

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071217\
 Data File : BF096697.D
 Acq On : 12 Jul 2017 17:47
 Operator : SJ/JU
 Sample : I4126-05
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PP-SW-1

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	4.857	467	471	482	rBV	385323	619919	18.36%	2.437%
2	5.281	538	543	547	rBV	2846203	3375888	100.00%	13.270%
3	6.316	713	719	722	rBV	2746486	3176460	94.09%	12.486%
4	6.439	735	740	743	rBV	3009498	3112811	92.21%	12.236%
5	6.669	775	779	782	rBV	798168	723924	21.44%	2.846%
6	6.828	801	806	809	rBV	2303209	2328917	68.99%	9.154%
7	7.233	869	875	878	rBV	1810731	1987827	58.88%	7.814%
8	7.951	992	997	1000	rBV	1005512	948955	28.11%	3.730%
9	9.027	1174	1180	1183	rBV	2985941	2872734	85.10%	11.292%
10	9.422	1243	1247	1250	rBV	313604	275877	8.17%	1.084%
11	9.698	1289	1294	1298	rBV2	975710	843884	25.00%	3.317%
12	10.145	1367	1370	1373	rVB	55168	44516	1.32%	0.175%
13	10.486	1423	1428	1431	rBV	1569425	1478308	43.79%	5.811%
14	10.616	1447	1450	1460	rBV	58872	70151	2.08%	0.276%
15	11.174	1542	1545	1549	rVB	791525	678061	20.09%	2.665%
16	12.762	1810	1815	1818	rBV	1866190	1769998	52.43%	6.957%
17	13.668	1965	1969	1976	rBV	127586	145398	4.31%	0.572%
18	13.804	1988	1992	1996	rBV	586874	522305	15.47%	2.053%
19	15.198	2224	2229	2234	rBV	398117	464276	13.75%	1.825%

