

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103017\
 Data File : BF099982.D
 Acq On : 31 Oct 2017 2:02
 Operator : SJ/JU
 Sample : I6083-08
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 102017-TIFR-F-U-B

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-BF102317.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	4.998	493	495	514	rBV	58570	91721	3.67%	0.630%
2	5.410	562	565	596	rBV	474046	686267	27.44%	4.716%
3	6.434	736	739	757	rBV	288721	461212	18.44%	3.169%
4	6.557	757	760	775	rVB	1409655	1311479	52.44%	9.013%
5	6.787	796	799	808	rBV	540087	469805	18.78%	3.229%
6	6.939	821	825	843	rBV	1917693	1802132	72.05%	12.384%
7	7.363	892	897	921	rBV	1257944	1348878	53.93%	9.270%
8	8.069	1014	1017	1035	rBV	764446	634410	25.37%	4.360%
9	9.145	1196	1200	1203	rBV	2907111	2501063	100.00%	17.188%
10	9.545	1265	1268	1277	rBB	30673	28616	1.14%	0.197%
11	9.828	1309	1316	1329	rVB	710970	719310	28.76%	4.943%
12	10.498	1426	1430	1434	rBV	78373	68877	2.75%	0.473%
13	10.539	1434	1437	1443	rBV	150559	121932	4.88%	0.838%
14	10.622	1447	1451	1466	rBV	923163	856027	34.23%	5.883%
15	11.322	1566	1570	1579	rBV	655103	616360	24.64%	4.236%
16	12.910	1835	1840	1843	rBV	1948730	2000117	79.97%	13.745%
17	13.980	2018	2022	2031	rBV	438617	441949	17.67%	3.037%
18	15.468	2270	2275	2284	rBV	286180	391473	15.65%	2.690%

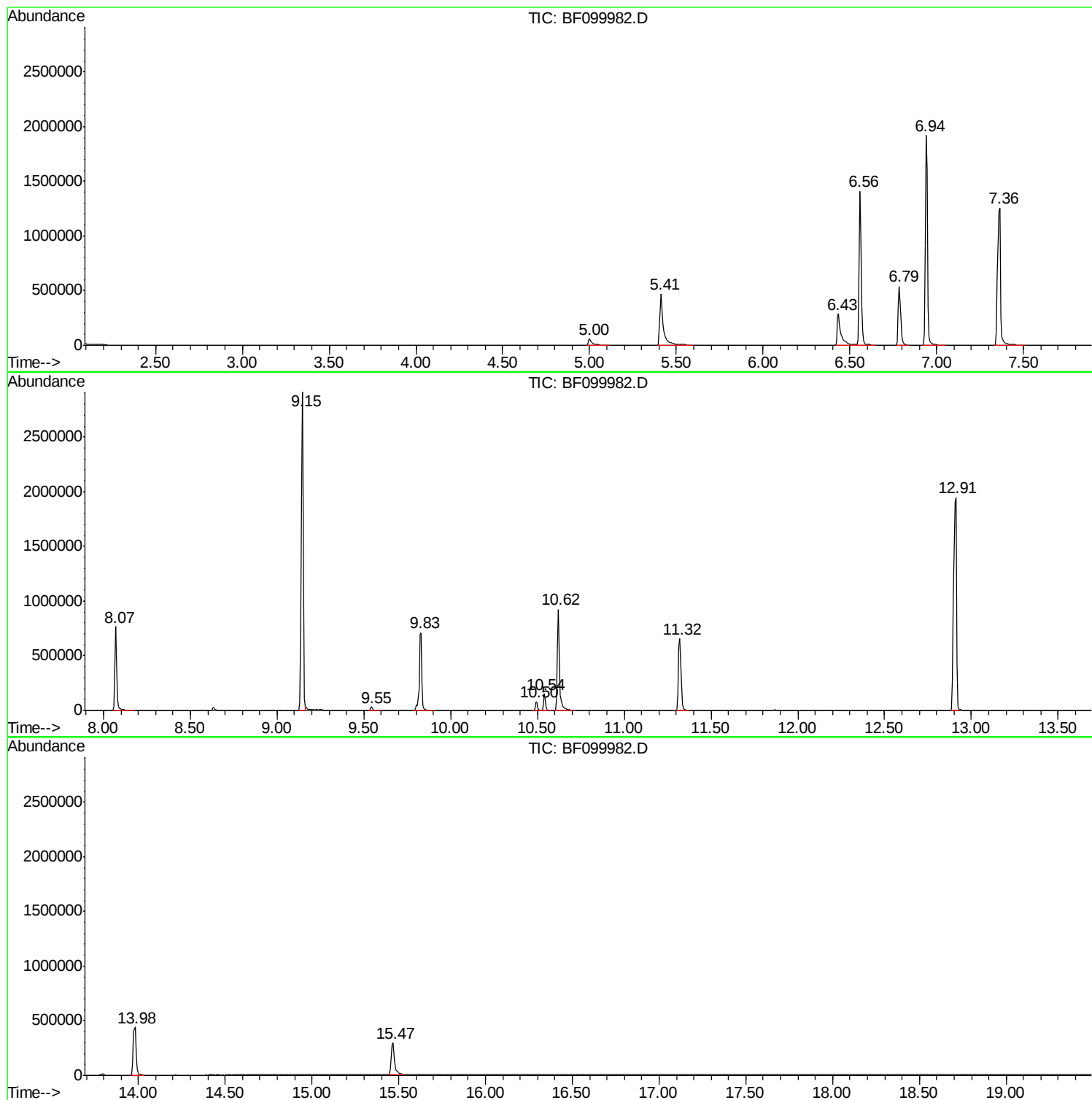
Sum of corrected areas: 14551628

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103017\
Data File : BF099982.D
Acq On : 31 Oct 2017 2:02
Operator : SJ/JU
Sample : I6083-08
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
102017-TIFR-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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\BF103017\
Data File : BF099982.D
Acq On : 31 Oct 2017 2:02
Operator : SJ/JU
Sample : I6083-08
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
