

## Supplementary Material

### Structures of 4-Iminopyrido[1,2-*a*]pyrimidines, Pyrido[1,2-*a*]pyrimidin-4-ones, Pyridopyrimidinium Olates, and Thiazolo[3,2-*a*]pyrimidine Analogs

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Tables of bond lengths and angles in 2-chloro-8-methyl-4-(2-(4-picolinyl)-imino)-4H-pyrido[1,2-*a*]pyrimidine **8**, 7-chloro-5-(2-thiazolylimino)-5*H*-thiazolo[3,2-*a*]pyrimidine **9**, 2-methylamino-4*H*-pyrido[1,2-*a*]pyrimidin-4-one **10**, 7-methylthio-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one **11**, 2,3-dihydro-7-methylthio-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one **12**, and 1-methyl-2-[(*o*-*tert*-butylphenyl)imino]-1,2-dihydropyrimidin-1-ium-4-olate **13**.

Table S1. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **8**

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C(2)-N(1)	1.303(3)
C(2)-C(3)	1.340(3)
C(2)-Cl(1)	1.718(3)
C(3)-C(4)	1.389(3)
C(4)-N(4)	1.279(3)
C(4)-N(5)	1.422(3)
C(6)-N(1)	1.318(3)
C(6)-N(5)	1.364(3)
C(6)-C(10)	1.391(4)
C(7)-C(8)	1.323(4)
C(7)-N(5)	1.353(3)
C(8)-C(9)	1.394(4)
C(9)-C(10)	1.331(4)
C(9)-C(11)	1.474(4)
C(12)-N(2)	1.325(3)
C(12)-C(13)	1.371(3)
C(12)-N(4)	1.377(3)
C(13)-C(14)	1.356(4)
C(14)-C(15)	1.366(4)
C(14)-C(17)	1.487(4)
C(15)-C(16)	1.354(4)
C(16)-N(2)	1.318(3)
N(1)-C(2)-C(3)	127.8(3)
N(1)-C(2)-Cl(1)	114.15(19)
C(3)-C(2)-Cl(1)	118.0(2)
C(2)-C(3)-C(4)	119.0(3)
N(4)-C(4)-C(3)	132.7(2)
N(4)-C(4)-N(5)	113.7(2)
C(3)-C(4)-N(5)	113.5(2)
N(1)-C(6)-N(5)	122.4(2)
N(1)-C(6)-C(10)	119.9(2)
N(5)-C(6)-C(10)	117.8(2)
C(8)-C(7)-N(5)	121.8(2)
C(7)-C(8)-C(9)	121.0(3)
C(10)-C(9)-C(8)	116.9(2)

C(10)-C(9)-C(11)	123.4(3)
C(8)-C(9)-C(11)	119.7(3)
C(9)-C(10)-C(6)	123.0(2)
N(2)-C(12)-C(13)	121.8(2)
N(2)-C(12)-N(4)	123.2(2)
C(13)-C(12)-N(4)	115.0(2)
C(14)-C(13)-C(12)	121.2(3)
C(13)-C(14)-C(15)	116.6(2)
C(13)-C(14)-C(17)	121.8(3)
C(15)-C(14)-C(17)	121.5(3)
C(16)-C(15)-C(14)	119.2(3)
N(2)-C(16)-C(15)	124.7(3)
C(2)-N(1)-C(6)	115.5(2)
C(16)-N(2)-C(12)	116.4(2)
C(4)-N(4)-C(12)	125.0(2)
C(7)-N(5)-C(6)	119.5(2)
C(7)-N(5)-C(4)	118.8(2)
C(6)-N(5)-C(4)	121.7(2)

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Table S2. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **9**

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C(2)-N(1)	1.325(4)
C(2)-C(3)	1.334(4)
C(2)-Cl(1)	1.712(3)
C(3)-C(4)	1.392(4)
C(4)-N(4)	1.284(4)
C(4)-N(5)	1.394(4)
C(6)-N(1)	1.290(4)
C(6)-N(5)	1.340(4)
C(6)-S(1)	1.701(3)
C(7)-C(8)	1.312(5)
C(7)-N(5)	1.372(4)
C(8)-S(1)	1.691(4)
C(9)-N(2)	1.291(4)
C(9)-N(4)	1.352(4)
C(9)-S(2)	1.716(3)
C(10)-C(11)	1.314(5)
C(10)-N(2)	1.356(4)
C(11)-S(2)	1.682(4)
N(1)-C(2)-C(3)	127.2(3)
N(1)-C(2)-Cl(1)	113.5(3)
C(3)-C(2)-Cl(1)	119.3(3)
C(2)-C(3)-C(4)	119.8(3)
N(4)-C(4)-C(3)	132.5(3)
N(4)-C(4)-N(5)	114.9(3)
C(3)-C(4)-N(5)	112.5(3)
N(1)-C(6)-N(5)	125.8(3)
N(1)-C(6)-S(1)	123.5(3)
N(5)-C(6)-S(1)	110.7(3)
C(8)-C(7)-N(5)	112.4(3)
C(7)-C(8)-S(1)	112.8(3)
N(2)-C(9)-N(4)	130.4(3)
N(2)-C(9)-S(2)	113.6(3)
N(4)-C(9)-S(2)	116.0(3)
C(11)-C(10)-N(2)	117.7(4)
C(10)-C(11)-S(2)	109.2(3)

