Supporting Information

Design and Synthesis of ERα/ERβ Seletive Coumarin and Chromene Derivatives as Potential Anti-Breast Cancer and Anti-Osteoporotic Agents

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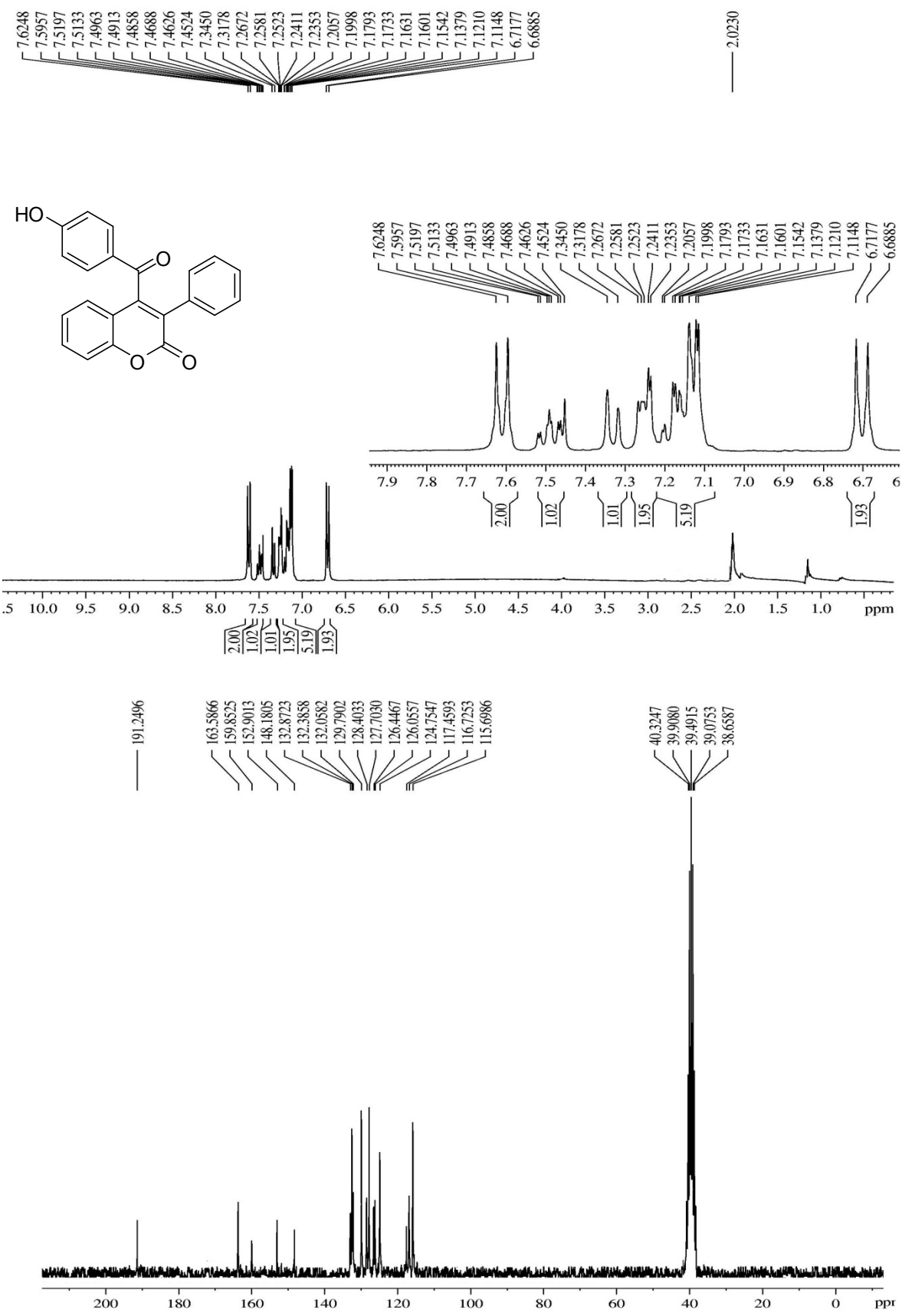
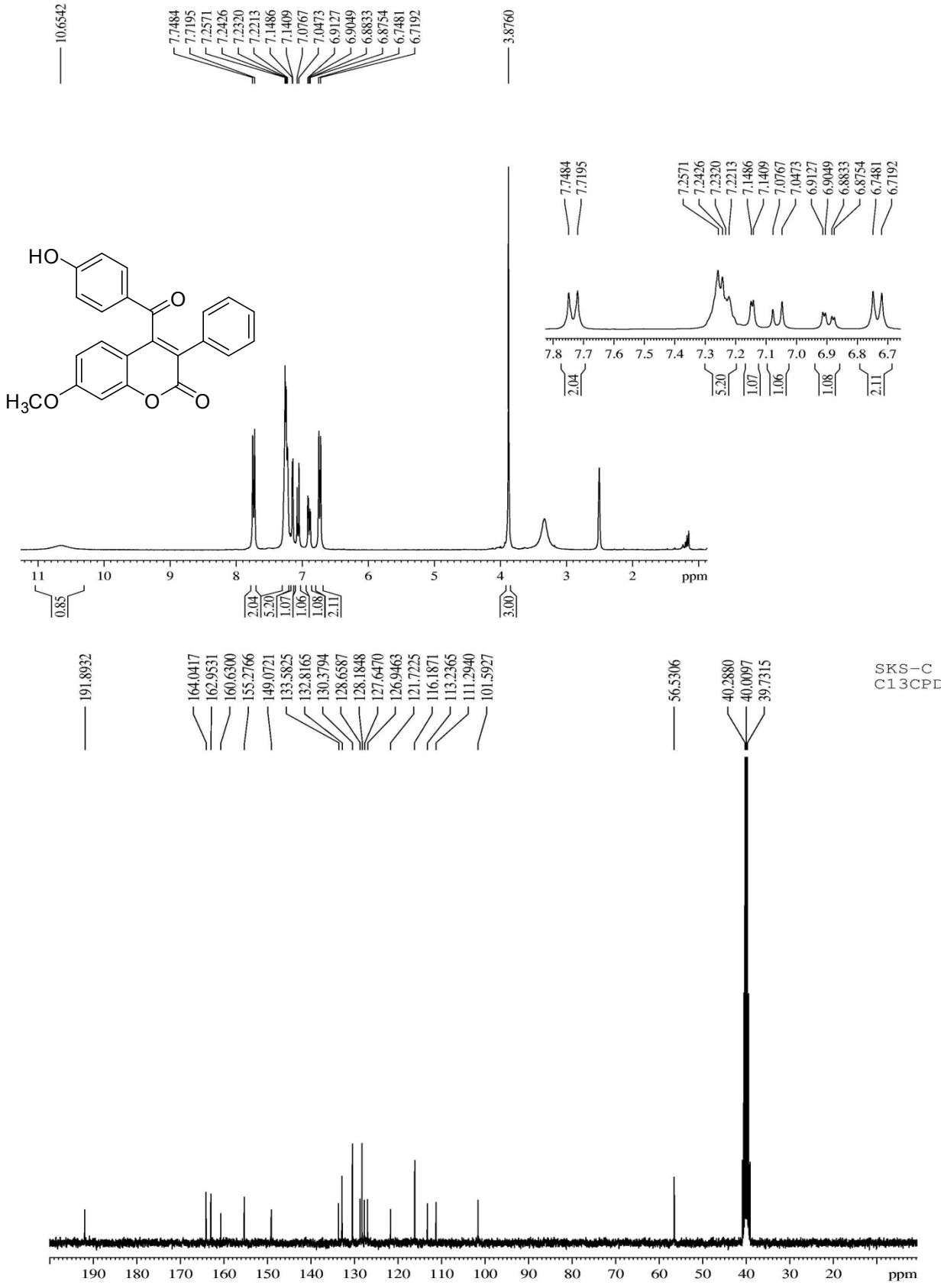
X-Ray Crystallographic data of compound 18

