Supplementary Material (ESI) for Organic & Biomolecular Chemistry

A new synthesis of fully phosphorylated flavones as potent pancreatic cholesterol esterase inhibitors

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Analytical data and graphs for determination of inhibitor IC50

Compounds **1a–1e, 2a–2e** were assayed according to the above procedure. The IC50 values are shown in Table 1, and Figures 1–7.

Table 1 Inhibitory effects on CEase of **1a**–**1e** and **2a**–**2e**

Compound	IC50/nM	Compound	IC50/μM
2a	3.89	**1a**	28.1
2b	26.1	**1b**	35.7
2c	3.76	**1c**	ni[a]
2d	2.44	**1d**	ni
2e	390	**1e**	ni

[a] ni, no inhibition at 100 μM.

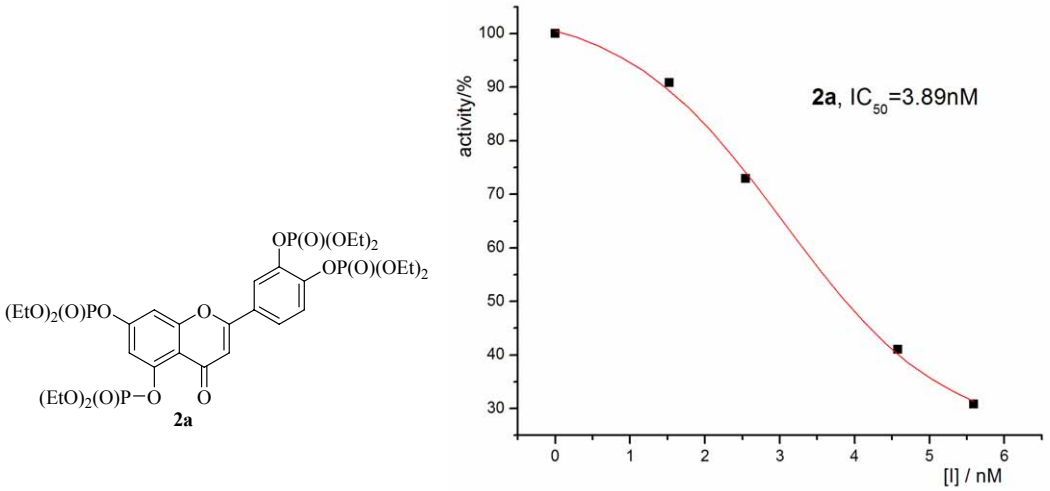


Figure 1. Graph for determining IC50 value of **2a** for CEase inhibition

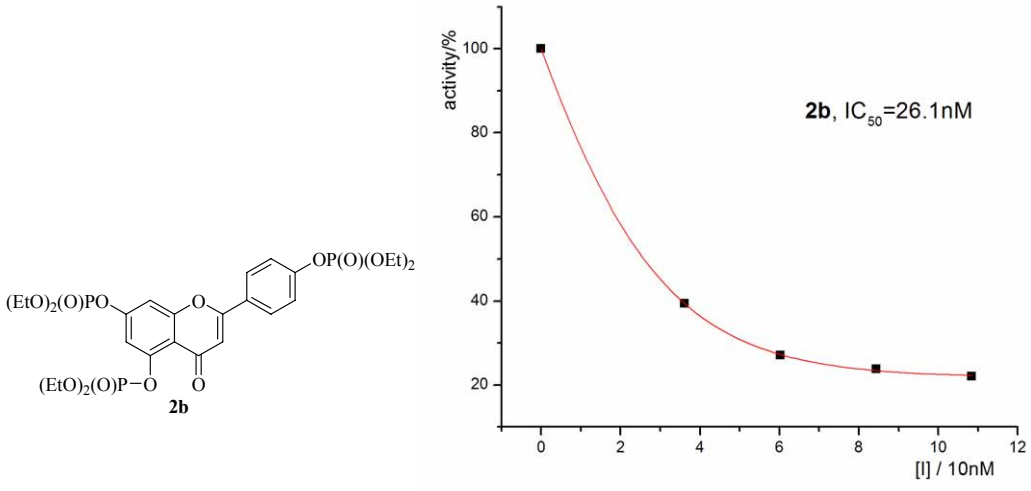
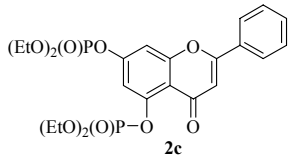


Figure 2. Graph for determining IC50 value of **2b** for CEase inhibition



2c

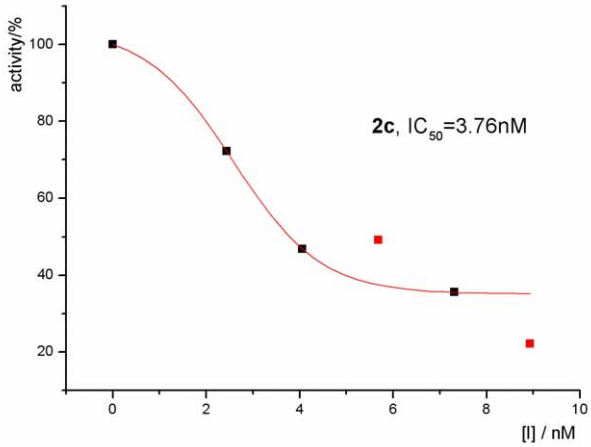
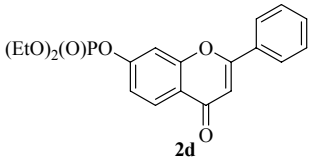


Figure 3. Graph for determining IC50 value of **2c** for CEase inhibition



2d

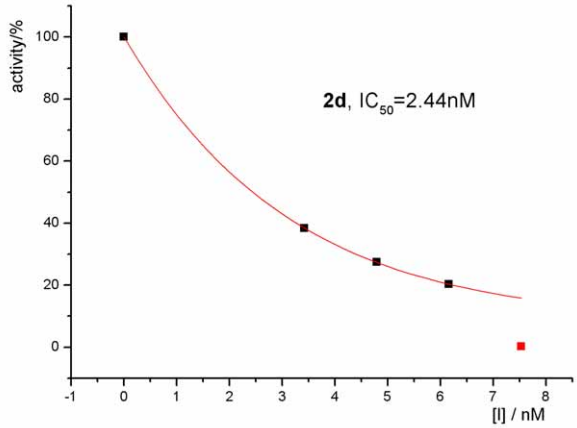
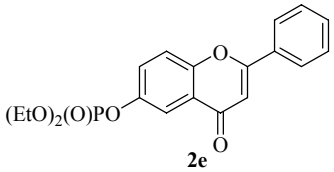


