

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040618\
 Data File : BF104347.D
 Acq On : 7 Apr 2018 9:50
 Operator : JU/SJ
 Sample : J2255-02
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 040418-JETB-E-D-M

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-BF040618.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	4.998	491	495	500	rVB	119627	117559	2.83%	0.487%
2	5.404	559	564	567	rBV	1318974	1129762	27.21%	4.677%
3	6.416	732	736	739	rBV	854451	675957	16.28%	2.798%
4	6.569	757	762	765	rBV	2377651	2139817	51.54%	8.858%
5	6.804	798	802	805	rBV	1053743	882478	21.26%	3.653%
6	6.963	824	829	832	rVB	3073150	2902612	69.92%	12.016%
7	7.369	892	898	901	rBV	2350750	2374346	57.19%	9.829%
8	8.086	1015	1020	1023	rBV	1441394	1177436	28.36%	4.874%
9	9.163	1198	1203	1207	rBV	3943855	4151367	100.00%	17.185%
10	9.557	1266	1270	1273	rBV	131814	120056	2.89%	0.497%
11	9.769	1303	1306	1309	rVB	72213	55994	1.35%	0.232%
12	9.839	1313	1318	1322	rVB2	1405684	1255875	30.25%	5.199%
13	10.269	1384	1391	1395	rBV2	72746	74088	1.78%	0.307%
14	10.627	1447	1452	1455	rBV	1675266	1479446	35.64%	6.124%
15	10.745	1469	1472	1480	rVB	57325	56885	1.37%	0.235%
16	11.327	1567	1571	1574	rBV	1179939	960061	23.13%	3.974%
17	12.739	1808	1811	1814	rBV	123920	95050	2.29%	0.393%
18	12.921	1837	1842	1845	rBV	2673229	2713560	65.37%	11.233%
19	13.445	1928	1931	1934	rBV	70389	55081	1.33%	0.228%
20	13.810	1990	1993	2005	rBV	178359	179859	4.33%	0.745%
21	13.968	2016	2020	2023	rBV	958857	823577	19.84%	3.409%
22	15.421	2262	2267	2271	rBV	613160	736187	17.73%	3.048%

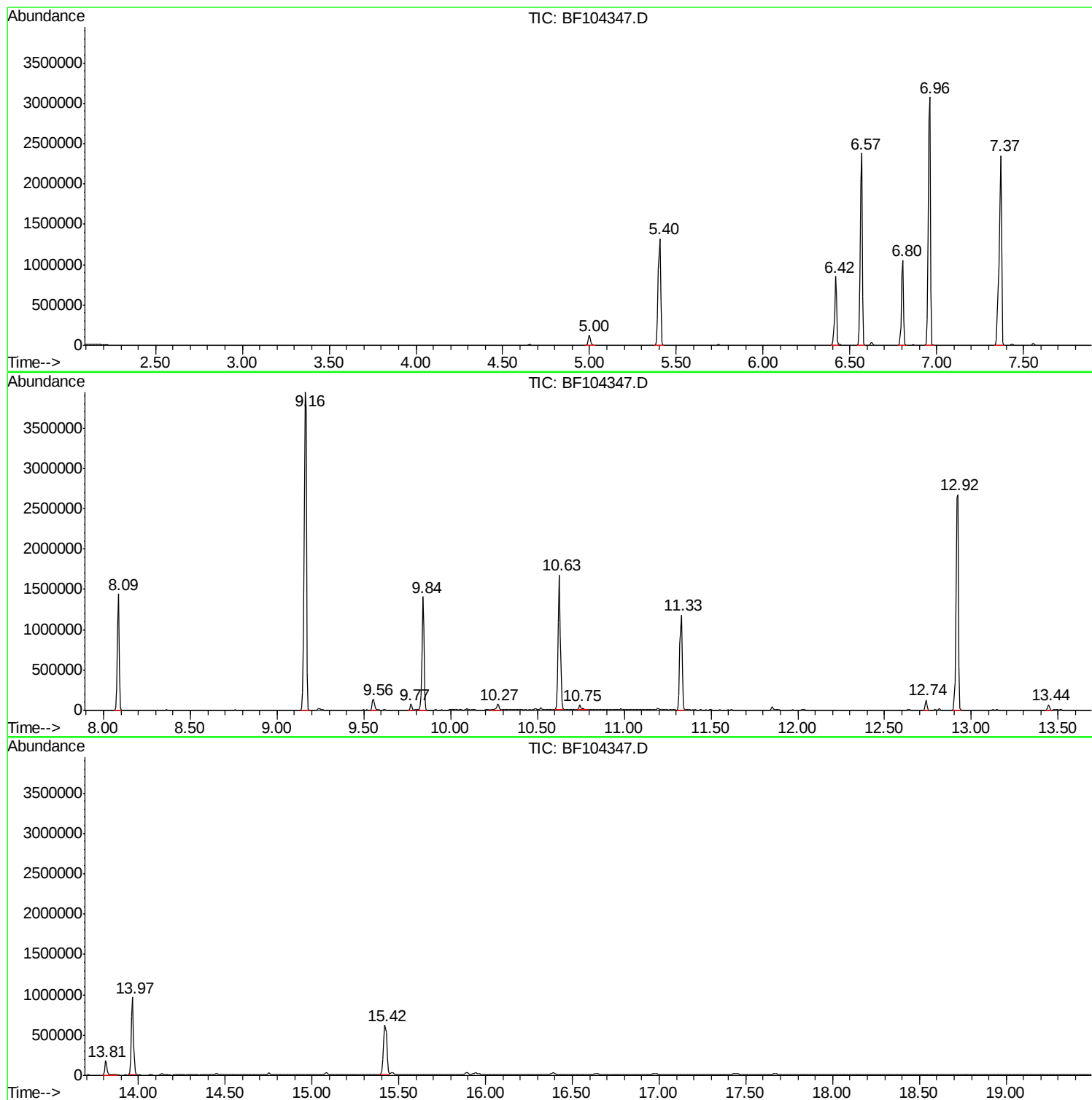
Sum of corrected areas: 24157053

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040618\
Data File : BF104347.D
Acq On : 7 Apr 2018 9:50
Operator : JU/SJ
Sample : J2255-02
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
