

Supplementary Materials

2,5-Diketopiperazine Derivatives as Potential Anti-Influenza (H5N2) Agents: Synthesis, Biological Evaluation, and Molecular Docking Study

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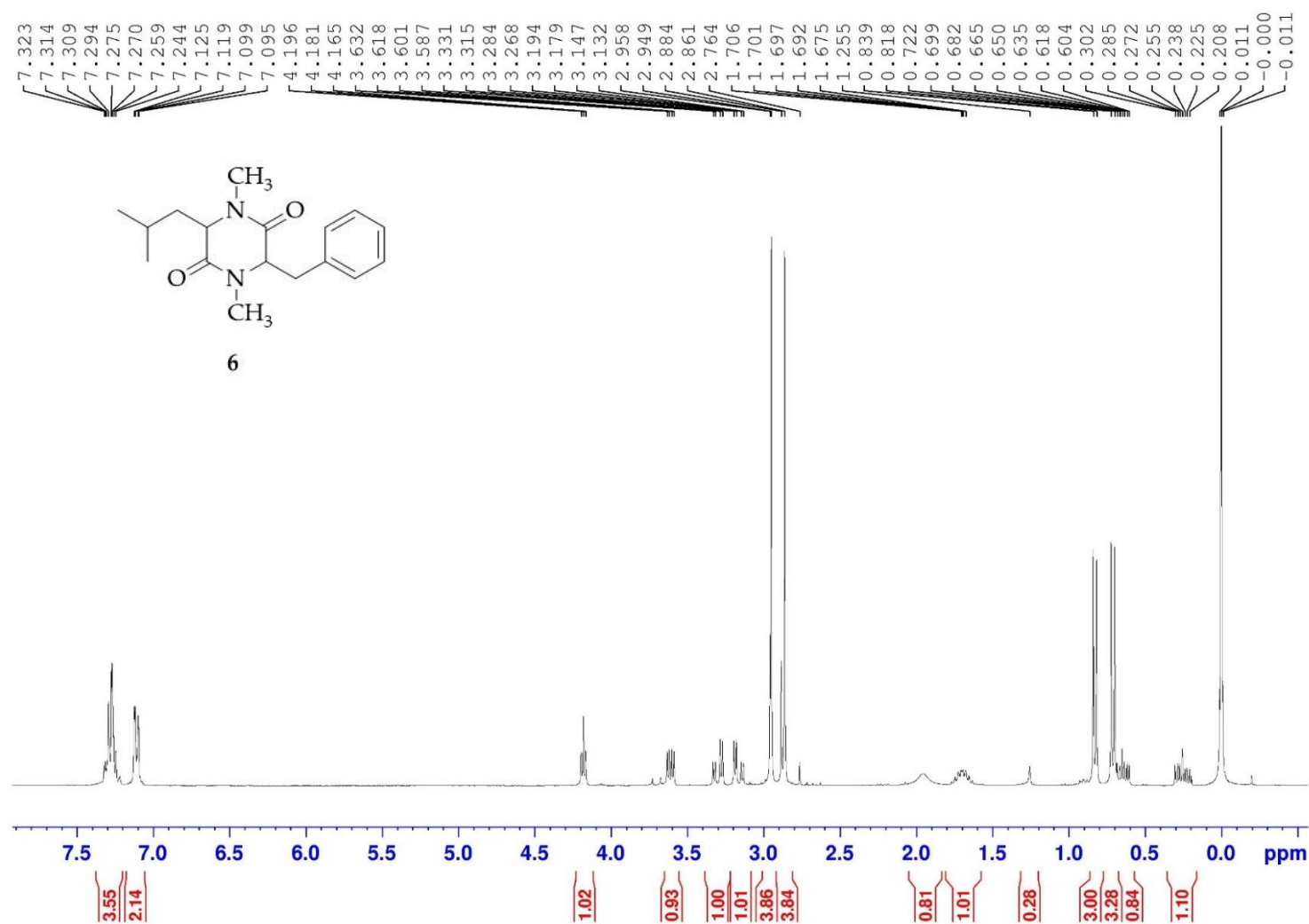


Figure S1. ¹H-NMR of the (3*S*,6*S*)-3-Benzyl-6-isobutyl-1,4-dimethyl-2,5-diketopiperazine (6).

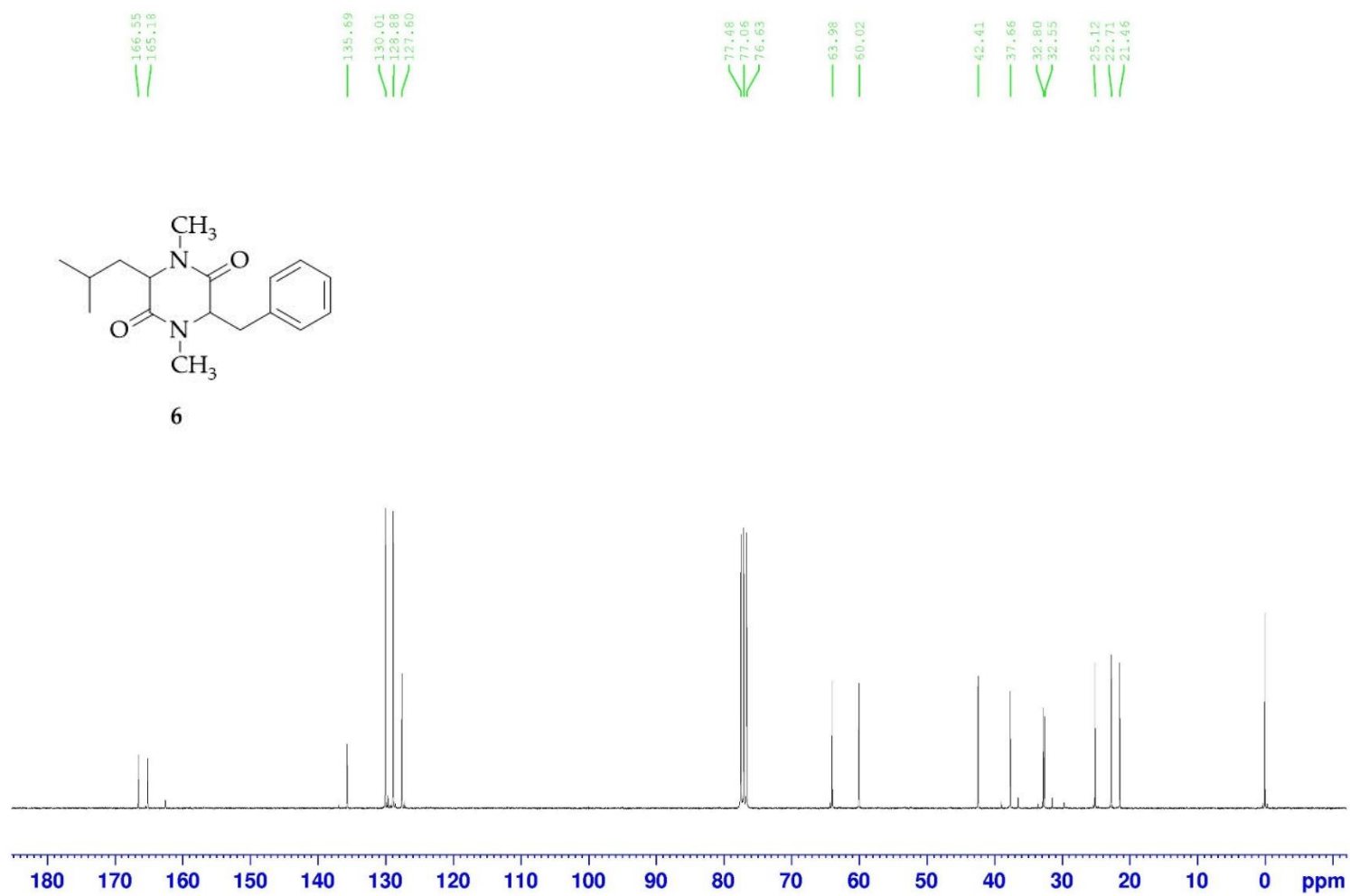
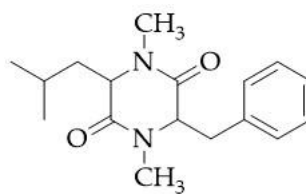


Figure S2. ¹³C-NMR of the (3*S*,6*S*)-3-Benzyl-6-isobutyl-1,4-dimethyl-2,5-diketopiperazine (6).



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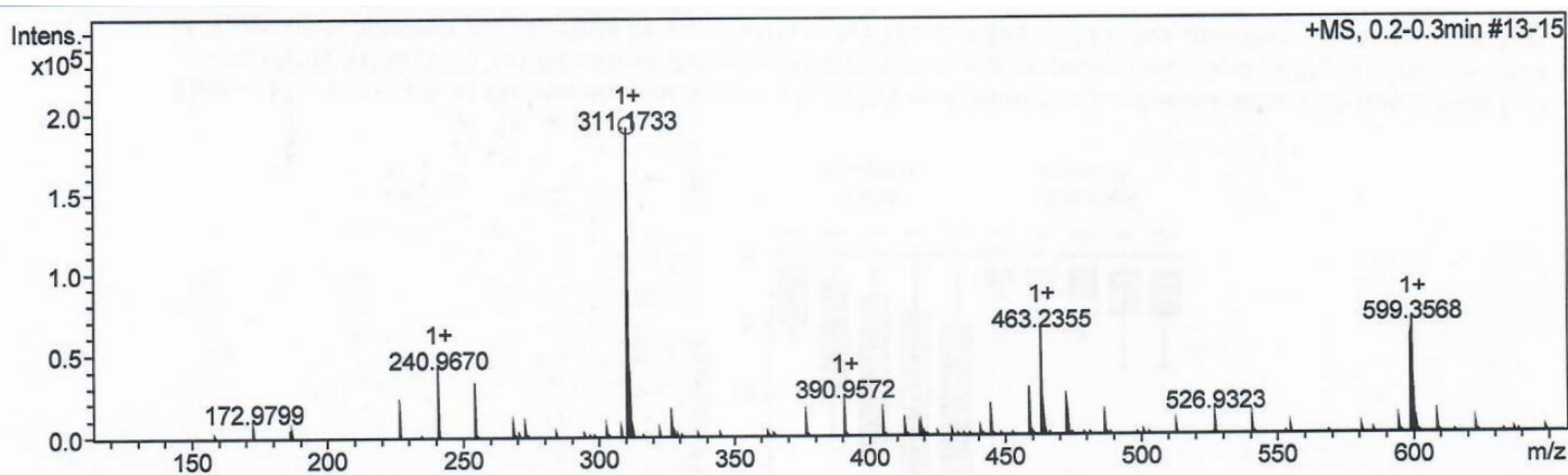


Figure S3. HRMS of the (3*S*,6*S*)-3-Benzyl-6-isobutyl-1,4-dimethyl-2,5-diketopiperazine (**6**).

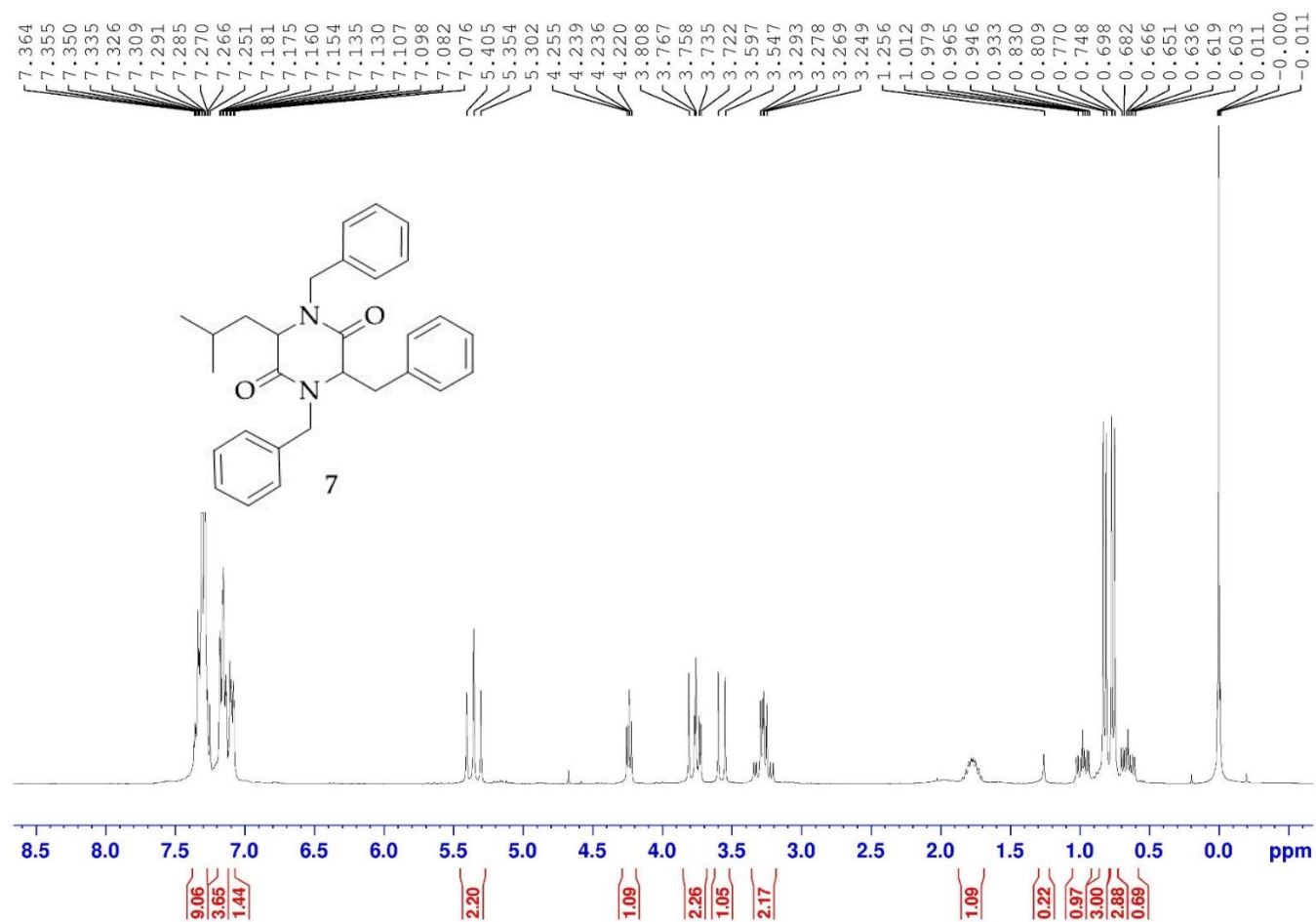


Figure S4. ¹H-NMR of the (3S,6S)-1,3,4-Tribenzyl-6-isobutyl-2,5-diketopiperazine (7).

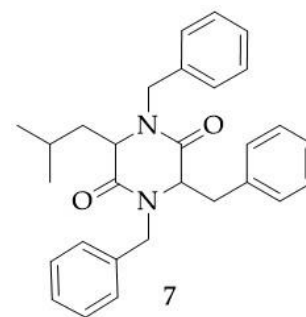
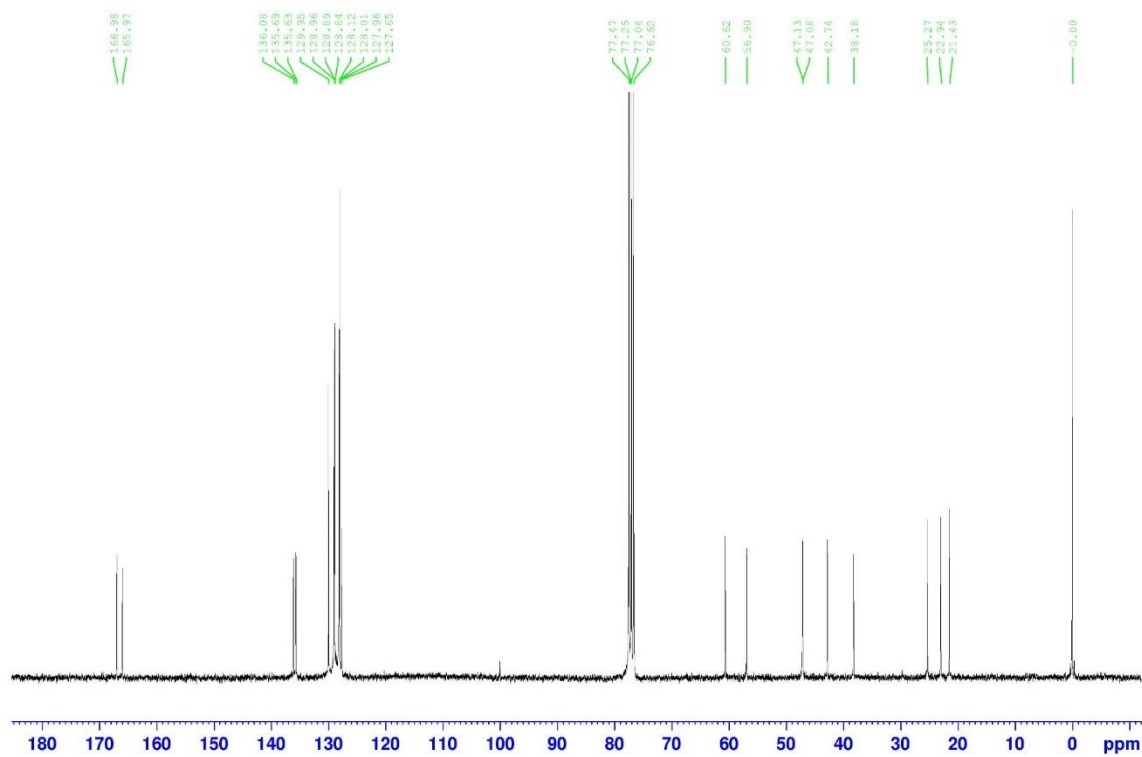


Figure S5. ^{13}C -NMR of the (3*S*,6*S*)-1,3,4-Tribenzyl-6-isobutyl-2,5-diketopiperazine (7).

