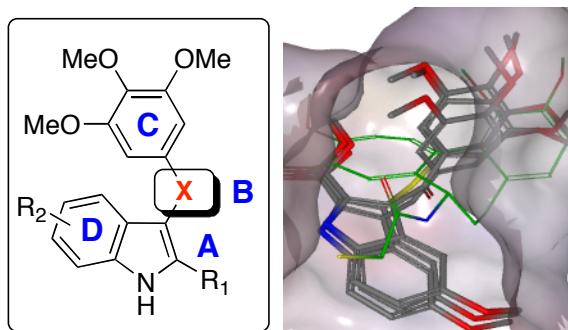


Supporting Information

New Arylthioindoles and Related Bioisosteres at the Sulfur Bridging Group. 4. Synthesis, Tubulin Polymerization, Cell Growth Inhibition, and Molecular Modeling Studies

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TOC graphics



R₁=H,COOMe,COOEt; R₂=H,5-Cl,5-Br,5-OMe;
X=S,SO,SO₂,CO,CH₂,COCH₂,COCO,CH₂CH₂.

Contents

- **Figure 1S.** Effects of compounds **24**, **27-29**, **36**, **39** and **41** on murine macrophage J744.1 cell morphology.
- **Table 1S.** Elemental analyses of new derivatives **7**, **8**, **10**, **11**, **13**, **14**, **16**, **17**, **19-23**, **25-32**, **35**, **37-41**, and **43-56**.

Murine Macrophage J744.1 (48 h)

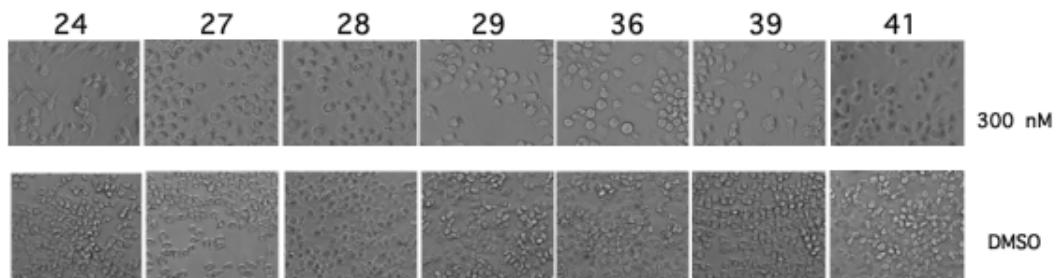


Figure 1S. Effects of compounds **24**, **27-29**, **36**, **39** and **41** on murine macrophage J744.1 cell morphology, as visualized by time-lapse microscopy (magnification 20 x)

Table 1S. Elemental Analyses of New Derivatives **7, 8, 10, 11, 13, 14, 16, 17, 19-23, 25-32, 35, 37-41**, and **43-56**.

