

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110116\
 Data File : BF090956.D
 Acq On : 1 Nov 2016 17:43
 Operator : UM/SJ
 Sample : H5478-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SD-3

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-BF102616.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	4.898	244	246	259	rBV	708801	1260000	21.87%	2.500%
2	5.333	281	284	287	rBV	3868667	5074110	88.05%	10.068%
3	6.384	373	376	378	rBV	4260825	4976364	86.36%	9.874%
4	6.510	384	387	389	rBV	4425938	5614209	97.43%	11.139%
5	6.739	405	407	409	rBV	893549	997778	17.32%	1.980%
6	6.887	418	420	423	rBV	3113997	3918006	67.99%	7.774%
7	7.310	454	457	459	rBV	2304794	3499619	60.73%	6.944%
8	7.413	463	466	474	rVB	79186	154577	2.68%	0.307%
9	8.019	517	519	522	rBV	1411984	1402202	24.33%	2.782%
10	9.105	611	614	616	rBV	5462322	5762474	100.00%	11.433%
11	9.505	646	649	651	rBV	1504507	1858315	32.25%	3.687%
12	9.699	663	666	670	rBV3	25581	58155	1.01%	0.115%
13	9.779	670	673	675	rBV	1324216	1681913	29.19%	3.337%
14	10.190	703	709	713	rBV3	58465	113205	1.96%	0.225%
15	10.568	739	742	744	rBV	3668690	3985107	69.16%	7.907%
16	10.693	751	753	759	rVB	61986	117171	2.03%	0.232%
17	11.139	790	792	793	rBV	59817	65777	1.14%	0.131%
18	11.253	800	802	805	rBV	1791764	1627283	28.24%	3.229%
19	11.493	820	823	827	rBV	102503	121978	2.12%	0.242%
20	12.842	938	941	944	rBV	4244298	5184939	89.98%	10.288%
21	13.745	1017	1020	1026	rBV	273151	348240	6.04%	0.691%
22	13.894	1030	1033	1035	rBV	947597	1361397	23.63%	2.701%
23	14.374	1073	1075	1081	rBV	45892	75618	1.31%	0.150%
24	14.739	1104	1107	1109	rBV	105144	148253	2.57%	0.294%
25	14.979	1125	1128	1133	rBV	42177	70471	1.22%	0.140%
26	15.288	1152	1155	1157	rBV	706328	922774	16.01%	1.831%

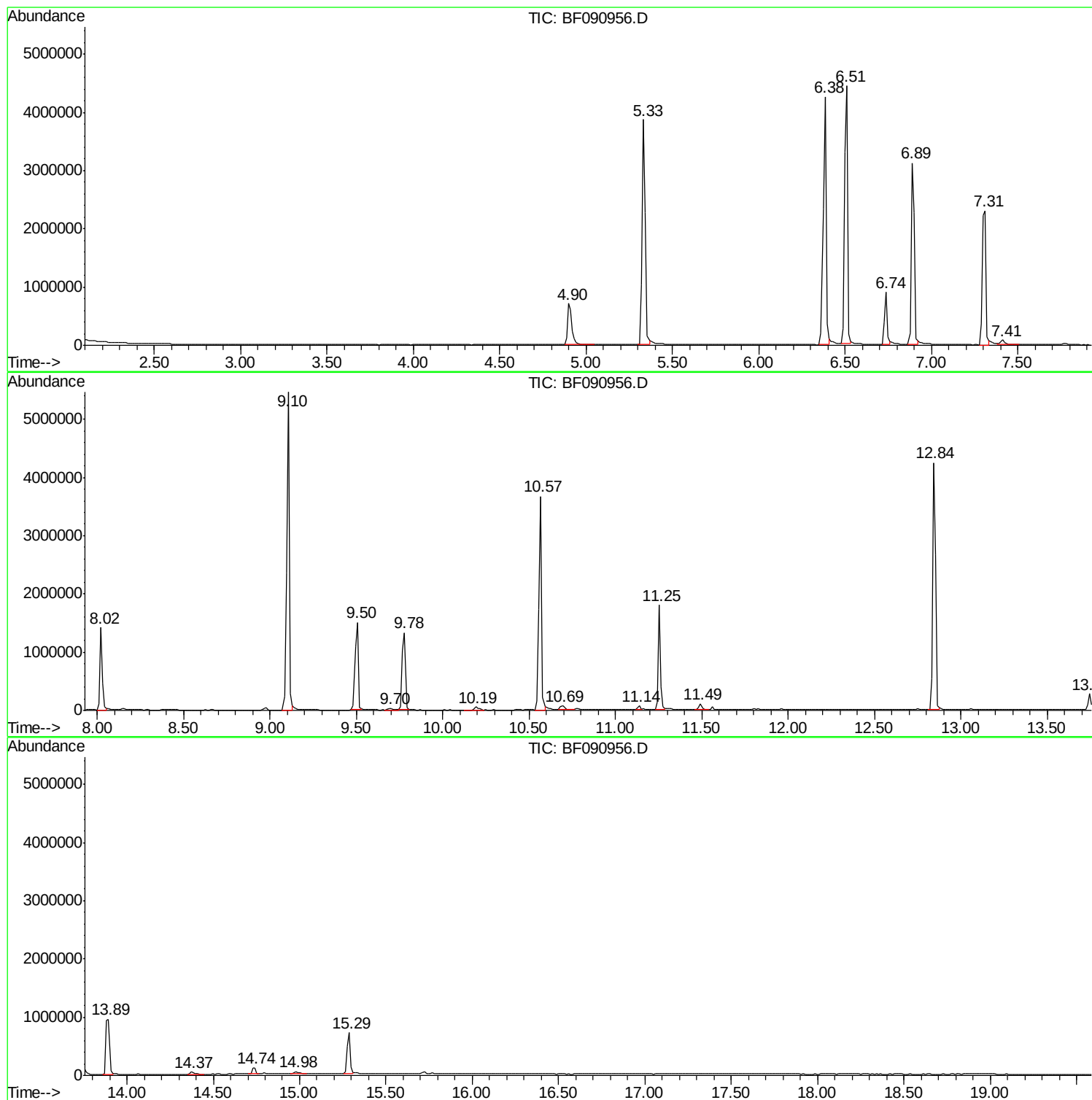
Sum of corrected areas: 50399935

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110116\
Data File : BF090956.D