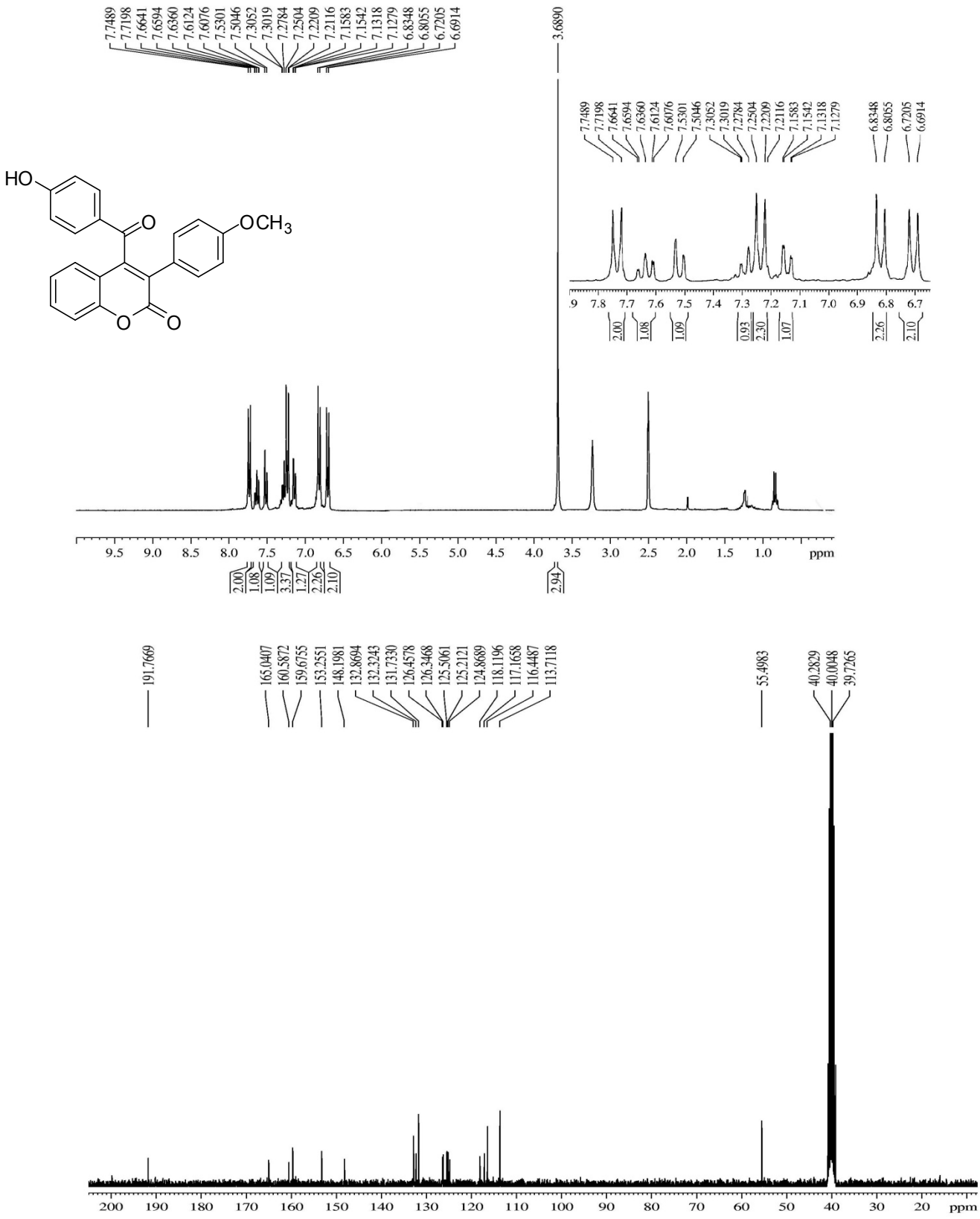
The crystal data of $C_{31}H_{31}NO_6$, M = 513.57, triclinic, P -1, a = 8.7579(8) Å,b = 10.0549(9) Å, c = 16.4135(15) Å, α = 104.343(2) β = 94.619(2)°, γ = 106.200(2), V = 1327.2(2) Å^3, Z = 2, D_c = 1.285 gcm^{-3}, μ (Mo-Kα) = 0.089 mm^{-1}, F(000) = 544, rectangular block, colourless, 15674 reflections measured (R_{int} = 0.0182), 6205 unique, wR_2 = 0.1548 for all data, conventional R = 0.0514 [$(\Delta/\sigma)_{max}$ = 000)] on F-values of 4610 reflections with $I>2\sigma(I)$, S = 1.034 for all data and 345 parameters. Unit cell determination and intensity data collection was performed on a Bruker SMART APEX CCD diffractometer at 293(2) K. Structure solutions by direct methods and refinements by full-matrix least-squares methods on F^2. Programs: SMART (Bruker, 2001), SAINT (Bruker, 2001), and SHELXTL-NT [Bruker AXS, Madison, WI, 1997]. CCDC (deposit No: 962314) contains the supplementary crystallographic data. These data can be obtained free of charge from www.ccdc.cam.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Center, 12 Union Road, Cambridge, CB2 1EZ, U. K; Fax: (internat.) + 44-1223/336-033; E-mail: deposit@ccdc.cam.ac.uk.



