

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
 Data File : BF088601.D
 Acq On : 2 Jul 2016 4:31
 Operator : UM/SJ
 Sample : H3831-02
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-03-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-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	1.667	3	7	9	rVB	4677511	6644803	100.00%	17.591%
2	1.735	12	13	23	rVB	536358	832088	12.52%	2.203%
3	1.872	23	25	39	rVB	2261074	5256686	79.11%	13.916%
4	2.055	39	41	83	rVB2	143473	824500	12.41%	2.183%
5	4.981	294	297	301	rBV	218165	294783	4.44%	0.780%
6	5.404	331	334	337	rBV	2403775	2495334	37.55%	6.606%
7	6.444	421	425	427	rBV	2546607	3068962	46.19%	8.124%
8	6.570	433	436	439	rBV	2086841	2733125	41.13%	7.235%
9	6.810	454	457	459	rBV	815206	767668	11.55%	2.032%
10	6.970	468	471	473	rVB	1604184	2245486	33.79%	5.944%
11	7.370	503	506	508	rBV	1776963	1710816	25.75%	4.529%
12	8.090	567	569	571	rVB	1126625	963383	14.50%	2.550%
13	9.176	661	664	666	rVB	2250721	3031008	45.61%	8.024%
14	9.565	696	698	700	rBV	146959	157523	2.37%	0.417%
15	9.839	720	722	725	rVB	973353	939355	14.14%	2.487%
16	10.628	788	791	793	rBV	1439475	1437512	21.63%	3.806%
17	11.199	839	841	843	rBV	70088	70653	1.06%	0.187%
18	11.313	849	851	854	rVB	621612	769728	11.58%	2.038%
19	12.902	987	990	993	rBV	2253863	2038445	30.68%	5.396%
20	13.828	1068	1071	1078	rBV	58258	108323	1.63%	0.287%
21	13.942	1078	1081	1084	rBV	779917	707427	10.65%	1.873%
22	14.799	1153	1156	1158	rBV	123566	123442	1.86%	0.327%
23	15.348	1201	1204	1206	rBV	388645	553375	8.33%	1.465%

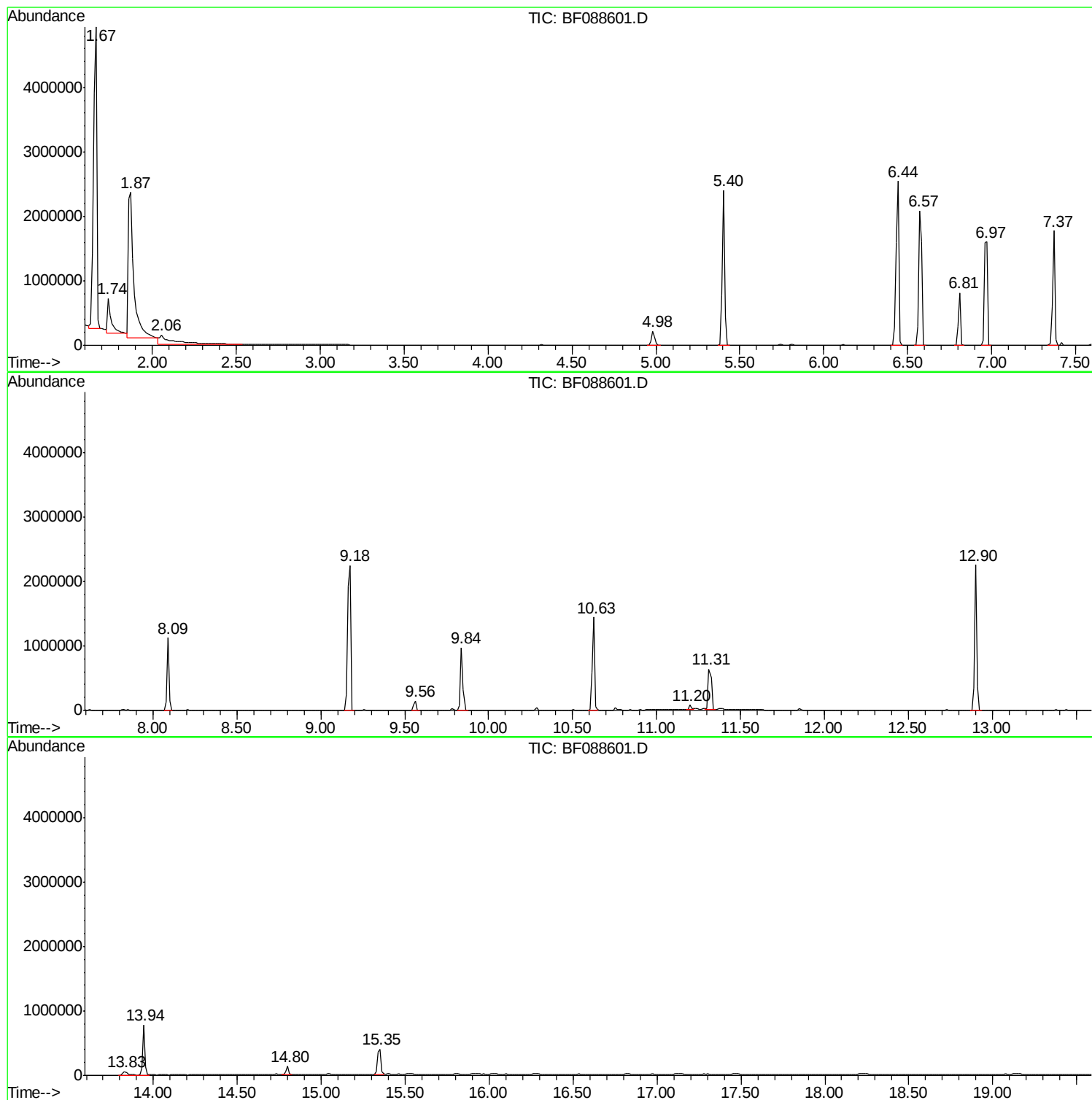
Sum of corrected areas: 37774425

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088601.D
Acq On : 2 Jul 2016 4:31
Operator : UM/SJ
