LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF103017\
Data File : BF099980.D
Acq On : 31 Oct 2017 1:11
Operator : SJ/JU
Sample : I6083-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102017-TIFR-F-D-M

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	4.992	492	494	510	rBV	66100	98379	3.76%	0.640%
2	5.410	562	565	589	rBV	456999	709359	27.12%	4.613%
3	6.428	736	738	751	rBV	325111	496481	18.98%	3.229%
4	6.557	757	760	772	rVB	1443654	1311367	50.14%	8.529%
5	6.786	796	799	809	rBV	547467	483758	18.49%	3.146%
6	6.939	822	825	845	rVB	1884679	1800412	68.83%	11.709%
7	7.357	892	896	920	rBV	1267164	1357025	51.88%	8.825%
8	8.069	1014	1017	1033	rBV	791324	660342	25.25%	4.295%
9	8.627	1109	1112	1121	rBB	46274	44923	1.72%	0.292%
10	9.145	1196	1200	1203	rBV	2915827	2615646	100.00%	17.011%
11	9.545	1265	1268	1277	rBB	63227	57090	2.18%	0.371%
12	9.827	1309	1316	1326	rVB	786852	750566	28.70%	4.881%
13	10.239	1383	1386	1390	rVB	243635	177020	6.77%	1.151%
14	10.498	1426	1430	1434	rBV	65572	51186	1.96%	0.333%
15	10.539	1434	1437	1447	rVB	247377	199032	7.61%	1.294%
16	10.621	1447	1451	1465	rBV	959846	900897	34.44%	5.859%
17	11.321	1566	1570	1578	rBV	724598	636199	24.32%	4.138%
18	12.910	1835	1840	1843	rBV	2211630	2085908	79.75%	13.566%
19	13.792	1986	1990	2000	rBV	37321	50424	1.93%	0.328%
20	13.980	2018	2022	2030	rBV	470348	464296	17.75%	3.020%
21	15.468	2270	2275	2284	rBV	336253	425914	16.28%	2.770%

