

Supporting Information
for
A novel and practical asymmetric synthesis of dapoxetine hydrochloride

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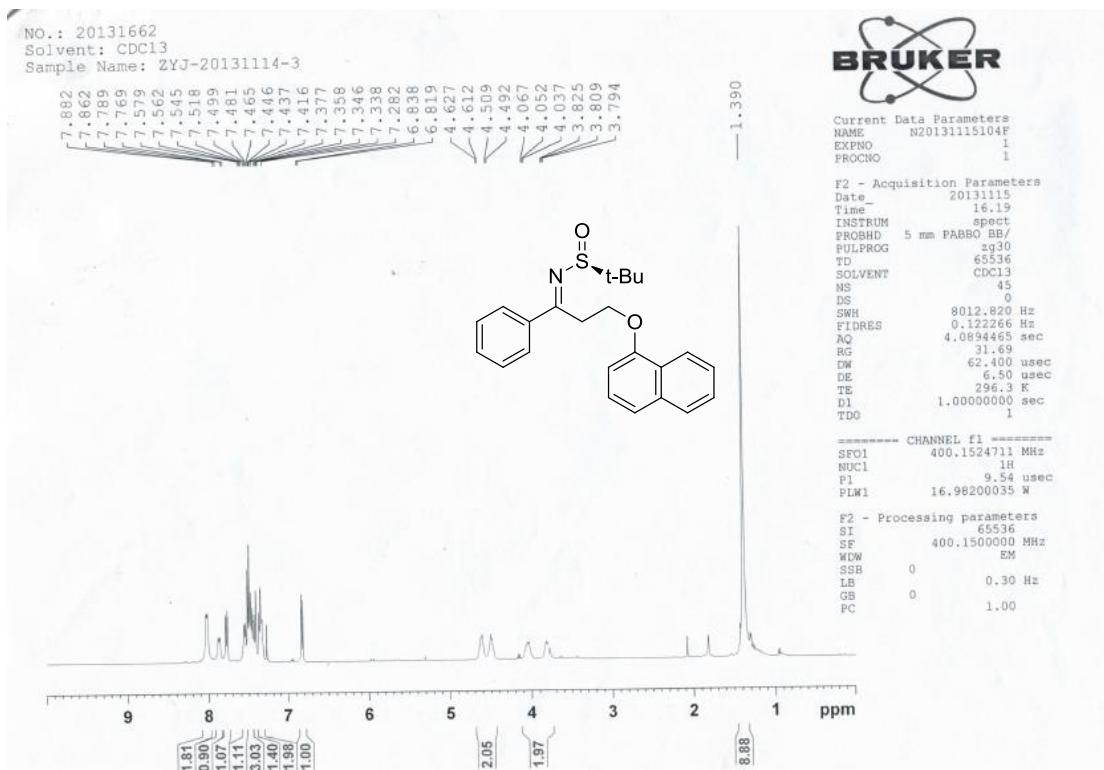
Email: Deyong Ye - dyye@shmu.edu.cn;
Weicheng Zhou - zhouweicheng58@163.com

* Corresponding author

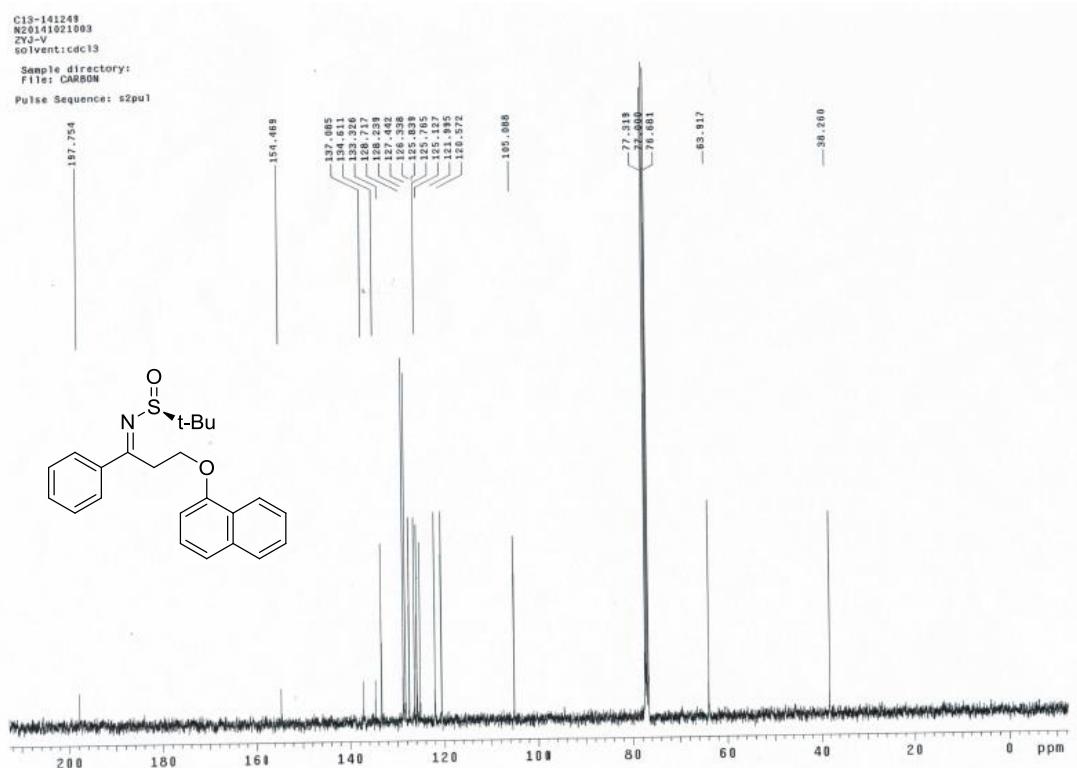
¹H NMR, ¹³C NMR and ESIMS spectra of compounds 1, 4, 5, 5”, 6 and 7 and chiral HPLC diagrams of 1 and 7

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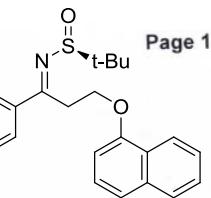


¹H NMR spectrum of compound 4



¹³C NMR spectrum of compound **4**

Elemental Composition Report



Page 1

Single Mass Analysis

Tolerance = 30.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

15 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 10-40 H: 10-40 N: 0-1 O: 0-2 Na: 1-1 S: 1-1

