© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 1

REVISED

Supporting Information

Title: *"A simple and efficient approach for the synthesis of fluorinated and non-fluorinated octaethylporphyrin-based benzochlorins with variable lipophilicity, their in vivo tumor uptake and the preliminary in vitro photosensitizing efficacy."*

Manuscript No: JO001541+

Authors: Guolin Li, Andrew Graham, William Potter, Zachary D. Grossman, Allan Oseroff, Thomas J. Dougherty and Ravindra K. Pandey*

Figure 1: ^{1}H NMR spectrum of porphyrin **3**.

Figure 2: ^{19}F NMR spectrum of porphyrin **3**.

Figure 3: ^{1}H NMR spectrum of porphyrin **4**.

Figure 4: ^{19}F NMR spectrum of porphyrin **4**.

Figure 5: ^{1}H NMR spectrum of benzochlorin **5**.

Figure 6: ^{19}F NMR spectrum of benzochlorin **5**.

Figure 7: ^{13}C NMR spectrum of benzochlorin **5**.

Figure 8: ^{1}H NMR spectrum of porphyrin **6a**.

Figure 9: ^{1}H NMR spectrum of porphyrin **6b**.

Figure 10: ^{1}H NMR spectrum of porphyrin **6c**.

Figure 11: ^{1}H NMR spectrum of porphyrin **6d**.

Figure 12: ^{1}H NMR spectrum of porphyrin **6e**.

Figure 13: ^{1}H NMR spectrum of porphyrin **7a**.

Figure 14: ^{1}H NMR spectrum of porphyrin **7b**.

Figure 15: ^{1}H NMR spectrum of porphyrin **7c**.

Figure 16: ^{1}H NMR spectrum of porphyrin **7d**.

Figure 17: ^{1}H NMR spectrum of porphyrin **7e**.

Figure 18: ^{1}H NMR spectrum of porphyrin **8**.

Figure 19: ^{1}H NMR spectrum of benzochlorin **9**.

Figure 20: ^{19}F NMR spectrum of benzochlorin **9**.

Figure 21: ^{1}H NMR spectrum of porphyrin **10**.

Figure 22: ^{1}H NMR spectrum of benzochlorin **11**.

Figure 23: ^{1}H NMR spectrum of benzochlorin **12**.

Figure 24: ^{1}H NMR spectrum of benzochlorin **13a**.

Figure 25: ^{1}H NMR spectrum of benzochlorin **13b**.

Figure 26: ^{1}H NMR spectrum of benzochlorin **13c**.

Figure 27: ^{1}H NMR spectrum of benzochlorin **13d**.

Figure 28: ^{1}H NMR spectrum of porphyrin **14**.

Figure 29: ^{1}H NMR spectrum of benzochlorin **15**.

Figure 30: ^{1}H NMR spectrum of porphyrin **16**.

© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 3

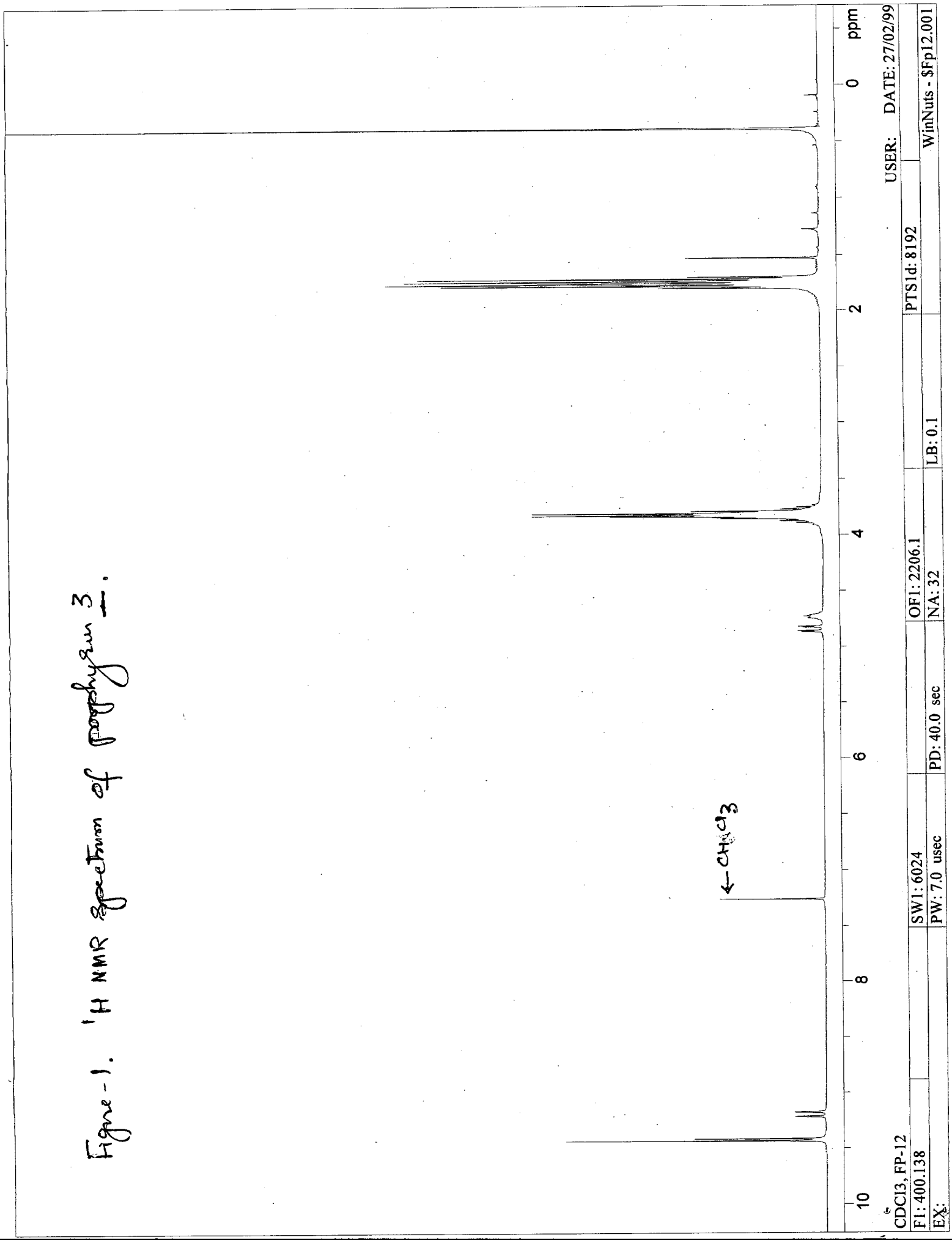
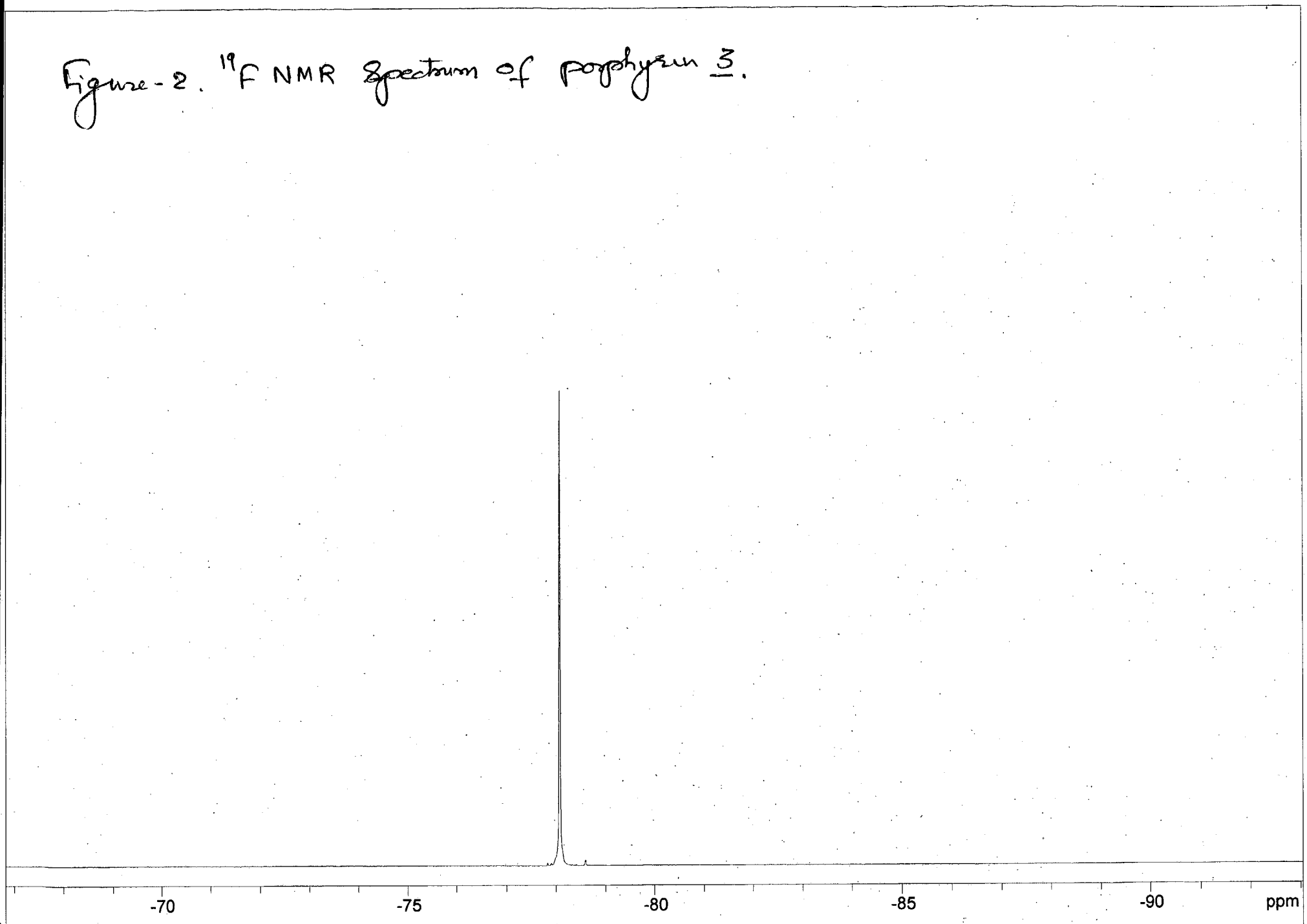


Figure-1. ^1H NMR spectrum of porphyrin 3.

Figure-2. ^{19}F NMR Spectrum of porphyrin 3.



CDCl3, FP-12, F-19 NMR USER: DATE: 27/02/99

F1: 376.471		SW1: 26315		OF1: -24724.4		PTS1d: 8192	
EX:		PW: 8.0 usec	PD: 20.0 sec	NA: 40	LB: 2.0		WinNuts - $Ffp12.001

© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 4

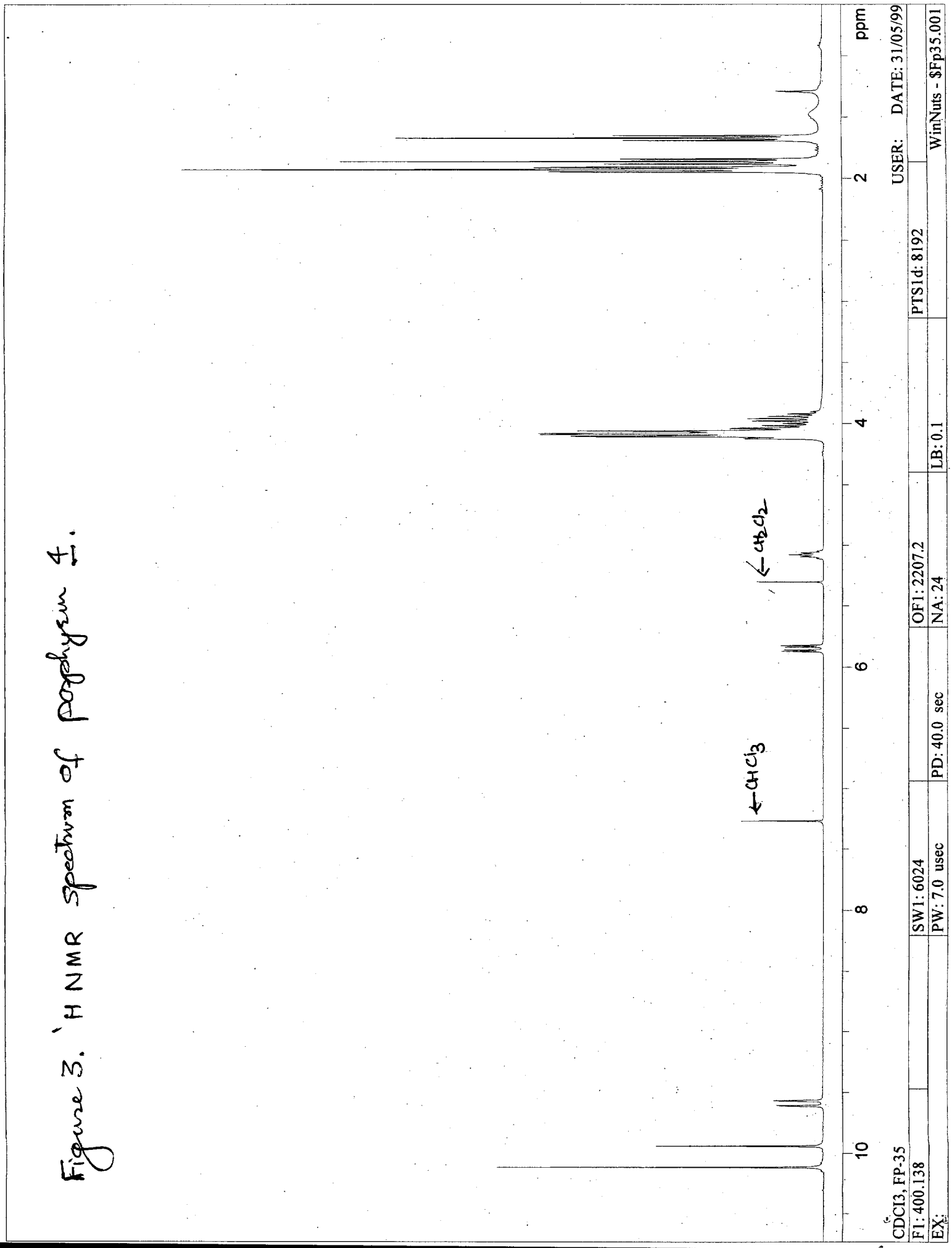


Figure 3. ^1H NMR spectrum of porphyrin 4.

© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 6

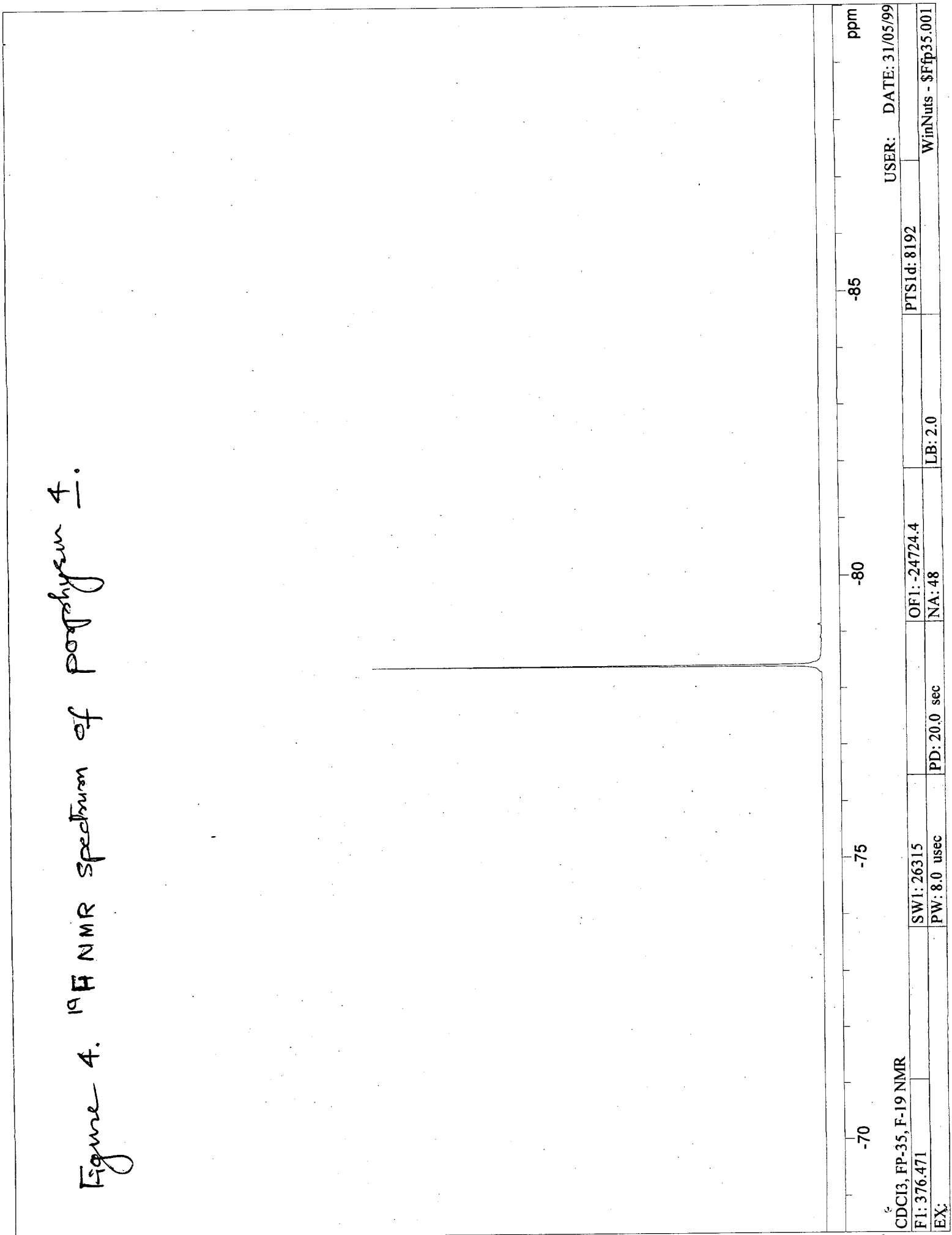


Figure 4. ^{19}F NMR spectrum of porphyrin 4.

© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 7

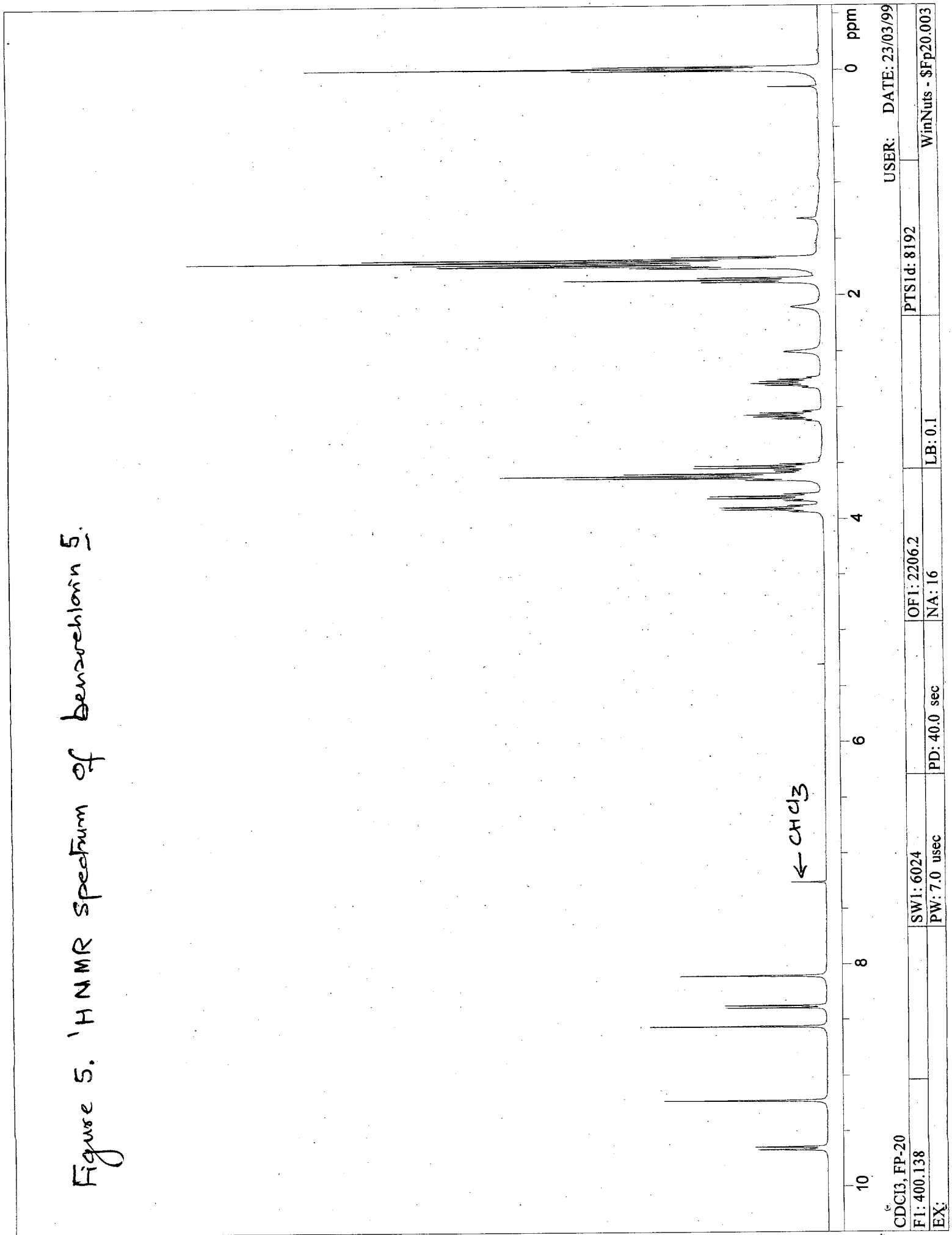
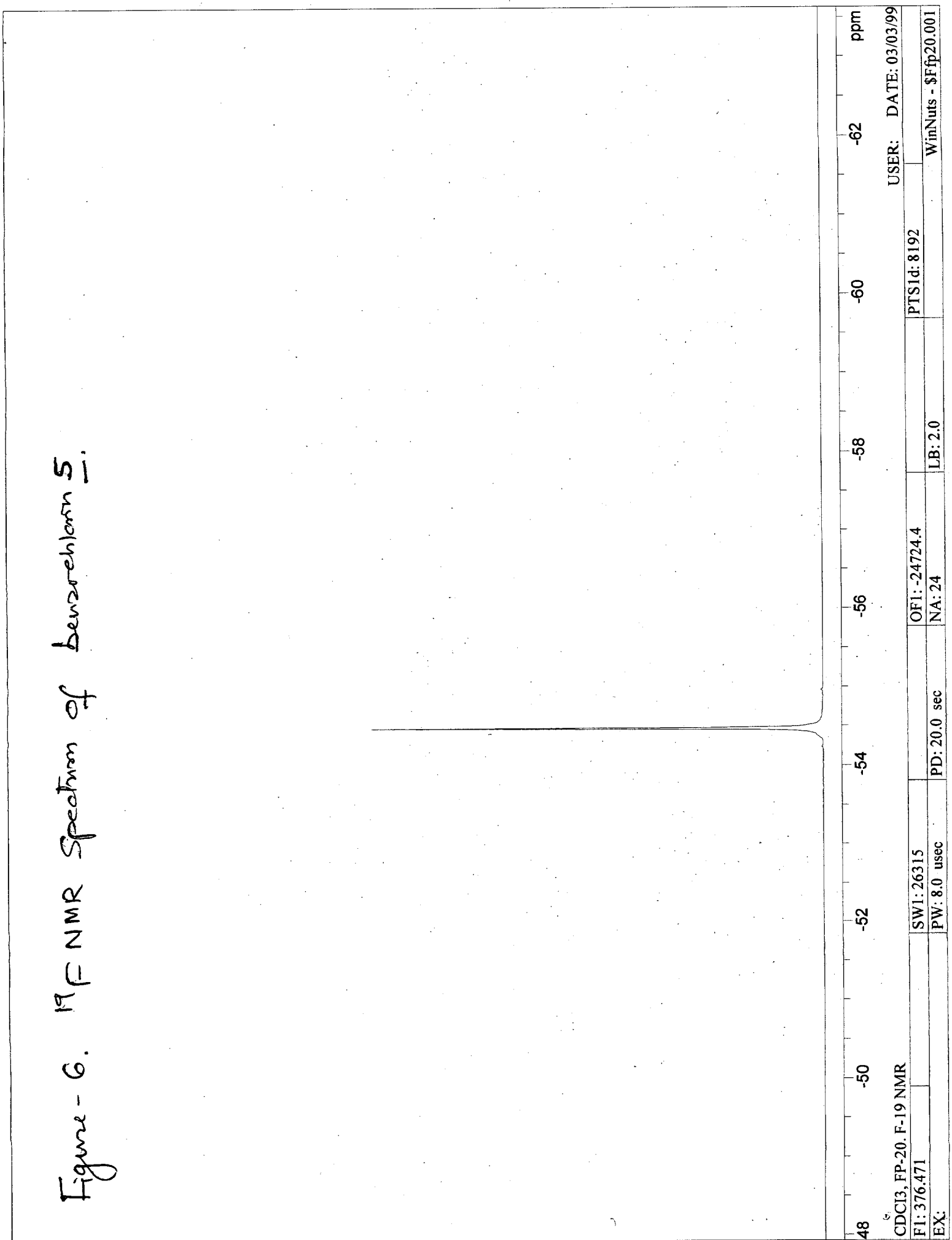


Figure 5. ^{1}H NMR spectrum of benzochlorin 5.

© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 8

Figure - 6. ^{19}F NMR Spectrum of benzochloam 5i.



© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 9

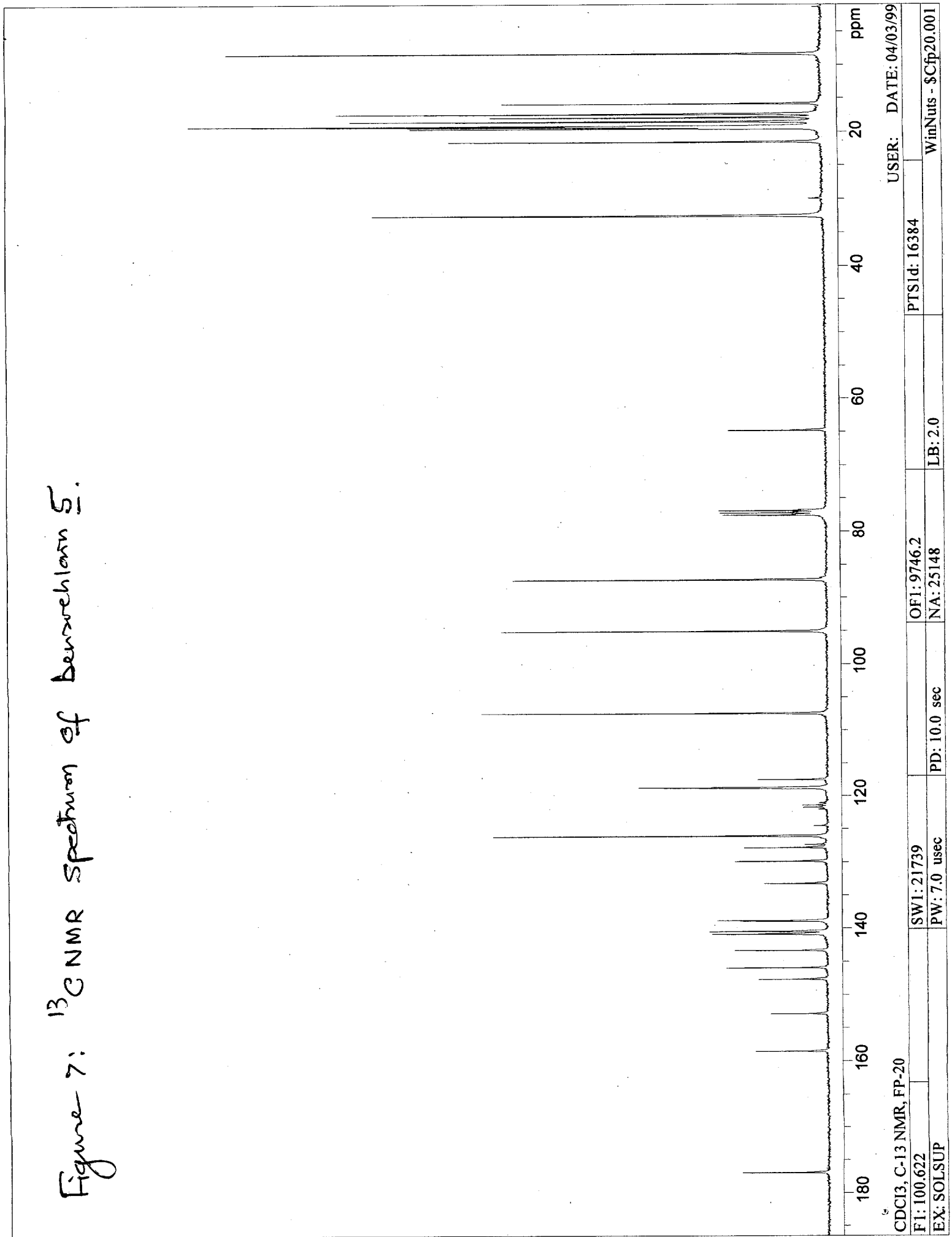


Figure 7: ^{13}C NMR spectrum of benzochlam 5.

