# **Supporting information**

Robust leishmanicidal upshot of some new diphenyl triazine-based molecules

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# 1. General procedure for the synthesis of compounds 6a–6j (Scheme S1)

A mixture of 4,6-dichloropyrimidine **5** (10 mmol), different amines (**R**<sub>3</sub>) (10 mmol) and K<sub>2</sub>CO<sub>3</sub> (13 mmol) in anhydrous dimethylformamide (DMF) in round bottom flask was refluxed at 100 °C overnight. The reaction completion as well as formation of desired product was preliminarily confirmed by TLC. The reaction mixture was cooled to room temperature and diluted by ethyl acetate (100 mL) and the organic layer was washed with water and then with brine solution. The organic layer was dried over sodium sulphate, concentrated and purified by column chromatography using 15–20% EtOAc/Hexane to obtain compounds **6a–6j**.

#### Scheme S1.

Scheme 2.



Reagents and conditions: K<sub>2</sub>CO<sub>3</sub>, DMF, reflux 100 °C, overnight.

#### 2. General procedure for the synthesis of compound 8 (Scheme S2)

A mixture of aluminium chloride (5.3 g, 39.7 mol) and 25 mL DCM was allowed for stirring at room temperature. 3-chloropropionylchloride (5.5 g, 43.3 mol) dissolved in 20 mL DCM was added dropwise to the stirring solution of AlCl<sub>3</sub>. After half an hour 1,2-dimethoxybenzene (5.0 g, 36.1 mol) was added to the reaction mixture and the mixture was allowed for stirring for 24 h at room temperature. On the completion of the reaction, the reaction mixture was poured into ice-cold water and the organic part was extracted with DCM (50 mL x 3). The organic layer was washed with sodium bicarbonate and brine solutions and was dried over Na<sub>2</sub>SO<sub>4</sub>. The crude product **8** was purified by column chromatography using ethyl acetate hexane 25:75.

Scheme S2.



Reagents and conditions: (i)3-chloropropanoyl chloride, AlCl<sub>3</sub>, CH<sub>2</sub>Cl<sub>2</sub>, 24h, room temperature

# 3. General procedure for the synthesis of compounds 13a and 13b (Scheme S3)

A solution of **3** (85 mmol) in POCl<sub>3</sub> (1.34 mole) could reflux for 18 h. On the completion of the reaction, the reaction mixture was cooled and concentrated under vacuum. The resulting brown oil was obtained in CH<sub>2</sub>Cl<sub>2</sub> (500 mL) and was washed with water (250 mL x 3). The organic extract received was dried through Na<sub>2</sub>SO<sub>4</sub> and concentrated in vacuum to give a brown oil. The crude product (**5a–5d**) was chromatographed on silica gel eluting with 15% EtOAc/ Hexane.[1]

# Scheme S3.



*Reagents and conditions. (i) Benzene, 83 °C reflux ,1.5h (ii) Acetic acid, 110 C reflux 4-5h; (iii) POCl<sub>3</sub>,110 C,18h.* 



ctral data of the synthesized compounds



Figure S1: <sup>1</sup>H NMR spectrum of Molecule (T1)

# Generic Display Report





Figure S3: Mass spectrum of Molecule (T1)

Figure S4: <sup>1</sup>H NMR spectrum of Molecule (T2)



Figure S5: <sup>13</sup>C NMR spectrum of Molecule (T2)



#### Figure S6: Mass spectrum of Molecule (T2)



Figure S8: <sup>13</sup>C NMR spectrum of Molecule (T3)



Figure S9: Mass spectrum of Molecule (T3)



Figure S10: <sup>1</sup>H NMR spectrum of Molecule (T4)



Figure S11: <sup>13</sup>C NMR spectrum of Molecule (T4)







Figure S14: <sup>13</sup>C NMR spectrum of Molecule (T5)







Figure S17: <sup>13</sup>C NMR spectrum of Molecule (T6)



Figure S18: Mass spectrum of Molecule (T6)



Figure S20: <sup>13</sup>C NMR spectrum of Molecule (T7)



Figure S21: Mass spectrum of Molecule (T7)



Figure S22: <sup>1</sup>H NMR spectrum of Molecule (T8)



Figure S23: <sup>13</sup>C NMR spectrum of Molecule (T8)

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Figure S24: Mass spectrum of Molecule (T8)