Figure 4. Graph for determining IC50 value of **2d** for CEase inhibition



2e

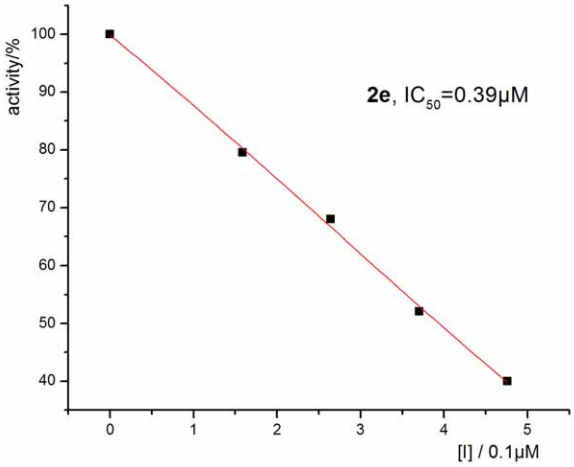


Figure 5. Graph for determining IC50 value of **2e** for CEase inhibition

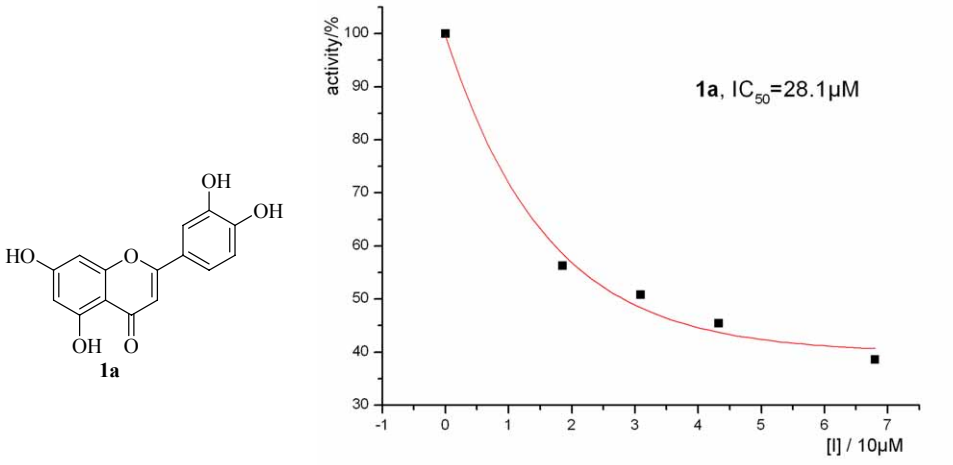


Figure 6. Graph for determining IC50 value of **1a** for CEase inhibition

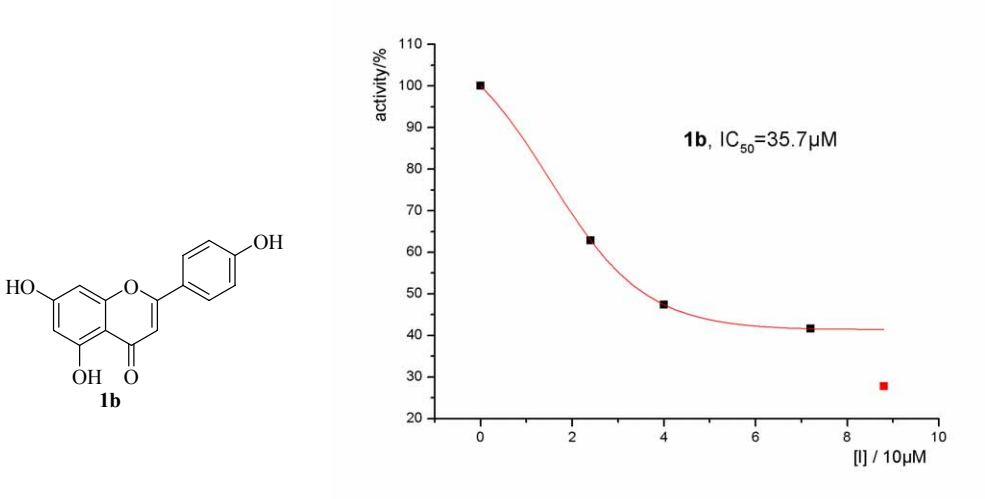
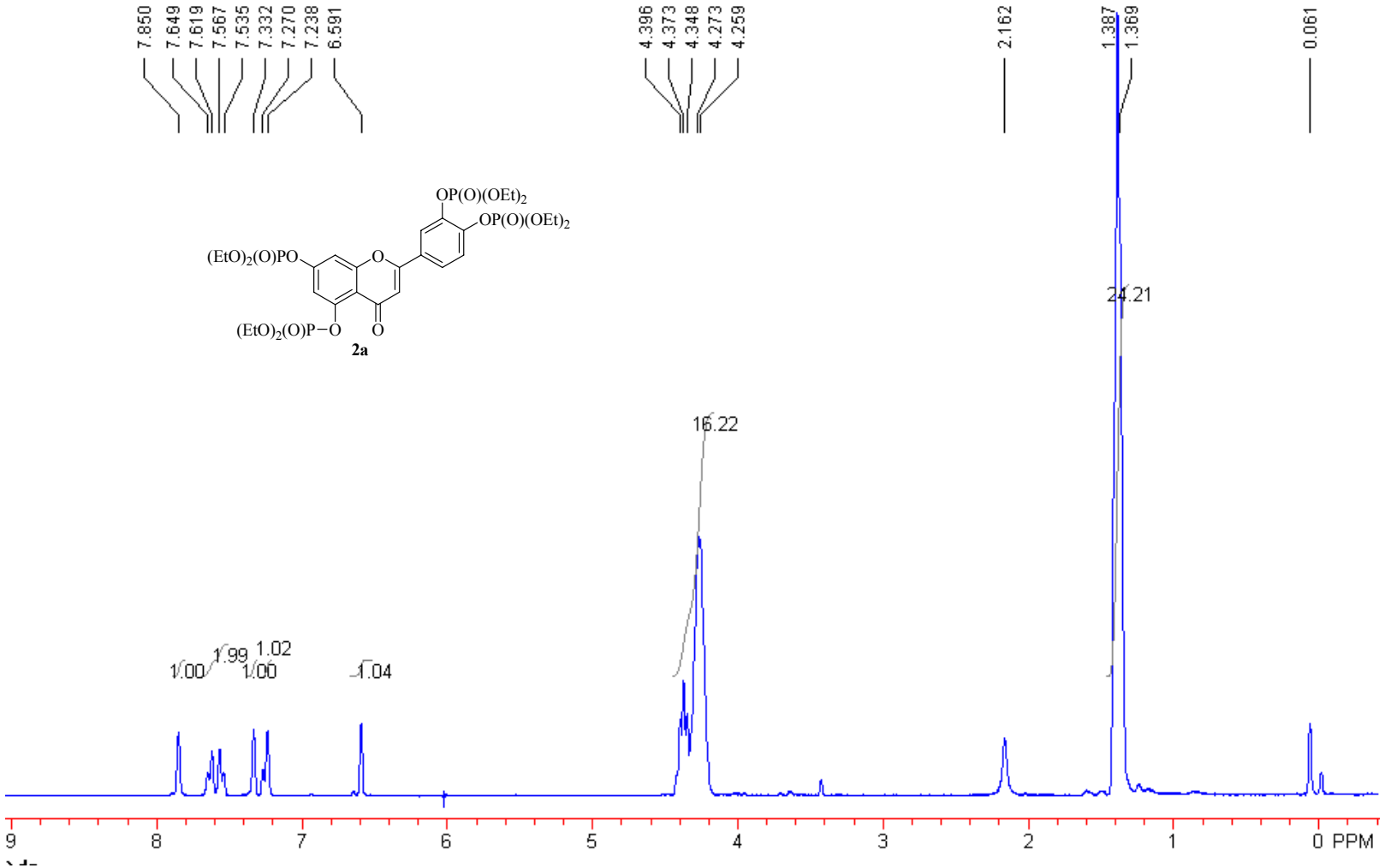


