LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085899.D
Acq On : 30 Mar 2016 21:18
Operator : UM/SJ
Sample : H2023-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

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-BF032416.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	4.984	234	236	244	rBV	76032	113961	3.65%	0.459%
2	5.396	269	272	275	rBV	2487746	2615569	83.86%	10.535%
3	6.436	361	363	366	rBV	2072498	2790808	89.48%	11.241%
4	6.562	372	374	377	rBV	2154048	2892091	92.73%	11.649%
5	6.802	392	395	397	rBV	476543	620651	19.90%	2.500%
6	6.950	406	408	411	rBV	2109738	2092464	67.09%	8.428%
7	7.362	441	444	447	rBV	1480013	1818474	58.30%	7.325%
8	8.082	505	507	510	rBV	974129	836843	26.83%	3.371%
9	9.168	599	602	604	rBV	2342042	3118944	100.00%	12.563%
10	9.556	634	636	638	rBV	570500	469079	15.04%	1.889%
11	9.773	652	655	657	rBV	119682	99859	3.20%	0.402%
12	9.842	658	661	663	rVB	683918	854250	27.39%	3.441%
13	10.002	672	675	679	rBV3	20017	45230	1.45%	0.182%
14	10.276	697	699	700	rVB	80568	109582	3.51%	0.441%
15	10.493	715	718	721	rBV	40019	71411	2.29%	0.288%
16	10.631	727	730	732	rBV	1720924	1790481	57.41%	7.212%
17	10.745	737	740	744	rVV	124115	150425	4.82%	0.606%
18	10.939	755	757	761	rVB2	15131	35175	1.13%	0.142%
19	11.191	777	779	780	rBV	57885	48290	1.55%	0.195%
20	11.316	788	790	793	rBV	796323	772169	24.76%	3.110%
21	12.905	926	929	931	rBV	2315060	2067484	66.29%	8.328%
22	13.808	1005	1008	1012	rBV	29605	56717	1.82%	0.228%
23	13.957	1018	1021	1023	rBV	665840	601661	19.29%	2.423%
24	14.700	1084	1086	1091	rBV	88520	104933	3.36%	0.423%
25	14.791	1091	1094	1096	rVV	31276	35057	1.12%	0.141%
26	15.374	1142	1145	1151	rBV	461066	614655	19.71%	2.476%