102017-TIFR-F-U-B

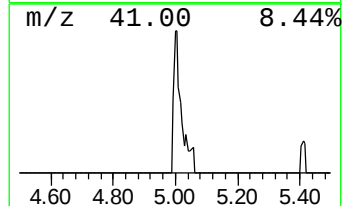
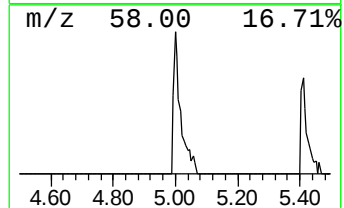
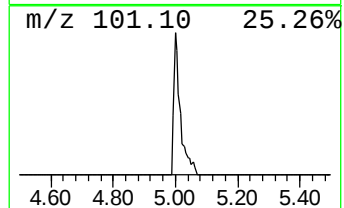
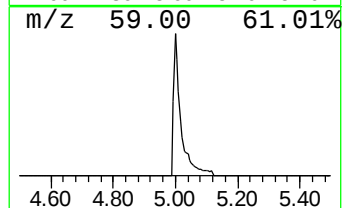
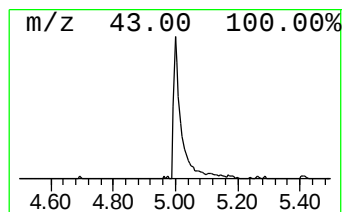
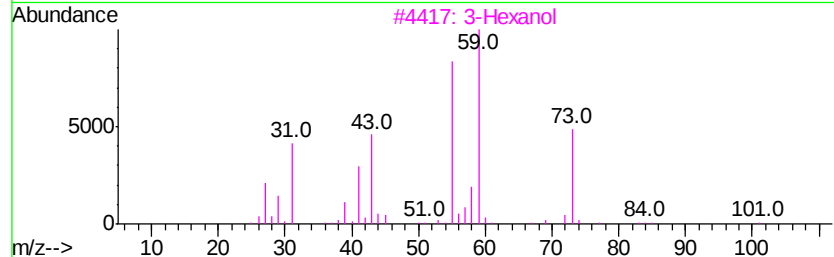
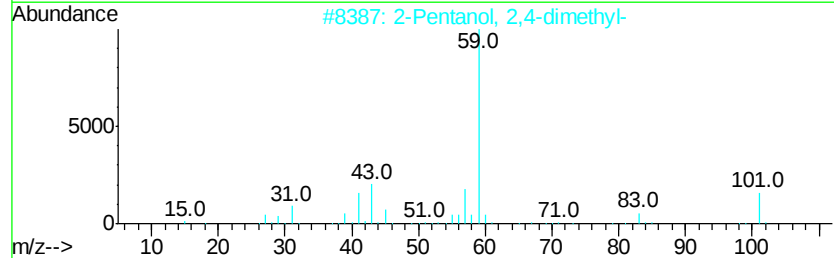
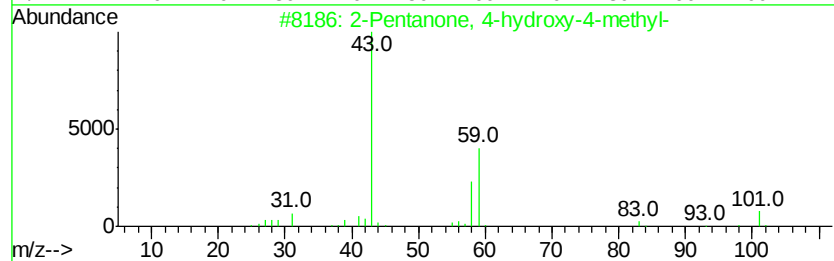
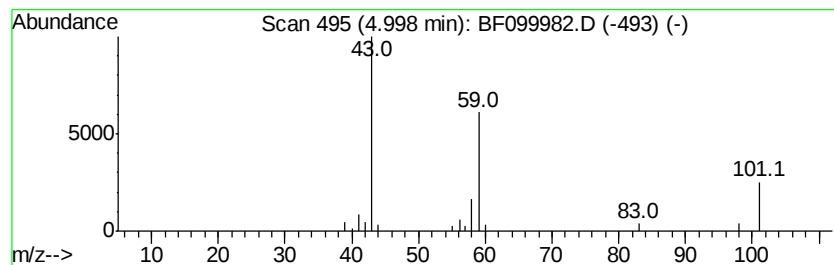
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.00	3.90 ng	91721	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25
3			3-Hexanol	102	C6H14O	000623-37-0	25
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103017\
Data File : BF099982.D
Acq On : 31 Oct 2017 2:02
Operator : SJ/JU
Sample : I6083-08
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
102017-TIFR-F-U-B

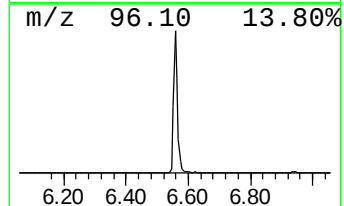
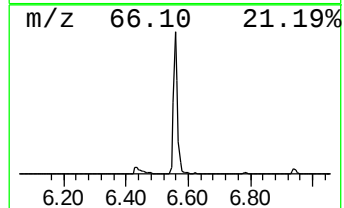
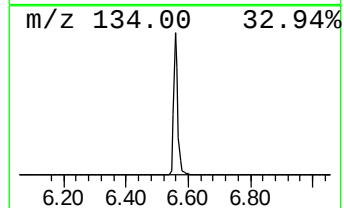
