

Supporting Information

Substituent Effects on the Photorearrangements of Unsymmetrically Substituted Diazinobarrelenes

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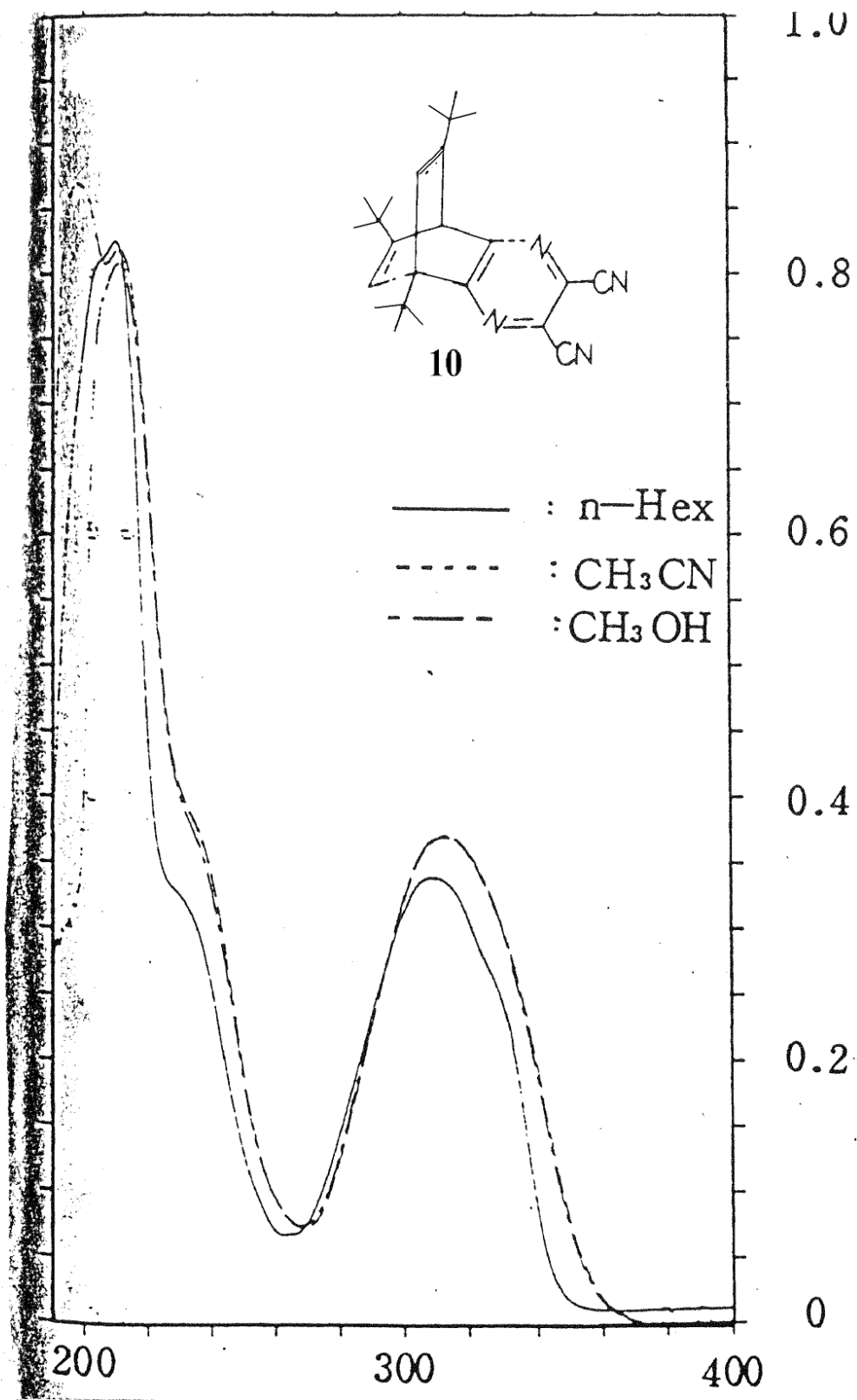
Table of Contents

1. General Procedures.....	S4
2. UV Spectra (10).....	S5
3. UV Spectra (13).....	S6
4. UV Spectra (14).....	S7
5. UV Spectra (15).....	S8
6. UV Spectra (16c).....	S9
7. UV Spectra (quinoxaline).....	S10
8. UV Spectra (40).....	S11
9. UV Spectra (41).....	S12
10. UV Spectra (47).....	S13
11. UV Spectra (48).....	S14
12. UV Spectra (49).....	S15
13. UV Spectra(50).....	S16
14. UV Spectra (51).....	S17
15. UV Spectra (52).....	S18
16. ¹³ C NMR (10).....	S19
17. ¹³ C NMR (13).....	S20
18. ¹³ C NMR (14).....	S21
19. ¹³ C NMR (15).....	S22
20. ¹³ C NMR (40).....	S23
21. ¹³ C NMR (41).....	S24

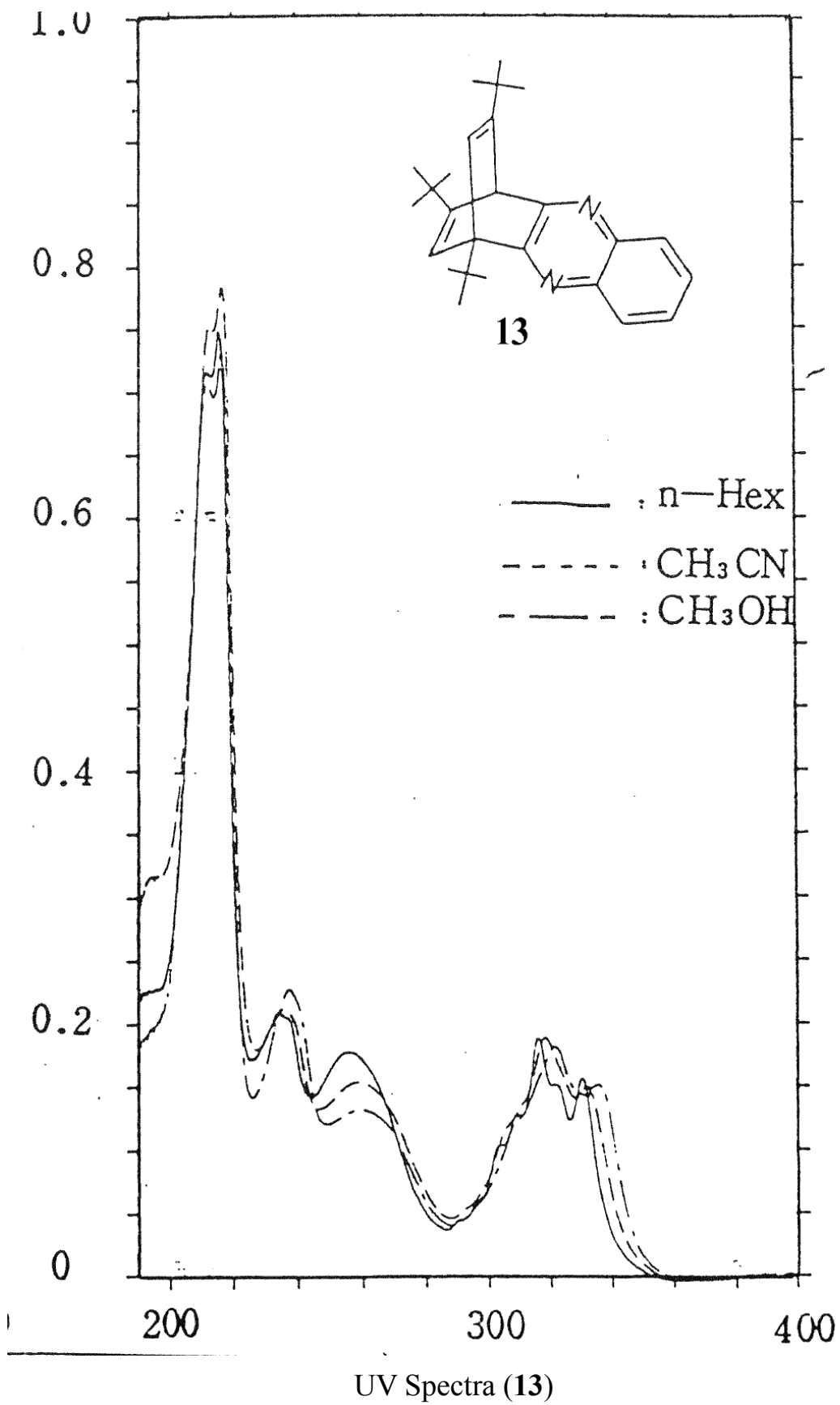
22.	¹³ C NMR (47)	S25
23.	¹³ C NMR (48)	S26
24.	¹³ C NMR (49)	S27
25.	¹³ C NMR (50)	S28
26.	¹³ C NMR (51)	S29
27.	¹³ C NMR (52)	S30
28.	¹ H NMR (8)	S31
29.	¹ H NMR (9)	S32
30.	¹ H NMR (10)	S33
31.	¹ H NMR (11)	S34
32.	¹ H NMR (12)	S35
33.	¹ H NMR (13)	S36
34.	¹ H NMR (14)	S37
35.	¹ H NMR (15)	S38
36.	¹ H NMR (16a)	S39
37.	¹ H NMR (16b)	S40
38.	¹ H NMR (16c)	S41
39.	¹ H NMR (22b)	S42
40.	¹ H NMR (24a)	S43
41.	¹ H NMR (25a)	S44
42.	¹ H NMR (25b)	S45
46.	¹ H NMR (40)	S46
47.	¹ H NMR (41)	S47
48.	¹ H NMR (47)	S48
49.	¹ H NMR (48)	S49

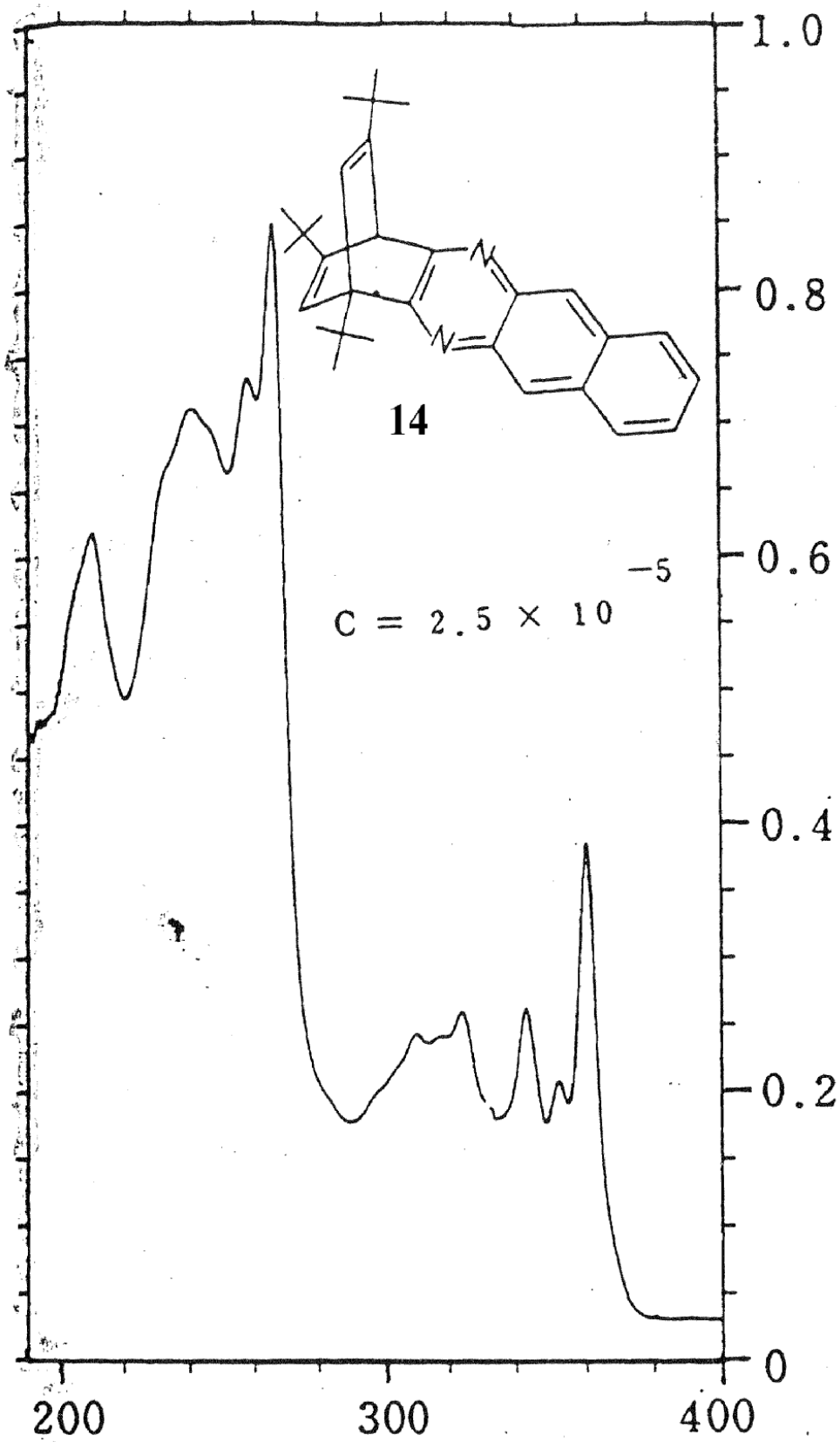
50.	^1H NMR (49)	S50
51.	^1H NMR (50)	S51
52.	^1H NMR (51)	S52
53.	^1H NMR (52)	S53
54.	2D-COSY (13)	S54
55.	2D-COSY(41)	S55
56.	2D-COSY (47, 48, 49)	S56

General Procedures. Unless stated otherwise, reagents were obtained from commercial sources and used without further purification. Reactions were monitored using Thin-Layer Chromatographic plates (0.25 mm – silica gel plates, 60F-254) with 7% ethanolic phosphomolybdic acid (H_2SO_4 , CeSO_4 , $(\text{NH}_4)_6\text{Mo}_7\text{O}_{24}\cdot 4\text{H}_2\text{O}$) as developing reagent. Standard column chromatography was conducted using 70–230 mesh silica gel. IR spectra were recorded as films on NaCl plates. Unless otherwise specified ^1H , ^{13}C NMR and DEPT spectra were recorded in CDCl_3 and chemical shifts were reported in δ (ppm) using solvent resonance as the internal reference. The high resolution mass spectra (HRMS) were recorded on JEOL JMS-HX 110 mass spectrometer. Photochemical reactions were carried out in spectroscopic grade solvents. All the starting materials dissolved in specific solvents were degassed either by bubbling with argon or by sonication for 1 h. Irradiation of samples were performed in a Rayonet photoreactor using RPR 3500 ($\lambda = 350$ nm). UV spectra of the starting materials were determined using a double-beam UV-Vis spectrophotometer.

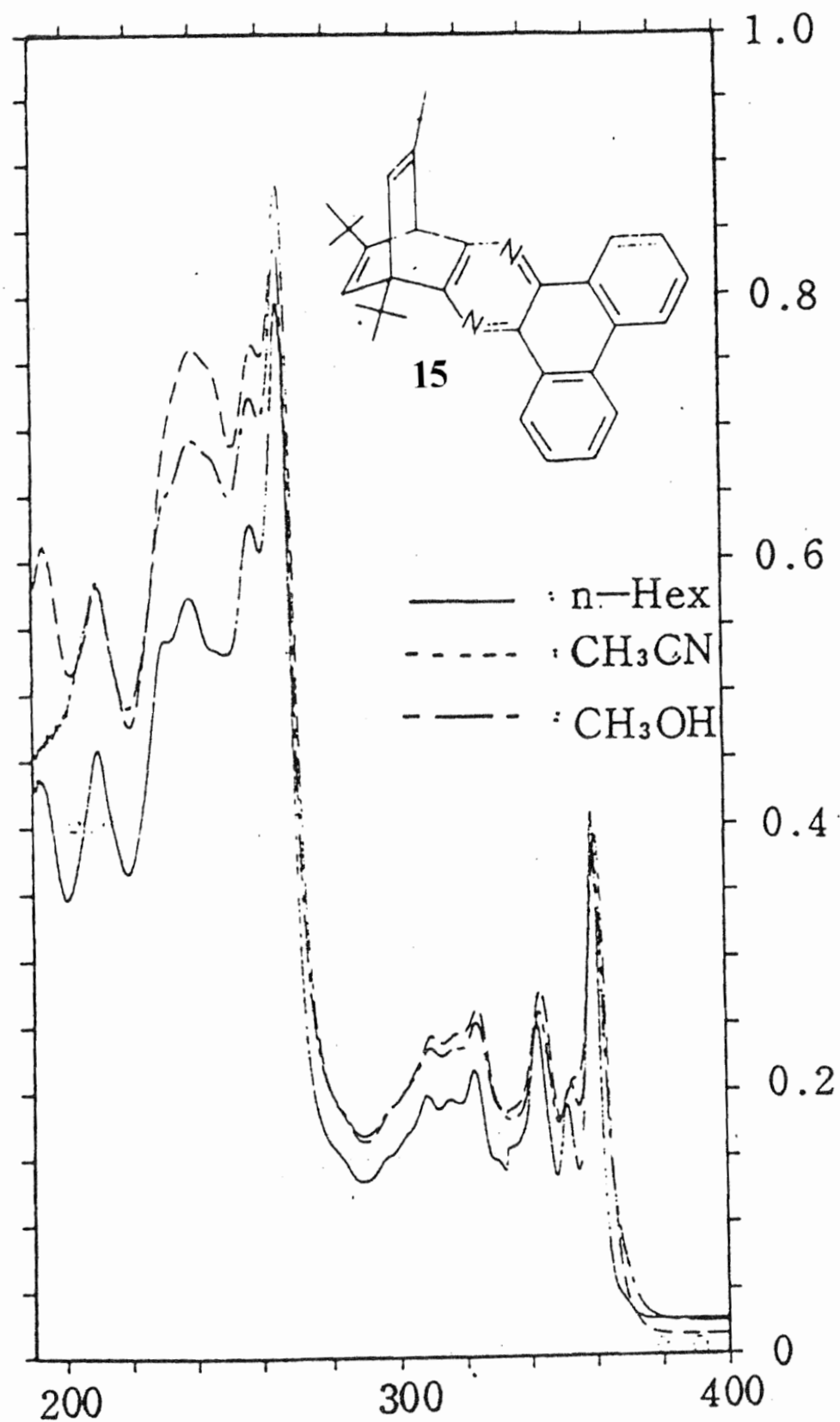


UV Spectra (**10**)

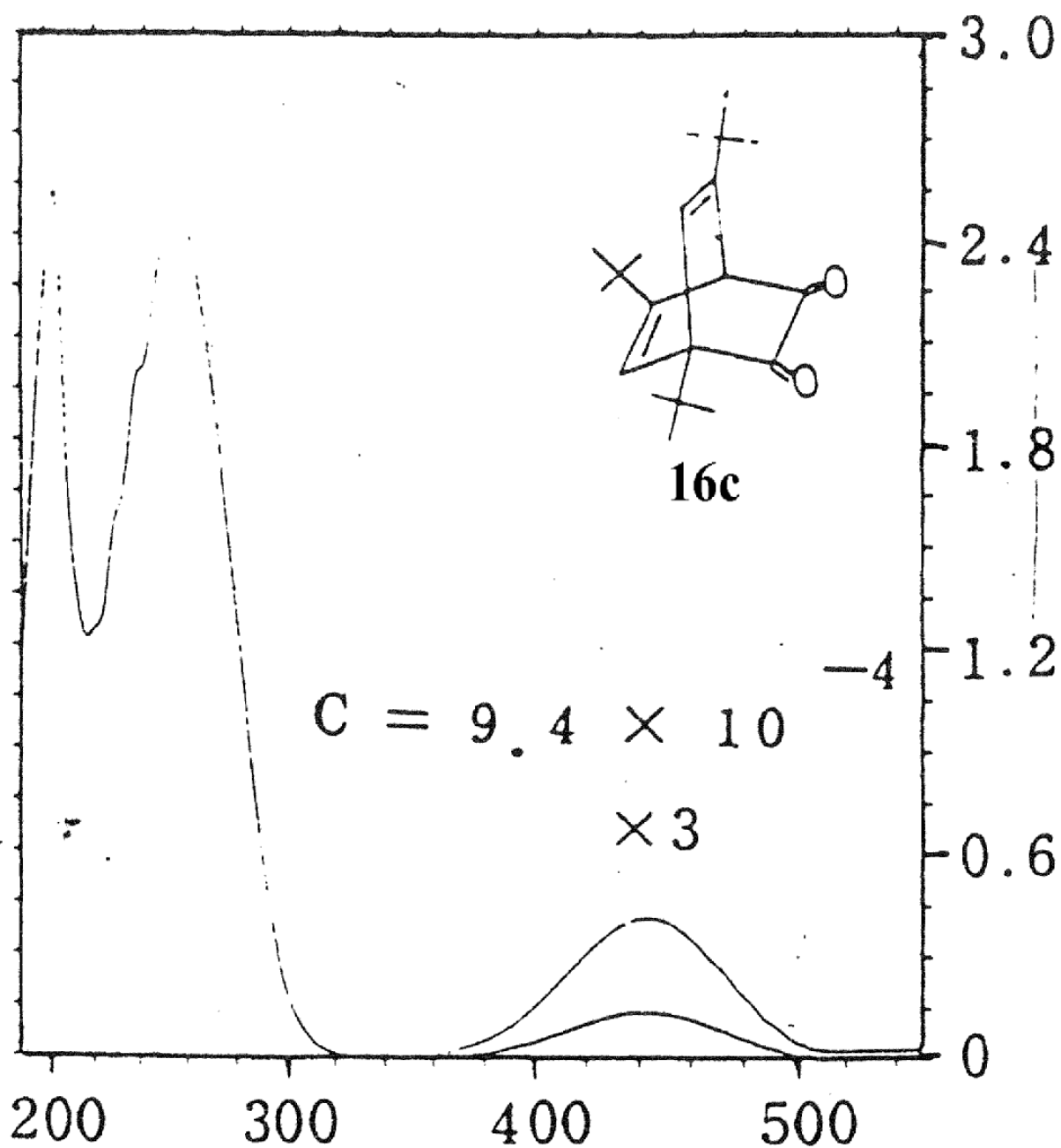




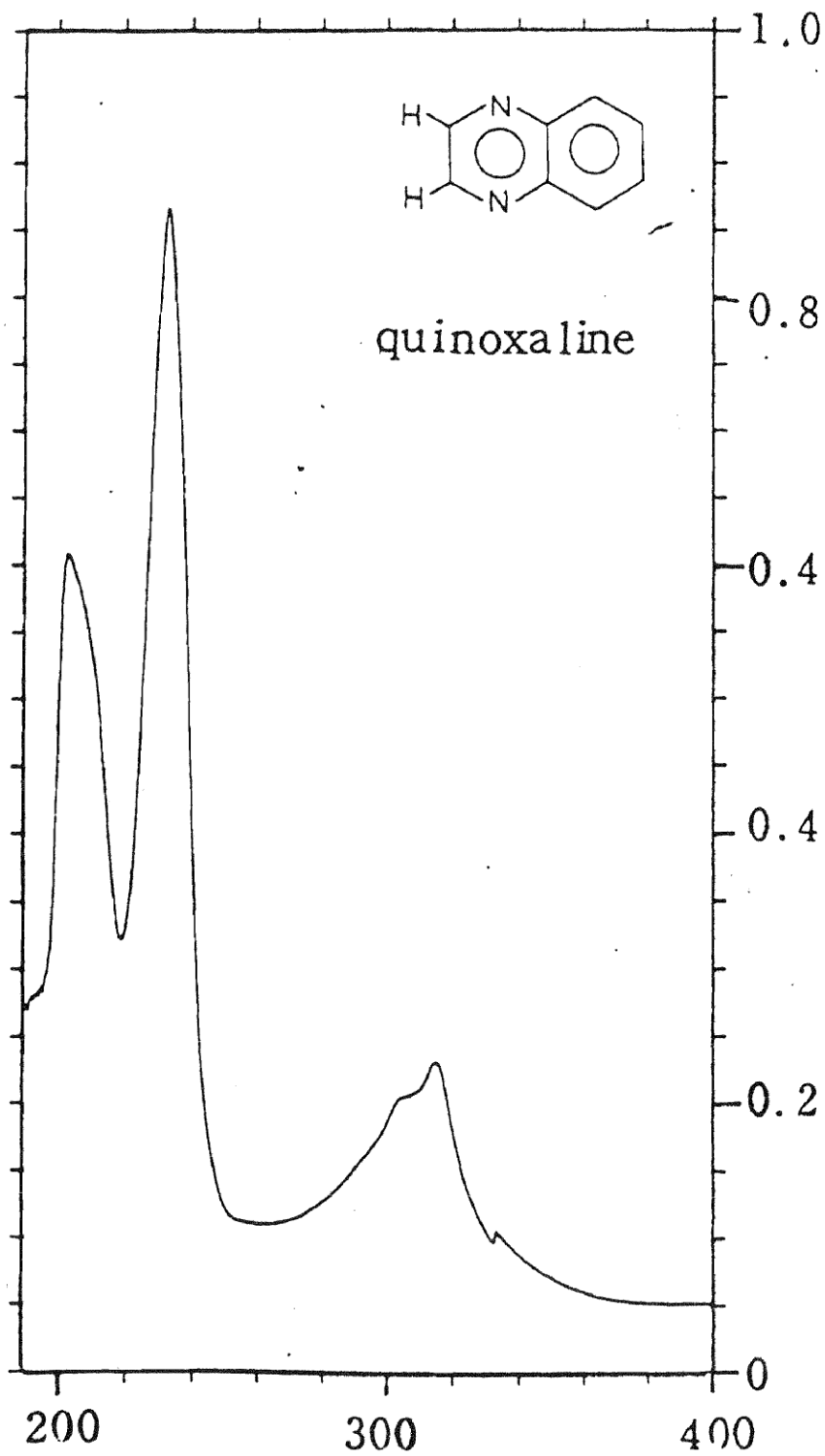
UV Spectra (14)



