

Supporting Information

Synthesis and Neurotoxicity Profile of 2,4,5-Trihydroxymethamphetamine and its 6-(*N*-Acetylcystein-*S*-yl) Conjugate

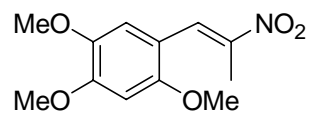
Anne Neudörffer,[†] Melanie Mueller,[‡] Claire-Marie Martinez,[†] Annis Mehan,[‡] Una McCann,[§]
George A. Ricaurte^{*‡} and Martine Langeron^{*†}

[†]*UMR 8638 CNRS - Université Paris Descartes, Synthèse et Structure de Molécules d'Intérêt Pharmacologique, Faculté des Sciences Pharmaceutiques et Biologiques, 4 Avenue de l'Observatoire, 75270 Paris cedex 06, France,* [‡]*Department of Neurology and* [§]*Department of Psychiatry and Behavioral Sciences, Johns Hopkins University School of Medicine, 5501 Hopkins Bayview Circle, Baltimore, Maryland 21224*

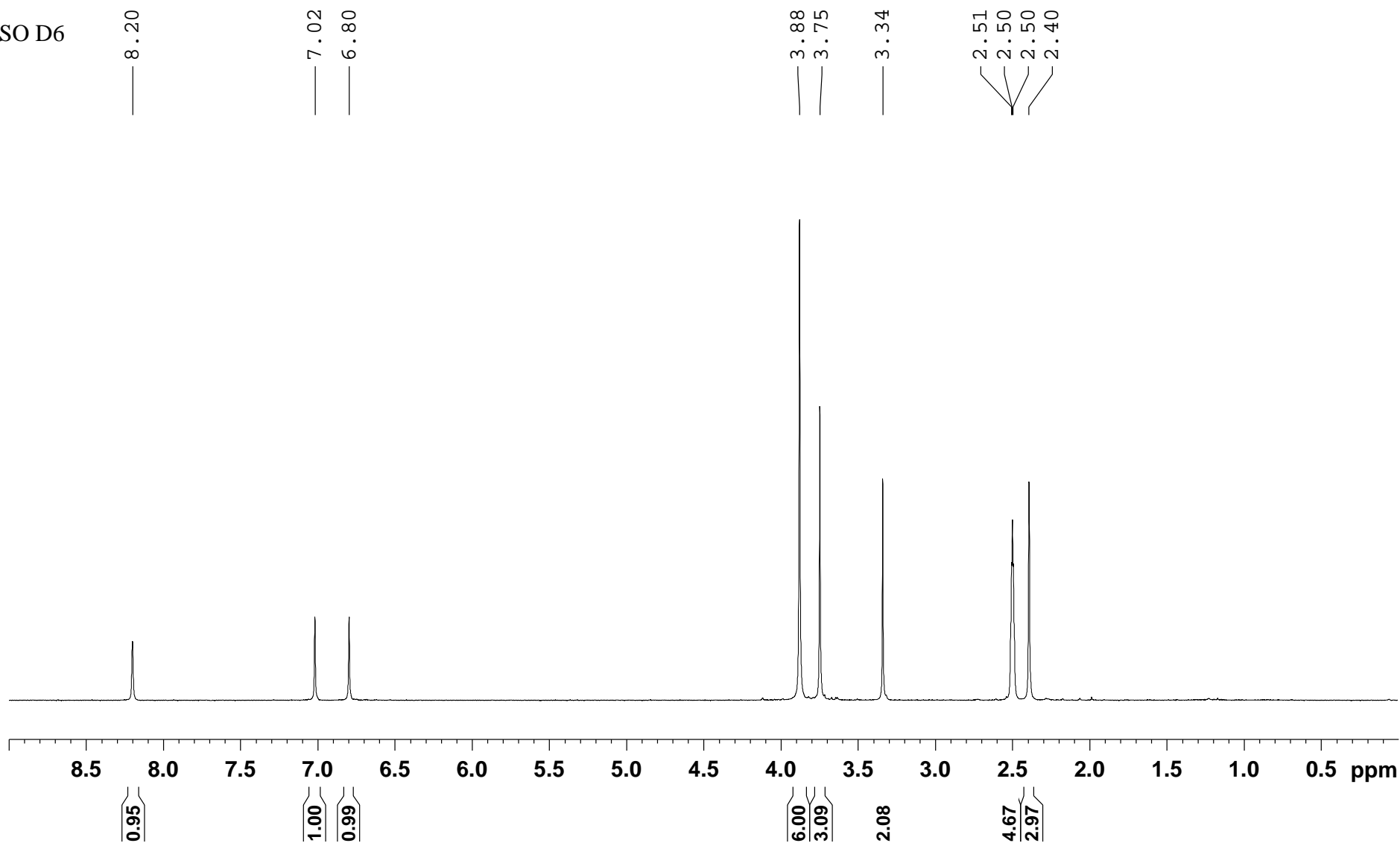
E-mail: martine.langeron@parisdescartes.fr (M.L.); ricaurte@jhmi.edu (G.A.R.)

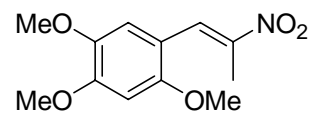
Table of Contents

- I. ¹H and ¹³C NMR spectra of THMA **4** and its synthetic intermediates, together with 6-(*N*-acetylcystein-*S*-yl)-THMA **5**
- II. Analytical HPLC chromatograms of THMA **4** and of 6-(*N*-acetylcystein-*S*-yl)-THMA **5**

