

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101617\
 Data File : BF099540.D
 Acq On : 16 Oct 2017 13:17
 Operator : SJ/JU
 Sample : I5776-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ENV-104-2(0-5)

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-BF092317.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	5.069	504	507	518	rBV	264226	356968	15.11%	1.834%
2	5.469	571	575	598	rBV	2111443	2066081	87.43%	10.617%
3	6.481	742	747	750	rBV	2034961	2022115	85.57%	10.391%
4	6.616	766	770	773	rBV	2423968	2134223	90.32%	10.967%
5	6.845	805	809	816	rBV	657425	572516	24.23%	2.942%
6	6.998	831	835	839	rBV	1960503	1683920	71.26%	8.653%
7	7.410	900	905	908	rBV	1418164	1292011	54.68%	6.639%
8	8.122	1023	1026	1037	rBV	866053	781780	33.08%	4.017%
9	9.198	1204	1209	1212	rBV	2643842	2363041	100.00%	12.143%
10	9.592	1273	1276	1284	rBV	363459	276517	11.70%	1.421%
11	9.880	1321	1325	1332	rVB	996846	826835	34.99%	4.249%
12	10.669	1456	1459	1469	rBV	1197973	1199706	50.77%	6.165%
13	10.769	1473	1476	1485	rVB	29363	32076	1.36%	0.165%
14	11.369	1574	1578	1582	rBV	913857	753081	31.87%	3.870%
15	12.951	1843	1847	1850	rBV	1942371	1720606	72.81%	8.842%
16	13.833	1993	1997	2010	rBV2	49606	80156	3.39%	0.412%
17	14.010	2023	2027	2031	rBV	547450	510352	21.60%	2.623%
18	15.486	2272	2278	2286	rVB	399139	531178	22.48%	2.730%
19	15.898	2342	2348	2354	rBV2	32288	51531	2.18%	0.265%
20	16.398	2427	2433	2438	rBV2	36788	67773	2.87%	0.348%
21	16.980	2527	2532	2539	rVB2	28430	55084	2.33%	0.283%
22	17.668	2643	2649	2658	rVB4	24356	56318	2.38%	0.289%
23	18.492	2783	2789	2796	rBV5	12191	25727	1.09%	0.132%

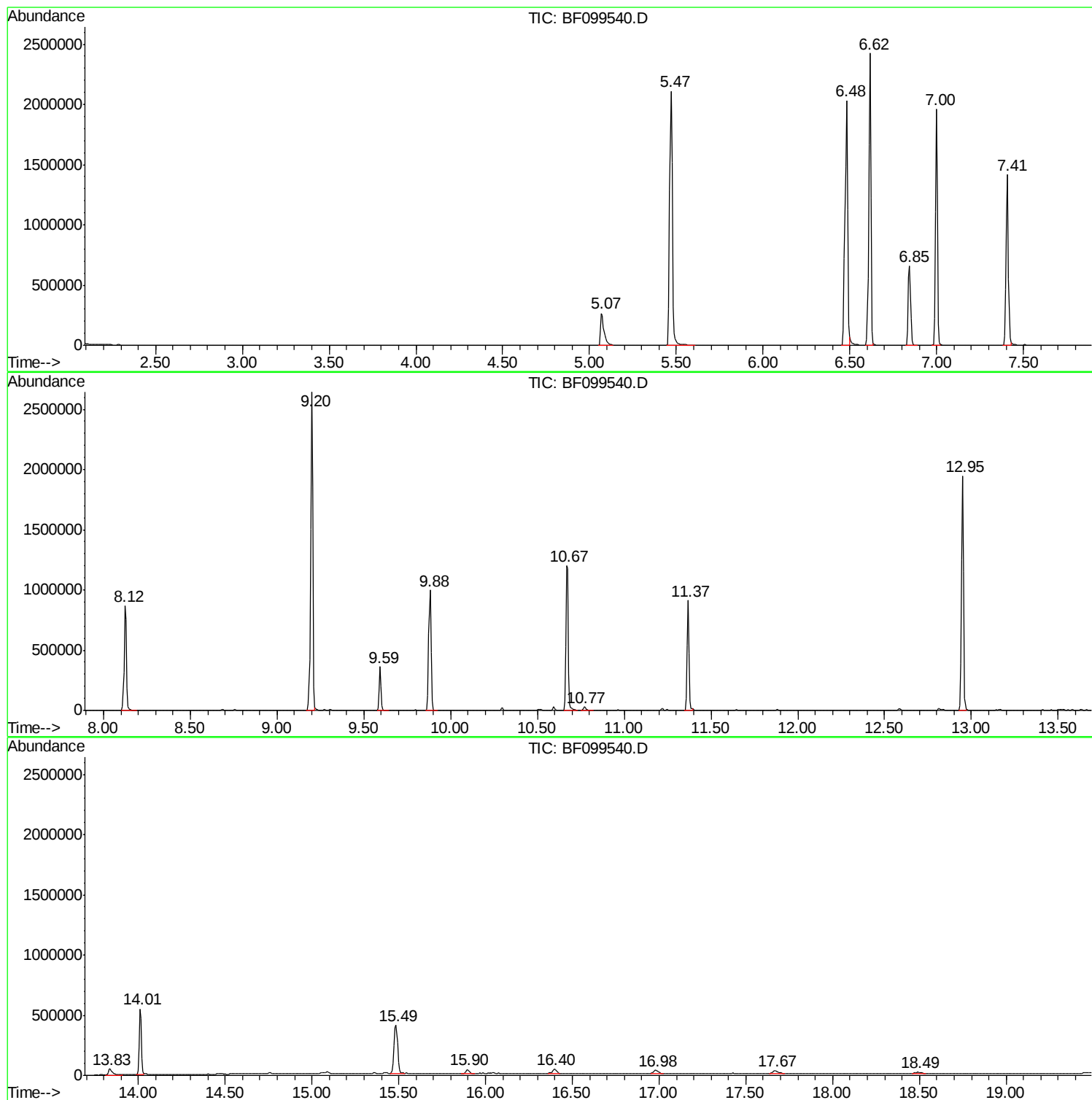
Sum of corrected areas: 19459595

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099540.D