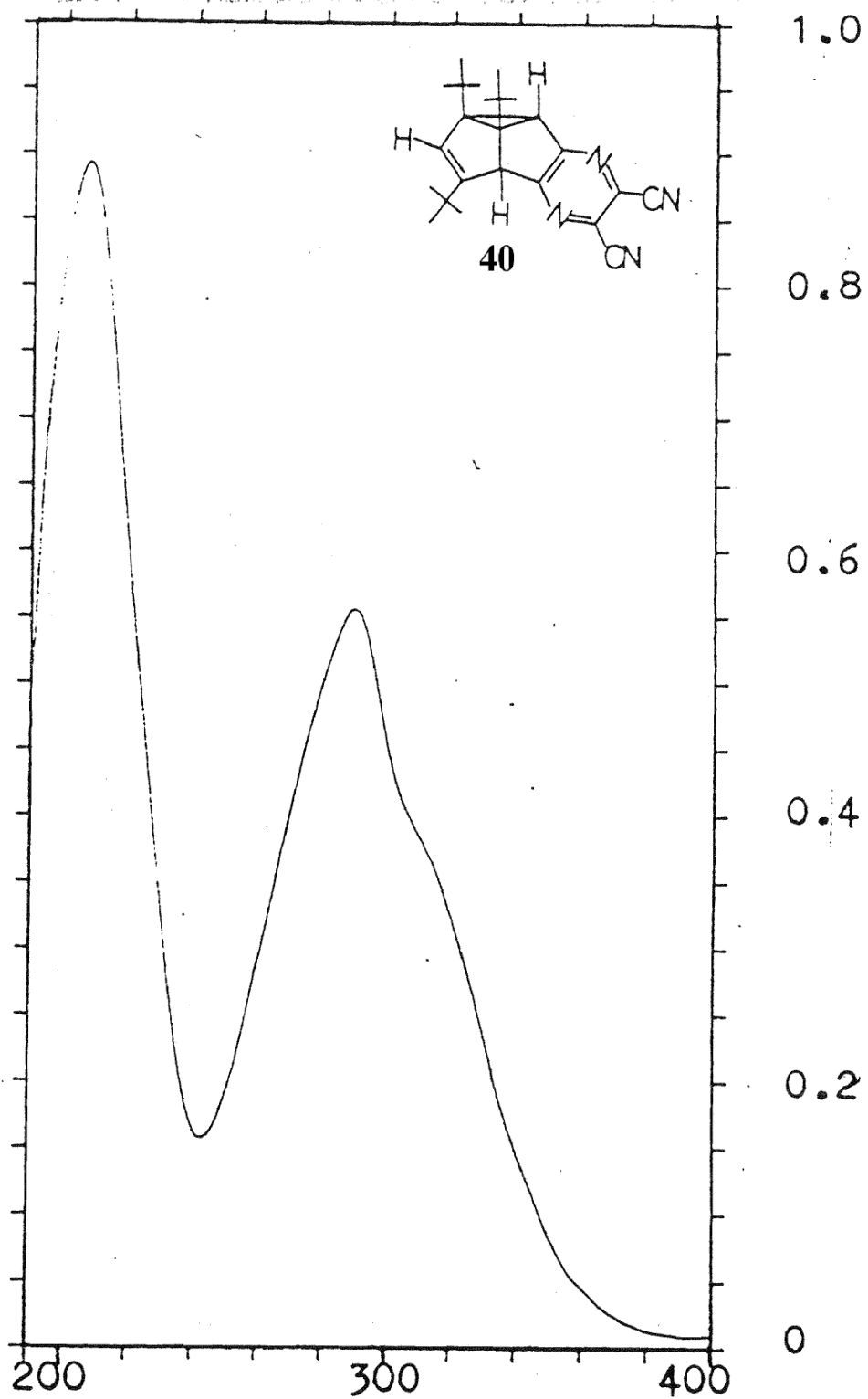
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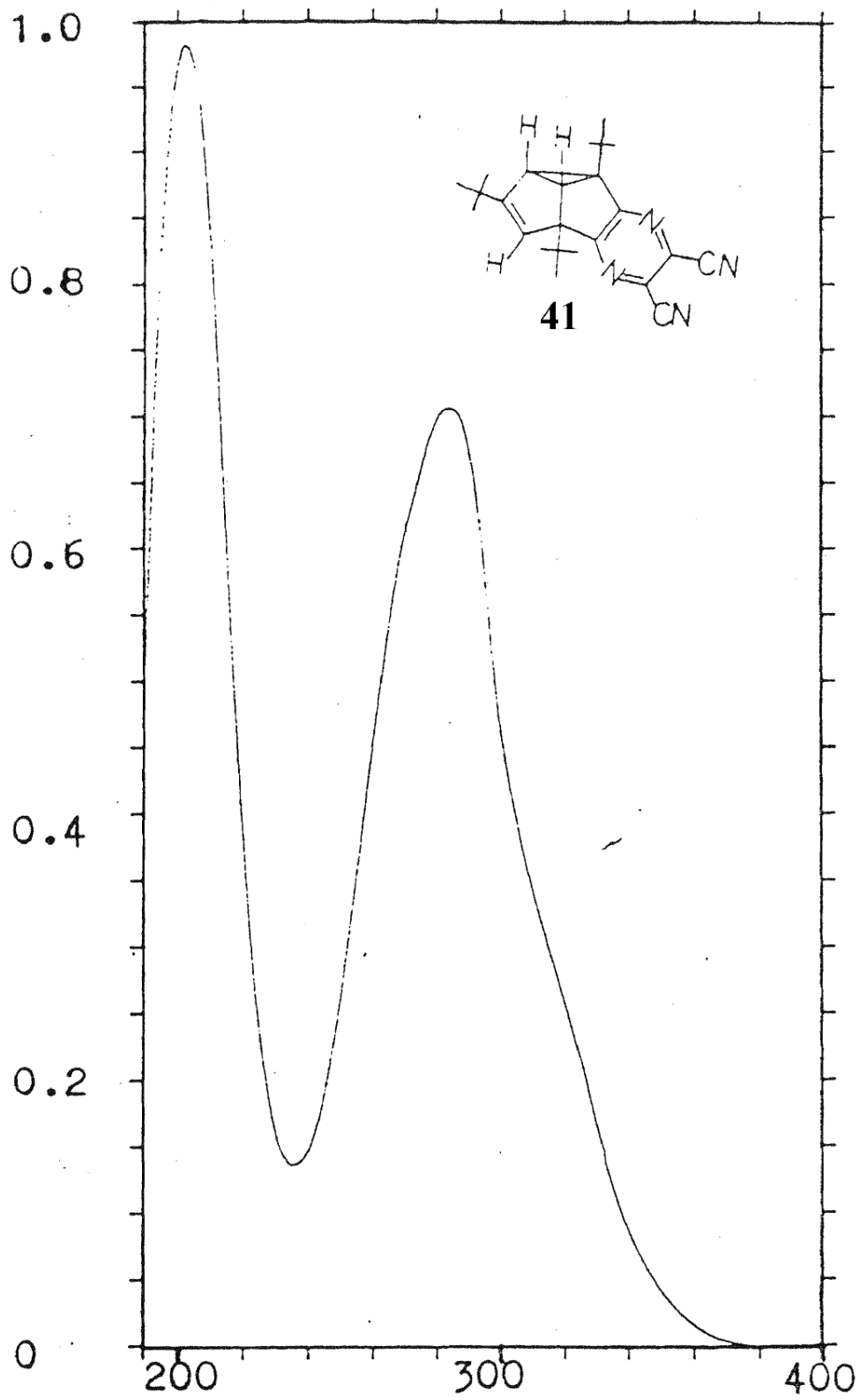
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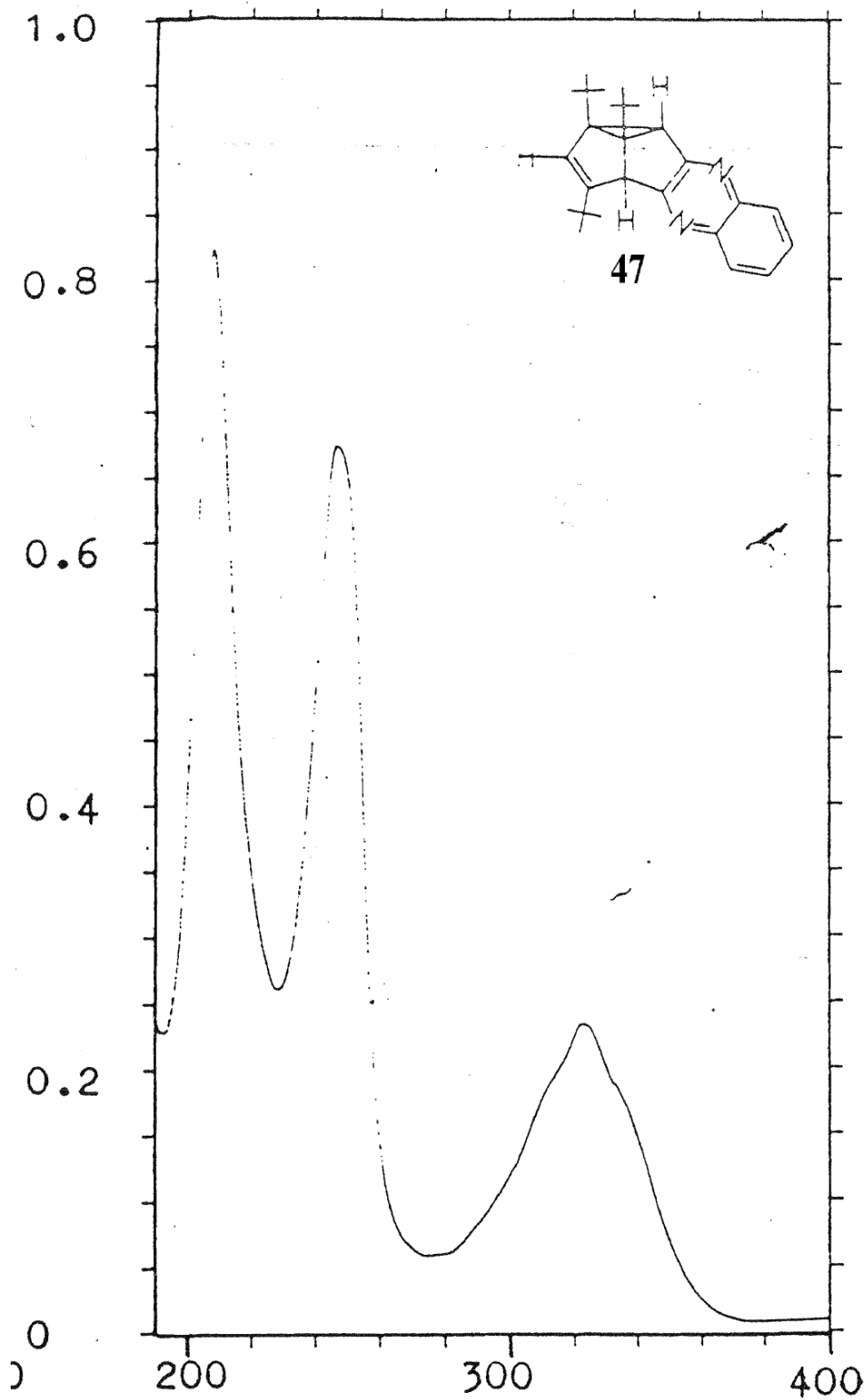
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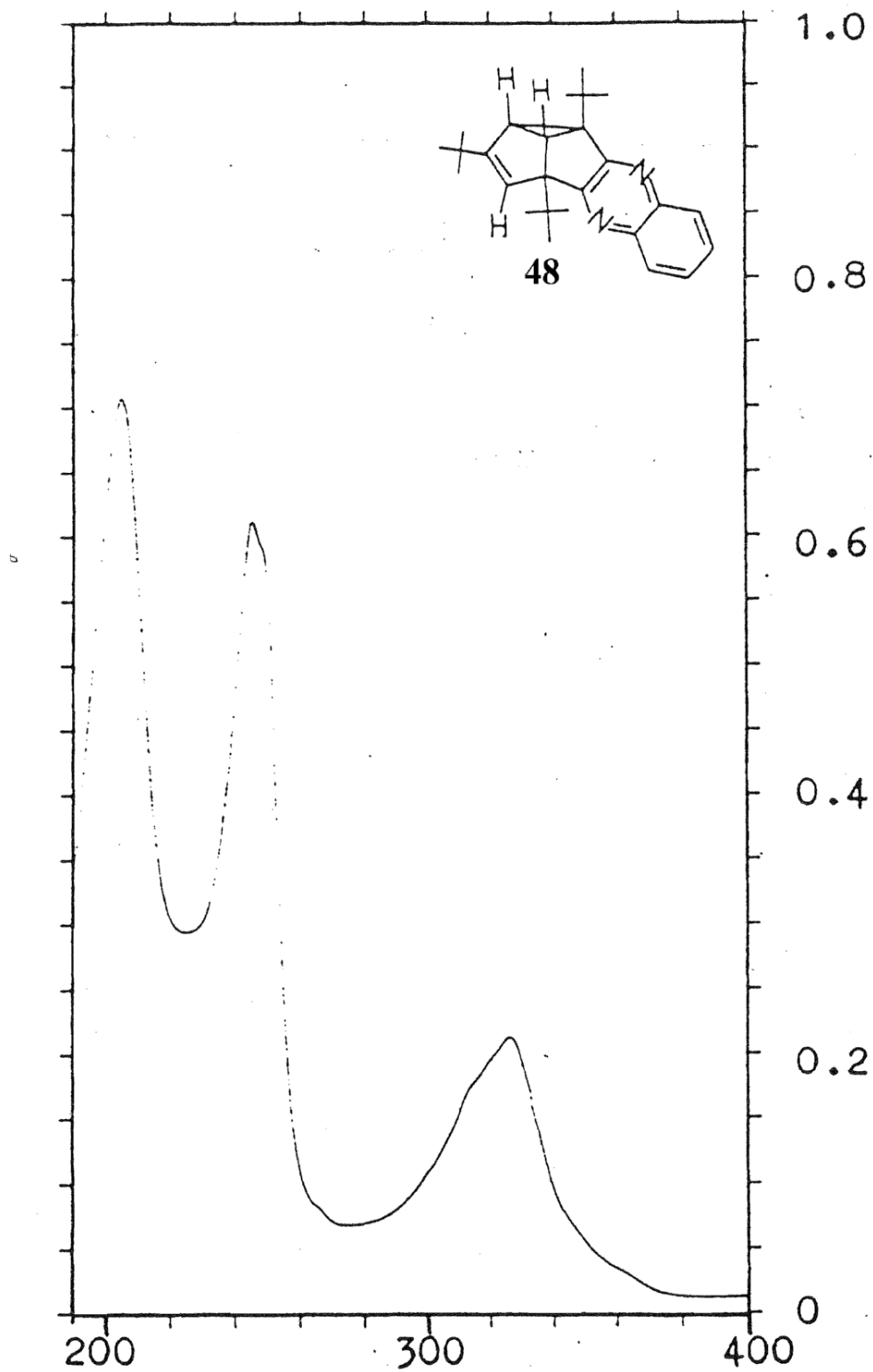
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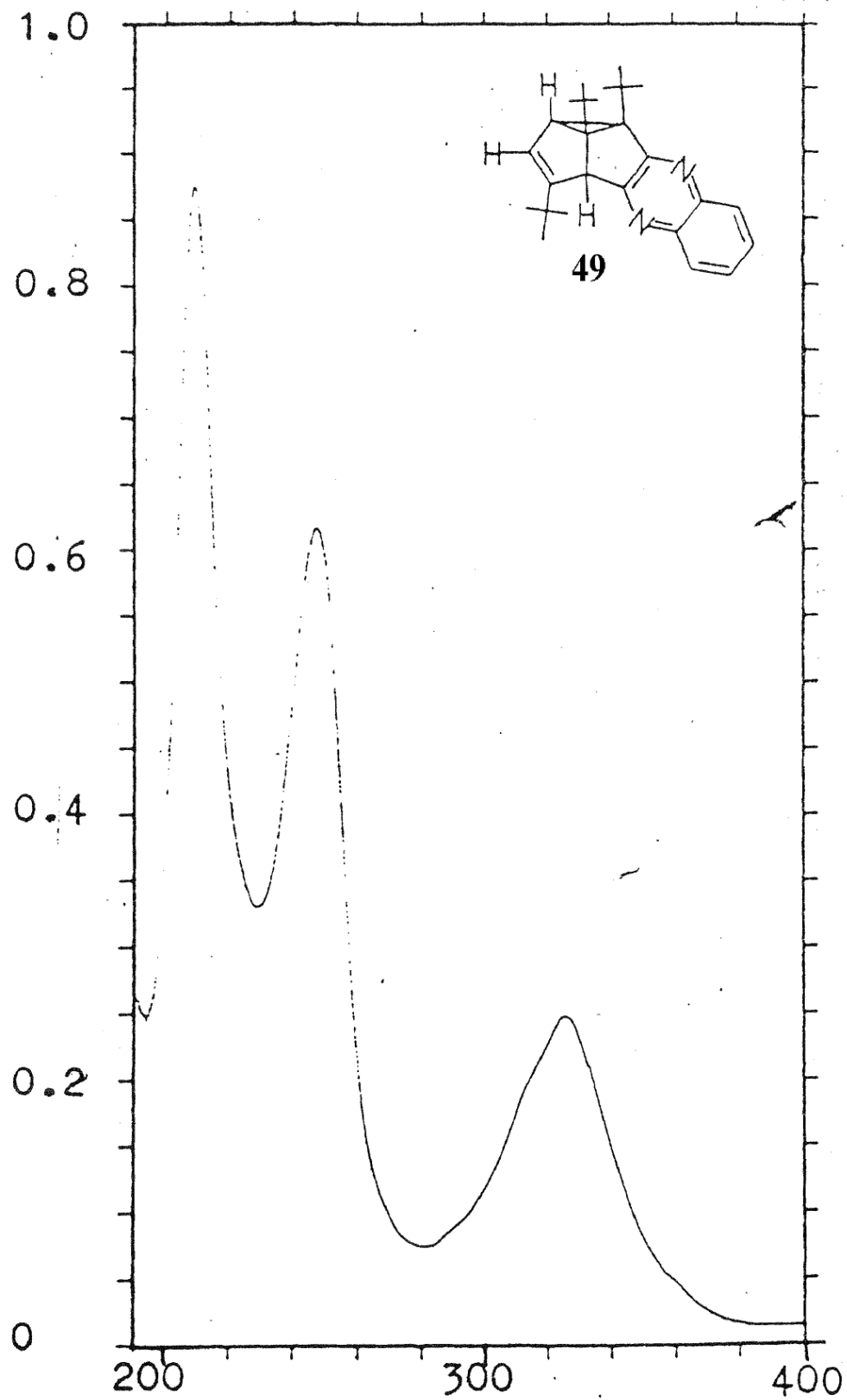
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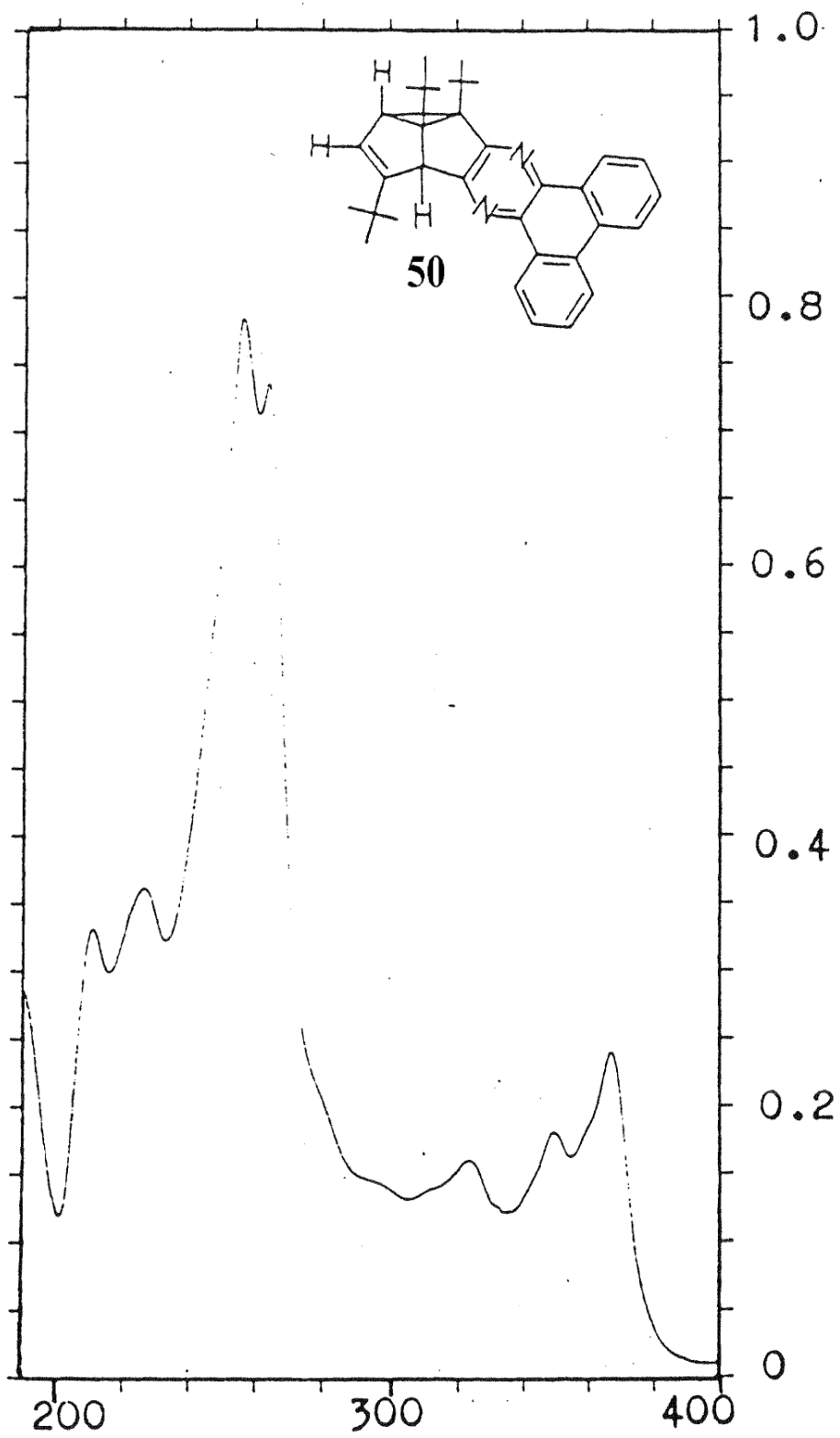
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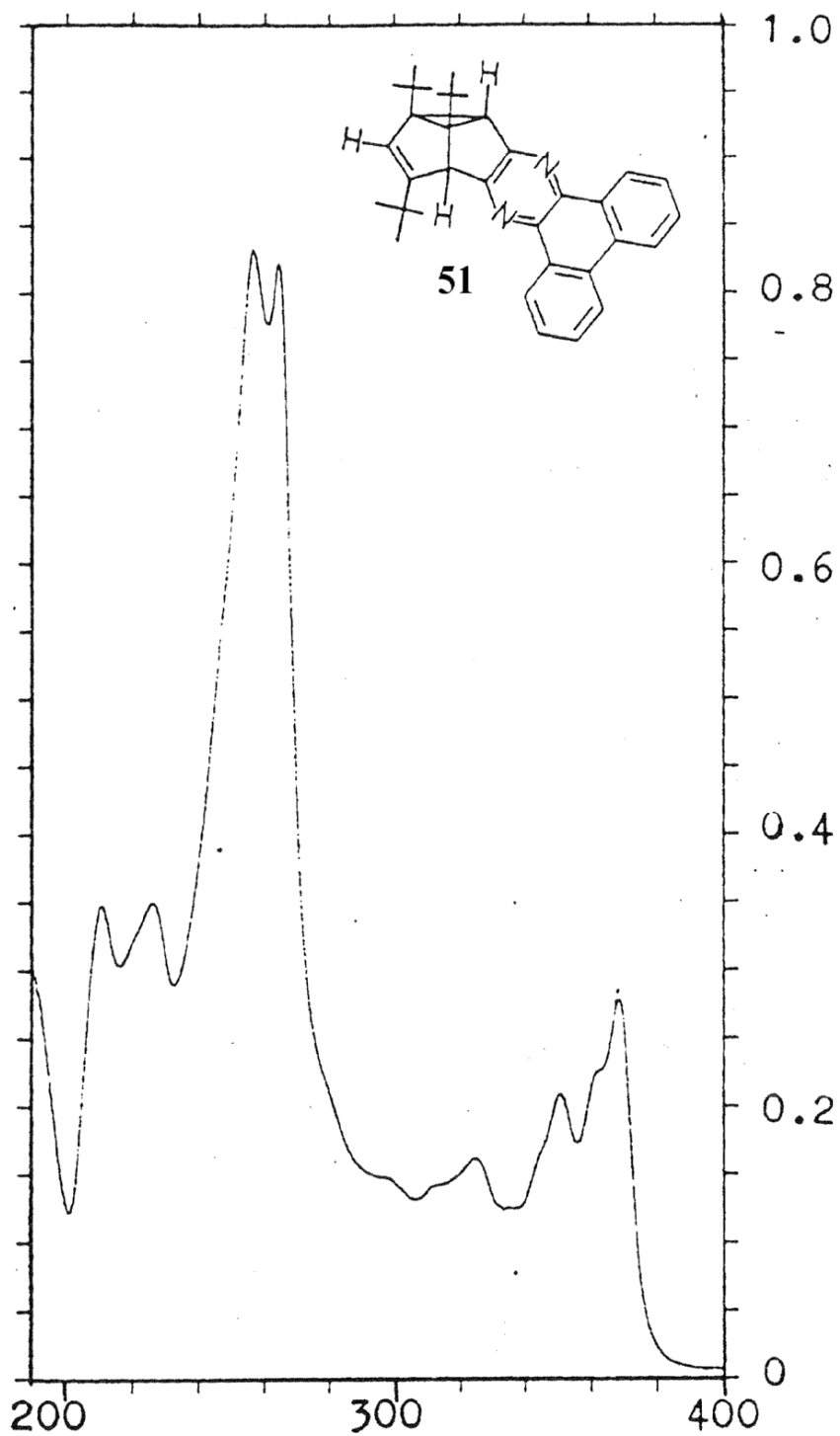
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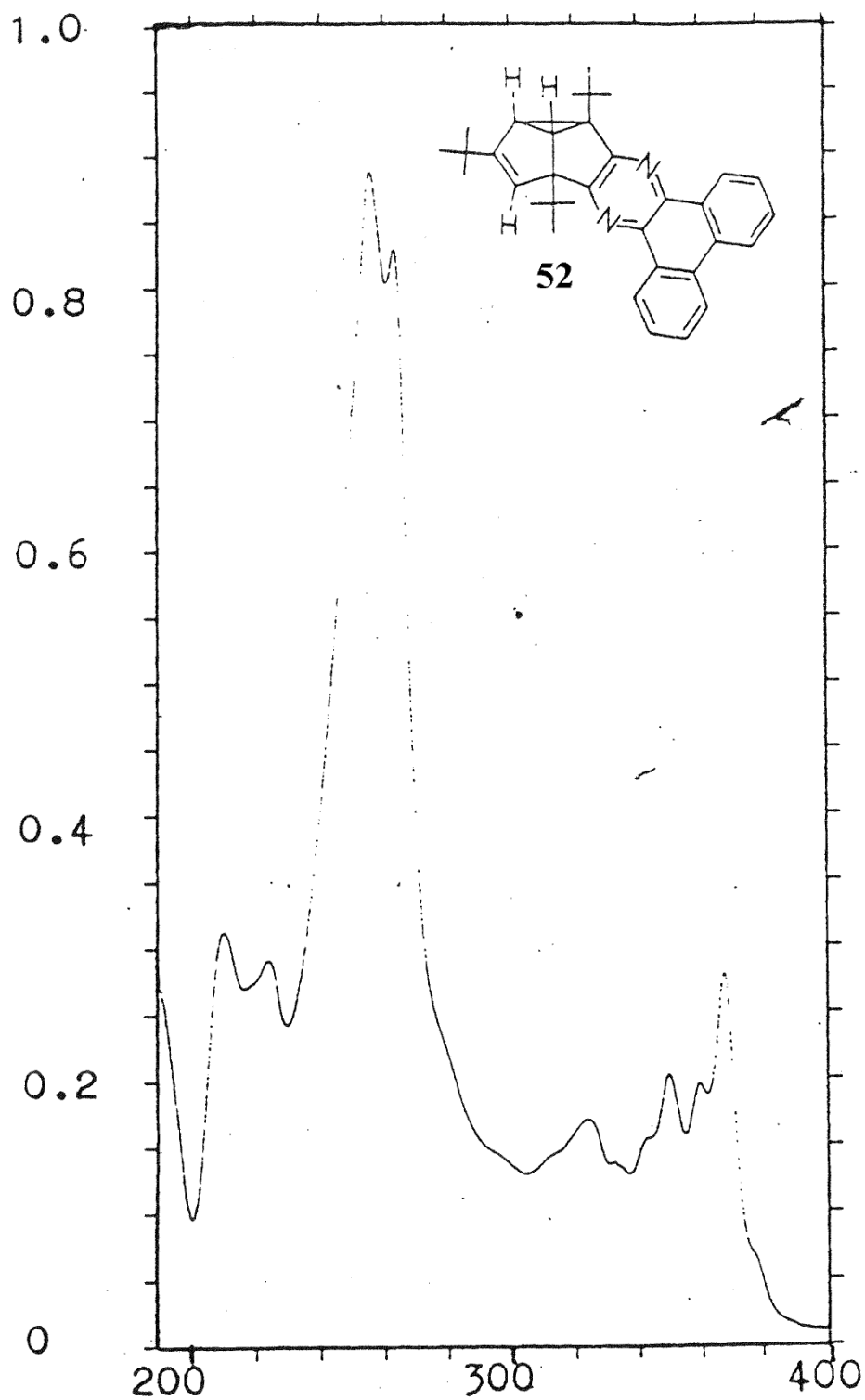
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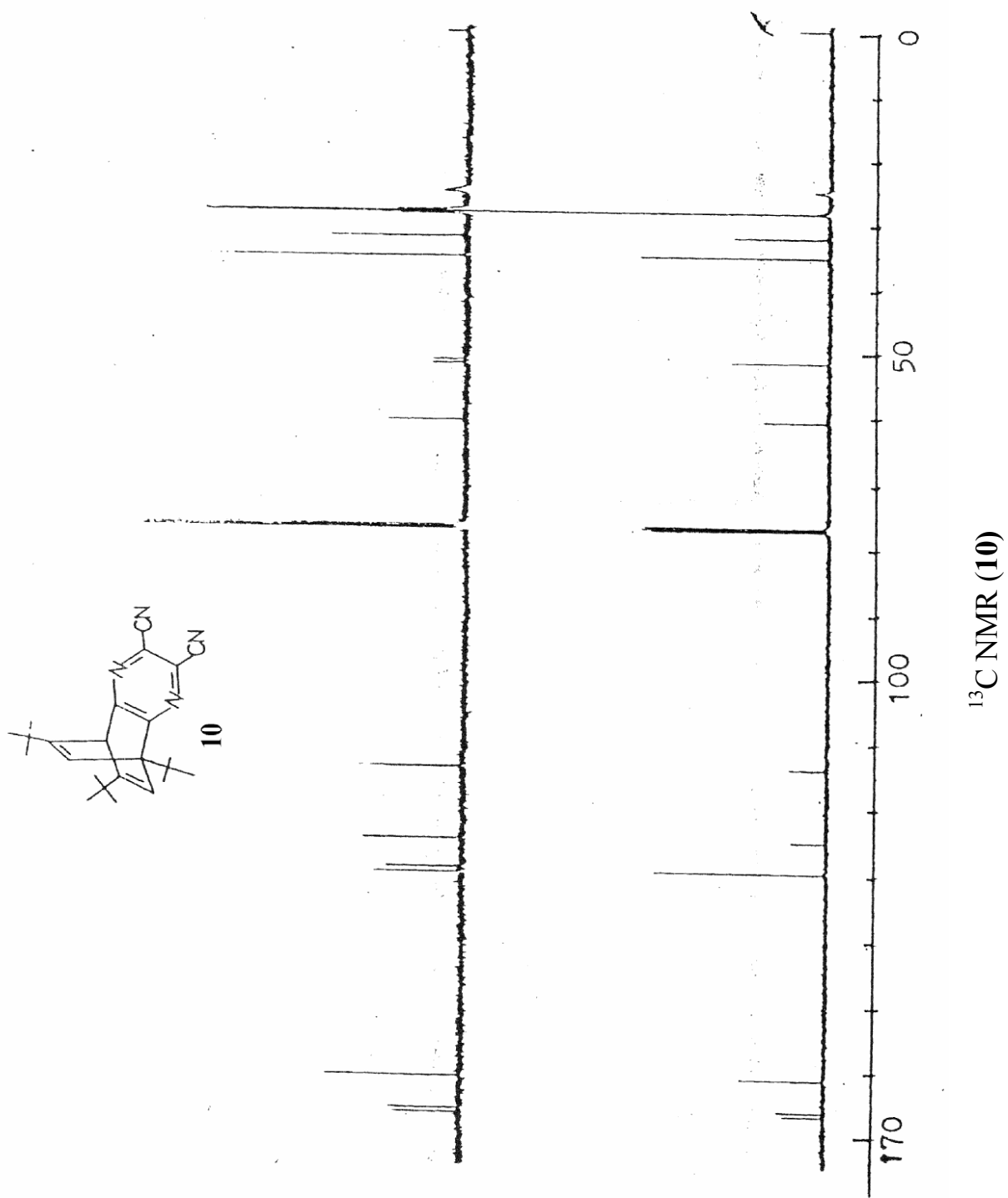
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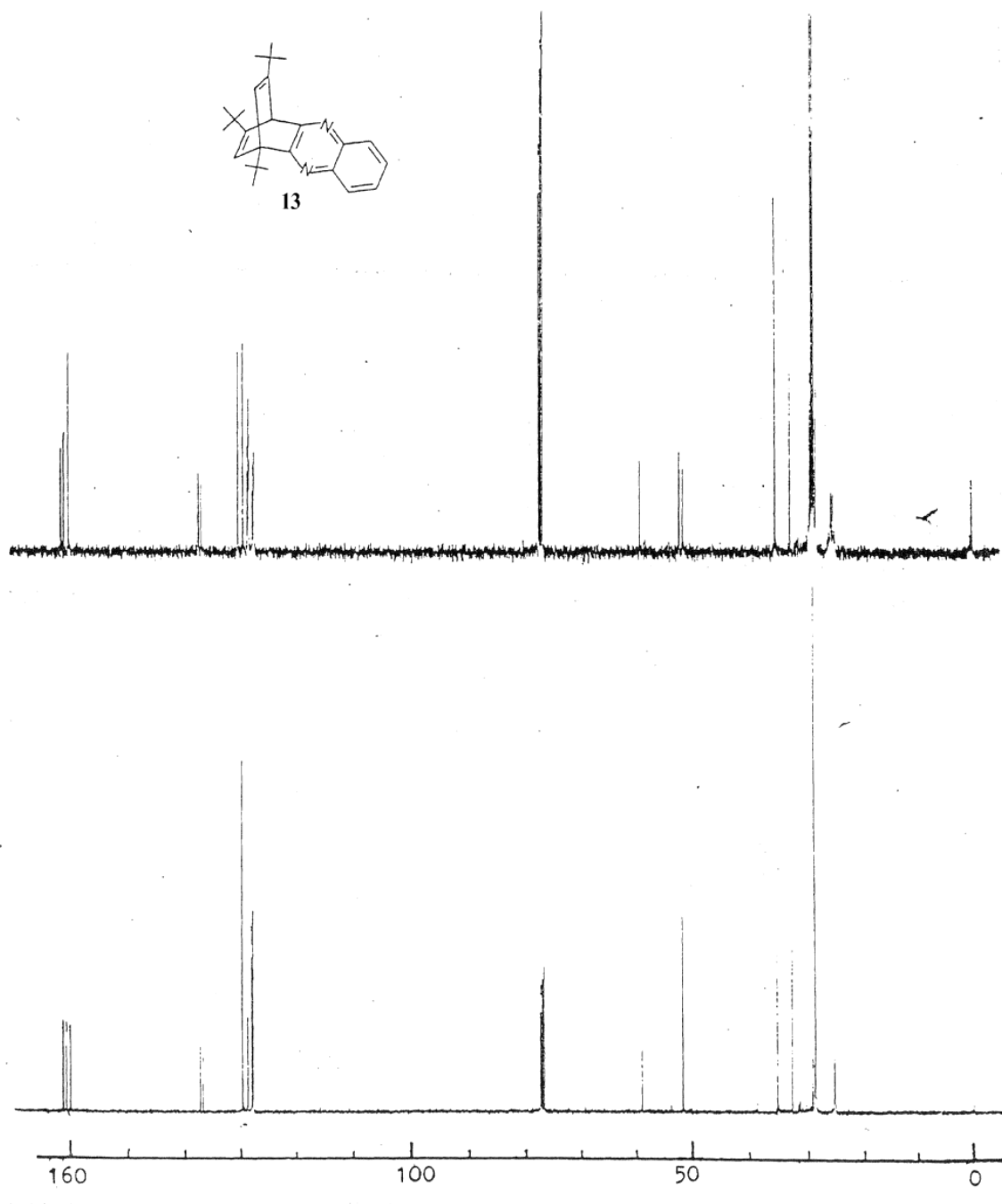


