LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011389.D
Acq On : 01 Sep 2017 01:33
Operator : SJ/JU
Sample : I4963-15
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 3834-CC5

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_M\METHODS\8270-BM083117.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	3.057	41	46	56	rBV	2022248	3558317	11.22%	2.264%
2	3.134	56	59	69	rVB	894043	1133292	3.57%	0.721%
3	5.081	382	390	400	rBV	736460	1123981	3.54%	0.715%
4	5.546	460	469	478	rBV	3961078	5858876	18.47%	3.728%
5	7.134	733	739	748	rVB	2397932	3704805	11.68%	2.357%
6	7.516	796	804	813	rBV	7527541	11690697	36.86%	7.438%
7	7.987	875	884	890	rBV	1857578	3027696	9.55%	1.926%
8	8.310	932	939	946	rBV	7038488	11599298	36.57%	7.380%
9	9.151	1074	1082	1091	rBV	5709516	9344622	29.46%	5.946%
10	10.798	1353	1362	1374	rBV	2710260	4563772	14.39%	2.904%
11	11.639	1496	1505	1515	rVB	135173	327459	1.03%	0.208%
12	11.992	1553	1565	1571	rBV	370617	671493	2.12%	0.427%
13	13.063	1743	1747	1760	rVB2	344100	588016	1.85%	0.374%
14	13.245	1768	1778	1786	rBV	15140267	21953446	69.22%	13.968%
15	14.621	2005	2012	2020	rVB2	3890239	5889470	18.57%	3.747%
16	16.104	2257	2264	2280	rBV	10633420	15024987	47.37%	9.560%
17	17.357	2471	2477	2487	rBV	4886259	7067193	22.28%	4.497%
18	18.233	2622	2626	2636	rBV	288601	467096	1.47%	0.297%
19	19.509	2839	2843	2853	rBV	305434	470909	1.48%	0.300%
20	19.968	2915	2921	2927	rBV	25503003	31716702	100.00%	20.180%
21	21.427	3165	3169	3174	rBV	429823	495268	1.56%	0.315%
22	21.521	3180	3185	3191	rBV	7241589	8879940	28.00%	5.650%
23	23.903	3583	3590	3599	rVB	3879427	8008395	25.25%	5.096%