Figure 7. Graph for determining IC50 value of **1b** for CEase inhibition

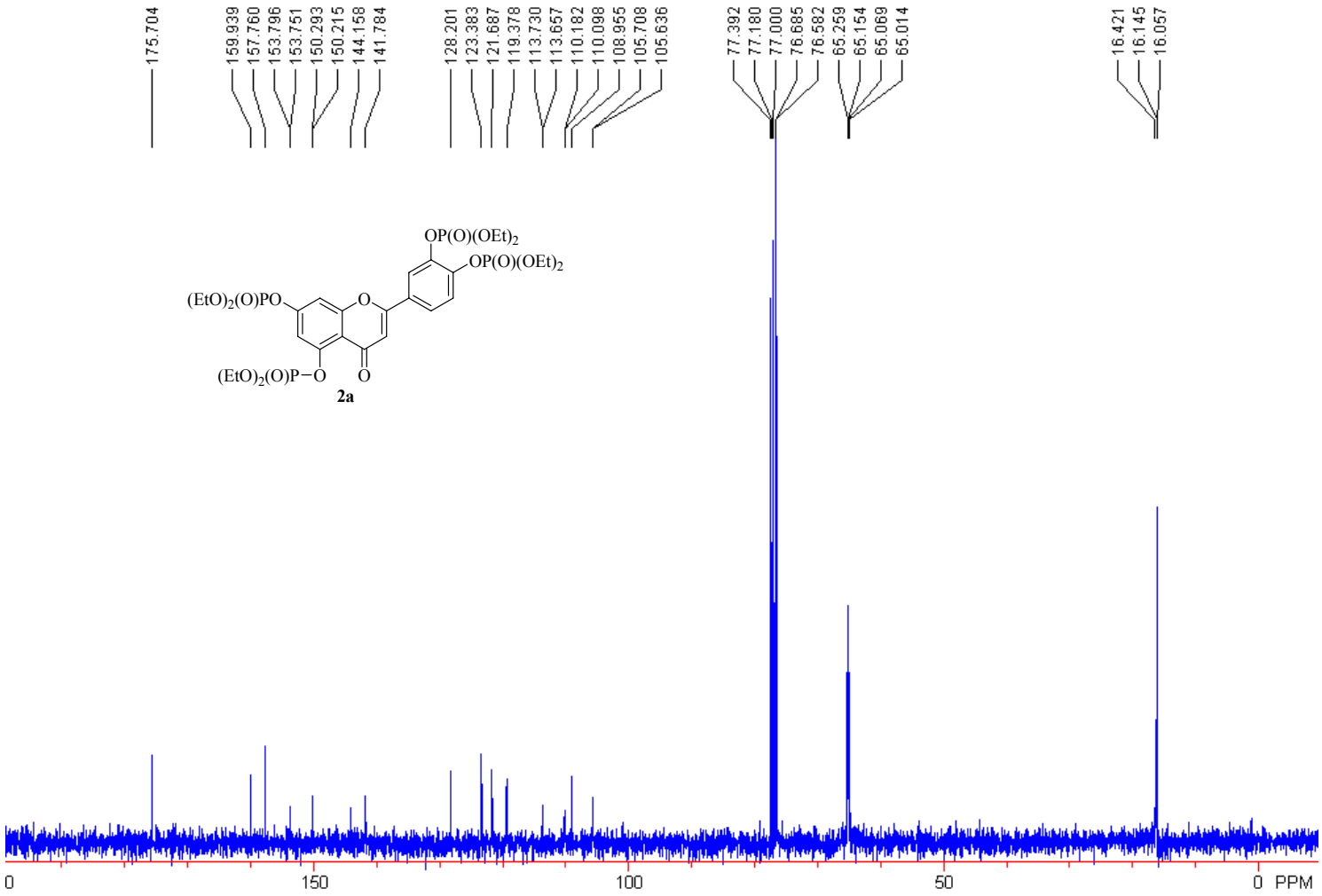
References

(1) X.-L. Chen, L. -B. Qu, T. Zhang, H. -X. Liu, F. Yu, Y. Yu, X. Cheng, Y.-F. Zhao, *Anal. Chem.* 2004, **71**, 211–217.
(2) X. Chen, T. Zhang, H. X. Liu, L. B. Qu, Y. Z. Yu, Y. Zhao, *Chin. Chem. Lett.* 2004, **15**, 343–346.
(3) L. Hosie, L. D. Sutton, D. M. Quinn, *J. Biol. Chem*. 1987, **262**, 260–264.

