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ELECTRONIC SUPPORTING INFORMATION

New tricyclic pyridazinone derivatives as potential STAT3 inhibitors

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δ_H (300 MHz; Me_4Si)

Table: ^{1}H-NMR Data of Compounds 1-4, 6, 9-13 ($CDCl_3$; chemical shift in ppm)

Compd	^{1}H NMR
1c	1.29 (t, 3H, CH_3), 2.0-2.10 (m, 2H, CH_2), 2.25-2.40 (m, 3H, CH, CH_2), 2.65-2.80 (m, 1H, CH_2), 2.85-2.95 (m, 1H, CH_2), 3.0-3.20 (m, 1H, CH_2), 3.35-45 (m, 1H, CH), 3.75-3.90 (m, 1H, CH), 3.95-4-15 (m, 3H, CH, CH_2), 7.30-7.45 (m, 3H, ArH), 7.70-7.80 (m, 1H, ArH)
2a	1.29 (t, 3H, CH_3), 1.41 (dq, 1H, CH), 1.7-1.5 (dd, 2H, CH_2), 2.3-2.1 (dd, 2H, CH_2), 2.85-2.75 (dd, 2H, CH_2), 4.13 (q, 2H, CH_2), 4.16 (d, 2H, CH2), 7.30-7.78 (m, 4H, ArH)
2b	1.29 (t, 3H, CH_3), 1.41 (dq, 1H, CH), 1.7-1.5 (dd, 2H, CH_2), 2.3-2.1 (dd, 2H, CH_2), 2.65 (d, 2H, CH_2), 2.85-2.75 (d, 2H, CH_2), 3.59 (dd, 2H, CH_2), 4.13 (dq, 2H, CH_2), 7.30-7.78 (m, 4H, ArH)
(±)-2c	1.29 (t, 3H, CH_3), 1.41 (dq, 1H, CH), 1.7-1.5 (dd, 2H, CH_2), 2.04 (d, 2H, CH_2), 2.3-2.1 (dd, 2H, CH_2), 2.47 (d, 2H, CH_2), 2.85-2.75 (dd, 2H, CH_2), 3.20 (q, 2H, CH_2), 4.13 (dq, 2H, CH_2), 7.30-7.78 (m, 4H, ArH)
2d	1.25 (t, 3H, CH_3), 1.45 (m, 1H, CH), 2.0-2.40 (m, 6H, CH_2), 2.60-2.80 (m, 2H, CH_2), 3.15 (m, 2H, CH_2), 3.81 (s, 3H, CH_3), 3.85 (s, 3H, CH_3), 3.95 (m, 2H, CH_2), 4.15 (q, 2H, CH_2), 6.45 (s, 1H, ArH), 7.25 (s, 1H, ArH)
2e	1.25 (t, 3H, CH_3), 1.50 (m, 1H, CH), 2.20-2.40 (m, 6H, CH_2), 2.60-2.95 (m, 4H, CH_2), 3.80-4.0 (m, 2H, CH_2), 4.10 (q, 2H, CH_2), 7.10-7.25 (m, 3H, ArH), 8.05 (d, 1H, ArH)
2f	1.29 (t, 3H,CH_3), 1.41 (dq, 1H, CH), 1.52 (d, 2H, CH_2), 1.64 (d, 2H, CH_2), 1.7-1.5 (dd, 2H, CH_2), 2.3-2.1 (dd, 2H, CH_2), 2.32 (d, 2H, CH_2), 2.85-2.75 (dd, 2H, CH_2), 3.20 (q, 2H, CH_2), 4.13 (dq, 2H, CH_2), 7.30-7.78 (m, 4H, ArH)
2g	1.29 (t, 5H, CH3, CH_2), 1.41 (dq, 1H, CH), 1.52 (t, 2H, CH_2), 1.64 (t, 2H, CH_2), 1.7-1.5 (dd, 2H, CH_2), 2.3-2.1 (dd, 2H, CH_2), 2.32 (dd, 2H, CH_2), 2.85-2.75 (dd, 2H, CH_2), 3.20 (t, 2H, CH_2), 4.13 (dq, 2H, CH_2), 7.30-7.78 (m, 4H, ArH)
2h	1.29 (m, 7H, CH_3, CH_2, CH_2), 1.41 (dq, 1H, CH), 1.52 (d, 2H, CH_2), 1.64 (d, 2H, CH_2), 1.7-1.5 (dd, 2H, CH_2), 2.3-2.1 (dd, 2H, CH_2), 2.32 (d, 2H, CH_2), 2.85-2.75 (dd, 2H, CH_2), 3.20 (t, 2H, CH_2), 4.13 (dq, 2H, CH_2), 7.30-7.78 (m, 4H, ArH)
2i	1.41 (dq, 1H, CH), 1.7-1.5 (t, 2H, CH_2), 1.92 (d, 2H, CH_2) , 2.3-2.1 (t, 2H, CH_2), 2.3 (d, 2H, CH_2), 2.85-2.75 (dd, 2H, CH_2) 3.20 (d, 2H, CH_2), 7.30-7.78 (m, 4H, ArH), 11 (s, 1H, OH).
2j	1.55-1.70 (m, 1H, CH), 2.0-2.50 (m, 6H, CH_2), 2.70-3.0 (m, 4H, CH_2), 3.90-4.0 (m, 2H, CH_2), 7.15-7.35 (m, 3H, ArH), 8.15 (d, 1H, ArH)
2k	1.04 (m, 3H, CH_3), 1.41 (dq,1H, CH), 1.7-1.5 (dd, 2H, CH_2), 1.93 (m, 2H, CH_2), 2.3-2.1 (dd, 2H, CH_2), 2.34 (dd, 2H, CH_2), 2.85-2.75 (m, 2H, CH_2), 3.11 (t, 2H, CH_2), 3.20 (dq, 2H, CH_2), 7.30-7.78 (m, 4H, ArH), 8.03 (br s, 1H, NH)
2l	1.02 (t, 3H, CH_3), 1.38 (m, 2H, CH_2), 1.41 (dq, 1H, CH), 1.52 (dd, 2H, CH_2), 1.7-1.5 (dd, 2H, CH_2), 2.0 (br s, 1H, NH), 2.3-2.1 (dd, 2H, CH_2), 2.55 (d, 2H, CH_2), 2.59 (d, 2H, CH_2), 2.85-2.75 (dd, 2H, CH_2), 3.20 (dq, 2H, CH_2), 7.30-7.78 (m, 4H, ArH)
2m	0.95 (t, 3H, CH_3), 1.30-1.45 (m, 2H, CH_2), 1.50-1.75 (m, 5H, CH), 2.15-2.30 (m, 2H, CH_2), 2.60-3.95 (m, 4H, CH_2), 3.75-4.0 (m, 2H, CH_2), 7.15-7.35 (m, 3H, ArH), 8.15 (d, 1H, ArH)
2n	0.95 (t, 3H, CH_3), 1.20-1.35 (m, 4H, CH_2), 1.50-1.80 (m, 4H, CH), 2.15-2.30 (m, 2H, CH_2), 2.60-3.95 (m, 4H, CH_2), 3.75-4.0 (m, 2H, CH_2), 7.15-7.35 (m, 3H, ArH), 8.15 (d,

