

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111017\
 Data File : BF100417.D
 Acq On : 11 Nov 2017 3:28
 Operator : SJ/JU
 Sample : I6355-07
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 110317-TIFR-F-D-S

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-BF110817.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	2.205	17	20	45	rVB4	109867	286706	6.49%	1.041%
2	5.122	512	516	525	rVB	286622	297395	6.73%	1.080%
3	5.516	579	583	586	rBV	1883442	1643098	37.18%	5.965%
4	6.516	749	753	756	rBV	1258349	1088798	24.64%	3.953%
5	6.545	756	758	762	rVB	72310	58877	1.33%	0.214%
6	6.669	774	779	782	rBV	2945453	2654839	60.07%	9.638%
7	6.904	815	819	822	rBV	1016726	904737	20.47%	3.285%
8	7.063	841	846	849	rBV	3312836	3257770	73.71%	11.827%
9	7.469	909	915	918	rBV	2597626	2791801	63.17%	10.135%
10	8.181	1032	1036	1040	rBV	1275568	1103428	24.97%	4.006%
11	9.263	1214	1220	1223	rBV	4414361	4419616	100.00%	16.045%
12	9.645	1282	1285	1289	rBV	62671	51615	1.17%	0.187%
13	9.939	1329	1335	1343	rVB	1210322	1096644	24.81%	3.981%
14	10.604	1445	1448	1452	rBV	74434	51715	1.17%	0.188%
15	10.722	1464	1468	1472	rBV	1574728	1523459	34.47%	5.531%
16	11.422	1583	1587	1591	rBV	1022687	887891	20.09%	3.223%
17	12.821	1822	1825	1829	rBV	227395	178118	4.03%	0.647%
18	12.898	1831	1838	1842	rBV4	54018	77906	1.76%	0.283%
19	13.010	1852	1857	1860	rBV	3384907	3330238	75.35%	12.090%
20	13.527	1942	1945	1949	rBV	150616	119134	2.70%	0.432%
21	13.898	2004	2008	2015	rBV2	57580	73687	1.67%	0.268%
22	14.063	2032	2036	2039	rBV	880197	786006	17.78%	2.853%
23	15.545	2282	2288	2300	rBV	465538	668709	15.13%	2.428%
24	16.009	2363	2367	2372	rBV	42436	62147	1.41%	0.226%
25	16.533	2451	2456	2462	rVB2	40689	71978	1.63%	0.261%
26	17.139	2555	2559	2566	rVB4	30428	59331	1.34%	0.215%

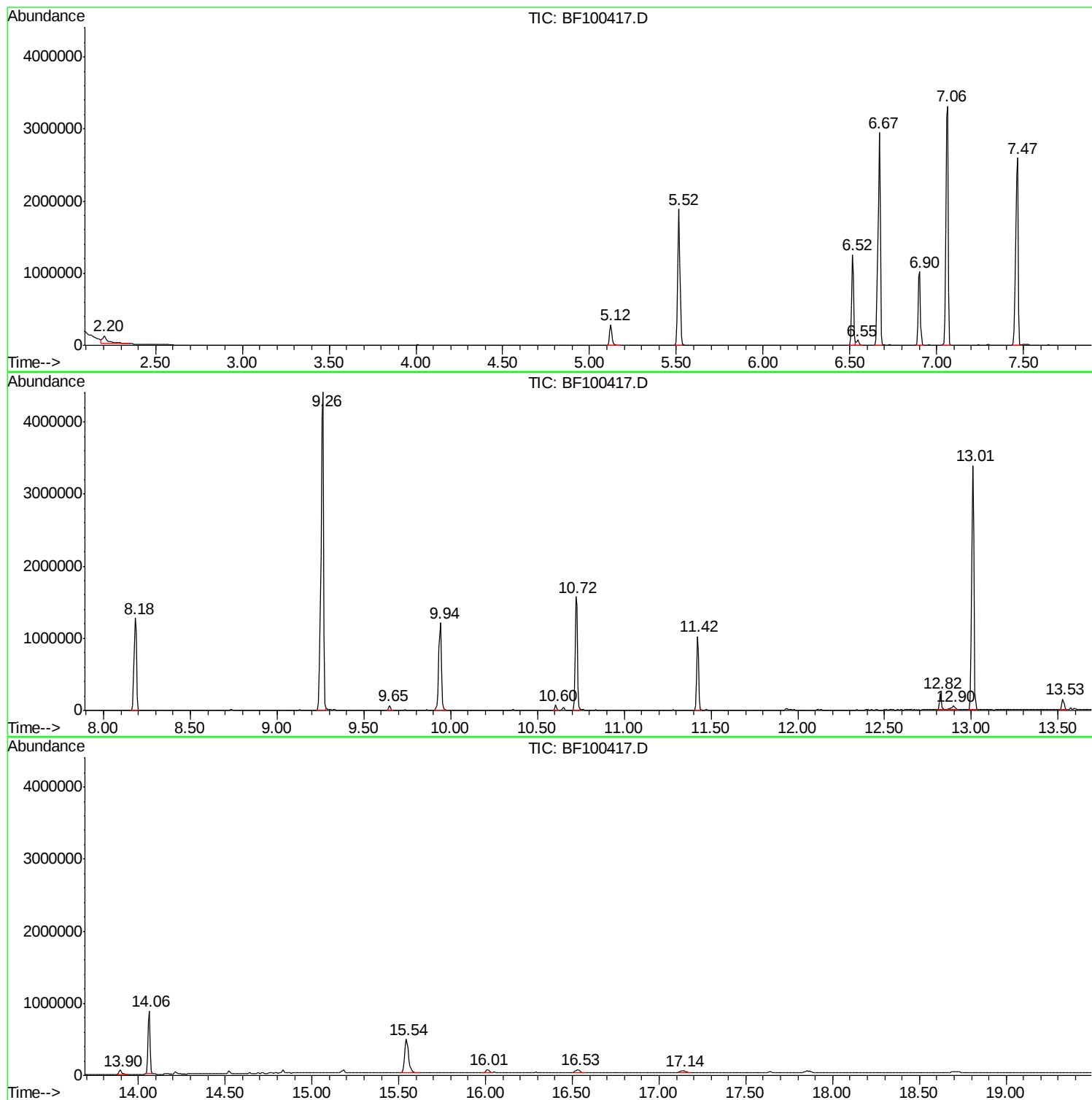
Sum of corrected areas: 27545643

