

Supporting Information for

Anti-lymphangiogenesis Components from Taiwanese Zoanthid *Palythoa tuberculosa*

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Figure S1. ¹H NMR spectrum of tuberazine A (**1**) (CD₃OD, 700 MHz)

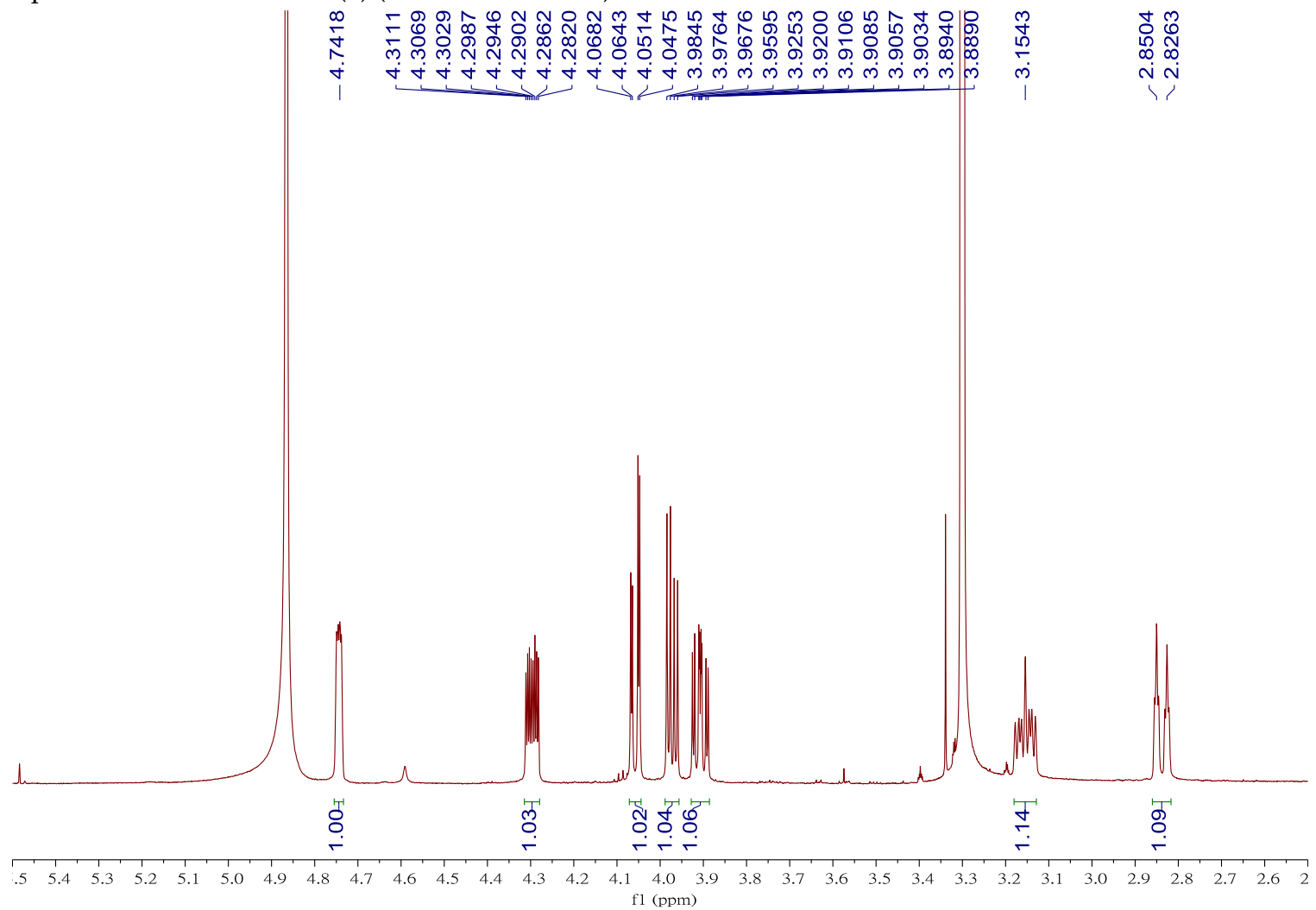


Figure S2. ^{13}C NMR spectrum of tuberazine A (**1**) (CD_3OD , 175 MHz)

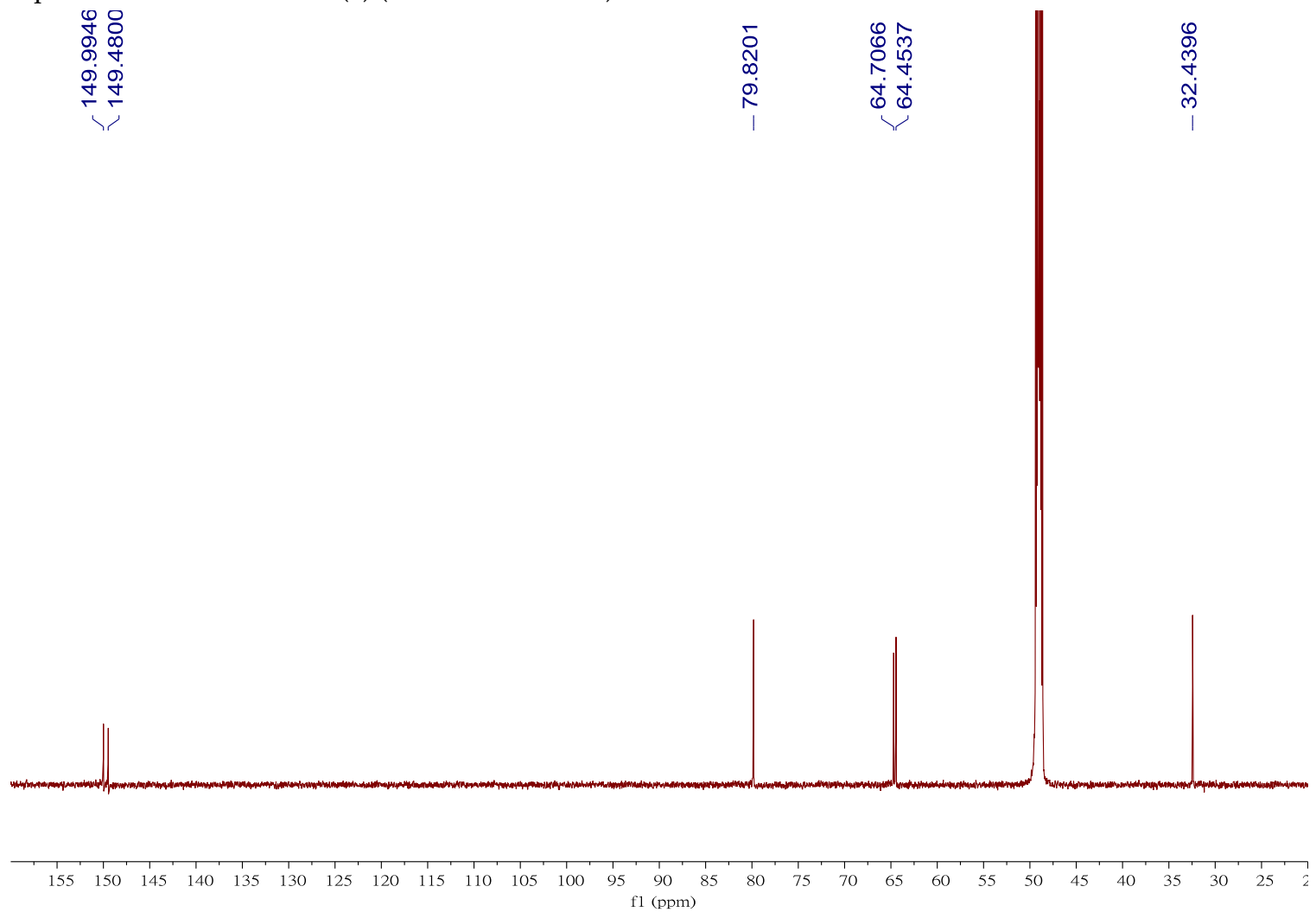


Figure S3. COSY spectrum of tuberazine A (1)

