

Supplementary Material

Discovery of Highly Potent Triazole Antifungal Agents with Piperdine-oxadiazole Side Chains

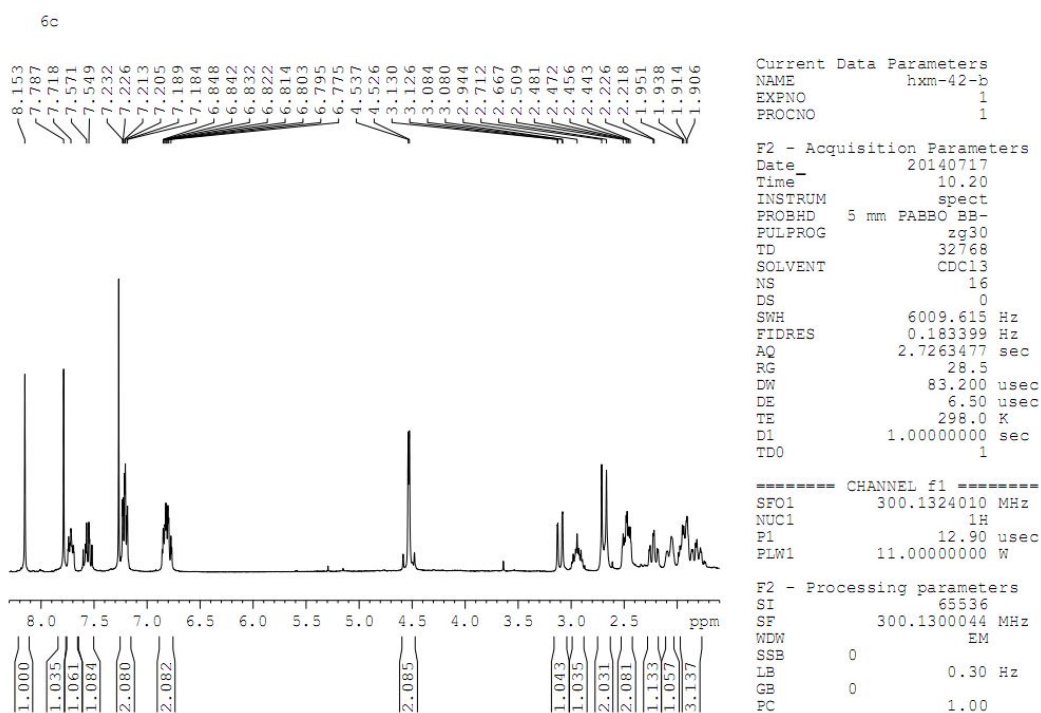
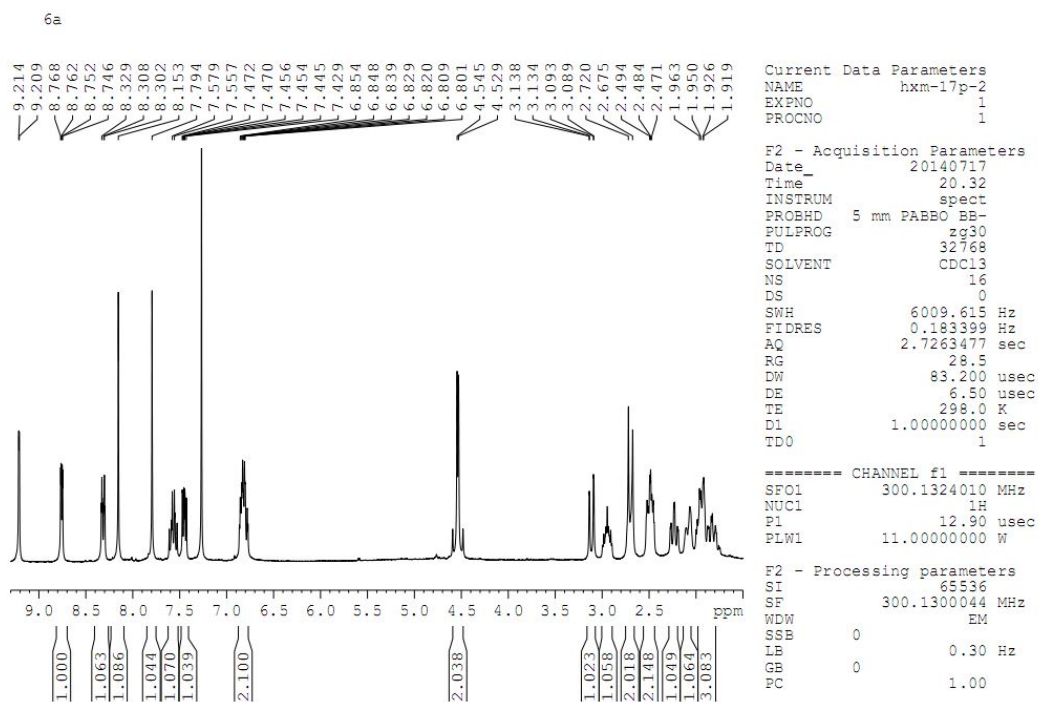
Xiaomeng He[§], Yan Jiang[§], Yongqiang Zhang, Shanchao Wu, Guoqiang Dong, Na Liu, Yang Liu, Jianzhong Yao, Zhenyuan Miao, Yan Wang*, Wannian Zhang* and Chunquan Sheng*

