

# Electronic Supplementary Information

## Strigolactones: A plant phytohormone as novel anti-inflammatory agents

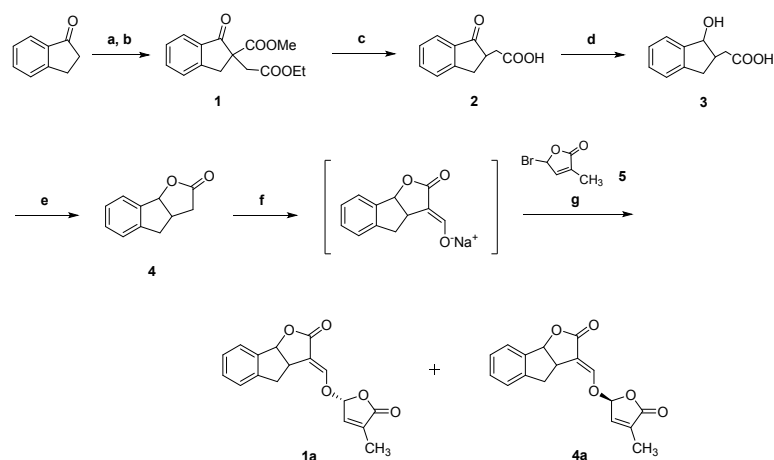
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## Scheme S1. Synthesis of GR24



**Scheme S1.** Synthesis of GR24: (a) NaH, DMC, THF, reflux, 1.5 h; (b) BrCH<sub>2</sub>COOEt, reflux, 1.5 h; (c) HCl/AcOH, reflux, 3 h; (d) NaBH<sub>4</sub>, NaOH, rt, 5 h; (e) p-TsOH, benzene, reflux, 3 h; (f) Na, HCO<sub>2</sub>Me, THF, rt, 1 h; (g) THF, rt, 5 h.

## Spectral data

Compounds	Spectral data
<b>2a</b>	[ $\alpha$ ] <sub>20</sub> D +440° ( <i>c</i> 0.5, CH <sub>3</sub> Cl <sub>3</sub> ), white solid; <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) $\delta$ 7.49 (t, <i>J</i> = 5.5 Hz, 2H), 7.38-7.21 (m, 4H), 6.99- 6.95 (m, 1H), 6.20- 6.16 (m, 1H), 5.95 (d, <i>J</i> = 7.8 Hz, 1H), 4.11 (q, <i>J</i> = 7.1 Hz, 1H), 3.99 – 3.89 (m, 1H), 3.44 (dd, <i>J</i> = 16.9, 9.3 Hz, 1H), 3.11 (dd, <i>J</i> = 16.9, 3.3 Hz, 1H), 2.04 (d, <i>J</i> = 2.4 Hz, 5H), 1.25 (t, <i>J</i> = 7.1 Hz, 7H), 0.86 (dd, <i>J</i> = 13.9, 6.6 Hz, 3H). <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) $\delta$ 171.43, 170.33, 151.12, 142.69, 141.02, 138.93, 136.18, 130.16, 127.64, 126.59, 125.25, 113.41, 100.70, 86.06, 38.98, 37.43, 29.82, 10.90. HRMS (ESI) Found MNa <sup>+</sup> 321.07326
<b>3a</b>	[ $\alpha$ ] <sub>20</sub> D -288° ( <i>c</i> 0.5, CH <sub>3</sub> Cl <sub>3</sub> ), Other spectral date was similar to <b>2a</b>
<b>5a</b>	[ $\alpha$ ] <sub>20</sub> D +290° ( <i>c</i> 0.5, CH <sub>3</sub> Cl <sub>3</sub> ), Other spectral date was similar to <b>2a</b>
<b>6a</b>	[ $\alpha$ ] <sub>20</sub> D -450° ( <i>c</i> 0.5, CH <sub>3</sub> Cl <sub>3</sub> ), Other spectral date was similar to <b>2a</b>
<b>2b</b>	[ $\alpha$ ] <sub>20</sub> D +401° ( <i>c</i> 0.5, CH <sub>3</sub> Cl <sub>3</sub> ), white solid; <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) $\delta$ : 7.50 (2 H, dd, <i>J</i> 8.1, 5.0), 7.40 – 7.21 (4 H, m), 5.98 (1 H, d, <i>J</i> 7.9), 5.87 (1 H, dt, <i>J</i> 16.1, 8.0), 4.01 – 3.88 (1 H, m), 3.45 (1 H, dd, <i>J</i> 16.8, 9.3), 3.15 – 3.04 (1 H, m), 2.91 – 2.76 (2 H, m), 2.19 – 2.01 (1 H, m), 1.46 (1 H, s). <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) $\delta$ : 177.39, 171.45, 152.16, 142.52, 138.76, 130.08, 127.50, 126.38, 125.31, 112.83, 103.02, 85.89, 38.67, 37.48, 35.72, 33.59, 17.01. HRMS (ESI) Found MNa <sup>+</sup> 321.07326

