LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF020617\
Data File : BF092805.D
Acq On : 6 Feb 2017 19:37
Operator : SJ/MA
Sample : I1692-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-15-40-COMP

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-BF013017.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	3.310	106	107	122	rBV	41671	160679	3.23%	0.388%
2	5.104	261	264	274	rBV	1200378	1752141	35.27%	4.235%
3	5.527	298	301	304	rBV	3714414	3937466	79.25%	9.516%
4	5.847	328	329	332	rBV	60330	61879	1.25%	0.150%
5	6.556	388	391	393	rBV	3813822	4275170	86.05%	10.333%
6	6.682	399	402	405	rBV	3875422	3940261	79.31%	9.523%
7	6.910	419	422	424	rBV	1041513	851654	17.14%	2.058%
8	7.070	433	436	438	rBV	3422773	3371887	67.87%	8.149%
9	7.482	468	472	474	rBV	2112996	2873424	57.84%	6.945%
10	8.190	532	534	537	rBV	947637	1072643	21.59%	2.592%
11	9.276	625	629	631	rBV	4340128	4968155	100.00%	12.007%
12	9.665	660	663	666	rBV	1215672	1069453	21.53%	2.585%
13	9.870	677	681	685	rBV2	39764	77425	1.56%	0.187%
14	9.950	685	688	690	rVB	1548592	1356757	27.31%	3.279%
15	10.373	722	725	727	rVB2	32653	54352	1.09%	0.131%
16	10.739	754	757	760	rBV	2248877	2670880	53.76%	6.455%
17	10.853	764	767	772	rVB	75194	109799	2.21%	0.265%
18	11.299	804	806	807	rBV	91172	79831	1.61%	0.193%
19	11.436	815	818	820	rBV	1577418	1393010	28.04%	3.367%
20	11.722	841	843	846	rVB	59064	55795	1.12%	0.135%
21	12.648	921	924	926	rBV	60281	53961	1.09%	0.130%
22	12.876	942	944	946	rBV	62338	54746	1.10%	0.132%
23	13.025	954	957	960	rBV	3832037	4415866	88.88%	10.673%
24	13.917	1033	1035	1042	rBV	81733	138208	2.78%	0.334%
25	14.077	1046	1049	1051	rBV	1438338	1415937	28.50%	3.422%
26	15.105	1136	1139	1143	rBV	26199	53320	1.07%	0.129%
27	15.528	1173	1176	1182	rBV	834165	1111037	22.36%	2.685%