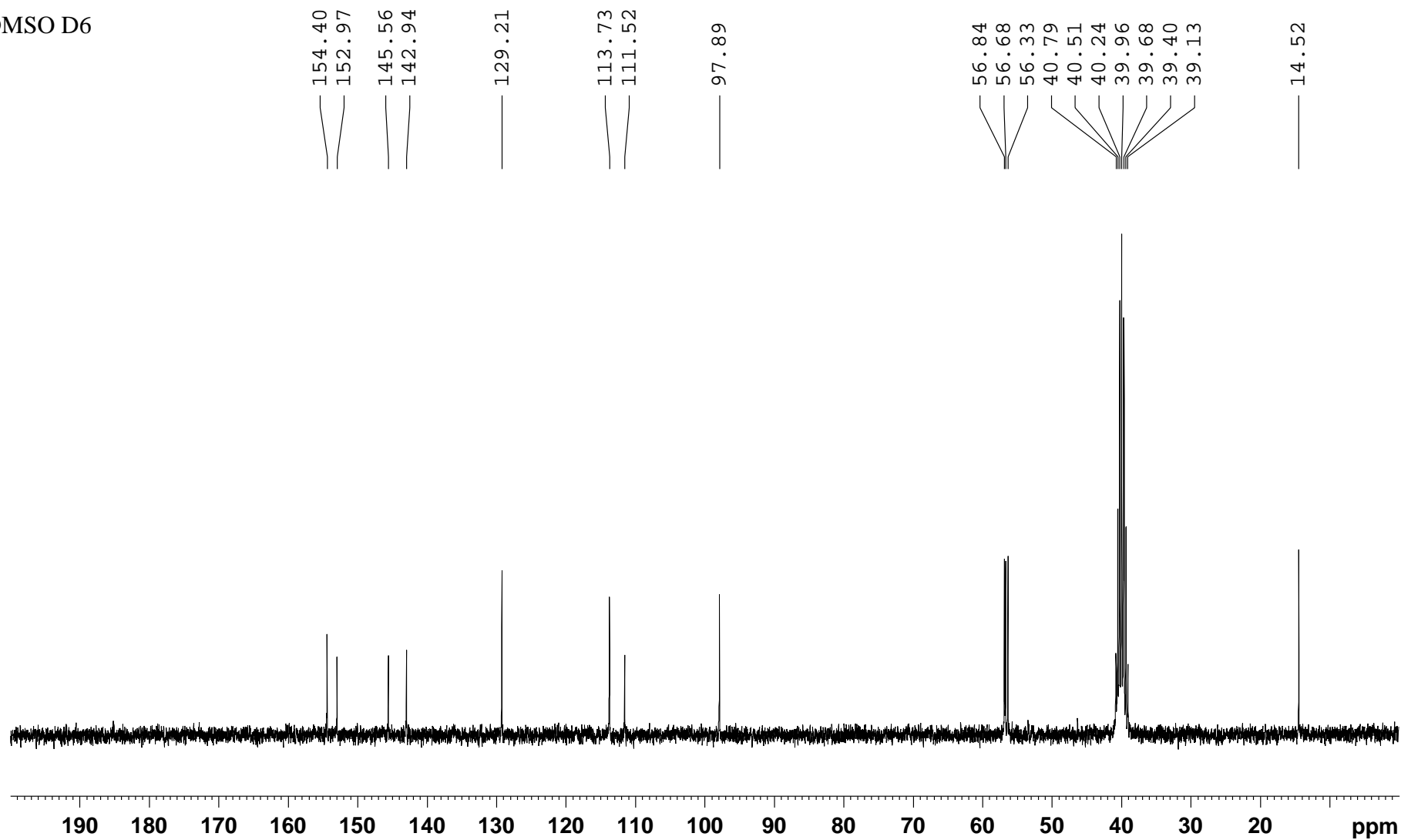


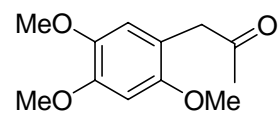
DMSO D6





DMSO D6



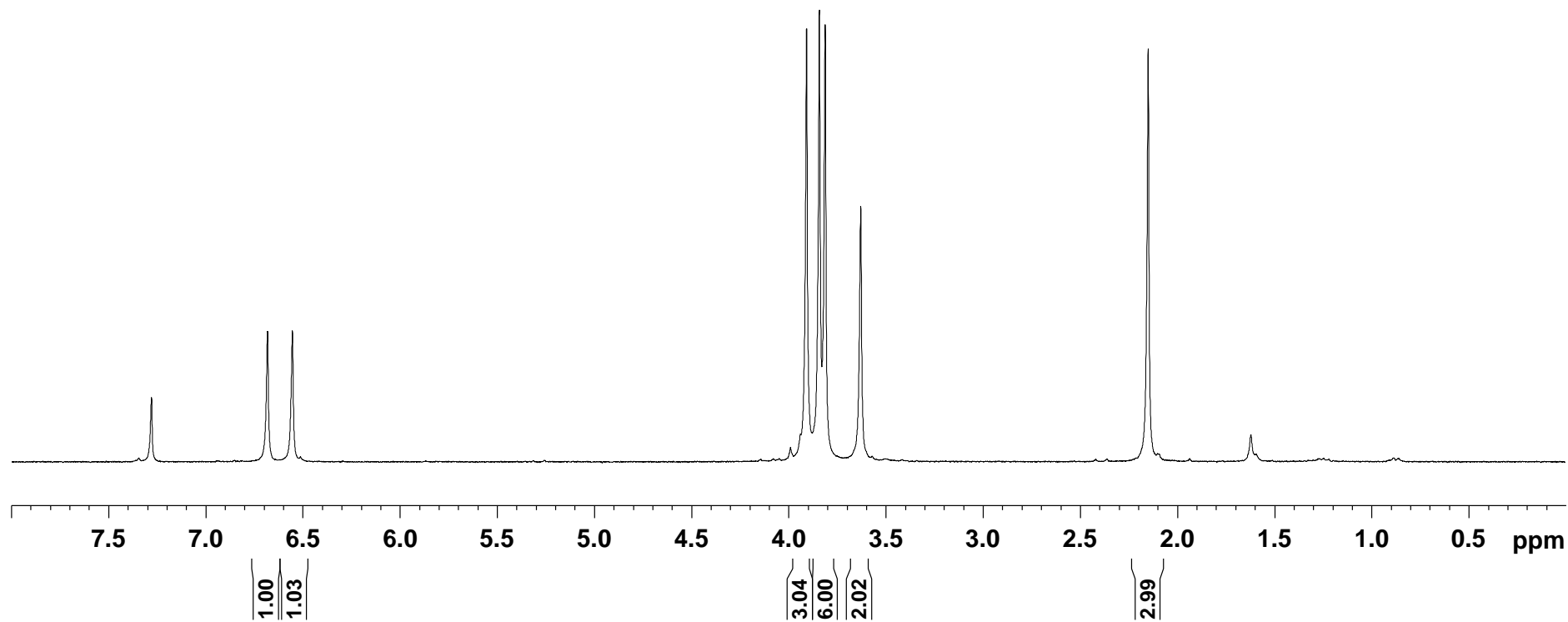


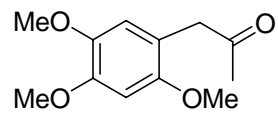