Sum of corrected areas: 15376224

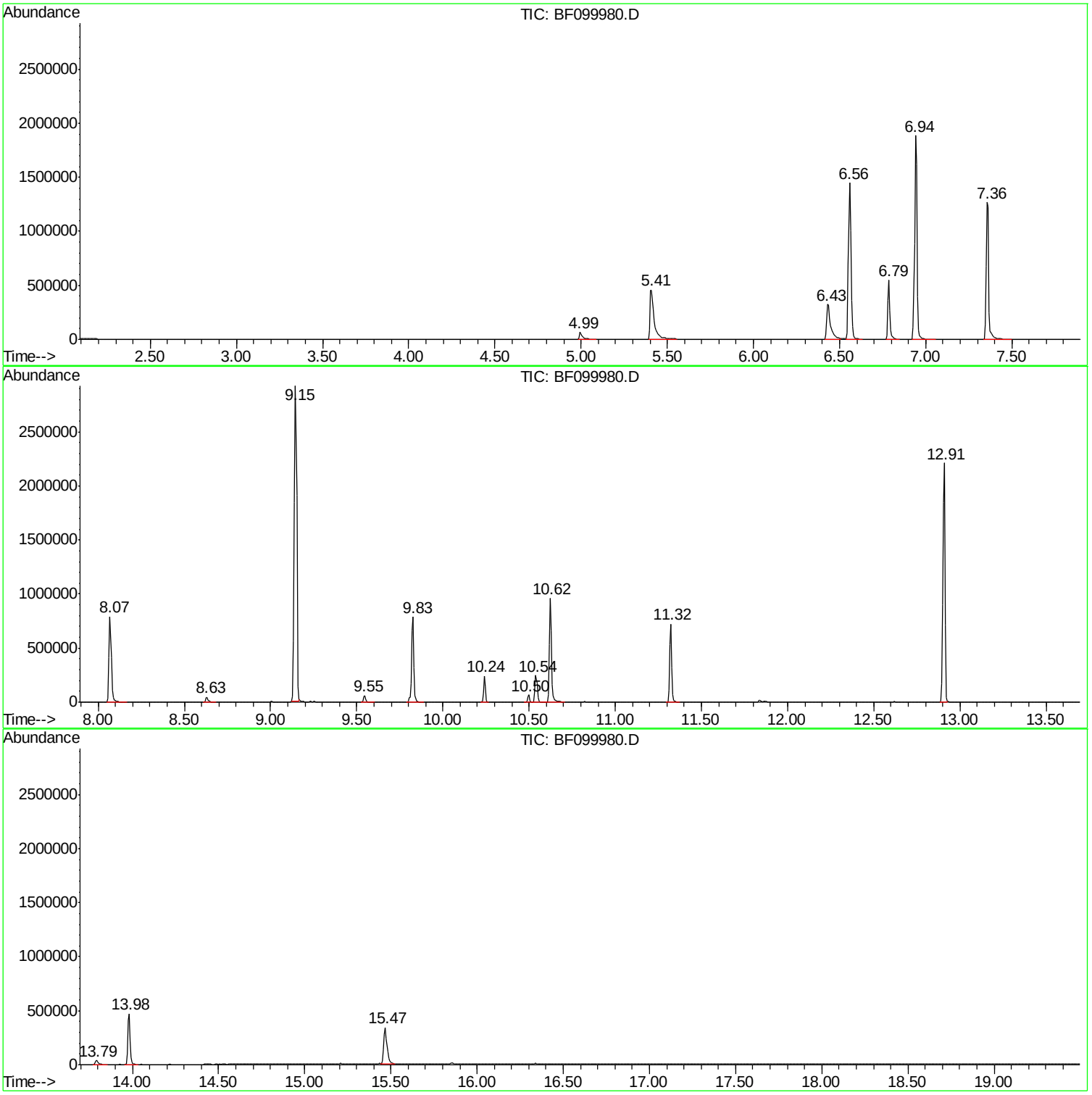
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF103017\
Data File : BF099980.D
Acq On : 31 Oct 2017 1:11
Operator : SJ/JU
Sample : I6083-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102017-TIFR-F-D-M

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 : BF099980.D
Acq On : 31 Oct 2017 1:11
Operator : SJ/JU
Sample : I6083-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
102017-TIFR-F-D-M

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

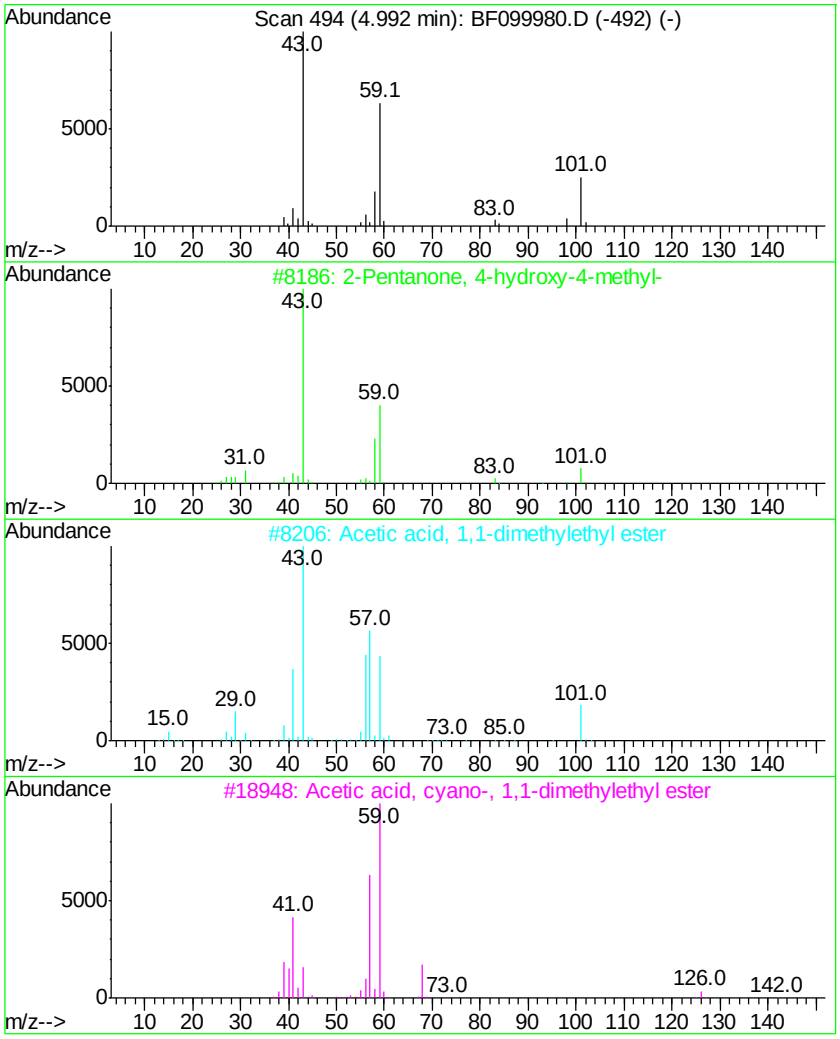
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

