

Supporting Information

Design, Synthesis and Biological Evaluation of Novel androst-17 β -amide structurally related compounds as Dual 5 α -reductase Inhibitors and Androgen Receptor Antagonists

Kejing Lao^{a,b,c}, Guoliang Xun^d, Xingchun Gou^{a*}, Hua Xiang^{b,c*}

^a*Institute of Basic and Translational Medicine & Shaanxi Key Laboratory of Brain Disorders, Xi'an Medical University, No.1 Xinwang Road, Xi'an, 710021, PR China*

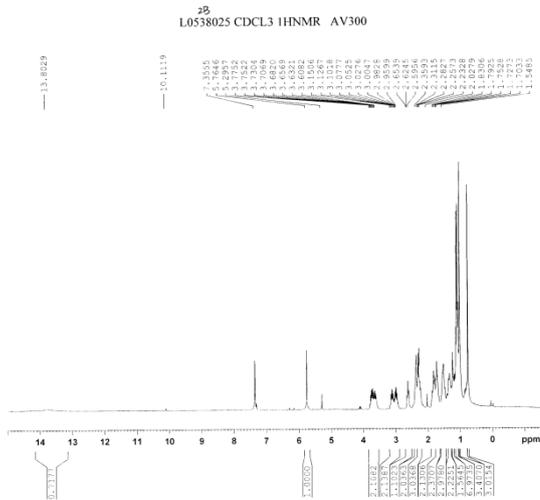
^b*Jiangsu Key Laboratory of Drug Design and Optimization, China Pharmaceutical University, 24 Tongjiaxiang, Nanjing 210009, PR China*

^c*Department of Medicinal Chemistry, School of Pharmacy, China Pharmaceutical University, 24 Tongjiaxiang, Nanjing 210009, PR China*

^d*Shanghai Abbisko Therapeutics Co., Ltd*

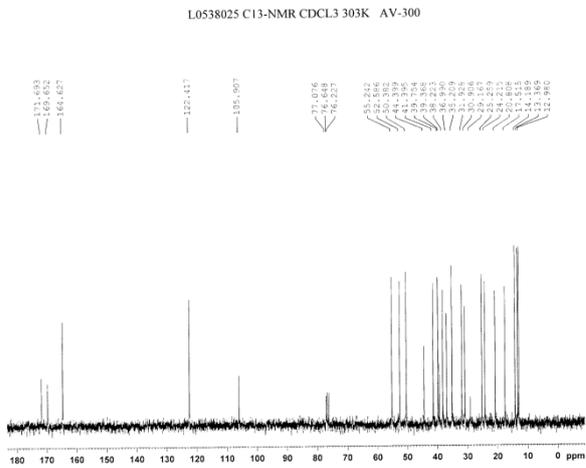
* Corresponding author. Tel.: +86 29 86177603; Fax:+86 29 86177603 (X. Gou) and Tel.: +86 025 83271096; Fax: +86 025 83271096 (H. Xiang). E-mail addresses: gxchun@126.com (X. Gou) and xianghua@cpu.edu.cn (H. Xiang).