C(6)-N(1)-C(2)	112.8(3)
C(9)-N(2)-C(10)	109.7(3)
C(4)-N(4)-C(9)	121.3(3)
C(6)-N(5)-C(7)	113.5(3)
C(6)-N(5)-C(4)	121.7(3)
C(7)-N(5)-C(4)	124.7(3)
C(8)-S(1)-C(6)	90.50(18)
C(11)-S(2)-C(9)	89.90(19)

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Table S3. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **10**

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C(2)-N(2)	1.321(3)
C(2)-N(1)	1.333(3)
C(2)-C(3)	1.376(3)
C(3)-C(4)	1.352(3)
C(4)-O(4)	1.238(2)
C(4)-N(5)	1.421(3)
C(6)-N(1)	1.303(3)
C(6)-N(5)	1.364(2)
C(6)-C(10)	1.397(3)
C(7)-C(8)	1.325(3)
C(7)-N(5)	1.353(3)
C(8)-C(9)	1.382(3)
C(9)-C(10)	1.332(3)
C(11)-N(2)	1.424(3)
N(2)-C(2)-N(1)	117.42(19)
N(2)-C(2)-C(3)	119.9(2)
N(1)-C(2)-C(3)	122.7(2)
C(4)-C(3)-C(2)	121.2(2)
O(4)-C(4)-C(3)	127.9(2)
O(4)-C(4)-N(5)	117.0(2)
C(3)-C(4)-N(5)	115.17(18)
N(1)-C(6)-N(5)	123.66(19)
N(1)-C(6)-C(10)	119.97(19)
N(5)-C(6)-C(10)	116.4(2)
C(8)-C(7)-N(5)	121.3(2)
C(7)-C(8)-C(9)	119.2(2)
C(10)-C(9)-C(8)	120.0(2)
C(9)-C(10)-C(6)	121.6(2)
C(6)-N(1)-C(2)	117.40(17)
C(2)-N(2)-C(11)	123.5(2)
C(7)-N(5)-C(6)	121.53(19)
C(7)-N(5)-C(4)	118.62(18)
C(6)-N(5)-C(4)	119.85(18)

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Table S4. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **11**

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C(2)-N(1)	1.339(3)
C(2)-C(3)	1.352(4)
C(2)-S(1)	1.729(3)
C(3)-C(4)	1.382(4)
C(4)-O(4)	1.213(3)
C(4)-N(5)	1.410(3)
C(6)-N(1)	1.285(3)
C(6)-N(5)	1.349(3)
C(6)-S(2)	1.705(3)
C(7)-C(8)	1.302(4)
C(7)-N(5)	1.377(3)
C(8)-S(2)	1.700(3)
C(9)-S(1)	1.757(4)
N(1)-C(2)-C(3)	123.9(3)
N(1)-C(2)-S(1)	117.9(2)
C(3)-C(2)-S(1)	118.2(2)
C(2)-C(3)-C(4)	122.1(3)
O(4)-C(4)-C(3)	128.9(3)
O(4)-C(4)-N(5)	118.7(3)
C(3)-C(4)-N(5)	112.3(3)
N(1)-C(6)-N(5)	126.1(3)
N(1)-C(6)-S(2)	123.9(2)
N(5)-C(6)-S(2)	109.9(2)
C(8)-C(7)-N(5)	112.5(3)
C(7)-C(8)-S(2)	113.0(2)
C(6)-N(1)-C(2)	114.6(3)
C(6)-N(5)-C(7)	113.9(2)
C(6)-N(5)-C(4)	120.8(2)
C(7)-N(5)-C(4)	125.3(3)
C(2)-S(1)-C(9)	102.38(16)
C(8)-S(2)-C(6)	90.65(14)

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Table S5. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **12**