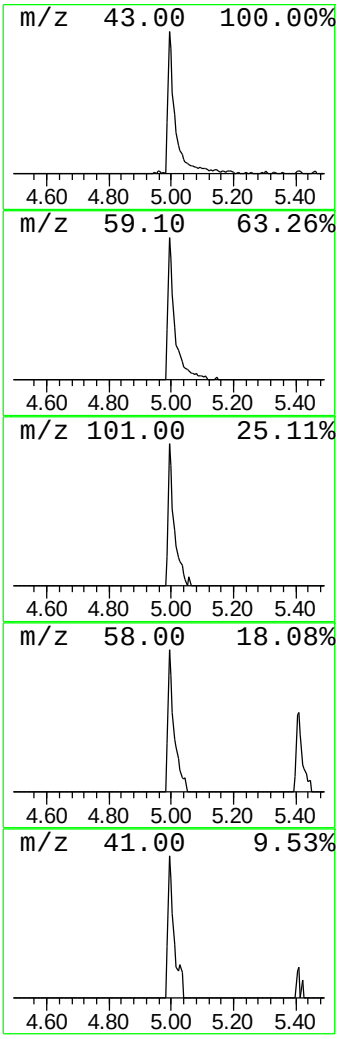
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	4.07 ng	98379	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	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Acetone	58	C3H6O	000067-64-1	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF103017\
Data File : BF099980.D
Acq On : 31 Oct 2017 1:11
Operator : SJ/JU
Sample : I6083-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102017-TIFR-F-D-M

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

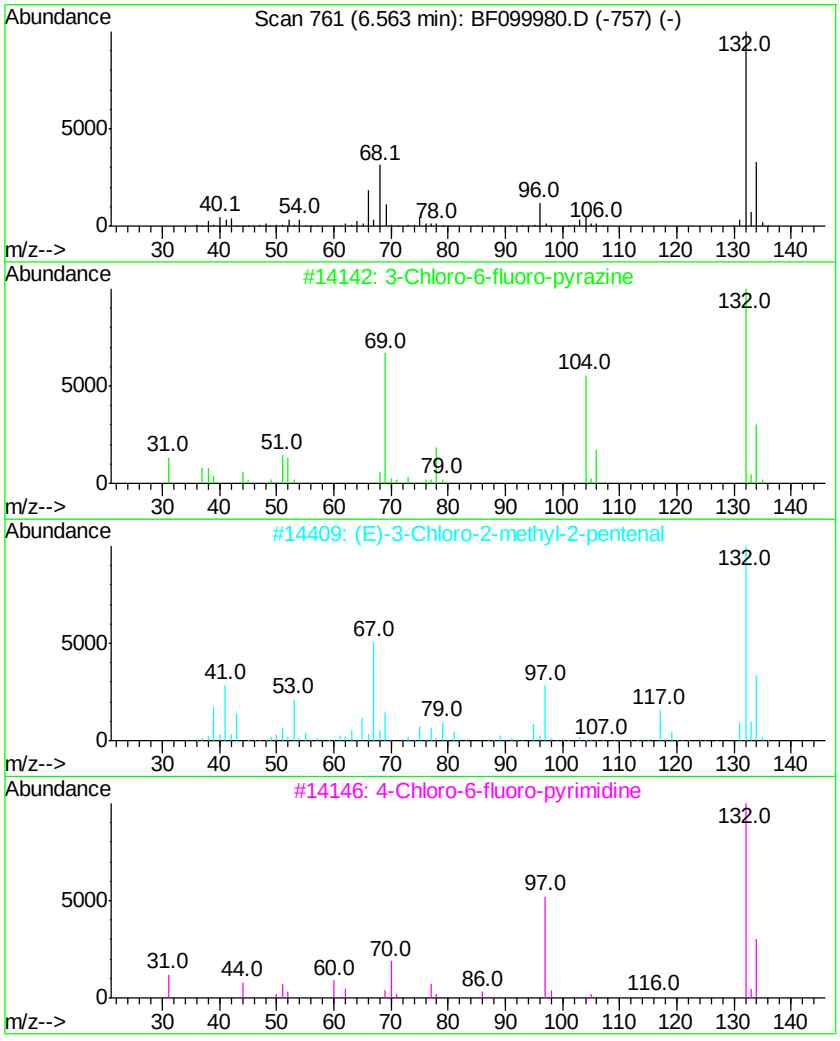
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