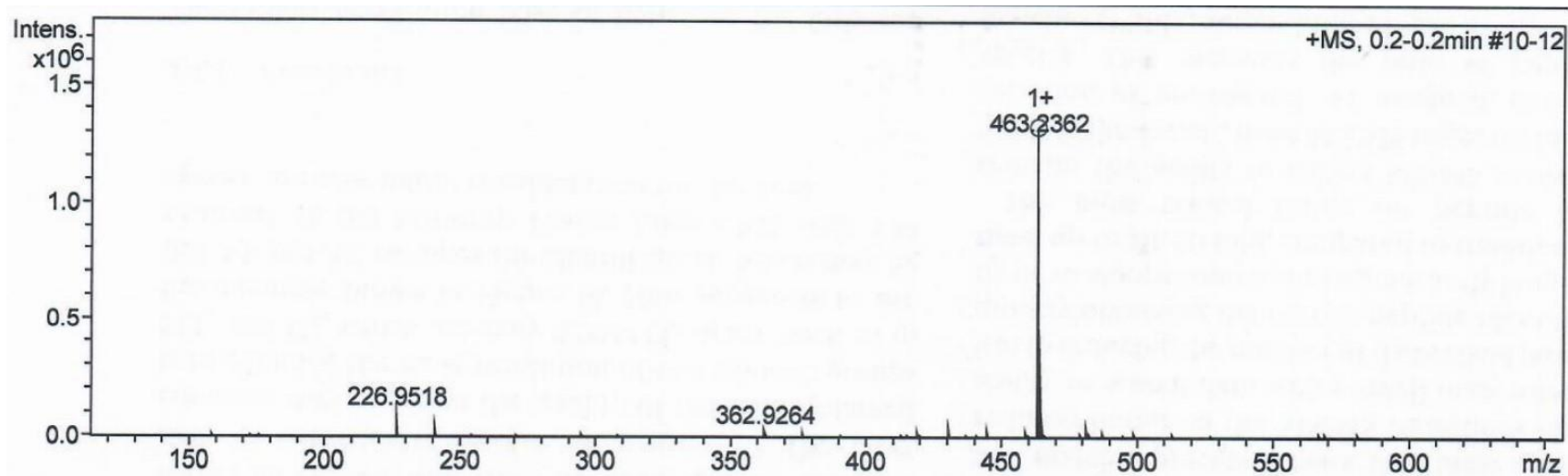
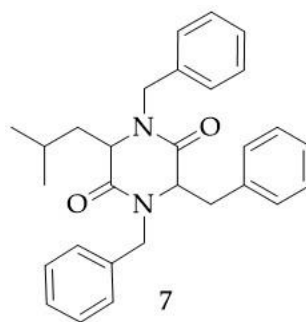


Figure S6. HRMS of the (3*S*,6*S*)-1,3,4-Tribenzyl-6-isobutyl-2,5-diketopiperazine (7).

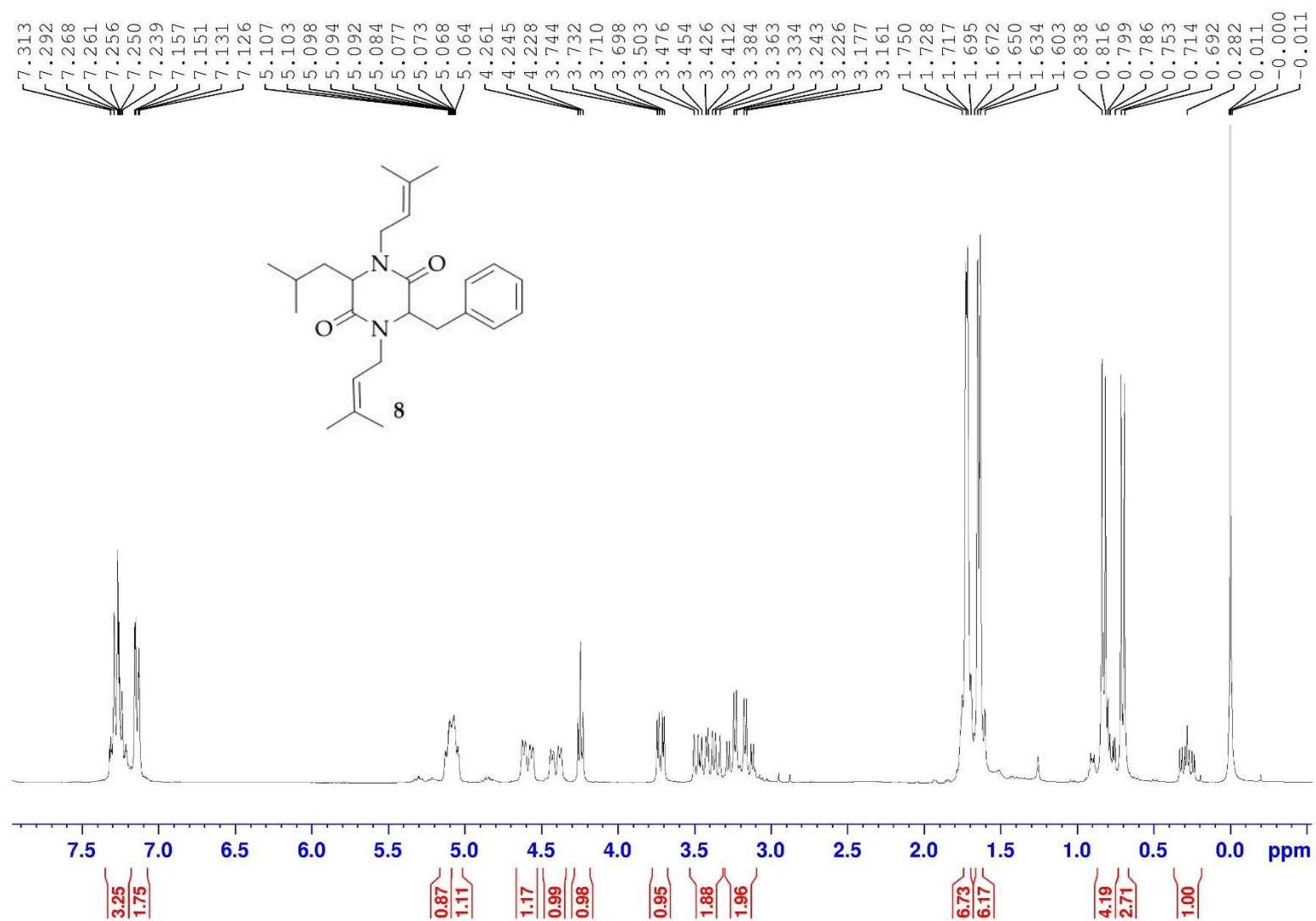


Figure S7. ¹H-NMR of the (3*S*,6*S*)-3-Benzyl-6-isobutyl-1,4-bis(3-methylbut-2-en-1-yl)-2,5-diketopiperazine (8).

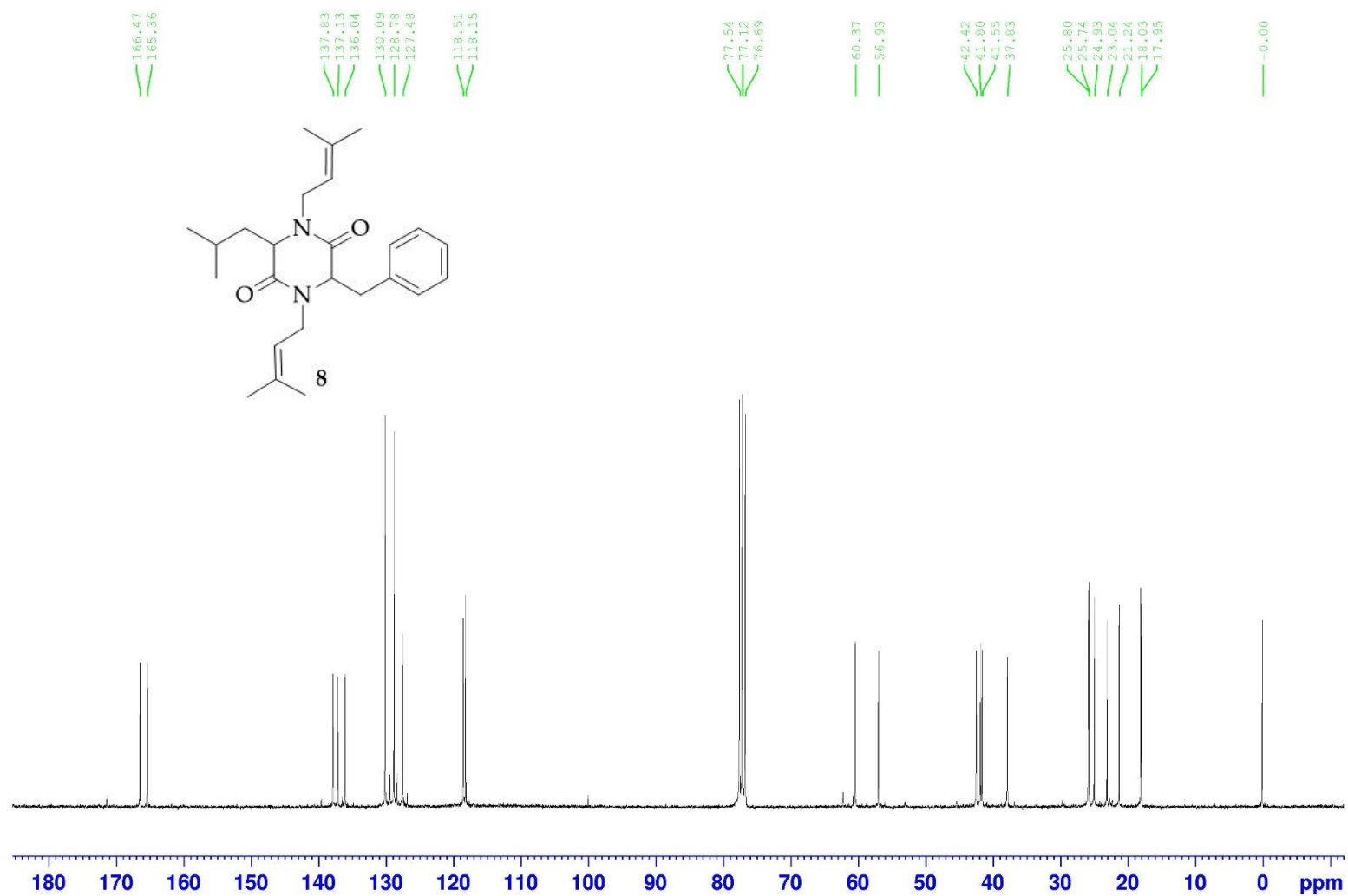


Figure S8. ¹³C-NMR of the (3*S*,6*S*)-3-Benzyl-6-isobutyl-1,4-bis(3-methylbut-2-en-1-yl)-2,5-diketopiperazine (8).

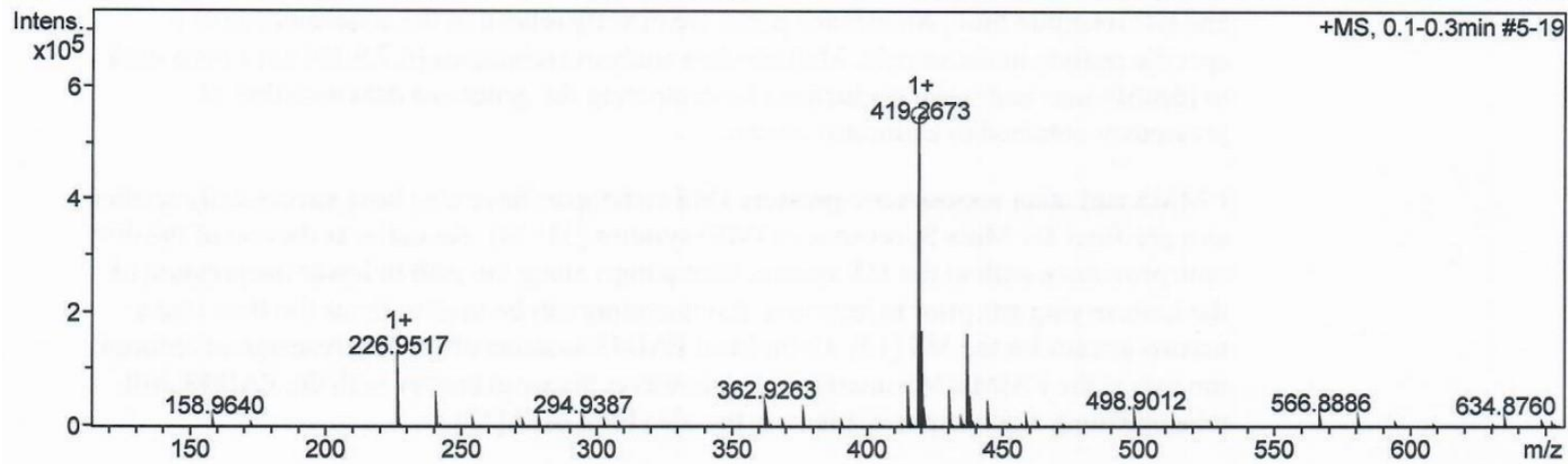
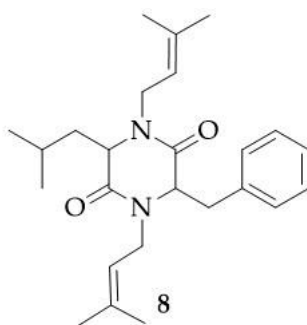


Figure S9. HRMS of the (3*S*,6*S*)-3-Benzyl-6-isobutyl-1,4-bis(3-methylbut-2-en-1-yl)-2,5-diketopiperazine (8).

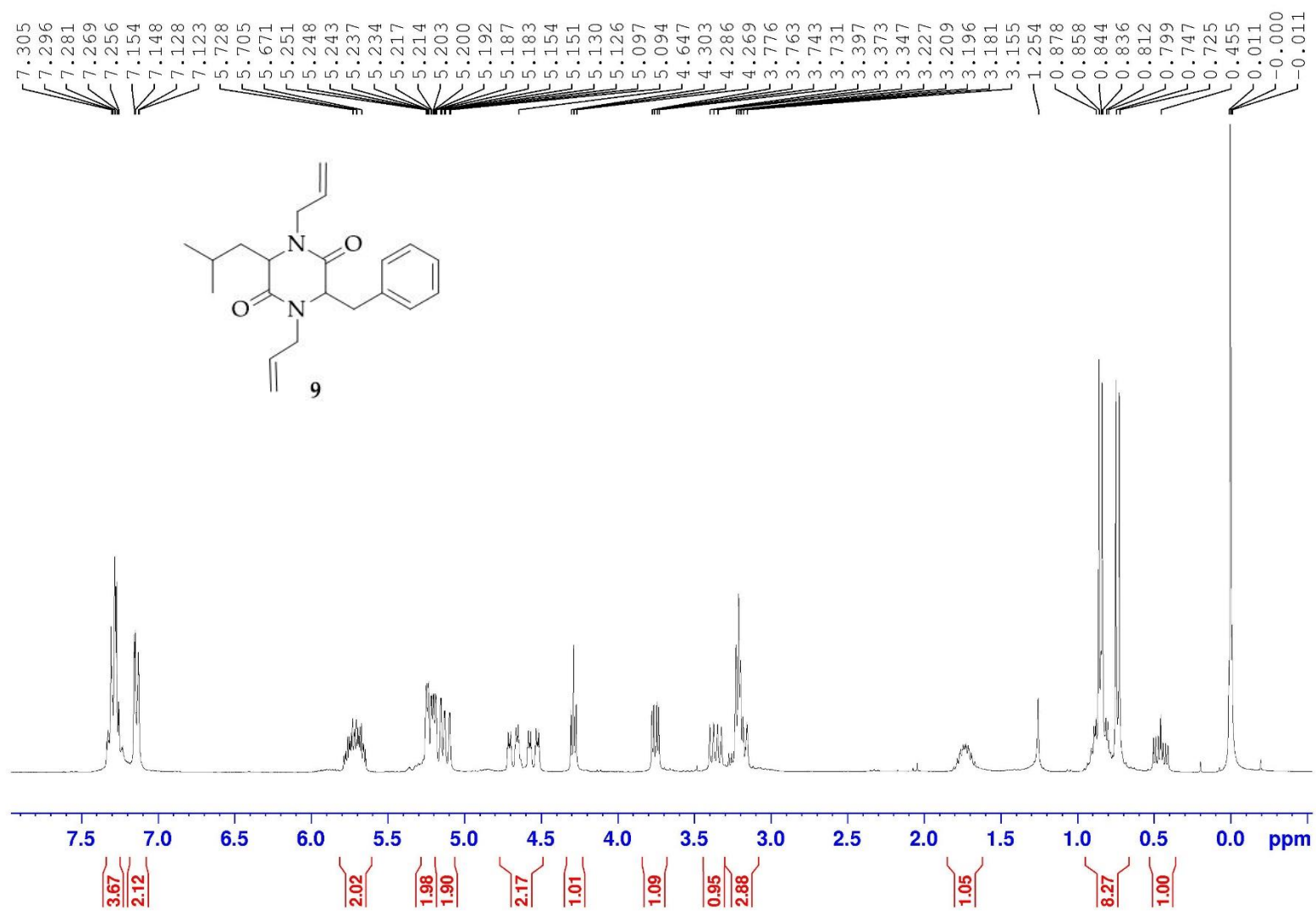


Figure S10. ¹H-NMR of the (3S,6S)-1,4-Diallyl-3-benzyl-6-isobutyl-2,5-diketopiperazine (9).