*School of Pharmacy, Second Military Medical University, 325 Guohe Road, Shanghai
200433, China*

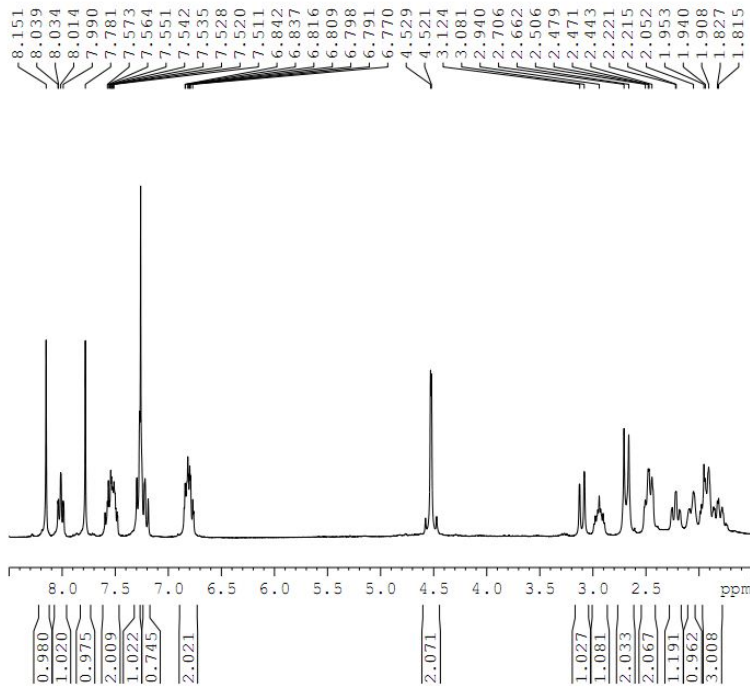
[§]These authors contributed equally to this work.

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Representative ¹H NMR spectra for the target compounds



