

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
 Data File : BF087263.D
 Acq On : 21 May 2016 10:35
 Operator : UM/SJ
 Sample : H3151-03
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SED-5-0-2

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-BF051716.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	1.701	8	10	48	rVB	2894844	5826925	100.00%	13.327%
2	4.684	269	271	289	rBV	233074	584840	10.04%	1.338%
3	5.141	309	311	334	rBV	3345991	3994406	68.55%	9.136%
4	6.227	403	406	413	rBV	3696348	4097714	70.32%	9.372%
5	6.330	413	415	417	rBV	4479036	4359693	74.82%	9.971%
6	6.559	433	435	441	rVB	675976	838157	14.38%	1.917%
7	6.707	446	448	451	rBV	3121009	2892247	49.64%	6.615%
8	7.130	483	485	488	rBV	2339155	2494732	42.81%	5.706%
9	7.839	545	547	550	rBV	921359	1117169	19.17%	2.555%
10	8.925	639	642	644	rBV	4558768	4751075	81.54%	10.866%
11	9.325	675	677	681	rBV	817098	695237	11.93%	1.590%
12	9.530	693	695	697	rBV	72562	72967	1.25%	0.167%
13	9.588	697	700	703	rBV	1509342	1335194	22.91%	3.054%
14	10.033	735	739	740	rBV	147513	147391	2.53%	0.337%
15	10.250	755	758	761	rBV	46454	75621	1.30%	0.173%
16	10.376	767	769	772	rBV	2570444	2731921	46.88%	6.248%
17	10.502	778	780	787	rVB	170717	217410	3.73%	0.497%
18	10.948	817	819	820	rBV	106341	92926	1.59%	0.213%
19	11.062	827	829	832	rBV	1286686	1243427	21.34%	2.844%
20	12.651	965	968	970	rBV	4200286	4204501	72.16%	9.616%
21	13.576	1042	1049	1057	rBV	46348	139720	2.40%	0.320%
22	13.691	1057	1059	1066	rVV	962245	948463	16.28%	2.169%
23	14.525	1129	1132	1135	rBV	200990	184476	3.17%	0.422%
24	15.039	1175	1177	1187	rBV	485047	677385	11.63%	1.549%

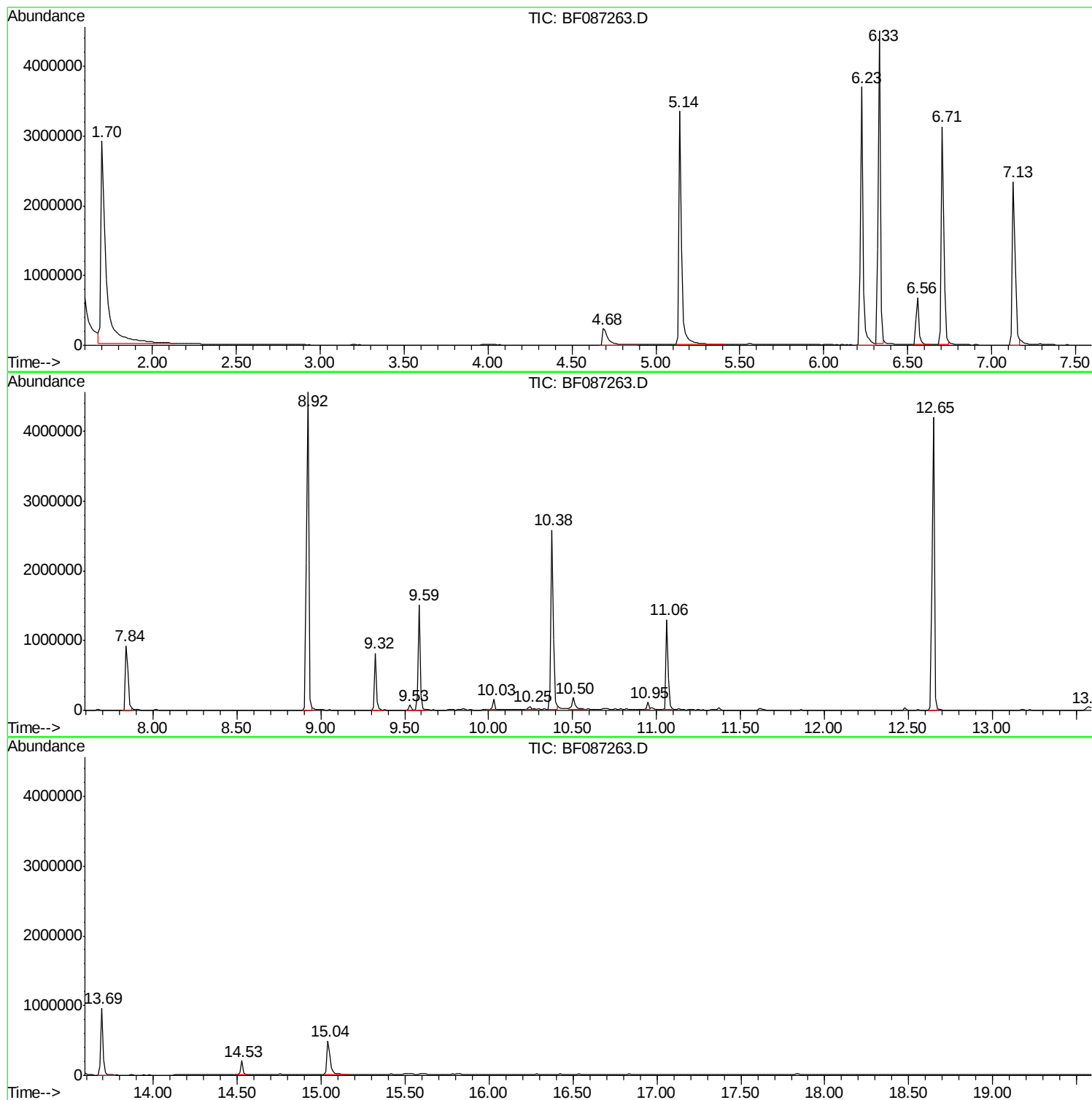
Sum of corrected areas: 43723597

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052016\
Data File : BF087263.D
Acq On : 21 May 2016 10:35
Operator : UM/SJ