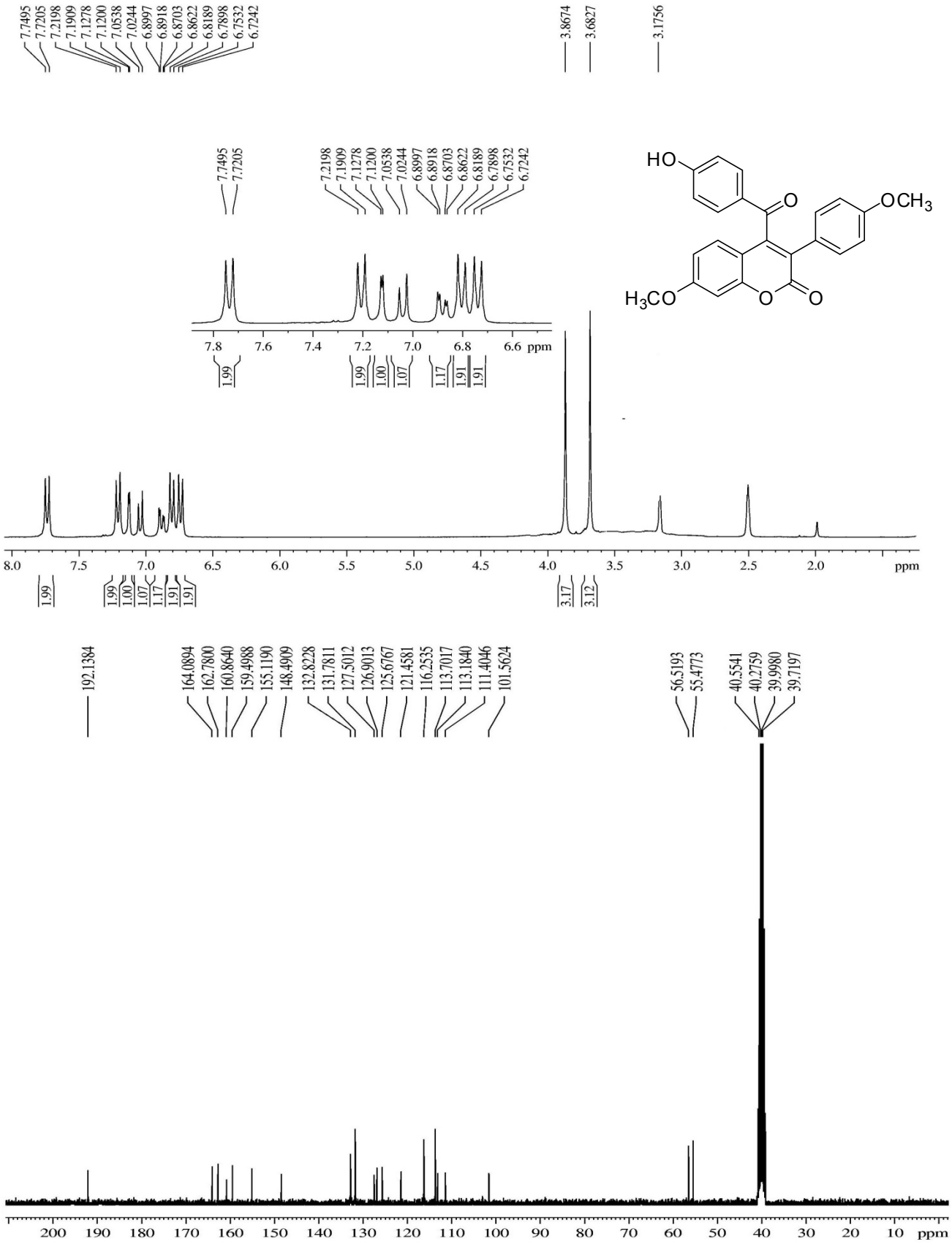
^{1}H and ^{13}C spectra of compound 8



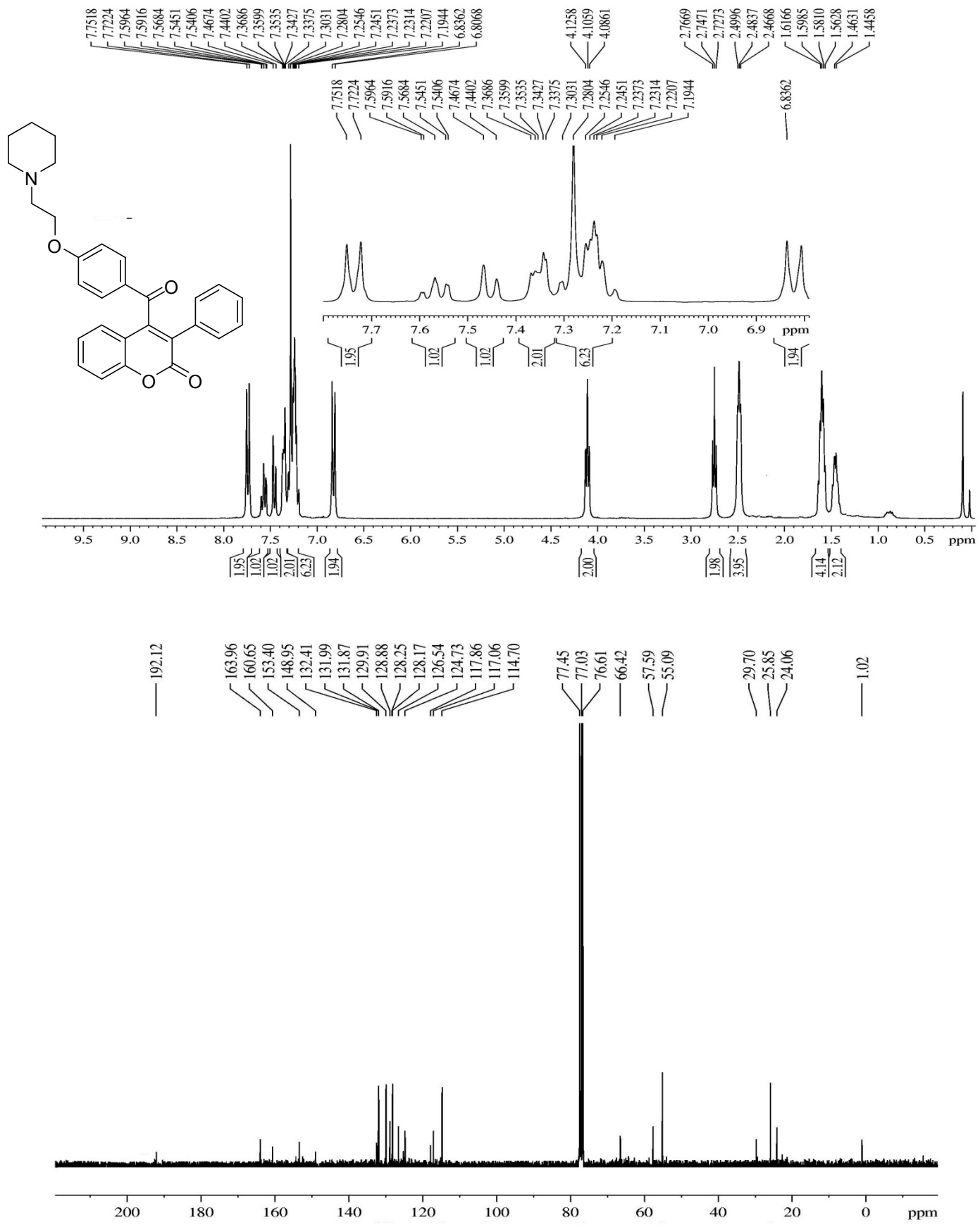
^{1}H and ^{13}C spectra of compound 9



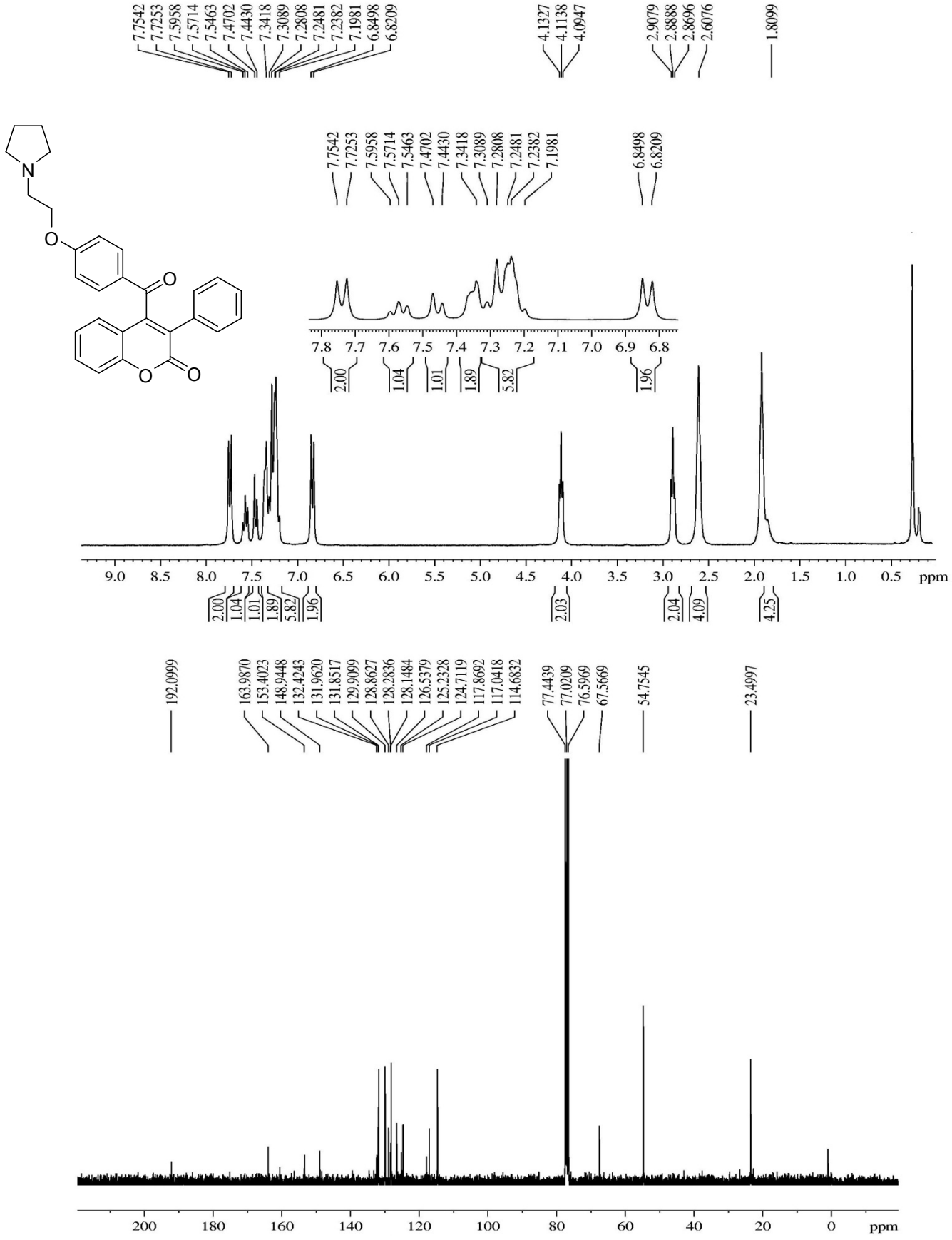
^{1}H and ^{13}C spectra of compound 10



^{1}H and ^{13}C spectra of compound 11



^{1}H and ^{13}C spectra of compound 12



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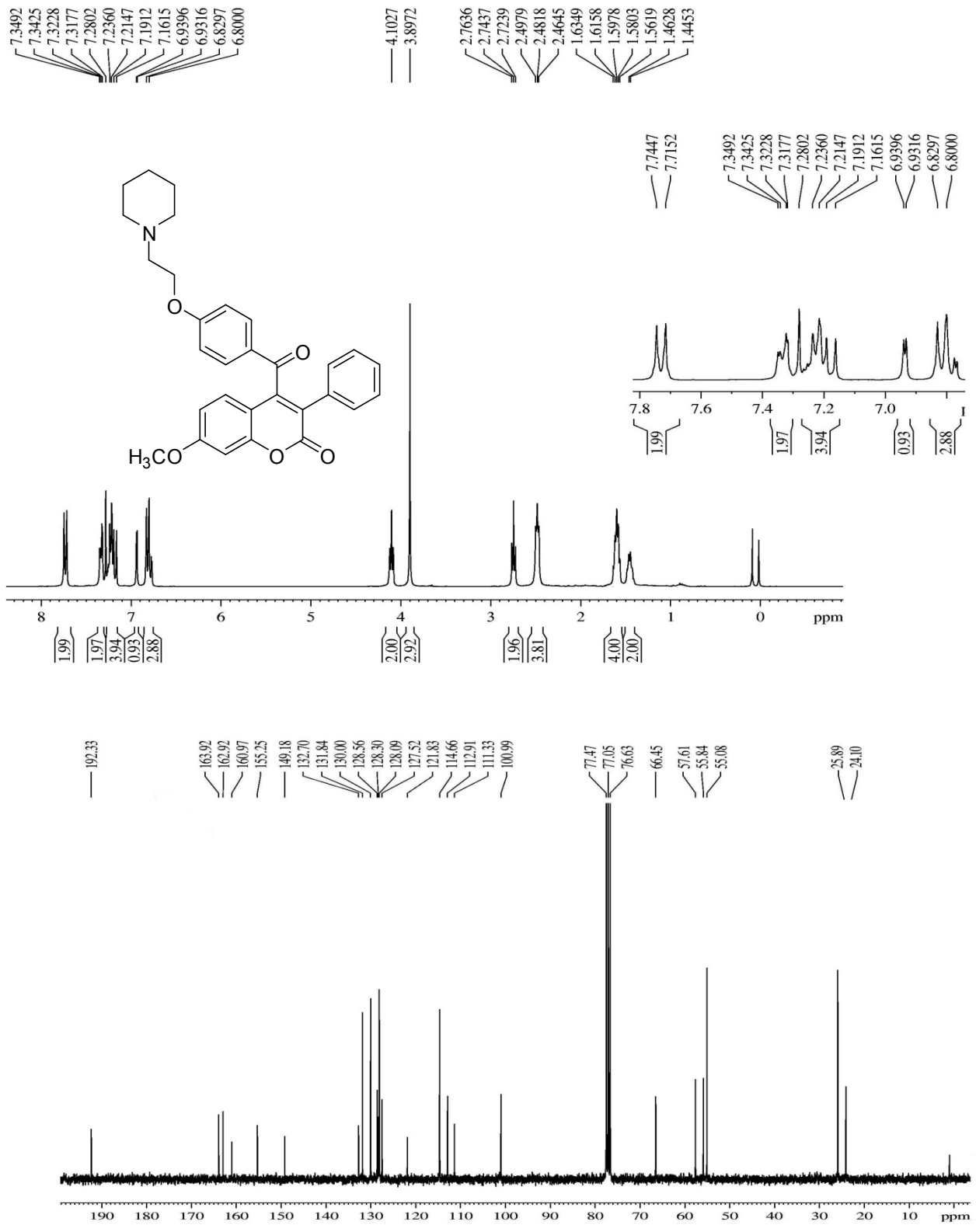