Sample : H3831-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

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\BF070116\
Data File : BF088601.D
Acq On : 2 Jul 2016 4:31
Operator : UM/SJ
Sample : H3831-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
SB-03-COMP

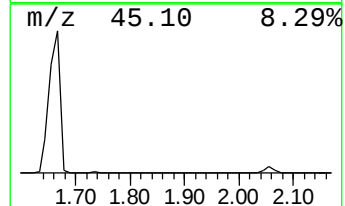
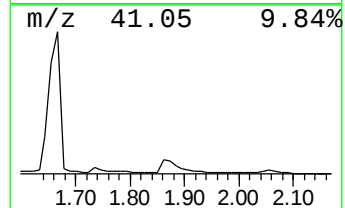
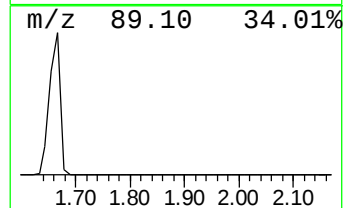
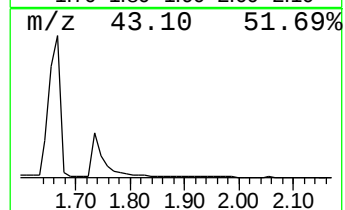
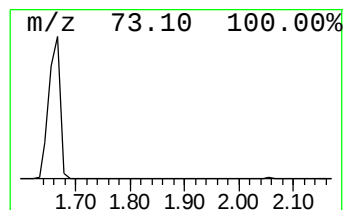
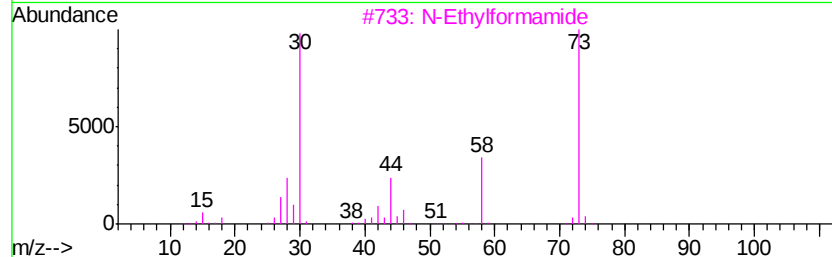
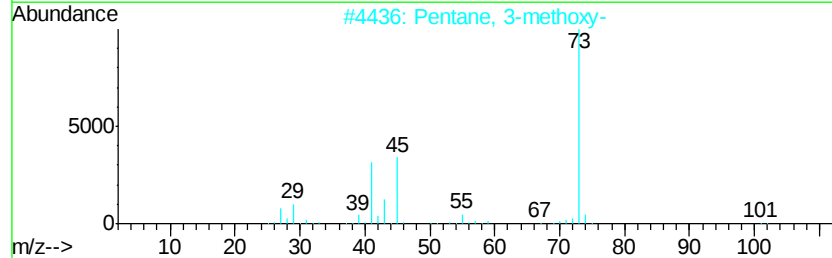
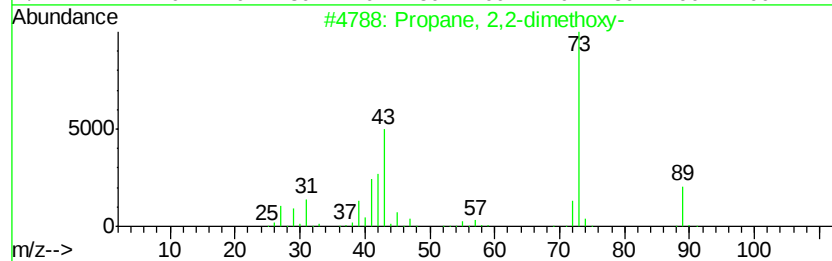
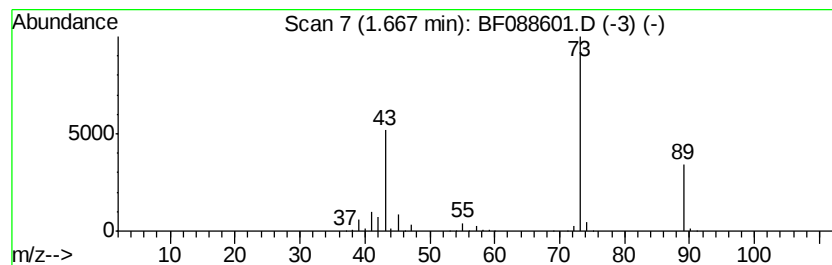
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	173.12 ng	6644800	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3			N-Ethylformamide	73	C3H7NO	000627-45-2	9
4			1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5			1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088601.D