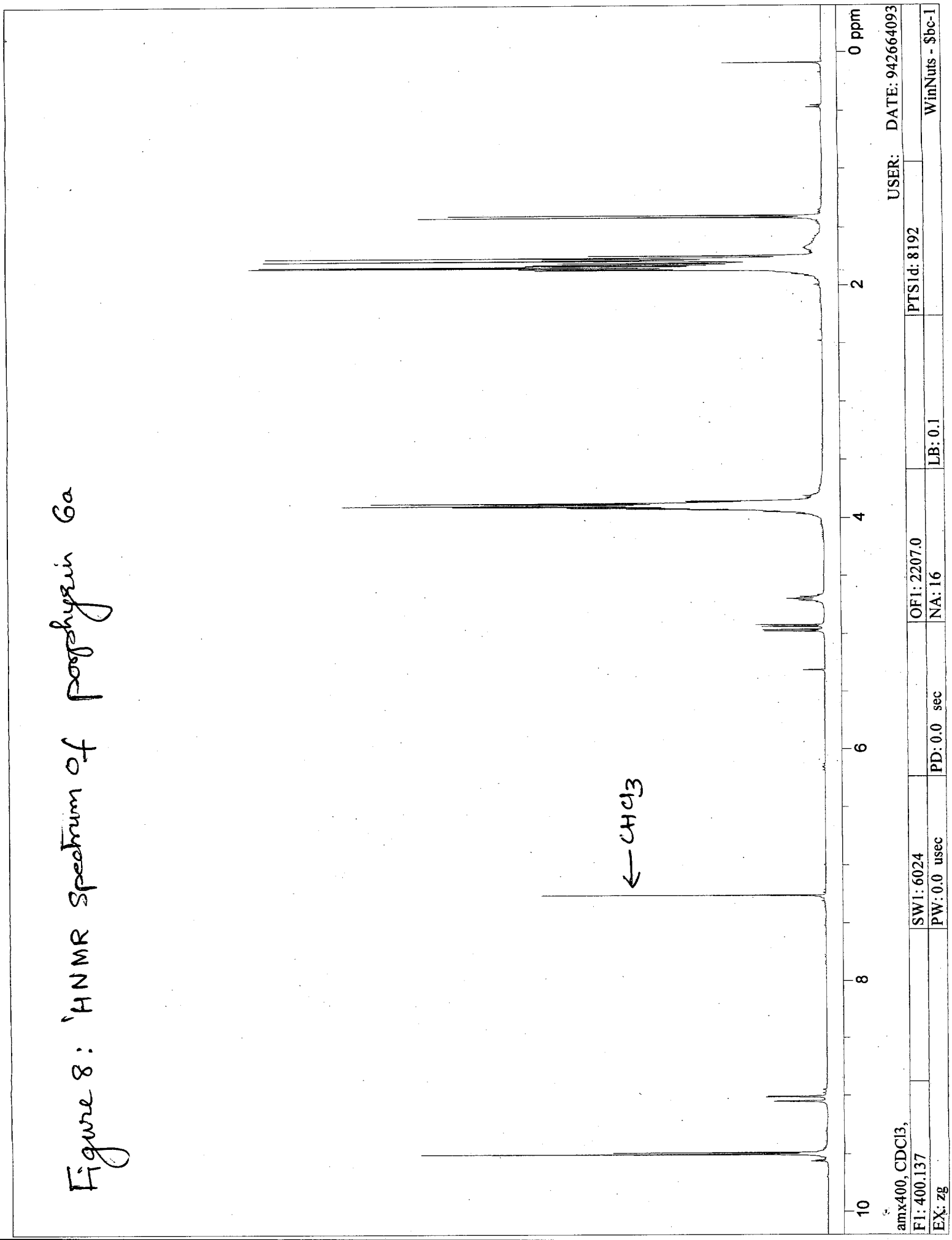
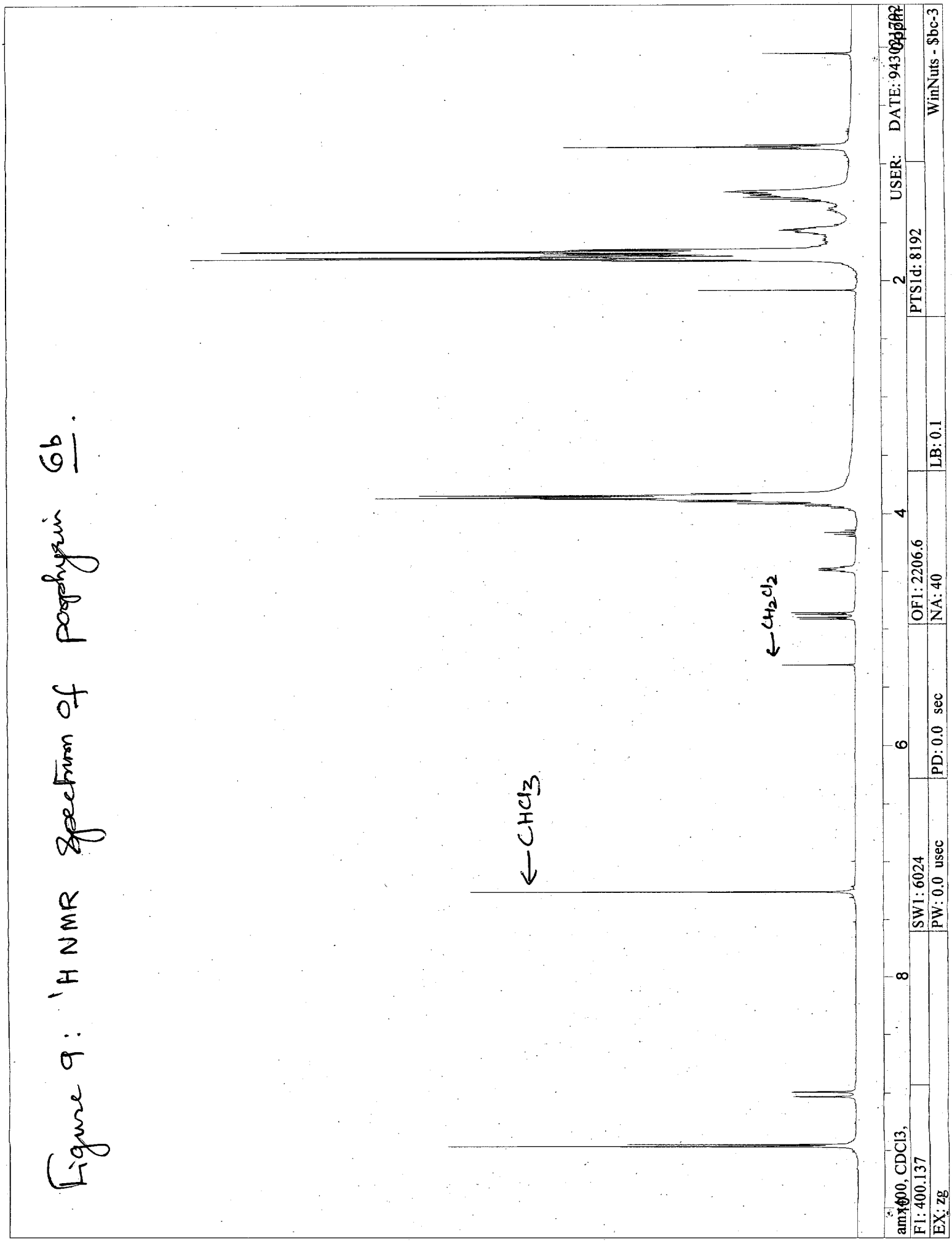


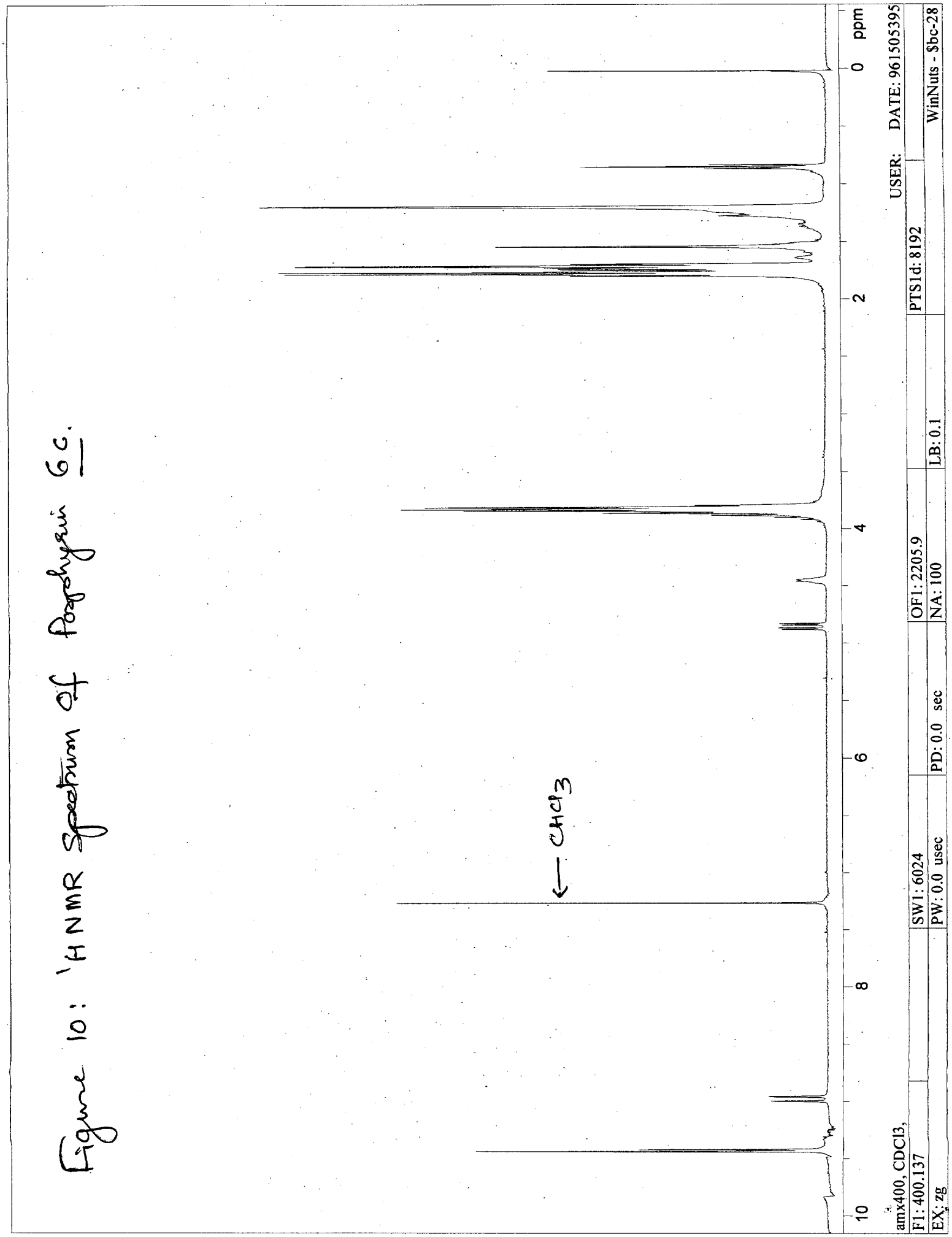
Figure 8: ^{1}HNMR spectrum of porphyrin 6a

Figure 9: ^{1}H NMR Spectrum of porphyrin 6b.



© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 12

Figure 10: ^{1}H NMR Spectrum of Porphyrin 6c.



© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 13

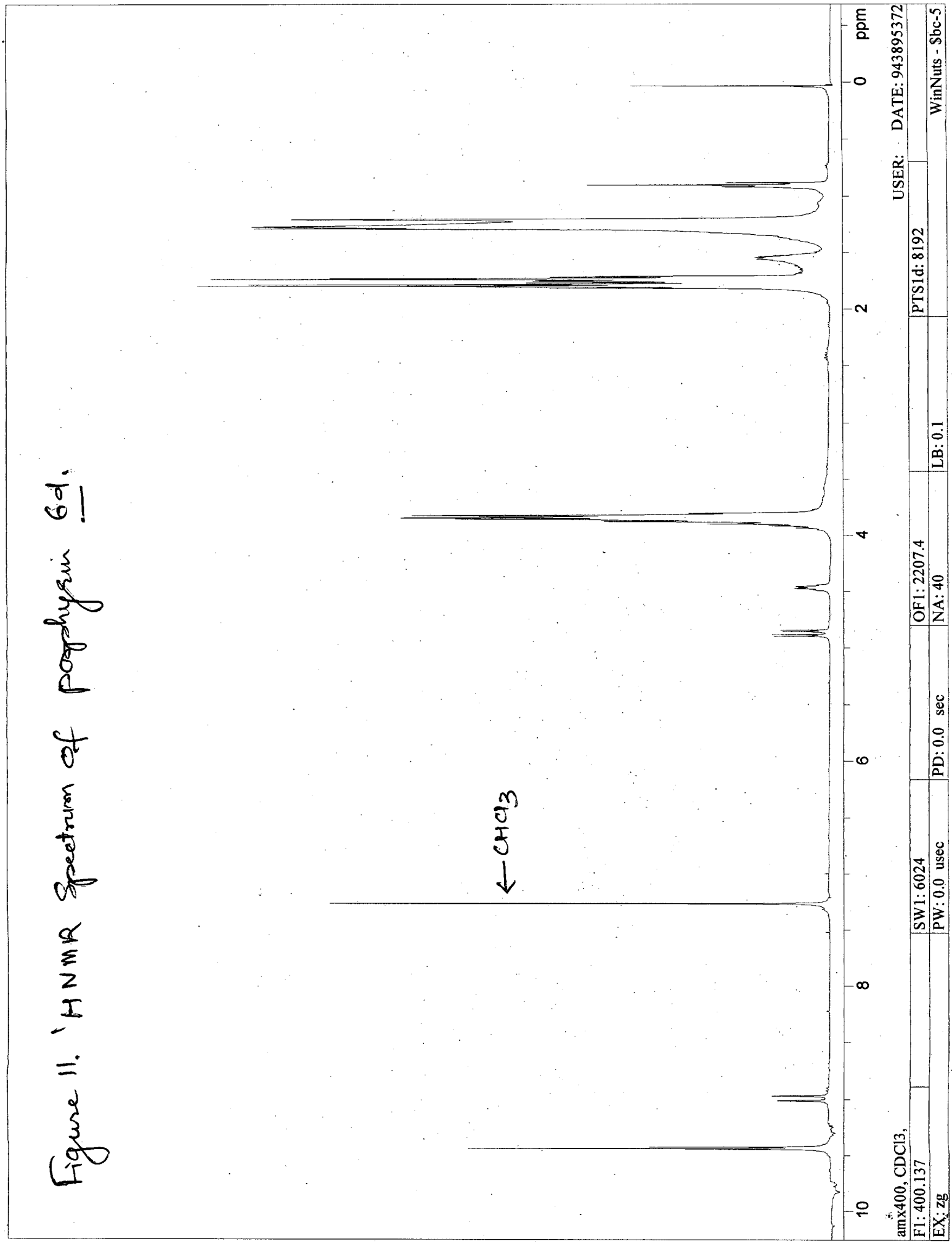


Figure 11. ^{1}HNMR Spectrum of Porphyrin 6d.

© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 14

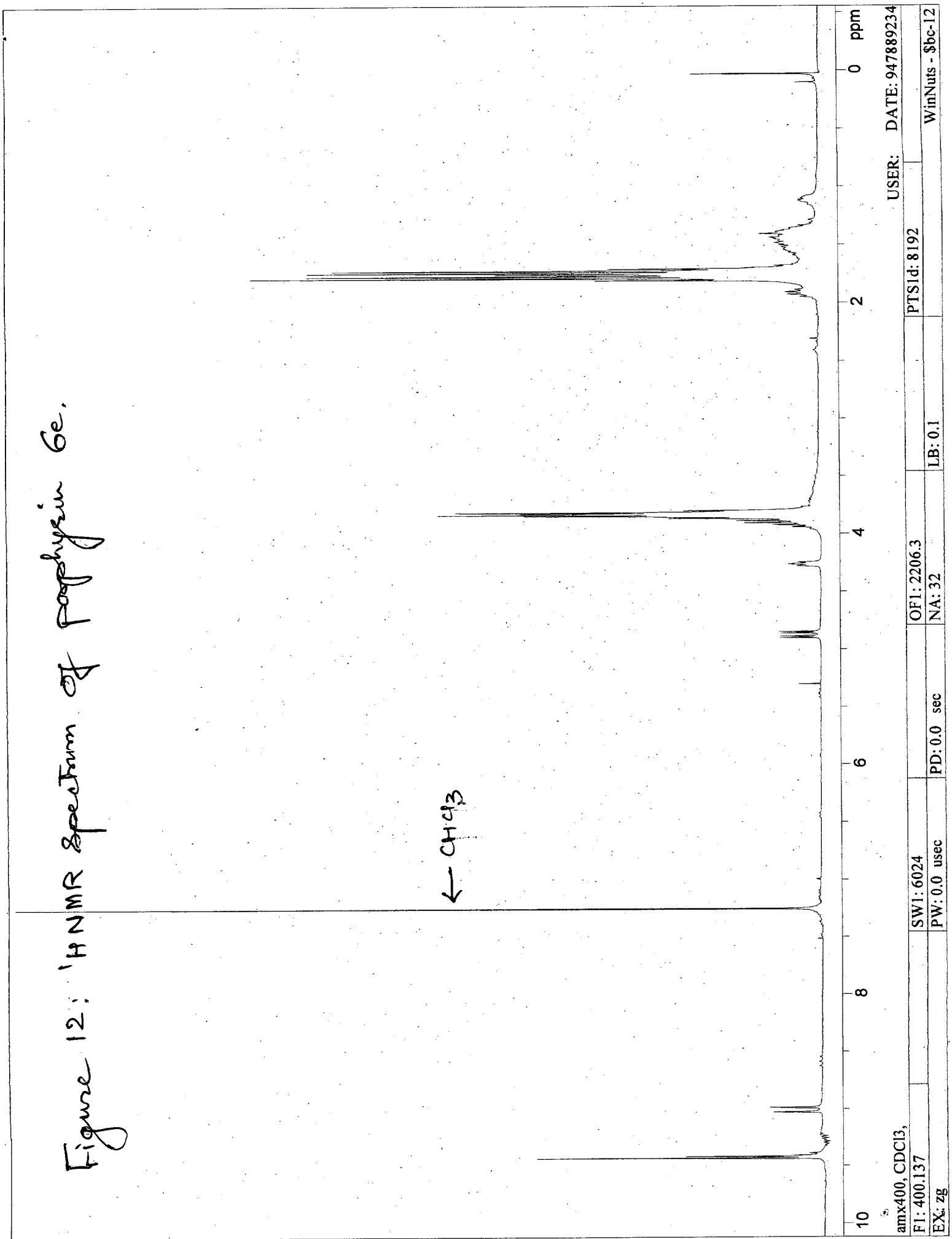
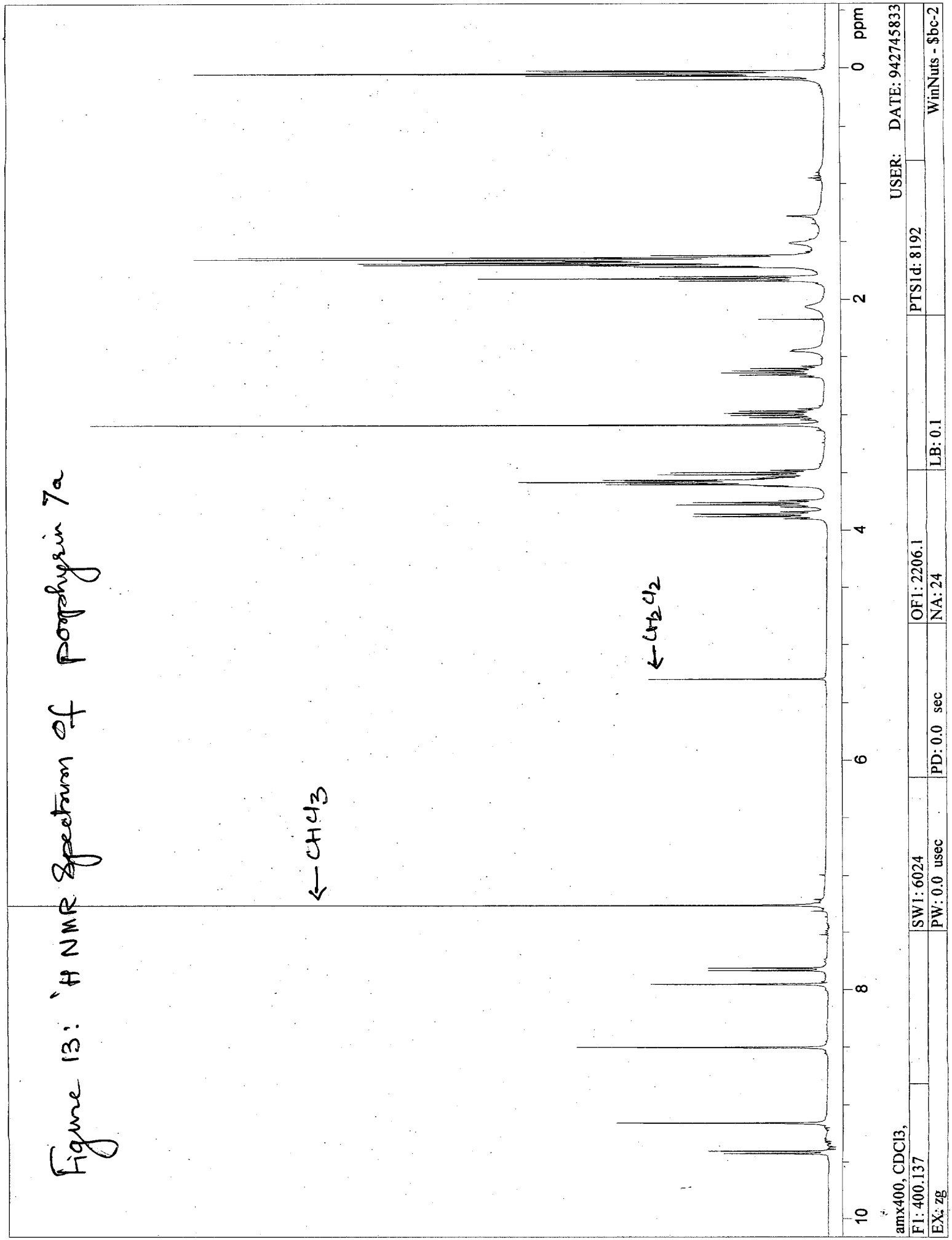


Figure 12: ^{1}H NMR spectrum of Porphyrin 6e.

© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 15



© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 16

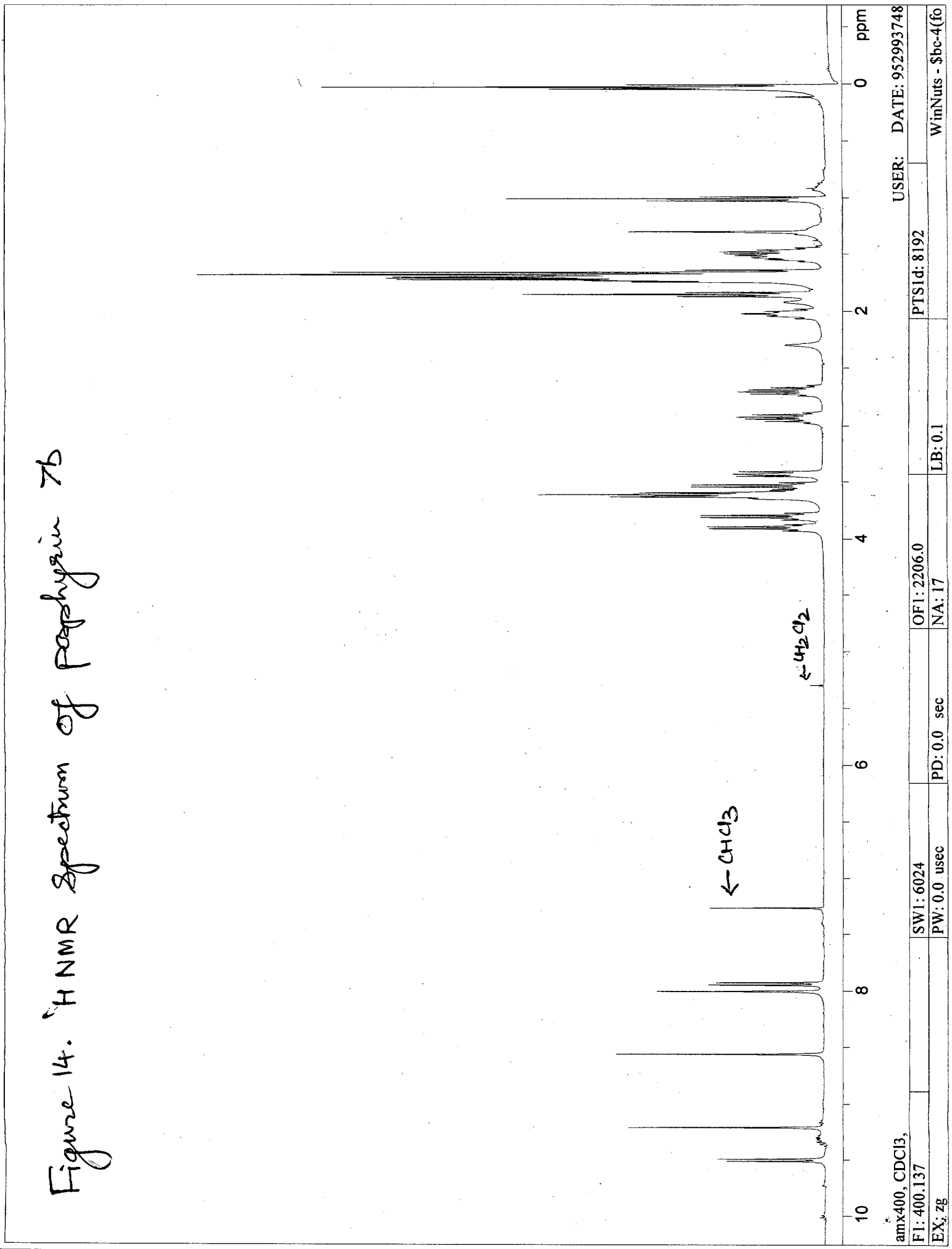


Figure 14. ^{1}H NMR Spectrum of Porphyrin 7b

© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 17

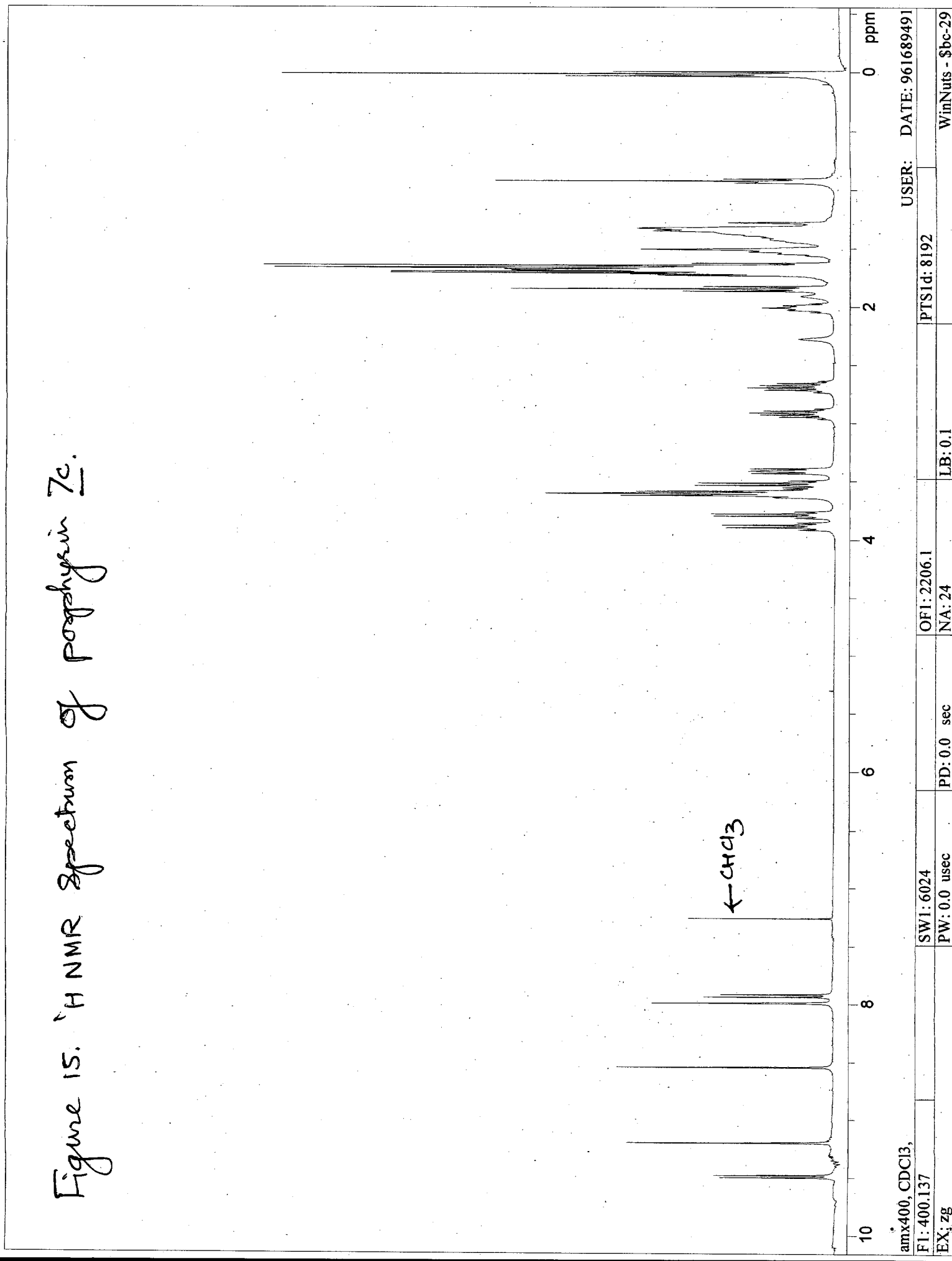


Figure 15. ^{1}H NMR Spectrum of porphyrin 7c.

© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 18

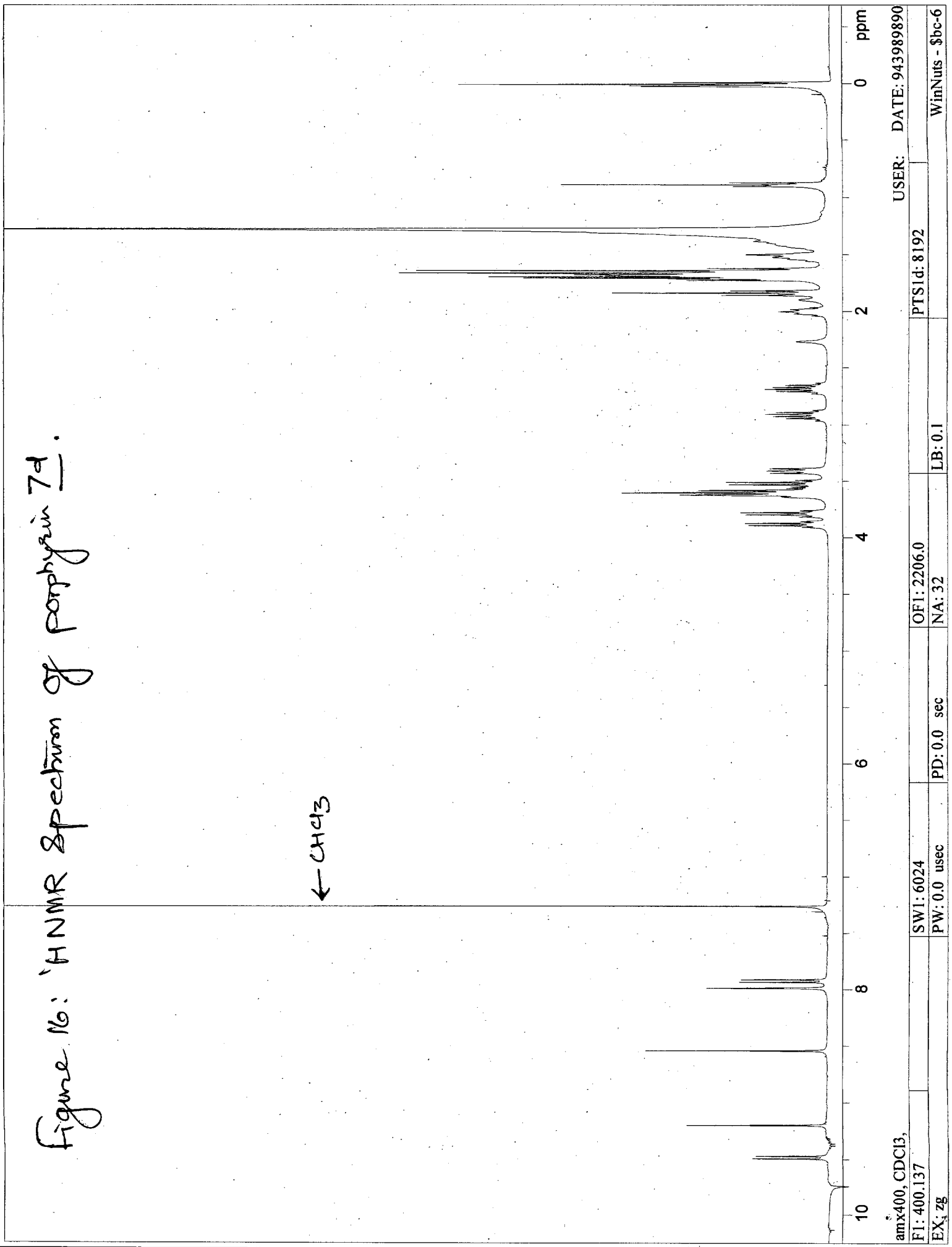


Figure 16: ^{1}H NMR Spectrum of Porphyrin 7d.

© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 19

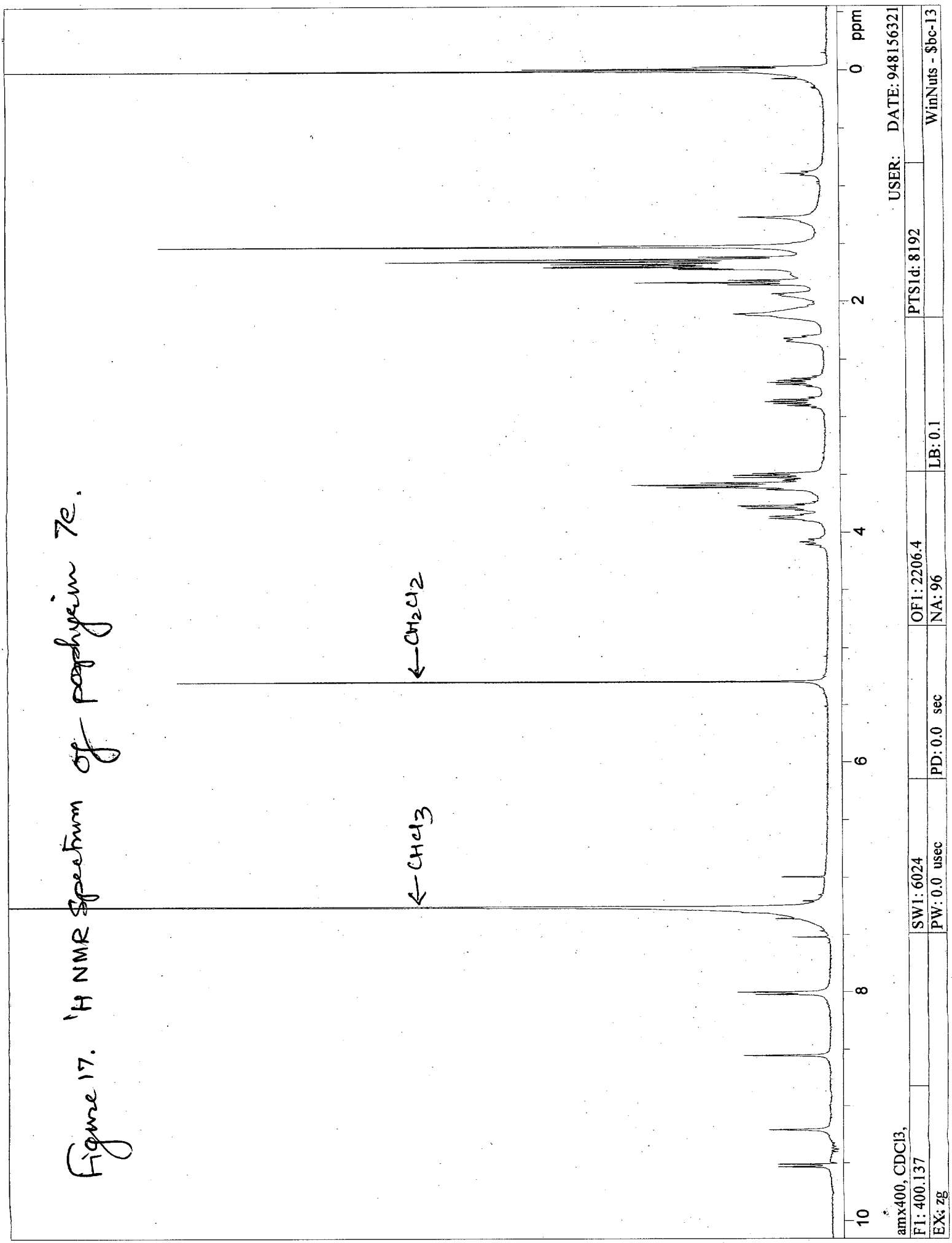


Figure 17. ^1H NMR spectrum of porphycin 7e.

© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 20

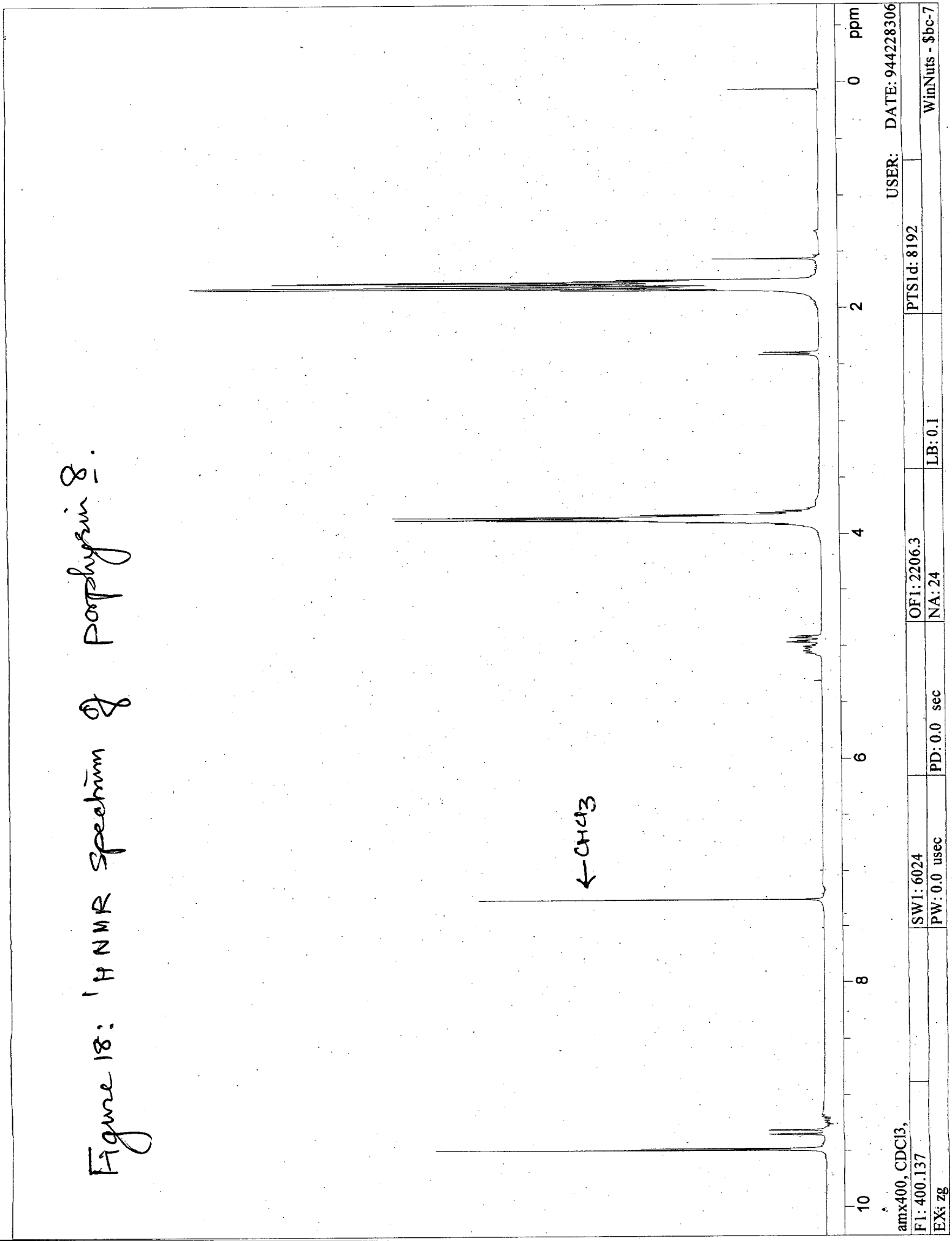


Figure 18: ^{1}H NMR spectrum of Porphyrin 8.

© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 21

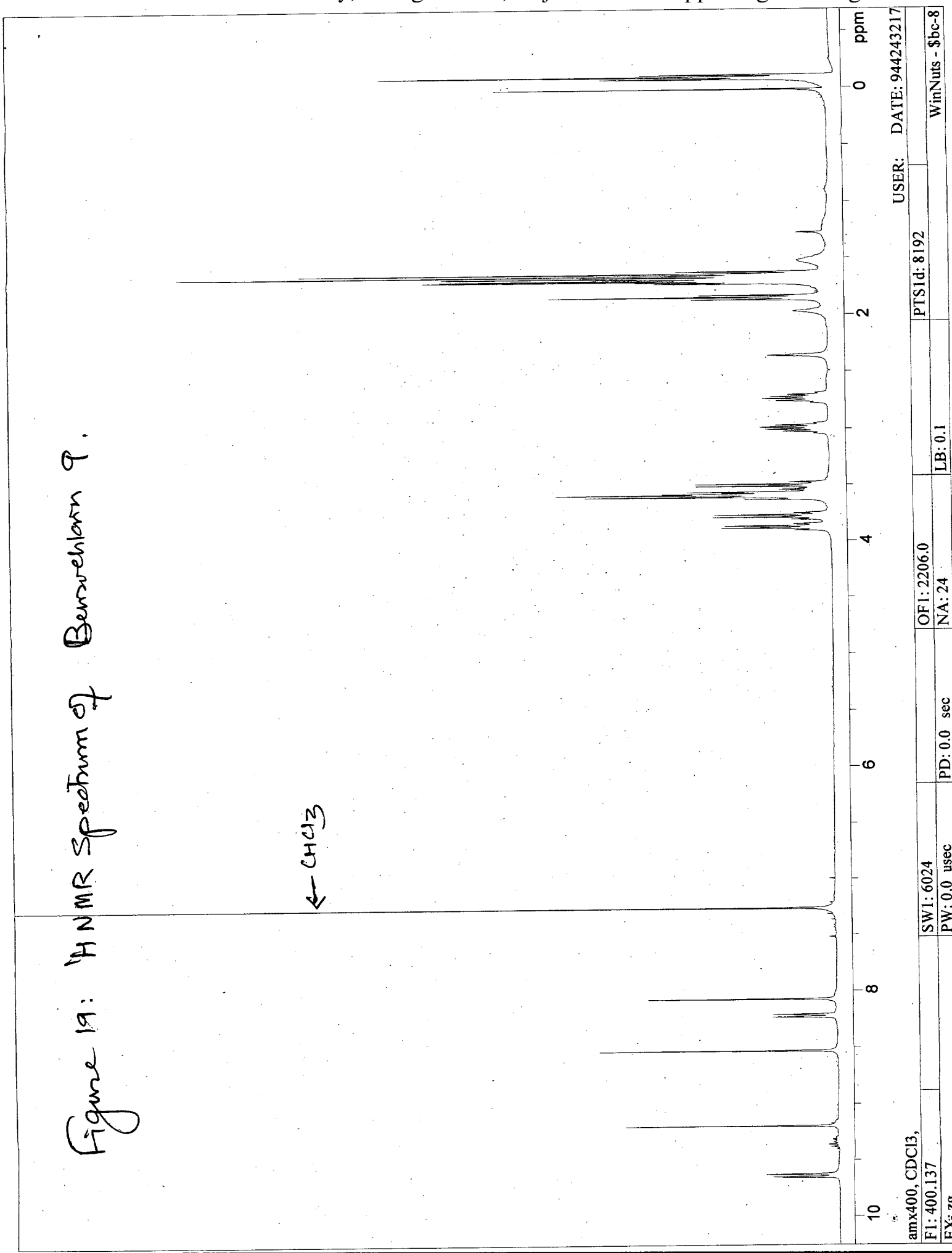


Figure 19: ^{1}H NMR Spectrum of Benzenlam 9.

© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 22

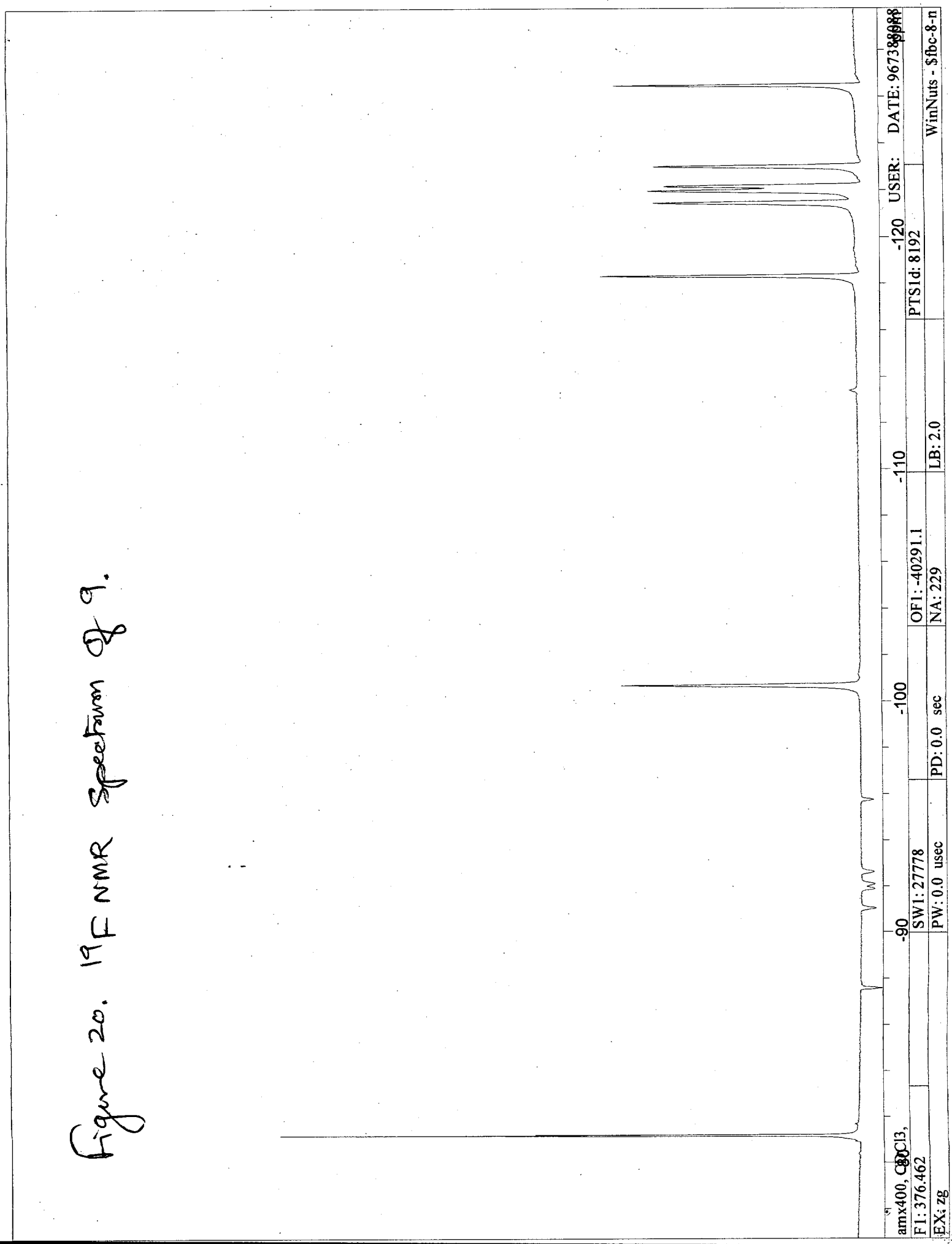
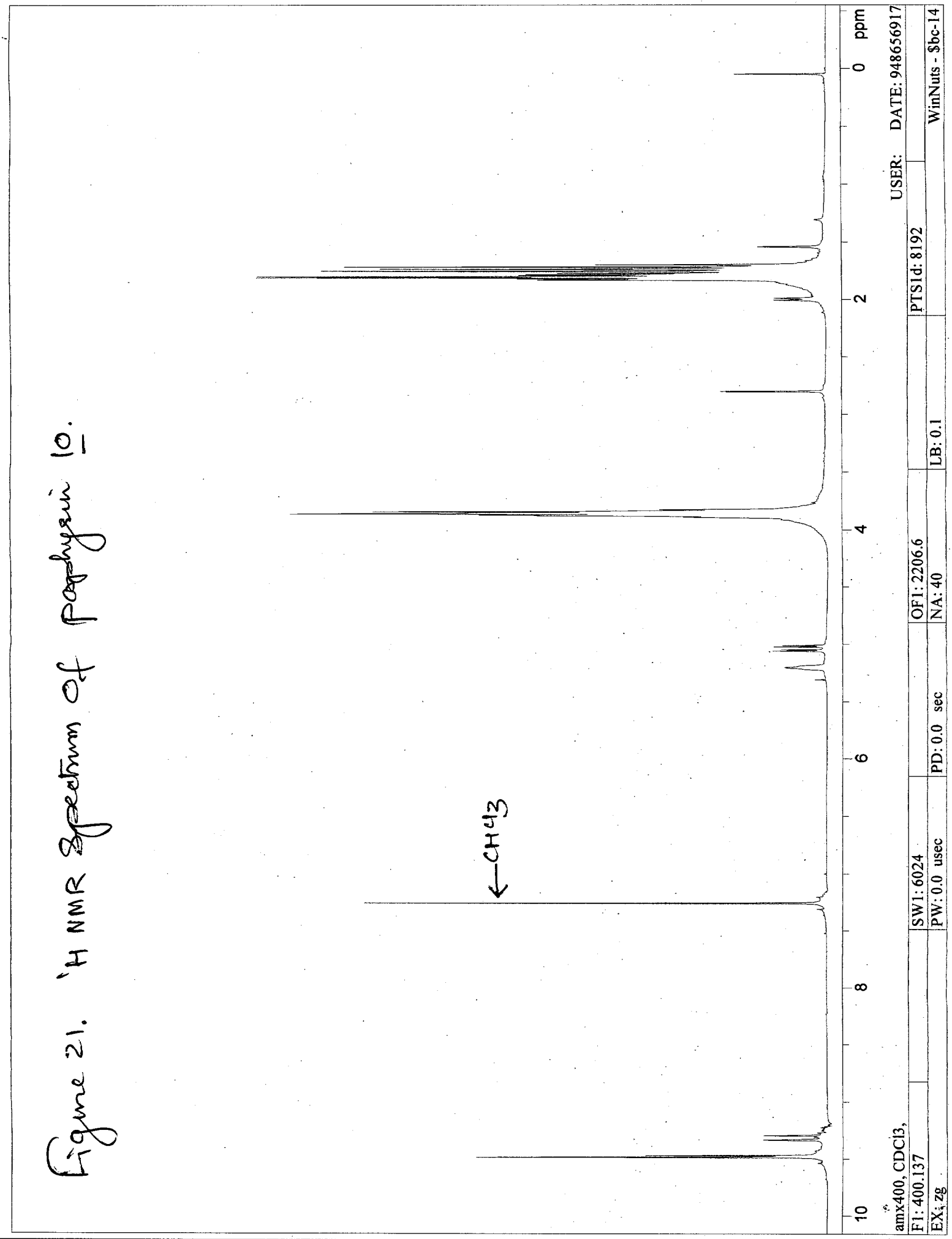


Figure 20. ^{19}F NMR Spectrum of 9.

© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 23

Figure 21. ^{1}H NMR Spectrum of Pogbyzii 10.



© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 24

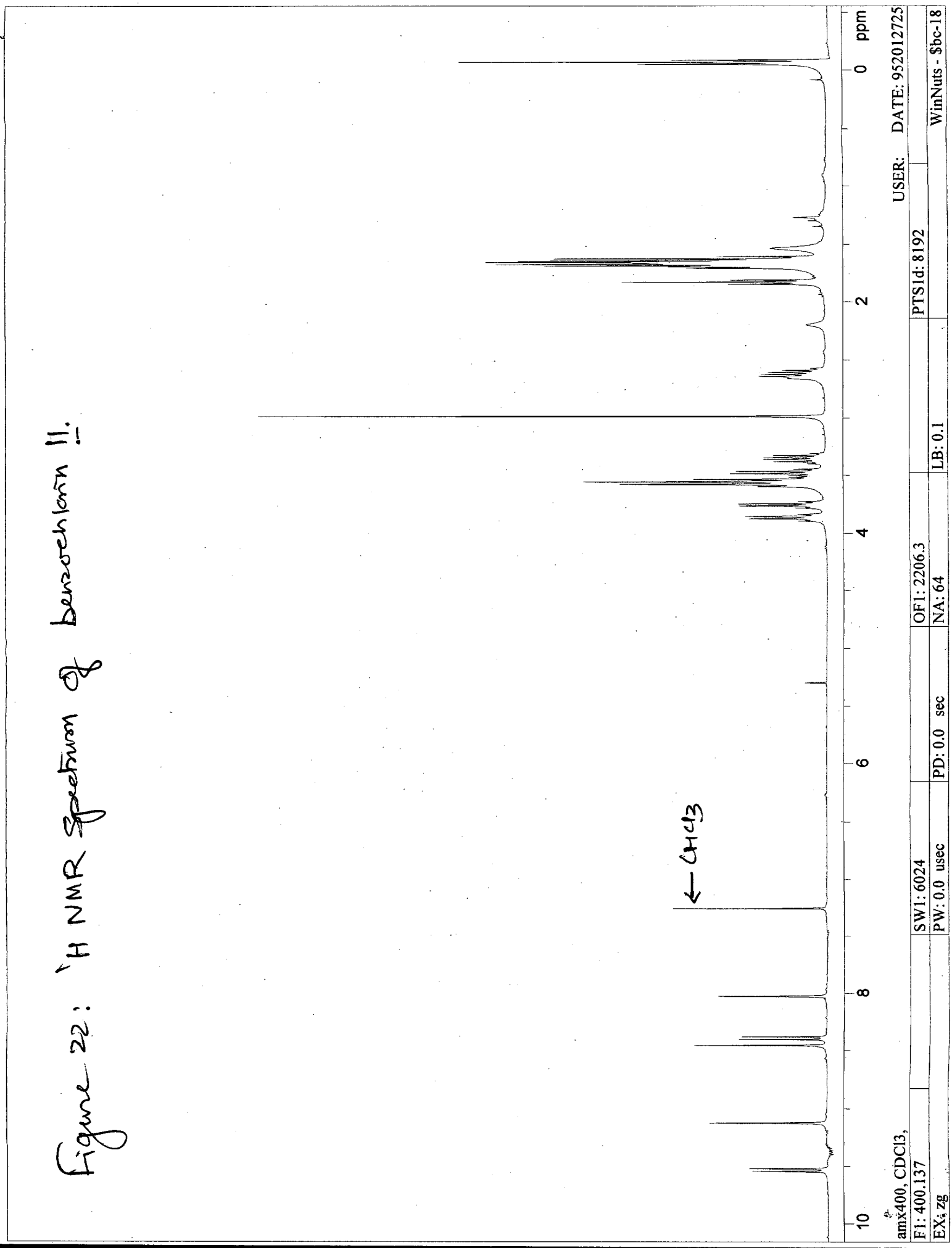


Figure 22: ^{1}H NMR Spectrum of benzenlorin II.

© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 25

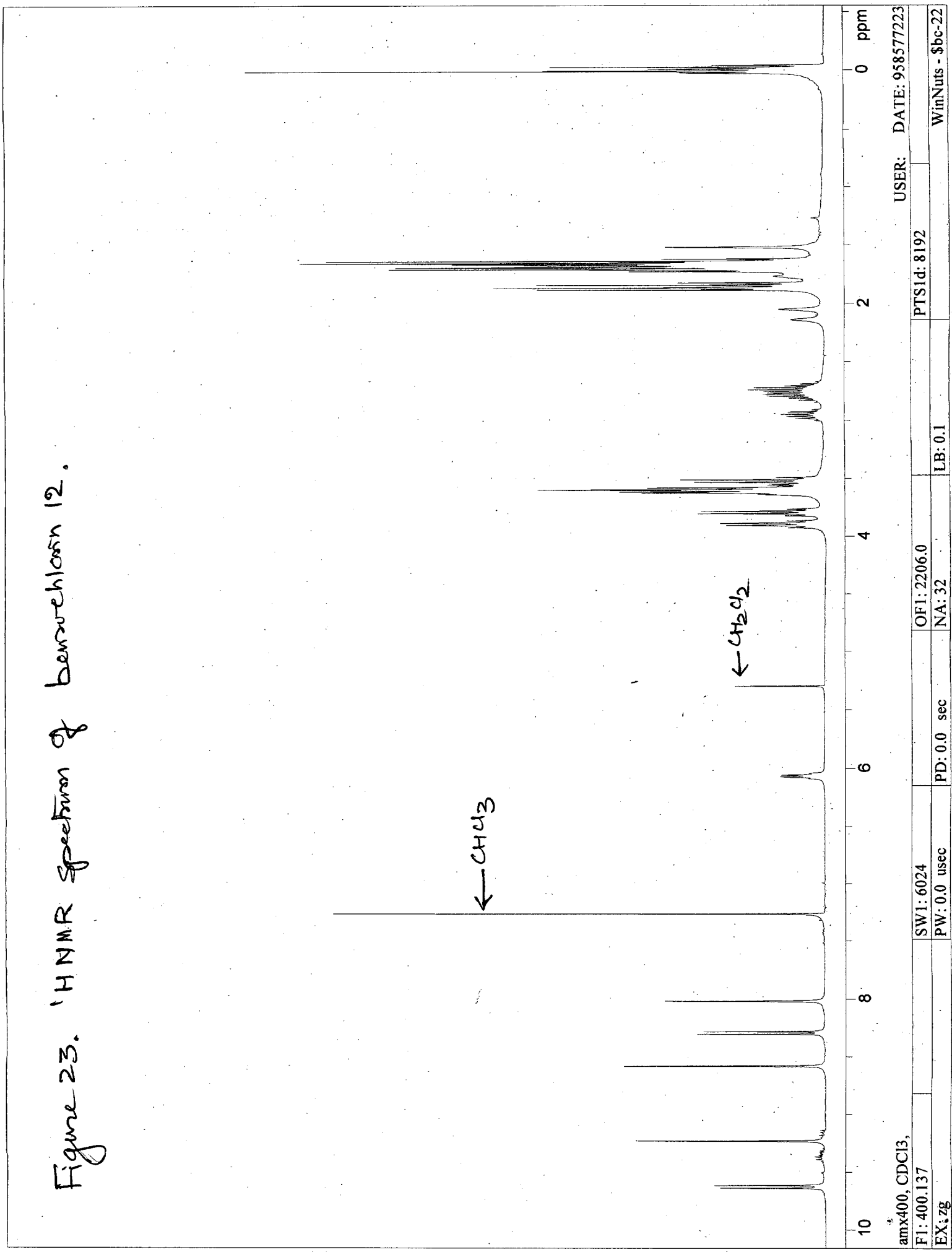


Figure 23. ^1H NMR spectrum of benzochloran 12.

© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 26

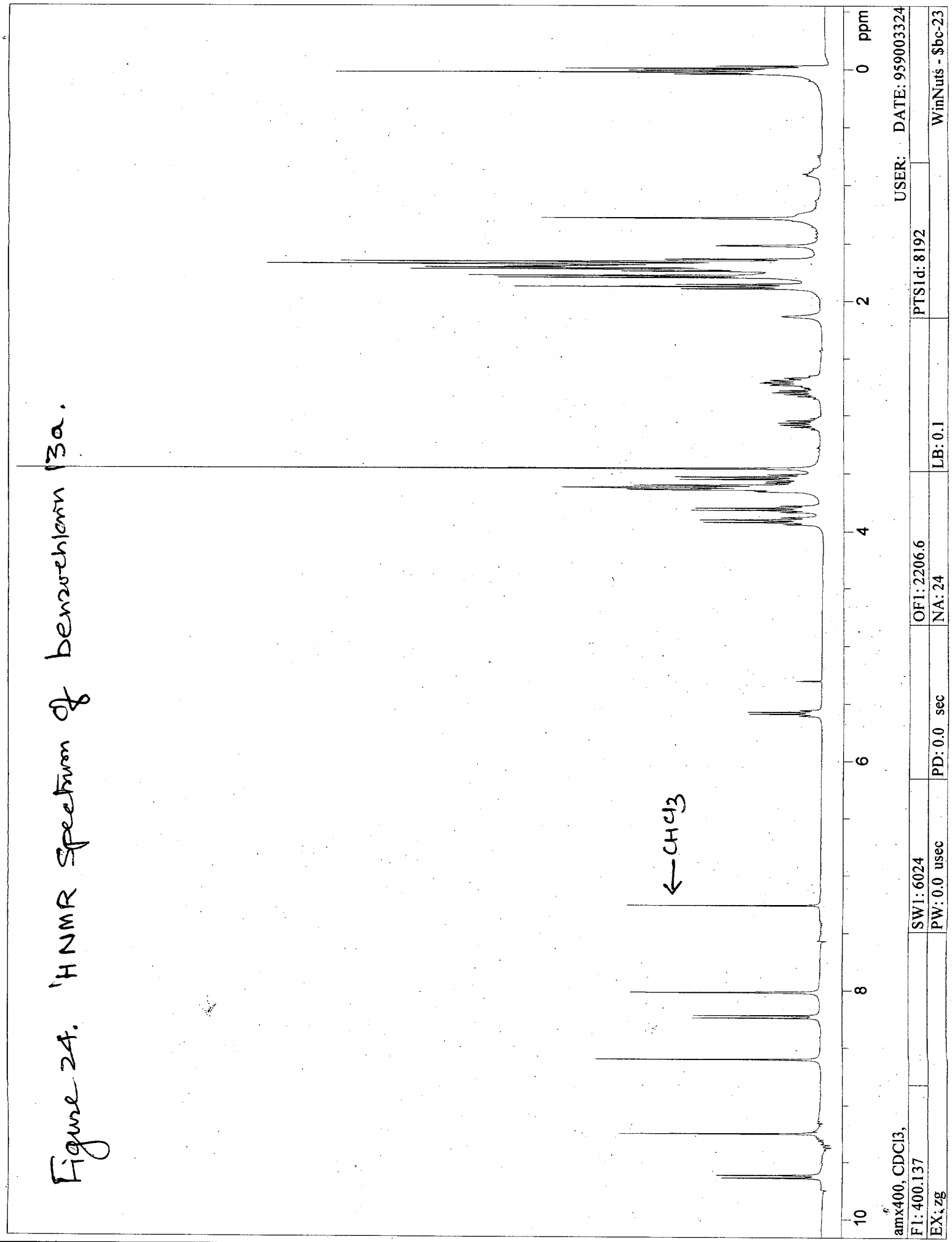
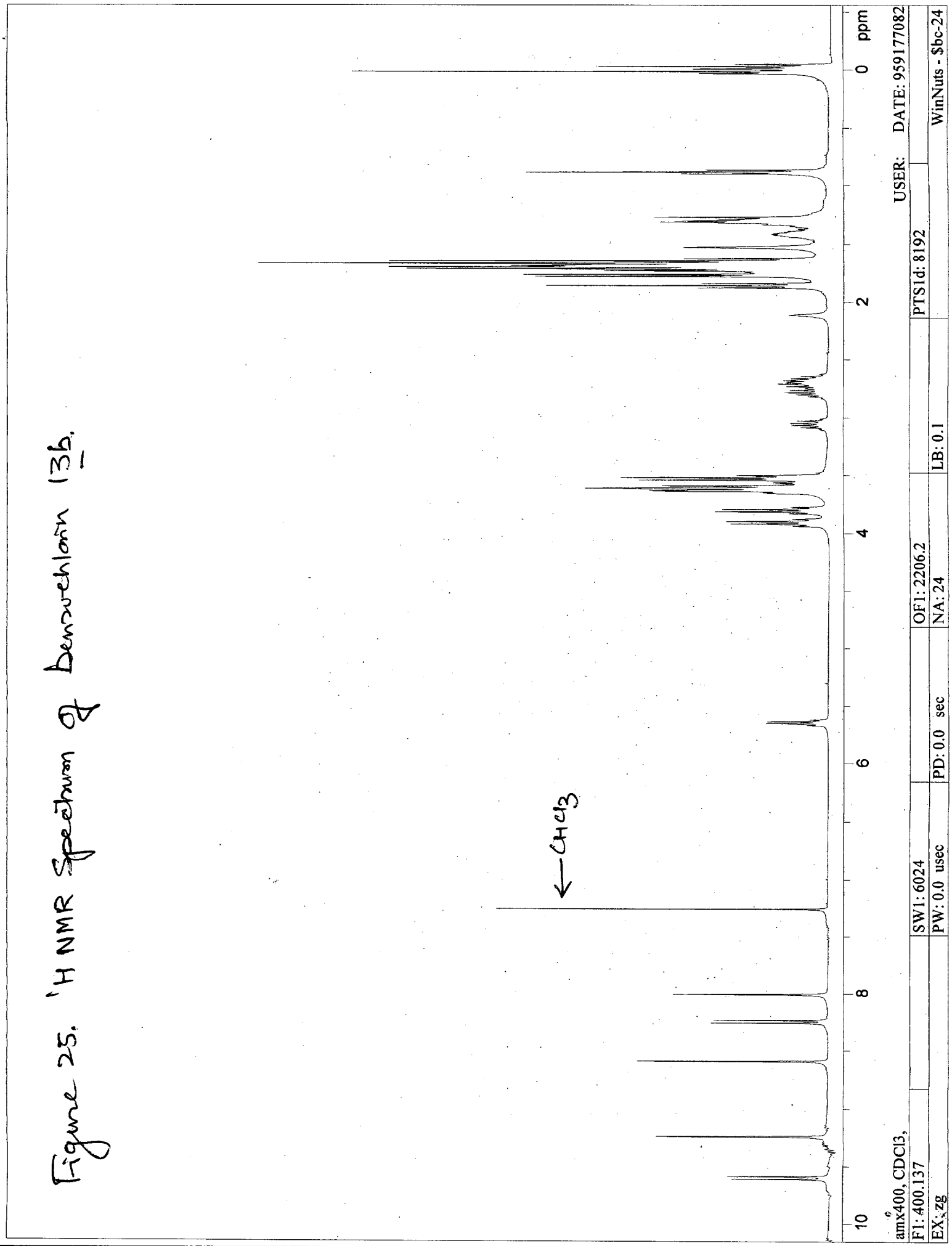


Figure 24. ^{1}H NMR Spectrum of benzothiazole 13a.

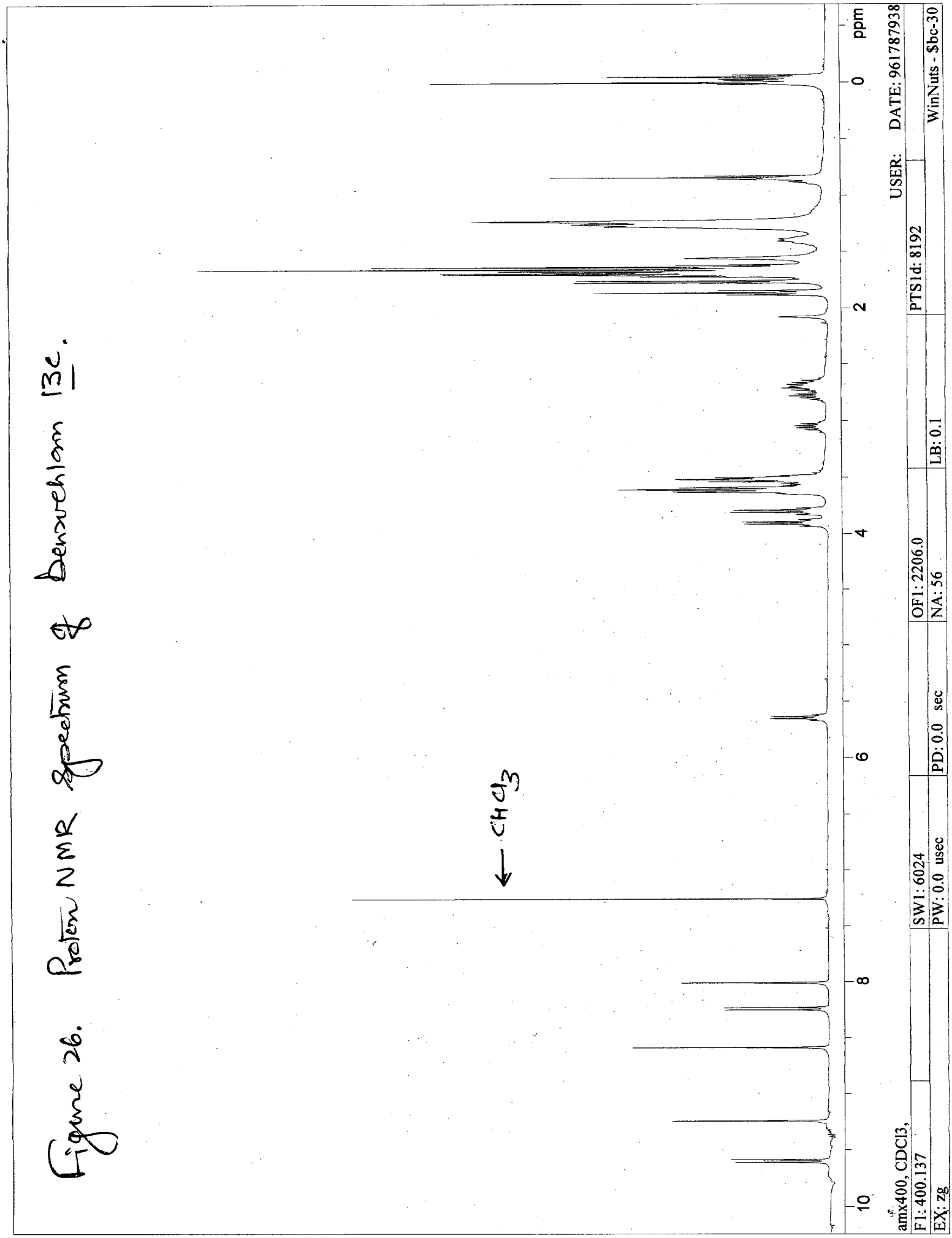
© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 27

Figure 25. ^{1}H NMR Spectrum of Benzochlorin 13b.