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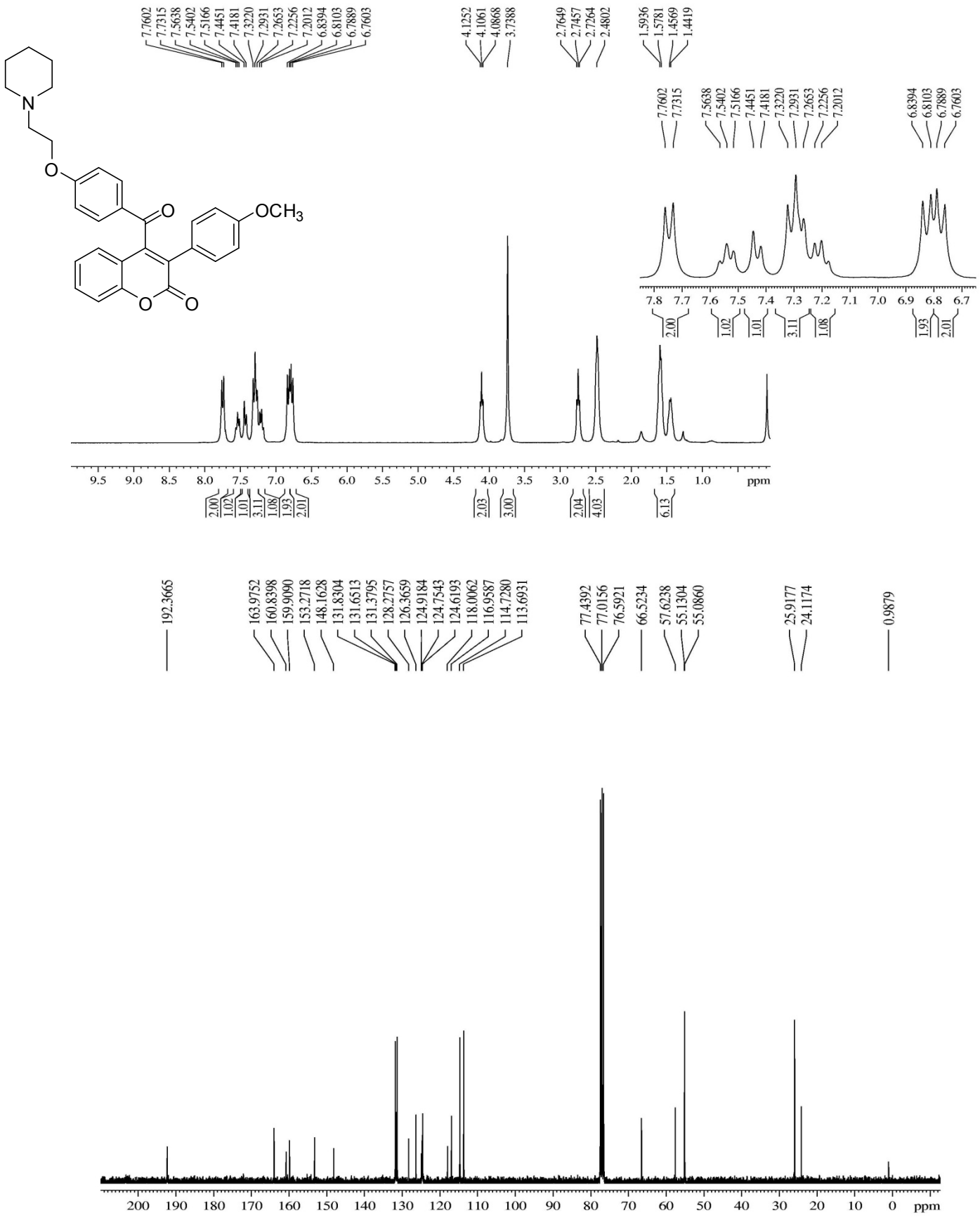
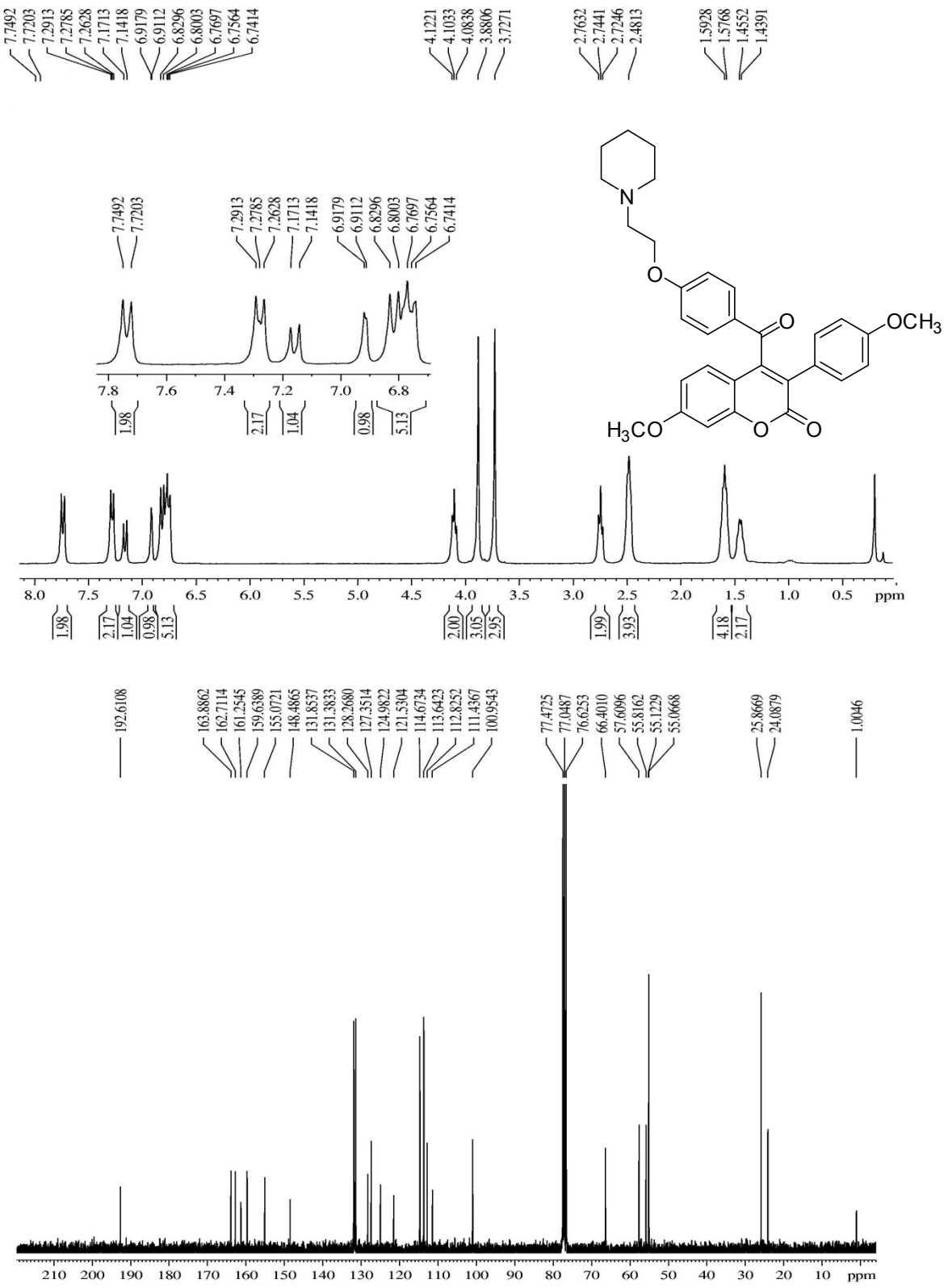
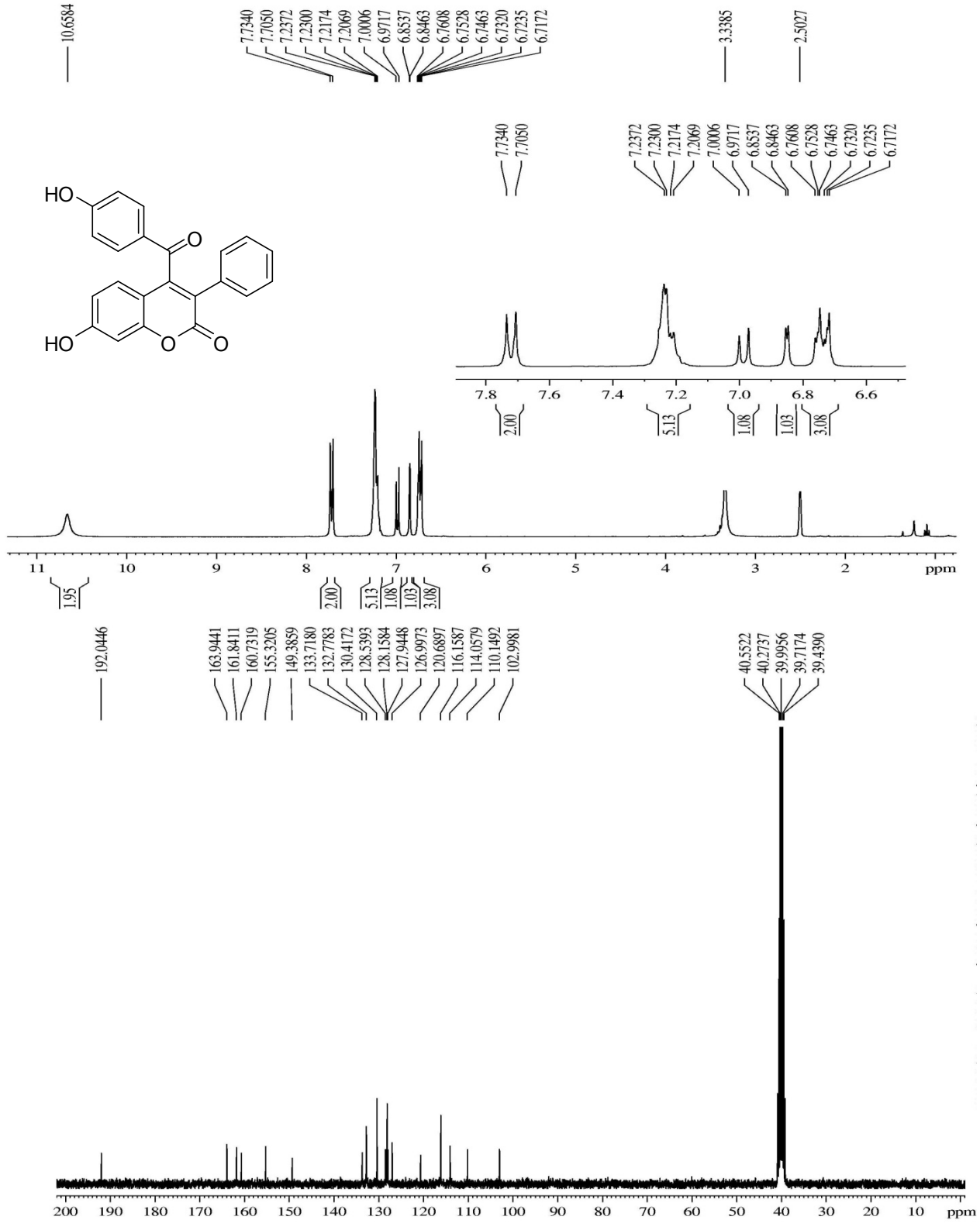