CDCl₃

6.68
6.55

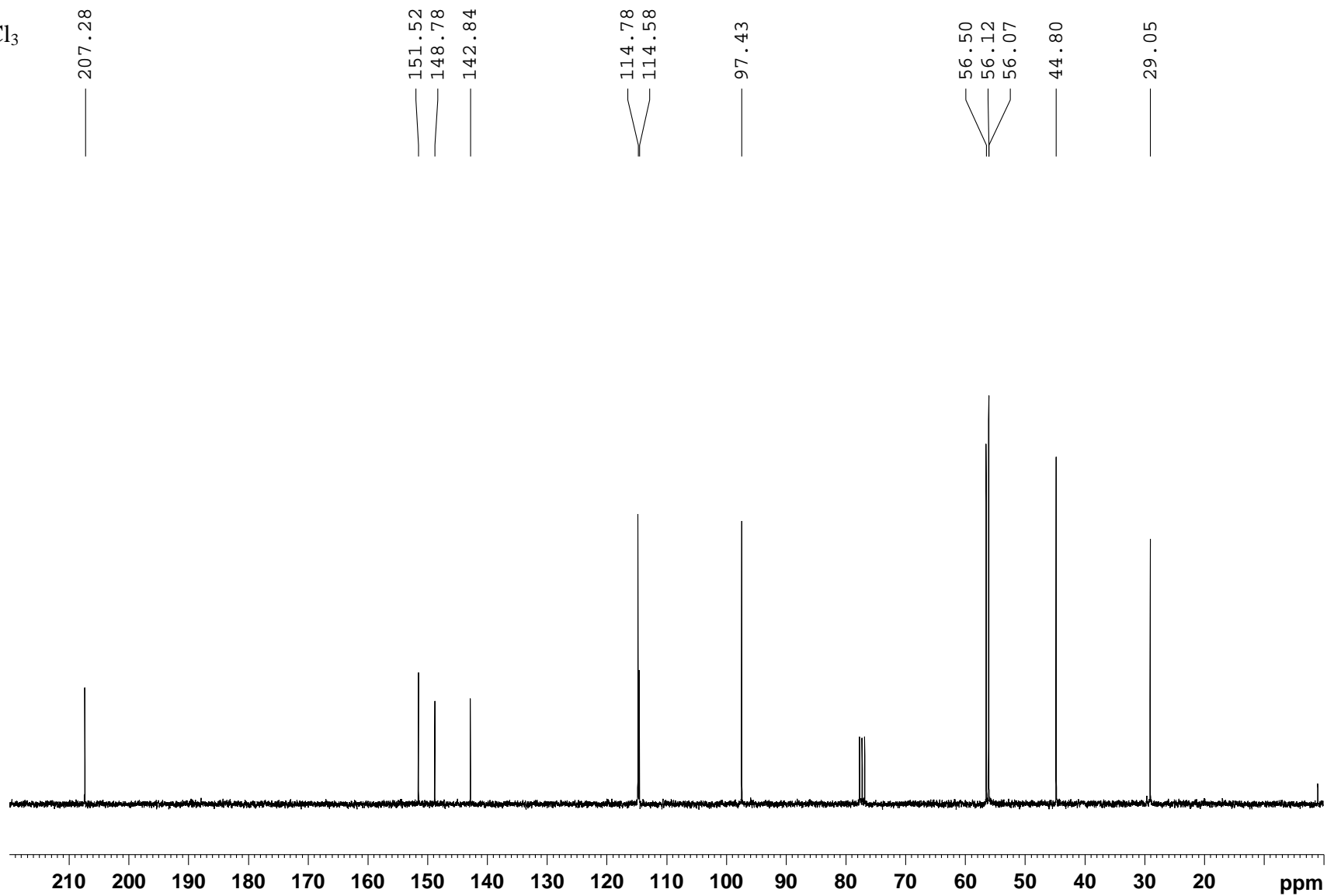
3.91
3.84
3.81
3.63

2.15

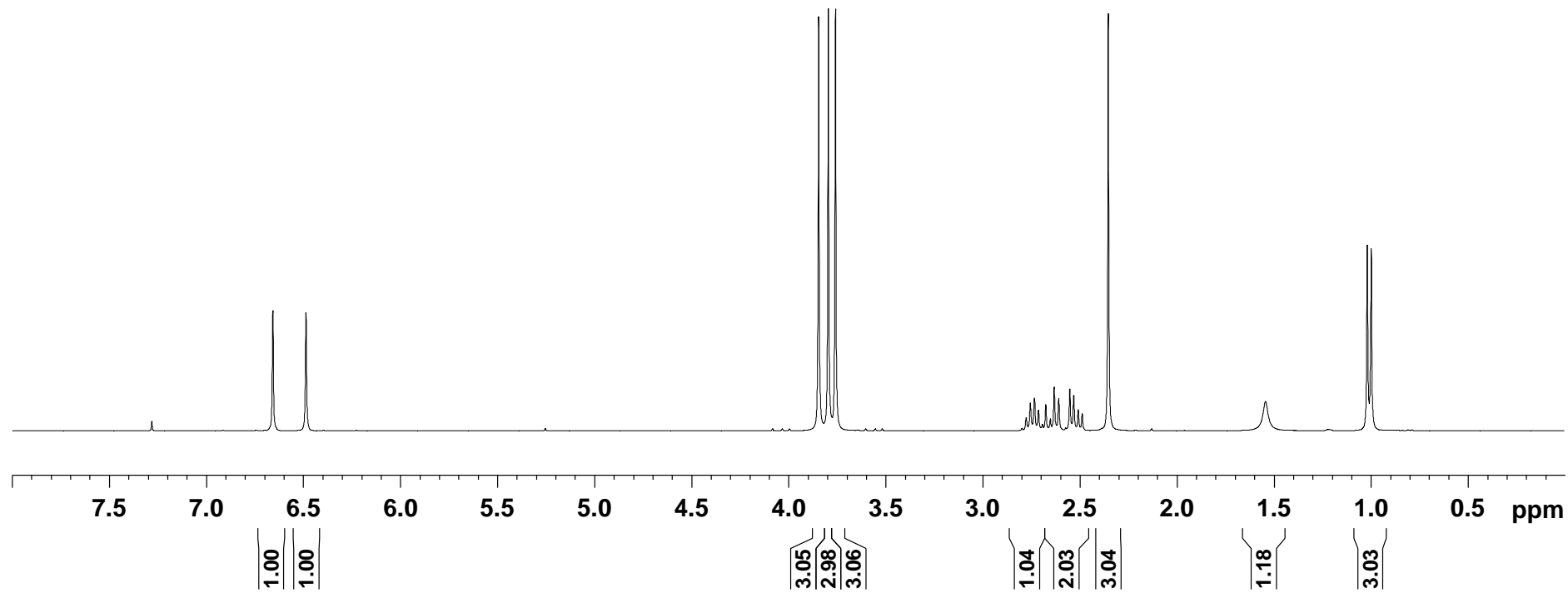
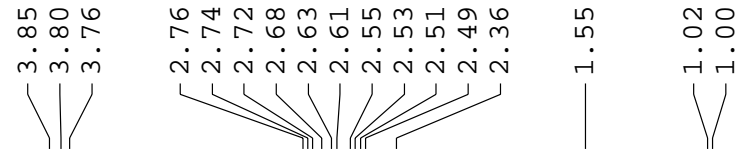
