Supporting Information

Chemical components from the seeds of *Catalpa bungei* and their inhibition of soluble epoxide hydrolase, cholinesterase and nuclear factor kappa B activities

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Mumhar	1					
number	¹³ C	¹ H	¹ H- ¹ HCOSY	HMBC	NOESY	
1	93.1	5.70 d, <i>J</i> = 2.1 Hz	Н-9	C-5, C-8	H-6, H-10, H-1	
3	95.9	5.35 d, <i>J</i> = 2.8 Hz	H_{α} , H_{β} -4	C-1, C-5		
4	34.4	2.49 dd, <i>J</i> = 13.5, 8.3 Hz	H-5	C-6, C-5		
		2.13 dd, <i>J</i> = 13.9, 3.2 Hz	Н-3	C-9, C-6	Н-6	
5	34.8	2.40, m	H-9, H-6	C-8	H-7	
6	87.7	5.05 dd, <i>J</i> = 8.3, 2.7 Hz	H-5, H-7	C-7, C-9, C-5	H-1	
7	70.4	4.46 d, <i>J</i> = 8.3 Hz	H-6	C-6, C-8	H-5, H-9	
8	79.9					
9	48.3	2.65 br. d, <i>J</i> = 9.9 Hz	H-5, H-1	C-4, C-8	H-7	
10	62.1	4.08 d, <i>J</i> = 12.0 Hz		C-3, C-7, C-9	H-1	
		3.72 d, <i>J</i> = 11.8 Hz		C-3, C-7		
1'	99.0	4.73 d, <i>J</i> = 8.0 Hz	H-2'	C-1	H-1	
2'	74.7	3.19 dd, <i>J</i> = 9.1, 8.1 Hz	H-3', H-2'			
3'	78.2	3.41, m	H-2',H-4'			
4'	71.6	3.31, m	Overlap			
5'	78.1	3.31, m	Overlap			
6'	62.7	3.70, m	H-5'			
		3.90, m	H-5'			
1"	127.6					
2"	111.9	7.25 d, <i>J</i> = 1.8 Hz		C-4"	H-10"	
3"	149.4					
4"	150.8					
5"	116.5	6.85 d, <i>J</i> = 8.2 Hz	H-6"	C-3", C-1"		
6"	124.3	7.13 dd, <i>J</i> = 8.2, 1.9 Hz	H-5"	C-2", C-4"		
7"	147.5	7.68 d, <i>J</i> = 15.9 Hz	H-7"	C-9", C-6",		
				C-2"		
8"	114.9	6.45 d, <i>J</i> = 15.9 Hz	H-8"	C-1"		
9"	168.8					
10"	56.5	3.93, s		C-3"	H-2"	

Table S1. NMR data of 1 (CH₃OH- d_4)

NT 1			2		
Number	¹³ C	$^{1}\mathrm{H}$	¹ H- ¹ HCOSY	HMBC	NOESY
1	93.1	5.64 d, <i>J</i> = 2.0 Hz	H-9	C-5, C-8	H-6, H-10, H-1'
3	95.9	5.30 d, <i>J</i> = 2.7 Hz	H _α , H _β -4	C-1, C-5	
4	34.4	2.43 dd, <i>J</i> =13.4, 8.5 Hz	Н-5	C-6, C-5	
		2.07 dd, <i>J</i> = 13.9, 3.2 Hz	Н-3	C-9, C-6	H-6
5	34.7	2.34 m	H-9, H-6	C-8	H-7
6	87.7	4.99 dd, J = 8.3, 2.7	H-5, H-7	C-7, C-9, C-5	H-1
		Hz			
7	70.4	4.41 d, <i>J</i> = 8.1 Hz	H-6	C-6, C-8	H-5, H-9
8	79.9				
9	48.3	2.59 br. d, <i>J</i> = 9.9 Hz	H-5, H-1	C-4, C-8	H-7
10	62.1	4.02 d, <i>J</i> = 11.8 Hz		C-3, C-7, C-9	H-1
		3.65 m		C-3, C-7	
1'	98.9	4.67 d, <i>J</i> = 8.0 Hz	H-2'	C-1	H-1
2'	74.7	3.14 t, <i>J</i> = 8.6 Hz	H-3', H-2'		
3'	78.1	3.35, m	H-2',H-4'		
4'	71.6	3.26, m	H-3', H-5'		
5'	78.1	3.28, m	H-4', H-6'		
6'	62.7	3.85, m	H-5'		
		3.65, m	H-5'		
1"	127.0				
2"	131.3	7.46 d, <i>J</i> = 8.6 Hz	H-3"	C-4", C-7"	
3"	116.9	6.79 d, <i>J</i> = 8.6 Hz	H-2"	C-1", C-5"	
4"	161.5				
5"	116.9	6.79 d, <i>J</i> = 8.6 Hz	H-6"	C-1", C-3"	
6"	131.3	7.46 d, <i>J</i> = 8.6 Hz	H-5"	C-2", C-7"	
7"	147.2	7.62 d, <i>J</i> = 15.8 Hz	H-8"	C-9", C-2"	
8"	114.5	6.36 d, <i>J</i> = 15.9 Hz	H-7"	C-1"	
9"	168.9				
10"					

