

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121517\
 Data File : BF101454.D
 Acq On : 15 Dec 2017 20:21
 Operator : SJ/JU
 Sample : I6889-02
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GIS-1(0-3)

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-BF121417.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	5.046	499	503	525	rBV	540563	964806	20.44%	2.519%
2	5.446	566	571	599	rBV	3630887	4479798	94.90%	11.694%
3	5.781	625	628	641	rBV	27106	61214	1.30%	0.160%
4	6.457	738	743	761	rBV	3432514	4720516	100.00%	12.323%
5	6.593	761	766	769	rBV	3746397	4072591	86.27%	10.631%
6	6.816	800	804	812	rBV	1153315	1091145	23.11%	2.848%
7	6.969	826	830	843	rBV	3194992	3249899	68.85%	8.484%
8	7.387	896	901	919	rBV	2668519	2888116	61.18%	7.539%
9	8.098	1018	1022	1045	rVB	1335962	1455873	30.84%	3.800%
10	8.657	1113	1117	1129	rBV	166133	180902	3.83%	0.472%
11	9.175	1199	1205	1208	rBV	4053429	4070736	86.23%	10.626%
12	9.569	1268	1272	1283	rBV	326585	347728	7.37%	0.908%
13	9.851	1316	1320	1334	rVB2	1426615	1401264	29.68%	3.658%
14	10.569	1438	1442	1447	rBV	454777	422764	8.96%	1.104%
15	10.651	1451	1456	1469	rBV	2056233	2300195	48.73%	6.005%
16	11.345	1570	1574	1583	rBV	1298047	1298954	27.52%	3.391%
17	11.857	1658	1661	1664	rBV3	51449	55864	1.18%	0.146%
18	12.810	1816	1823	1826	rVB2	39845	63954	1.35%	0.167%
19	12.927	1839	1843	1847	rBV	3052665	3116271	66.02%	8.135%
20	13.810	1990	1993	2005	rBV	122819	188958	4.00%	0.493%
21	13.951	2013	2017	2020	rVB	79886	78023	1.65%	0.204%
22	13.992	2020	2024	2032	rBV	952941	1012600	21.45%	2.643%
23	15.468	2270	2275	2283	rVB	551930	785604	16.64%	2.051%

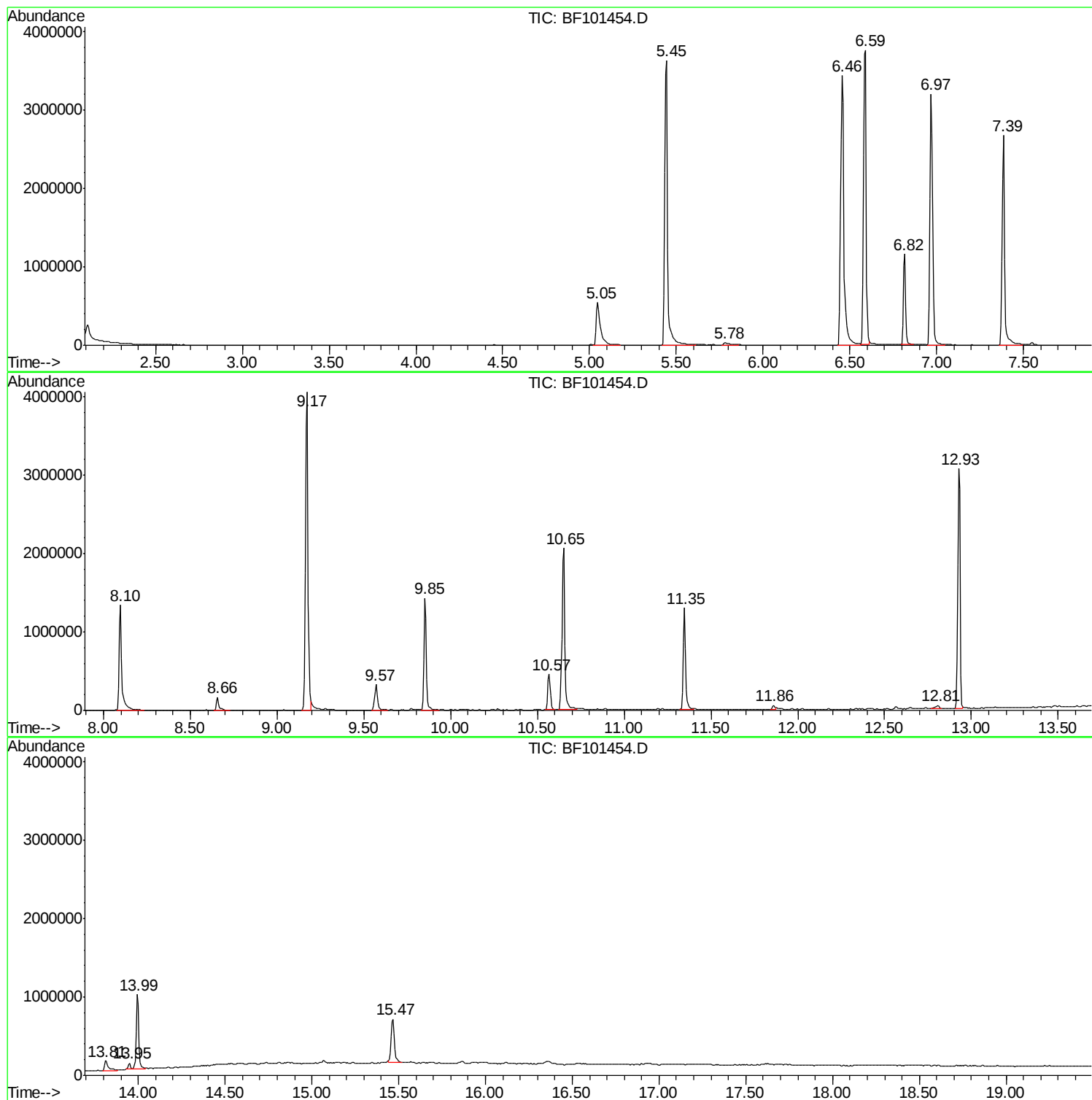
Sum of corrected areas: 38307775

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121517\
Data File : BF101454.D
Acq On : 15 Dec 2017 20:21
Operator : SJ/JU
