

***N*³-Alkylation during formation of quinazolin-4-ones from condensation of anthranilamides and *ortho*amides**

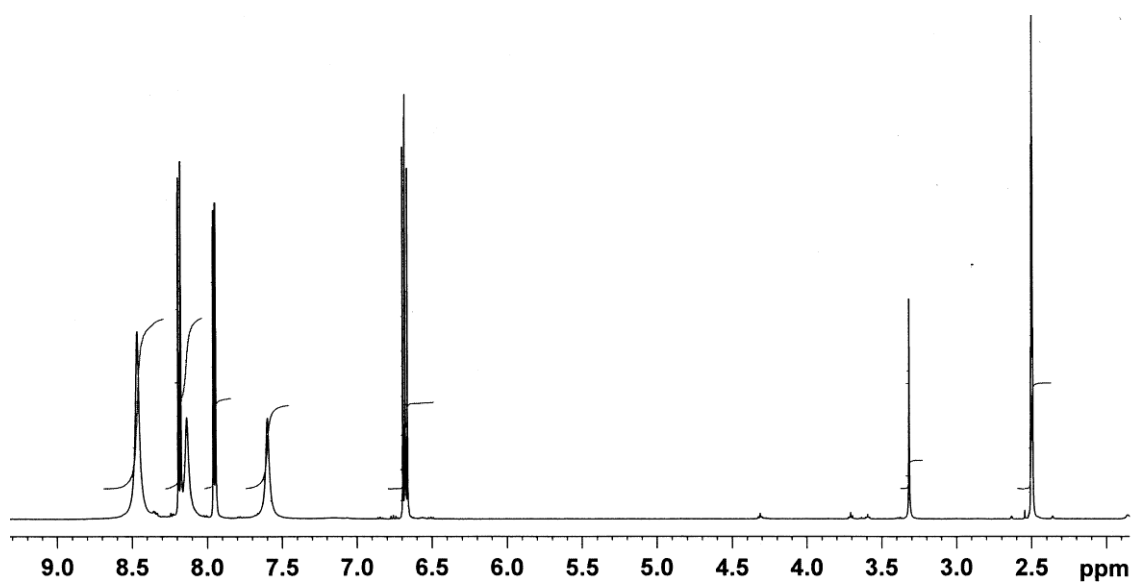
Amit Nathubhai, Richard Patterson, Timothy J. Woodman, Harriet E. C. Sharp, Miranda T. Y. Chui, Hugo H. K. Chung, Stephanie W. S. Lau, Jun Zheng, Matthew D. Lloyd, Andrew S. Thompson and Michael D. Threadgill

Medicinal Chemistry, Department of Pharmacy & Pharmacology, University of Bath, Claverton Down, Bath BA2 7AY, UK

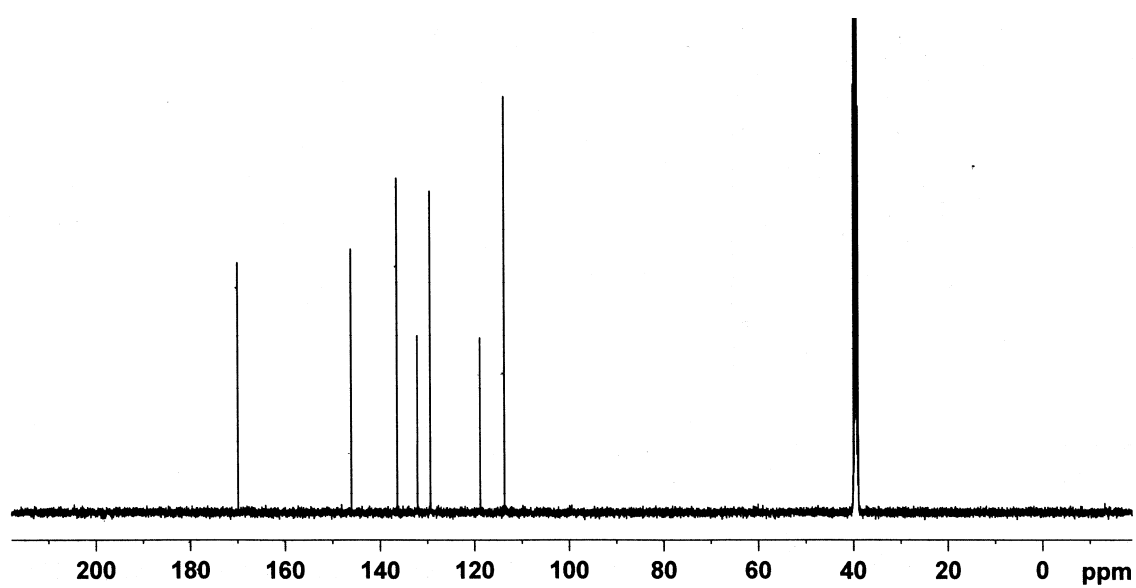
ELECTRONIC SUPPLEMENTARY INFORMATION

NMR spectra of isolated compounds.	2
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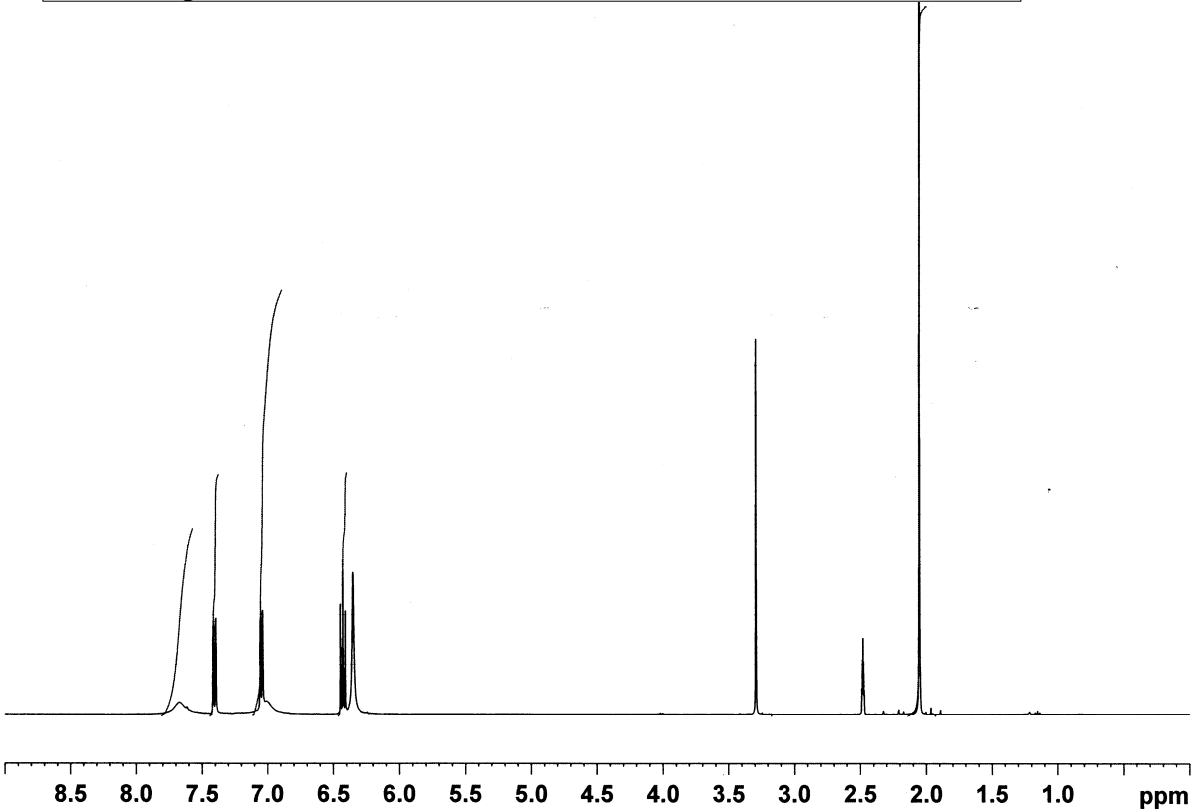
^1H NMR spectrum of 8.



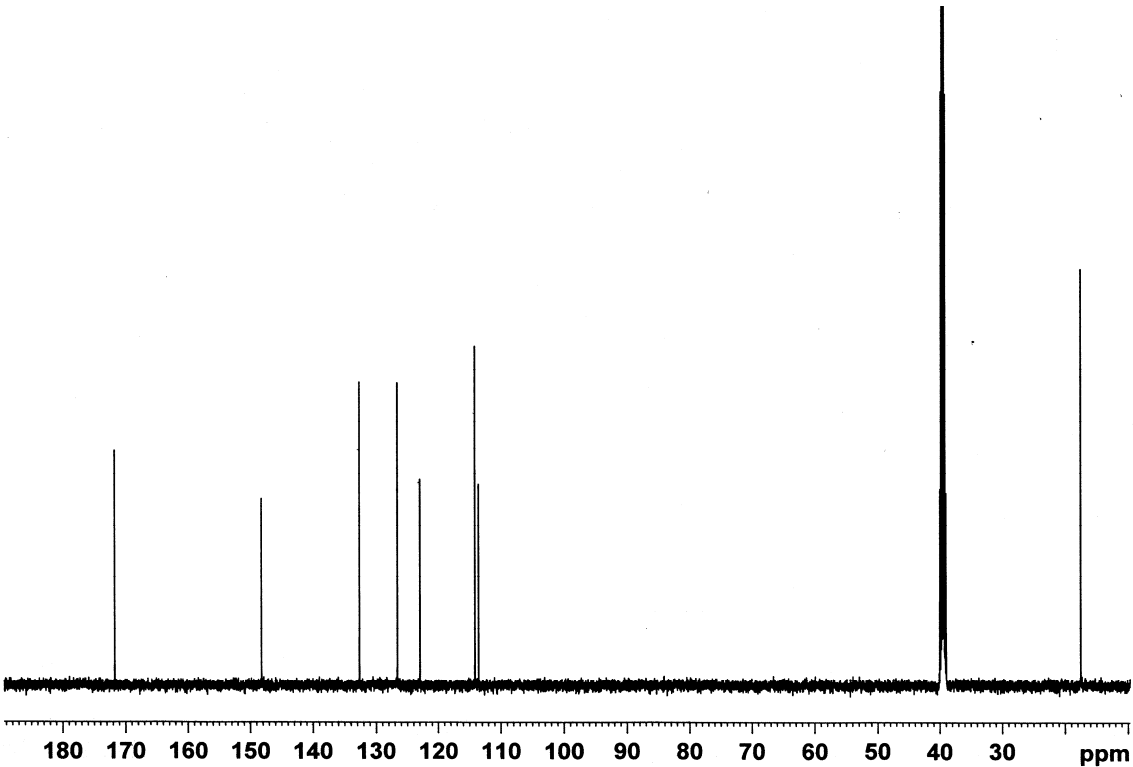
^{13}C NMR spectrum of 8.



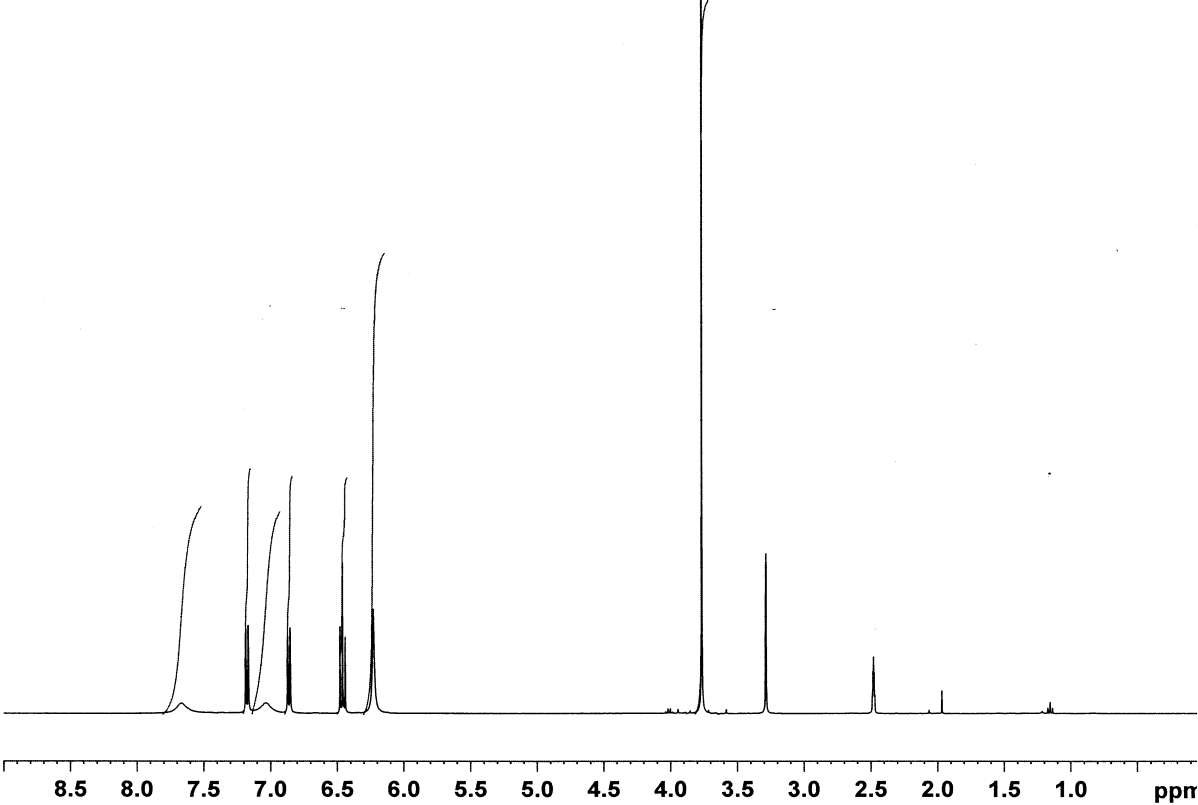
¹H NMR spectrum of 9.



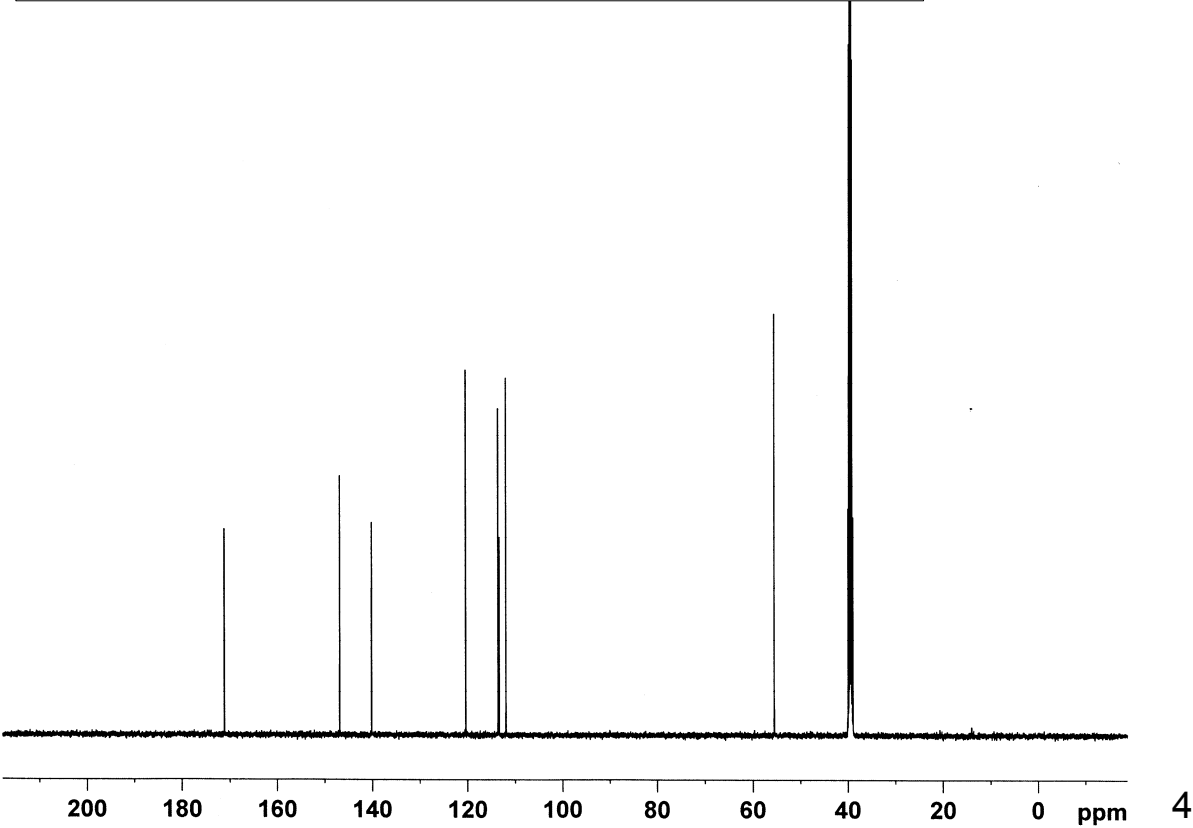
¹³C NMR spectrum of 9.

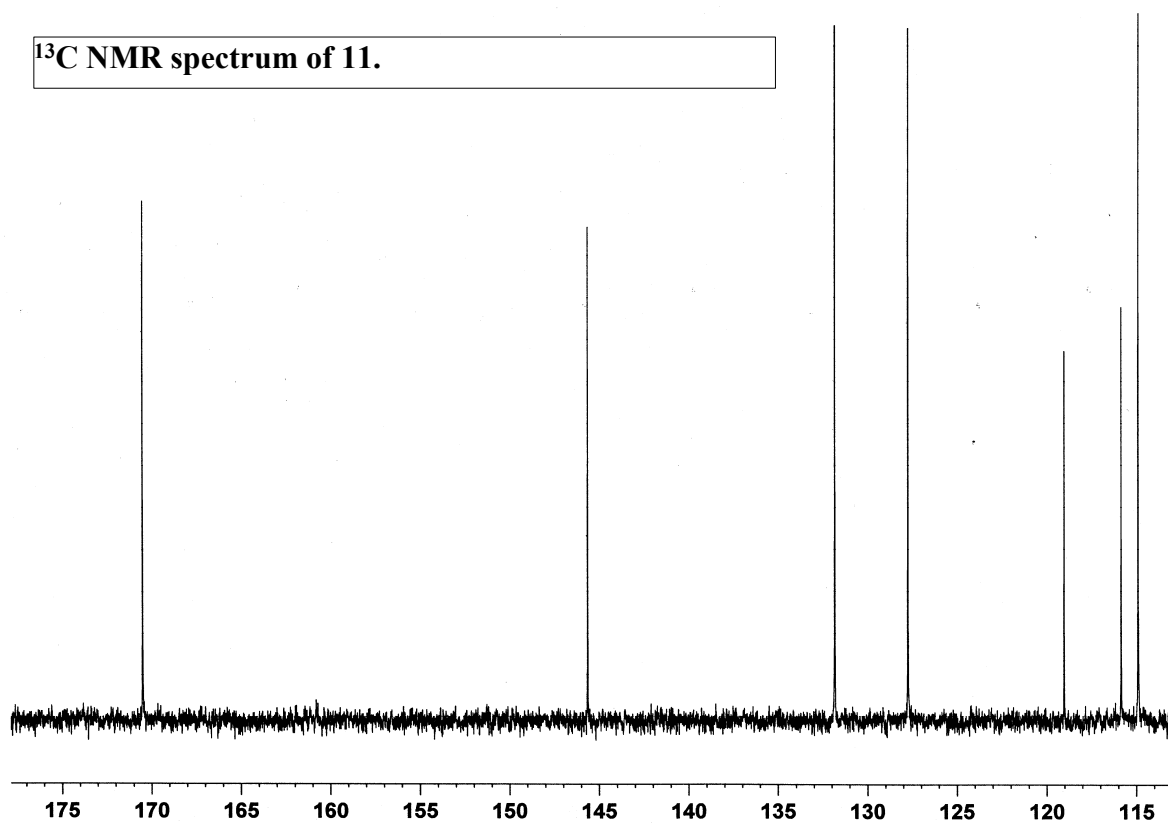
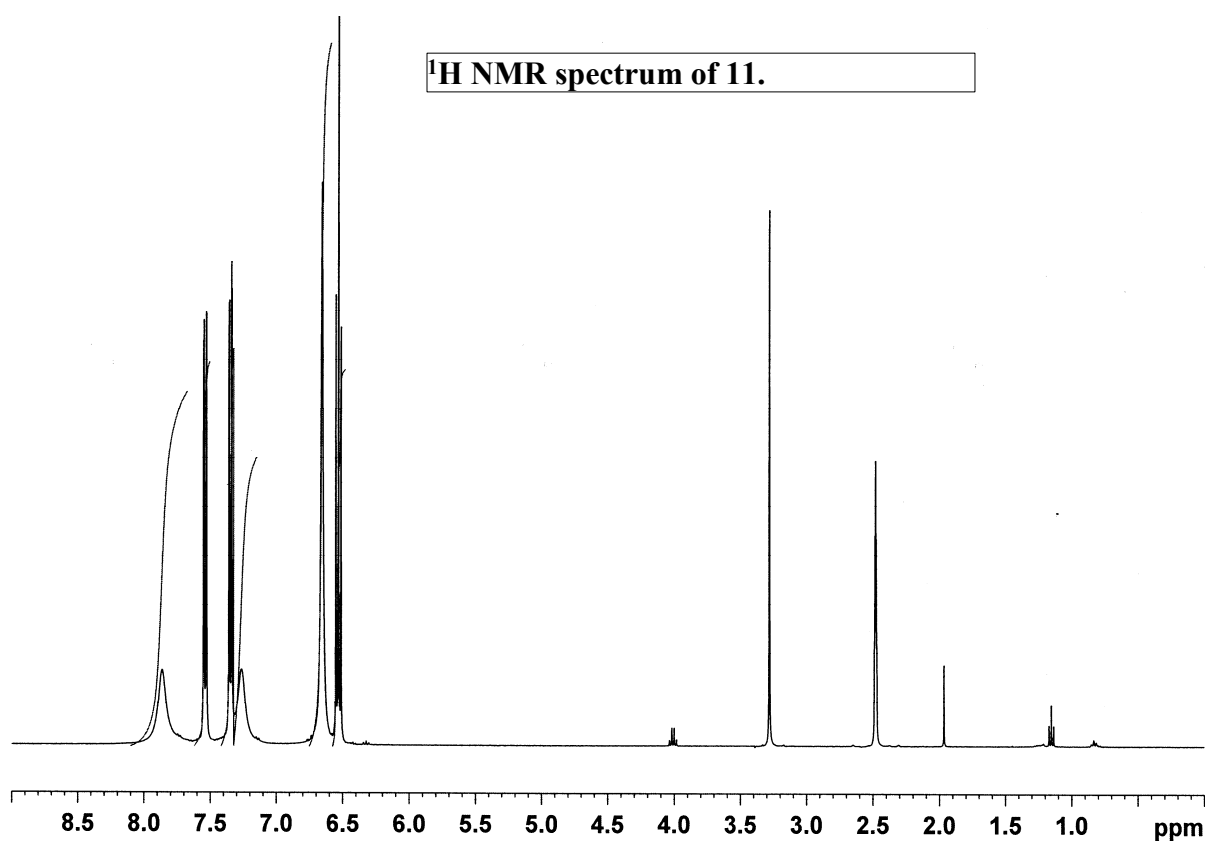


¹H NMR spectrum of 10.

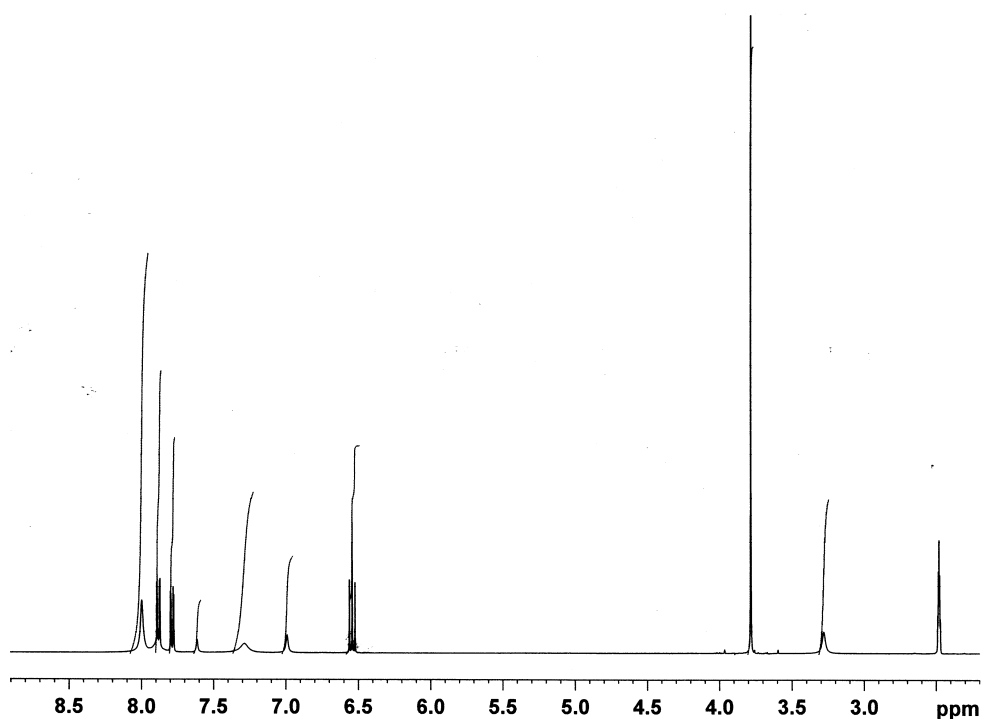


¹³C NMR spectrum of 10.

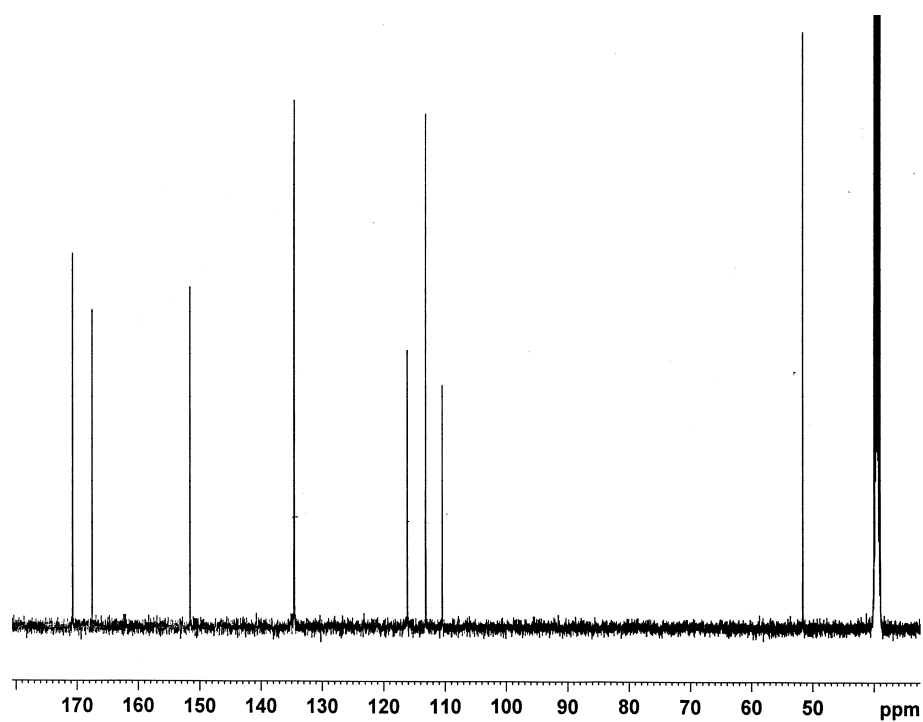




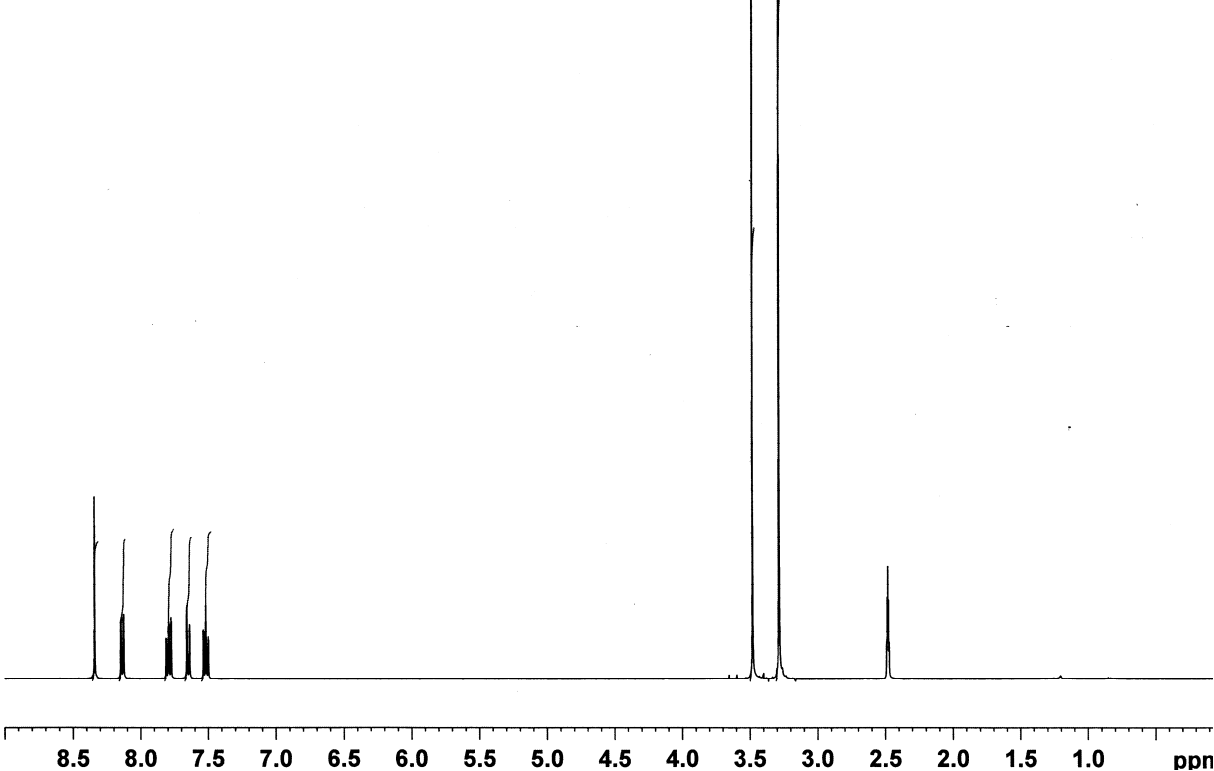
^1H NMR spectrum of 12.



