

Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
 Data File : BF085366.D
 Acq On : 11 Mar 2016 6:59
 Operator : UM/SJ
 Sample : H1731-16
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-29-COMP

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-BF030316.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	5.144	248	250	256	rBV	229310	305256	6.77%	0.814%
2	5.544	282	285	287	rBV	3647119	3846312	85.25%	10.253%
3	6.573	371	375	377	rBV	2828838	4498849	99.71%	11.993%
4	6.710	384	387	389	rBV	4039720	4511954	100.00%	12.028%
5	6.939	404	407	409	rBV	1211357	993390	22.02%	2.648%
6	7.099	418	421	423	rBV	3590637	3445467	76.36%	9.185%
7	7.499	453	456	459	rBV	2325575	2610263	57.85%	6.958%
8	8.219	517	519	522	rBV	1179053	1151208	25.51%	3.069%
9	9.305	611	614	616	rBV	3409734	4288444	95.05%	11.432%
10	9.693	646	648	650	rBV	767777	728629	16.15%	1.942%
11	9.910	664	667	669	rBV	116506	101926	2.26%	0.272%
12	9.979	671	673	675	rVB	1432066	1227414	27.20%	3.272%
13	10.402	709	710	712	rVB	109318	132412	2.93%	0.353%
14	10.630	727	730	733	rBV	52374	88391	1.96%	0.236%
15	10.768	739	742	744	rBV	2406523	2341962	51.91%	6.243%
16	10.882	749	752	757	rVV	155737	192299	4.26%	0.513%
17	11.328	789	791	792	rBV	87402	73729	1.63%	0.197%
18	11.465	800	803	805	rBV	1118932	1067270	23.65%	2.845%
19	11.991	846	849	851	rBV	76726	121190	2.69%	0.323%
20	12.768	915	917	920	rBV	47519	56683	1.26%	0.151%
21	13.042	939	941	944	rBV	2245780	3150477	69.83%	8.398%
22	13.934	1017	1019	1028	rBV	472001	686847	15.22%	1.831%
23	14.094	1031	1033	1036	rBV	794379	822215	18.22%	2.192%
24	14.574	1072	1075	1082	rBV2	46235	98923	2.19%	0.264%
25	15.557	1158	1161	1164	rBV	619147	810643	17.97%	2.161%
26	16.082	1204	1207	1211	rBV	44209	107131	2.37%	0.286%
27	17.614	1337	1341	1346	rVB5	19620	54055	1.20%	0.144%

