LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090434.D
Acq On : 6 Oct 2016 22:37
Operator : UM/SJ
Sample : H5121-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1

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-BF100516.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	3.457	96	98	112	rBV2	106179	232700	2.82%	0.367%
2	5.205	248	251	256	rBV	1277613	1802893	21.84%	2.840%
3	5.606	283	286	289	rBV	5790822	6284722	76.15%	9.899%
4	6.577	368	371	372	rBV	69594	104364	1.26%	0.164%
5	6.623	372	375	377	rVB	6148739	7125106	86.33%	11.223%
6	6.760	384	387	390	rBV	5644720	6536986	79.20%	10.296%
7	6.989	405	407	410	rBV	1063163	1306042	15.82%	2.057%
8	7.149	419	421	424	rVB	4553427	4927714	59.70%	7.762%
9	7.560	453	457	459	rBV	4147503	4749418	57.54%	7.481%
10	8.280	517	520	522	rBV	2148544	1844912	22.35%	2.906%
11	9.366	611	615	617	rBV	8153614	8253590	100.00%	13.000%
12	9.754	646	649	651	rBV	2022766	1690947	20.49%	2.663%
13	10.040	672	674	676	rVB	2123589	1961996	23.77%	3.090%
14	10.840	740	744	746	rBV2	3098402	4580511	55.50%	7.215%
15	10.943	751	753	758	rVB	67684	125584	1.52%	0.198%
16	11.400	791	793	794	rBV	113054	100815	1.22%	0.159%
17	11.538	802	805	807	rBV	1547245	1873438	22.70%	2.951%
18	12.052	848	850	860	rBV	344509	463199	5.61%	0.730%
19	12.841	917	919	925	rBV	161802	221962	2.69%	0.350%
20	13.126	941	944	946	rBV	7208352	6506489	78.83%	10.248%
21	14.018	1020	1022	1029	rBV	366631	430767	5.22%	0.678%
22	14.178	1034	1036	1039	rVV	1365485	1222190	14.81%	1.925%
23	15.675	1164	1167	1170	rBV	764165	1142834	13.85%	1.800%