6d



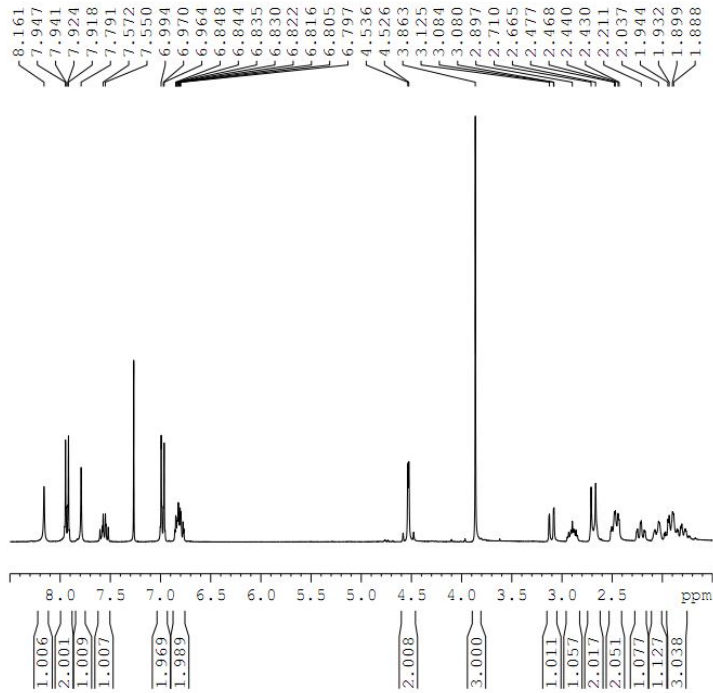
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 PROCNO 1

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 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 16
 DS 0
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 FIDRES 0.183399 Hz
 AQ 2.7263477 sec
 RG 28.5
 DW 83.200 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

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 NUC1 1H
 P1 12.90 usec
 PLW1 11.00000000 W

F2 - Processing parameters
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 PC 1.00

6e



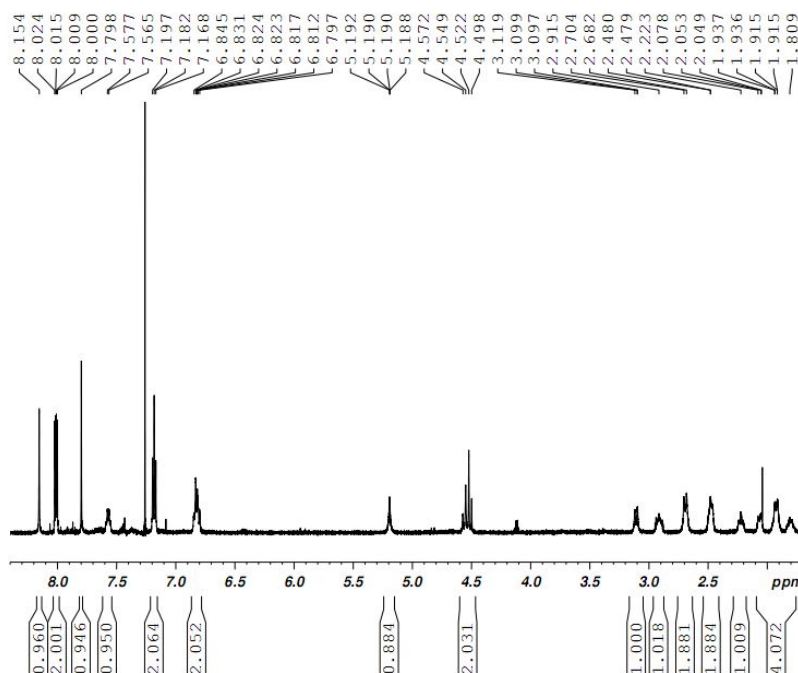
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 AQ 2.7263477 sec
 RG 28.5
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 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
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 NUC1 1H
 P1 12.90 usec
 PLW1 11.00000000 W