Acq On : 2 Jul 2016 4:31
Operator : UM/SJ
Sample : H3831-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

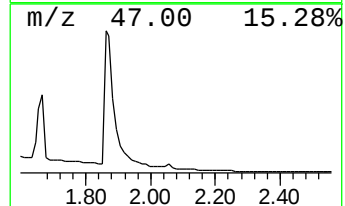
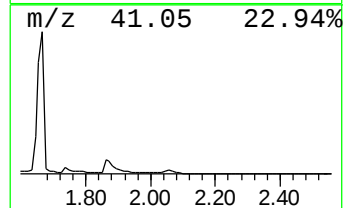
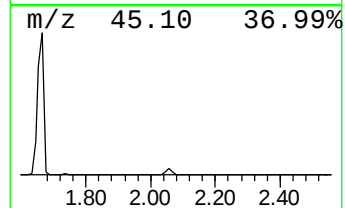
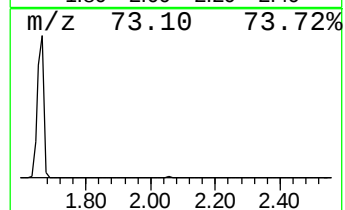
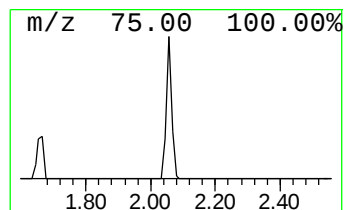
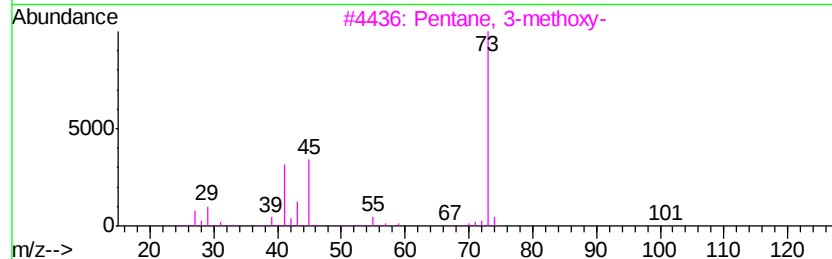
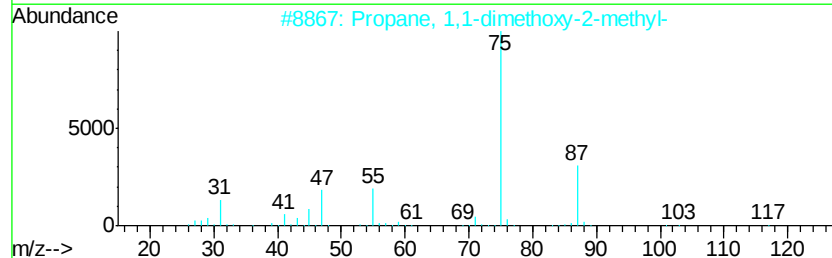
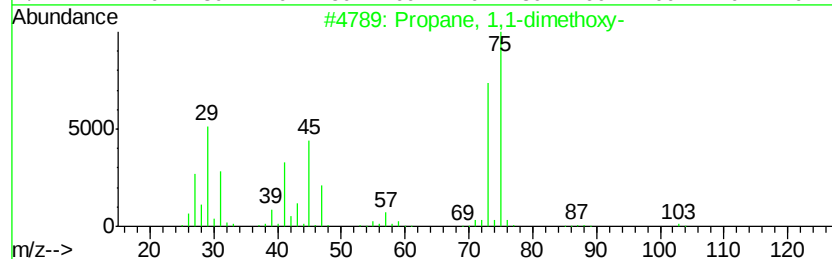
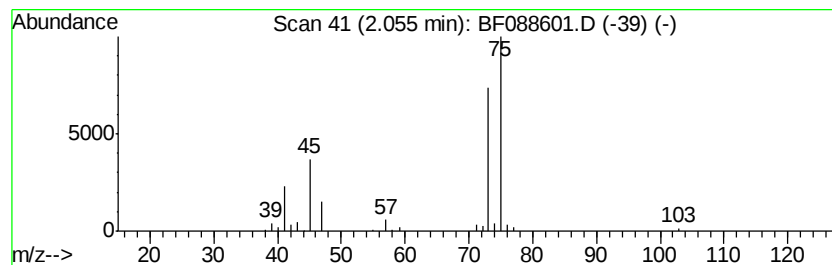
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.06	21.48 ng	824500	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	36
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
4		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	12
5		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088601.D
Acq On : 2 Jul 2016 4:31