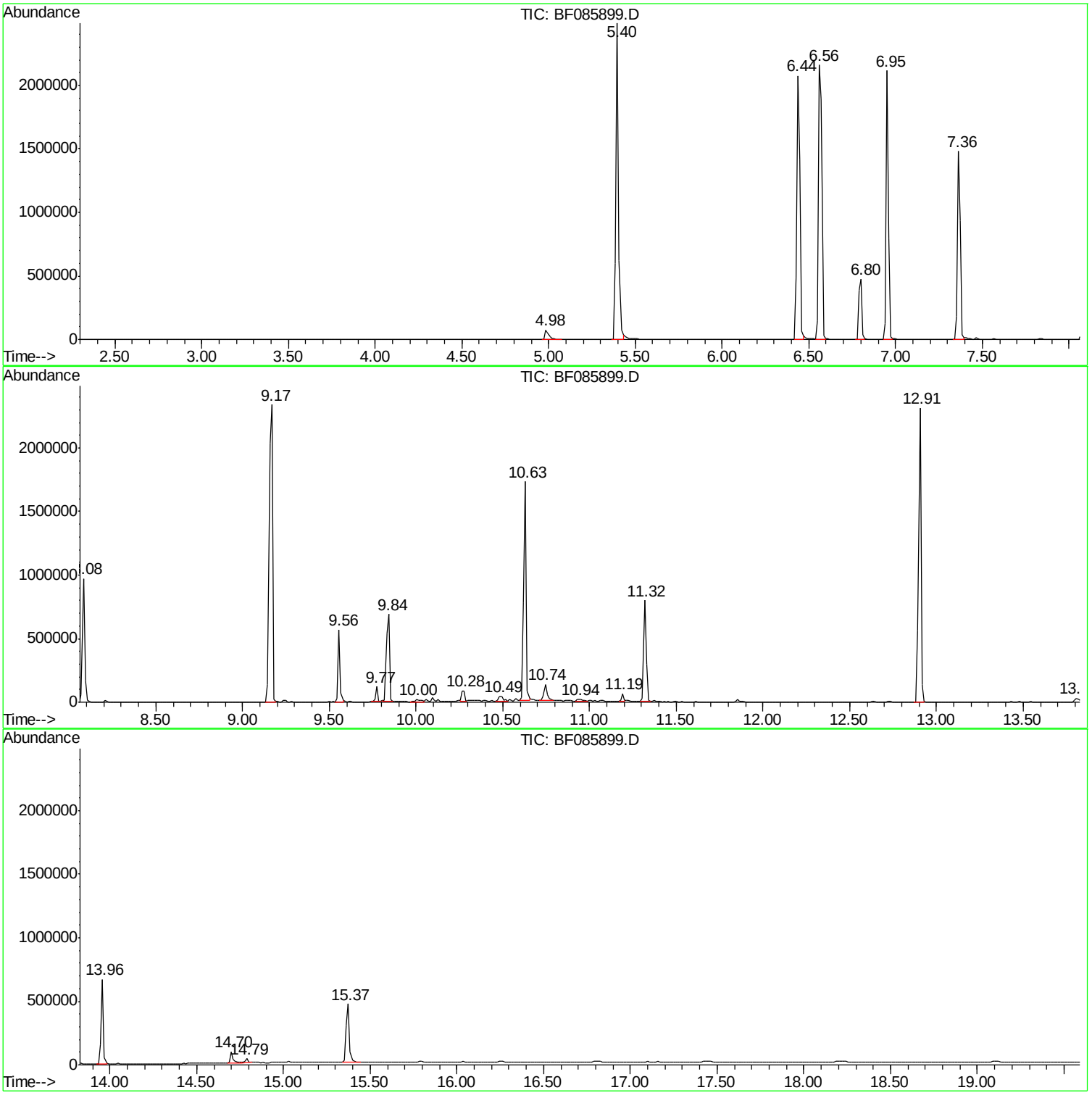
Sum of corrected areas: 24826263

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085899.D
Acq On : 30 Mar 2016 21:18
Operator : UM/SJ
Sample : H2023-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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\BF033016\
Data File : BF085899.D
Acq On : 30 Mar 2016 21:18
Operator : UM/SJ
Sample : H2023-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

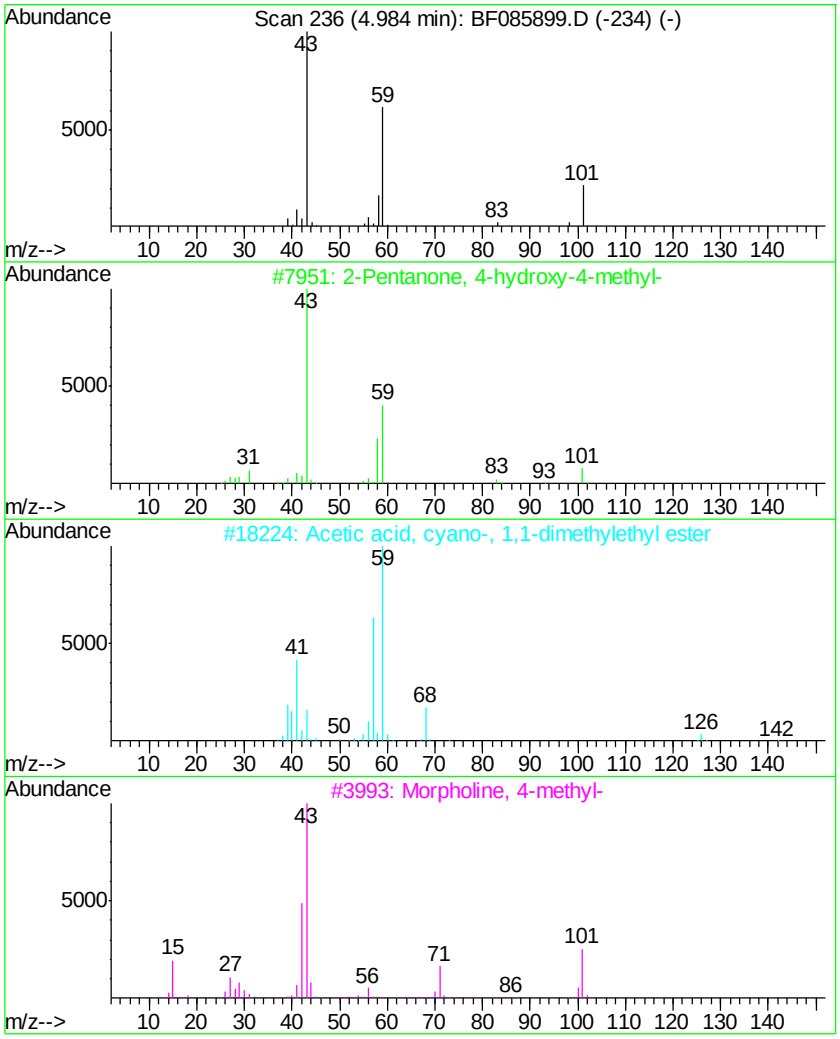
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