Sample : H3151-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SED-5-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.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\BF052016\
Data File : BF087263.D
Acq On : 21 May 2016 10:35
Operator : UM/SJ
Sample : H3151-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SED-5-0-2

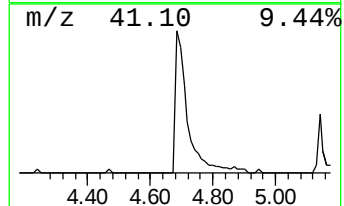
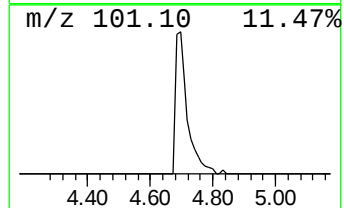
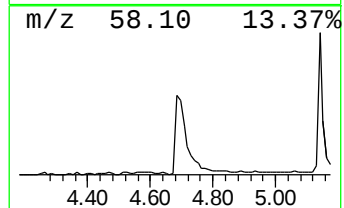
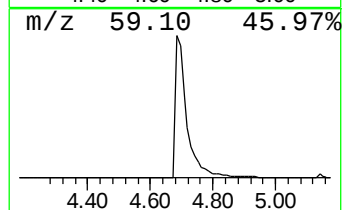
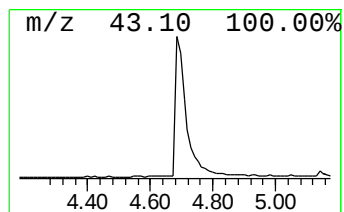
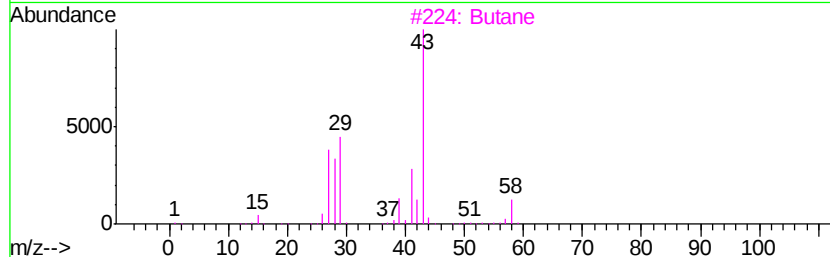
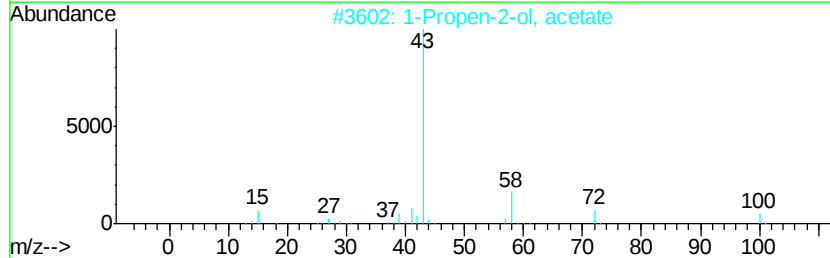
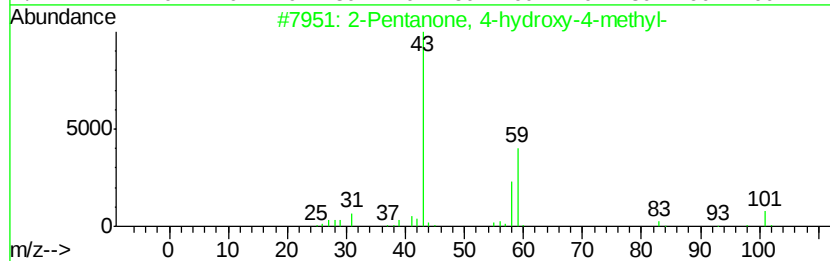
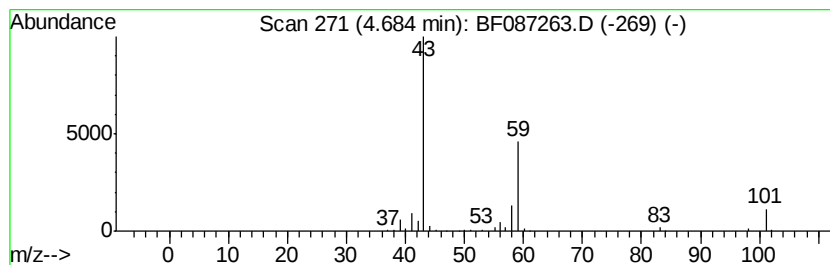
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
4.68	13.96 ng	584840	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		Butane	58	C4H10	000106-97-8	9
4		Diacetamide	101	C4H7NO2	000625-77-4	9
5		Acetic acid, 2-propenyl ester	100	C5H8O2	000591-87-7	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052016\
Data File : BF087263.D