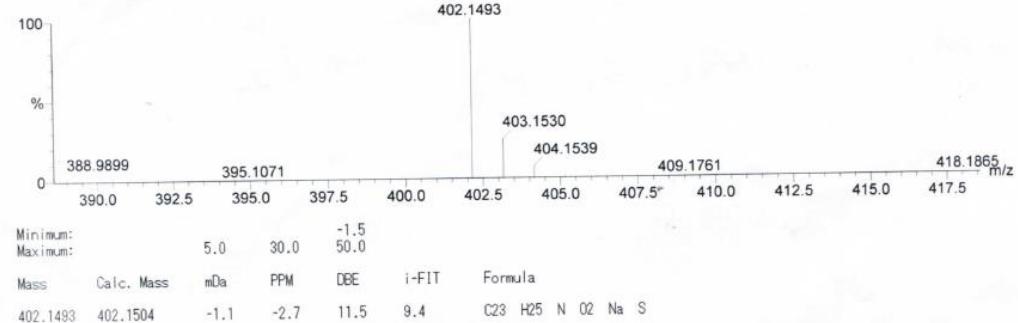
SIPI

ZYJ-V

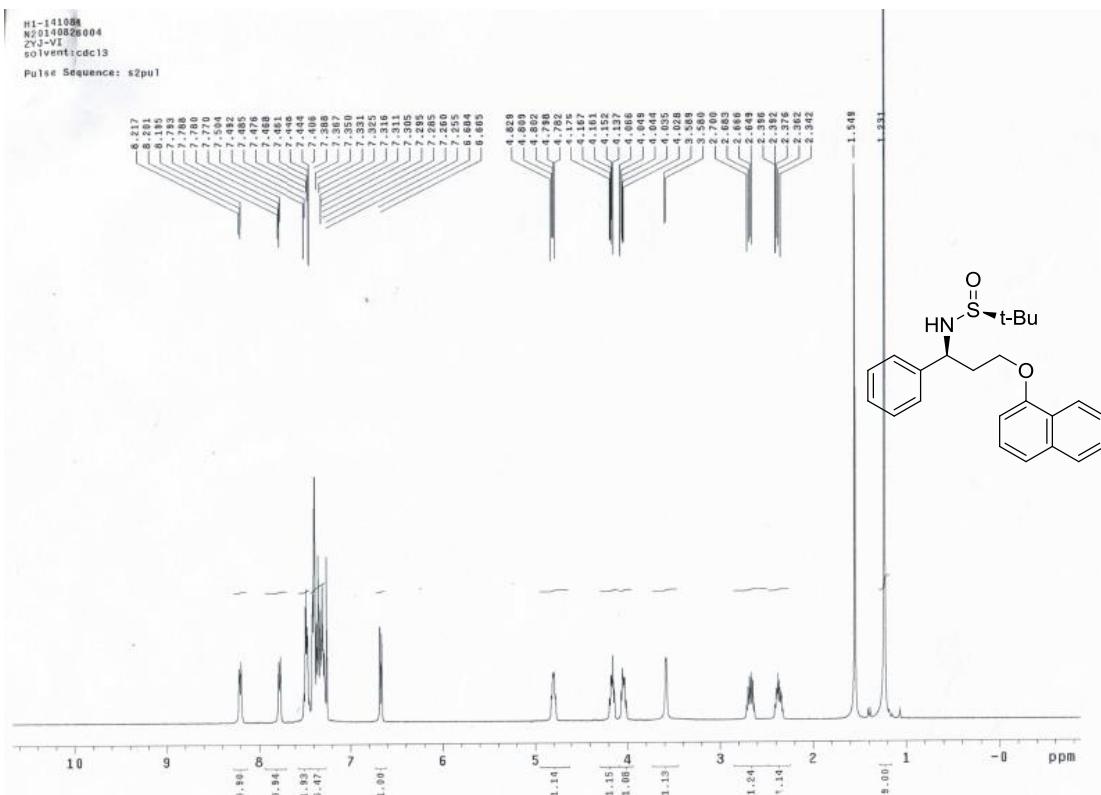
Q15-1893HR 22 (0.407) AM (Cen,2, 80.00, Ar,5000.0,360.29,1.00); Sm (Mn, 2x3.00); Sb (1,40.00); Cm (9:22)

14:10:51,13-Nov-2015

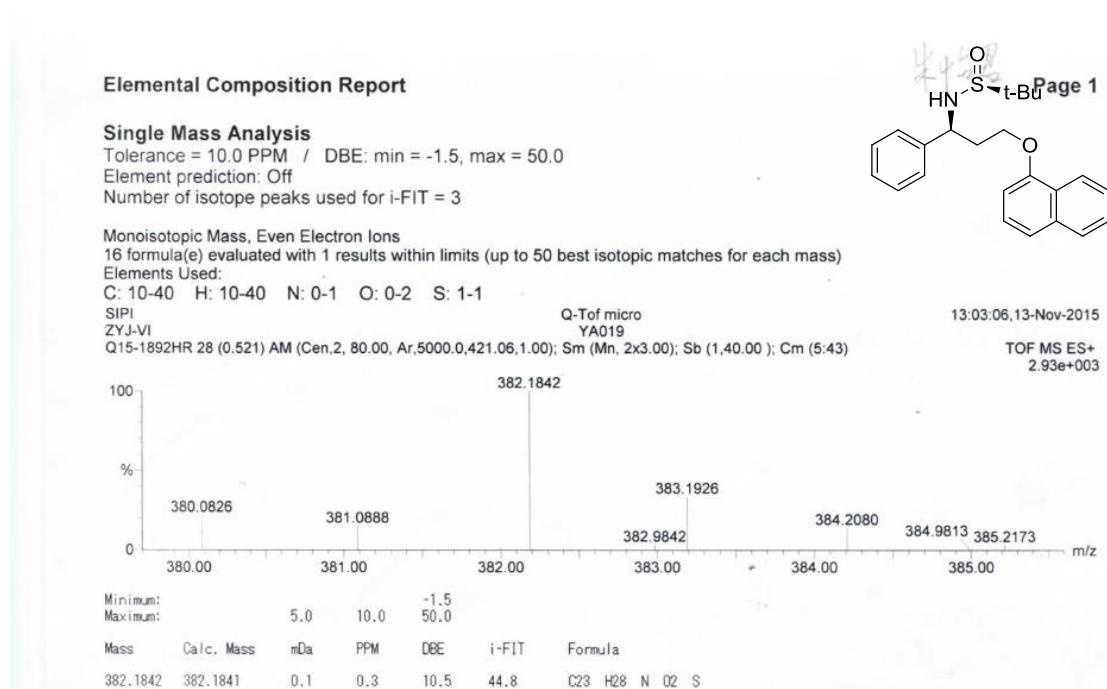
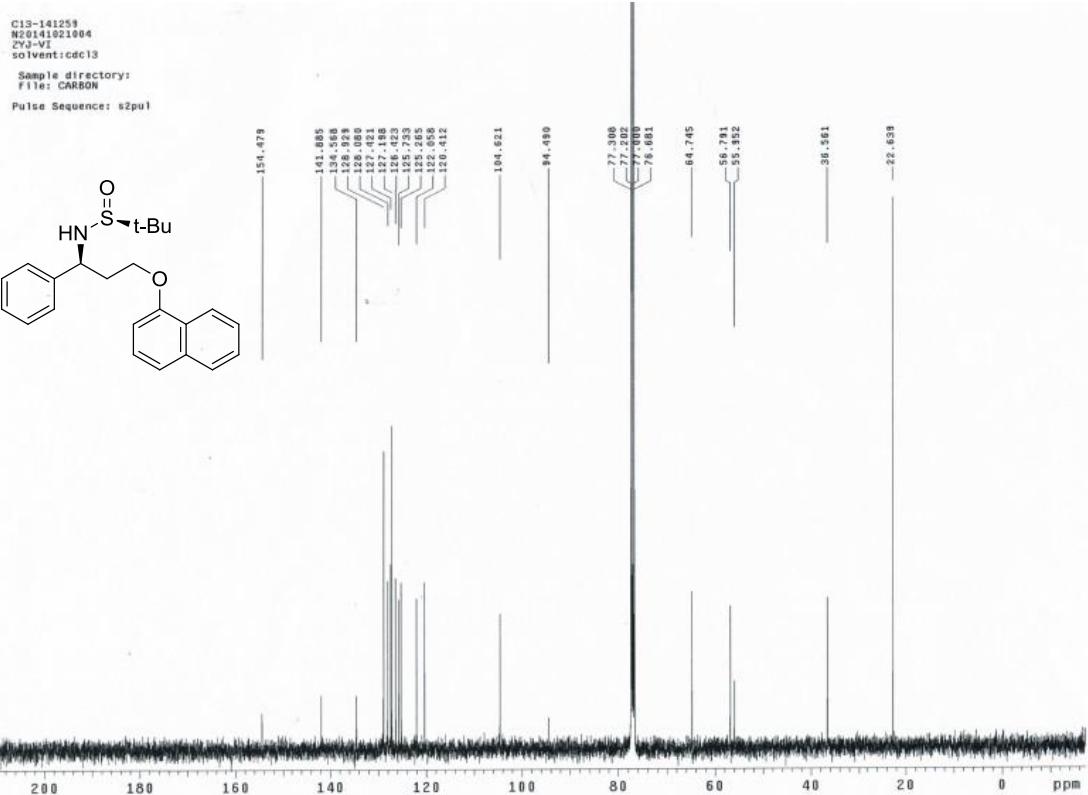
TOF MS ES+
3.42e+003