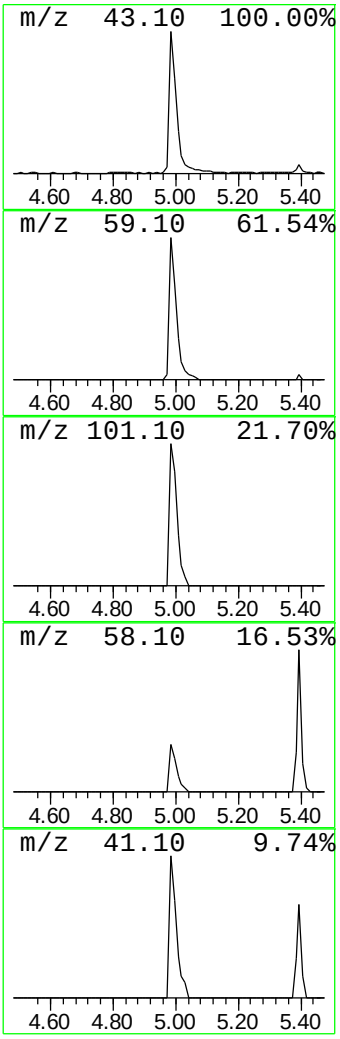
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	3.67 ng	113961	1,4-Dichlorobenzene-d4	6.80

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085899.D
Acq On : 30 Mar 2016 21:18
Operator : UM/SJ
Sample : H2023-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

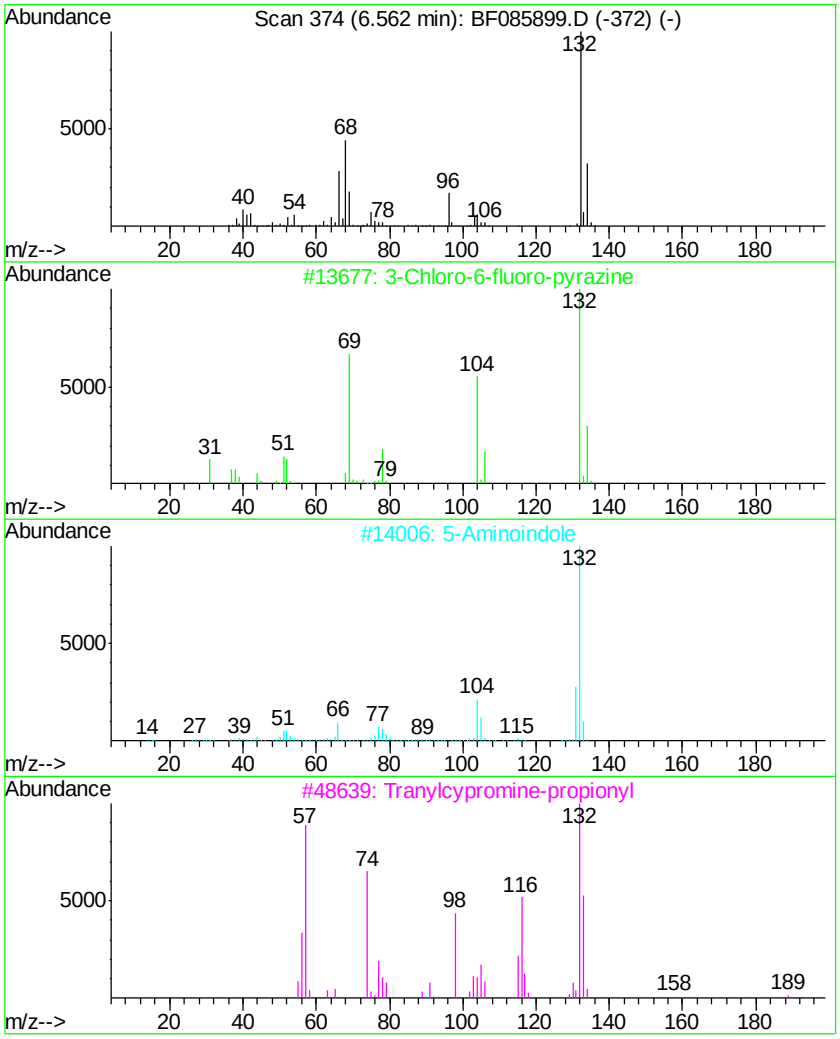
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