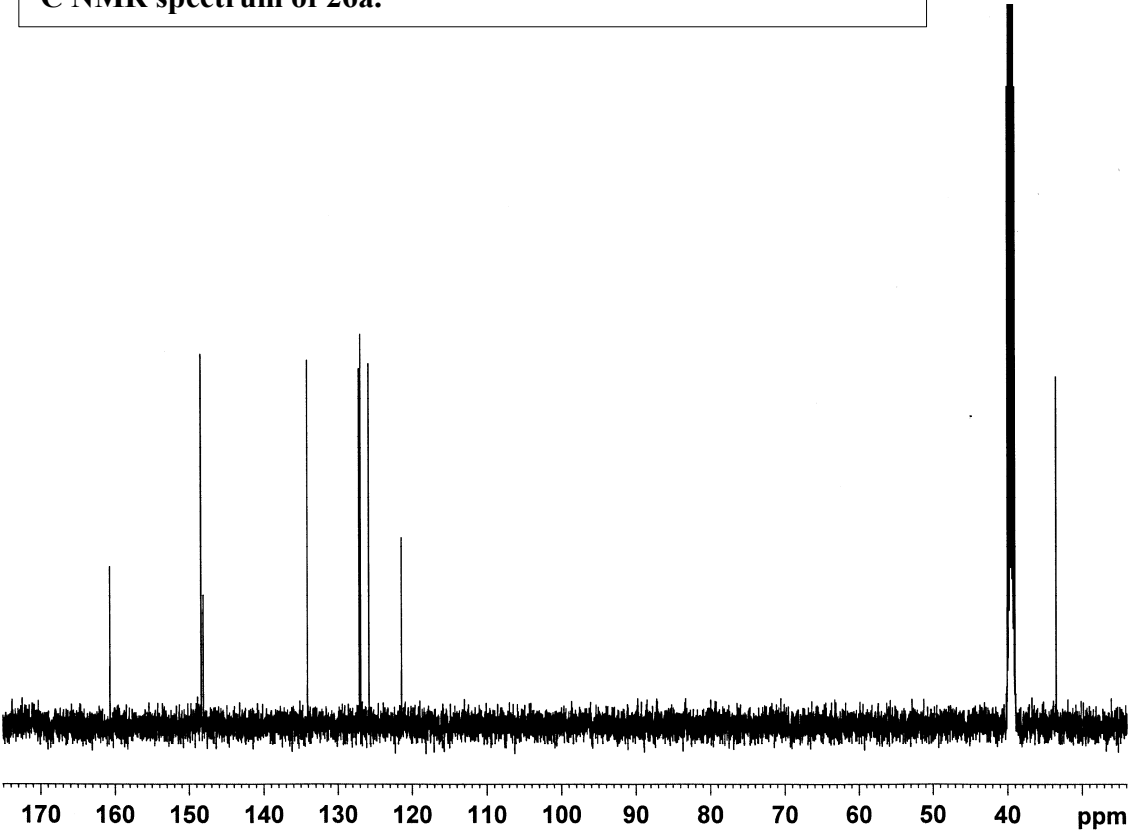
^{13}C NMR spectrum of 12.



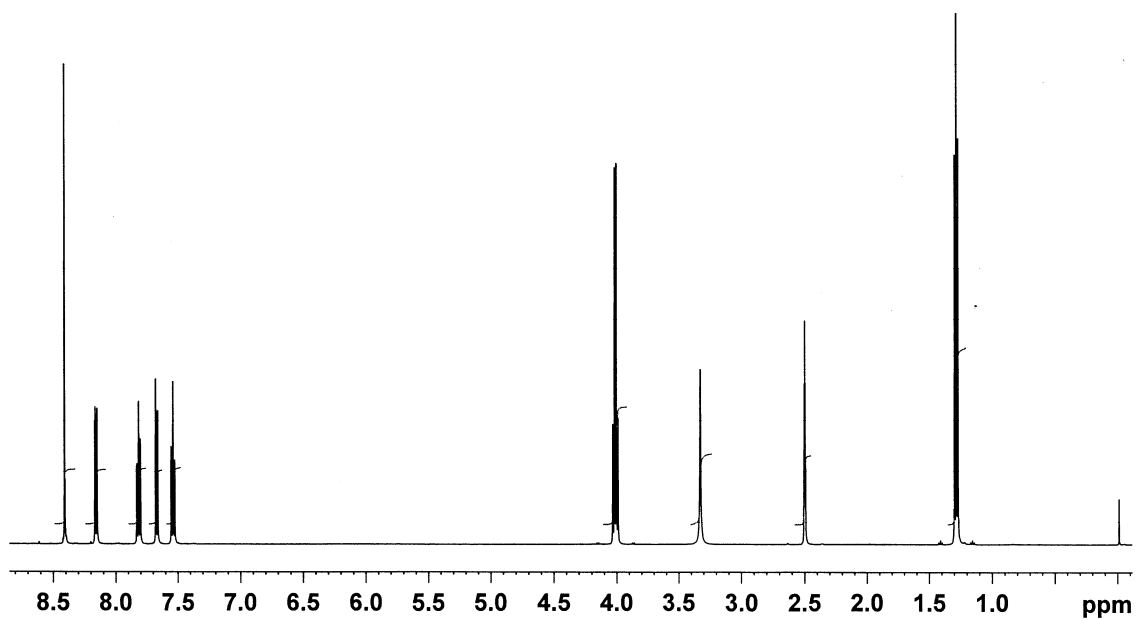
¹H NMR spectrum of 26a.



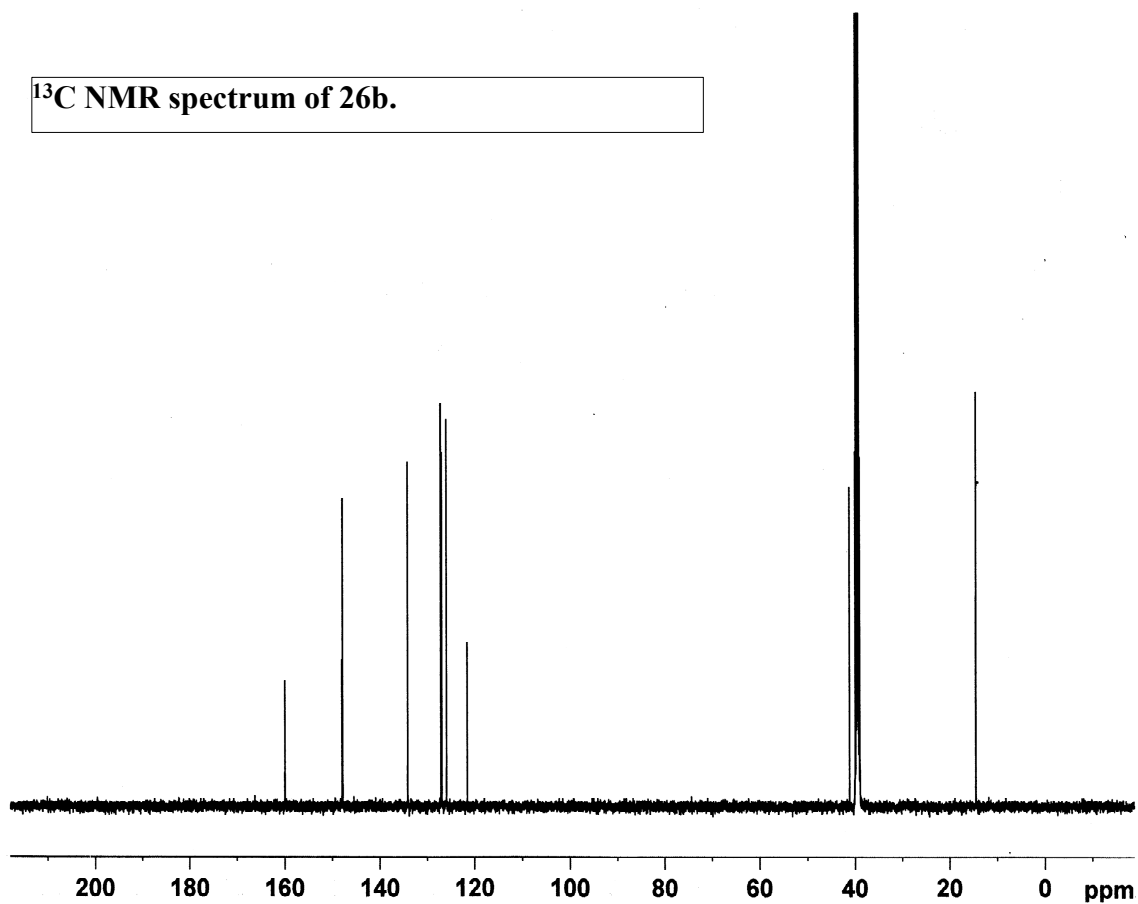
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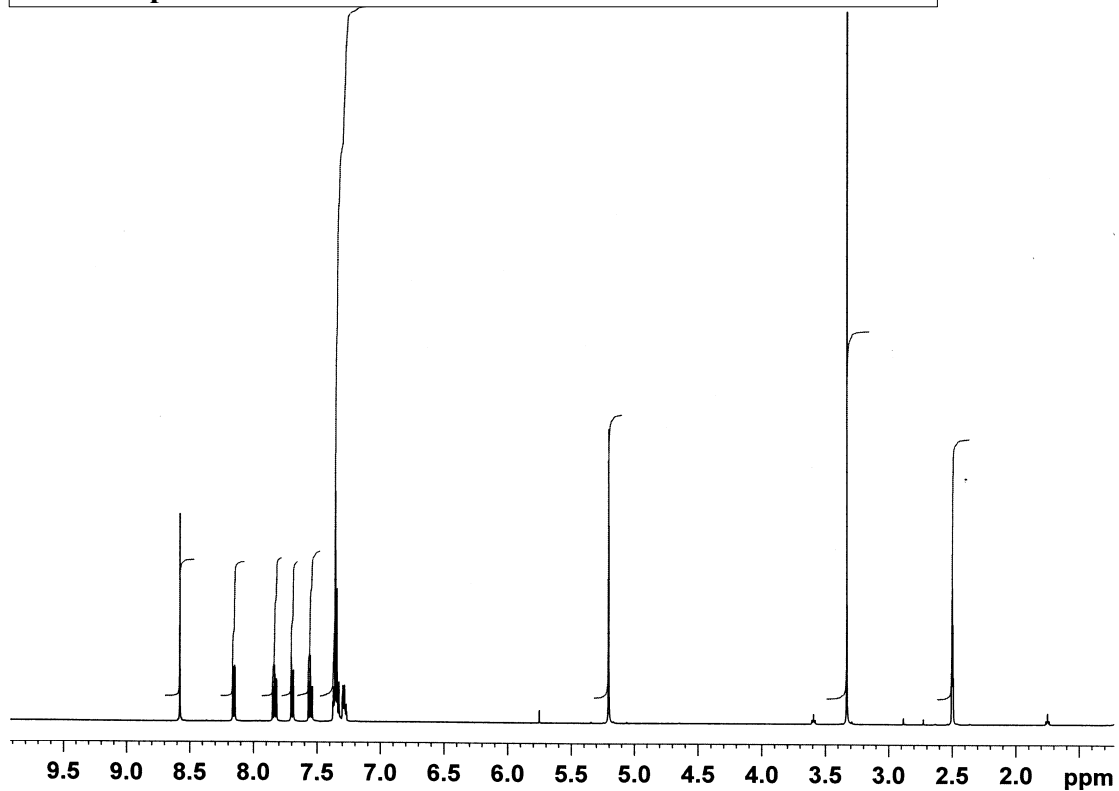
^1H NMR spectrum of 26b.



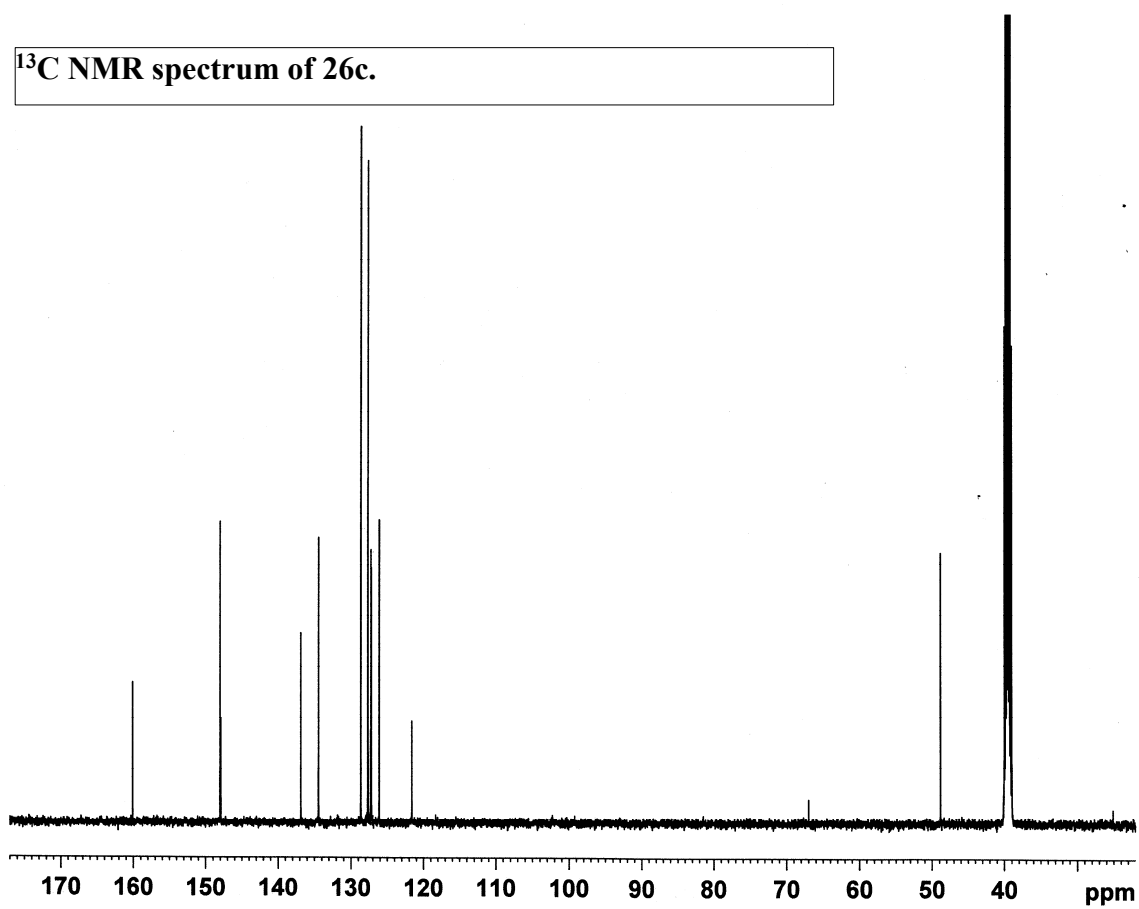
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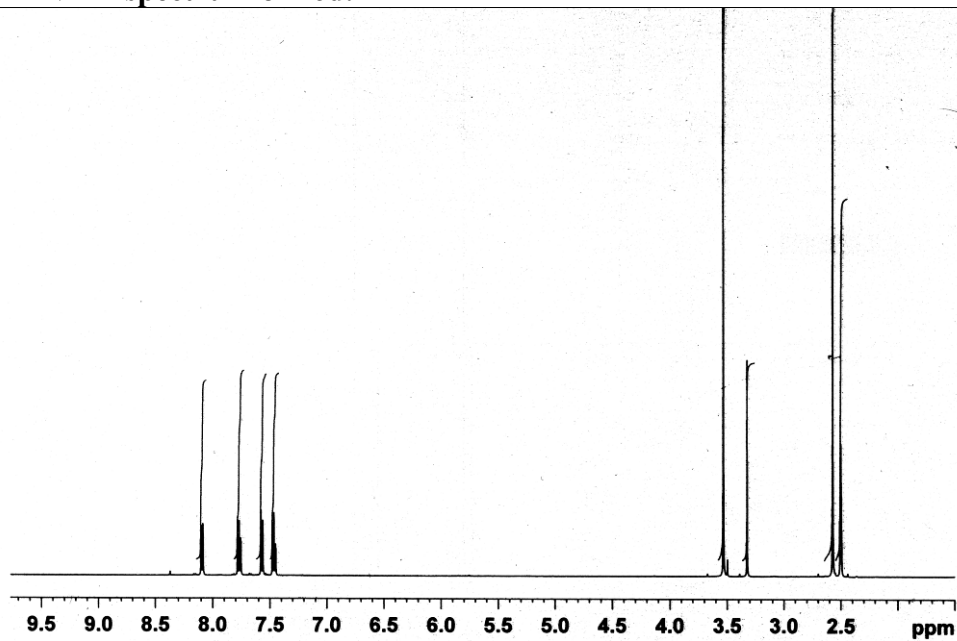
¹H NMR spectrum of 26c.



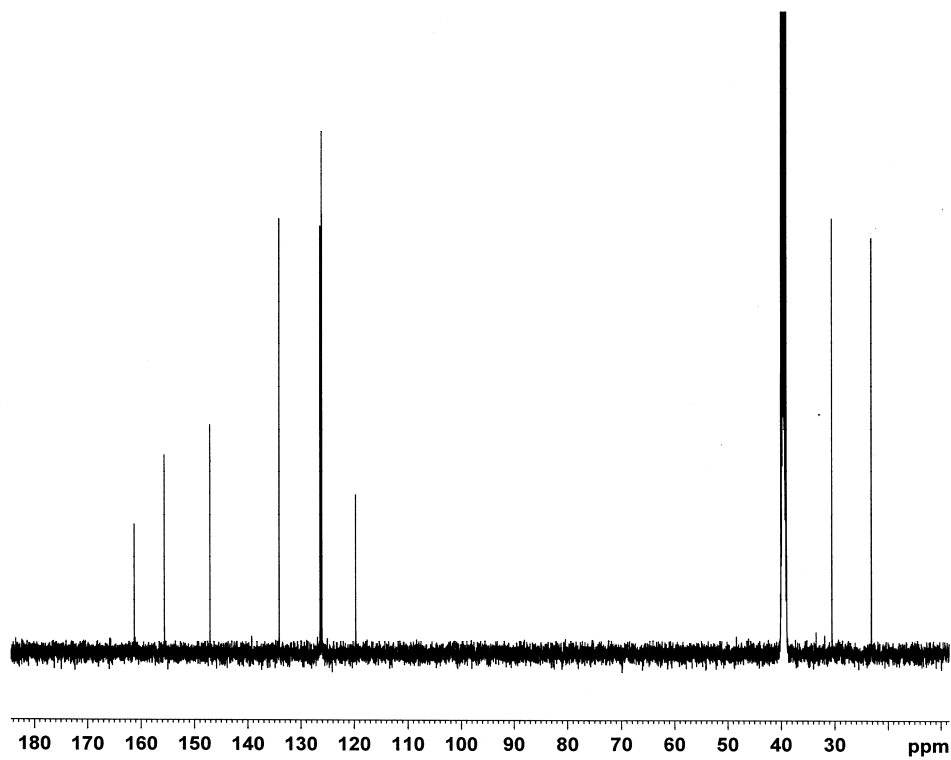
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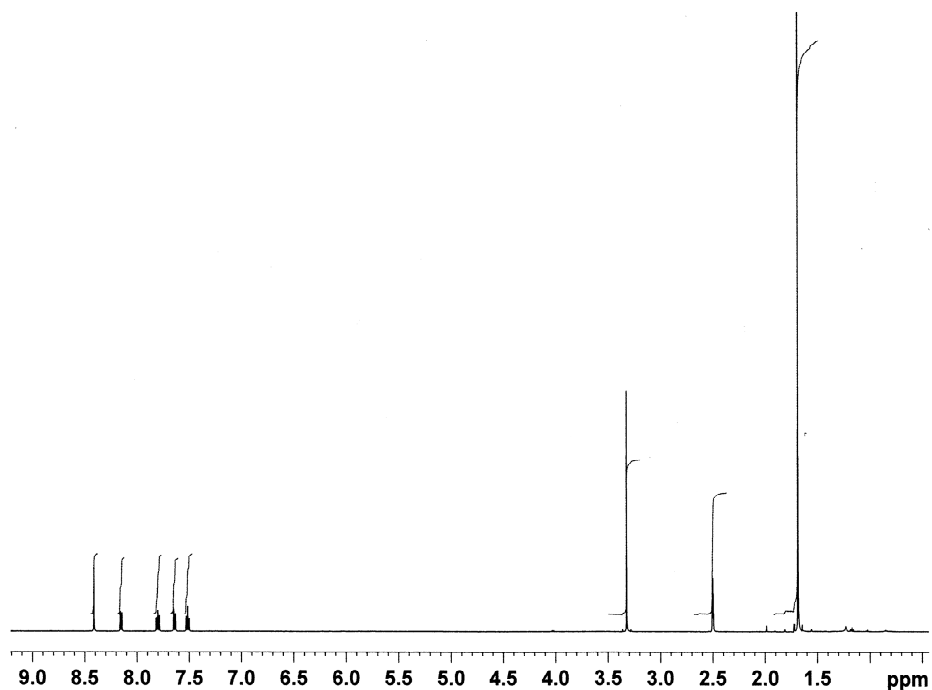
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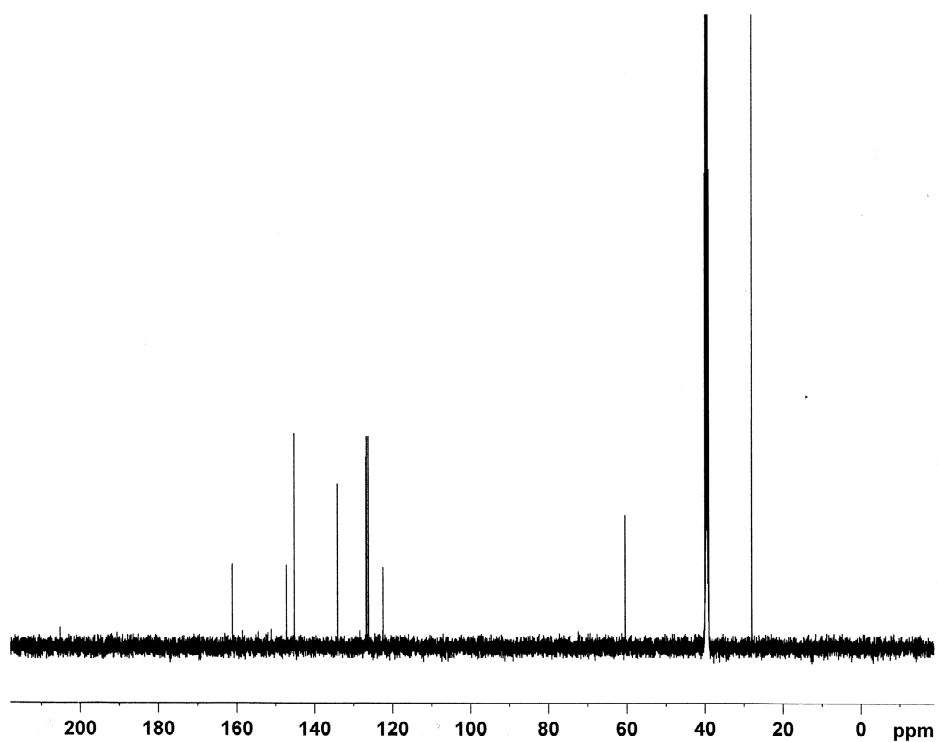
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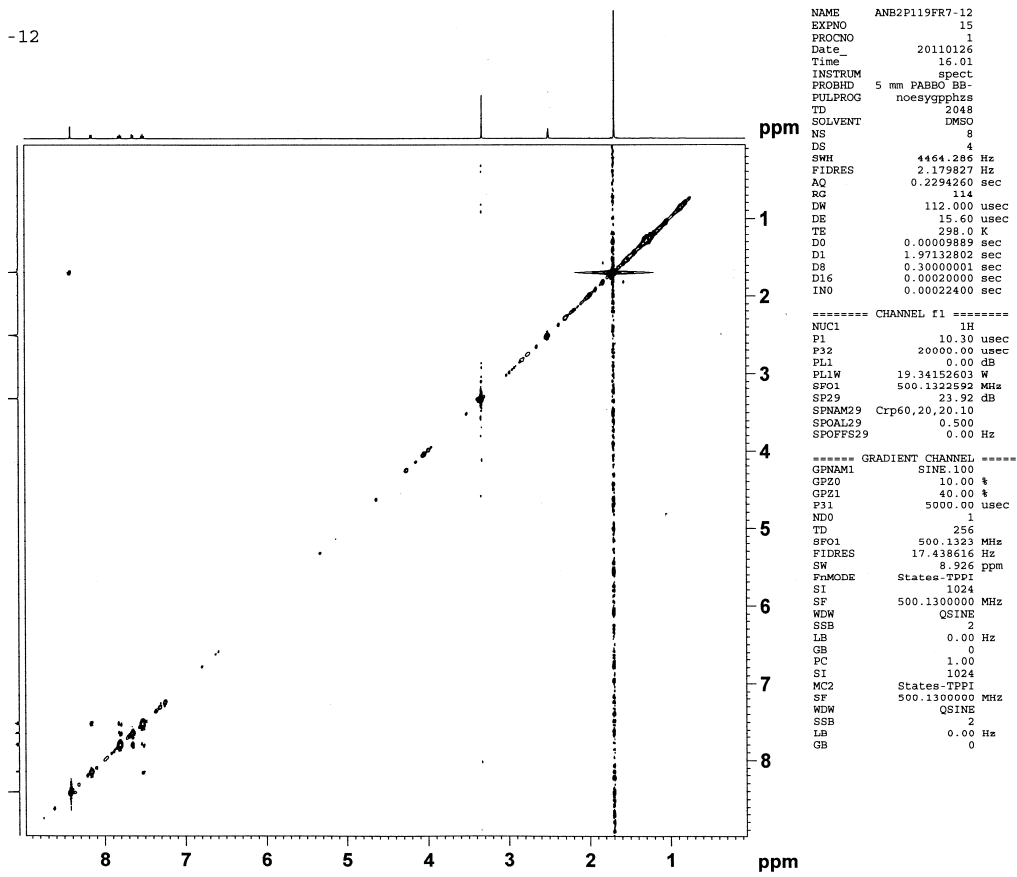
^1H NMR spectrum of 26f.



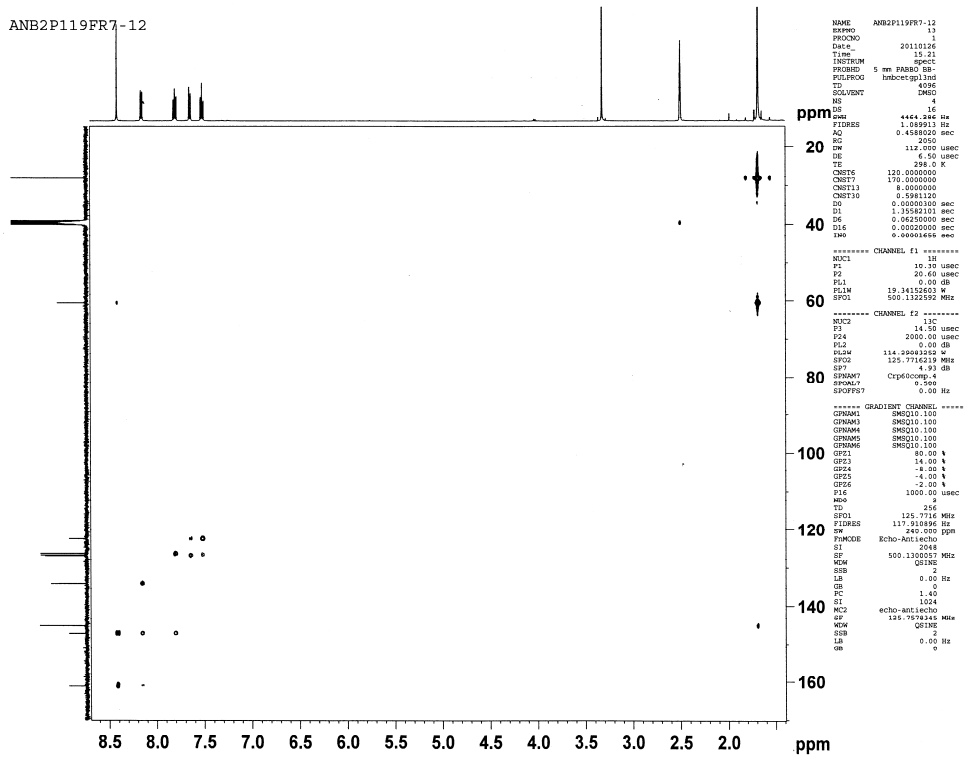
^{13}C NMR spectrum of 26f.



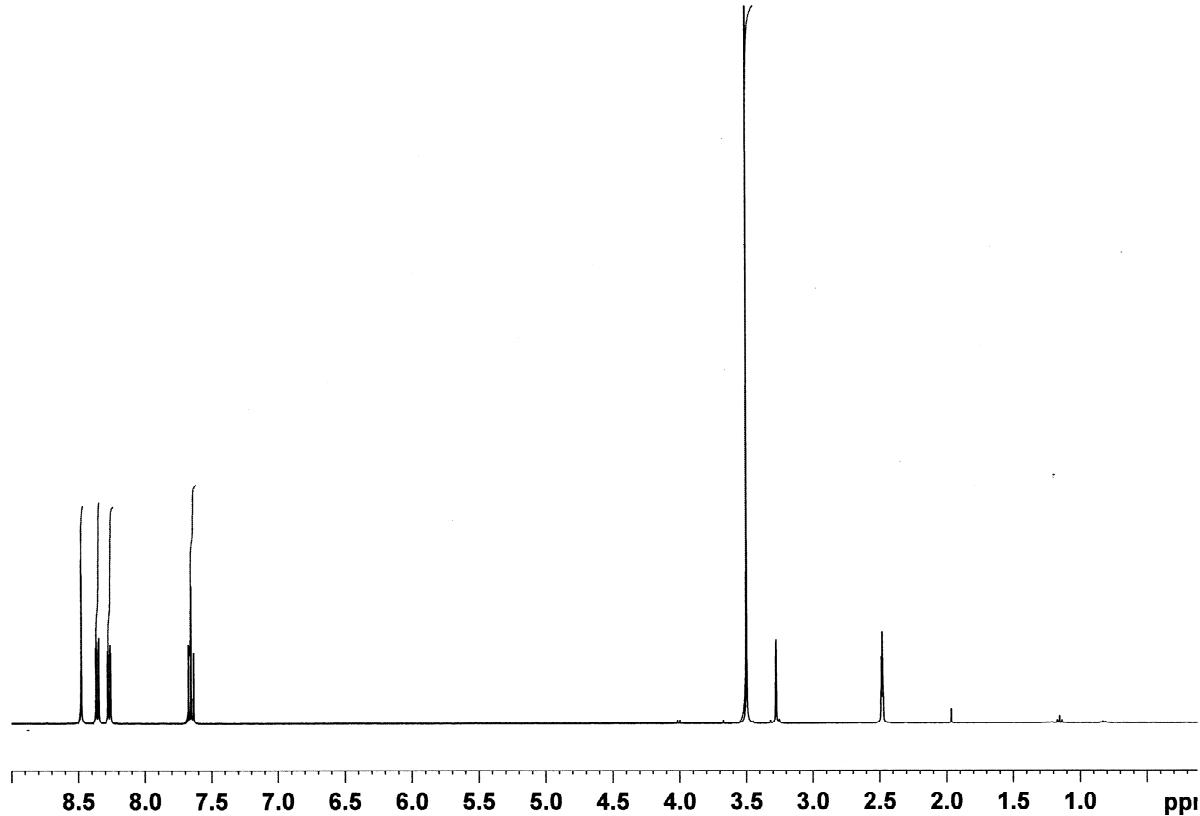
¹H-¹H NOESY spectrum of 26f.