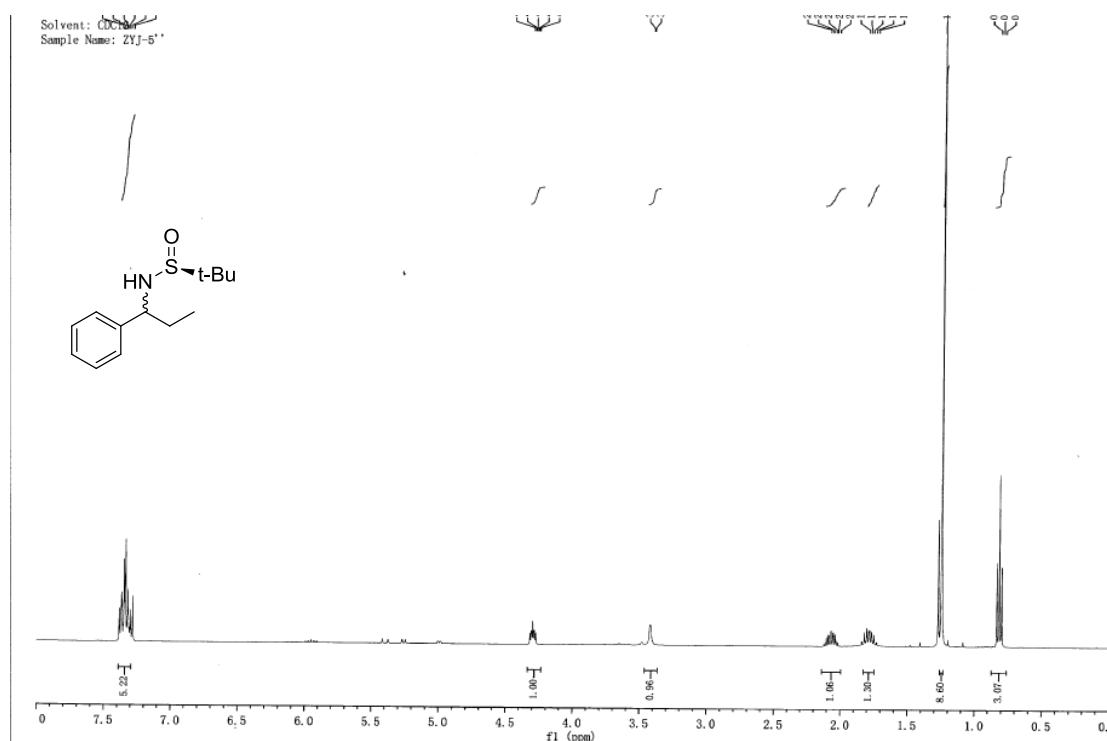
HRMS spectrum of compound 4



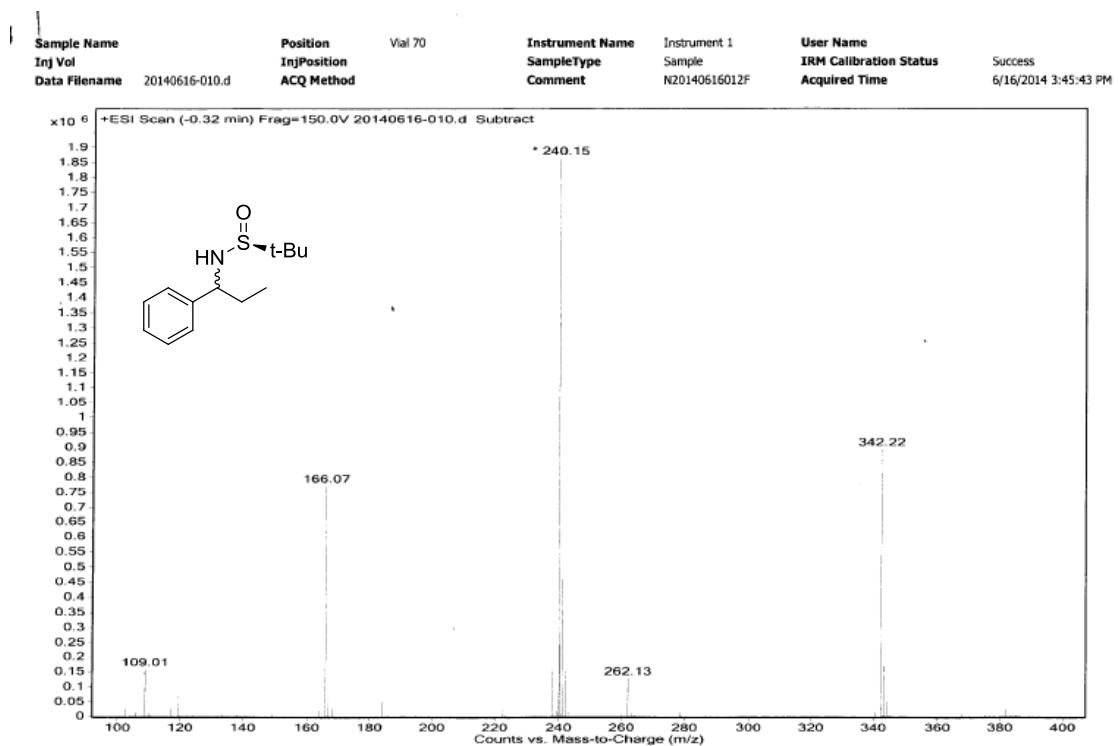
