

Supporting Information for

**Iodine-Catalysed Regioselective Thiolation of Flavonoids Using
Sulfonyl Hydrazides as Sulfenylation Reagents**

Xia Zhao, ^{*a} Zhijie Deng, ^a Aoqi Wei, ^a Boyang Li ^a and Kui Lu ^{*b}

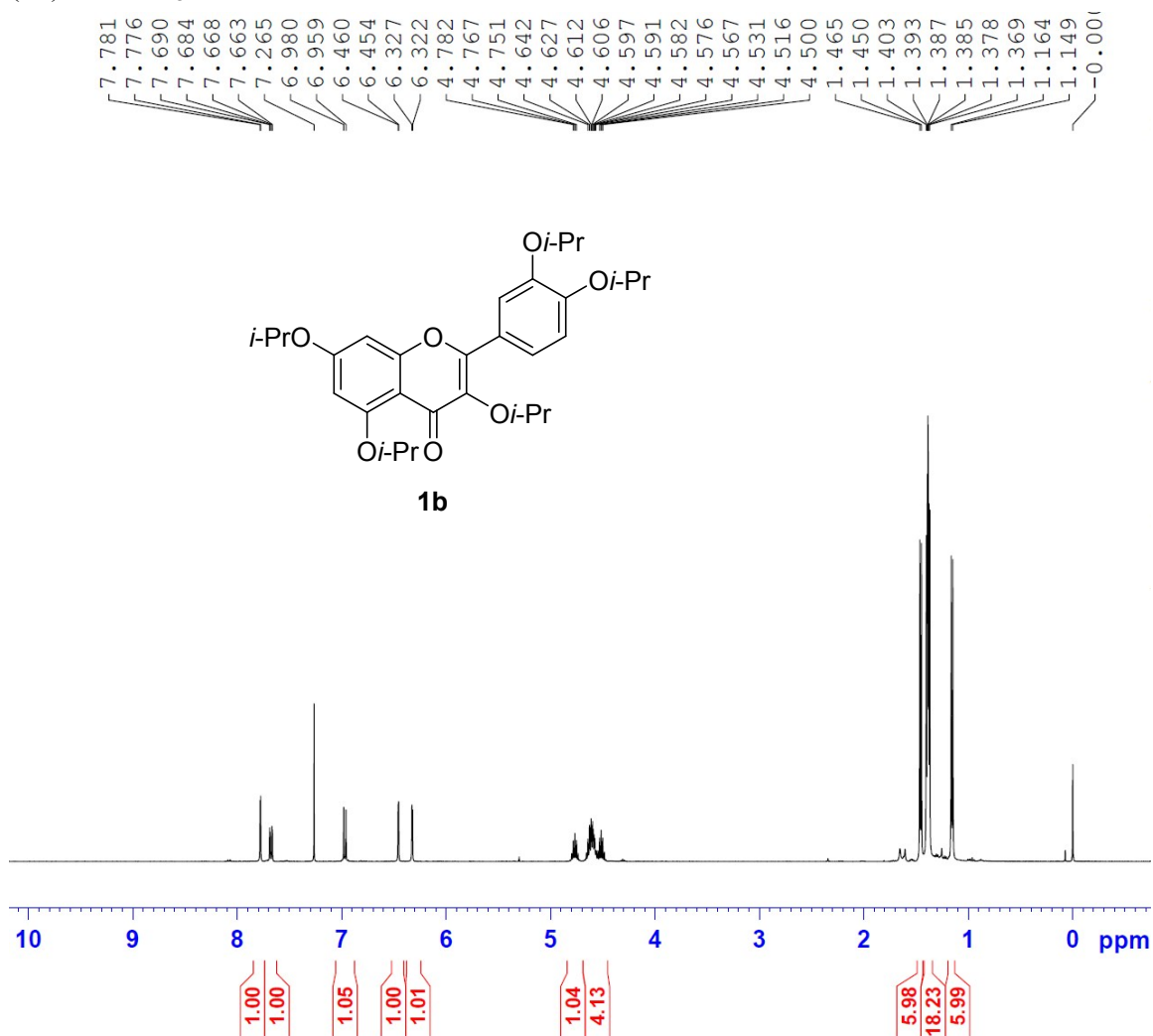
^a *College of Chemistry, Tianjin Key Laboratory of Structure and Performance for Functional Molecules, Key laboratory of Inorganic-organic Hybrid Functional Material Chemistry, Ministry of Education, Tianjin Normal University, Tianjin 300387, China*

^b *College of Biotechnology, Tianjin University of Science & Technology, Tianjin 300457, China*

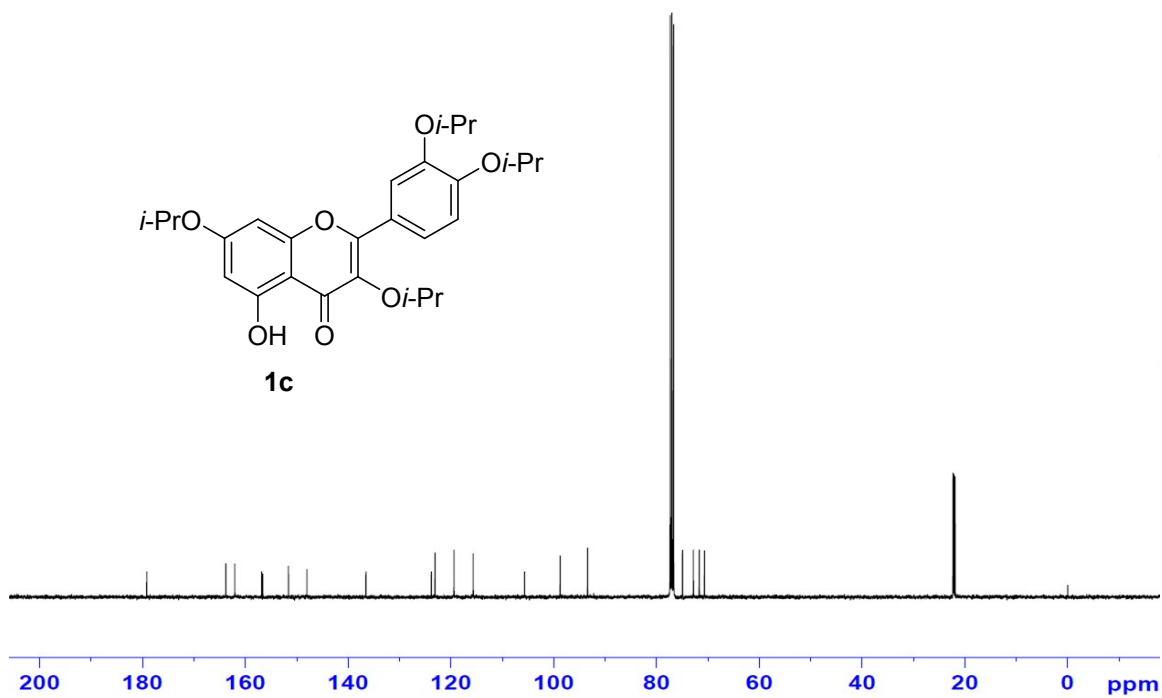
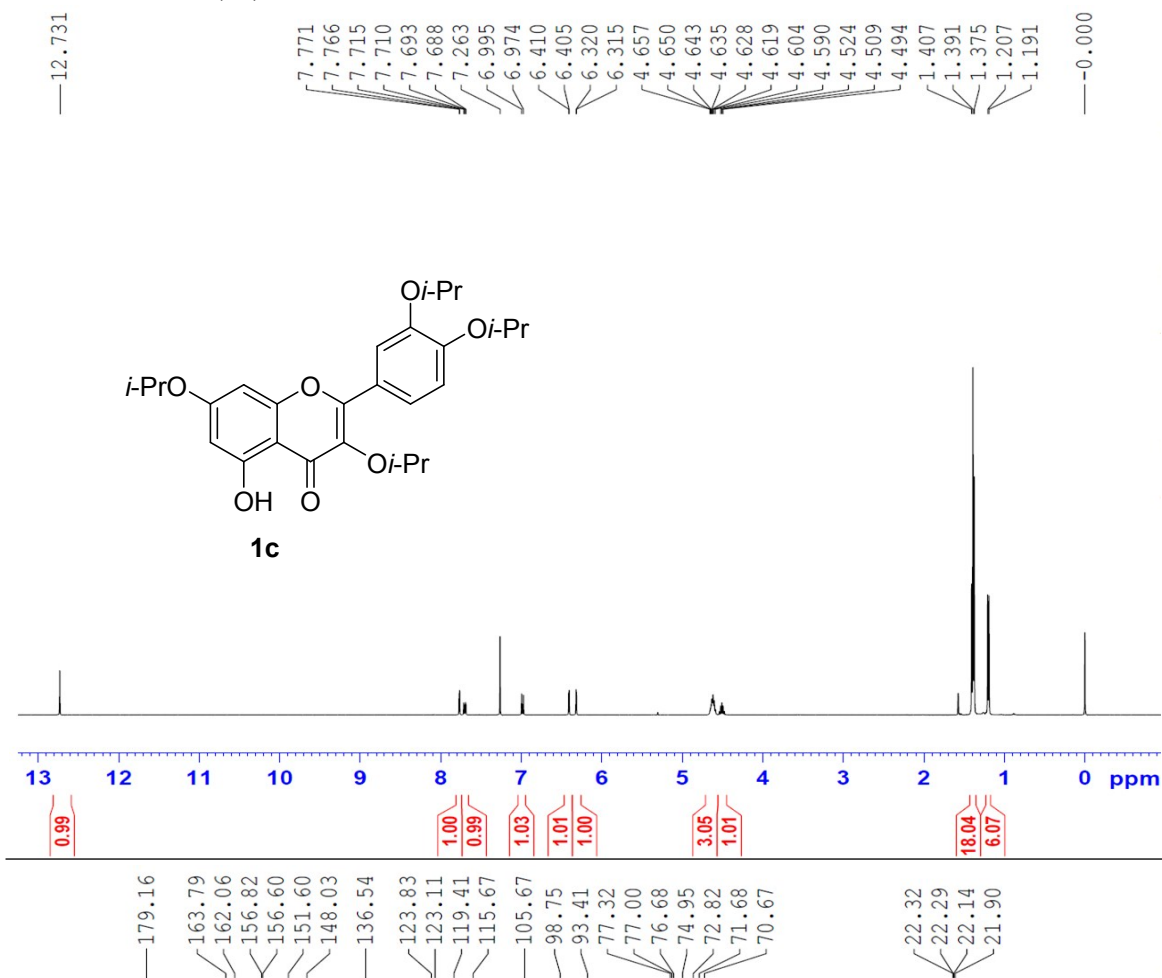
*E-mail: hxyzhx@mail.tjnu.edu.cn; lukui@tust.edu.cn