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6h



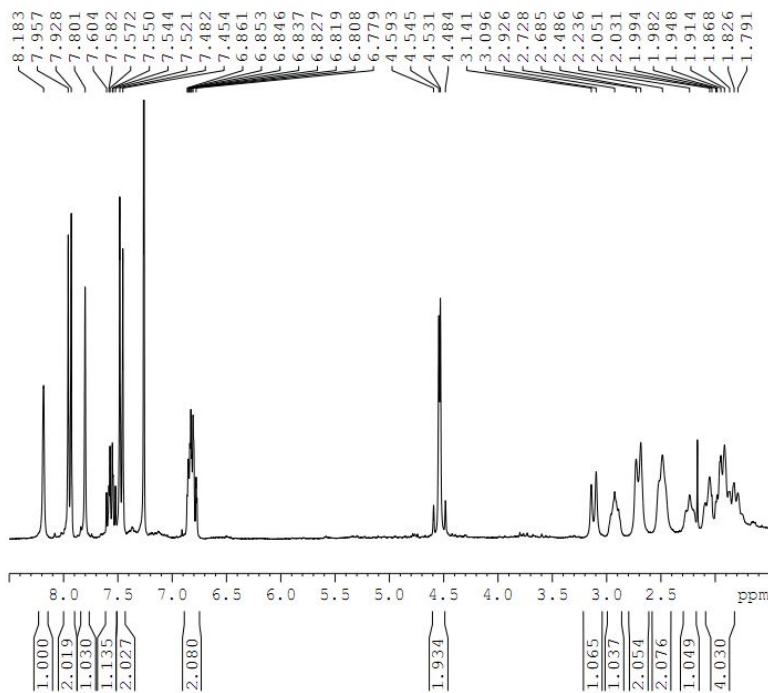
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PROCNO 1

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NS 16
DS 0
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FIDRES 0.146719 Hz
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TE 295.2 K
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NUC1 1H
P1 13.70 usec
PLW1 19.34000015 W

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GB 0
PC 1.00

6j



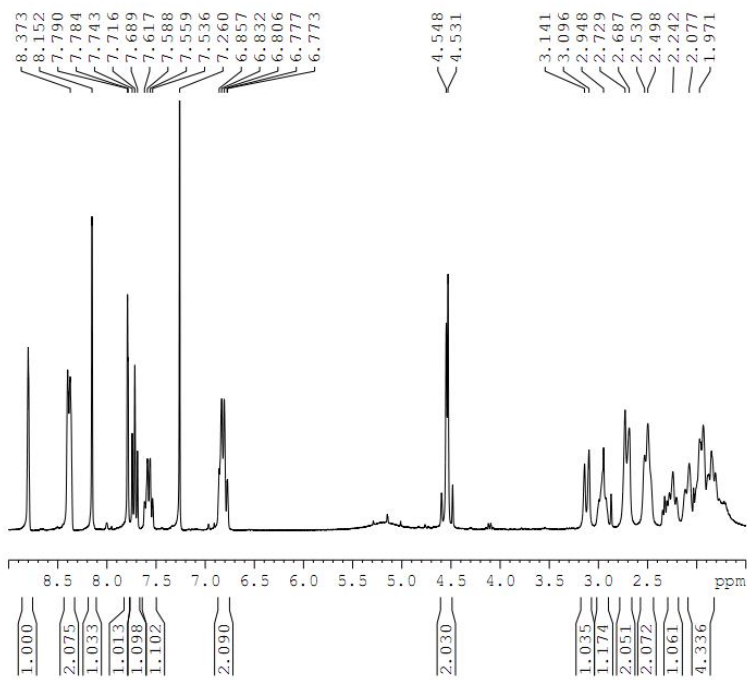
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EXPNO 1
PROCNO 1

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SOLVENT CDC13
NS 128
DS 0
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 45.2
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
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NUC1 1H
P1 12.90 usec
PLW1 11.00000000 W

F2 - Processing parameters
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SF 300.1300066 MHz
WDW EM
SSB 0
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GB 0
PC 1.00