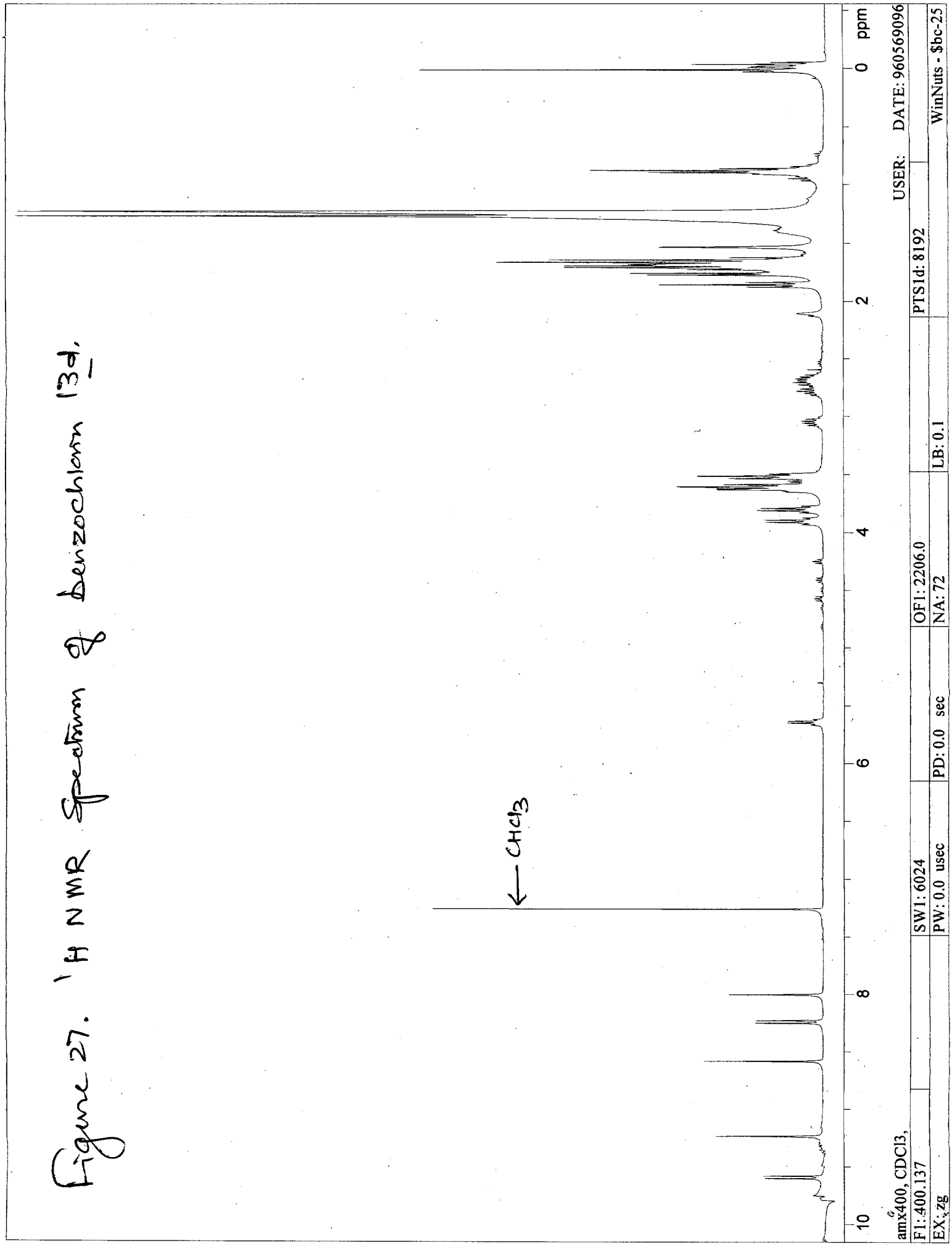


© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 28

Figure 26. Proton NMR spectrum of Benzochlam 13c.



© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 29



© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 30

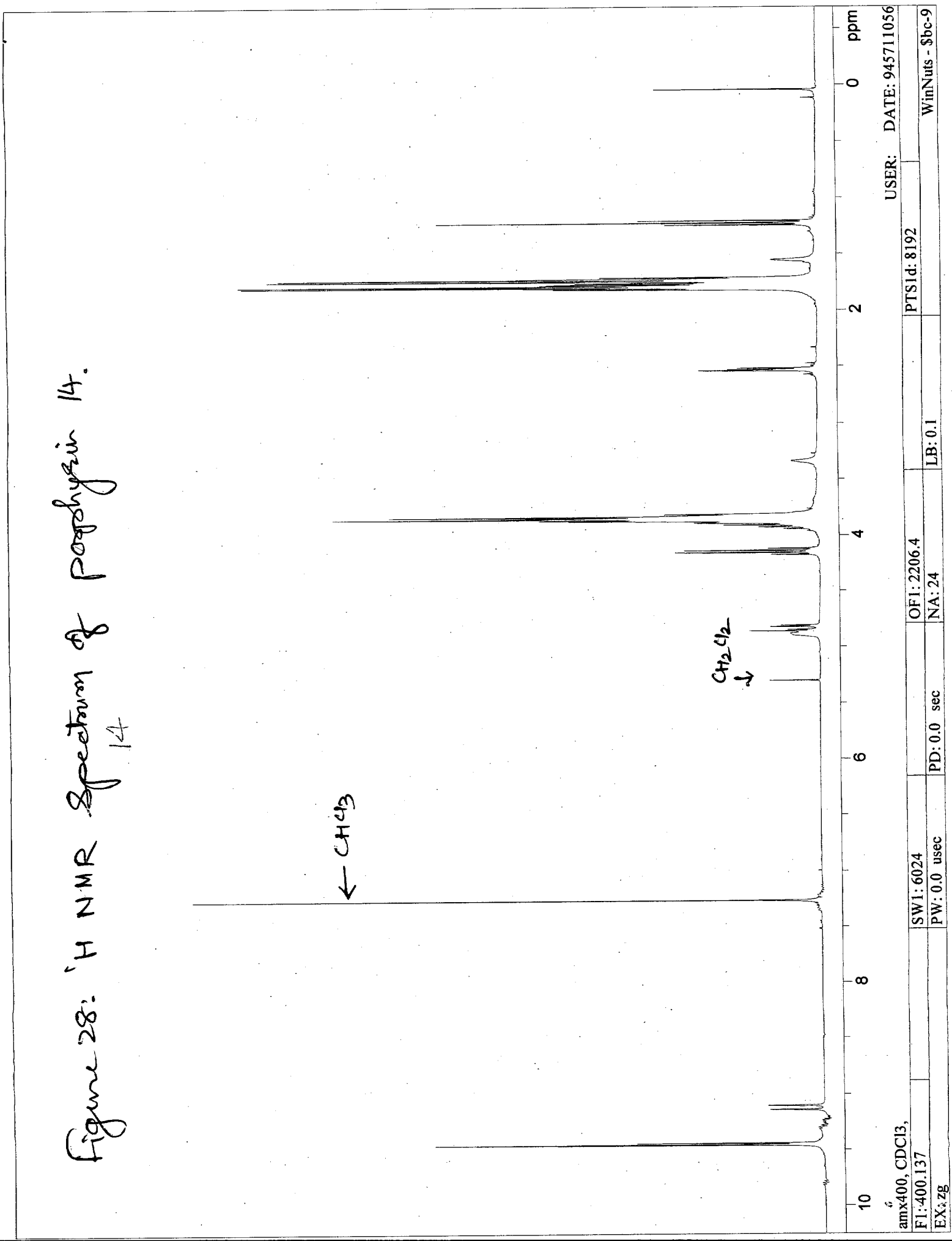
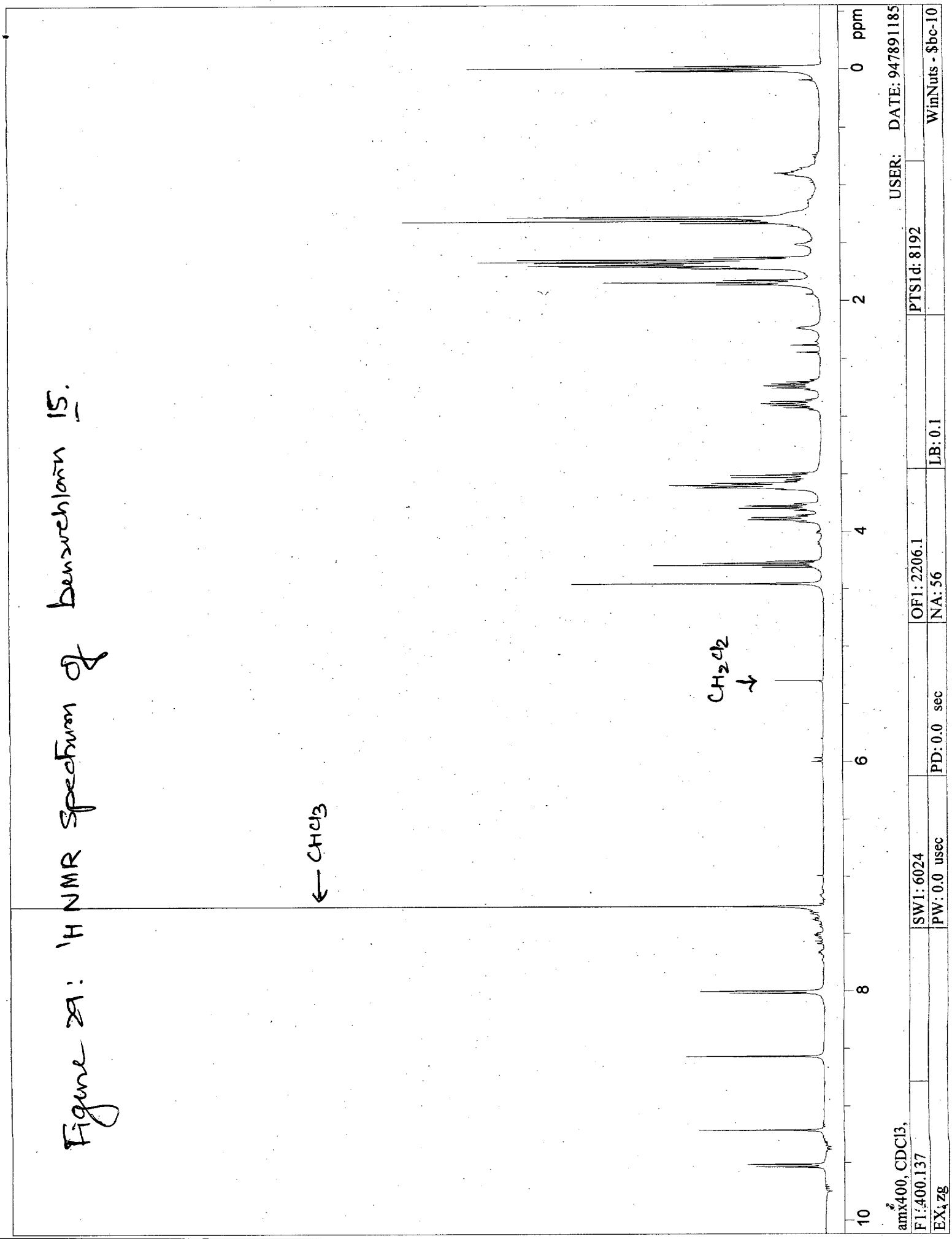


Figure 28: ^1H NMR Spectrum of porphyrin 14.
14

© 2001 American Chemical Society, J. Org. Chem., Li jo001541+ Supporting Info Page 31

Figure 29: ^1H NMR spectrum of benzochlorin 15.



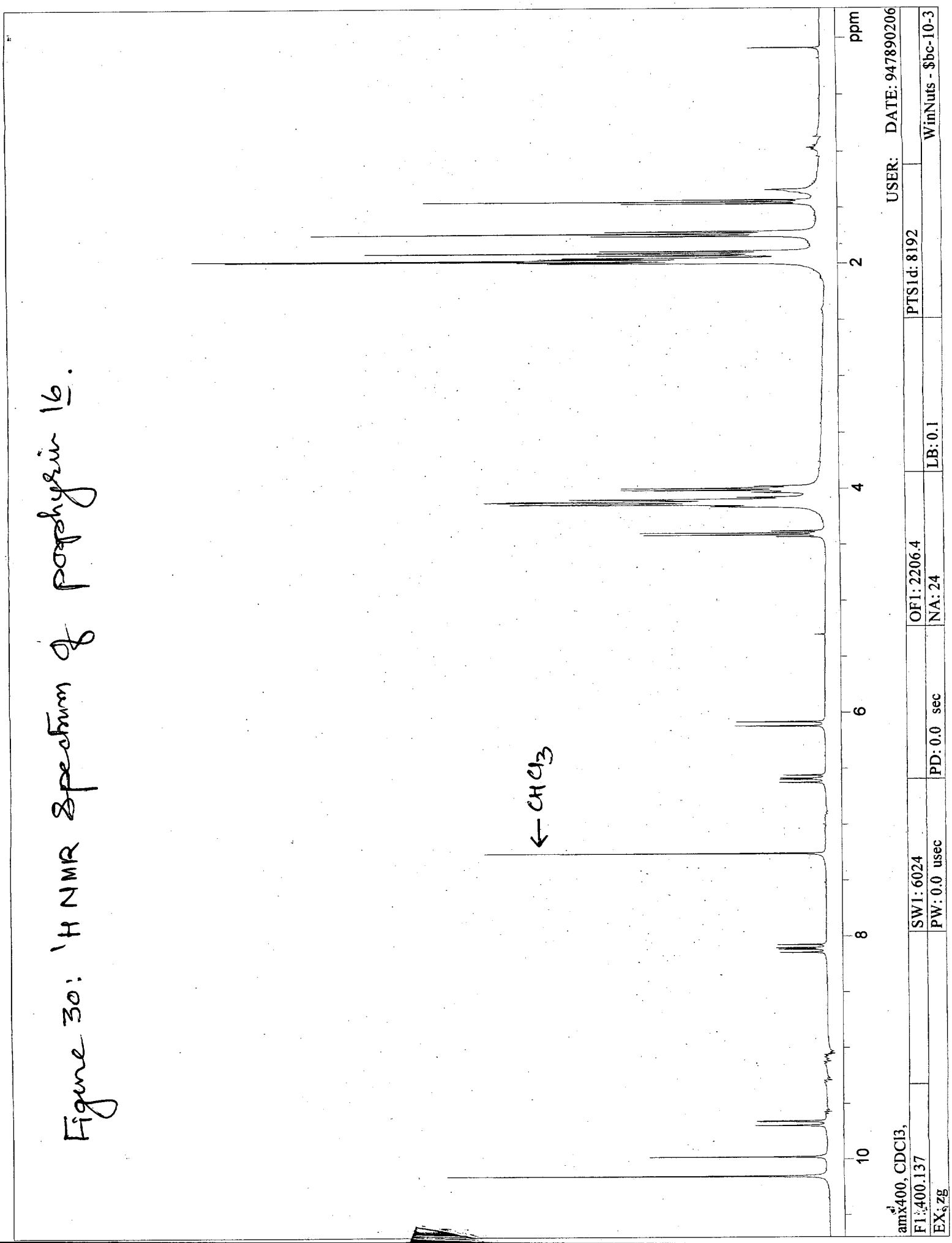


Figure 30: ^{1}H NMR Spectrum of porphyrin 16.