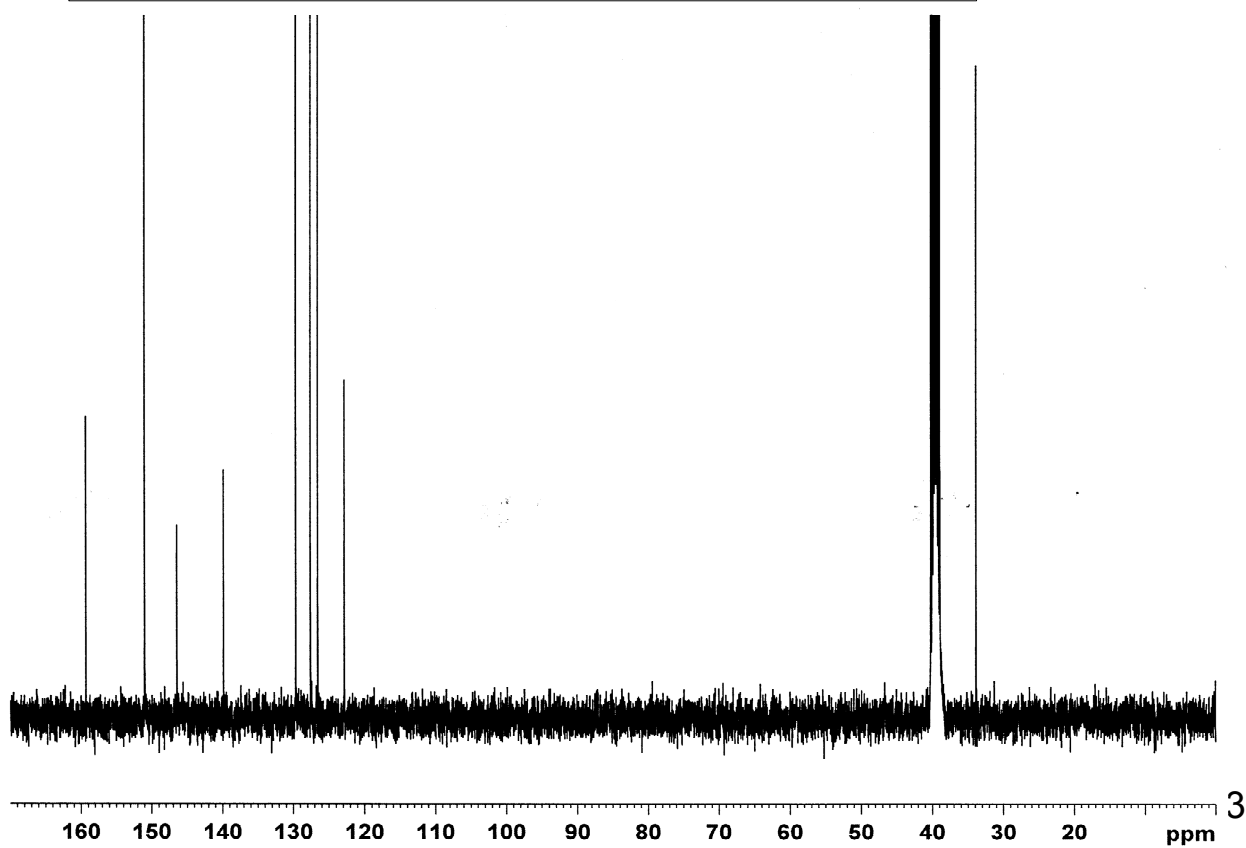
HMBC spectrum of 26f.



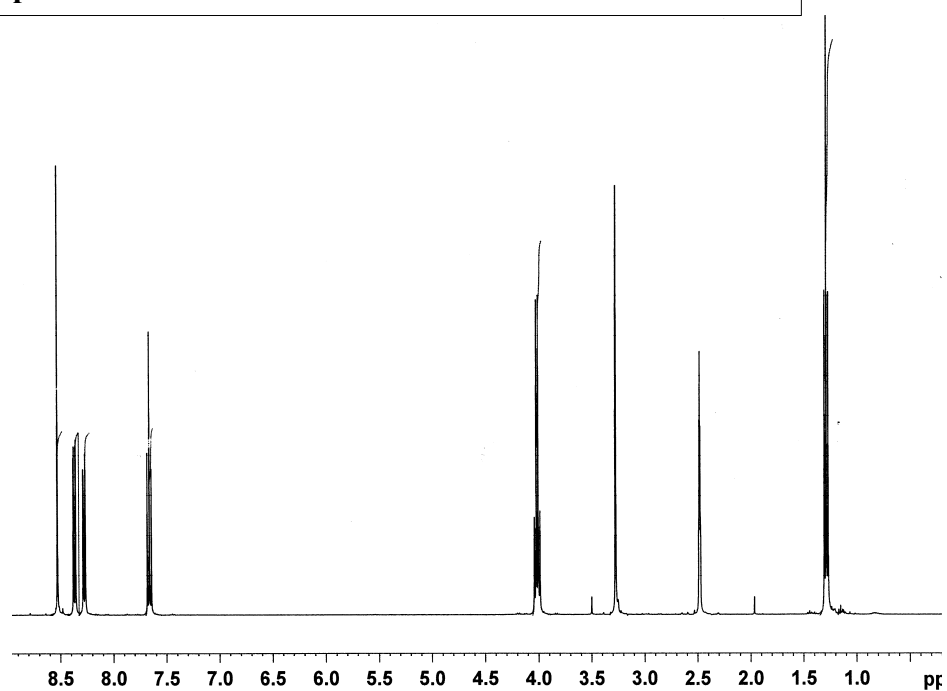
¹H NMR spectrum of 27a.



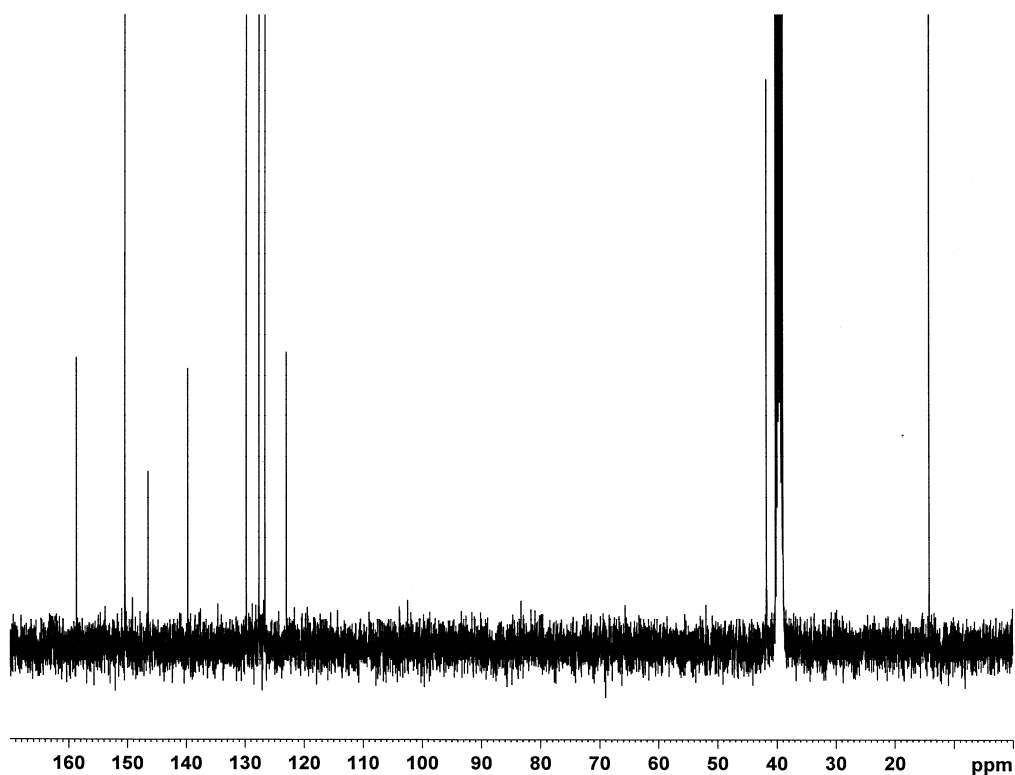
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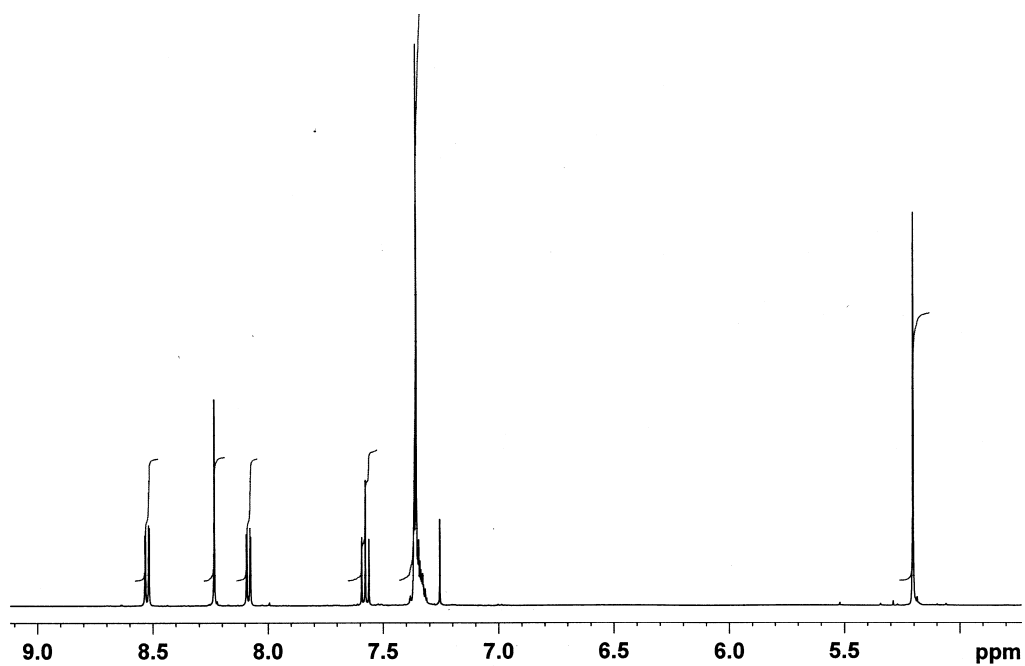
¹H NMR spectrum of 27b.



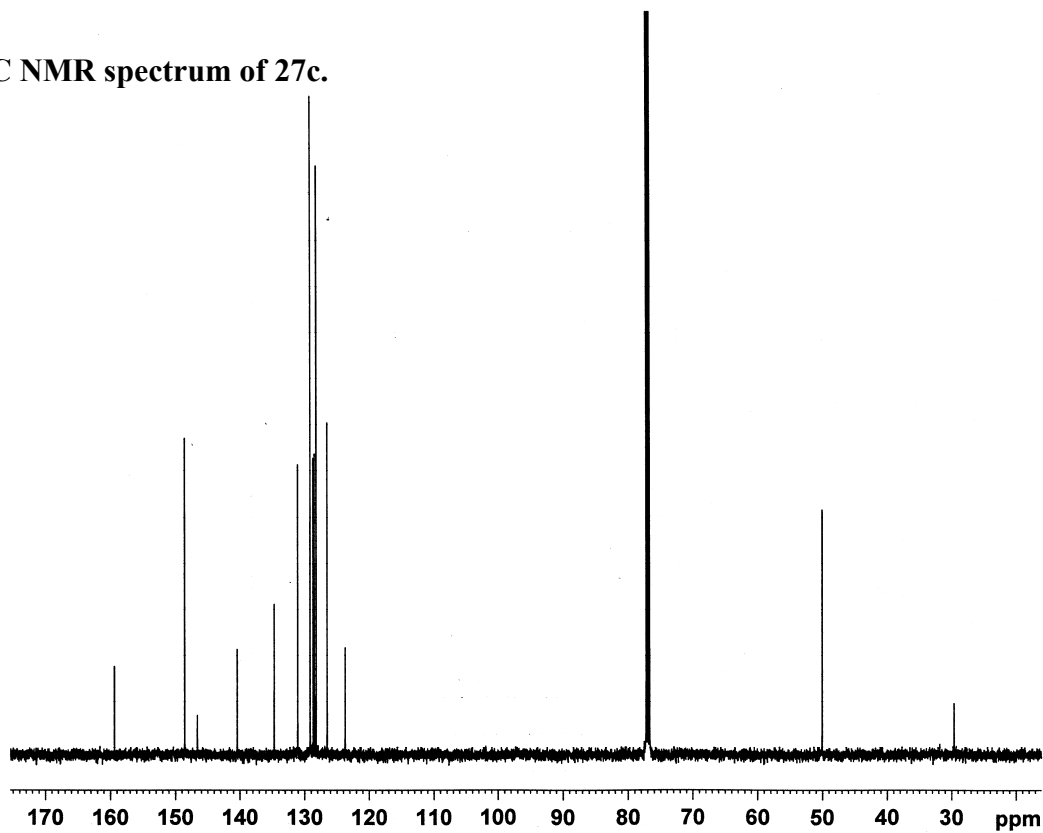
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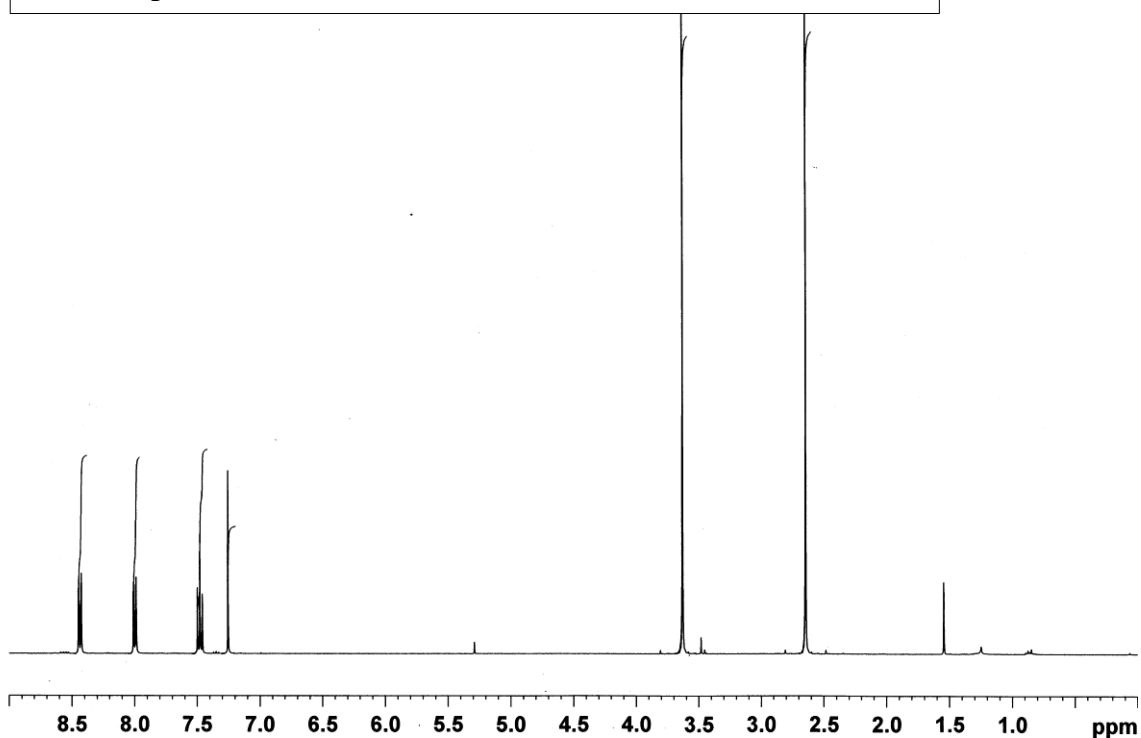
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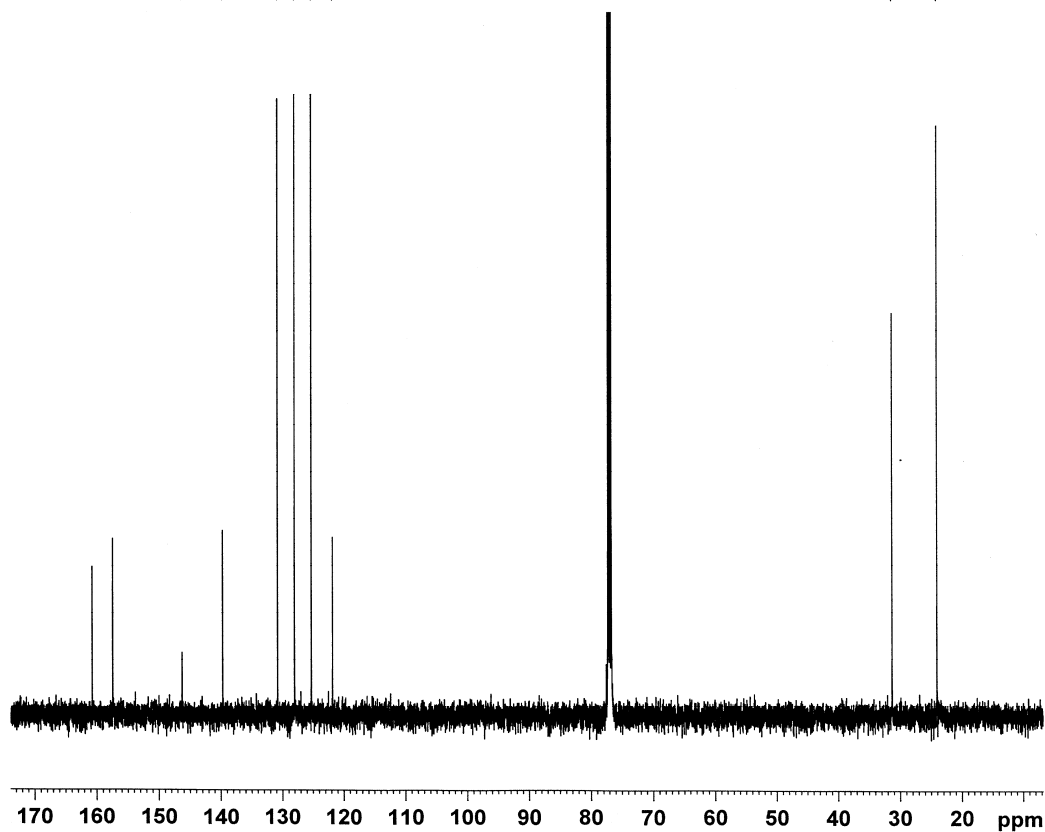
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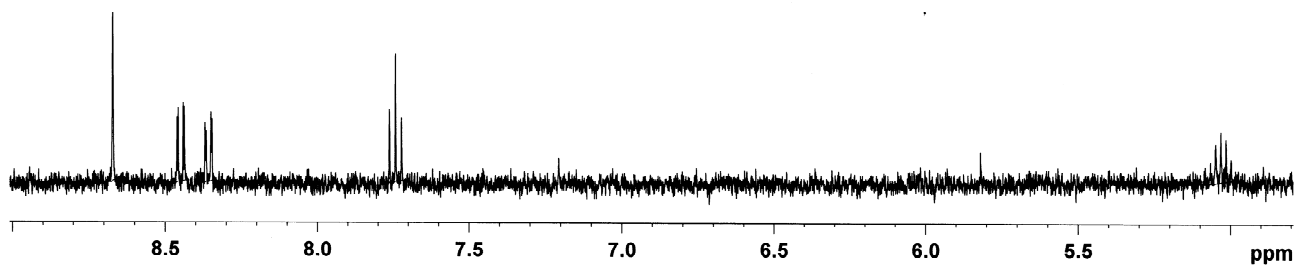
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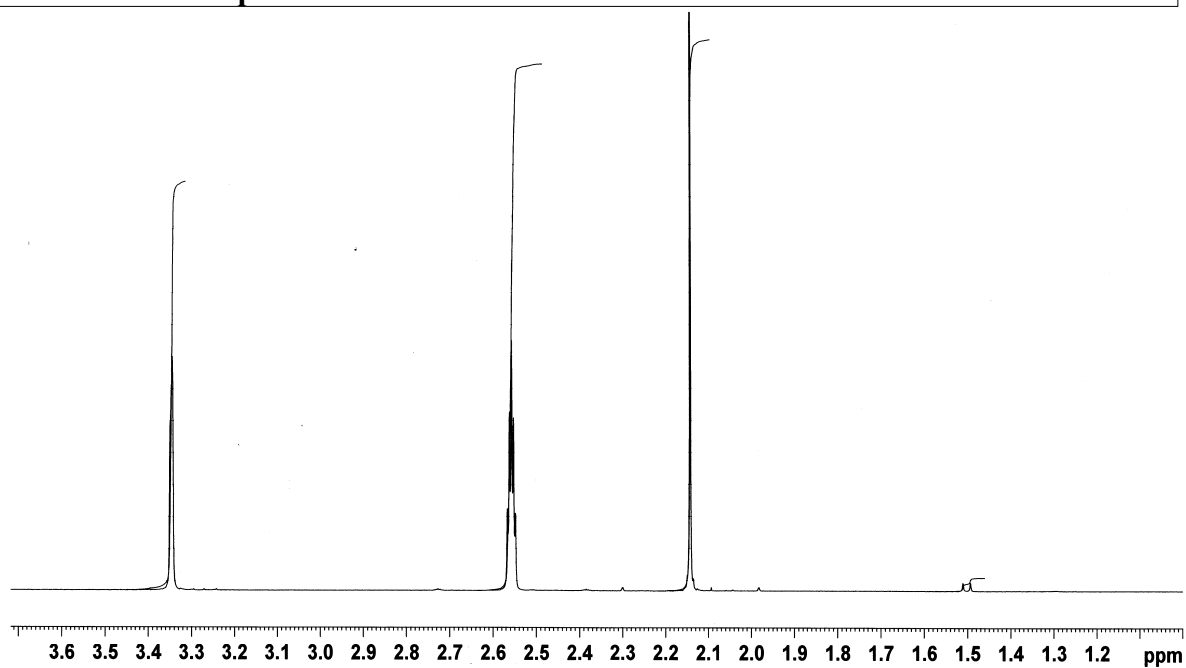
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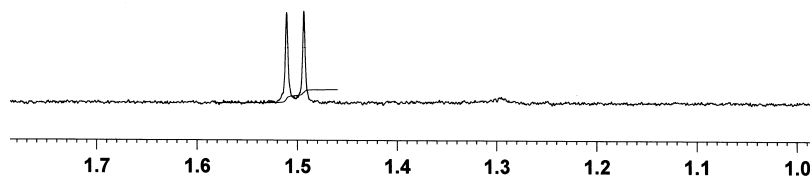
Part of ^1H NMR spectrum of 27e.



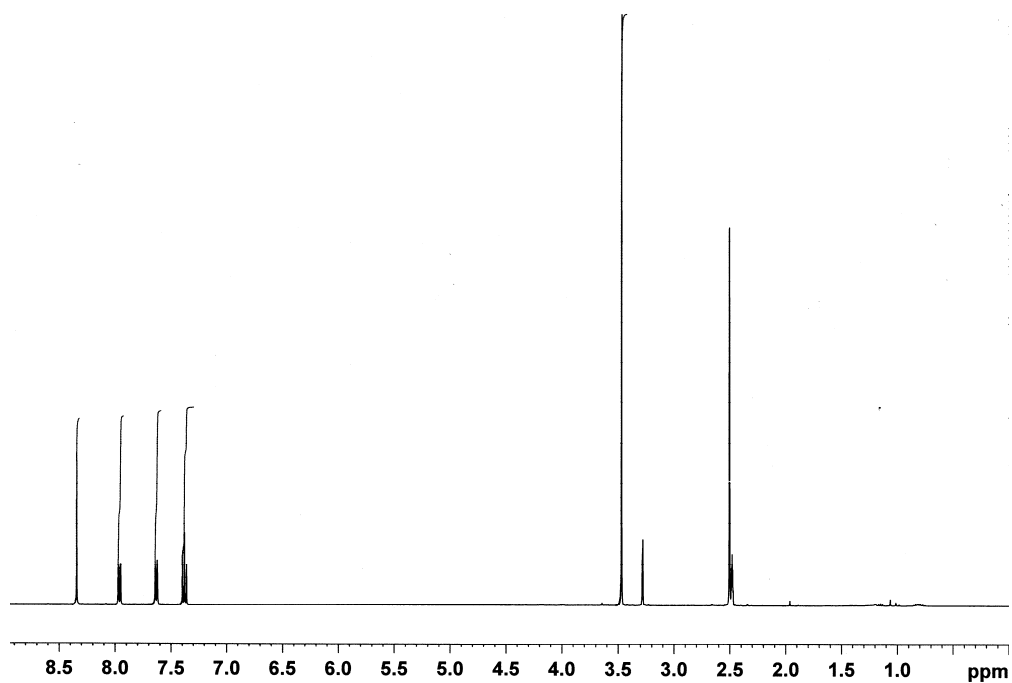
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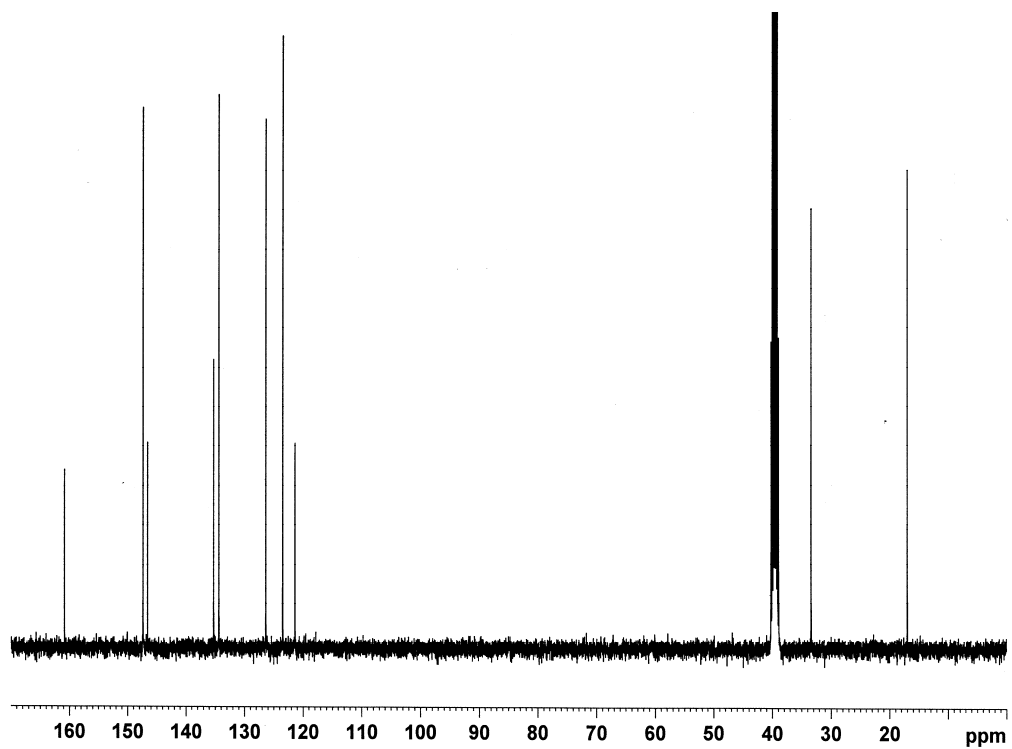
Part of ^1H NMR spectrum of 27e.



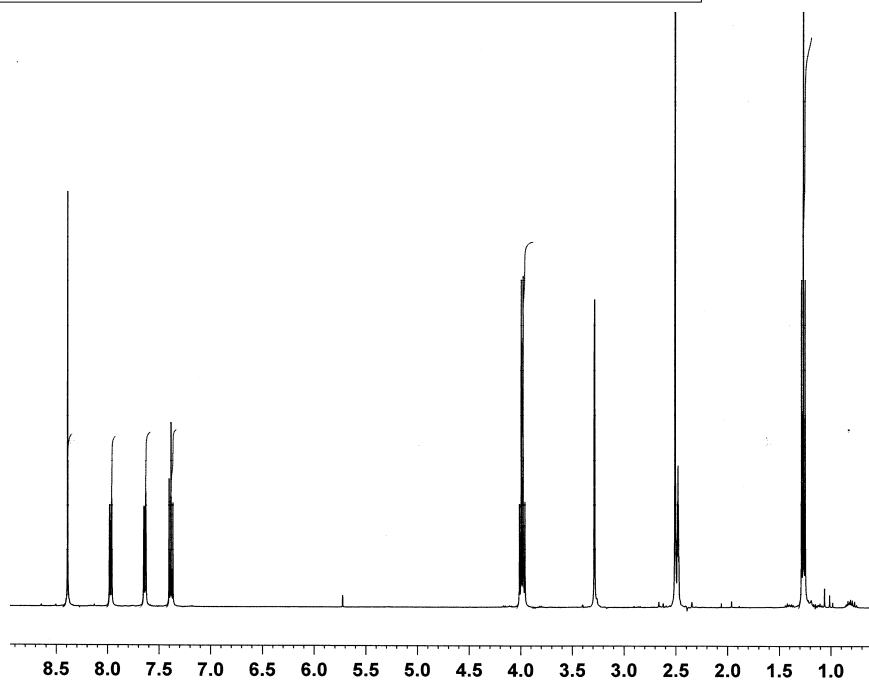
^1H NMR spectrum of 28a.