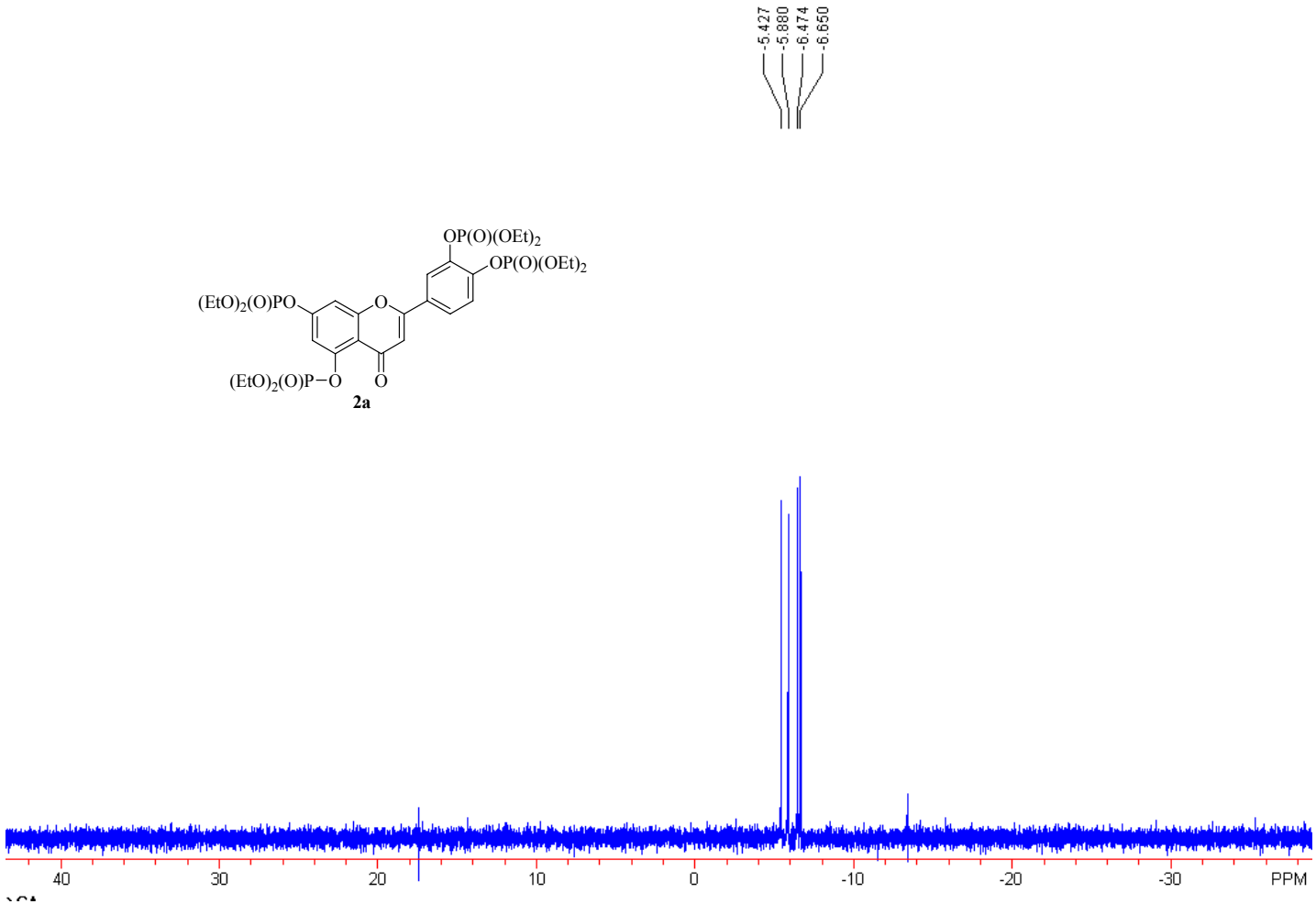
^{1}H NMR (300 MHz, $CDCl_3$) of **2a**



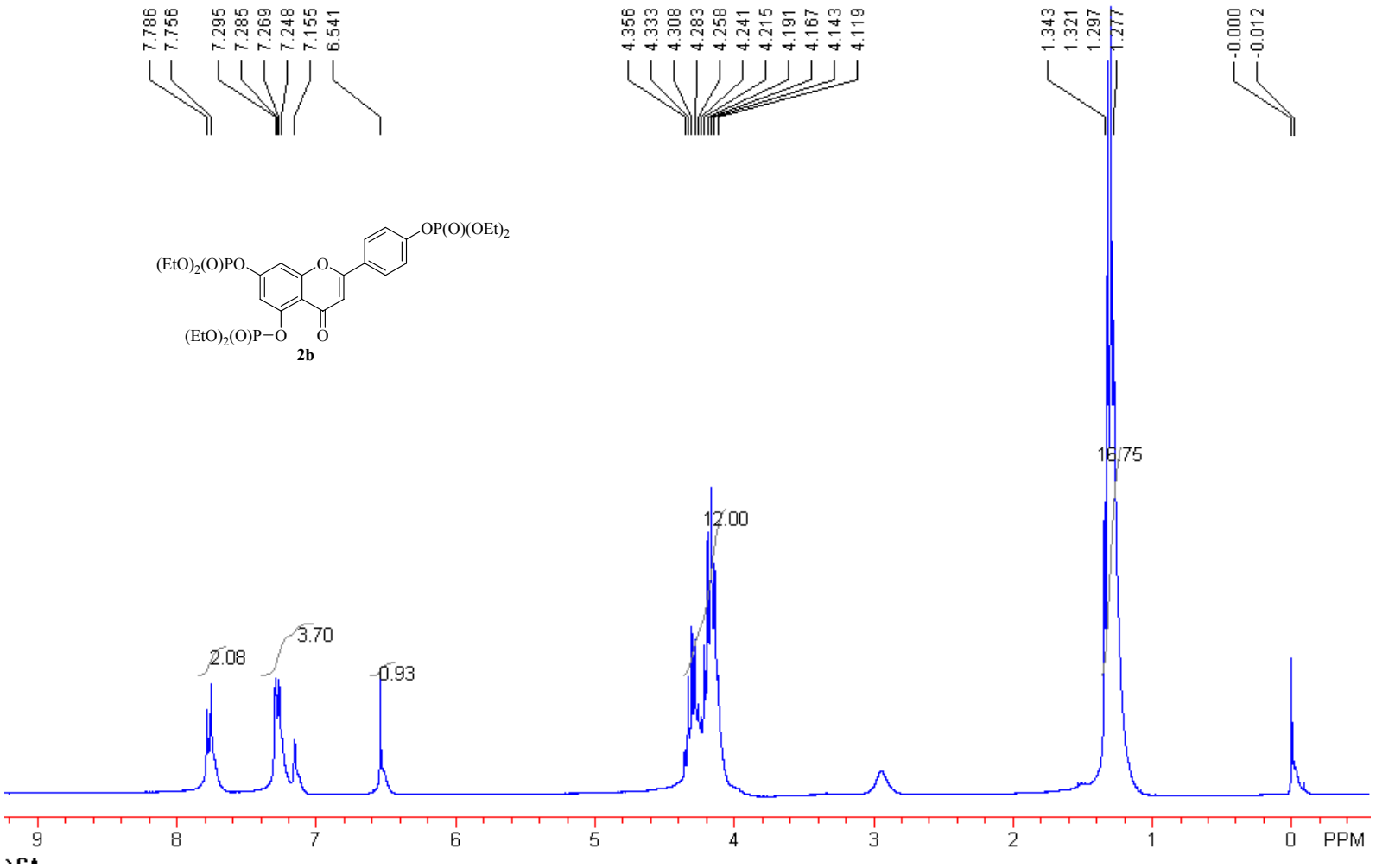
^{13}C NMR (75.4 MHz, $CDCl_3$) of **2a**