Acq On : 16 Oct 2017 13:17
Operator : SJ/JU
Sample : I5776-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-2(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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\BF101617\
Data File : BF099540.D
Acq On : 16 Oct 2017 13:17
Operator : SJ/JU
Sample : I5776-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-2(0-5)

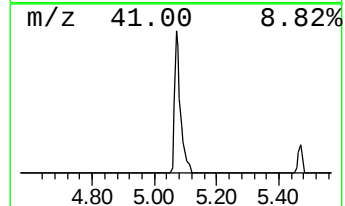
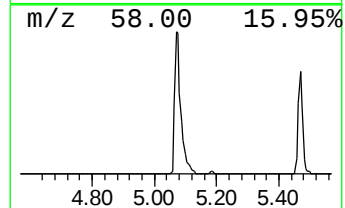
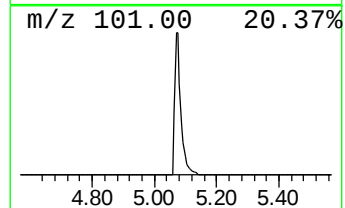
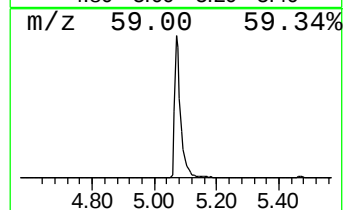
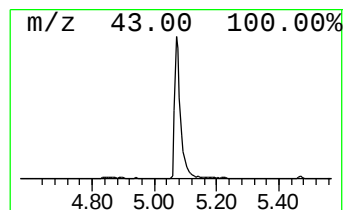
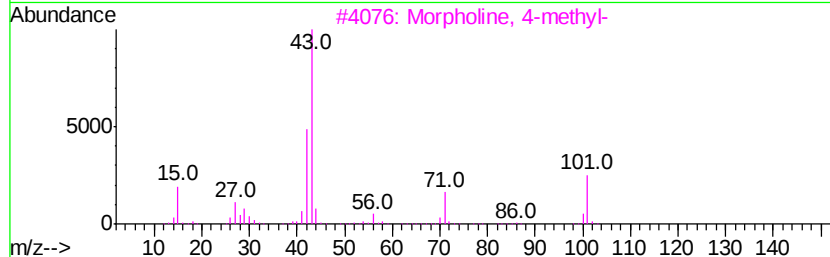
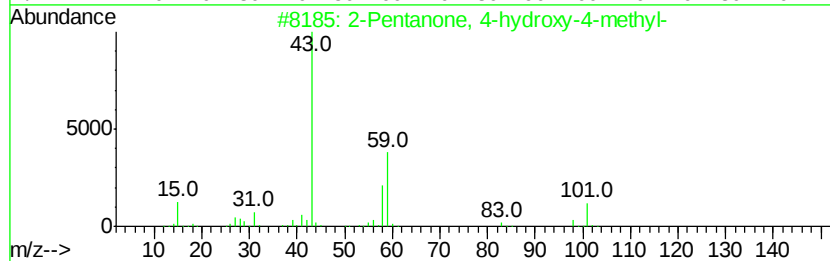
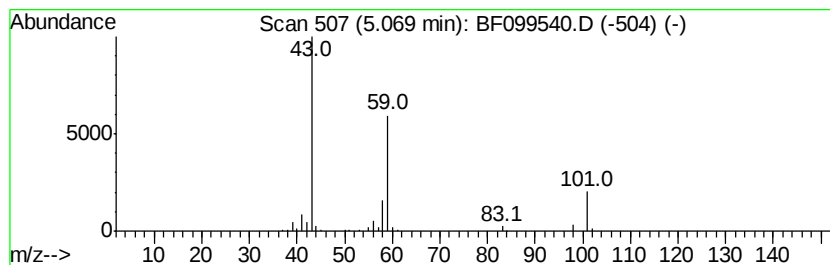
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.07	12.47 ng	356968	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099540.D
Acq On : 16 Oct 2017 13:17
Operator : SJ/JU