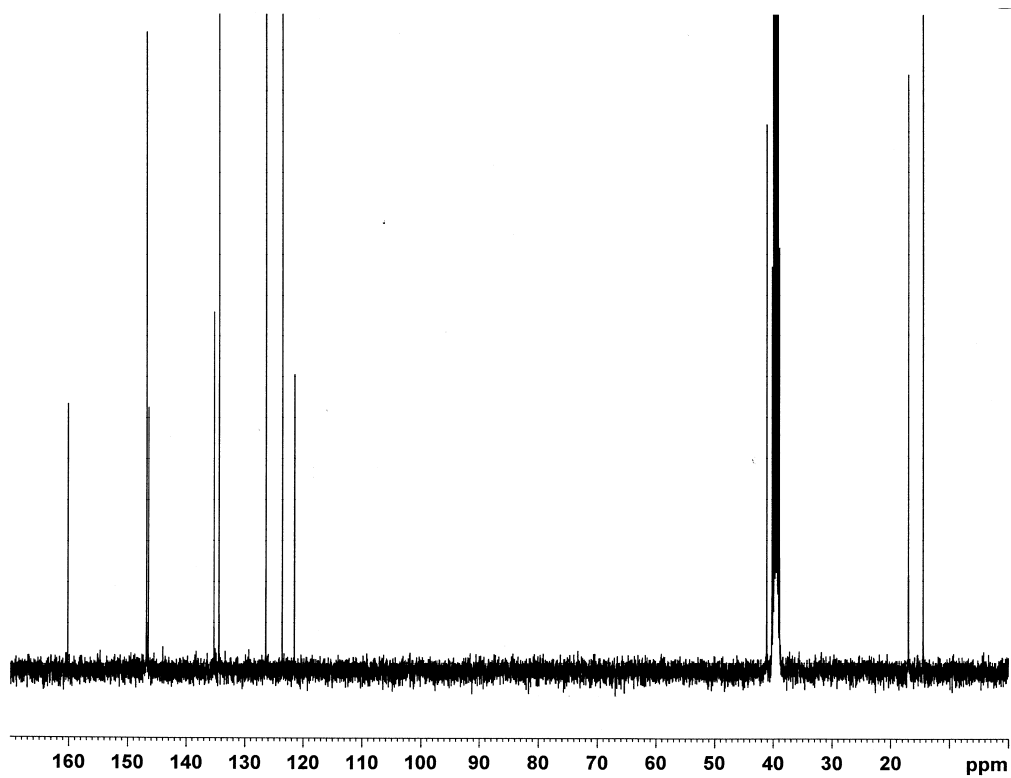
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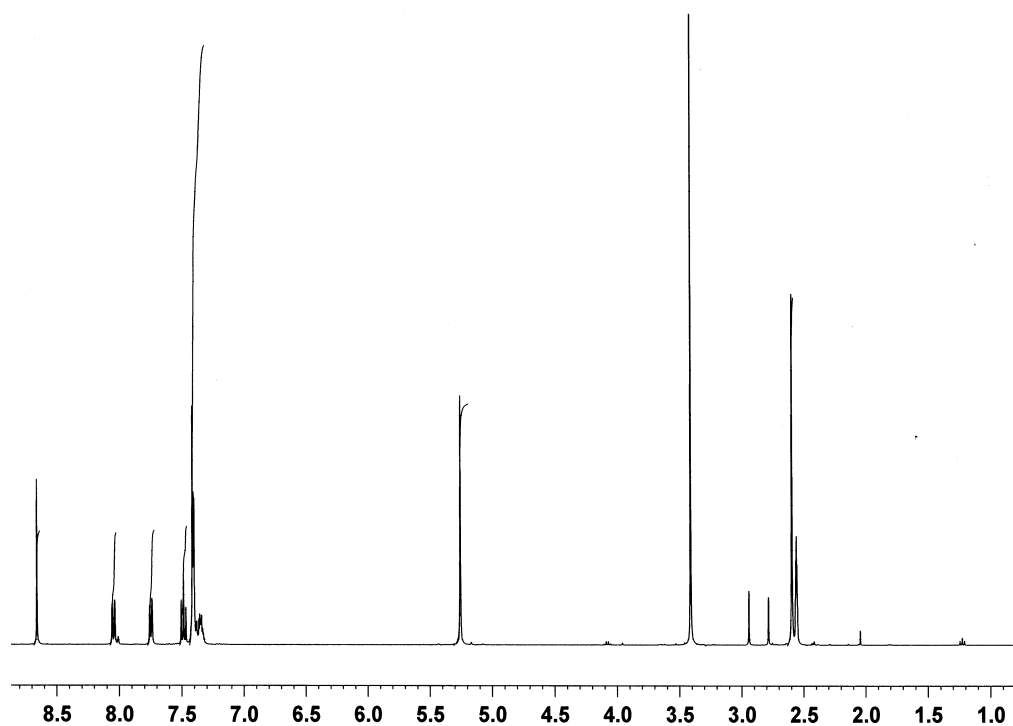
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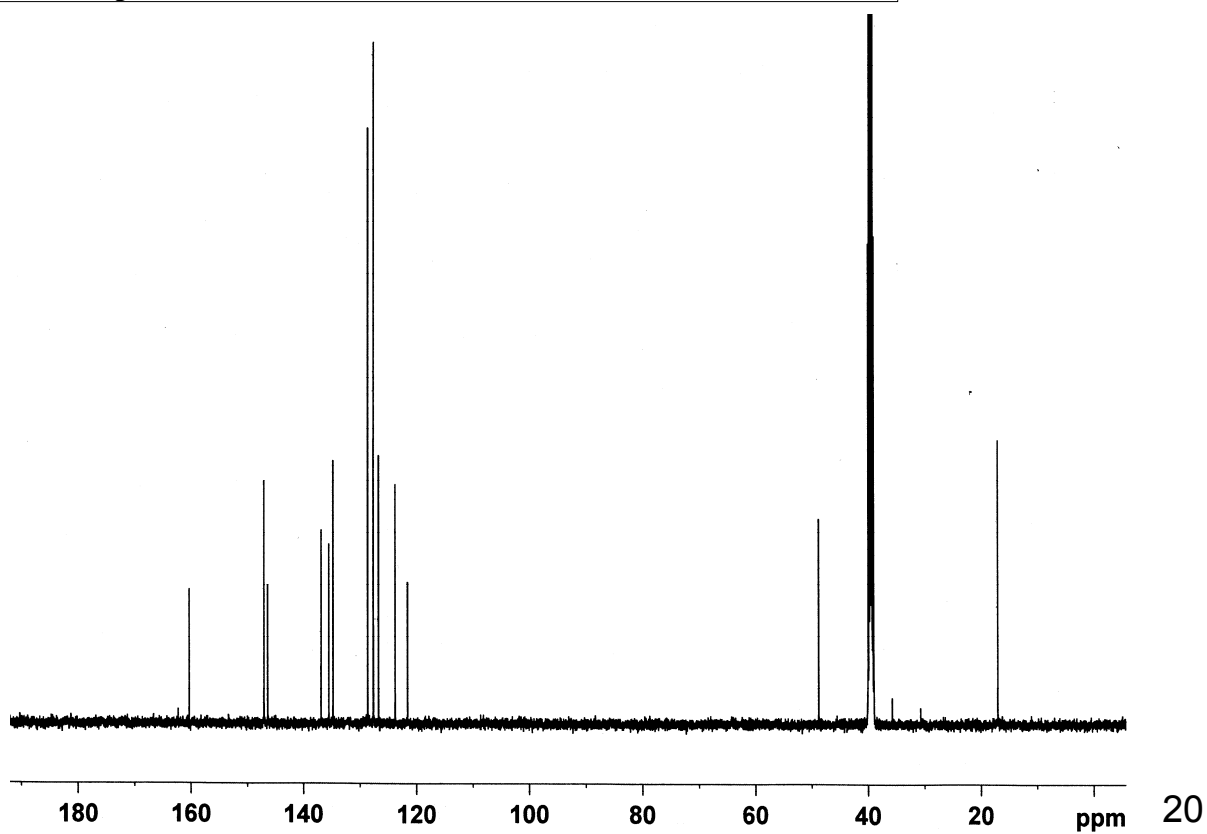
^{13}C NMR spectrum of 28b.



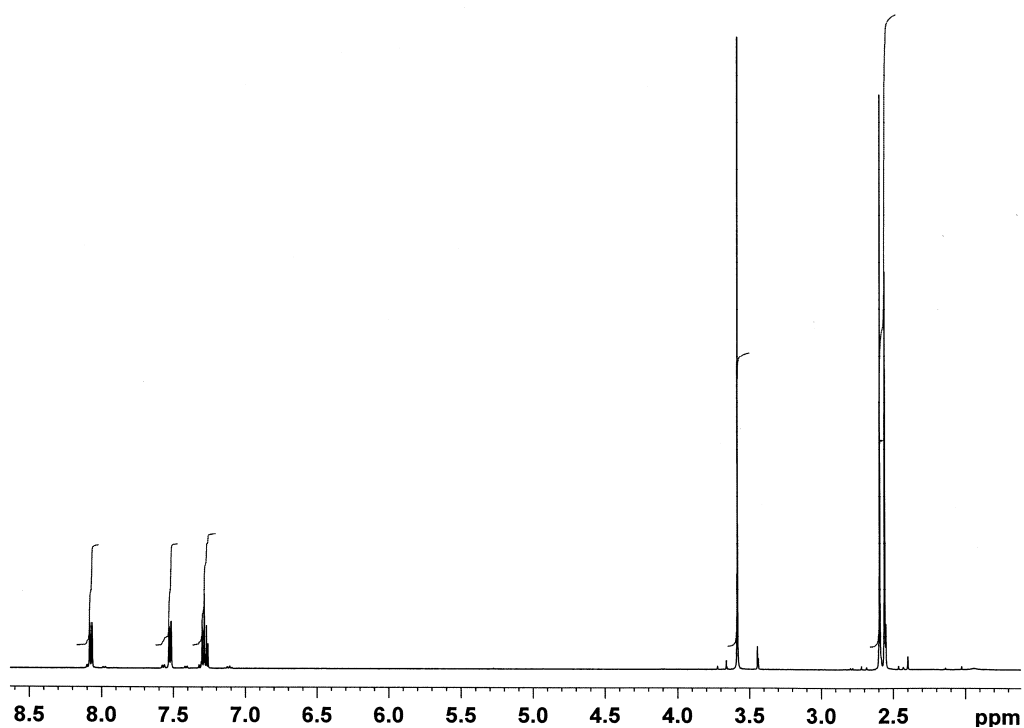
^1H NMR spectrum of 28c.



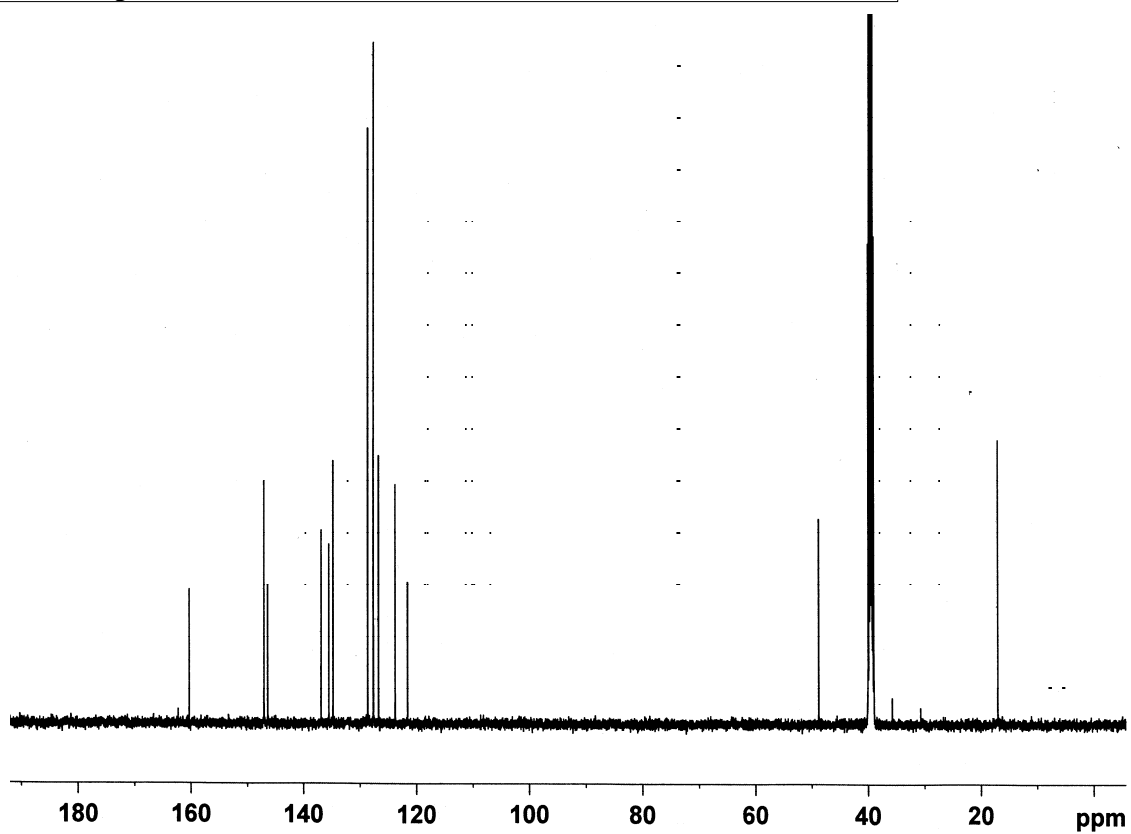
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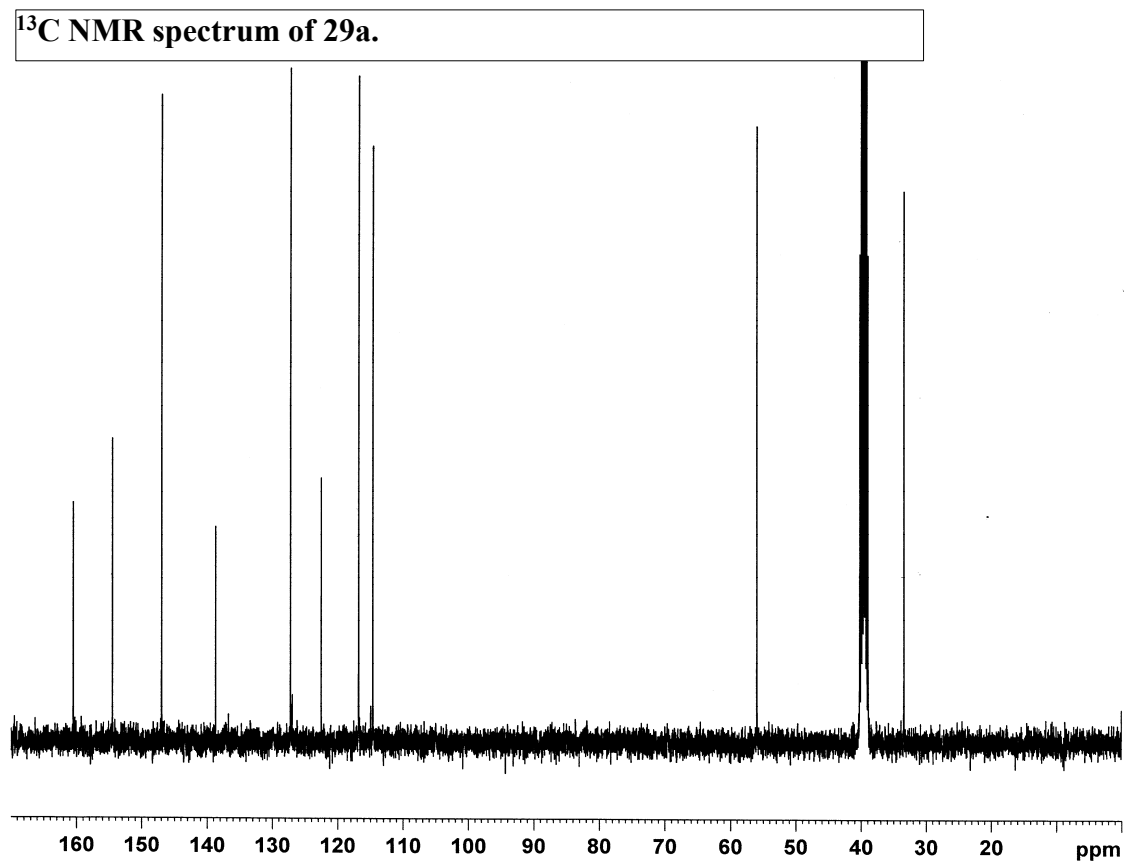
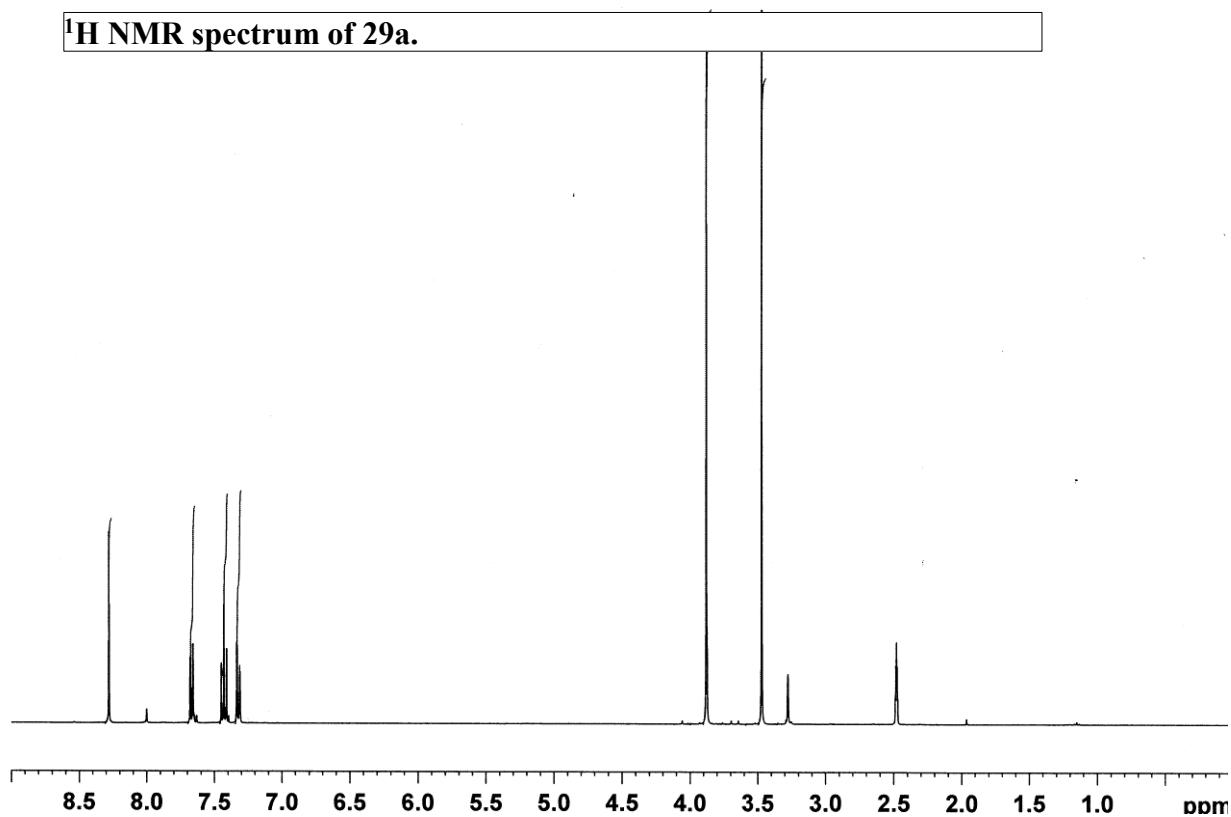


¹H NMR spectrum of 28d.

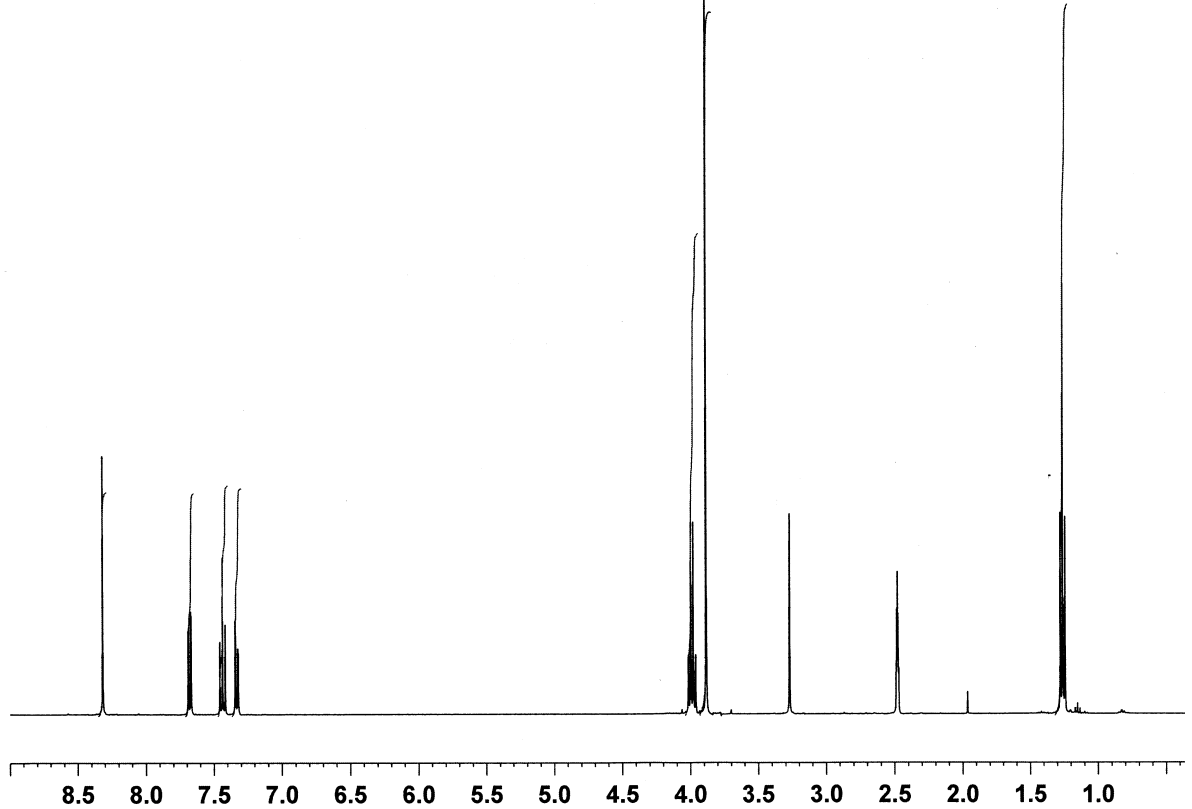


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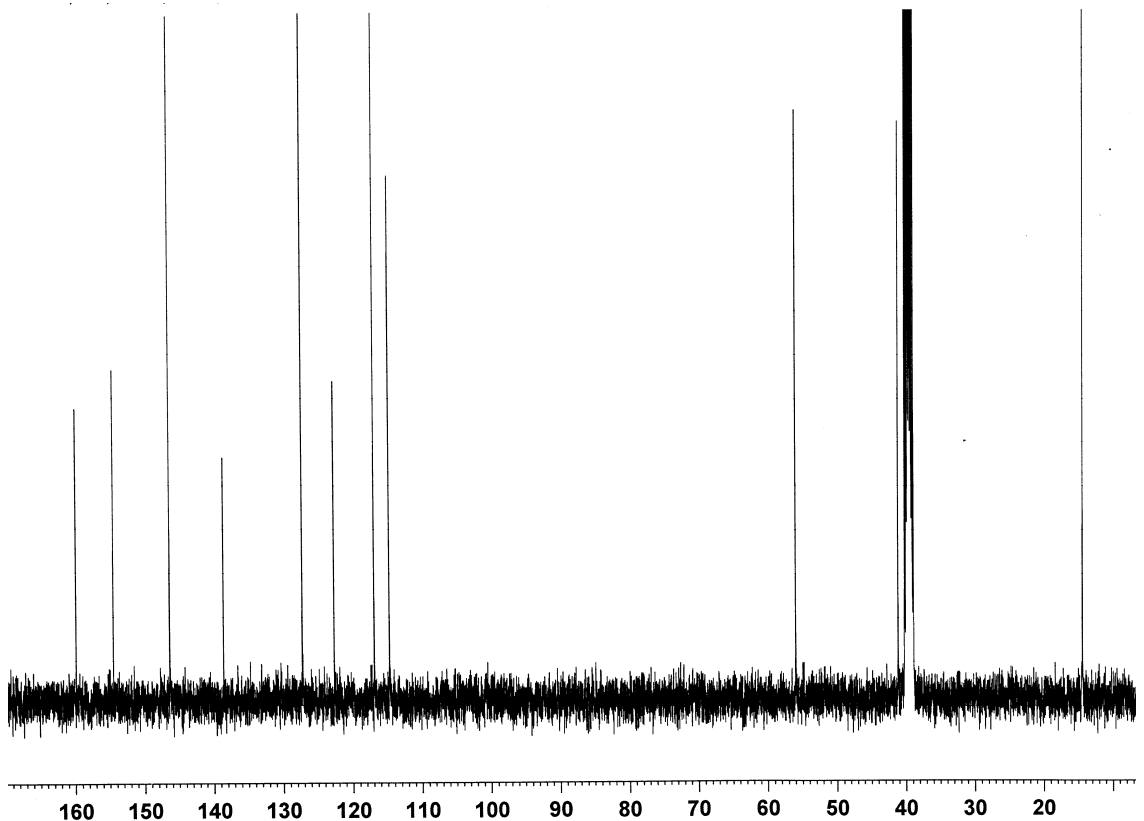




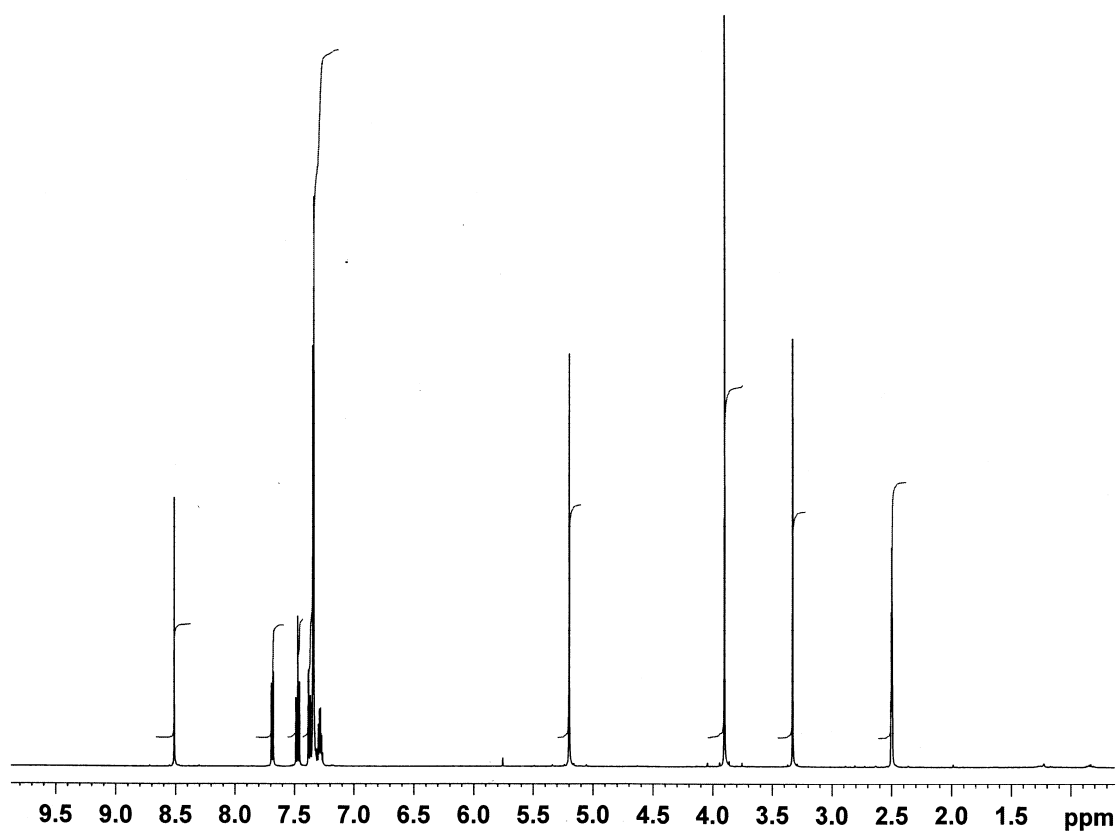
¹H NMR spectrum of 29b.



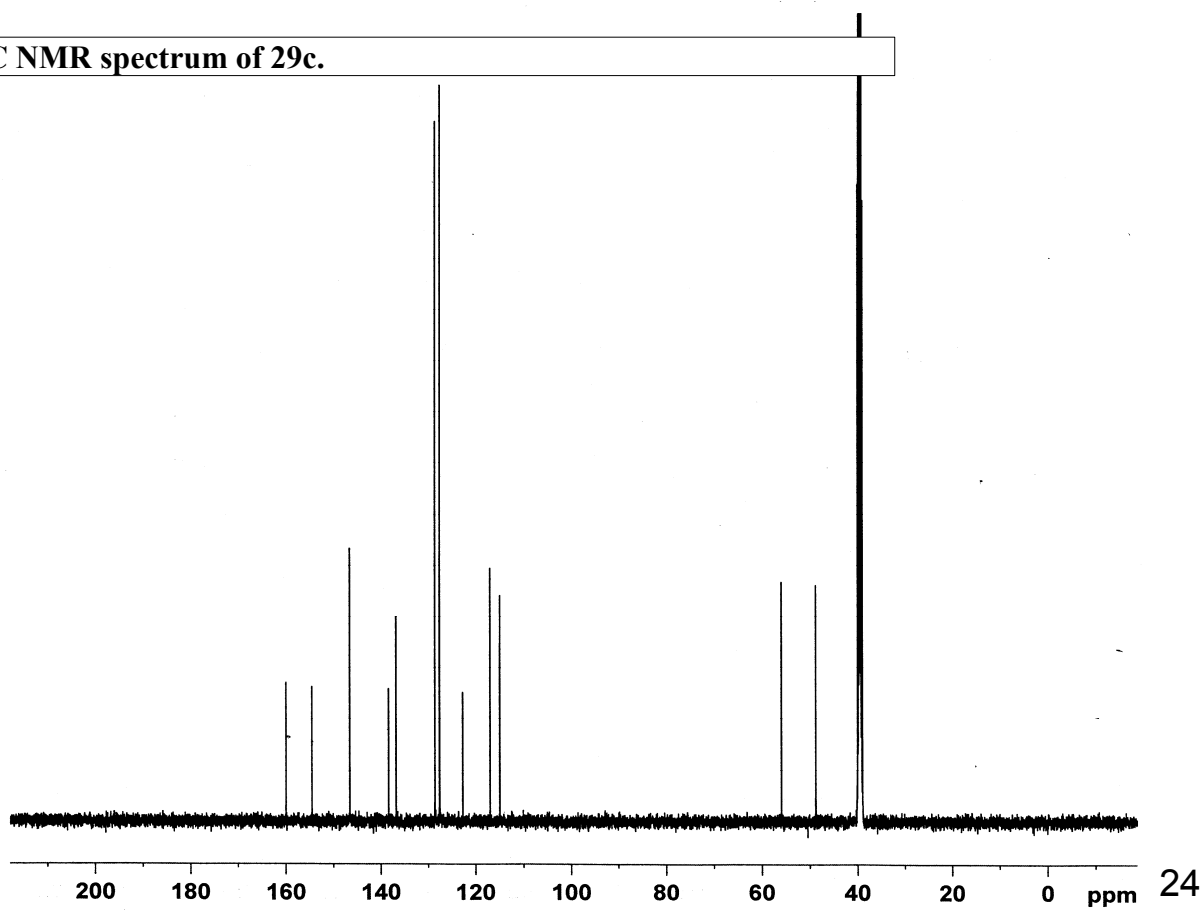
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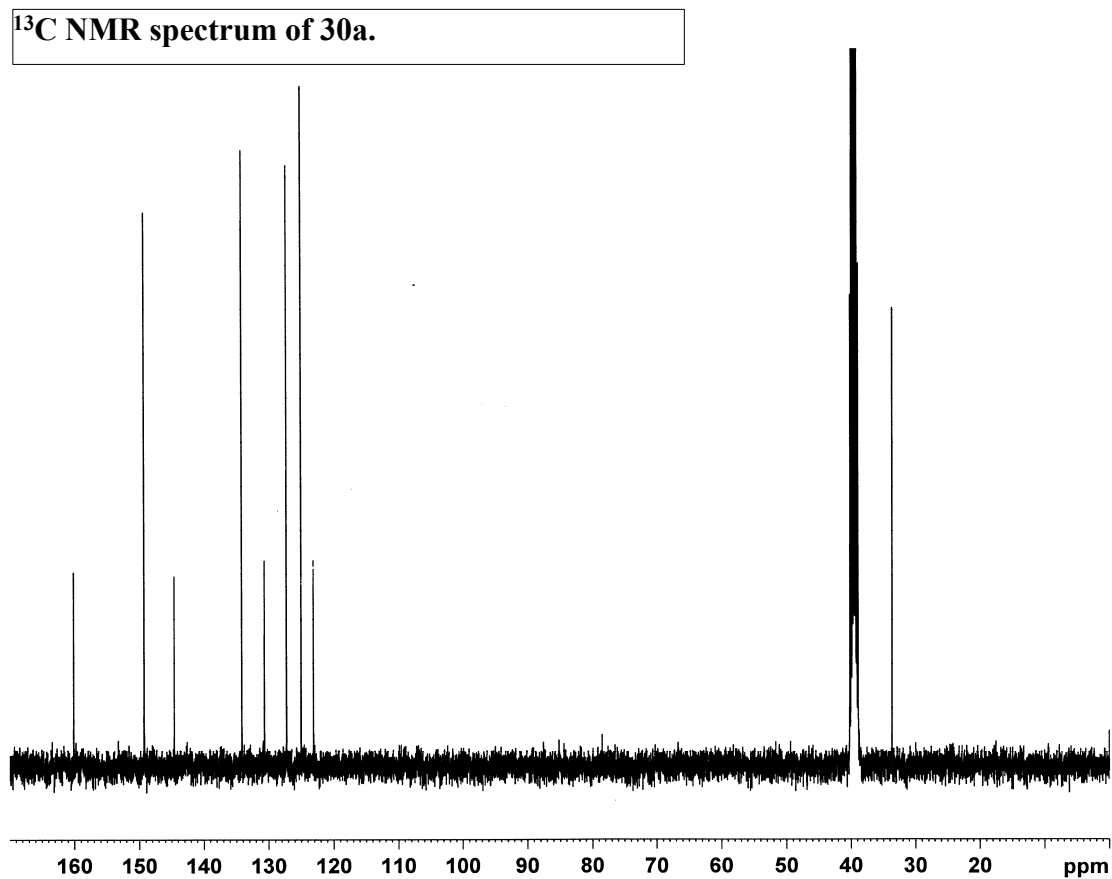
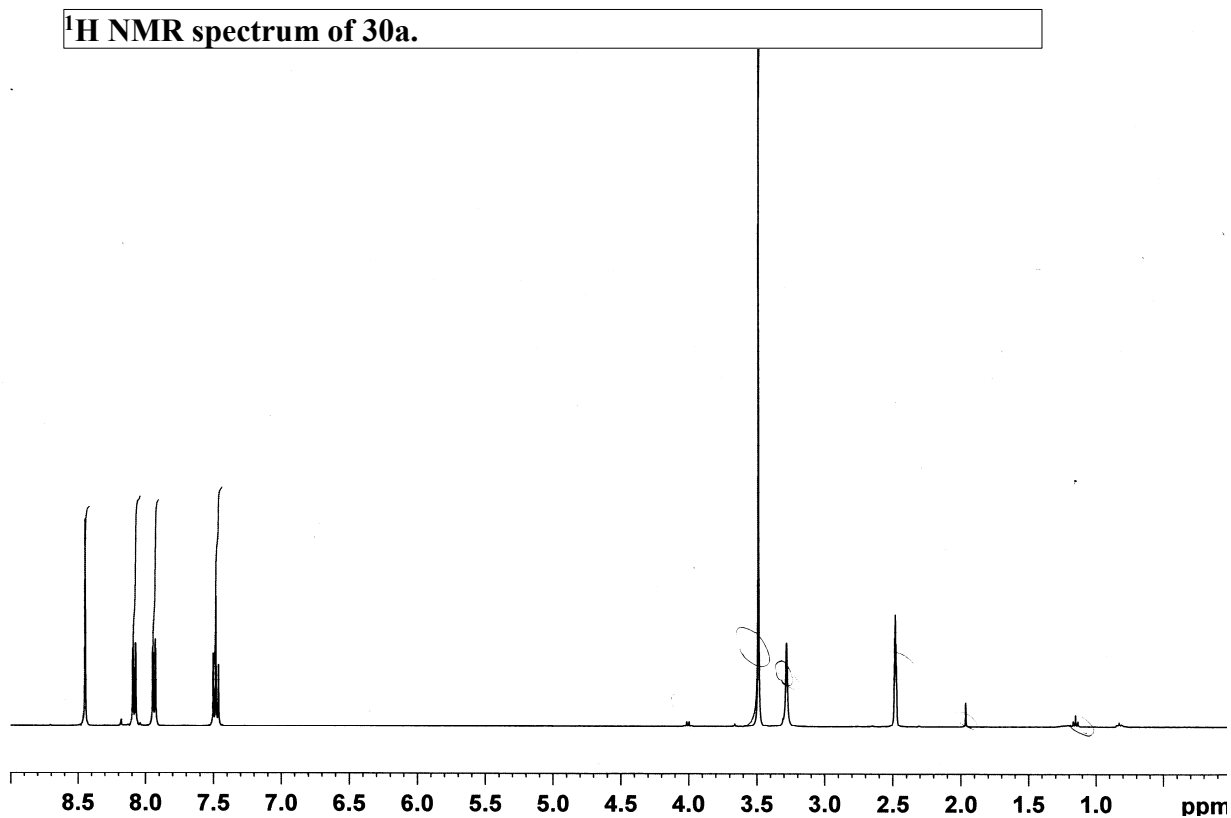


^1H NMR spectrum of 29c.