040418-JETB-E-D-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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\BF040618\
Data File : BF104347.D
Acq On : 7 Apr 2018 9:50
Operator : JU/SJ
Sample : J2255-02
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
040418-JETB-E-D-M

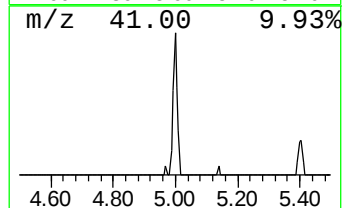
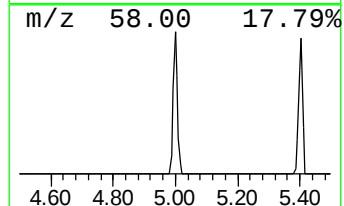
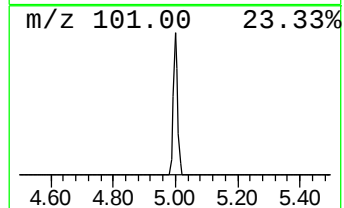
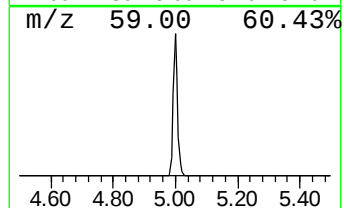
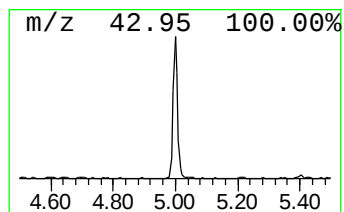
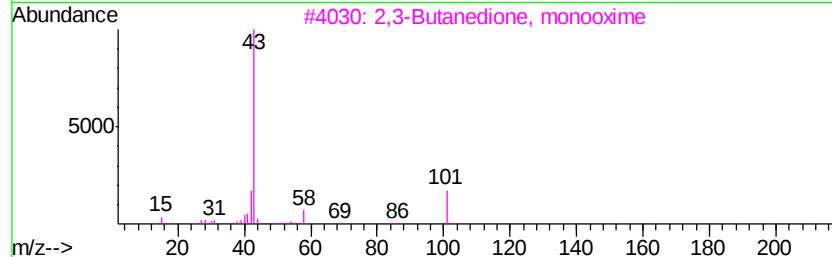
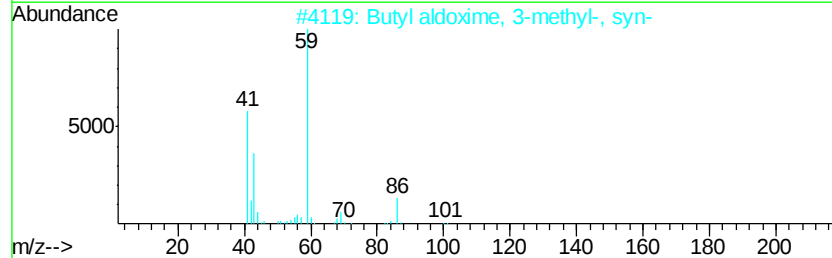
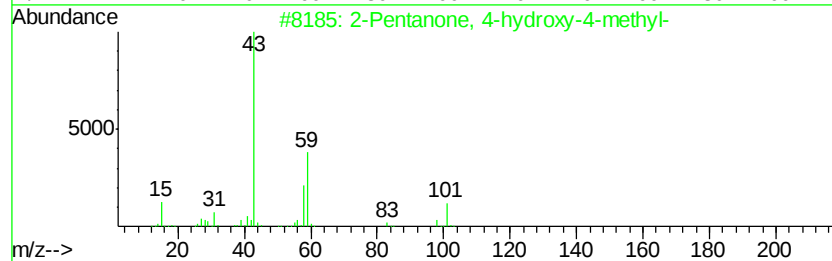
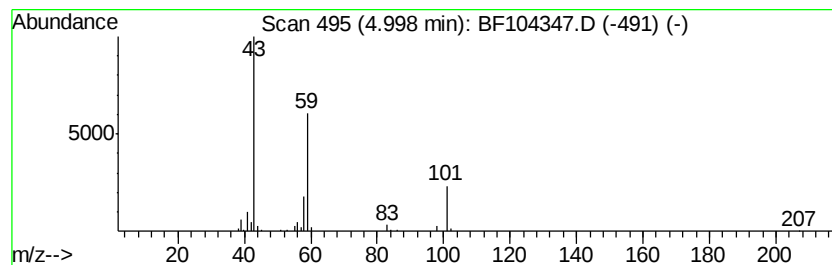
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
5.00	2.66 ng	117559	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
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\BF040618\
Data File : BF104347.D
Acq On : 7 Apr 2018 9:50
Operator : JU/SJ
Sample : J2255-02
