

Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
 Data File : BF096561.D
 Acq On : 7 Jul 2017 16:09
 Operator : SJ/MA
 Sample : I4064-09
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PET-BF006-01

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-BF070117.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	4.887	472	476	487	rVB	468702	638403	21.03%	2.443%
2	5.316	543	549	552	rBV	2739398	2956760	97.38%	11.315%
3	6.339	717	723	731	rBV	2755646	3036167	100.00%	11.619%
4	6.469	740	745	748	rBV	2914000	2858526	94.15%	10.939%
5	6.698	780	784	787	rBV	761395	695855	22.92%	2.663%
6	6.851	806	810	814	rBV	2330559	2209422	72.77%	8.455%
7	7.257	873	879	882	rBV	1757225	1721344	56.69%	6.587%
8	7.975	997	1001	1005	rBV	1042420	976781	32.17%	3.738%
9	9.057	1179	1185	1188	rBV	2969778	2990417	98.49%	11.444%
10	9.445	1247	1251	1254	rBV	263354	206483	6.80%	0.790%
11	9.727	1294	1299	1303	rBV	1180698	1041206	34.29%	3.985%
12	10.174	1371	1375	1378	rVB	66091	52254	1.72%	0.200%
13	10.392	1407	1412	1415	rBV2	20395	31539	1.04%	0.121%
14	10.516	1428	1433	1436	rBV	1602215	1559785	51.37%	5.969%
15	10.645	1452	1455	1462	rBV	61401	60467	1.99%	0.231%
16	11.204	1546	1550	1554	rBV	1072678	949905	31.29%	3.635%
17	12.792	1815	1820	1823	rBV2	2453142	2481780	81.74%	9.497%
18	13.692	1969	1973	1988	rBV	188720	218712	7.20%	0.837%
19	13.833	1993	1997	2004	rVB	709677	638904	21.04%	2.445%
20	14.592	2122	2126	2134	rBV	219332	237400	7.82%	0.908%
21	14.686	2139	2142	2145	rVB	35166	34007	1.12%	0.130%
22	15.233	2230	2235	2240	rBV	440856	497806	16.40%	1.905%
23	15.727	2315	2319	2326	rBV6	15765	37154	1.22%	0.142%

