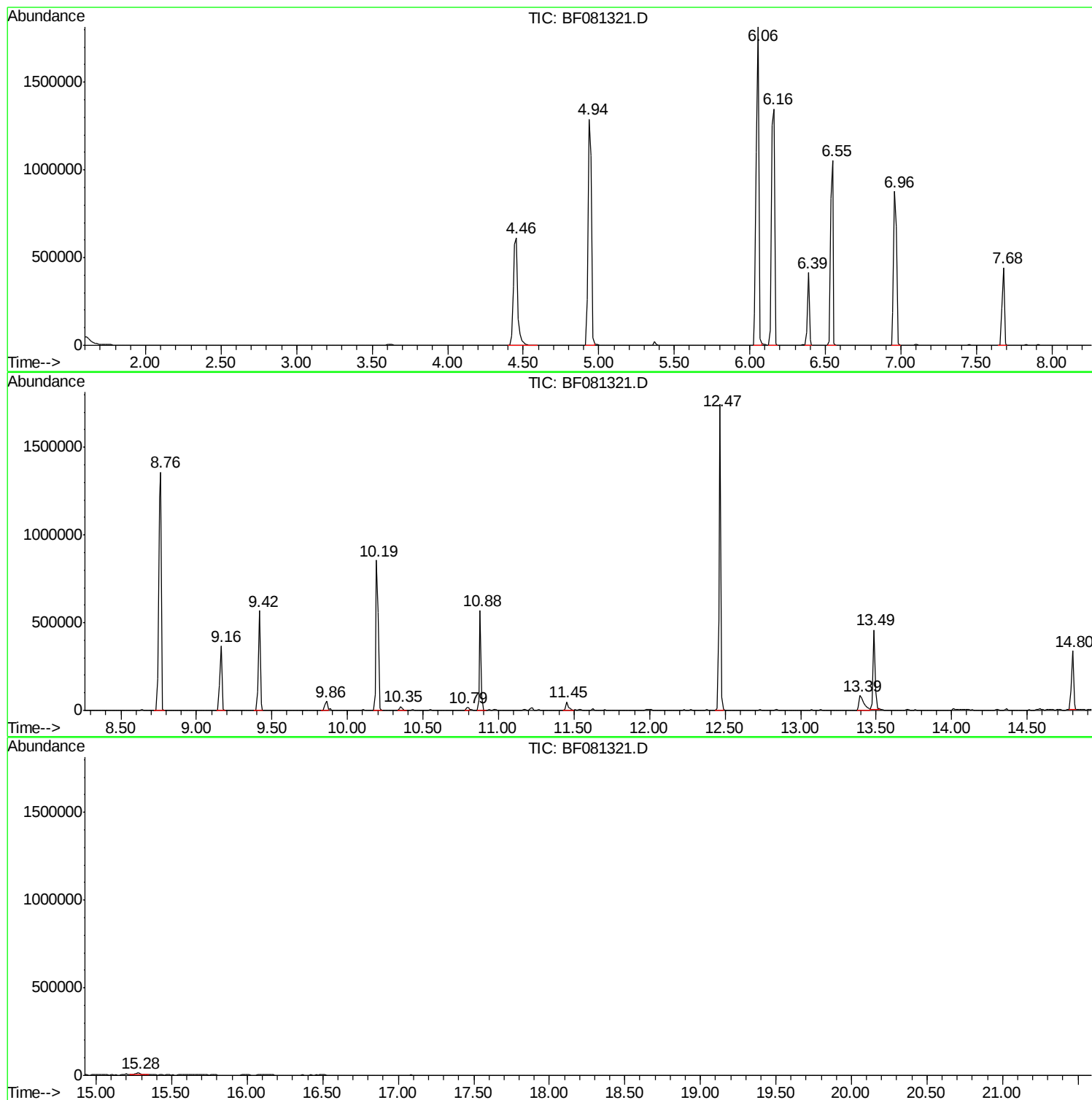
Sum of corrected areas: 17441868

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
Data File : BF081321.D
Acq On : 2 Sep 2015 00:13
Operator : UM/IZ
Sample : G3479-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COFF-3-4(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
Data File : BF081321.D
Acq On : 2 Sep 2015 00:13
Operator : UM/IZ
Sample : G3479-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COFF-3-4(0-2)

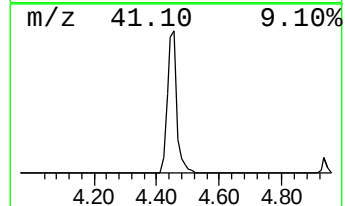
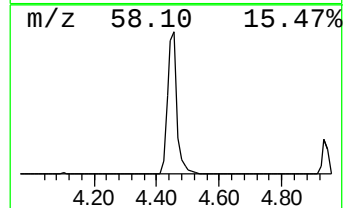
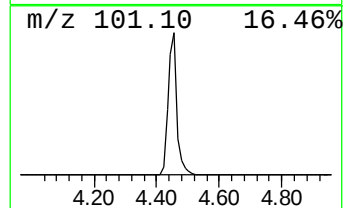
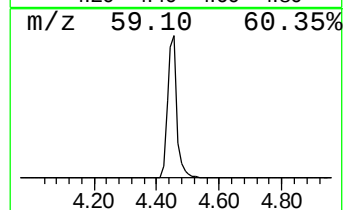
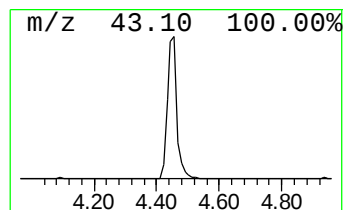
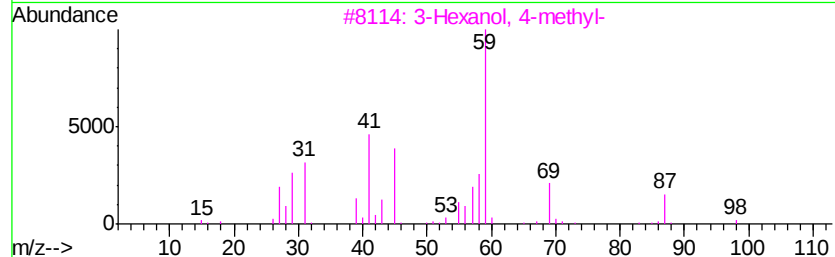