60



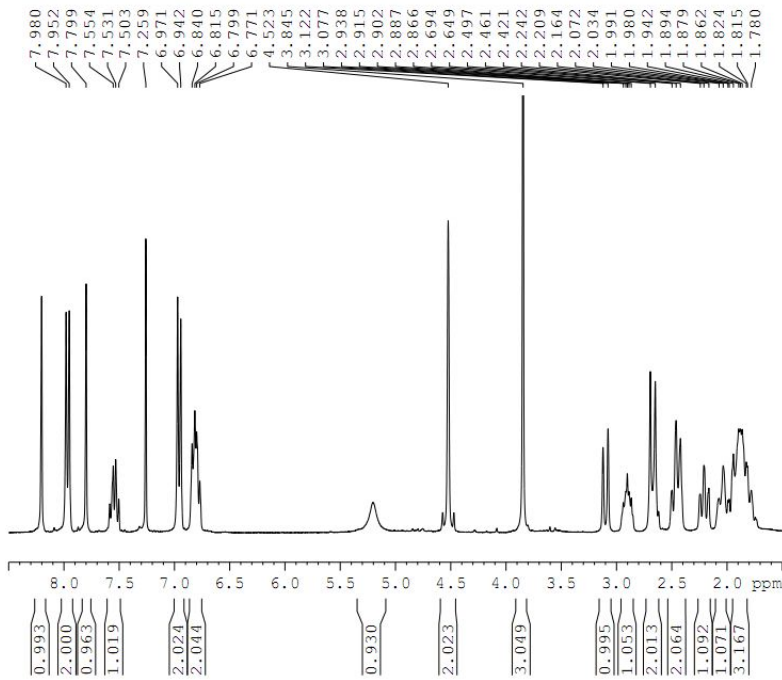
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 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6009.615 Hz
 FIDRES 0.183399 Hz
 AQ 2.7263477 sec
 RG 28.5
 DW 83.200 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 300.1324010 MHz
 NUC1 1H
 P1 12.90 usec
 PLW1 11.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1300066 MHz
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 SSB 0
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 GB 0
 FC 1.00

11b

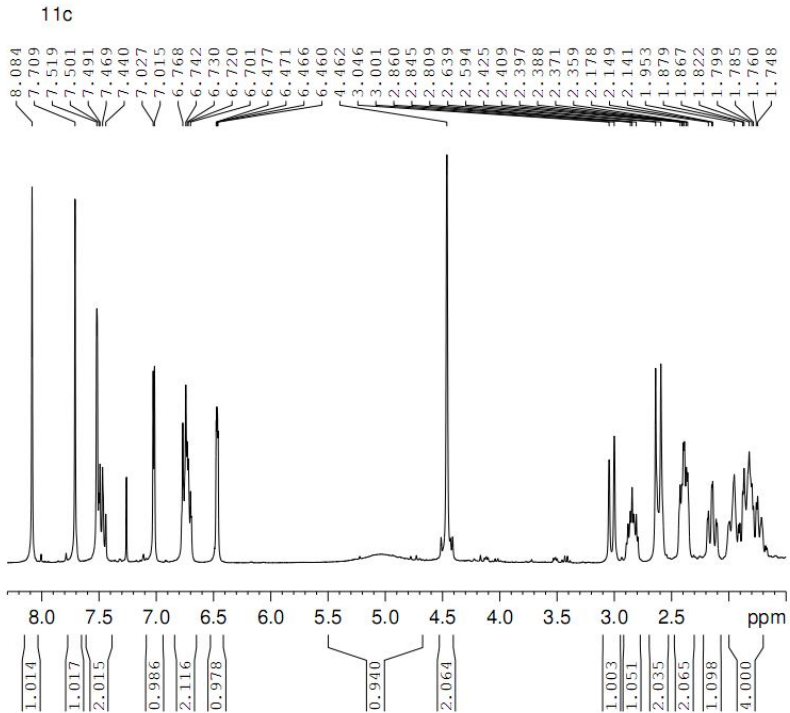


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 NAME hxm-70-1
 EXPNO 11
 PROCNO 1

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 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6009.615 Hz
 FIDRES 0.183399 Hz
 AQ 2.7263477 sec
 RG 28.5
 DW 83.200 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
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 NUC1 1H
 P1 12.90 usec
 PLW1 11.00000000 W