Table S2. NMR data of 2 (CH_3OH-d_4)

$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Nu	imber	3		
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		¹³ C	$^{1}\mathrm{H}$	¹ H- ¹ HCOSY	HMBC
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1	93.1	5.70 d, <i>J</i> = 2.1 Hz	Н-9	C-5, C-8
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3	95.9	5.36 d, J = 2.8 Hz	$H_{\alpha}, H_{\beta}-4$	C-1, C-5
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	34.4	2.49 dd, <i>J</i> = 13.3, 8.5 Hz	H-5	C-6, C-5
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$			2.16 dd, <i>J</i> = 13.8, 3.2 Hz	H-3	C-9, C-6
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	5	34.7	2.43, m	H-9, H-6	C-8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	6	87.9	5.13 dd, <i>J</i> = 8.3, 2.7 Hz	H-5, H-7	C-7, C-9,
7 70.4 $4.54 \text{ dd}, J = 8.3, 0.9 \text{ Hz}$ $H-6$ $C-6, C-8$ 8 79.9 9 48.3 $2.67 \text{ br. d}, J = 9.8 \text{ Hz}$ $H-5, H-1$ $C-4, C-8$ 10 62.1 $4.09 \text{ dd}, J = 12.1, 0.8 \text{ Hz}$ $C-3, C-7, C-9$ $C-3$ $3.72 \text{ d}, J = 12.4 \text{ Hz}$ $C-3, C-7$ 1' 98.9 $4.73 \text{ d}, J = 8.0 \text{ Hz}$ $H-2'$ $C-1$ 2' 74.2 $3.18 \text{ dd}, J = 9.0, 8.1 \text{ Hz}$ $H-3', H-2'$ $C-1$ 3' 78.1 $3.40, \text{ m}$ $H-2', H-4'$ H' 4' 71.6 $3.31, \text{ m}$ $H-3', H-5'$ S' 5' 78.1 $3.30, \text{ m}$ $H-4', H-6'$ $6'$ 6' 62.7 $3.70, \text{ m}$ $H-5'$ $H-5'$ 1'' 121.4 Z'' 132.9 $7.92 \text{ d}, J = 8.8 \text{ Hz}$ $H-3''$ 4'' 116.4 $6.87 \text{ d}, J = 8.8 \text{ Hz}$ $H-6'''$ $H-6'''$ 6'' 132.9 $7.92 \text{ d}, J = 8.8 \text{ Hz}$ $H-6'''$ $H-6''''$ 7''' $168.$					C-5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	7	70.4	4.54 dd, <i>J</i> = 8.3, 0.9 Hz	H-6	C-6, C-8
9 48.3 2.67 br. d, $J = 9.8$ Hz H-5, H-1 C-4, C-8 10 62.1 4.09 dd, $J = 12.1$, 0.8 Hz C-3, C-7, C-9 3.72 d, $J = 12.4$ Hz C-3, C-7 1' 98.9 4.73 d, $J = 8.0$ Hz H-2' C-1 2' 74.2 3.18 dd, $J = 9.0$, 8.1 Hz H-3', H-2' C-1 3' 78.1 3.40, m H-2', H-4' H-3', H-5' 5' 78.1 3.30, m H-4', H-6' H-6' 6' 62.7 3.70, m H-5' H-3'' 1'' 121.4 2'' 164.3 6.87 d, $J = 8.8$ Hz H-3'' 4'' 164.3 5'' 116.4 6.87 d, $J = 8.8$ Hz H-6'' 6'' 132.9 7.92 d, $J = 8.8$ Hz H-6'' H-5'' 7''' 168.6 164.5 16.87 d, $J = 8.8$ Hz H-6'''	8	79.9			