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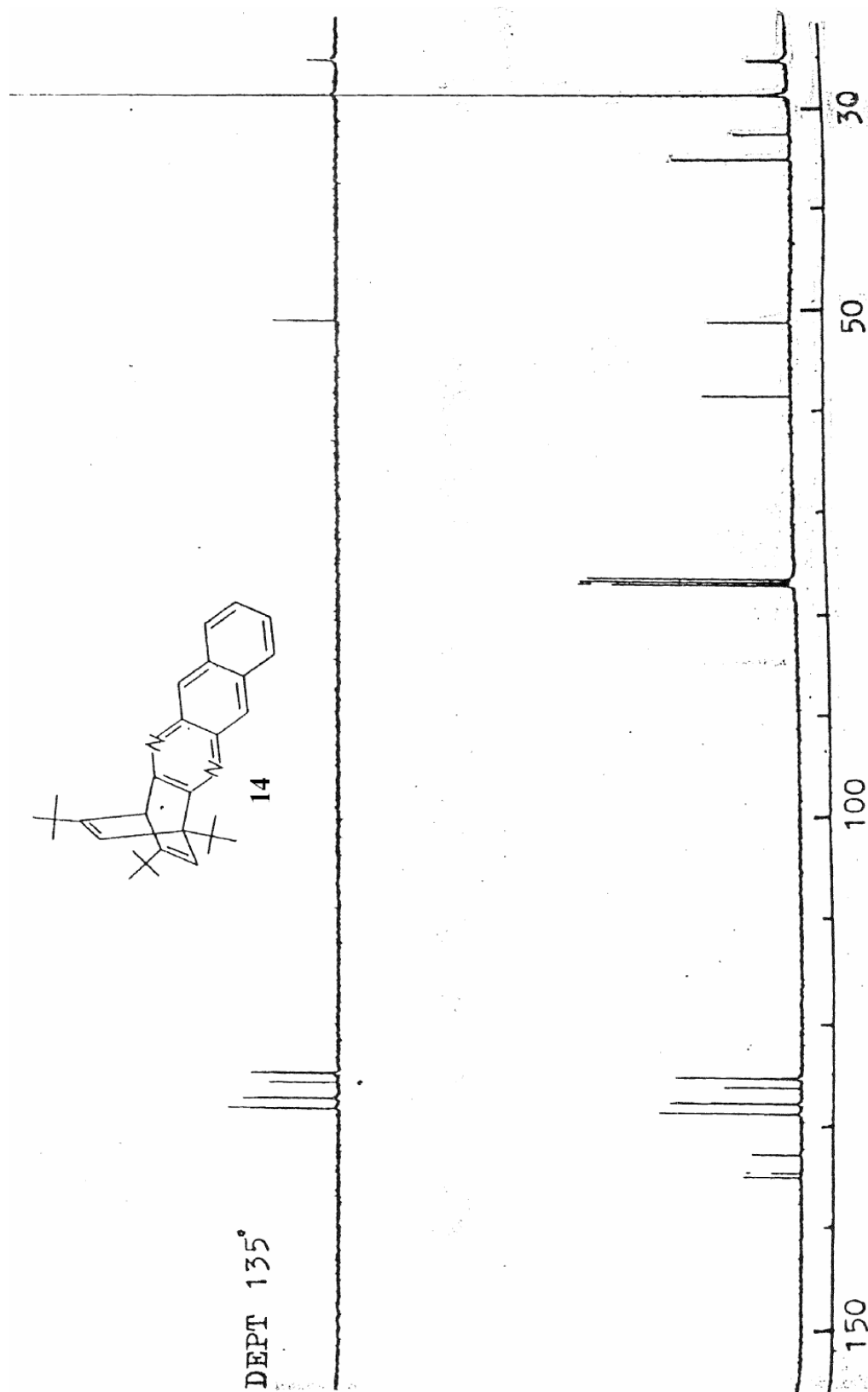


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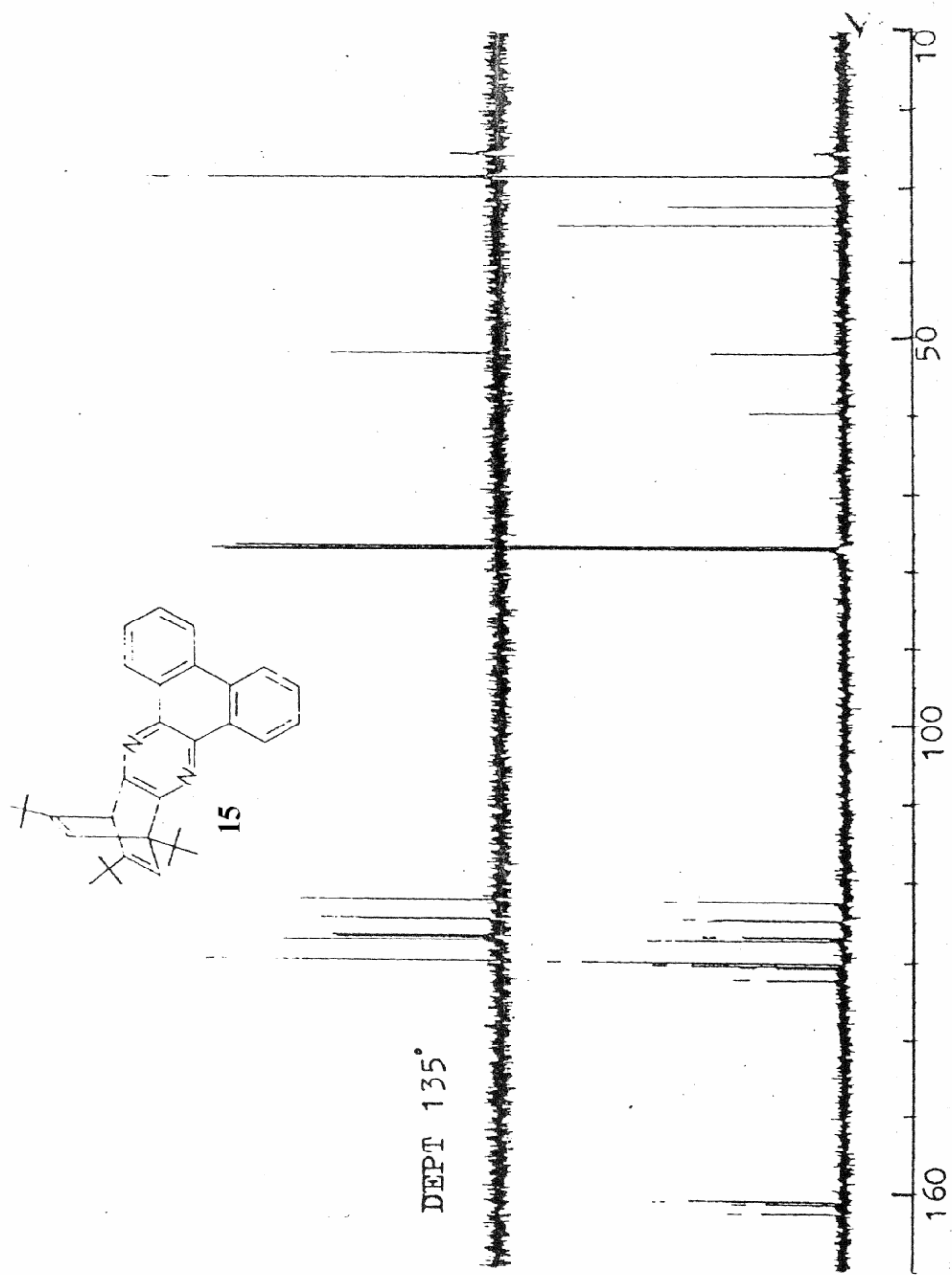