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111017\
Data File : BF100417.D
Acq On : 11 Nov 2017 3:28
Operator : SJ/JU
Sample : I6355-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110317-TIFR-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111017\
Data File : BF100417.D
Acq On : 11 Nov 2017 3:28
Operator : SJ/JU
Sample : I6355-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110317-TIFR-F-D-S

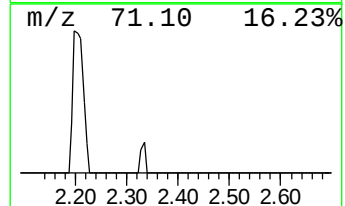
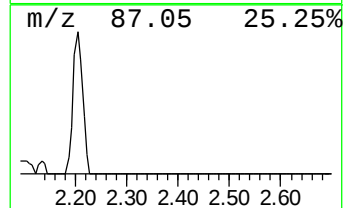
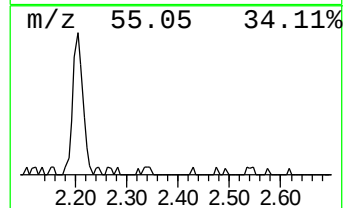
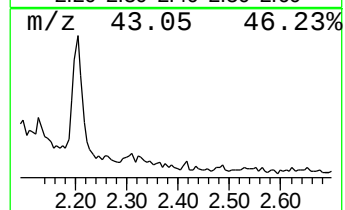
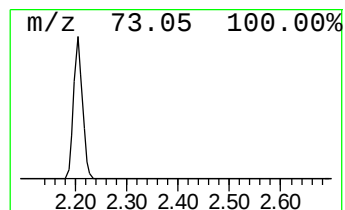
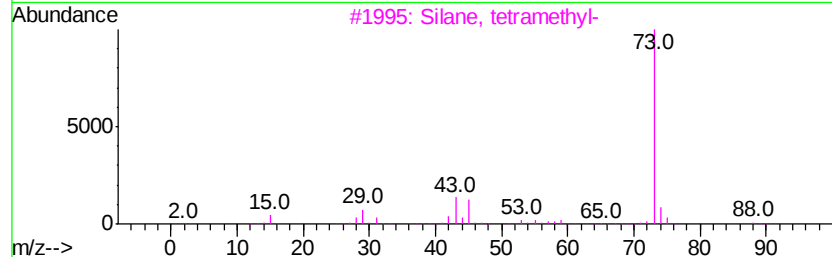
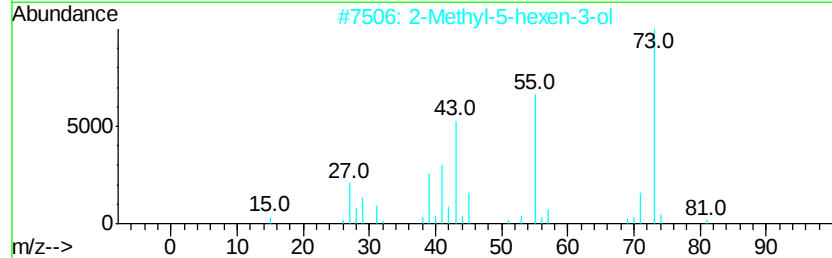
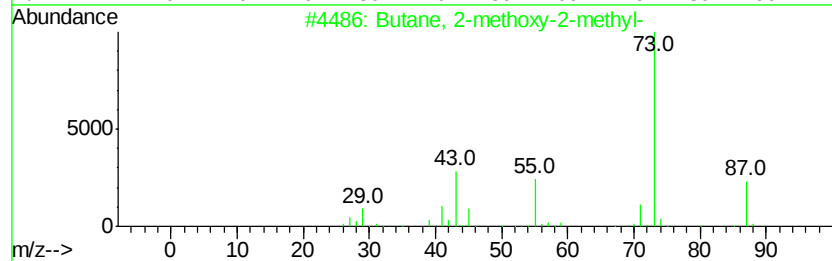
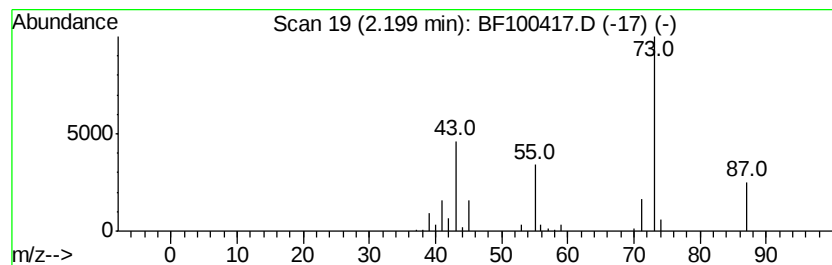
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	6.34 ng	286706	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111017\
Data File : BF100417.D