The spectrum of flavonoid isopropyl ethers

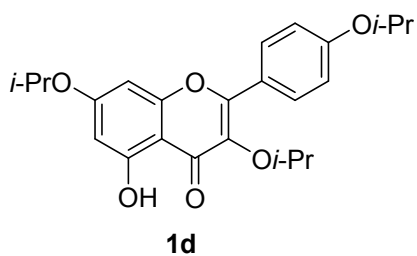
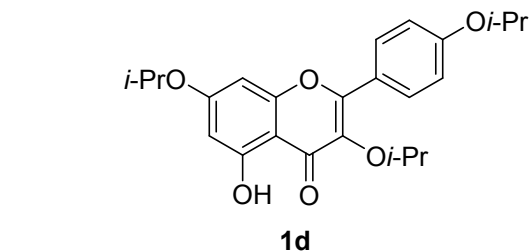
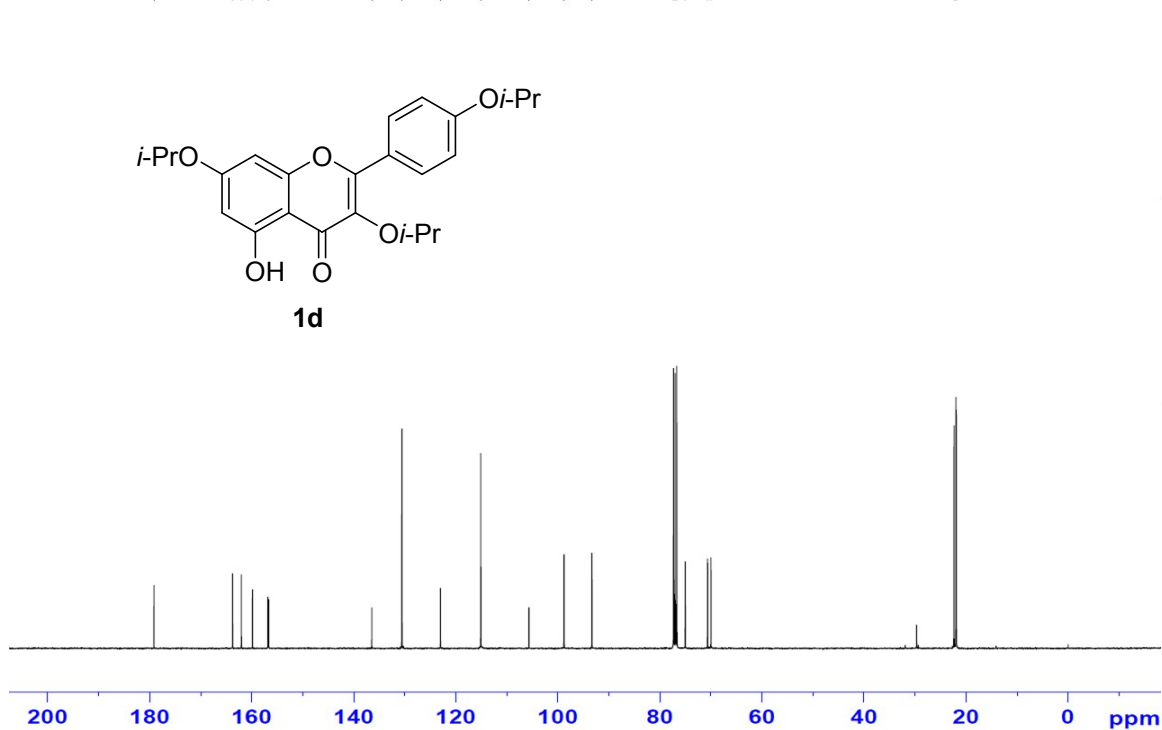
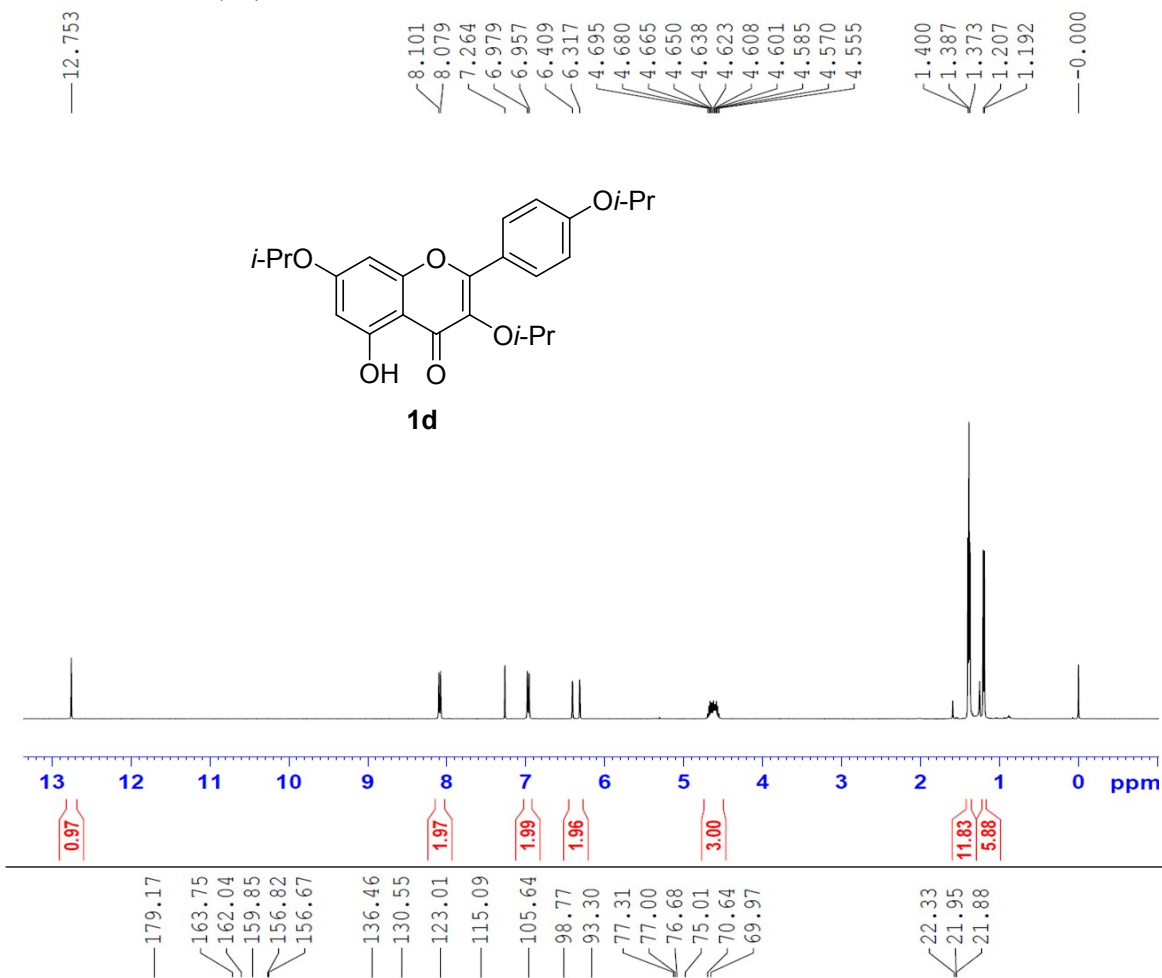
¹H NMR spectra of 2-(3,4-diisopropoxyphenyl)-3,5,7-triisopropoxy-4H-chromen-4-one (1b) in CDCl₃



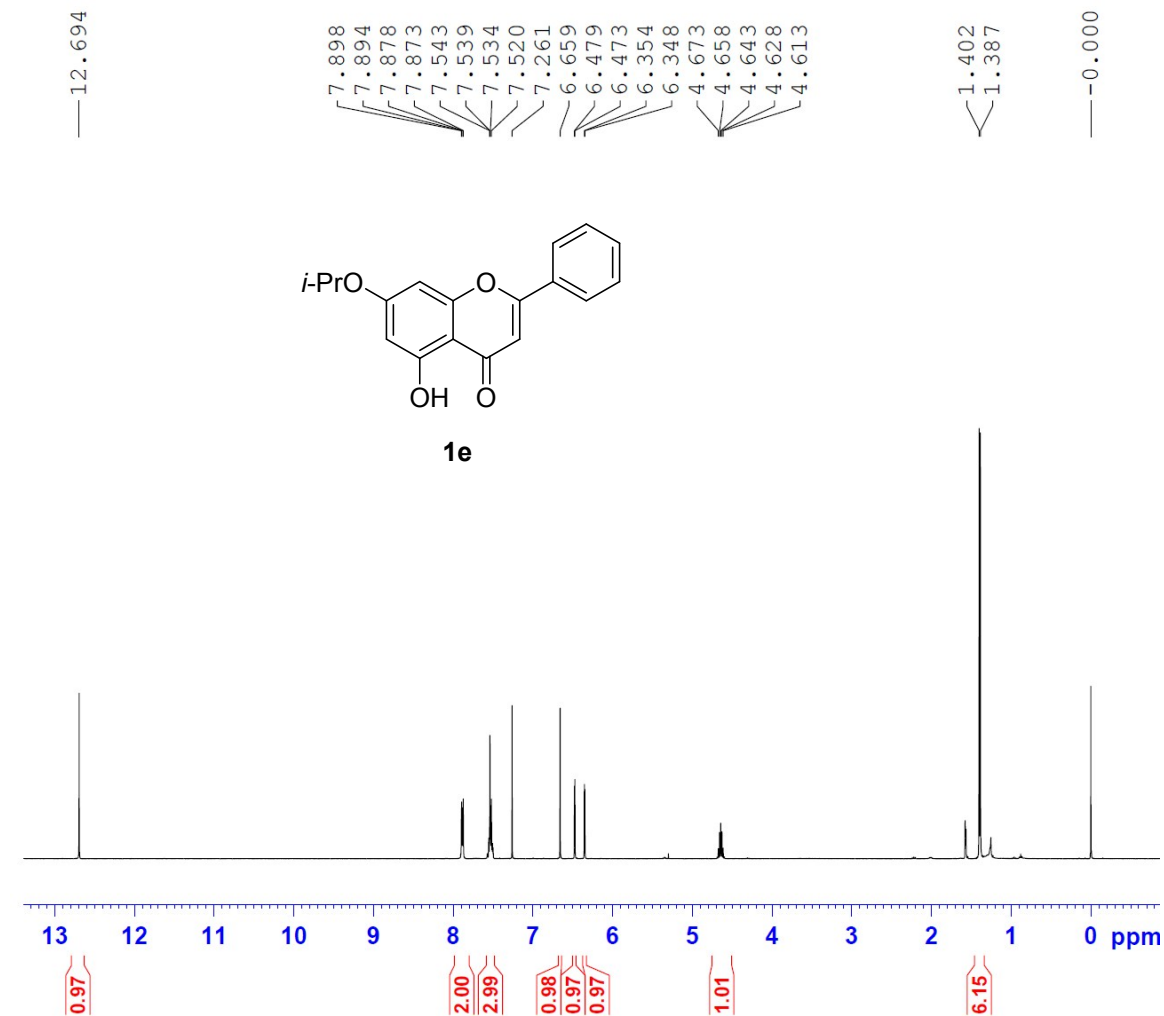
^1H and ^{13}C NMR spectra of 2-(3,4-diisopropoxyphenyl)-5-hydroxy-3,7-diisopropoxy-4H-chromen-4-one (**1c**) in CDCl_3