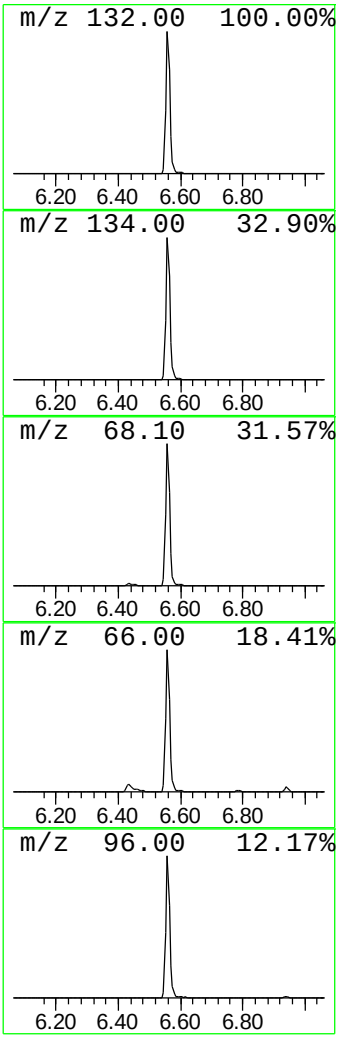
****

Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	54.22 ng	1311370	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF103017\
Data File : BF099980.D
Acq On : 31 Oct 2017 1:11
Operator : SJ/JU
Sample : I6083-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102017-TIFR-F-D-M