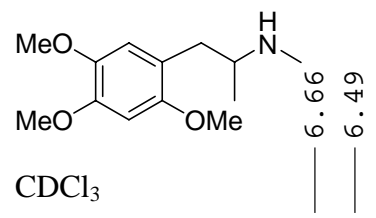


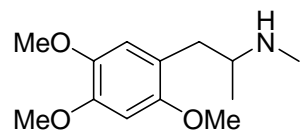


CDCl₃

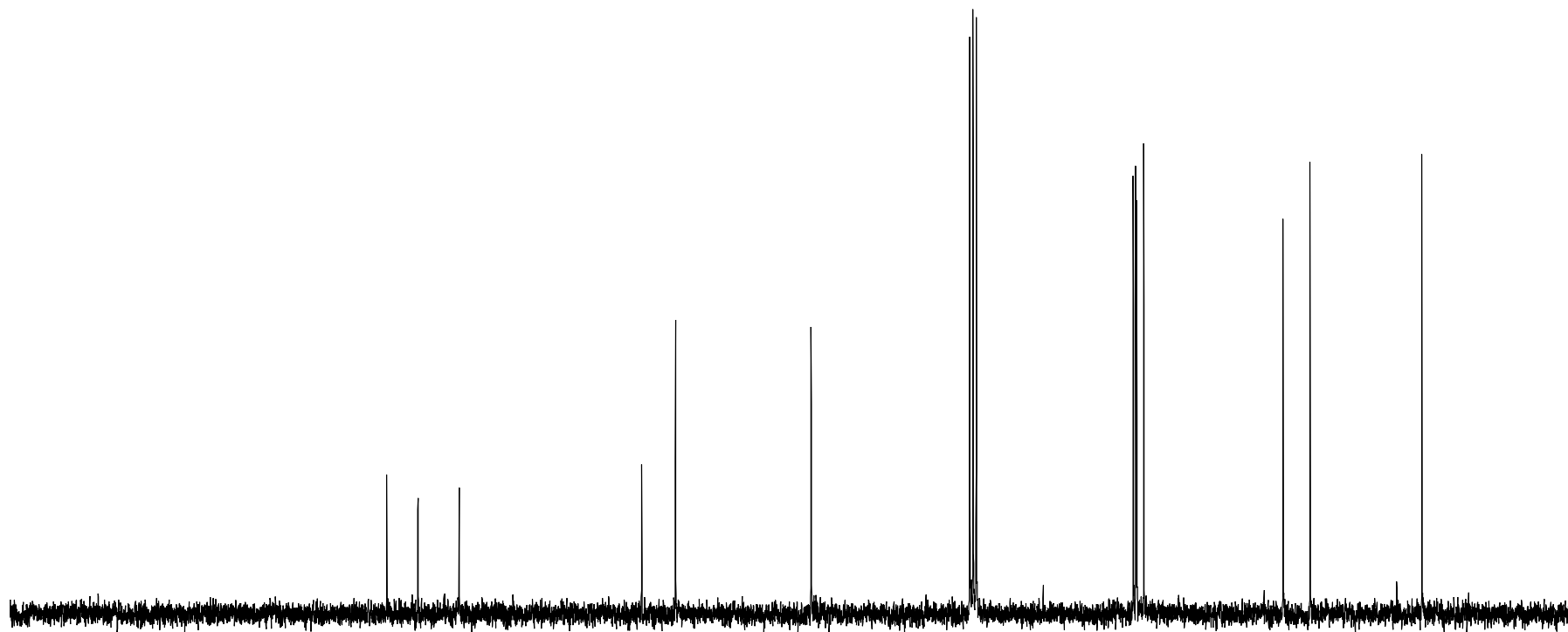
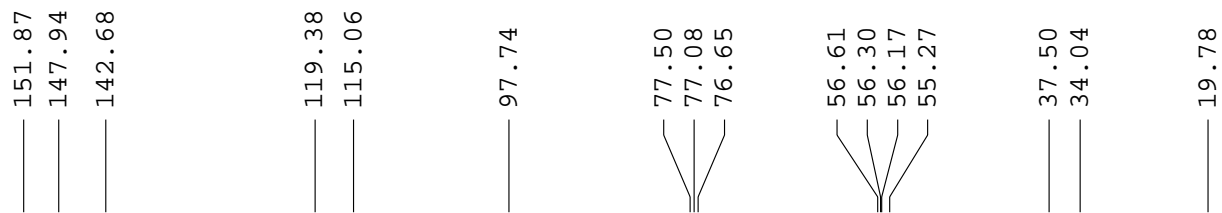