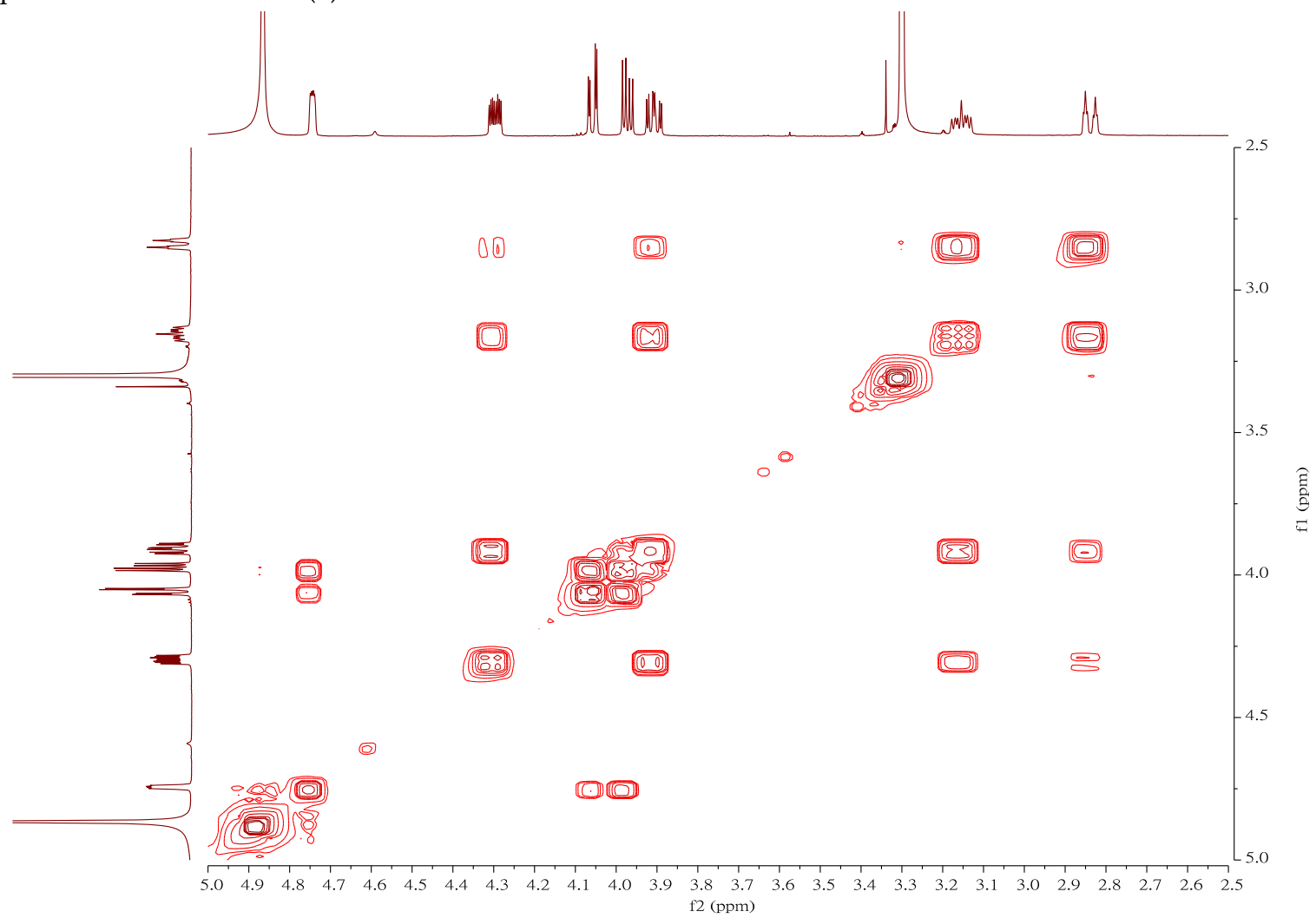


Figure S4. HSQC spectrum of tuberazine A (1)

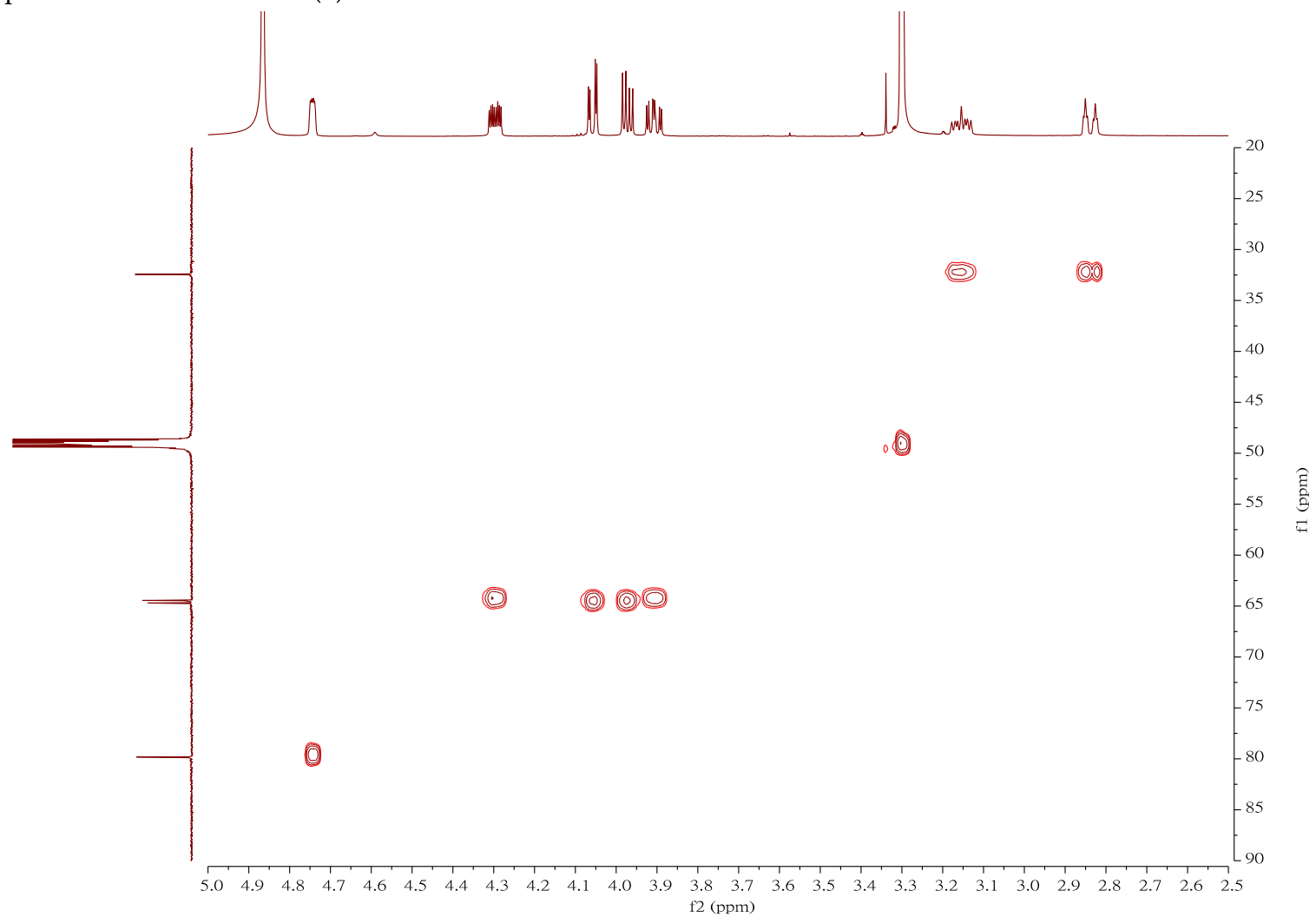


Figure S5. HMBC spectrum of tuberazine A (1)

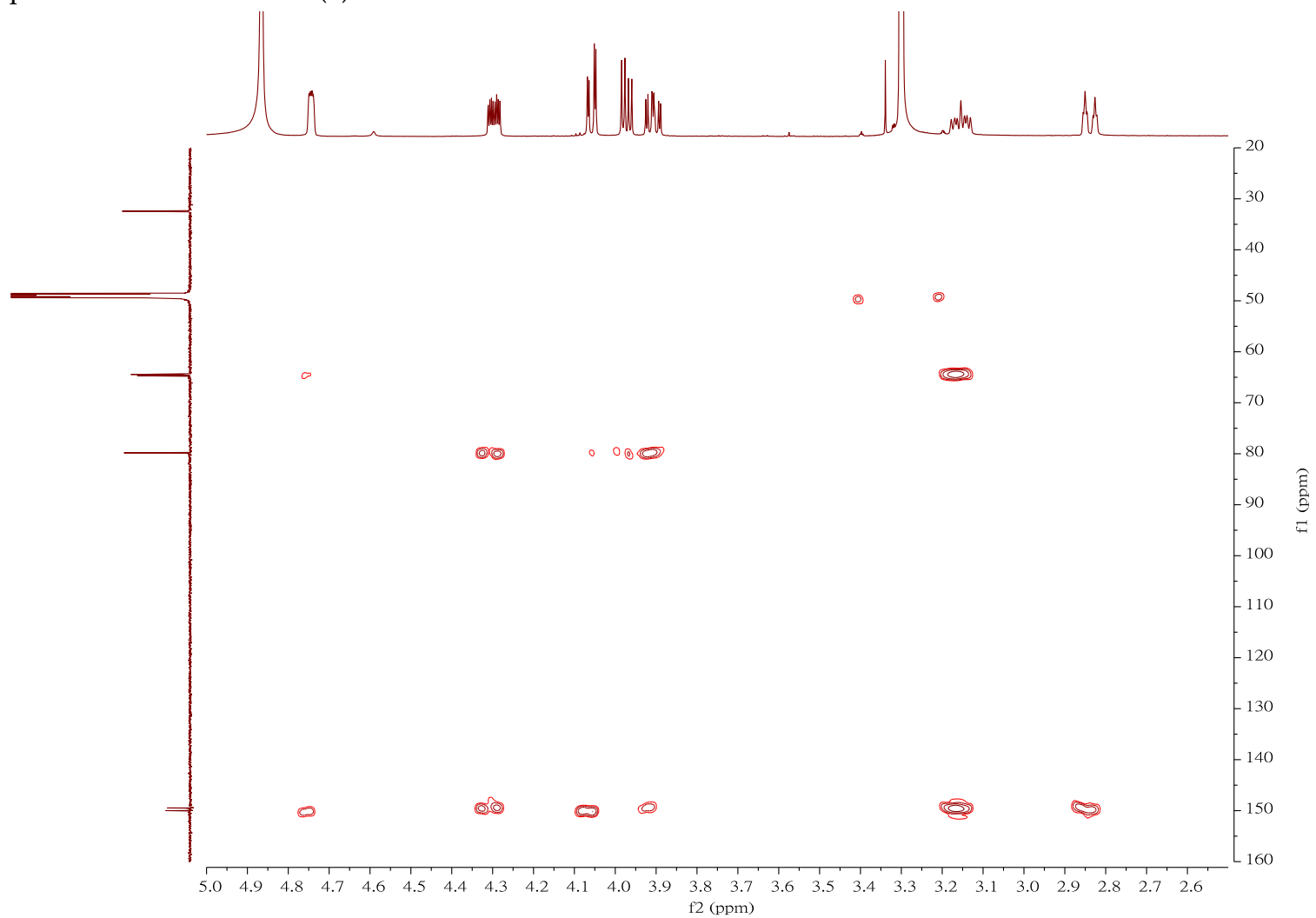


Figure S6. ^1H - ^{15}N HMBC spectrum of tuberazine A (1)