F2 - Processing parameters
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 SF 300.1300072 MHz
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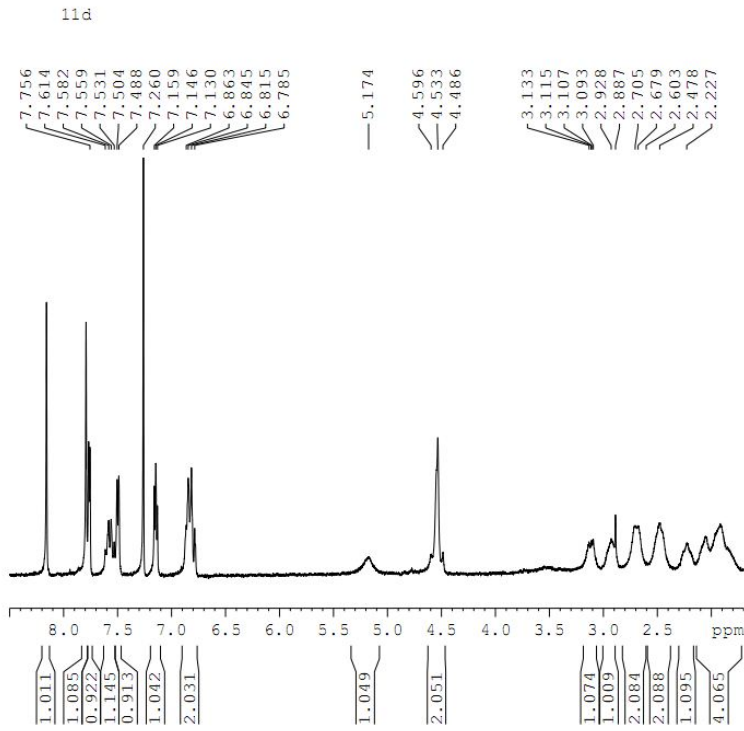


Current Data Parameters
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 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
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 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6009.615 Hz
 FIDRES 0.183399 Hz
 AQ 2.7263477 sec
 RG 28.5
 DW 83.200 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1324010 MHz
 NUC1 1H
 P1 12.90 usec
 PLW1 11.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1300066 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

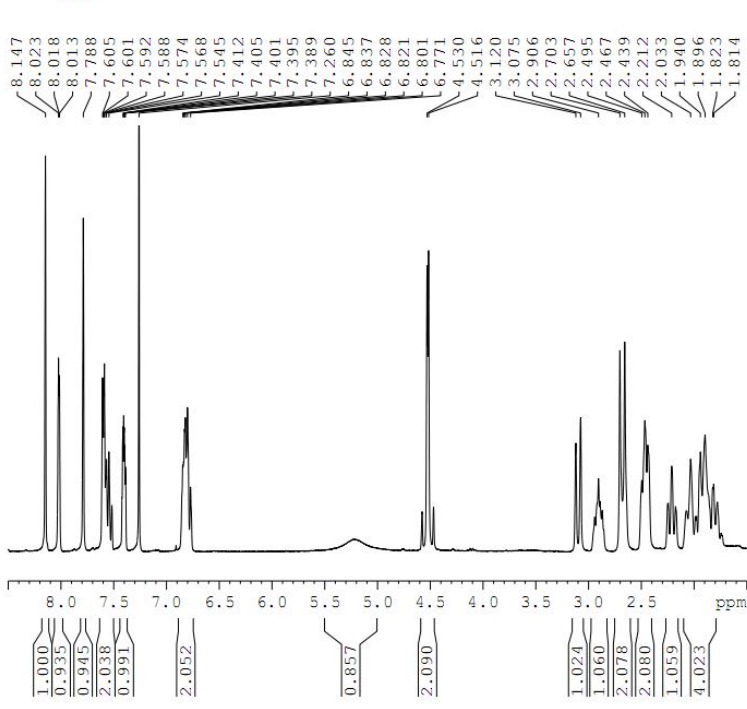


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 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
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 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6009.615 Hz
 FIDRES 0.183399 Hz
 AQ 2.7263477 sec
 RG 28.5
 DW 83.200 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1324010 MHz
 NUC1 1H
 P1 12.90 usec
 PLW1 11.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1300067 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME hxm-105b
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20140610
 Time 14.43
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 16
 DS 0
 SWH 6009.615 Hz
 FIDRES 0.183399 Hz
 AQ 2.7263477 sec
 RG 28.5
 DW 83.200 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 300.1324010 MHz
 NUC1 1H
 P1 12.90 usec
 PLW1 11.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1300067 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 FC 1.00

Determination of the purity of target compounds by HPLC analysis. Representative data was provided for compound 11b.