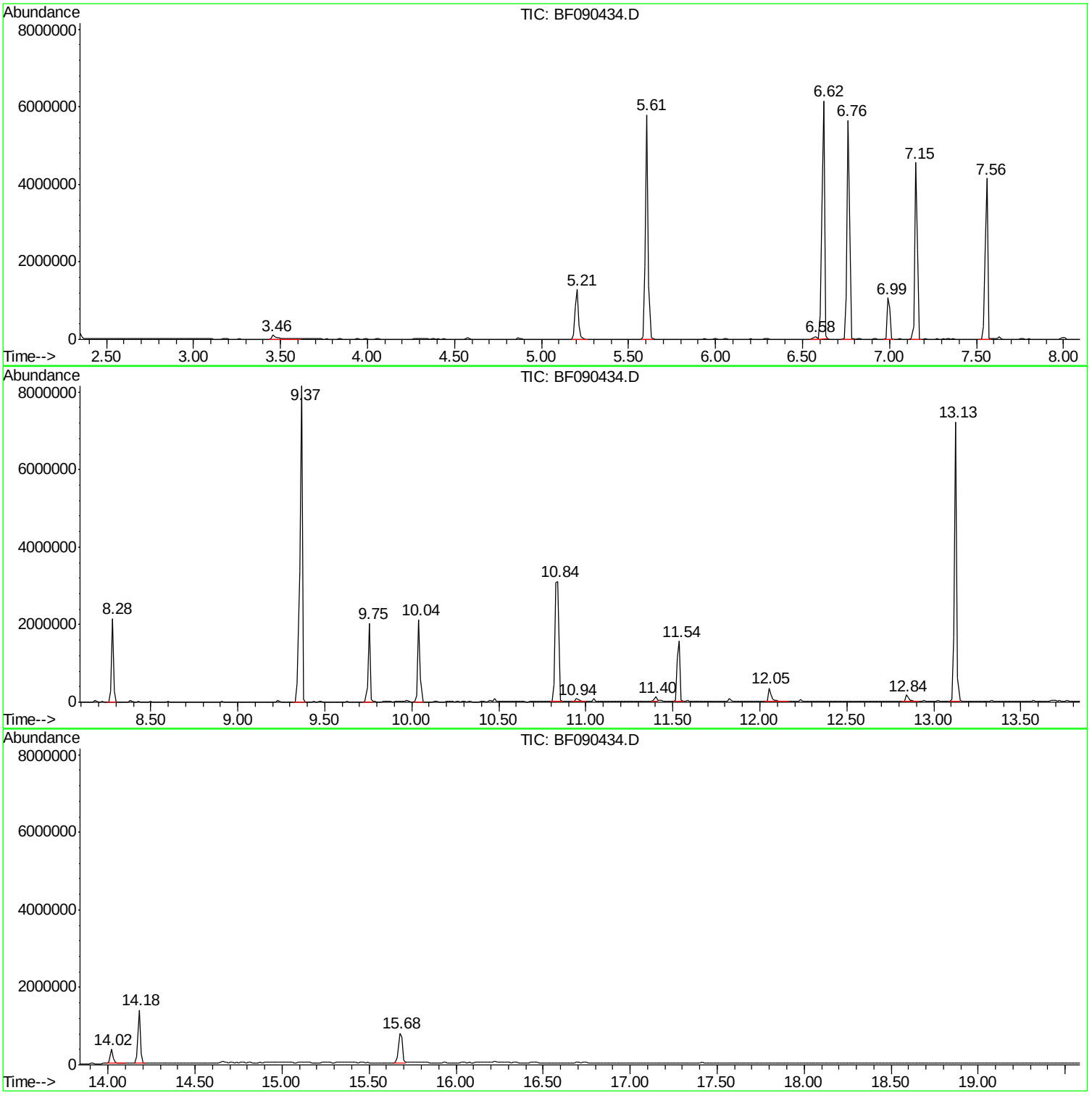
Sum of corrected areas: 63489179

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090434.D
Acq On : 6 Oct 2016 22:37
Operator : UM/SJ
Sample : H5121-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090434.D
Acq On : 6 Oct 2016 22:37
Operator : UM/SJ
Sample : H5121-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

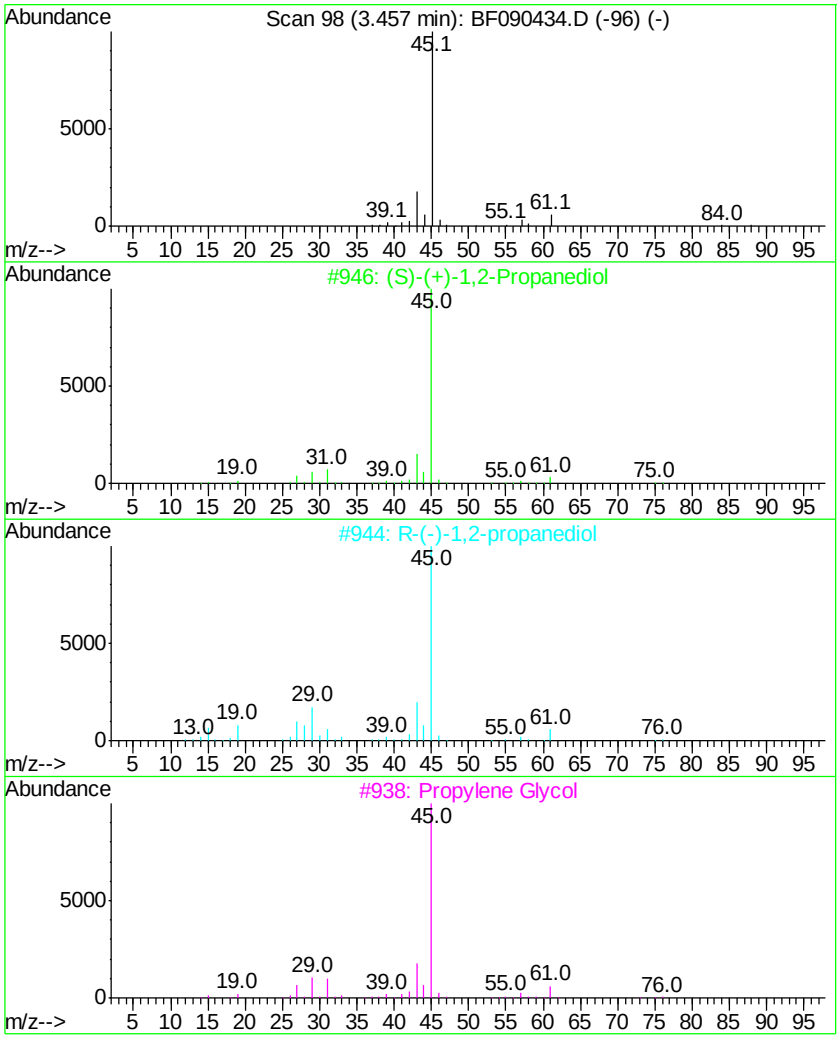
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