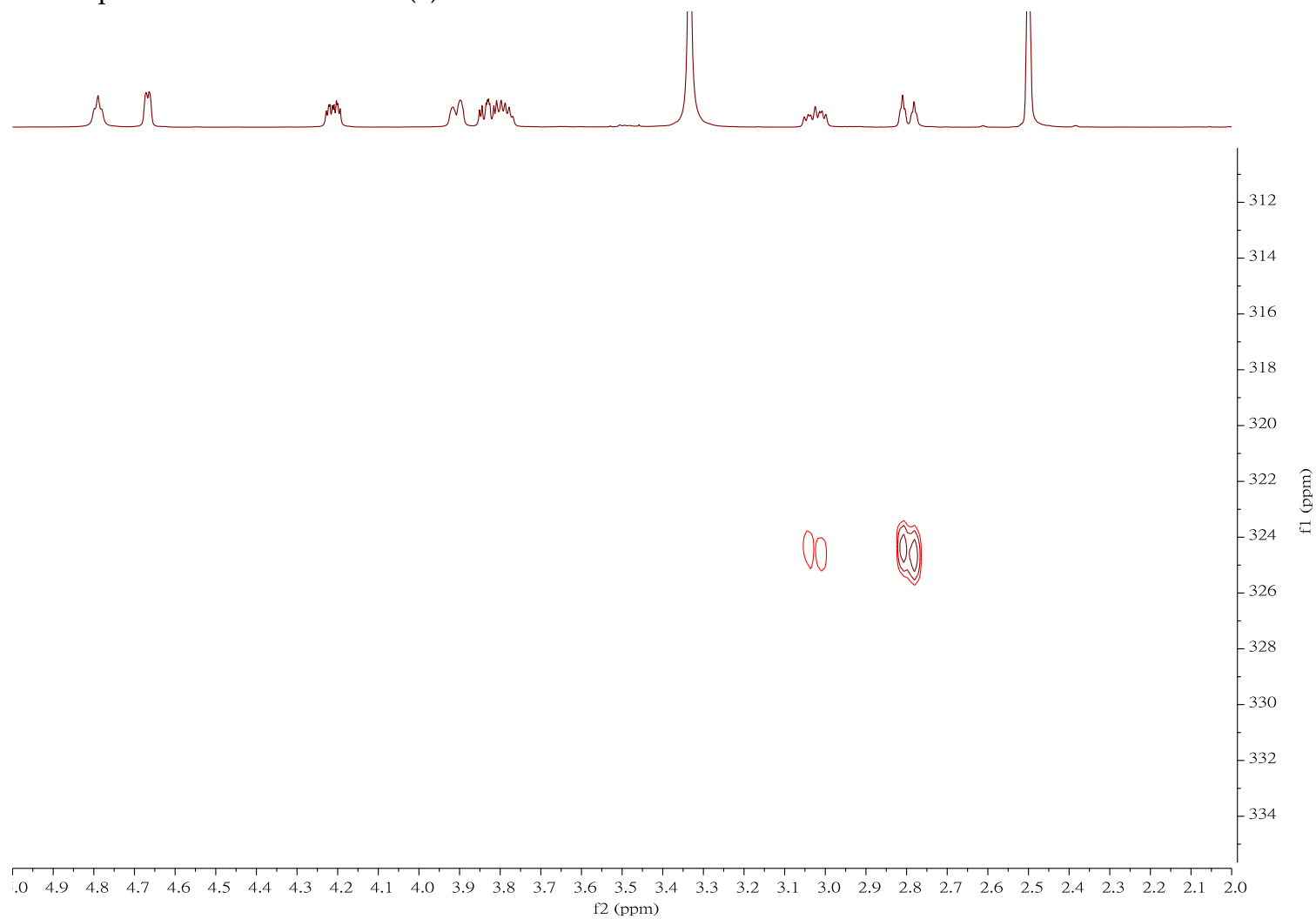


Figure S7. ¹H NMR spectrum of tuberazine B (2) (CD₃OD, 700 MHz)

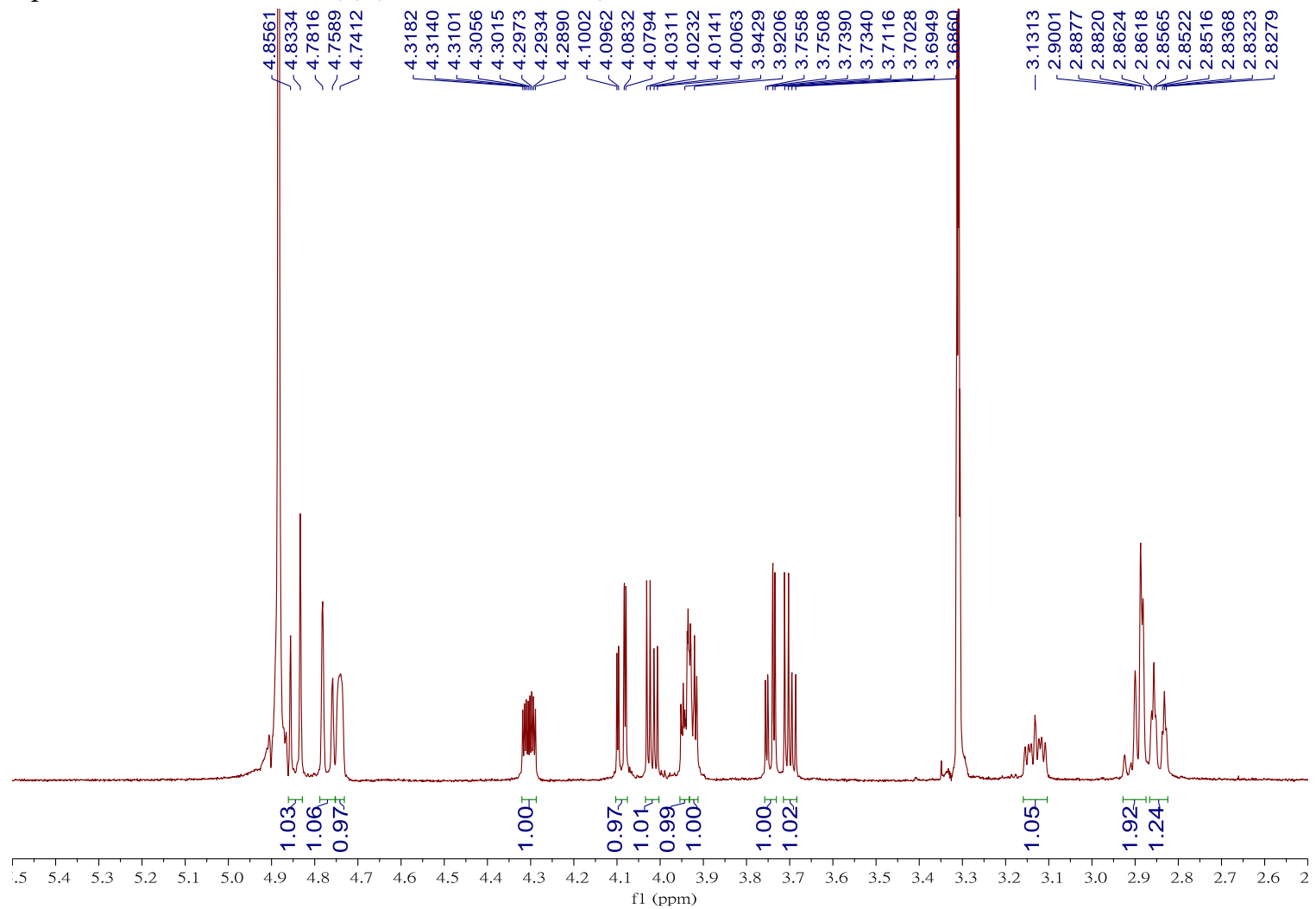


Figure S8. ^{13}C NMR spectrum of tuberazine B (**2**) (CD_3OD , 175 MHz)

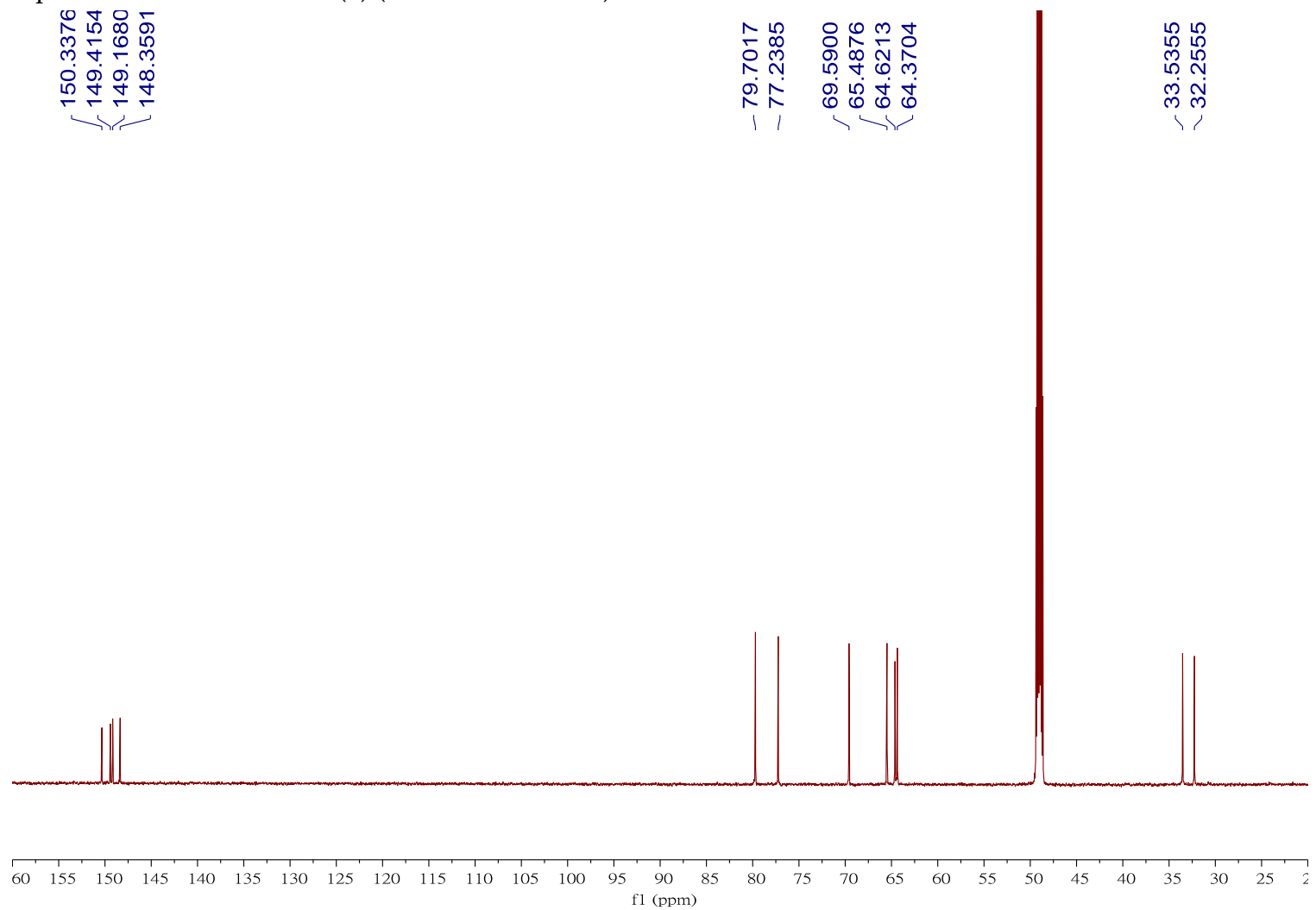


Figure S10. HSQC spectrum of tuberazine B (2)