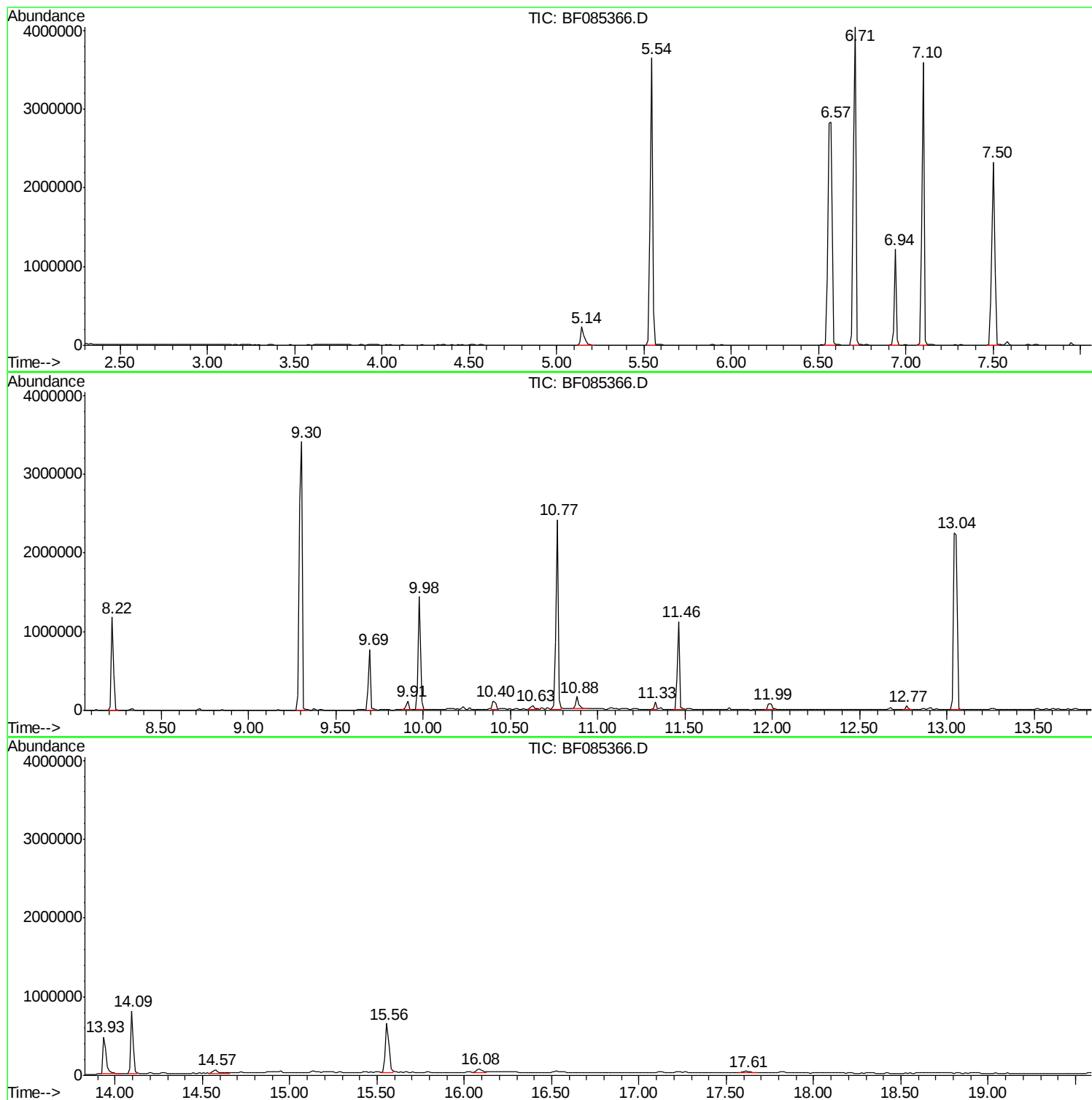
Sum of corrected areas: 37513339

Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085366.D
Acq On : 11 Mar 2016 6:59
Operator : UM/SJ
Sample : H1731-16
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085366.D
Acq On : 11 Mar 2016 6:59
Operator : UM/SJ
Sample : H1731-16
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-COMP

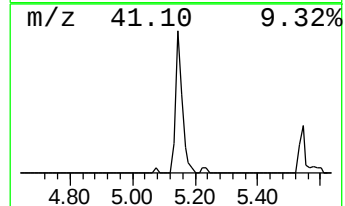
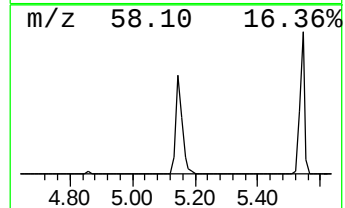
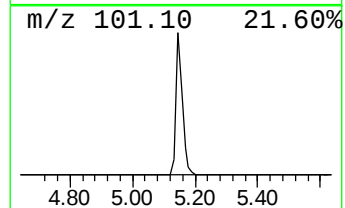
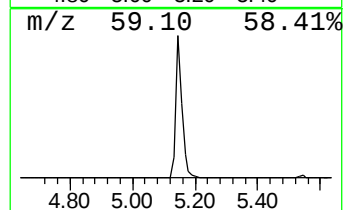
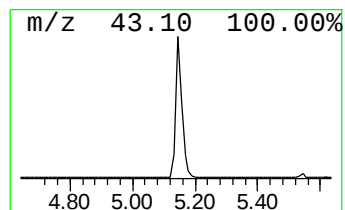
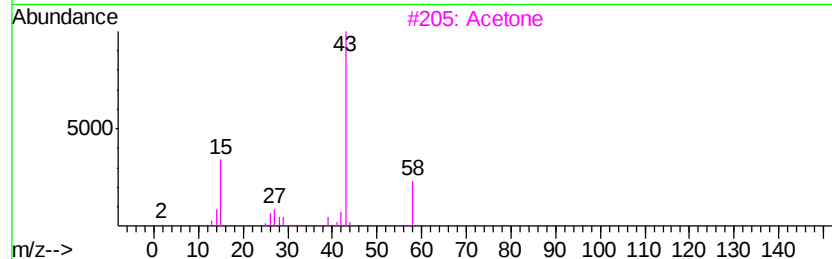
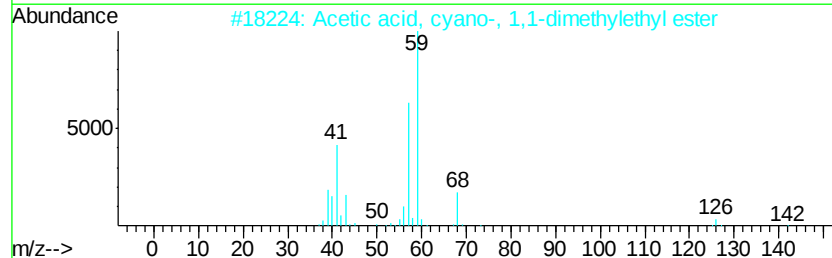
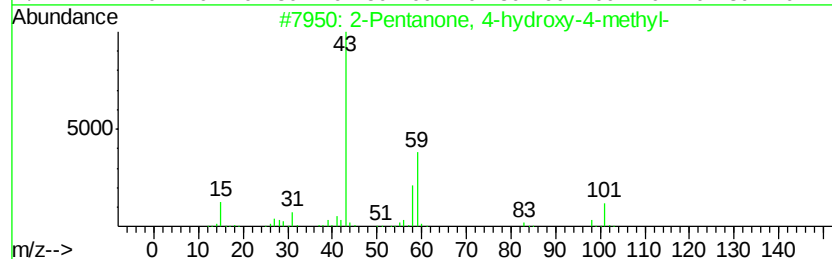
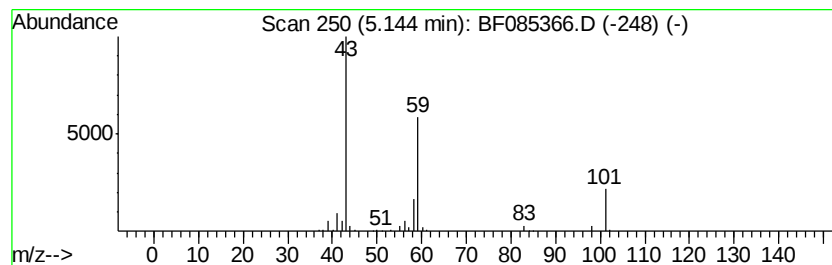
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	6.15 ng	305256	1,4-Dichlorobenzene-d4	6.94

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-dimethy...	141	C7H11NO2	001116-98-9	23	
3	Acetone	58	C3H6O	000067-64-1	10	
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085366.D
Acq On : 11 Mar 2016 6:59
Operator : UM/SJ
Sample : H1731-16
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-COMP