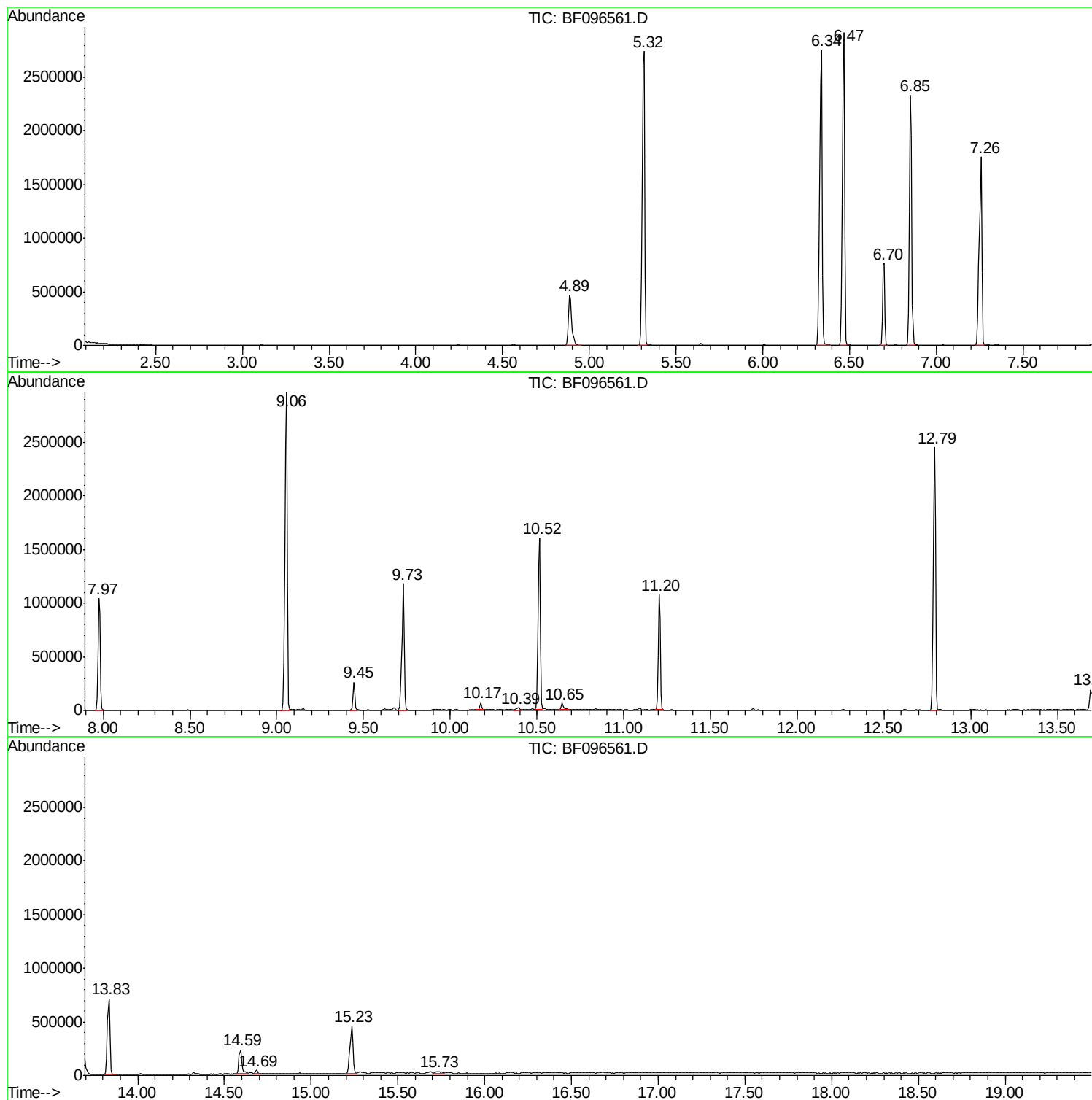
Sum of corrected areas: 26131077

Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
Data File : BF096561.D
Acq On : 7 Jul 2017 16:09
Operator : SJ/MA
Sample : I4064-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PET-BF006-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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\BF070717\
Data File : BF096561.D
Acq On : 7 Jul 2017 16:09
Operator : SJ/MA
Sample : I4064-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PET-BF006-01