Acq On : 1 Nov 2016 17:43
Operator : UM/SJ
Sample : H5478-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SD-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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\BF110116\
Data File : BF090956.D
Acq On : 1 Nov 2016 17:43
Operator : UM/SJ
Sample : H5478-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SD-3

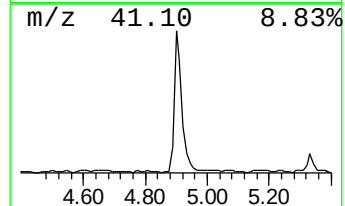
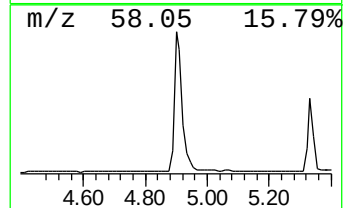
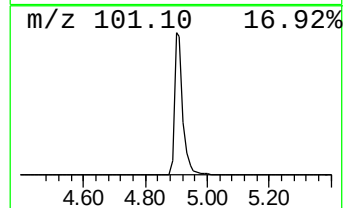
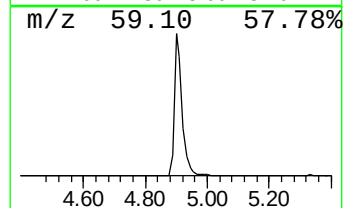
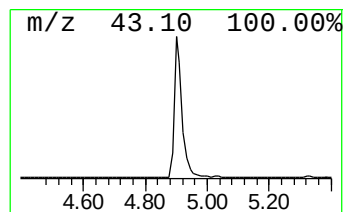
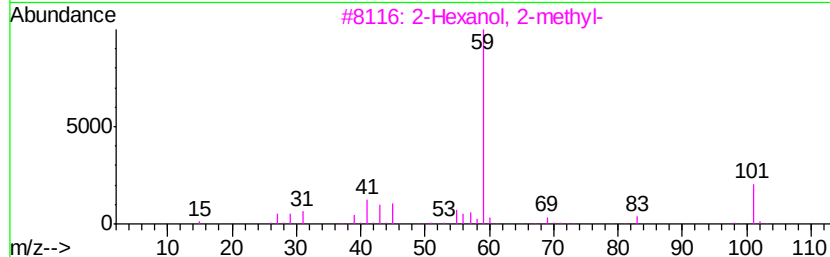
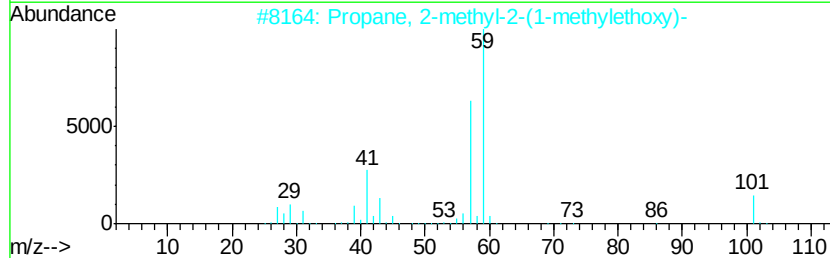
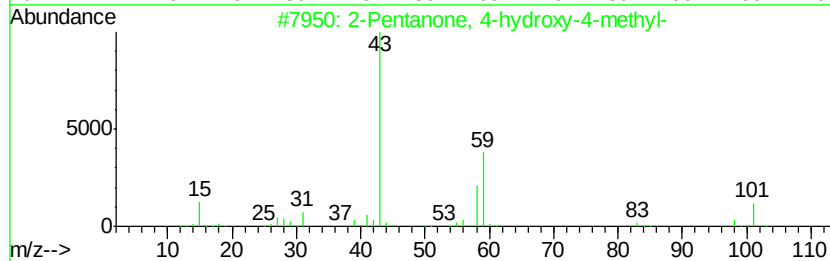
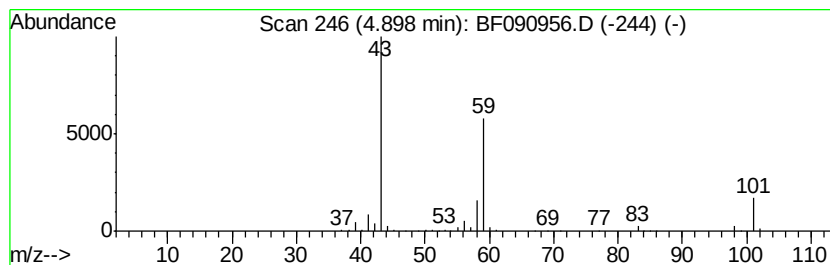
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.90	25.26 ng	1260000	1,4-Dichlorobenzene-d4	6.74

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110116\
Data File : BF090956.D
Acq On : 1 Nov 2016 17:43