Acq On : 11 Nov 2017 3:28
Operator : SJ/JU
Sample : I6355-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110317-TIFR-F-D-S

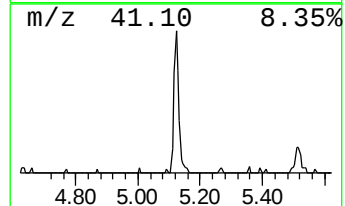
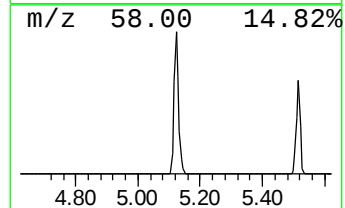
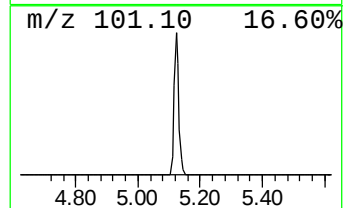
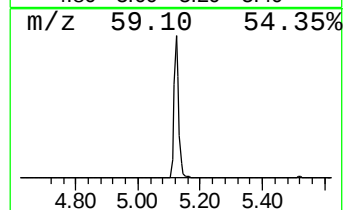
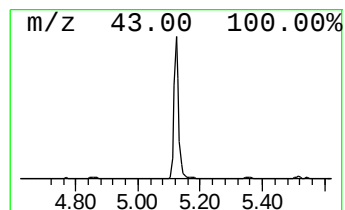
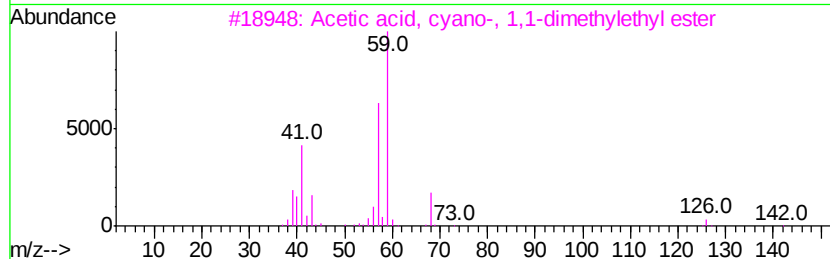
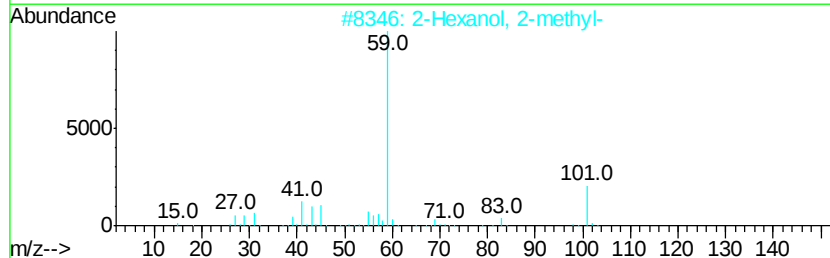
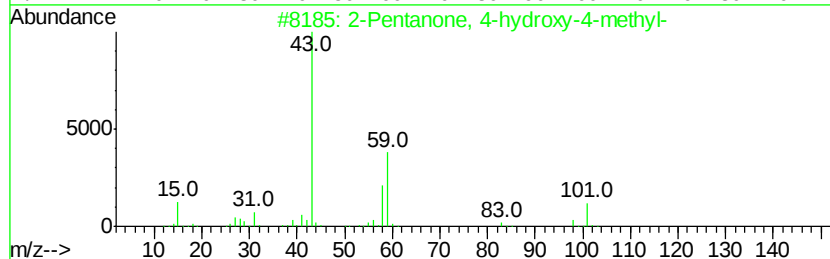
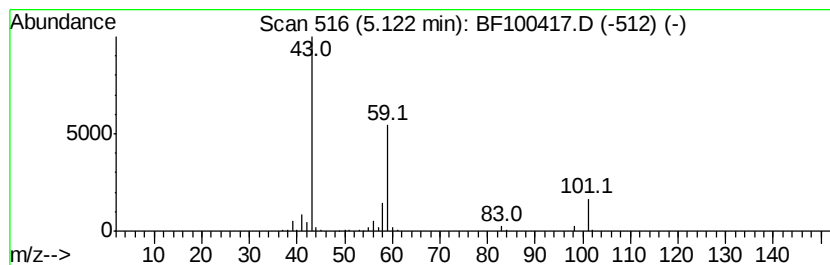
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	6.57 ng	297395	1,4-Dichlorobenzene-d4	6.90

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	28
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111017\
Data File : BF100417.D
Acq On : 11 Nov 2017 3:28
Operator : SJ/JU
Sample : I6355-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110317-TIFR-F-D-S

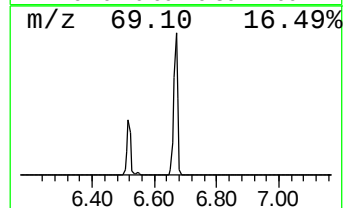
