

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
 Data File : BF095566.D
 Acq On : 31 May 2017 16:23
 Operator : SJ/MA
 Sample : I3329-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-13(5-8)

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-BF050217.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	4.825	504	508	529	rBV	95448	301255	8.13%	0.992%
2	5.472	614	618	652	rBV	1848517	3266797	88.15%	10.762%
3	7.107	890	896	909	rBV	1929118	3169010	85.51%	10.440%
4	7.213	909	914	939	rVB	2439185	3598696	97.10%	11.855%
5	7.548	968	971	986	rBV	423660	588721	15.88%	1.939%
6	7.789	1006	1012	1039	rBV	1868854	2607122	70.35%	8.589%
7	8.466	1121	1127	1147	rBV	1218228	1829506	49.36%	6.027%
8	9.583	1312	1317	1334	rBV	565124	834561	22.52%	2.749%
9	11.360	1612	1619	1634	rBV	2623357	3706156	100.00%	12.209%
10	12.048	1731	1736	1752	rBV	656374	834066	22.50%	2.748%
11	12.407	1791	1797	1810	rBV2	672869	882115	23.80%	2.906%
12	13.707	2012	2018	2033	rBV	1393966	2116110	57.10%	6.971%
13	14.024	2067	2072	2083	rBV	41176	73620	1.99%	0.243%
14	14.806	2200	2205	2217	rVB	732926	1031218	27.82%	3.397%
15	15.795	2365	2373	2381	rBV	120987	169904	4.58%	0.560%
16	16.624	2511	2514	2523	rVB	28421	40798	1.10%	0.134%
17	16.924	2562	2565	2571	rVB	30281	42845	1.16%	0.141%
18	17.165	2599	2606	2609	rBV	2589408	3411986	92.06%	11.240%
19	18.400	2811	2816	2829	rBV	106497	190071	5.13%	0.626%
20	18.506	2829	2834	2843	rBV	752960	965596	26.05%	3.181%
21	20.177	3114	3118	3126	rBV	504525	654773	17.67%	2.157%
22	20.671	3197	3202	3209	rBV7	19811	40570	1.09%	0.134%