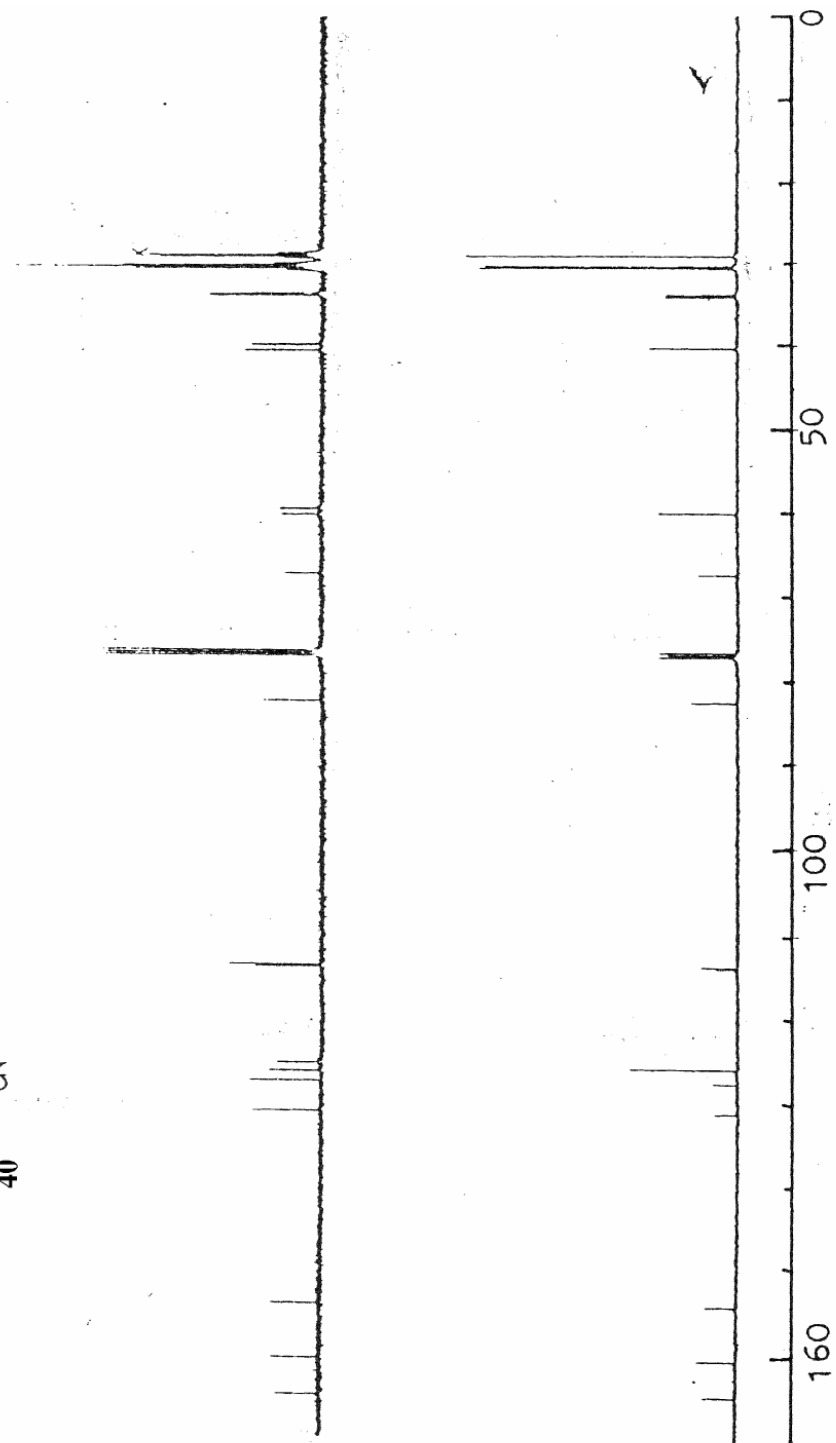
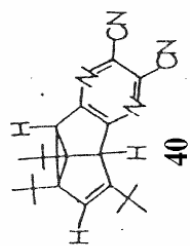
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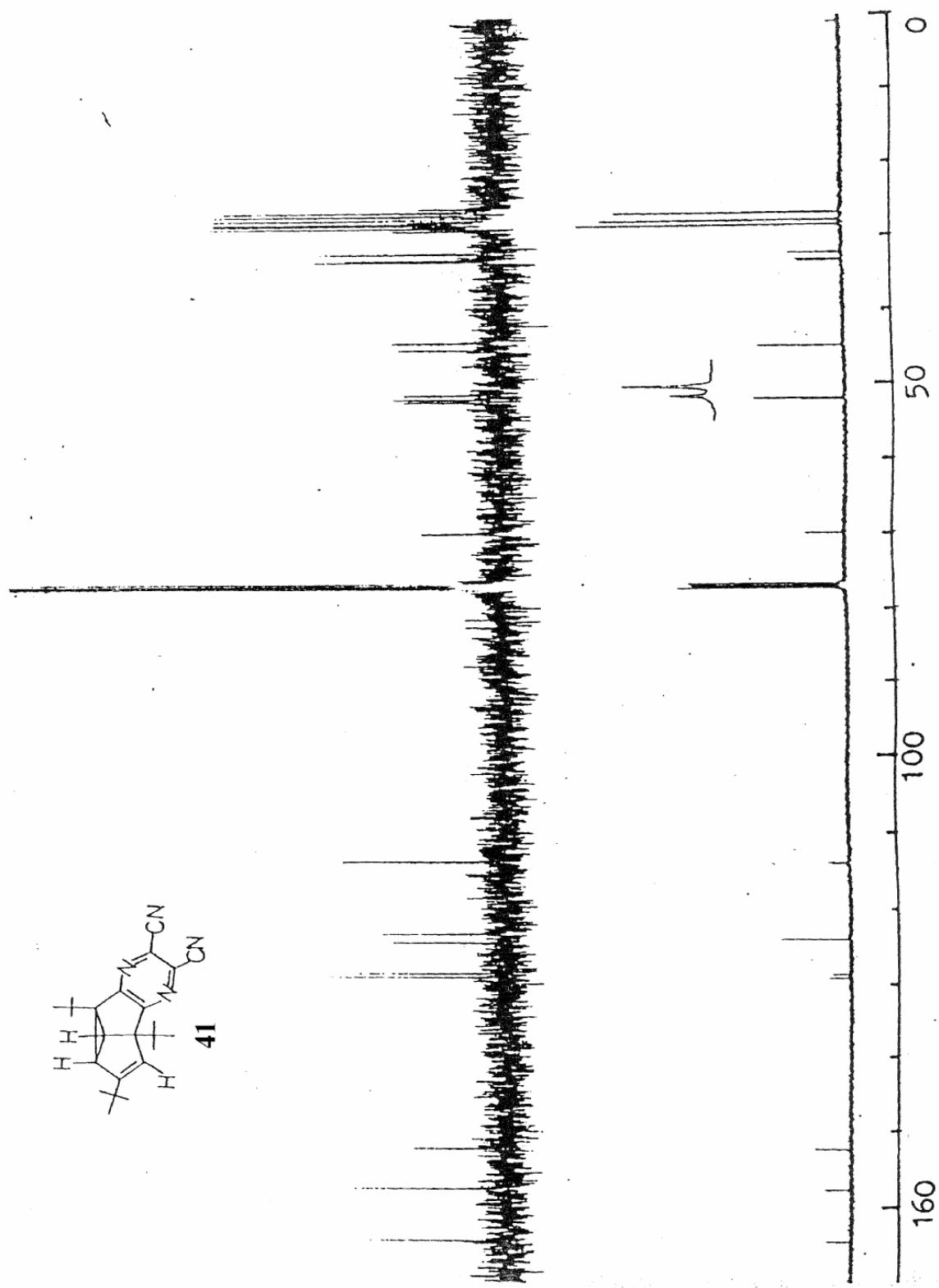
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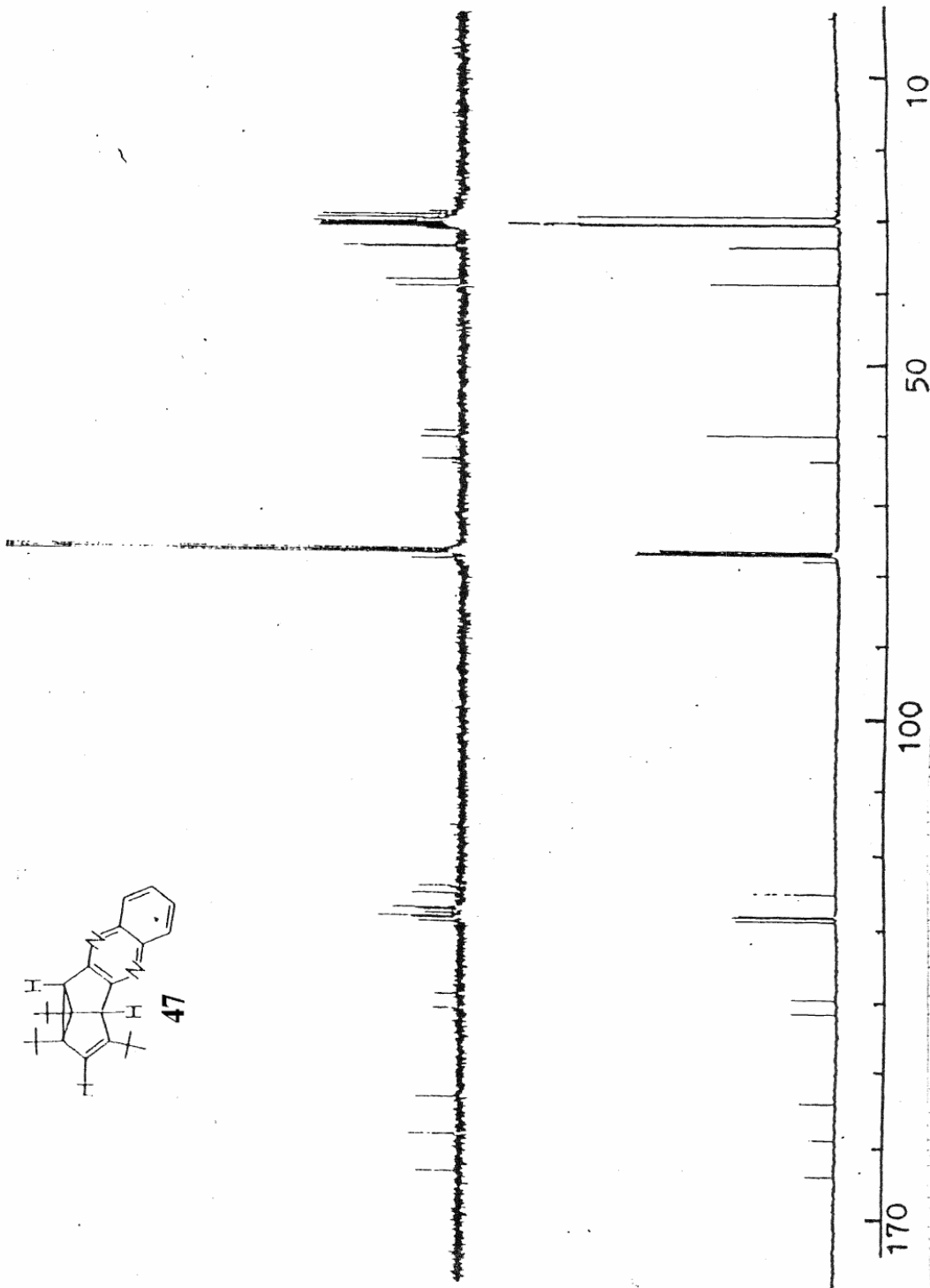
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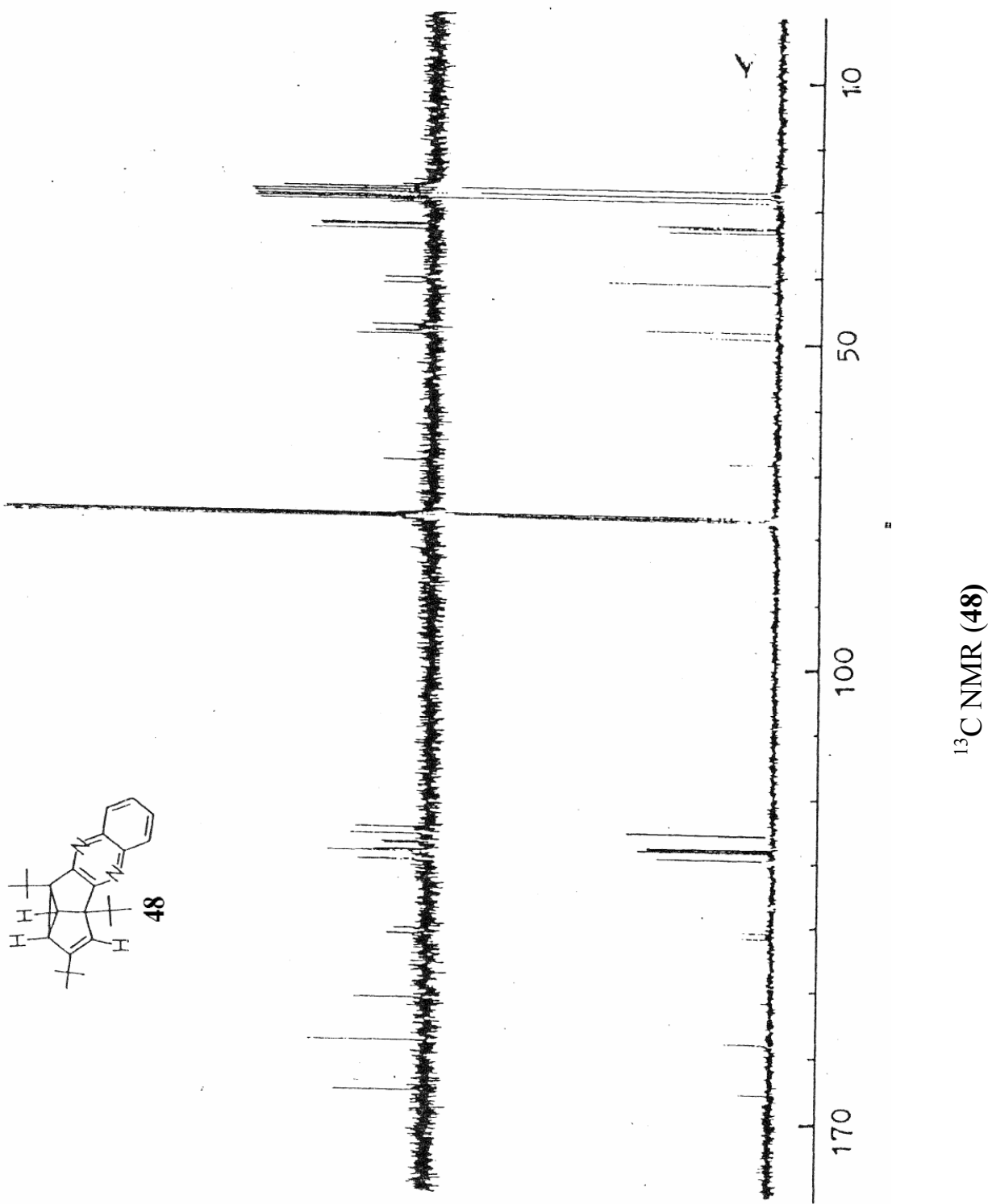
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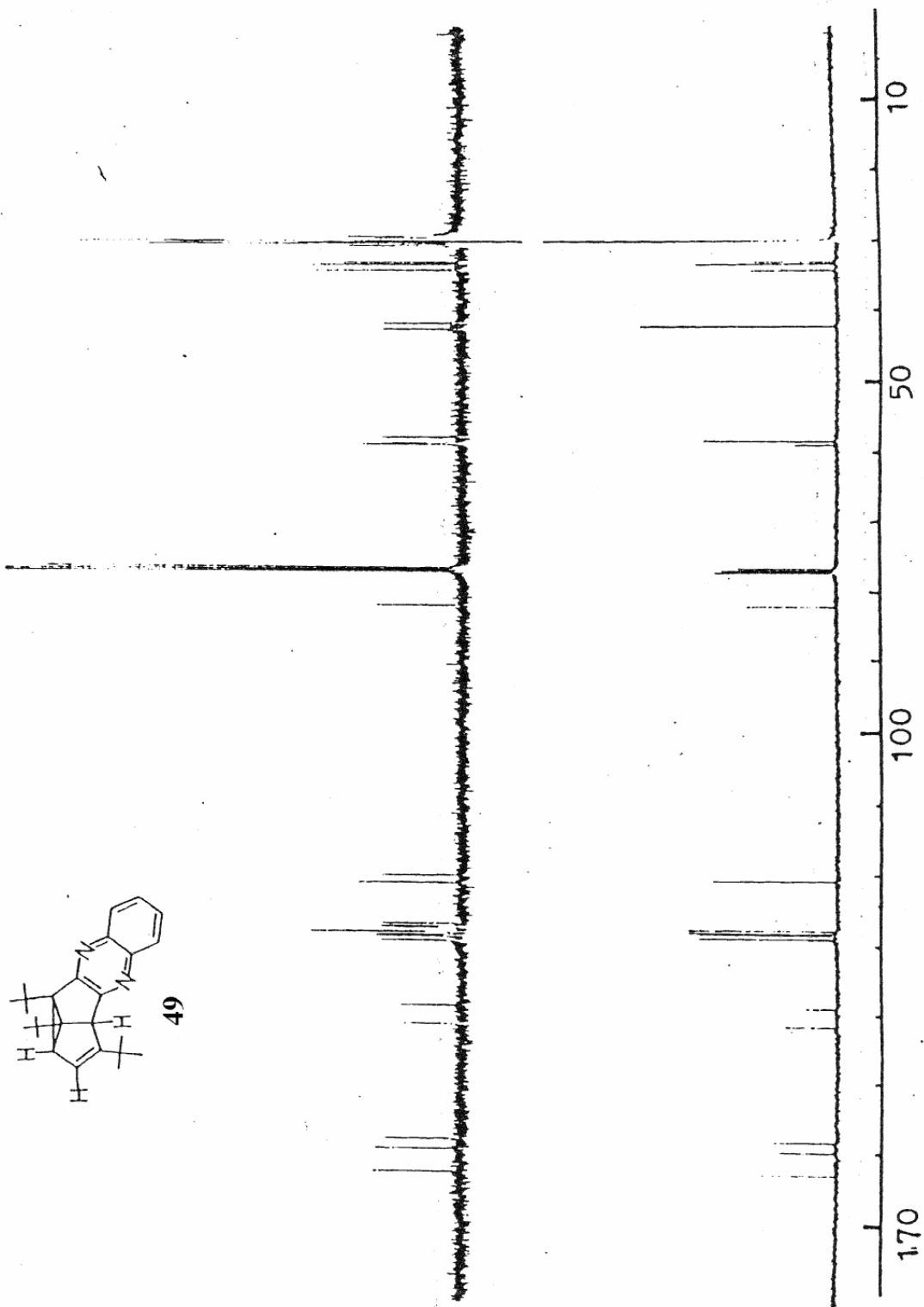


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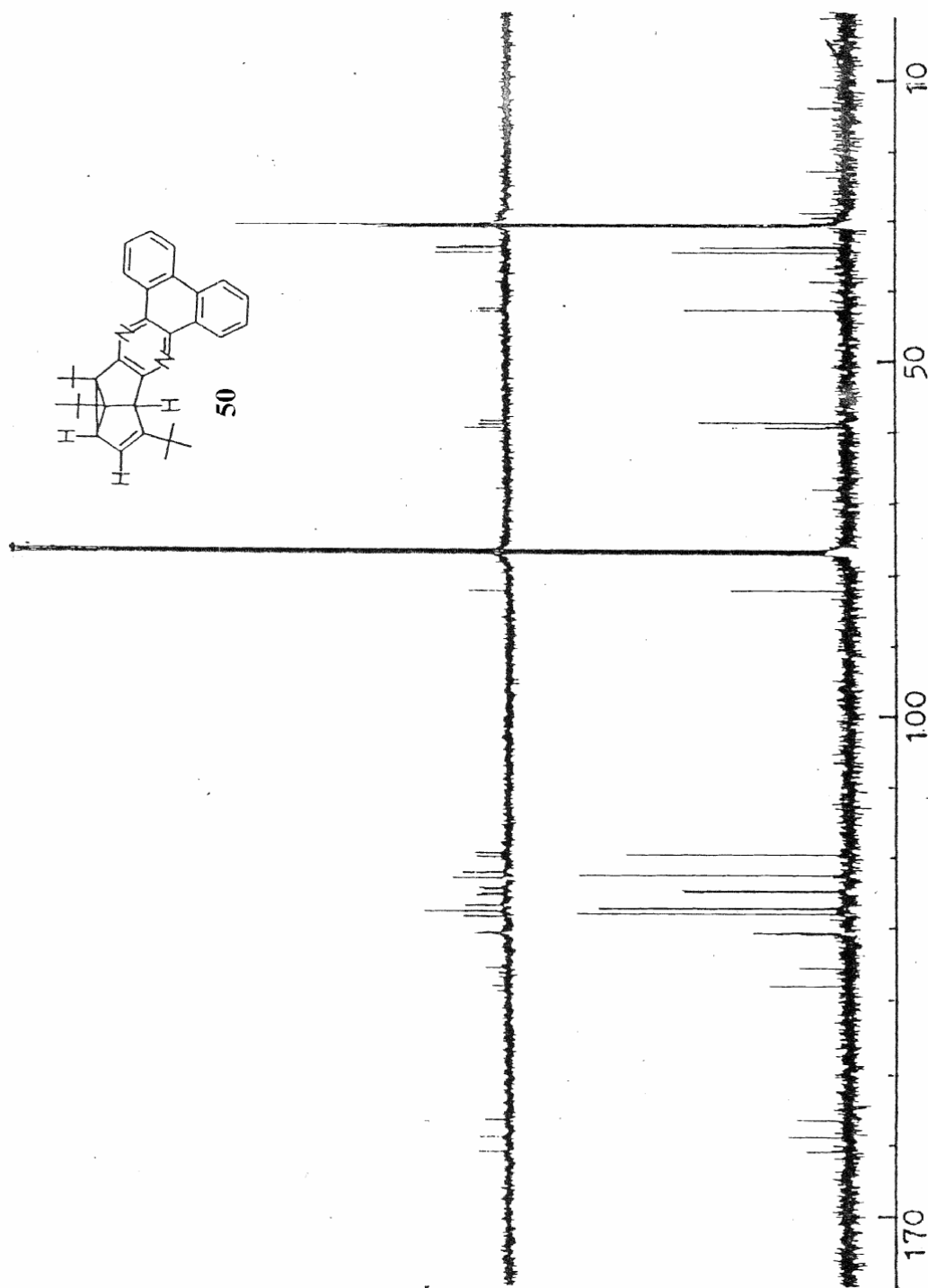


