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Synthesis, X-ray Crystal Structure and Theoretical Calculations of Antileishmanial Neolignan Analogues

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CCDC 703864 and CCDC 703867 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.can.ac.uk/conts/retrieving.html or from the Cambridge Crystallographic Data Center (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(1233)336-033; e-mail: deposit@ccdc.can.ac.uk.

Table S1. Scan step number and energy of the conformers calculated by DFT B3LYP/6-31G* for molecules **12** and **20**

Molecule **12**		Molecule **20**	
Scan step number	Energy (Hartree)	Scan step number	Energy (Hartree)
0.86[a]	–1742.08	0.83[a]	–1150.74
1.84	–1742.08	1.80	–1150.74
2.82	–1742.08	2.91	–1150.74
3.93	–1742.08	3.88	−1150.74
4.91	–1742.08	4.98	–1150.74
6.14	–1742.08	5.67	–1150.74
7.00	–1742.07	7.06	–1150.74
7.98	–1742.08	7.89	–1150.74
8.84	–1742.06	9.00	–1150.74
9.82	–1742.03	9.97	–1150.74
11.05	–1742.05	10.93	–1150.74
12.16	–1742.07	11.90	–1150.74
13.02	–1741.93	13.01	–1150.74
14.12	–1742.03	13.98	–1150.74
14.86	–1742.05	14.81	–1150.74
15.84	–1742.06	15.78	–1150.74
16.82	–1742.06	16.89	–1150.74
18.05	–1742.06	17.99	–1150.74
19.04	–1742.04	18.82	–1150.74
19.89	–1741.91	20.07	–1150.74
20.88	–1742.07	21.18	–1150.74
22.11	–1742.04	22.01	–1150.74
22.96	–1742.03	23.11	–1150.74
23.70	–1742.04	24.08	–1150.74
24.93	–1742.05	24.91	–1150.73
26.16	–1742.05	25.88	–1150.73
26.89	–1742.06	26.99	–1150.73
28.12	–1742.06	27.96	–1150.74
28.86	–1742.05	28.93	–1150.73
29.96	–1742.06	29.90	–1150.72
30.95	–1742.07	30.87	–1150.71
32.18	–1742.06	31.70	–1150.72
33.16	–1742.06	33.08	–1150.73
33.89	–1742.05	34.05	–1150.73
		35.02	–1150.73
		36.26	–1150.73

[a] Structures optimized with the 6-311++G(*d*,*p*) basis sets using X-ray diffraction data.

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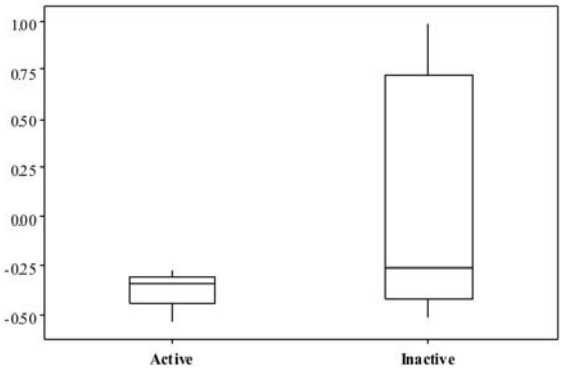

Figure S1. Box plot of *L. donovani* activity for O or S atom considering nineteen neolignan compounds.

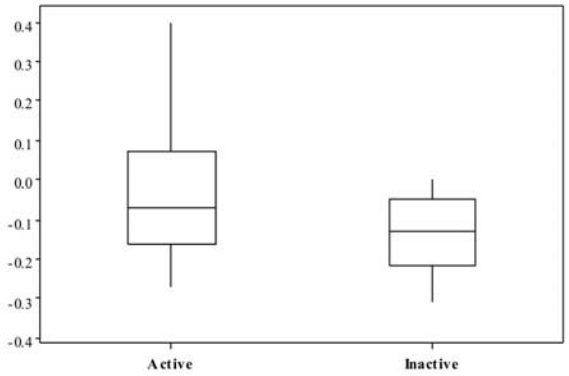

Figure S2. Box plot of *L. donovani* activity for Q5' considering nineteen neolignan compounds.

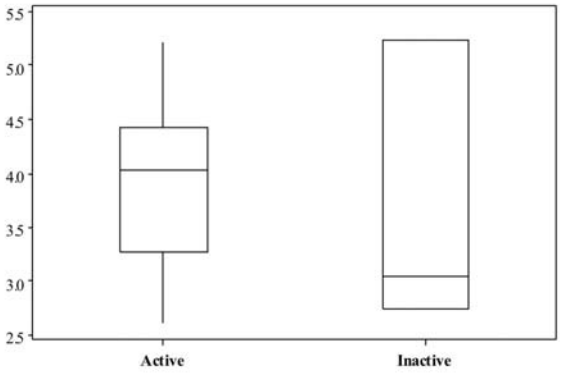

Figure S3. Box plot of *L. amazonensis* activity for ClogP considering nineteen neolignan compounds.

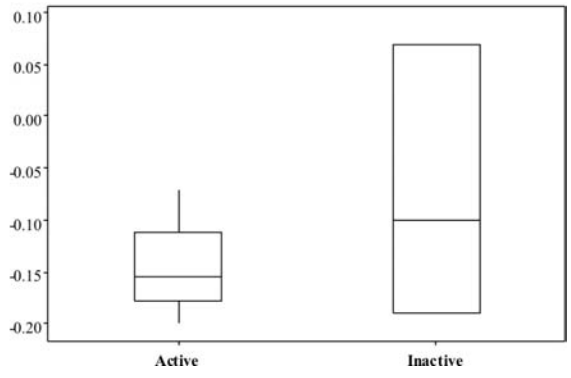

Figure S4. Box plot of *L. amazonensis* activity for Q2 considering nineteen neolignan compounds.

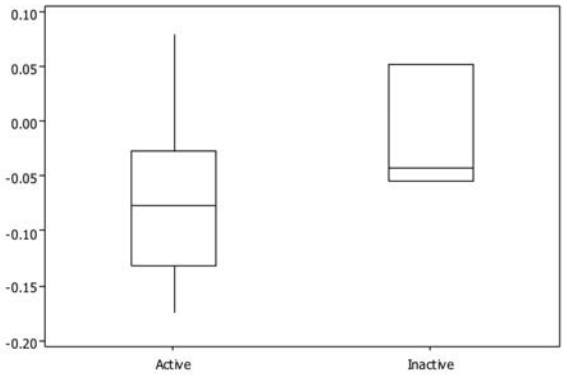

Figure S5. Box plot of *L. amazonensis* activity for Q1 considering nineteen neolignan compounds.