Figure S26: <sup>13</sup>C NMR spectrum of Molecule (T9)



Figure S27: Mass spectrum of Molecule (T9)



Figure S29: <sup>13</sup>C NMR spectrum of Molecule (T10)



Figure S30: Mass spectrum of Molecule (T10)



Figure S32: <sup>13</sup>C NMR spectrum of Molecule (T11)



Figure S33: Mass spectrum of Molecule (T11)



Figure S35: <sup>13</sup>C NMR spectrum of Molecule (T12)

	n-202013:15:18	3: Sca
090620-TBZ-12 154 (2.565	5) Cm (154.159)	
100	301.02	
· *-	325.27 339.21	
108.87	255.05 340.25 422.43 651.14	916 82 962 4
157.05	423.31 473.16 634.25 676.08 738.49 757.58 823.27 885.94	hartreptore
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090620-TBZ-12 157 (2.610	230 300 350 400 450 500 550 800 650 700 100 100 100 100 100 100 100 100 10	2. Sca
100	534.18	
2		
	535.21	
148.94	391 43 475 37 520 14 536.23 603 22 708.29 783 82 24 859.36	931.21 994
205.01	274.18.288.25.304.32 410.21 617.24.655.33 783.02 900	950 1
090620-TBZ-12 117 (1.949	200 300 300 400 400 500 500 600 850 700 750 550 955 ) Cm (115.118)	3: Sca
100	247.97	- 12
	446.19	
8°-	258.88 519.13	
138.07 171.10 183.34	305.91 357.01 403.43 455.81 520.96558.32 647.21 678.38 720.10 754.02 832.40 855.42	947.91966.1
0		950
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28-		
100.15	251.07	
163.99 194.06	286.09 344.12 394.24 448.11 518.10 536.11 589.25 649.21 711.40 770.34 825.42 872.04908.	71 977.91
150 200	250 300 350 400 450 500 550 600 650 700 750 800 850 900	950 10
090620-TBZ-12 117 (1.943)	Cm (105:121)	
		2: Scan
100-	250.07	2: Scan 2
100-	250.07	2: Scan 2
100-	250.07	2: Scan 2
100 .8-	250.07	2: Scan 2
100- 38- 100.16 148.95 193.07	251.08	2: Scan 2
100- 2 <sup>8-</sup> 100.16 146.95 193.07 0	250.07 251.08 286.08 344.12 424.31 448.11 518.09 589.18 649.21 708.22 770.38 833.80969.74.907.3	2: Scan 2 34 959.81
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100- 3 <sup>8</sup> 100.16 148.95 193.07 0 150 200 090620-TBZ-12 120 (1.993) 100- 2	250.07 251.08 286.08 344.12 424.31 448.11 518.09 589.18 649.21 708.22 770.38 833.80869.74.907.3 250 300 350 400 450 500 550 600 650 700 750 800 850 900 250.03	2: Scan 2 34 959.81 98 950 10 2: Scan 1
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100- 100.16 148.95 193.07 0 150 200 090620-TBZ-12 120 (1.993) 100- 193.03 36- 100.14 149.03 194.10 0 150 200	251.08 251.08 2550 300 350 400 450 500 550 600 650 700 750 800 850 900 250.03 251.27 285.92 344.21 377.83 424.01 483.06 535.98 589.28.604.29 690.35 756.46 786.35 818.25 a52.21 250 300 350 400 450 500 550 600 650 700 750 800 80 900 250.03	2: Scan 2 34 959.81 98/ 950 10 2: Scan 1 959.66 982.8
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Figure S36: Mass spectrum of Molecule (T12)



Figure S38: <sup>13</sup>C NMR spectrum of Molecule (T13)



CS Scanned with CamScanner

Figure S39: Mass spectrum of Molecule (T13)



Figure S41: <sup>13</sup>C NMR spectrum of Molecule (T14)







Figure S44: <sup>13</sup>C NMR spectrum of Molecule (T15)



Figure S45: Mass spectrum of Molecule (T15)

# References

[1] J. Kumar, P. Meena, A. Singh, E. Jameel, M. Maqbool, M. Mobashir, et al., Synthesis and screening of triazolopyrimidine scaffold as multi-functional agents for Alzheimer's disease therapies, European Journal of Medicinal Chemistry. (2016). doi:10.1016/j.ejmech.2016.04.053.