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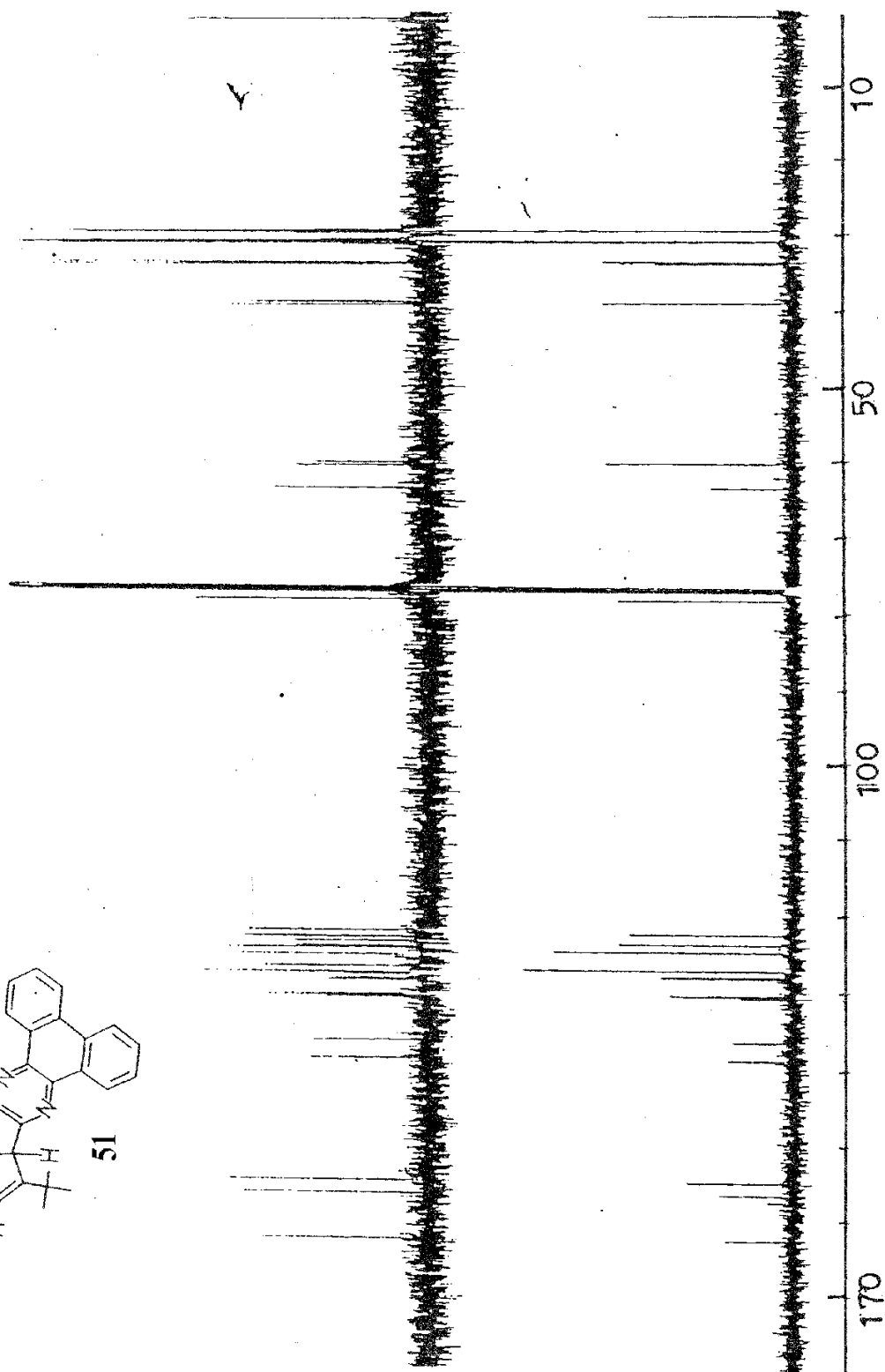
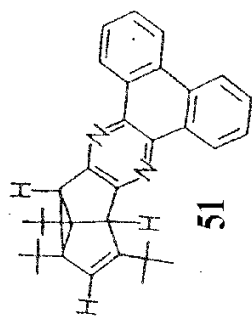




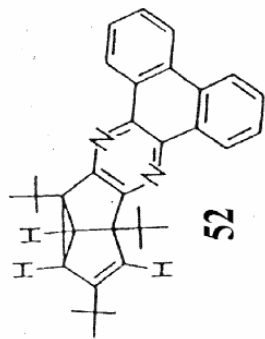
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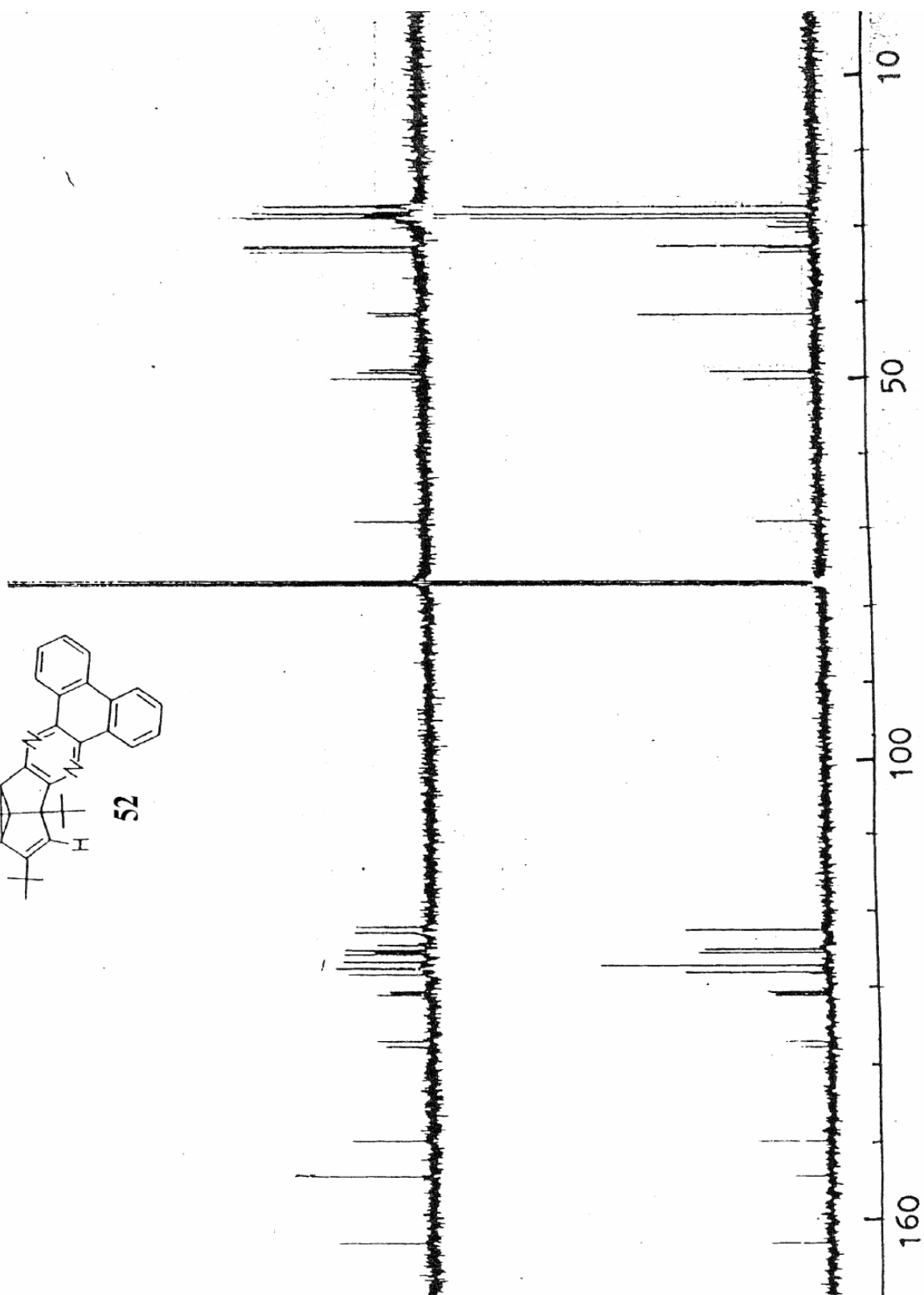
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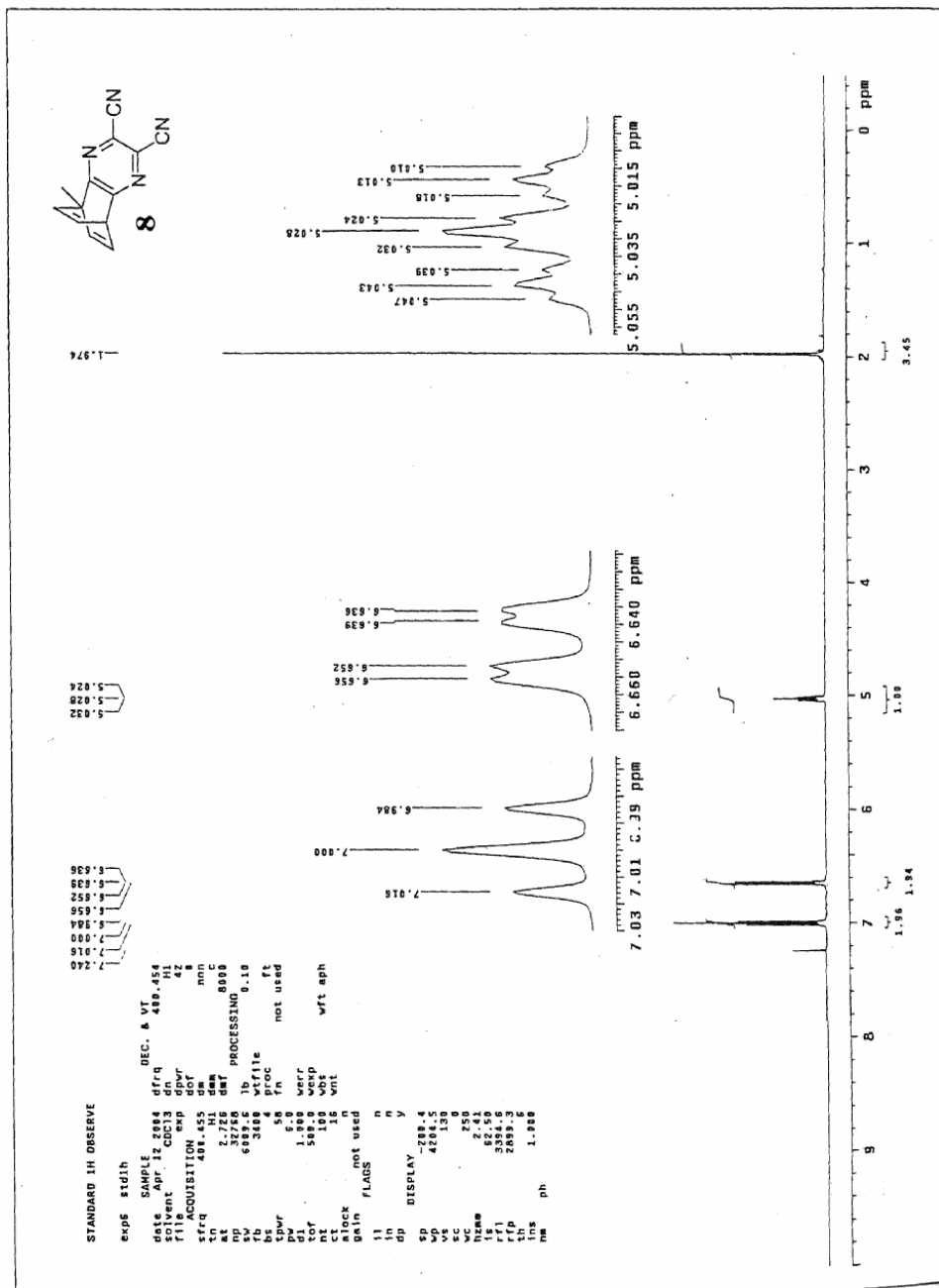
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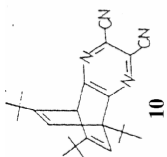
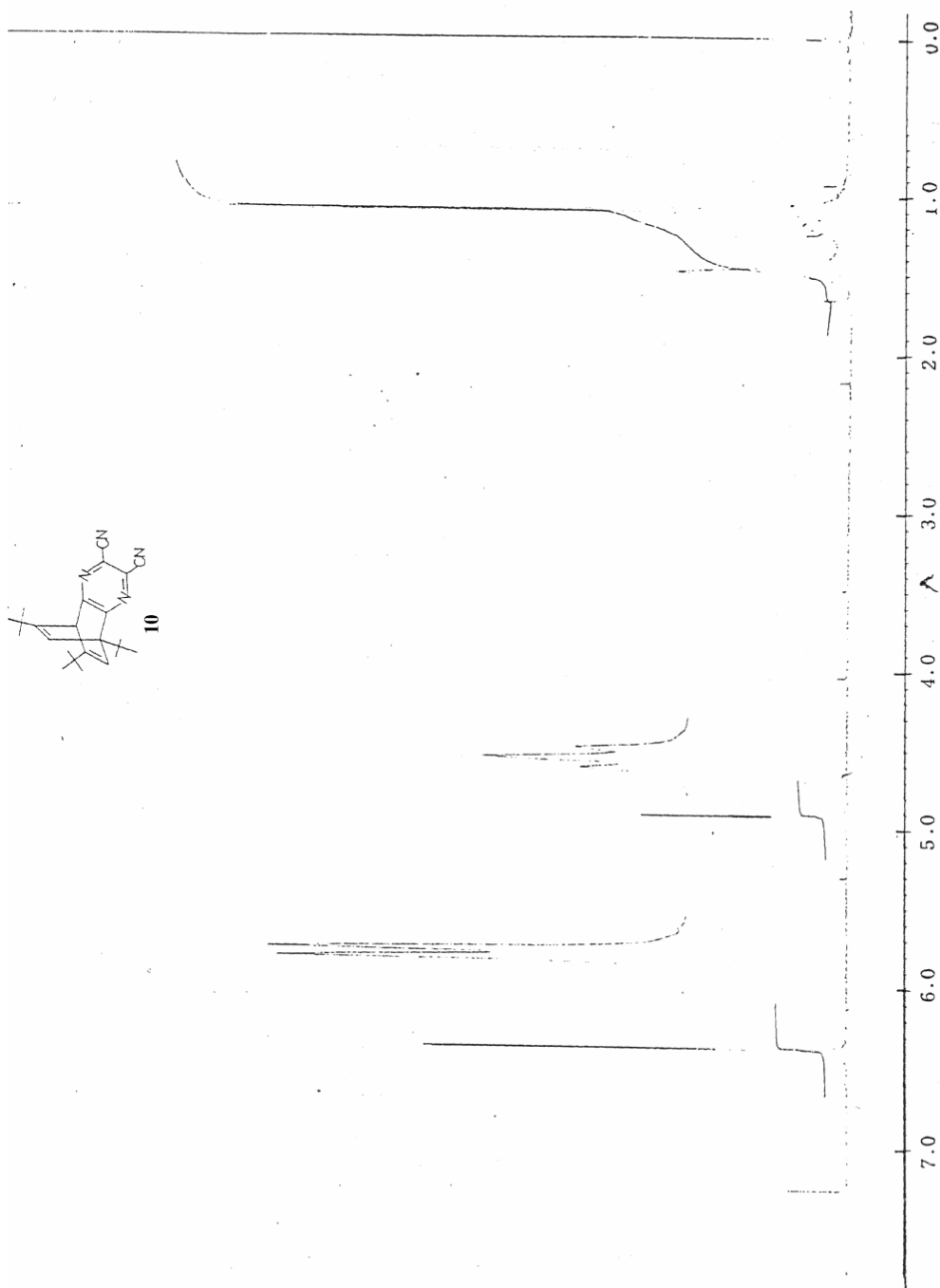
52



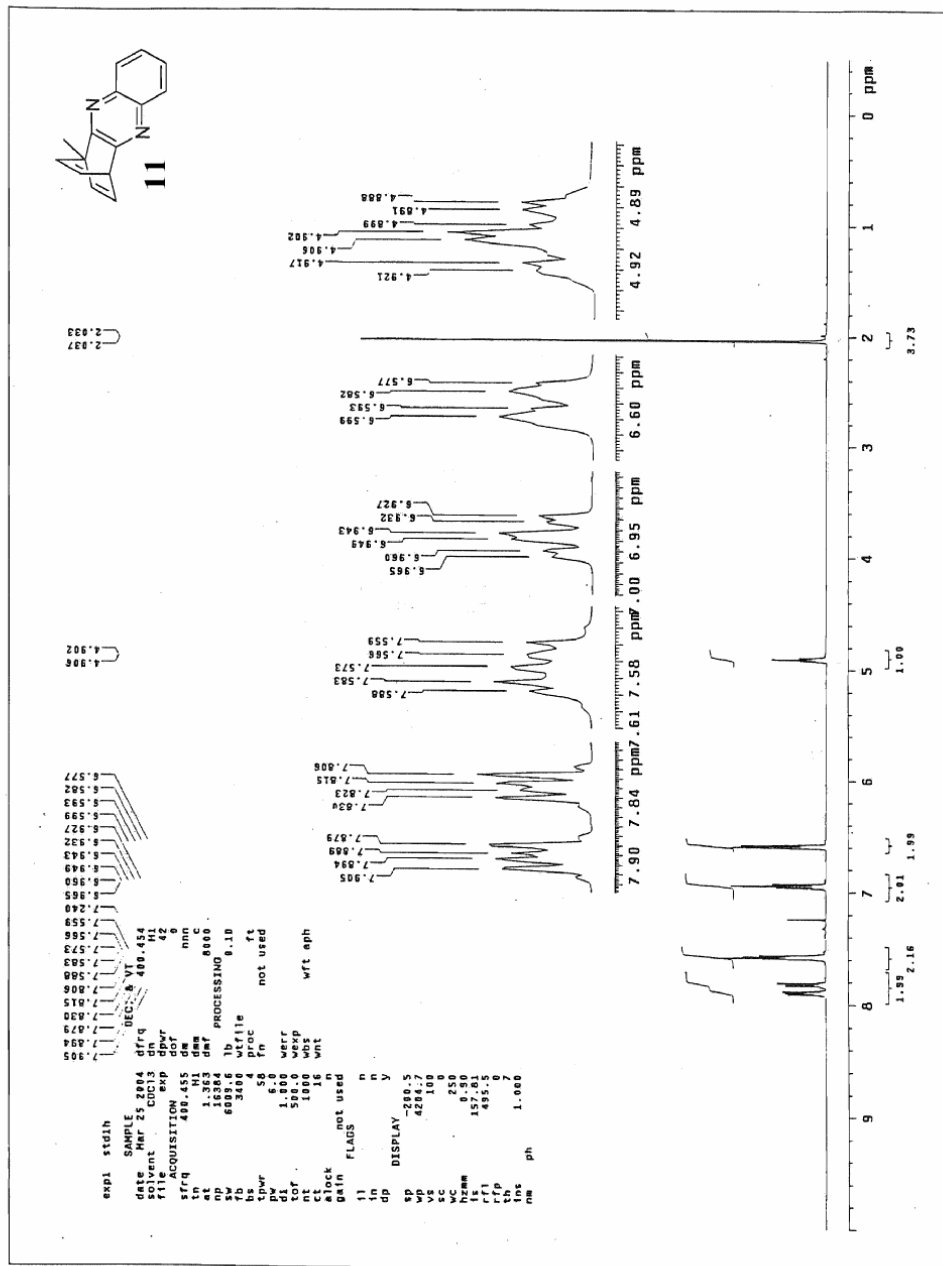
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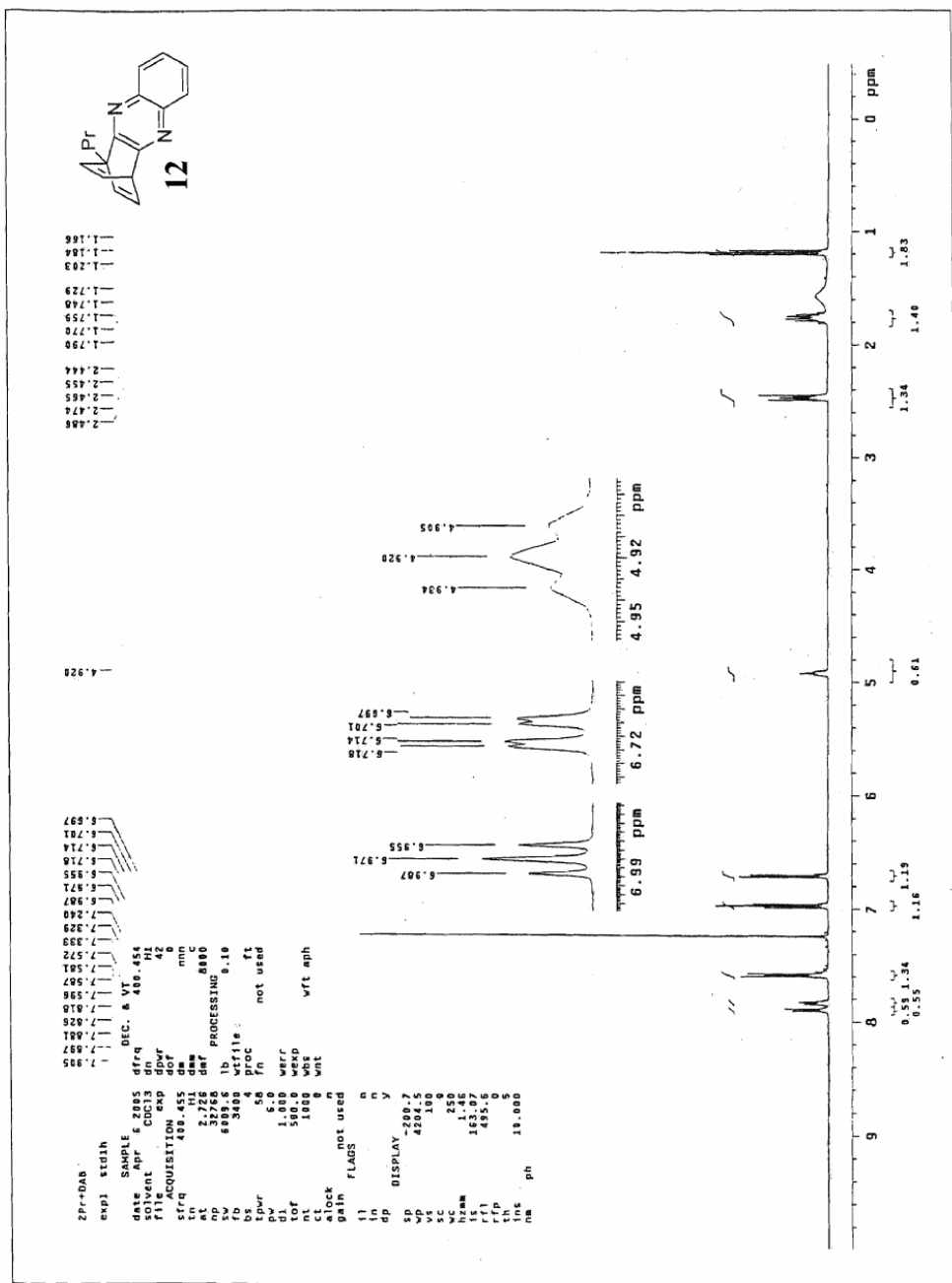