Operator : UM/SJ
Sample : H3831-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

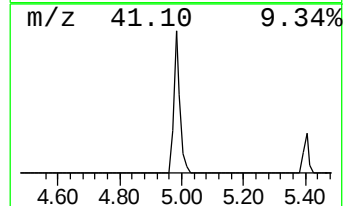
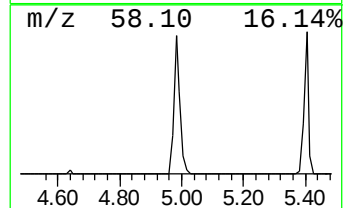
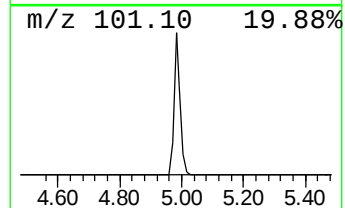
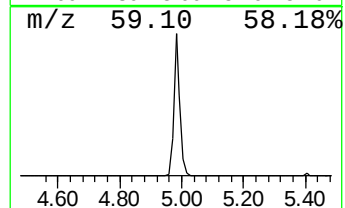
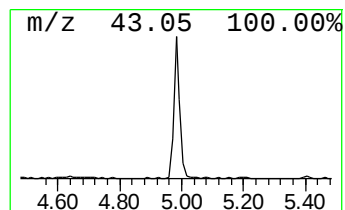
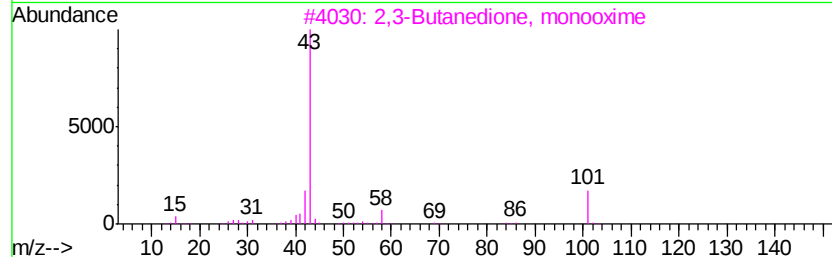
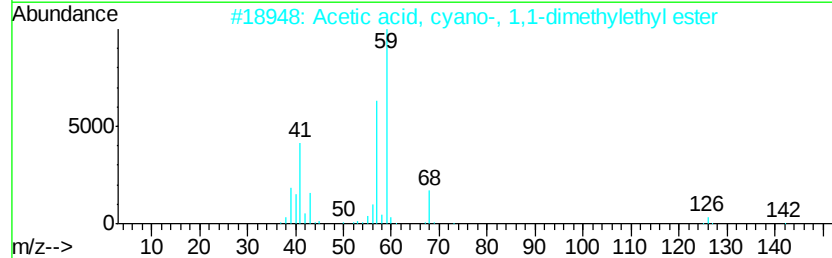
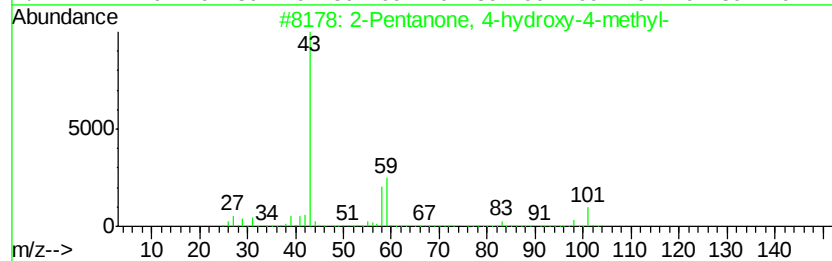
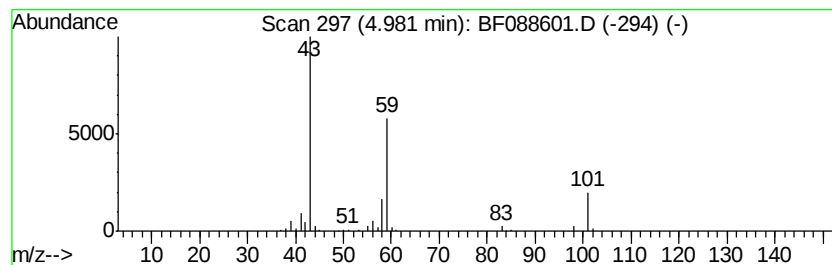
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	7.68 ng	294783	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088601.D
Acq On : 2 Jul 2016 4:31
Operator : UM/SJ
Sample : H3831-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

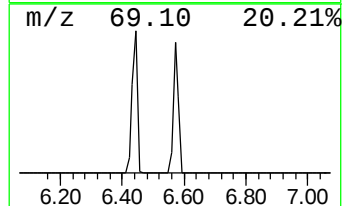
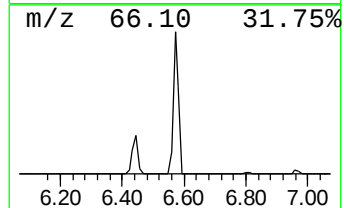
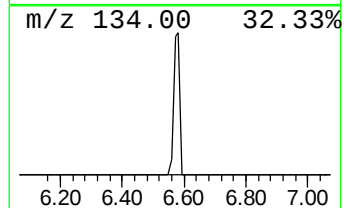
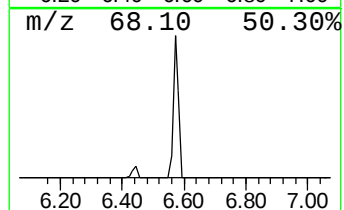