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

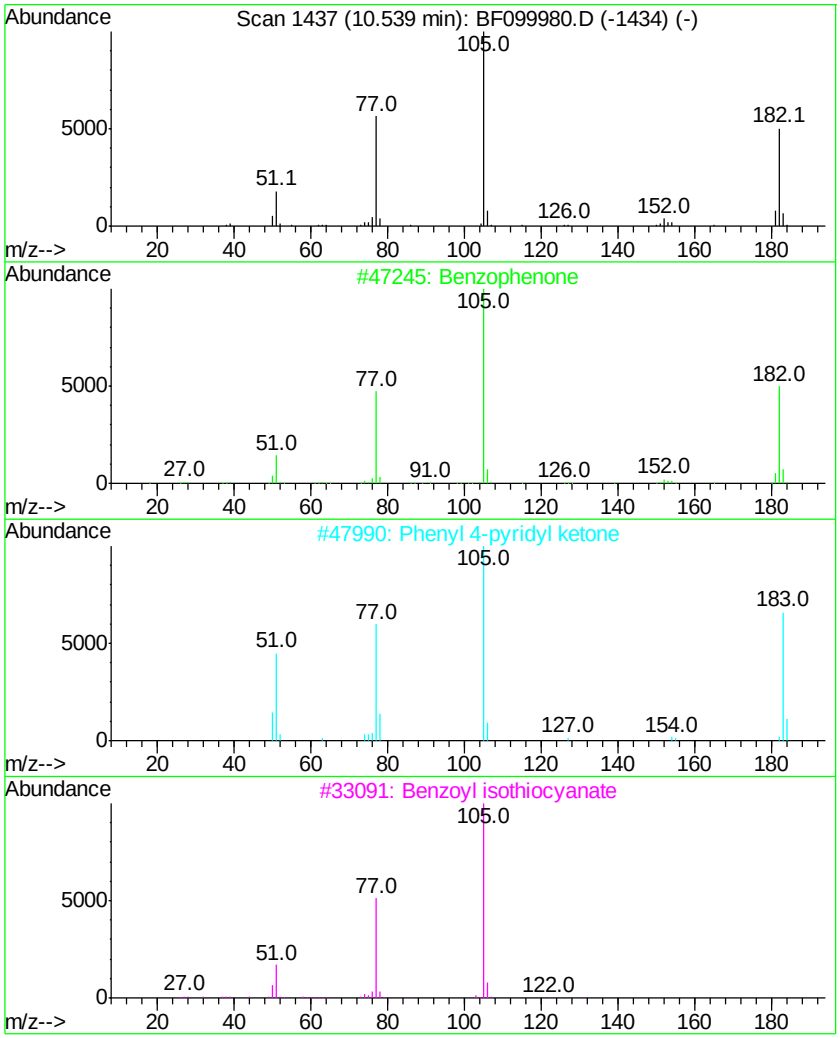
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

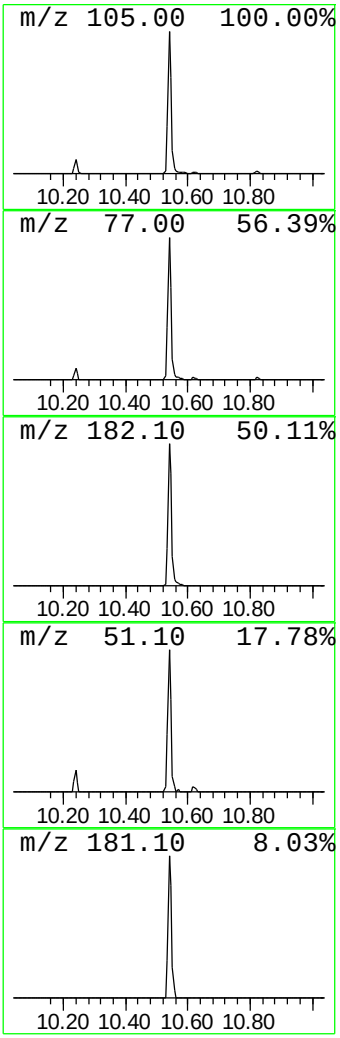
****

Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.54	5.30 ng	199032	Acenaphthene-d10	9.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	47
3	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	46
4	5-[N-Benzoylaminomethyl]tetrazole	203	C9H9N5O	1000227-36-3	43
5	Cyclobutyl phenyl ketone	160	C11H12O	005407-98-7	43





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF103017\
Data File : BF099980.D
Acq On : 31 Oct 2017 1:11
Operator : SJ/JU
Sample : I6083-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102017-TIFR-F-D-M