¹H NMR spectrum of compound 5



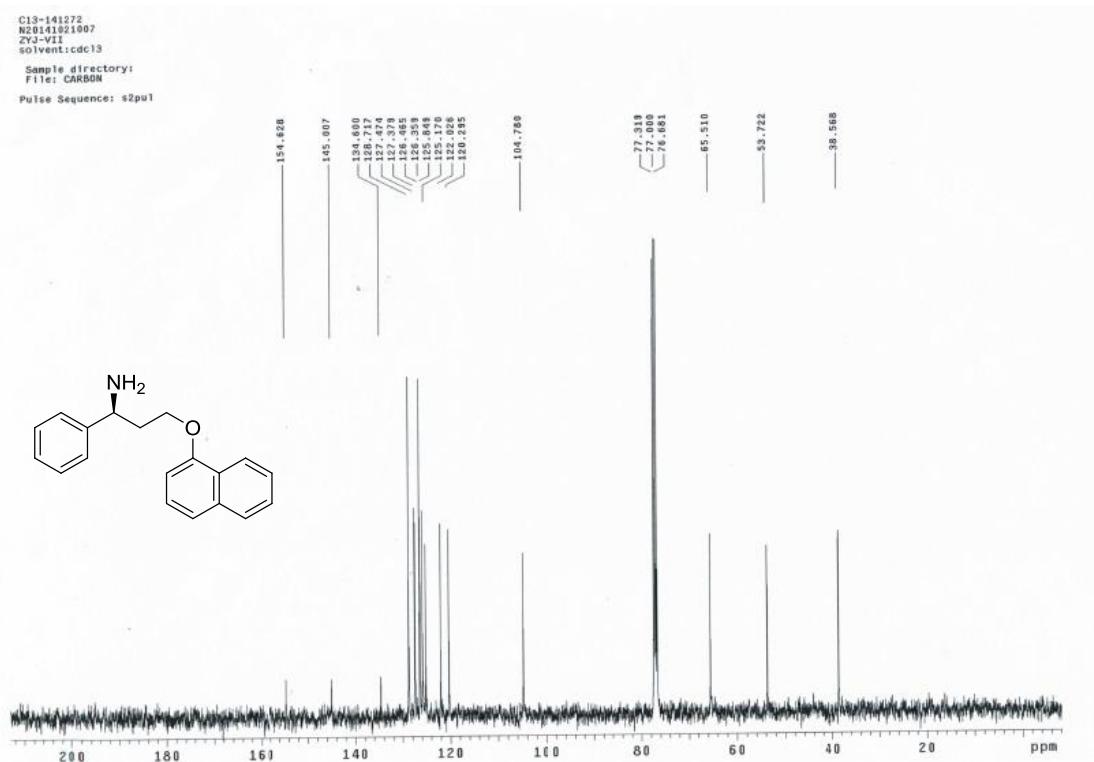
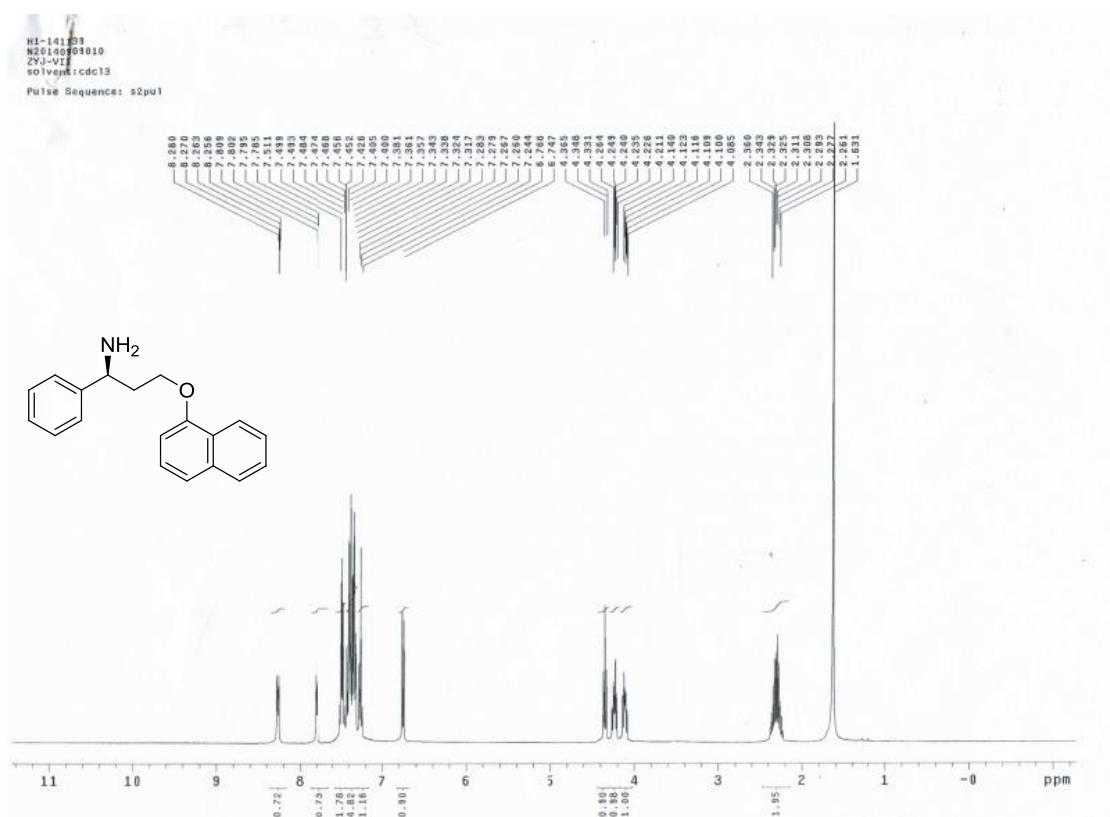
HRMS spectrum of compound 5