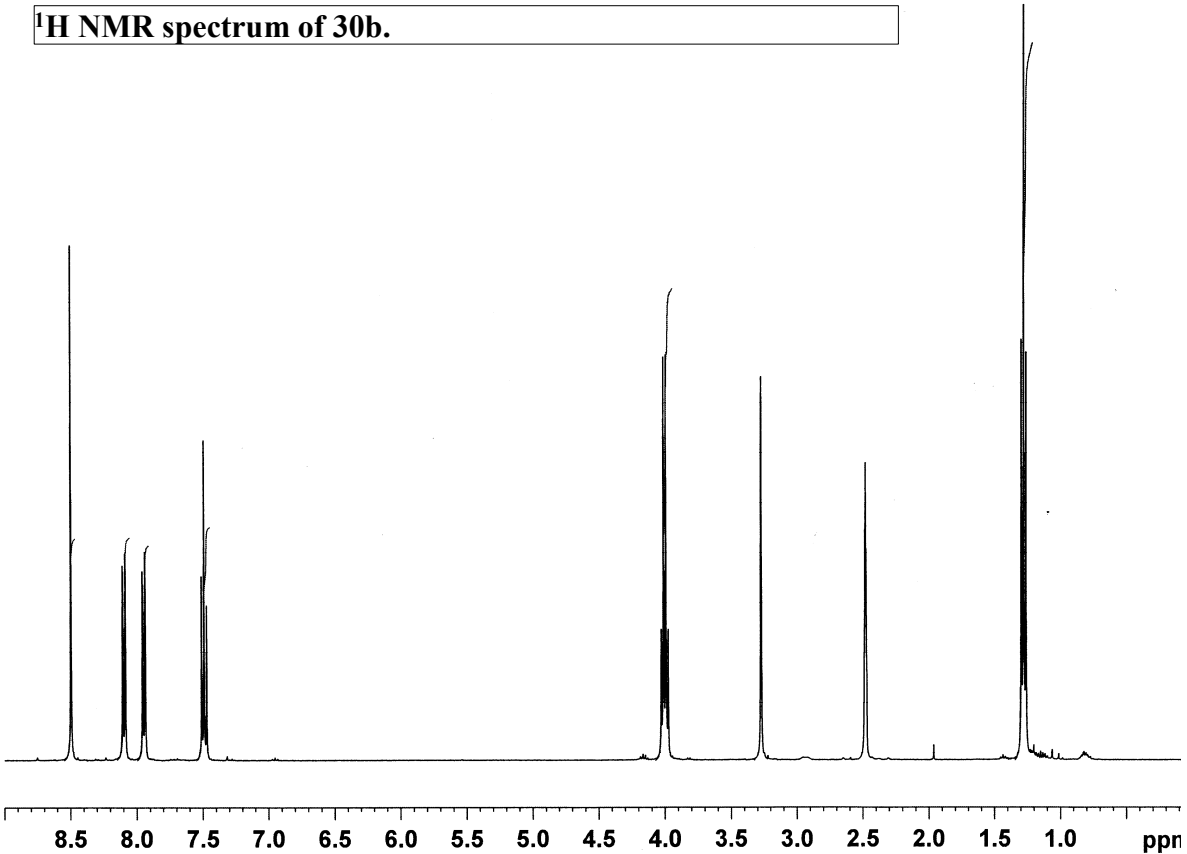


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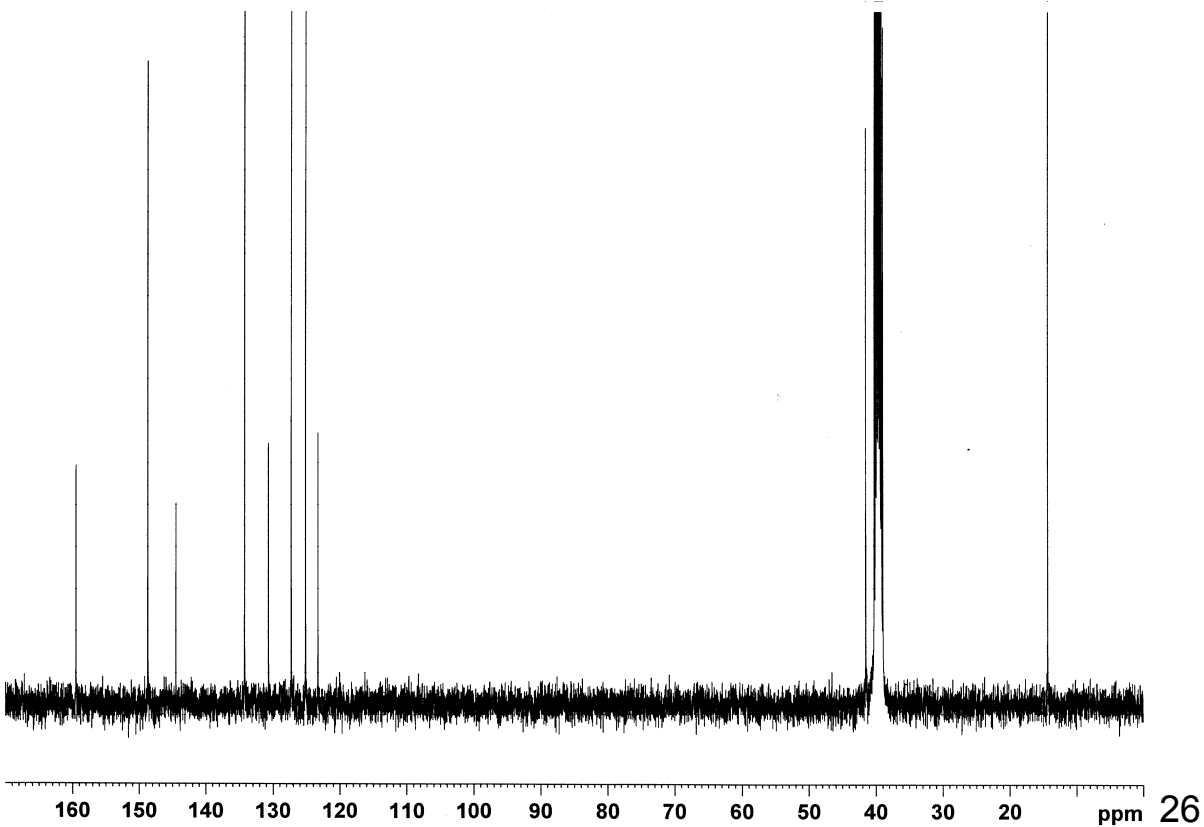




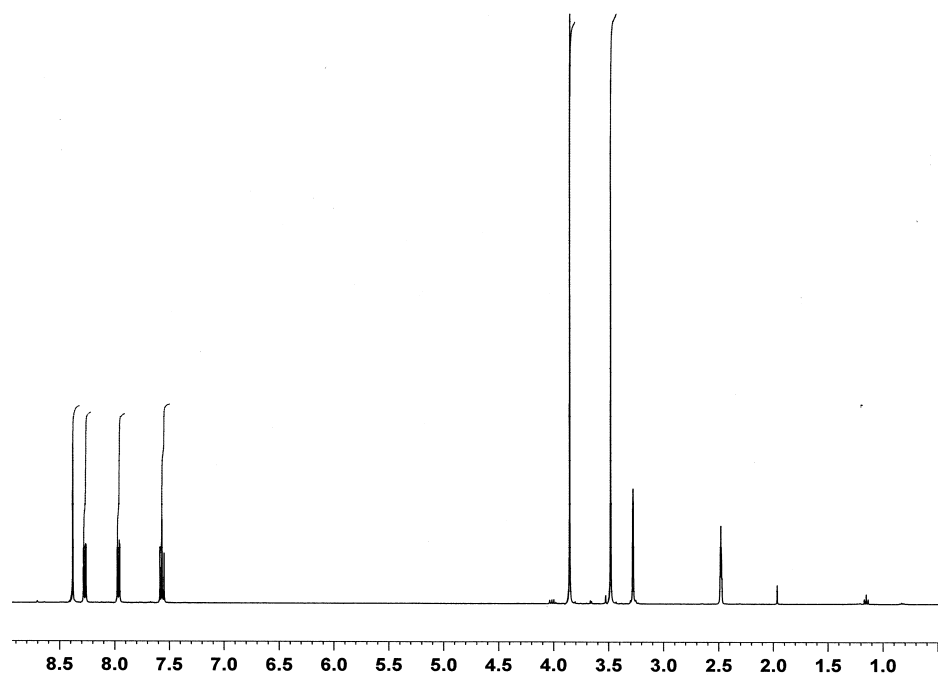
¹H NMR spectrum of 30b.



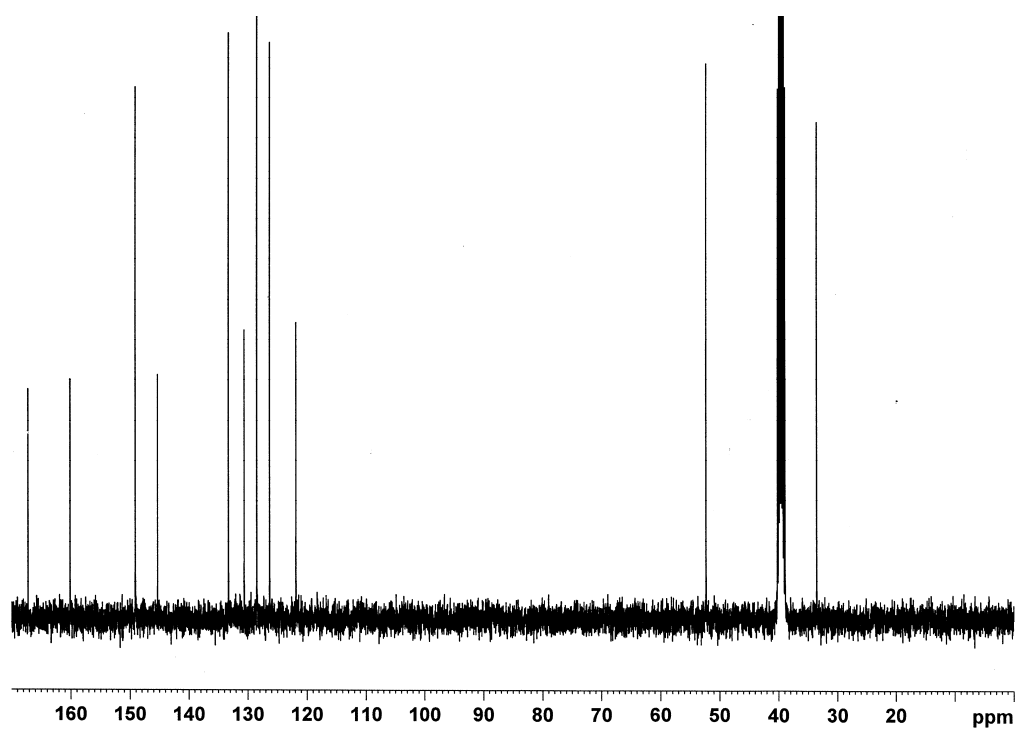
¹³C NMR spectrum of 30b.



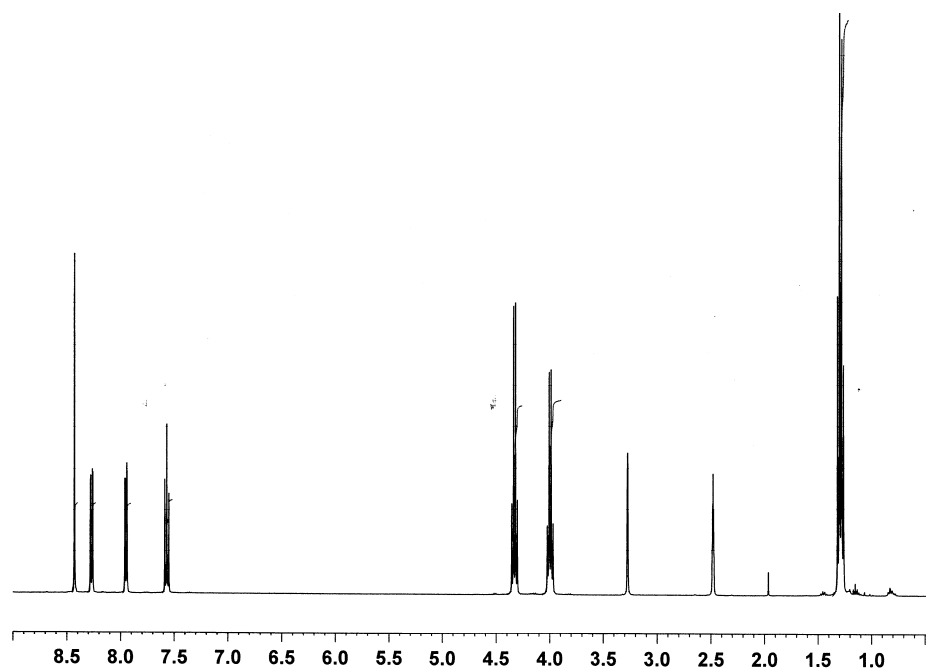
¹H NMR spectrum of 31a.



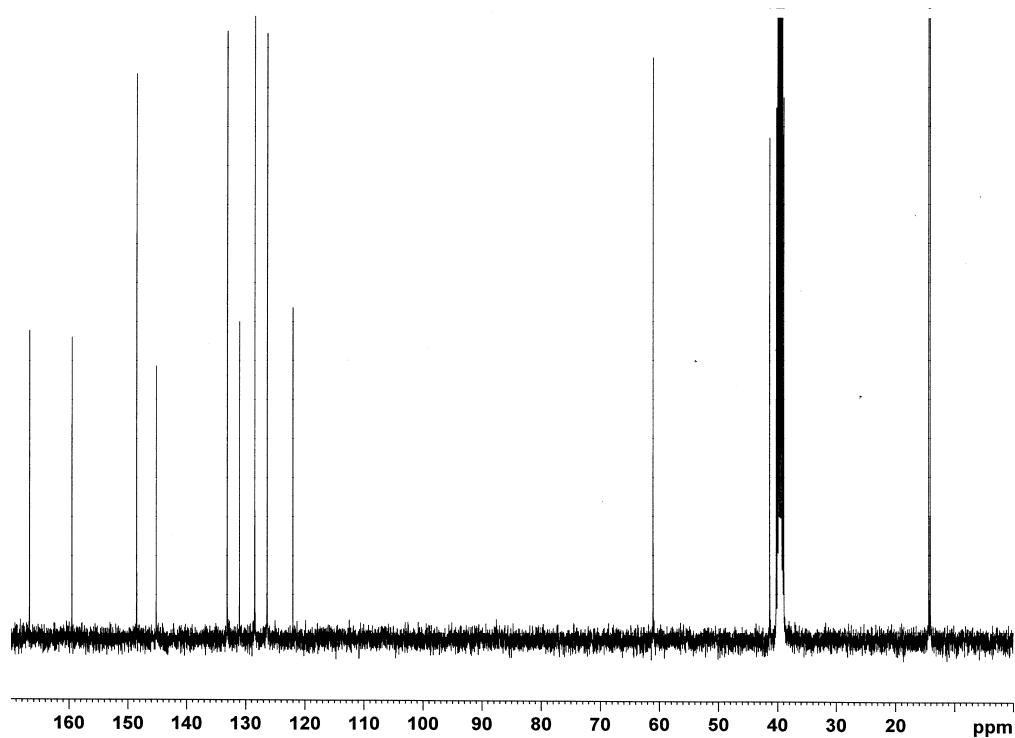
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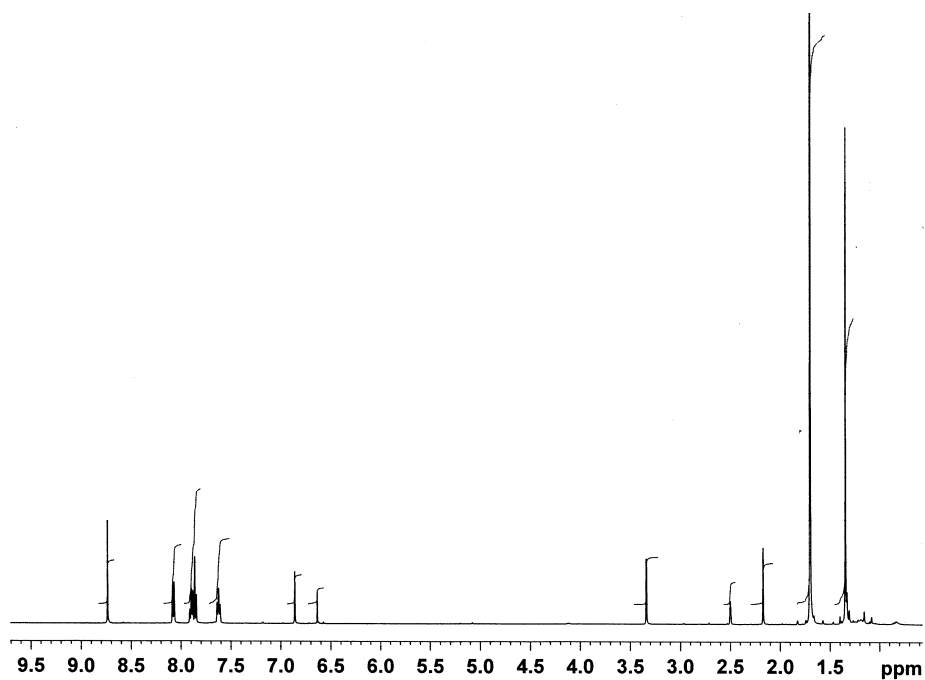
¹H NMR spectrum of 32b.



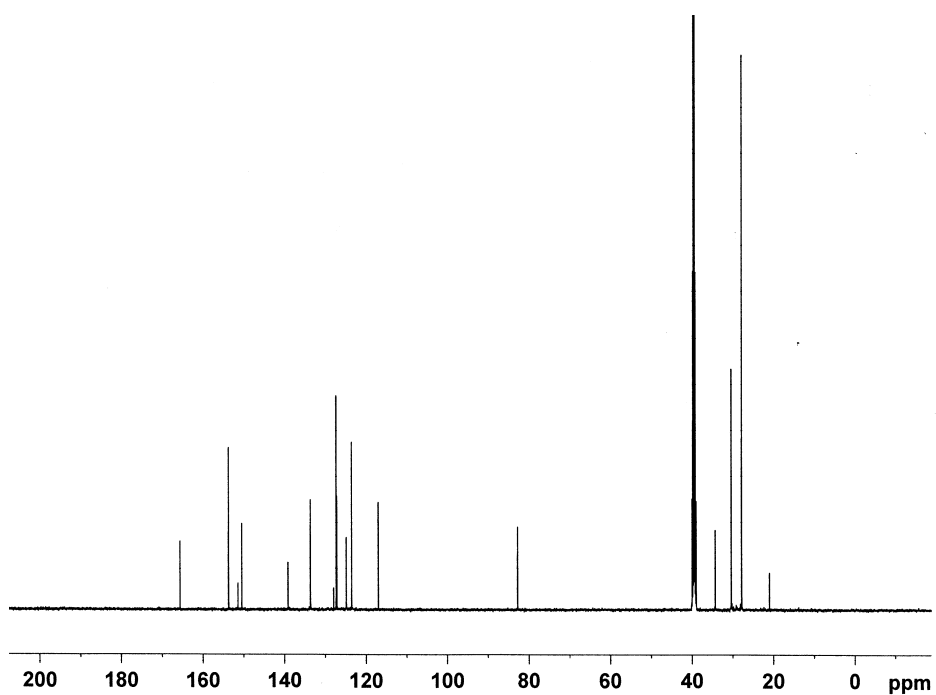
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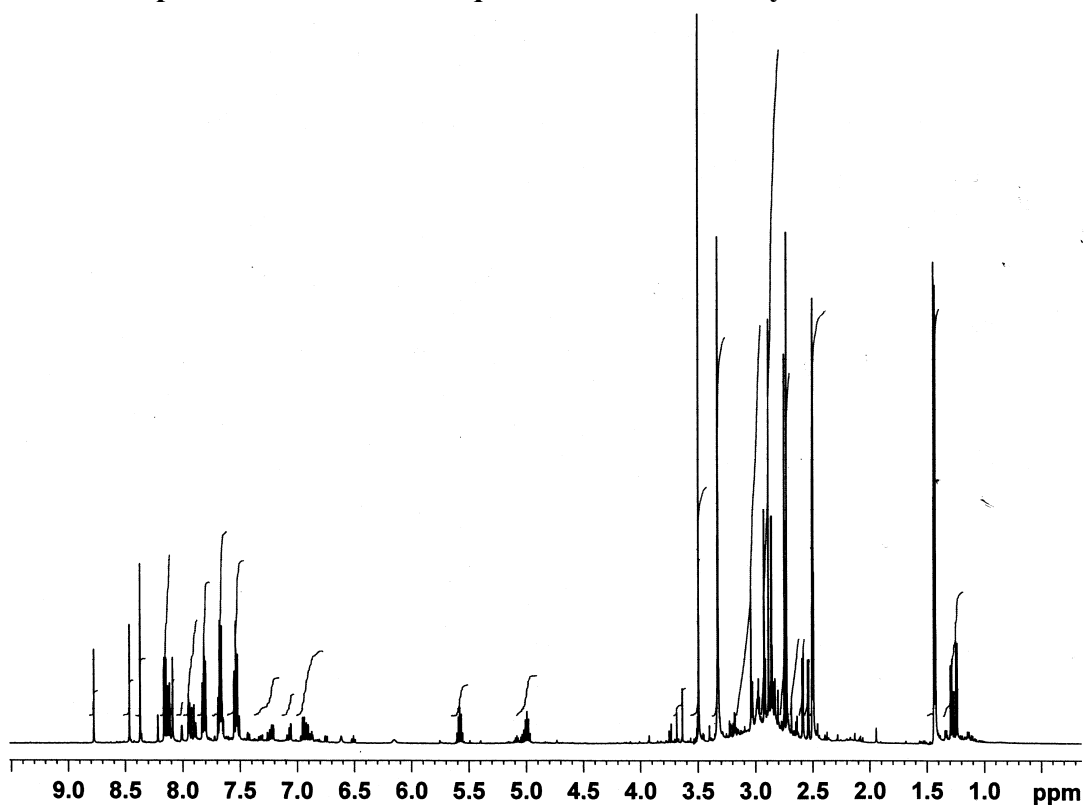
^1H NMR spectrum of crude 47f.



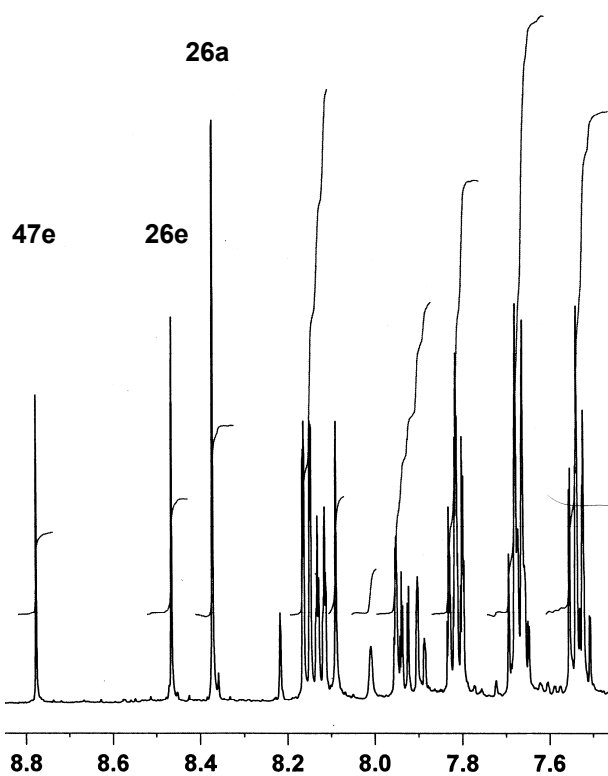
^{13}C NMR spectrum of crude 47f.



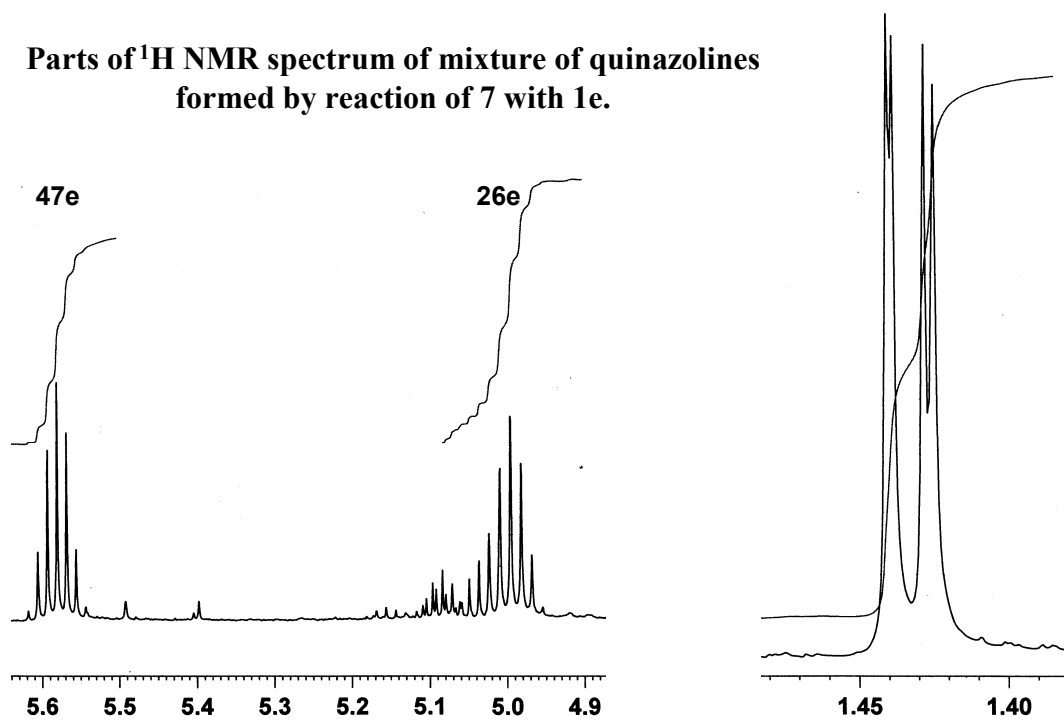
^1H NMR spectrum of mixture of quinazolines formed by reaction of 7 with 1e.



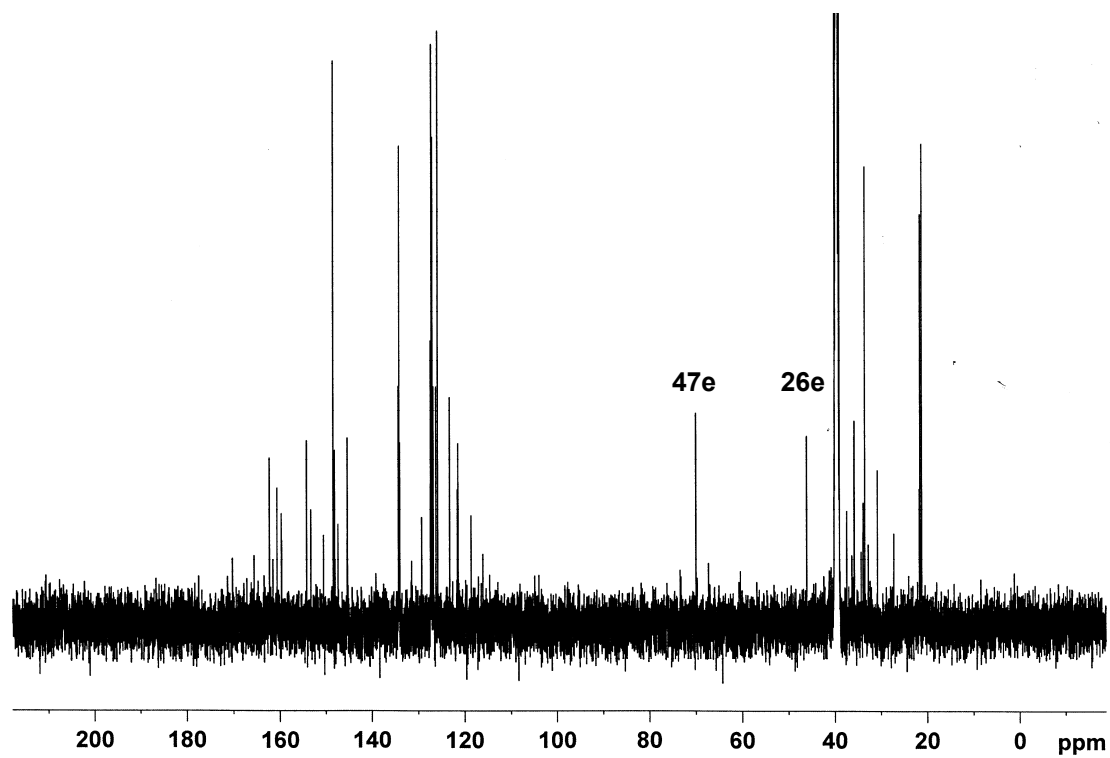
Part of ^1H NMR spectrum of mixture of quinazolines formed by reaction of 7 with 1e.



