

Synthesis of Novel PETT Analogues: 3,4-Dimethoxy Phenyl Ethyl 1,3,5-Triazinyl Thiourea Derivatives and their Antibacterial and Anti-HIV Studies

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Table S1. Elemental analyses data of **8a-o** and **9a-o**

| Compound | Molecular Formula | Elemental analyses | | |
|-----------|--|--------------------|--------|---------|
| | | %C | %H | %N |
| 8a | C ₃₀ H ₂₇ N ₇ O ₆ S | 58.72 | 4.40 | 15.98 |
| | | (58.50) | (4.11) | (15.69) |
| 8b | C ₃₁ H ₂₉ N ₇ O ₆ S | 59.31 | 4.62 | 15.62 |
| | | (59.07) | (4.33) | (15.35) |
| 8c | C ₃₄ H ₂₉ N ₇ O ₆ S | 61.53 | 4.37 | 14.78 |
| | | (61.25) | (4.12) | (14.49) |
| 8d | C ₃₁ H ₂₉ N ₇ O ₇ S | 57.83 | 4.51 | 15.23 |
| | | (57.59) | (4.28) | (15.00) |
| 8e | C ₃₁ H ₂₉ N ₇ O ₇ S | 57.83 | 4.51 | 15.23 |
| | | (57.55) | (4.30) | (15.01) |
| 8f | C ₃₁ H ₂₉ N ₇ O ₆ S | 59.31 | 4.62 | 15.62 |
| | | (59.07) | (4.32) | (15.32) |
| 8g | C ₃₁ H ₂₉ N ₇ O ₆ S | 59.31 | 4.62 | 15.62 |
| | | (59.10) | (4.25) | (15.35) |
| 8h | C ₃₁ H ₂₉ N ₇ O ₆ S | 59.31 | 4.62 | 15.62 |
| | | (59.01) | (4.35) | (15.37) |
| 8i | C ₃₀ H ₂₆ N ₈ O ₈ S | 54.69 | 3.95 | 17.01 |
| | | (54.40) | (3.67) | (16.75) |
| 8j | C ₃₀ H ₂₆ N ₈ O ₈ S | 54.69 | 3.95 | 17.01 |
| | | (54.45) | (3.66) | (16.80) |
| 8k | C ₃₀ H ₂₆ N ₈ O ₈ S | 54.69 | 3.95 | 17.01 |
| | | (54.39) | (3.65) | (16.31) |
| 8l | C ₃₀ H ₂₆ N ₇ O ₆ SCl | 55.59 | 4.01 | 15.13 |
| | | (55.29) | (3.70) | (14.97) |
| 8m | C ₃₀ H ₂₆ N ₇ O ₆ SCl | 55.59 | 4.01 | 15.13 |
| | | (55.30) | (3.72) | (14.95) |
| 8n | C ₃₀ H ₂₆ N ₇ O ₆ SCl | 55.59 | 4.01 | 15.13 |
| | | (55.31) | (3.75) | (15.00) |
| 8o | C ₃₀ H ₂₆ N ₇ O ₆ SF | 57.03 | 4.12 | 15.53 |
| | | (56.83) | (4.00) | (15.25) |
| 9a | C ₃₀ H ₂₇ N ₇ O ₅ S ₂ | 57.21 | 4.29 | 15.57 |
| | | (57.01) | (4.00) | (15.30) |
| 9b | C ₃₁ H ₂₉ N ₇ O ₅ S ₂ | 57.83 | 4.51 | 15.23 |
| | | (57.45) | (4.30) | (15.00) |
| 9c | C ₃₄ H ₂₉ N ₇ O ₅ S ₂ | 60.06 | 4.27 | 14.43 |
| | | (59.70) | (4.01) | (14.12) |
| 9d | C ₃₁ H ₂₉ N ₇ O ₆ S ₂ | 56.42 | 4.39 | 14.86 |
| | | (56.16) | (4.15) | (14.59) |

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Table S1. cont.

| Compound | Molecular Formula | Elemental analyses | | |
|-----------|---------------------------|--------------------|----------------|------------------|
| | | %C | %H | %N |
| 9e | $C_{31}H_{29}N_7O_6S_2$ | 56.42 (56.12) | 4.39 (4.10) | 14.86 (14.57) |
| 9f | $C_{31}H_{29}N_7O_5S_2$ | 57.83 (57.60) | 4.51 (4.30) | 15.23 (14.98) |
| 9g | $C_{31}H_{29}N_7O_5S_2$ | 57.83 (57.54) | 4.51 (4.21) | 15.23 (15.03) |
| 9h | $C_{31}H_{29}N_7O_5S_2$ | 57.83 (57.57) | 4.51 (4.27) | 15.23 (15.00) |
| 9i | $C_{30}H_{26}N_8O_7S_2$ | 53.39 (53.11) | 3.86 (3.59) | 16.61 (16.30) |
| 9j | $C_{30}H_{26}N_8O_7S_2$ | 53.39 (53.19) | 3.86 (3.56) | 16.61 (16.35) |
| 9k | $C_{30}H_{26}N_8O_7S_2$ | 53.39 (53.09) | 3.86 (3.55) | 16.61 (16.40) |
| 9l | $C_{30}H_{26}N_7O_5S_2Cl$ | 54.24 (54.00) | 3.92 (3.66) | 14.76 (14.49) |
| 9m | $C_{30}H_{26}N_7O_5S_2Cl$ | 54.24 (54.02) | 3.92 (3.62) | 14.76 (14.50) |
| 9n | $C_{30}H_{26}N_7O_5S_2Cl$ | 54.24 (53.97) | 3.92 (3.70) | 14.76 (14.54) |
| 9o | $C_{30}H_{26}N_7O_5S_2F$ | 55.62 (55.33) | 4.02 (3.82) | 15.14 (14.95) |