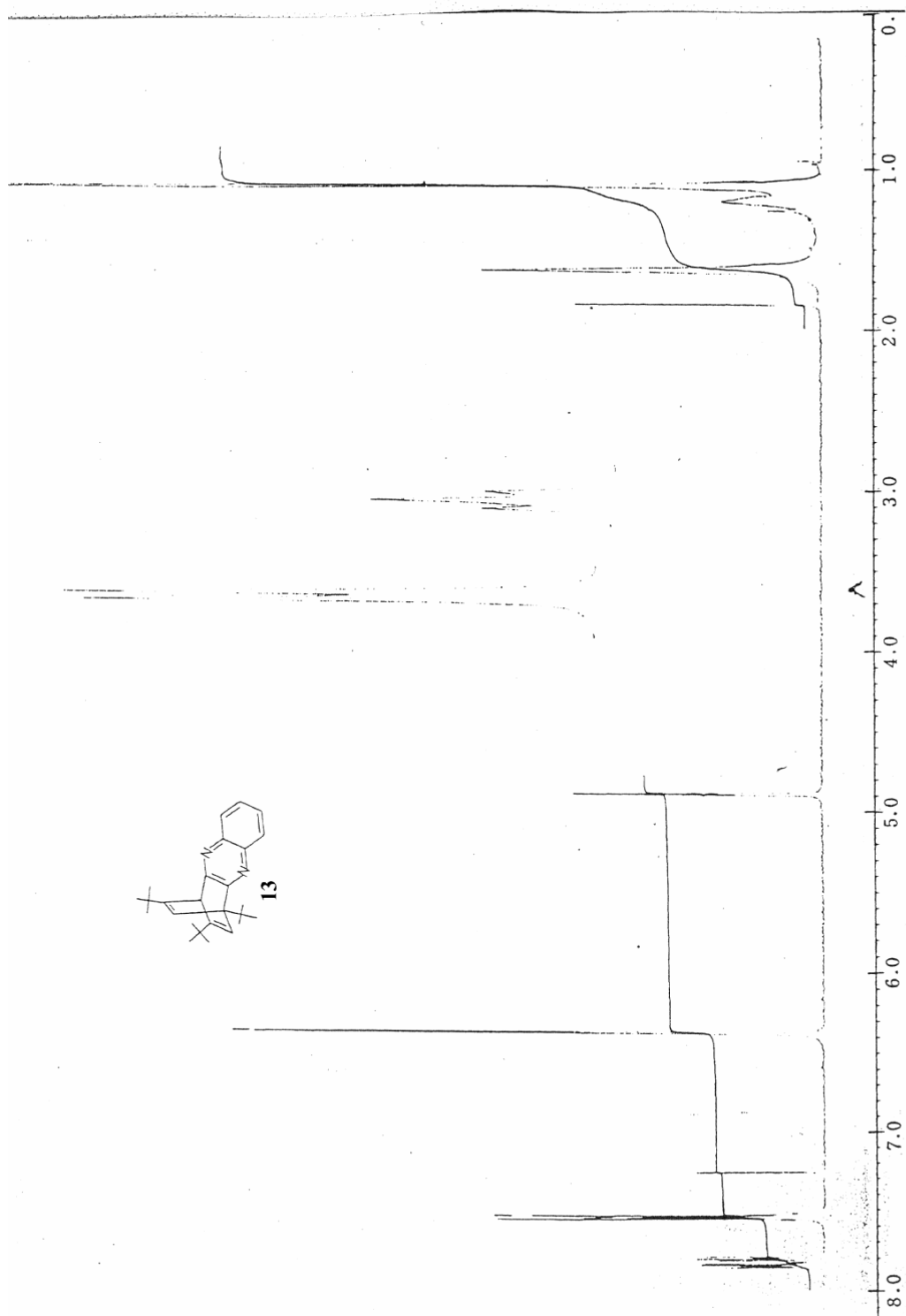
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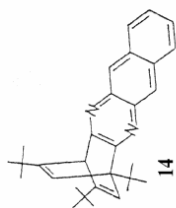
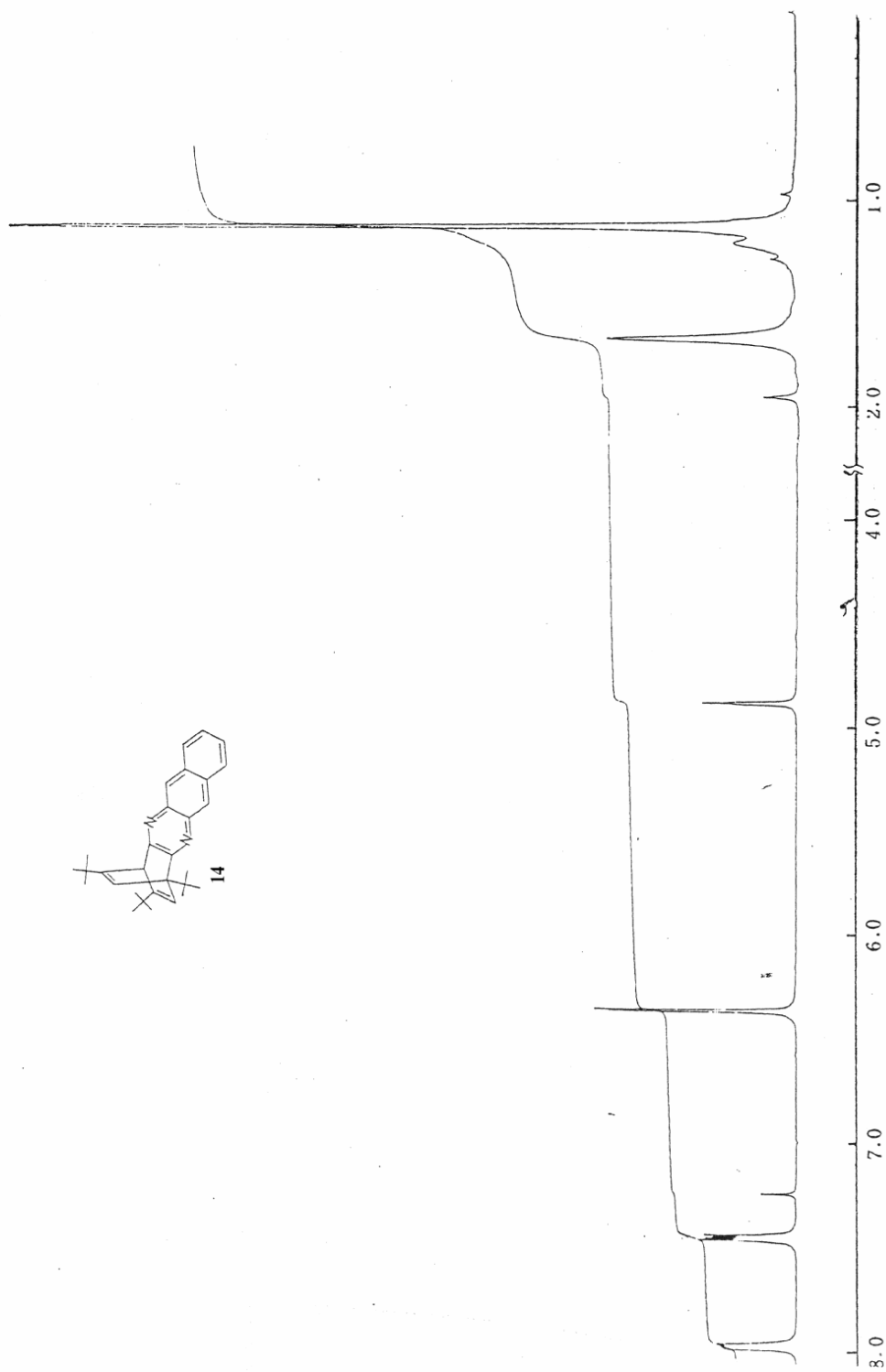
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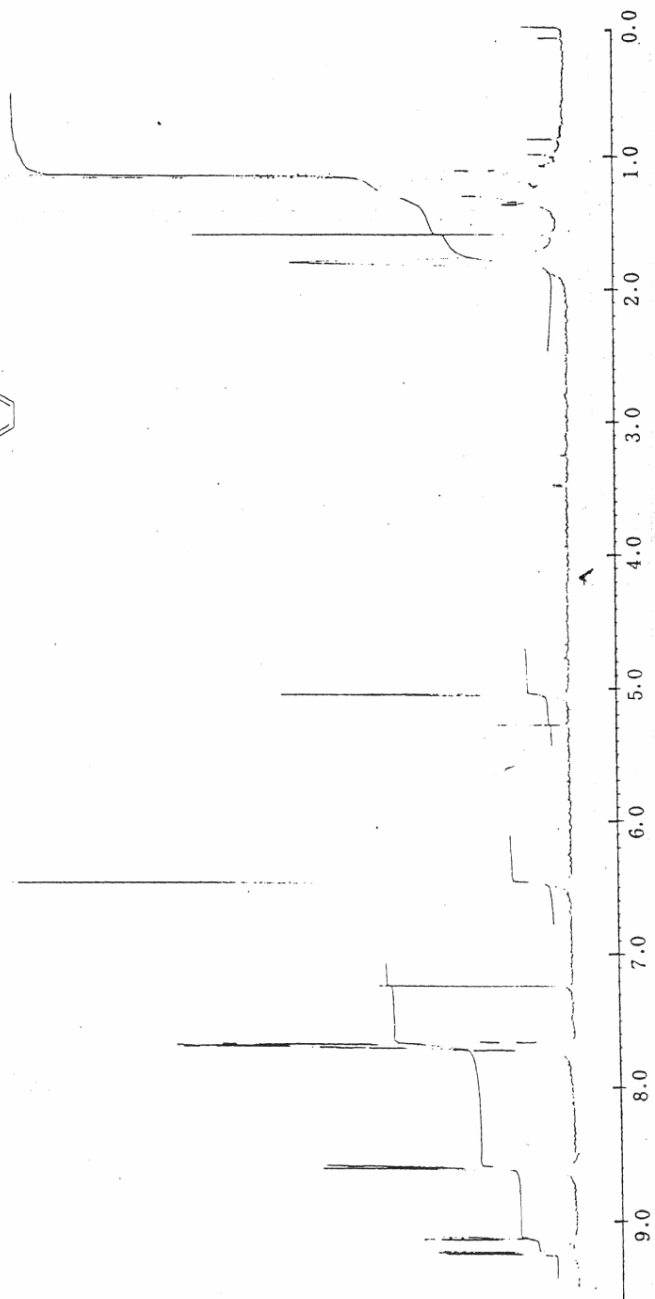
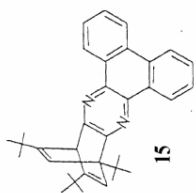




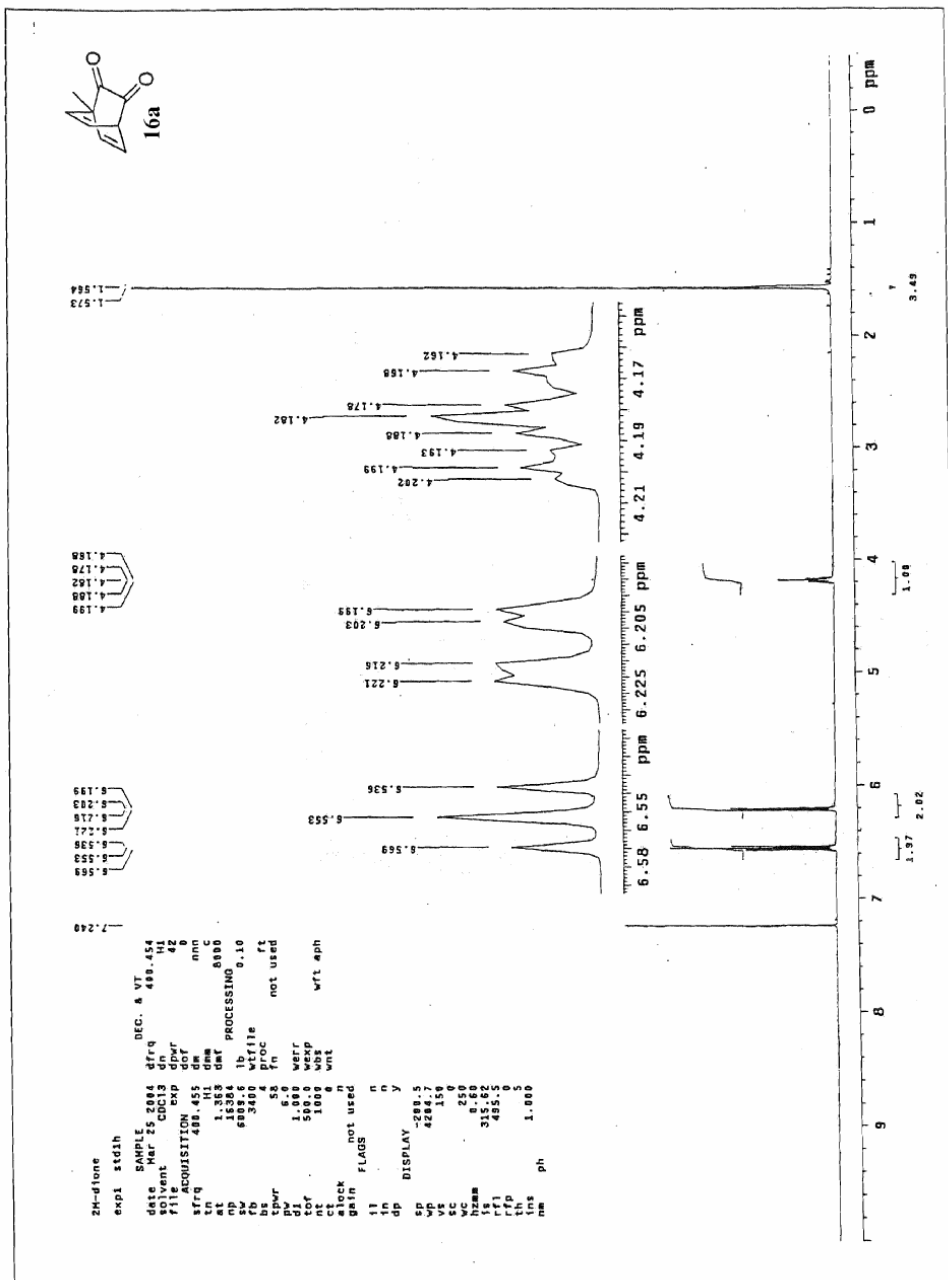
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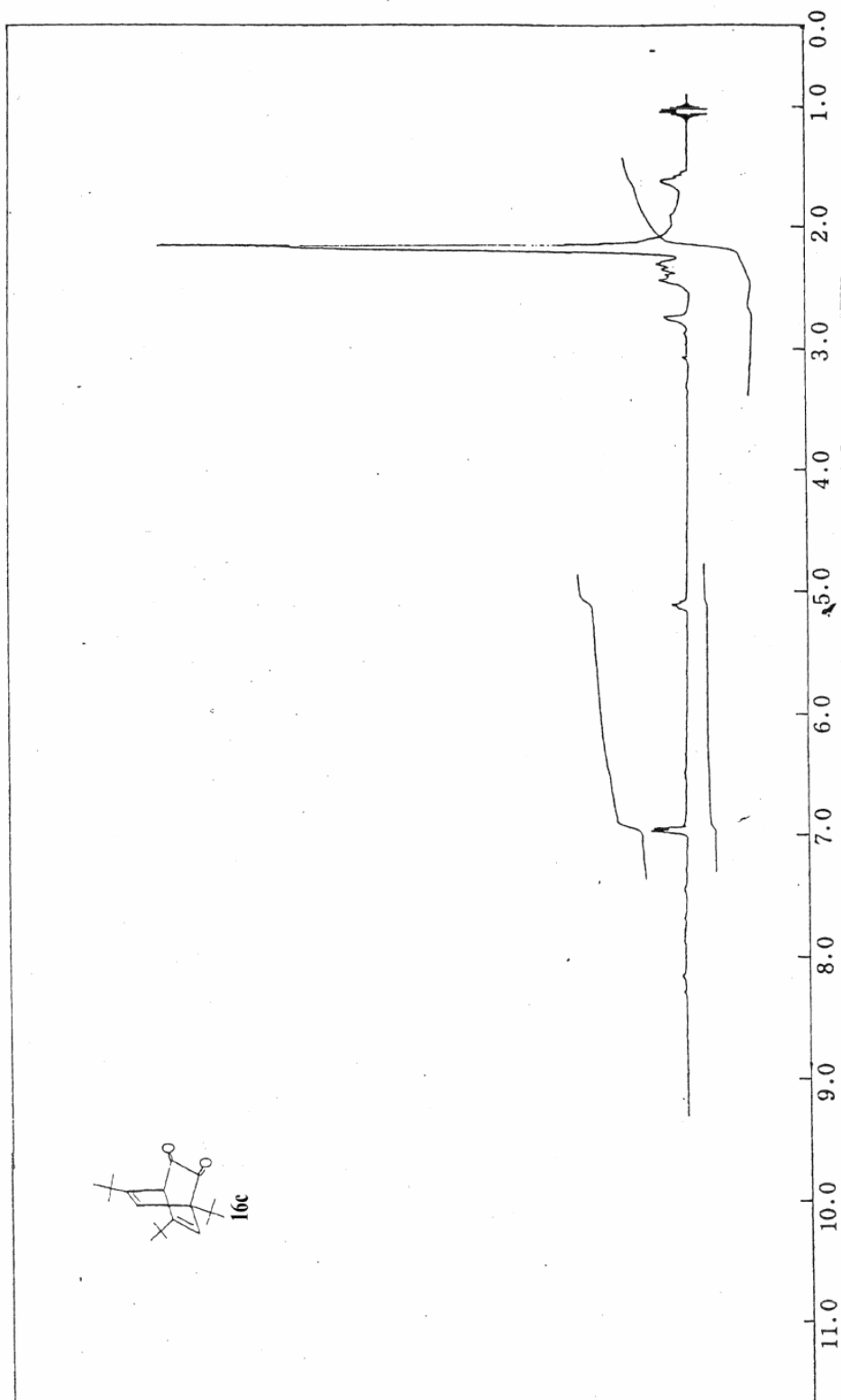
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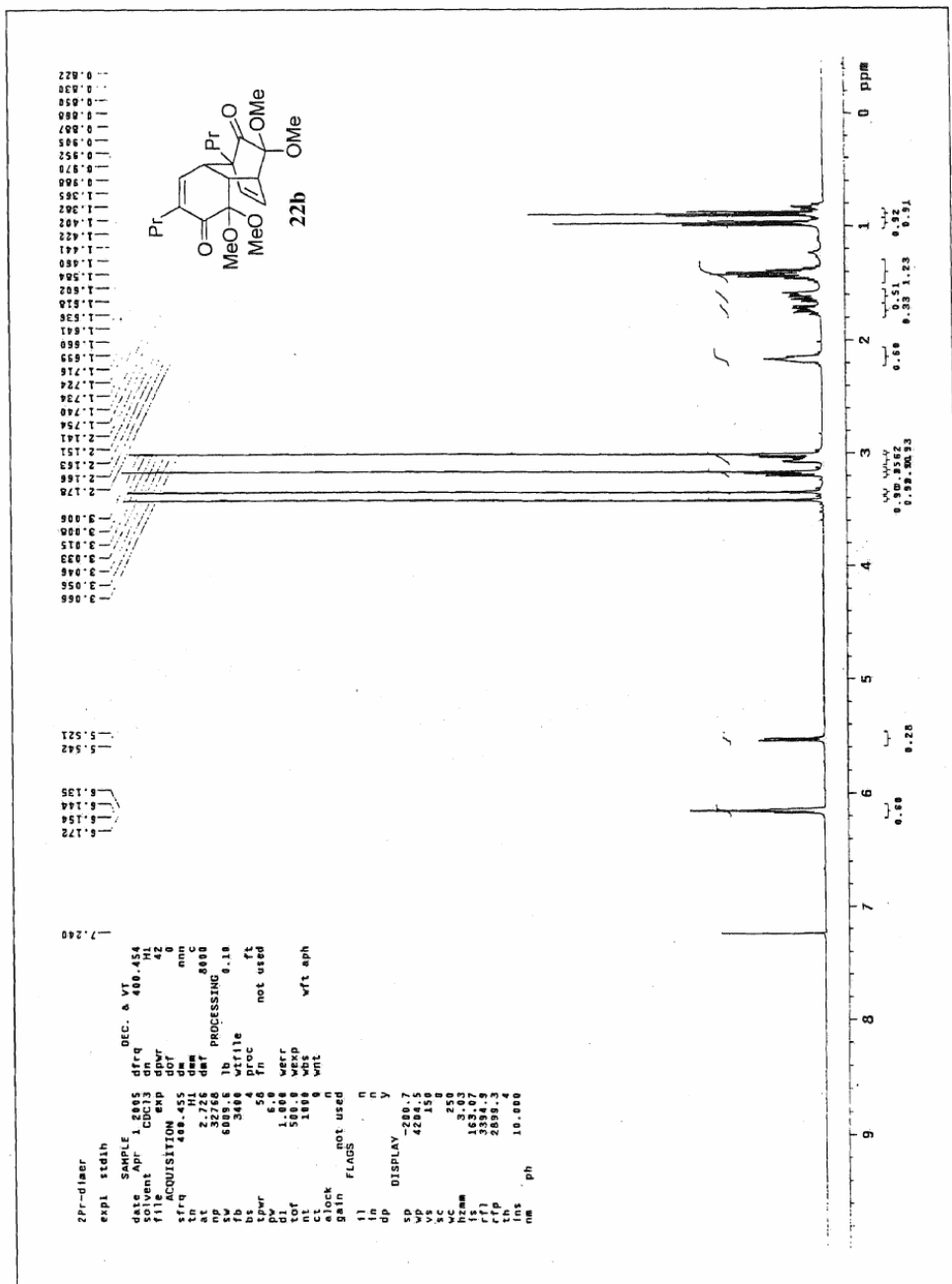
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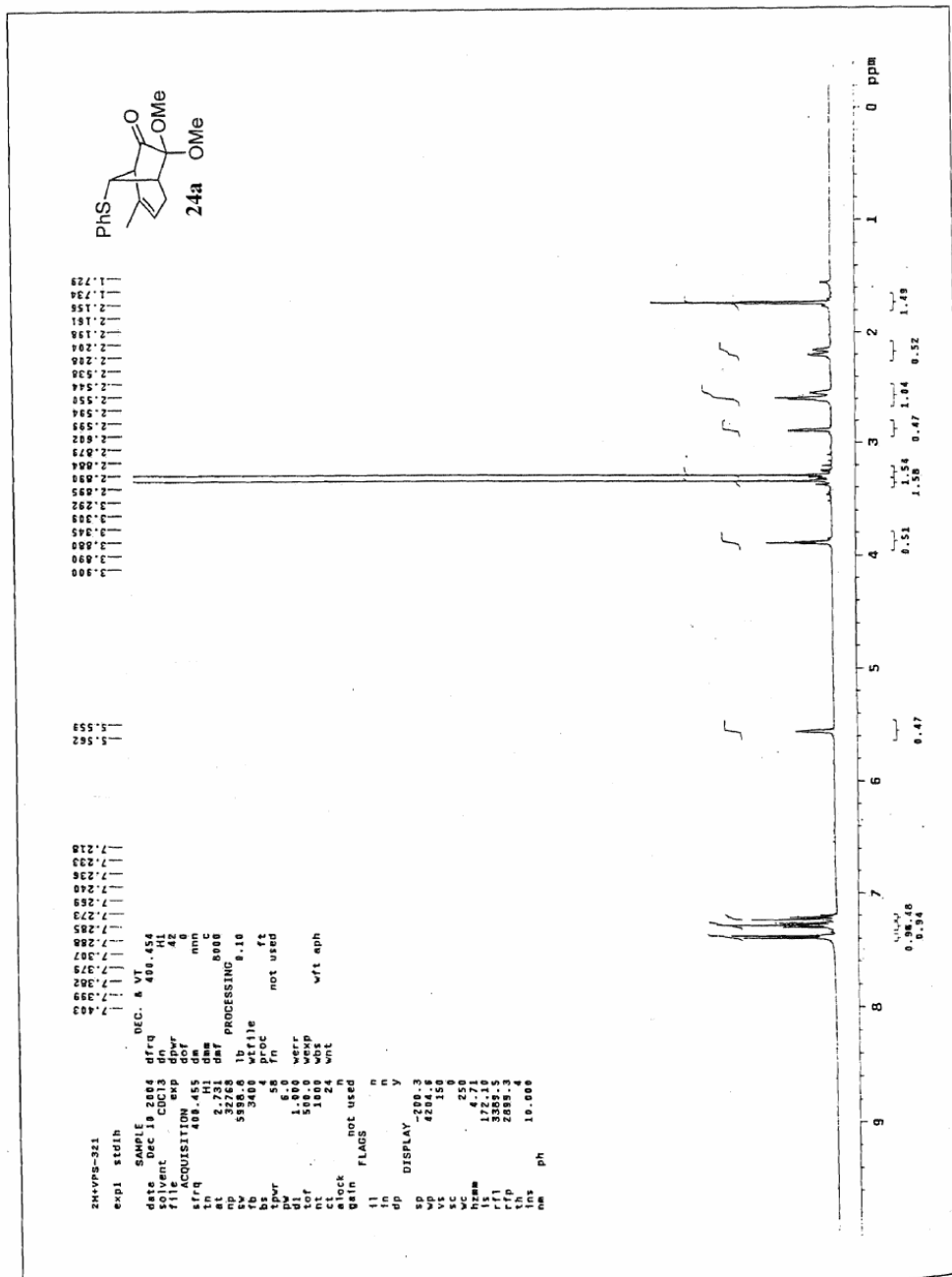


¹H NMR (16a)