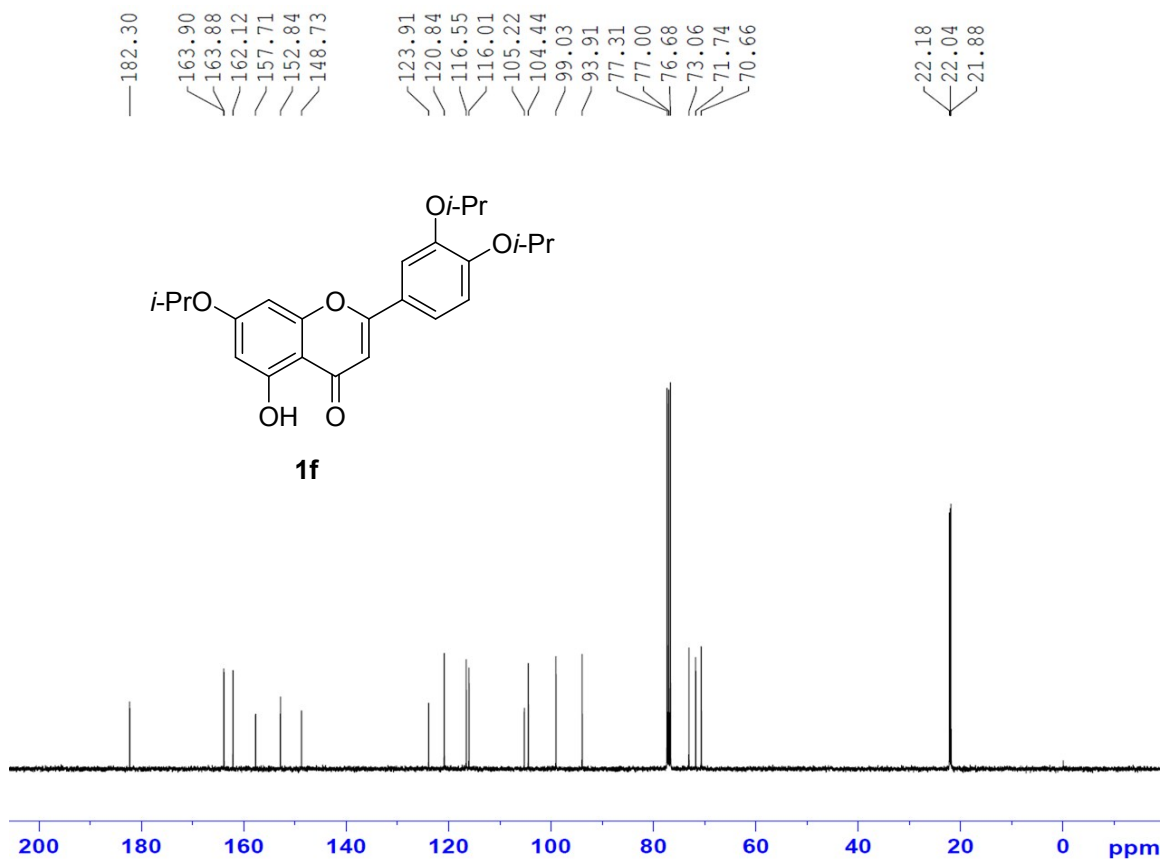
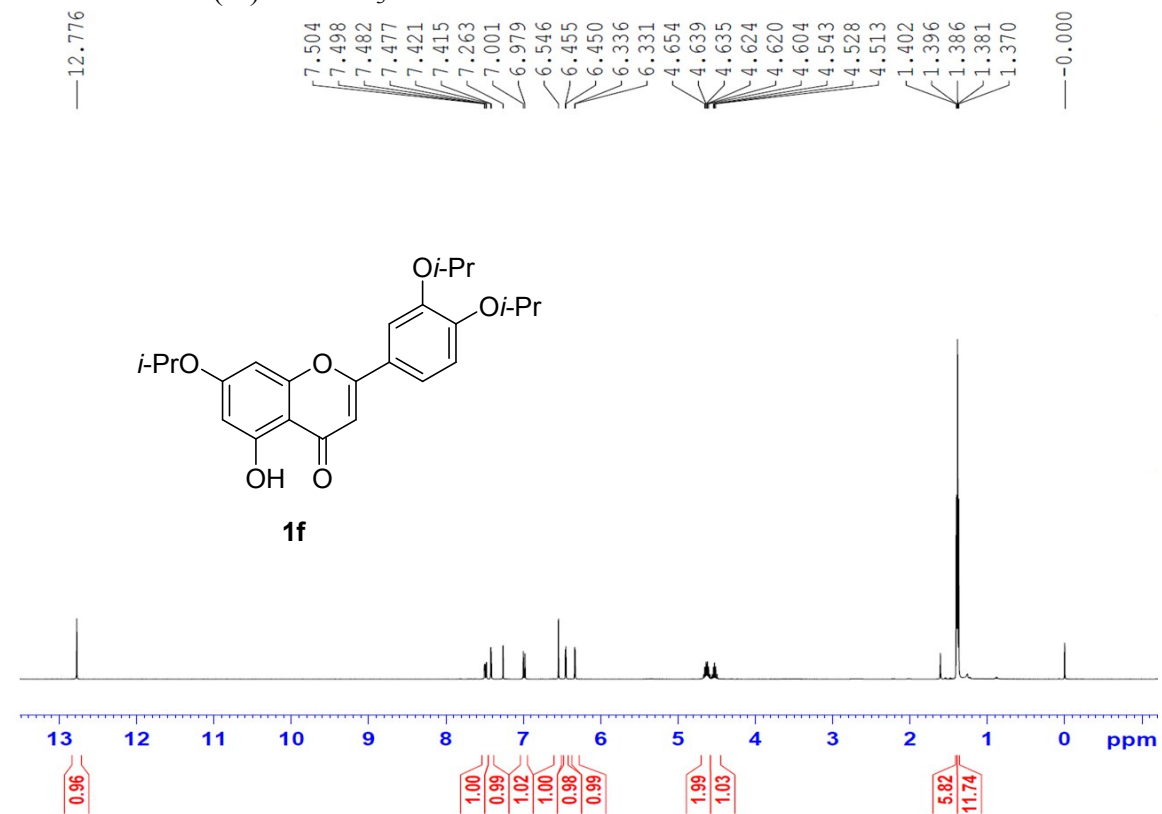
^1H and ^{13}C NMR spectra of 5-hydroxy-3,7-diisopropoxy-2-(4-isopropoxyphenyl)-4H-chromen-4-one (1d) in CDCl_3



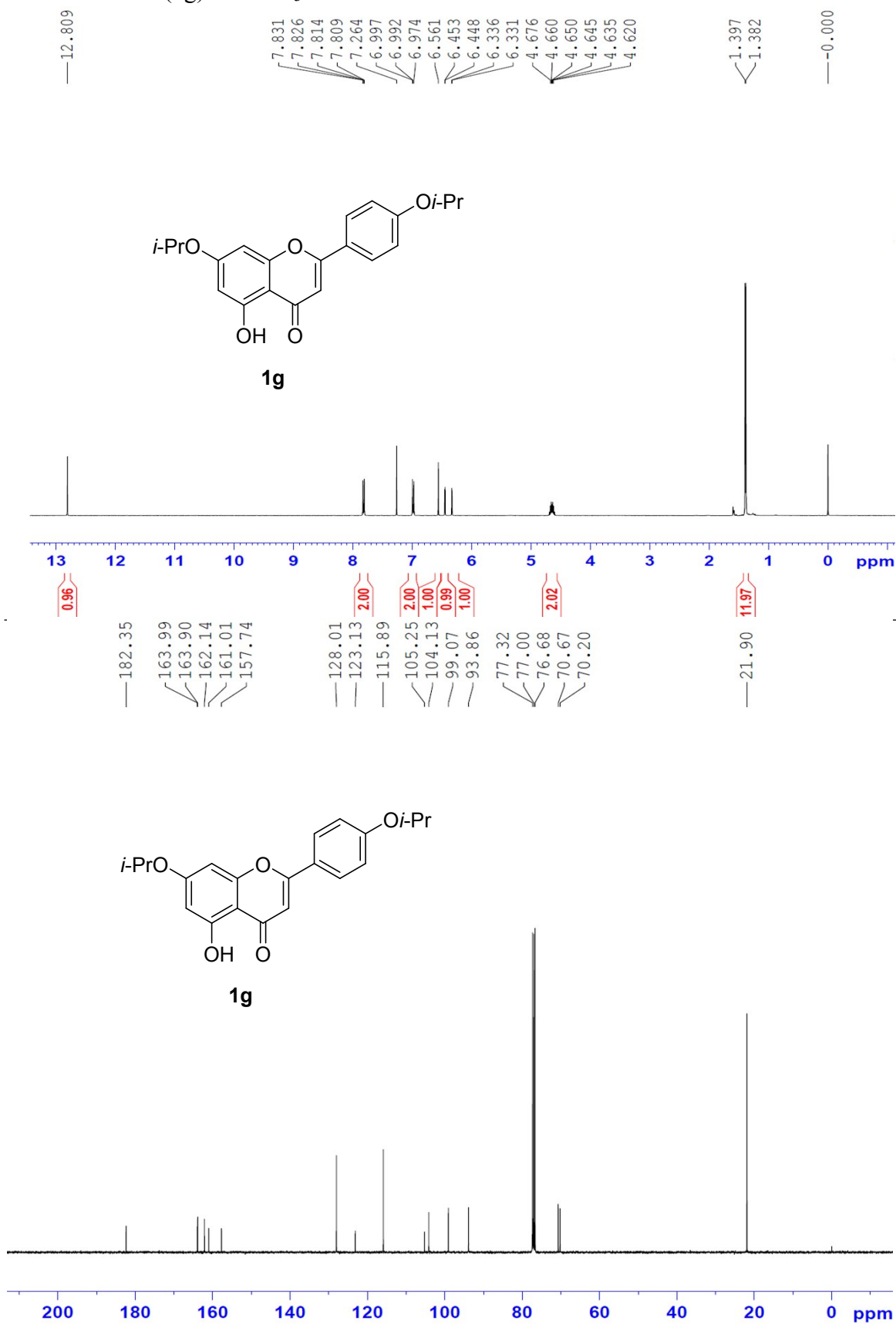
^1H NMR spectra of 5-hydroxy-7-isopropoxy-2-phenyl-4H-chromen-4-one (1e) in CDCl_3