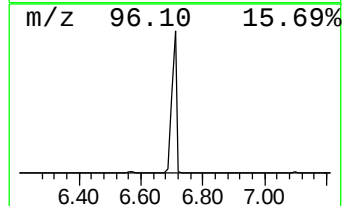
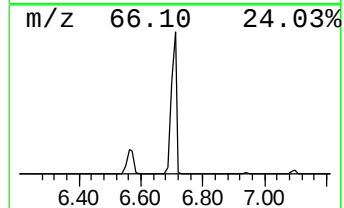
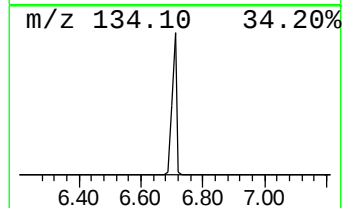
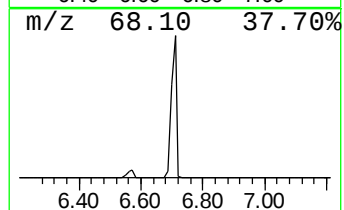
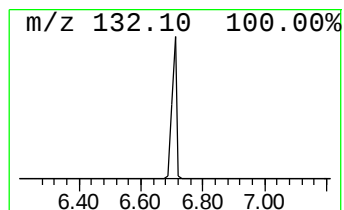
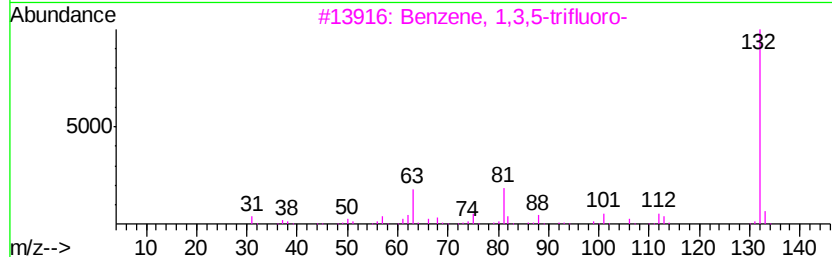
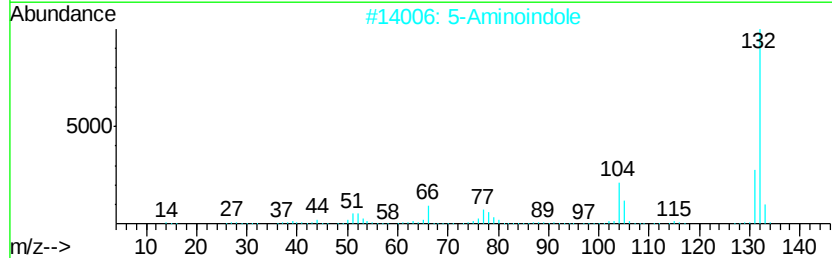
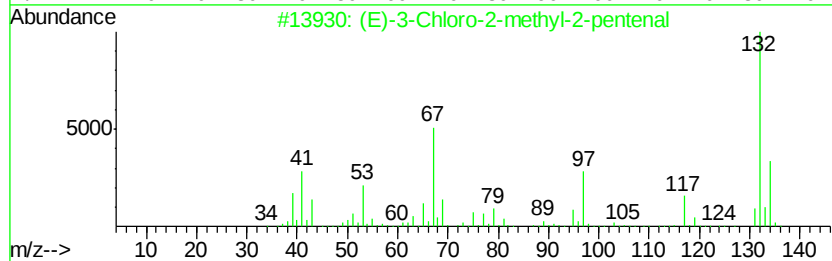
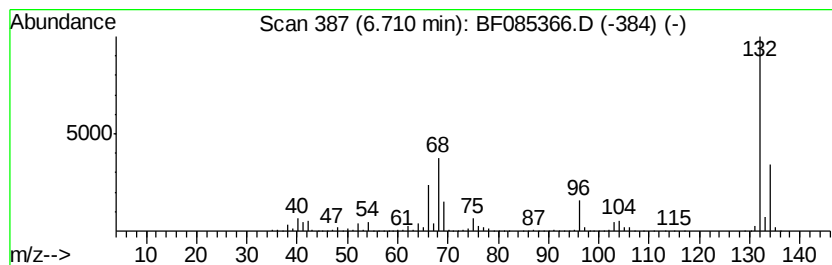
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	90.84 ng	4511950	1,4-Dichlorobenzene-d4	6.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085366.D
Acq On : 11 Mar 2016 6:59
Operator : UM/SJ
Sample : H1731-16
Misc :
ALS Vial : 36 Sample Multiplier: 1