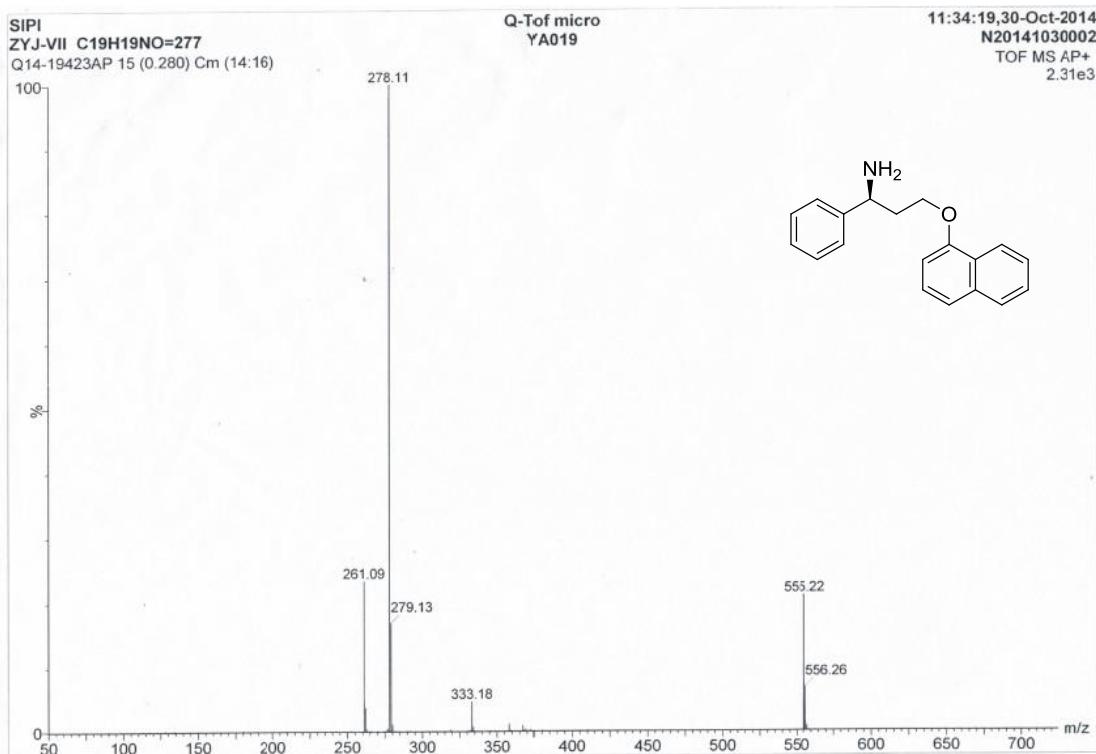


^1H NMR spectrum of compound 5"

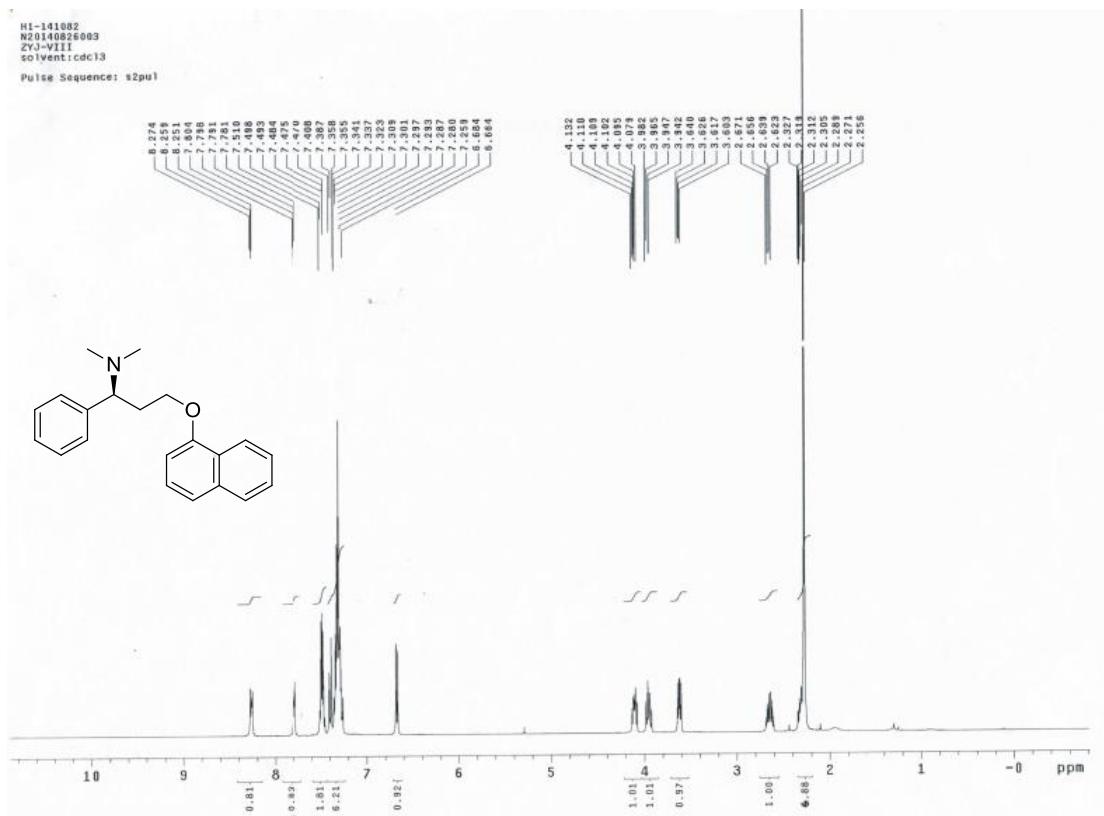


ESIMS spectrum of compound 5"