^{1}H and ^{13}C spectra of compound 16



^{1}H and ^{13}C spectra of compound 18



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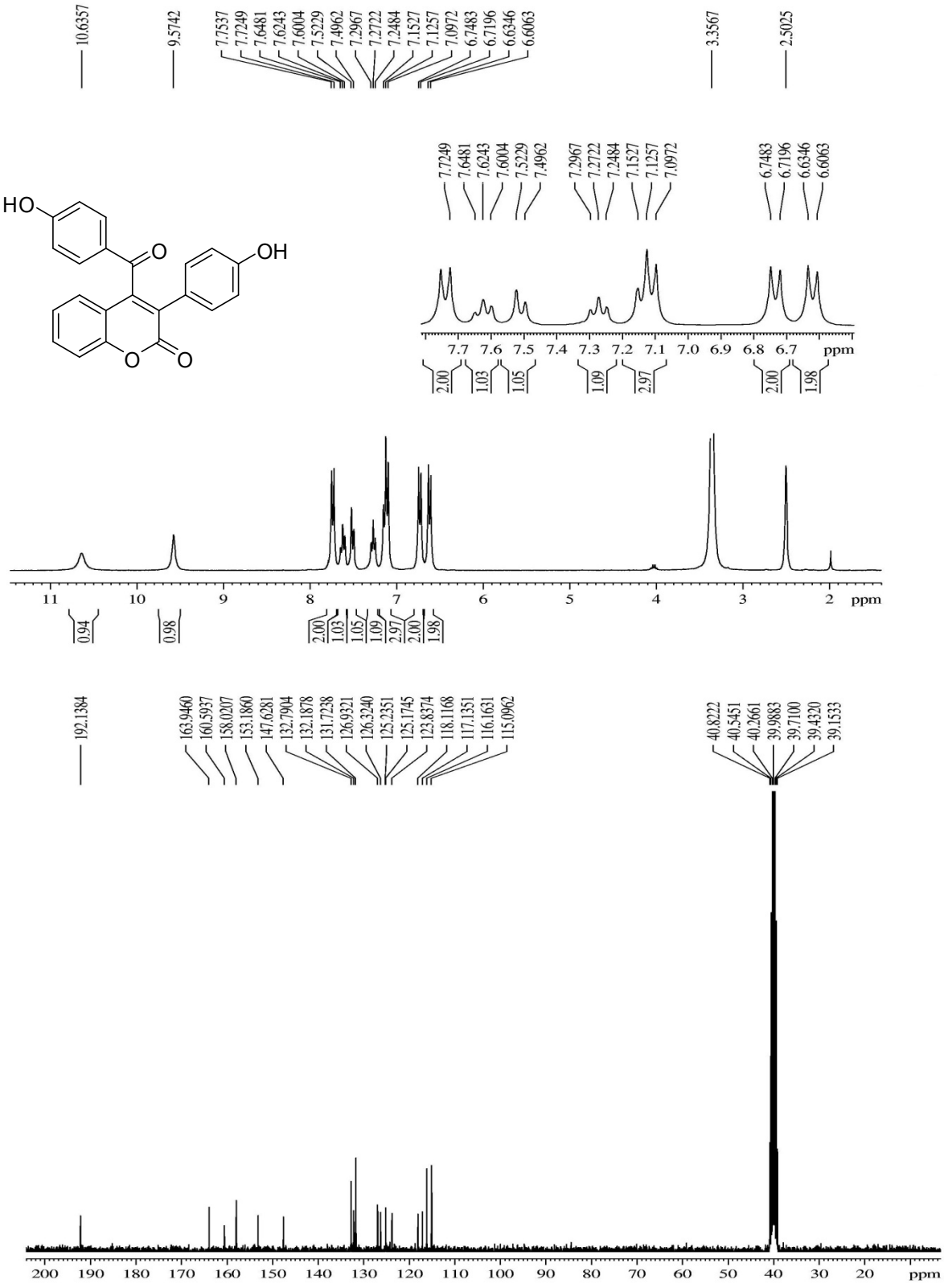
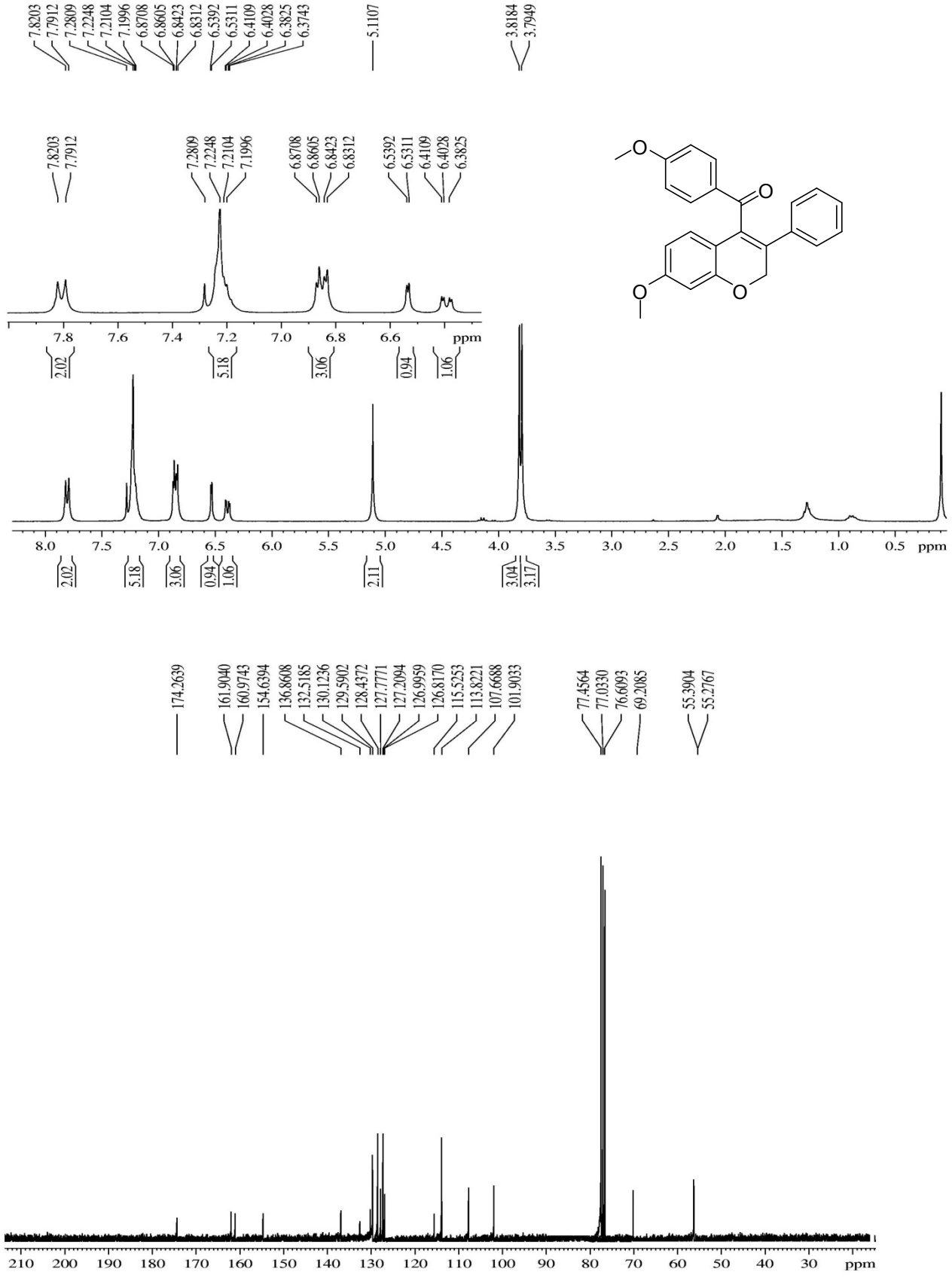
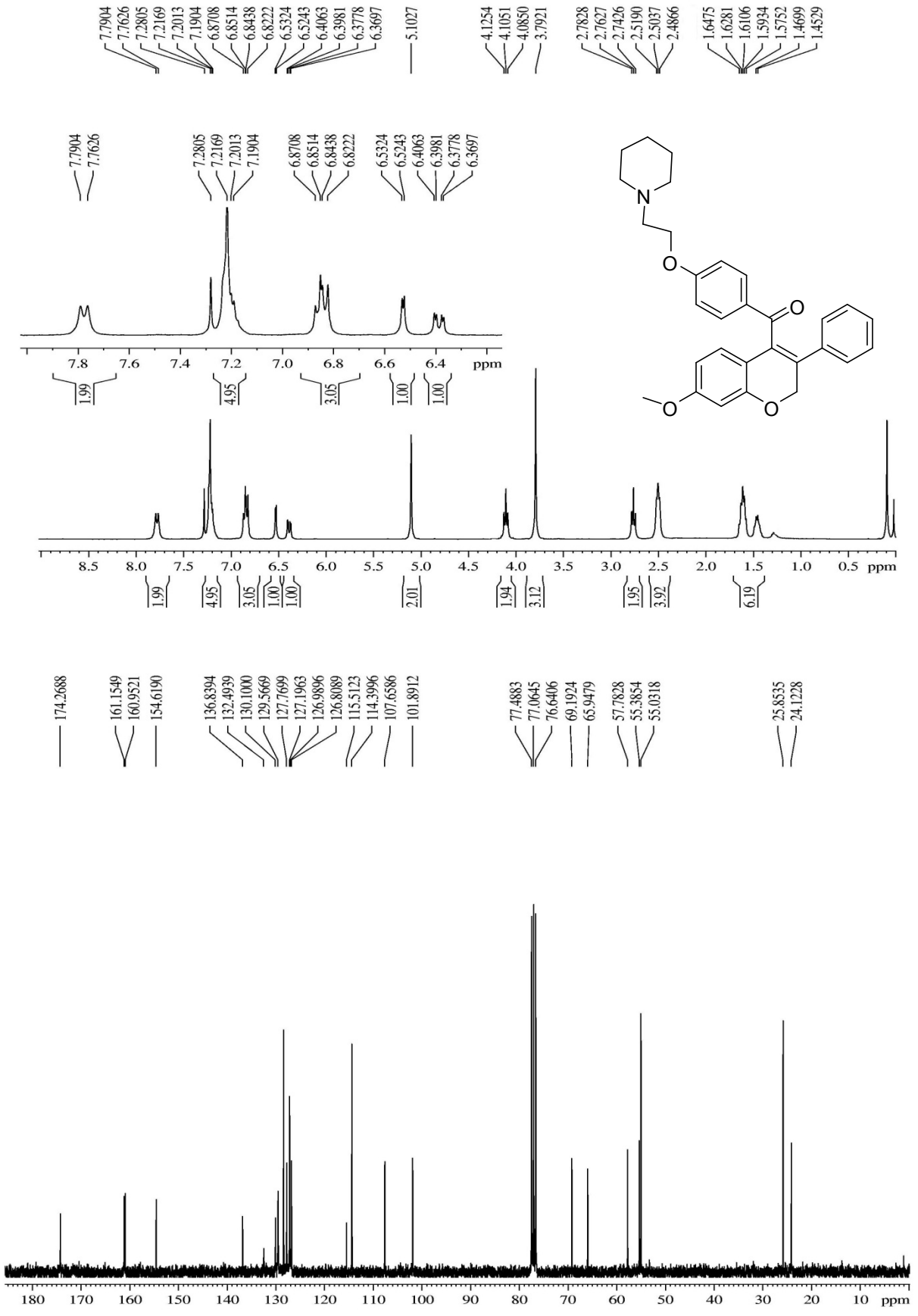