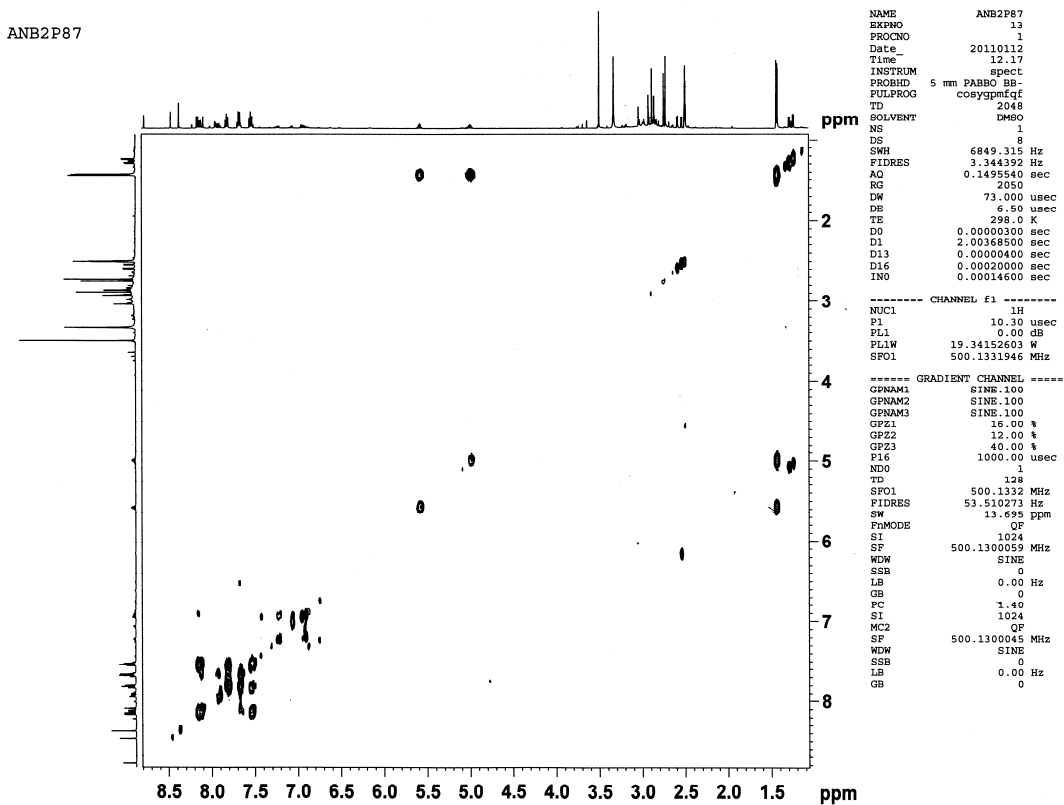
**Parts of ^1H NMR spectrum of mixture of quinazolines
formed by reaction of 7 with 1e.**



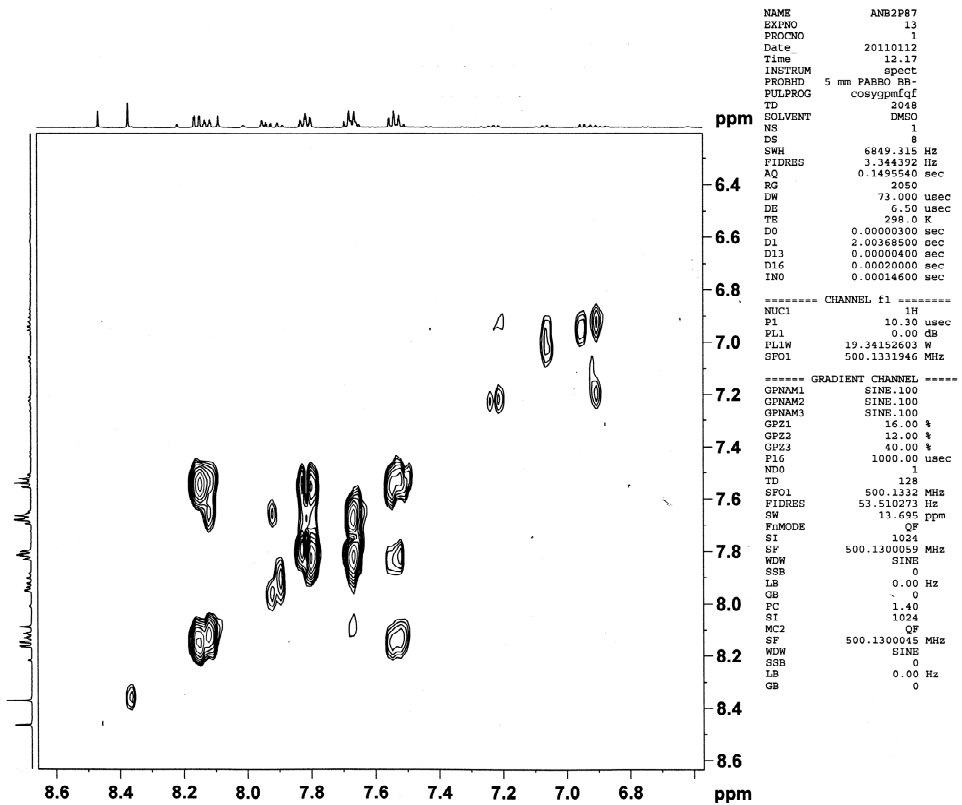
^{13}C NMR spectrum of mixture of quinazolines formed by reaction of 7 with 1e.



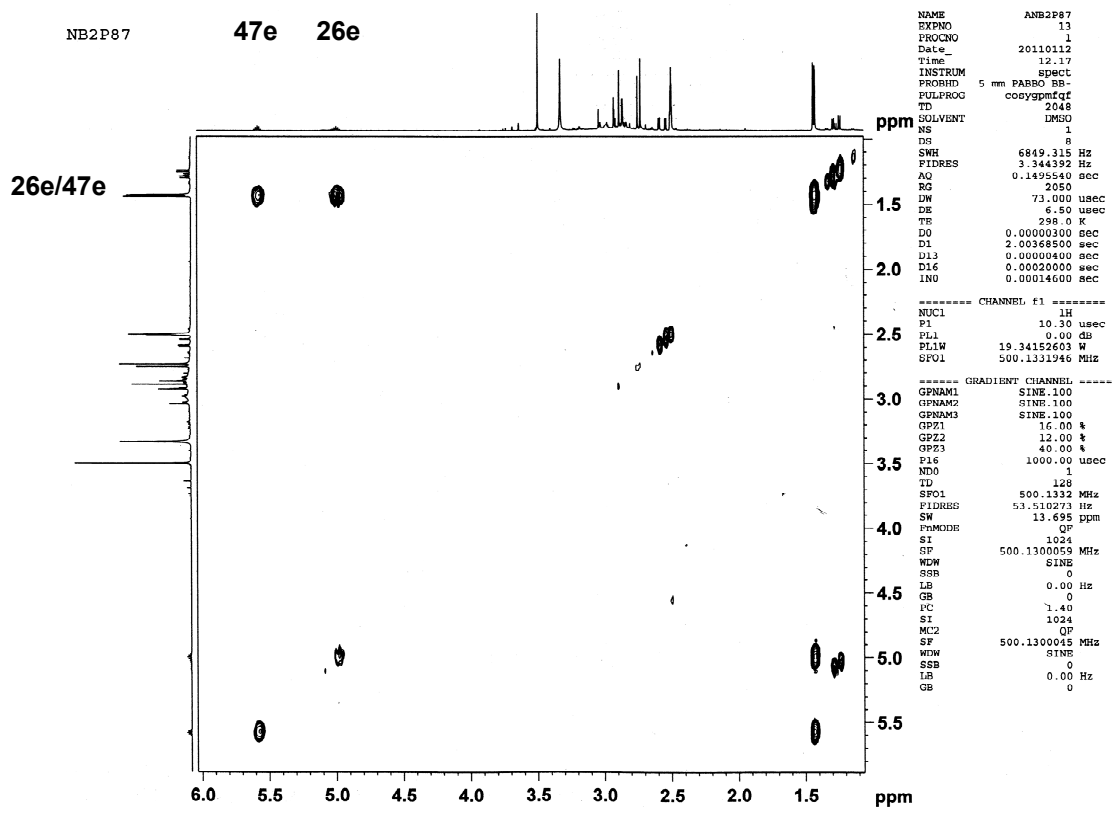
¹H-¹H COSY spectrum of mixture of quinazolines formed by reaction of 7 with 1e.



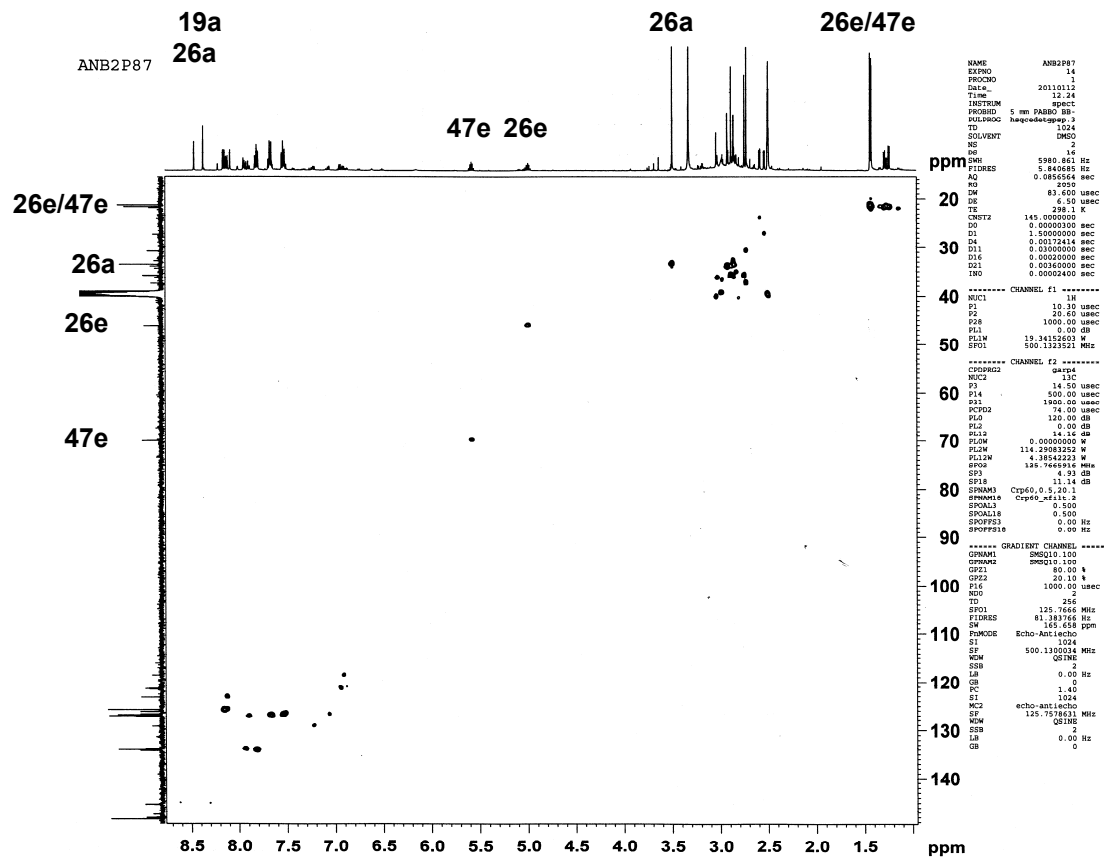
Part of ¹H-¹H COSY spectrum of mixture of quinazolines formed by reaction of 7 with 1e.



Part of ¹H-¹H COSY spectrum of mixture of quinazolines formed by
reaction of 7 with 1e.

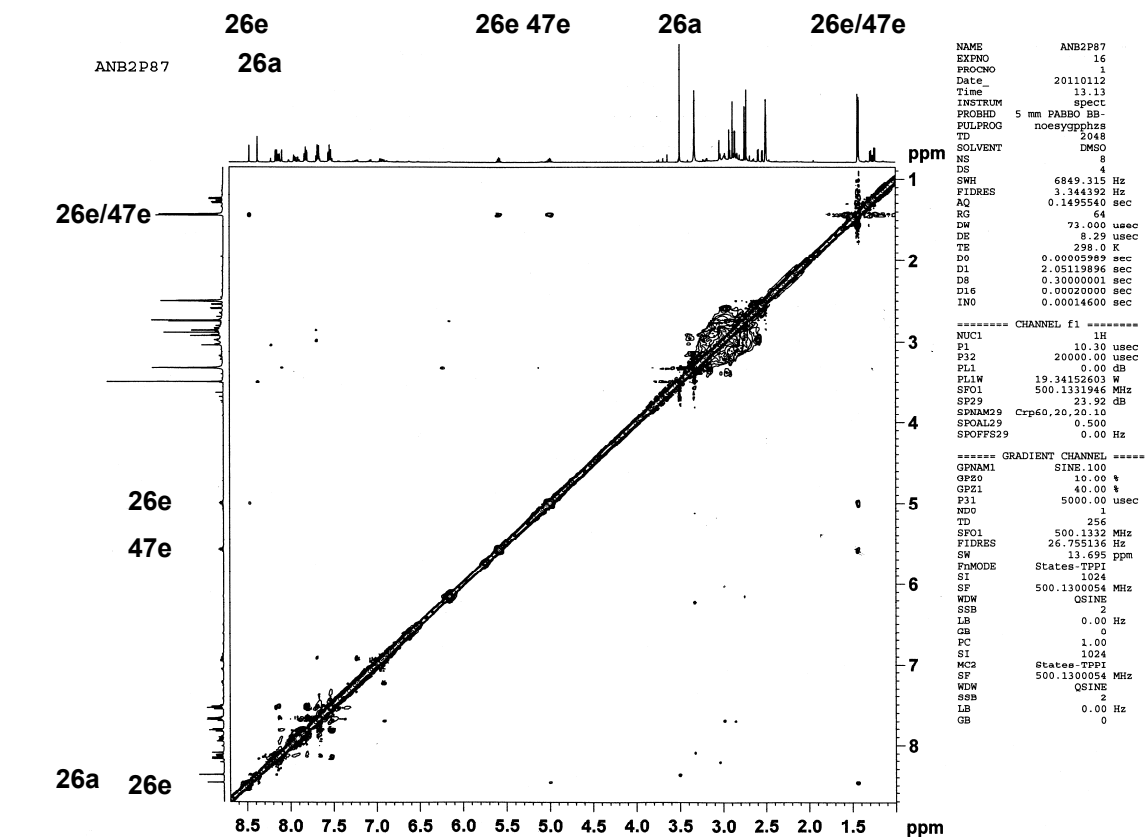


HSQC spectrum of mixture of quinazolines formed by reaction of 3a with 1e.

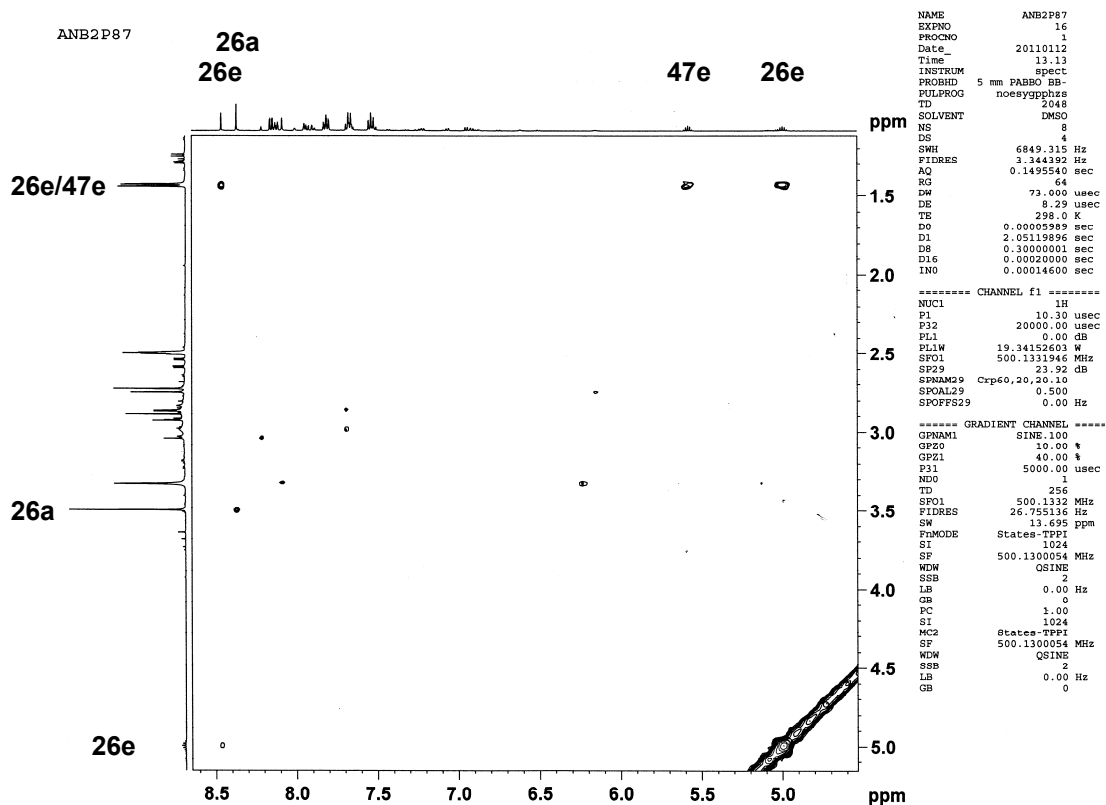




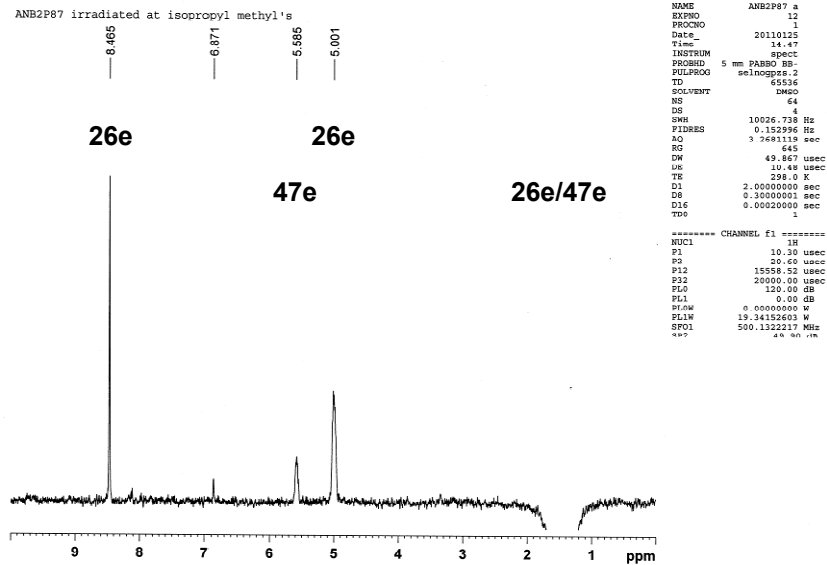
¹H-¹H NOESY spectrum of mixture of quinazolines formed by reaction of 7 with 1e.



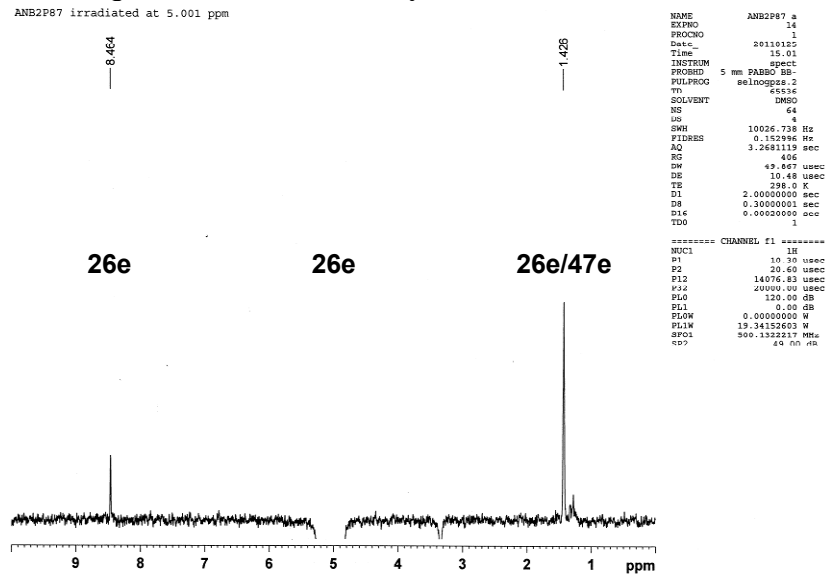
Part of ¹H-¹H NOESY spectrum of mixture of quinazolines formed by reaction of 7 with 1e.



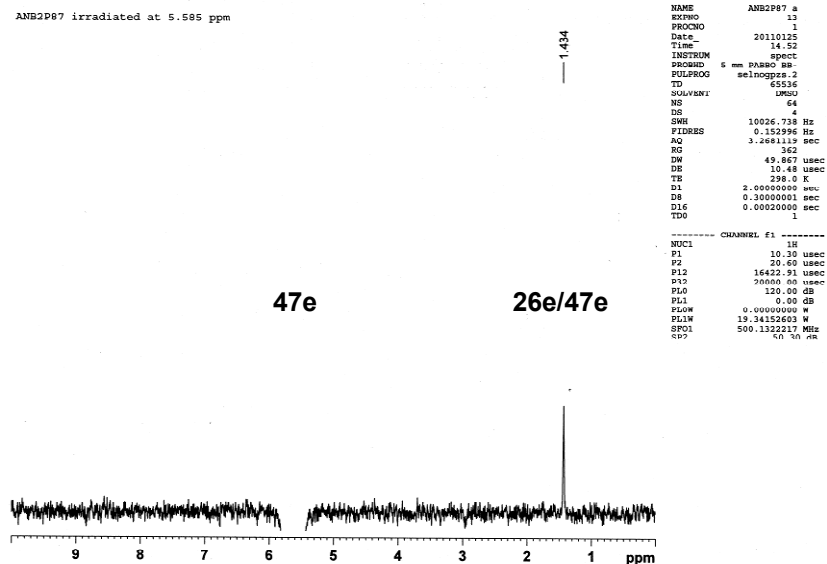
¹H NOE difference spectrum (irradiation at δ 1.5) of mixture of quinazolines formed by reaction of 7 with 1e.



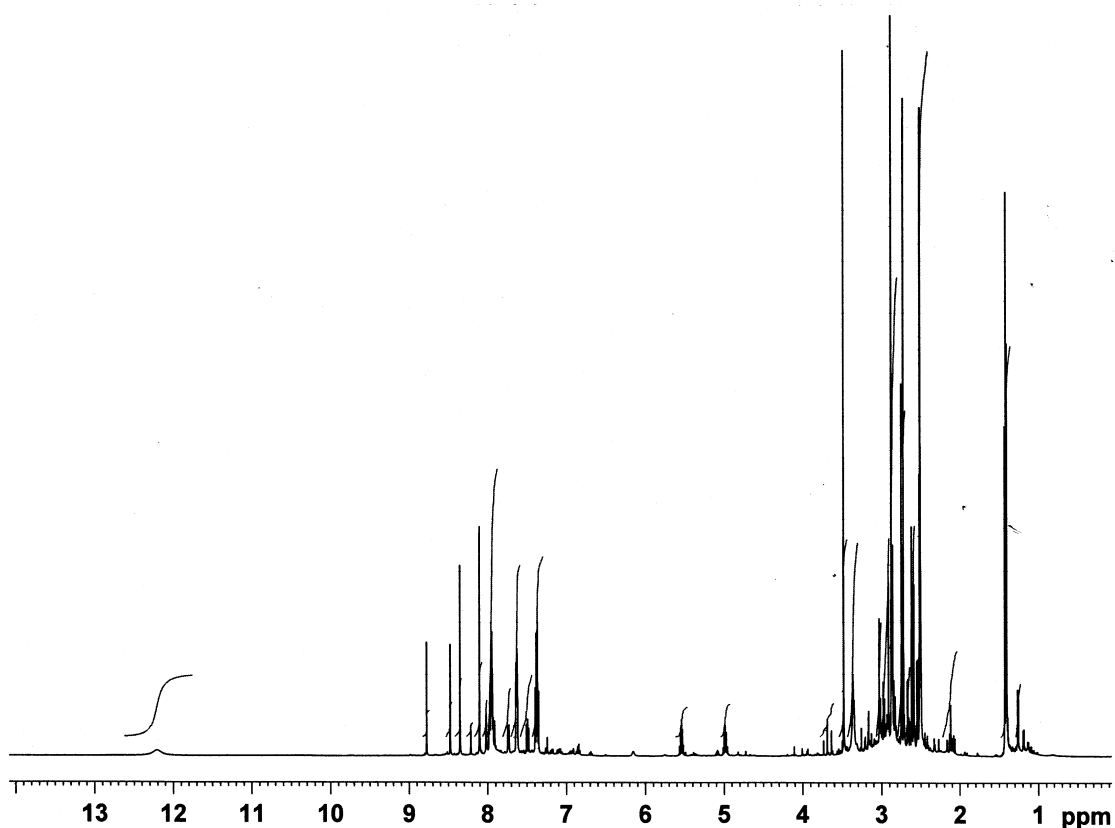
¹H NOE difference spectrum (irradiation at δ 5.00) of mixture of quinazolines formed by reaction of 7 with 1e.



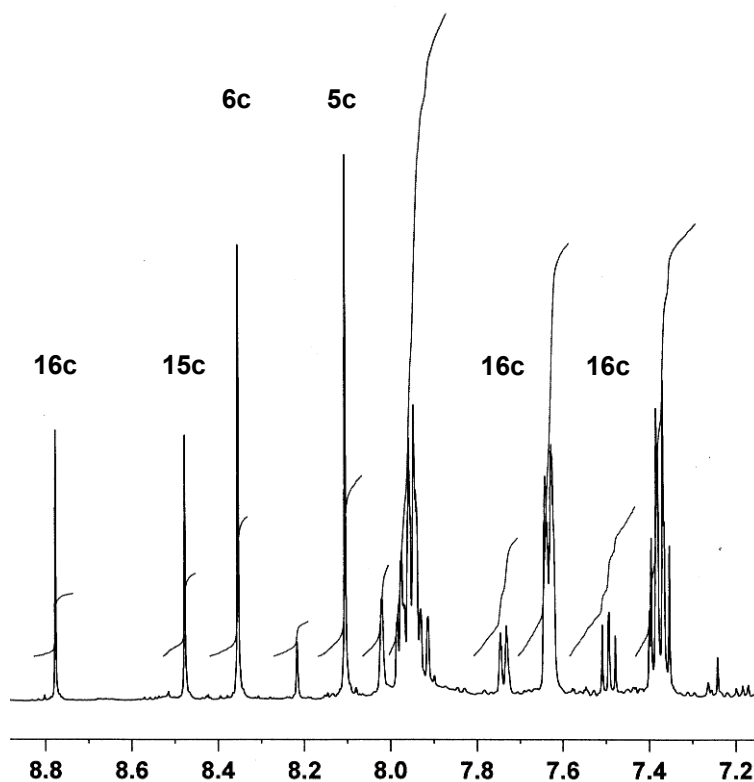
¹H NOE difference spectrum (irradiation at δ 5.58) of mixture of quinazolines formed by reaction of 7 with 1e.



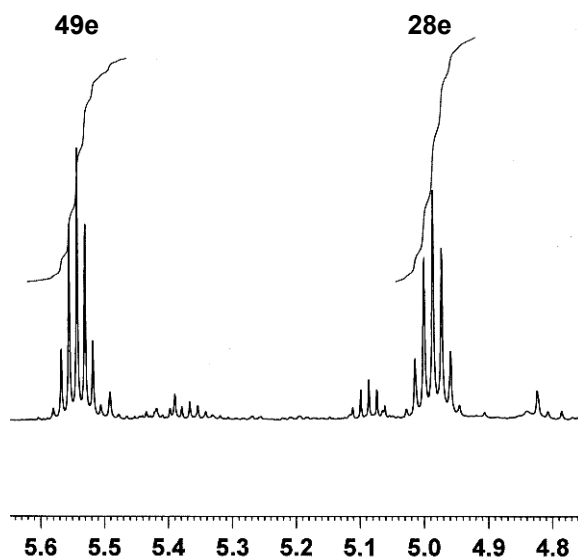
^1H NMR spectrum of mixture of quinazolines formed by reaction of 9 with 1e.



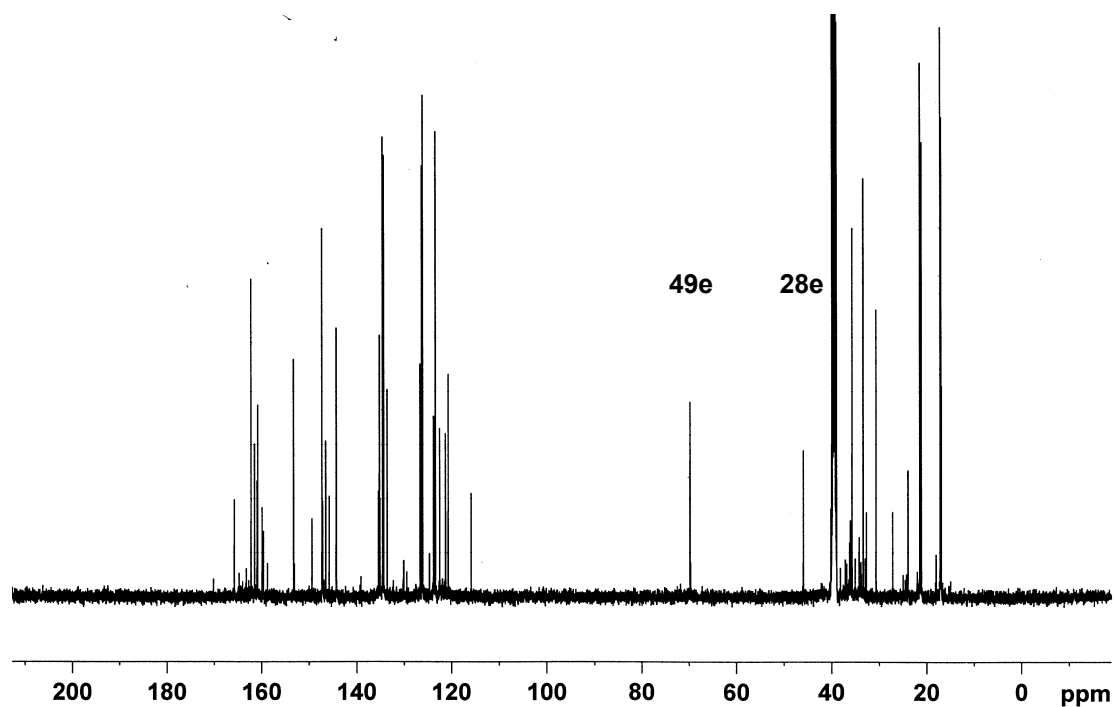
Part of ^1H NMR spectrum of mixture of quinazolines formed by reaction of 9 with 1e.