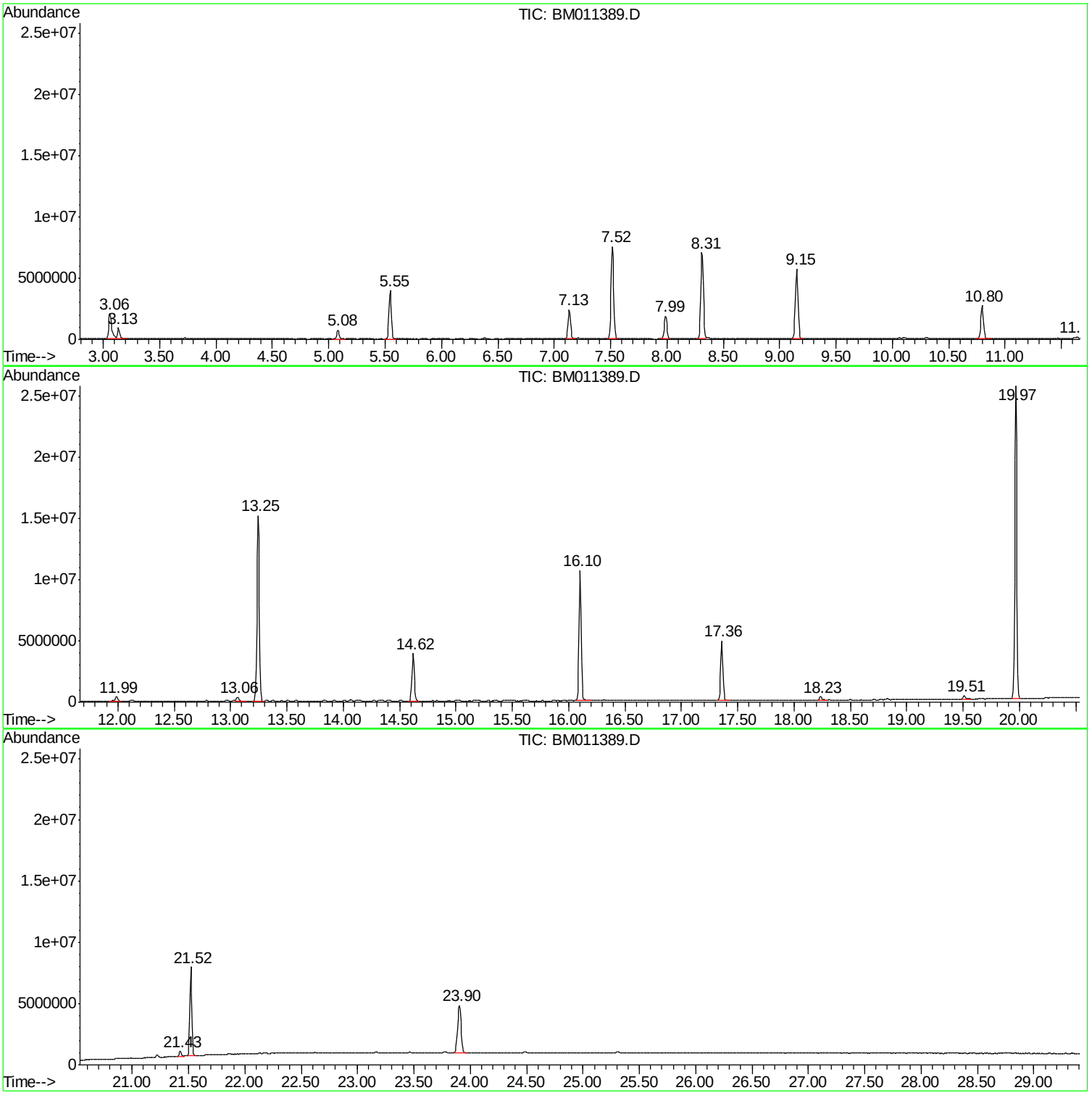
Sum of corrected areas: 157165730

Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011389.D
Acq On : 01 Sep 2017 01:33
Operator : SJ/JU
Sample : I4963-15
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3834-CC5

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM083117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011389.D
Acq On : 01 Sep 2017 01:33
Operator : SJ/JU
Sample : I4963-15
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 3834-CC5

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM083117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

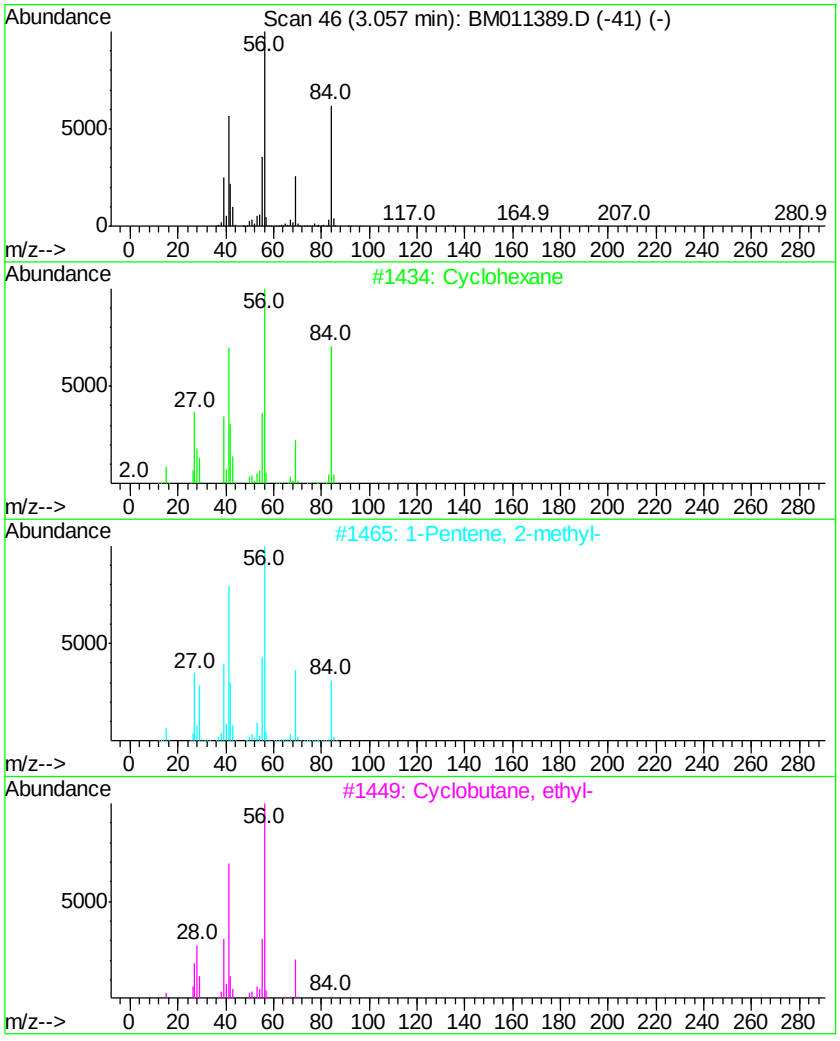
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