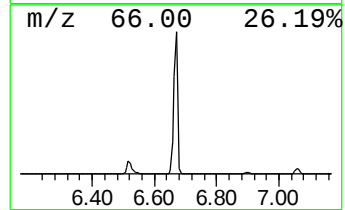
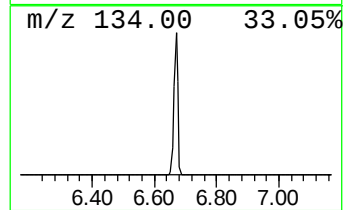
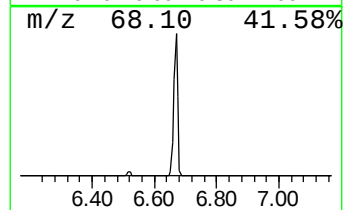
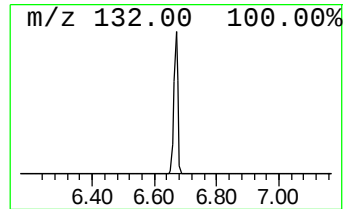
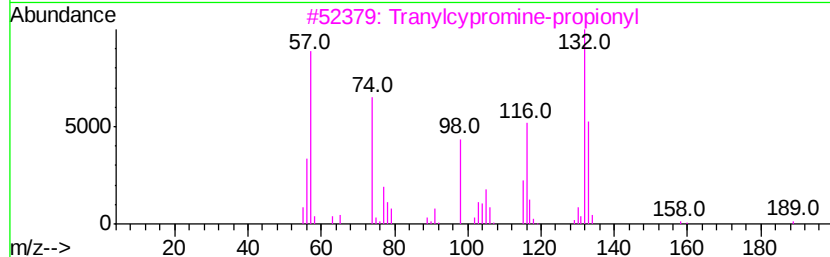
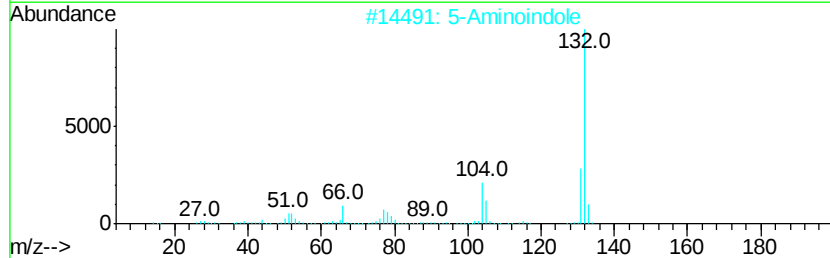
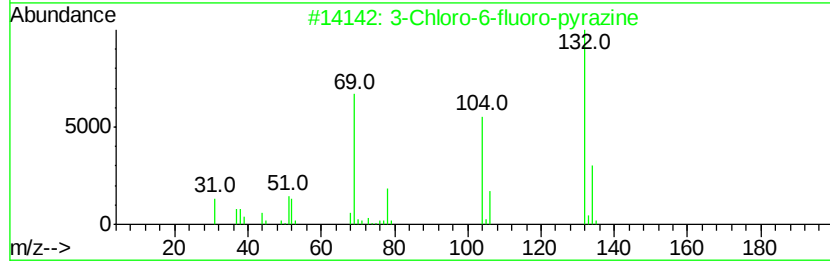
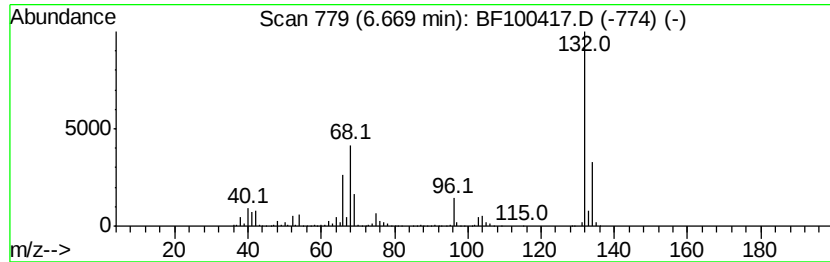
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	58.69 ng	2654840	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111017\
 Data File : BF100417.D
 Acq On : 11 Nov 2017 3:28
 Operator : SJ/JU
 Sample : I6355-07
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 110317-TIFR-F-D-S

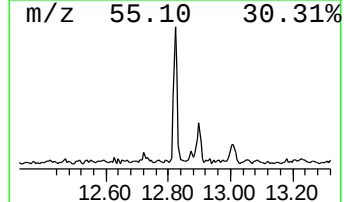
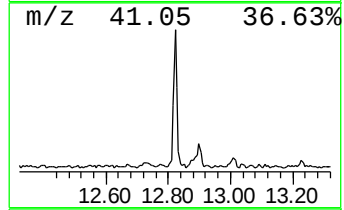
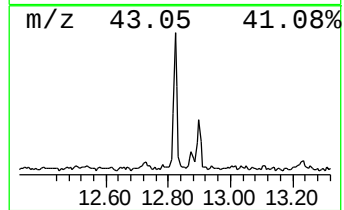
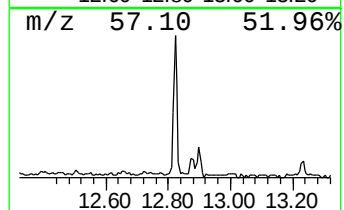
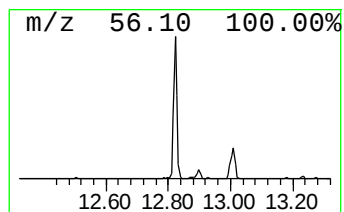
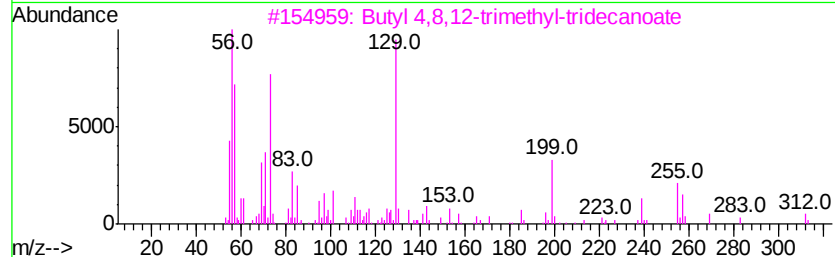
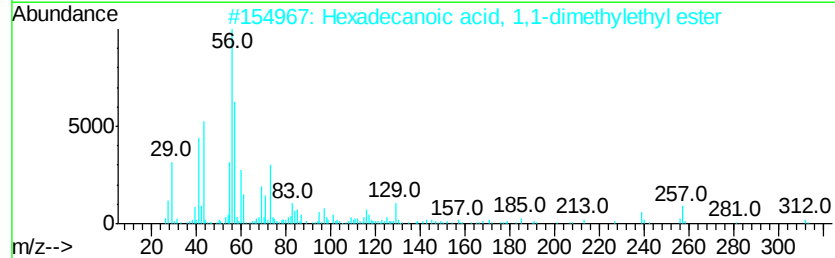
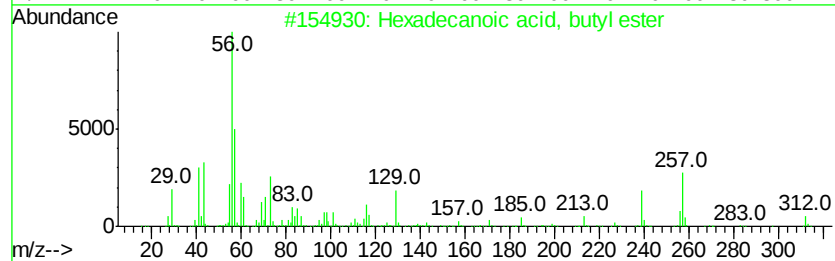