Sample : I6889-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GIS-1(0-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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\BF121517\
Data File : BF101454.D
Acq On : 15 Dec 2017 20:21
Operator : SJ/JU
Sample : I6889-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GIS-1(0-3)

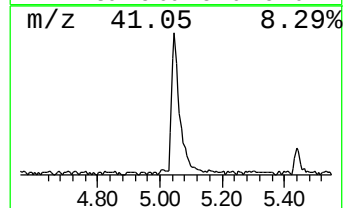
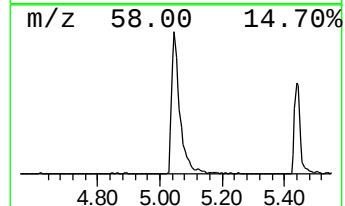
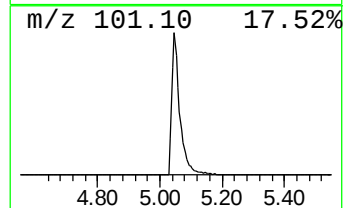
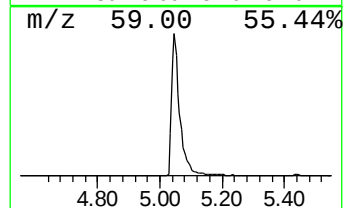
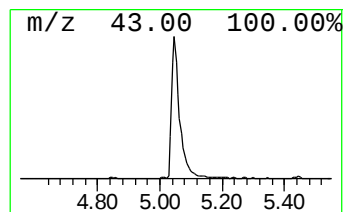
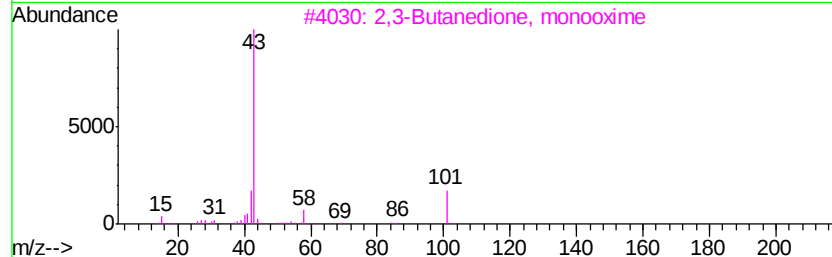
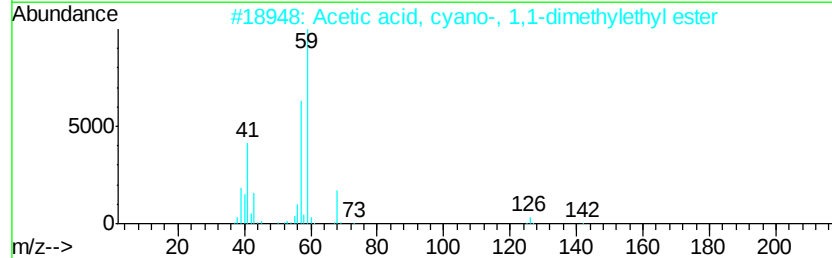
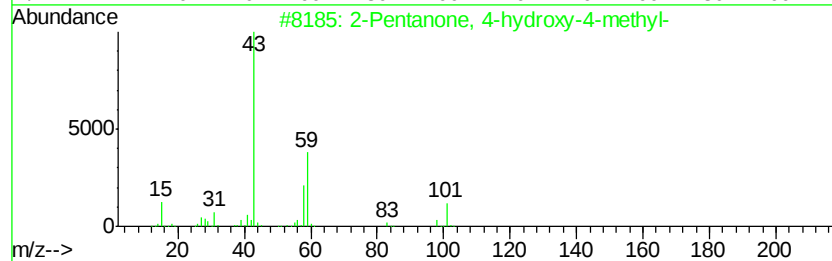
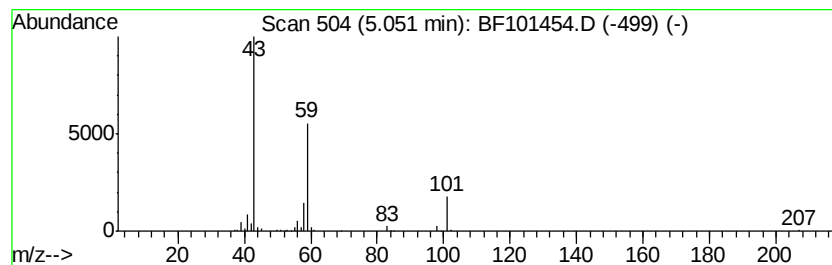
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.05	17.68 ng	964806	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		1,2-Butanediol	90	C4H10O2	000584-03-2	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121517\