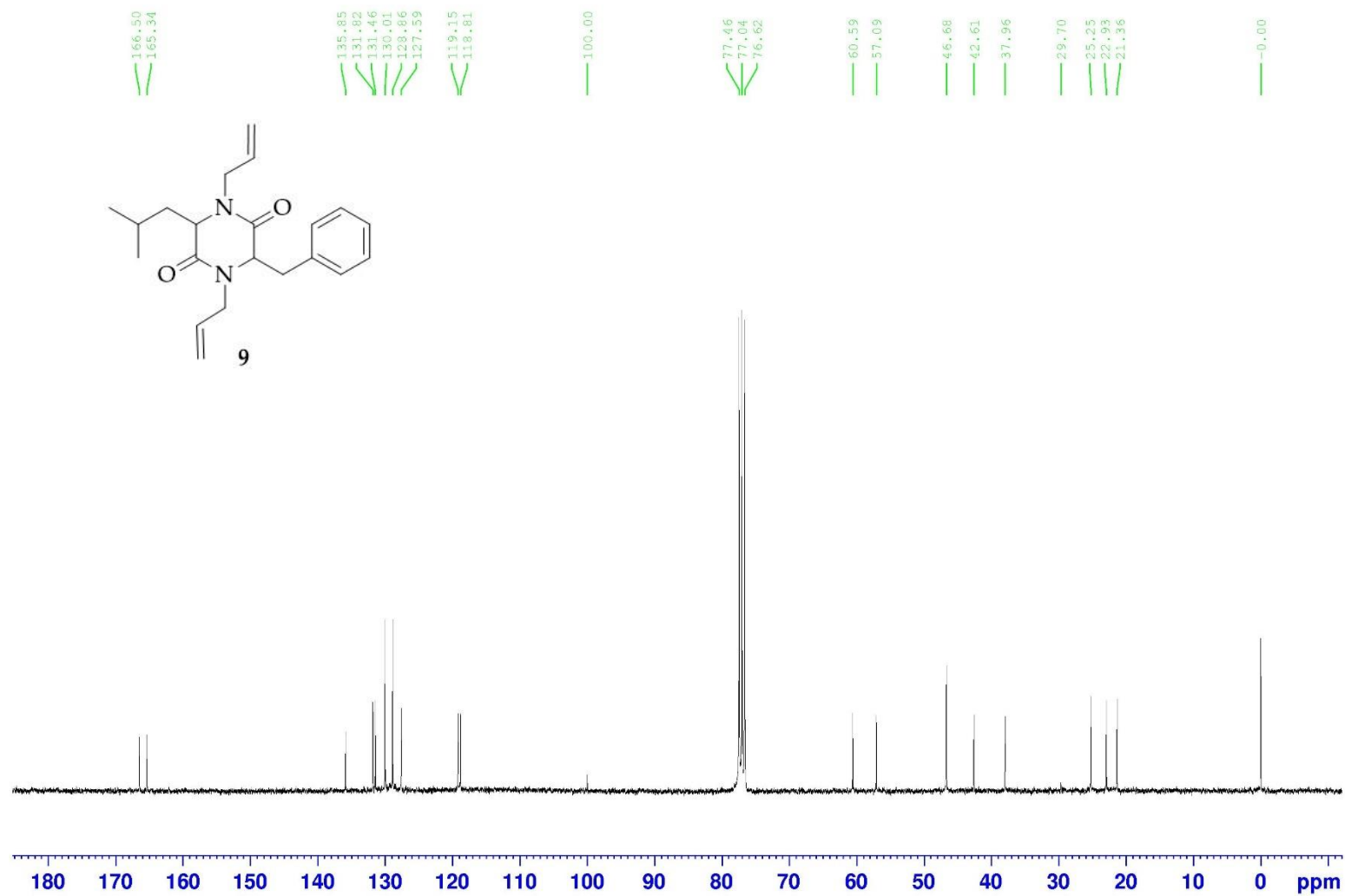


Figure S11. ¹³C-NMR of the (3S,6S)-1,4-Diallyl-3-benzyl-6-isobutyl-2,5-diketopiperazine (9).

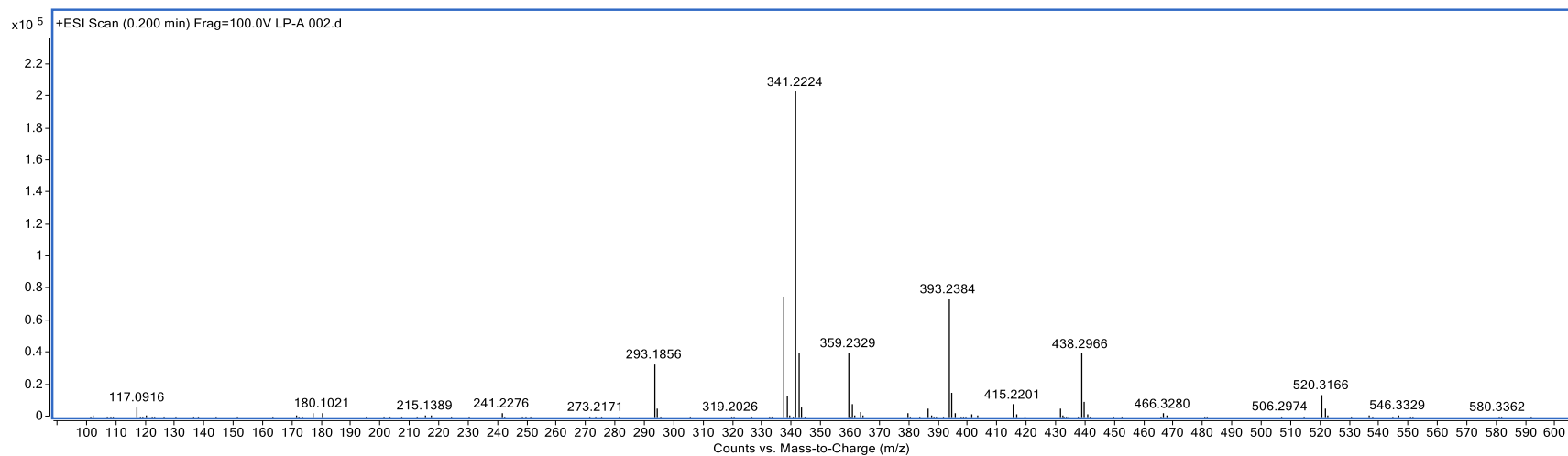
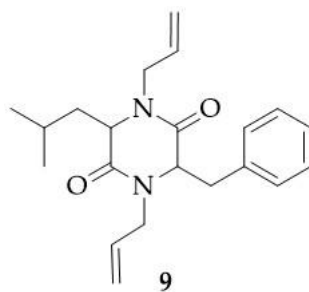


Figure S12. HRMS of the (3S,6S)-1,4-Diallyl-3-benzyl-6-isobutyl-2,5-diketopiperazine (**9**).

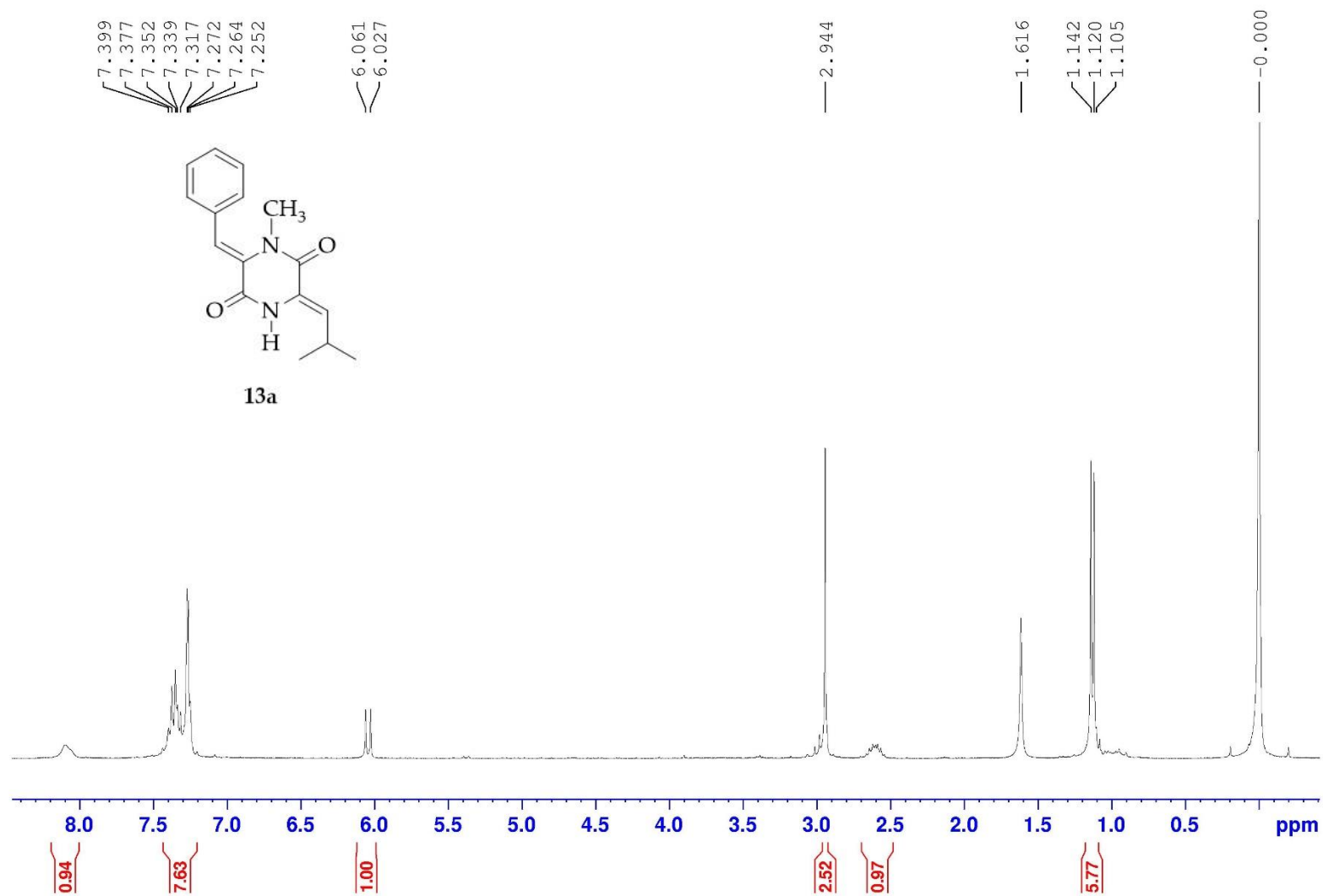


Figure S13. ¹H-NMR of the (3Z,6Z)-3-Benzylidene-6-(2-methylpropylidene)-4-methyl-2,5-diketopiperazine (**13a**).

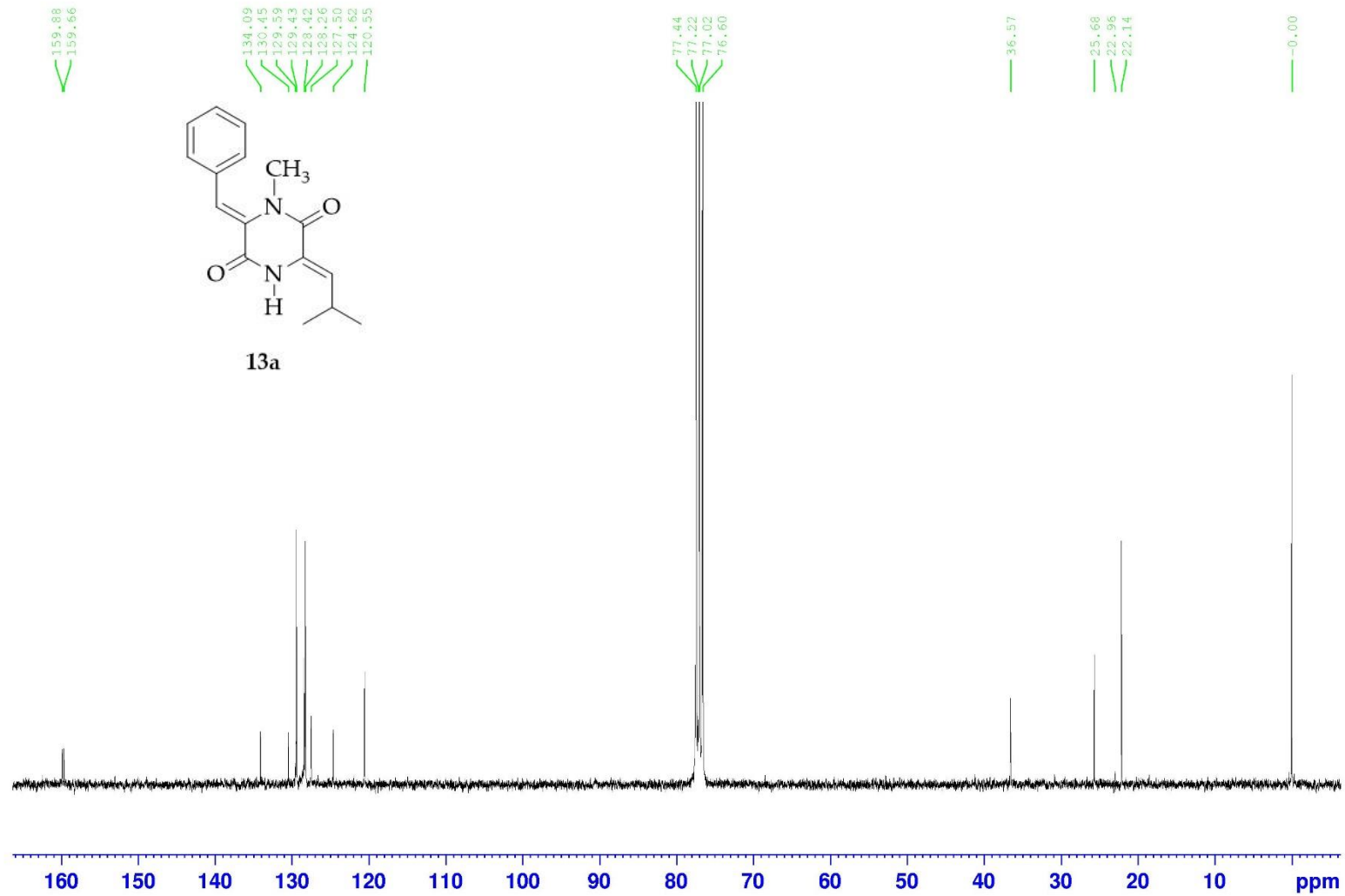
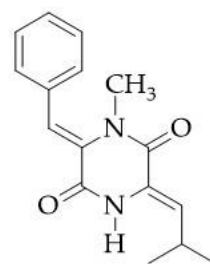


Figure S14. ¹³C-NMR of the (3Z,6Z)-3-Benzylidene-6-(2-methylpropylidene)-4-methyl-2,5-diketopiperazine (**13a**).



13a

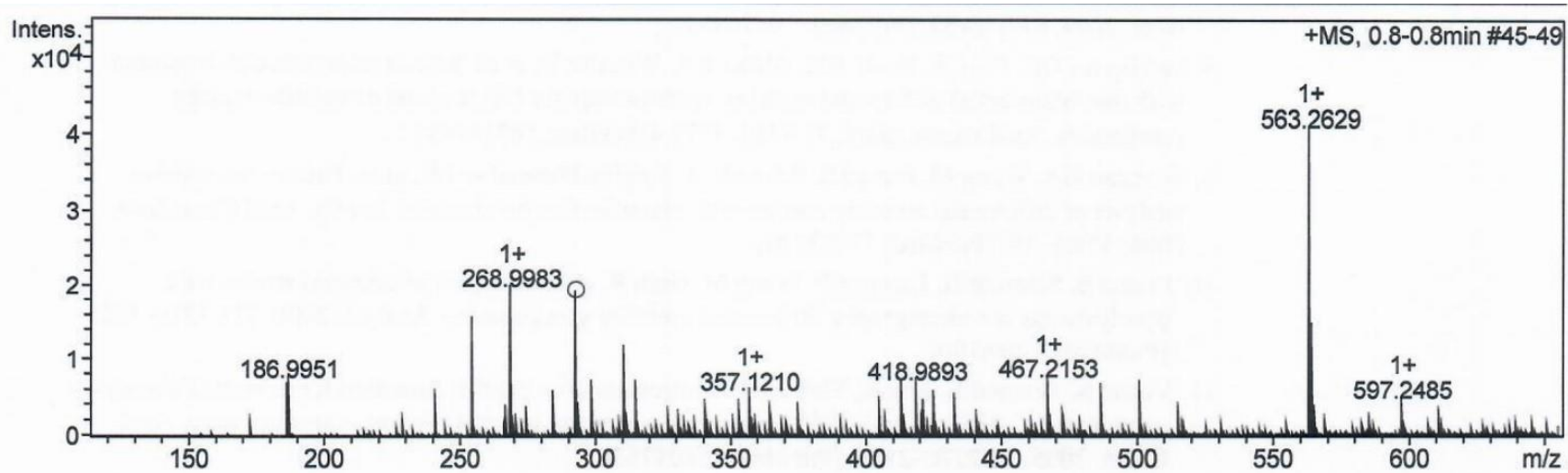


Figure S15. HRMS of the (3Z,6Z)-3-Benzylidene-6-(2-methylpropylidene)-4-methyl-2,5-diketopiperazine (**13a**).