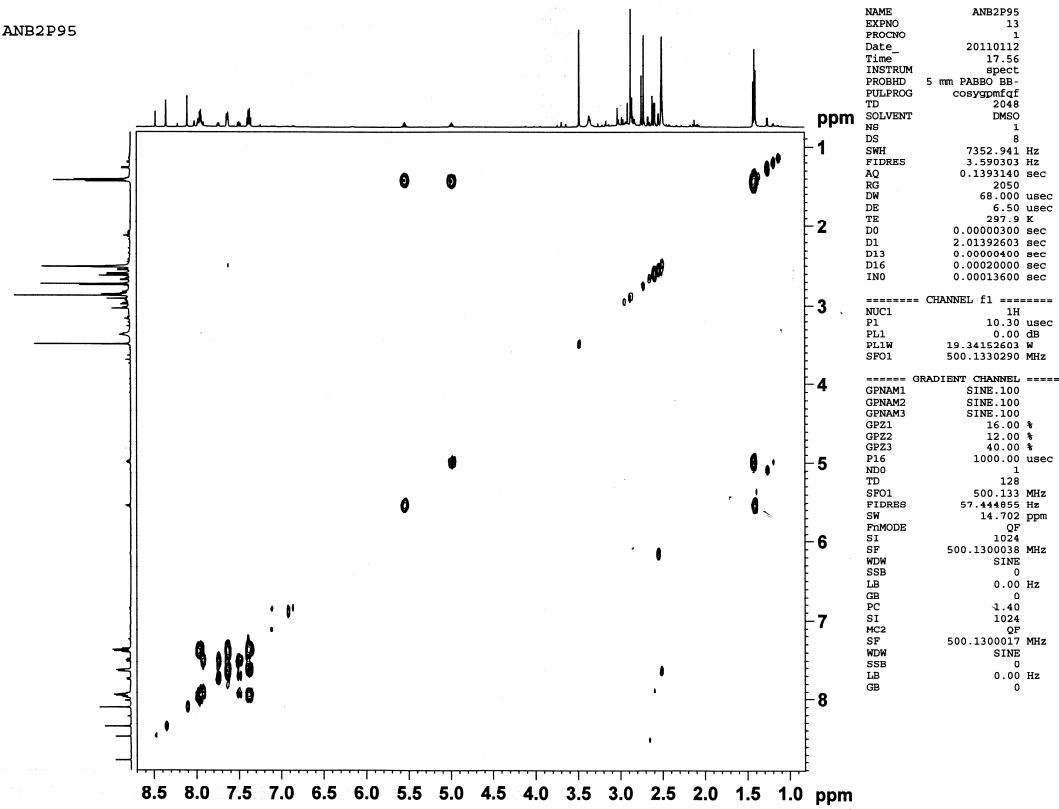
**Part of ^1H NMR spectrum of mixture of quinazolines
formed by reaction of 9 with 1e.**



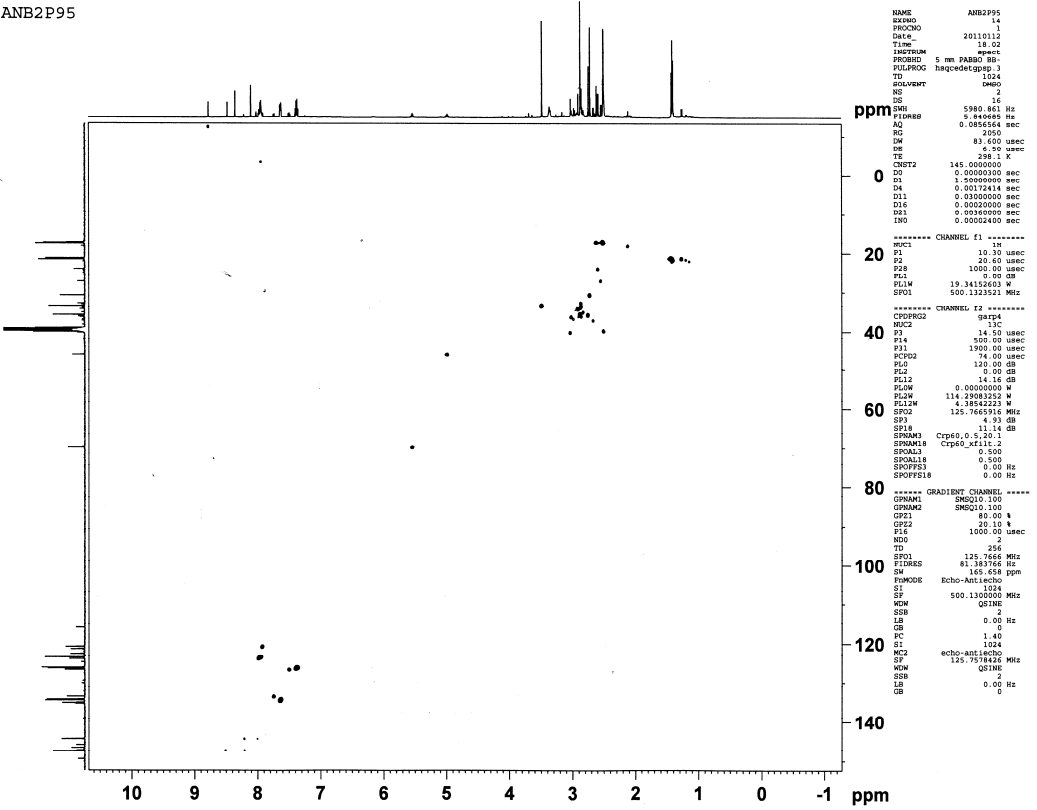
^{13}C NMR spectrum of mixture of quinazolines formed by reaction of 9 with 1e.



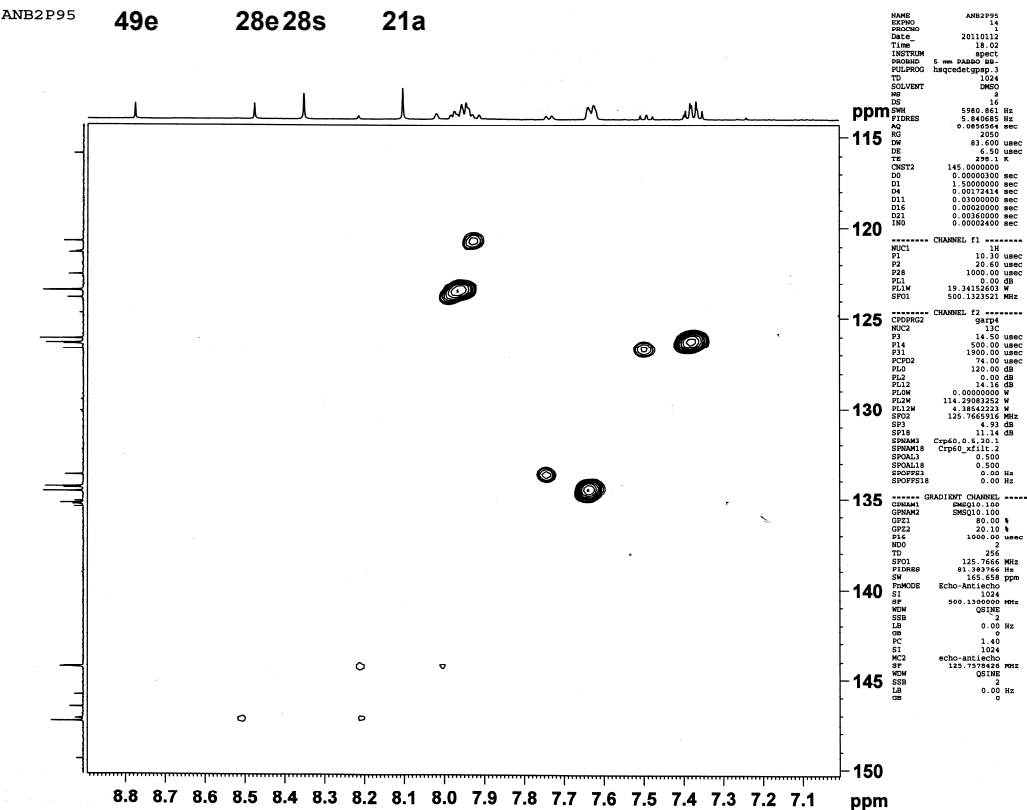
¹H-¹H COSY spectrum of mixture of quinazolines formed by reaction of 9 with 1e.



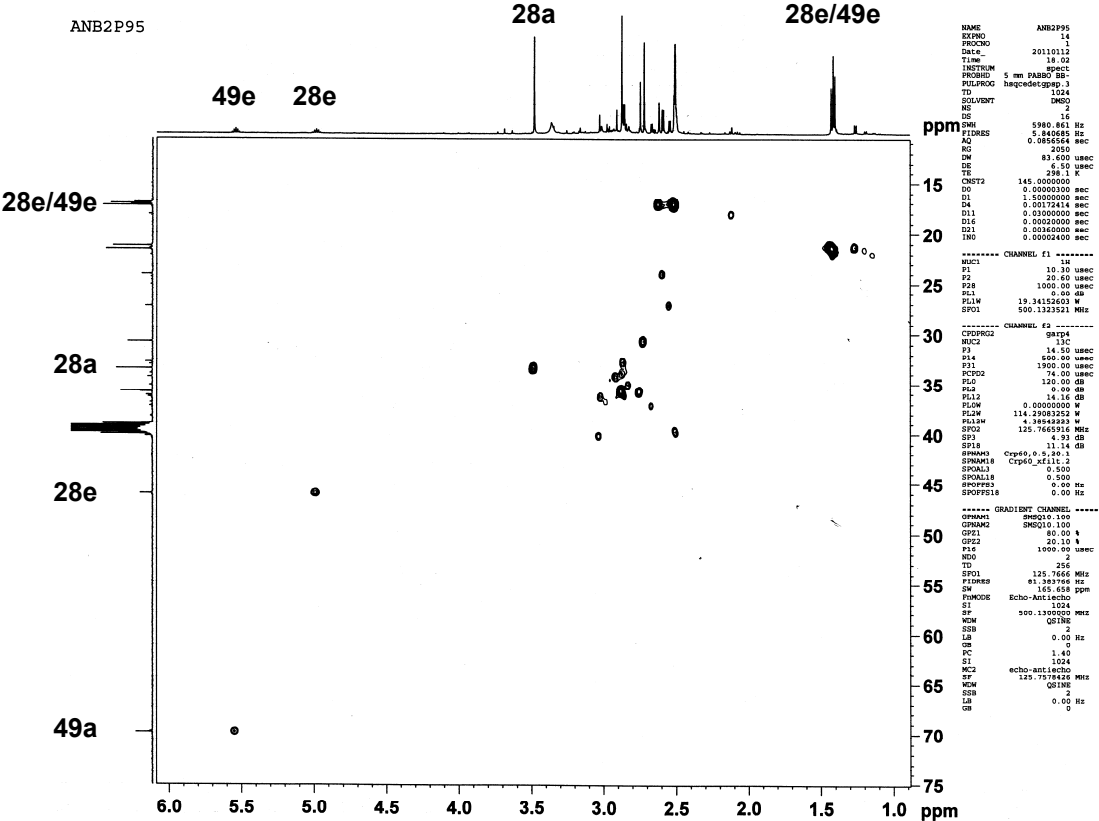
HSQC spectrum of mixture of quinazolines formed by reaction of 9 with 1e.



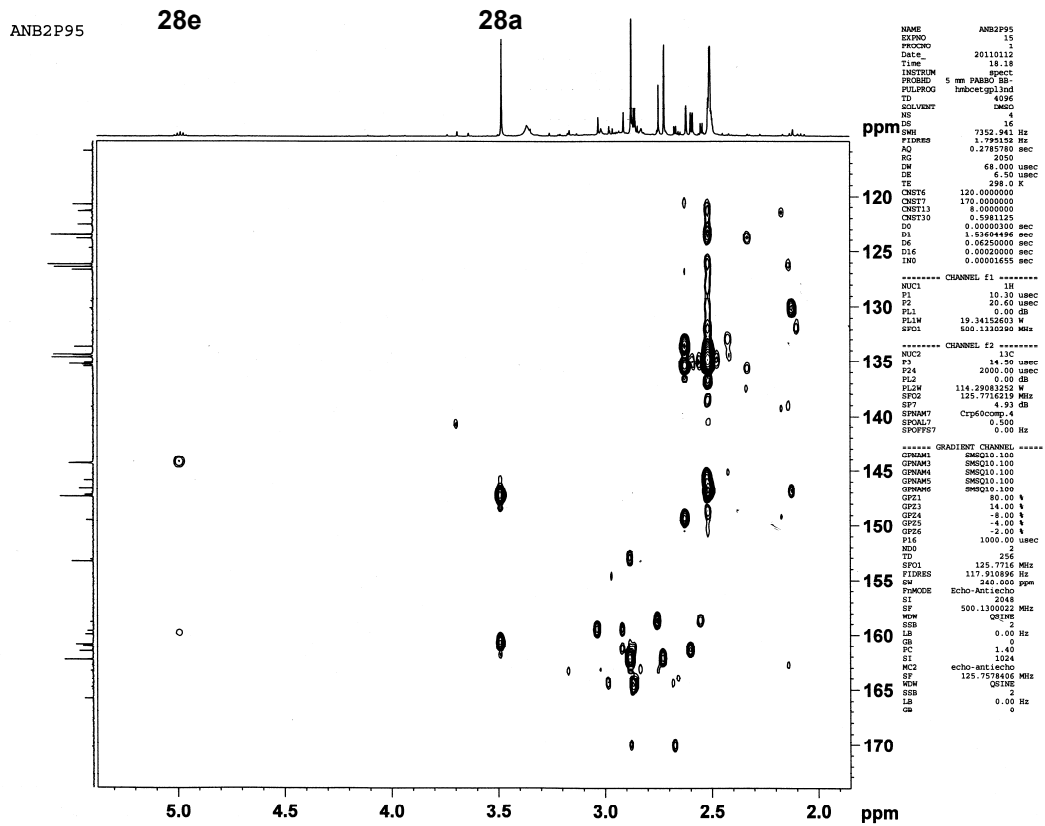
Part of HSQC spectrum of mixture of quinazolines formed by reaction of
9 with 1e.



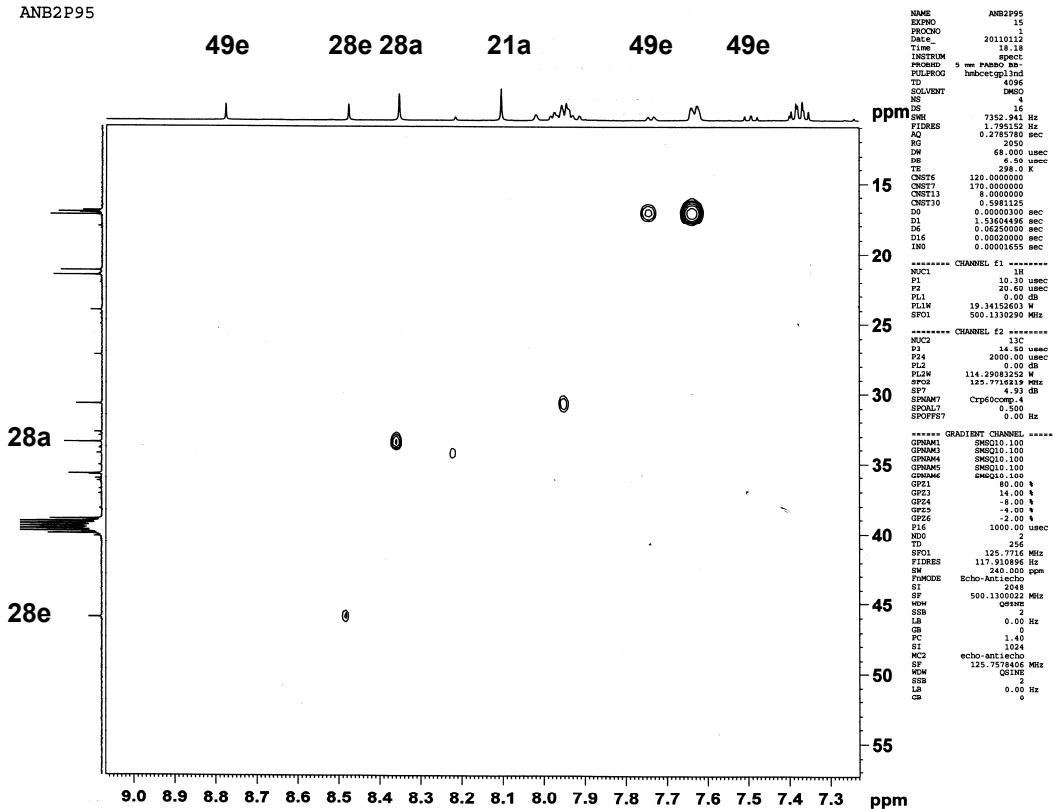
Part of HSQC spectrum of mixture of quinazolines formed by reaction of
9 with 1e.



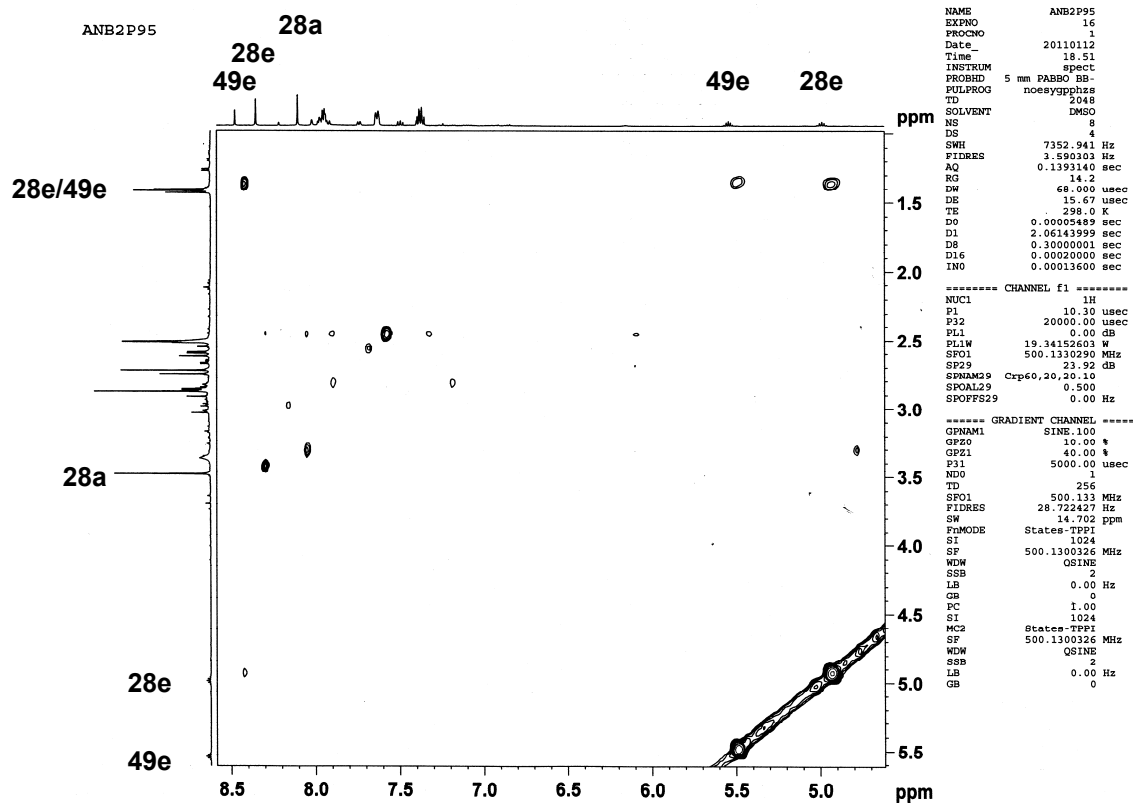
Part of HMBC spectrum of mixture of quinazolines formed by reaction of 9 with 1e.



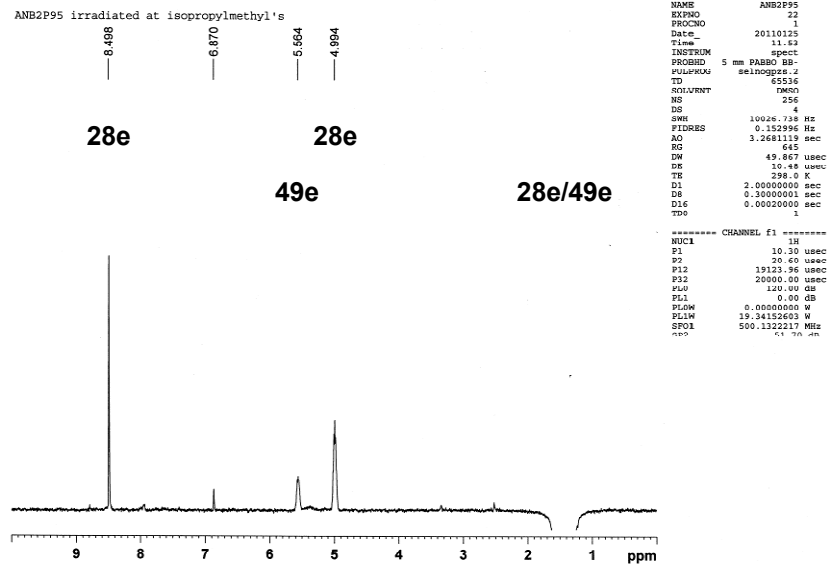
Part of HMBC spectrum of mixture of quinazolines formed by reaction of 9 with 1e.



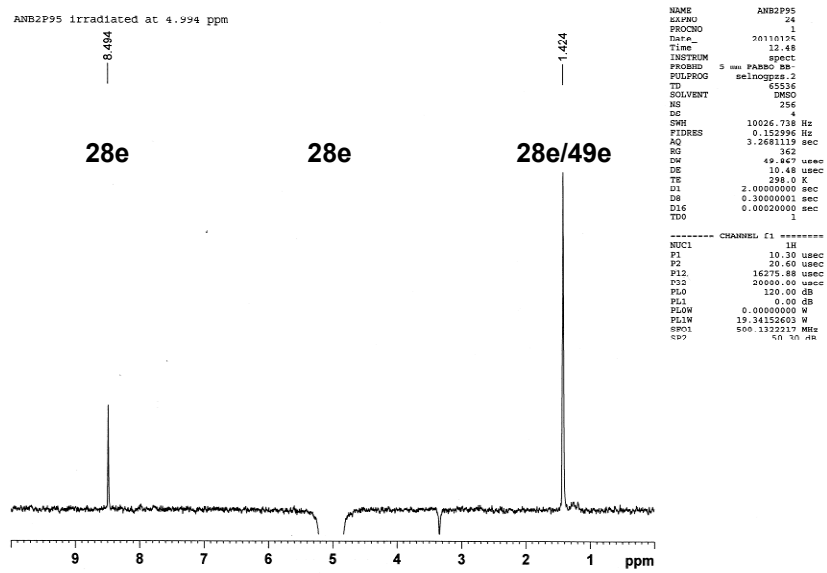
Part of ¹H-¹H NOESY spectrum of mixture of quinazolines formed by
reaction of 9 with 1e.



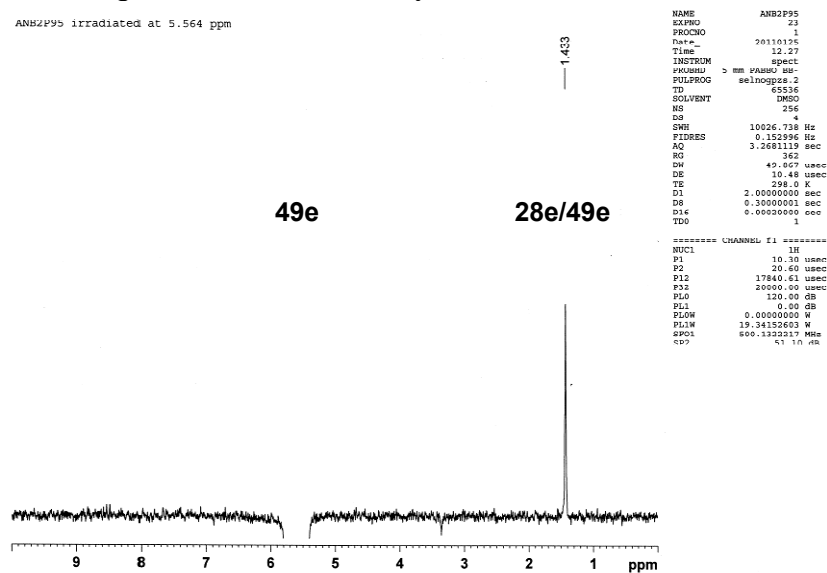
¹H NOE difference spectrum (irradiation at δ 1.5) of mixture of quinazolines formed by reaction of 9 with 1e.



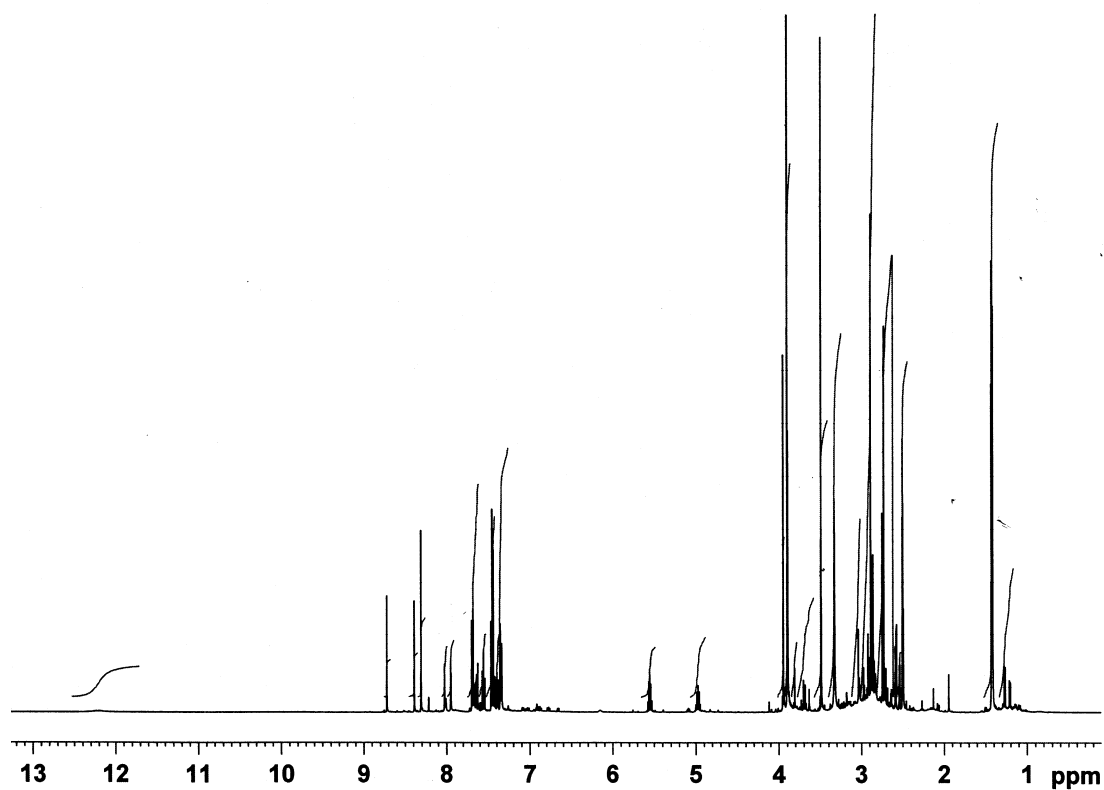
¹H NOE difference spectrum (irradiation at δ 4.99) of mixture of quinazolines formed by reaction of 9 with 1e.



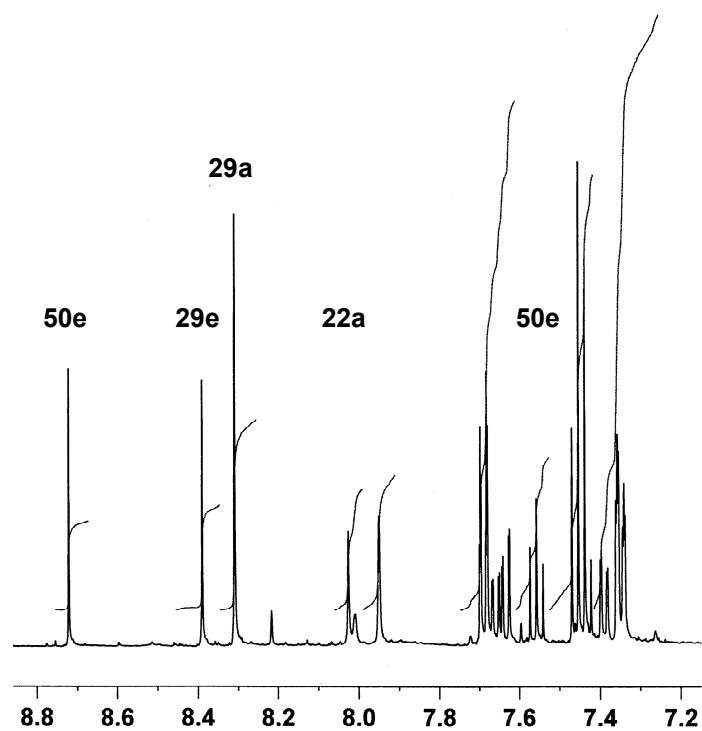
¹H NOE difference spectrum (irradiation at δ 5.56) of mixture of quinazolines formed by reaction of 9 with 1e.



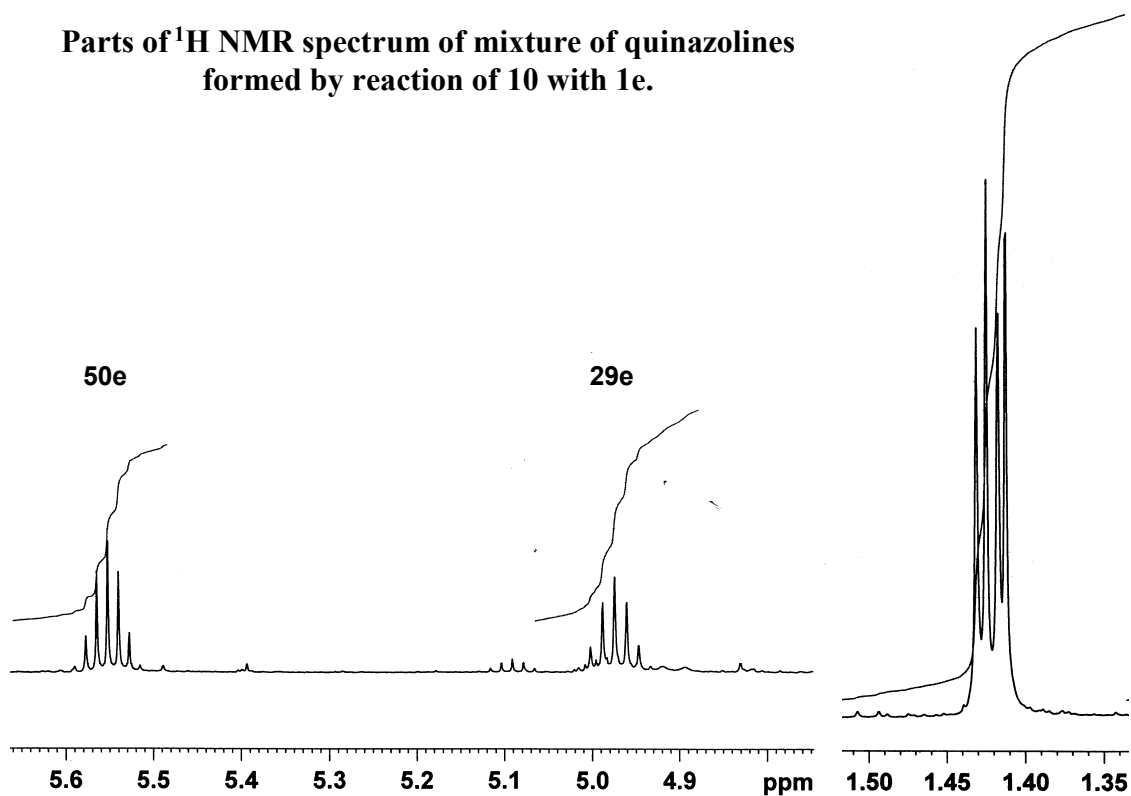
^1H NMR spectrum of mixture of quinazolines formed by reaction of 10 with 1e.