7b



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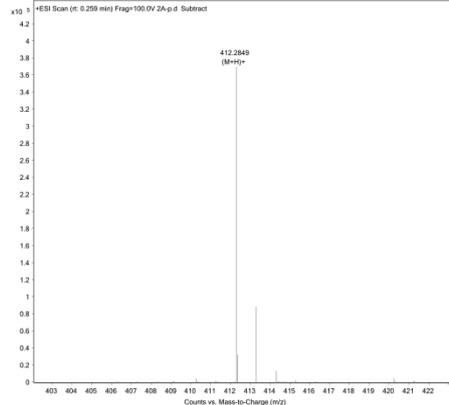
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TD         32768
SOLVENT   CDCL3
DS         4
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RG         0.320019 Hz
AQ         2.77844 sec
RG         69.333
DE         0.00 usec
TE         300.2 K
D1         1.0000000 sec
D11        0
TD0        1
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NUC1       13
P1         12.48 usec
PC1        0.00 dB
PL1W      12.36450577 dB
SFO1       100.628114 MHz
NUC2       1
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PC2        0.00 dB
PL2W      0.00000000 MHz
SFO2       0.00000000 MHz
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EXPNO     2
PROCNO    1
DATE_     20160405
TIME      8.41
INSTRUM   spect
PROBHD    5 mm QNP1H 13C
PULPROG   zgpg30
TD         65536
SOLVENT   CDCL3
DS         8
AQ         1.9531200 sec
RG         0.238023 Hz
RG         1.6737316 sec
AQ         46.3
DE         23.600 usec
TE         300.2 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1
----- CHANNEL f1 -----
NUC1       13C
P1         12.48 usec
PC1        0.00 dB
PL1W      12.36450577 dB
SFO1       100.628114 MHz
----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2       13
P2         60.00 usec
PC2        0.00 dB
PL2W      11.80000000 dB
PL2W      12.36450577 dB
SFO2       0.31876211 MHz
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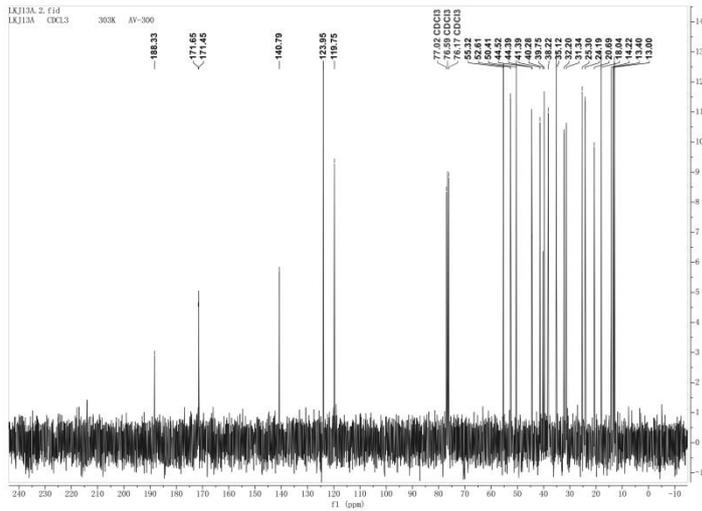


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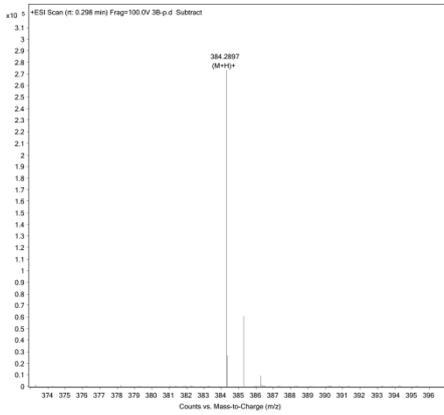
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TIME      8.41
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TD         65536
SOLVENT   CDCL3
DS         8
AQ         1.9531200 sec
RG         0.238023 Hz
RG         1.6737316 sec
AQ         46.3
DE         23.600 usec
TE         300.2 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1
----- CHANNEL f1 -----
NUC1       13C
P1         12.48 usec
PC1        0.00 dB
PL1W      12.36450577 dB
SFO1       100.628114 MHz
----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2       13
P2         60.00 usec
PC2        0.00 dB
PL2W      11.80000000 dB
PL2W      12.36450577 dB
SFO2       0.31876211 MHz
SFO2       300.1312000 MHz
SI         32768
SF         75.4678607 MHz
NS         500
DSB        0
LB         1.00 Hz
DD         0.50
  
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ACQ Method	Comment		Acquired Time