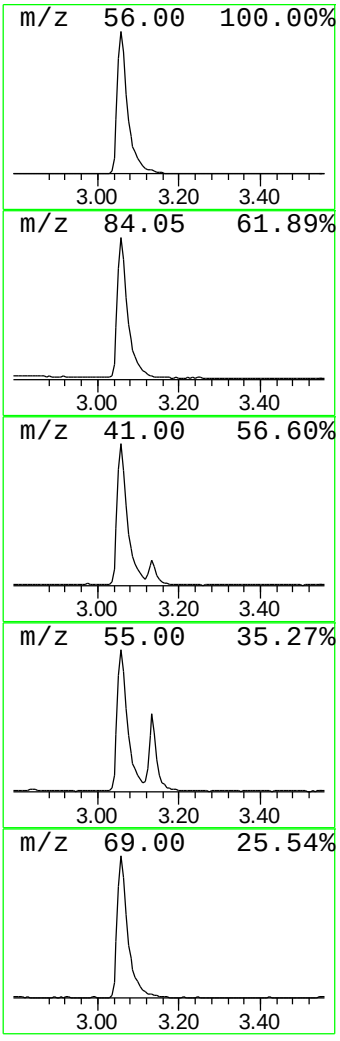
****

Peak Number 1 Cyclohexane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.06	23.51 ng	3558320	1,4-Dichlorobenzene-d4	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	91
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	50
4	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	47
5	Cyclopentane, methyl-	84	C6H12	000096-37-7	45





Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011389.D
Acq On : 01 Sep 2017 01:33
Operator : SJ/JU
Sample : I4963-15
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 3834-CC5

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM083117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

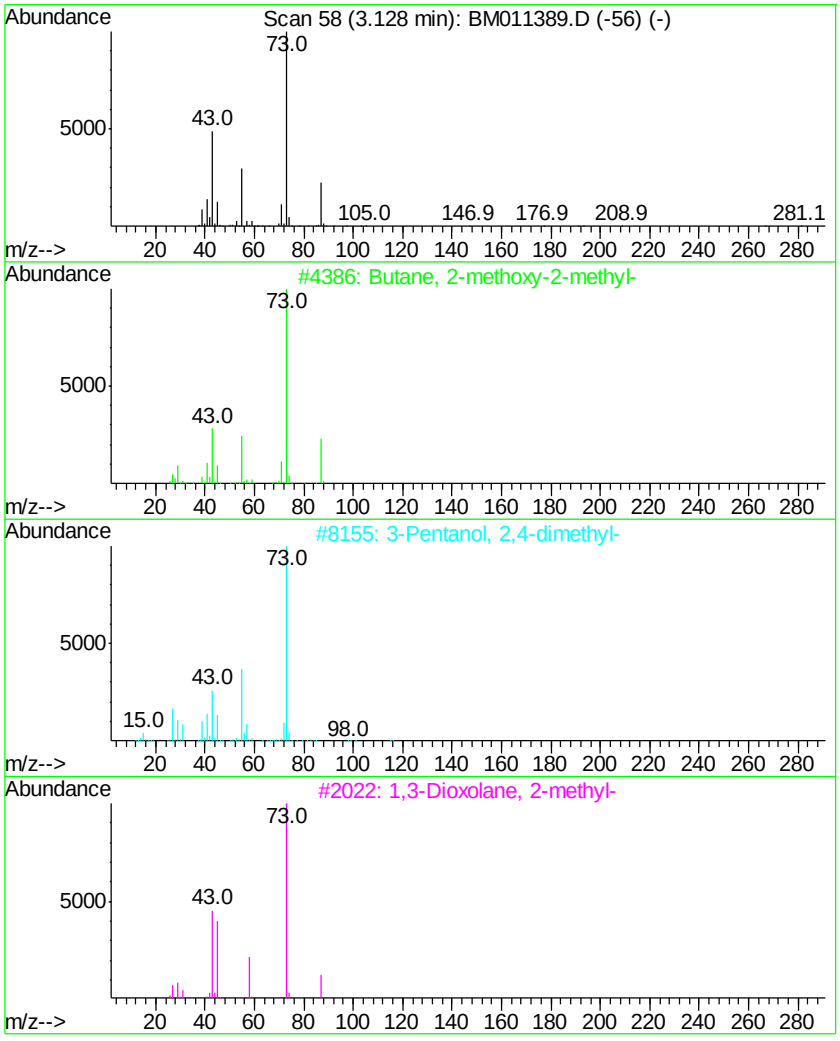
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