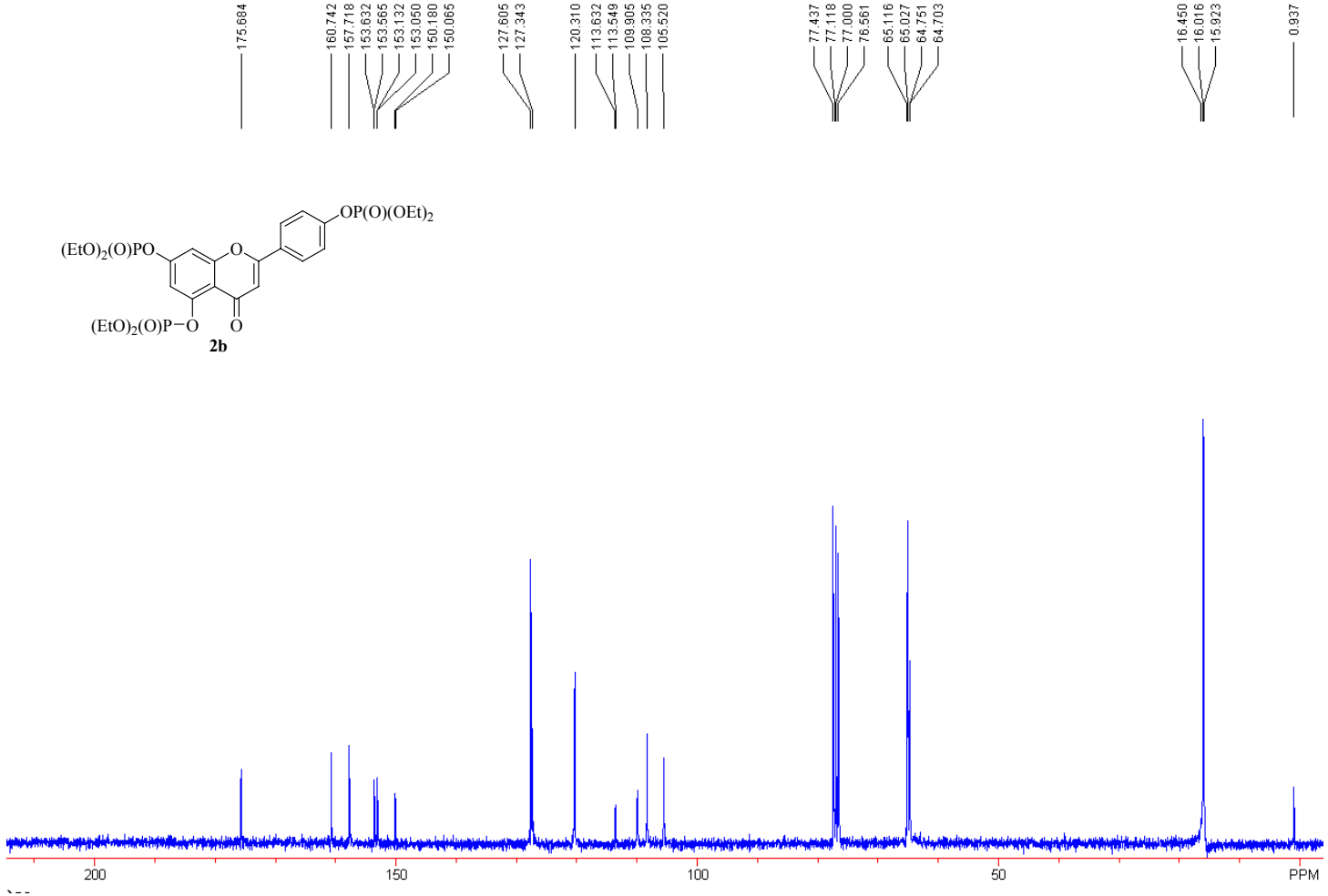
^{31}P NMR (121 MHz, $CDCl_3$) of **2a**