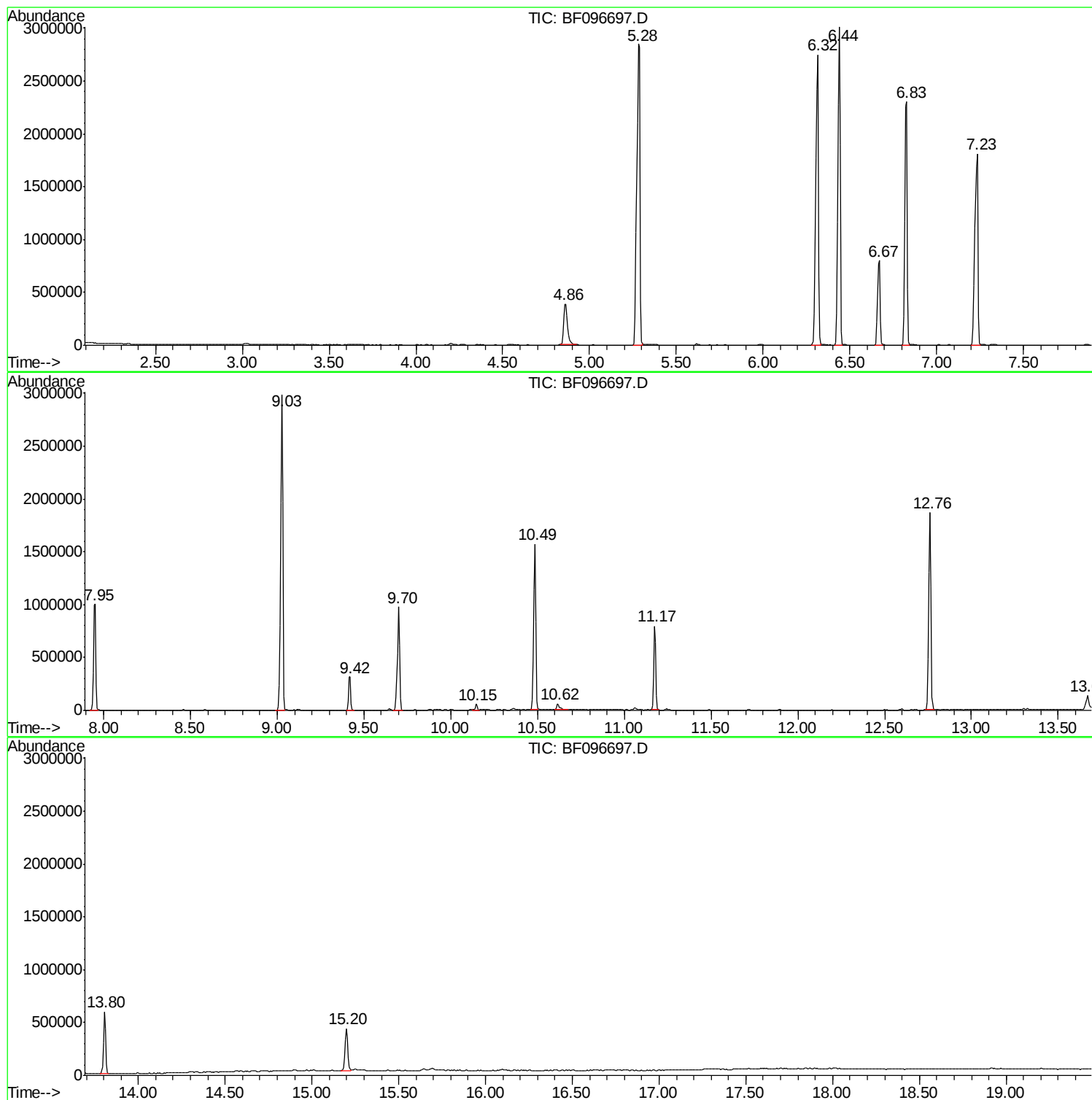
Sum of corrected areas: 25440209

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071217\
Data File : BF096697.D
Acq On : 12 Jul 2017 17:47
Operator : SJ/JU
Sample : I4126-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PP-SW-1

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\BF071217\
Data File : BF096697.D
Acq On : 12 Jul 2017 17:47
Operator : SJ/JU
Sample : I4126-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PP-SW-1

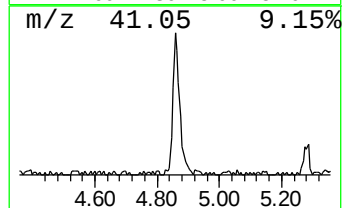