^{1}H and ^{13}C spectra of compound 21

^{1}H and ^{13}C spectra of compound 27



^{1}H and ^{13}C spectra of compound 34



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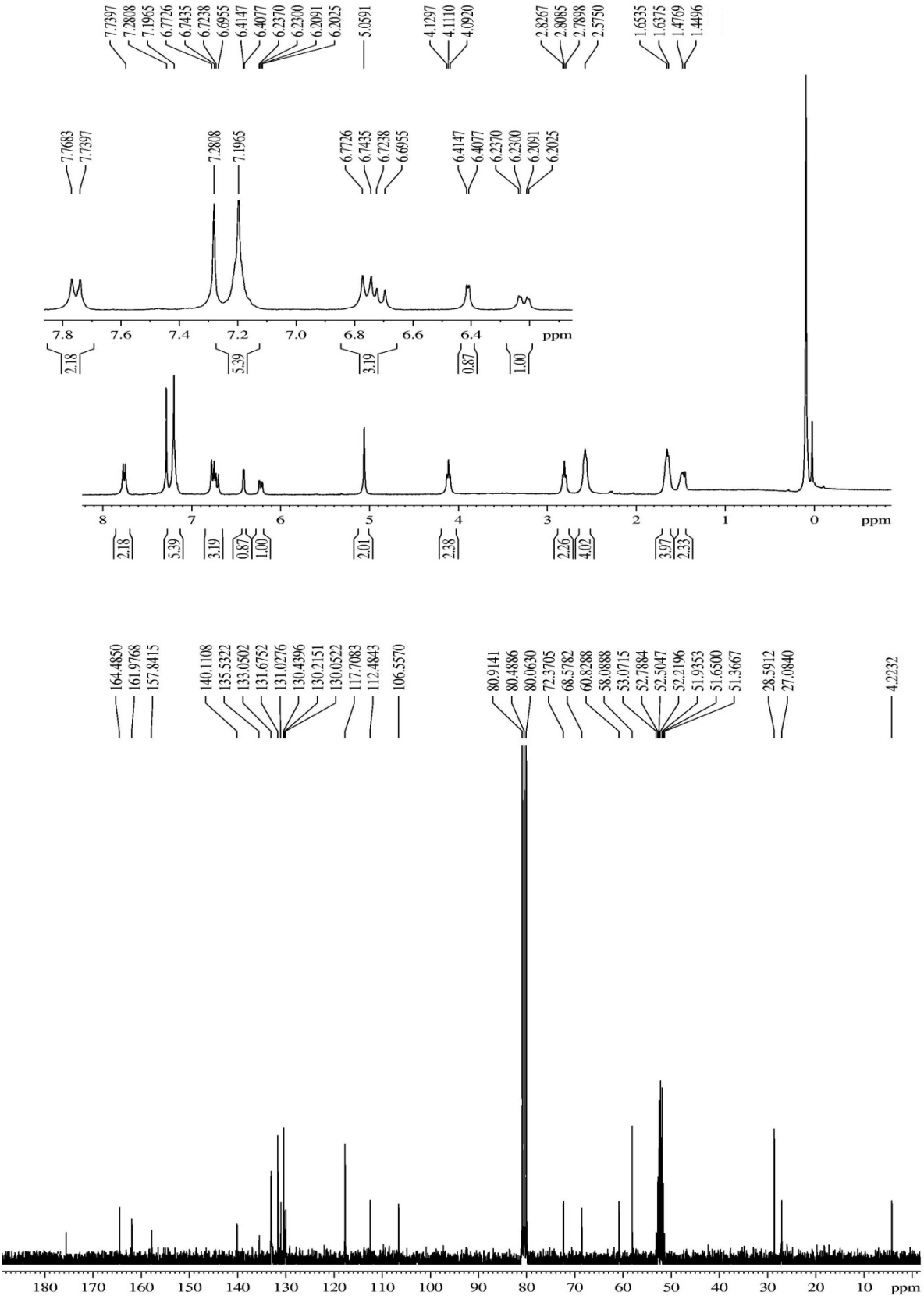