| Compd | Calcd | Found |
|-----------|--|--|
| 7 | C, 65.02; H, 5.19; N, 3.79. | C, 65.01; H, 5.18; N, 3.79. |
| 8 | C, 67.58; H, 5.95; N, 3.94. | C, 67.57; H, 5.95; N, 3.92. |
| 10 | C, 65.77; H, 5.52; N, 3.65. | C, 65.77; H, 5.53; N, 3.64. |
| 11 | C, 68.23; H, 6.28; N, 3.79. | C, 68.22; H, 6.25; N, 3.79. |
| 13 | C, 65.29; H, 4.67; Cl, 10.13; N, 4.06. | C, 65.30; H, 4.67; Cl, 10.14; N, 4.05. |
| 14 | C, 65.24; H, 5.48; Cl, 10.56; N, 4.23. | C, 65.24; H, 5.49; Cl, 10.58; N, 4.21. |
| 16 | C, 59.54; H, 4.50; Cl, 8.67; N, 3.47. | C, 59.53; H, 4.51; Cl, 8.66; N, 3.47. |
| 17 | C, 61.68; H, 5.18; Cl, 8.99; N, 3.60. | C, 61.69; H, 5.17; Cl, 8.98; N, 3.60. |
| 19 | C, 60.42; H, 4.83; Cl, 8.38; N, 3.36. | C, 60.44; H, 4.83; Cl, 8.37; N, 3.35. |
| 20 | C, 62.51; H, 5.50; Cl, 8.67; N, 3.47. | C, 62.51; H, 5.51; Cl, 8.66; N, 3.46. |
| 21 | C, 61.24; H, 5.14; Cl, 8.11; N, 3.25. | C, 61.25; H, 5.13; Cl, 8.11; N, 3.26. |
| 22 | C, 59.31; H, 4.53; Cl, 7.86; N, 3.15. | C, 59.31; H, 4.54; Cl, 7.85; N, 3.14. |
| 23 | C, 62.29; H, 5.80; Cl, 8.38; N, 3.36. | C, 62.30; H, 5.81; Cl, 8.38; N, 3.36. |
| 25 | C, 55.52; H, 4.14; Br, 20.28; N, 3.59. | C, 55.51; H, 4.13; Br, 20.28; N, 3.59. |
| 26 | C, 57.59; H, 4.84; Br, 21.04; N, 3.73. | C, 57.60; H, 4.85; Br, 21.04; N, 3.73. |
| 27 | C, 50.55; H, 4.02; Br, 17.50; N, 3.10. | C, 50.54; H, 4.01; Br, 17.50; N, 3.11. |
| 28 | C, 53.69; H, 4.06; Br, 17.65; N, 3.13. | C, 53.69; H, 4.07; Br, 17.64; N, 3.14. |
| 29 | C, 55.42; H, 4.65; Br, 18.22; N, 3.23. | C, 55.43; H, 4.64; Br, 18.22; N, 3.22. |
| 30 | C, 51.61; H, 4.33; Br, 16.97; N, 3.01; S, 6.87 | C, 51.61; H, 4.32; Br, 16.97; N, 3.00; S, 6.87 |
| 31 | C, 54.66; H, 4.37; Br, 17.12; N, 3.04. | C, 54.65; H, 4.36; Br, 17.12; N, 3.04. |
| 32 | C, 54.42; H, 7.79; Br, 17.04; N, 3.02. | C, 54.43; H, 7.79; Br, 17.05; N, 3.02. |
| 35 | C, 69.69; H, 6.47; N, 4.28. | C, 69.69; H, 6.48; N, 4.29. |
| 37 | C, 57.26; H, 5.05; N, 3.34; S, 7.63. | C, 57.27; H, 5.06; N, 3.34; S, 7.63. |
| 38 | C, 55.15; H, 4.86; N, 3.22; S, 7.35. | C, 55.14; H, 4.85; N, 3.22; S, 7.35. |
| 39 | C, 63.14; H, 5.30; N, 3.51. | C, 63.13; H, 5.31; N, 3.51. |
| 40 | C, 62.82; H, 5.78; N, 3.49. | C, 62.83; H, 5.79; N, 3.49. |
| 41 | C, 65.43; H, 6.01; N, 3.63. | C, 65.44; H, 6.02; N, 3.63. |
| 43 | C, 63.90; H, 5.61; N, 3.39. | C, 63.91; H, 5.62; N, 3.40. |
| 44 | C, 63.59; H, 6.07; N, 3.37. | C, 63.60; H, 6.06; N, 3.38. |
| 45 | C, 66.14; H, 6.31; N, 3.51. | C, 66.13; H, 6.32; N, 3.50. |
| 46 | C, 63.94; H, 6.63; N, 4.39. | C, 63.92; H, 6.61; N, 4.39. |
| 47 | C, 65.69; H, 7.25; N, 4.03. | C, 65.69; H, 7.24; N, 4.03. |
| 48 | C, 66.46; H, 7.53; N, 3.88. | C, 66.46; H, 7.53; N, 3.87. |
| 49 | C, 67.84; H, 8.02; N, 3.60. | C, 67.83; H, 8.01; N, 3.60. |
| 50 | C, 59.99; H, 6.29; N, 8.74. | C, 60.00; H, 6.30; N, 8.74. |
| 51 | C, 61.25; H, 5.75; N, 4.20. | C, 61.24; H, 5.74; N, 4.20. |
| 52 | C, 57.48; H, 5.43; N, 8.38. | C, 57.49; H, 5.42; N, 8.38. |
| 53 | C, 57.48; H, 5.43; N, 8.38. | C, 57.49; H, 5.44; N, 8.38. |
| 54 | C, 61.85; H, 5.88; N, 4.81. | C, 61.84; H, 5.86; N, 4.81. |
| 55 | C, 62.69; H, 7.41; N, 3.32. | C, 62.70; H, 7.42; N, 3.32. |
| 56 | C, 51.15; H, 5.21; Cl, 10.78; N, 8.52. | C, 51.16; H, 5.22; Cl, 10.78; N, 8.53. |