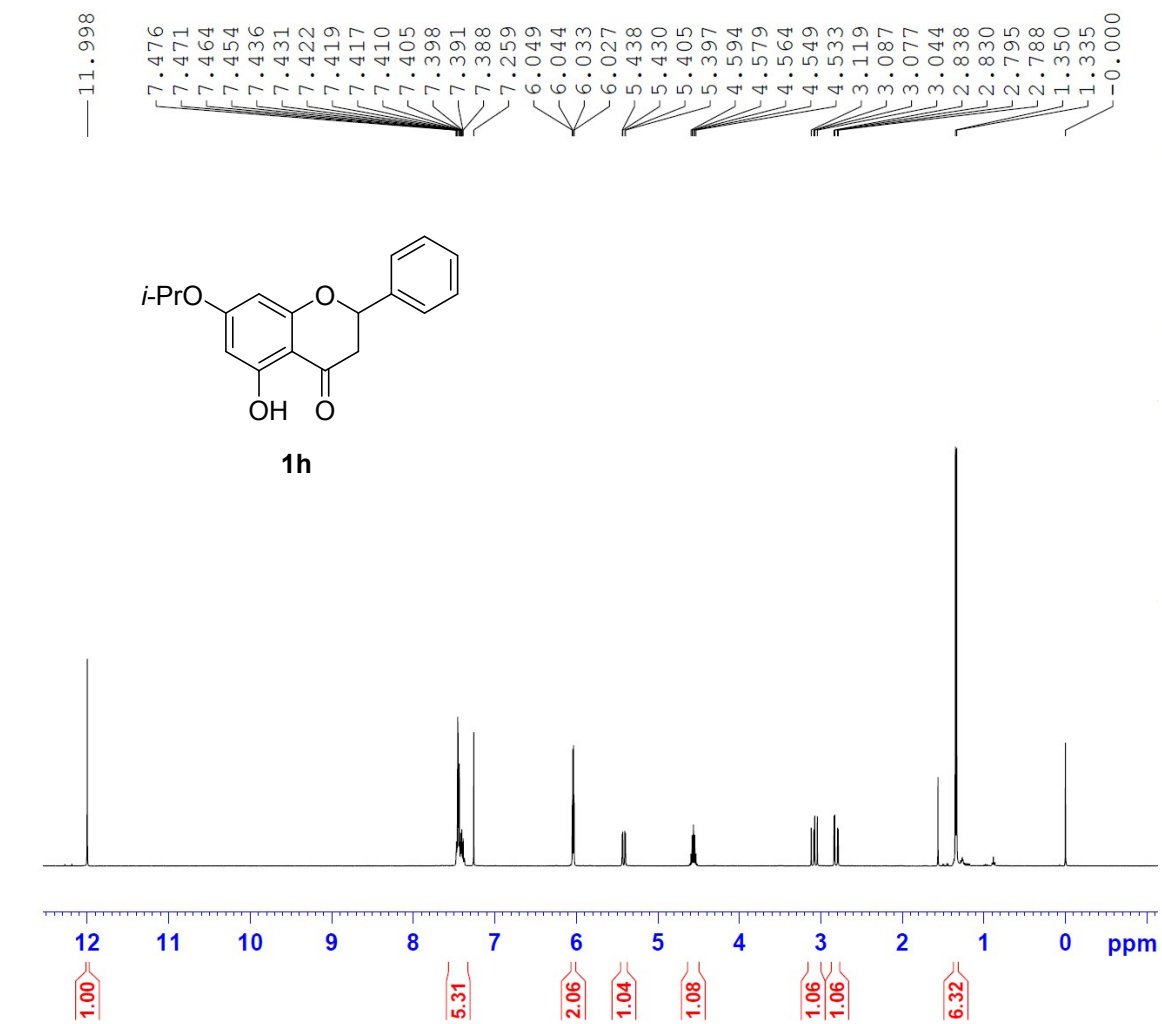
^1H and ^{13}C NMR spectra of 2-(3,4-diisopropoxyphenyl)-5-hydroxy-7-isopropoxy-4H-chromen-4-one (1f) in CDCl_3



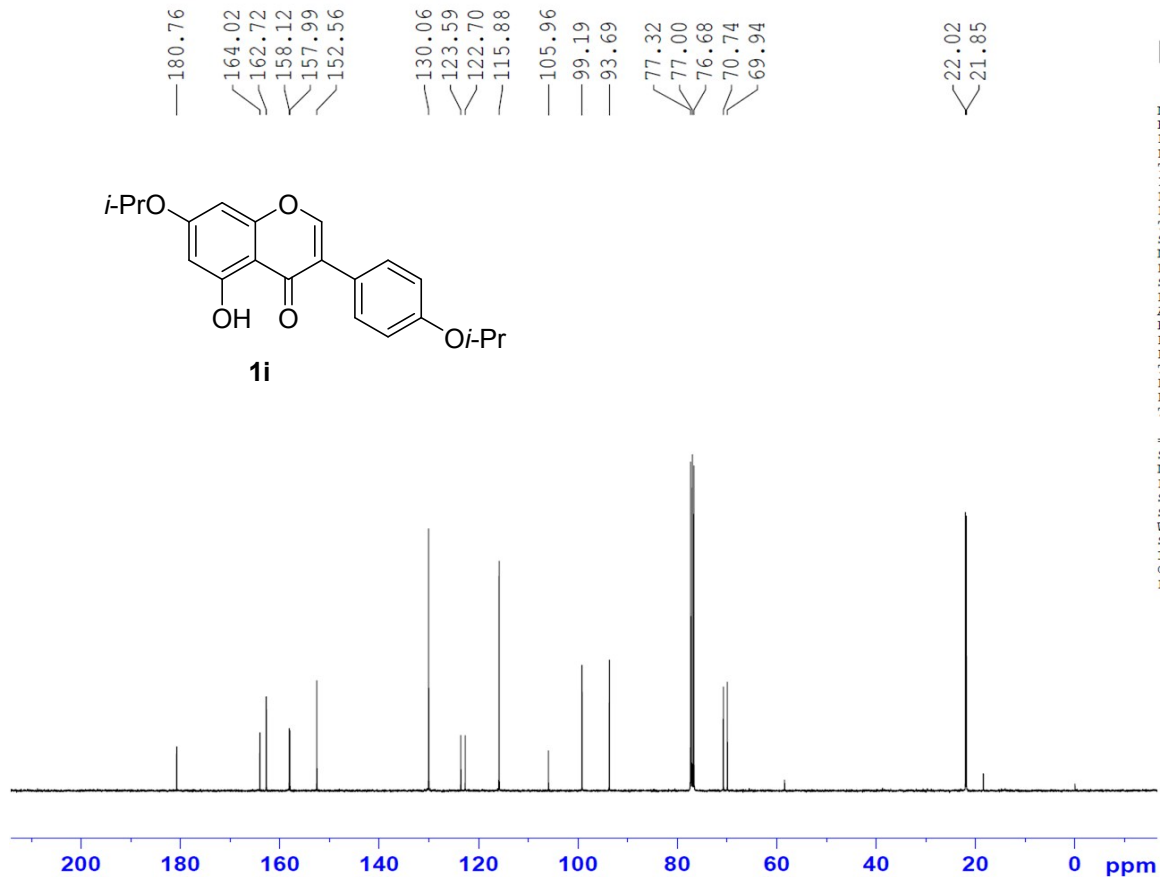
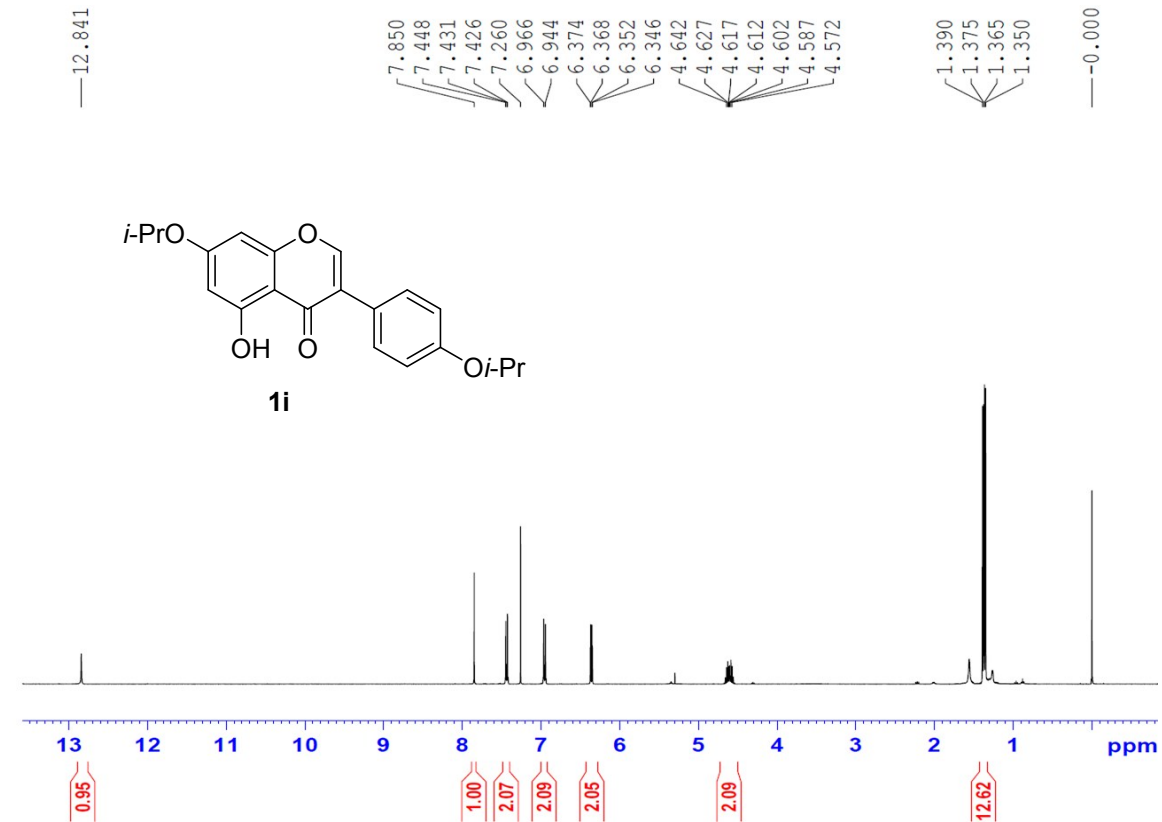
^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 5-hydroxy-7-isopropoxy-2-(4-isopropoxyphenyl)-4H-chromen-4-one (**1g**) in CDCl_3