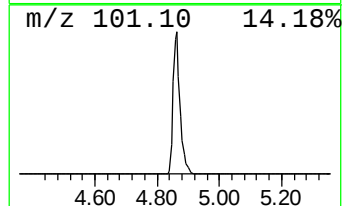
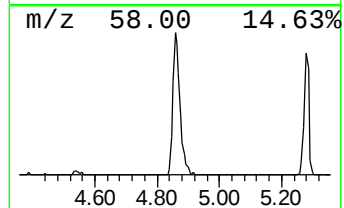
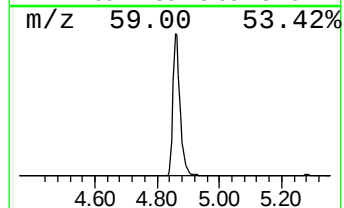
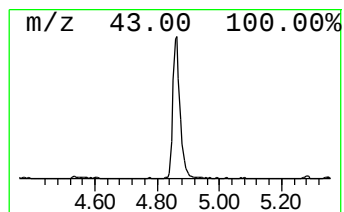
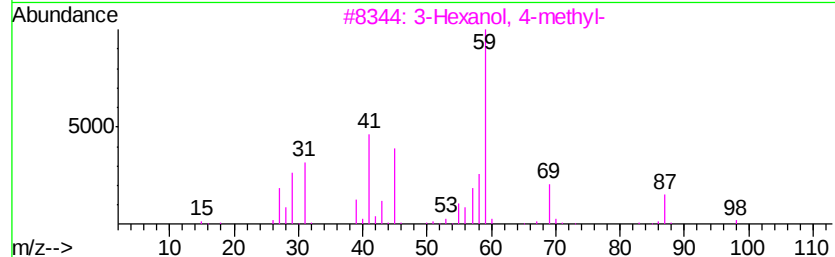
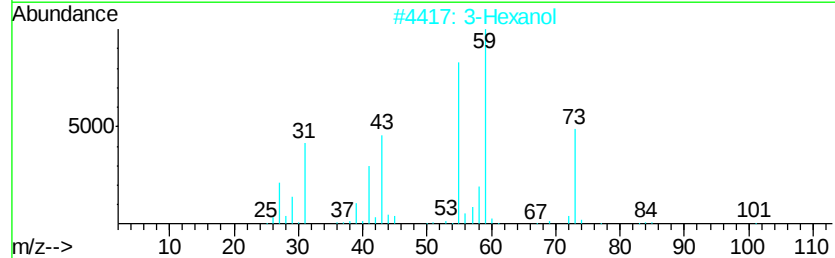
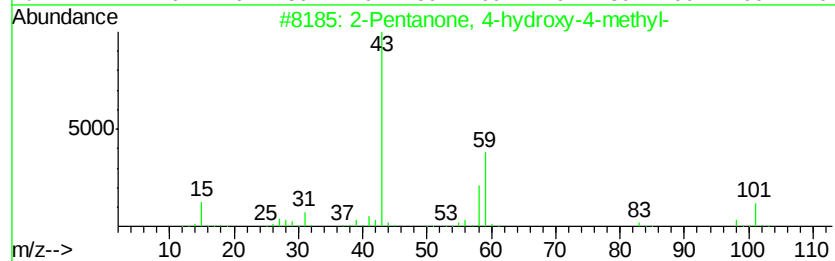
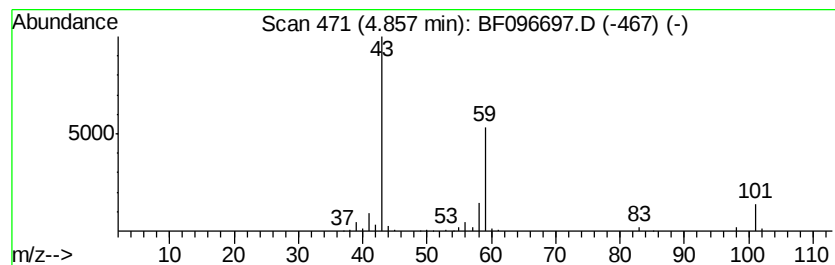
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.86	17.13 ng	619919	1,4-Dichlorobenzene-d4	6.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol	102	C6H14O	000623-37-0	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