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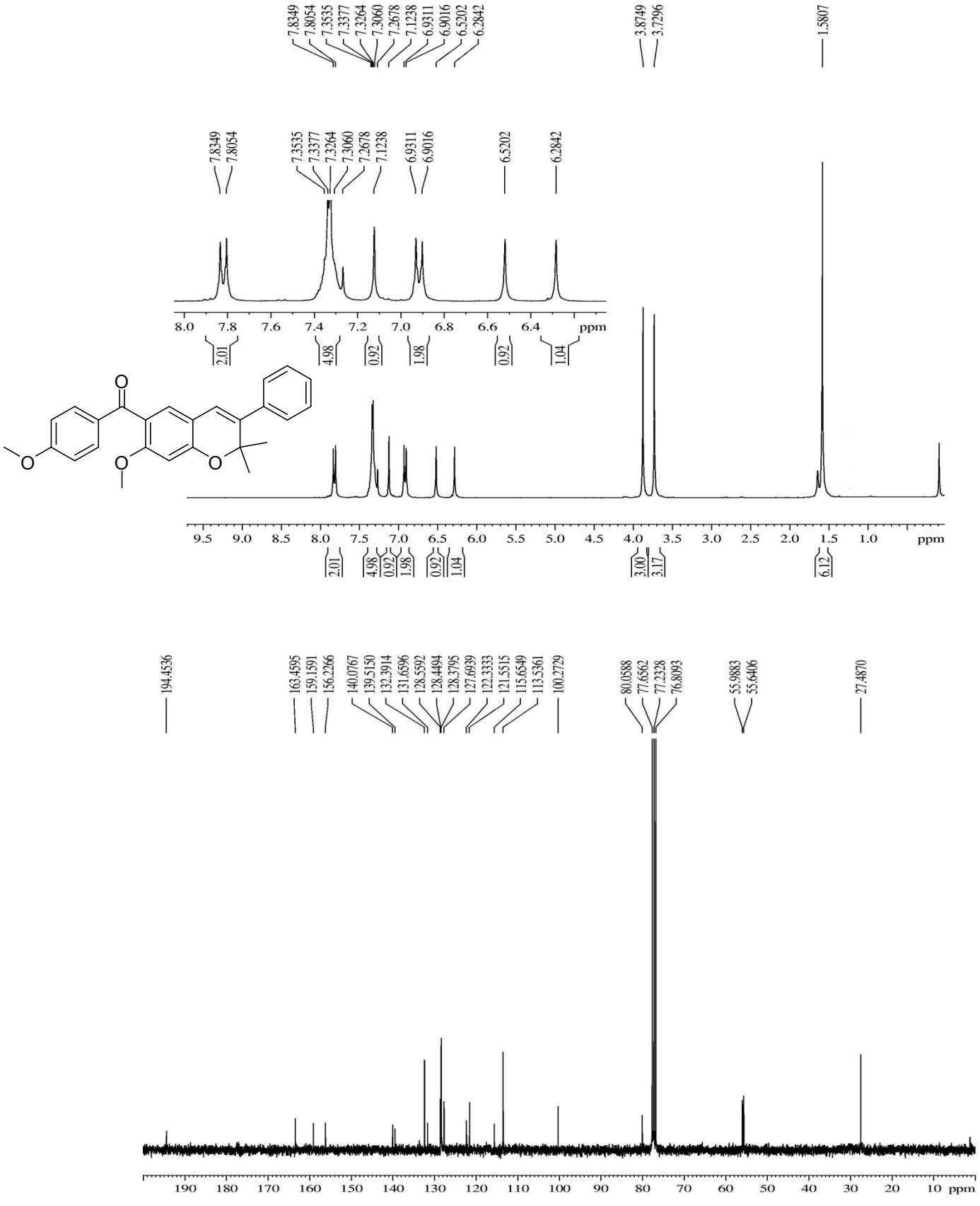
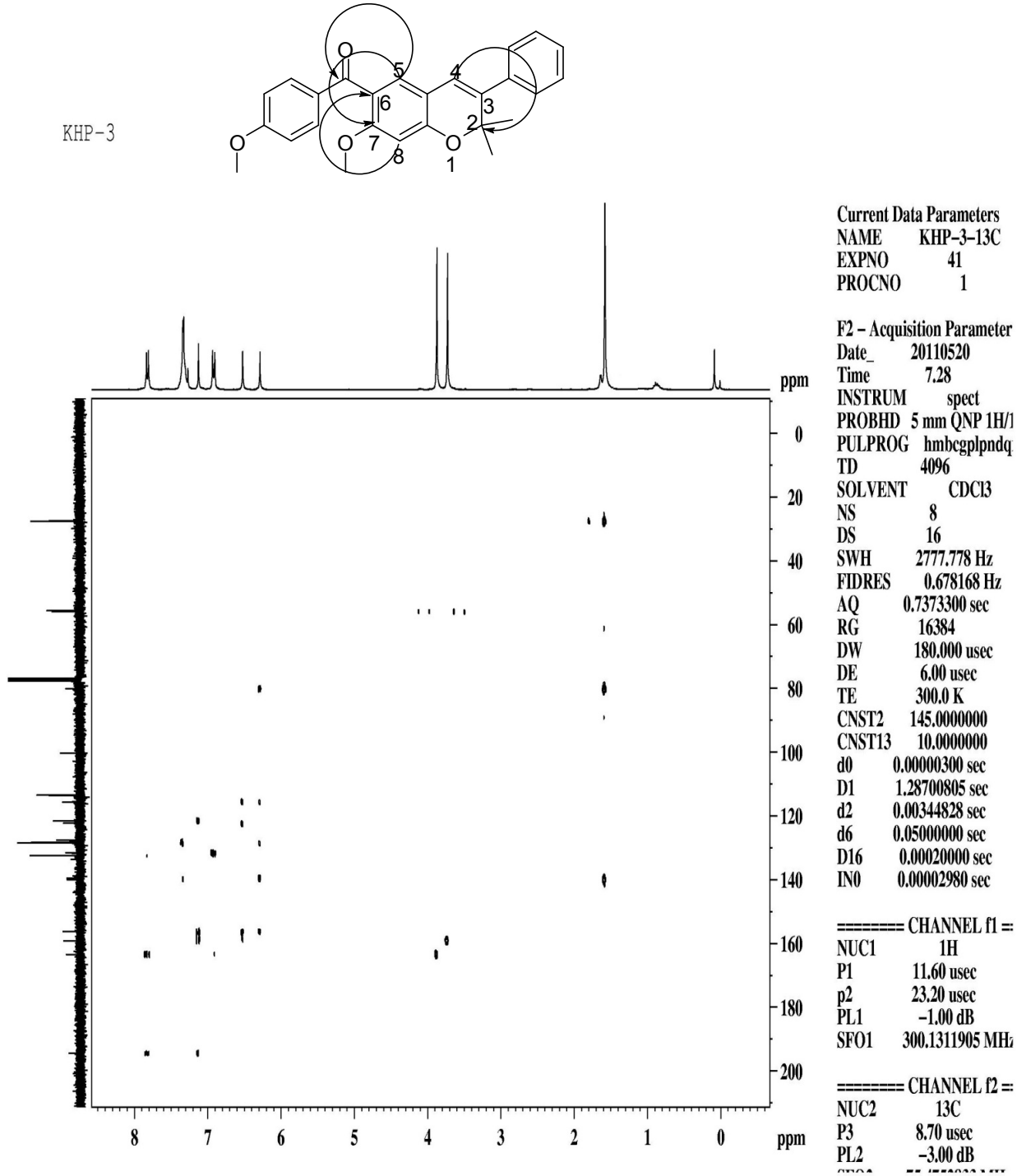
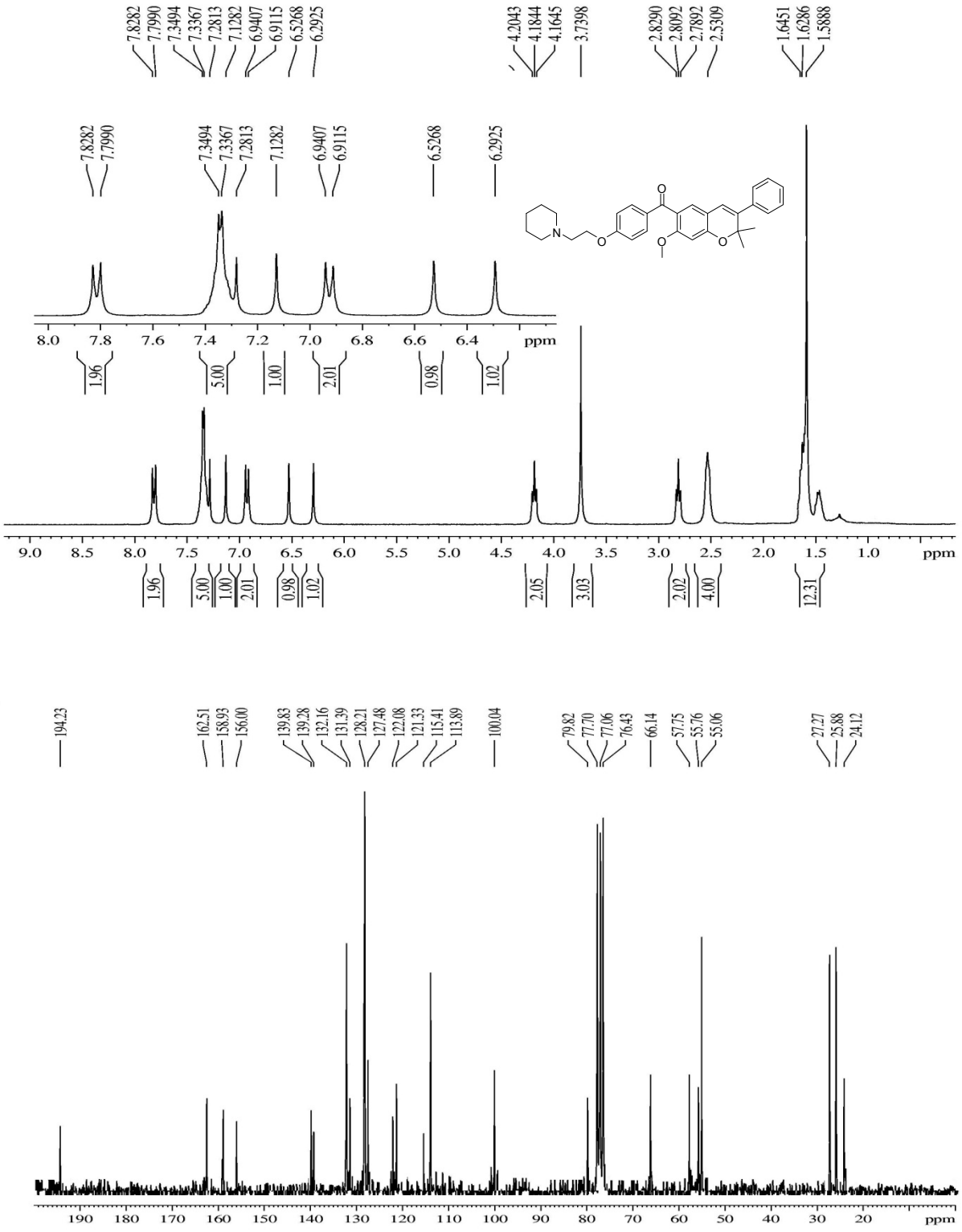


^{1}H and ^{13}C spectra of compound 43



HMBC spectrum of compound 43



^{1}H and ^{13}C spectra of compound 45

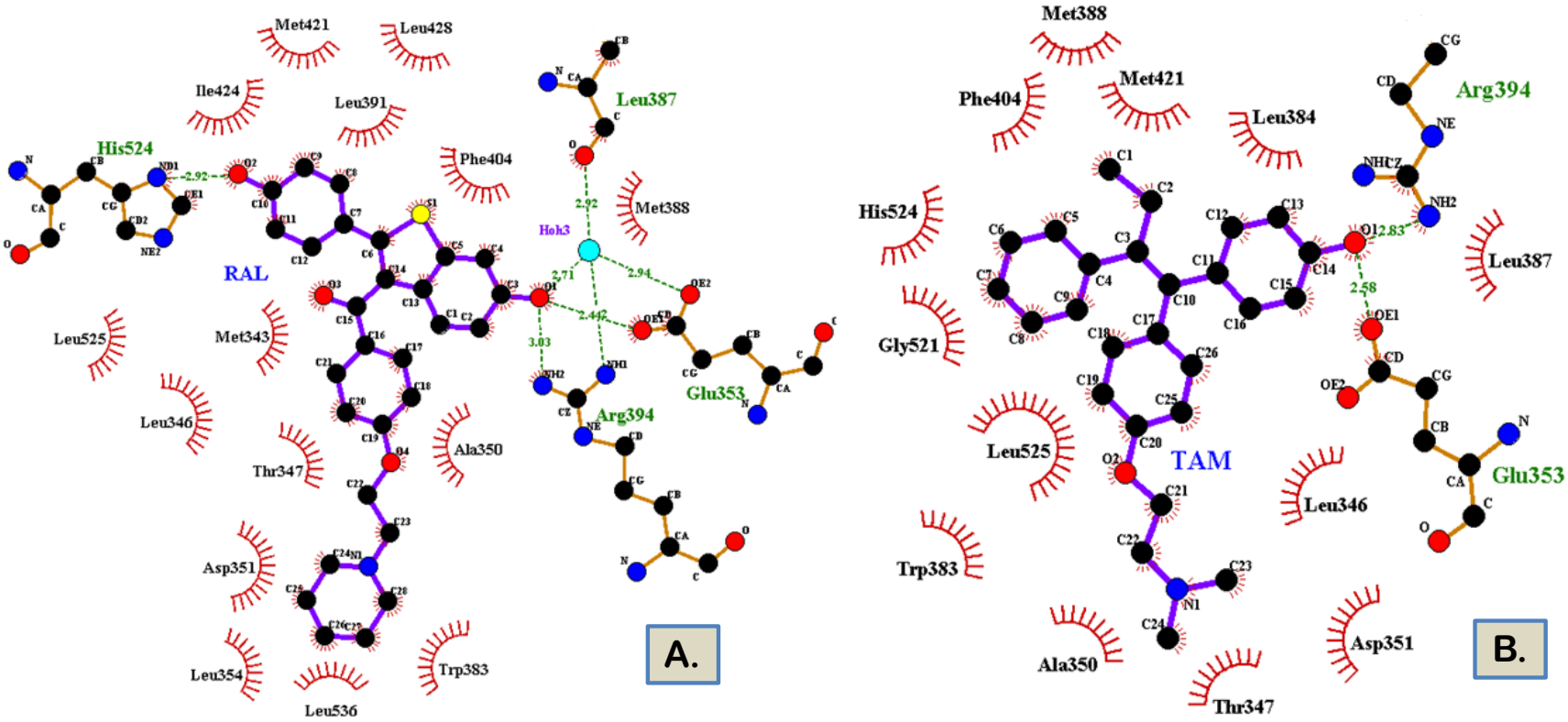


Figure S1. 2D Binding pose analysis of compound **(A).** RAL **(B).** TAM at the binding site of human ER- α.