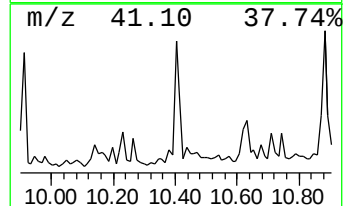
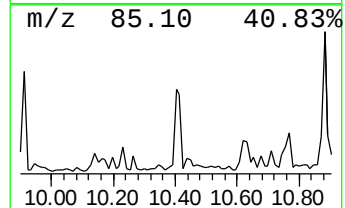
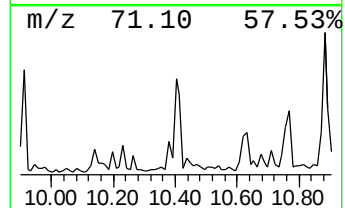
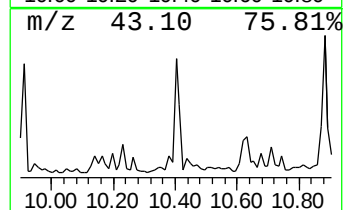
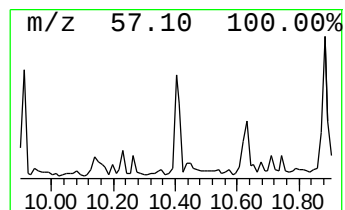
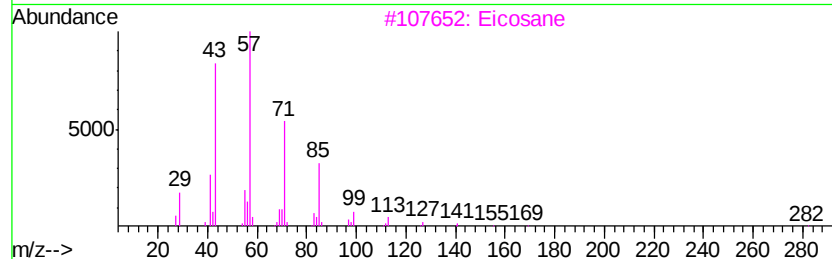
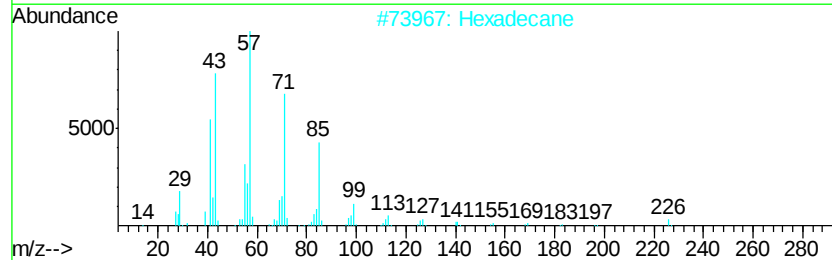
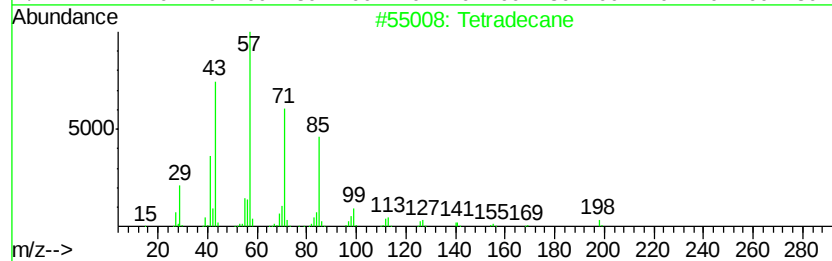
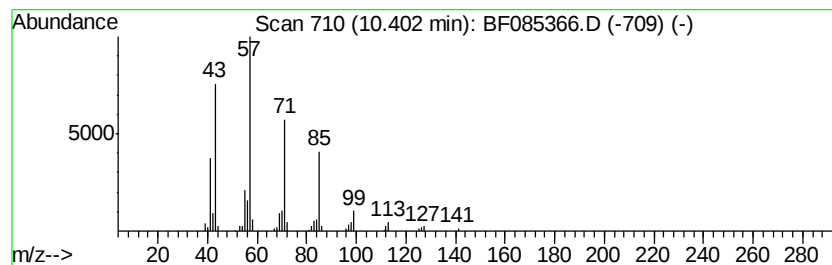
Instrument :
BNA_F
ClientSampleId :
SB-29-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.40	2.16 ng	132412	Acenaphthene-d10	9.98
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tetradecane	198 C14H30	000629-59-4 90
2		Hexadecane	226 C16H34	000544-76-3 87
3		Eicosane	282 C20H42	000112-95-8 83
4		Pentadecane	212 C15H32	000629-62-9 83
5		Decane, 2,3,5-trimethyl-	184 C13H28	062238-11-3 83



Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085366.D
Acq On : 11 Mar 2016 6:59
Operator : UM/SJ
Sample : H1731-16
Misc :
ALS Vial : 36 Sample Multiplier: 1