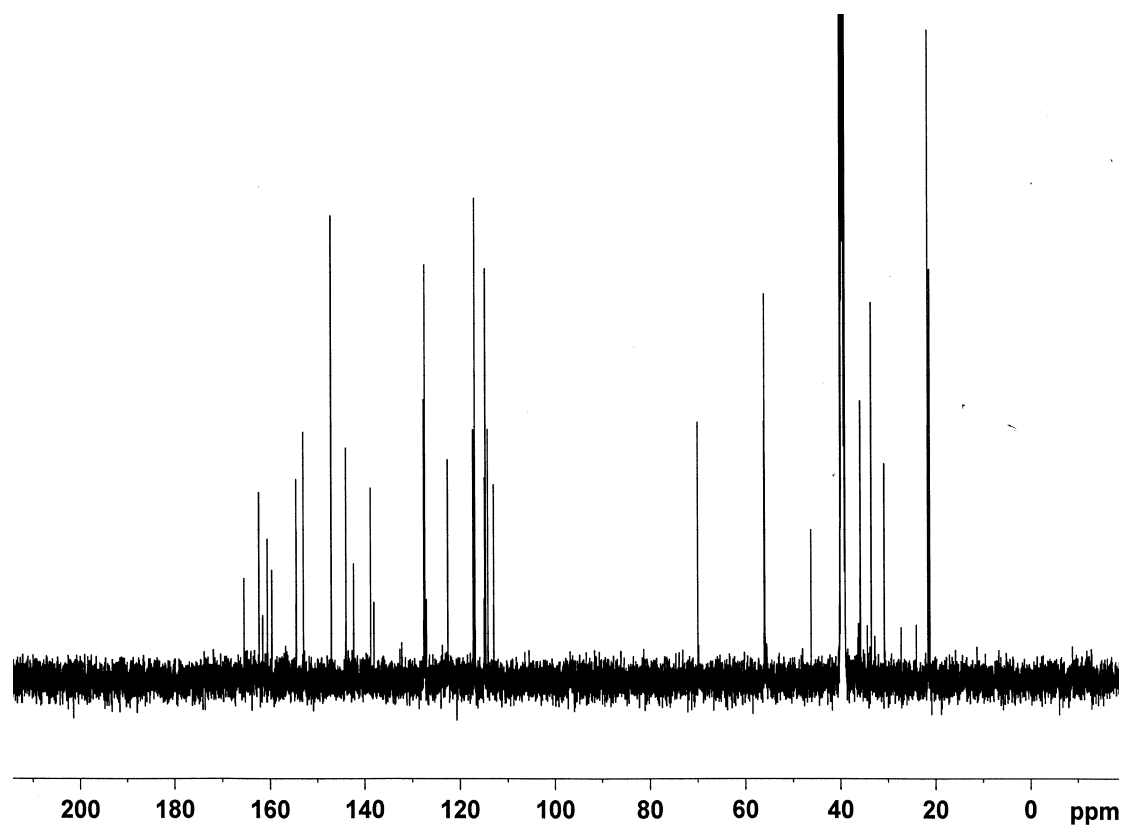
Part of ^1H NMR spectrum of mixture of quinazolines formed by reaction of 10 with 1e.



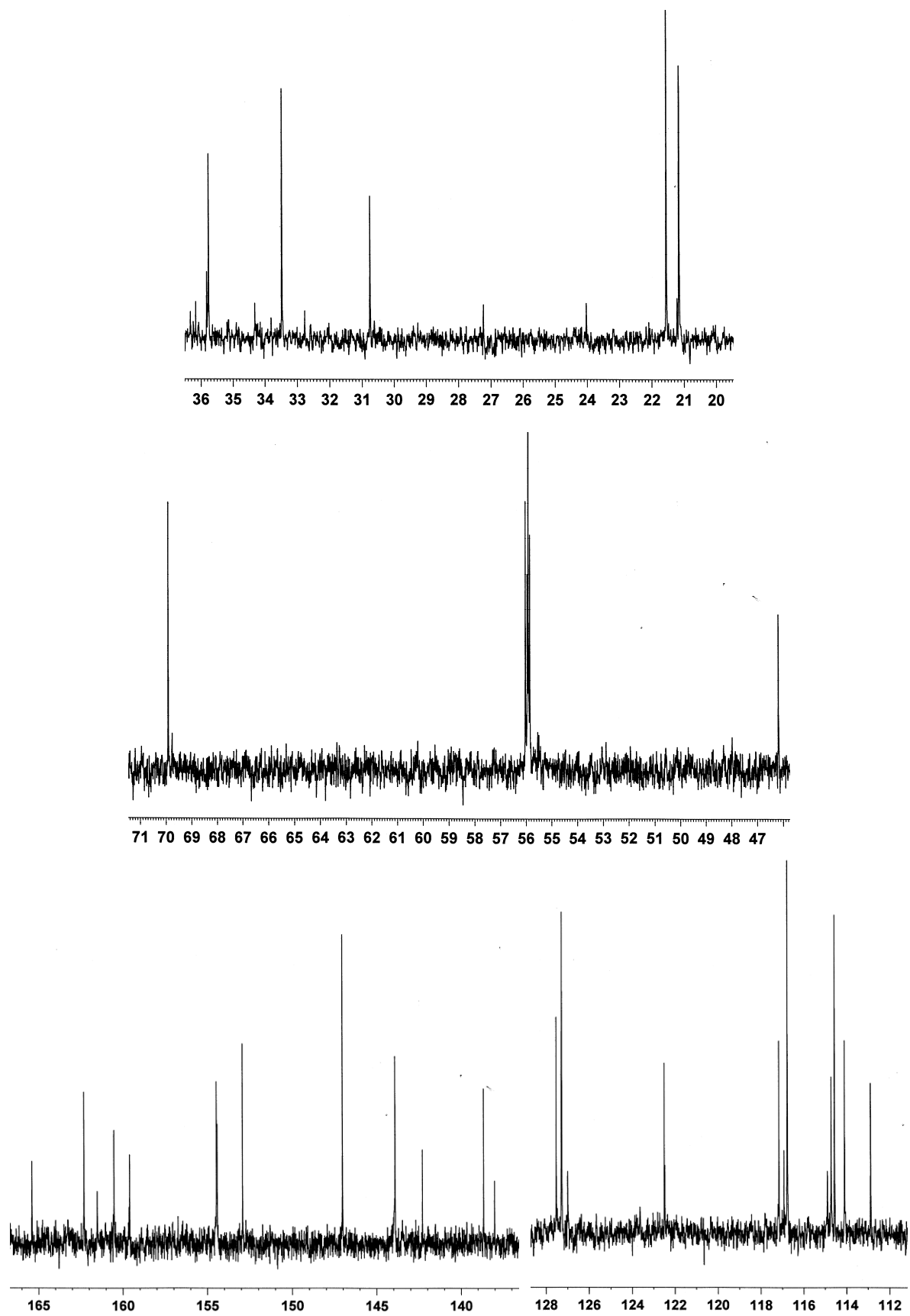
**Parts of ^1H NMR spectrum of mixture of quinazolines
formed by reaction of 10 with 1e.**



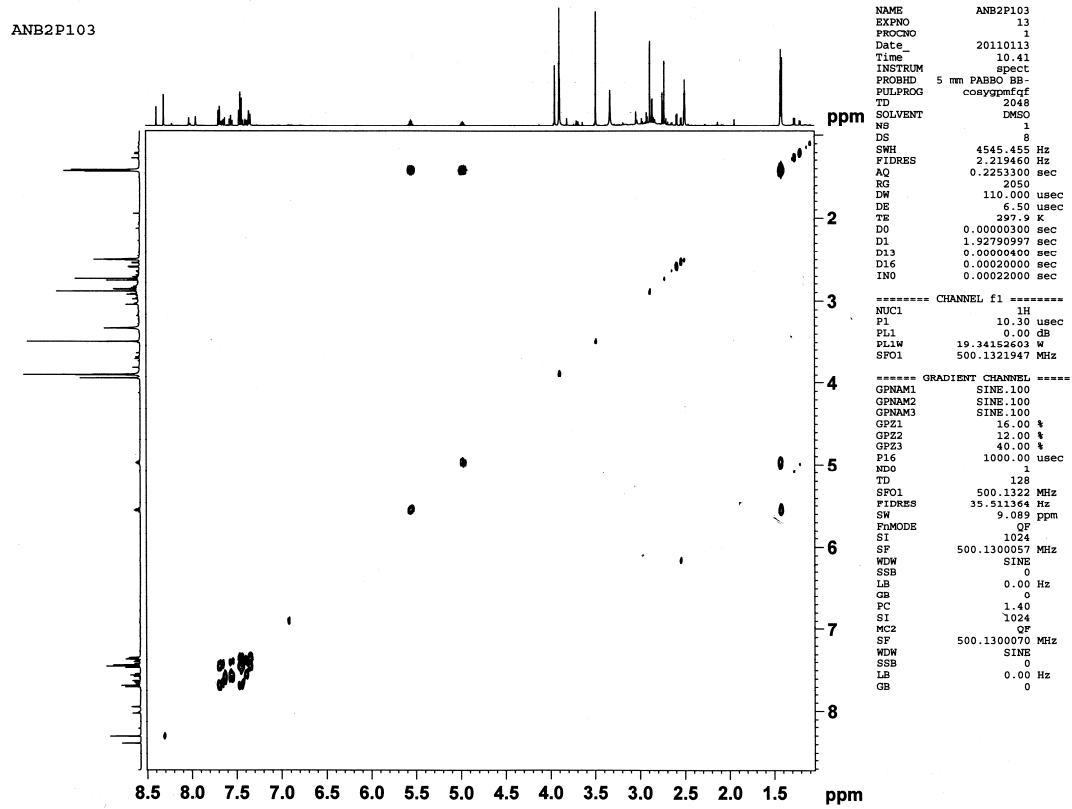
^{13}C NMR spectrum of mixture of quinazolines formed by reaction of 10 with 1e.



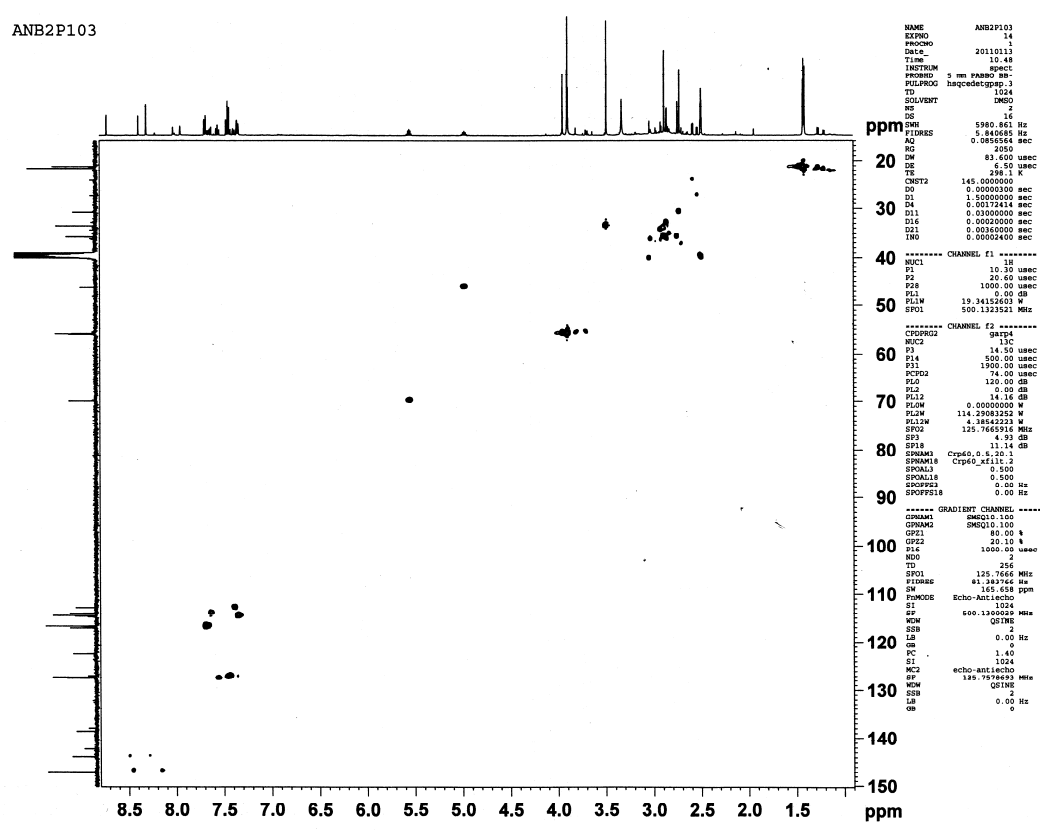
Parts of ¹³C NMR spectrum of mixture of quinazolines formed by reaction of 10 with 1e.



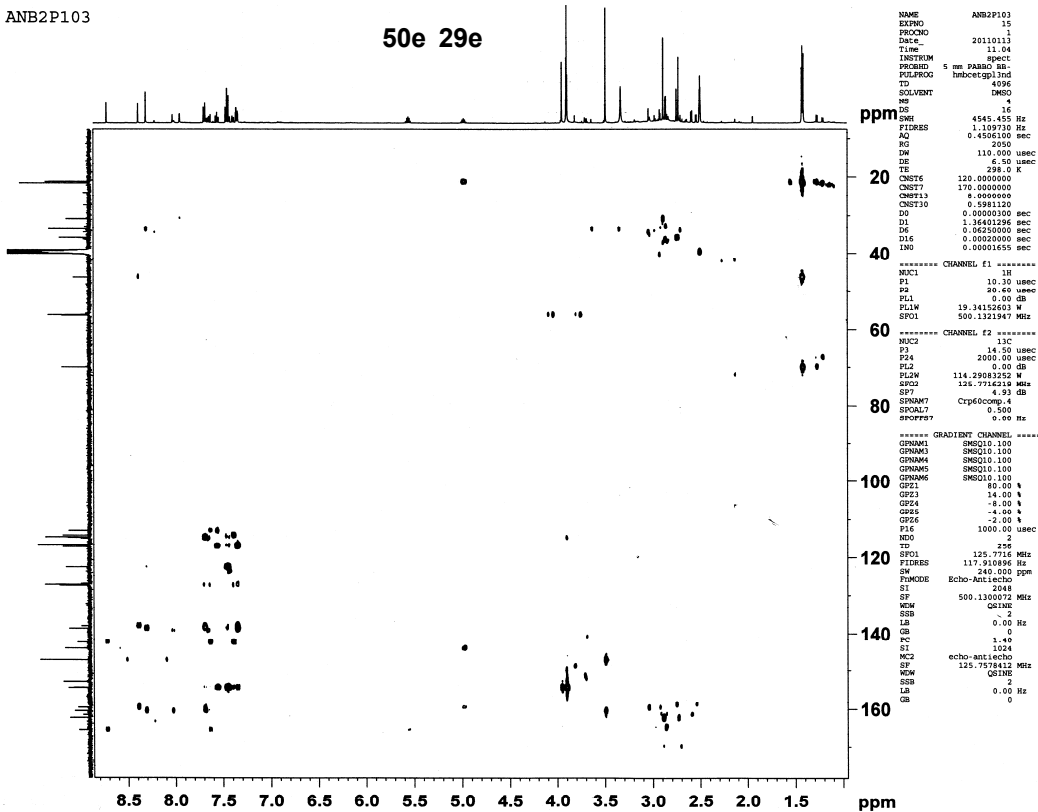
¹H-¹H COSY spectrum of mixture of quinazolines formed by reaction of 10 with 1e.



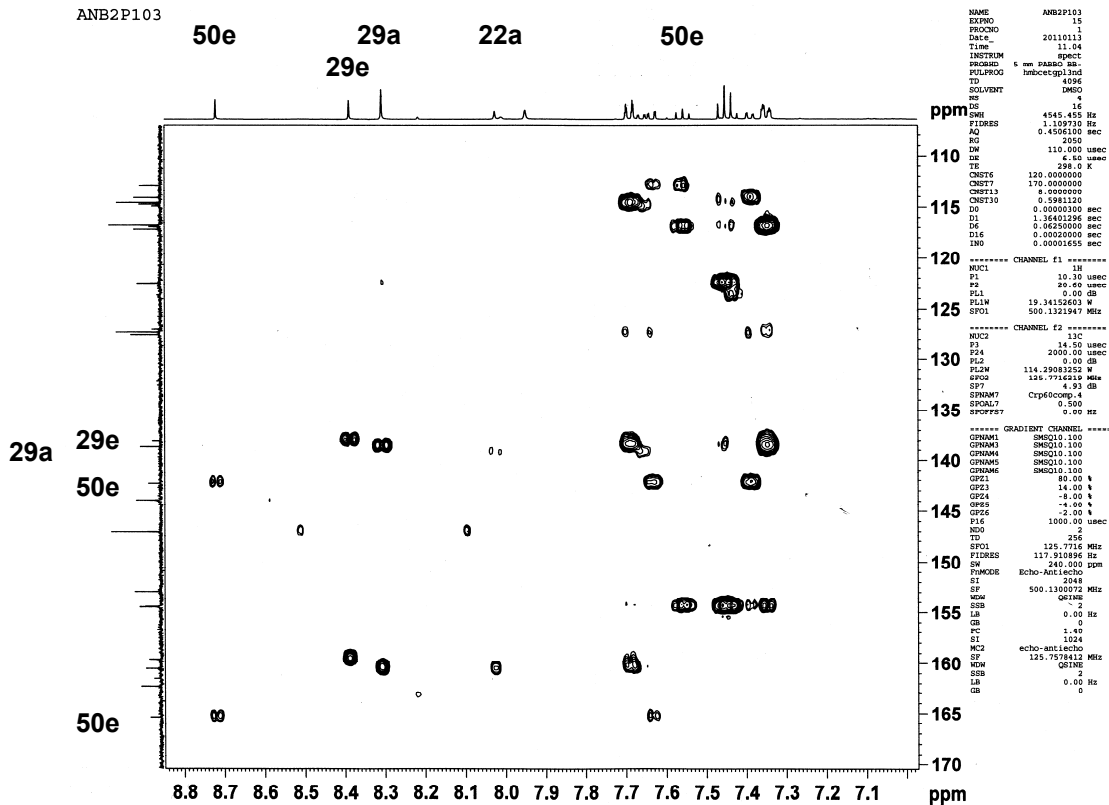
HSQC spectrum of mixture of quinazolines formed by reaction of 10 with 1e.



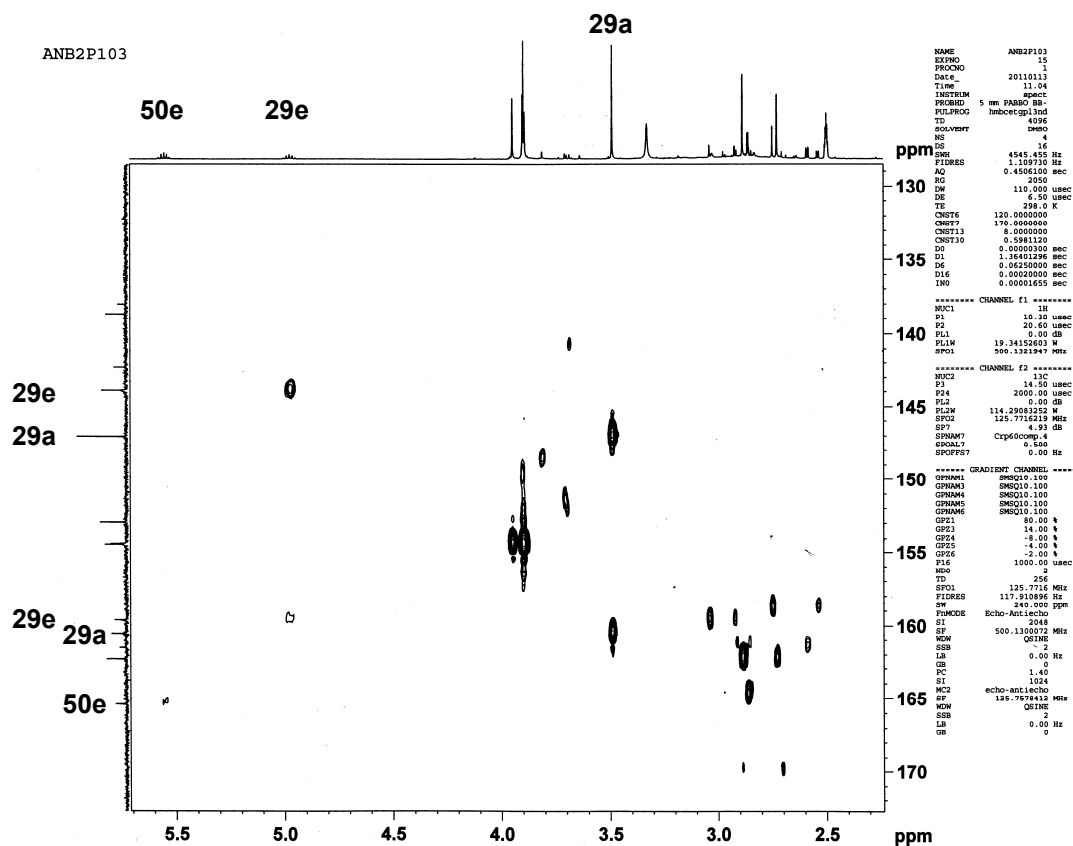
HMBC spectrum of mixture of quinazolines formed by reaction of 10 with 1e.



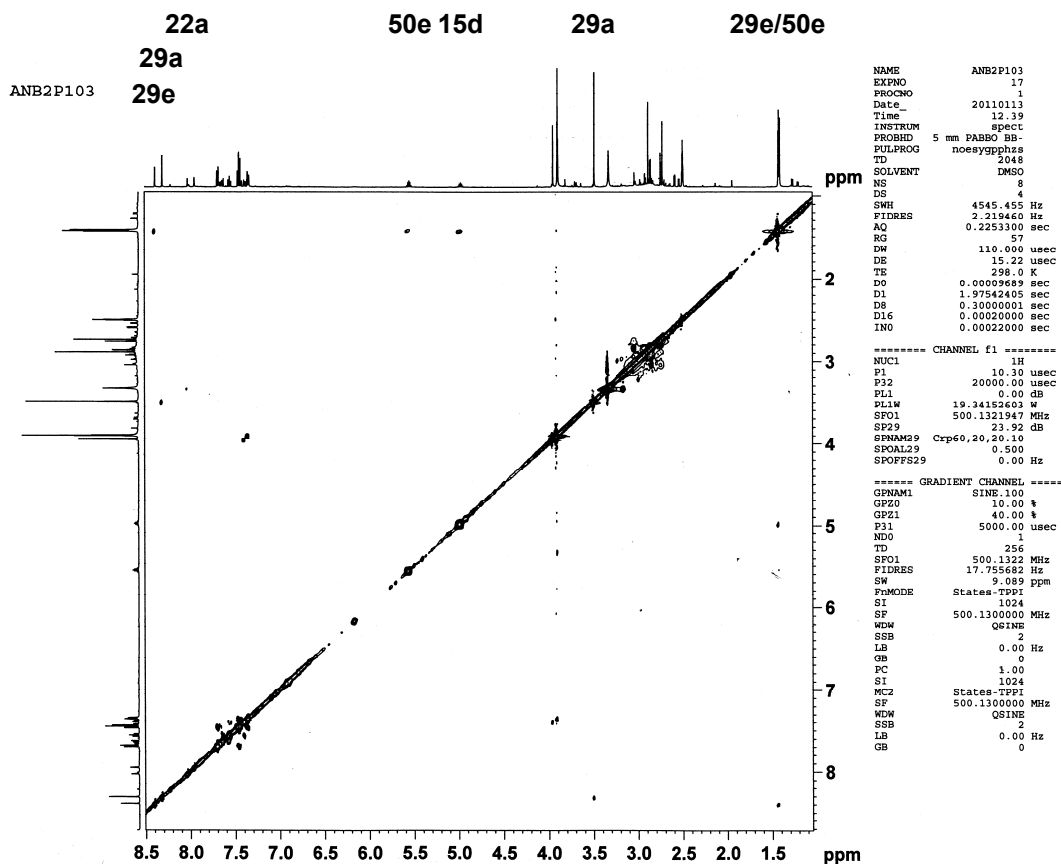
Part of HMBC spectrum of mixture of quinazolines formed by reaction of 10 with 1e.



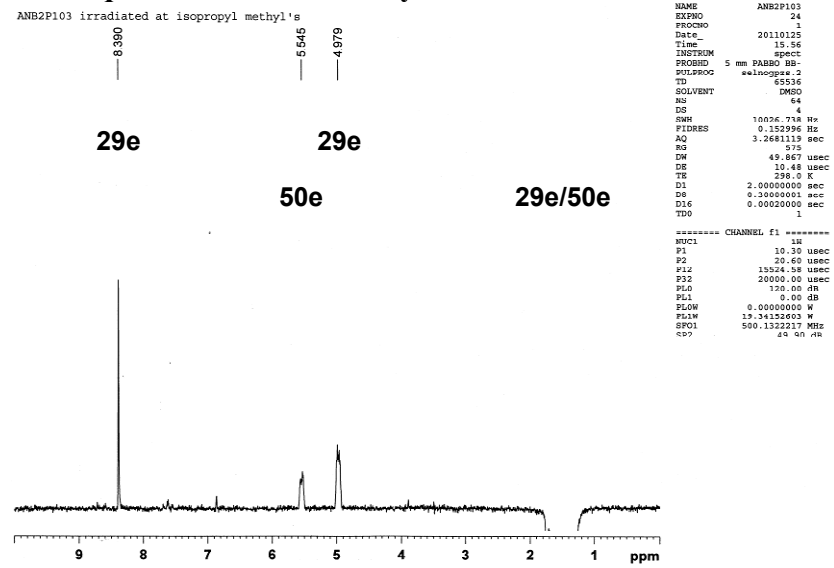
Part of HMBC spectrum of mixture of quinazolines formed by reaction of
10 with 1e.



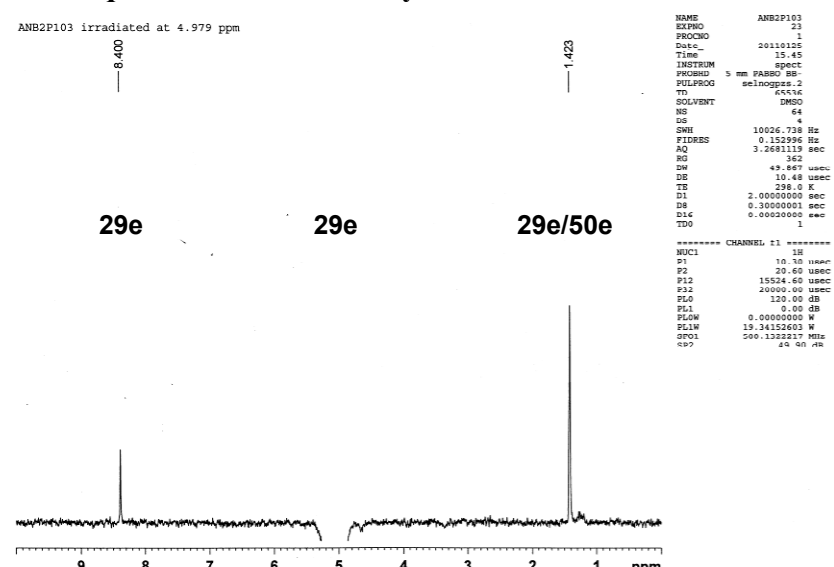
^1H - ^1H NOESY spectrum of mixture of quinazolines formed by reaction of
10 with 1e.



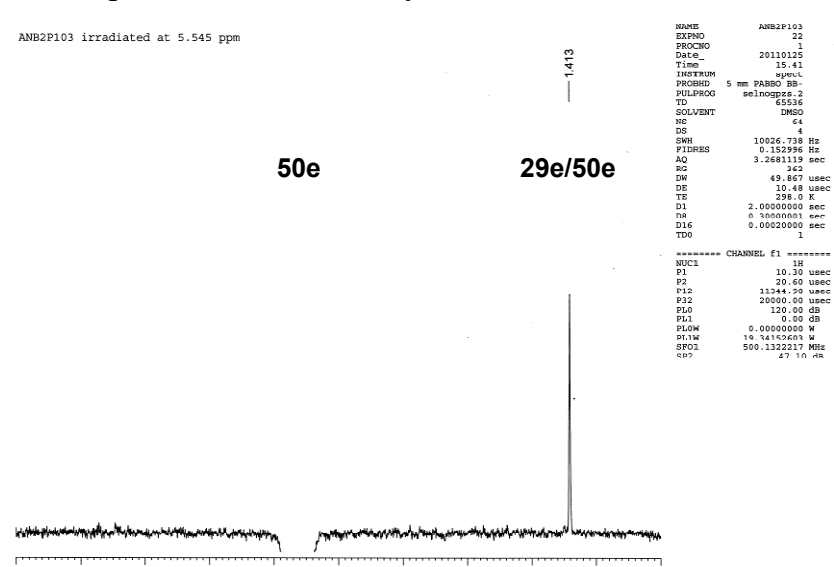
¹H NOE difference spectrum (irradiation at δ 1.5) of mixture of quinazolines formed by reaction of 10 with 1e.



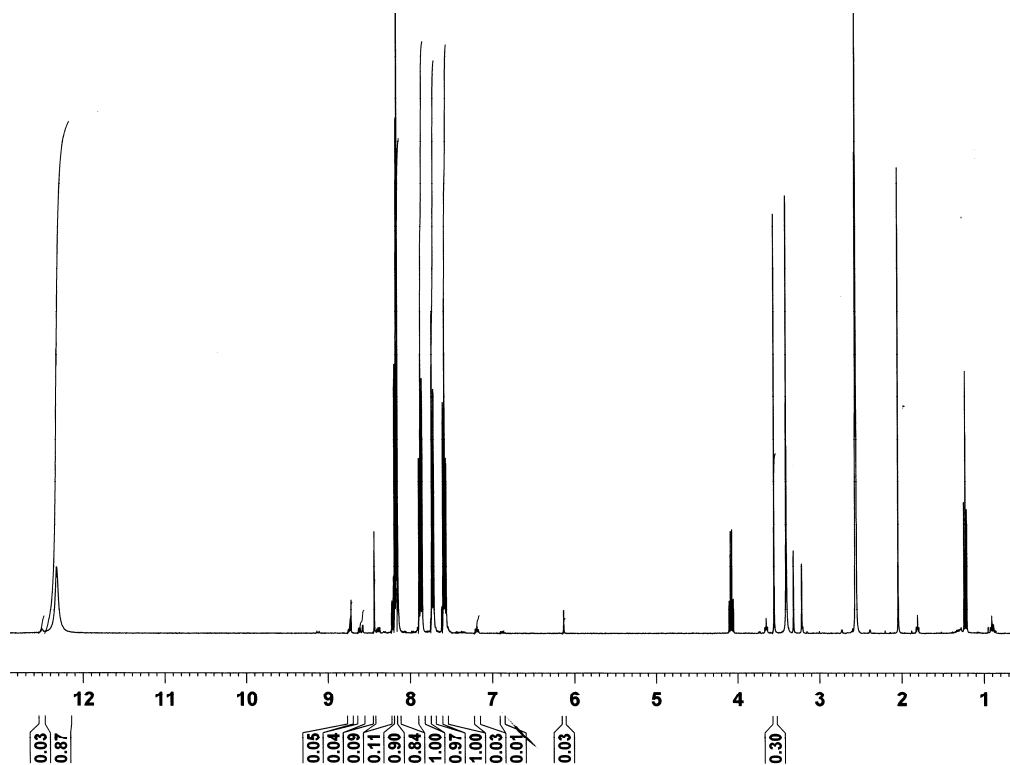
¹H NOE difference spectrum (irradiation at δ 4.98) of mixture of quinazolines formed by reaction of 10 with 1e.



¹H NOE difference spectrum (irradiation at δ 5.55) of mixture of quinazolines formed by reaction of 10 with 1e.



¹H NMR spectrum of mixture of quinazolin-4-ones formed by reaction of 7 with 1g.



Part of ¹H NMR spectrum of mixture of quinazolines formed by reaction of 7 with 1g.