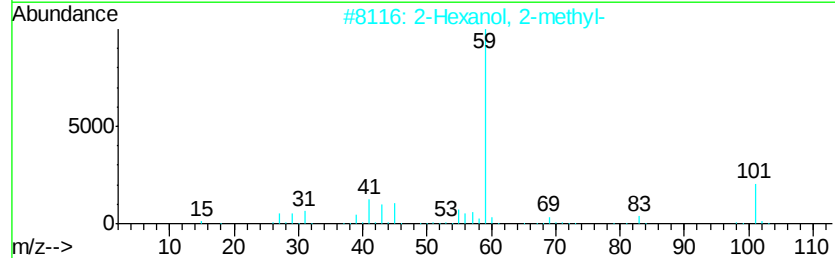
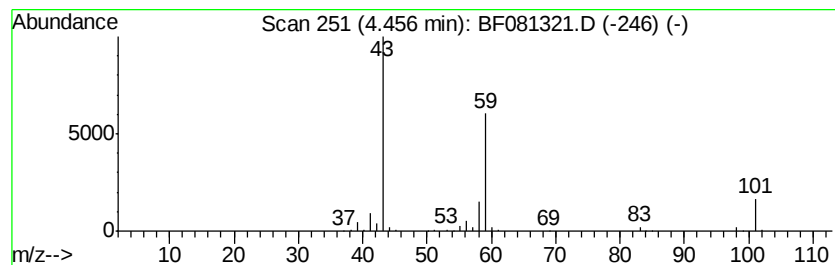
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
4.46	72.03 ng	1269140	1,4-Dichlorobenzene-d4	6.39

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
Data File : BF081321.D
Acq On : 2 Sep 2015 00:13
Operator : UM/IZ
Sample : G3479-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COFF-3-4(0-2)

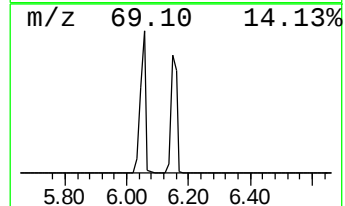
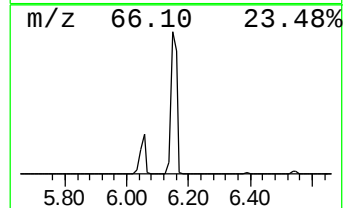
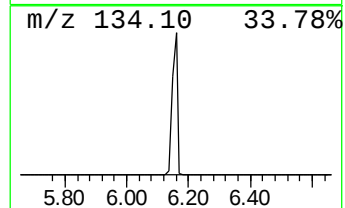
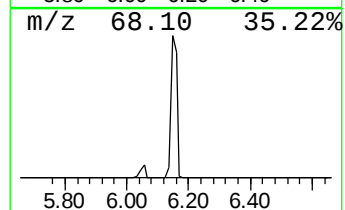
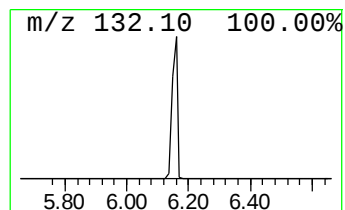
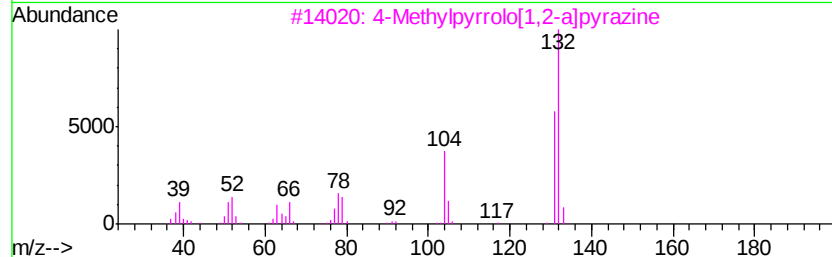
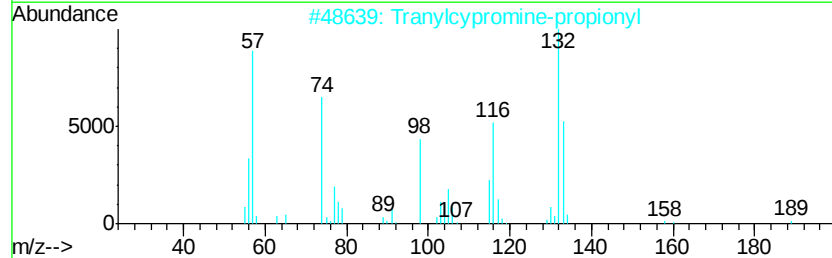
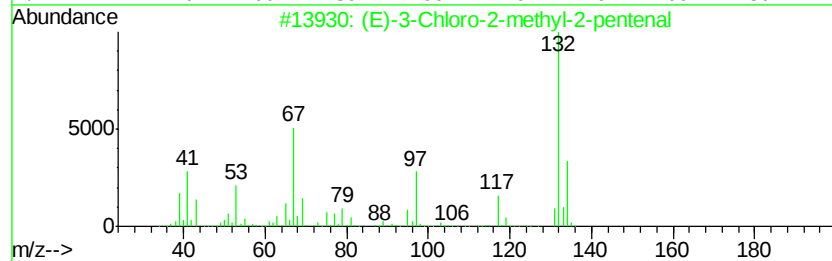
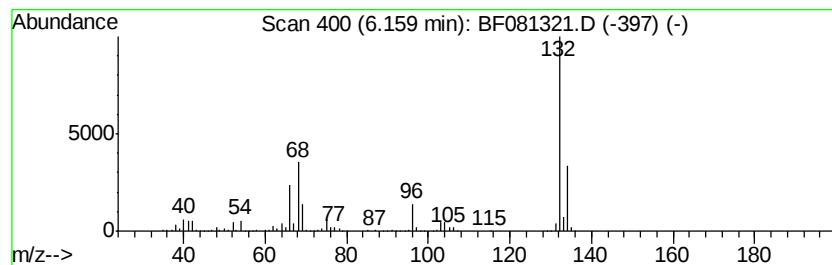