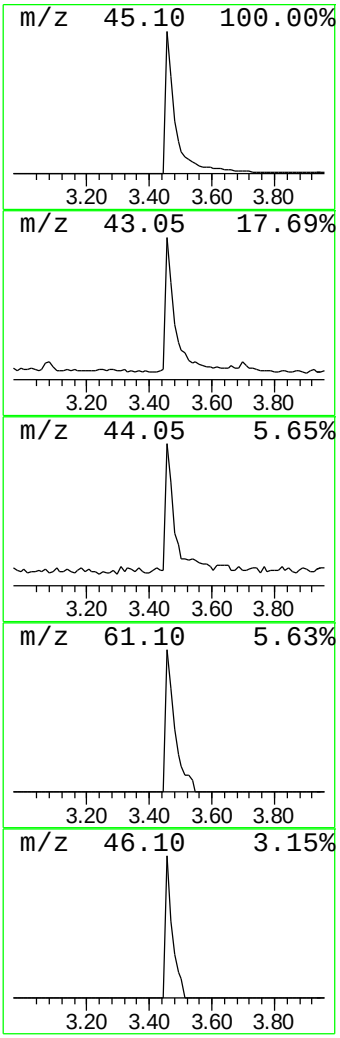
****

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.46	3.56 ng	232700	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	Propylene Glycol	76	C3H8O2	000057-55-6	43
4	2-Butanol, 3-methyl-, (S)-	88	C5H12O	001517-66-4	9
5	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090434.D
Acq On : 6 Oct 2016 22:37
Operator : UM/SJ
Sample : H5121-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

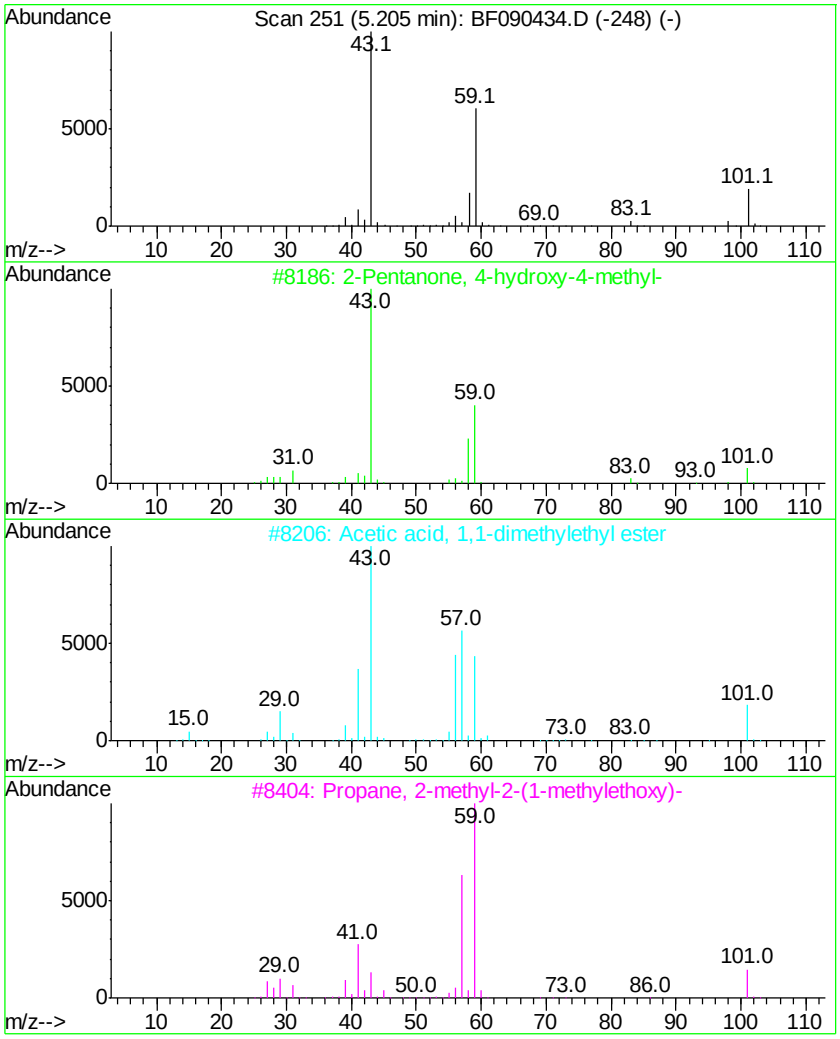
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