Data Path : Z:\HPCHEM1\BNA_F\Data\BF071217\
Data File : BF096697.D
Acq On : 12 Jul 2017 17:47
Operator : SJ/JU
Sample : I4126-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PP-SW-1

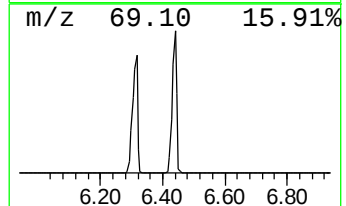
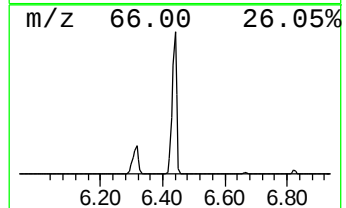
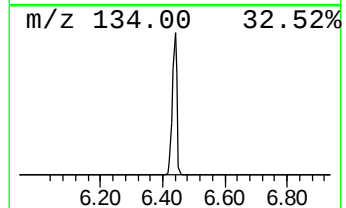
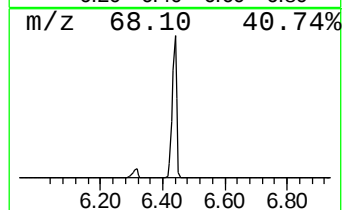
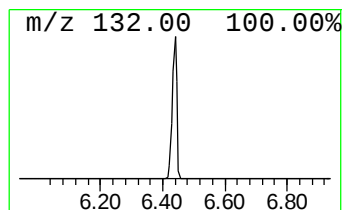
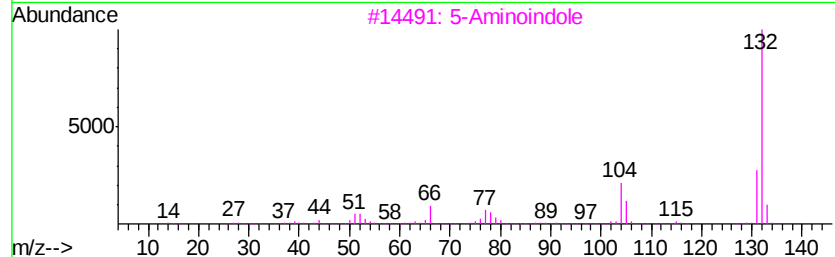
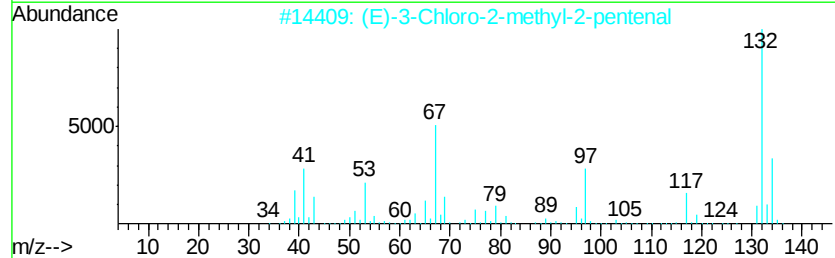
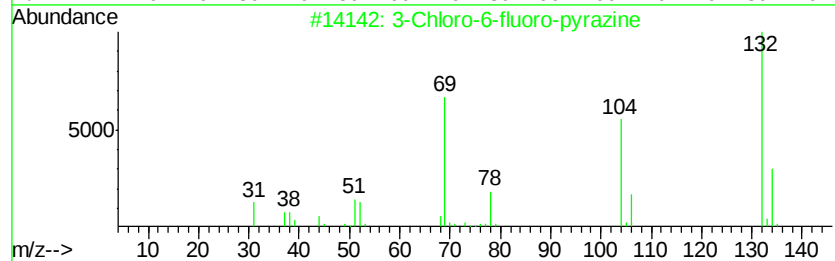
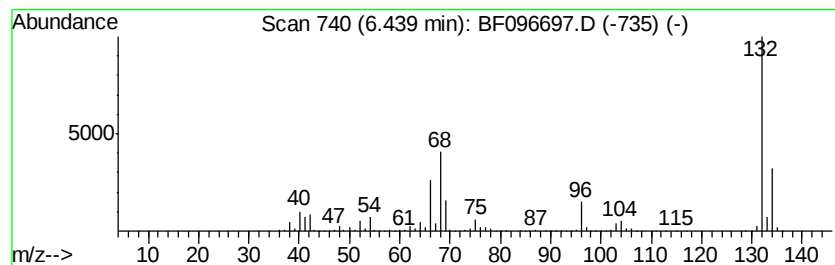
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	86.00 ng	3112810	1,4-Dichlorobenzene-d4	6.67

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		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA_F\Data\BF071217\
Data File : BF096697.D
Acq On : 12 Jul 2017 17:47
Operator : SJ/JU
Sample : I4126-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PP-SW-1

