Electronic Supplementary Material (ESI) for MedChemComm.

Antiprotozoal activity of dehydroabietic acid derivatives against *Leishmania donovani* and *Trypanosoma cruzi*

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Supplementary Information

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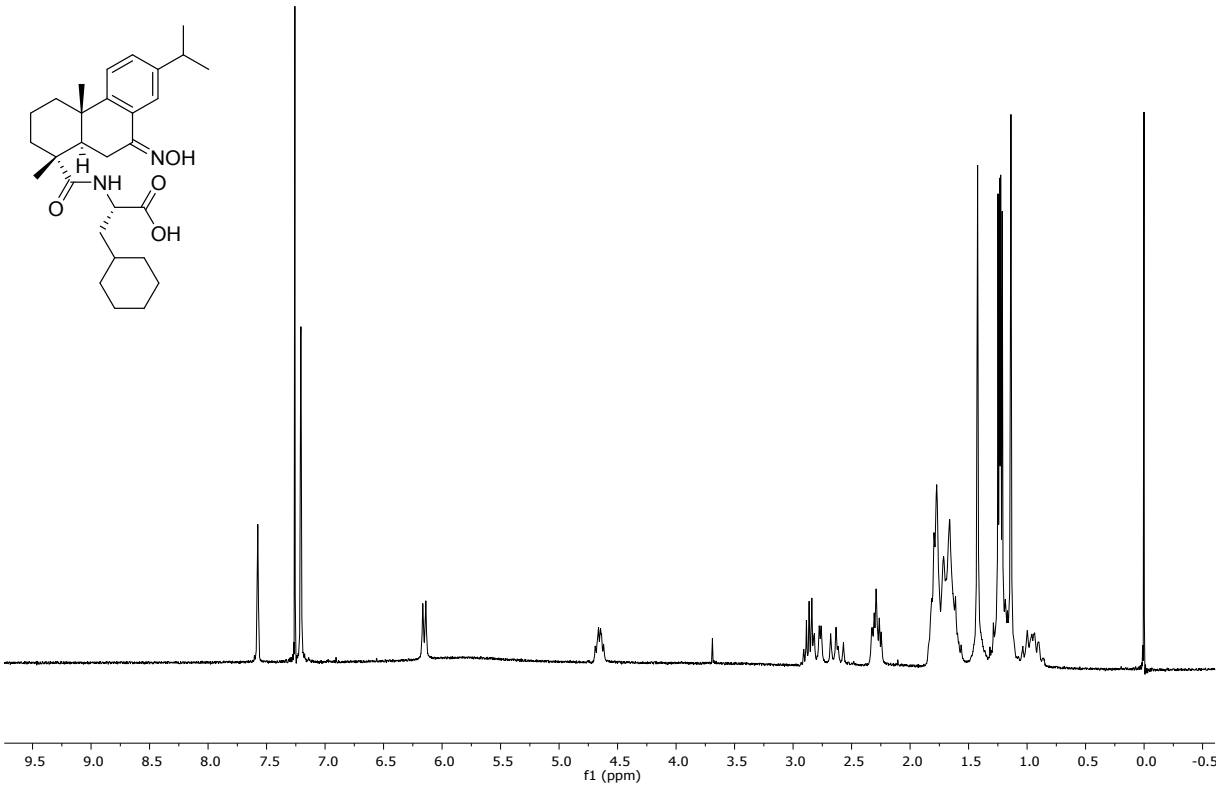
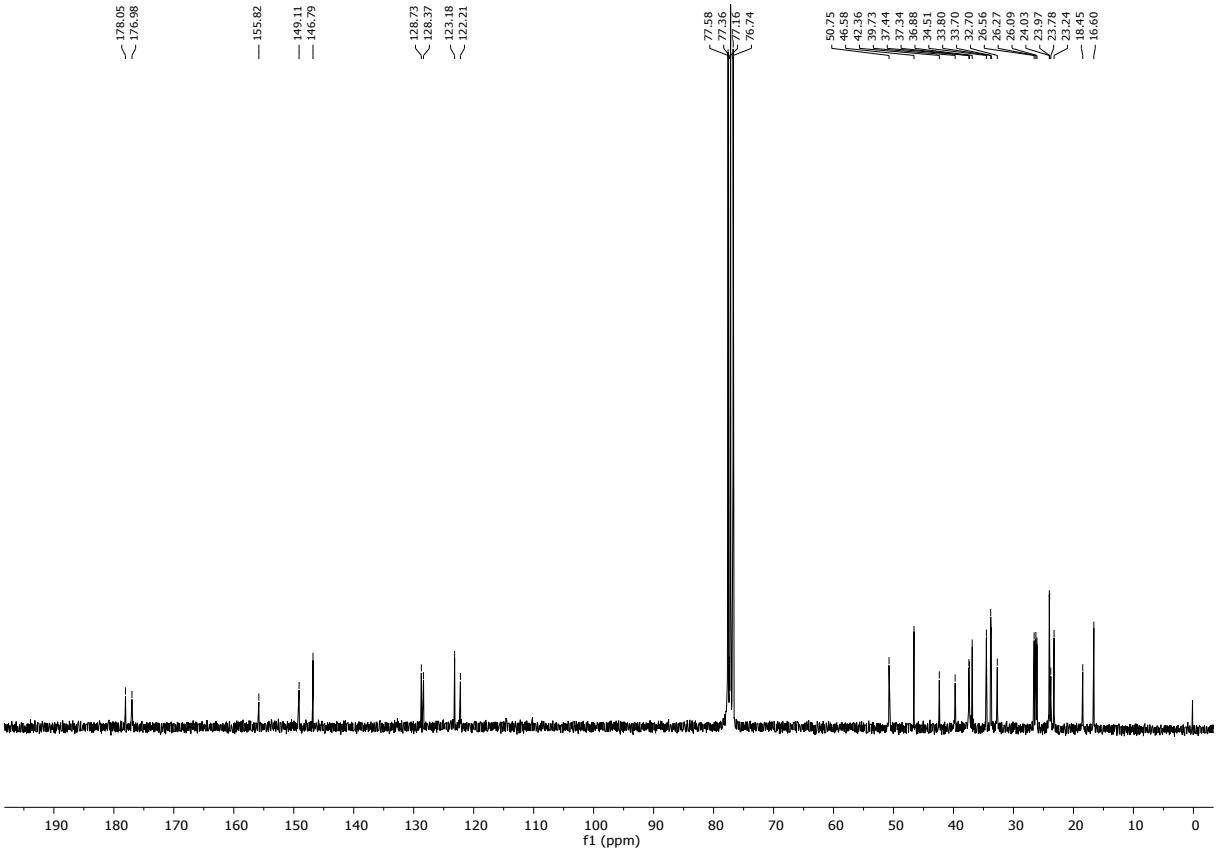
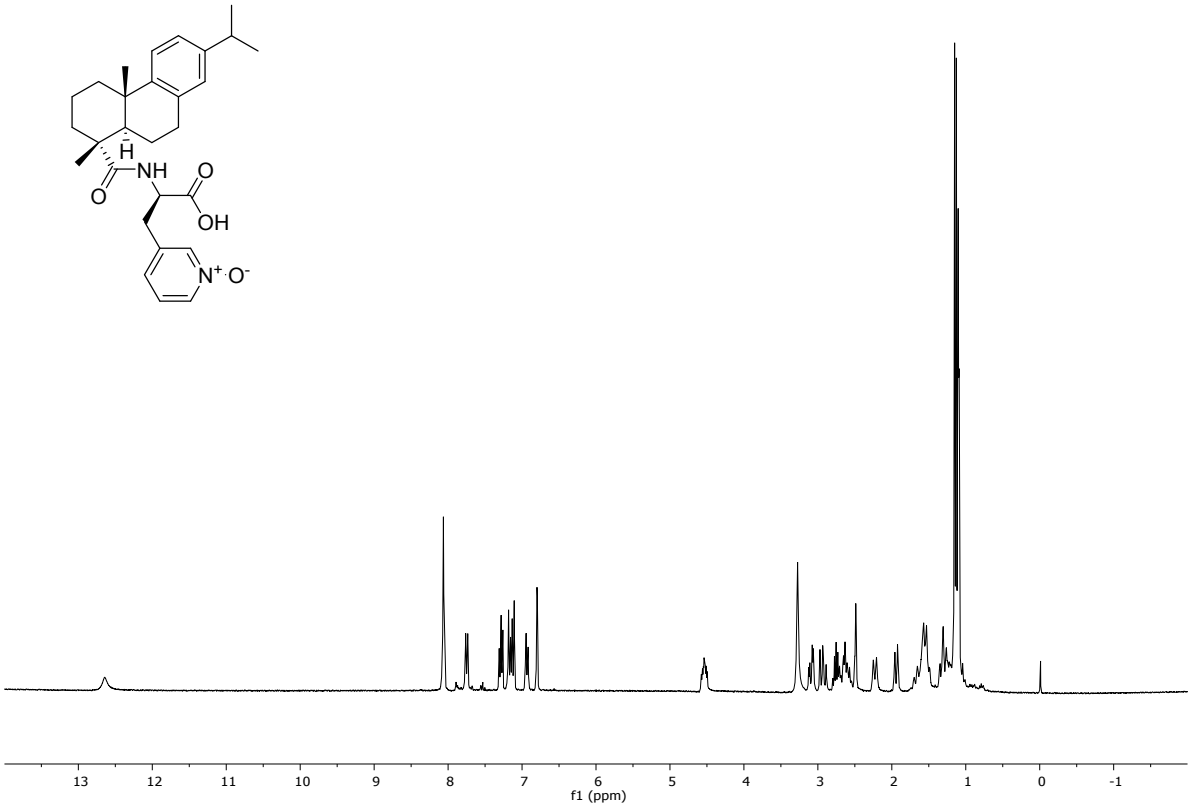
Compound spectra