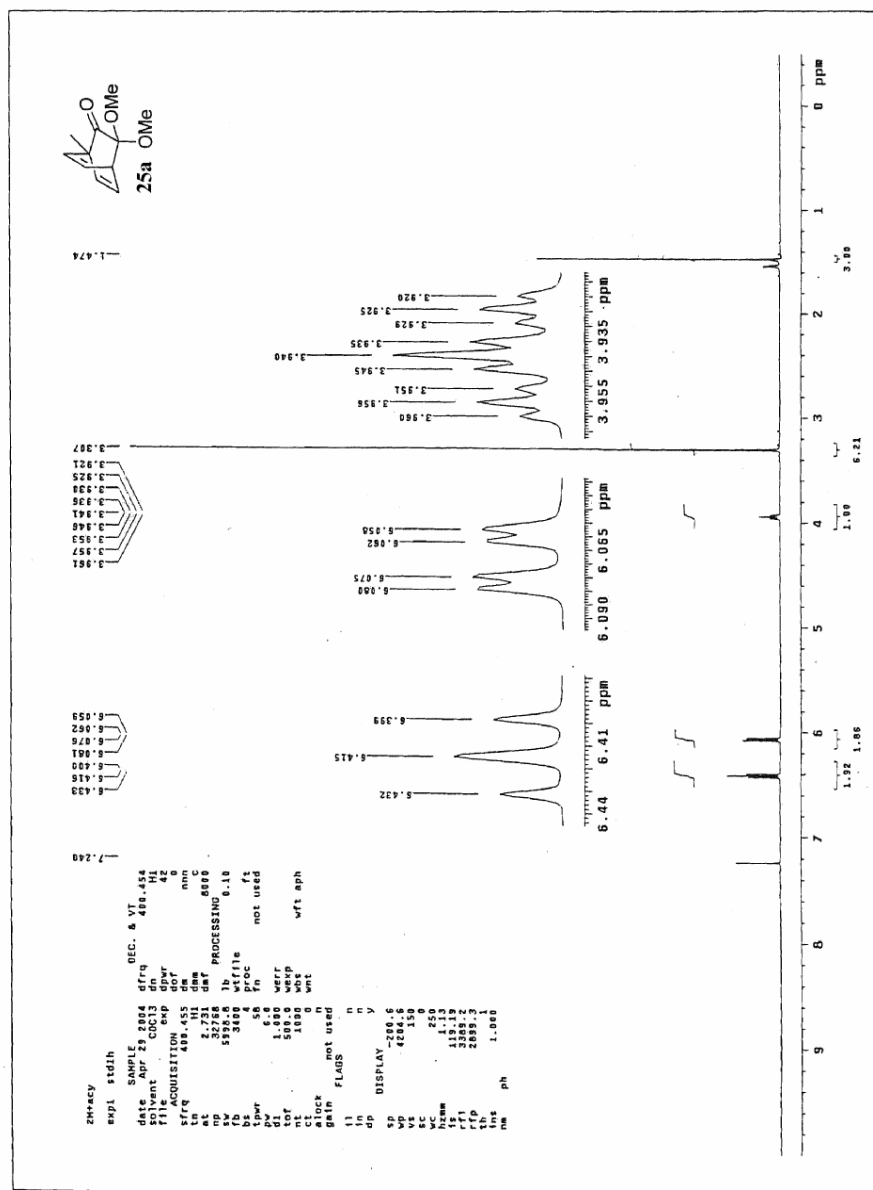


^1H NMR (**16c**)

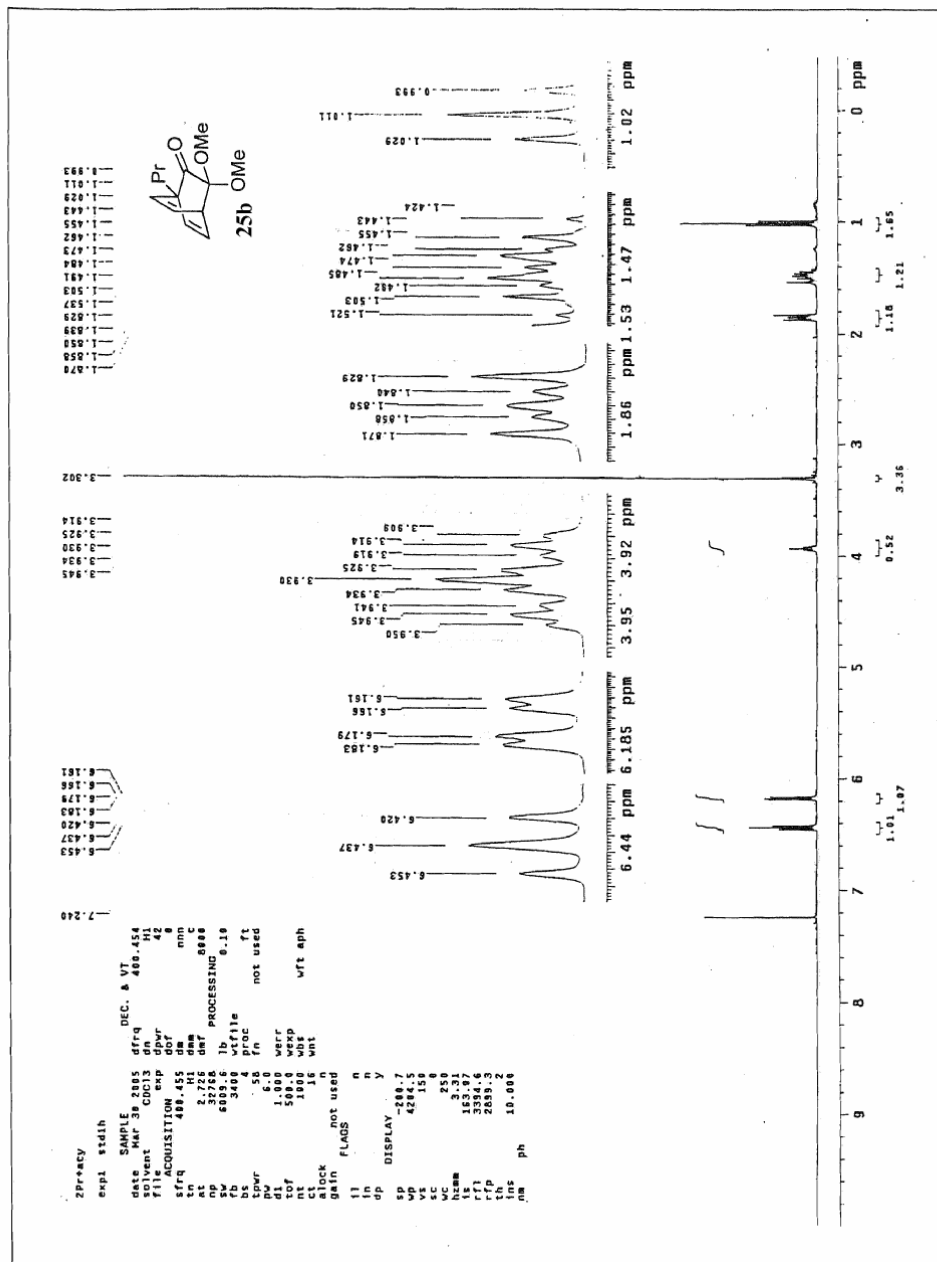




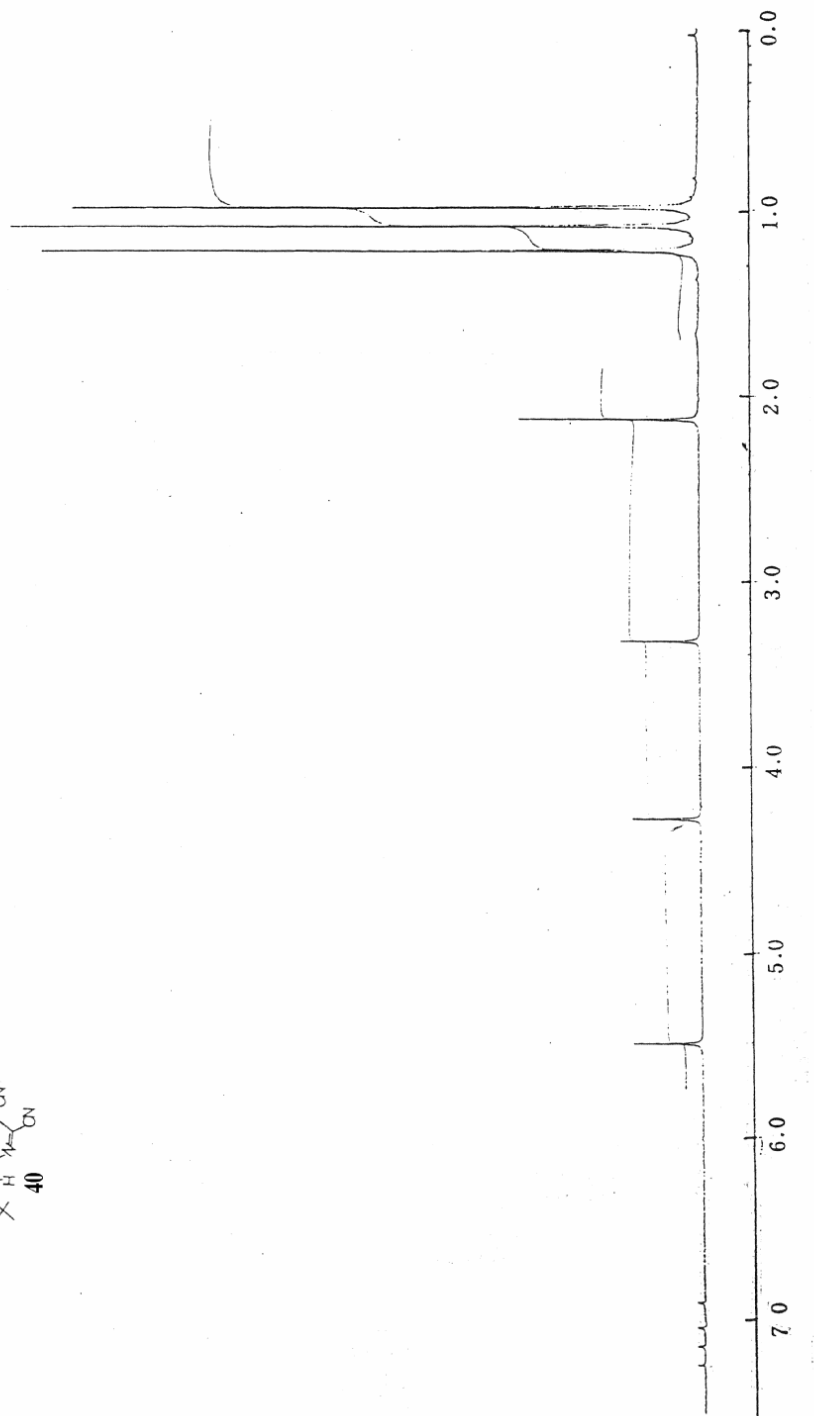
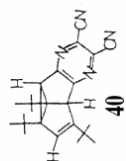
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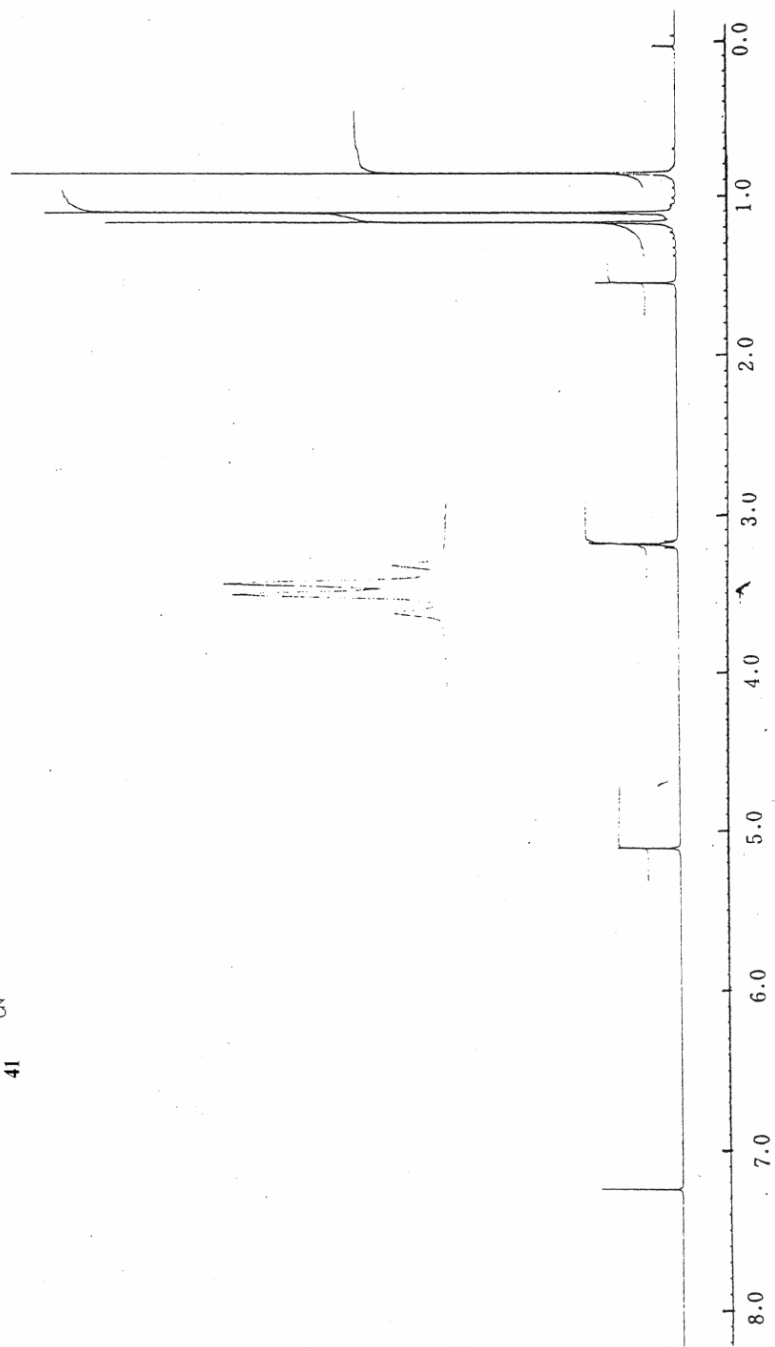
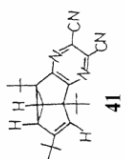
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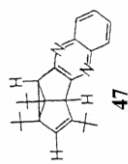
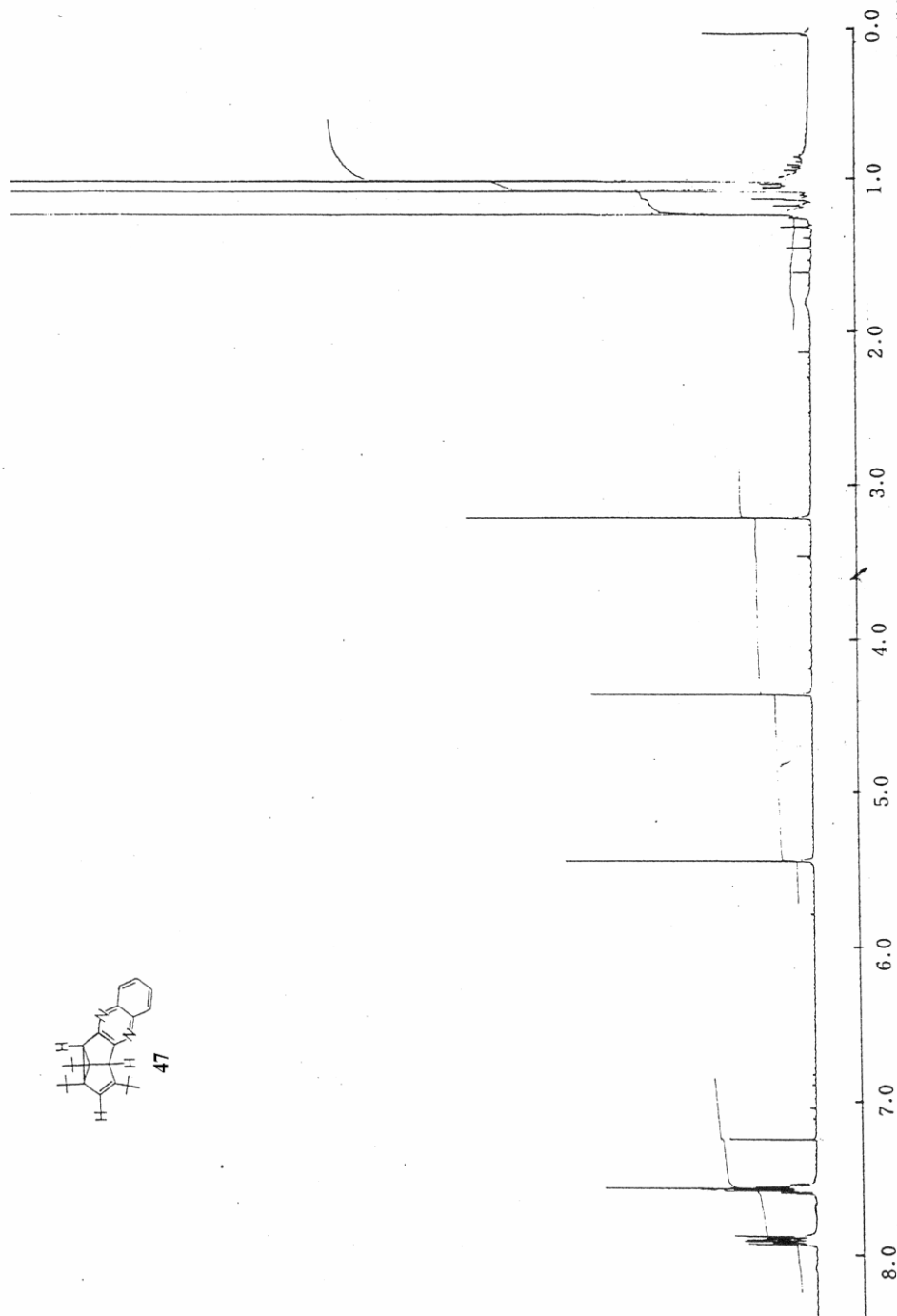
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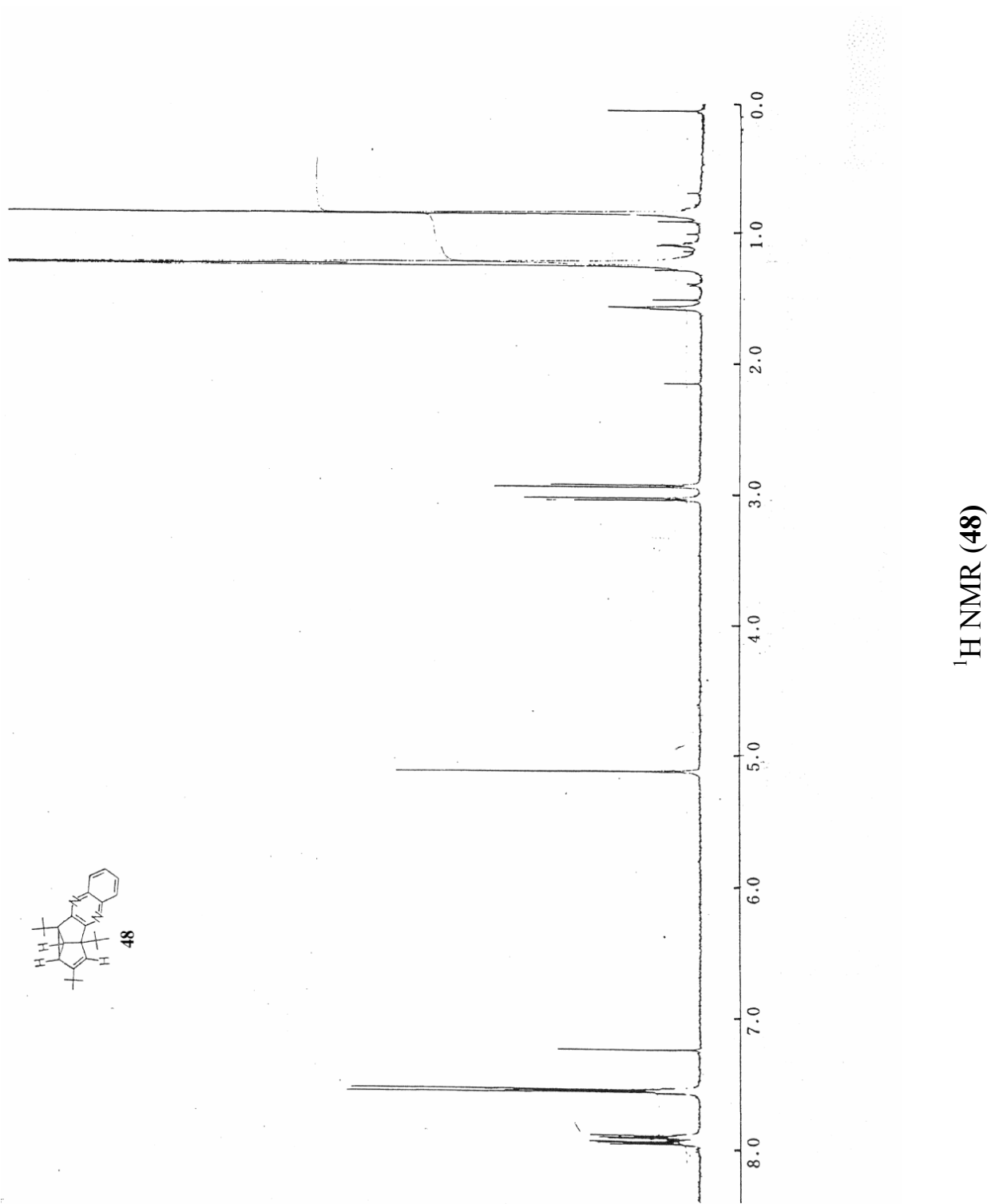
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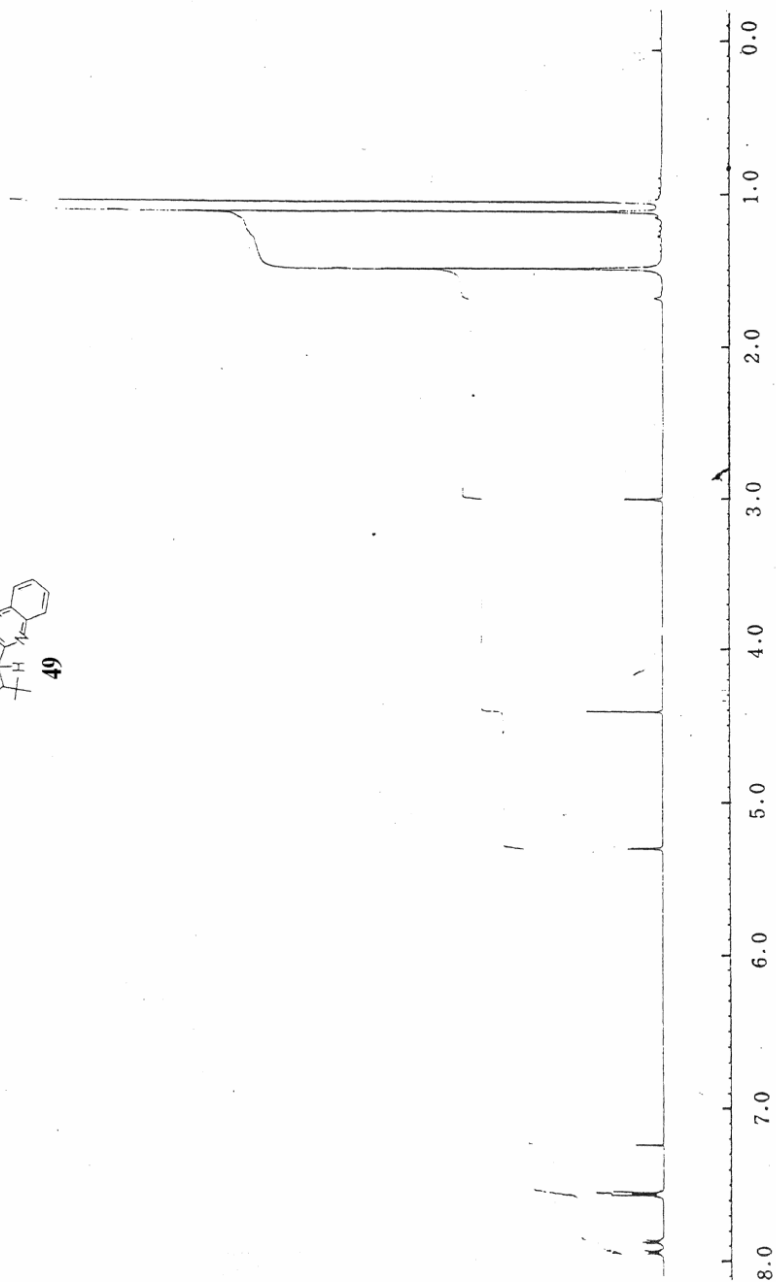
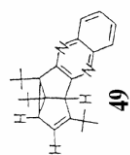