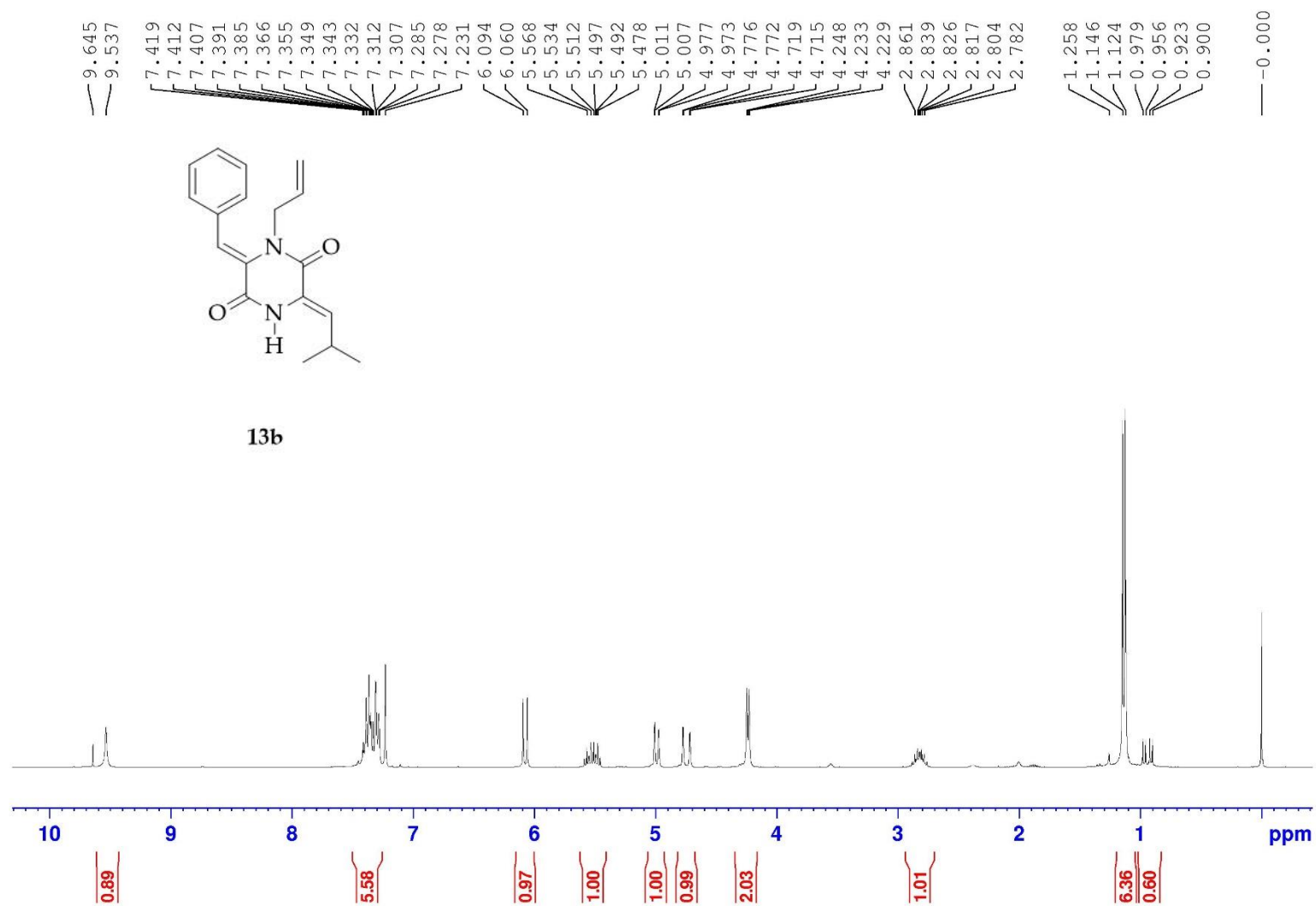


Figure S16. ¹H-NMR of the (3Z,6Z)-4-Allyl-3-benzylidene-6-(2-methylpropylidene)-2,5-diketopiperazine (**13b**).

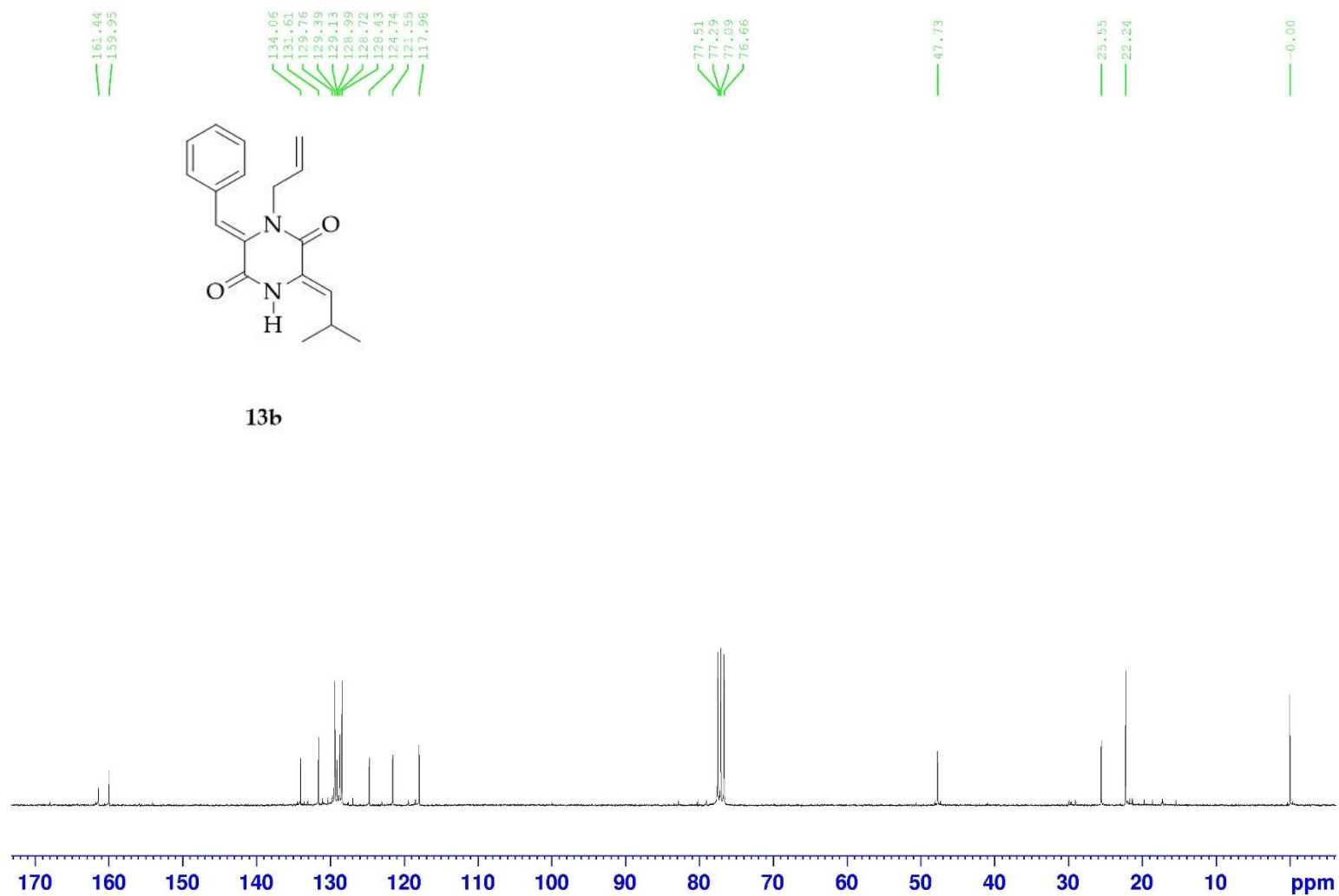
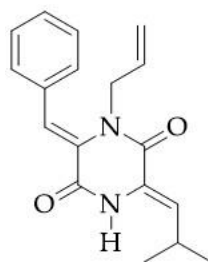


Figure S17. ¹³C-NMR of the (3Z,6Z)-4-Allyl-3-benzylidene-6-(2-methylpropylidene)-2,5-diketopiperazine (13b).



13b

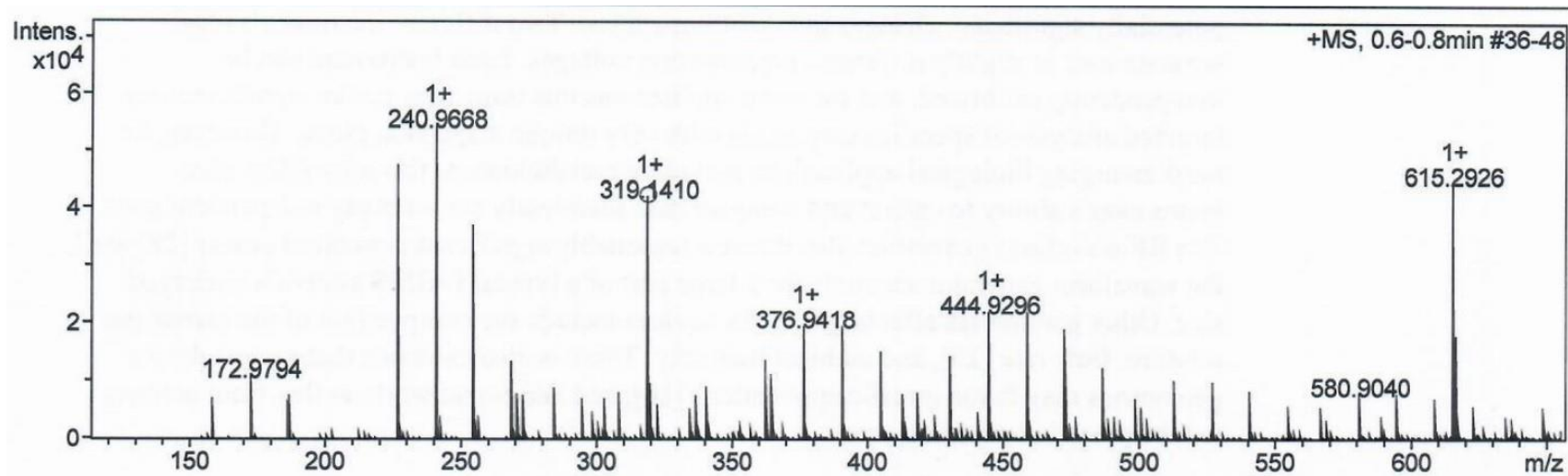


Figure S18. HRMS of the (3Z,6Z)-4-Allyl-3-benzylidene-6-(2-methylpropylidene)-2,5-diketopiperazine (13b).

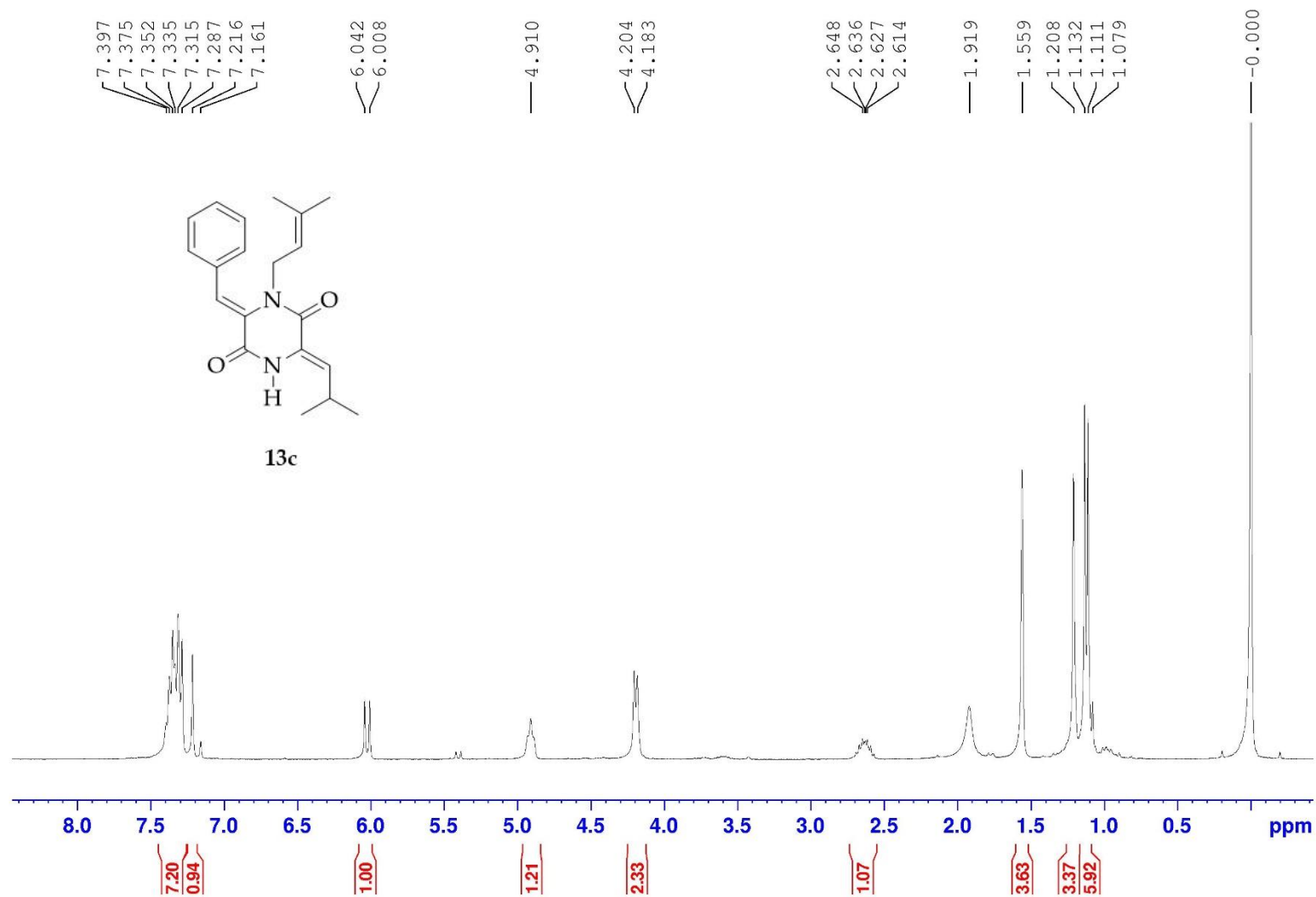


Figure S19. ¹H-NMR of the (3Z,6Z)-3-Benzylidene-6-(2-methylpropylidene)-4-(3-methyl but-2-en-1-yl)-2,5-diketopiperazine (**13c**).