Sample : I5776-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-2(0-5)

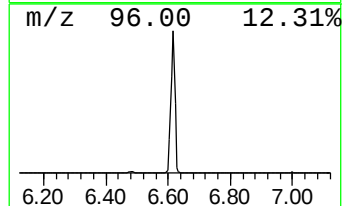
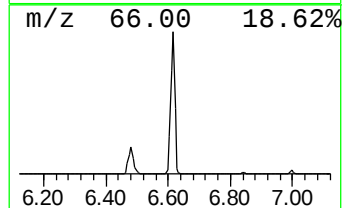
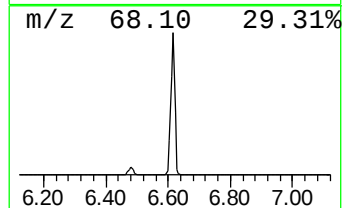
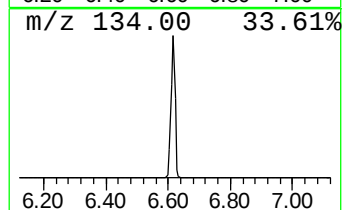
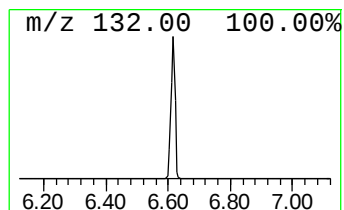
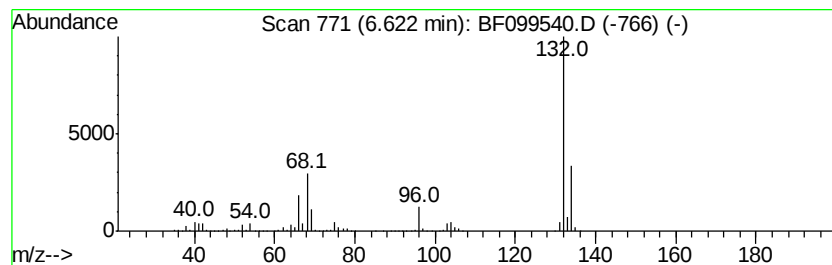
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	74.56 ng	2134220	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099540.D
Acq On : 16 Oct 2017 13:17
Operator : SJ/JU
Sample : I5776-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-2(0-5)

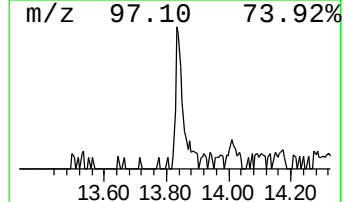
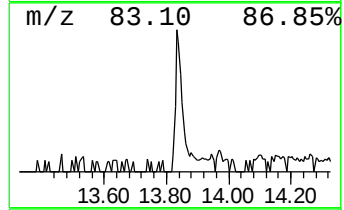
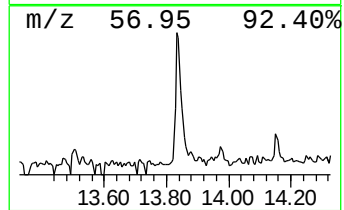
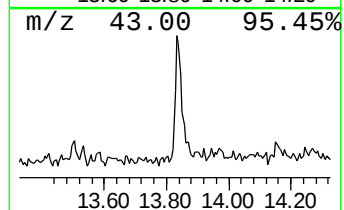
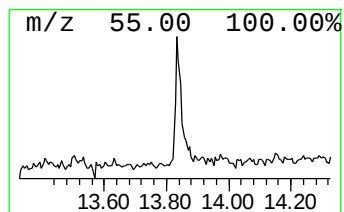
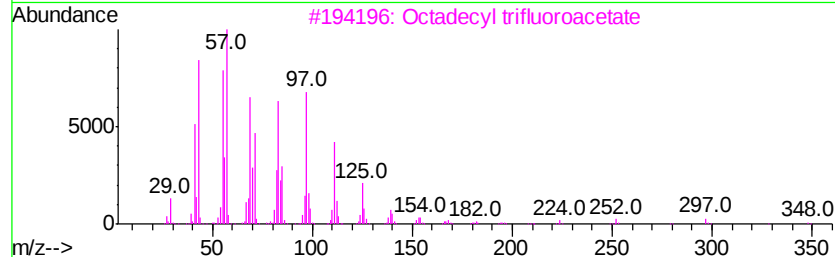
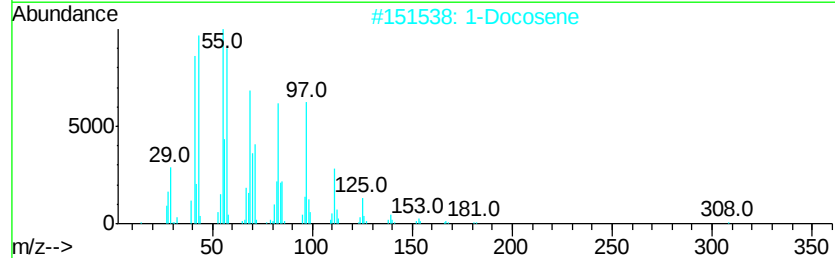