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.16 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	105.16 ng	1852740	1,4-Dichlorobenzene-d4	6.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2		Tranlylcypropine-propionyl	189	C12H15NO	1000123-86-3	16
3		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
Data File : BF081321.D
Acq On : 2 Sep 2015 00:13
Operator : UM/IZ
Sample : G3479-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COFF-3-4(0-2)

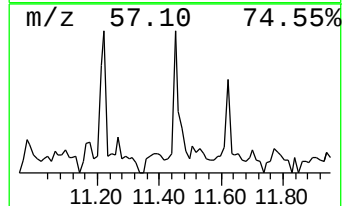
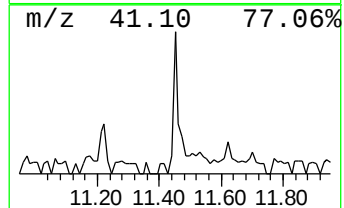
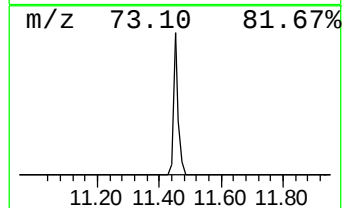
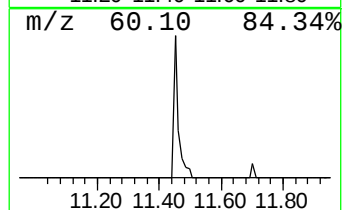
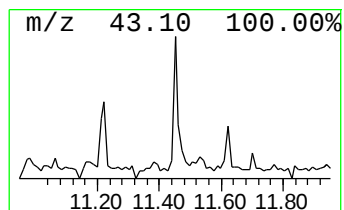
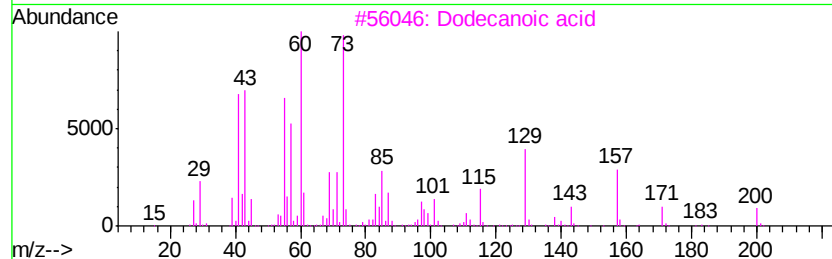