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
040418-JETB-E-D-M

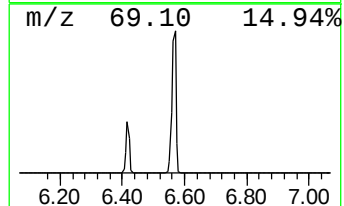
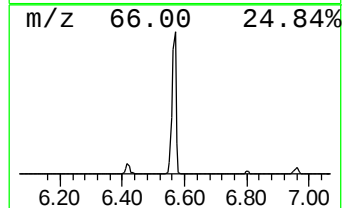
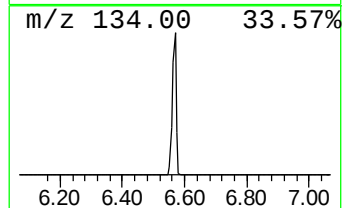
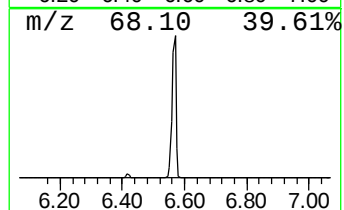
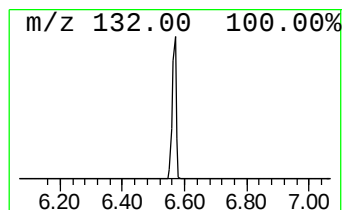
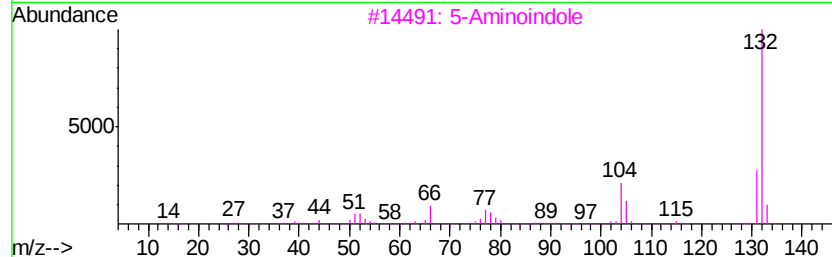
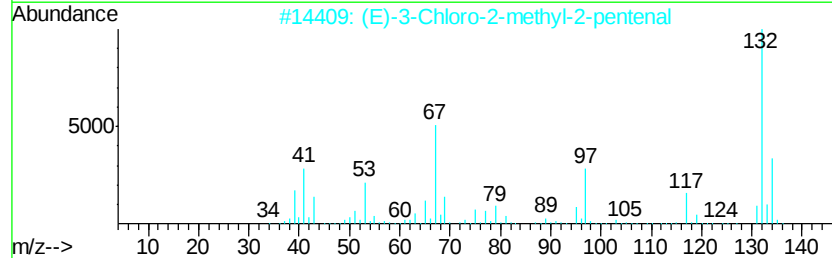
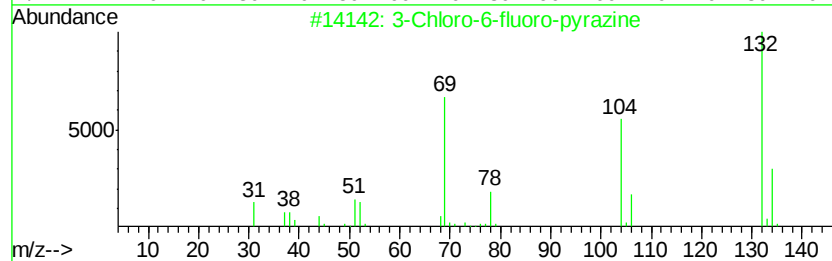
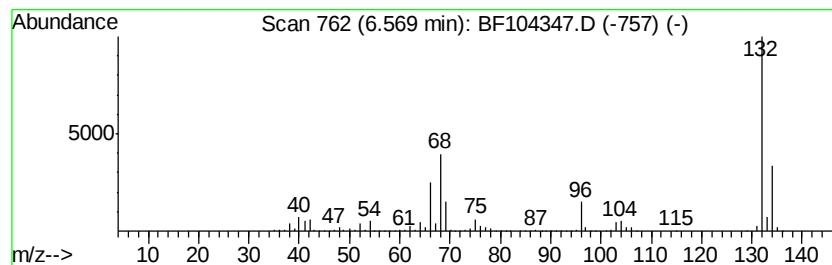
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	48.50 ng	2139820	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040618\
Data File : BF104347.D
Acq On : 7 Apr 2018 9:50
Operator : JU/SJ
Sample : J2255-02
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
040418-JETB-E-D-M

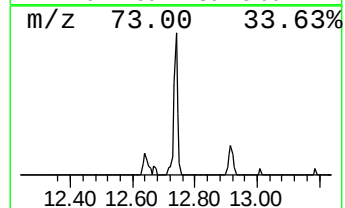
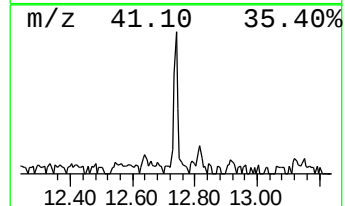
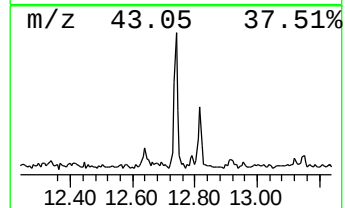
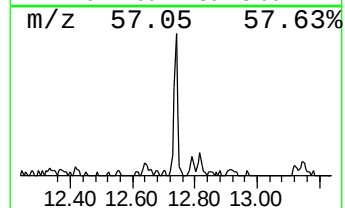
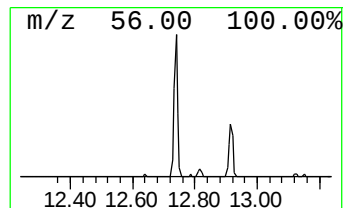