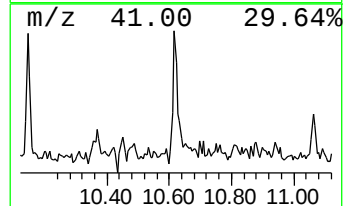
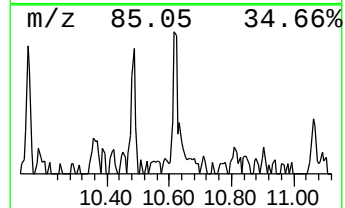
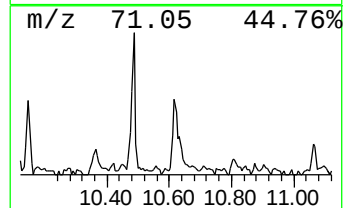
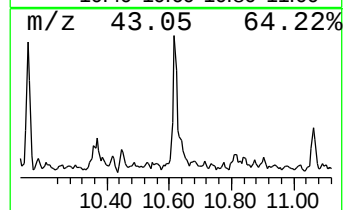
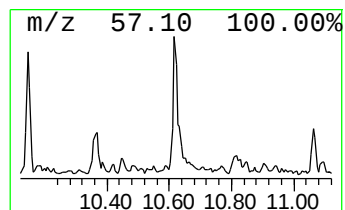
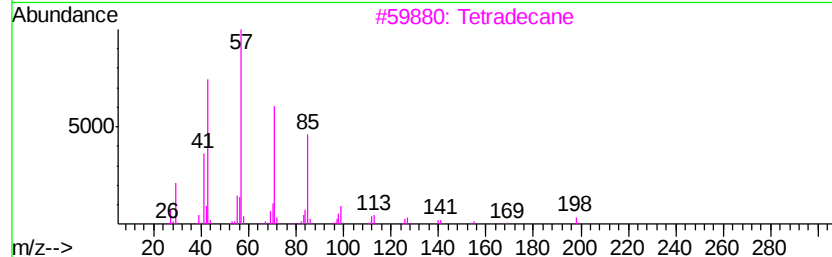
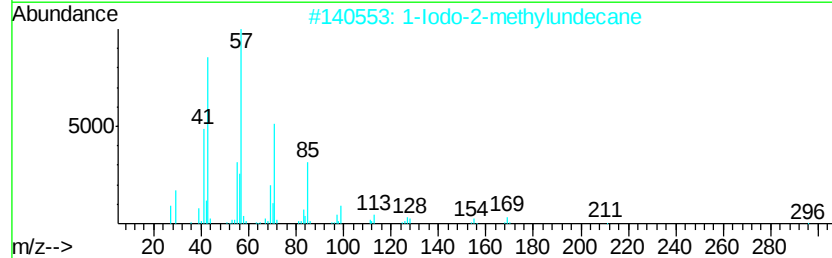
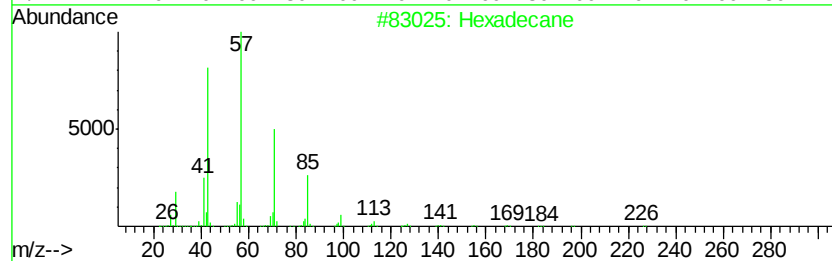
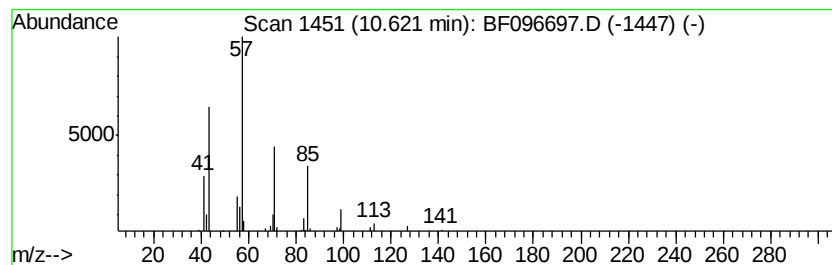
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	2.07 ng	70151	Phenanthrene-d10	11.17

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	90
2	1-Iodo-2-methylundecane		296	C12H25I	073105-67-6	90
3	Tetradecane		198	C14H30	000629-59-4	83
4	Pentadecane		212	C15H32	000629-62-9	78
5	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	72



Data Path : Z:\HPCHEM1\BNA_F\Data\BF071217\
Data File : BF096697.D
Acq On : 12 Jul 2017 17:47
Operator : SJ/JU
Sample : I4126-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PP-SW-1