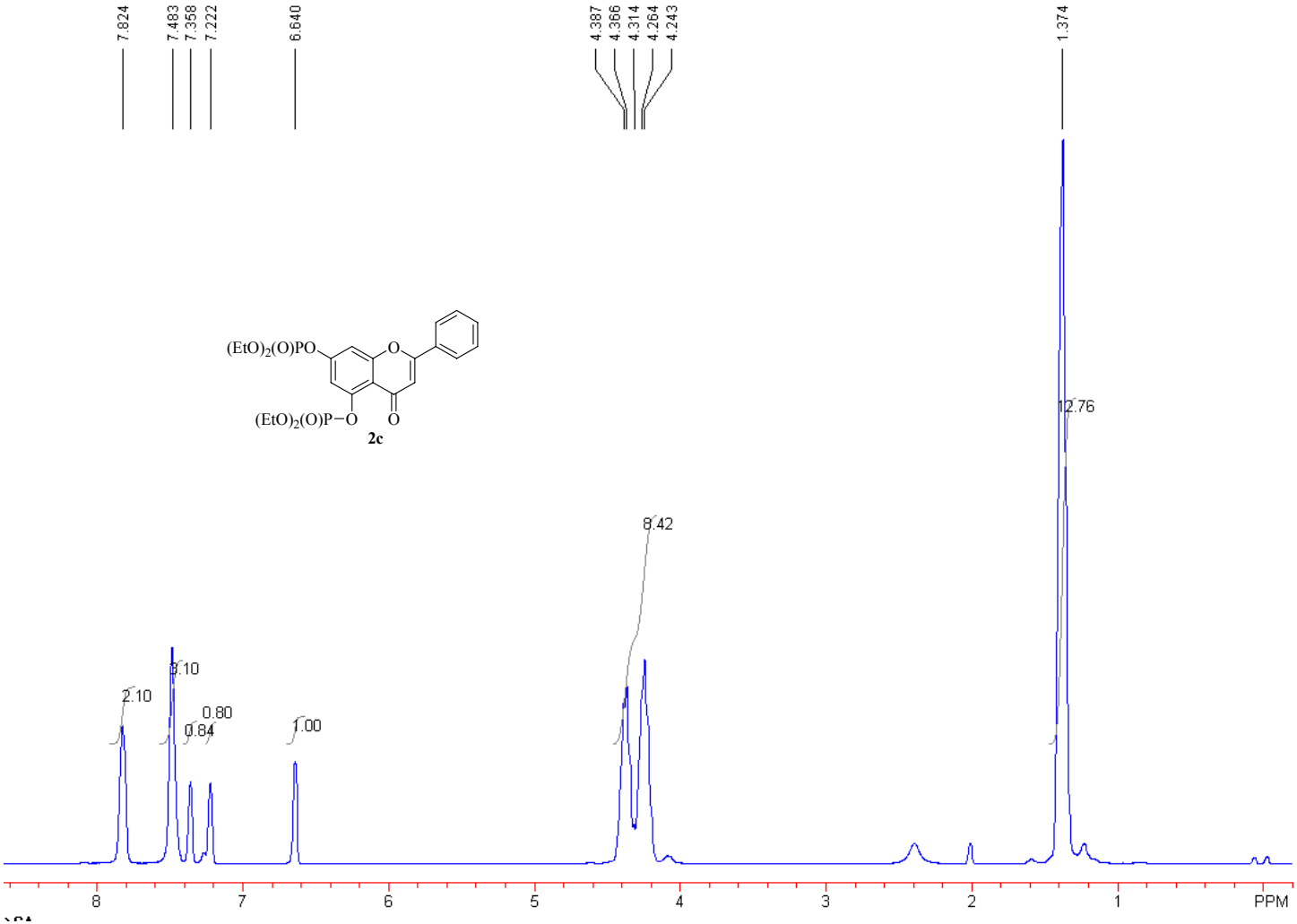
^{1}H NMR (300 MHz, $CDCl_3$) of **2b**



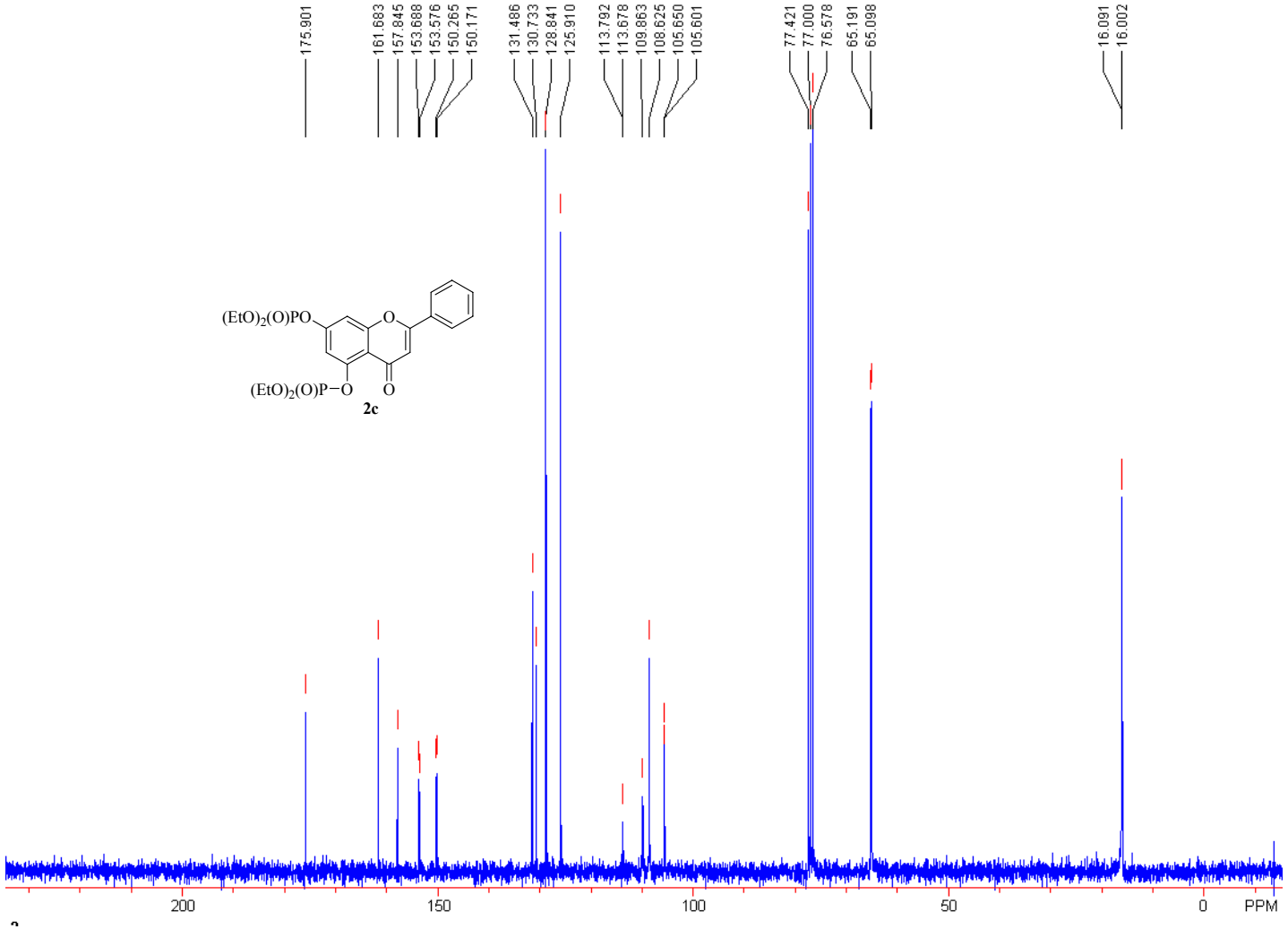
^{13}C NMR (75.4 MHz, $CDCl_3$) of **2b**