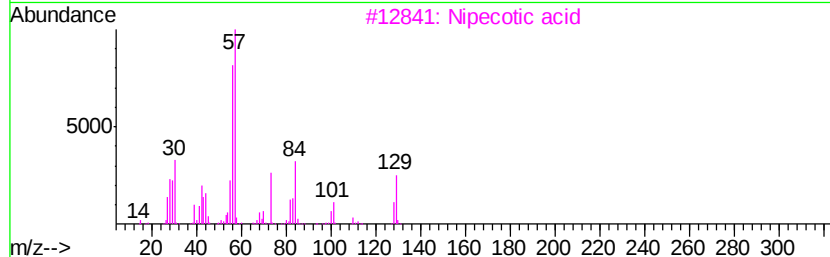
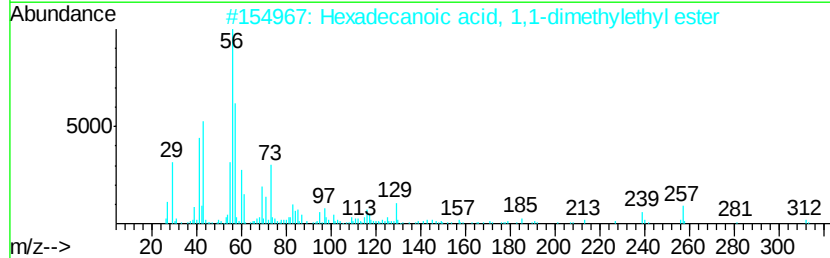
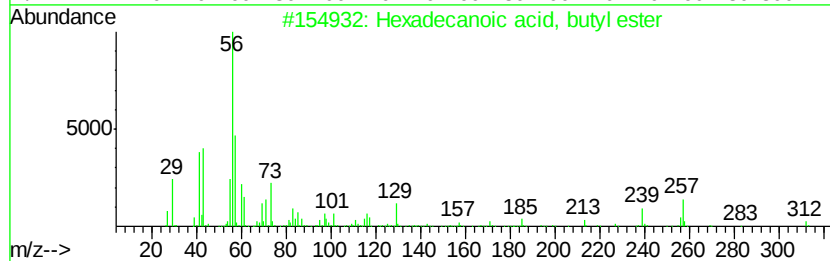
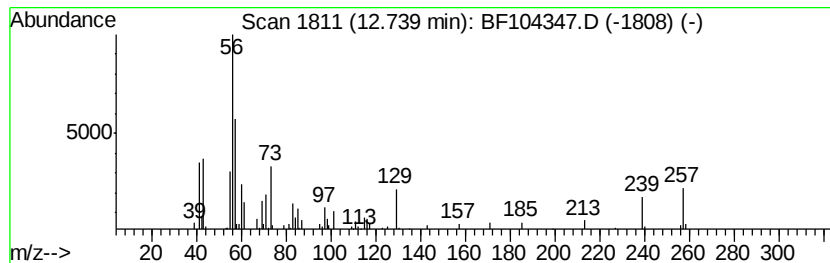
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.31 ng	95050	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
3		Nipecotic acid	129	C6H11NO2	000498-95-3	47
4		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35
5		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040618\
Data File : BF104347.D
Acq On : 7 Apr 2018 9:50
Operator : JU/SJ
Sample : J2255-02
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
040418-JETB-E-D-M

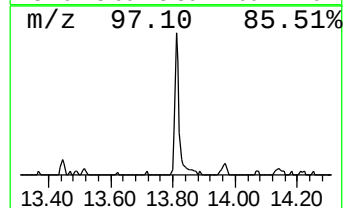
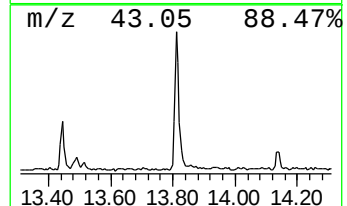
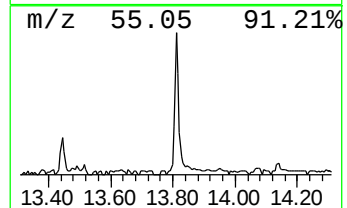
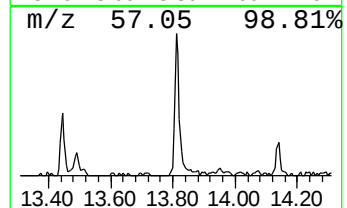
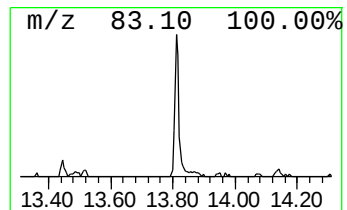
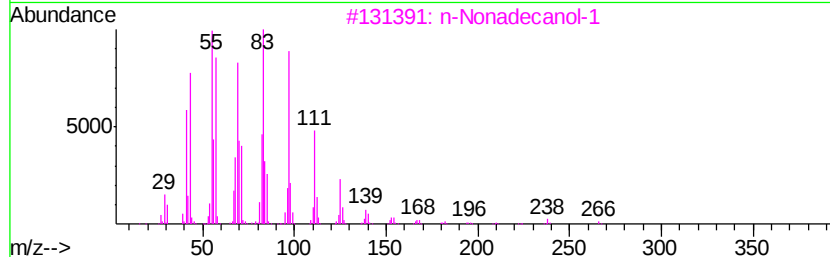
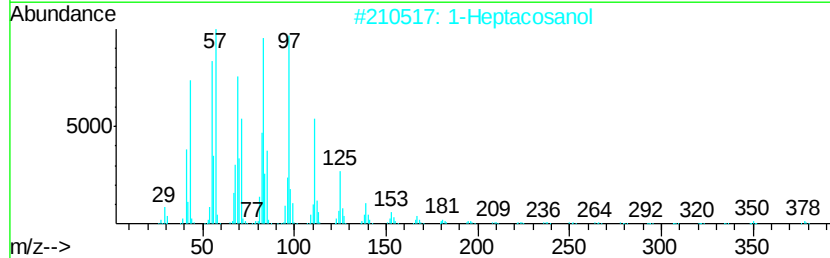
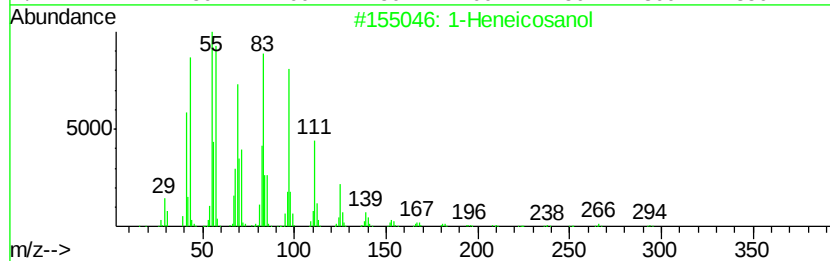