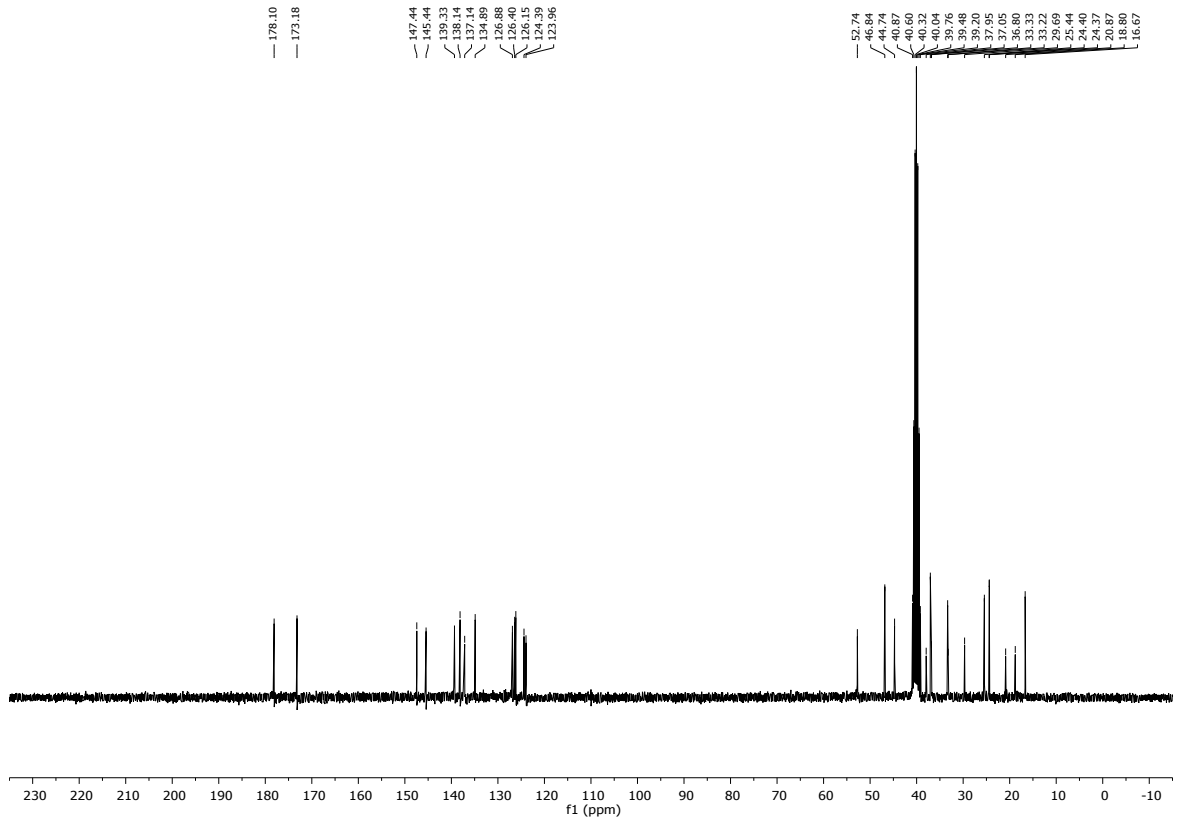
^{1}H-NMR spectrum of compound **17** in $CDCl_3$.



^{13}C-NMR spectrum of compound **17** in $CDCl_3$.



^{1}H-NMR spectrum of compound **29** in DMSO-d_6.



^{13}C-NMR spectrum of compound **29** in DMSO-d_6.

Table 1. Calculated Lipinski parameters and drug scores of compounds **13-16, 19, 23-26** and **28**.[1,2]

Compound	MW[a]	logP[b]	HBAs[c]	HBDs[d]	Drug score
Rule[3]	≤ 500	≤ 5	≤ 10	≤ 5	--
13	453	6.25	3	2	0.16
14	467	6.55	2	1	0.15
15	467	5.19	4	2	0.17
16	496	5.19	4	2	0.14
19	447	6.32	3	2	0.18
23	447	6.32	3	2	0.18
24	462	5.04	3	1	0.33
25	448	5.01	4	2	0.24
26	477	6.07	3	2	0.23
28	478	3.50	3	1	0.20

[a]MW: molecular weight
[b] log *P*: logarithm of partition coefficient between *n*-octanol and water
[c] HBA: hydrogen bond acceptor
[d] HBD: hydrogen bond donor

Table 2. Predicted toxicity of compounds **13-16, 19, 23-26** and **28** (1 = safe).[1]

Compound	Mutagenic	Tumorigenic	Irritant	Reproductive Effect
13	1	1	1	1
14	1	1	1	1
15	1	1	1	1
16	1	1	1	1
19	1	1	1	1
23	1	1	1	1
24	1	1	1	1
25	1	1	1	1
26	1	1	1	1
28	1	1	1	1

References

1. OSIRIS Property Explorer. Available online from: http://www.organicchemistry. org/prog/peo/.

2. Marvin Sketch 6.3.0. Available online from: http://www.chemaxon.com/products/marvin/marvinsketch.

3. P. Lesson, *Nature*, 2012, **481**, 455-456.