Data File : BF101454.D
Acq On : 15 Dec 2017 20:21
Operator : SJ/JU
Sample : I6889-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GIS-1(0-3)

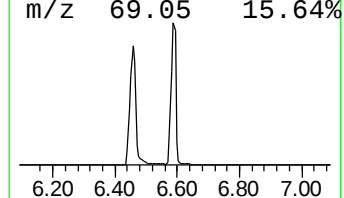
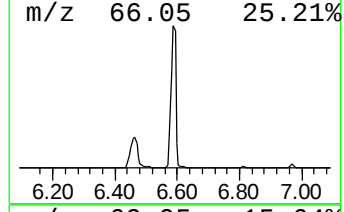
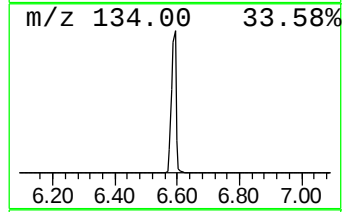
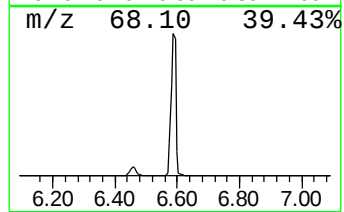
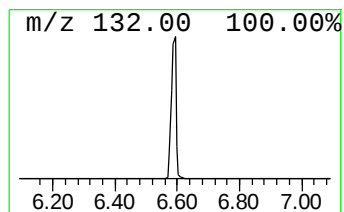
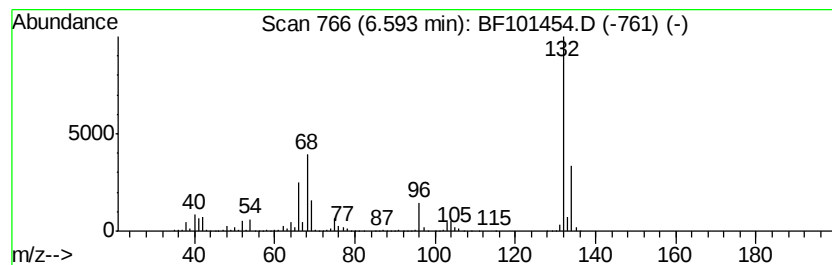
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	74.65 ng	4072590	1,4-Dichlorobenzene-d4	6.82

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121517\
Data File : BF101454.D
Acq On : 15 Dec 2017 20:21
Operator : SJ/JU
Sample : I6889-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GIS-1(0-3)

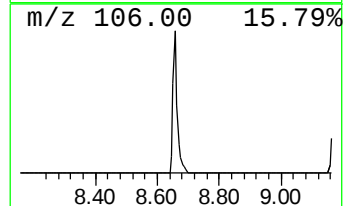
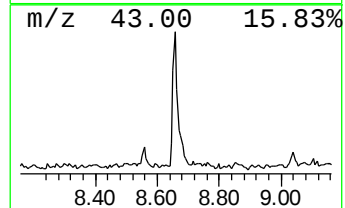
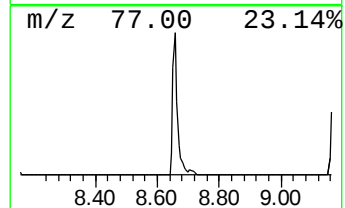
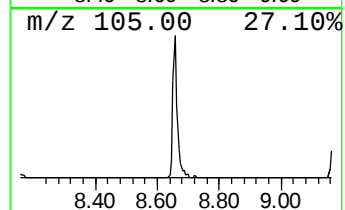