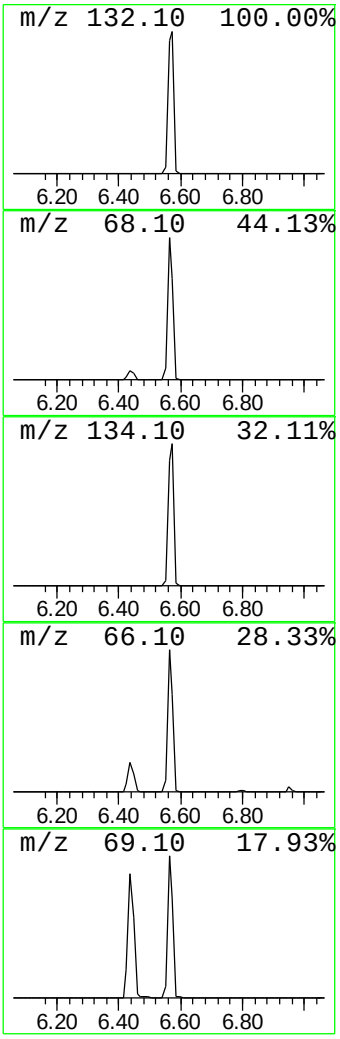
****

Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	93.20 ng	2892090	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085899.D
Acq On : 30 Mar 2016 21:18
Operator : UM/SJ
Sample : H2023-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

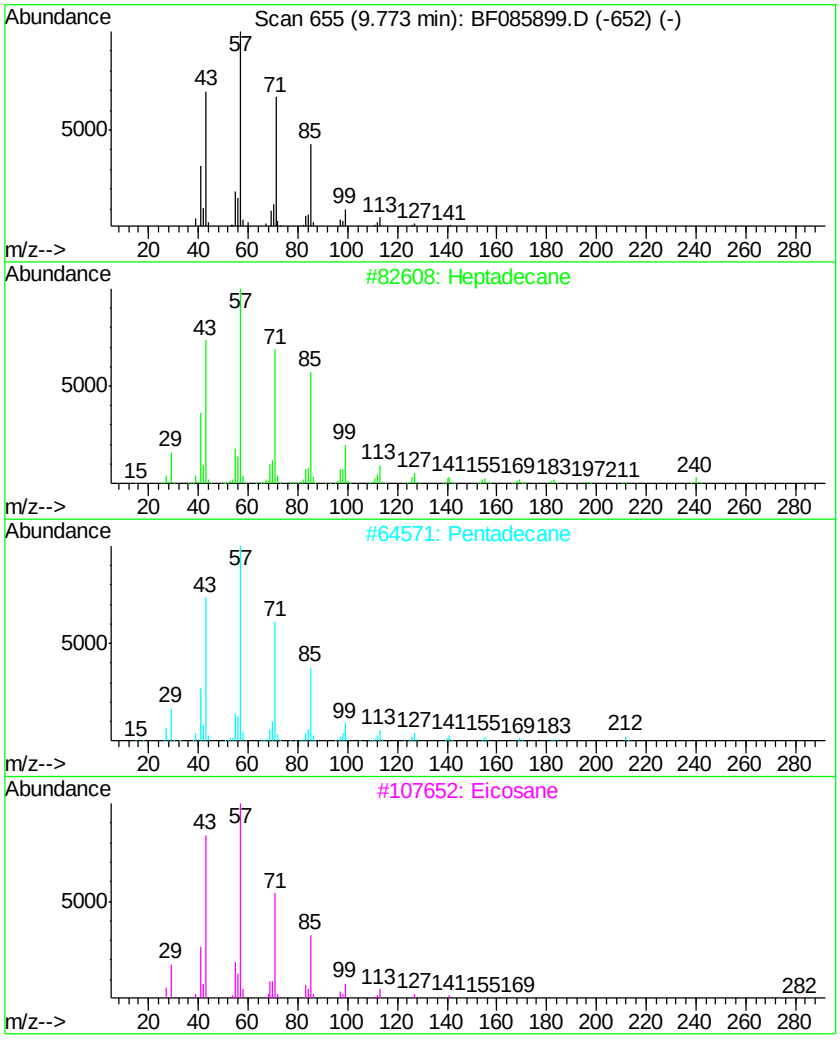
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