S5

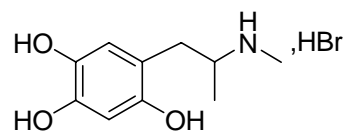




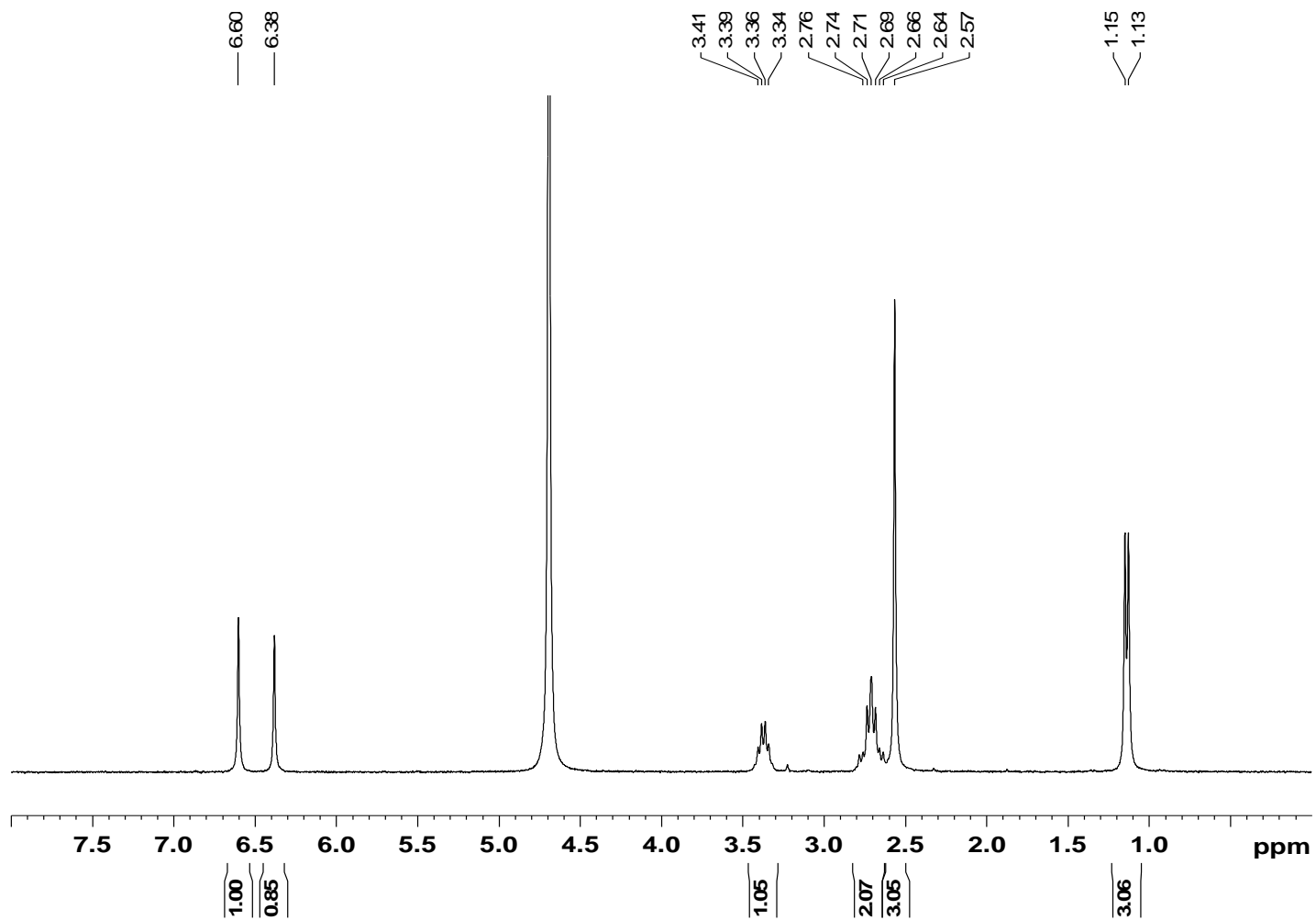
CDCl₃

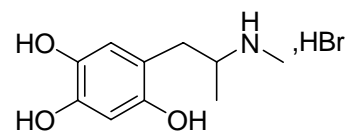