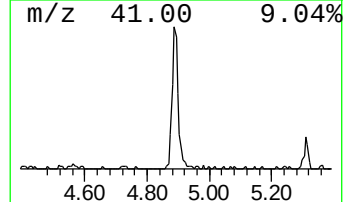
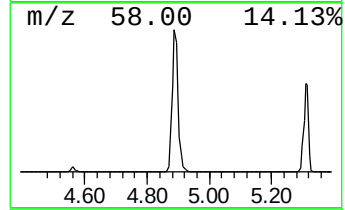
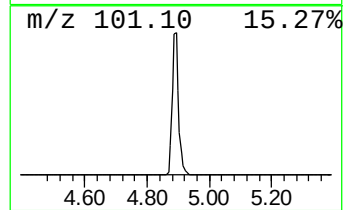
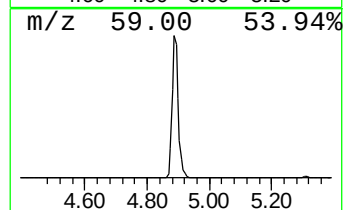
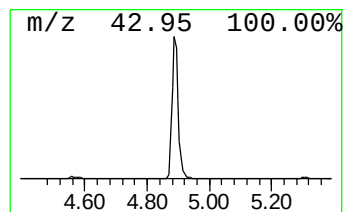
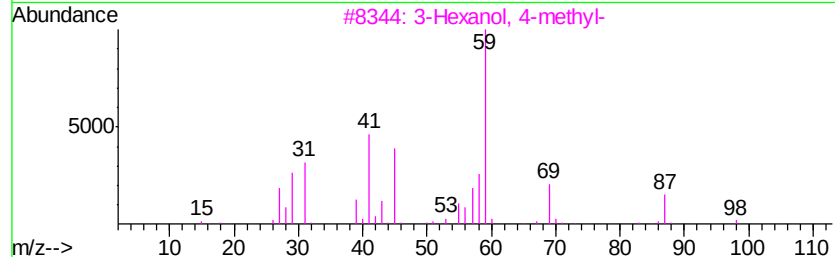
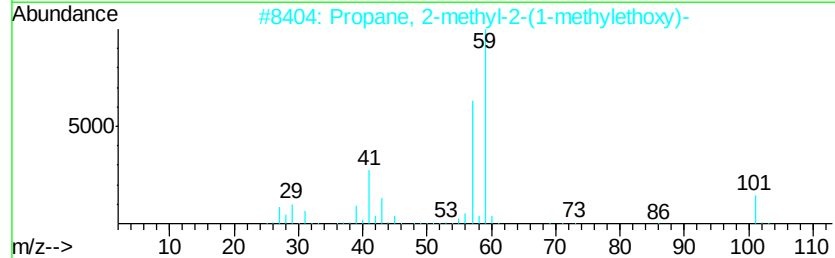
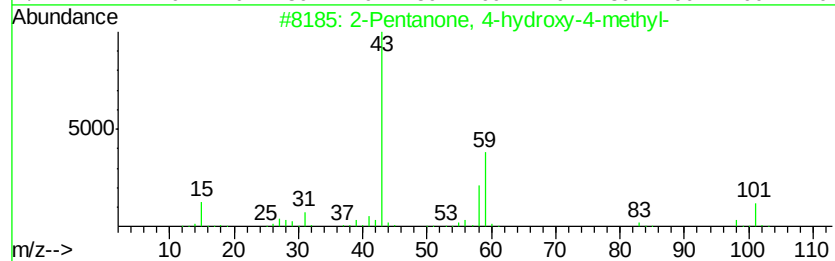
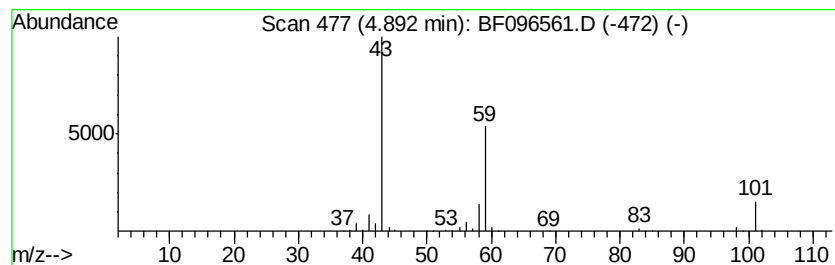
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.89	18.35 ng	638403	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
Data File : BF096561.D
Acq On : 7 Jul 2017 16:09
Operator : SJ/MA
Sample : I4064-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PET-BF006-01