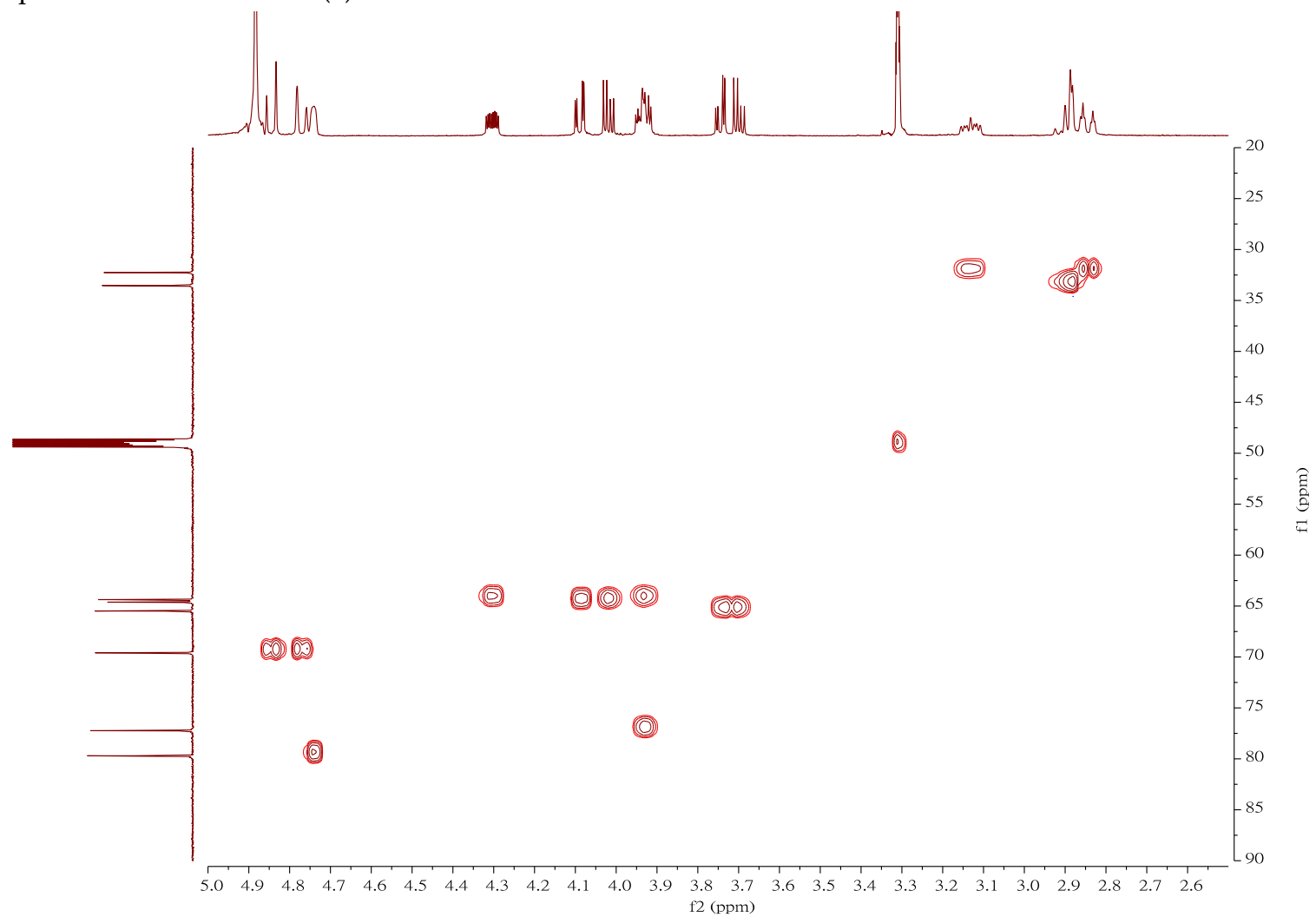


Figure S11. HMBC spectrum of tuberazine B (2)

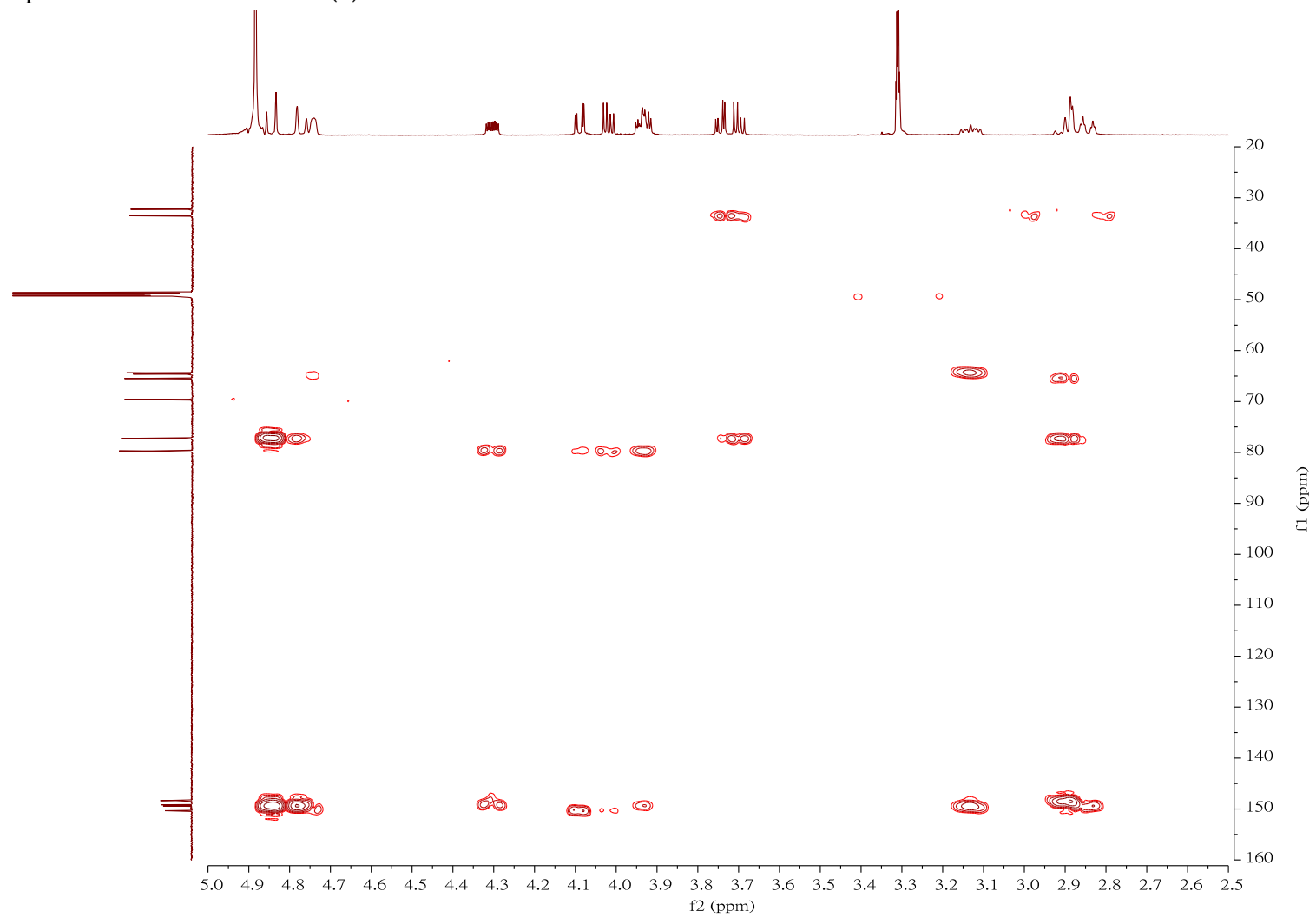


Figure S12. ^1H - ^{15}N HMBC spectrum of tuberazine B (2)