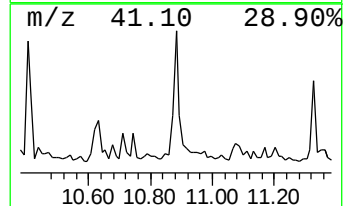
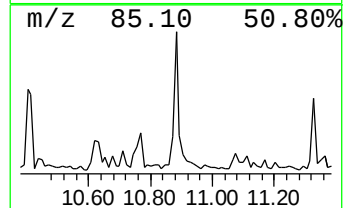
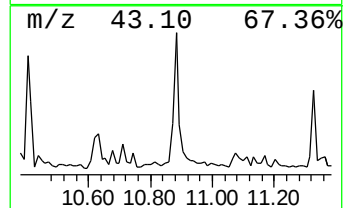
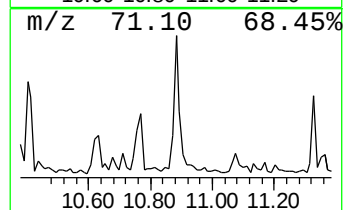
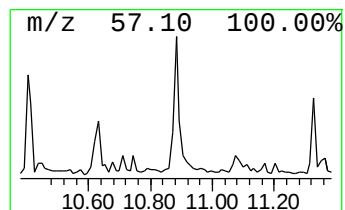
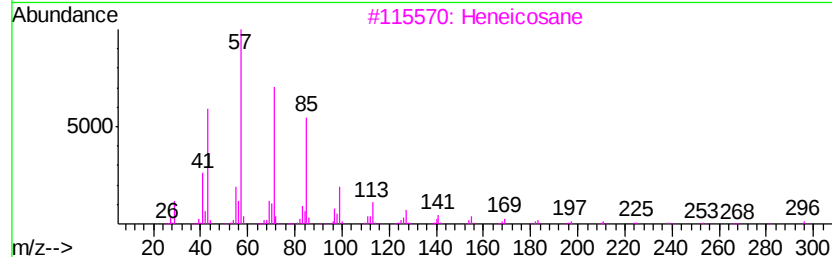
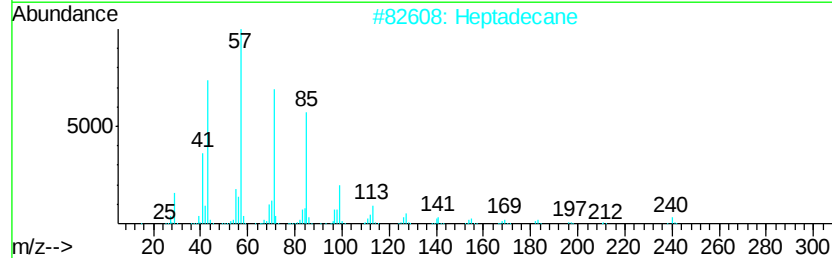
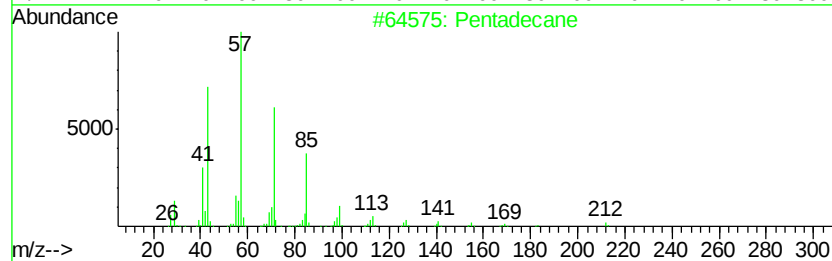
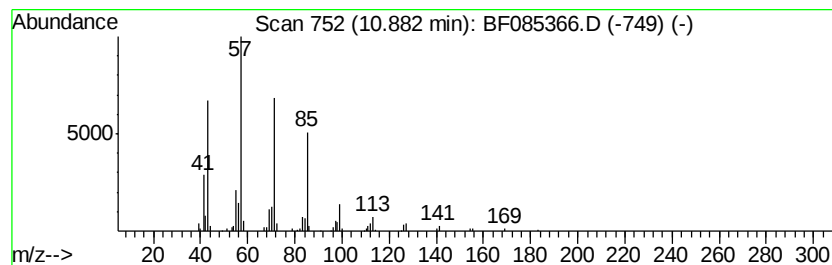
Instrument :
BNA_F
ClientSampleId :
SB-29-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.88	3.60 ng	192299	Phenanthrene-d10		11.46
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tetradecane	198	C14H30	000629-59-4	91
5	Nonadecane	268	C19H40	000629-92-5	90



Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085366.D
Acq On : 11 Mar 2016 6:59
Operator : UM/SJ
Sample : H1731-16
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-COMP

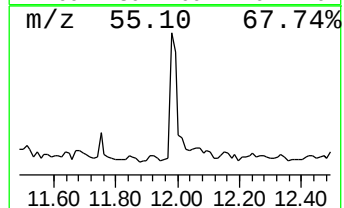
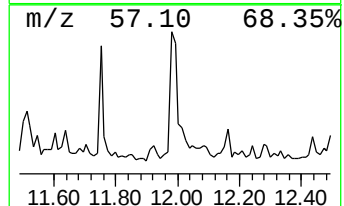
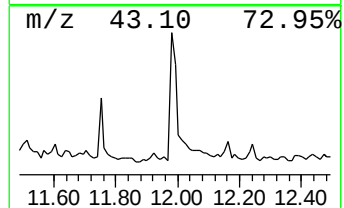
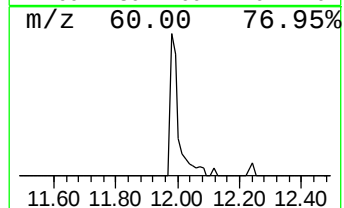
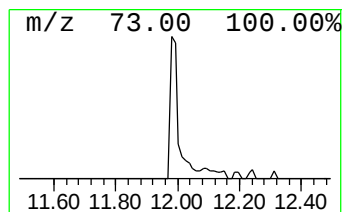
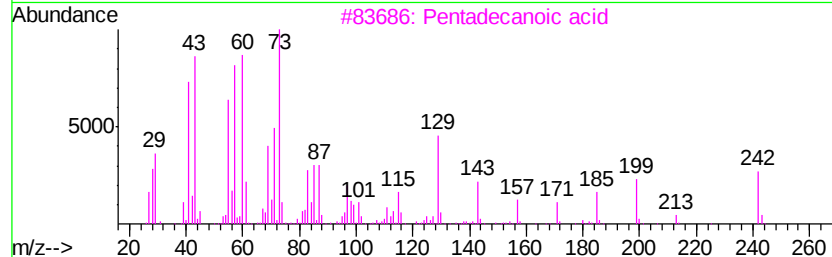
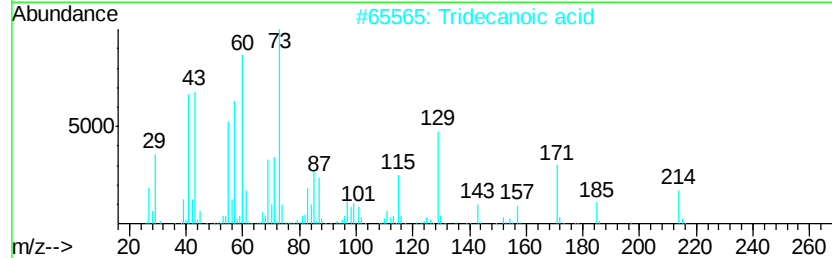
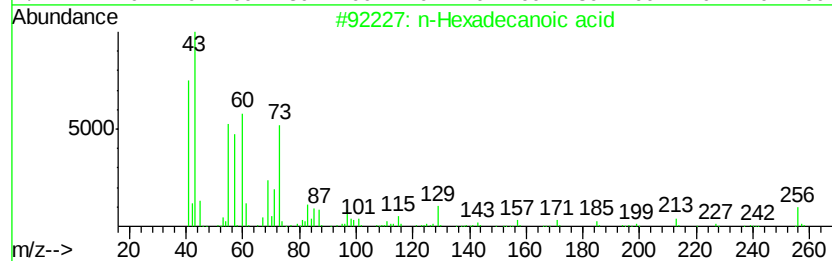
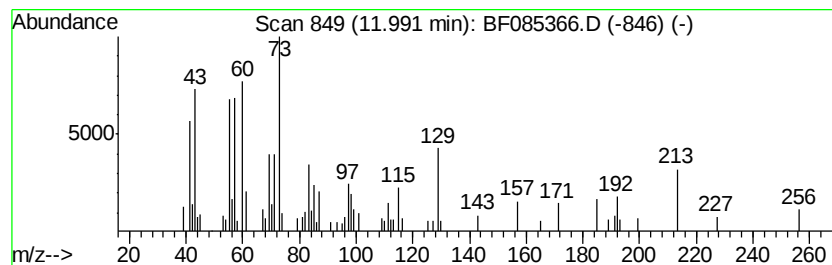
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.27 ng	121190	Phenanthrene-d10	11.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tridecanoic acid	214	C13H26O2	000638-53-9	74
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		d-Glucohexodialdose	178	C6H10O6	1000149-19-1	27



Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085366.D
Acq On : 11 Mar 2016 6:59
Operator : UM/SJ
Sample : H1731-16
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-COMP

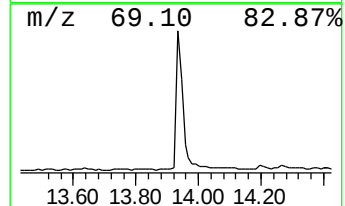
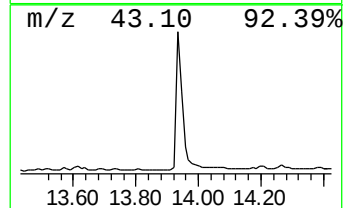
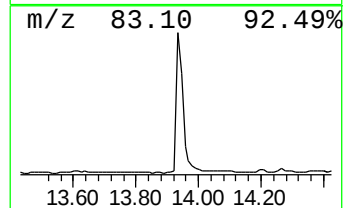
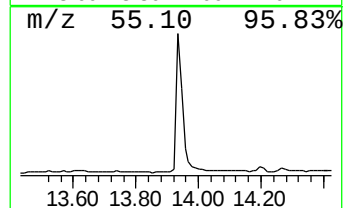
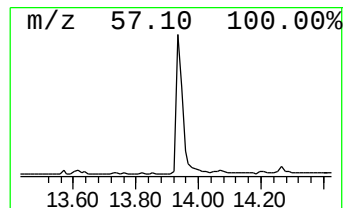
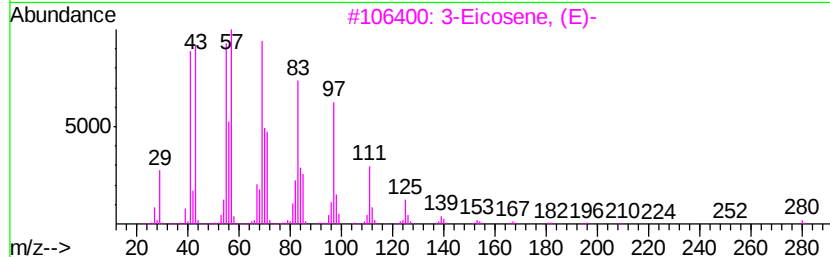
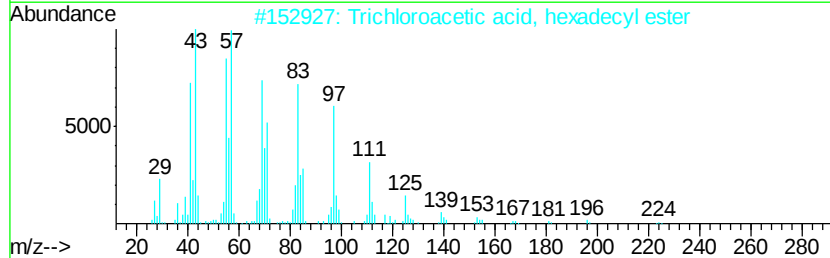
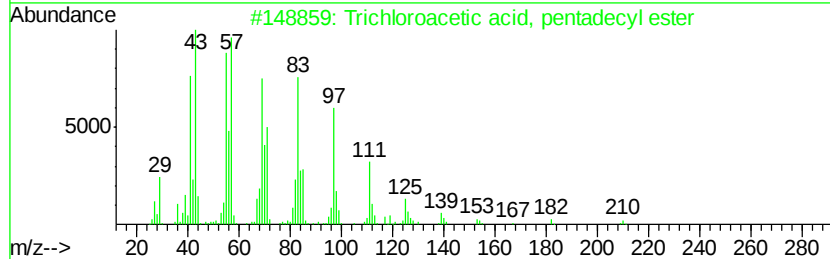
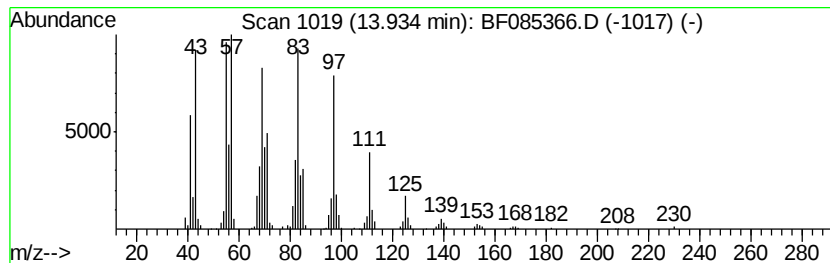
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trichloroacetic acid, penta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	16.71 ng	686847	Chrysene-d12	14.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91



Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085366.D
Acq On : 11 Mar 2016 6:59
Operator : UM/SJ
Sample : H1731-16
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-COMP

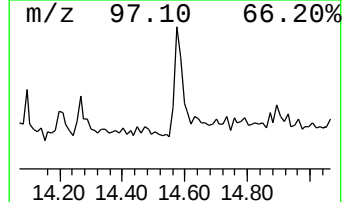
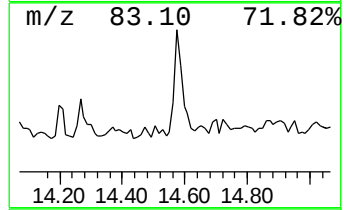
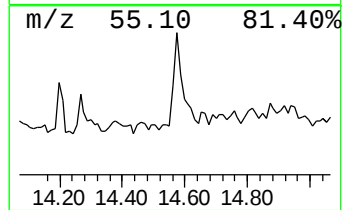
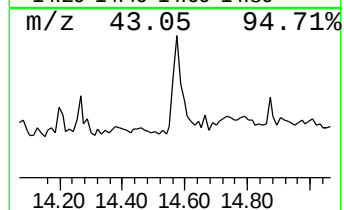
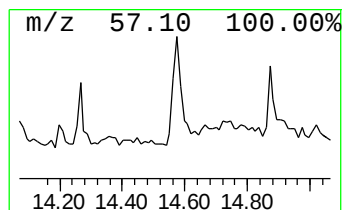
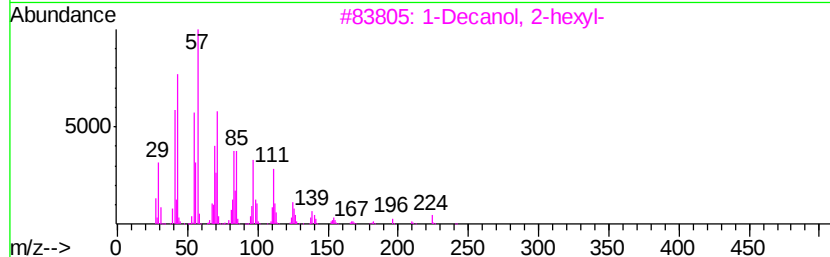
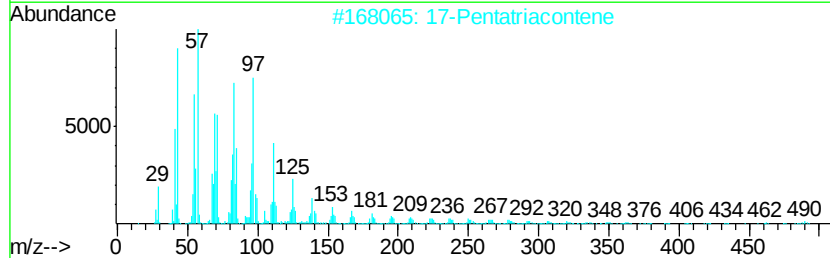
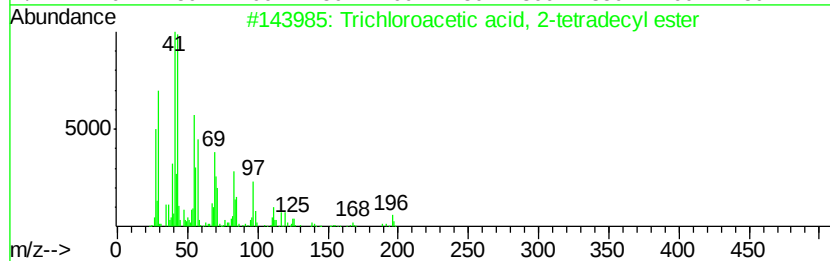
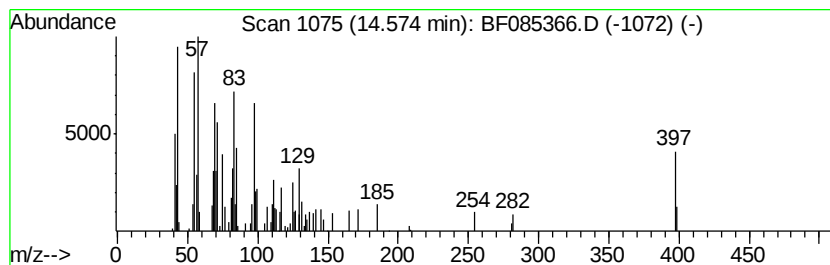
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.57 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	2.41 ng	98923	Chrysene-d12	14.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, 2-tetradec...	358	C16H29Cl3O2	1000282-06-6	46
2		17-Pentatriacontene	491	C35H70	006971-40-0	38
3		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	30
4		Nonahexacontanoic acid	999	C69H138O2	040710-32-5	27
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	25



Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085366.D
Acq On : 11 Mar 2016 6:59
Operator : UM/SJ
Sample : H1731-16
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-COMP