Operator : UM/SJ
Sample : H5478-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SD-3

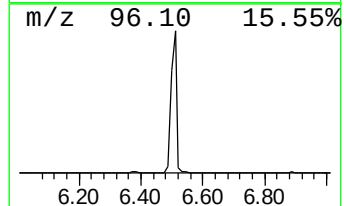
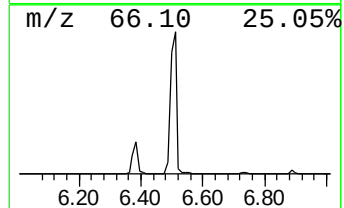
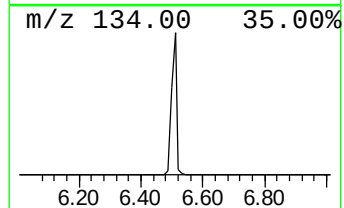
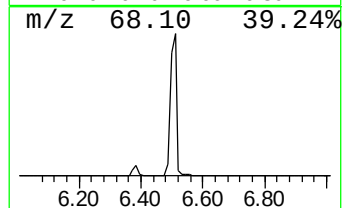
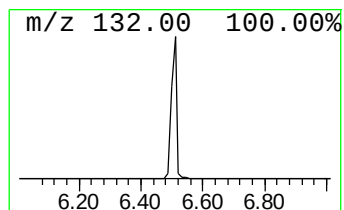
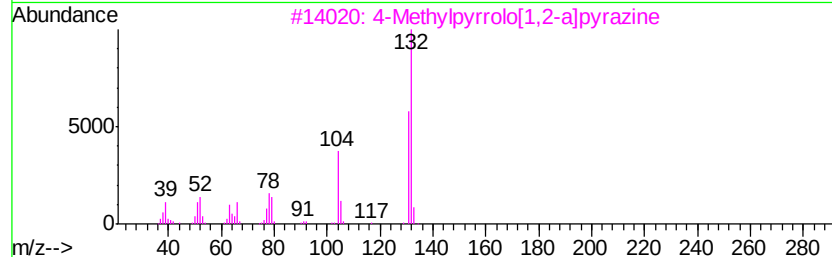
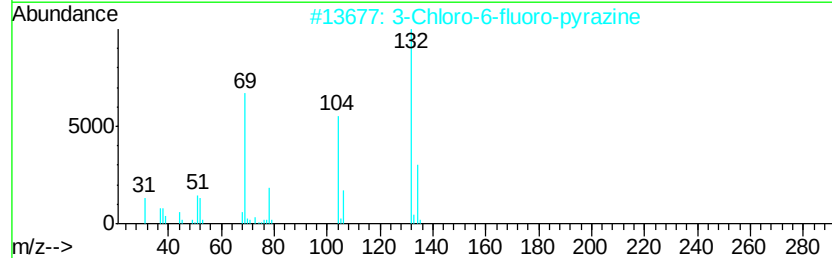
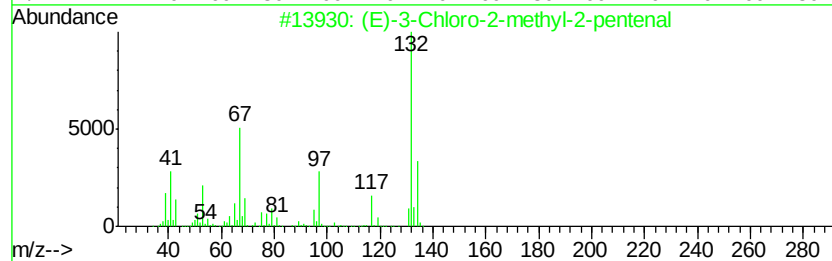
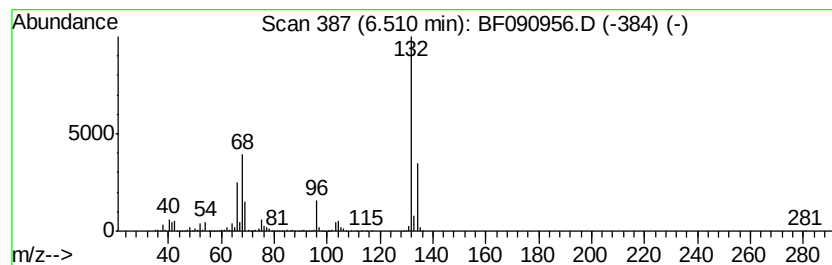
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	112.53 ng	5614210	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	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\BF110116\
Data File : BF090956.D
Acq On : 1 Nov 2016 17:43
Operator : UM/SJ
Sample : H5478-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SD-3

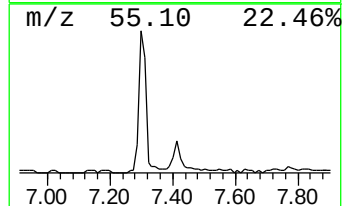
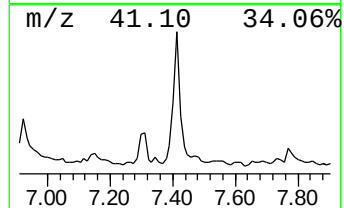
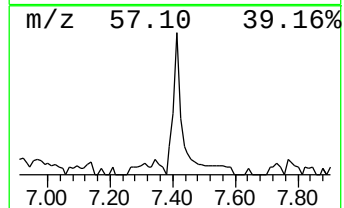
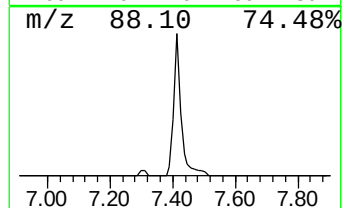