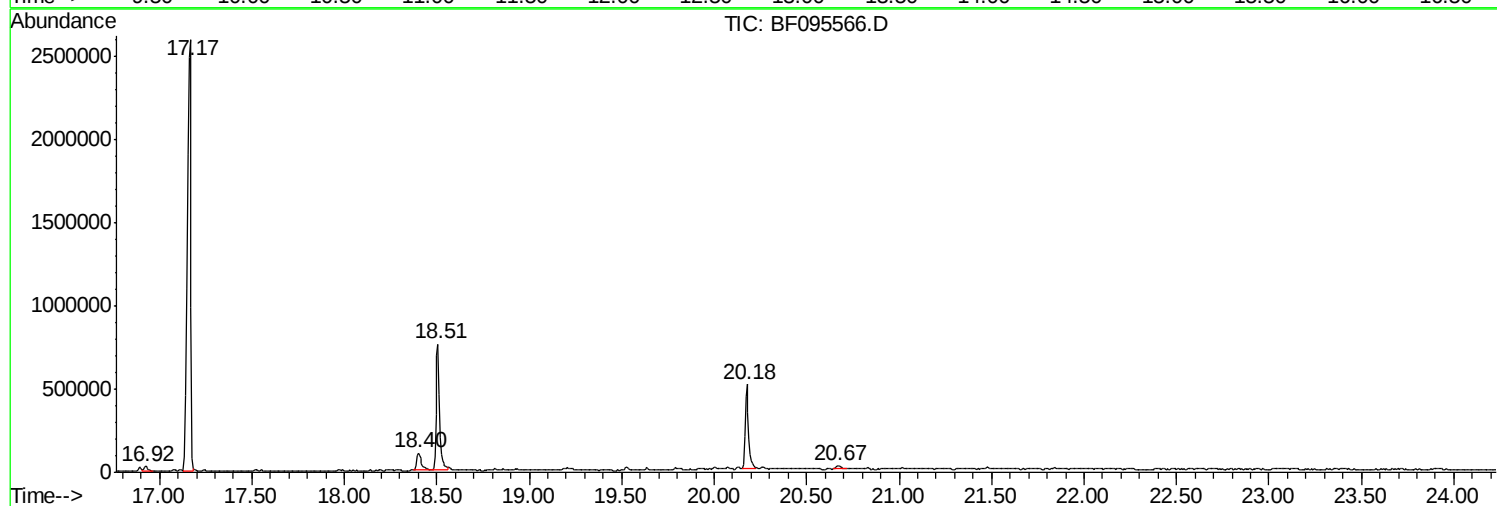
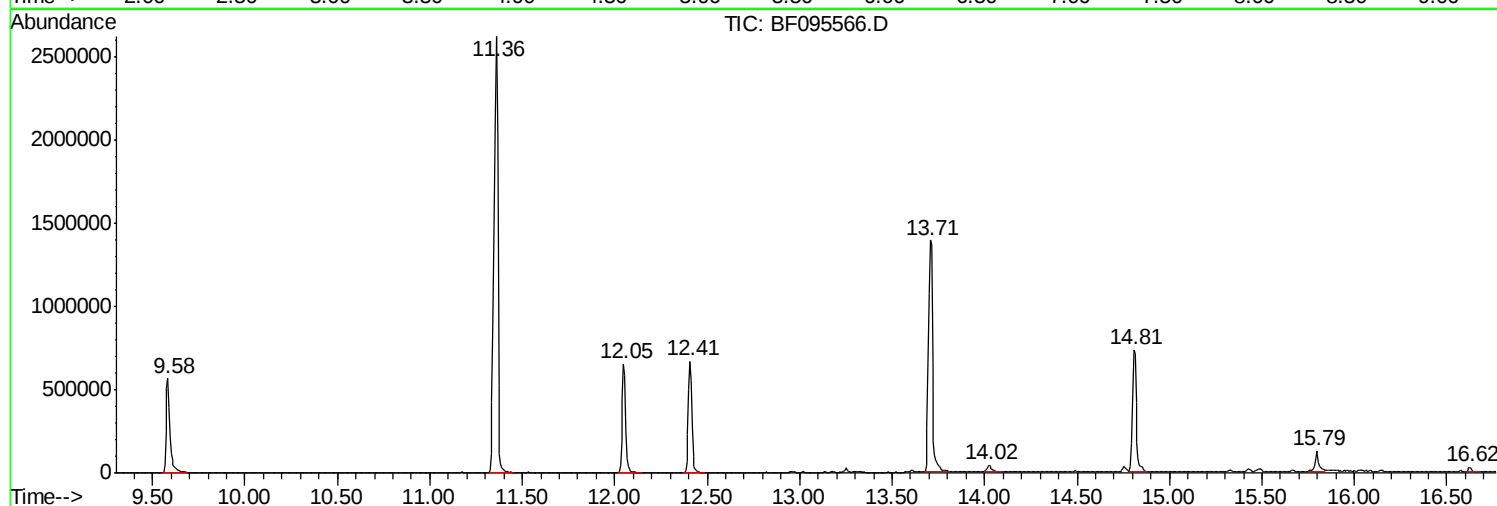
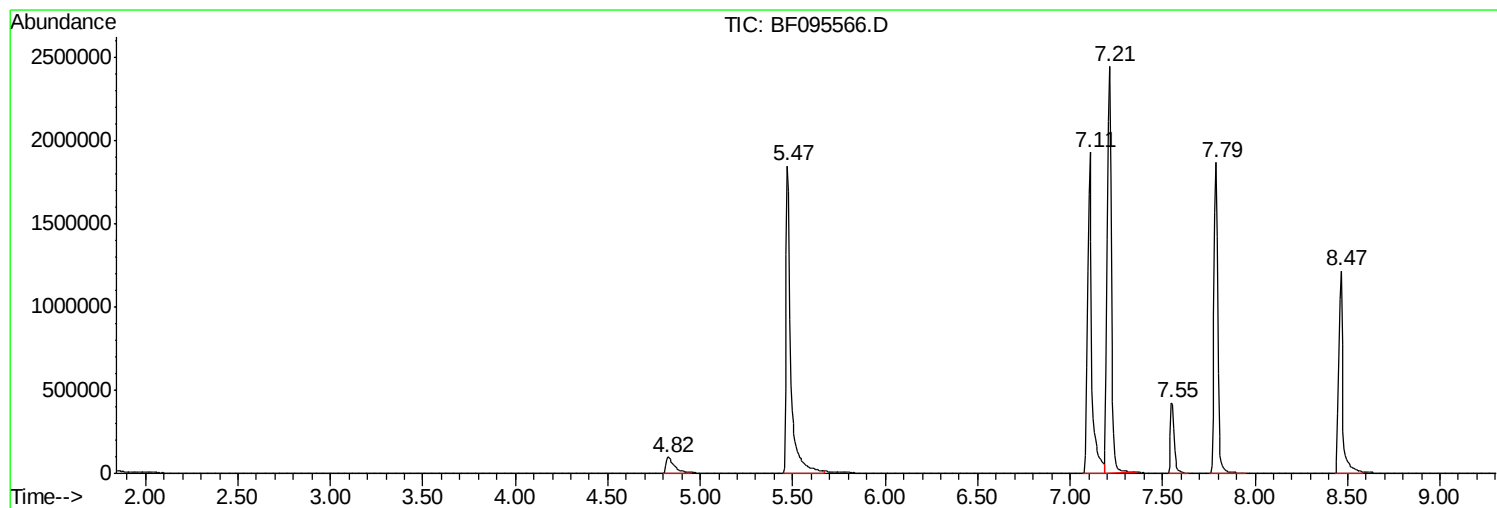
Sum of corrected areas: 30355496

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
Data File : BF095566.D
Acq On : 31 May 2017 16:23
Operator : SJ/MA
Sample : I3329-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-13(5-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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\BF053117\
Data File : BF095566.D
Acq On : 31 May 2017 16:23
Operator : SJ/MA
Sample : I3329-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-13(5-8)

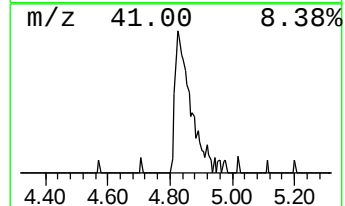
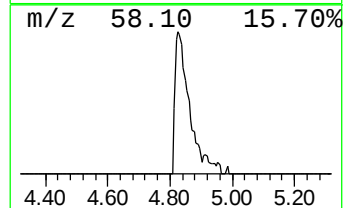
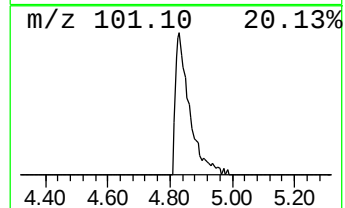
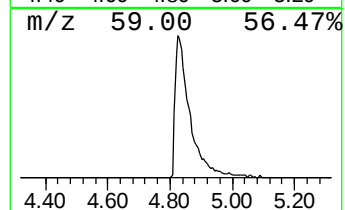