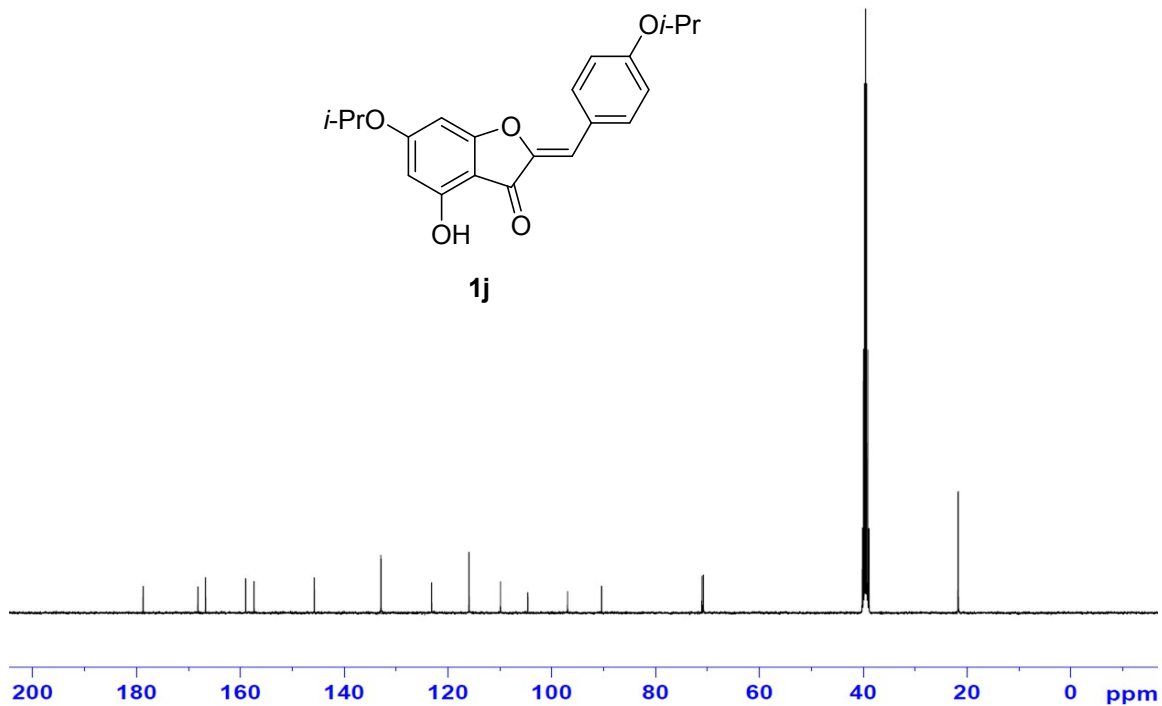
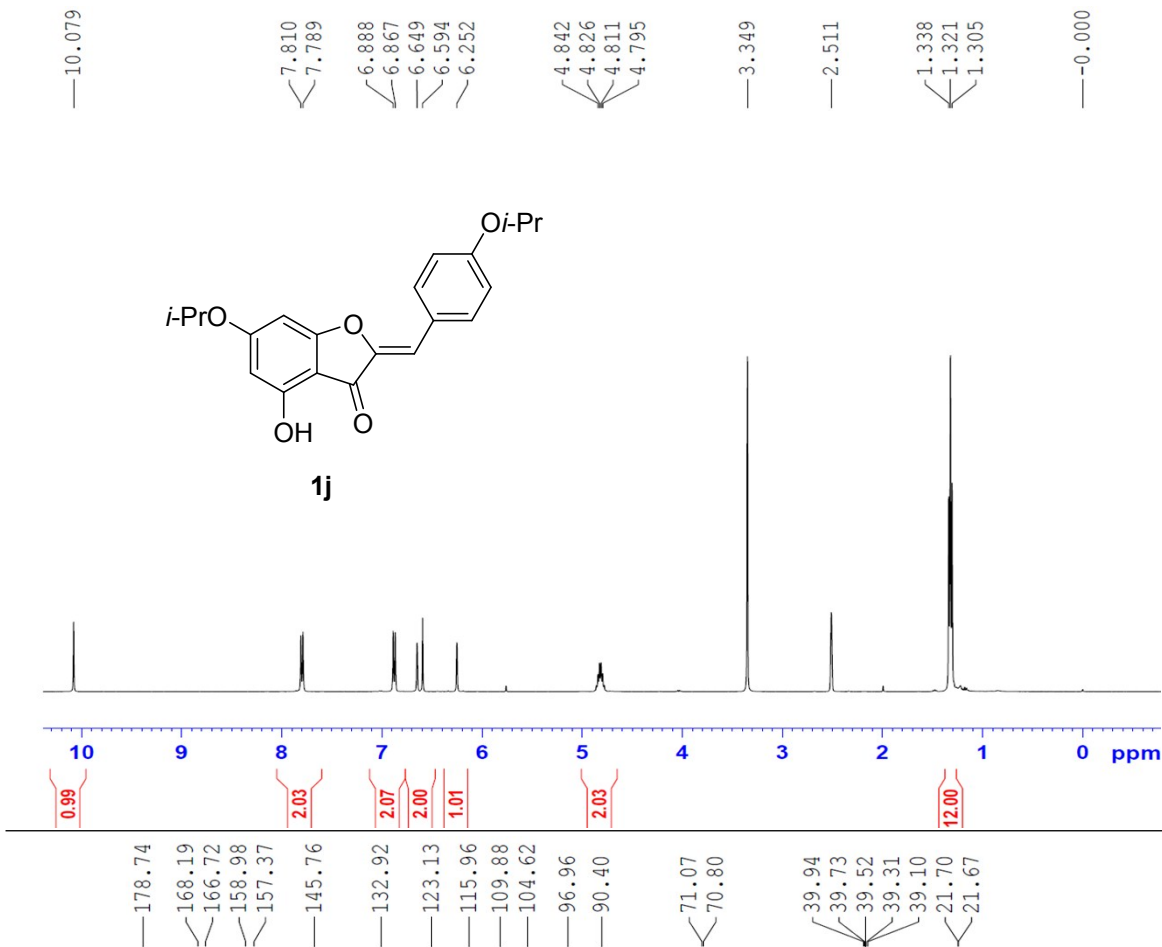
^1H NMR spectra of 5-hydroxy-7-isopropoxy-2-phenylchroman-4-one (1h) in CDCl_3



^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 5-hydroxy-7-isopropoxy-3-(4-isopropoxyphenyl)-4H-chromen-4-one (**1i**) in CDCl_3

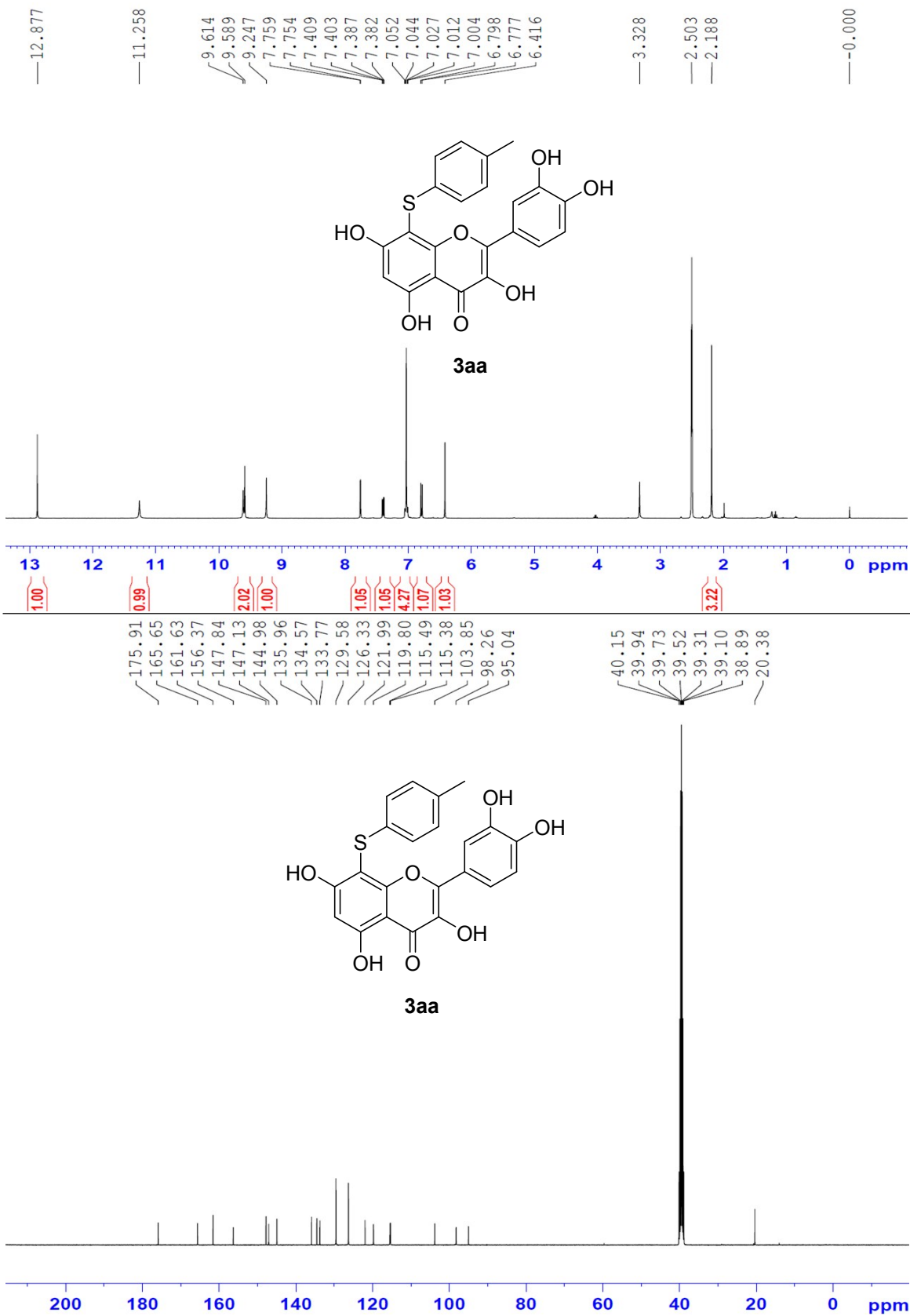


^1H and ^{13}C NMR spectra of (Z)-4-hydroxy-6-isopropoxy-2-(4-isopropoxybenzylidene)benzofuran-3(2H)-one (**1j**) in DMSO-d_6