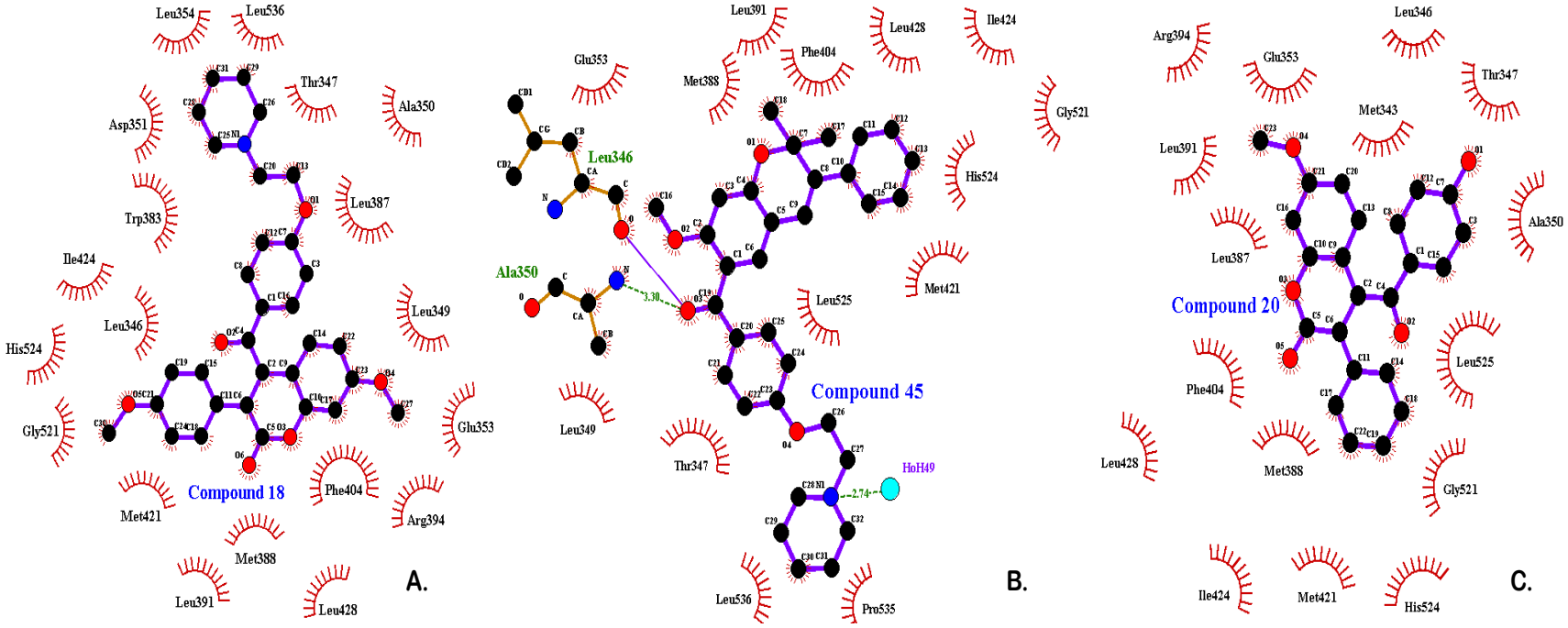


Figure S2. 2D Binding pose analysis of compound **(A). 18, (B). 45 , (C) 20** at the binding site of human ER- α.

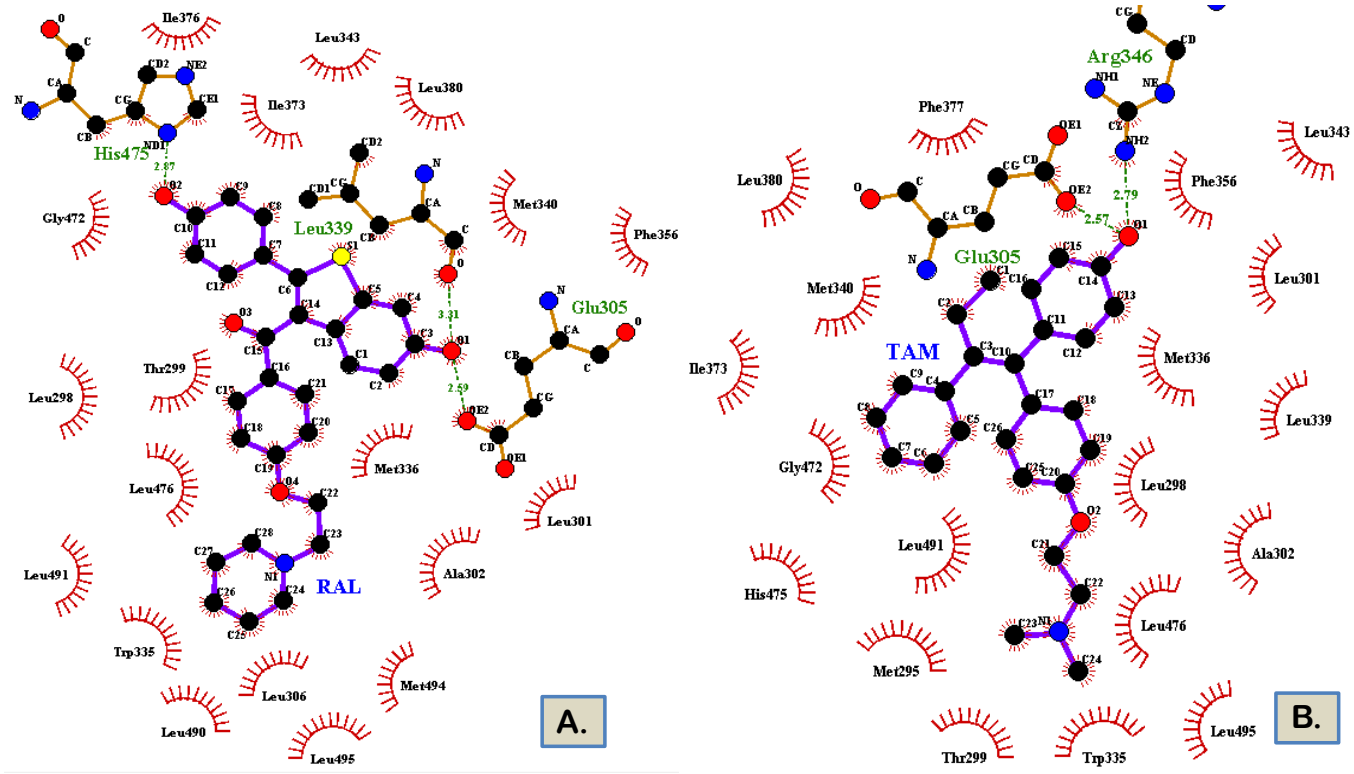


Figure S3. 2D Binding pose analysis of compound **(A).** RAL **(B).** TAM at the binding site of human ER- β.

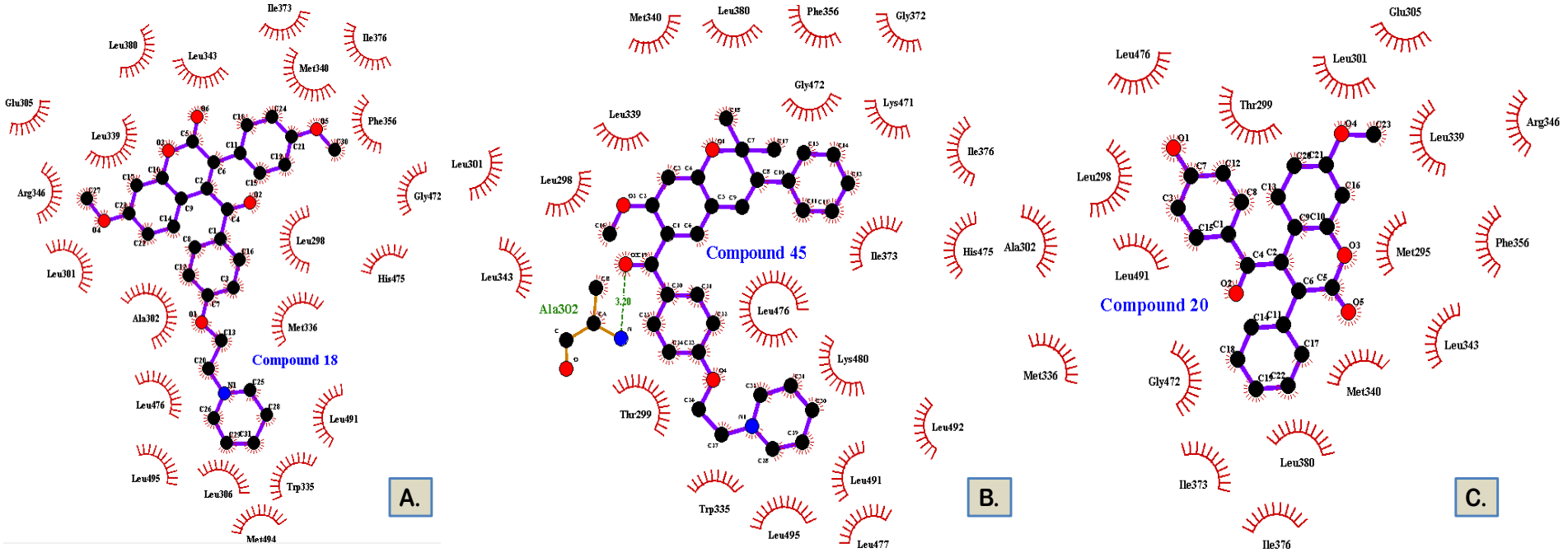


Figure S4. 2D Binding pose analysis of compound **(A). 18, (B). 45 , (C) 20** at the binding site of human ER- β.