

Supporting Information

Identification and Development of Novel Inhibitors of *Toxoplasma gondii* Enoyl Reductase

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Table Sd1: HPLC Purity Analysis Data of the tested TgENR inhibitors.

Compd	Gradient Method	Wavelength (nM)	t_R (min)	Purity (%)	HPLC column
2	C	280	18.16	99	WATERS Bondapak TM C ₁₈ (3.9 × 300 mm)
3	A	280	13.69	97	Synergi 4um (150 x 4.6 mm)
4	D	280	9.47	99	ACE 3.5 AQ (100 x 4.6 mm)
6	C	280	12.27	100	WATERS Bondapak TM C ₁₈ (3.9 × 300 mm)
7	A	254	8.40	99	Synergi 4um (150 x 4.6 mm)
8	C	280	16.83	98	WATERS Bondapak TM C ₁₈ (3.9 × 300 mm)
9	C	280	16.06	97	WATERS Bondapak TM C ₁₈ (3.9 × 300 mm)
10	C	280	11.02	96	WATERS Bondapak TM C ₁₈ (3.9 × 300 mm)
11	C	280	7.47	99	WATERS Bondapak TM C ₁₈ (3.9 × 300 mm)
13	A	280	12.31	99	Synergi 4um (150 x 4.6 mm)
14	C	254	3.68	98	WATERS Bondapak TM C ₁₈ (3.9 × 300 mm)
15	C	280	4.97	100	WATERS Bondapak TM C ₁₈ (3.9 × 300 mm)
16	C	280	13.58	99	WATERS Bondapak TM C ₁₈ (3.9 × 300 mm)
17	C	280	2.97	100	WATERS Bondapak TM C ₁₈ (3.9 × 300 mm)
18	C	280	3.88	99	WATERS Bondapak TM C ₁₈ (3.9 × 300 mm)
19	C	280	11.22	99	WATERS Bondapak TM C ₁₈ (3.9 × 300 mm)
20	C	280	11.66	96	WATERS Bondapak TM C ₁₈ (3.9 × 300 mm)
21	C	280	10.86	98	WATERS Bondapak TM C ₁₈ (3.9 × 300 mm)
22	C	280	11.55	99	WATERS Bondapak TM C ₁₈ (3.9 × 300 mm)
23	C	280	10.53	98	WATERS Bondapak TM C ₁₈ (3.9 × 300 mm)
24	C	280	3.78	99	WATERS Bondapak TM C ₁₈ (3.9 × 300 mm)

25	C	280	18.99	97	WATERS Bondapak™C ₁₈ (3.9 × 300 mm)
26	A	280	9.66	99	Synergi 4um (150 x 4.6 mm)
27	A	280	11.91	95	Synergi 4um (150 x 4.6 mm)
28	B	254	6.85	98	Synergi 4um (150 x 4.6 mm)
29	C	280	18.61	99	WATERS Bondapak™C ₁₈ (3.9 × 300 mm)
30	A	280	11.33	97	Synergi 4um (150 x 4.6 mm)
31	C	280	12.15	99	WATERS Bondapak™C ₁₈ (3.9 × 300 mm)
32	B	254	8.85	98	Synergi 4um (150 x 4.6 mm)
33	A	280	12.59	99	Synergi 4um (150 x 4.6 mm)
34	A	254	9.23	96	Synergi 4um (150 x 4.6 mm)
35	B	254	7.78	98	Synergi 4um (150 x 4.6 mm)
38	A	280	12.17	96	Synergi 4um (150 x 4.6 mm) Hydro-RP
39	A	280	10.32	100	Synergi 4um (150 x 4.6 mm) Hydro-RP
40	A	280	10.96	100	Synergi 4um (150 x 4.6 mm) Hydro-RP
41	A	280	10.83	97	Synergi 4um (150 x 4.6 mm) Hydro-RP
42	A	280	9.72	98	Synergi 4um (150 x 4.6 mm) Hydro-RP
43	A	280	8.64	98	Synergi 4um (150 x 4.6 mm) Hydro-RP
44	A	280	9.66	96	Synergi 4um (150 x 4.6 mm) Hydro-RP
45	A	254	10.89	96	Synergi 4um (150 x 4.6 mm)
46	A	280	11.41	98	Synergi 4um (150 x 4.6 mm)
47	A	280	2.34	97	Synergi 4um (150 x 4.6 mm)
48	A	254	6.85	100	Synergi 4um (150 x 4.6 mm)
49	A	254	8.97	100	Synergi 4um (150 x 4.6 mm)
50	A	280	6.75	99	Synergi 4um (150 x 4.6 mm) Hydro-RP
51	A	280	8.62	99	Synergi 4um (150 x 4.6 mm) Hydro-RP

52	A	280	7.60	96	Synergi 4um (150 x 4.6 mm) Hydro-RP
53	A	280	1.59	97	Synergi 4um (150 x 4.6 mm)
54	A	280	5.23	100	Synergi 4um (150 x 4.6 mm)

The HPLC Analysis was carried out by using Shimadzu HPLC Prominence Series components with a two-mobile phase system (0.05% TFA in water (sol.A) and 0.05% TFA in acetonitrile (sol. B) or Methanol (sol. C) with a gradient.

Gradient A: (flow rate: 1.3 ml/min) from 30% sol.C in sol.A to 100% sol.B in 25 min.

Gradient B: (flow rate: 1.3 ml/min) from 50% sol.C in sol.A to 100% sol.B in 25 min.

Gradient C: (flow rate: 1.3 ml/min) from 50% sol.B in sol.A to 100% sol.B in 25 min.