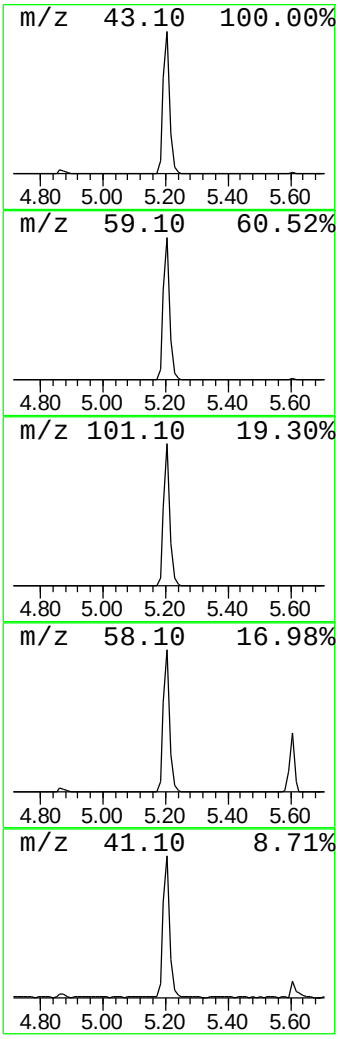
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	27.61 ng	1802890	1,4-Dichlorobenzene-d4	7.00

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	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090434.D
Acq On : 6 Oct 2016 22:37
Operator : UM/SJ
Sample : H5121-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

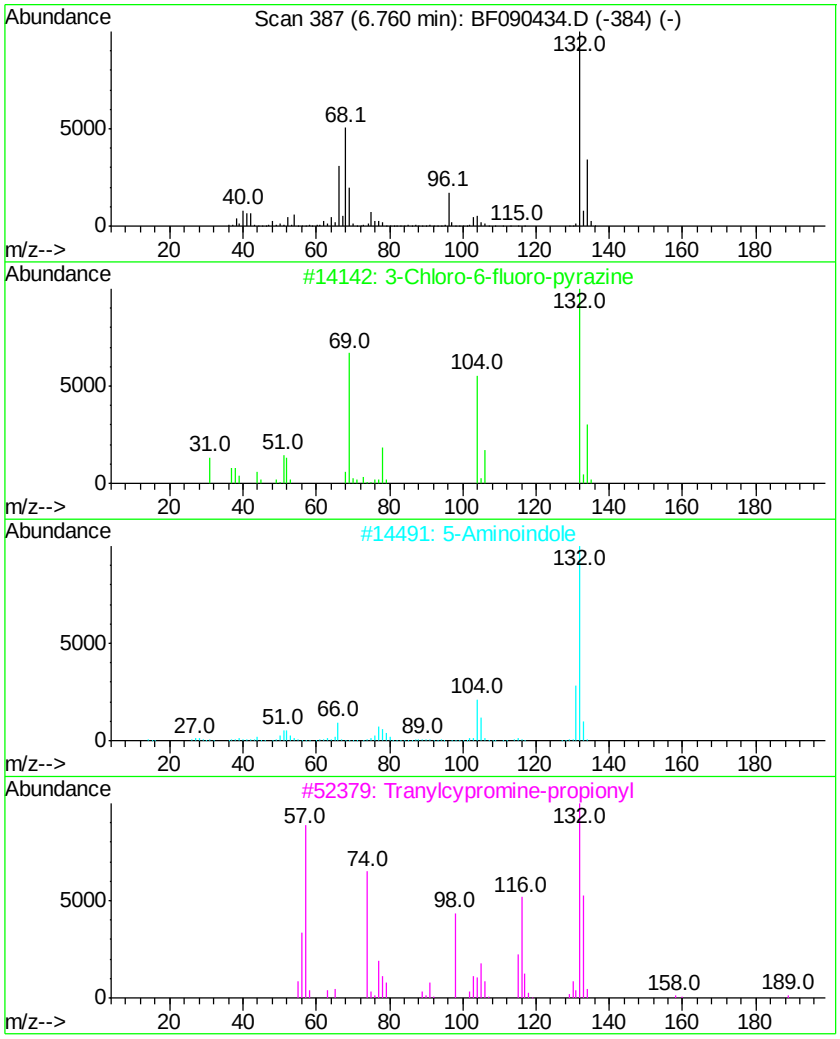
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