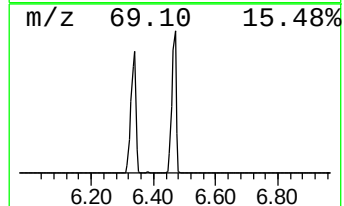
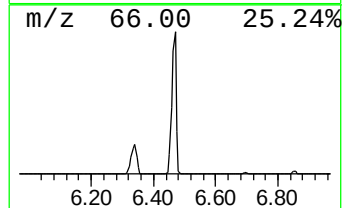
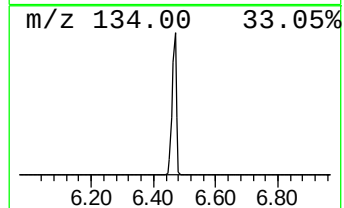
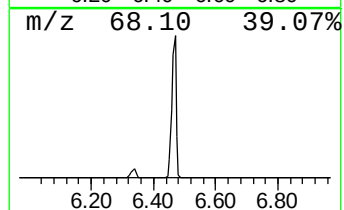
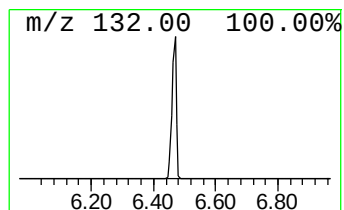
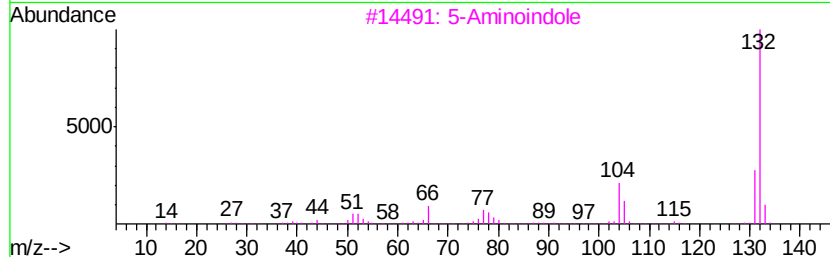
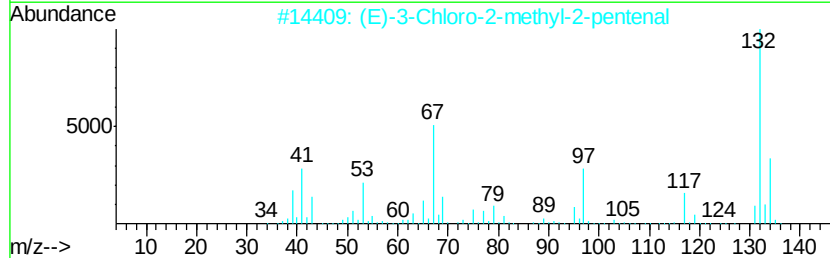
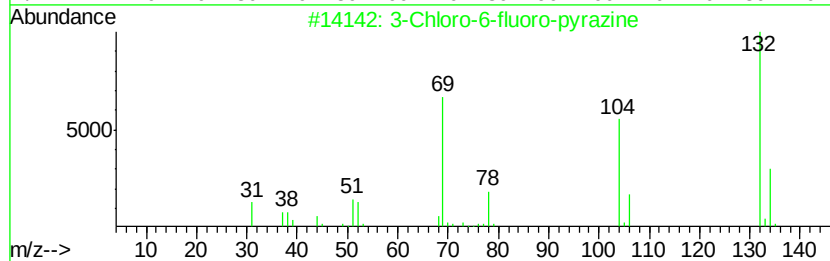
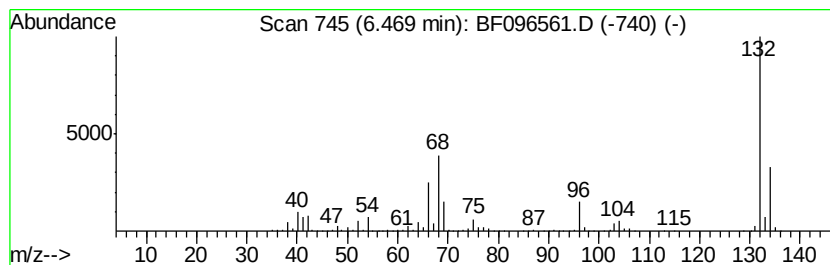
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	82.16 ng	2858530	1,4-Dichlorobenzene-d4	6.70

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	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
Data File : BF096561.D
Acq On : 7 Jul 2017 16:09
Operator : SJ/MA
Sample : I4064-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