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S(1)-C(2)	1.730(3)
S(1)-C(9)	1.774(3)
S(2)-C(6)	1.723(2)
S(2)-C(8)	1.785(3)
N(5)-C(6)	1.343(3)
N(5)-C(4)	1.378(3)
N(5)-C(7)	1.443(3)
N(1)-C(6)	1.282(3)
N(1)-C(2)	1.360(3)
O(4)-C(4)	1.216(3)
C(7)-C(8)	1.478(4)
C(2)-C(3)	1.344(3)
C(3)-C(4)	1.401(3)
C(2)-S(1)-C(9)	103.69(13)
C(6)-S(2)-C(8)	92.26(13)
C(6)-N(5)-C(4)	121.1(2)
C(6)-N(5)-C(7)	117.0(2)
C(4)-N(5)-C(7)	121.7(2)
C(6)-N(1)-C(2)	114.6(2)
N(5)-C(7)-C(8)	108.0(2)
C(3)-C(2)-N(1)	123.8(2)
C(3)-C(2)-S(1)	125.45(19)
N(1)-C(2)-S(1)	110.74(18)
N(1)-C(6)-N(5)	126.0(2)
N(1)-C(6)-S(2)	122.21(19)
N(5)-C(6)-S(2)	111.81(18)
C(2)-C(3)-C(4)	120.5(2)
O(4)-C(4)-N(5)	118.8(2)
O(4)-C(4)-C(3)	127.4(2)
N(5)-C(4)-C(3)	113.8(2)
C(7)-C(8)-S(2)	108.6(2)

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Table S6. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **13**

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C(1)-N(1)	1.472(3)
C(2)-N(2)	1.279(3)
C(2)-C(3)	1.423(3)
C(2)-N(1)	1.429(3)
C(3)-C(4)	1.352(3)
C(4)-O(4)	1.241(3)
C(4)-N(5)	1.499(3)
C(6)-N(1)	1.334(3)
C(6)-N(5)	1.366(3)
C(6)-C(10)	1.412(3)
C(7)-N(5)	1.356(3)
C(7)-C(8)	1.375(4)
C(8)-C(9)	1.391(4)
C(9)-C(10)	1.338(4)
C(11)-C(16)	1.395(4)
C(11)-C(12)	1.408(4)
C(11)-N(2)	1.413(3)
C(12)-C(13)	1.392(4)
C(12)-C(17)	1.527(4)
C(13)-C(14)	1.371(5)
C(14)-C(15)	1.360(5)
C(15)-C(16)	1.383(4)
C(17)-C(20)	1.528(4)
C(17)-C(18)	1.529(4)
C(17)-C(19)	1.542(4)
N(2)-C(2)-C(3)	129.4(2)
N(2)-C(2)-N(1)	115.5(2)
C(3)-C(2)-N(1)	115.1(2)
C(4)-C(3)-C(2)	125.8(2)
O(4)-C(4)-C(3)	130.7(2)
O(4)-C(4)-N(5)	115.5(2)
C(3)-C(4)-N(5)	113.8(2)
N(1)-C(6)-N(5)	120.1(2)
N(1)-C(6)-C(10)	122.5(2)
N(5)-C(6)-C(10)	117.4(2)

N(5)-C(7)-C(8)	120.4(3)
C(7)-C(8)-C(9)	118.5(3)
C(10)-C(9)-C(8)	120.9(3)
C(9)-C(10)-C(6)	120.8(3)
C(16)-C(11)-C(12)	119.4(2)
C(16)-C(11)-N(2)	118.9(3)
C(12)-C(11)-N(2)	121.4(2)
C(13)-C(12)-C(11)	117.0(3)
C(13)-C(12)-C(17)	120.5(3)
C(11)-C(12)-C(17)	122.5(2)
C(14)-C(13)-C(12)	122.8(3)
C(15)-C(14)-C(13)	120.0(3)
C(14)-C(15)-C(16)	119.5(3)
C(15)-C(16)-C(11)	121.3(3)
C(12)-C(17)-C(20)	112.4(2)
C(12)-C(17)-C(18)	109.3(2)
C(20)-C(17)-C(18)	106.7(3)
C(12)-C(17)-C(19)	110.7(2)
C(20)-C(17)-C(19)	107.4(3)
C(18)-C(17)-C(19)	110.3(3)
C(6)-N(1)-C(2)	123.01(19)
C(6)-N(1)-C(1)	119.3(2)
C(2)-N(1)-C(1)	117.7(2)
C(2)-N(2)-C(11)	120.5(2)
C(7)-N(5)-C(6)	122.0(2)
C(7)-N(5)-C(4)	116.2(2)
C(6)-N(5)-C(4)	121.8(2)

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