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1H, ArH)

2o 1.41 (dq, 1H, CH), 1.7-1.5 (m, 2H, CH_2), 1.84 (d, 2H, CH_2), 2.3-2.1 (dd, 2H, CH_2), 2.85-2.75 (dd, 2H, CH_2), 3.20 (t, 2H, CH_2N), 3.65 (dq, 1H, OH), 4.08 (m, 2H, CH_2O), 5.11 (br s, 2H, NH_2), 5.19 (s, 1H, COCH), 7.30-7.78 (m, 4H, ArH)

2p 1.50-1.65 (m, 1H, CH), 2.10-2-40 (m, 4H, CH_2), 2.55-2.65 (m, 1H, CH), 2.7-95 (m, 3H, CH_2), 3.0-3.1 (m, 2H, CH_2), 3.85-4.0 (m, 2H, CH_2), 7.20-7.40 (m, 3H, ArH), 8.0-8.10 (m, 1H, ArH)

3c 1.29 (t, 3H, CH_3), 1.4-1.2 (m, 2H, CH_2), 1.41 (m, 1H, CH), 1.90-1.80 (m, 2H, CH_2), 2.04 (q, 2H, CH_2), 2.3-2.1 (dd, 2H, CH_2), 2.47 (dd, 2H, CH_2CO), 2.88-2.84 (dd, 2H,CH_2), 3.20 (t, 2H, CH_2N), 4.13 (t, 2H, CH_2O), 7.30-7.78 (m, 4H, ArH)

4c 1.25 (t, 3H, CH_3), 2.15-2.27 (m, 2H, CH_2), 2.38-2.48 (m, 2H, CH_2), 2.80-2.95 (m, 4H, CH_2), 4.10 (q, 2H, CH_2), 4.25-4.32 (t, 2H, CH_2), 6.75 (s, 1H, CH), 7.20-7.40 (m, 3H, ArH), 8.0-8.10 (m, 1H, ArH)