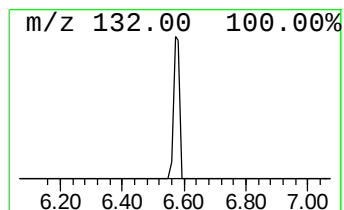
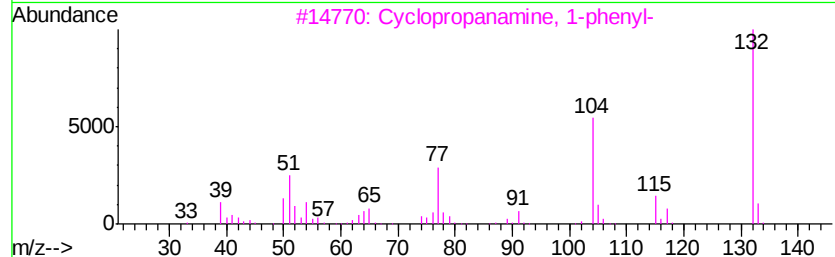
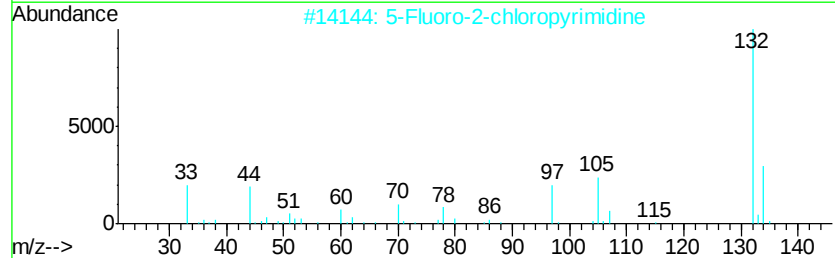
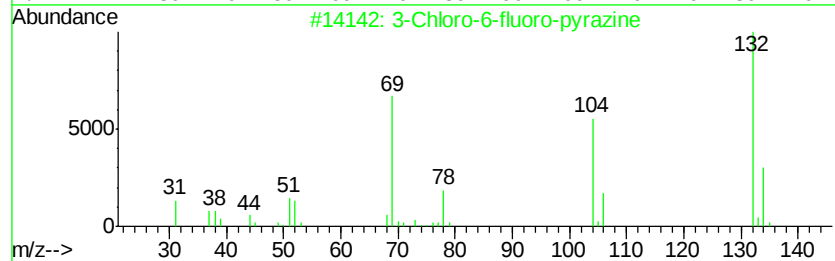
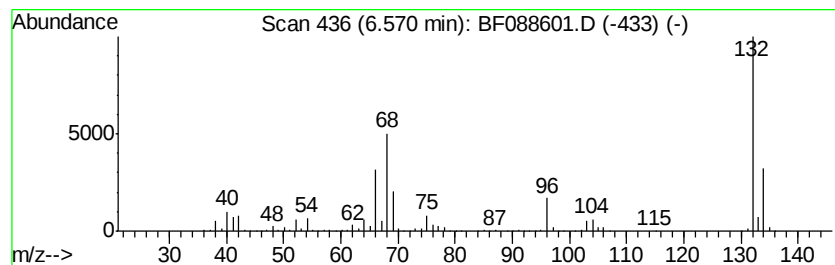
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown6.57 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	71.21 ng	2733130	1,4-Dichlorobenzene-d4	6.81

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	12
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088601.D
Acq On : 2 Jul 2016 4:31
Operator : UM/SJ
Sample : H3831-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

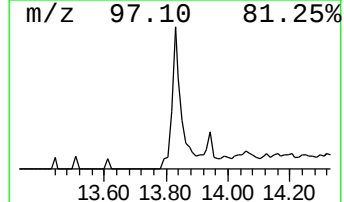
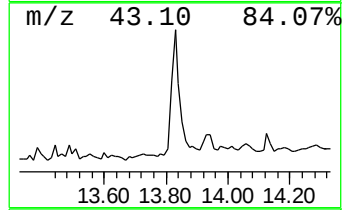
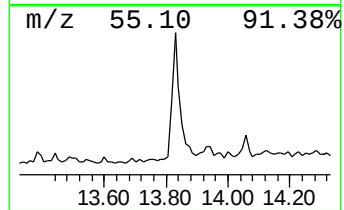
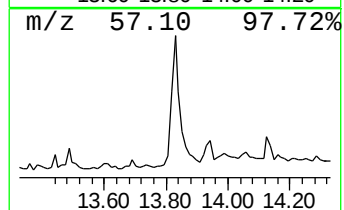
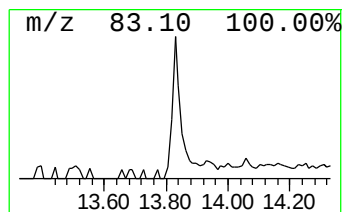
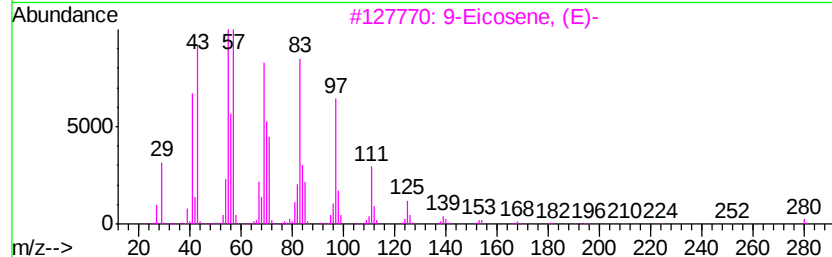
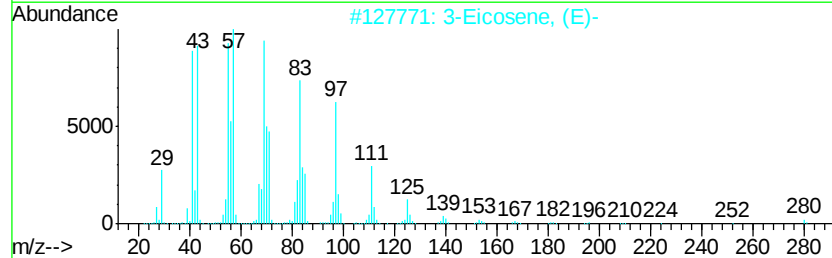