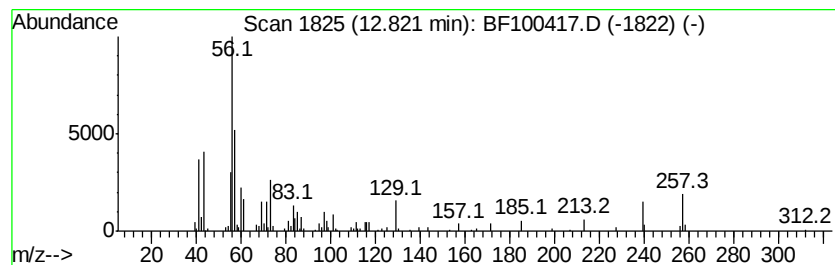
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.82	4.53 ng	178118	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	86
3		Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	50
4		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	37
5		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	35



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111017\
Data File : BF100417.D
Acq On : 11 Nov 2017 3:28
Operator : SJ/JU
Sample : I6355-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110317-TIFR-F-D-S

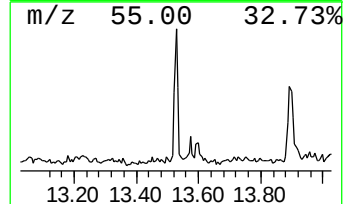
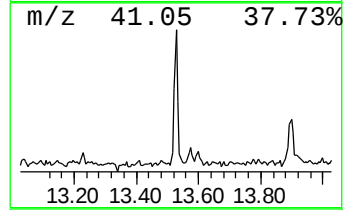
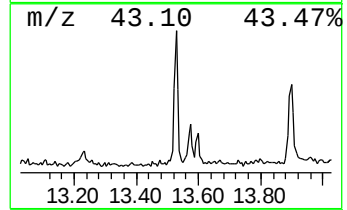
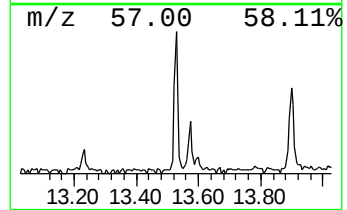
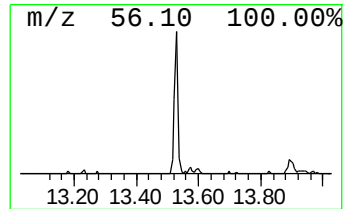
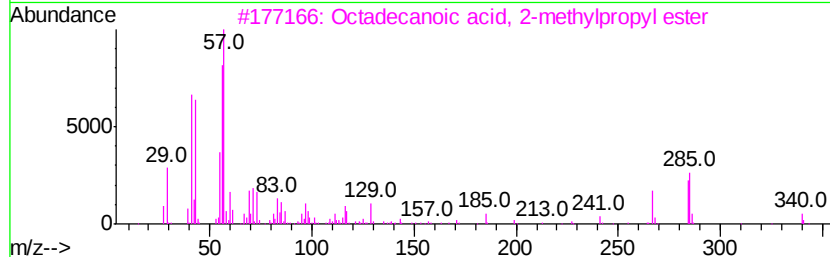
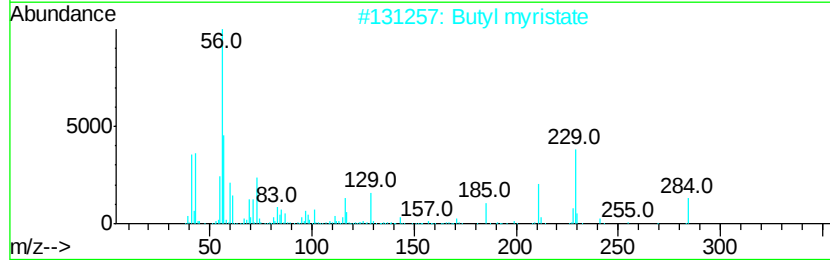
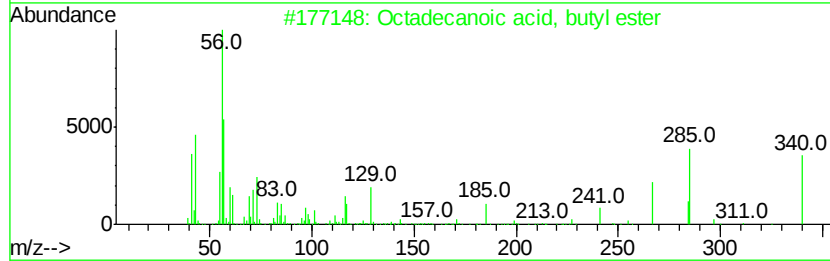
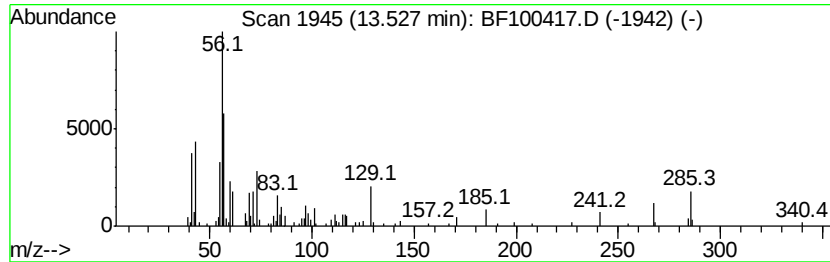