190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

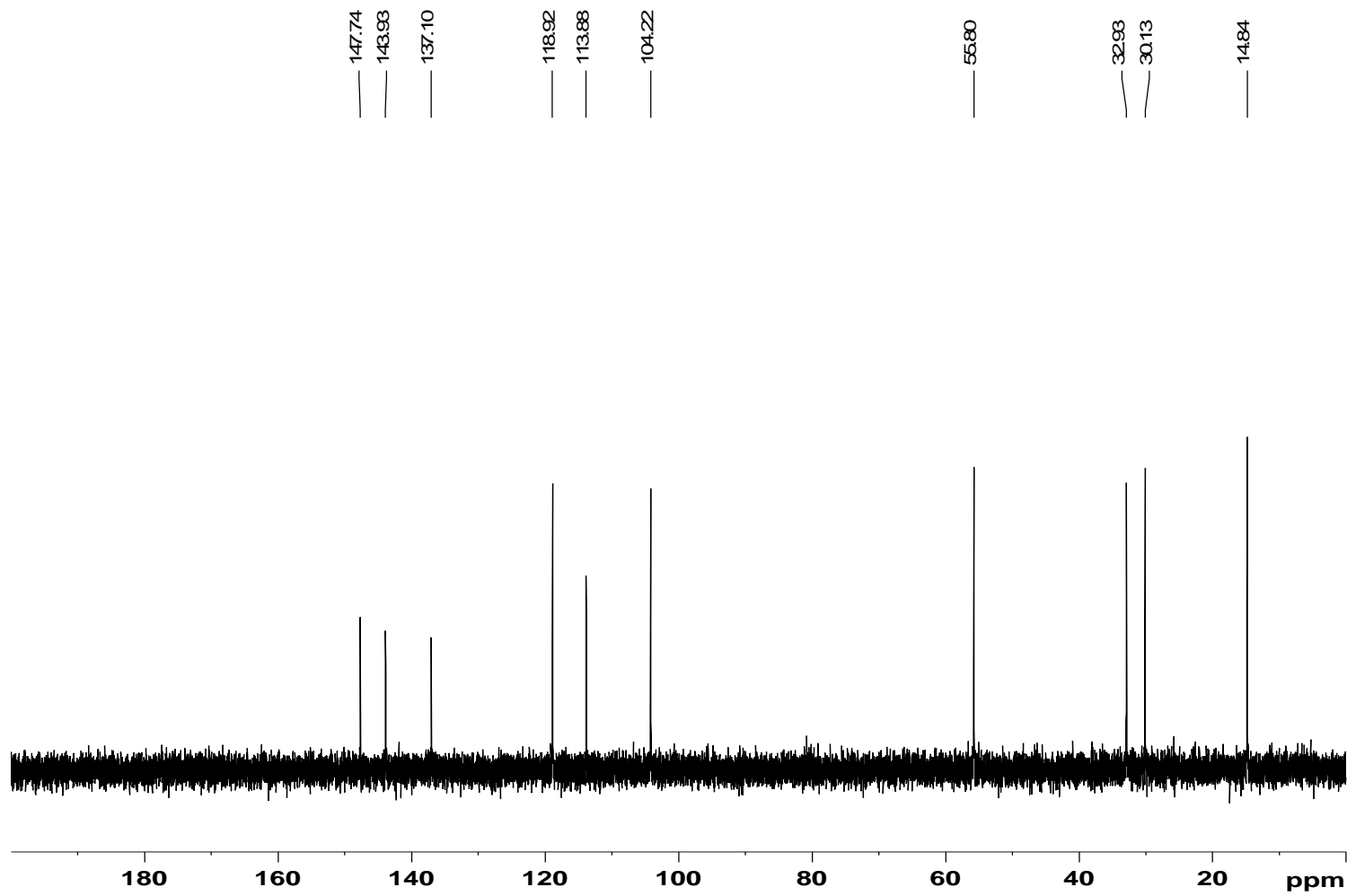


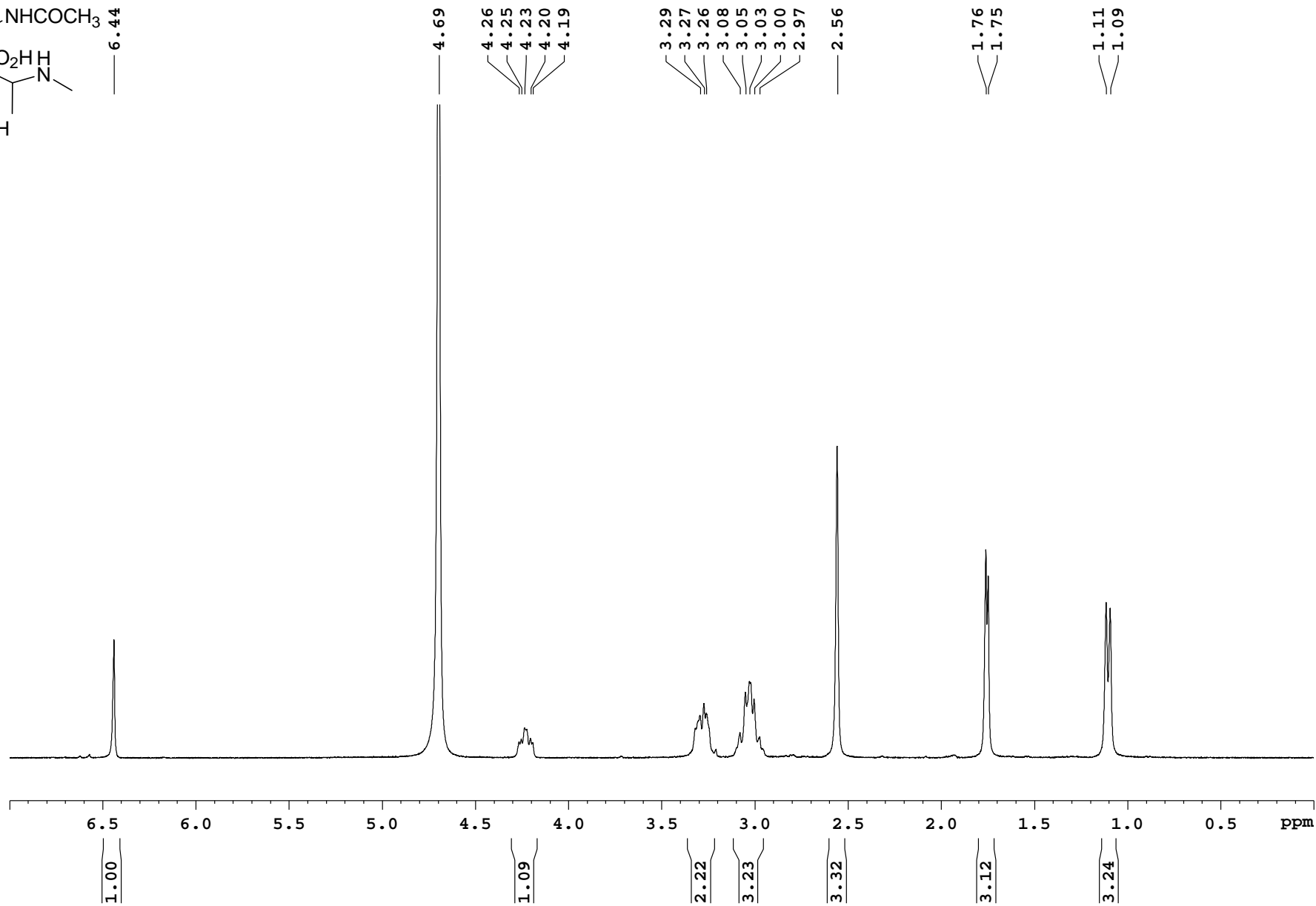
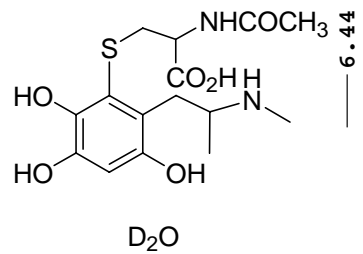
D₂O