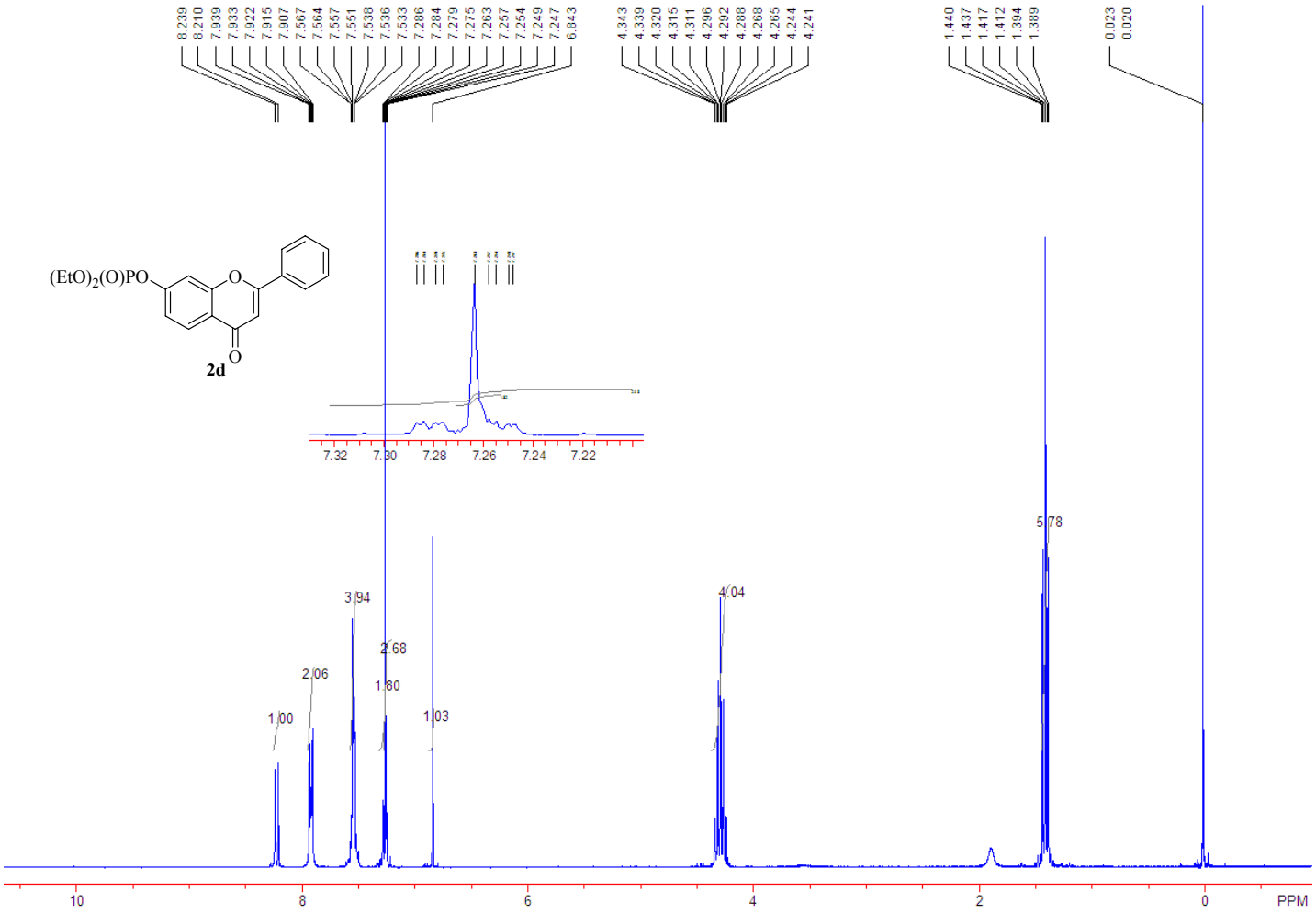
^{1}H NMR (300 MHz, $CDCl_3$) of **2c**



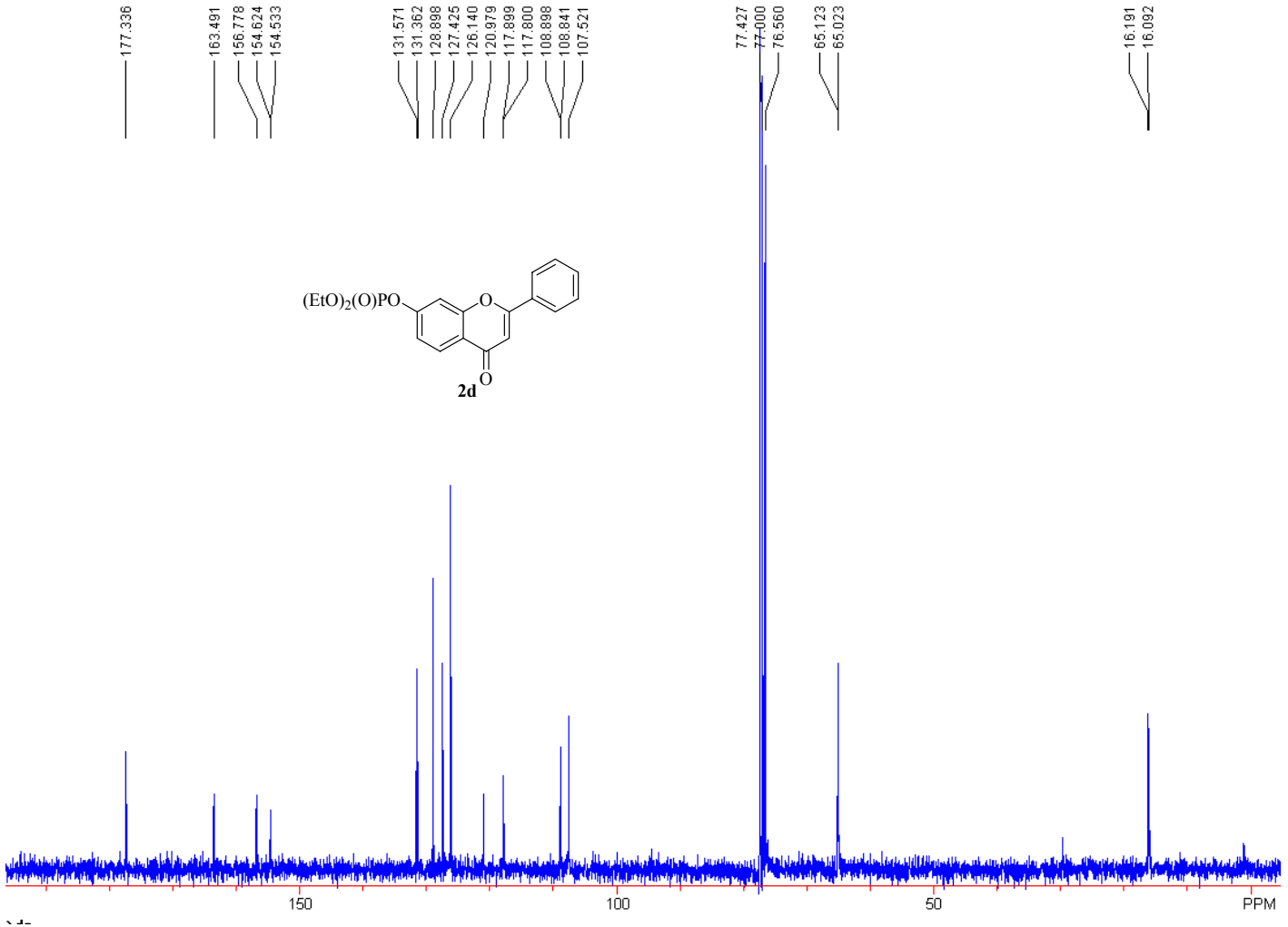
^{13}C NMR (75.4 MHz, $CDCl_3$) of **2c**