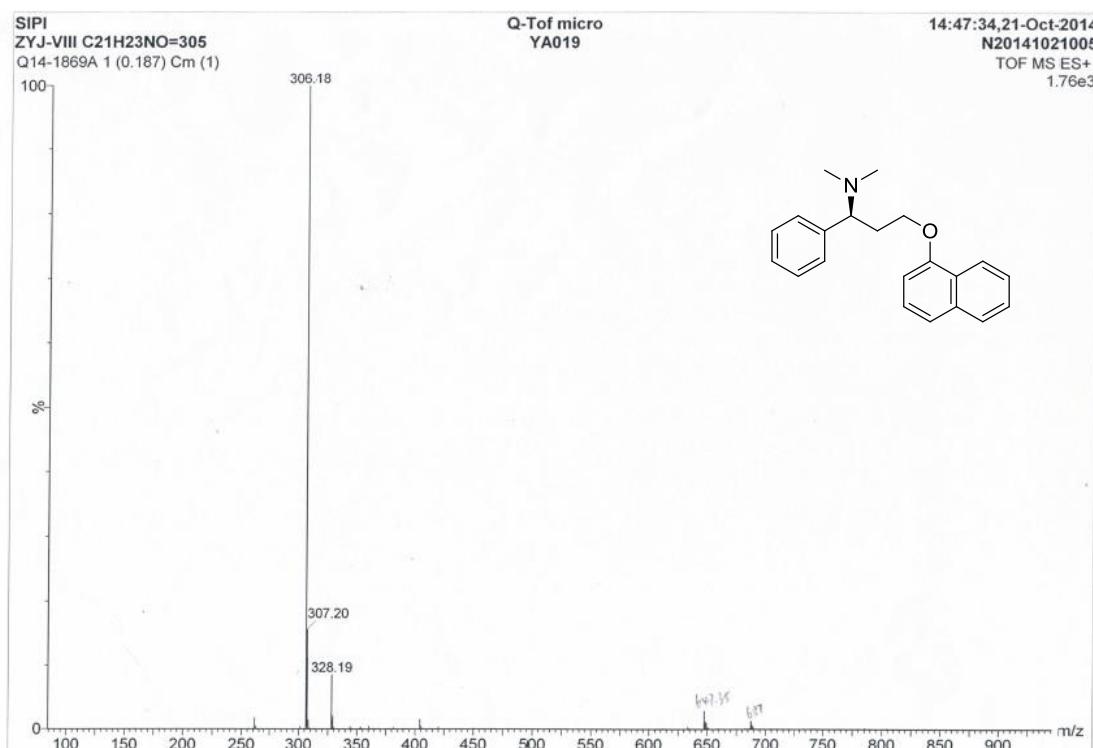
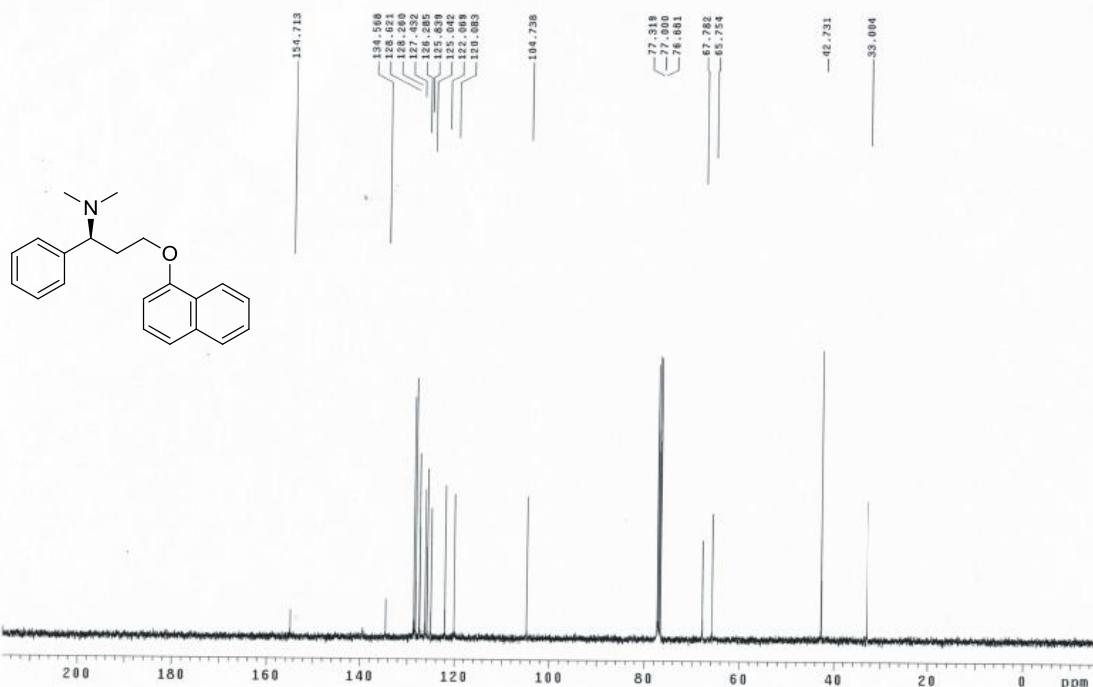


ESIMS spectrum of compound **6**



¹H NMR spectrum of compound 7

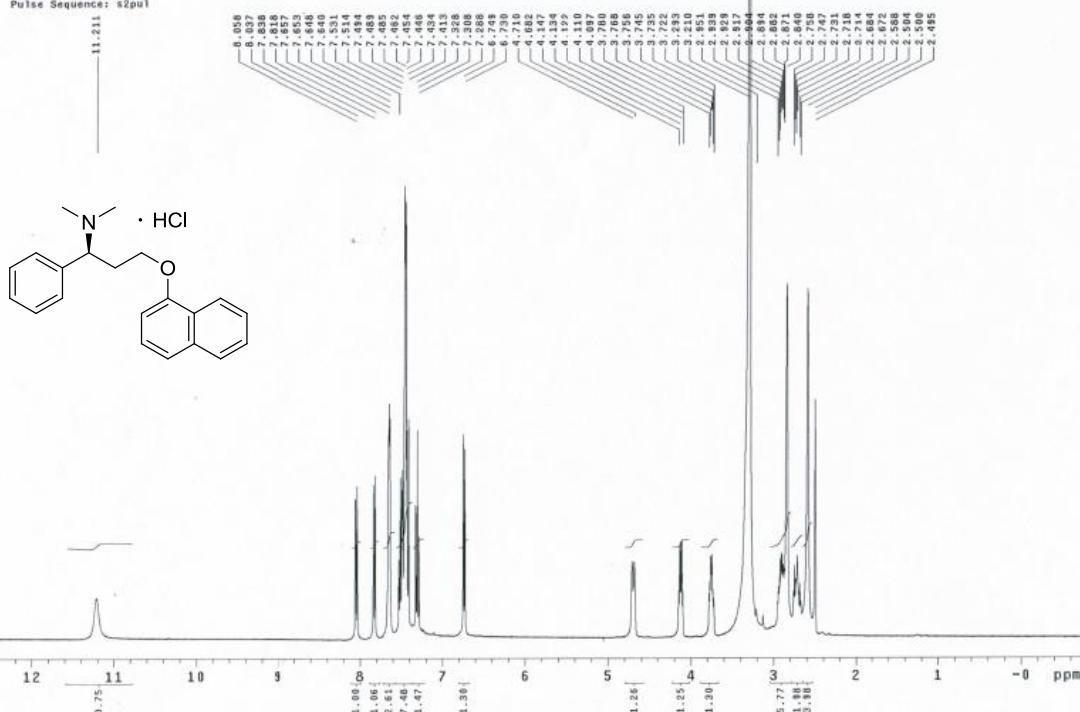
C13-141268
N20141021005
ZYJ-VIII
solventicdc13
Sample directory:
File: CARBON
Pulse Sequence: s2pul