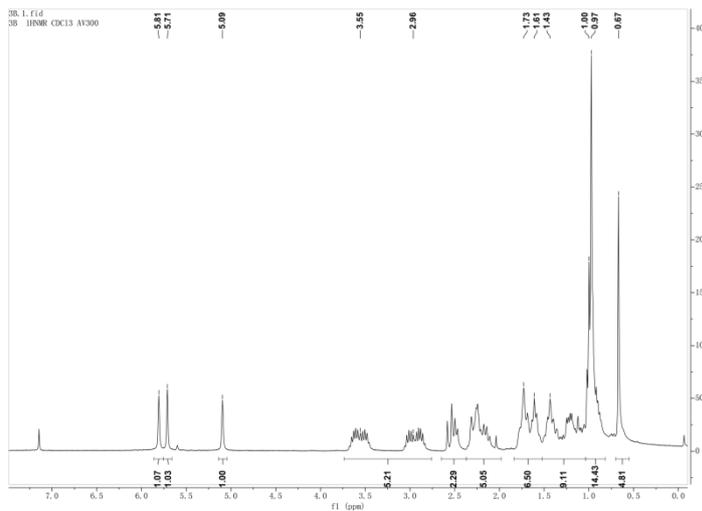


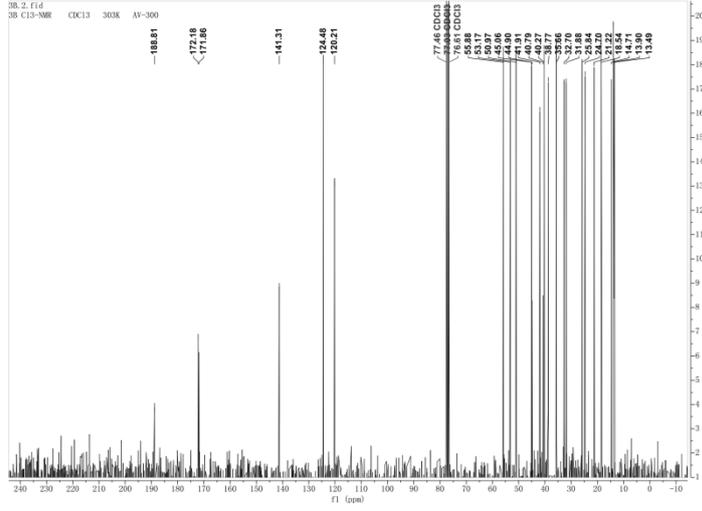


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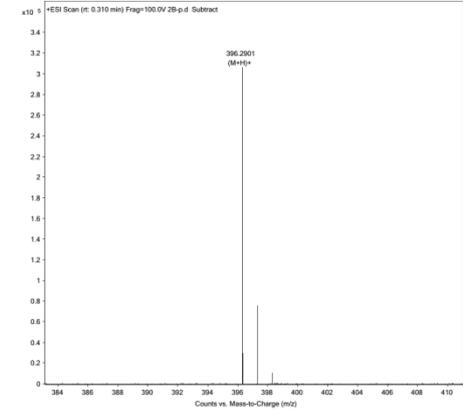


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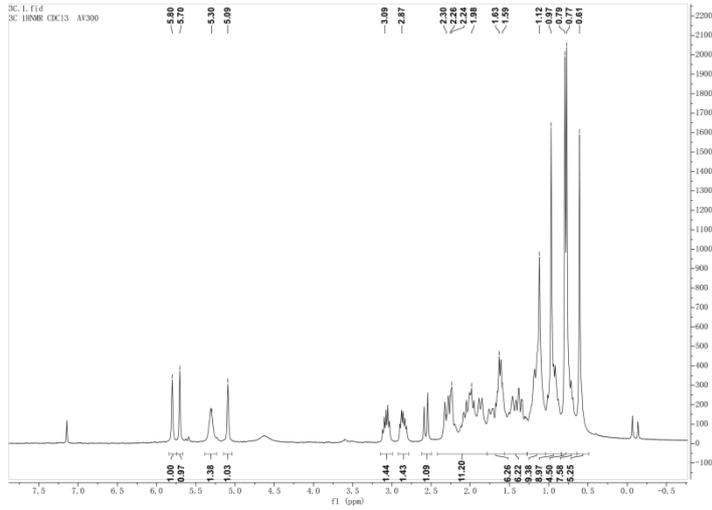