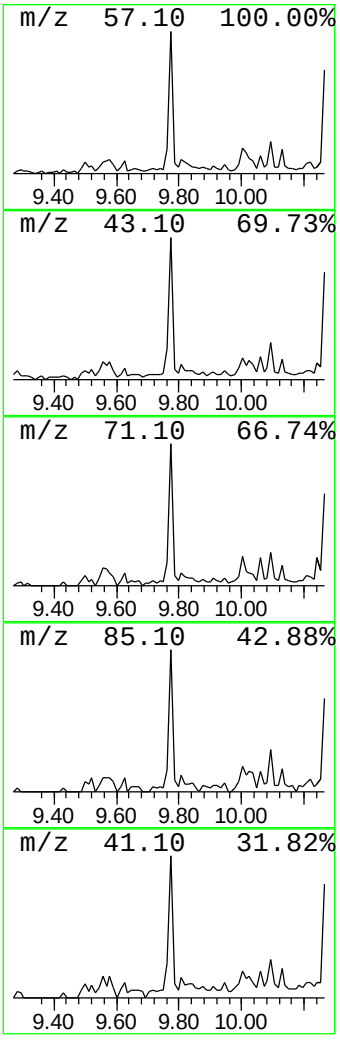
****

Peak Number 4 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.77	2.34 ng	99859	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Pentadecane	212	C15H32	000629-62-9	86
3	Eicosane	282	C20H42	000112-95-8	83
4	Tetracosane	338	C24H50	000646-31-1	83
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085899.D
Acq On : 30 Mar 2016 21:18
Operator : UM/SJ
Sample : H2023-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

