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Synthesis, Crystal Structure and Anti-ischemic Activity of (*E*)-1-(4-(Bis(4-methoxy-phenyl)methyl)piperazin-1-yl)-3-(4-chlorophenyl)-prop-2-en-1-one

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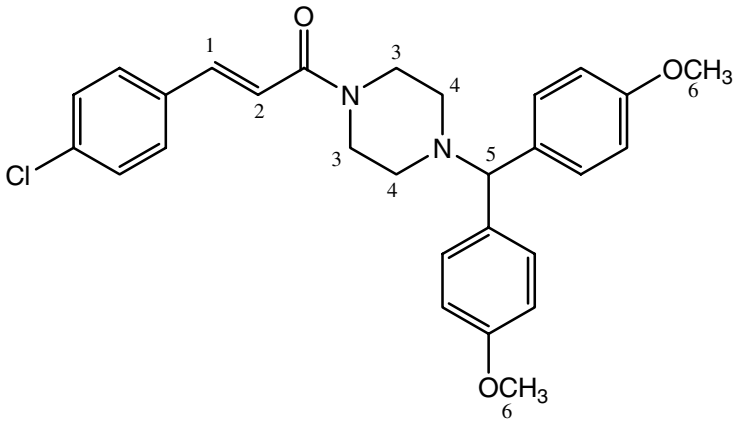
Material and Methods

^{1}H NMR and ^{13}C NMR were recorded on a Bruker ACF-300 MHz instrument (Bruker) with $CDCl_3$ as the solvent and tetramethylsilane as an internal standard (chemical shifts are expressed as δ values, J in hertz). High resolution mass spectra (HRMS) was recorded on a MALDI Micro MX instrument (Waters). IR spectra was recorded on a Bruker Tensor 27 FT-IR instrument (Bruker).



compound 5

Table 1: ^{1}H NMR Chemical Shifts (δ, ppm) and Coupling Constants (J, Hz) of compound **5**

No.	**Compound 5**
1	7.56 (d, J = 15.3 Hz)
2	6.77 (d, J = 15.0 Hz)
3	3.52 (m)
4	2.39 (m)
5	4.18 (s)
6	3.76 (s)