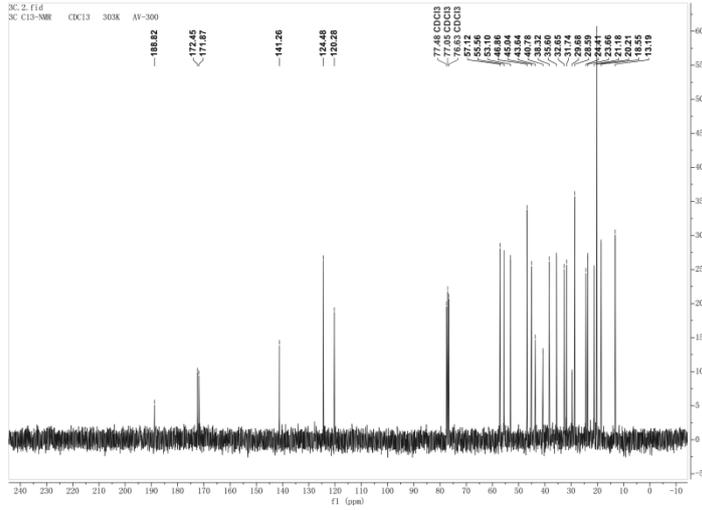


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Sample Type	SRM Calibration Status	Success	Data Filename
ACQ Method	Comment		Acquired Time

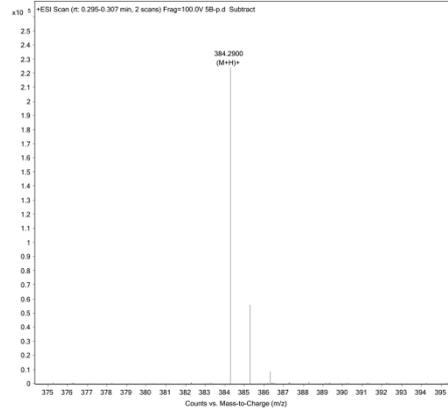


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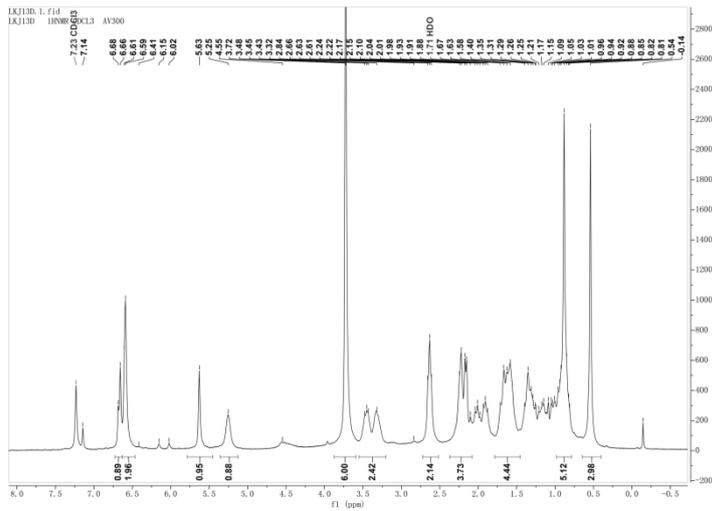