Sum of corrected areas: 41375736

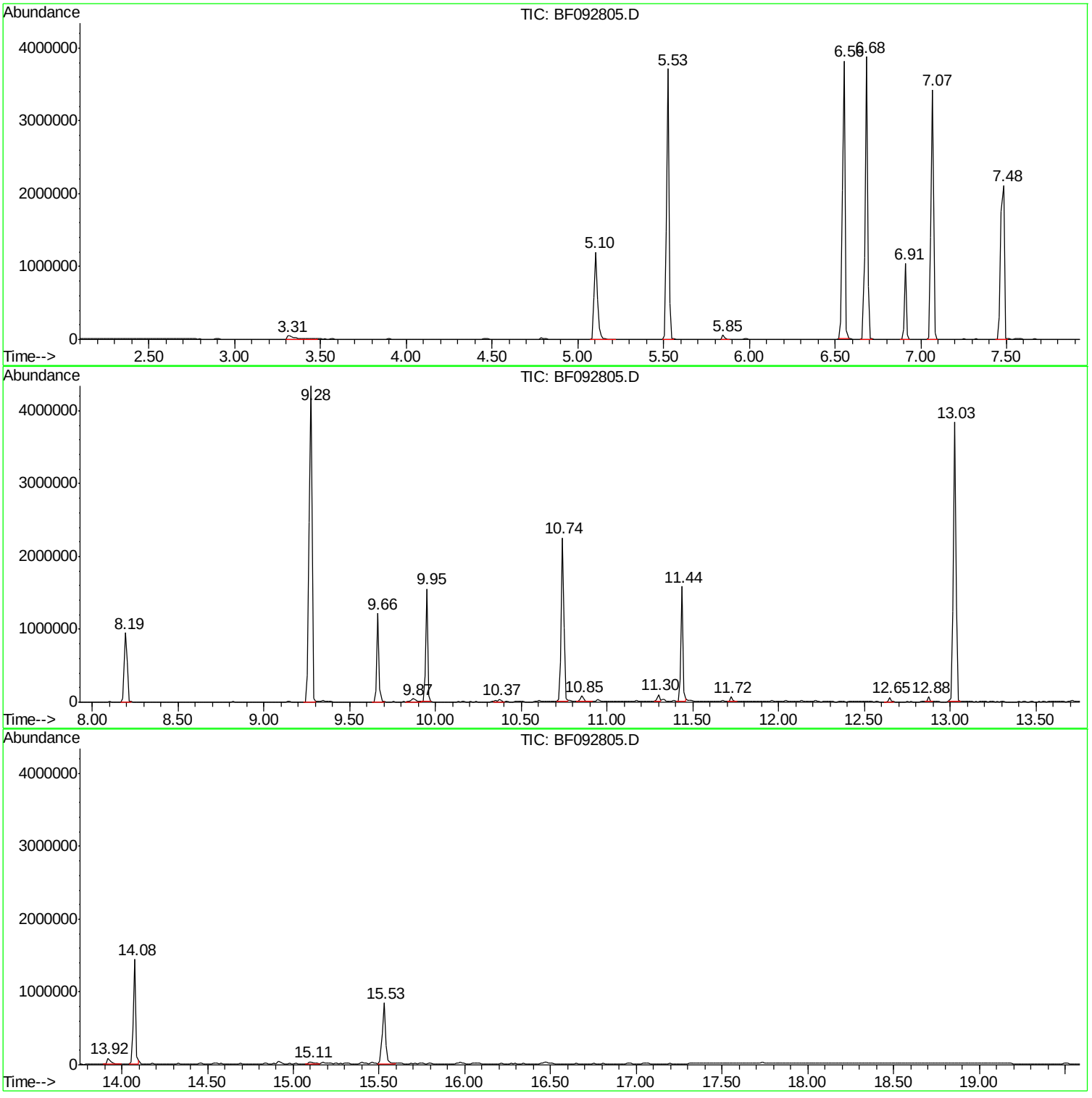
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\Data\BF020617\
Data File : BF092805.D
Acq On : 6 Feb 2017 19:37
Operator : SJ/MA
Sample : I1692-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-15-40-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\Data\BF020617\
Data File : BF092805.D
Acq On : 6 Feb 2017 19:37
Operator : SJ/MA
Sample : I1692-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-15-40-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