Figure 1 ^{1}H NMR spectrum of compound **5**

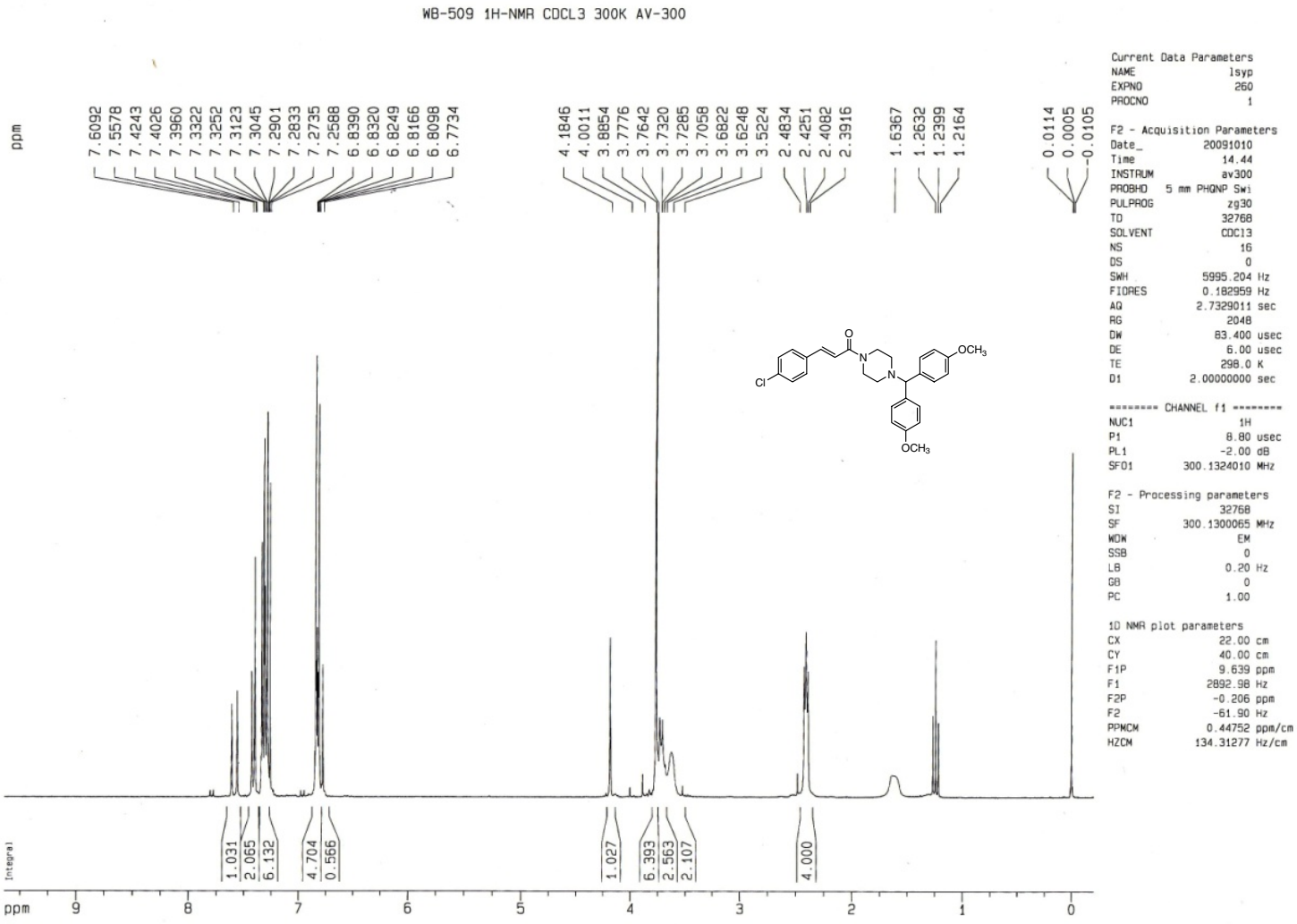
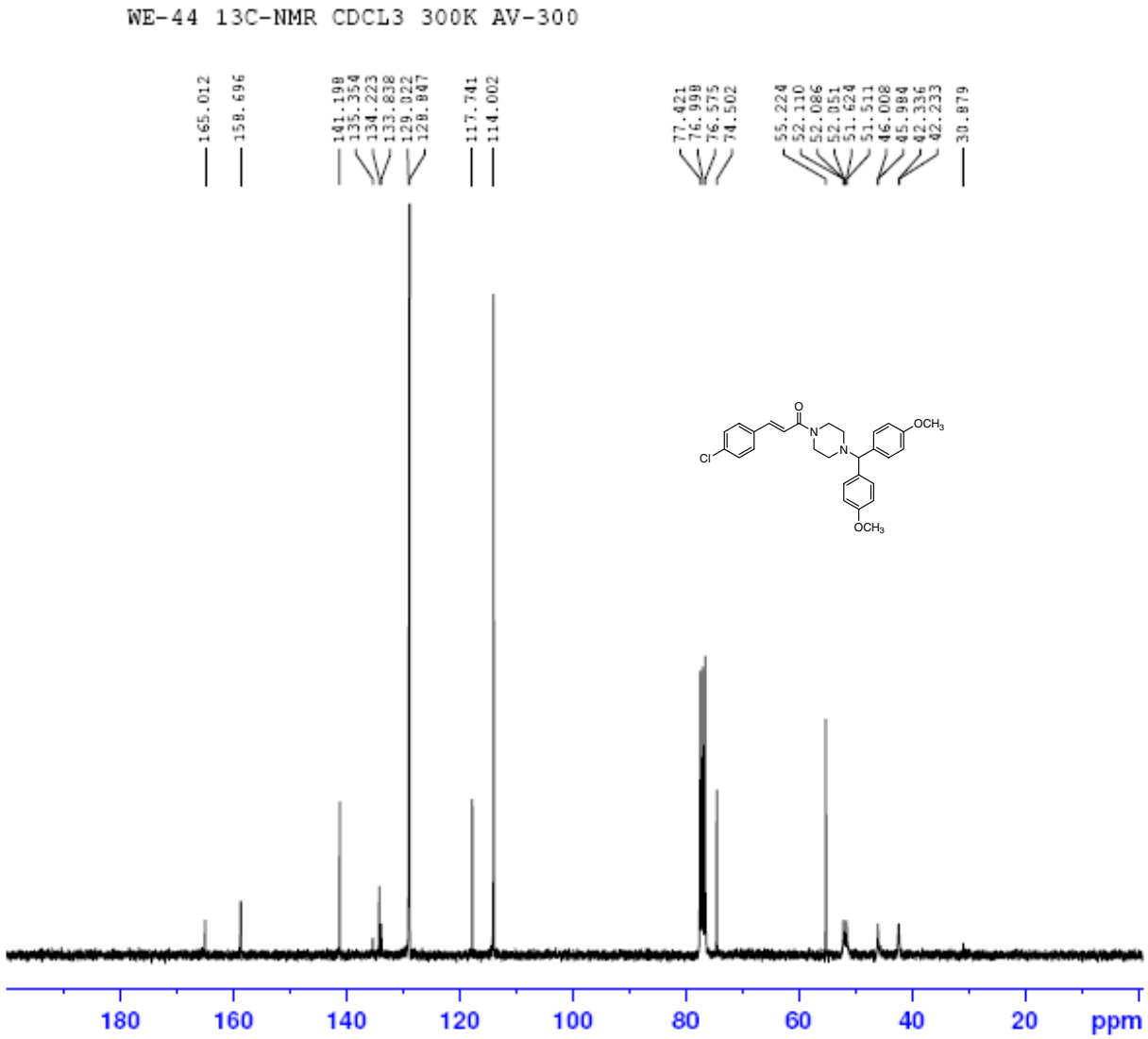
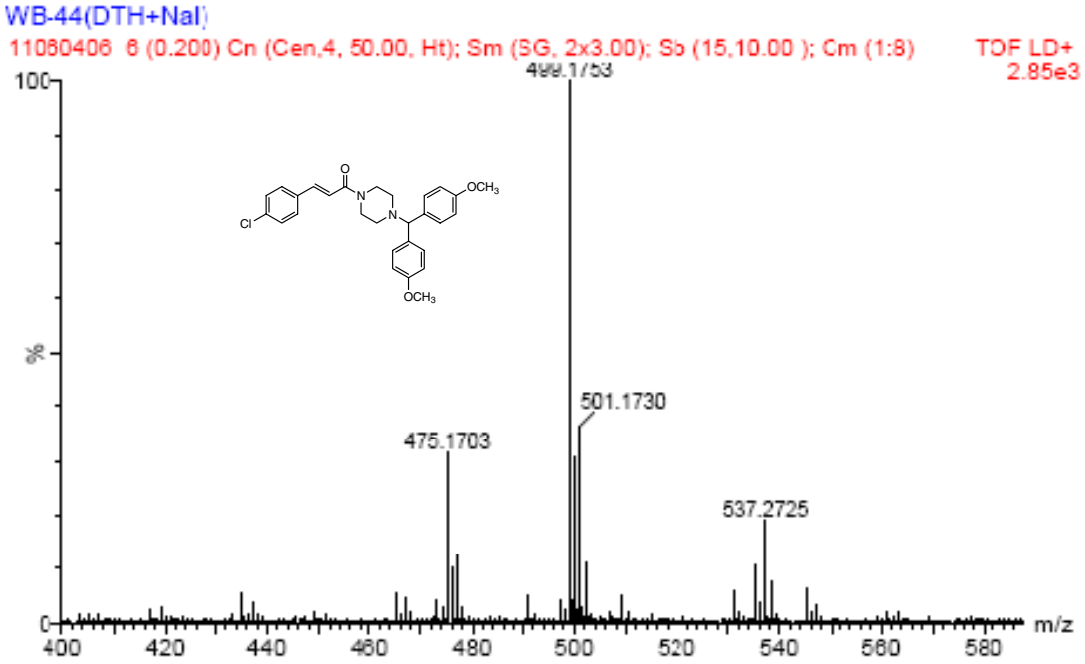


Figure 2 ^{13}C NMR spectrum of **5**



NAME	py300	
EXPNO	26	
PROCNO	1	
Date_	20140101	
Time	15.51	
INSTRUM	av300	
PROBHD	5 mm PHQNP Swi	
PULPROG	zgdc	
TD	32768	
SOLVENT	CDCl3	
NS	12804	
DS	2	
SWH	18115.941	Hz
FIDRES	0.552855	Hz
AQ	0.9044469	sec
RG	102400	
DW	27.600	usec
DE	6.00	usec
TE	300.0	K
D1	1.00000000	sec
d11	0.03000000	sec
========	CHANNEL f1	========
NUC1	13C	
P1	6.20	usec
PL1	-5.00	dB
SFO1	75.4763979	MHz
========	CHANNEL f2	========
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	-2.00	dB
PL12	19.00	dB
SFO2	300.1312005	MHz
SI	32768	
SF	75.4677486	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	0.20	

Figure 3 HRMS spectrum of **5**



Elemental Composition Report

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -10.0, max = 100.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
60 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Minimum:				-10.0		
Maximum:		50.0	10.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
499.1753	499.1764	-1.1	-2.3	14.5	1	C28 H29 N2 O3 Na Cl

Figure 4 IR spectrum of compound **5**