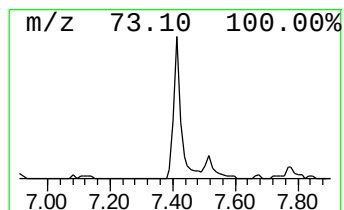
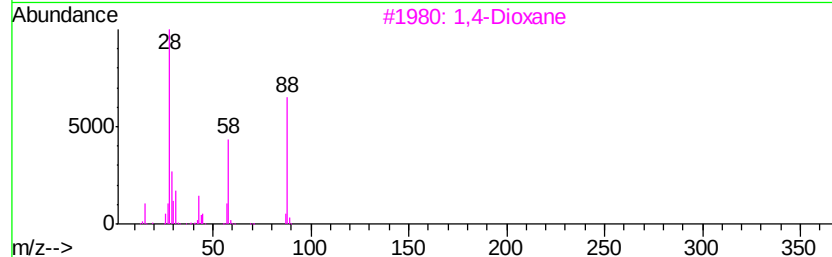
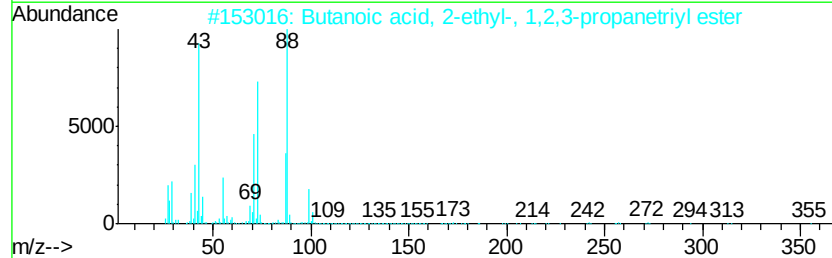
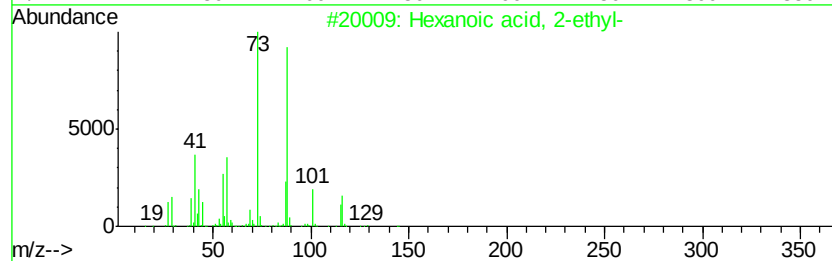
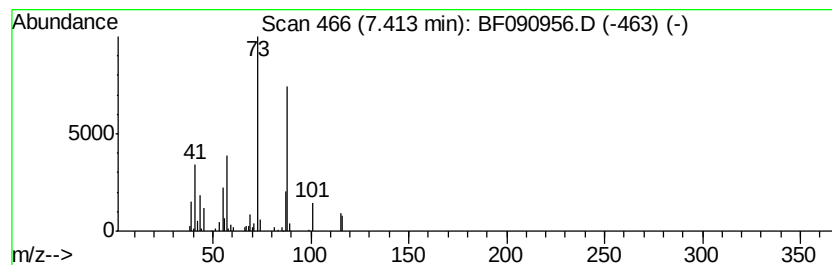
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	2.20 ng	154577	Naphthalene-d8	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	72
2		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
3		1,4-Dioxane	88	C4H8O2	000123-91-1	40
4		Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	36
5		Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	035939-74-3	33



Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090956.D
Acq On : 1 Nov 2016 17:43
Operator : UM/SJ
Sample : H5478-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

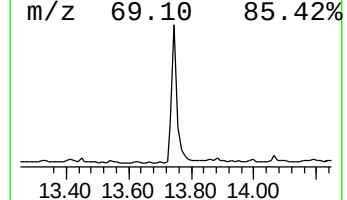
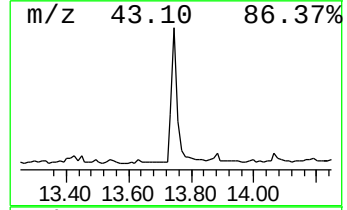
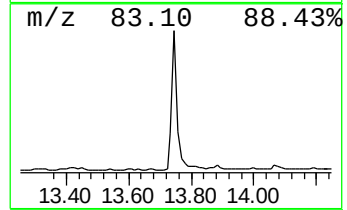
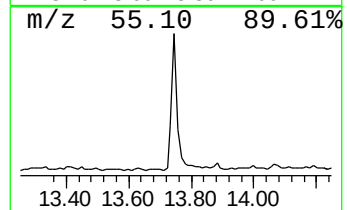
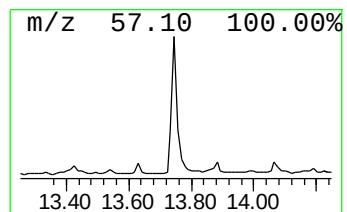