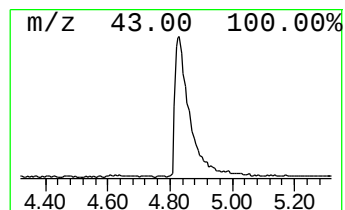
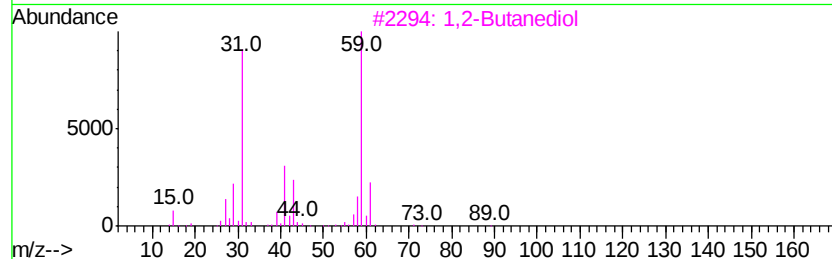
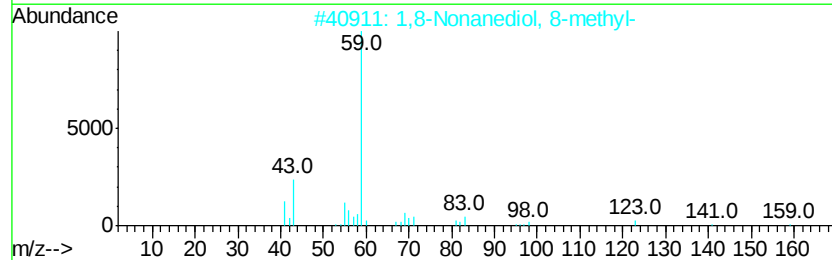
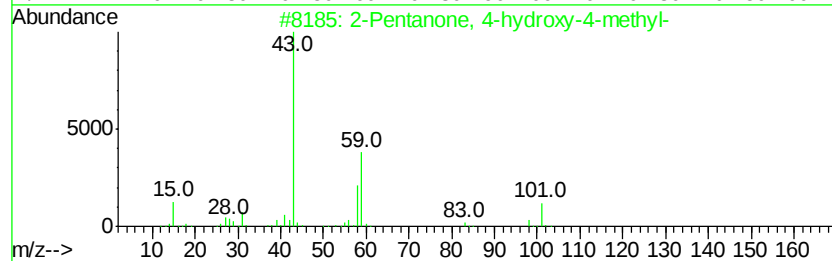
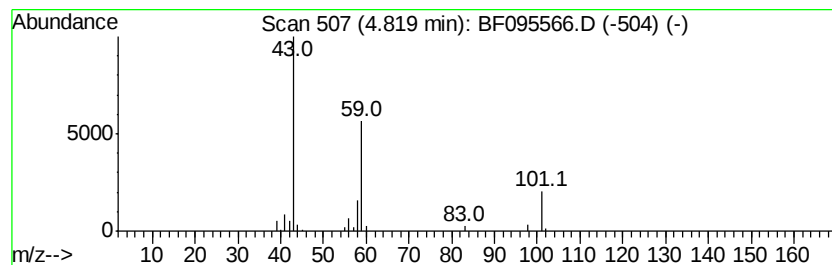
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	10.23 ng	301255	1,4-Dichlorobenzene-d4	7.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
3		1,2-Butanediol	90	C4H10O2	000584-03-2	23
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
Data File : BF095566.D
Acq On : 31 May 2017 16:23
Operator : SJ/MA
Sample : I3329-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-13(5-8)

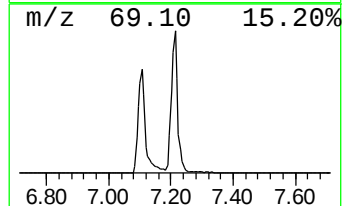
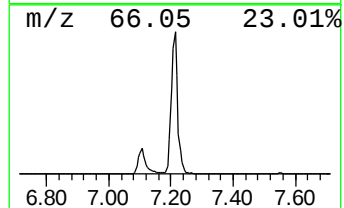
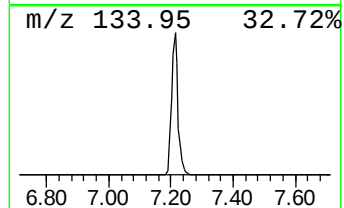
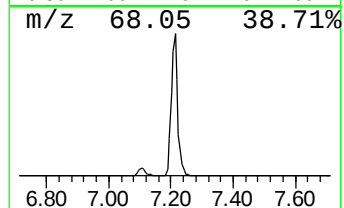
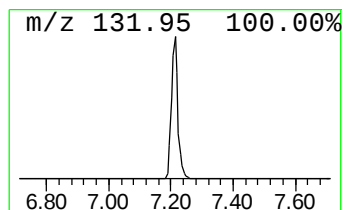