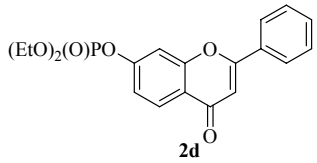


^{1}H NMR (300 MHz, $CDCl_3$) of **2d**



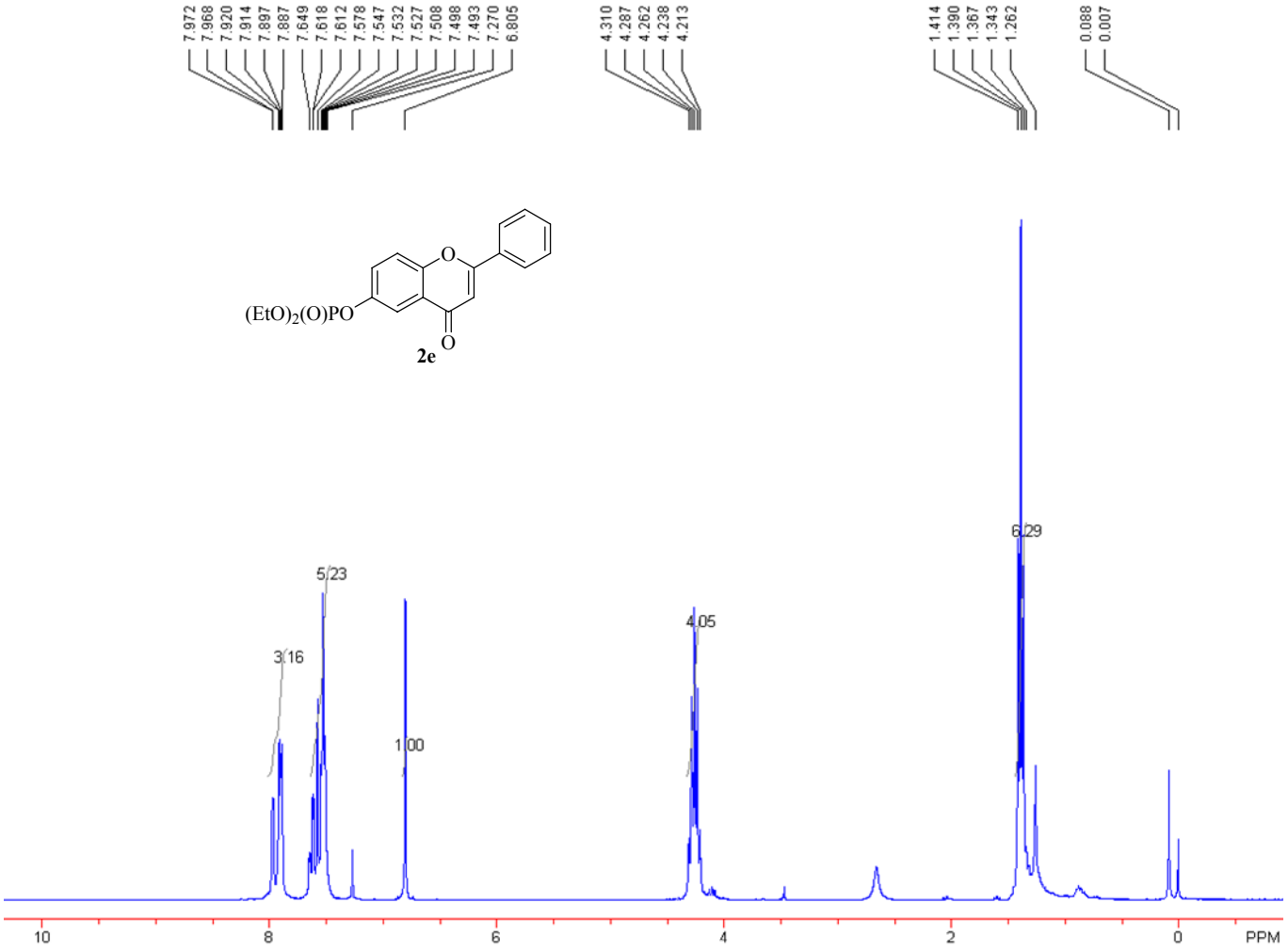
^{13}C NMR (75.4 MHz, $CDCl_3$) of **2d**





2d

^{1}H NMR (300 MHz, $CDCl_3$) of **2e**



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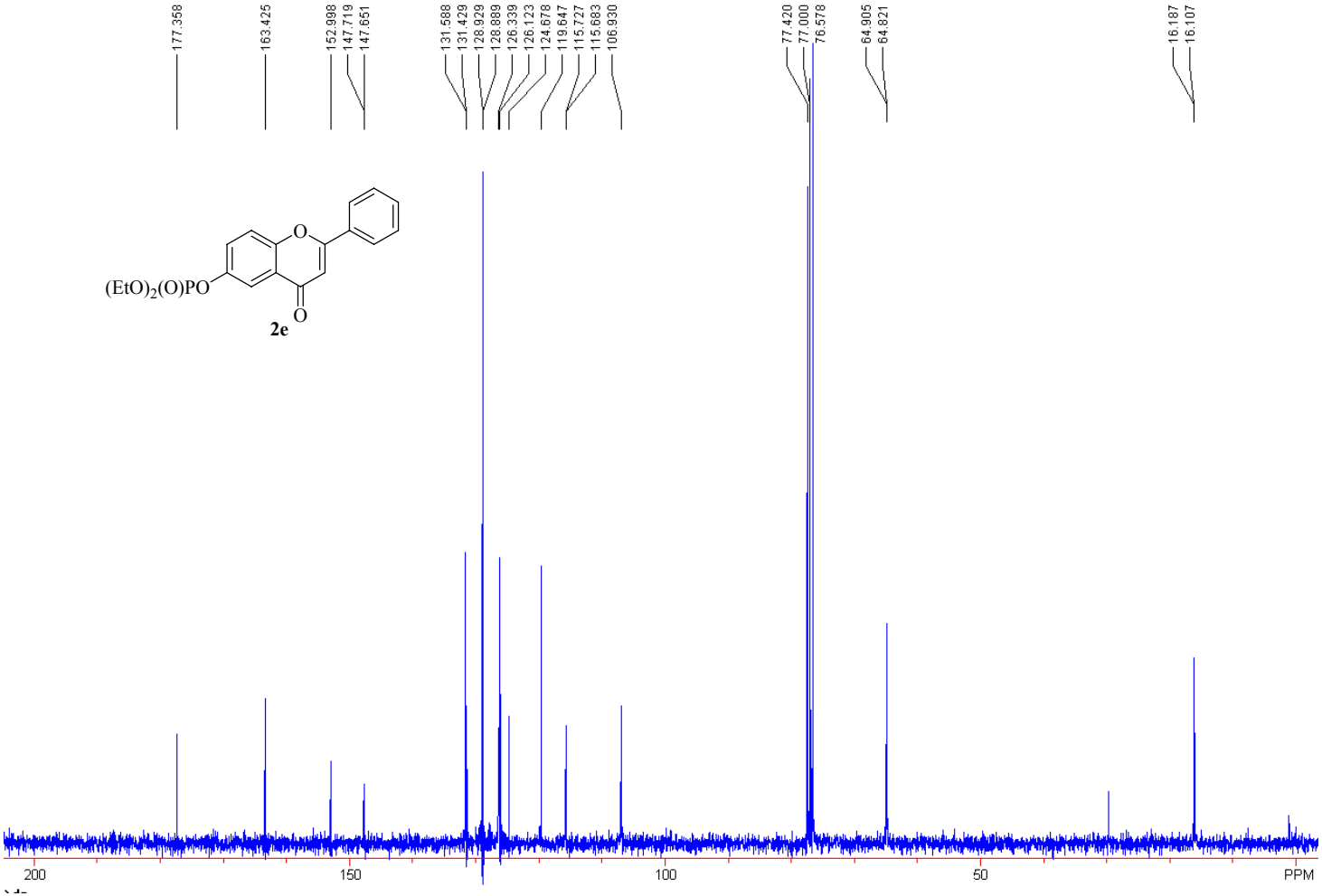

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