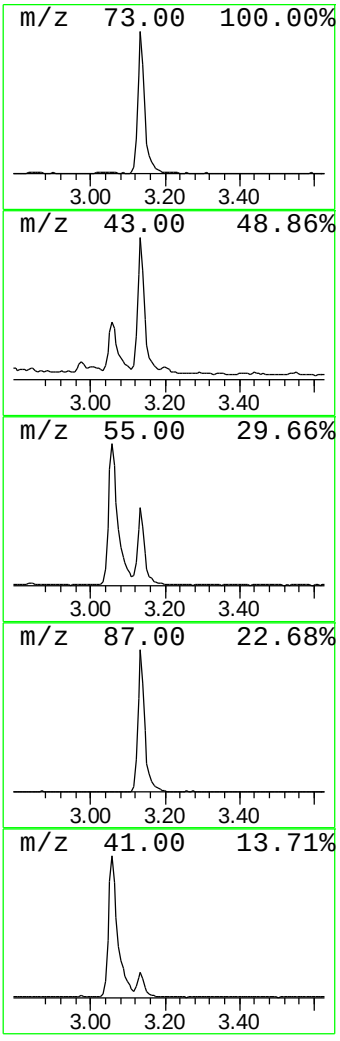
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	7.49 ng	1133290	1,4-Dichlorobenzene-d4	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011389.D
Acq On : 01 Sep 2017 01:33
Operator : SJ/JU
Sample : I4963-15
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 3834-CC5

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM083117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

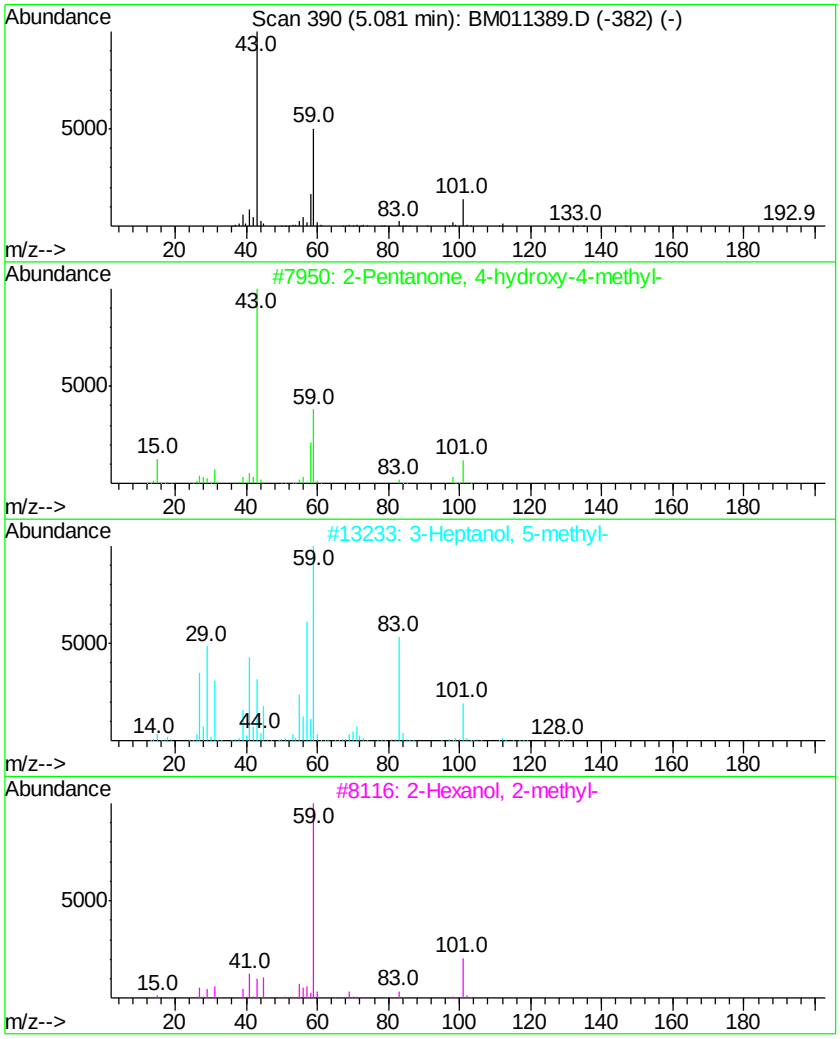
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