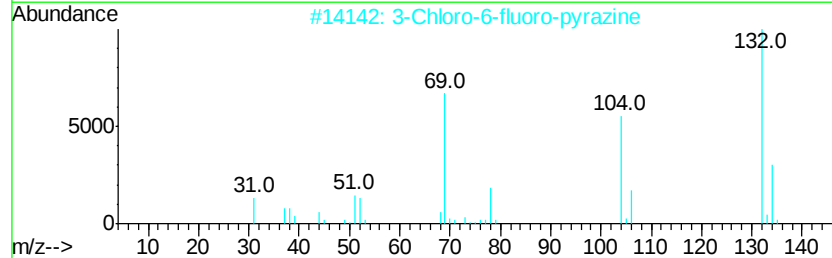
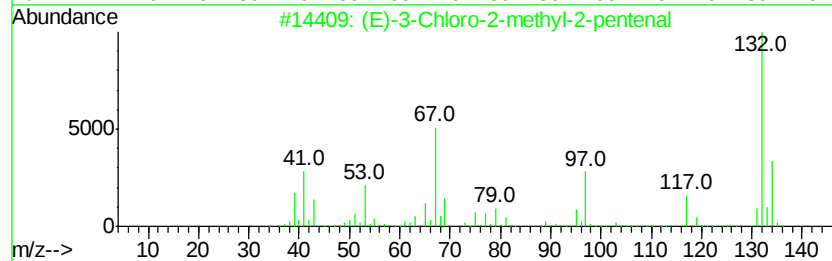
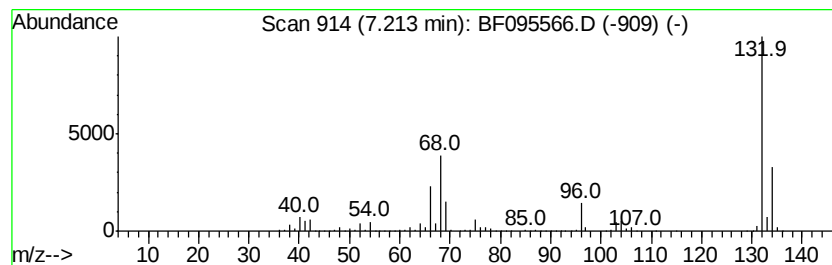
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	122.26 ng	3598700	1,4-Dichlorobenzene-d4	7.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
Data File : BF095566.D
Acq On : 31 May 2017 16:23
Operator : SJ/MA
Sample : I3329-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-13(5-8)

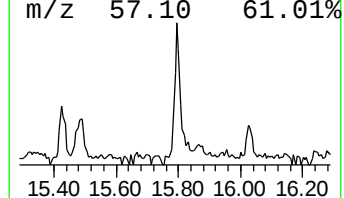
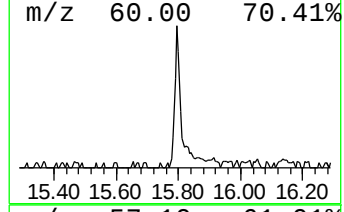
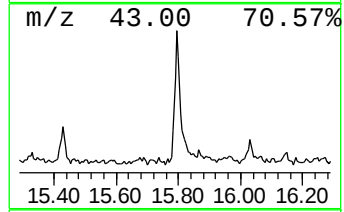
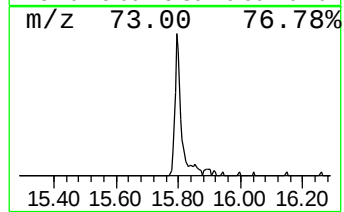
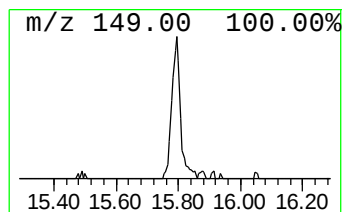
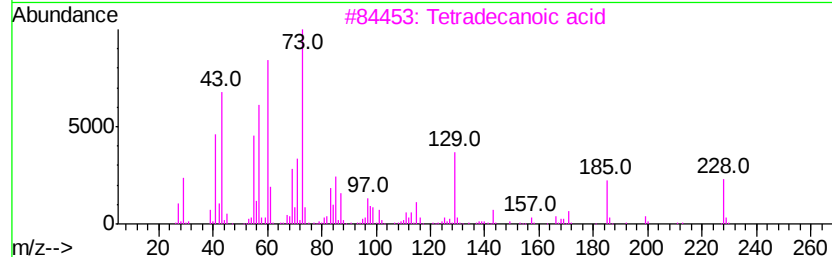
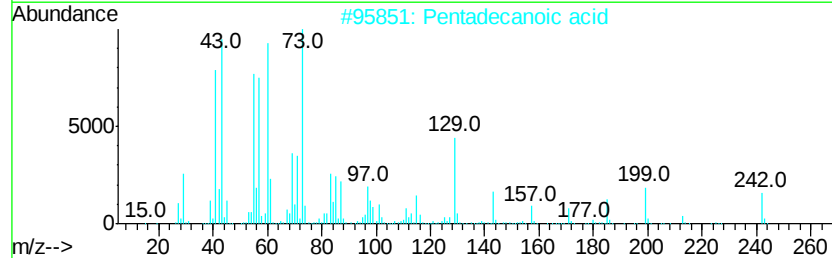
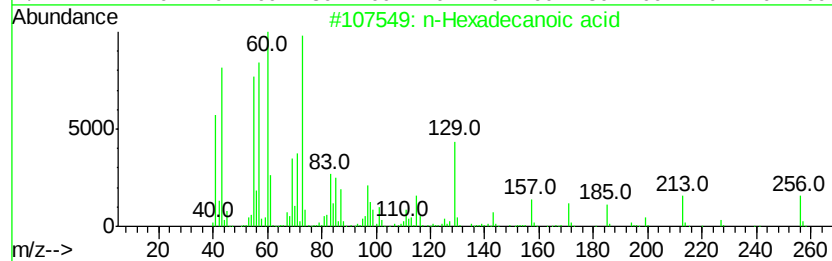
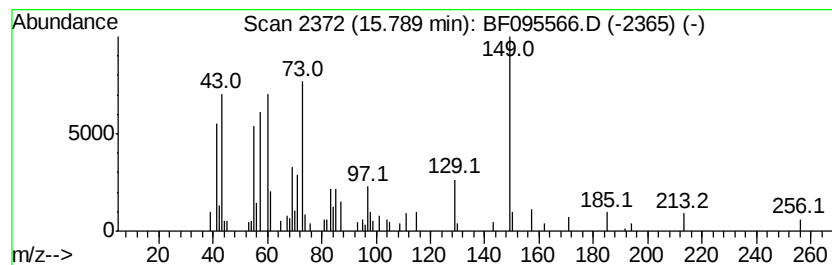