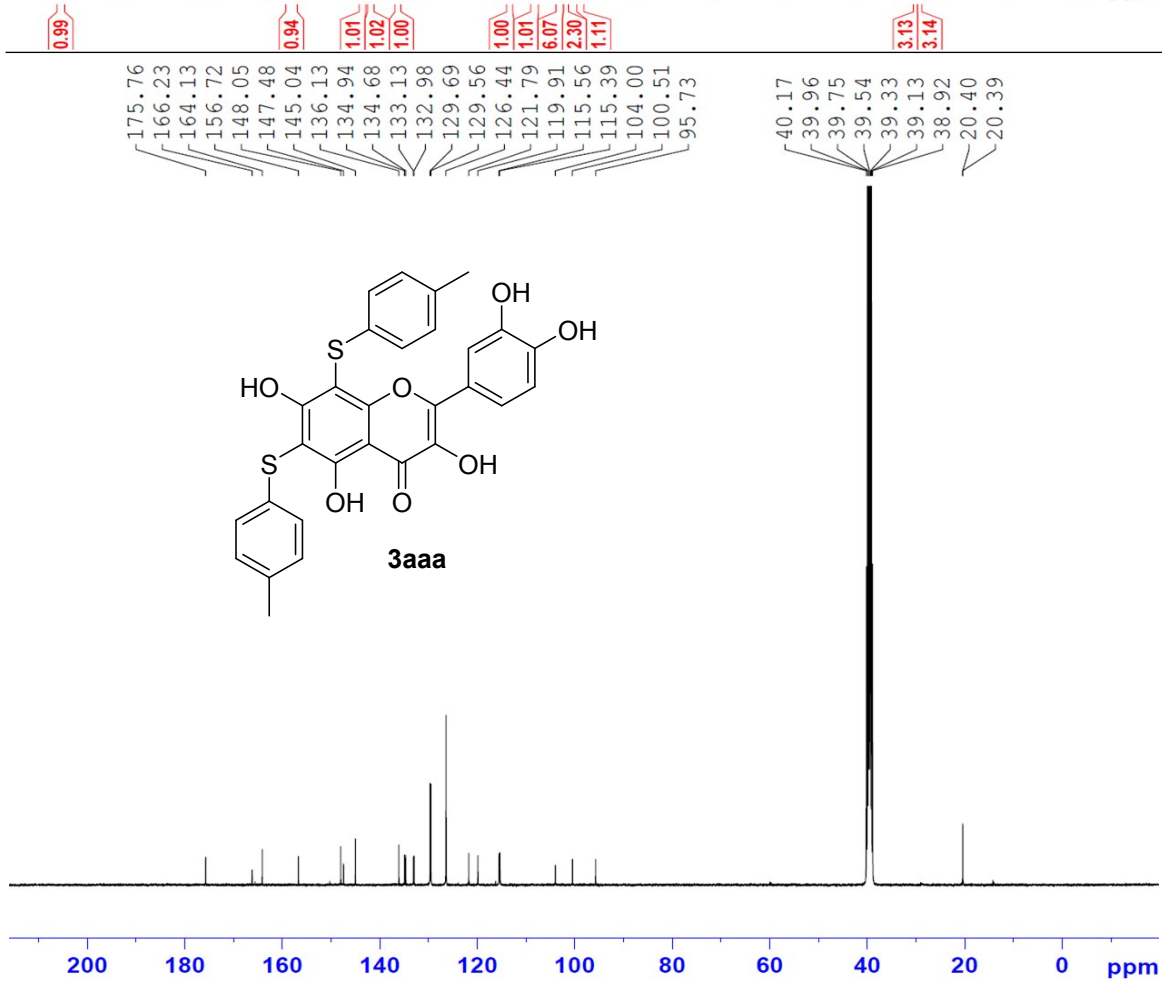
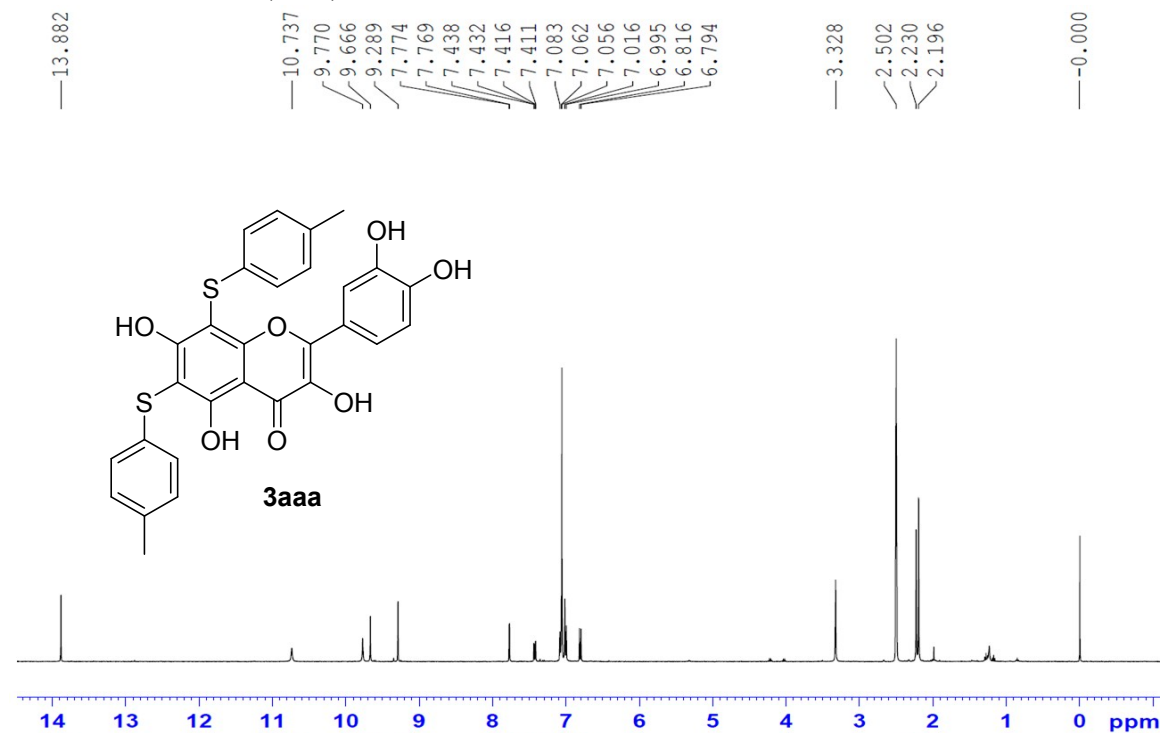