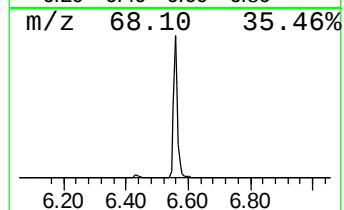
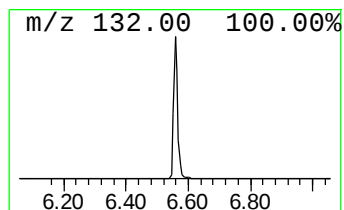
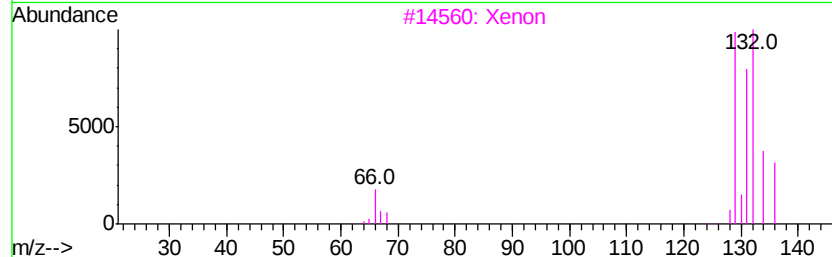
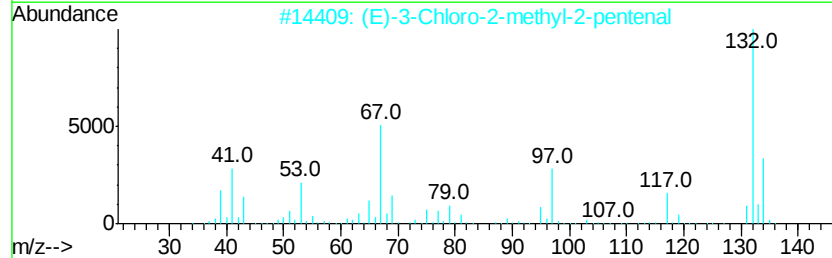
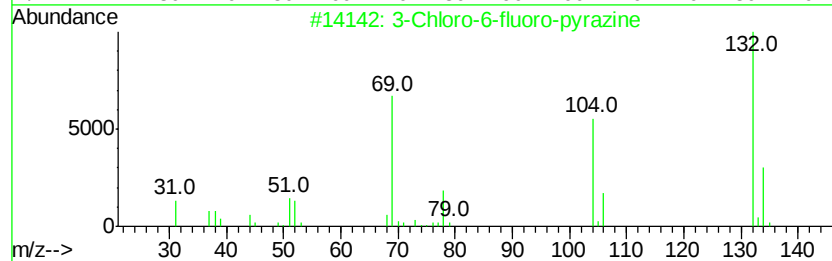
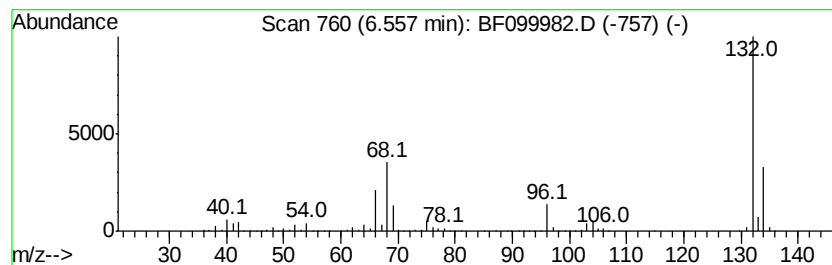
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	55.83 ng	1311480	1,4-Dichlorobenzene-d4	6.79

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		Xenon	132	Xe	007440-63-3	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF103017\
Data File : BF099982.D
Acq On : 31 Oct 2017 2:02
Operator : SJ/JU
Sample : I6083-08
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
102017-TIFR-F-U-B

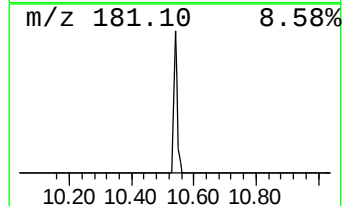
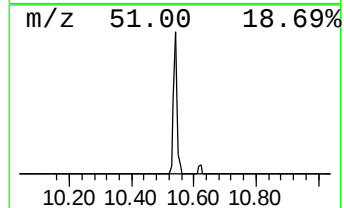
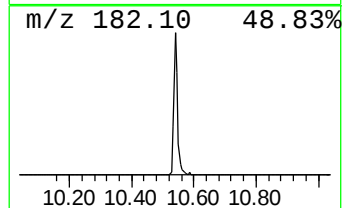
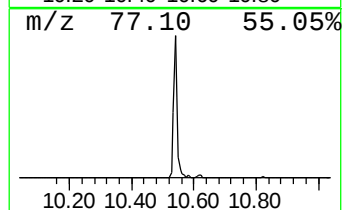
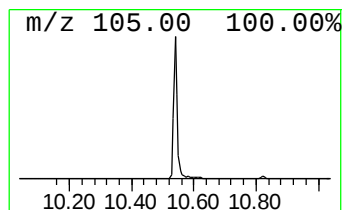
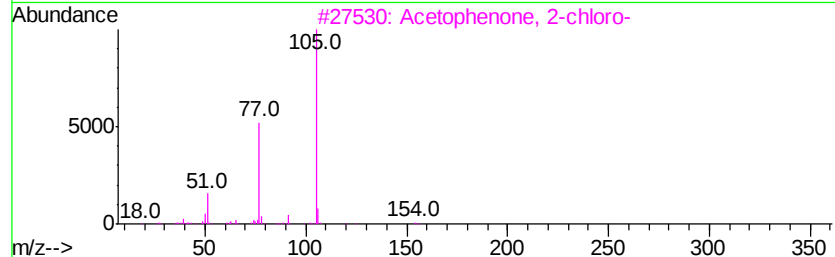
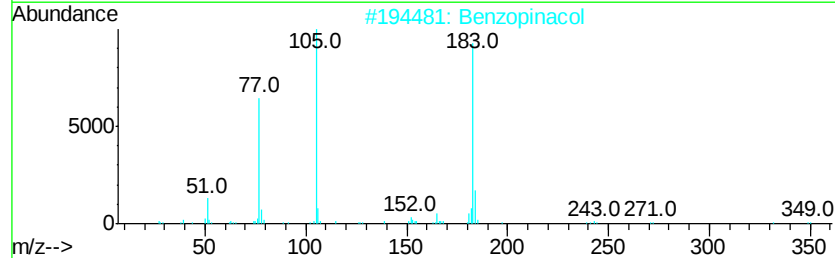