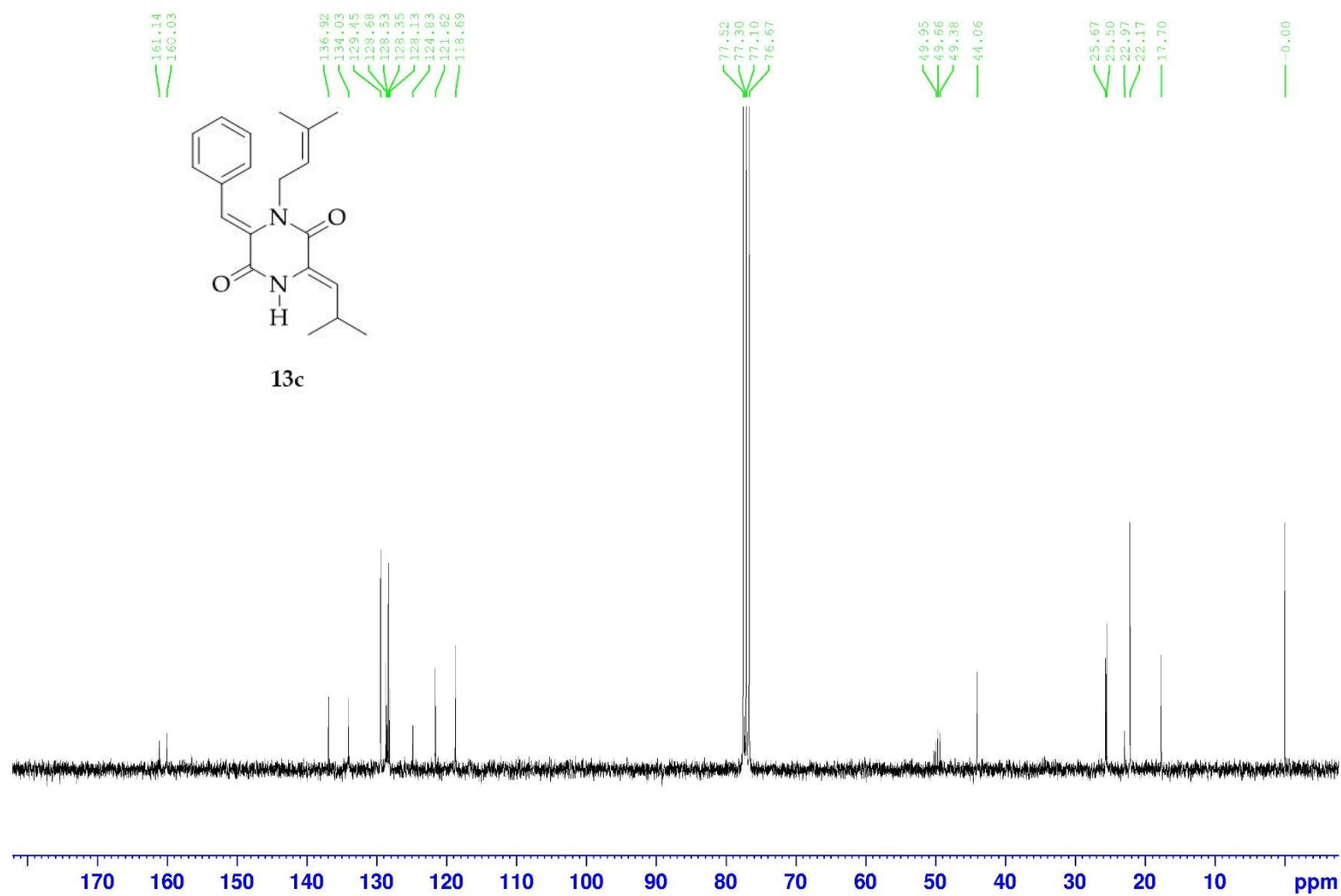
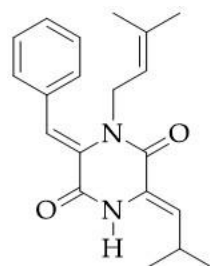


Figure S20. ¹³C-NMR of the (3Z,6Z)-3-Benzylidene-6-(2-methylpropylidene)-4-(3-methyl but-2-en-1-yl)-2,5-diketopiperazine (13c).



13c

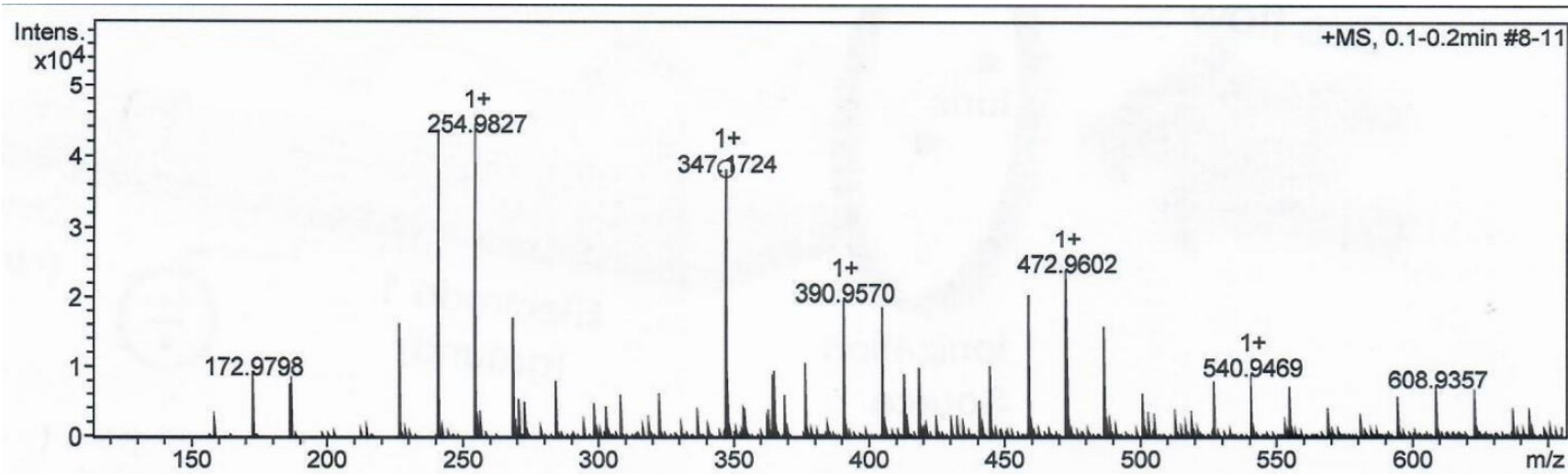


Figure S21. HRMS of the (3Z,6Z)-3-Benzylidene-6-(2-methylpropylidene)-4-(3-methyl but-2-en-1-yl)-2,5-diketopiperazine (**13c**).

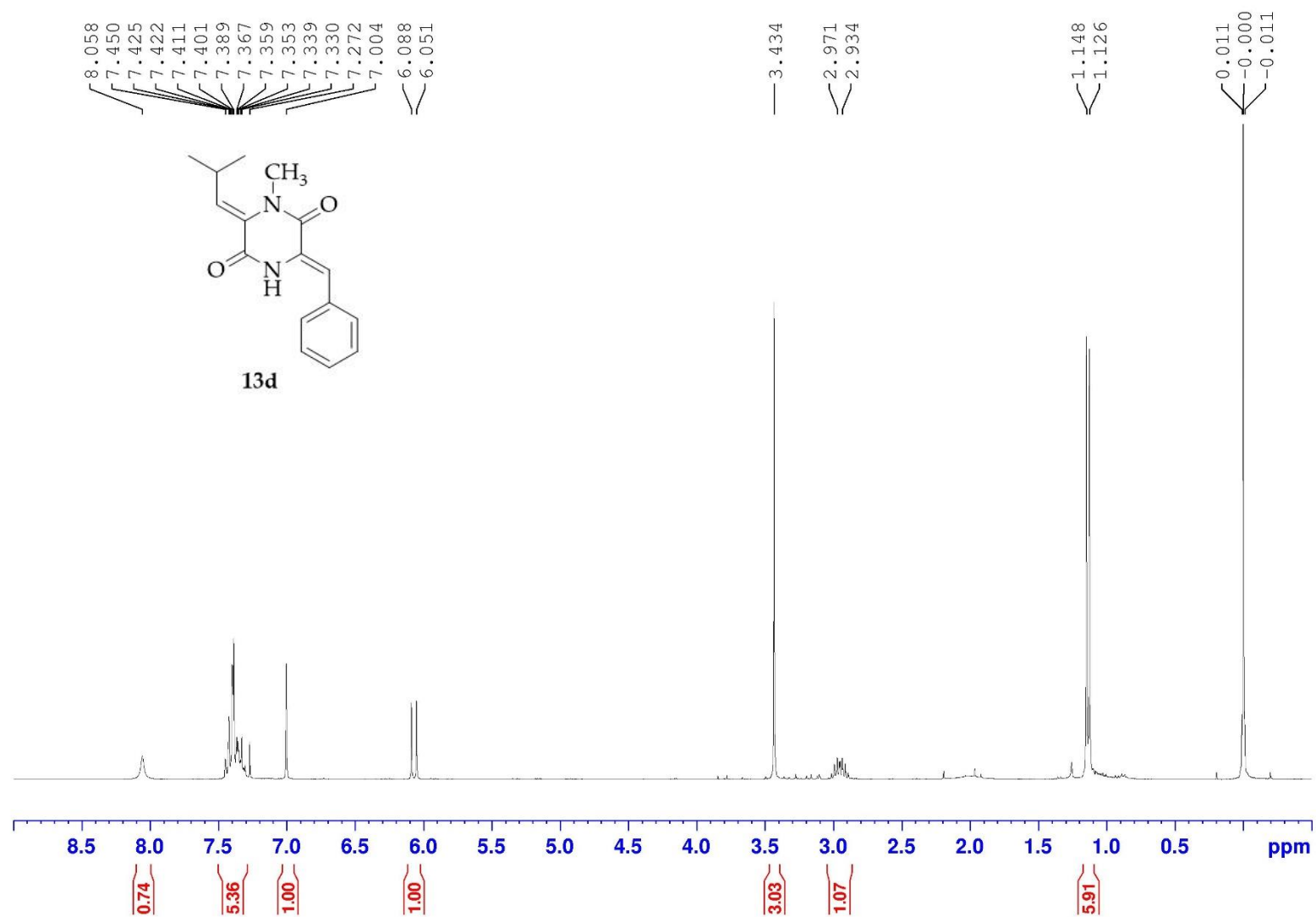


Figure S22. ¹H-NMR of the (3*Z*,6*Z*)-3-Benzylidene-6-(2-methylpropylidene)-1-methyl-2,5-diketopiperazine (**13d**).

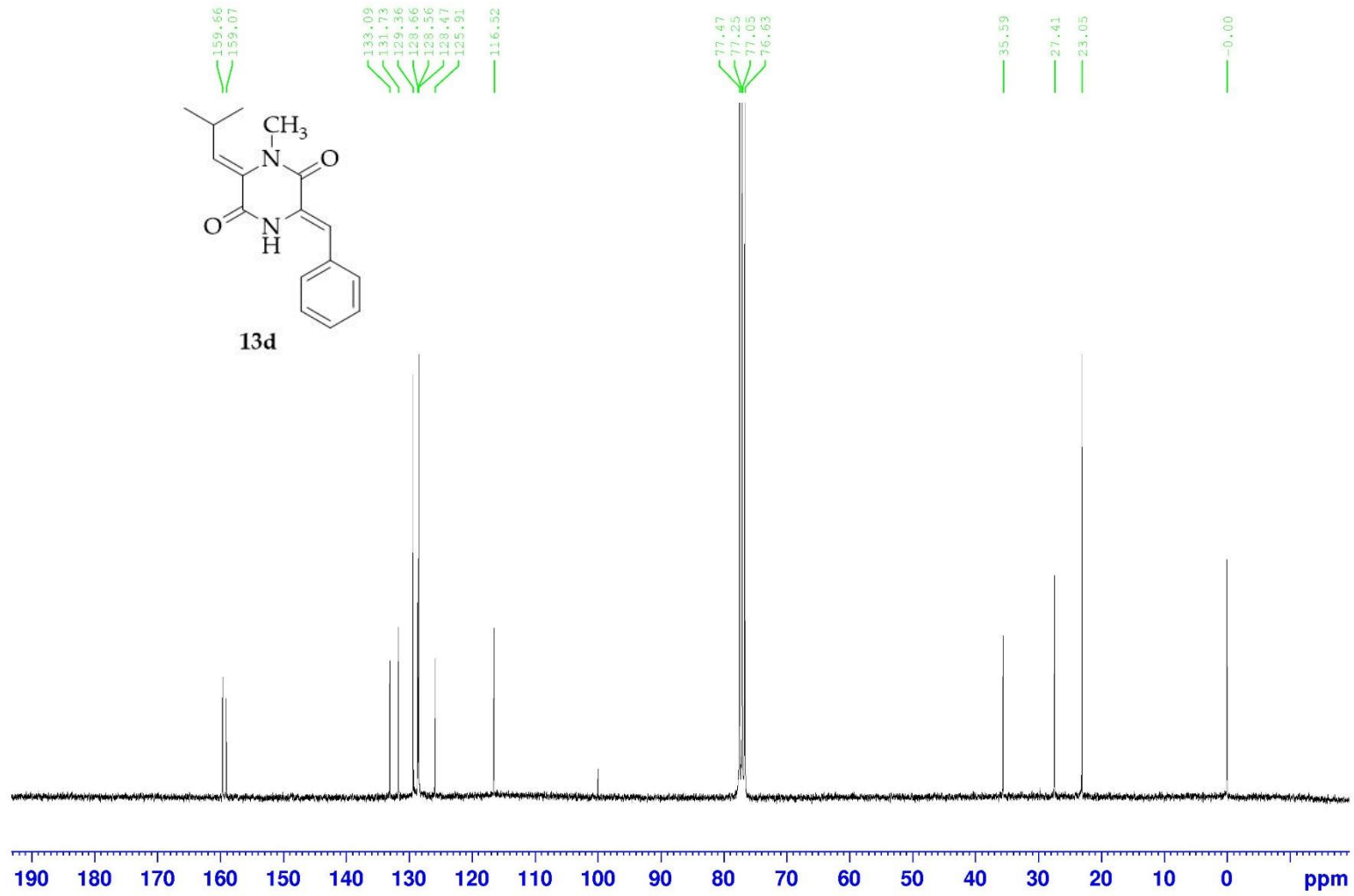


Figure S23. ¹³C-NMR of the (3*Z*,6*Z*)-3-Benzylidene-6-(2-methylpropylidene)-1-methyl-2,5-diketopiperazine (**13d**).

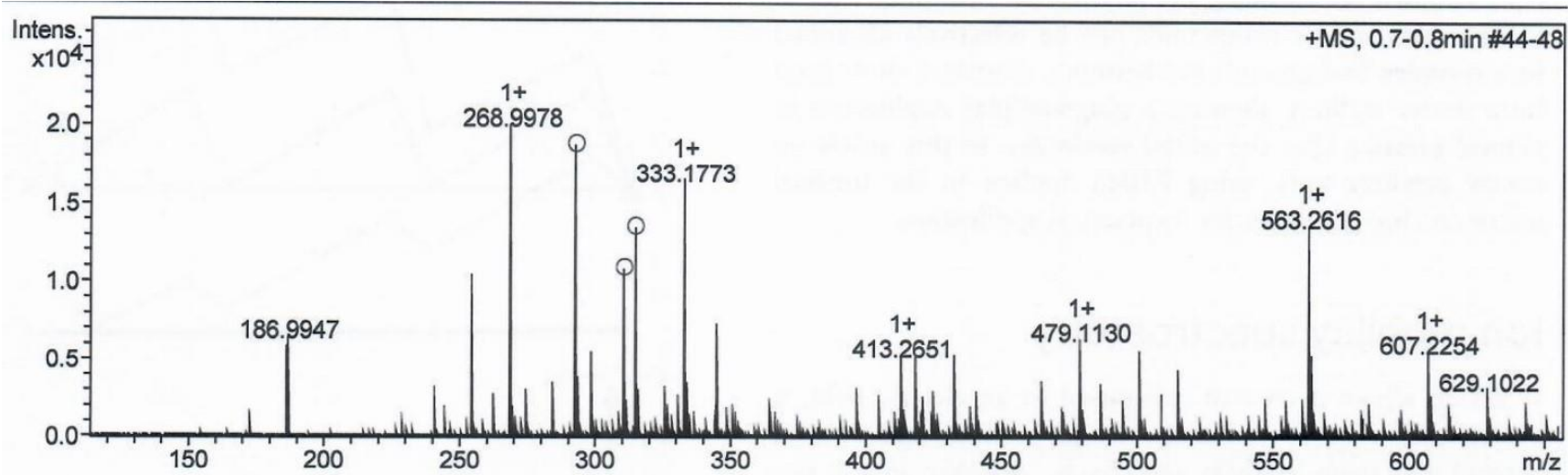
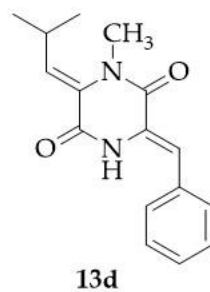


Figure S24. HRMS of the (3Z,6Z)-3-Benzylidene-6-(2-methylpropylidene)-1-methyl-2,5-diketopiperazine (**13d**).

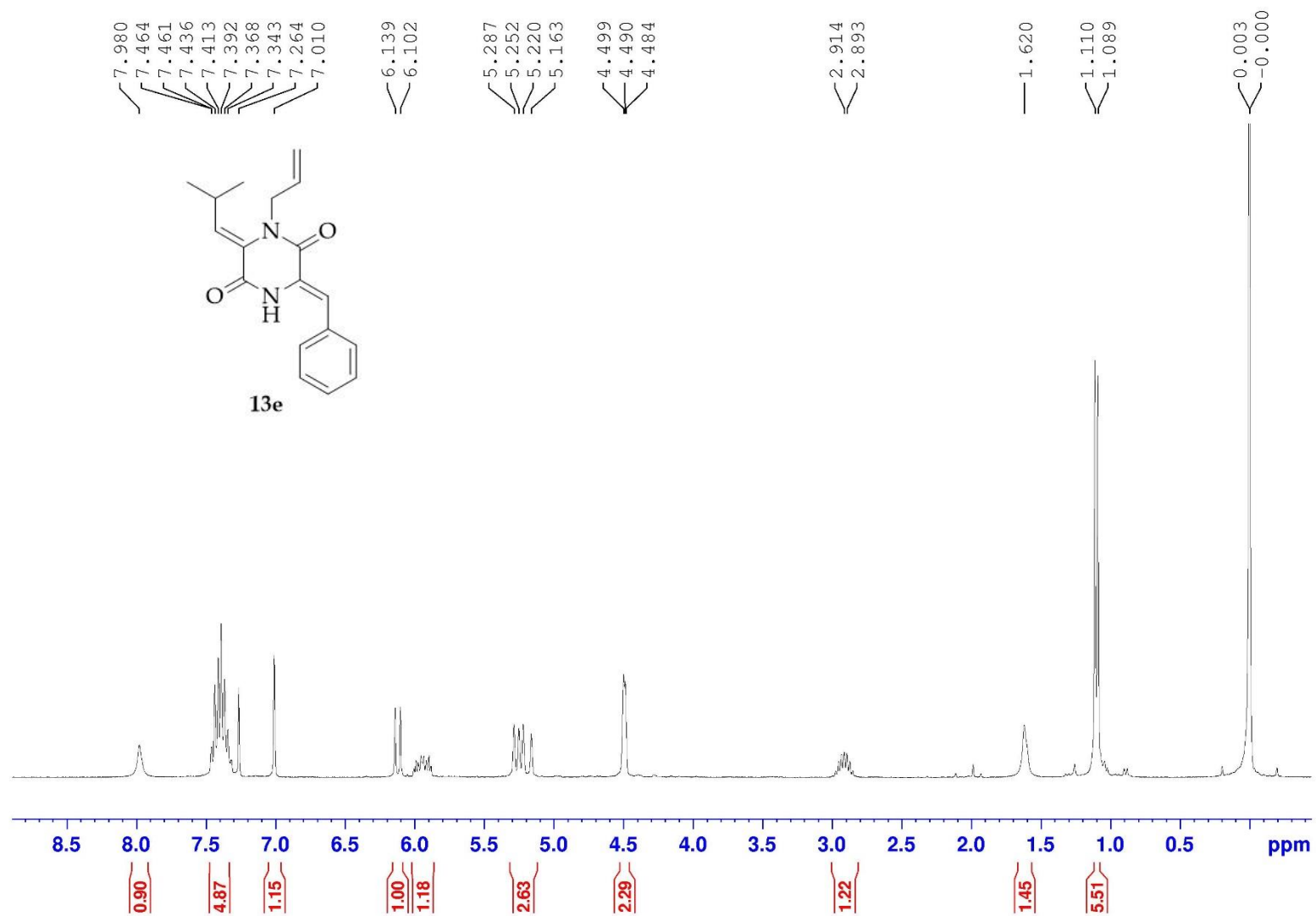


Figure S25. ^1H -NMR of the (3Z,6Z)-1-Allyl-3-benzylidene-6-(2-methylpropylidene)-2,5-diketopiperazine (**13e**).