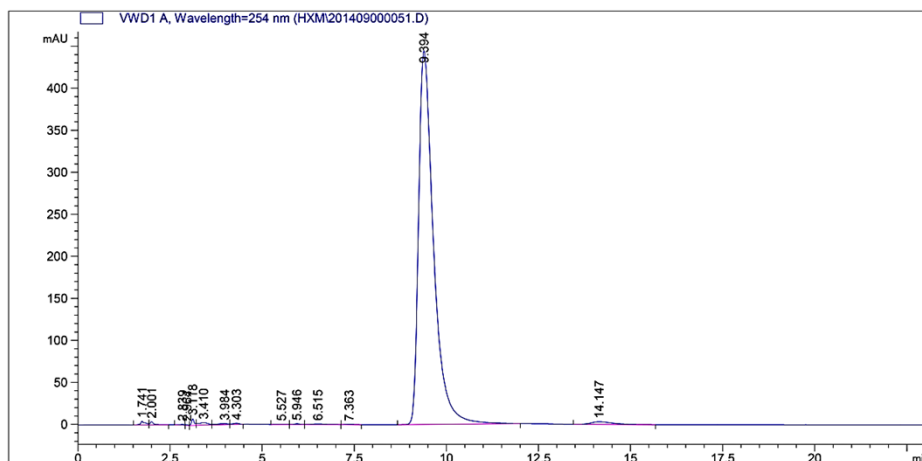
Data File D:\CHEM32\1\DATA\HXM\201409000051.D
 Sample Name: 70-1

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Acq. Instrument : HPLC1260
Injection Date  : 9/28/2014 8:12:23 PM
Location       : -
Inj Volume     : Manually

Acq. Method    : D:\CHEM32\1\DATA\HXM\201409000049.D\RUN.M
Last changed   : 9/28/2014 2:32:18 PM by hxm
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Last changed   : 9/28/2014 9:09:13 PM by hxm
Method Info    : MeOH/H2O=70:30,254nm,0.8ml/min,460*250MM

Sample Info    : CH3OH/H2O=78/22 254nm, 1ml/min
                  C18 460*250MM
  
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Area Percent Report

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Sorted By      : Signal
Multiplier:    : 1.0000
Dilution:      : 1.0000
Sample Amount: : 1.00000 [ng/ul] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs
  
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Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
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2	2.001	VB	0.0922	24.27445	3.79013	0.1881
3	2.839	BV	0.1169	7.09739	8.45329e-1	0.0550
4	2.964	VB	0.0775	4.24229	8.45386e-1	0.0329

HPLC1260 11/7/2014 11:10:29 AM hyh

Page 1 of 2

5	3.118	BV	0.0693	37.93463	8.07766	0.2940
6	3.410	VV	0.2672	53.70966	2.91793	0.4162
7	3.984	VV	0.3029	27.80171	1.19122	0.2154
8	4.303	VB	0.1705	16.53780	1.42304	0.1282
9	5.527	BV	0.2908	3.65873	1.95762e-1	0.0284
10	5.946	VV	0.1659	8.34250	7.59918e-1	0.0646
11	6.515	VB	0.3889	16.40956	6.05643e-1	0.1272
12	7.363	BB	0.2212	4.01097	2.82065e-1	0.0311
13	9.394	BB	0.4233	1.25316e4	444.89804	97.1083
14	14.147	BB	0.6030	132.45390	3.26435	1.0264

Totals : 1.29048e4 473.56069

*** End of Report ***