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	3.30 ng	169904	Phenanthrene-d10	14.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Undecanoic acid	186	C11H22O2	000112-37-8	50
5	Tridecanoic acid	214	C13H26O2	000638-53-9	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
Data File : BF095566.D
Acq On : 31 May 2017 16:23
Operator : SJ/MA
Sample : I3329-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

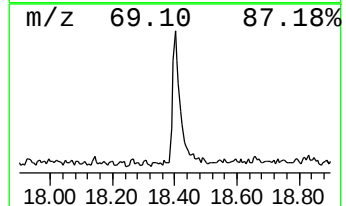
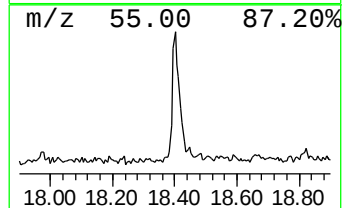
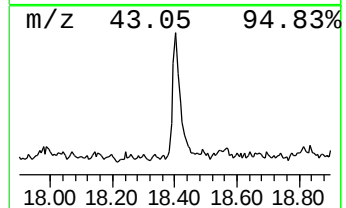
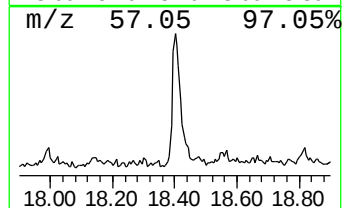
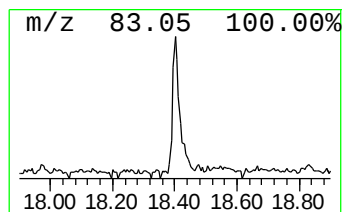
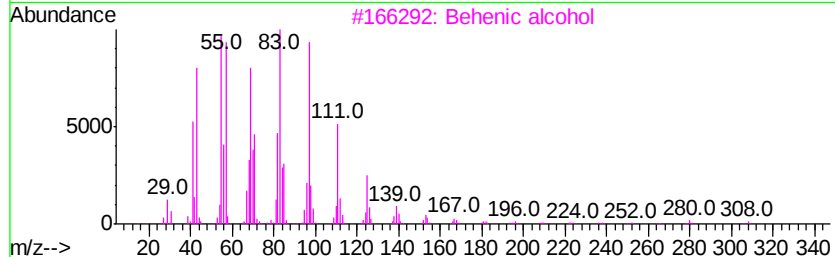
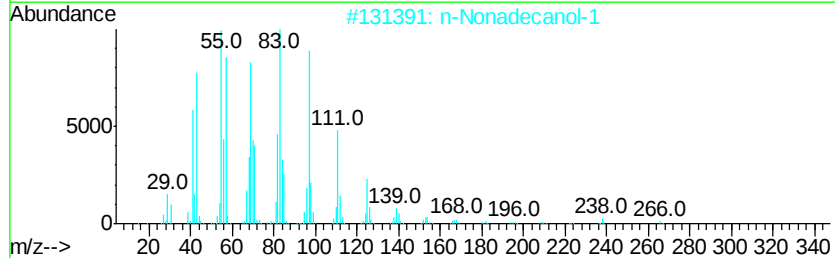
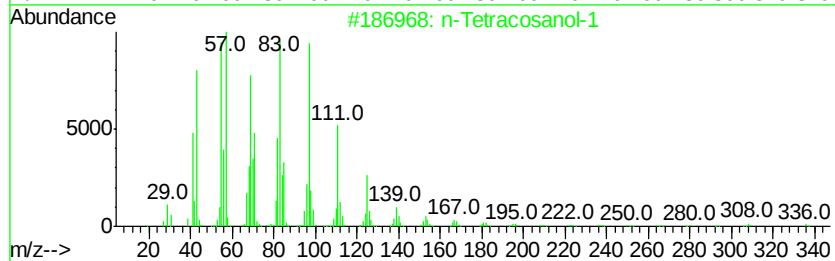