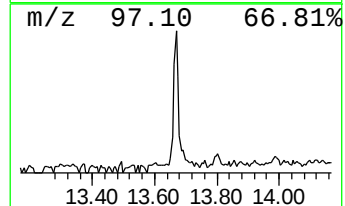
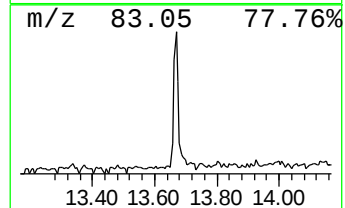
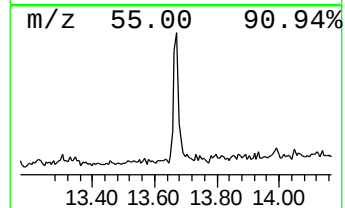
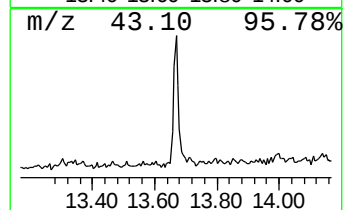
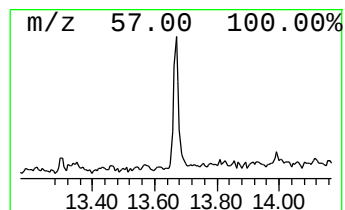
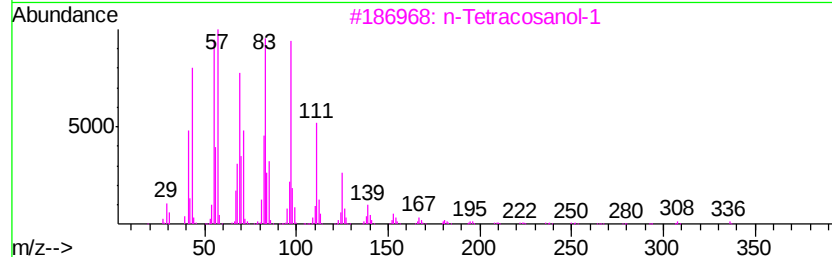
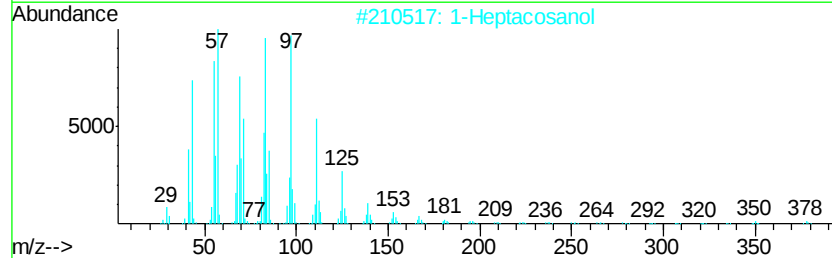
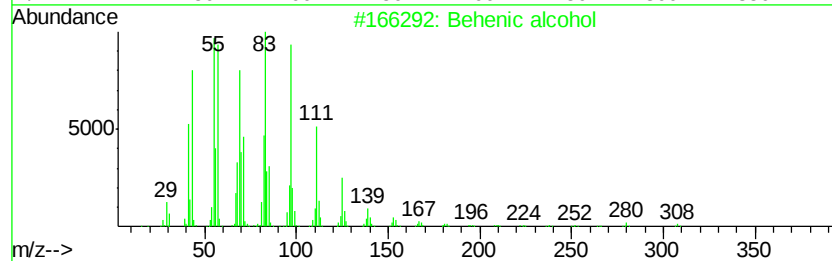
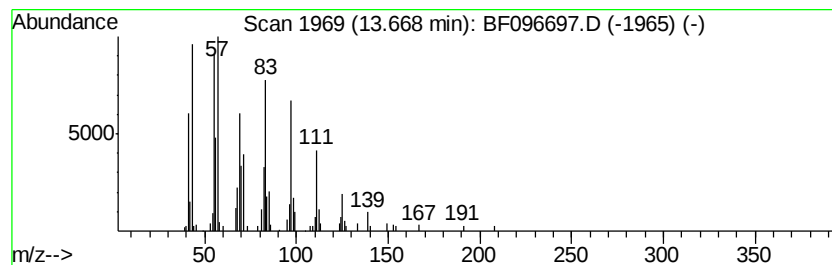
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	5.57 ng	145398	Chrysene-d12	13.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	93
2		1-Heptacosanol	396	C27H56O	002004-39-9	90
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4		1-Octadecanol	270	C18H38O	000112-92-5	87
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	83



Data Path : Z:\HPCHEM1\BNA_F\Data\BF071217\
Data File : BF096697.D
Acq On : 12 Jul 2017 17:47
Operator : SJ/JU
Sample : I4126-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PP-SW-1

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...	4.86	17.1	ng	619919	1	6.67	723924	20.0
unknown6.44	6.44	86.0	ng	3112810	1	6.67	723924	20.0
Hexadecane	10.62	2.1	ng	70151	4	11.17	678061	20.0
Behenic alcohol	13.67	5.6	ng	145398	5	13.80	522305	20.0