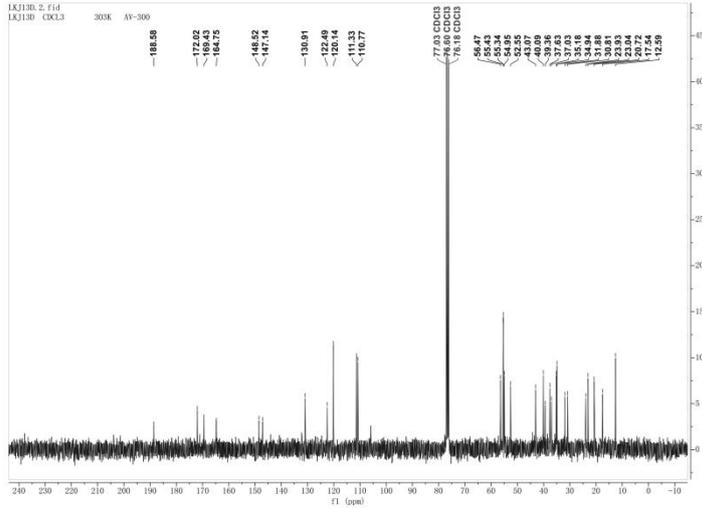


Sample Name	Position	PID#	Instrument Name	Instrument 1
User Name	log Met	0.05	HighResolution	
Sample Type	Sample	SRM Calibration Status	Success	
ACQ Method	2011010-HSonly.p.m	Comment		
			Data Filename	SR.p.d
			Acquired Time	5/9/2017 2:39:13 PM (UTC+08:00)

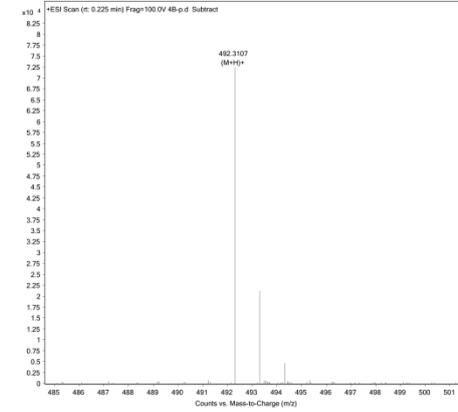


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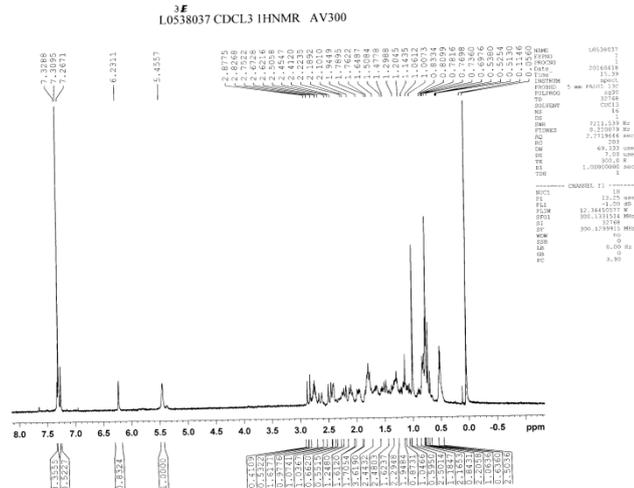


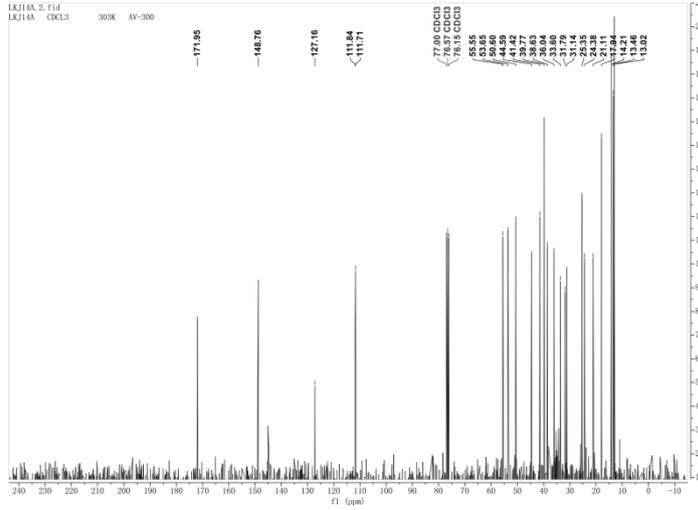


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User Name	Exp No.	026	HighResolution	
Sample Type	IRN Calibration Status	Success	Data Filename	46.p.d
Acq Method	Comment		Acquired Time	5/9/2017 2:29:38 PM (UTC+08:00)