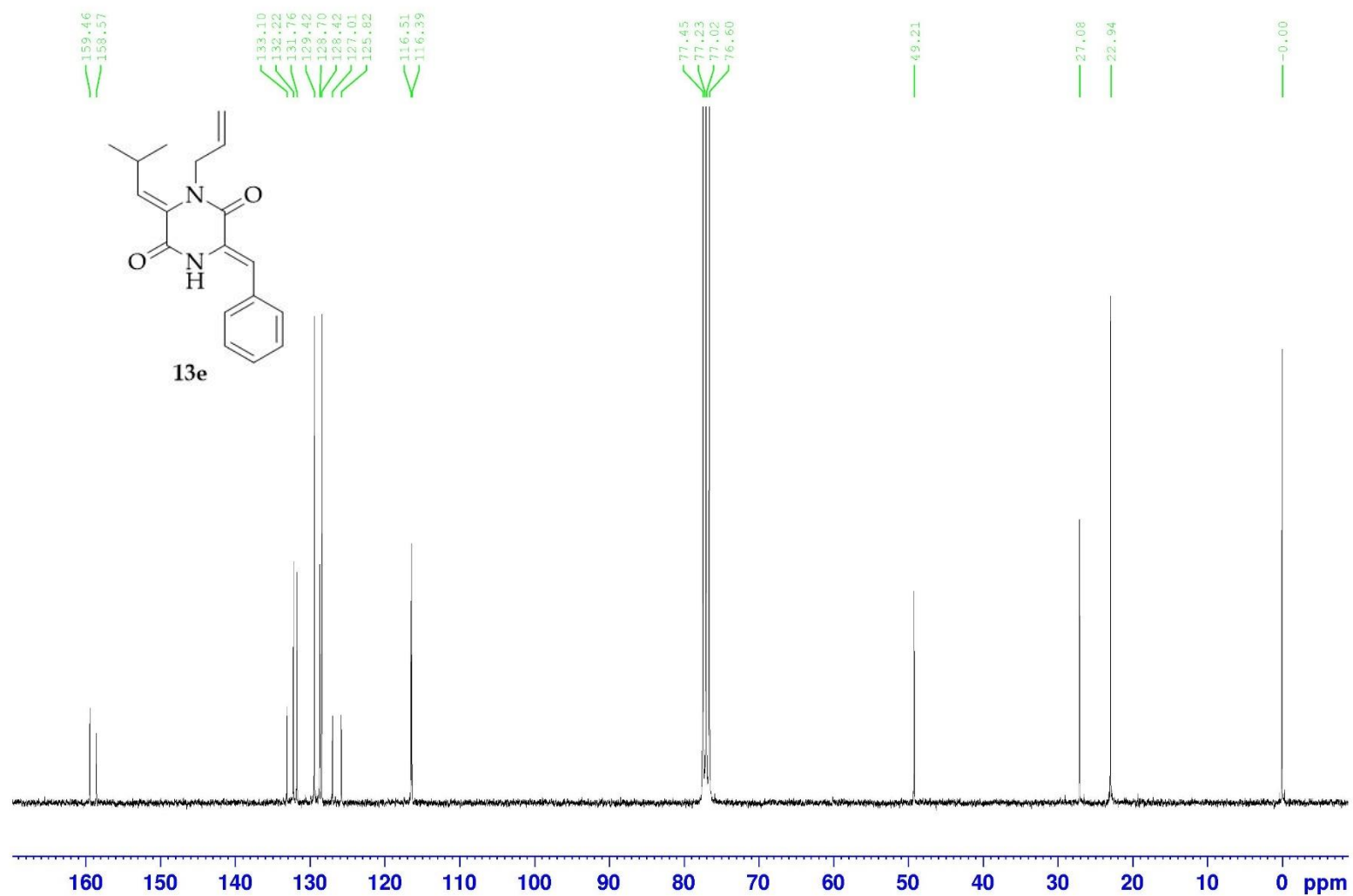


Figure S26. ¹³C-NMR of the (3Z,6Z)-1-Allyl-3-benzylidene-6-(2-methylpropylidene)-2,5-diketopiperazine (**13e**).

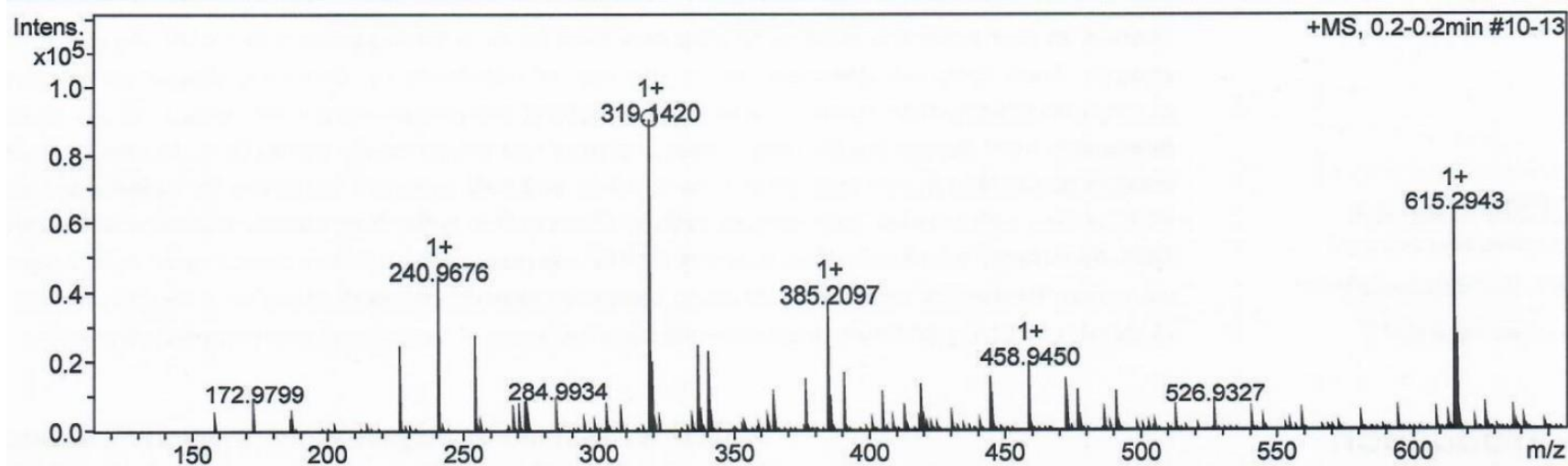
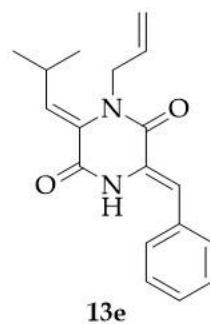


Figure S27. HRMS of the (3Z,6Z)-1-Allyl-3-benzylidene-6-(2-methylpropylidene)-2,5-diketopiperazine (**13e**).

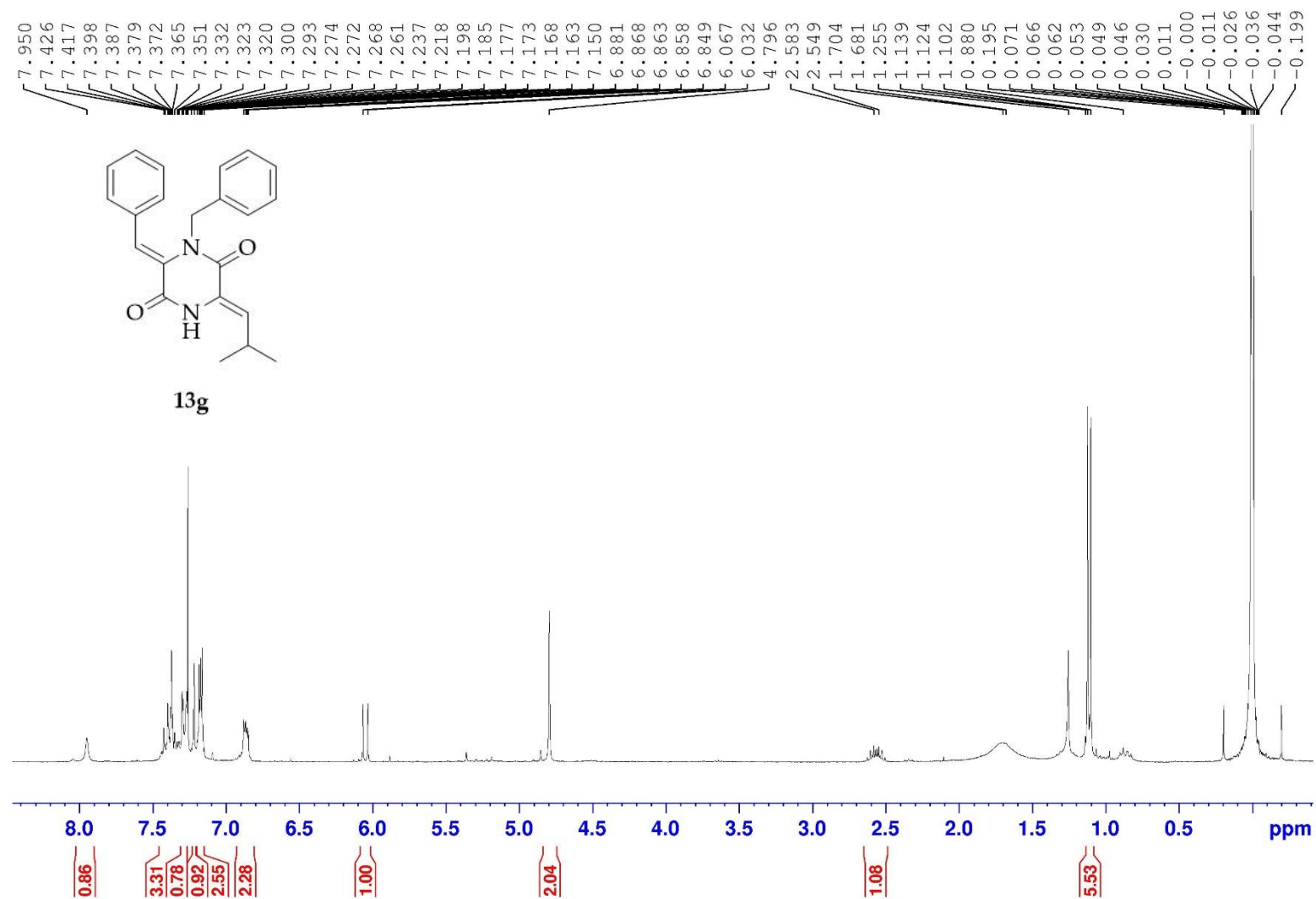


Figure S28. ¹H-NMR of the (3*Z*,6*Z*)-4-Benzyl-3-benzylidene-6-(2-methylpropylidene)-2,5-diketopiperazine (**13g**).

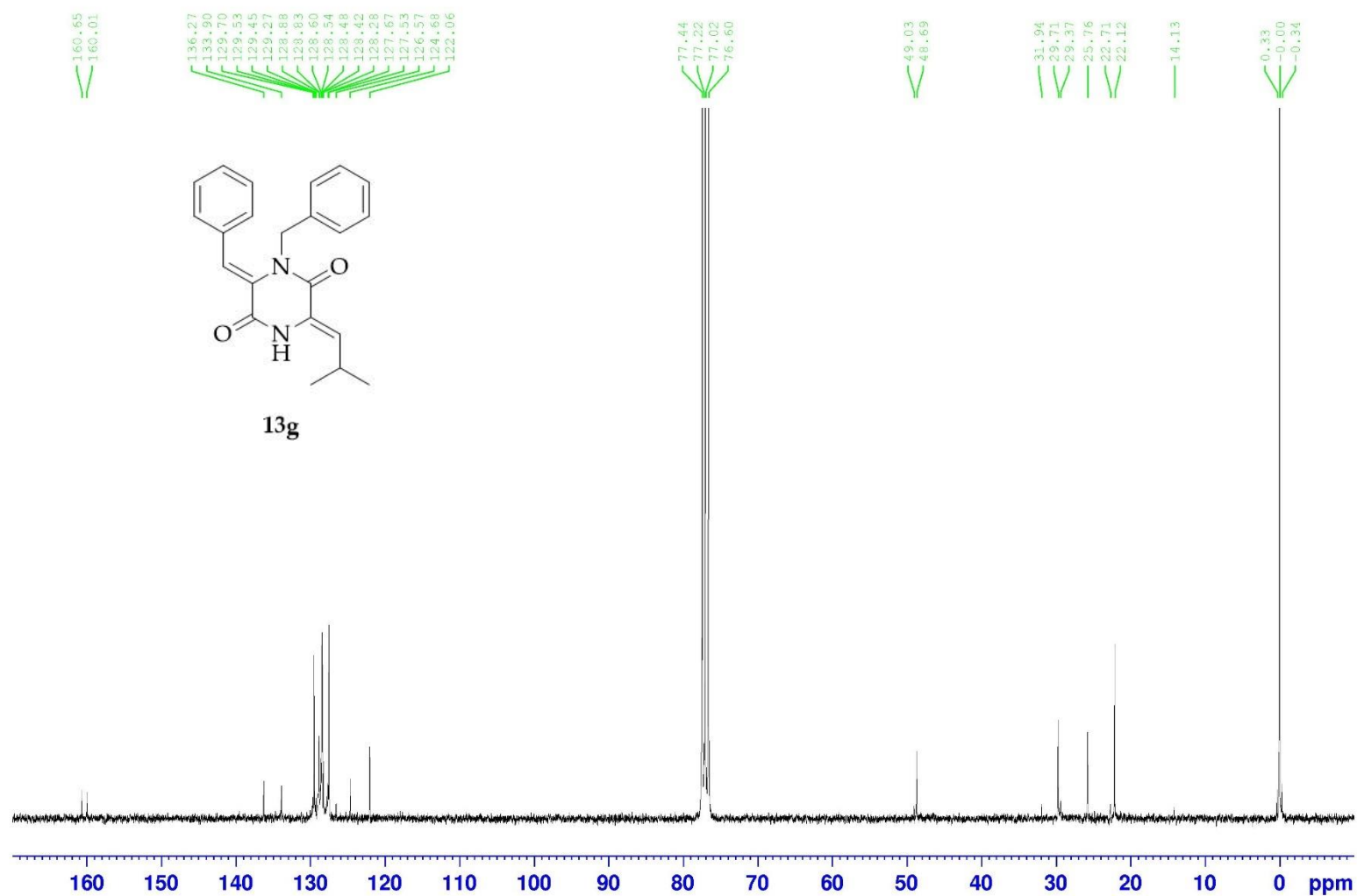
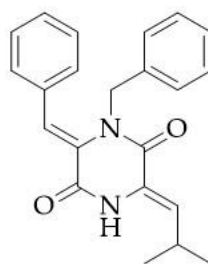


Figure S29. ¹³C-NMR of the (3*Z*,6*Z*)-4-Benzyl-3-benzylidene-6-(2-methylpropylidene)-2,5-diketopiperazine (**13g**).