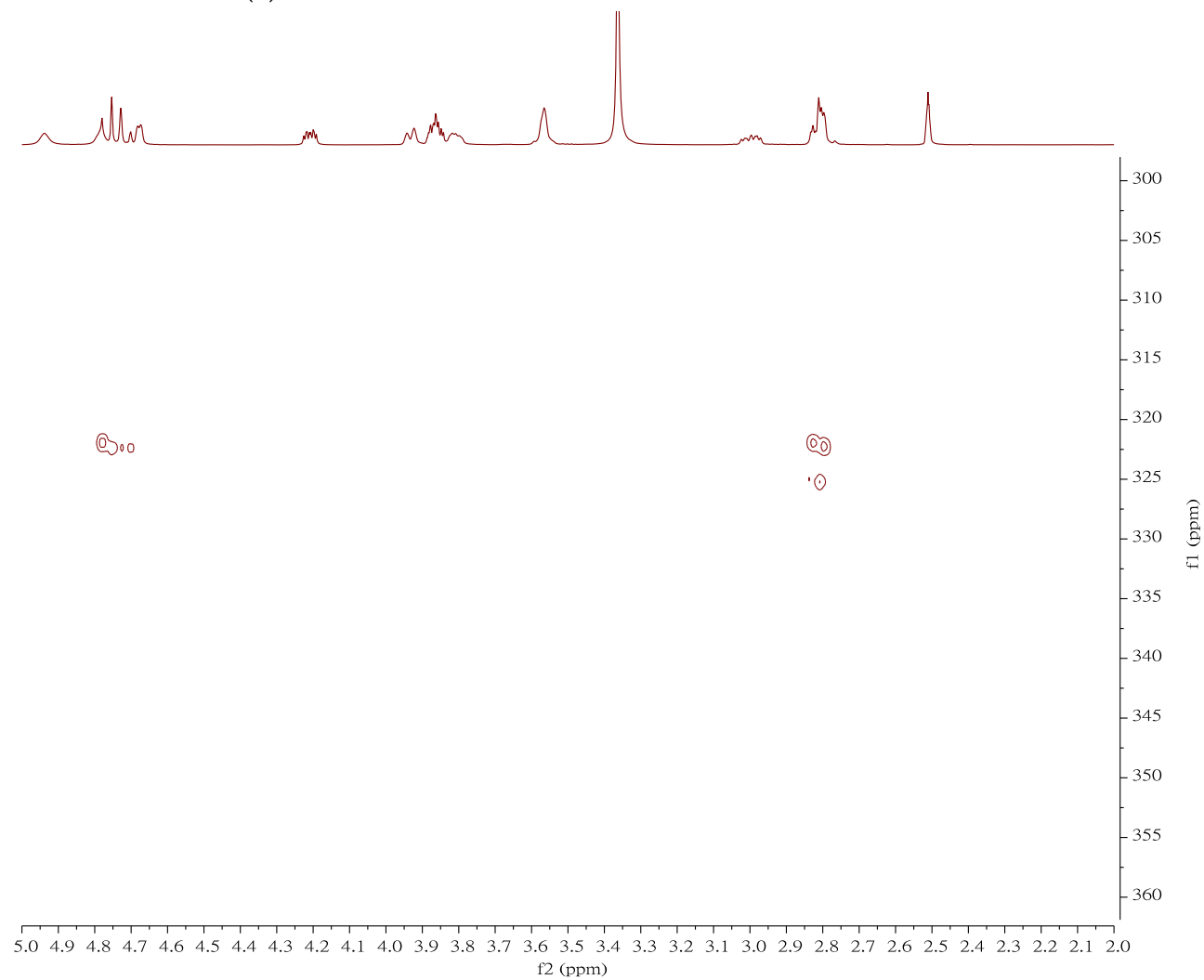


Figure S13. ¹H NMR spectrum of tuberazine C (3) (CD₃OD, 700 MHz)

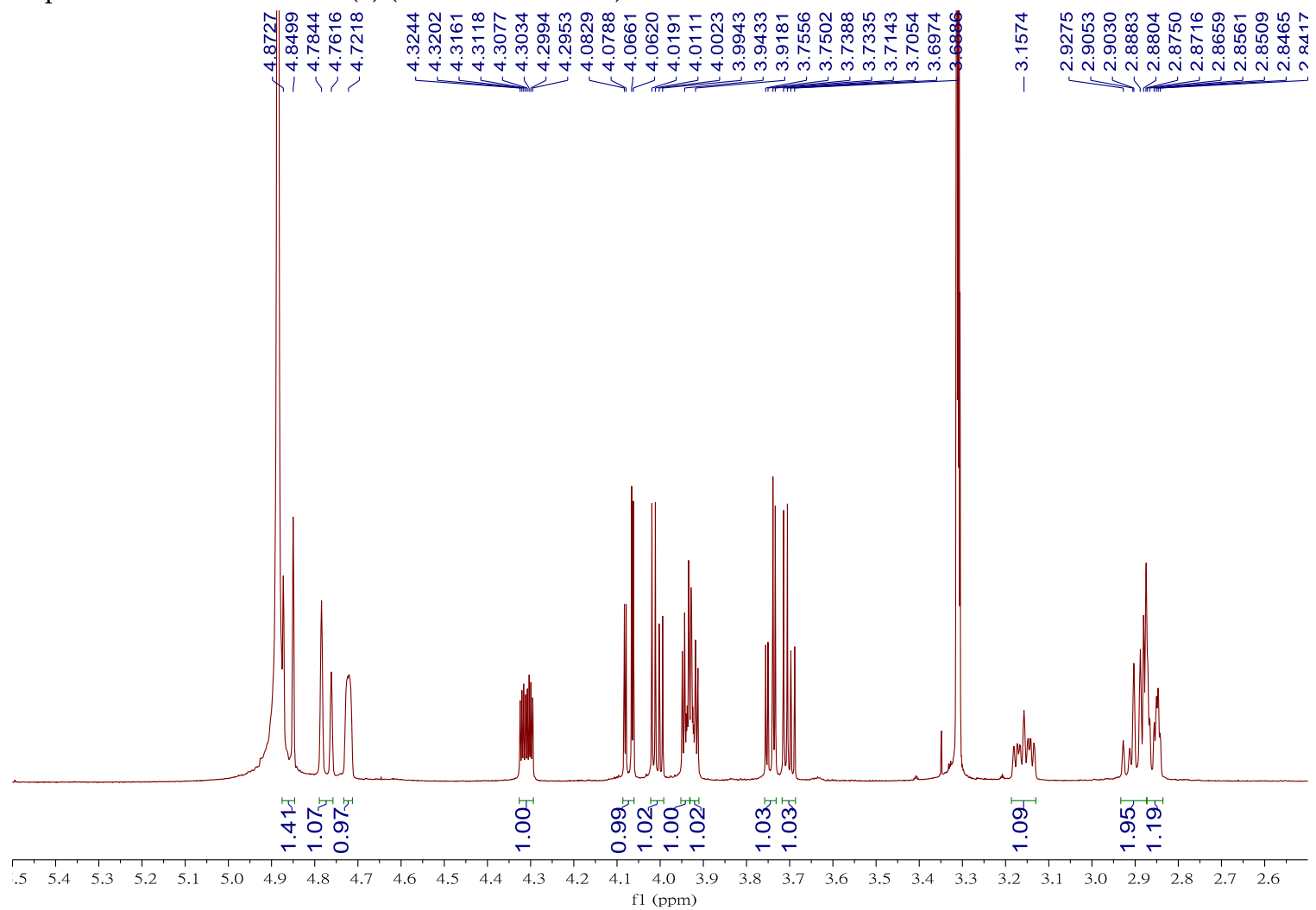


Figure S14. ^{13}C NMR spectrum of tuberazine C (**3**) (CD_3OD , 175 MHz)

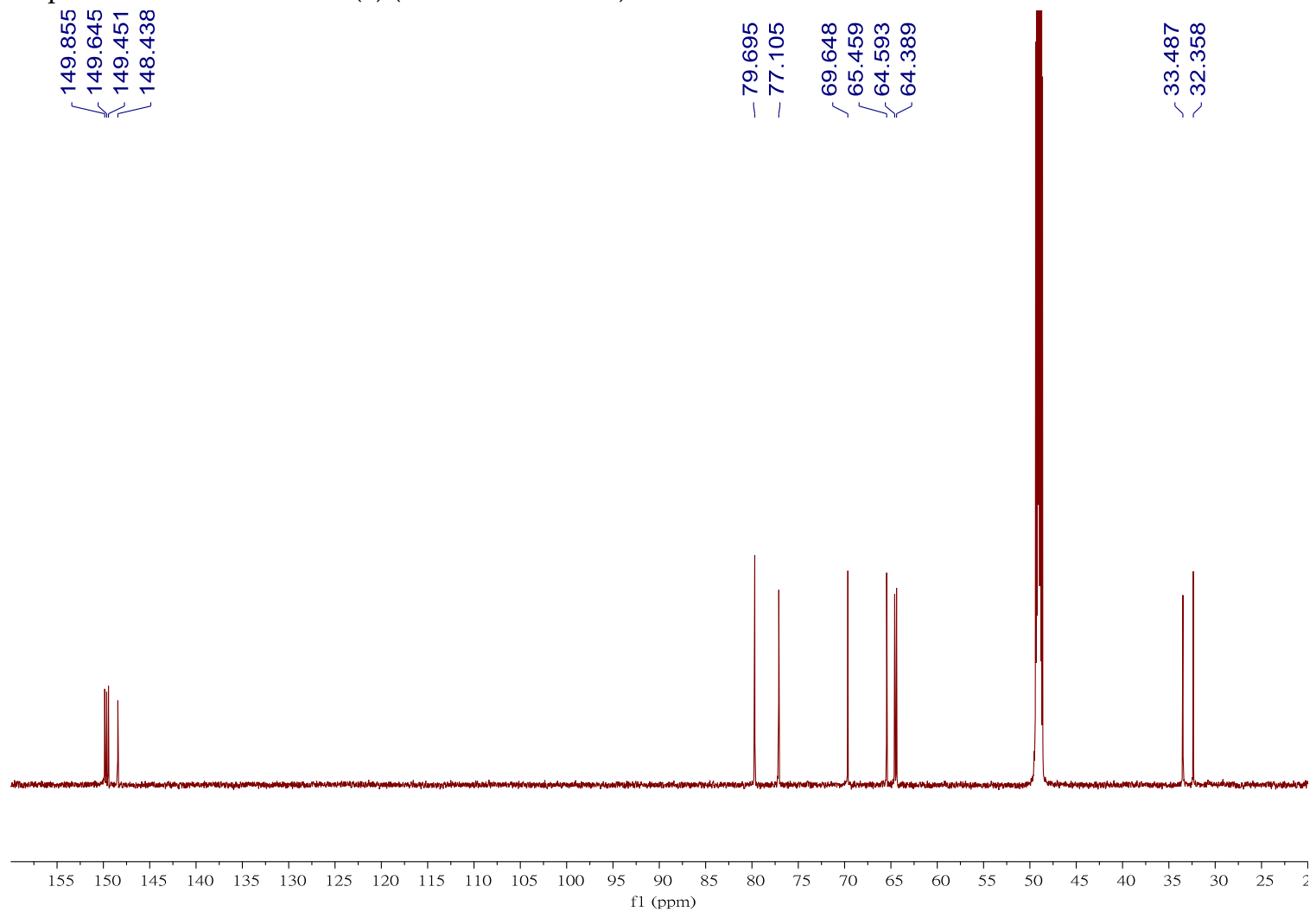


Figure S15. COSY spectrum of tuberazine C (3)