ESIMS spectrum of compound 7

H1-141241
N20141021008
ZYJ-Dapoxetine
solvent: DMSO-d6

DRIVER: 0430-06

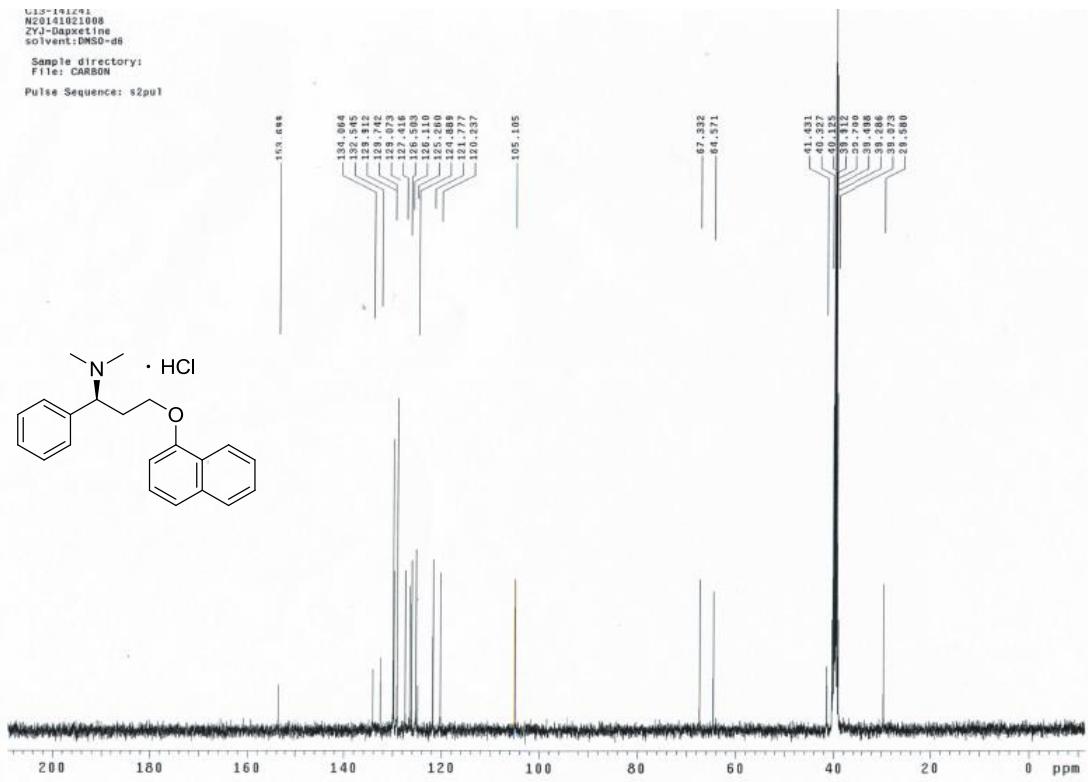


¹H NMR spectrum of compound 1

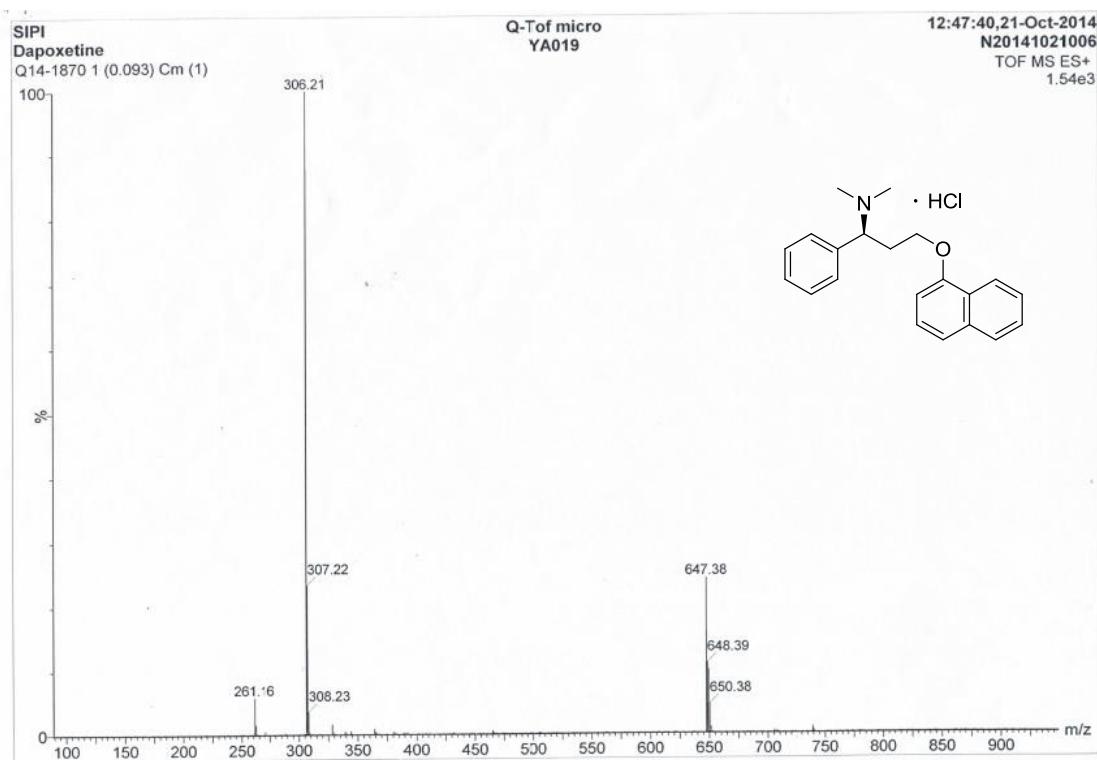
U15-141291
N20141021008
ZYJ-Dapoxetine
solvent:DMSO-d6