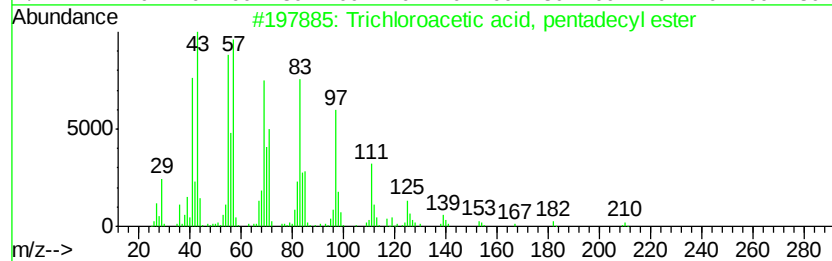
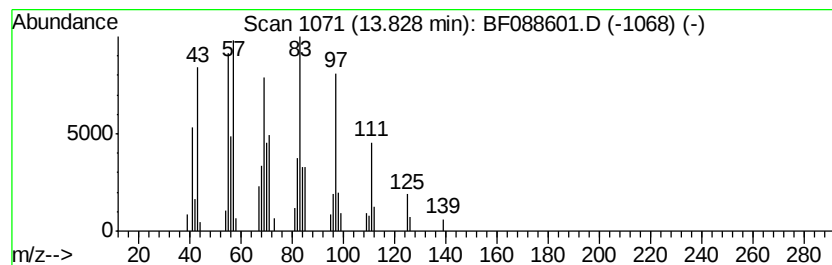
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trichloroacetic acid, penta... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	3.06 ng	108323	Chrysene-d12	13.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3		9-Eicosene, (E)-	280	C20H40	074685-29-3	90
4		1-Hexadecanol	242	C16H34O	036653-82-4	87
5		11-Tricosene	322	C23H46	052078-56-5	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088601.D
Acq On : 2 Jul 2016 4:31
Operator : UM/SJ
Sample : H3831-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

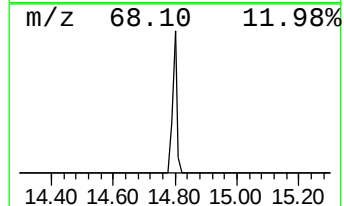
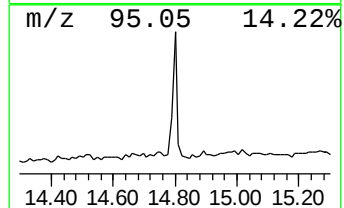
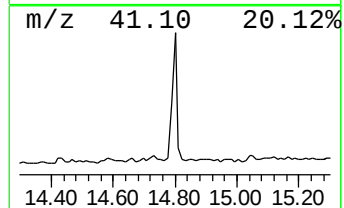
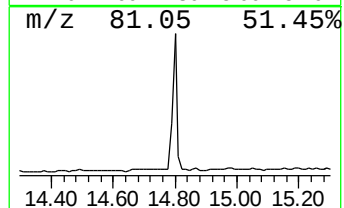
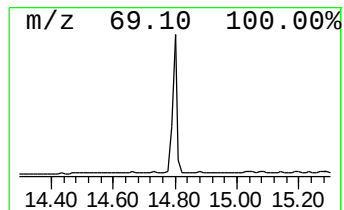
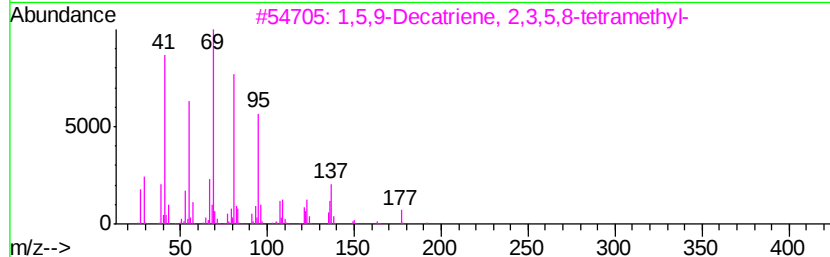
