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NOTE

Study on the Monocrystal of Rifampicin

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A monocrystal of rifampicin is obtained at the solvent condition as methanol:water (2:1). Besides we analyzed its structure. Finally we confirmed the spatial configuration of rifampicin.

Key Words: Rifampicin monocrystal structure crystal.

There is no literature on the research on the monocrystal of rifampicin[1]. The direct way on analyzing the spatial configuration of compound was to obtain the monocrystal.

All reagents and spectroscopic solvents pure grade employed for test are AR. The raw material of rifampicin was obtained in our laboratory.

Monocrystal cultivation: We adopted the solvent evaporation method on cultivating the monocrystal of rifampicin. The schematic diagram of principle of the solvent evaporation method was shown at Fig. 1. 1 mL benign solvent was added into moderate amount of rifampicin. After it was dissolved, 1 mL poor solvent was added on the surface of the solution carefully. Then the solution was closed with the sealing film. We made several pores on the sealing film with syringe needle at room temperature and observed its change everyday.

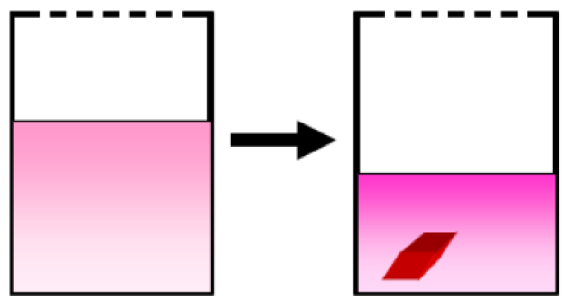

Fig. 1. Schematic diagram of principle of the solvent evaporation method

Determination on the monocrystal of rifampicin: The obtained monocrystal of rifampicin was analyzed at the Institute of Materia Medica (IMM), Chinese Academy of Medical Sciences and Peking Union Medical College.

Structure of monocrystal of rifampicin: We analyzed the structure of monocrystal of rifampicin by SHELXS 97 and obtained 55 non-hydrogen atoms' position from E figure. We also obained the other non-hydrogen atoms' position by least squares and difference Fourier method and obtained all hydrogen atoms' position by geometric calculation and difference fourier method. The final reliable factor was 0.0537. The wR^2 was 0.1288. The S was 1.028. The stoichiometric asymmetric unit type was $C_{43}H_{58}N_4O_{12}\cdot(H_2O)_5$. The molecular weight was 822.95. The density of crystal was 1.255 g cm^3. The relative molecular configuration diagram is shown at Fig. 2. Three-dimensional structure of the molecular ellipsoid map is shown at Fig. 3. The cell stacked figure by b axis is shown at Fig. 4.

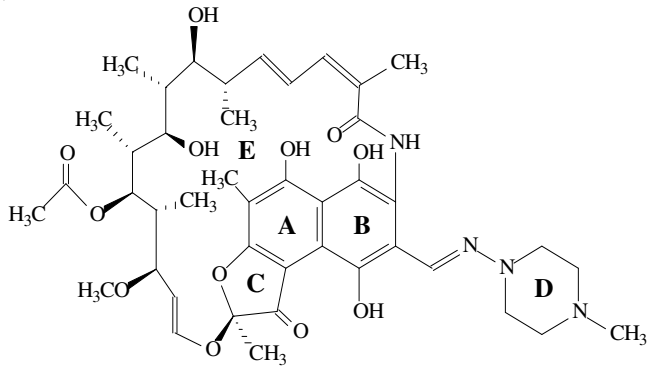

Fig. 2. Relative molecular configuration diagram

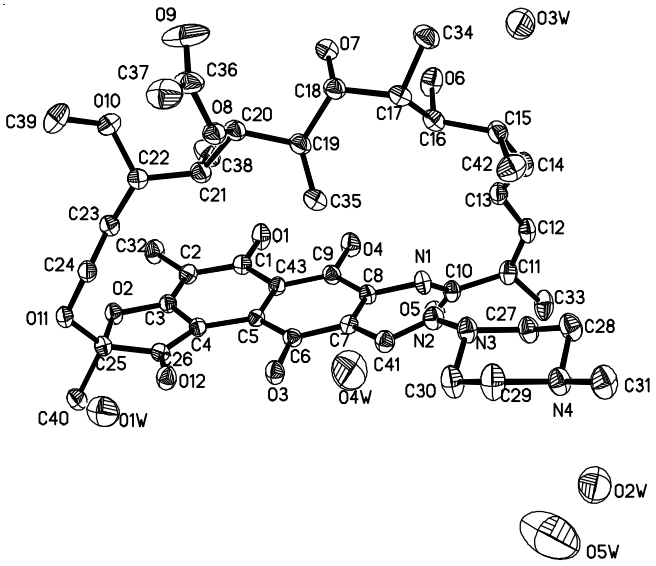

Fig. 3. Three-dimensional structure of the molecular ellipsoid map

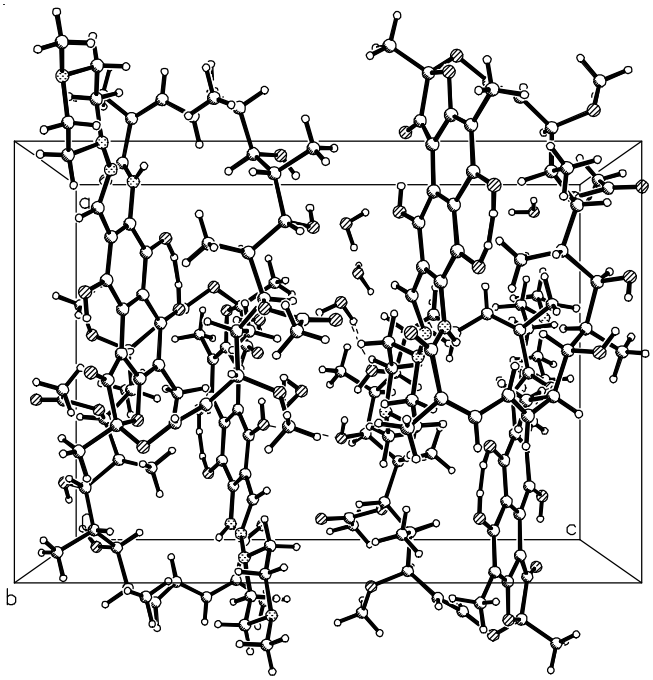

Fig. 4. Cell stacked figure by b-axis

Conclusion

A monocrystal of rifampicin is obtained at the solvent condition as methanol:water (2:1) and also analyzed its structure.

REFERENCES

1. S. Agrawal, Y. Ashokraj, P.V. Bharatam, O. Pillai and R. Panchagnula, *Eur. J. Pharm. Sci.*, **22**, 127 (2004).