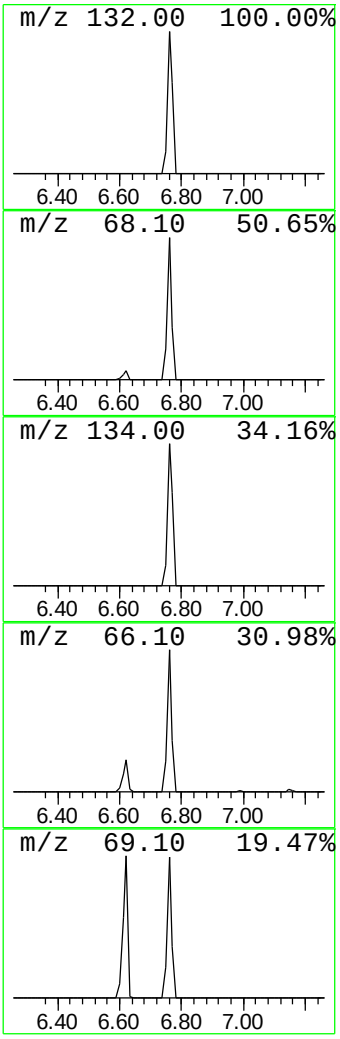
****

Peak Number 3 unknown6.76 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	100.10 ng	6536990	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090434.D
Acq On : 6 Oct 2016 22:37
Operator : UM/SJ
Sample : H5121-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

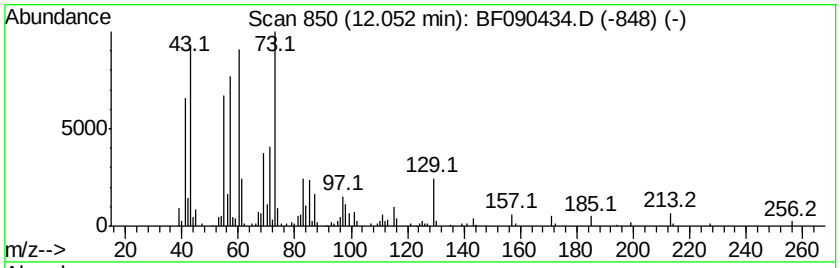
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