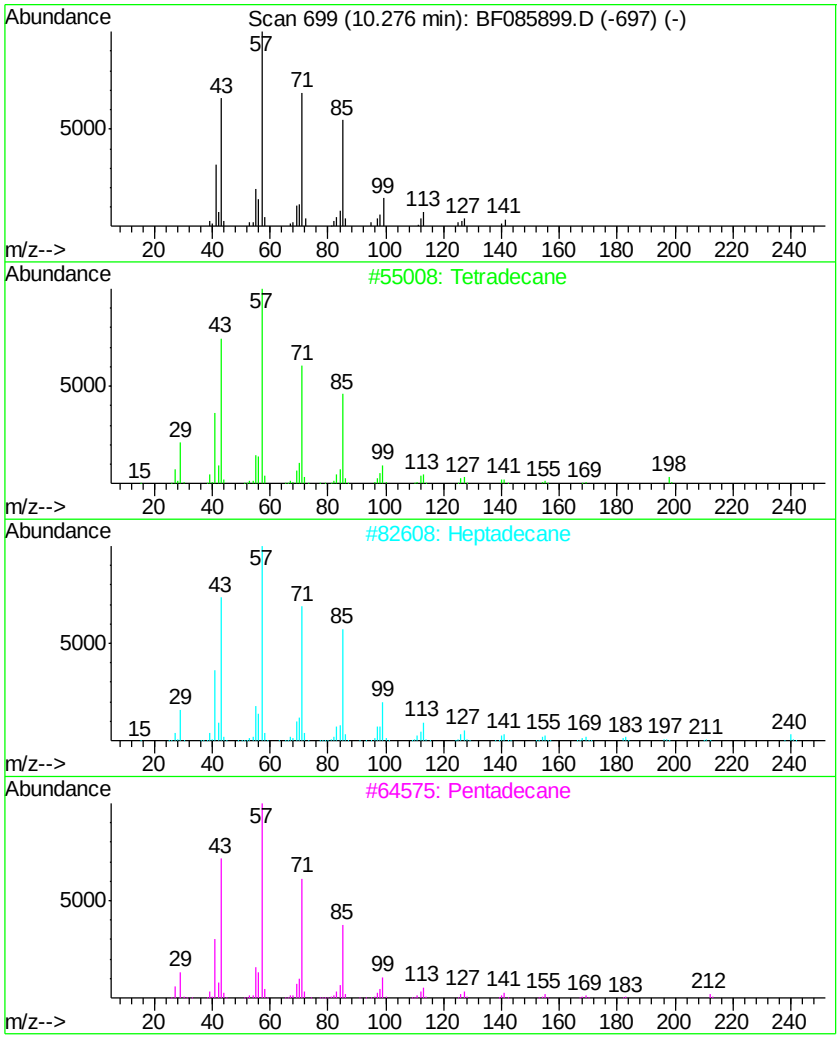
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

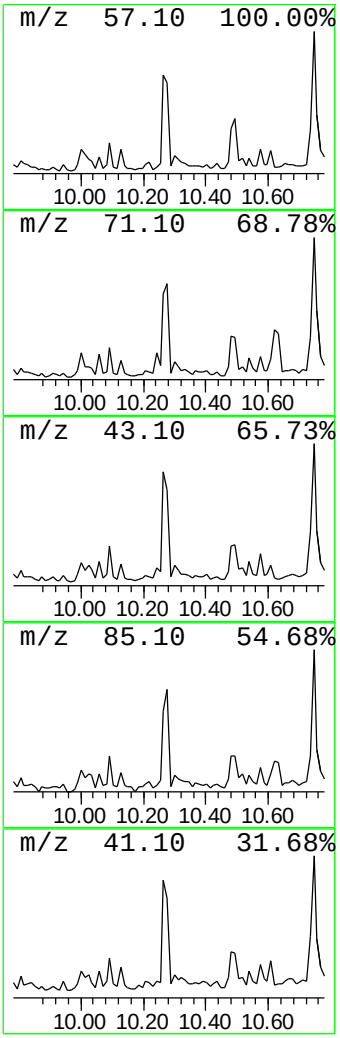
****

Peak Number 5 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.28	2.57 ng	109582	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Pentadecane	212	C15H32	000629-62-9	90
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	86
5	Octadecane	254	C18H38	000593-45-3	80





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085899.D
Acq On : 30 Mar 2016 21:18
Operator : UM/SJ
Sample : H2023-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