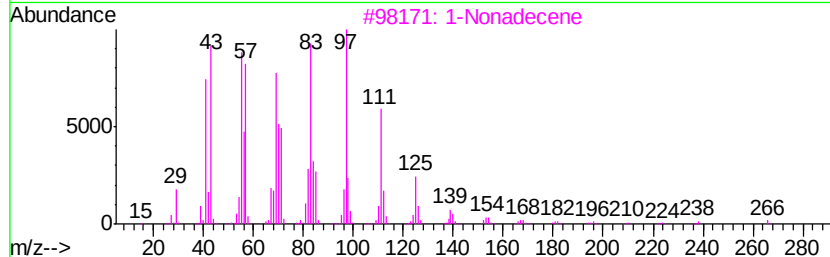
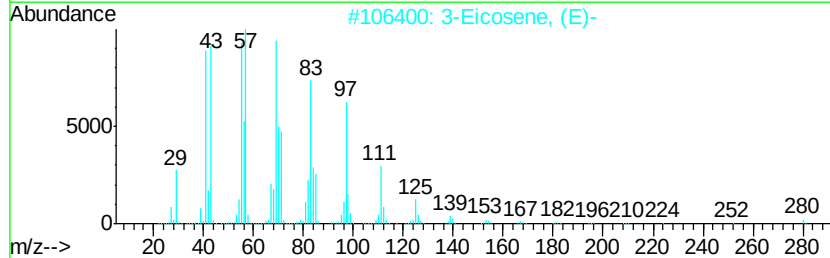
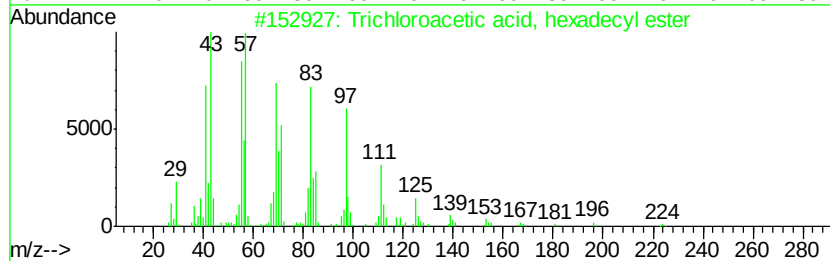
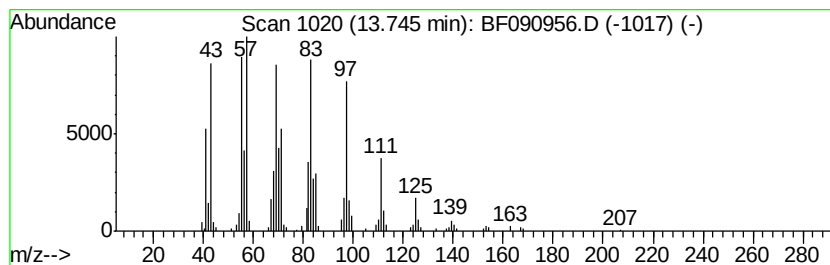
Instrument :
BNA_F
ClientSampleId :
SD-3

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.75	5.12 ng	348240	Chrysene-d12	13.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	90
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110116\
Data File : BF090956.D
Acq On : 1 Nov 2016 17:43
Operator : UM/SJ
Sample : H5478-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

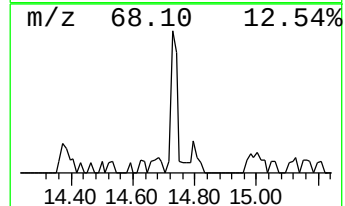
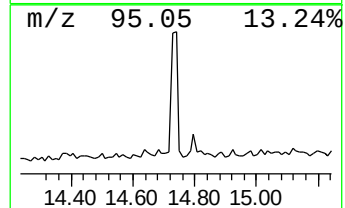
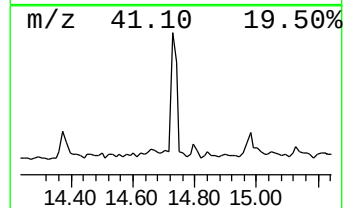
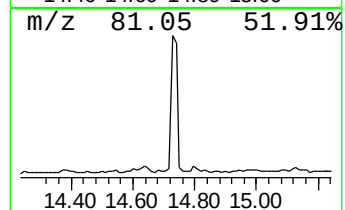
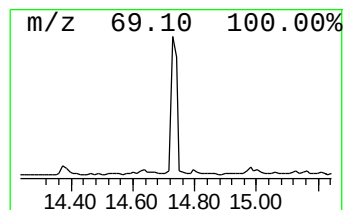
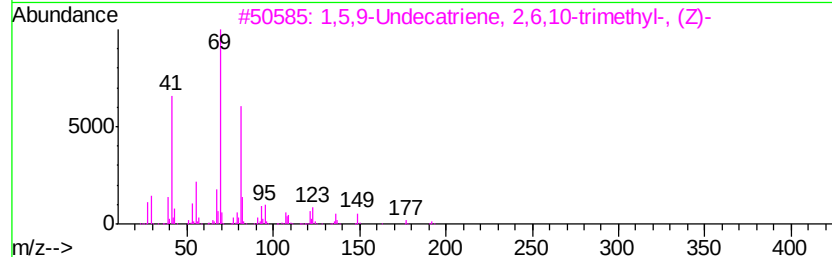
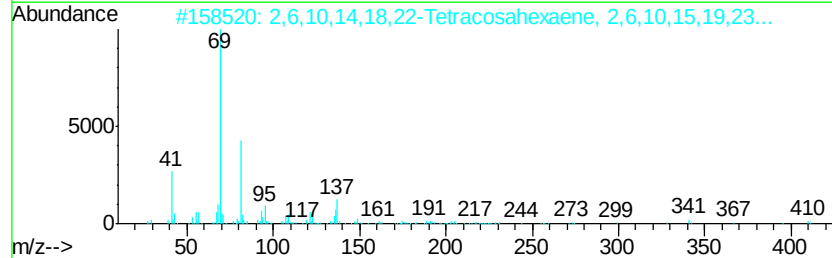
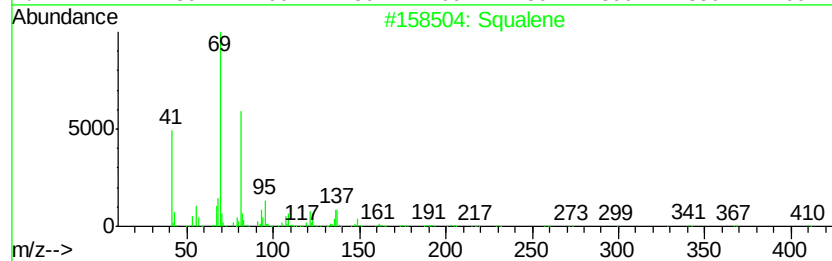
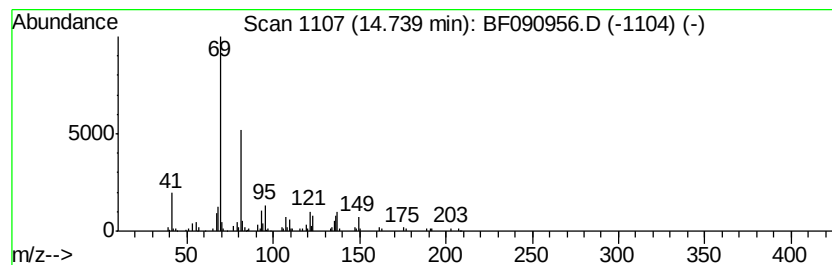
Instrument :
BNA_F
ClientSampleId :
SD-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	3.21 ng	148253	Perylene-d12	15.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	86
3	1,5,9-Undecatriene, 2,6,10-trime...	192 C14H24	062951-96-6	86
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222 C15H26O	000106-28-5	64
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264 C17H28O2	004128-17-0	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110116\
Data File : BF090956.D
Acq On : 1 Nov 2016 17:43
Operator : UM/SJ
Sample : H5478-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SD-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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...	4.90	25.3	ng	1260000	1	6.74	997778	20.0
unknown6.51	6.51	112.5	ng	5614210	1	6.74	997778	20.0
Hexanoic acid, 2-...	7.41	2.2	ng	154577	2	8.02	1402200	20.0
Trichloroacetic a...	13.75	5.1	ng	348240	5	13.89	1361400	20.0
Squalene	14.74	3.2	ng	148253	6	15.29	922774	20.0