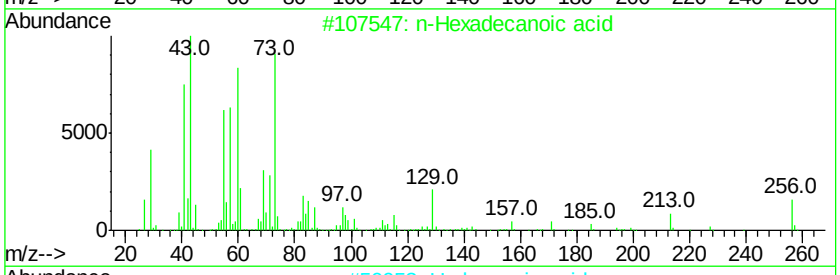
****

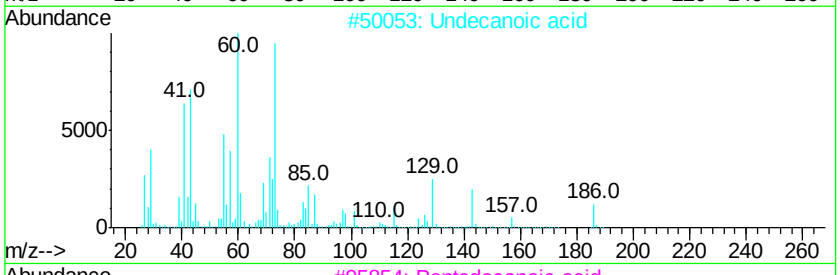
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

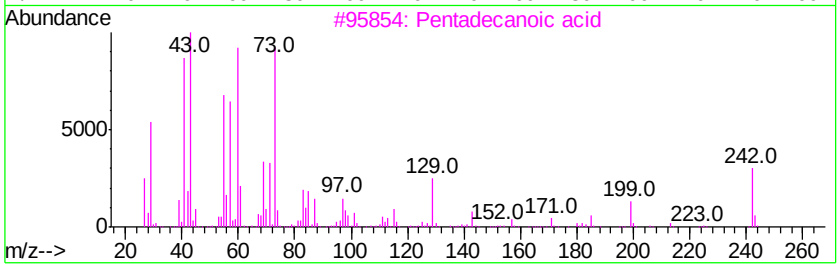
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	4.94 ng	463199	Phenanthrene-d10	11.54

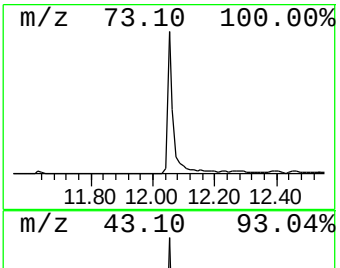
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Undecanoic acid	186	C11H22O2	000112-37-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	30

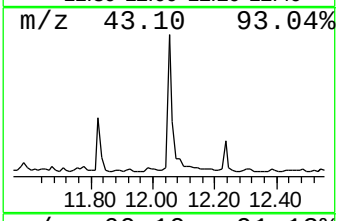


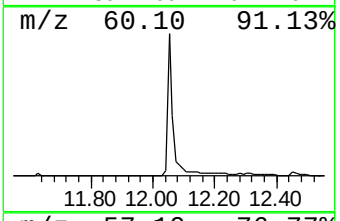


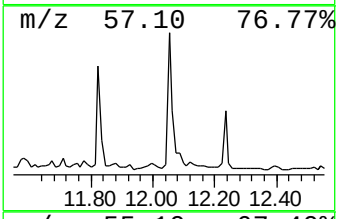


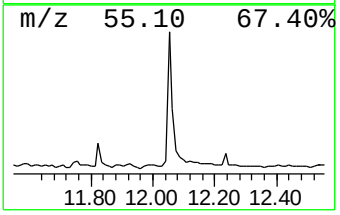












Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090434.D
Acq On : 6 Oct 2016 22:37
Operator : UM/SJ
Sample : H5121-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