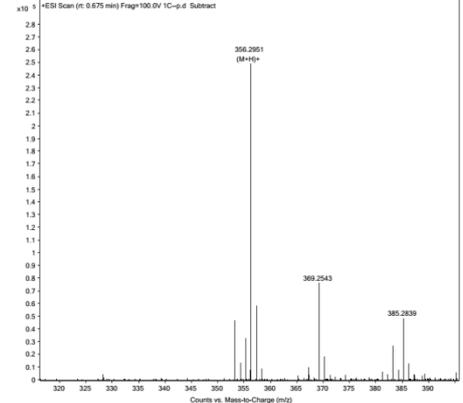


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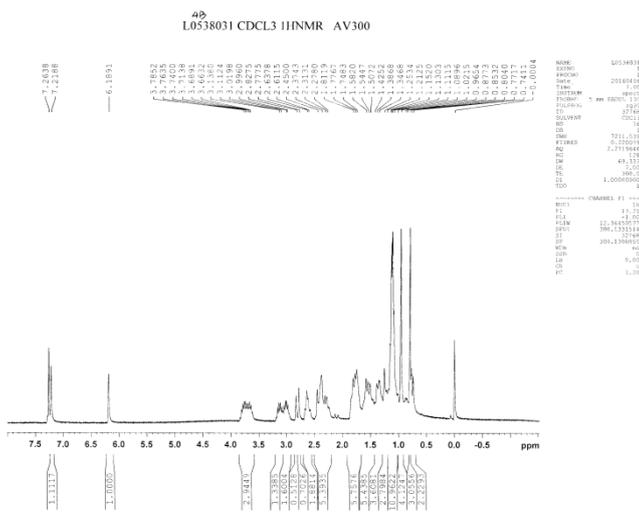




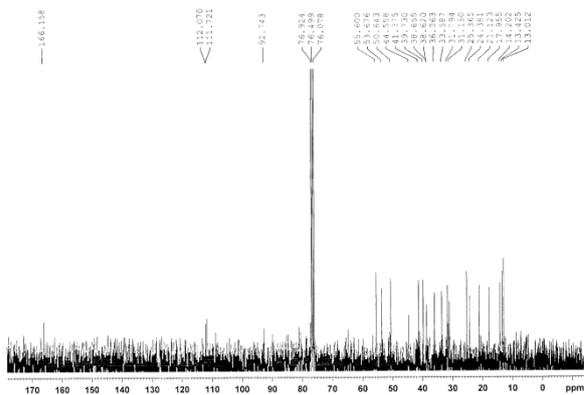
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User Name	log file	0.03	HighResolution	IC-p.d
Sample Type	IBM Calibration Status	Success	Data Filename	Acquired Time
ACQ Method	20110418-HSonly-p.d	Comment	5/9/2017 2:05:39 PM (UTC+08:00)	



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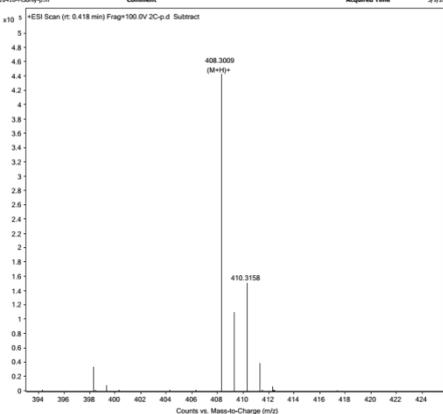
L0538031 C13-NMR CDCL3 303K AV-300