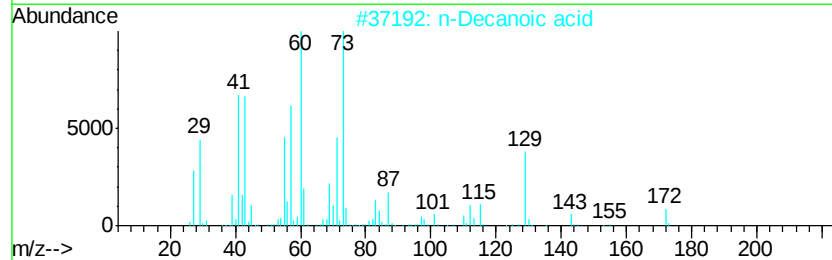
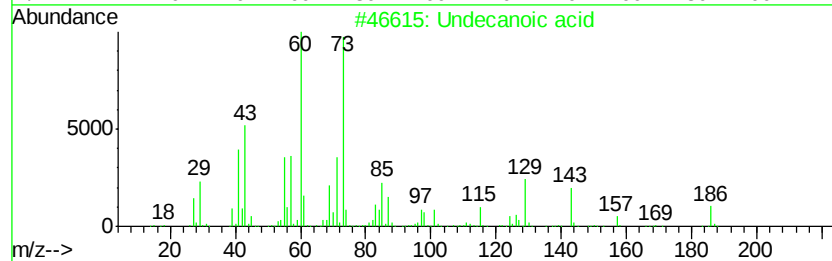
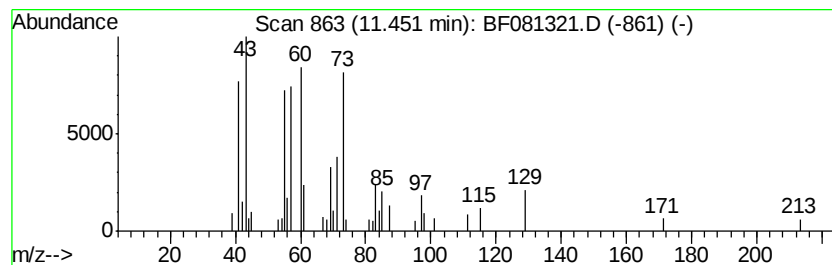
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Undecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.45	2.35 ng	57074	Phenanthrene-d10		10.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	86
2			n-Decanoic acid	172	C10H20O2	000334-48-5	59
3			Dodecanoic acid	200	C12H24O2	000143-07-7	53
4			Amyl Nitrite	117	C5H11NO2	000110-46-3	38
5			Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
Data File : BF081321.D
Acq On : 2 Sep 2015 00:13
Operator : UM/IZ
Sample : G3479-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COFF-3-4(0-2)

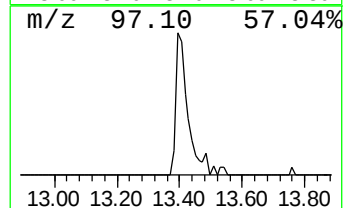