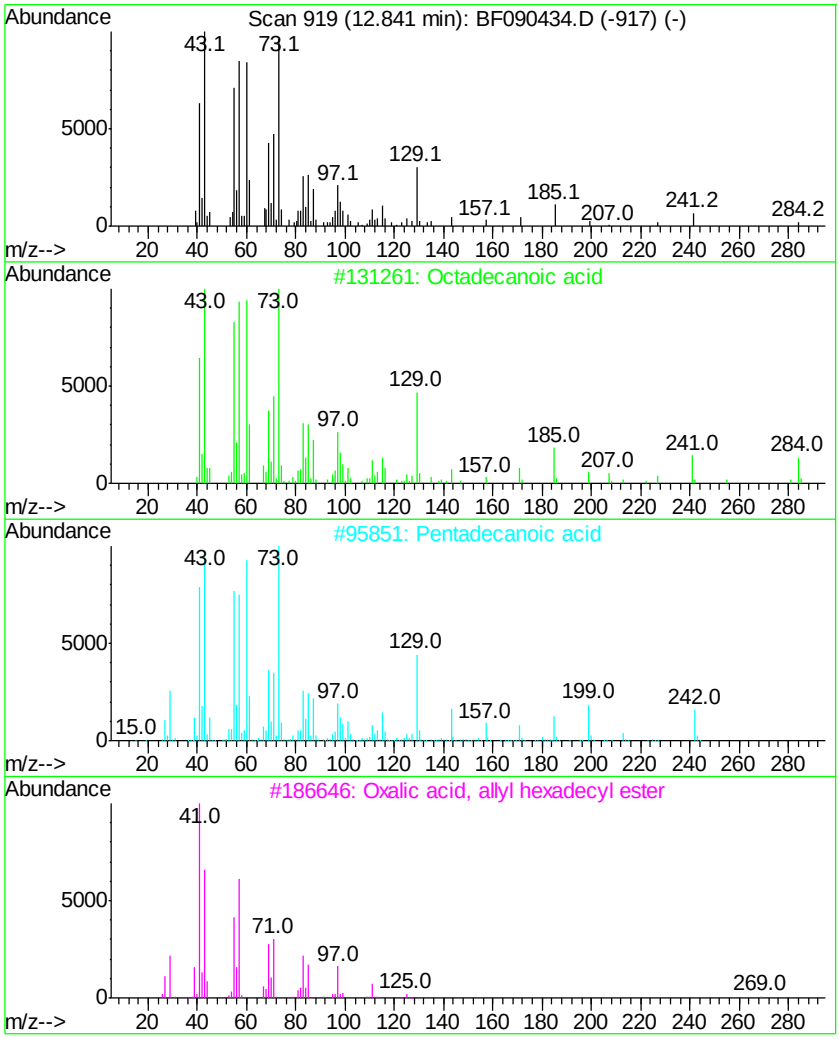
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

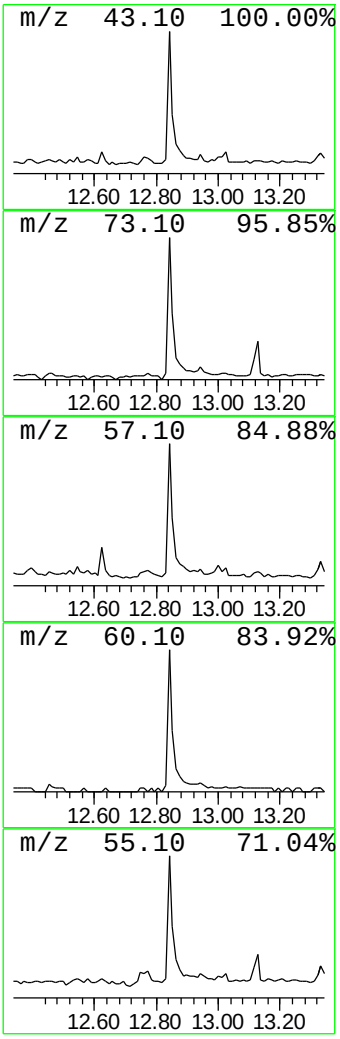
****

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	2.37 ng	221962	Phenanthrene-d10	11.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20
4	Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	18
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090434.D
Acq On : 6 Oct 2016 22:37
Operator : UM/SJ
Sample : H5121-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