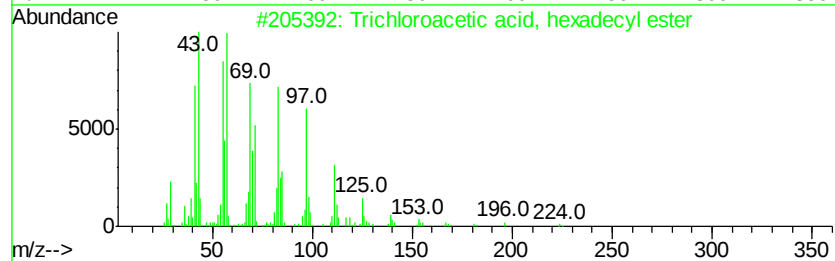
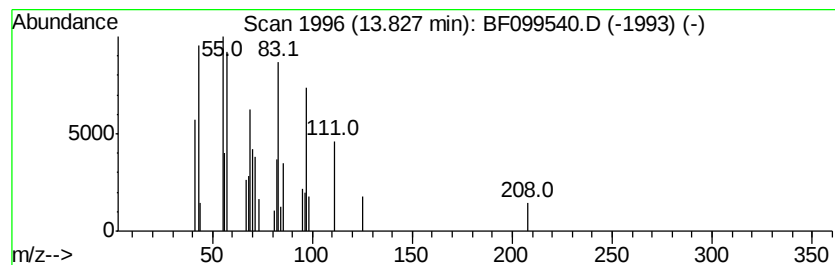
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	3.14 ng	80156	Chrysene-d12	14.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		1-Docosene	308	C22H44	001599-67-3	91
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4		Behenic alcohol	326	C22H46O	000661-19-8	91
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099540.D
Acq On : 16 Oct 2017 13:17
Operator : SJ/JU
Sample : I5776-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-2(0-5)

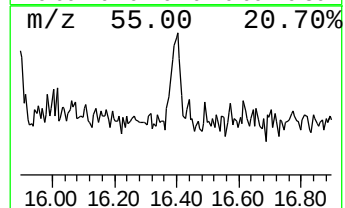
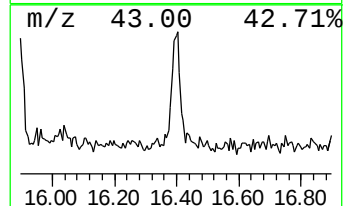
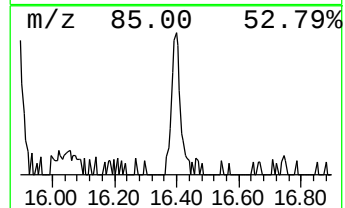
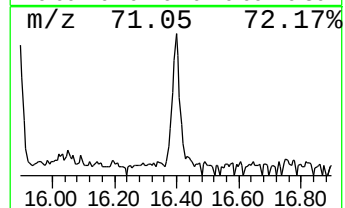
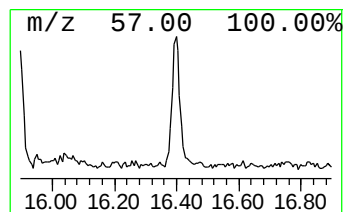
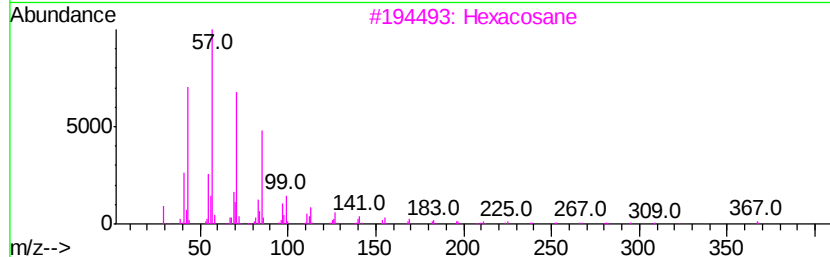
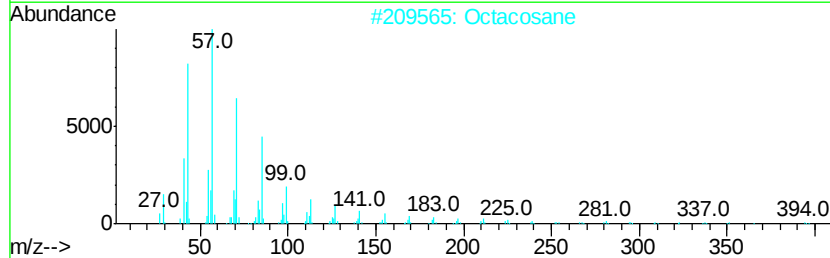
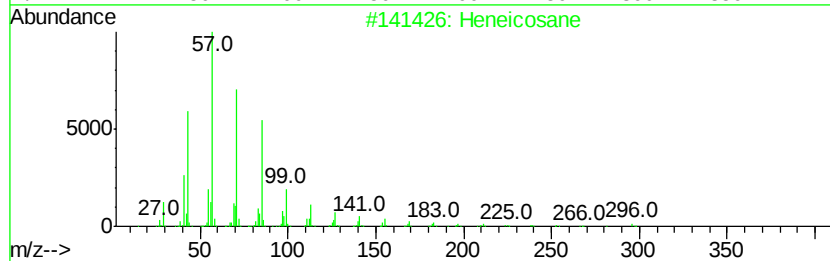