<b>3b</b>	[ $\alpha$ ]20 D -310° ( <i>c</i> 0.5, CH <sub>3</sub> Cl <sub>3</sub> ), Other spectral date was similar to <b>2b</b>
<b>5b</b>	[ $\alpha$ ]20 D +252° ( <i>c</i> 0.5, CH <sub>3</sub> Cl <sub>3</sub> ), Other spectral date was similar to <b>2b</b>
<b>6b</b>	[ $\alpha$ ]20 D -490° ( <i>c</i> 0.5, CH <sub>3</sub> Cl <sub>3</sub> ), Other spectral date was similar to <b>2b</b>

### Docking scores

**Table S1.** Result of the molecular docking scores.

Target No.	Structural No.	Receptor	PDB code	Resolution (Å)	Score
1.1	1	JNK-1	4w4w	1.9	-8.5
1.2	2	JNK-2	4y46	2.04	-9.1
1.3	3	JNK-3	4qtd	1.5	-9.4
1.4	4	JNK-4	4awi	1.91	-8.8
1.5	5	JNK-5	3rip	2.3	-8.8
2.1	6	P38-1	2ewa	2.1	-9.2
2.2	7	P38-2	4zth	2.15	-9.2
2.3	8	P38-3	2bak	2.2	-9.1
2.4	9	P38-4	4l8m	2.1	-6.7
2.5	10	P38-5	4dli	1.91	-7.9
3.1	11	CK2-1	5m4f	1.52	-8.9
3.2	12	CK2-2	5h8g	2	-9.5
3.3	13	CK2-3	5cqu	2.35	-8.8
3.4	14	CK2-4	4ub7	2.1	-7.9
3.5	15	CK2-5	3wik	2	-9.9
4.1	16	HDAC-1	5lgt	3	-9.3
4.2	17	HDAC-2	5l3e	2.8	-9.4
4.3	18	HDAC-3	5iwg	1.66	-7.5
4.4	19	HDAC-4	5l3d	2.6	-9
4.5	20	HDAC-5	4ly1	1.57	-7.6
5.1	21	PARP1-1	5ws1	1.9	-10.1
5.2	22	PARP1-2	5ds3	2.6	-9.3
5.3	23	PARP1-3	4rv6	3.19	-9.5
5.4	24	PARP1-4	5wrz	2.2	-10
5.5	25	PARP1-5	4r6e	2.2	-6.5

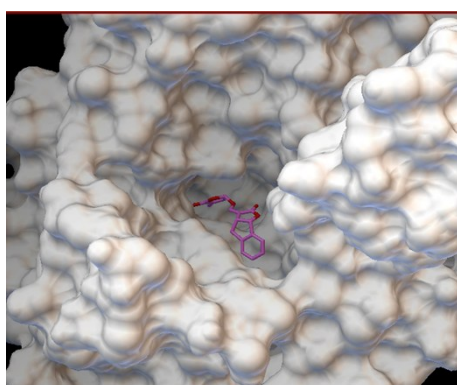
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6.1	26	PKA C-1	5bx6	1.89	-7.6
6.2	27	PKA C-2	5izj	1.85	-9.3
6.3	28	PKA C-3	4z84	1.55	-9.1
6.4	29	PKA C-4	4wb8	1.55	-7.7
6.5	30	PKA C-5	4ib1	1.63	-8.3
7	31	NIK	4dn5	2.5	-8.6
8.1	32	RSK1-1	4nif	2.15	-9.2
8.2	33	RSK1-2	2z7q	2	-7.9
9	34	MSK1	3kn5	2.4	-8.1
10.1	35	GSK-3beta-1	5k5n	2.2	-8.9
10.2	36	GSK-3beta-2	5hlp	2.45	-8.1
10.3	37	GSK-3beta-3	5f94	2.51	-8.5
10.4	38	GSK-3beta-4	4pte	2.03	-8.6
10.5	39	GSK-3beta-5	3f7z	2.4	-8.8
11	40	COT	4y85	2.33	-9.5
12.1	41	AKT-1	3ocb	2.7	-8.7
12.2	42	AKT-2	4ekl	2	-8.8
12.3	43	AKT-3	3qkm	2.2	-8.9
12.4	44	AKT-4	3cqw	2	-8.7
12.5	45	AKT-5	5kecv	2.7	-9.7
13.1	46	RIP-1	5hx6	2.23	-9.2
13.2	47	RIP-2	4itj	1.8	-8.9
13.3	48	RIP-3	5j7b	2.53	-9.2
13.4	49	RIP-4	5ar5	2.66	-9.1
14.1	50	PI3K-1	5swg	3.11	-8
14.2	51	PI3K-2	5ubr	2.4	-8.2
14.3	52	PI3K-3	5t8f	2.91	-8.8
14.4	53	PI3K-4	4urk	2.9	-9.4
14.5	54	PI3K-5	4wwo	2.3	-9.3
15.1	55	PDK1-1	5lvo	1.09	-9
15.2	56	PDK1-2	5hkm	2.1	-8.7