13g

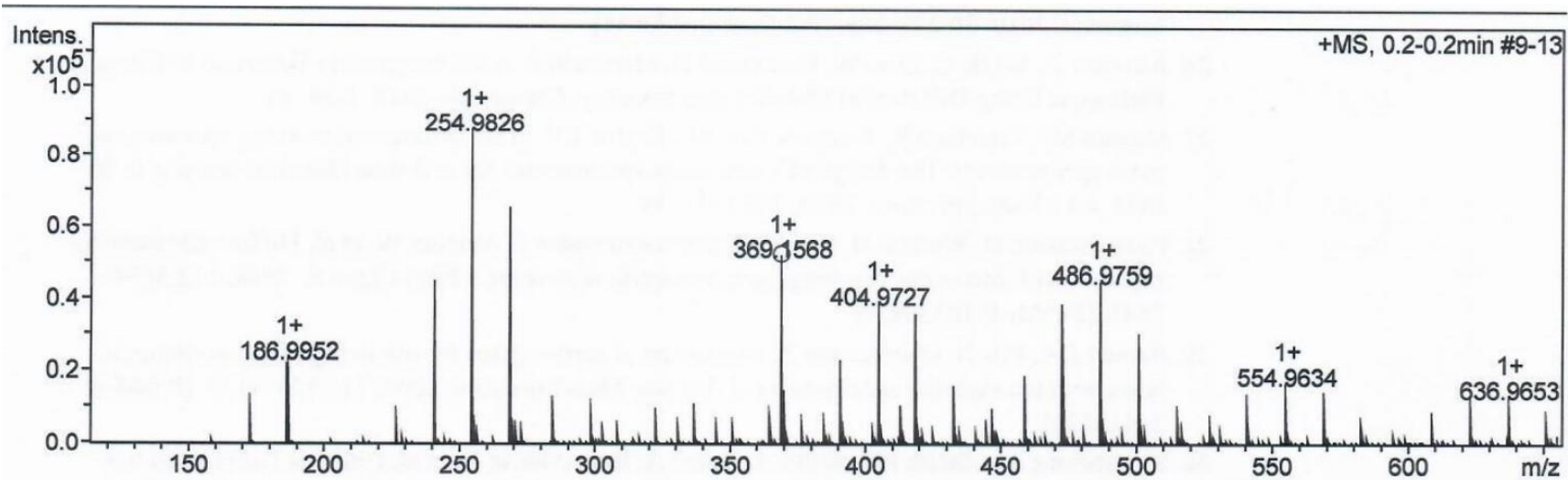


Figure S30. HRMS of the (3Z,6Z)-4-Benzyl-3-benzylidene-6-(2-methylpropylidene)-2,5-diketopiperazine (13g).

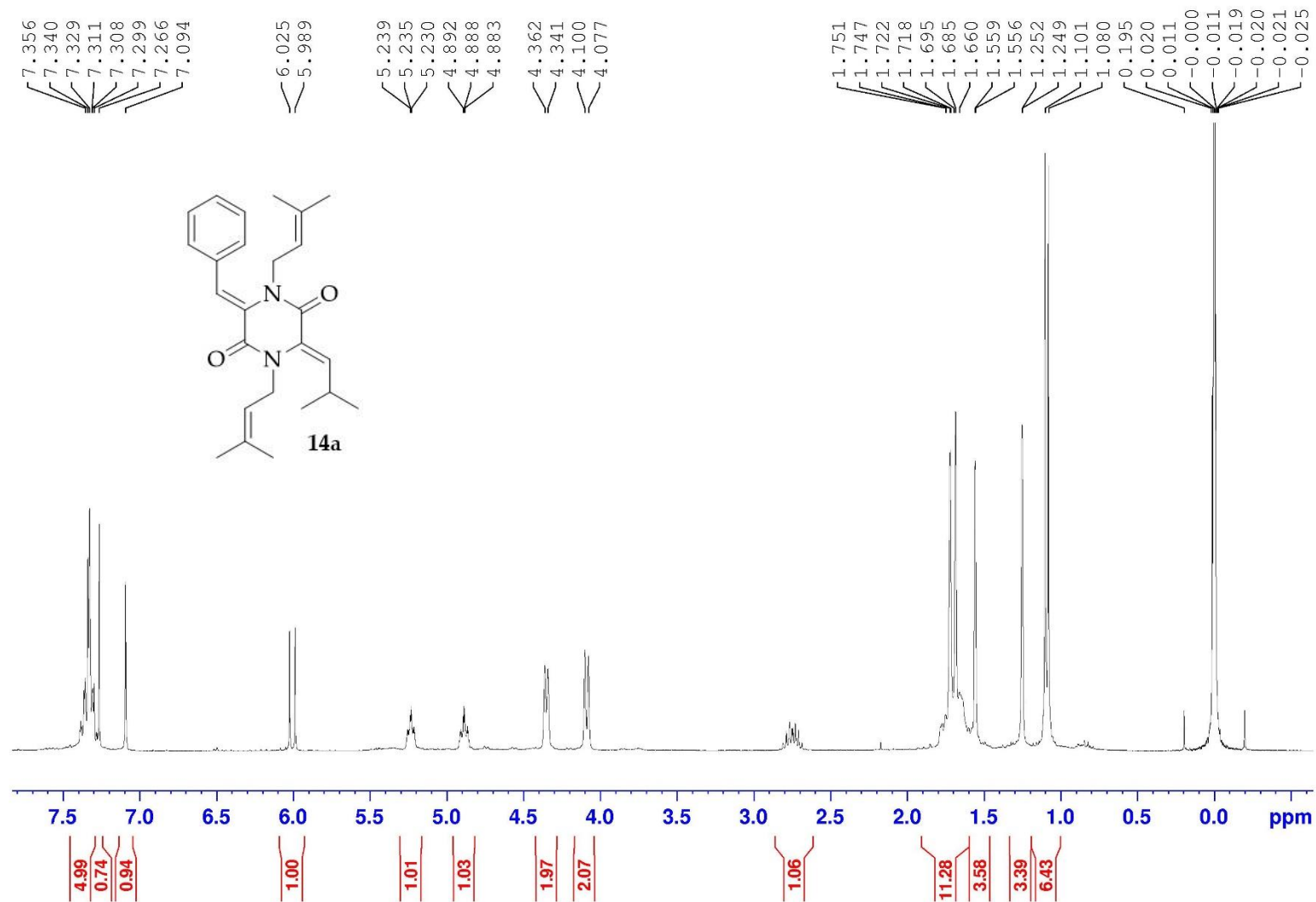


Figure S31. ¹H-NMR of the (3Z,6Z)-3-Benzylidene-6-(2-methylpropylidene)-1,4-bis(-3-methylbut-2-en-1-yl)-2,5-diketopiperazine (**14a**).

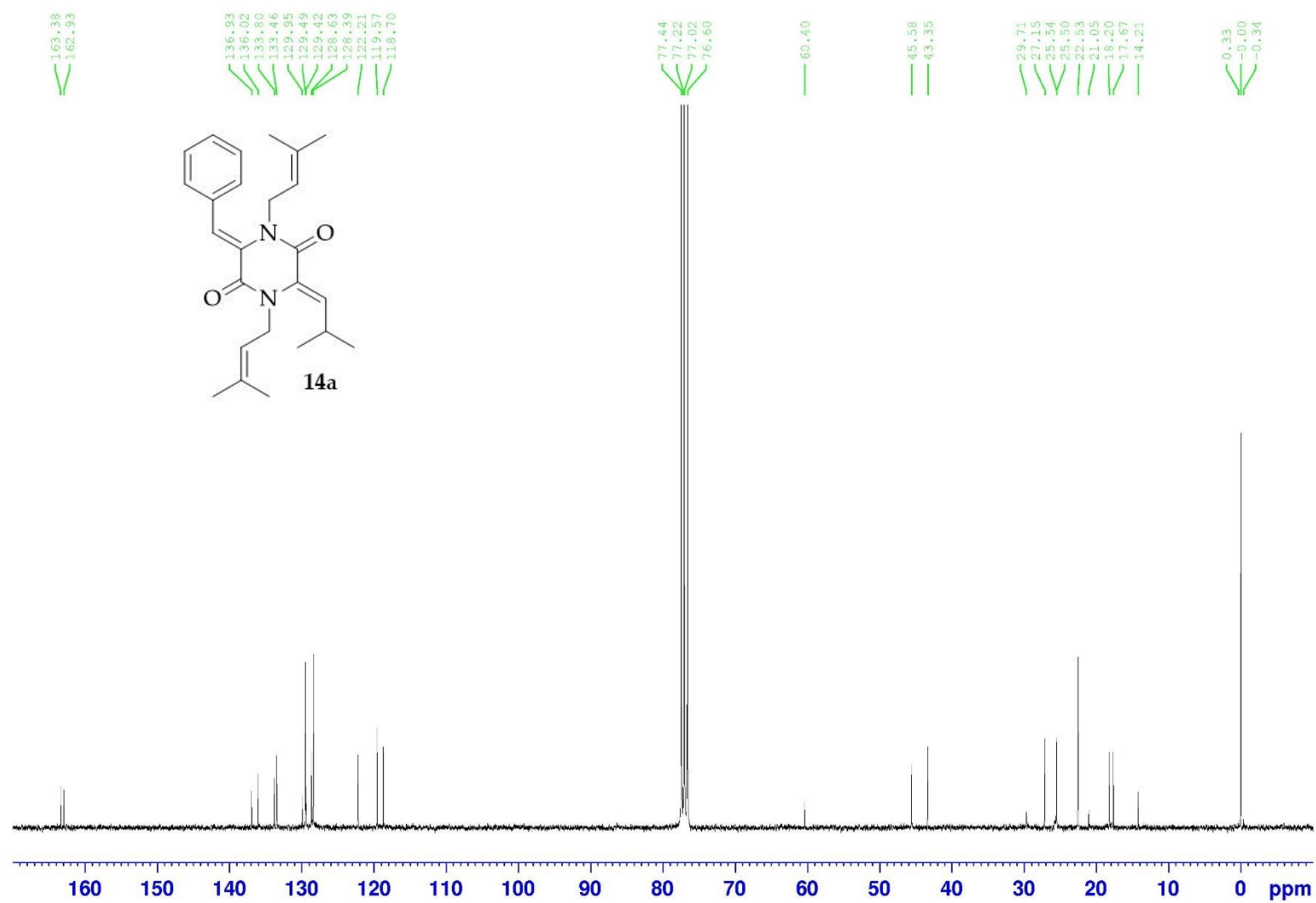


Figure S32. ^{13}C -NMR of the (3*Z*,6*Z*)-3-Benzylidene-6-(2-methylpropylidene)-1,4-bis(-3-methylbut-2-en-1-yl)-2,5-diketopiperazine (**14a**).

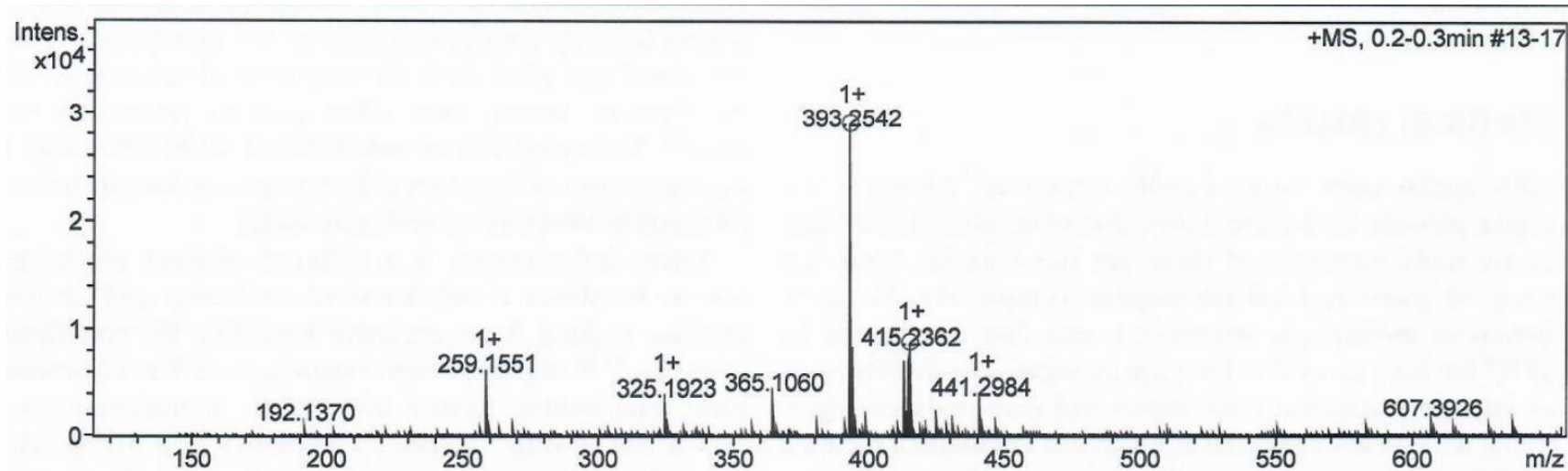
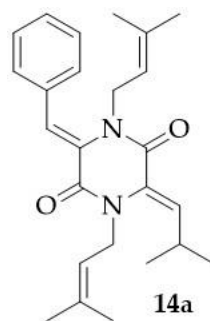


Figure S33. HRMS of the (3*Z*,6*Z*)-3-Benzylidene-6-(2-methylpropylidene)-1,4-bis(-3-methylbut-2-en-1-yl)-2,5-diketopiperazine (**14a**).

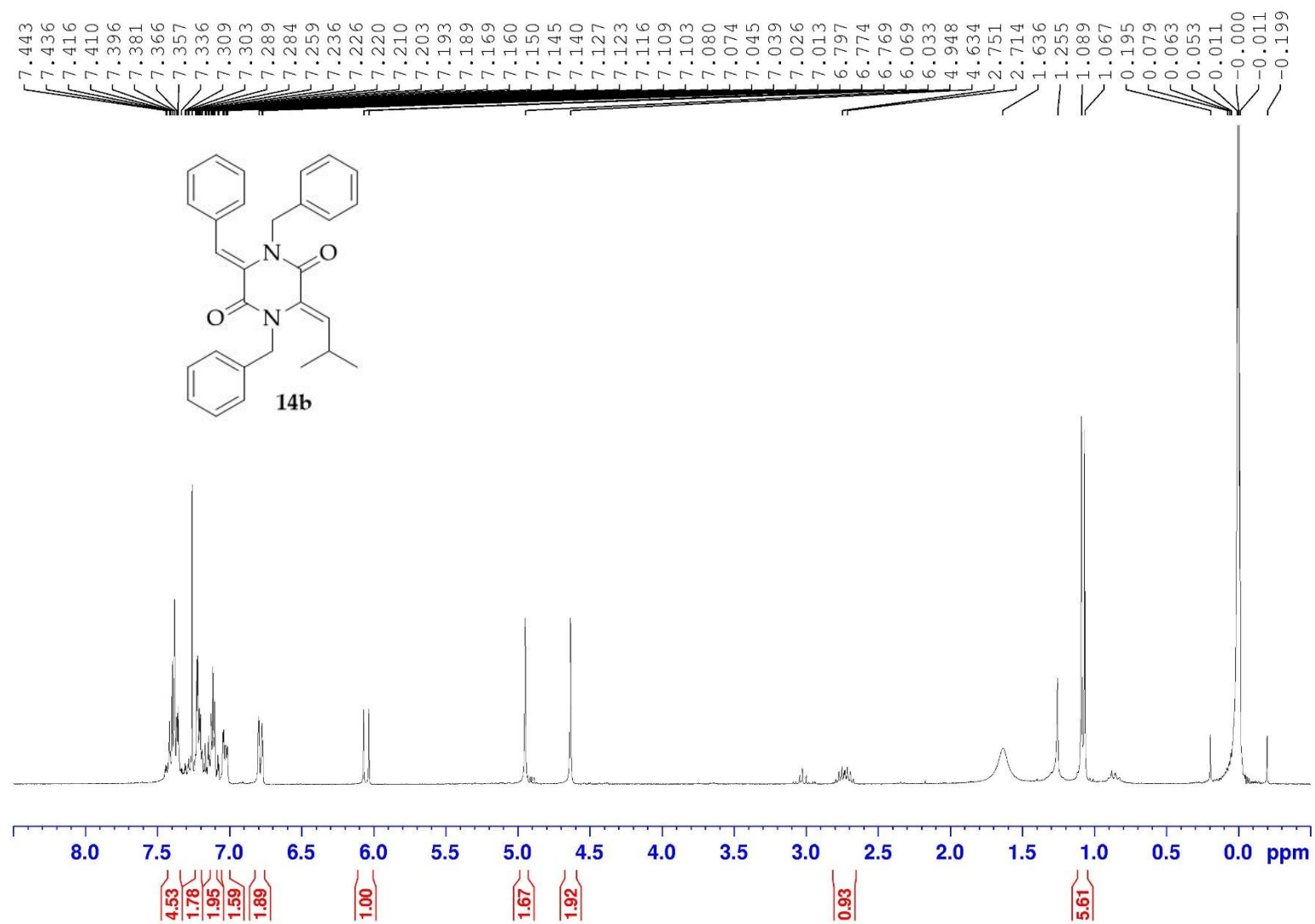


Figure S34. ¹H-NMR of the (3Z,6Z)-1,4-Dibenzyl-3-benzylidene-6-(2-methylpropylidene)-2,5-diketo piperazine (**14b**).