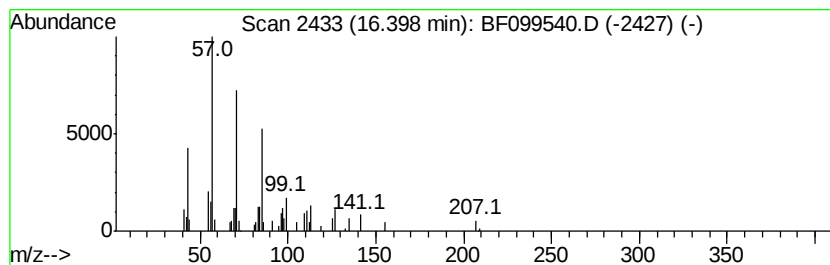
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	2.55 ng	67773	Perylene-d12	15.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	87
2	Octacosane		394	C28H58	000630-02-4	87
3	Hexacosane		366	C26H54	000630-01-3	87
4	Hentriacontane		437	C31H64	000630-04-6	83
5	Heptacosane		380	C27H56	000593-49-7	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099540.D
Acq On : 16 Oct 2017 13:17
Operator : SJ/JU
Sample : I5776-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-2(0-5)

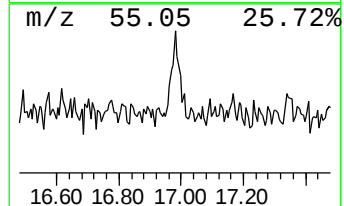
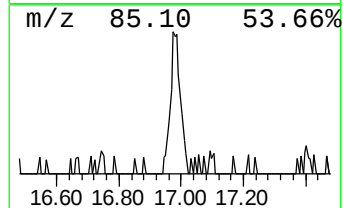
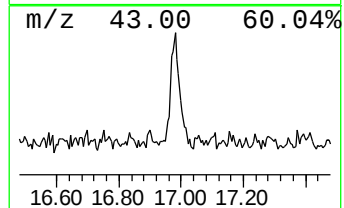
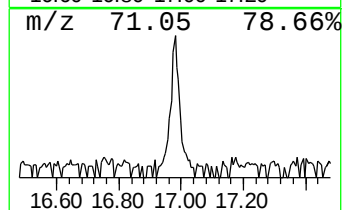
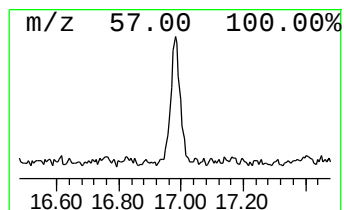
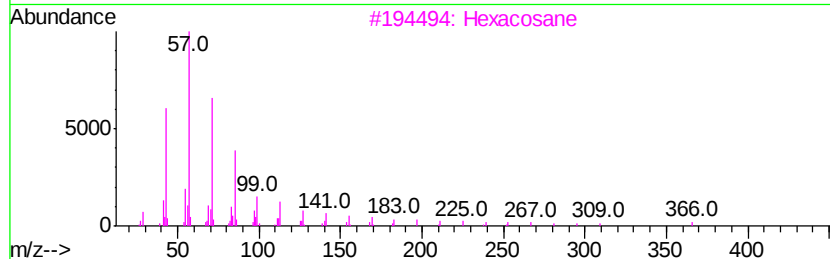
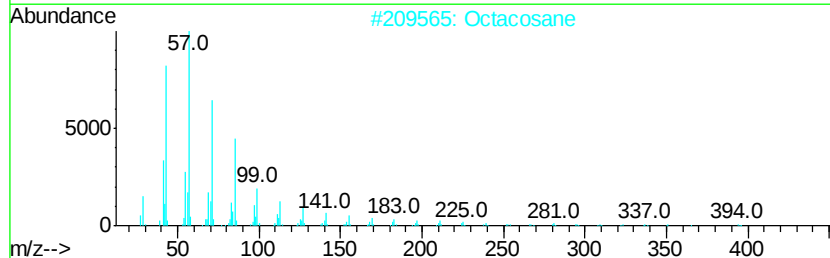
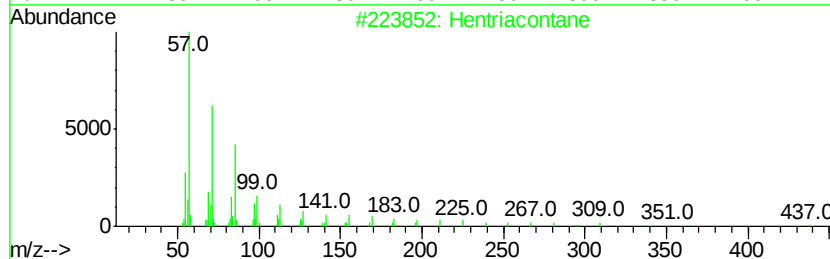
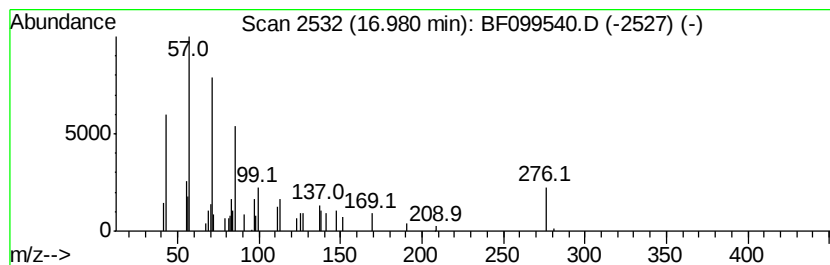