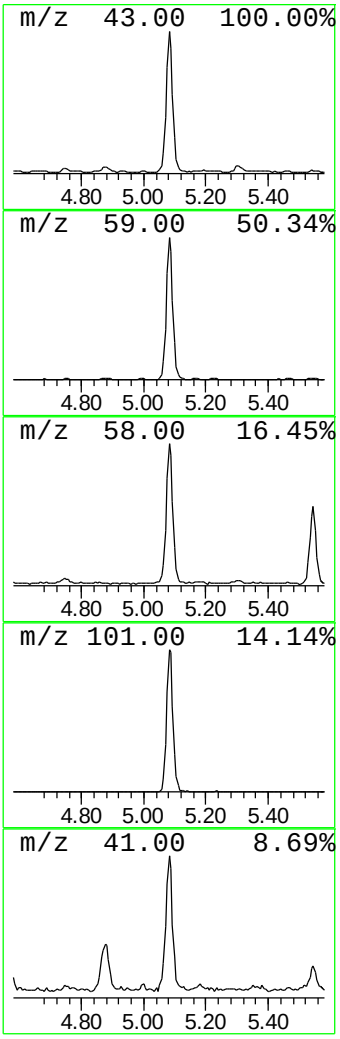
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	7.42 ng	1123980	1,4-Dichlorobenzene-d4	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Heptanol, 5-methyl-	130	C8H18O	018720-65-5	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5	2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	25





Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011389.D
Acq On : 01 Sep 2017 01:33
Operator : SJ/JU
Sample : I4963-15
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 3834-CC5

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM083117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

