

Supporting Information

Elemental Analysis

High-Resolution Mass Spectra (HRMS) (EI)

Design, Synthesis, and X-ray Crystal Structure of Classical and Nonclassical 2-Amino-4-oxo-5-substituted-6-ethyl-thieno[2,3-*d*]pyrimidines as Dual Thymidylate Synthase and Dihydrofolate Reductase Inhibitors and as Potential Antitumor Agents

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Elemental Analysis

Compd	Formula	Calcd, %					Found, %				
		C	H	N	S	I	C	H	N	S	I
5	C ₈ H ₉ N ₃ OS• 0.09CH ₃ COCH ₃	49.54	4.79	20.95	15.99		49.47	4.69	20.72	16.20	
6	C ₈ H ₈ IN ₃ OS• 0.34CH ₂ Cl ₂	28.61	2.49	12.00	9.15	36.24	28.61	2.45	11.62	8.83	36.45
8	C ₁₅ H ₁₃ N ₃ O ₃ S ₂ • 1.94CH ₃ COCH ₃	54.32	5.36	9.12	13.90		54.62	5.28	9.18	13.99	
9	C ₂₄ H ₂₈ N ₄ O ₆ S ₂ • 0.59CH ₃ COCH ₃	54.60	5.60	9.88	11.30		54.66	5.46	9.94	11.23	
2	C ₂₀ H ₂₀ N ₄ O ₆ S ₂ • 0.31CH ₃ COCH ₃ • .79HCl	48.01	4.36	10.68	12.23		47.97	4.75	10.67	12.37	

High-Resolution Mass Spectra (HRMS) (EI)

Compound	Formula	Calcd mass	Found mass
7	C ₁₆ H ₁₅ N ₃ O ₃ S ₂	361.0554	361.0556
9	C ₂₄ H ₂₈ N ₄ O ₆ S ₂	532.1450	532.1444
2a	C ₁₄ H ₁₃ N ₃ OS ₂	303.0500	303.0503
2b	C ₁₄ H ₁₂ N ₃ OCIS ₂	337.0110	337.0093
2c	C ₁₄ H ₁₃ N ₄ O ₃ S ₂	349.0429	349.0403
2d	C ₁₆ H ₁₇ N ₃ O ₃ S ₂	363.0711	363.0706
2e	C ₁₄ H ₁₁ C ₁₂ N ₃ OS ₂	370.9715	370.9720
2f	C ₁₄ H ₁₁ Cl ₂ N ₃ OS ₂	370.9708	370.9720
2g	C ₁₈ H ₁₅ N ₃ OS ₂	353.0656	353.0653
2h	C ₁₃ H ₁₃ N ₄ OS ₂	305.0531	305.0528
2i	C ₁₄ H ₁₂ FN ₃ OS ₂	321.0405	321.0404
2j	C ₁₄ H ₁₂ BrN ₃ OS ₂	380.9605	380.9611
2k	C ₁₄ H ₁₂ ClN ₃ OS ₂	337.0119	337.0110
2l	C ₁₆ H ₁₇ N ₃ O ₃ S ₂	363.0711	363.0721
2m	C ₁₄ H ₁₂ ClN ₃ OS ₂	337.0110	337.0113