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.98	2.07 ng	55084	Perylene-d12	15.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	68
2	Octacosane		394	C28H58	000630-02-4	64
3	Hexacosane		366	C26H54	000630-01-3	64
4	Pentacosane		352	C25H52	000629-99-2	64
5	triacontane		422	C30H62	000638-68-6	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101617\
Data File : BF099540.D
Acq On : 16 Oct 2017 13:17
Operator : SJ/JU
Sample : I5776-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-2(0-5)

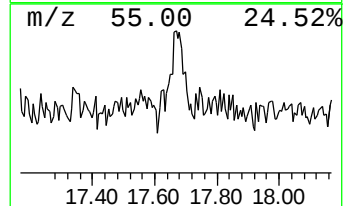
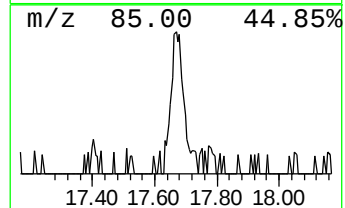
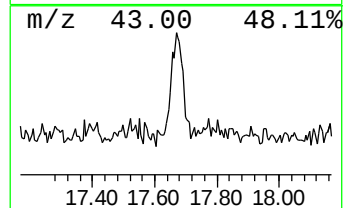
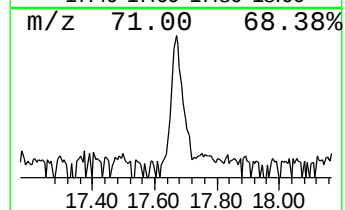
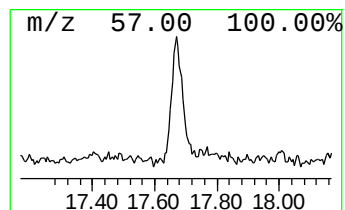
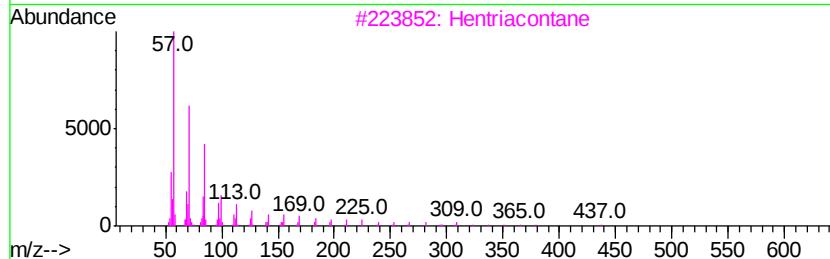
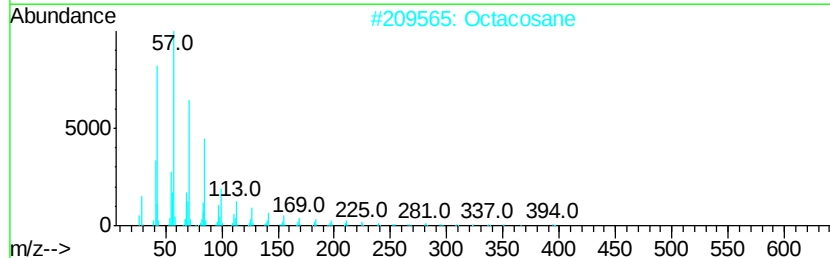
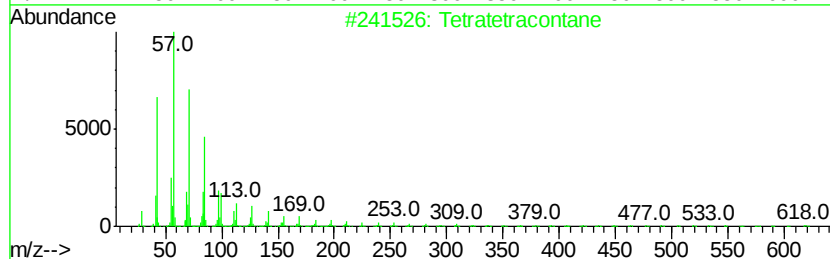
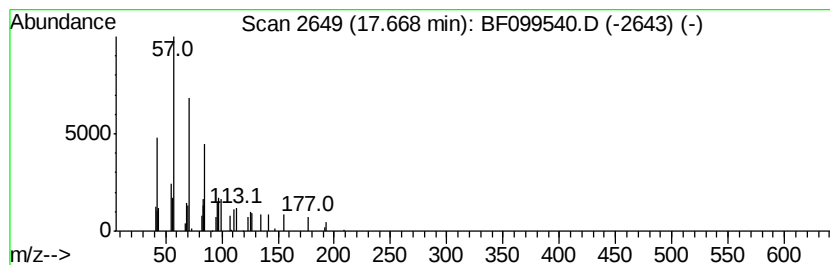
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.67	2.12 ng	56318	Perylene-d12	15.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	80
2		Octacosane	394	C28H58	000630-02-4	80
3		Hentriacontane	437	C31H64	000630-04-6	72
4		Hexacosane	366	C26H54	000630-01-3	72
5		Pentacosane	352	C25H52	000629-99-2	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101617\
Data File : BF099540.D
Acq On : 16 Oct 2017 13:17
Operator : SJ/JU
Sample : I5776-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-2(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	5.07	12.5	ng	356968	1	6.85	572516	20.0
unknown6.62	6.62	74.6	ng	2134220	1	6.85	572516	20.0
Trichloroacetic a...	13.83	3.1	ng	80156	5	14.01	510352	20.0
Heneicosane	16.40	2.5	ng	67773	6	15.49	531178	20.0
Hentriacontane	16.98	2.1	ng	55084	6	15.49	531178	20.0
Tetratetracontane	17.67	2.1	ng	56318	6	15.49	531178	20.0