Sample director

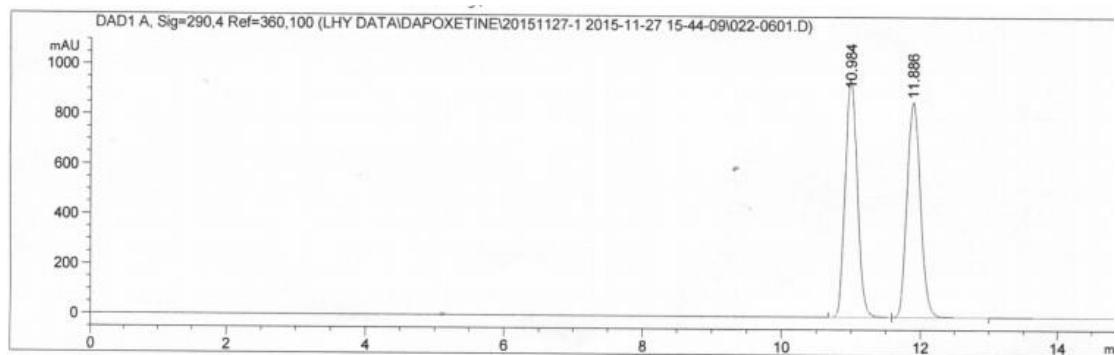
File: CARBON



¹³C NMR spectrum of compound 1



ESIMS spectrum of compound **1**



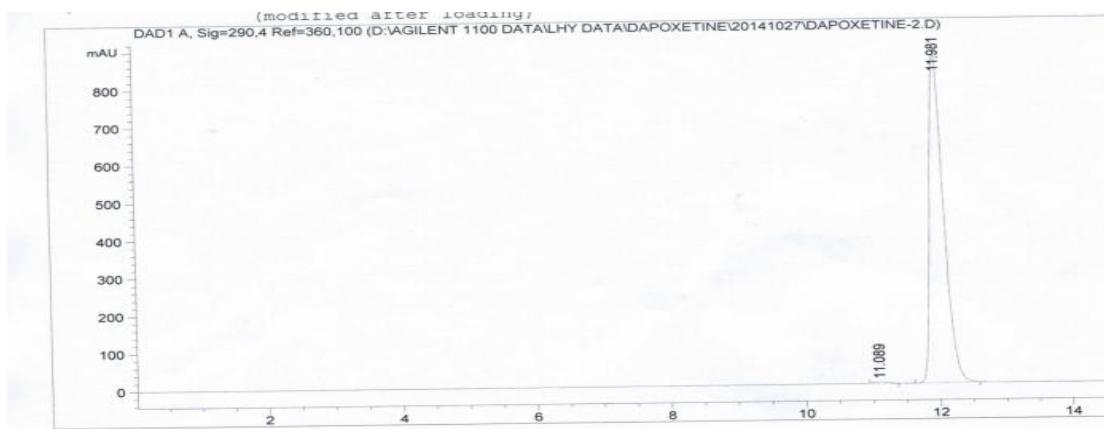
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Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=290.4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.984	BB	0.1886	1.14817e4	952.94586	49.9049
2	11.886	BB	0.2081	1.15254e4	861.45459	50.0951

Chiral HPLC of Racemic-7



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Area Percent Report
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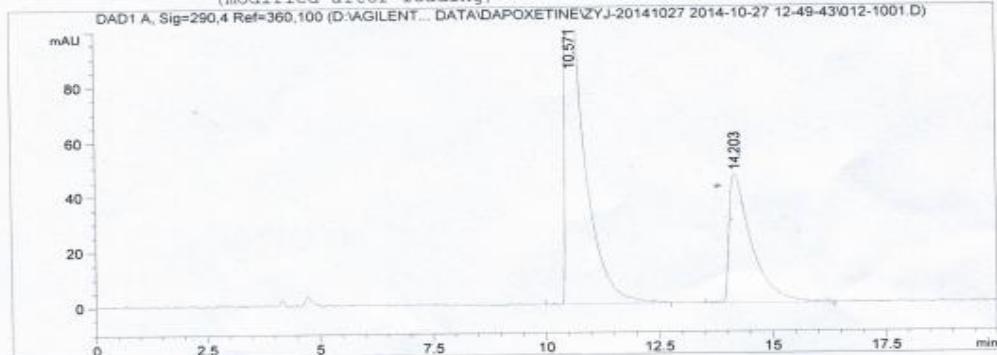
Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=290.4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.089	BB	0.1448	47.24658	4.21311	0.3667
2	11.981	BB	0.2249	1.28360e4	876.36298	99.6333

Chiral HPLC of 7

Last changed : 10/27/2014 12:48:24 PM by LHY
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 (modified after loading)



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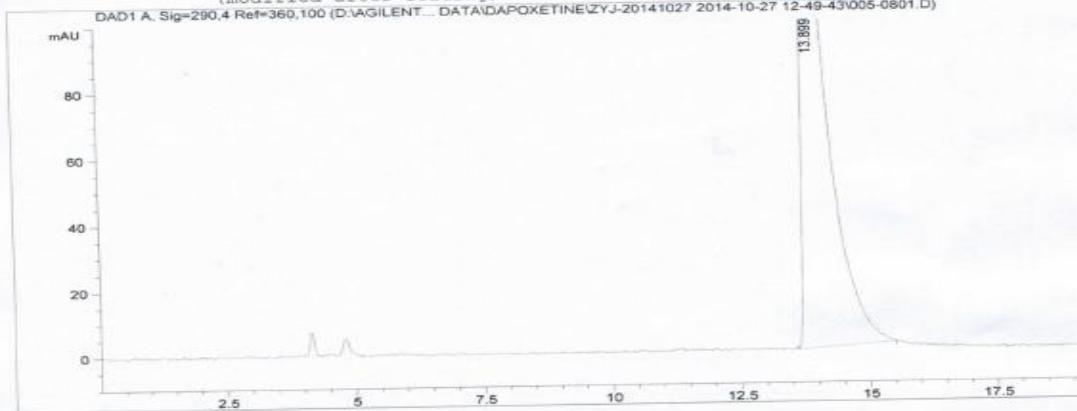
Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=290,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.571	BB	0.3648	3743.35107	145.16963	70.0842
2	14.203	BB	0.4891	1597.87012	46.47349	29.9158

Mixed Sample of (R)-1 and (S)-1

Last changed : 10/27/2014 12:48:24 PM by LHY
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 Last changed : 12/3/2014 8:49:13 AM by lzx
 (modified after loading)



 Area Percent Report

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=290,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.899	BB	0.4288	5424.02246	177.34618	100.0000

Chiral HPLC of 1