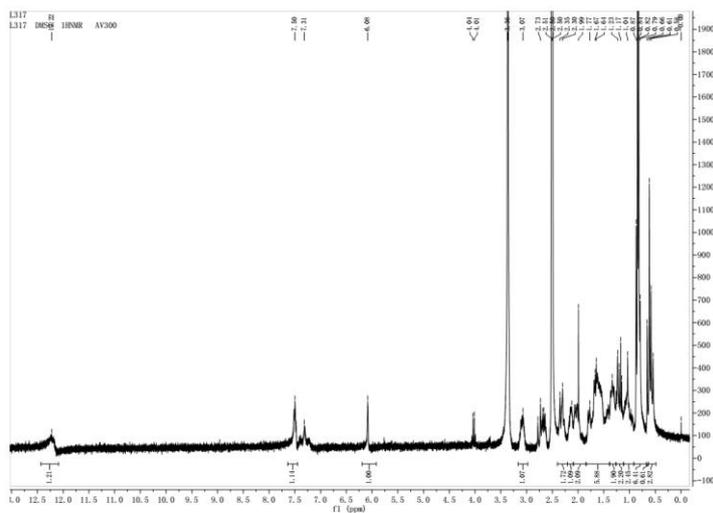
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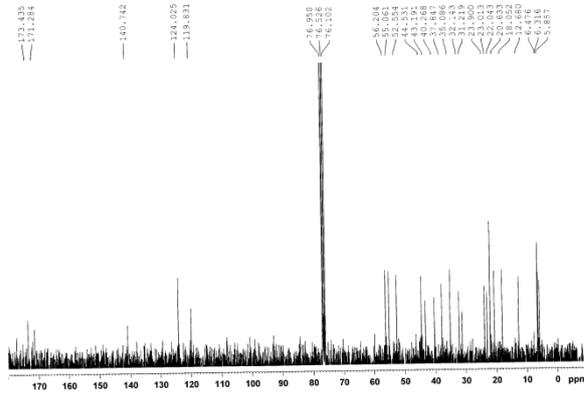
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PROCNO    1
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PULPROG   zgpg
TD         65536
SOLVENT   CDCl3
NS         4
DS         4
SWH        19331.258 Hz
FIDRES     0.298023 Hz
AQ         0.4777716 sec
RG         48.3
AQ         25.400 usec
DE         9.98 usec
TE         300.2 K
D1         2.0000000 sec
D11        0.0300000 sec
D20        1
----- CHANNEL f1 -----
NUC1       13C
P1         12.00 usec
PL1        0.00 dB
PL12       42.1745193 dB
SFO1       75.4764718 MHz
----- CHANNEL f2 -----
NAMEF2     waltz16
NUC2       1H
PCPD2      60.00 usec
PL2        1.00 dB
PL12       14.00 dB
PL12W      12.3643057 dB
PL12W      0.3389211 dB
SFO2       300.1362601 MHz
SF         375.0
RF         75.4487663 MHz
WDW         RM
SSB         0
LB          1.00 Hz
GB          0
PC          0.30
    
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Sample Name	Position	Instrument Name
20110418-HSonly-2.m	PC07	Instrument 1
User Name	log hcl	HighResolution
Sample Type	IBM Calibration Status	Success
ACQ Method	Comment	Data Filename
		Acquired Time



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NAME      L0538036
EXPNO    2
PROCNO   1
DATE_    20160413
Time     15.55
INSTRUM  spect
PROBHD   5 mm P4001
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        128
DS        4
SFORES   16666.666 Hz
FIDRES   0.254333 Hz
AQ        1.9641305 sec
RG        38
SWH       39.950 uspec
WDW       0.00 uspec
SS        300.0 K
TE        2.00000000 sec
D11       0.03000000 sec
TD0

===== CHANNEL f1 =====
NUC1      13C
P1        12.40 usec
PL1       0.00 dB
PL12      42.3745195 W
SFO1      75.4752213 MHz

===== CHANNEL f2 =====
C1P1PRG2  waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       1.00 dB
PL12      14.00 dB
PL13      17.3845077 W
PL14      0.3388211 W
PL15      0.34054621 W
SFO2      300.1312023 MHz
SI        32768
SF        75.4677843 MHz
WDW       0
SS        1.00 Hz
GB        0
PC        1.00
    
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Sample Name	Position	Instrument Name	Instrument 1
User Name	log H4	HighResolution	SC-p.d
Sample Type	IBM Calibration Status	Data Filename	5/9/2017 2:42:44 PM (UTC+08:00)
ACQ Method	20110413-HSonly-p.m	Acquired Time	