10 62.1 $4.09 \text{ dd}, J = 12.1, 0.8 \text{ Hz}$ C-3, C-7, C-9 $3.72 \text{ d}, J = 12.4 \text{ Hz}$ C-3, C-7 1' 98.9 $4.73 \text{ d}, J = 8.0 \text{ Hz}$ H-2' C-1 2' 74.2 $3.18 \text{ dd}, J = 9.0, 8.1 \text{ Hz}$ H-3', H-2' C-1 3' 78.1 $3.40, \text{ m}$ H-2', H-4' H-3', H-5' 5' 78.1 $3.30, \text{ m}$ H-4', H-6' 6' 62.7 $3.70, \text{ m}$ H-5' $3.91, \text{ m}$ H-5' H-3'' H-4'' 1'' 121.4 How H-2'' H-4'' 1'' 121.4 H-4', H-6' H-6'' H-5'' H-5'' 1'' 121.4 H-4'', H-6' H-5'' H-5'' H-4'', H-6'' H-4'', H-6'' 1'' 121.4 H-10'' H-2''' H-4'', H-6'' H-4'', H-6'' H-2''' H-4'', H-6'' H-4''	9	48.3	2.67 br. d, $J = 9.8$ Hz	H-5, H-1	C-4, C-8
C-9 $3.72 d, J = 12.4 Hz$ C-3, C-71'98.9 $4.73 d, J = 8.0 Hz$ H-2'2'74.2 $3.18 dd, J = 9.0, 8.1 Hz$ H-3', H-2'3'78.1 $3.40, m$ H-2',H-4'4'71.6 $3.31, m$ H-3', H-5'5'78.1 $3.30, m$ H-4', H-6'6'62.7 $3.70, m$ H-5'1"121.4121.42"132.97.92 d, $J = 8.8 Hz$ H-3"3"116.46.87 d, $J = 8.8 Hz$ H-2"4"164.35"116.46.87 d, $J = 8.8 Hz$ H-6"6"132.97.92 d, $J = 8.8 Hz$ H-6"6"132.97.92 d, $J = 8.8 Hz$ H-5"7"168.6168.6	10	62.1	4.09 dd, <i>J</i> = 12.1, 0.8 Hz		C-3, C-7,
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$					C-9
1' 98.9 4.73 d, $J = 8.0$ Hz H-2' C-1 2' 74.2 3.18 dd, $J = 9.0$, 8.1 Hz H-3', H-2' H-3', H-2' 3' 78.1 3.40 , m H-2', H-4' H-3', H-5' 4' 71.6 3.31 , m H-3', H-5' H-3', H-5' 5' 78.1 3.30 , m H-4', H-6' H-4', H-6' 6' 62.7 3.70 , m H-5' H-5' 1'' 121.4 H-5' H-5' H-4' 2'' 132.9 7.92 d, $J = 8.8$ Hz H-3'' 4'' 164.3 6.87 d, $J = 8.8$ Hz H-2'' 4'' 164.3 5'' 116.4 6.87 d, $J = 8.8$ Hz H-6'' 6'' 132.9 7.92 d, $J = 8.8$ Hz H-6'' H-5'' 7''' 168.6 168.6 H-5'' H-5''			3.72 d, <i>J</i> = 12.4 Hz		C-3, C-7
2' 74.2 $3.18 \text{ dd}, J = 9.0, 8.1 \text{ Hz}$ H-3', H-2' 3' 78.1 $3.40, \text{ m}$ H-2',H-4' 4' 71.6 $3.31, \text{ m}$ H-3', H-5' 5' 78.1 $3.30, \text{ m}$ H-4', H-6' 6' 62.7 $3.70, \text{ m}$ H-5' $3.91, \text{ m}$ H-5' H-5' 1" 121.4 110.4 6.87 d, $J = 8.8 \text{ Hz}$ H-3" 3" 116.4 6.87 d, $J = 8.8 \text{ Hz}$ H-2" 4" 164.3 116.4 6.87 d, $J = 8.8 \text{ Hz}$ H-6" 6" 132.9 7.92 d, $J = 8.8 \text{ Hz}$ H-6" 6" 132.9 7.92 d, $J = 8.8 \text{ Hz}$ H-5" 7" 168.6 168.6 168.7 d, $J = 8.8 \text{ Hz}$ H-5"	1'	98.9	4.73 d, J = 8.0 Hz	H-2'	C-1