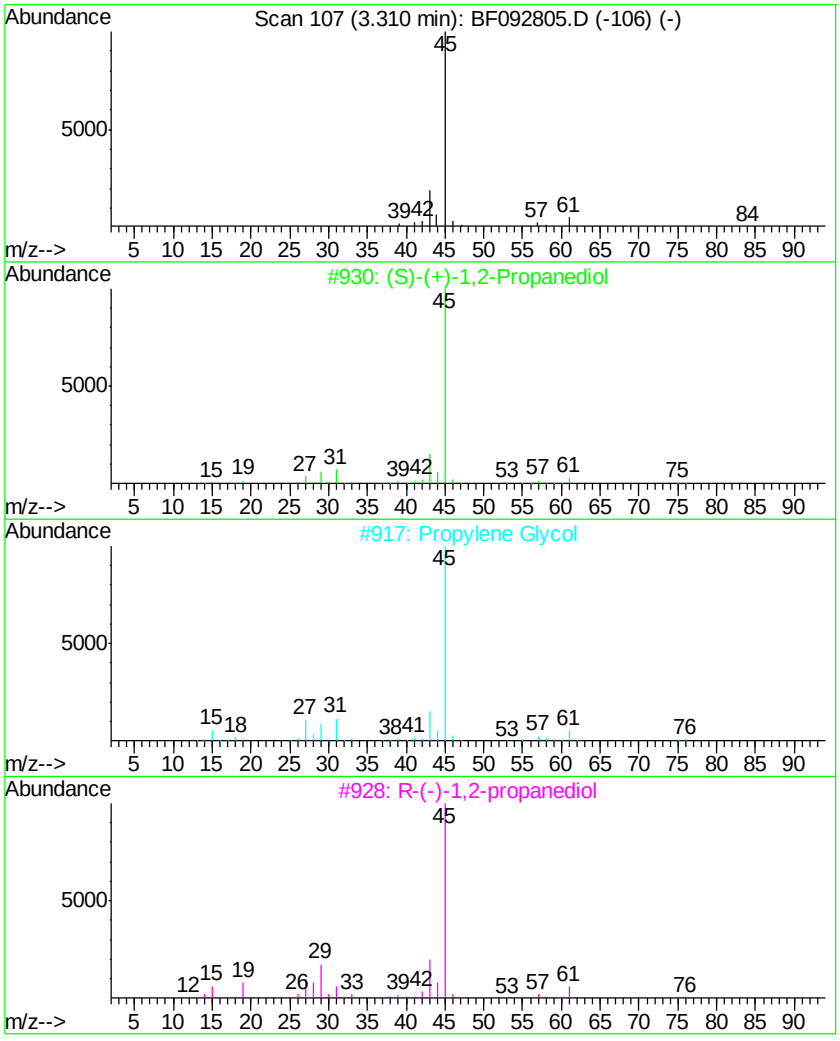
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

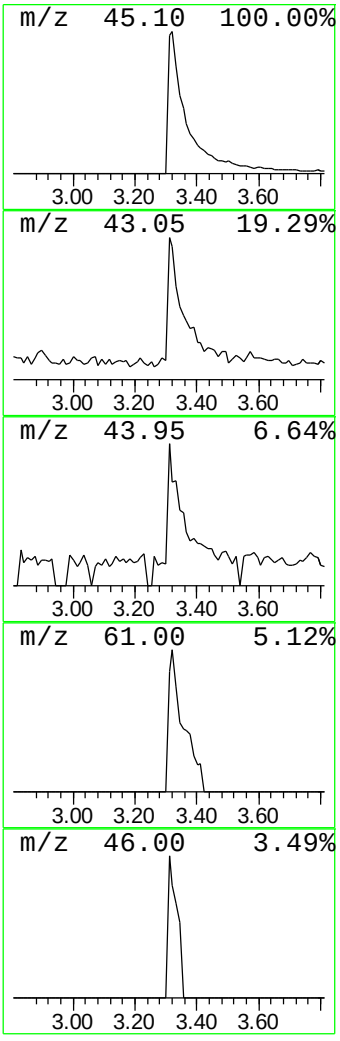
****

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.31	3.77 ng	160679	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	Propylene Glycol	76	C3H8O2	000057-55-6	64
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
4	Ethanol, 2,2'-oxybis-	106	C4H10O3	000111-46-6	9
5	Muramic acid	251	C9H17NO7	001114-41-6	9





Data Path : Z:\HPCHEM1\BNA F\Data\BF020617\
Data File : BF092805.D
Acq On : 6 Feb 2017 19:37
Operator : SJ/MA
Sample : I1692-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-15-40-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