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

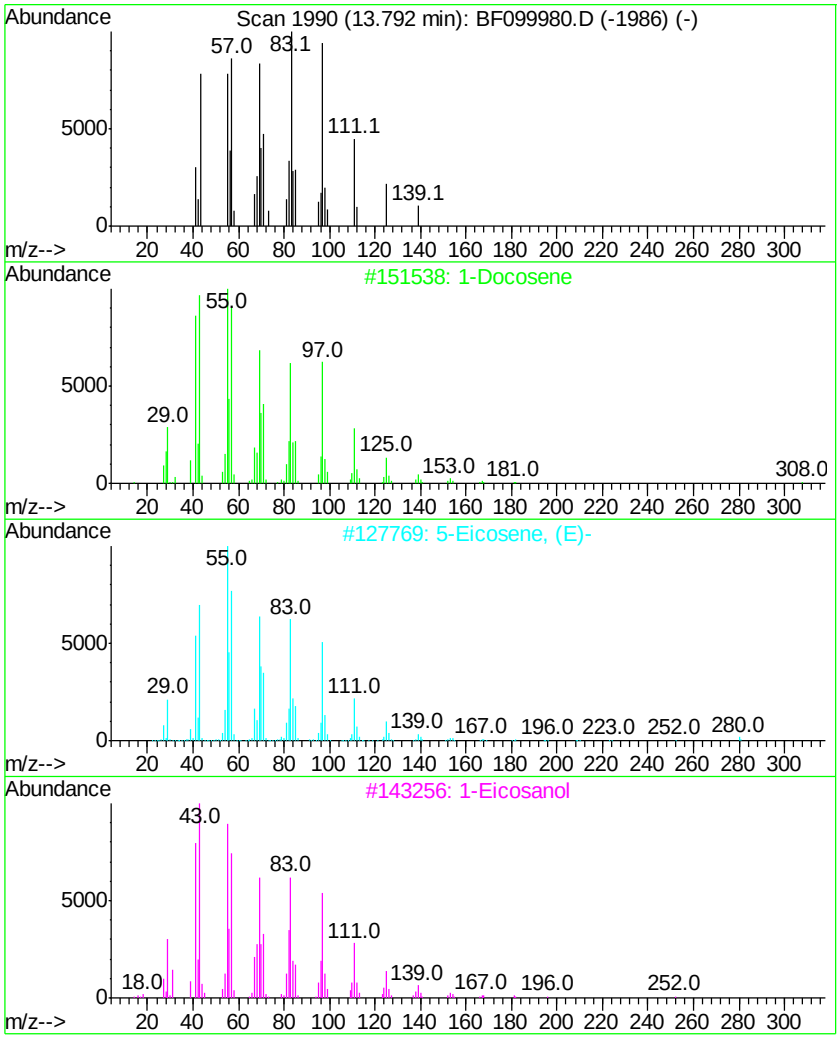
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

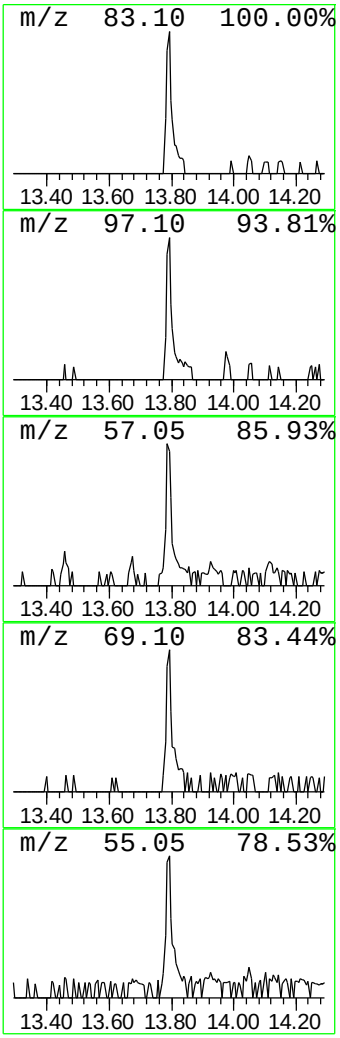
****

Peak Number 5 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	2.17 ng	50424	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	81
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	74
3	1-Eicosanol	298	C20H42O	000629-96-9	64
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	59
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103017\
Data File : BF099980.D
Acq On : 31 Oct 2017 1:11
Operator : SJ/JU
Sample : I6083-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102017-TIFR-F-D-M

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.99	4.1	ng	98379	1	6.79	483758	20.0
unknown6.56	6.56	54.2	ng	1311370	1	6.79	483758	20.0
Benzophenone	10.54	5.3	ng	199032	3	9.83	750566	20.0
1-Docosene	13.79	2.2	ng	50424	5	13.98	464296	20.0