The spectrum for sulfenylation product of flavonoid isopropyl ethers

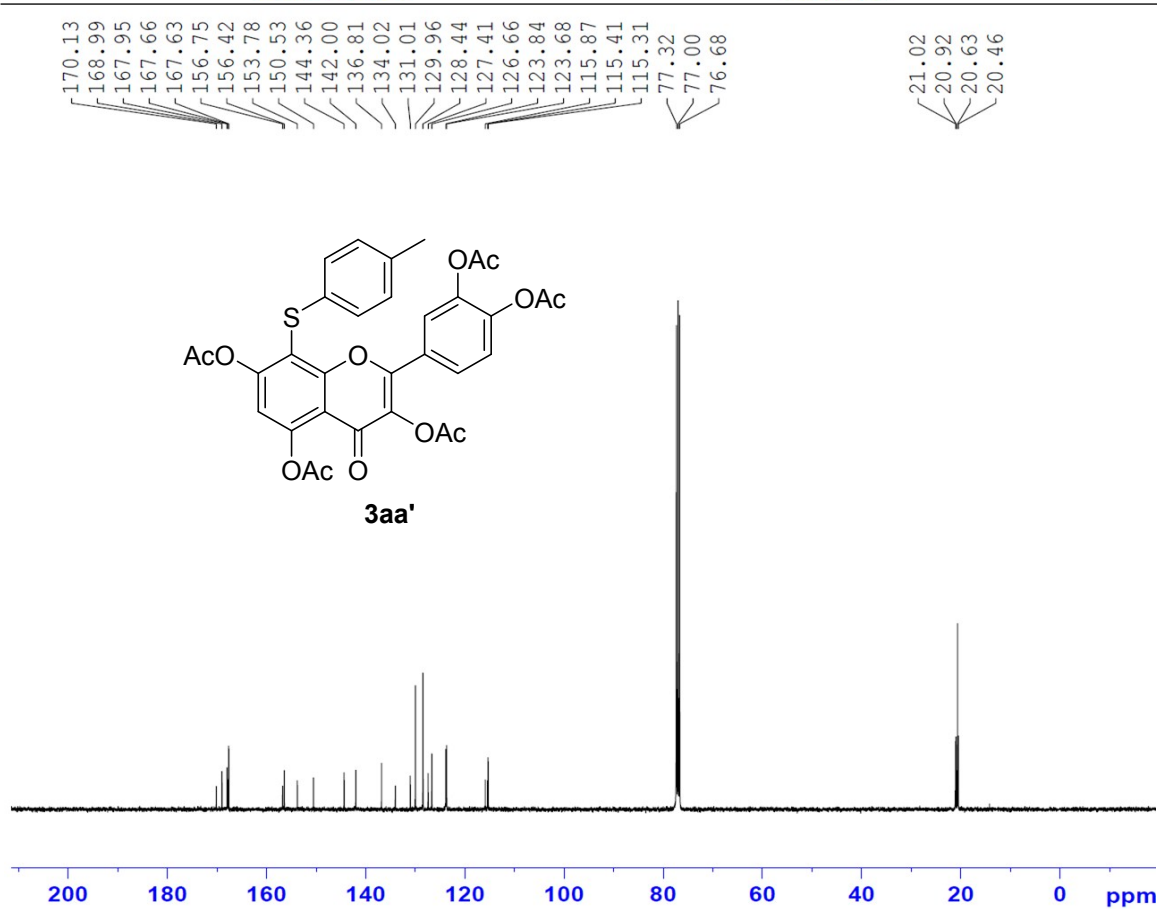
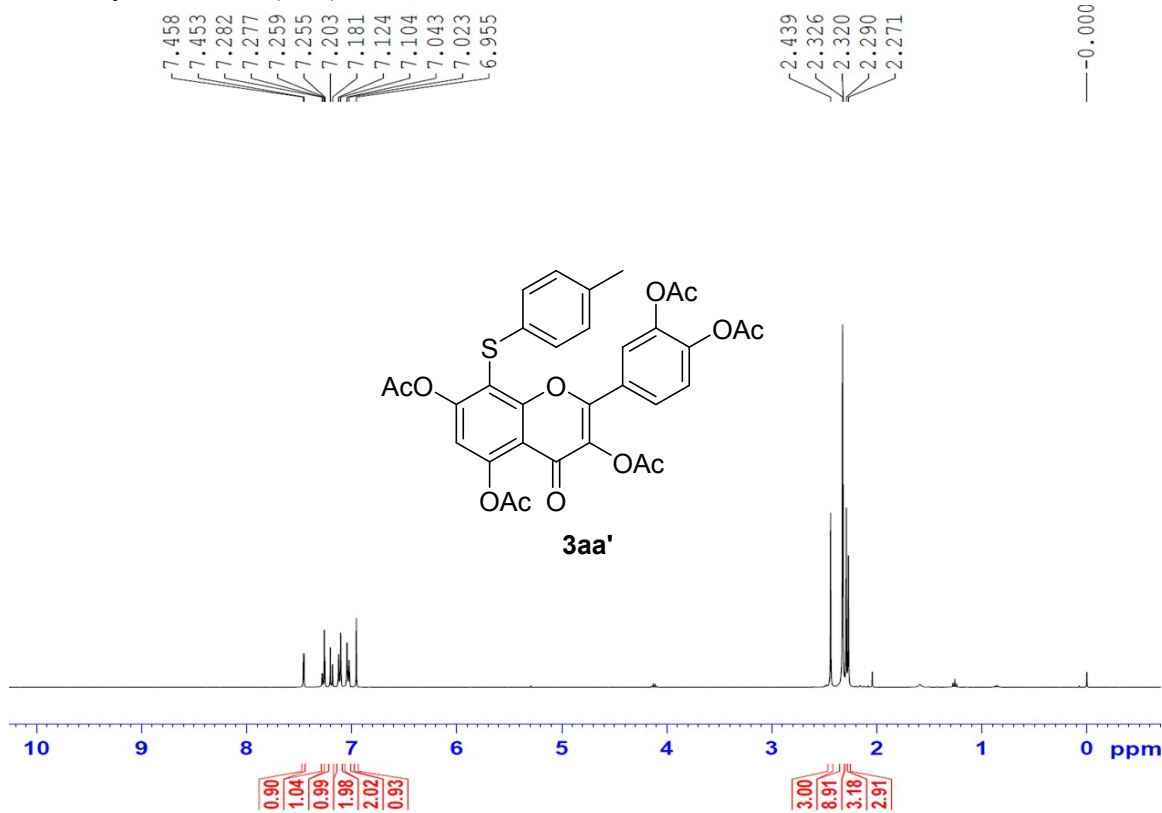
^1H and ^{13}C NMR spectra of 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-8-(p-tolylthio)-4H-chromen-4-one (3aa) in DMSO $^{\text{d6}}$



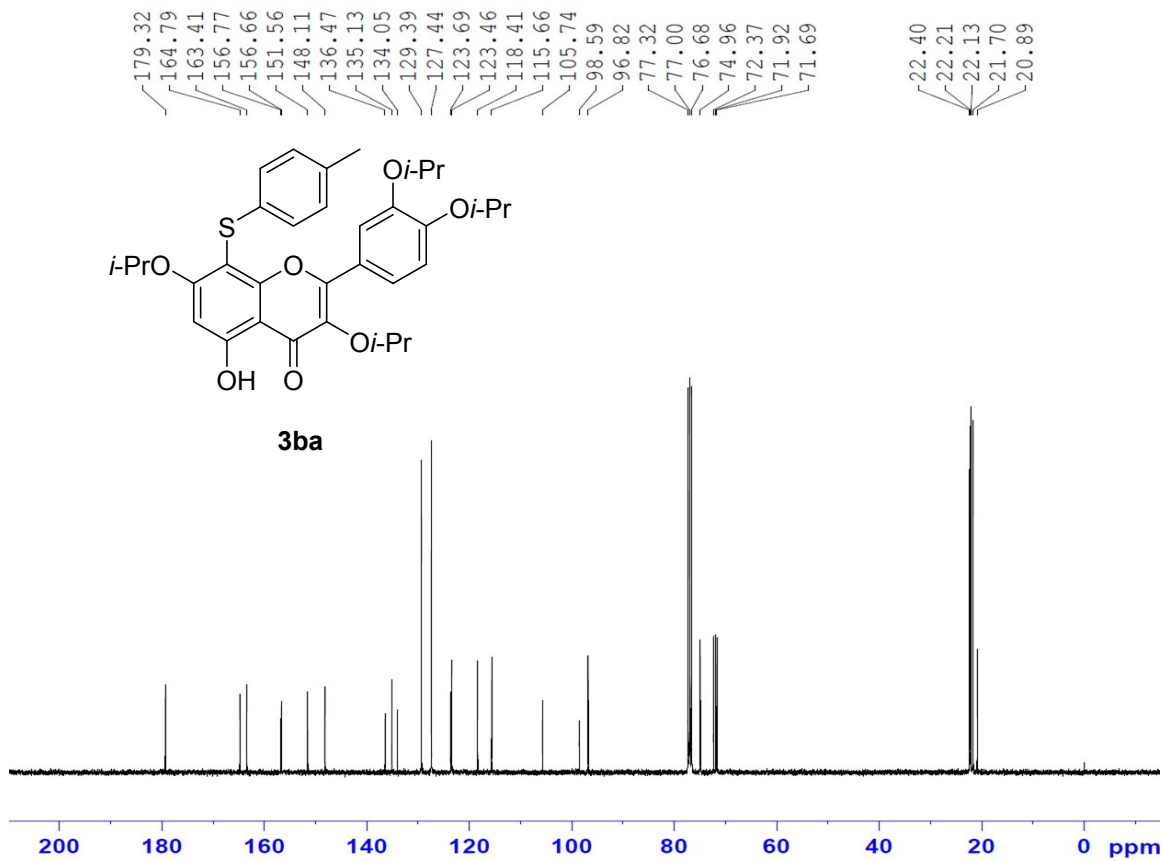
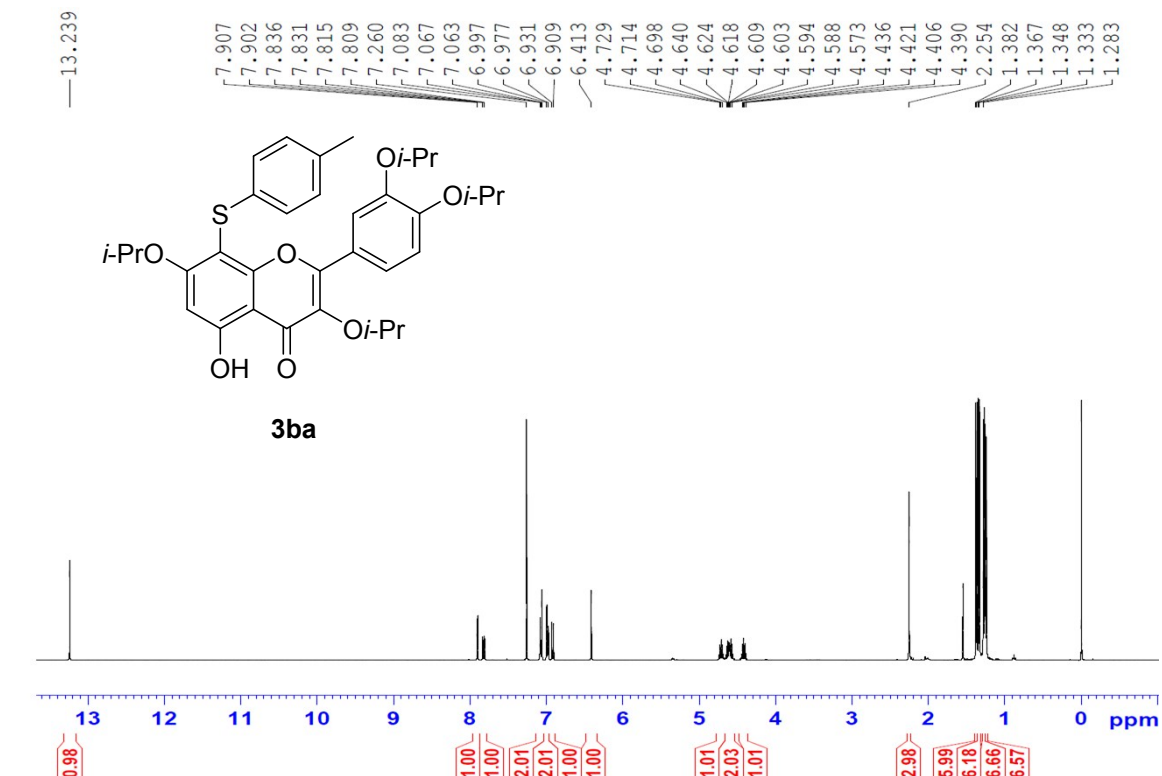
^1H and ^{13}C NMR spectra of 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-6,8-bis(p-tolylthio)-4H-chromen-4-one (3aaa) in DMSO-d_6