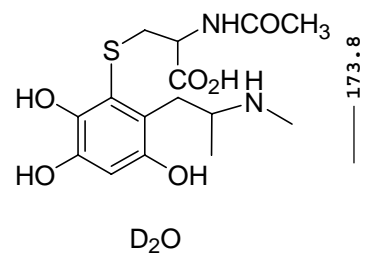




D₂O







147.9
147.9
143.9
139.9

120.4
120.3
117.7
117.6

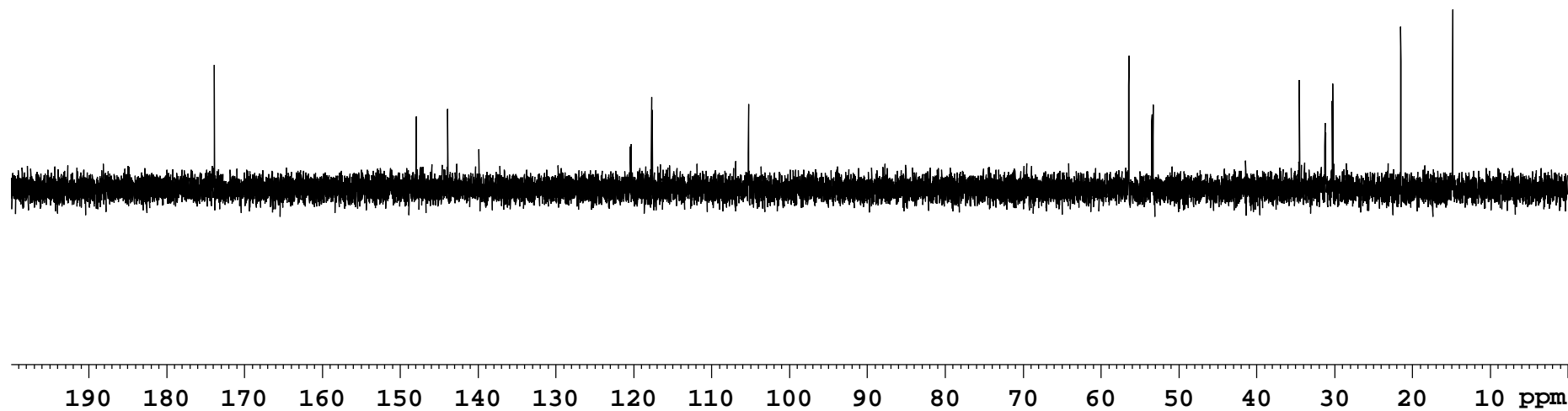
105.2

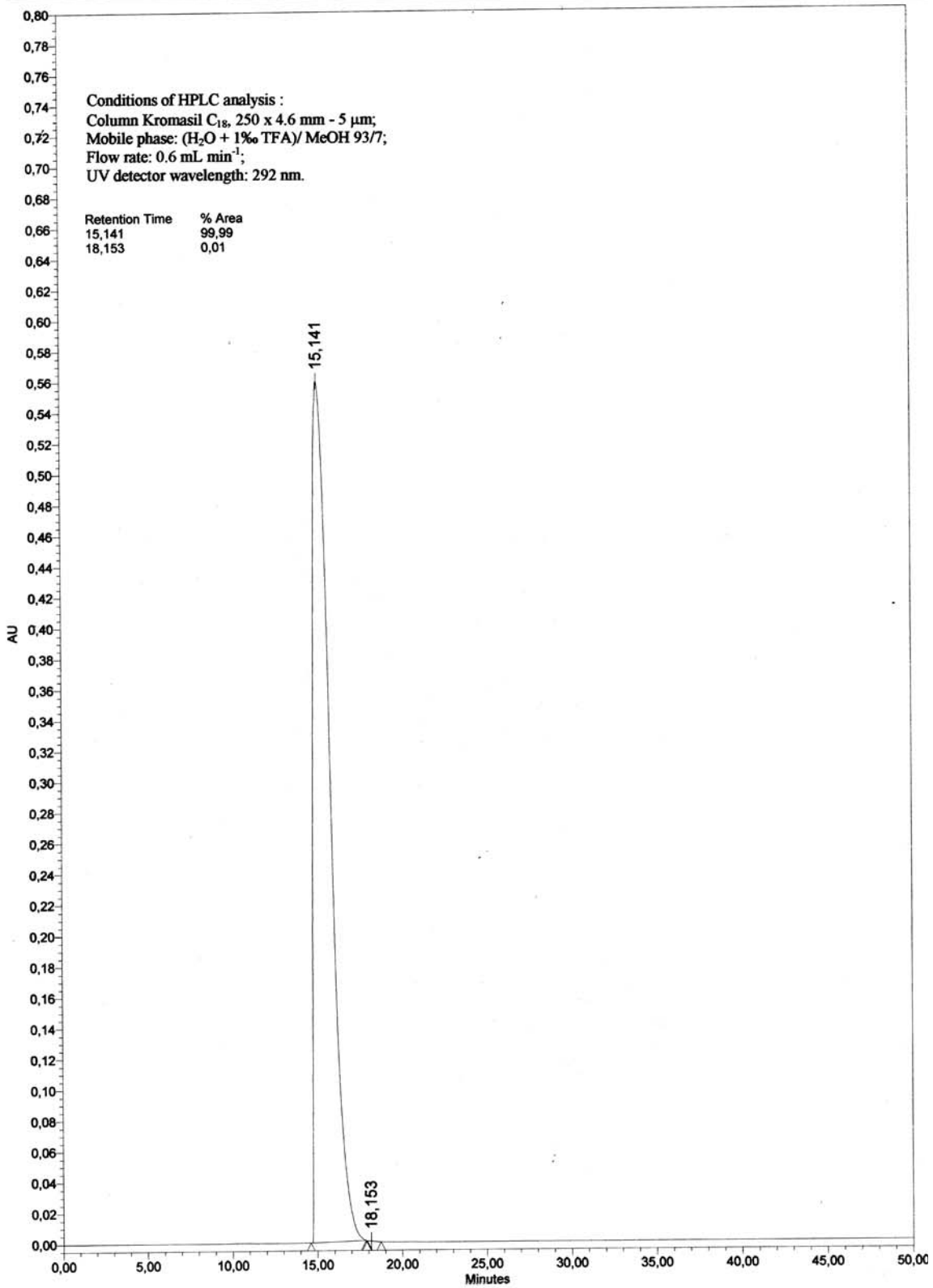
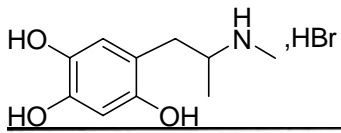
56.4
53.4
53.2