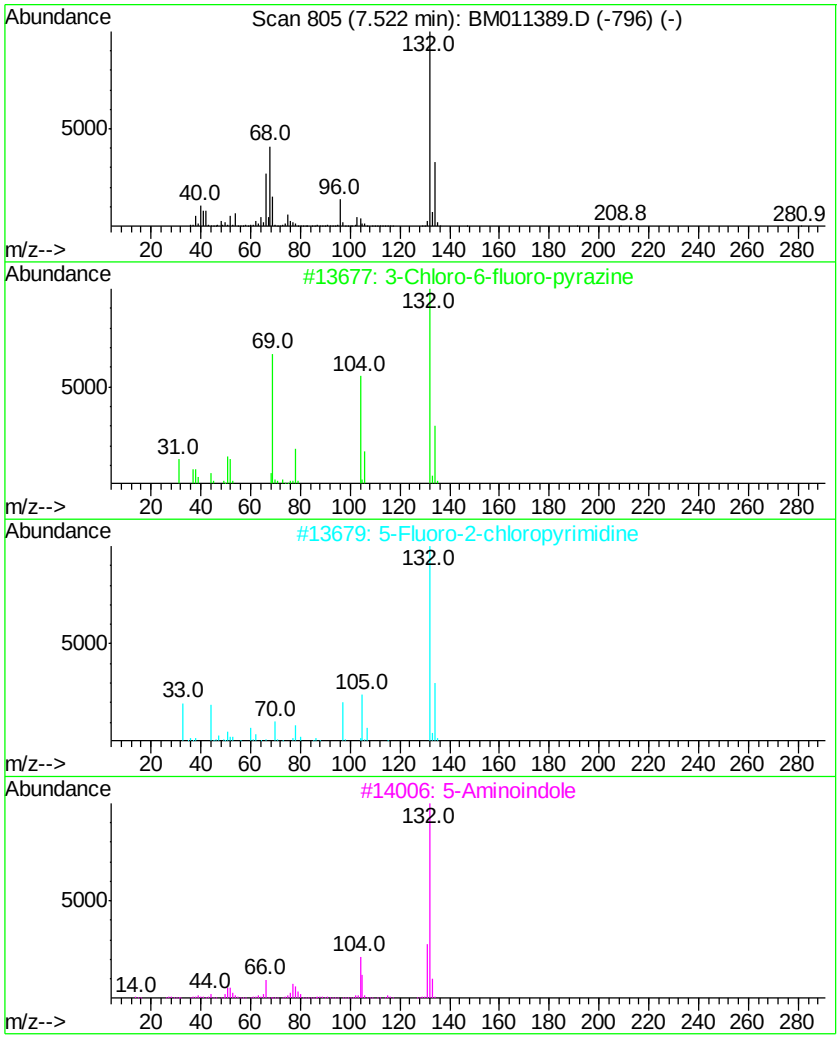
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

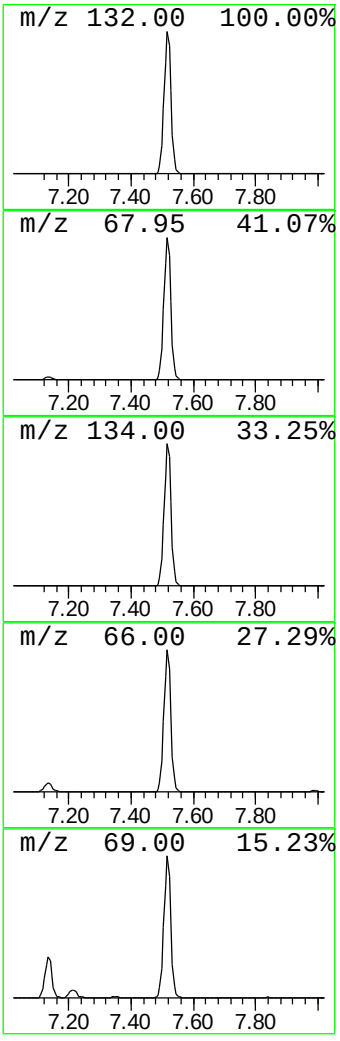
****

Peak Number 4 unknown7.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.52	77.23 ng	11690700	1,4-Dichlorobenzene-d4	7.99

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA M\DATA\BM083117\
Data File : BM011389.D
Acq On : 01 Sep 2017 01:33
Operator : SJ/JU
Sample : I4963-15
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 3834-CC5

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM083117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