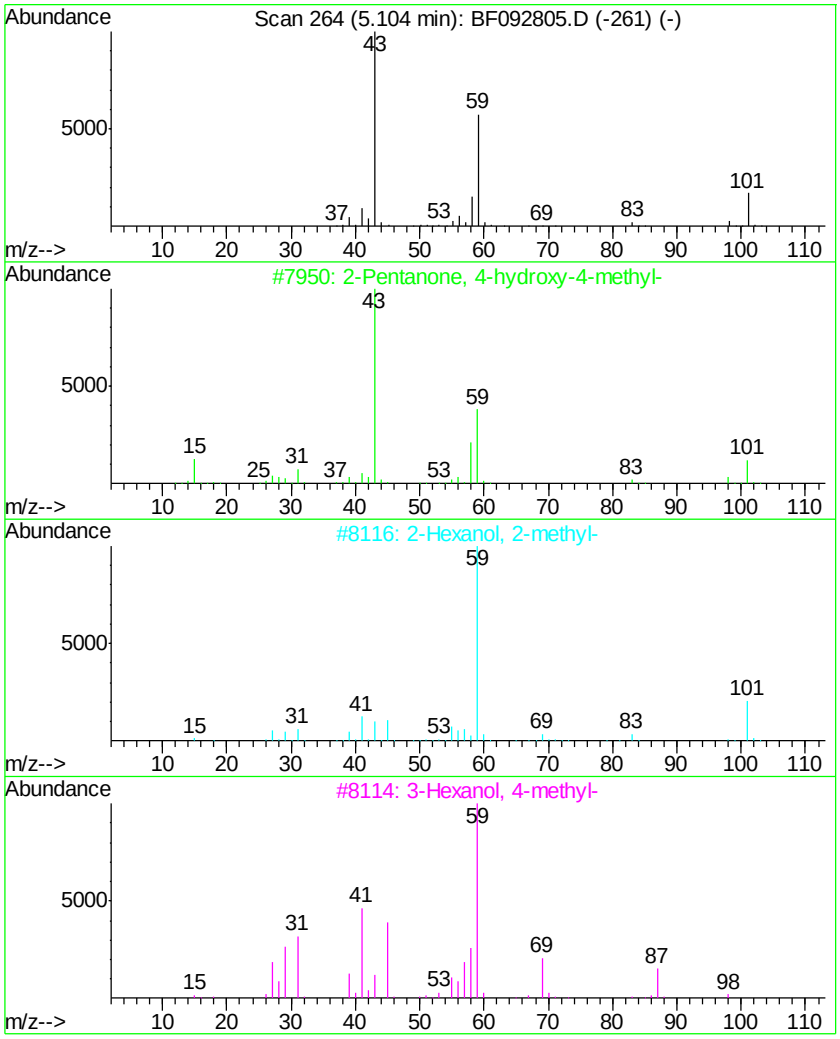
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

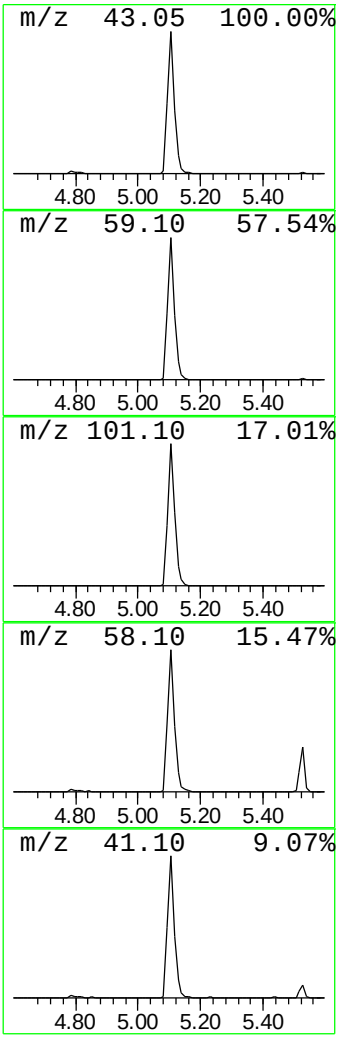
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	41.15 ng	1752140	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





Data Path : Z:\HPCHEM1\BNA F\Data\BF020617\
Data File : BF092805.D
Acq On : 6 Feb 2017 19:37
Operator : SJ/MA
Sample : I1692-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-15-40-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