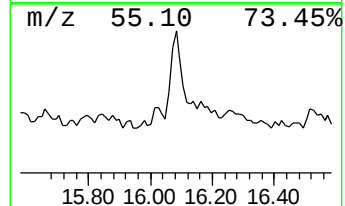
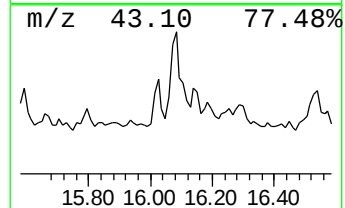
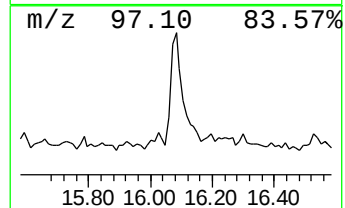
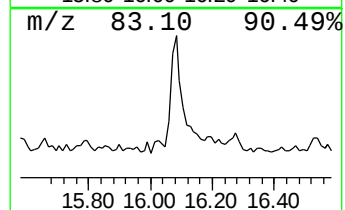
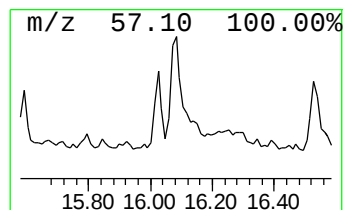
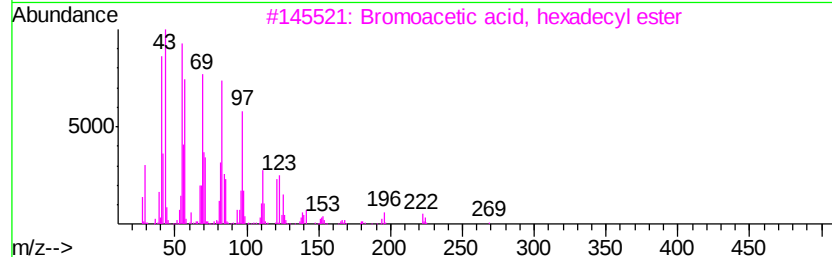
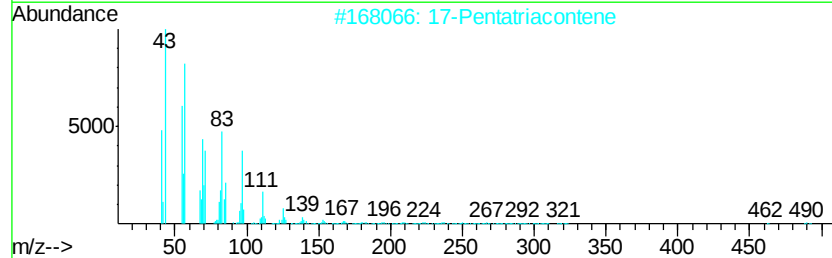
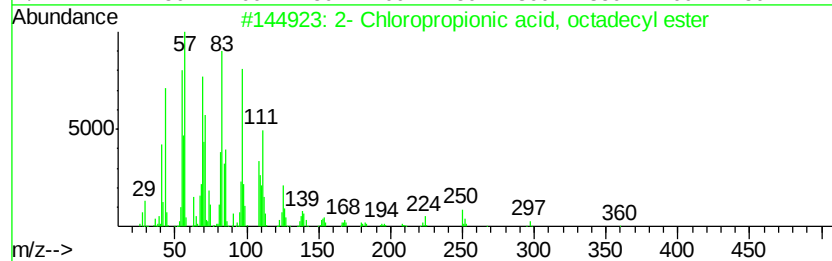
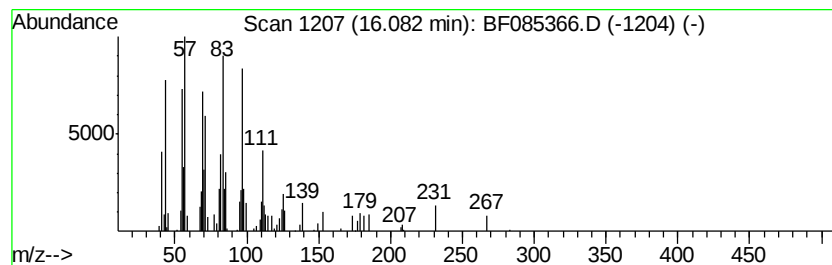
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2- Chloropropionic acid, oc... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	2.64 ng	107131	Perylene-d12	15.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	93
2	17-	Pentatriacontene	491	C35H70	006971-40-0	91
3	Bromoacetic acid, hexadecyl ester		362	C18H35BrO2	005454-48-8	91
4	Bacteriochlorophyll-c-stearyl		841	C52H72MgN4O4	1000164-49-7	87
5	Pentafluoropropionic acid, hepta...		402	C20H35F5O2	1000283-04-2	87



Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085366.D
Acq On : 11 Mar 2016 6:59
Operator : UM/SJ
Sample : H1731-16
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-29-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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...	5.14	6.2	ng	305256	1	6.94	993390	20.0
unknown6.71	6.71	90.8	ng	4511950	1	6.94	993390	20.0
Tetradecane	10.40	2.2	ng	132412	3	9.98	1227410	20.0
Pentadecane	10.88	3.6	ng	192299	4	11.46	1067270	20.0
n-Hexadecanoic acid	11.99	2.3	ng	121190	4	11.46	1067270	20.0
Trichloroacetic a...	13.93	16.7	ng	686847	5	14.09	822215	20.0
unknown14.57	14.57	2.4	ng	98923	5	14.09	822215	20.0
2- Chloropropioni...	16.08	2.6	ng	107131	6	15.56	810643	20.0