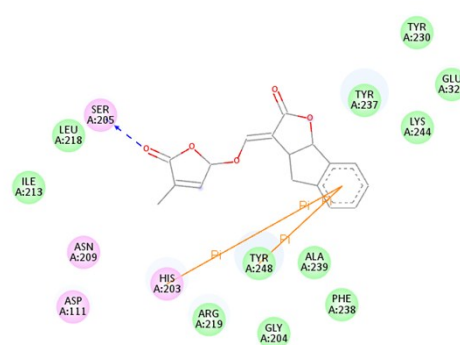
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15.3	57	PDK1-3	4xx9	1.4	-8.8
15.4	58	PDK1-4	5ack	1.24	-8.8
15.5	59	PDK1-5	4rrv	1.41	-8.7
16	60	UBC13	4onm	1.35	-7.8
17.1	61	MyD88-1	2y92	3.01	-7
17.2	62	MyD88-2	3ub2		

**Figures S1-S3. Docking informational interaction of 2a and PARP1/CK2/AKT.**

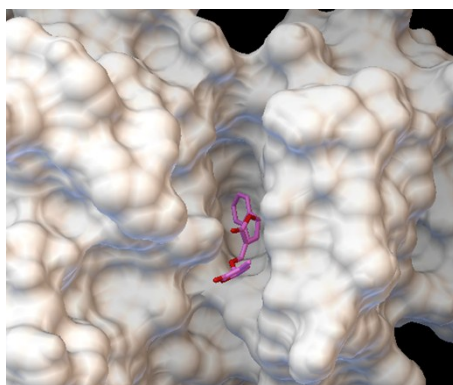


(a)

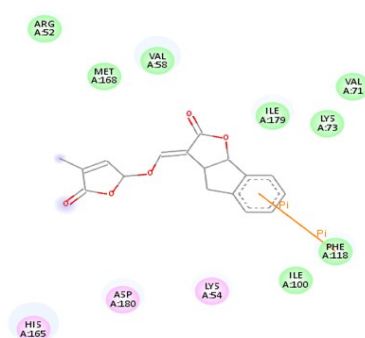


(b)

Figure S1. 2a and PARP1 combined mode (a) and 2D interaction diagram (b).

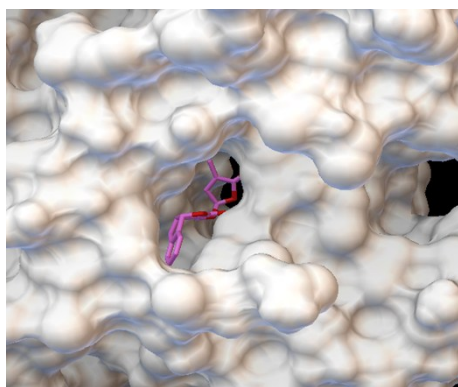


(a)

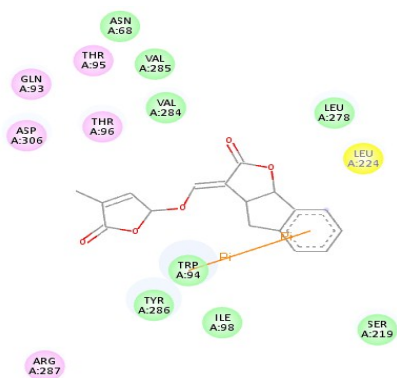


(b)

Figure S2. 2a and CK2 combined mode (a) and 2D interaction diagram (b).



(a)



(b)

Figure S3. 2a and AKT combined mode (a) and 2D interaction diagram (b).