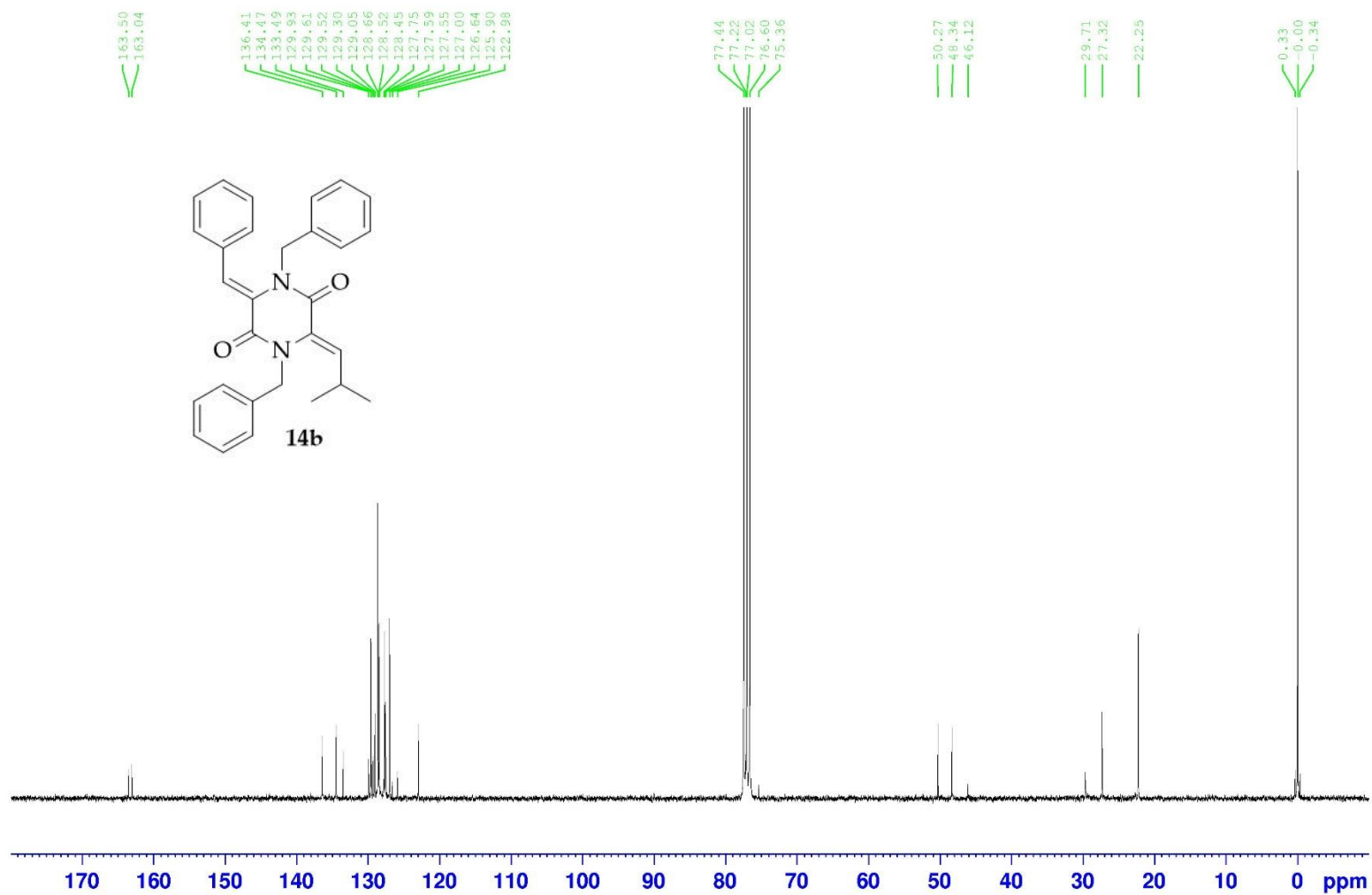


Figure S35. ¹³C-NMR of the (3Z,6Z)-1,4-Dibenzyl-3-benzylidene-6-(2-methylpropylidene)-2,5-diketo piperazine (**14b**).

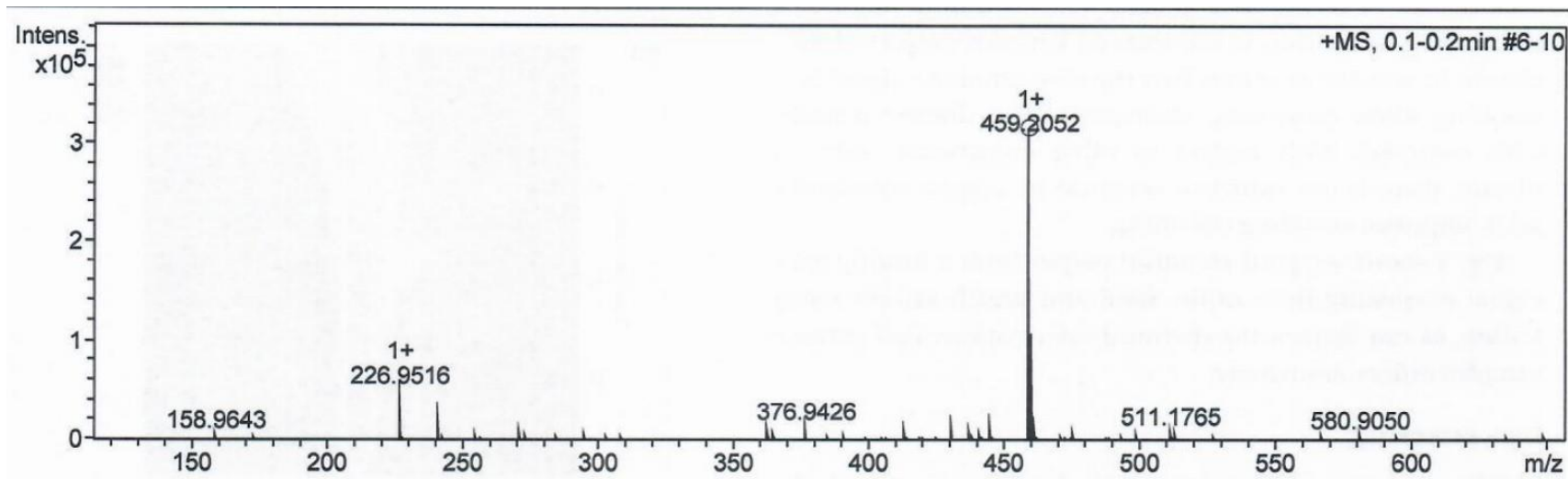
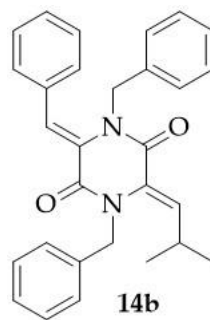


Figure S36. HRMS of the (3Z,6Z)-1,4-Dibenzyl-3-benzylidene-6-(2-methylpropylidene)-2,5-diketo piperazine (**14b**).

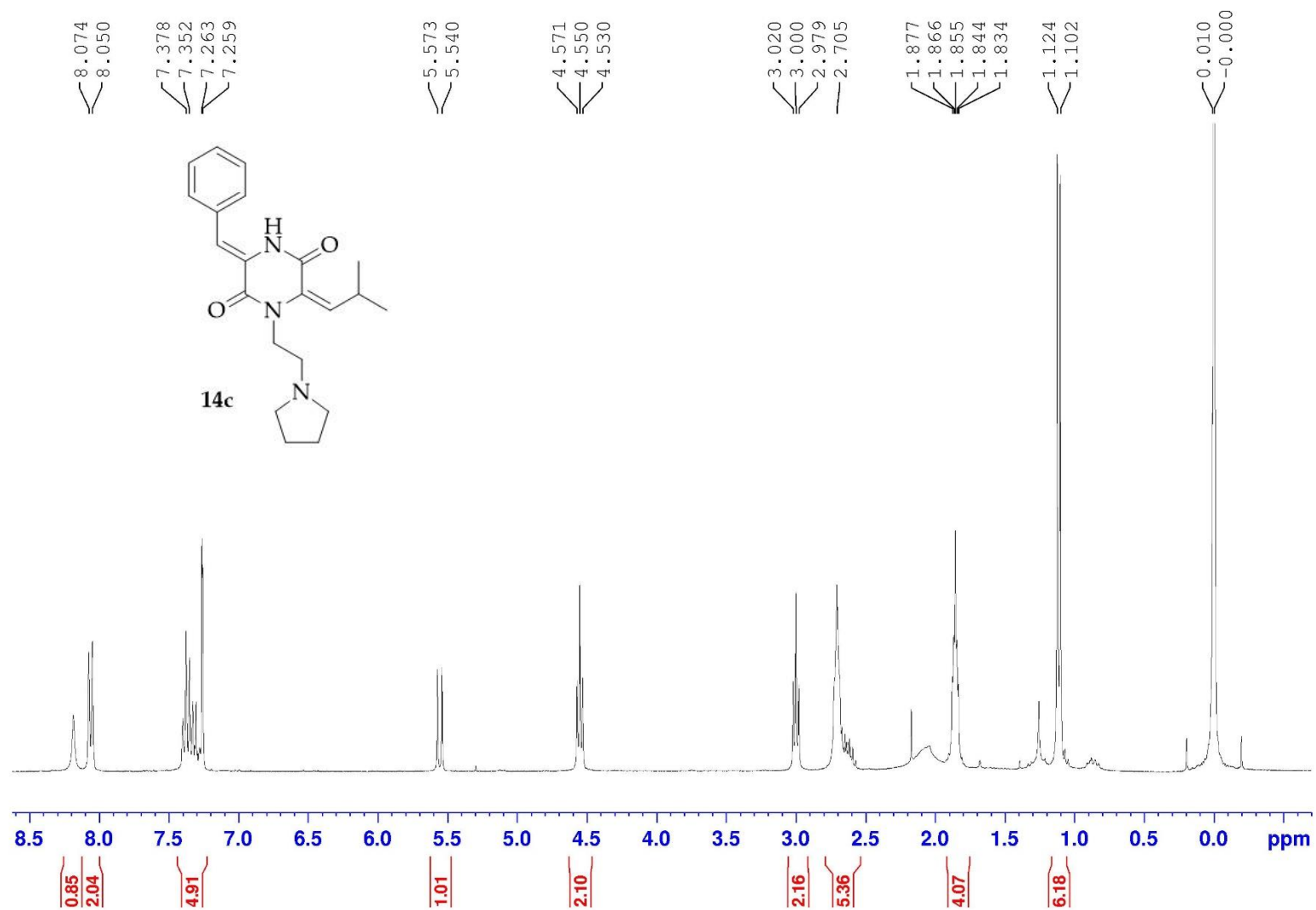


Figure S37. ¹H-NMR of the (3Z,6E)-3-Benzylidene-6-(2-methylpropylidene)-1-(1-ethyl pyrrolidine)-2,5-diketopiperazine (**14c**).

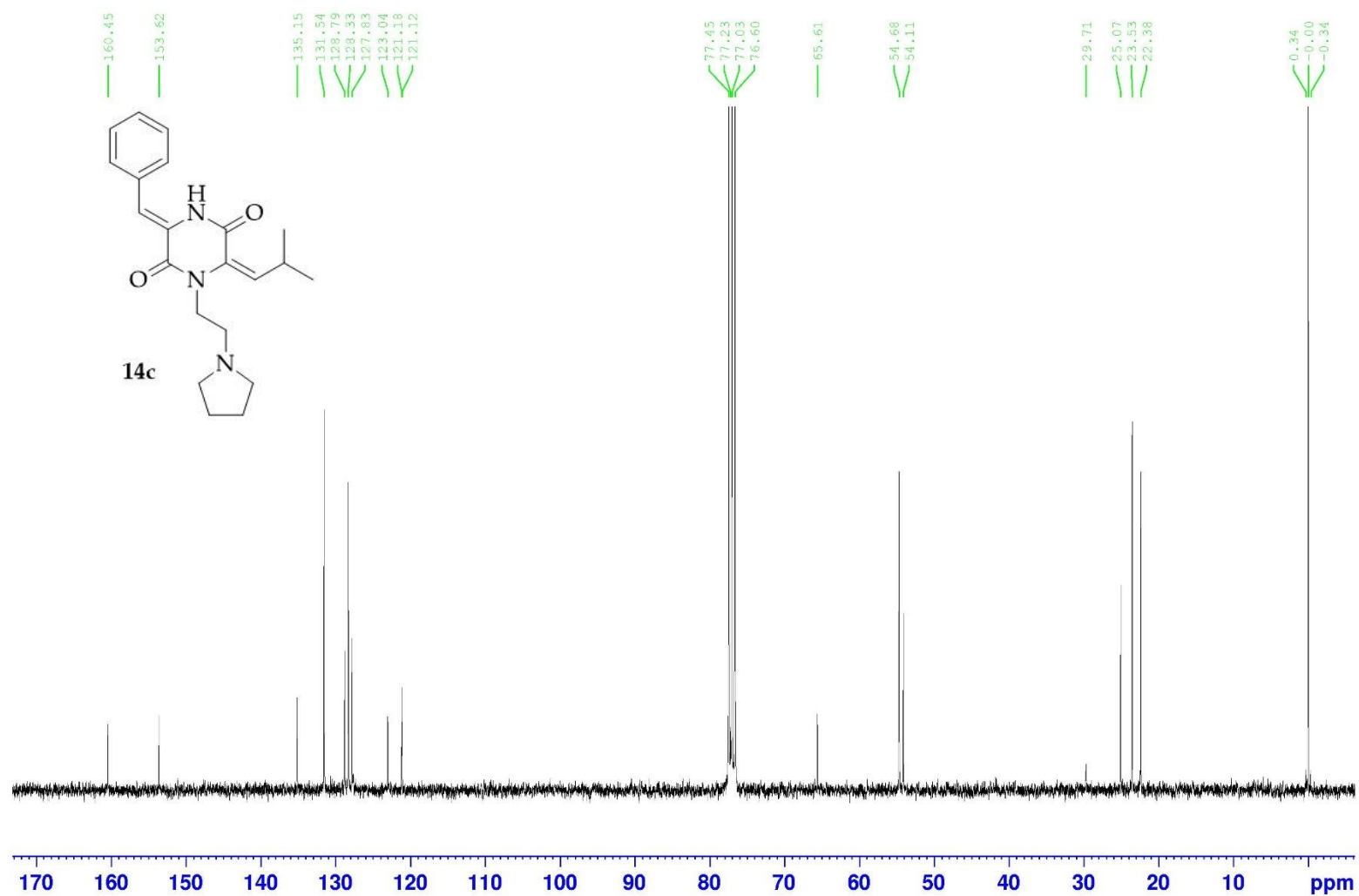


Figure S38. ¹³C-NMR of the (3*Z*,6*E*)-3-Benzylidene-6-(2-methylpropylidene)-1-(1-ethyl pyrrolidine)-2,5-diketopiperazine (**14c**).

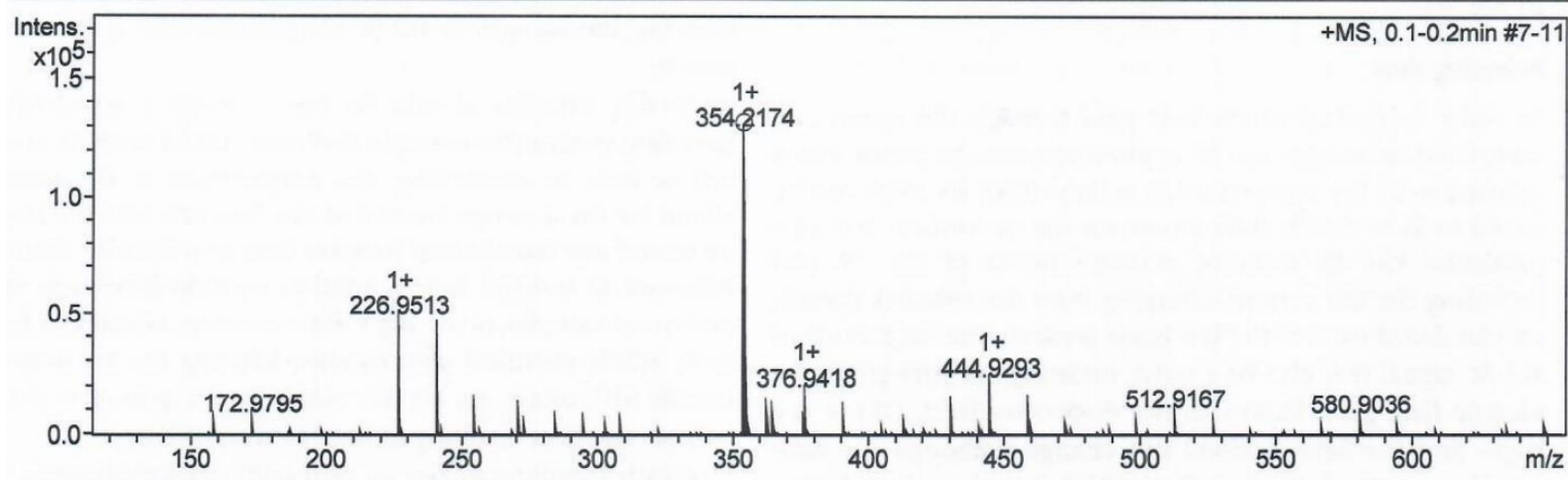
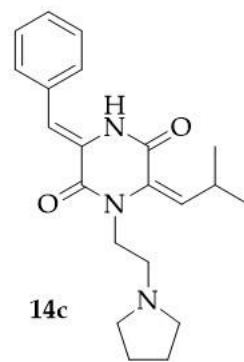


Figure S39. HRMS of the (3*Z*,6*E*)-3-Benzylidene-6-(2-methylpropylidene)-1-(1-ethyl pyrrolidine)-2,5-diketopiperazine (**14c**).