Acq On : 21 May 2016 10:35
Operator : UM/SJ
Sample : H3151-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SED-5-0-2

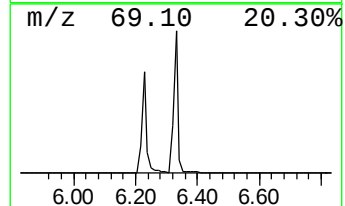
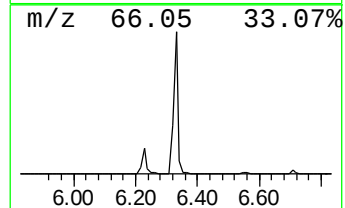
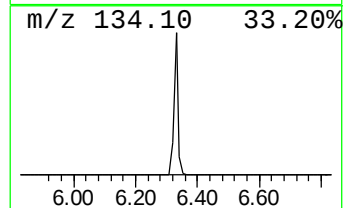
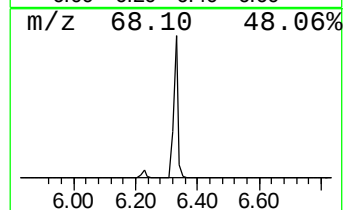
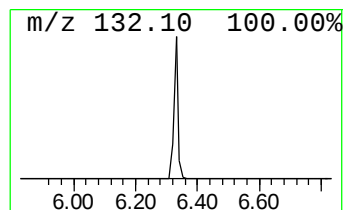
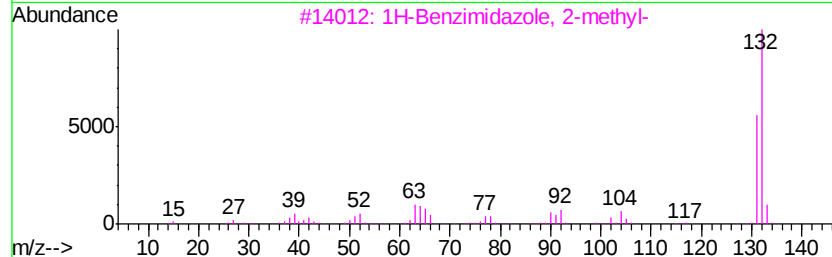
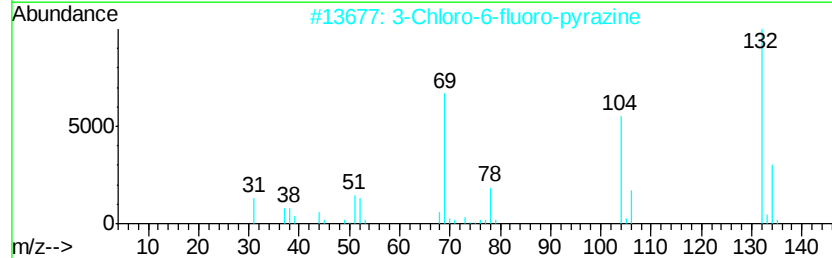
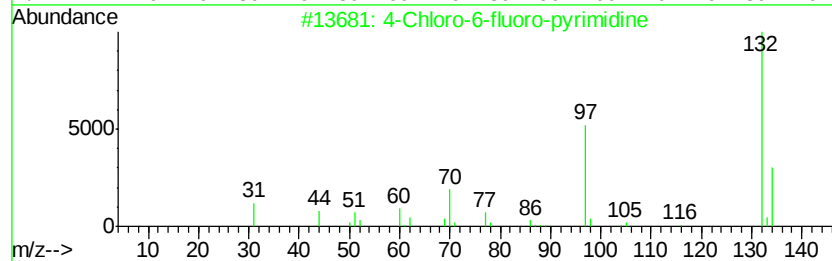
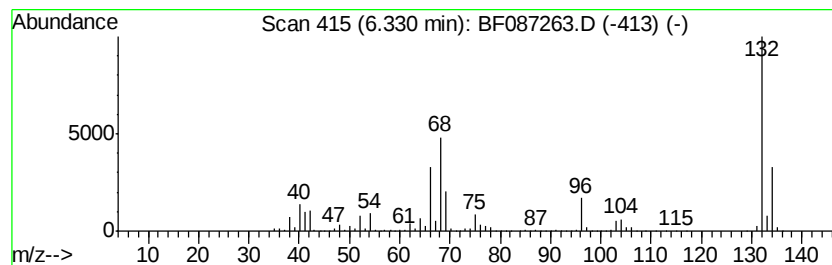
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.33 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	104.03 ng	4359690	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052016\
Data File : BF087263.D
Acq On : 21 May 2016 10:35
Operator : UM/SJ
Sample : H3151-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SED-5-0-2

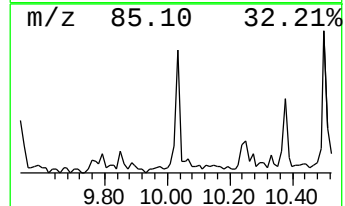
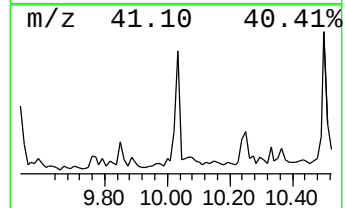
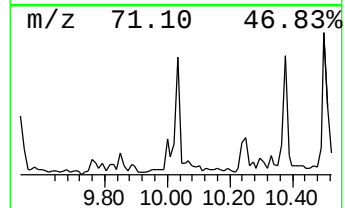
