Supplementary Information

Assessment of the Nematocidal Activity of Metallocenyl Analogues of Monepantel

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1) NMR spectra of compounds

Figure S1. 4a, ¹H, d⁶-acetone, 400 MHz





Figure S2. 4a, ¹³C, d⁶-acetone, 125 MHz

Figure S3. 5a, ¹H, d⁶-acetone, 500 MHz





Figure S4. 5a, ¹³C, d⁶-acetone, 125 MHz



Figure S6. 4b, ¹³C, d⁶-DMSO, 125 MHz



Figure S7. 5b, ¹H, d⁶-DMSO, 500 MHz









Figure S9. 6a, ¹H, d⁶-acetone, 500 MHz



Figure S10. 6a, ¹³C, d⁶-acetone, 125 MHz















Figure S15. 7, ¹H, CD₃CN, 500 MHz



Figure S16. 7, ¹³C, CD₃CN, 125 MHz



2) Figure S17. ORTEP plot of 7.



Figure S17. Molecular structures of 7 with atoms shown as thermal ellipsoids (drawn at 50% probability; hydrogen atoms are omitted for clarity).

3) Table S1. Antiparasitic activity of **4a/b**, **5a/b**, **6a/b** and **7** against *Ctenocephalides felis*, *Lucilia cuprina* and *Rhipicephalus sanguineus* and reference compounds (Dicyclanil for *Lucilia cuprina*; milbemycin oxime for *Rhipicephalus sanguineus* & thiamethoxam for *Ctenocephalides felis*) (n.d.i. = non-disclosable information¹ and n.d. = not determined). EC values are given in μ g/mL as well as in μ M. EC values are calculated as a mean of 2 series of triplicated dose responses. Experimental errors are not included as they are too low to influence the overall EC values.

Compound	EC ₈₀ value		EC ₈₀ value		EC ₈₀ value		EC ₈₀ value		EC ₈₀ value	
	<i>C. felis</i> oral test		<i>C. felis</i> tarsal test		L. cuprina		<i>R. sanguineus</i> immersion test		<i>R. sanguineus</i> tarsal test	
	[µg/mL]	[µM]	[µg/mL]	[µM]	[µg/mL]	[µM]	[µg/mL]	[µM]	[µg/mL]	[µM]
4a	>100.00	>320.37	>100.00	>320.37	>32.00	>102.52	>640.00	>2050.36	>100.00	>320.37
5a	>100.00	>190.78	>100.00	>190.78	>32.00	>61.05	>640.00	>1220.98	>100.00	>190.78
6a	>100.00	>207.79	>100.00	>207.79	>32.00	>66.49	>640.00	>1329.87	>100.00	>207.79
4b	>100.00	>279.82	>100.00	>279.82	>32.00	>89.54	>640.00	>1790.86	>100.00	>279.82
5b	>100.00	>162.70	>100.00	>162.70	>32.00	>52.06	>640.00	>1041.29	>100.00	>162.70
6b	>100.00	>189.94	>100.00	>189.94	>32.00	>60.78	>640.00	>1215.64	>100.00	>189.94
7	>100.00	>196.01	>100.00	>196.01	>32.00	>62.72	>640.00	>1254.43	>100.00	>196.01
CN CF ₃ ON NC AAD85	>100.00	>218.66	>100.00	>218.66	>32.00	>69.97	>640.00	>1399.43	>100.00	>218.66
$\overbrace{CF_3}^{CN} \cap \overbrace{CF_3}^{H} \cap \overbrace{O}^{S} \cap CF_3$ AAD96	n.d.i.	n.d.i.	n.d.i.	n.d.i.	n.d.i.	n.d.i.	n.d.i.	n.d.i.	n.d.i.	n.d.i.
Thiamethoxam	0.10	0.34	0.03	0.10	1.00	3.43	n.d.	n.d.	n.d.	n.d.
Milbemycin oxime	10.00	18.00	320.00	539.86	10.00	18.00	6.40	11.52	3.20	5.76
Dicyclanil	n.d.	n.d.	n.d.	n.d.	0.03	0.17	n.d.	n.d.	n.d.	n.d.