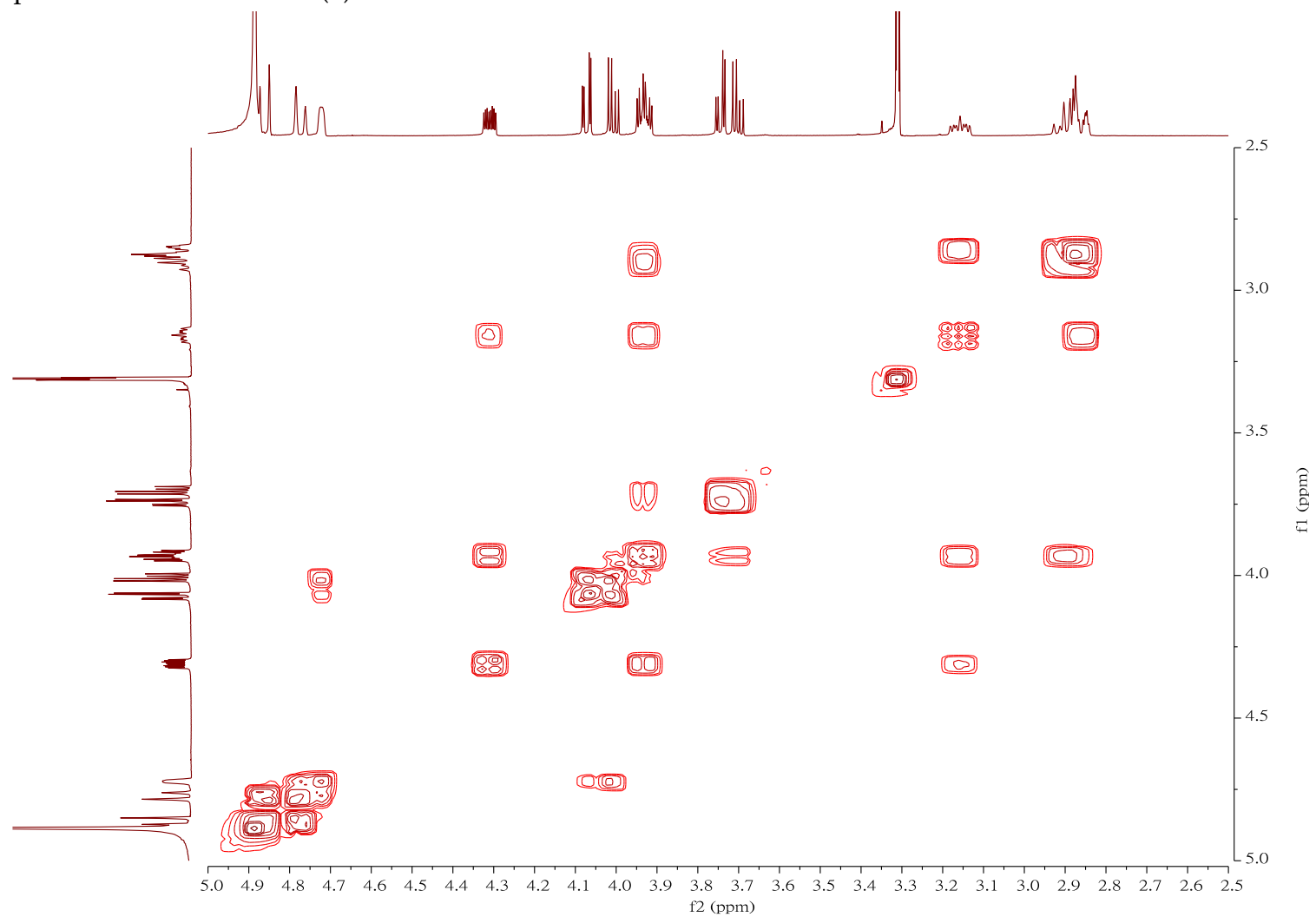


Figure S16. HSQC spectrum of tuberazine C (3)

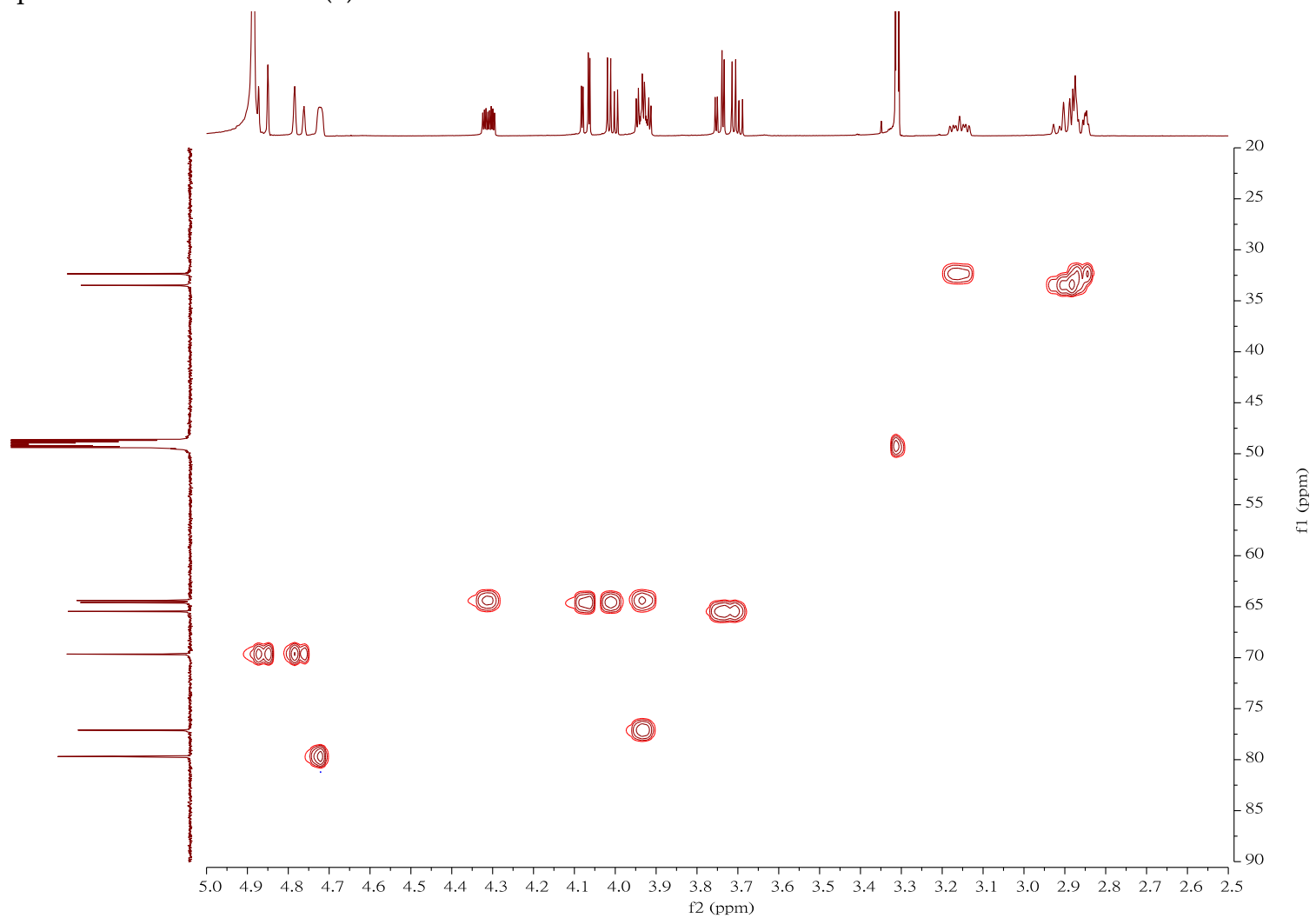


Figure S17. HMBC spectrum of tuberazine C (3)