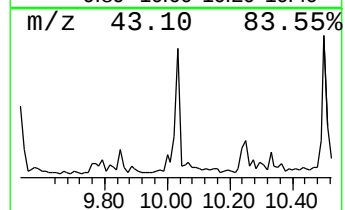
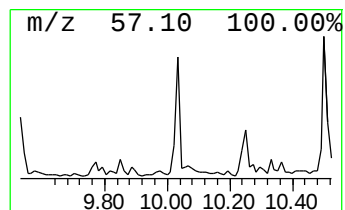
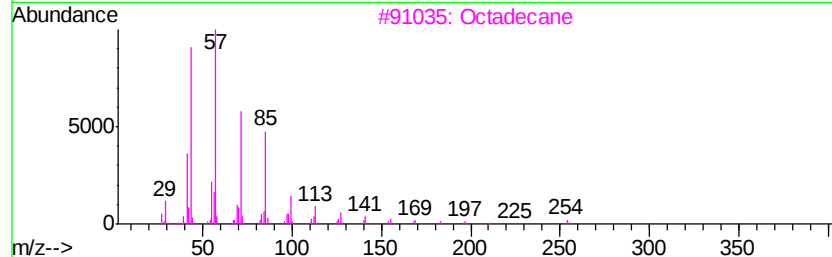
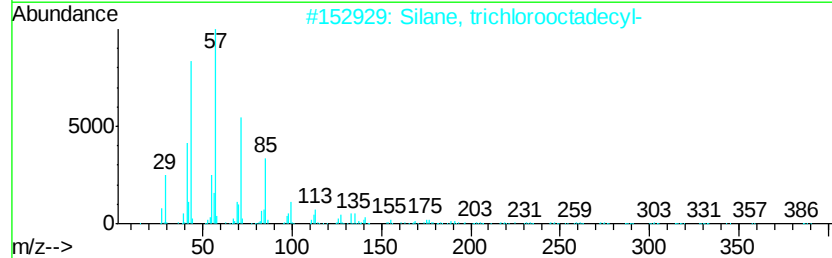
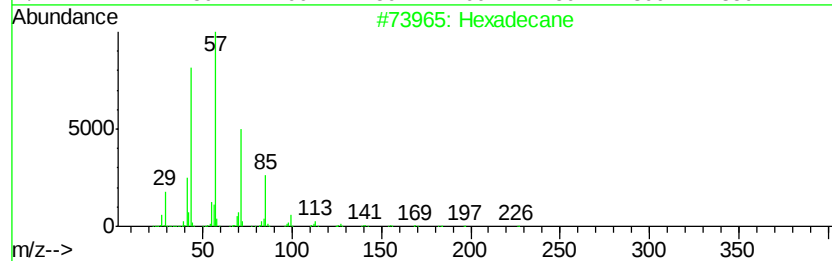
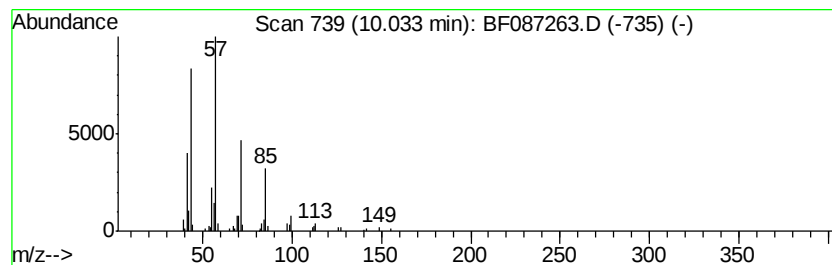
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.03	2.21 ng	147391	Acenaphthene-d10	9.59

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Silane, trichlorooctadecyl-		386	C18H37Cl3Si	000112-04-9	90
3	Octadecane		254	C18H38	000593-45-3	86
4	Pentadecane		212	C15H32	000629-62-9	86
5	Decane, 3-bromo-		220	C10H21Br	030571-71-2	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052016\
Data File : BF087263.D
Acq On : 21 May 2016 10:35
Operator : UM/SJ
Sample : H3151-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SED-5-0-2

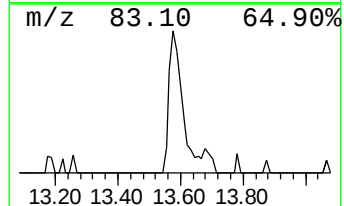
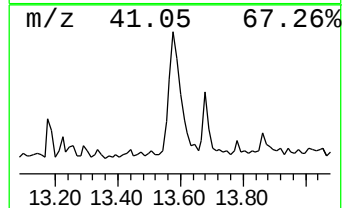
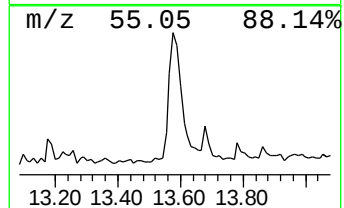
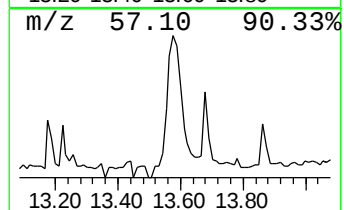