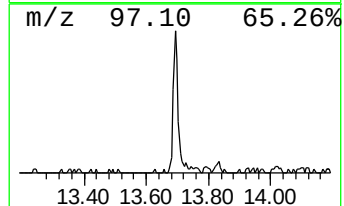
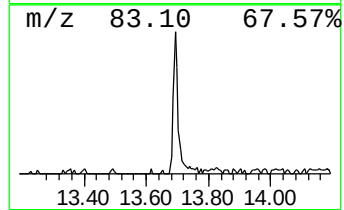
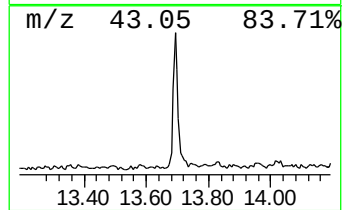
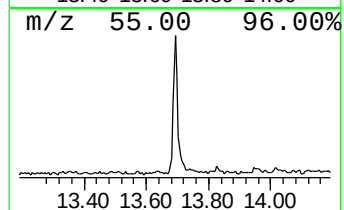
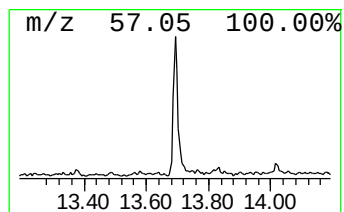
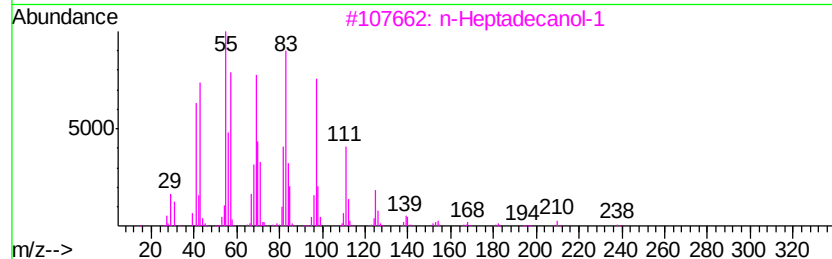
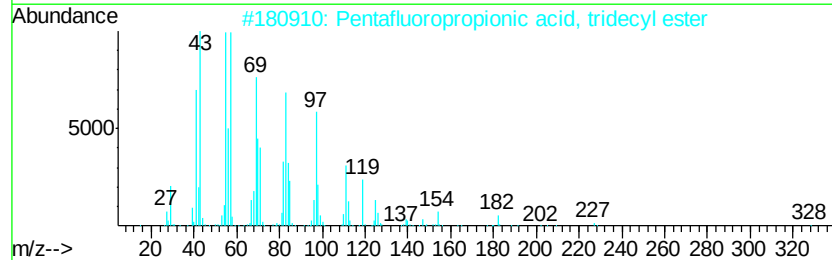
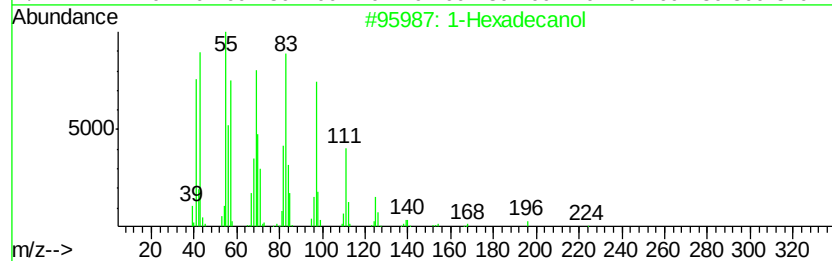
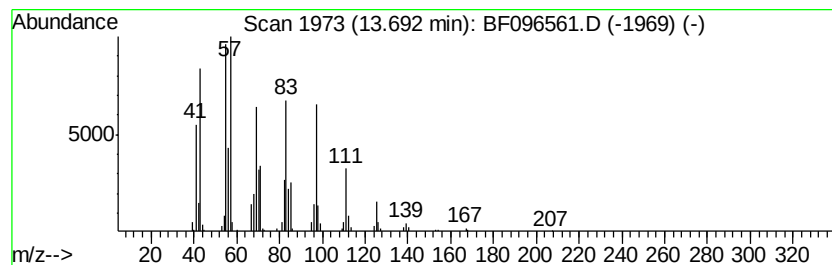
Instrument :
BNA_F
ClientSampleId :
PET-BF006-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Hexadecanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.69	6.85 ng	218712	Chrysene-d12		13.83		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexadecanol	242	C16H34O	036653-82-4	91
2			Pentafluoropropionic acid, tridecyl ester	346	C16H27F5O2	959261-22-4	91
3			n-Heptadecanol-1	256	C17H36O	001454-85-9	91
4			1-Nonadecene	266	C19H38	018435-45-5	91
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91



Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
Data File : BF096561.D
Acq On : 7 Jul 2017 16:09
Operator : SJ/MA
Sample : I4064-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PET-BF006-01