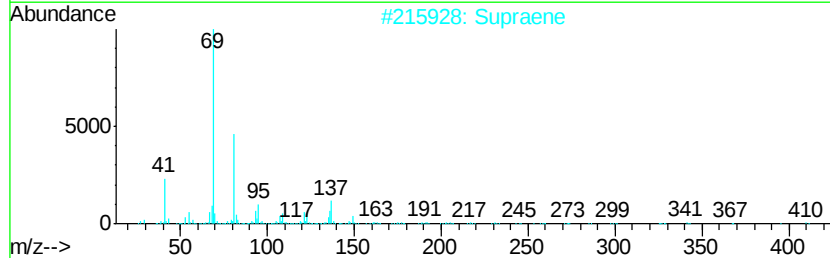
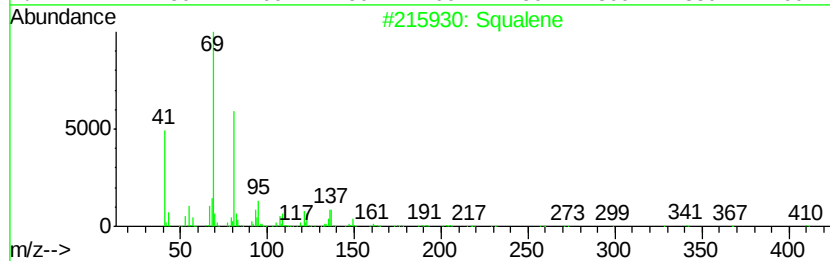
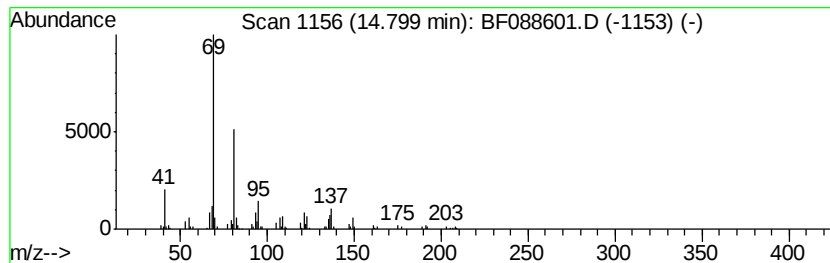
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	4.46 ng	123442	Perylene-d12	15.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5		Farnesol isomer a	222	C15H26O	1000108-92-4	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088601.D
Acq On : 2 Jul 2016 4:31
Operator : UM/SJ
Sample : H3831-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

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
Propane, 2,2-dime...	1.67	173.1	ng	6644800	1	6.81	767668	20.0
Propane, 1,1-dime...	2.06	21.5	ng	824500	1	6.81	767668	20.0
2-Pentanone, 4-hy...	4.98	7.7	ng	294783	1	6.81	767668	20.0
unknown6.57	6.57	71.2	ng	2733130	1	6.81	767668	20.0
Trichloroacetic a...	13.83	3.1	ng	108323	5	13.94	707427	20.0
Squalene	14.80	4.5	ng	123442	6	15.35	553375	20.0