3' 78.1 $3.40, m$ $H-2', H-4'$ $4'$ 71.6 $3.31, m$ $H-3', H-5'$ $5'$ 78.1 $3.30, m$ $H-4', H-6'$ $6'$ 62.7 $3.70, m$ $H-5'$ $3.91, m$ $H-5'$ $3.91, m$ $H-5'$ $1''$ 121.4 $H-3''$ $H-3''$ $2''$ 132.9 $7.92 d, J = 8.8 Hz$ $H-3''$ $3''$ 116.4 $6.87 d, J = 8.8 Hz$ $H-2''$ $4''$ 164.3 $5''$ 116.4 $6.87 d, J = 8.8 Hz$ $H-6''$ $6''$ 132.9 $7.92 d, J = 8.8 Hz$ $H-6''$ $H-5''$ $7''$ 168.6 $687 d, J = 8.8 Hz$ $H-5''$	2'	74.2	3.18 dd, <i>J</i> = 9.0, 8.1 Hz	H-3', H-2'	
4' 71.6 $3.31, m$ H-3', H-5' 5' 78.1 $3.30, m$ H-4', H-6' 6' 62.7 $3.70, m$ H-5' $3.91, m$ H-5' 1" 121.4 2" 132.9 7.92 d, $J = 8.8 \text{ Hz}$ H-3" 3" 116.4 6.87 d, $J = 8.8 \text{ Hz}$ H-2" 4" 164.3 5" 116.4 6.87 d, $J = 8.8 \text{ Hz}$ H-6" 6" 132.9 7.92 d, $J = 8.8 \text{ Hz}$ H-6" H-5" 7" 168.6 6.87 d, $J = 8.8 \text{ Hz}$ H-5"	3'	78.1	3.40, m	H-2',H-4'	
5' 78.1 3.30, m H-4', H-6' $6'$ 62.7 3.70, m H-5' $3.91, m$ H-5' $1"$ 121.4 $2"$ 132.9 7.92 d, $J = 8.8$ Hz H-3" $3"$ 116.4 6.87 d, $J = 8.8$ Hz H-2" $4"$ 164.3 5" 116.4 6.87 d, $J = 8.8$ Hz H-6" $6"$ 132.9 7.92 d, $J = 8.8$ Hz H-5" H-5" $7"$ 168.6 6.87 d, $J = 8.8$ Hz H-6"	4'	71.6	3.31, m	H-3', H-5'	
6' 62.7 $3.70, m$ $H-5'$ $3.91, m$ $H-5'$ $1"$ 121.4 $2"$ 132.9 $7.92 d, J = 8.8 Hz$ $H-3"$ $3"$ 116.4 $6.87 d, J = 8.8 Hz$ $H-2"$ $4"$ 164.3 $5"$ 116.4 $6.87 d, J = 8.8 Hz$ $H-6"$ $6"$ 132.9 $7.92 d, J = 8.8 Hz$ $H-6"$ $7"$ 168.6 168.6 168.6	5'	78.1	3.30, m	H-4', H-6'	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	6'	62.7	3.70, m	H-5'	
1" 121.4 2" 132.9 7.92 d, J = 8.8 Hz H-3" 3" 116.4 6.87 d, J = 8.8 Hz H-2" 4" 164.3 5" 116.4 6.87 d, J = 8.8 Hz H-6" 6" 132.9 7.92 d, J = 8.8 Hz H-5" 7" 168.6			3.91, m	H-5'	
2" 132.9 7.92 d, J = 8.8 Hz H-3" 3" 116.4 6.87 d, J = 8.8 Hz H-2" 4" 164.3 5" 116.4 6.87 d, J = 8.8 Hz H-6" 6" 132.9 7.92 d, J = 8.8 Hz H-5" 7" 168.6	1"	121.4			
3" 116.4 6.87 d, J = 8.8 Hz H-2" 4" 164.3 5" 116.4 6.87 d, J = 8.8 Hz H-6" 6" 132.9 7.92 d, J = 8.8 Hz H-5" 7" 168.6	2"	132.9	7.92 d, <i>J</i> = 8.8 Hz	Н-3"	
4" 164.3 5" 116.4 6.87 d, J = 8.8 Hz H-6" 6" 132.9 7.92 d, J = 8.8 Hz H-5" 7" 168.6	3"	116.4	6.87 d, <i>J</i> = 8.8 Hz	H-2"	
5" 116.4 6.87 d, J = 8.8 Hz H-6" 6" 132.9 7.92 d, J = 8.8 Hz H-5" 7" 168.6	4"	164.3			
6 " 132.9 7.92 d, J = 8.8 Hz H-5" 7 " 168.6	5"	116.4	6.87 d, <i>J</i> = 8.8 Hz	H-6"	
7" 168.6	6"	132.9	7.92 d, <i>J</i> = 8.8 Hz	H-5"	
	7''	168.6			