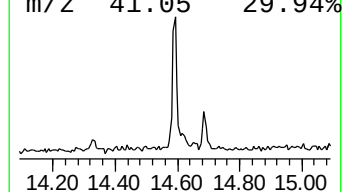
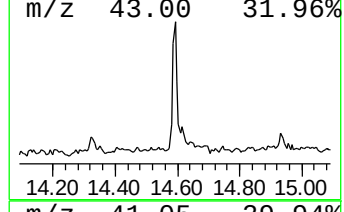
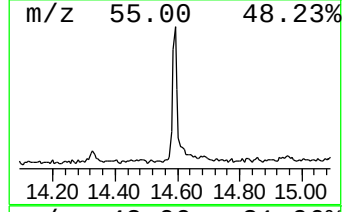
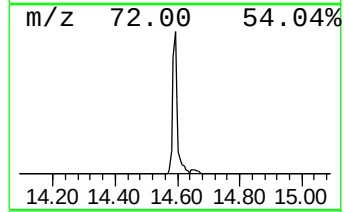
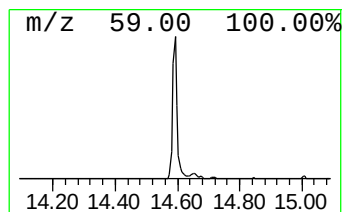
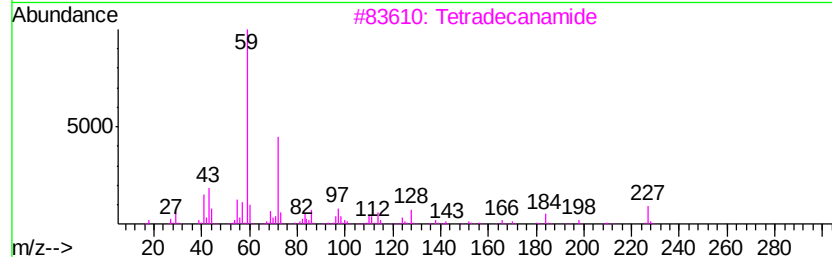
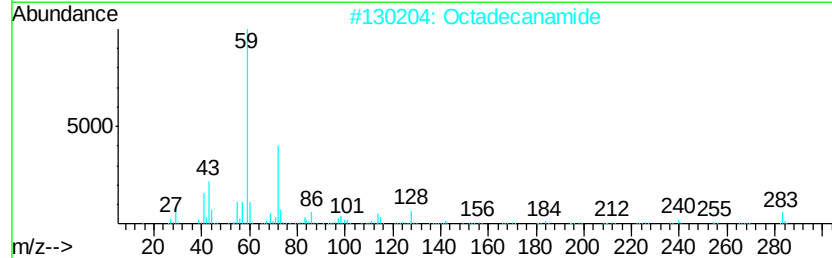
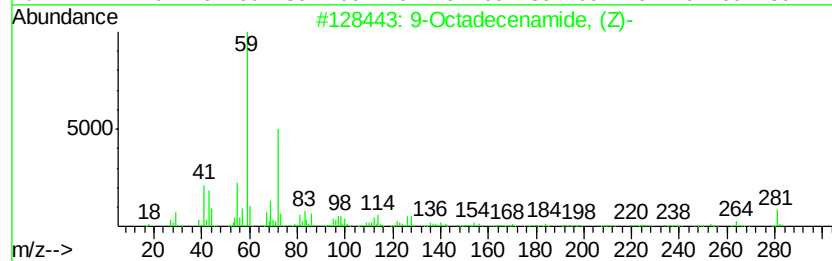
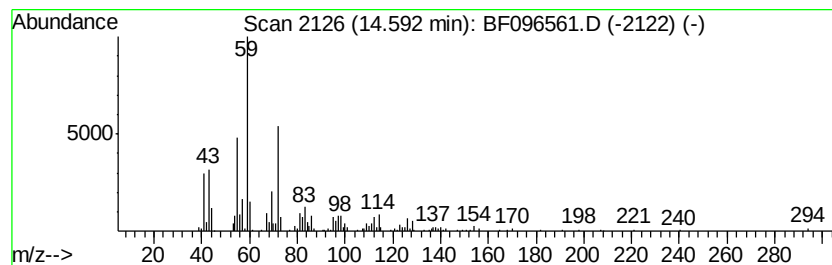
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	9.54 ng	237400	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		Octadecanamide	283	C18H37NO	000124-26-5	72
3		Tetradecanamide	227	C14H29NO	000638-58-4	72
4		7-Nonenamide	155	C9H17NO	090949-53-4	72
5		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64



Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
Data File : BF096561.D
Acq On : 7 Jul 2017 16:09
Operator : SJ/MA
Sample : I4064-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PET-BF006-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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...	4.89	18.4	ng	638403	1	6.70	695855	20.0
unknown6.47	6.47	82.2	ng	2858530	1	6.70	695855	20.0
1-Hexadecanol	13.69	6.8	ng	218712	5	13.83	638904	20.0
9-Octadecenamide,...	14.59	9.5	ng	237400	6	15.23	497806	20.0