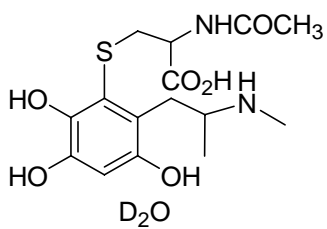
34.5
31.2
31.1
30.2
30.2

21.4

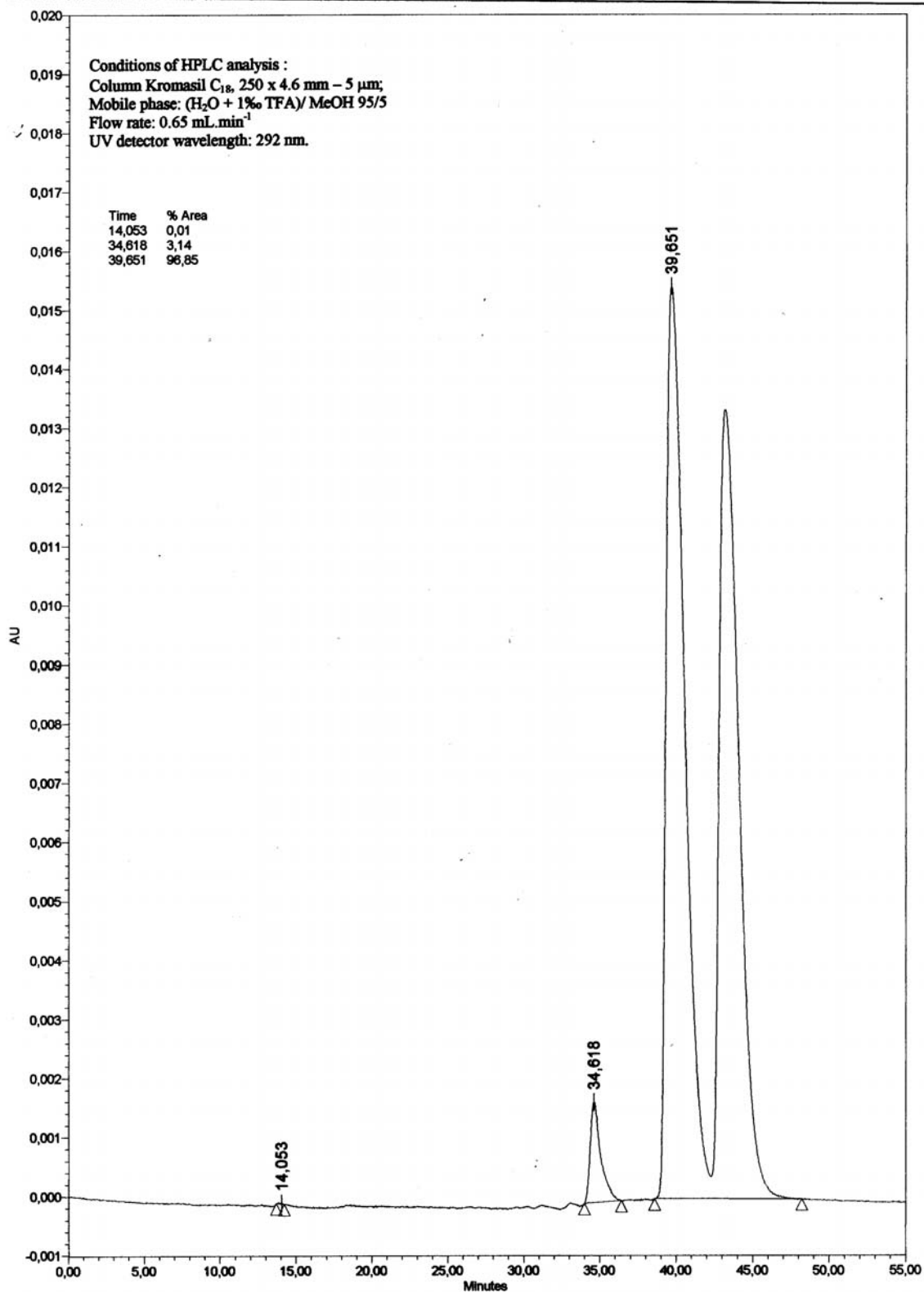
14.8

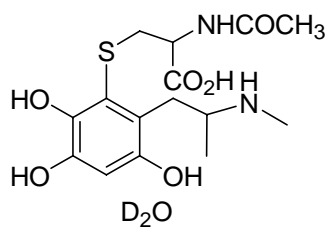






After the first semipreparative reversed-phase HPLC (96.5 % purity grade)





After the second semipreparative reversed-phase HPLC (99.5% purity grade)