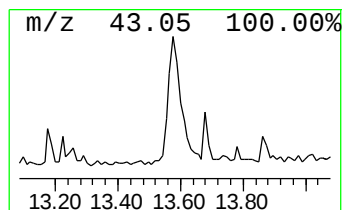
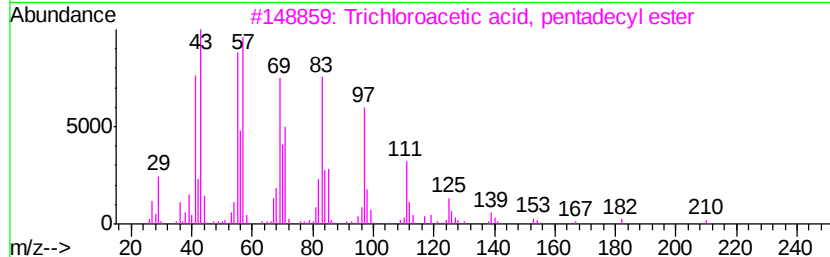
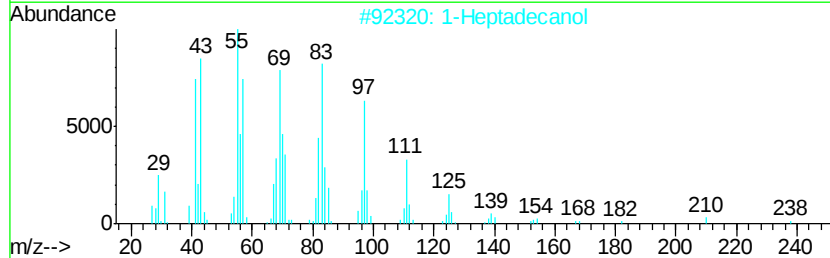
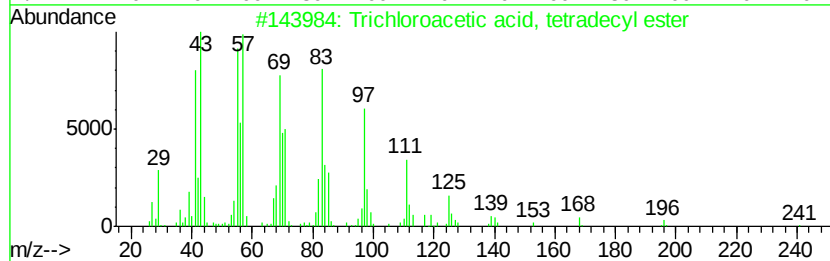
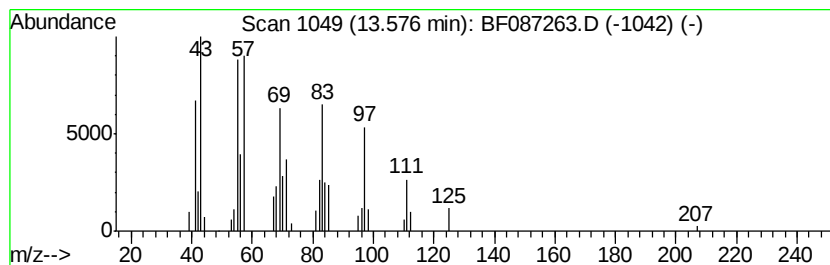
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trichloroacetic acid, tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.58	2.95 ng	139720	Chrysene-d12	13.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
2		1-Heptadecanol	256	C17H36O	001454-85-9	91
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4		1-Docosene	308	C22H44	001599-67-3	91
5		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052016\
Data File : BF087263.D
Acq On : 21 May 2016 10:35
Operator : UM/SJ
Sample : H3151-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SED-5-0-2

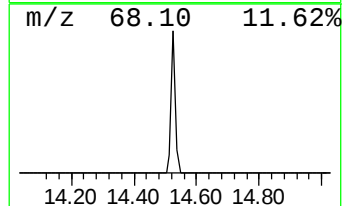
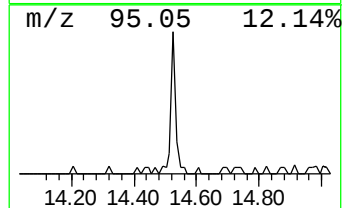
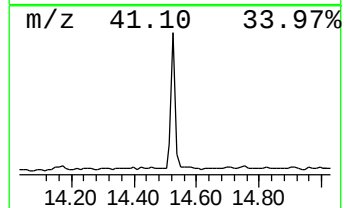
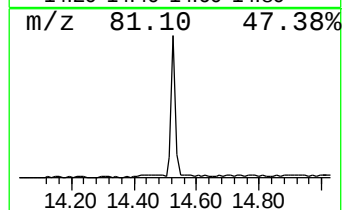