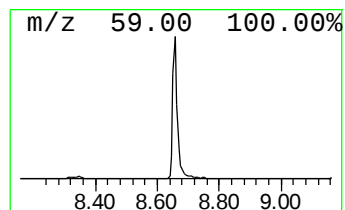
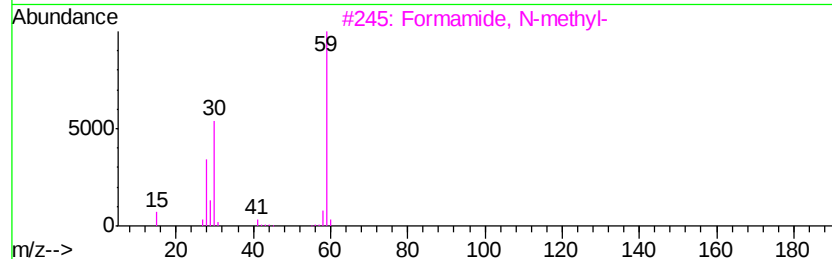
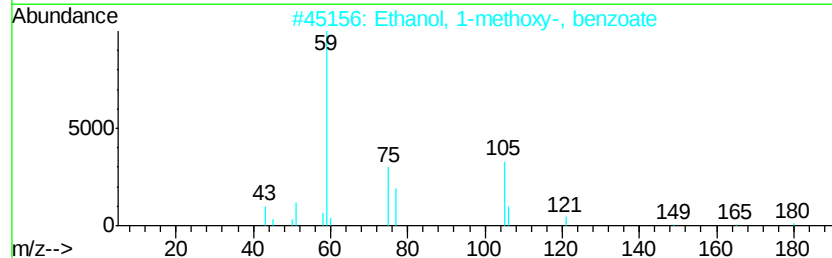
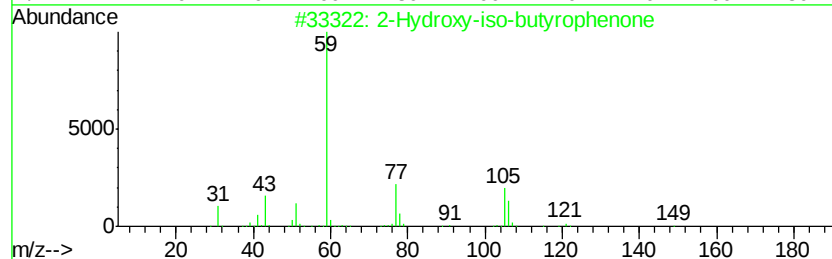
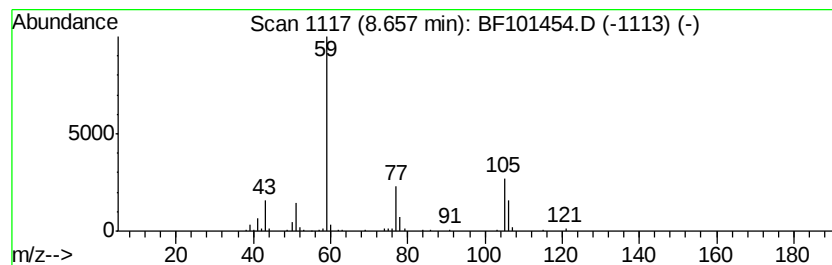
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.66	2.49 ng	180902	Napthalene-d8	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	72
3		Formamide, N-methyl-	59	C2H5NO	000123-39-7	9
4		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
5		Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121517\
Data File : BF101454.D
Acq On : 15 Dec 2017 20:21
Operator : SJ/JU
Sample : I6889-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

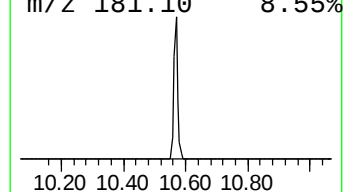
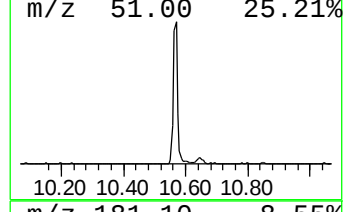
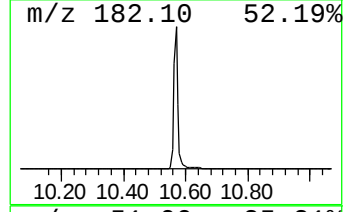
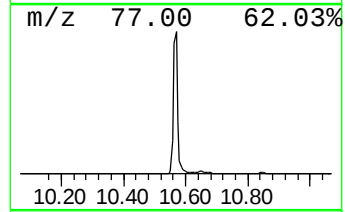
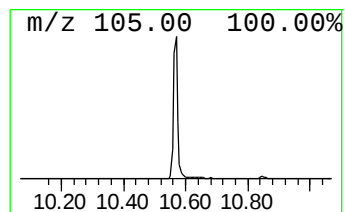
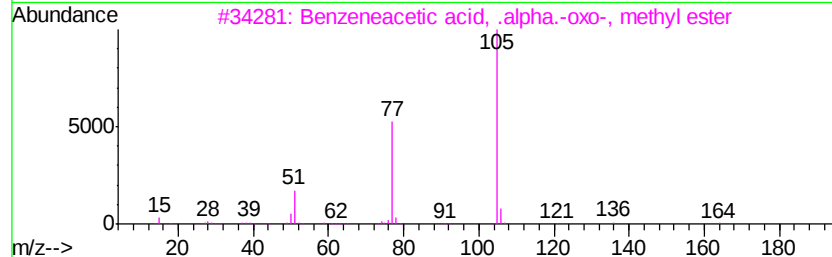