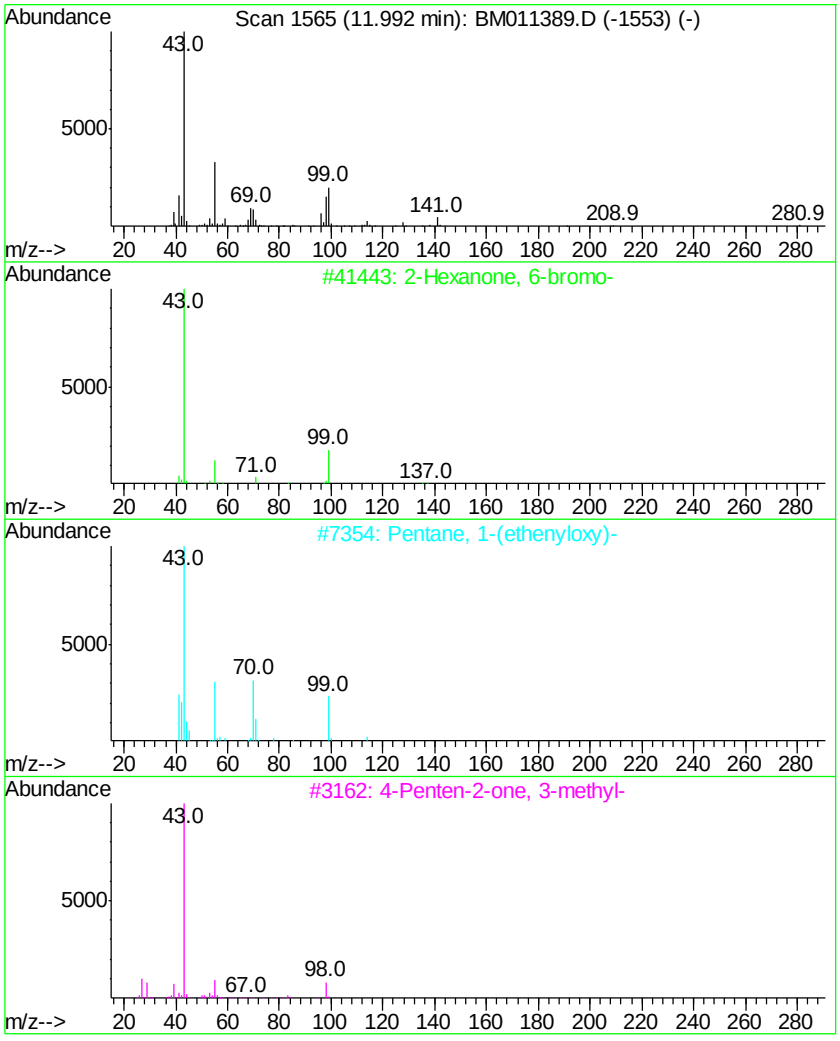
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

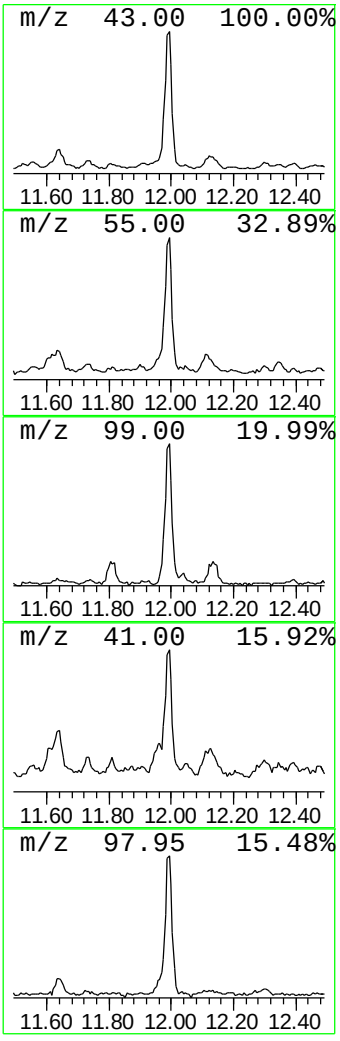
****

Peak Number 6 unknown11.99 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.94 ng	671493	Naphthalene-d8	10.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanone, 6-bromo-	178	C6H11BrO	010226-29-6	32
2	Pentane, 1-(ethenyloxy)-	114	C7H14O	005363-63-3	23
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	22
4	4-Hexen-2-one	98	C6H10O	025659-22-7	22
5	Acetic acid, 1,3,3-trimethyl-4-o...	198	C10H14O4	1000195-38-8	12





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM083117\
Data File : BM011389.D
Acq On : 01 Sep 2017 01:33
Operator : SJ/JU
Sample : I4963-15
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 3834-CC5

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM083117.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
Cyclohexane	3.06	23.5	ng	3558320	1	7.99	3027700	20.0
Butane, 2-methoxy...	3.13	7.5	ng	1133290	1	7.99	3027700	20.0
2-Pentanone, 4-hy...	5.08	7.4	ng	1123980	1	7.99	3027700	20.0
unknown7.52	7.52	77.2	ng	11690700	1	7.99	3027700	20.0
unknown11.99	11.99	2.9	ng	671493	2	10.80	4563770	20.0