$^1\text{H NMR}$ (41)

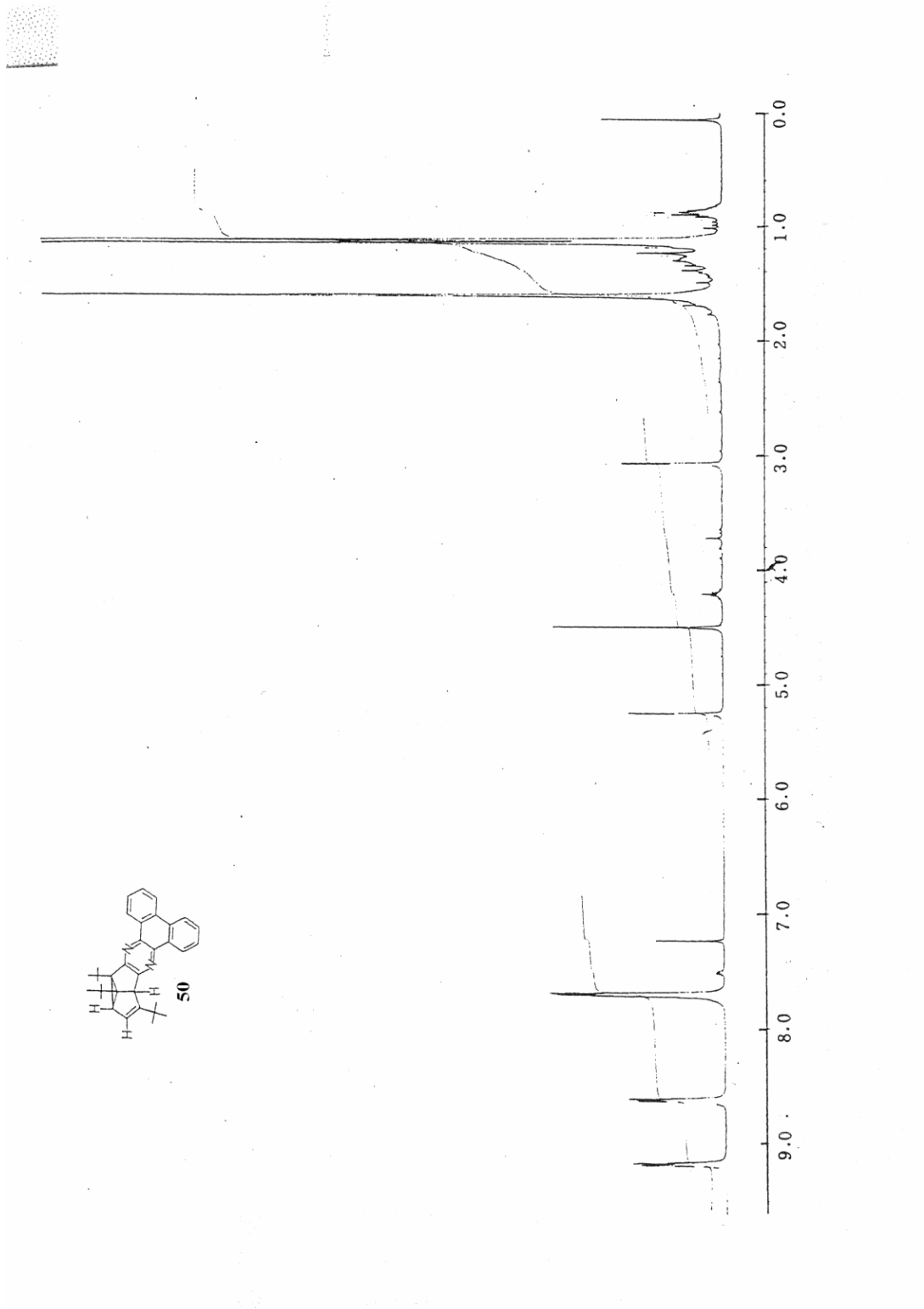


¹H NMR (47)

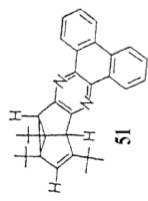
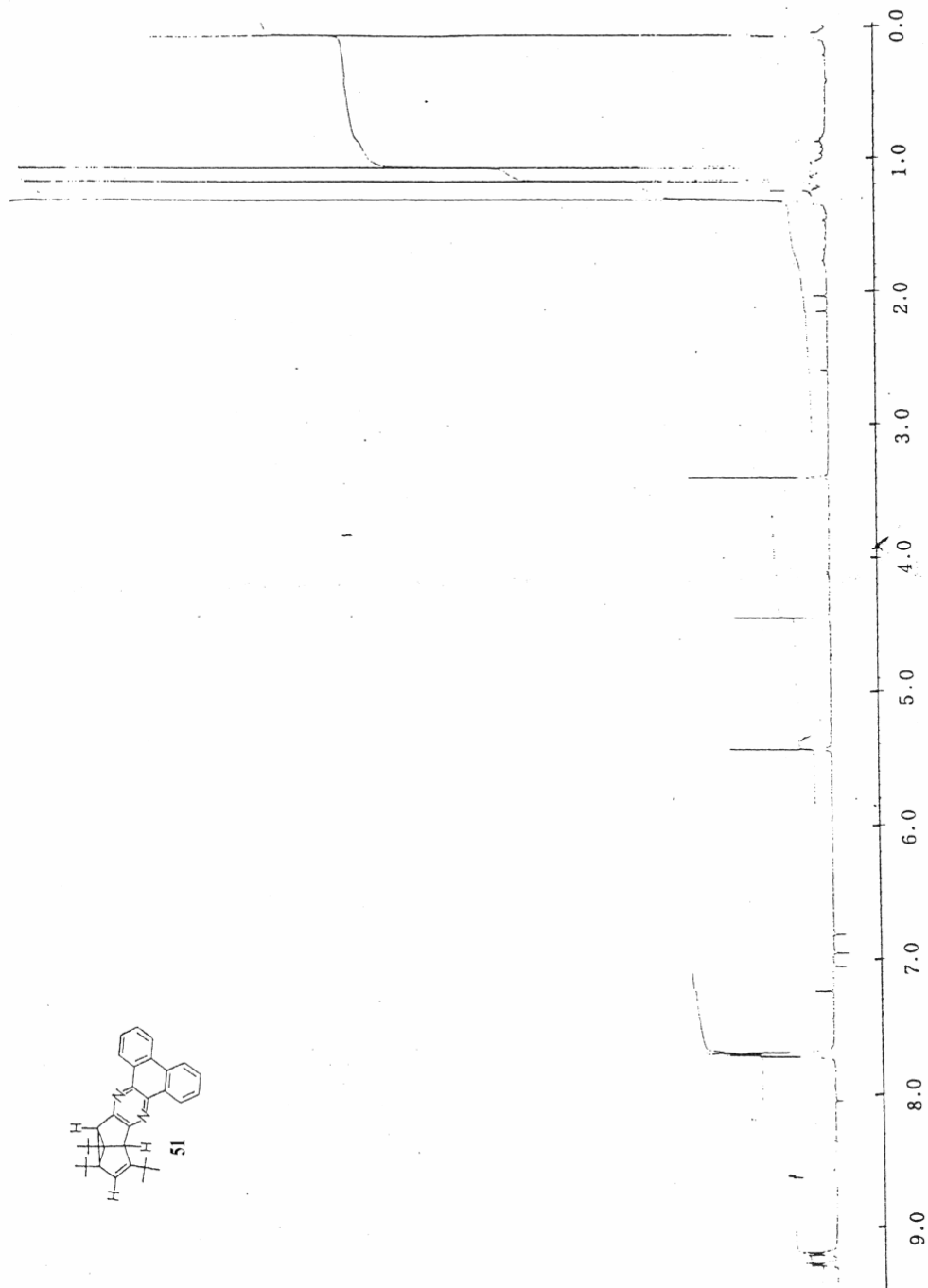




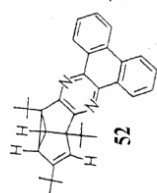
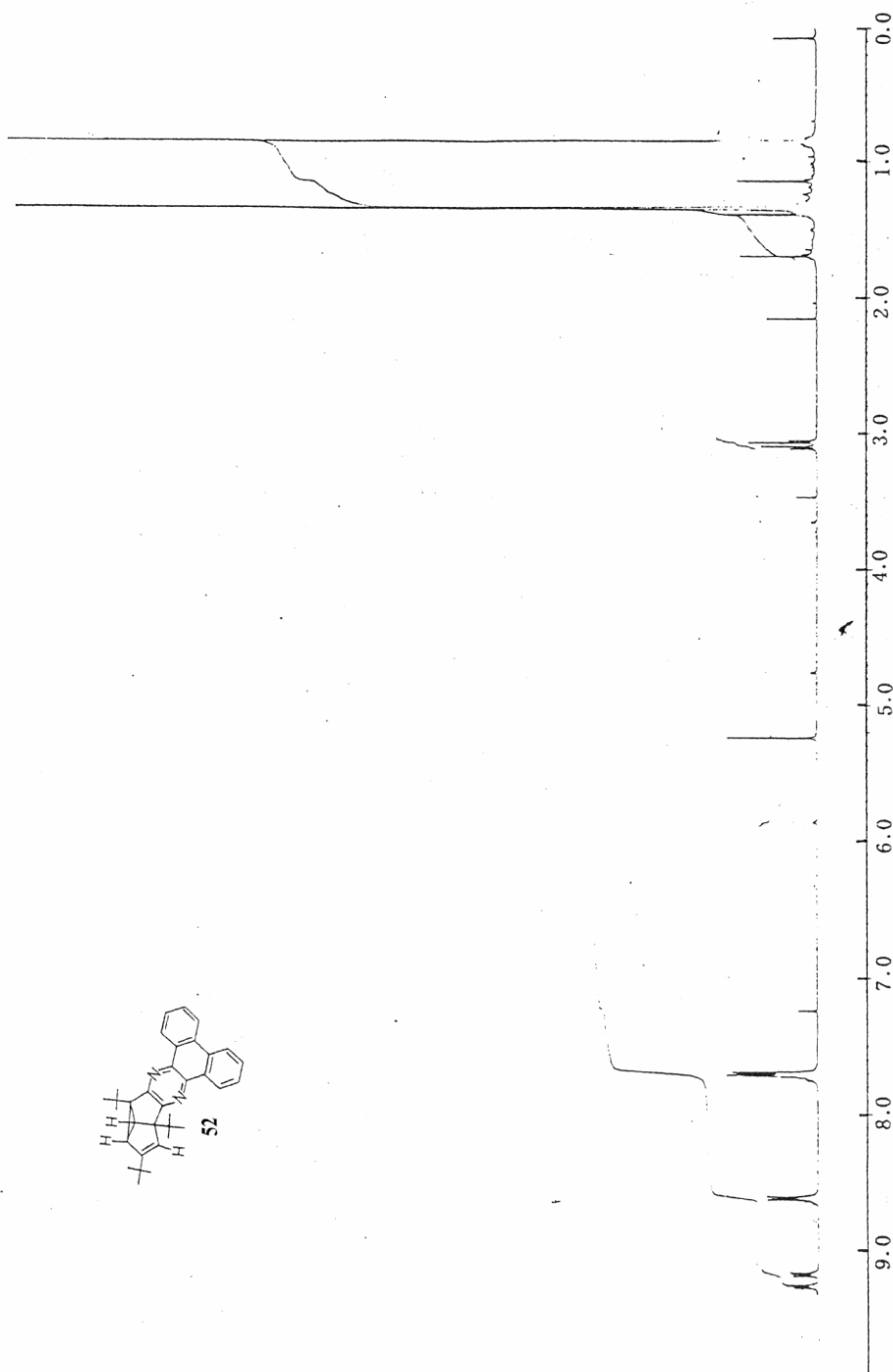
¹H NMR (49)



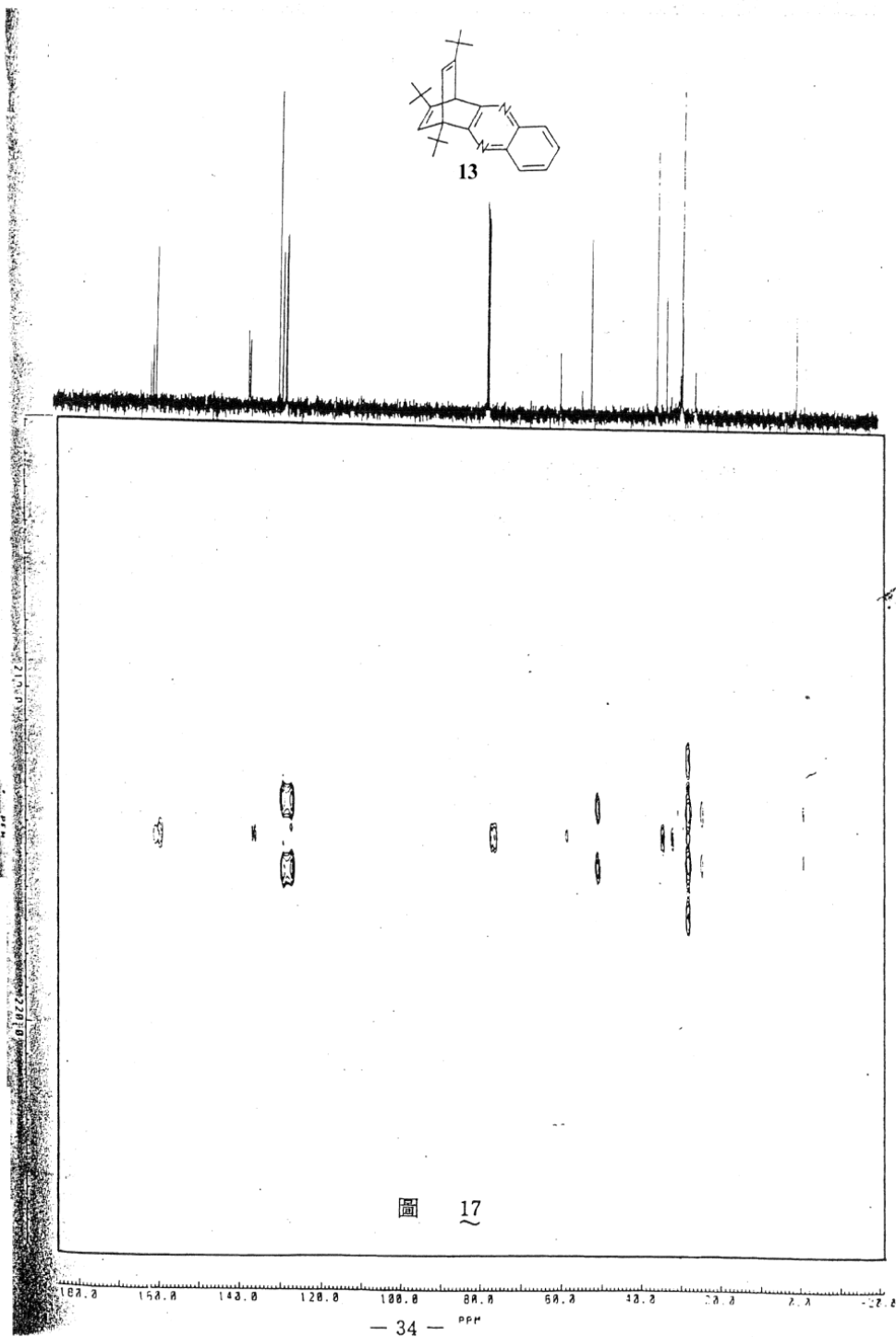
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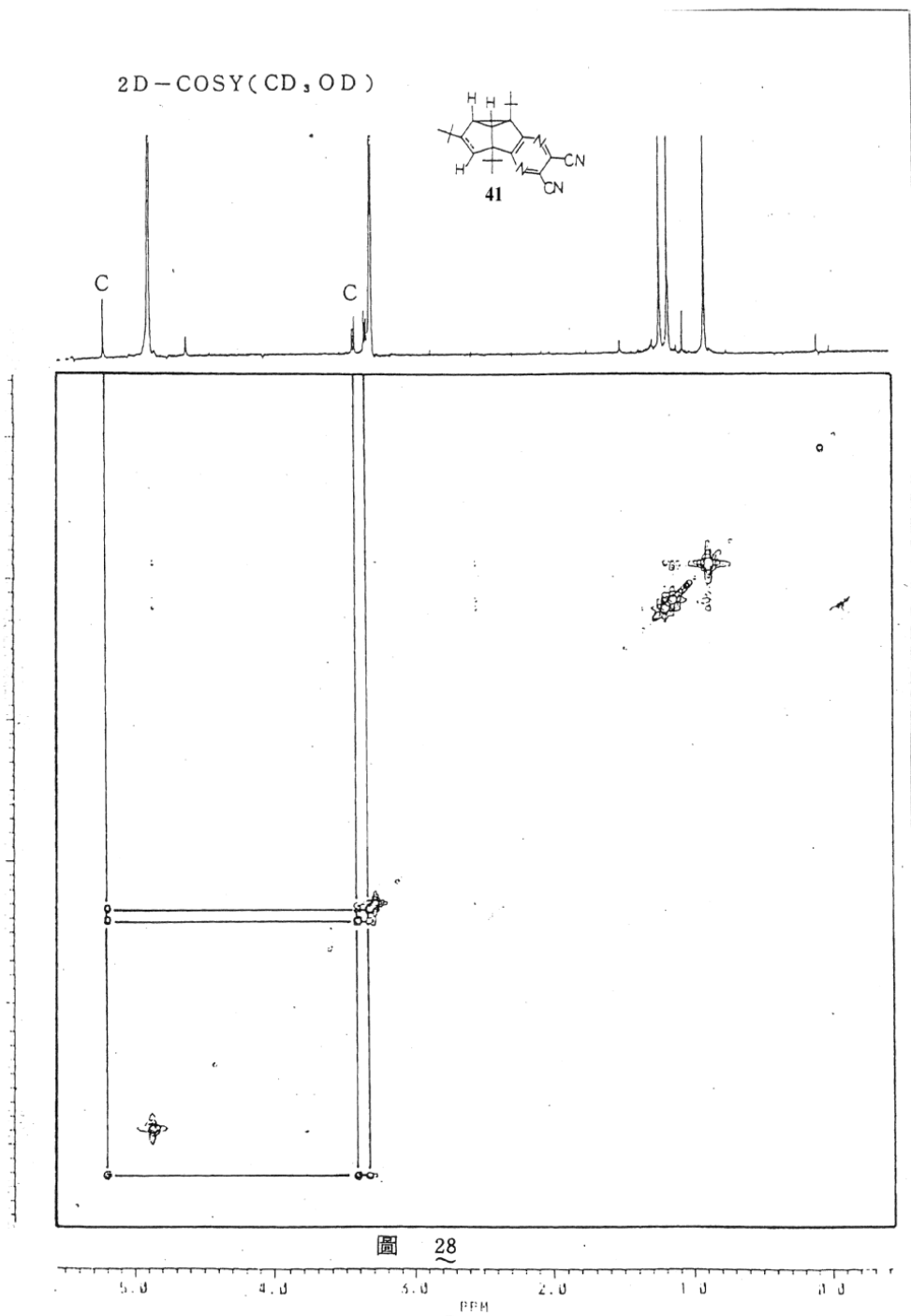
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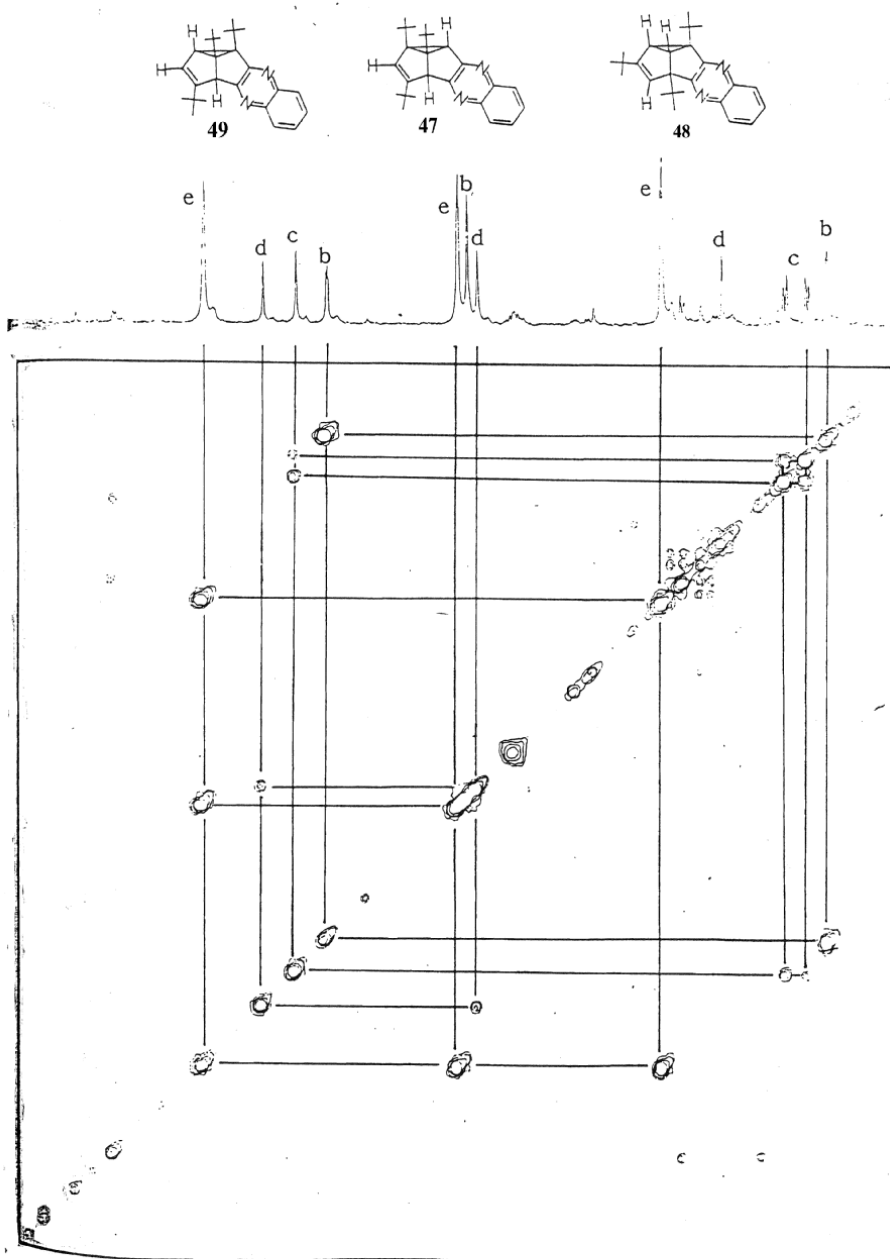
^1H NMR (52)



2D-COSY (13)



2D-COSY (41)



2D-COSY (47, 48, 49)