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	3.03 ng	119134	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	87
2		Butyl myristate	284	C18H36O2	000110-36-1	64
3		Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	43
4		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
5		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111017\
Data File : BF100417.D
Acq On : 11 Nov 2017 3:28
Operator : SJ/JU
Sample : I6355-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110317-TIFR-F-D-S

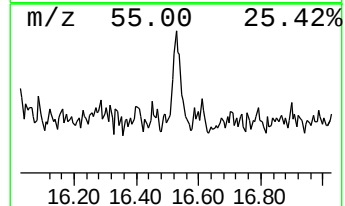
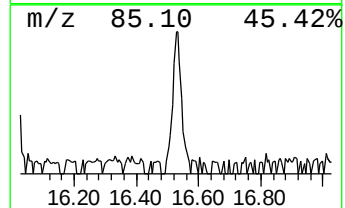
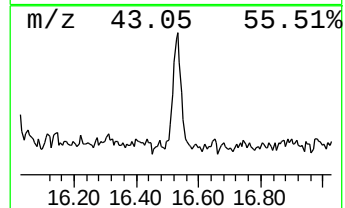
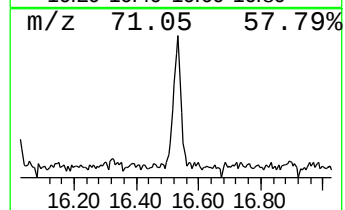
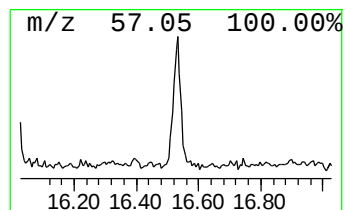
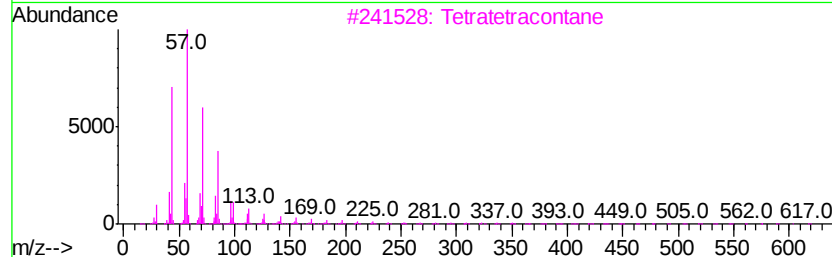
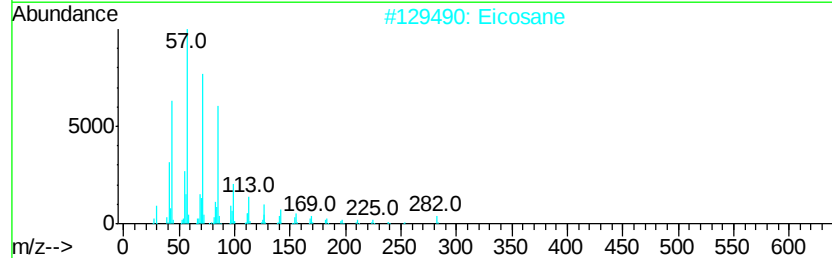
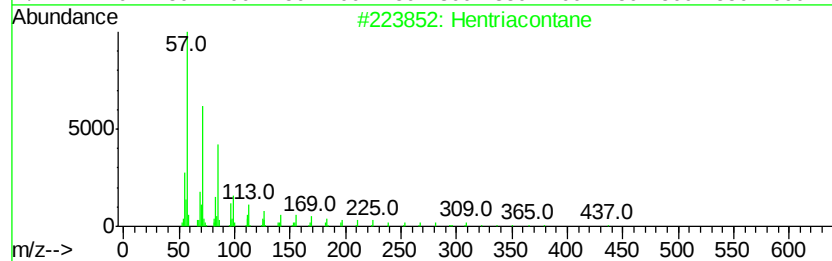
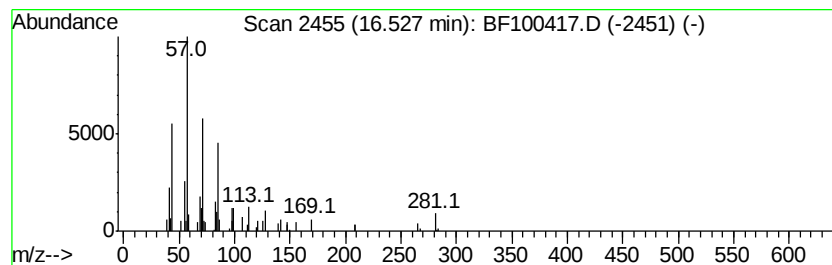
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.15 ng	71978	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	87
2		Eicosane	282	C20H42	000112-95-8	87
3		Tetratetracontane	619	C44H90	007098-22-8	87
4		Octacosane	394	C28H58	000630-02-4	87
5		Octadecane, 2-methyl-	268	C19H40	001560-88-9	86



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF111017\
Data File : BF100417.D
Acq On : 11 Nov 2017 3:28
Operator : SJ/JU
Sample : I6355-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110317-TIFR-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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
Butane, 2-methoxy...	2.20	6.3	ng	286706	1	6.90	904737	20.0
2-Pentanone, 4-hy...	5.12	6.6	ng	297395	1	6.90	904737	20.0
unknown6.67	6.67	58.7	ng	2654840	1	6.90	904737	20.0
Hexadecanoic acid...	12.82	4.5	ng	178118	5	14.06	786006	20.0
Octadecanoic acid...	13.53	3.0	ng	119134	5	14.06	786006	20.0
Hentriacontane	16.53	2.1	ng	71978	6	15.54	668709	20.0