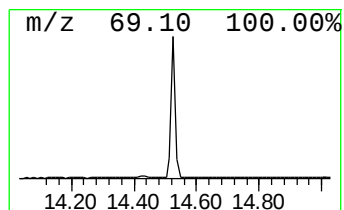
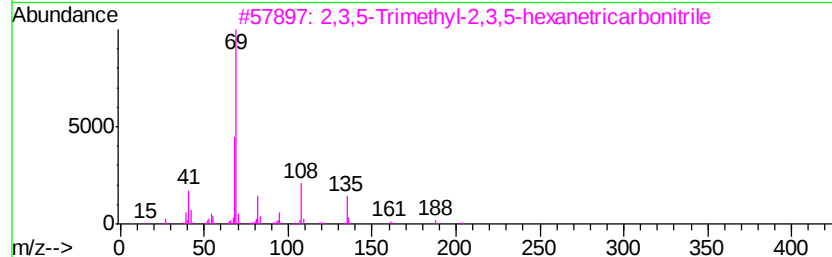
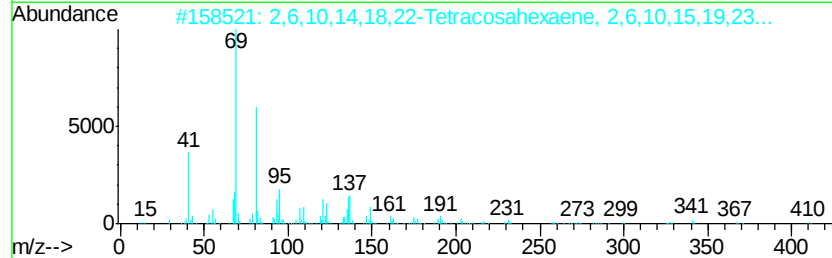
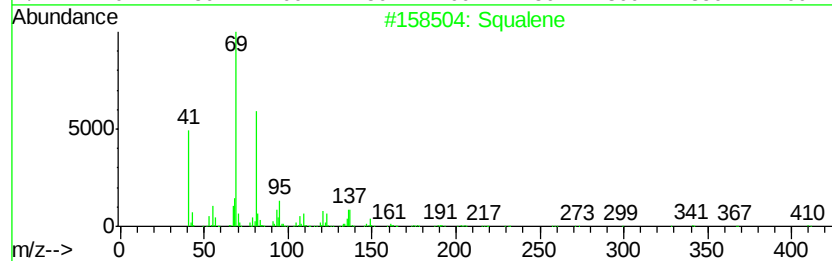
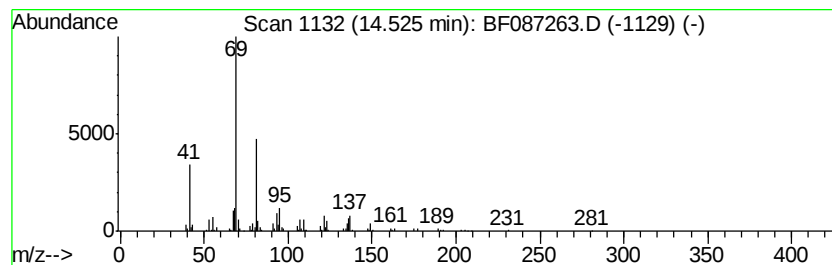
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	5.45 ng	184476	Perylene-d12	15.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	64
4		4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	58
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052016\
Data File : BF087263.D
Acq On : 21 May 2016 10:35
Operator : UM/SJ
Sample : H3151-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SED-5-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.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...	4.68	14.0	ng	584840	1	6.56	838157	20.0
unknown6.33	6.33	104.0	ng	4359690	1	6.56	838157	20.0
Hexadecane	10.03	2.2	ng	147391	3	9.59	1335190	20.0
Trichloroacetic a...	13.58	3.0	ng	139720	5	13.69	948463	20.0
Squalene	14.53	5.5	ng	184476	6	15.04	677385	20.0