6[a] 1.41 (m, 1H, CH), 1.7-1.5 (m, 2H, CH_2), 2.3-2.1 (m, 2H, CH_2), 2.85-2.75 (t, 2H, CH_2), 7.0 (br s, 1H, NH), 7.30-7.78 (m, 4H, ArH)

9 1.41 (dq, 1H, CH), 1.52 (d, 2H, CH_2), 1.7-1.5 (dd, 2H, CH_2), 1.82 (d, 2H, CH_2), 2.3-2.1 (dd, 2H, CH_2), 2.85-2.75 (m, 2H, CH_2), 3.20 (dq, 2H, CH_2), 3.51 (t, 2H, CH_2), 7.30-7.78 (m, 4H, ArH)

10 1.41 (dq, 1H, CH), 1.7-1.5 (m, 2H, CH_2), 1.75 (d, 2H, CH_2), 2.3-2.1 (dd, 2H, CH_2), 2.85-2.75 (dd, 2H, CH_2), 3.20 (t, 2H, CH_2), 3.50 (dq, 2H, CH_2), 3.65 (s, 1H, OH), 7.30-7.78 (m, 4H, ArH)

11 1.38 (m, 9H, $3CH_3$), 1.41 (dq, 1H, CH), 1.7-1.5 (t, 2H, CH_2), 1.84 (d, 2H, CH_2), 2.3-2.1 (dd, 2H, CH_2), 2.85-2.75 (dd, 2H, CH_2), 3.20 (dq, 2H, CH_2), 3.23-2.98 (dd, 2H, CH_2), 4.08 (t, 2H, CH_2), 4.68 (dq, 1H, CH), 7.27-7.40 (m, 5H, ArH), 7.30-7.78 (m, 4H, ArH), 8.03 (br s, 1H, NH)

12 1.50-1.65 (m, 1H, CH), 2.10-2-40 (m, 4H, CH_2), 2.40-2.50 (m, 2H, CH), 2.65-95 (m,4H, CH_2), 3.90-4.10 (m, 2H, CH_2), 7.10-7.40 (m, 3H, ArH), 8.10-8.20 (m, 1H, ArH)

(+)-13 1.55-1.70 (m, 1H, CH), 2.15-2.35 (m, 2H, CH_2), 2.65-2.95 (m, 4H, CH_2), 3.75-3.85 (m, 2H, CH_2), 4.10-4.30 (m, 2H, CH_2), 7.15-7.35 (m, 3H, ArH), 8.10-8.15 (m, 1H, ArH)

[a]CD_3OD

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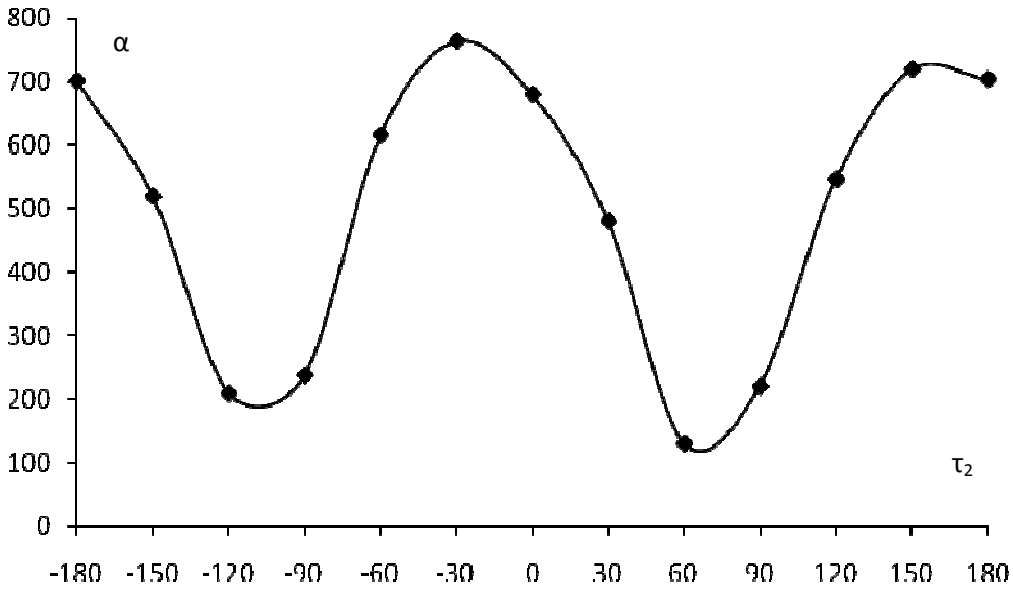

Figure S1. $[\alpha]_D$ values determined for the different points originating by the energy profile for rotation around the C-C bond between the two rings of compound **15**.