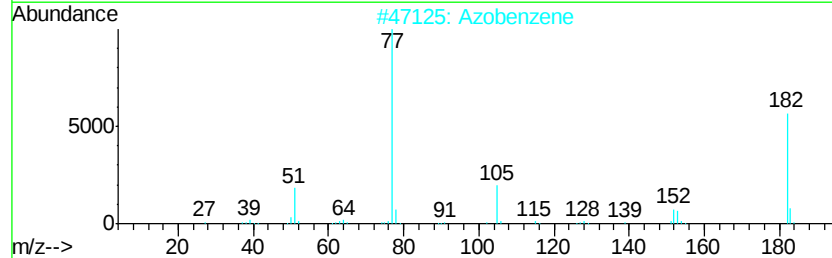
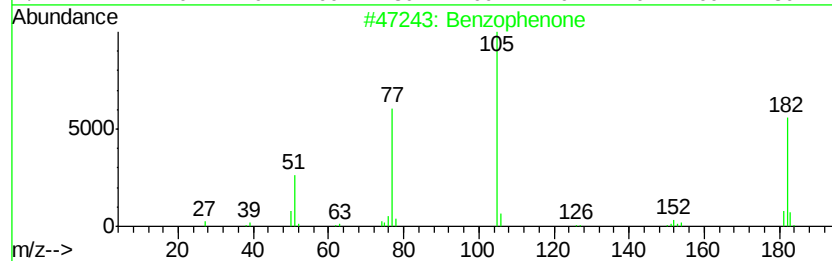
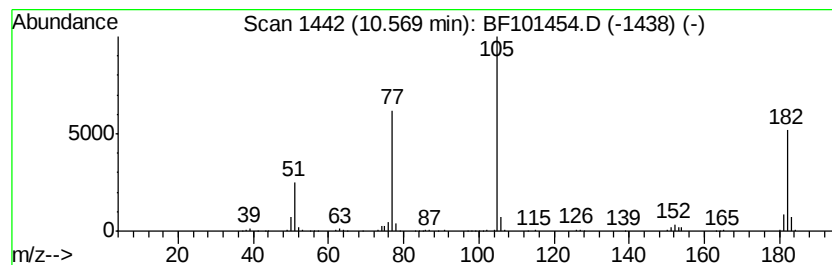
Instrument :
BNA_F
ClientSampleId :
GIS-1(0-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	6.03 ng	422764	Acenaphthene-d10	9.85
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 96
2		Azobenzene	182 C12H10N2	000103-33-3 64
3		Benzeneacetic acid, .alpha.-oxo-...	164 C9H8O3	015206-55-0 49
4		Benzenebutanoic acid, .gamma.-oxo-	178 C10H10O3	002051-95-8 47
5		Benzilamide	227 C14H13NO2	004746-87-6 47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121517\
Data File : BF101454.D
Acq On : 15 Dec 2017 20:21
Operator : SJ/JU
Sample : I6889-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GIS-1(0-3)

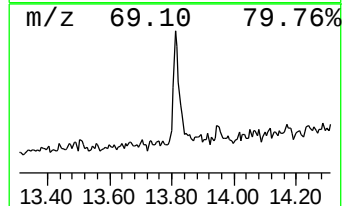
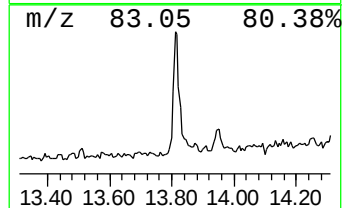
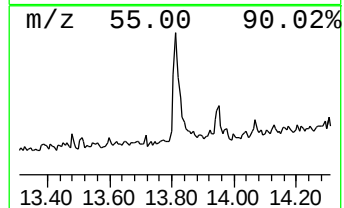
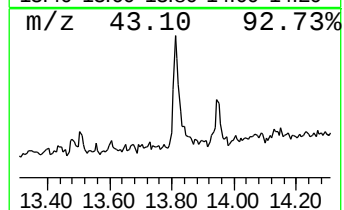