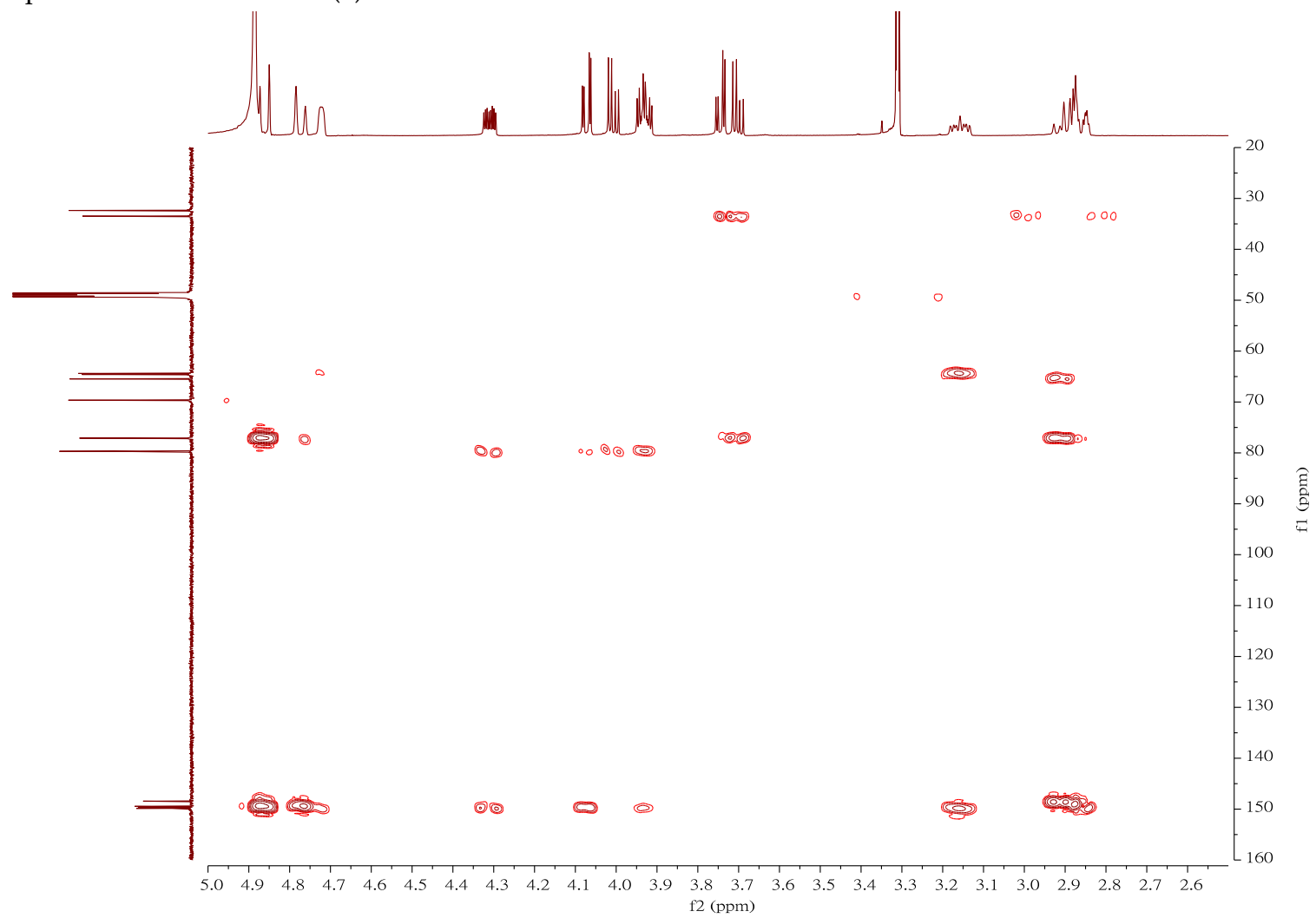


Figure S18. ^1H - ^{15}N HMBC spectrum of tuberazine C (3)

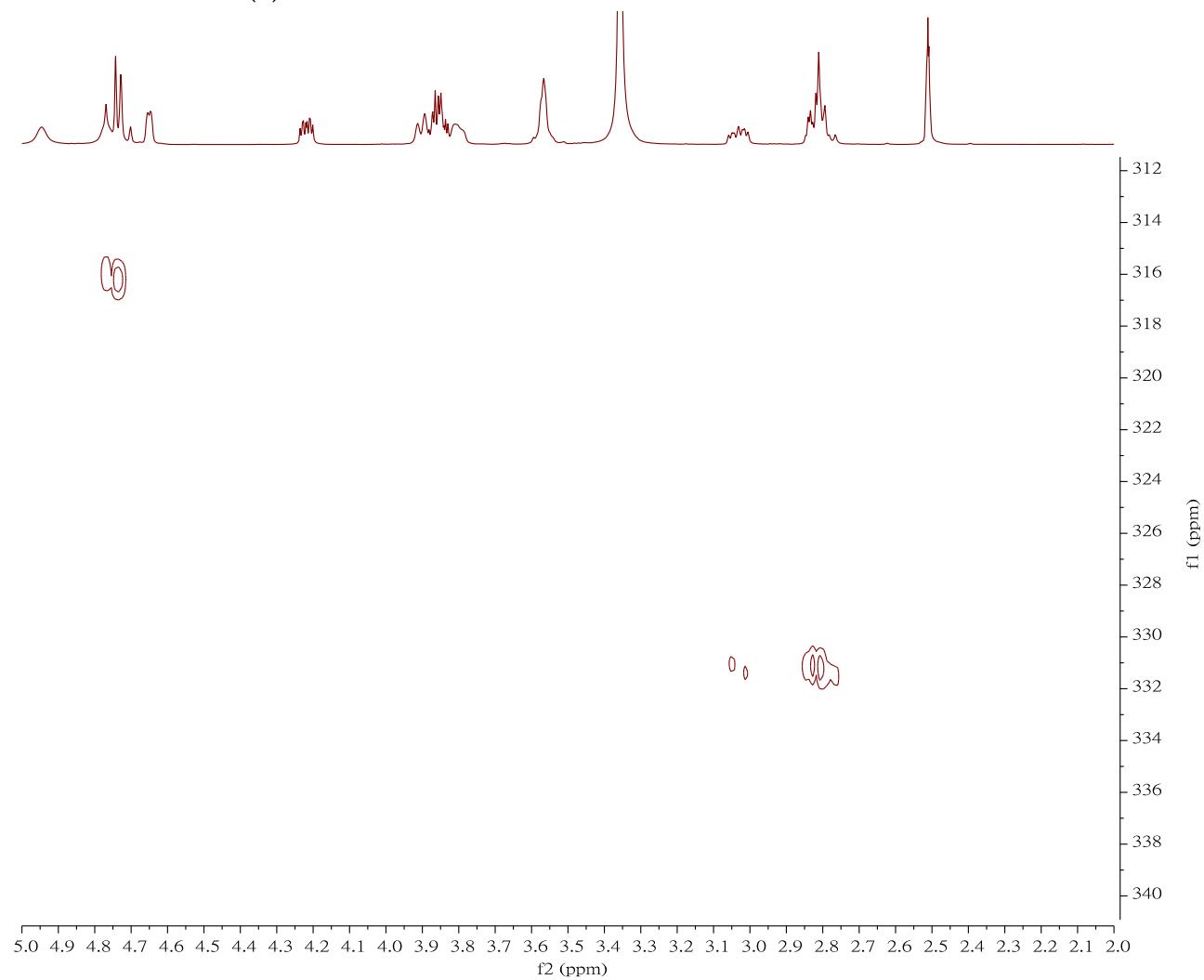
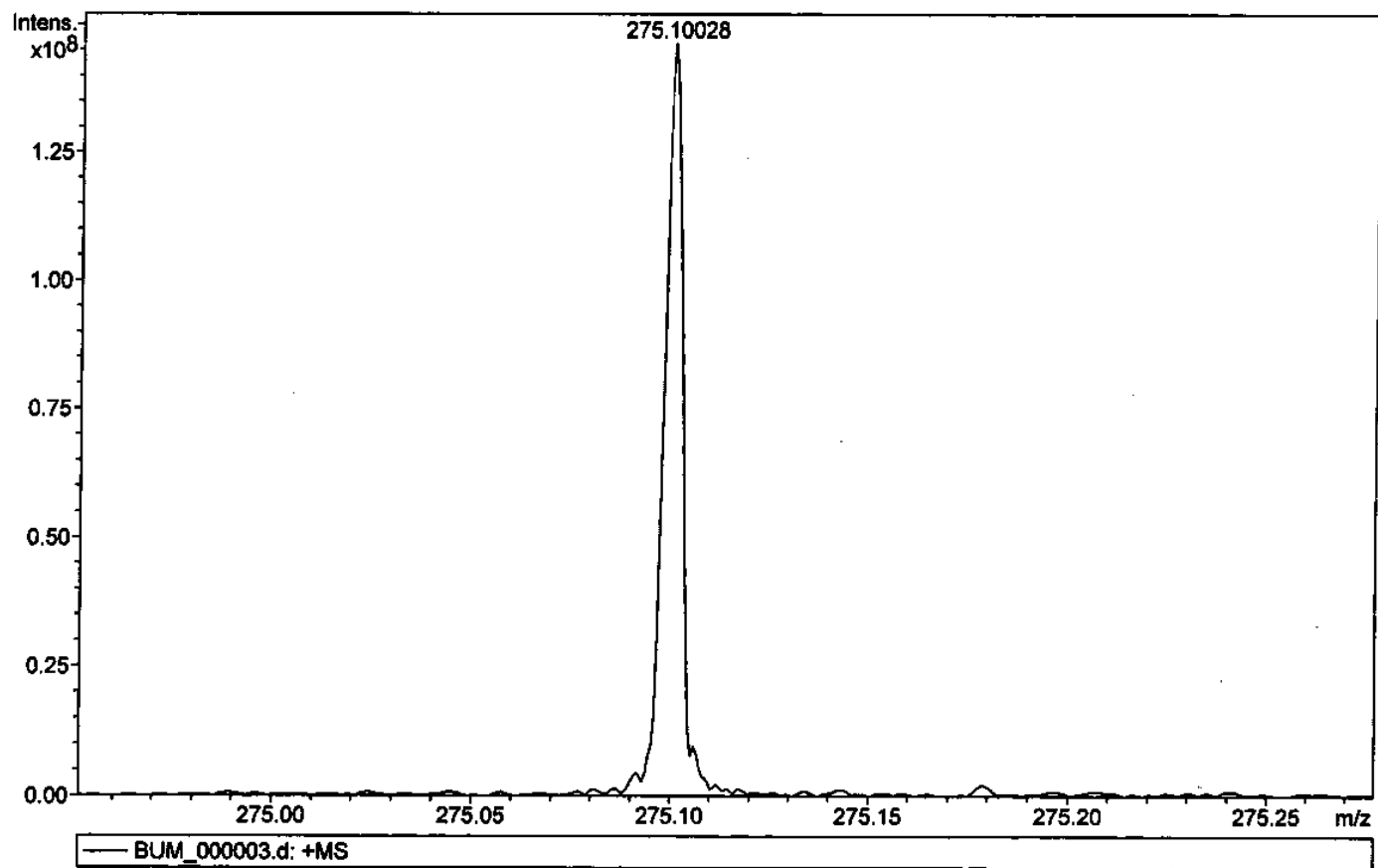
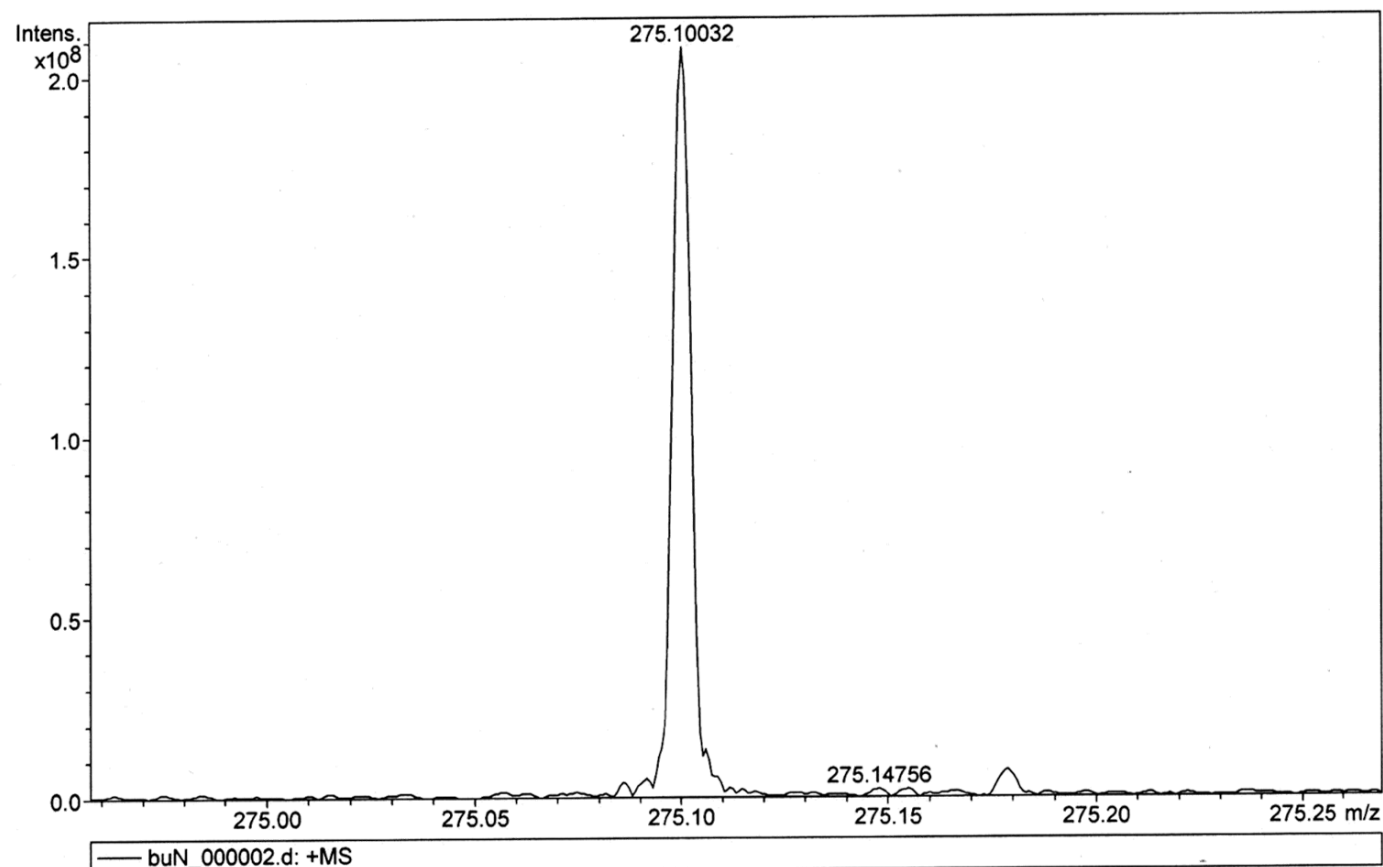