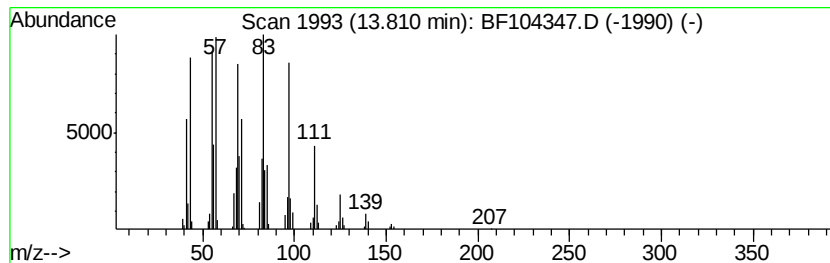
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	4.37 ng	179859	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol		312	C21H44O	015594-90-8	95
2	1-Heptacosanol		396	C27H56O	002004-39-9	93
3	n-Nonadecanol-1		284	C19H40O	001454-84-8	91
4	Behenic alcohol		326	C22H46O	000661-19-8	91
5	n-Tetracosanol-1		354	C24H50O	000506-51-4	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040618\
Data File : BF104347.D
Acq On : 7 Apr 2018 9:50
Operator : JU/SJ
Sample : J2255-02
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
040418-JETB-E-D-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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
2-Pentanone, 4-hy...	5.00	2.7	ng	117559	1	6.80	882478	20.0
unknown6.57	6.57	48.5	ng	2139820	1	6.80	882478	20.0
Hexadecanoic acid...	12.74	2.3	ng	95050	5	13.97	823577	20.0
1-Heneicosanol	13.81	4.4	ng	179859	5	13.97	823577	20.0