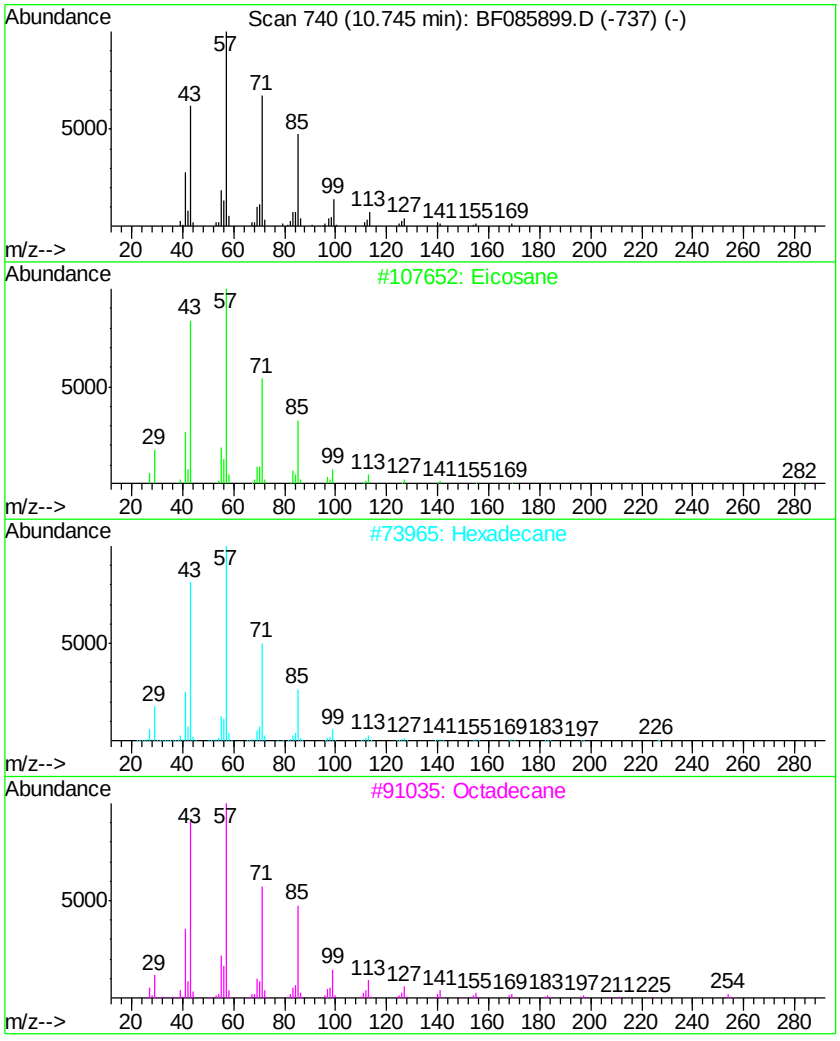
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

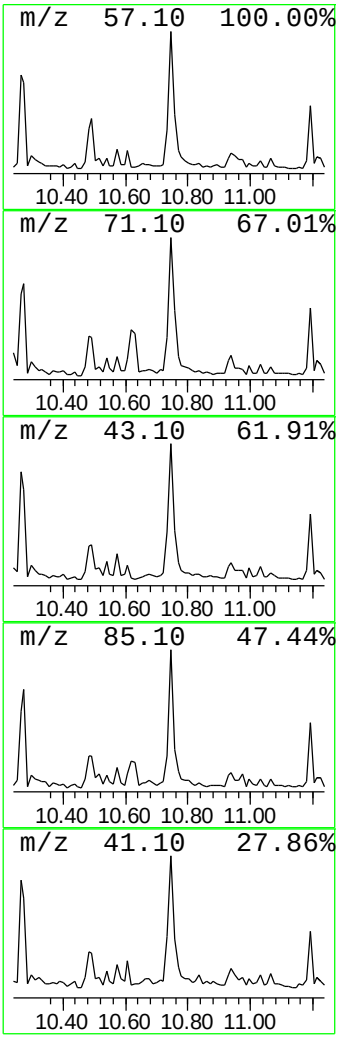
****

Peak Number 6 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	3.90 ng	150425	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Octadecane	254	C18H38	000593-45-3	90
4	Nonadecane	268	C19H40	000629-92-5	87
5	Heptadecane	240	C17H36	000629-78-7	87





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085899.D
Acq On : 30 Mar 2016 21:18
Operator : UM/SJ
Sample : H2023-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