Figure S19. HRESIMS spectrum of tuberazine A (1)



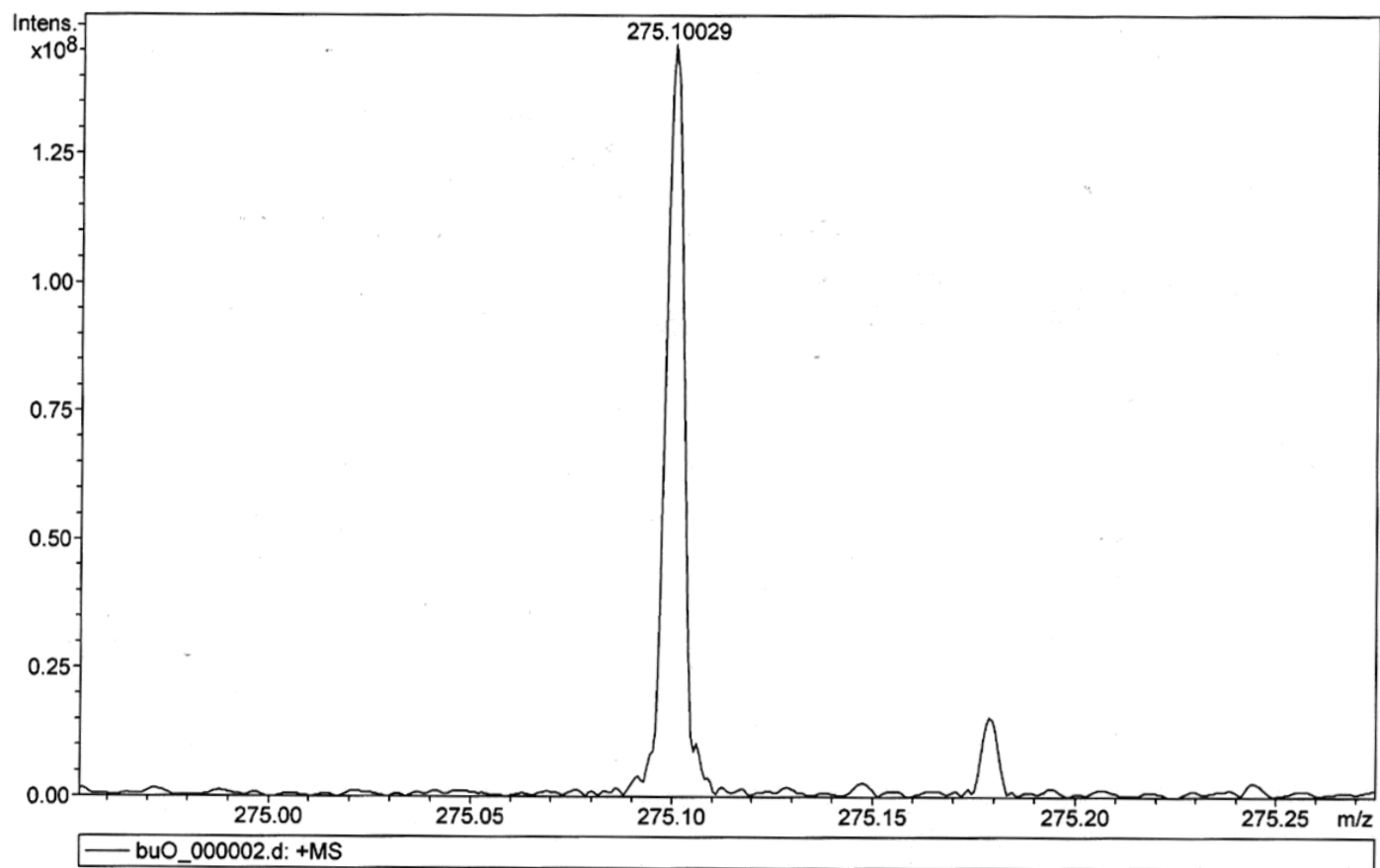
| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e ⁻ Conf | N-Rule |
|-----------|---|---|--------|-----------|-----------|-----------|--------|-----|---------------------|--------|
| 275.10028 | 1 | C ₁₂ H ₁₆ N ₂ NaO ₄ | 100.00 | 275.10023 | -0.05 | -0.19 | 7.3 | 5.5 | even | ok |

Figure S20. HRESIMS spectrum of tuberazine B (2)



| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e ⁻ Conf | N-Rule |
|-----------|---|---|--------|-----------|-----------|-----------|--------|-----|---------------------|--------|
| 275.10032 | 1 | C ₁₂ H ₁₆ N ₂ NaO ₄ | 100.00 | 275.10023 | -0.09 | -0.34 | 2.6 | 5.5 | even | ok |

Figure S21. HRESIMS spectrum of tuberazine C (3)



| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e ⁻ Conf | N-Rule |
|-----------|---|---|--------|-----------|-----------|-----------|--------|-----|---------------------|--------|
| 275.10029 | 1 | C ₁₂ H ₁₆ N ₂ NaO ₄ | 100.00 | 275.10023 | -0.06 | -0.22 | 3.7 | 5.5 | even | ok |

Figure S22. Possible structures of **1**

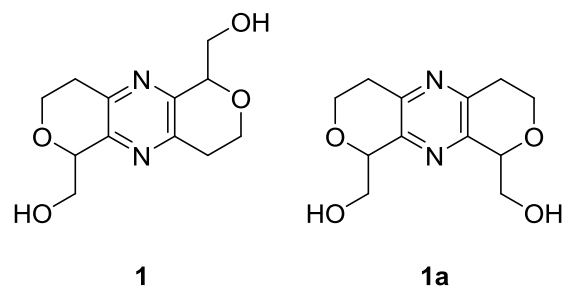


Figure S23. Possible structures of **2**

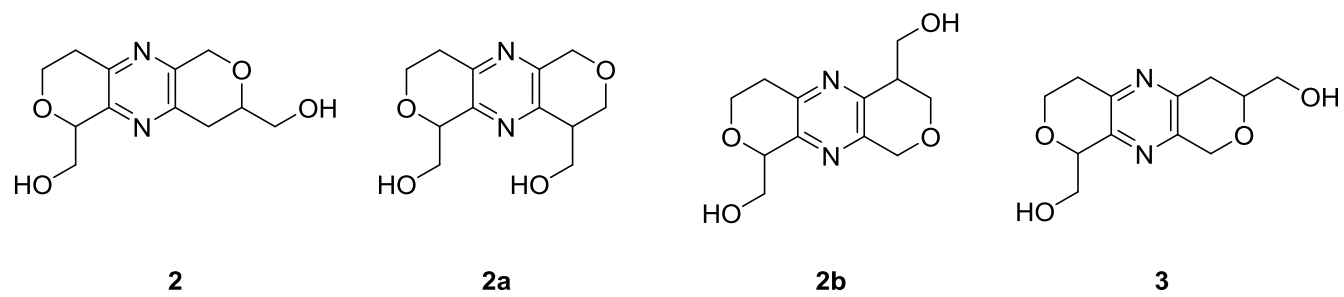


Table S1. Anti-lymphangiogenic activity of selected compounds

| Compound | IC ₅₀ (μg/ml) ^a |
|----------------------------|---------------------------------------|
| Tuberazines A (1) | 40 ± 2 |
| Tuberazines B (2) | 39 ± 2 |
| Tuberazines C (3) | 33 ± 1 |
| Rapamycin ^b | < 5 |

^aHalf maximal cytotoxicity concentration. ^bPositive control.