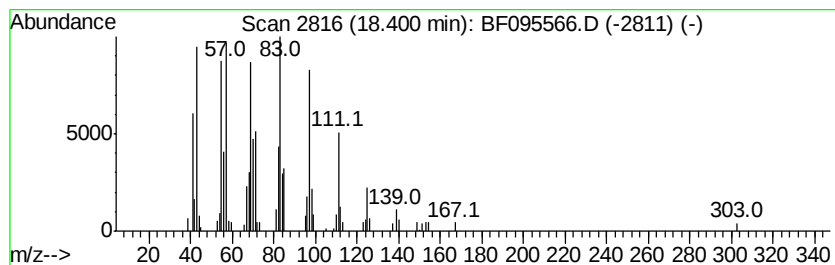
Instrument :
BNA_F
ClientSampleId :
B-13(5-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.40	3.94 ng	190071	Chrysene-d12	18.51	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	95
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
5	1-Heneicosanol	312	C21H44O	015594-90-8	95



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
Data File : BF095566.D
Acq On : 31 May 2017 16:23
Operator : SJ/MA
Sample : I3329-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-13(5-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	4.82	10.2	ng	301255	1	7.55	588721	20.0
unknown7.21	7.21	122.3	ng	3598700	1	7.55	588721	20.0
n-Hexadecanoic acid	15.79	3.3	ng	169904	4	14.81	1031220	20.0
n-Tetracosanol-1	18.40	3.9	ng	190071	5	18.51	965596	20.0