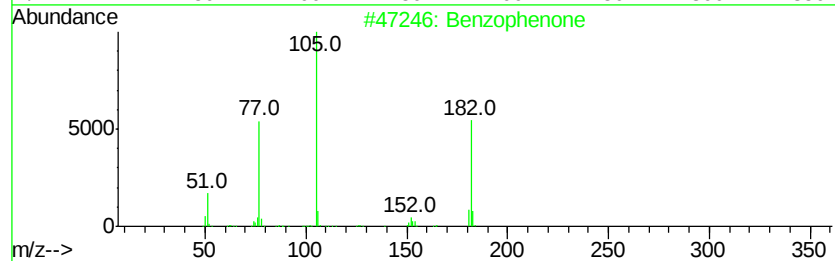
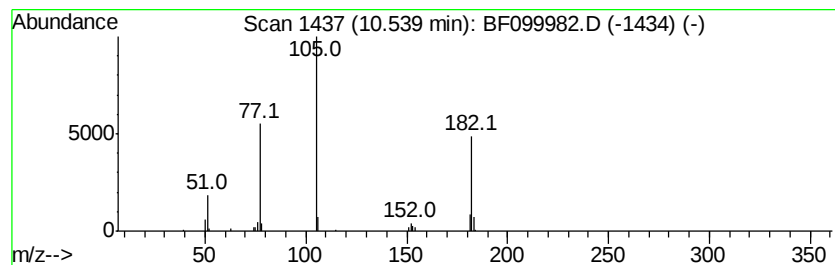
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.54	3.39 ng	121932	Acenaphthene-d10	9.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzophenone	182	C13H10O	000119-61-9	96
2		Benzopinacol	366	C26H22O2	000464-72-2	50
3		Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4		N-Benzovlimidazole	172	C10H8N2O	010364-94-0	43
5		Vinyl benzoate	148	C9H8O2	000769-78-8	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103017\
Data File : BF099982.D
Acq On : 31 Oct 2017 2:02
Operator : SJ/JU
Sample : I6083-08
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
102017-TIFR-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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...	5.00	3.9	ng	91721	1	6.79	469805	20.0
unknown6.56	6.56	55.8	ng	1311480	1	6.79	469805	20.0
Benzophenone	10.54	3.4	ng	121932	3	9.82	719310	20.0