Table S3. NMR data of **3** (CH₃OH- d_4)

01	cholinesterase inhibition (%)			
Compounds —	AChE	BChE		
1	39.61 ± 3.70 %	35.01 ± 2.55 %		
2	41.10 ± 1.03 %	36.77 ± 1.90 %		
3	42.34 ± 0.74 %	32.13 ± 1.31 %		
4	41.38 ± 4.27 %	34.29 ± 1.60 %		
5	37.53 ± 1.78 %	24.18 ± 2.00 %		
6	31.31 ± 3.02 %	31.77 ± 1.51 %		
7	27.06 ± 4.85 %	27.53 ± 3.34 %		
8	37.15 ± 0.44 %	30.05 ± 1.82 %		
10	46.49 ± 4.53 %	36.30 ± 3.29 %		
11	31.83 ± 3.23 %	19.98 ± 0.87 %		
12	25.42 ± 0.44 %	24.85 ± 1.04 %		
13	36.85 ± 3.08 %	39.05 ± 2.84 %		
14	48.51 ± 0.93 %	50.46 ± 2.89 %		
15	34.59 ± 2.06 %	17.06 ± 2.33 %		
16	36.09 ± 3.25 %	14.07 ± 0.19 %		
17	31.81 ± 3.35 %	24.73 ± 1.53 %		
18	35.88 ± 1.36 %	32.22 ± 0.33 %		
19	35.72 ± 2.79 %	72.32 ± 0.39 %		
20	51.25 ± 4.06 %	31.81 ± 0.33 %		
21	56.65 ± 0.79 %	75.90 ± 0.28 %		
22	37.72 ± 0.51 %	38.06 ± 1.36 %		

 Table S4. Cholinesterase inhibition of compounds



Figure S1. HR ESI MS spectra of compound 1



Figure S2. ¹H NMR spectra of compound 1



Figure S3. ¹³C NMR spectra of compound 1







Figure S6. HSQC spectra of compound 1



Figure S7. HMBC spectra of compound 1



Figure S8. NOESY spectra of compound 1



Figure S9. IR spectra of compound 1







Figure S11. ¹H NMR spectra of compound 2



Figure S12. ¹³C NMR spectra of compound 2



Figure S13. DEPT spectra of compound 2







Figure S18. IR spectra of compound 2