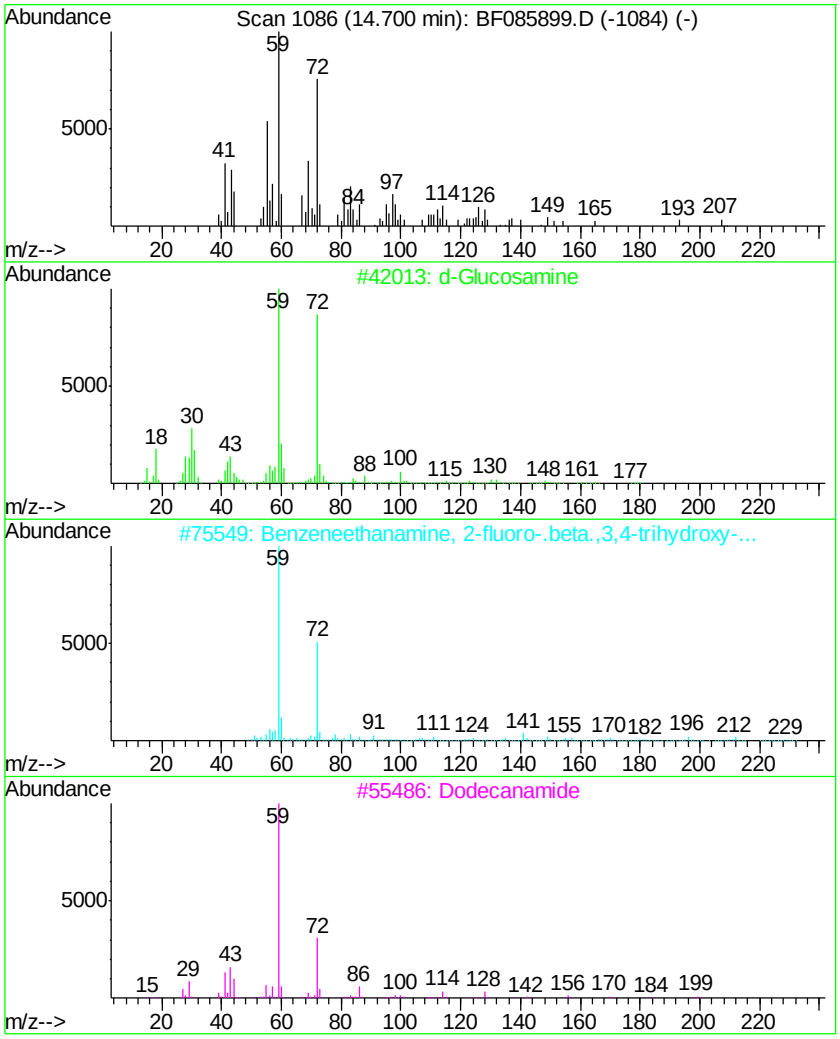
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

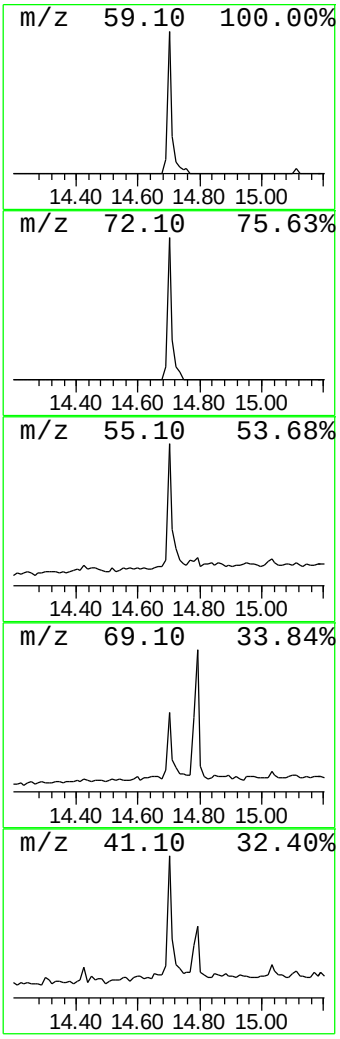
****

Peak Number 7 d-Glucosamine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	3.41 ng	104933	Perylene-d12	15.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	d-Glucosamine	179	C6H13NO5	000090-77-7	50
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	50
3	Dodecanamide	199	C12H25NO	001120-16-7	47
4	Tetradecanamide	227	C14H29NO	000638-58-4	47
5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085899.D
Acq On : 30 Mar 2016 21:18
Operator : UM/SJ
Sample : H2023-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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
2-Pentanone, 4-hy...	4.98	3.7	ng	113961	1	6.80	620651	20.0
unknown6.56	6.56	93.2	ng	2892090	1	6.80	620651	20.0
Heptadecane	9.77	2.3	ng	99859	3	9.84	854250	20.0
Tetradecane	10.28	2.6	ng	109582	3	9.84	854250	20.0
Eicosane	10.74	3.9	ng	150425	4	11.32	772169	20.0
d-Glucosamine	14.70	3.4	ng	104933	6	15.37	614655	20.0