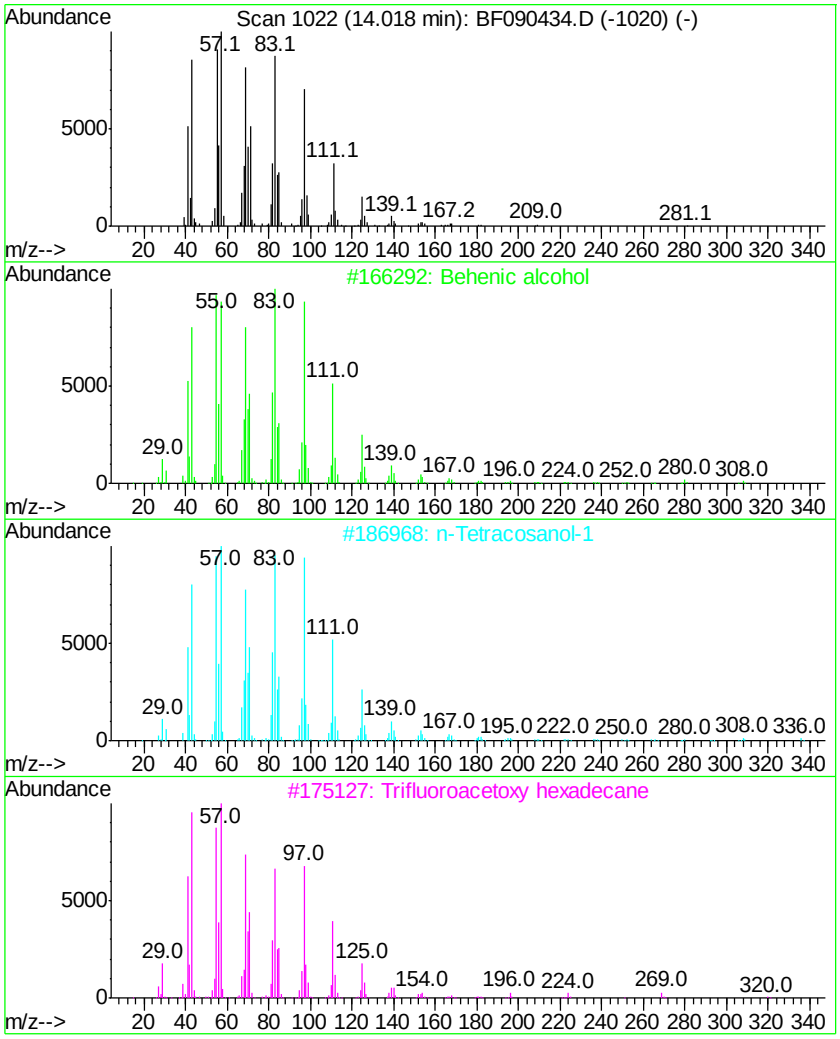
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

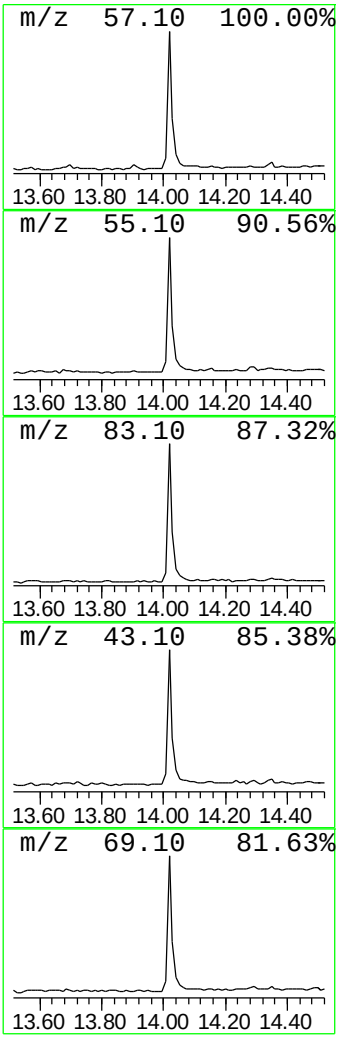
****

Peak Number 7 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.02	7.05 ng	430767	Chrysene-d12	14.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100616\
Data File : BF090434.D
Acq On : 6 Oct 2016 22:37
Operator : UM/SJ
Sample : H5121-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.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
(S)-(+)-1,2-Propa...	3.46	3.6	ng	232700	1	7.00	1306040	20.0
2-Pentanone, 4-hy...	5.21	27.6	ng	1802890	1	7.00	1306040	20.0
unknown6.76	6.76	100.1	ng	6536990	1	7.00	1306040	20.0
n-Hexadecanoic acid	12.05	4.9	ng	463199	4	11.54	1873440	20.0
Octadecanoic acid	12.84	2.4	ng	221962	4	11.54	1873440	20.0
Behenic alcohol	14.02	7.0	ng	430767	5	14.18	1222190	20.0