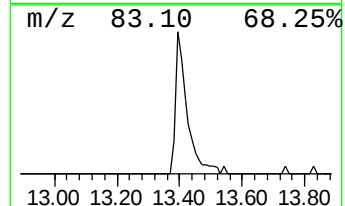
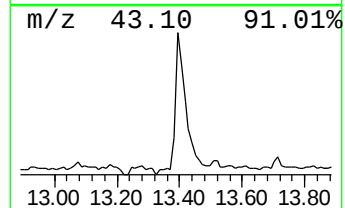
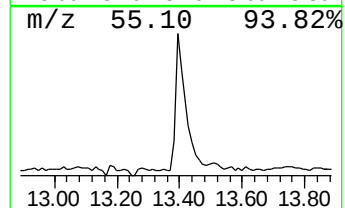
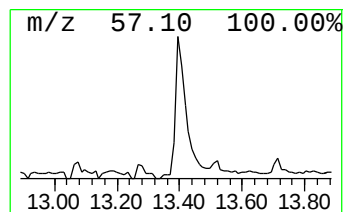
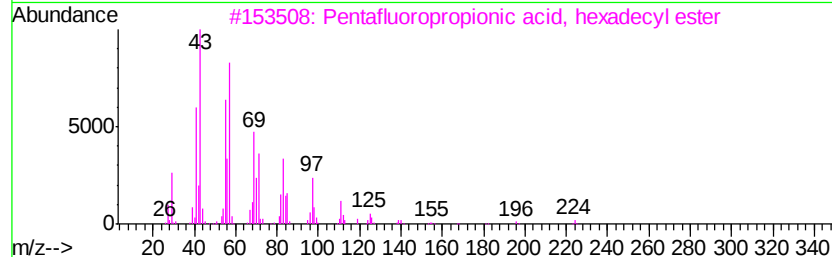
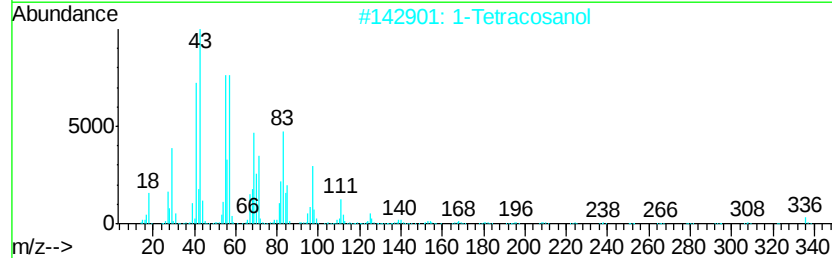
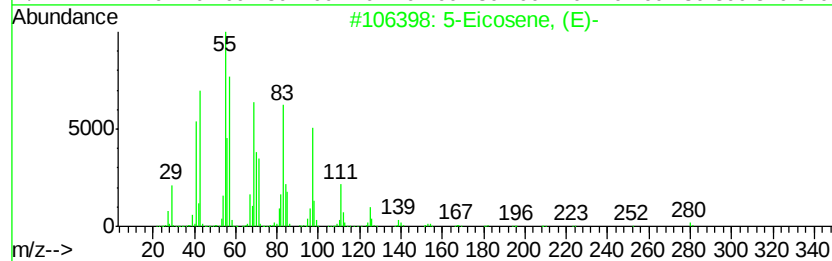
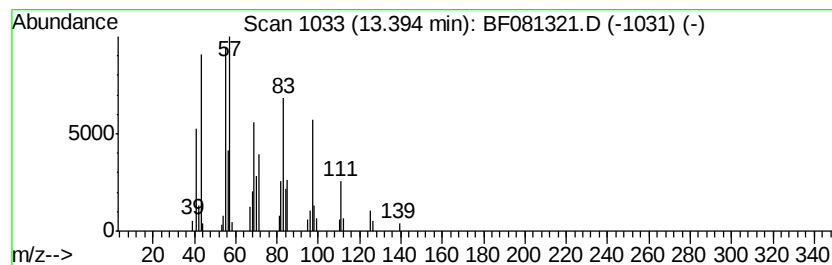
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.39	9.08 ng	184195	Chrysene-d12	13.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	91
2	1-Tetracosanol		354	C24H50O	000506-51-4	87
3	Pentafluoropropionic acid, hexadecyl ester		388	C19H33F5O2	006222-07-7	86
4	1-Hexacosanol		382	C26H54O	000506-52-5	83
5	Trifluoroacetic acid, n-heptadecyl ester		324	C17H31F3O2	1000216-79-2	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