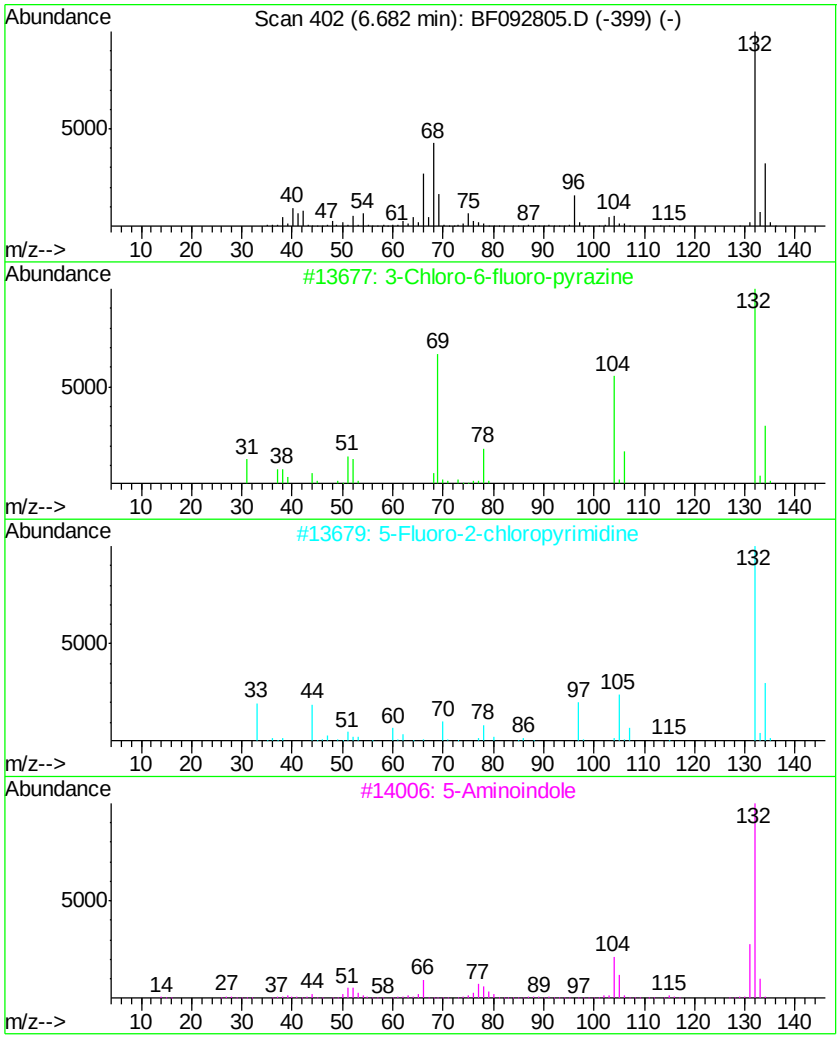
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

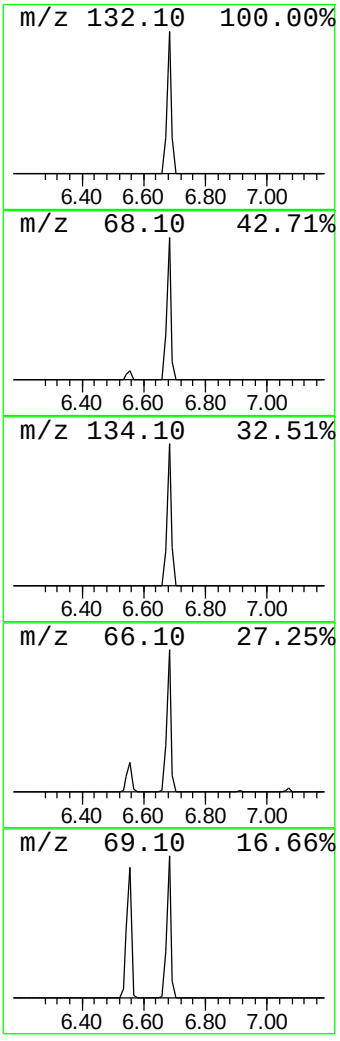
****

Peak Number 3 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	92.53 ng	3940260	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
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





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\Data\BF020617\
Data File : BF092805.D
Acq On : 6 Feb 2017 19:37
Operator : SJ/MA
Sample : I1692-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-15-40-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(S)-(+)-1,2-Propa...	3.31	3.8	ng	160679	1	6.91	851654	20.0
2-Pentanone, 4-hy...	5.10	41.1	ng	1752140	1	6.91	851654	20.0
unknown6.68	6.68	92.5	ng	3940260	1	6.91	851654	20.0