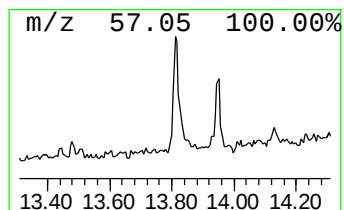
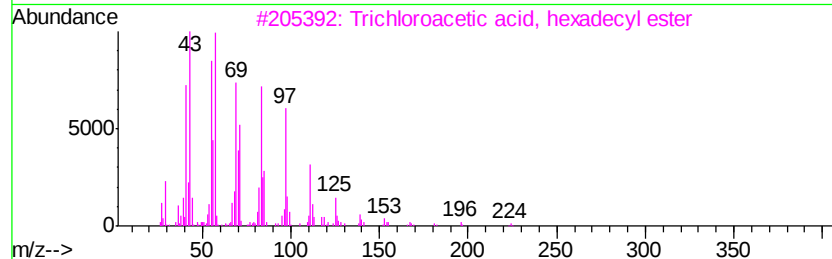
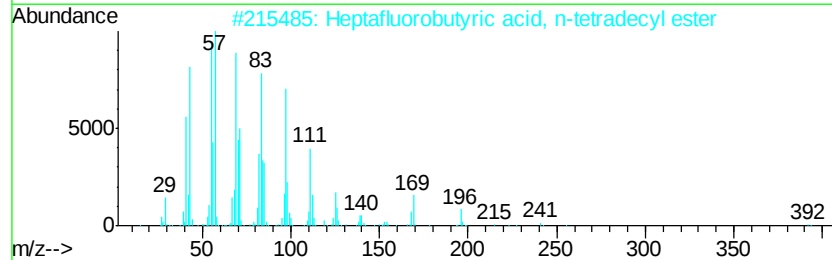
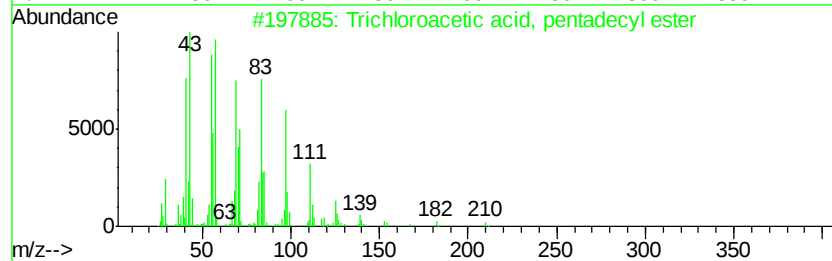
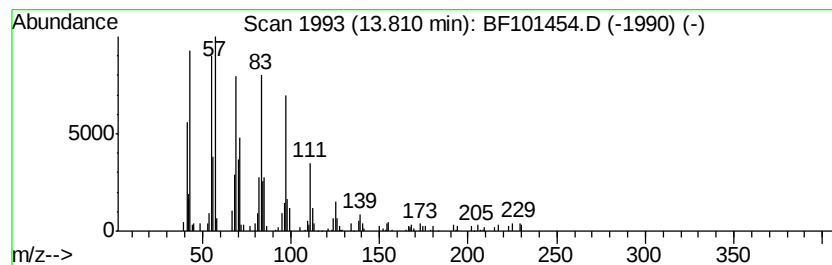
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	3.73 ng	188958	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	95
2		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121517\
Data File : BF101454.D
Acq On : 15 Dec 2017 20:21
Operator : SJ/JU
Sample : I6889-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GIS-1(0-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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...	5.05	17.7	ng	964806	1	6.82	1091150	20.0
unknown6.59	6.59	74.7	ng	4072590	1	6.82	1091150	20.0
2-Hydroxy-iso-but...	8.66	2.5	ng	180902	2	8.10	1455870	20.0
Benzophenone	10.57	6.0	ng	422764	3	9.85	1401260	20.0
Trichloroacetic a...	13.81	3.7	ng	188958	5	13.99	1012600	20.0