Data File : BF081321.D
Acq On : 2 Sep 2015 00:13
Operator : UM/IZ
Sample : G3479-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COFF-3-4(0-2)

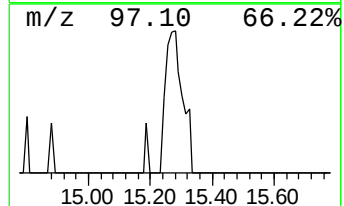
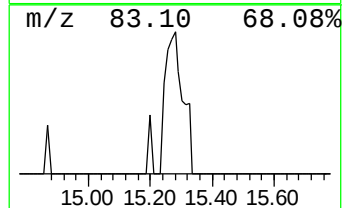
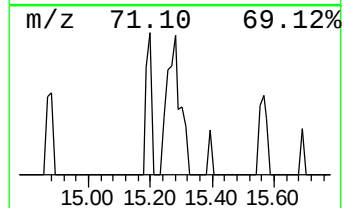
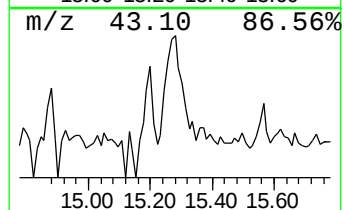
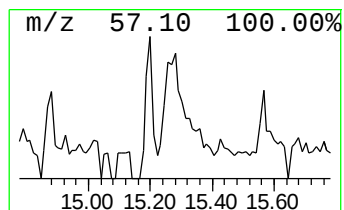
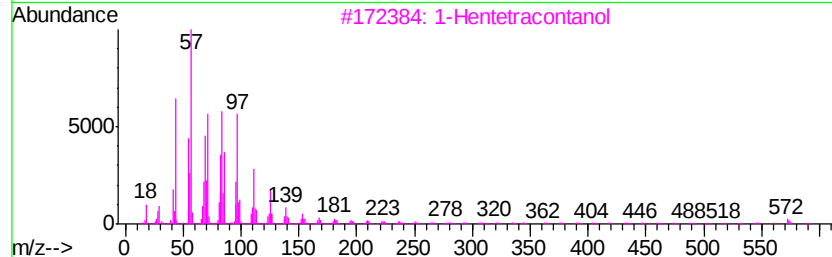
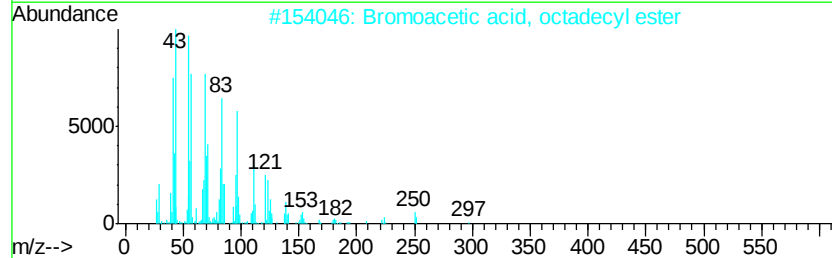
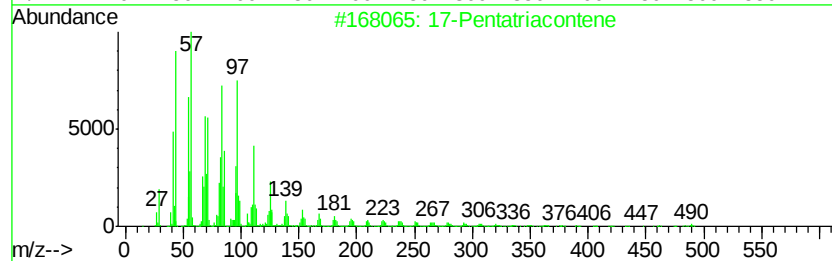
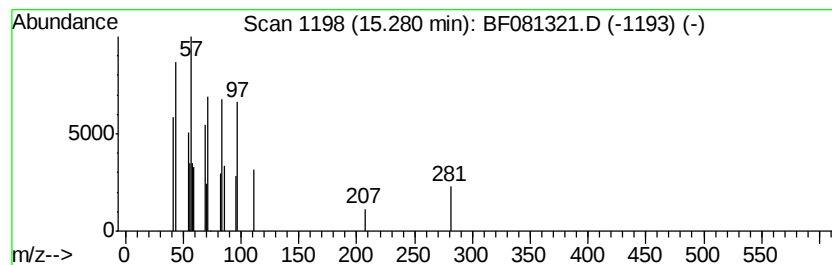
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 17-Pentatriacontene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	2.19 ng	36153	Perylene-d12	14.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-Pentatriacontene	491	C35H70	006971-40-0	72
2		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	64
3		1-Hentetracontanol	593	C41H84O	040710-42-7	59
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	53
5		Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
Data File : BF081321.D
Acq On : 2 Sep 2015 00:13
Operator : UM/IZ
Sample : G3479-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COFF-3-4(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.46	72.0	ng	1269140	1	6.39	352384	20.0
unknown6.16	6.16	105.2	ng	1852740	1	6.39	352384	20.0
Undecanoic acid	11.45	2.4	ng	57074	4	10.88	484948	20.0
5-Eicosene, (E)-	13.39	9.1	ng	184195	5	13.49	405877	20.0
17-Pentatriacontene	15.28	2.2	ng	36153	6	14.80	330148	20.0