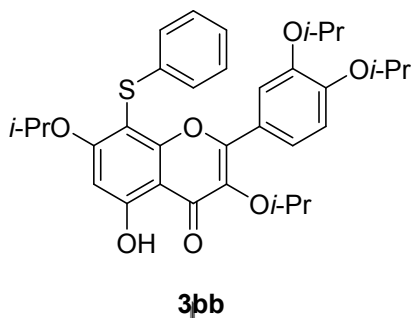
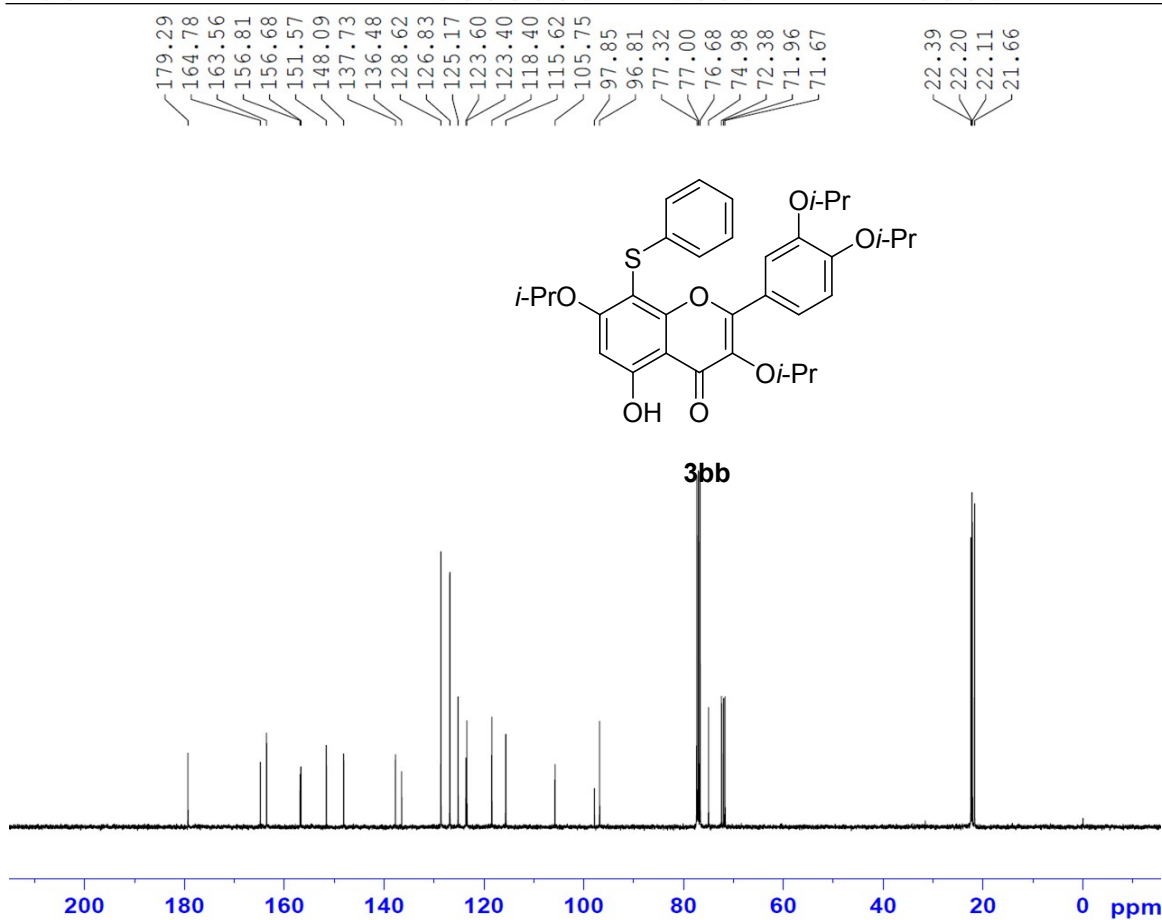
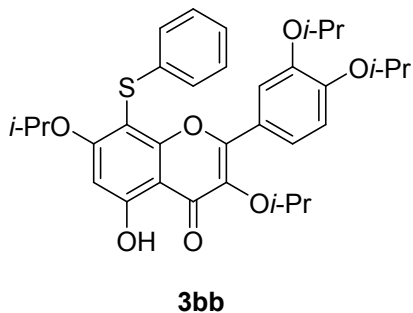
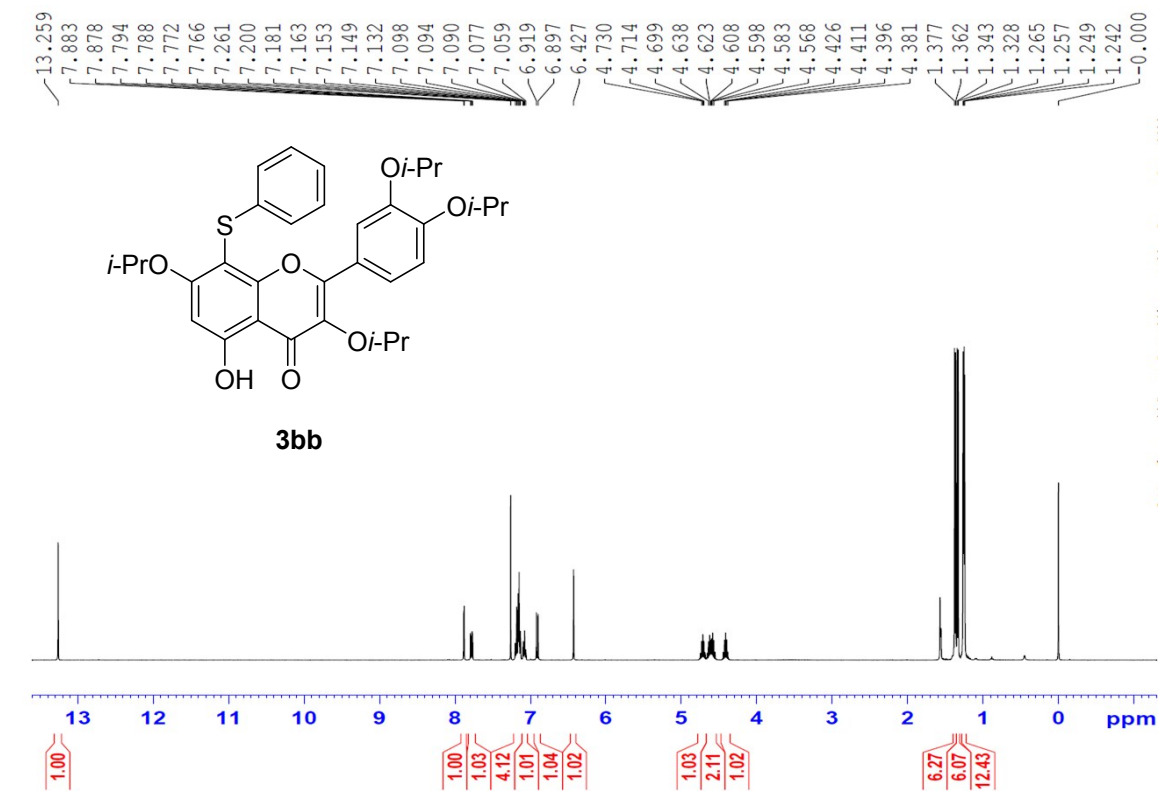
^1H and ^{13}C NMR spectra of 2-(3,4-diacetoxyphenyl)-4-oxo-8-(p-tolylthio)-4H-chromene-3,5,7-triyl triacetate (**3aa'**) in CDCl_3



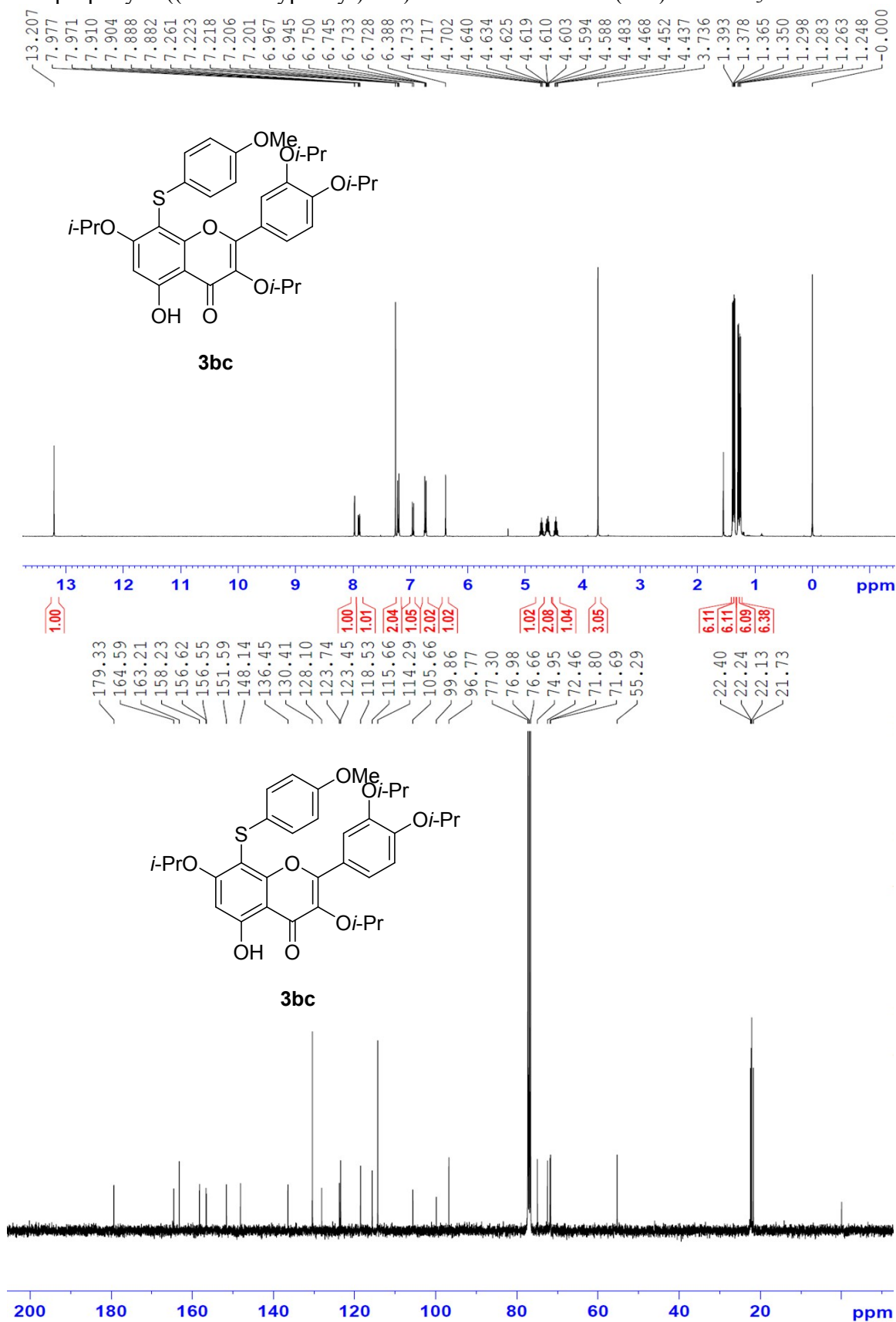
^1H and ^{13}C NMR spectra of 2-(3,4-diisopropoxyphenyl)-5-hydroxy-3,7-diisopropoxy-8-(p-tolylthio)-4H-chromen-4-one (3ba) in CDCl_3



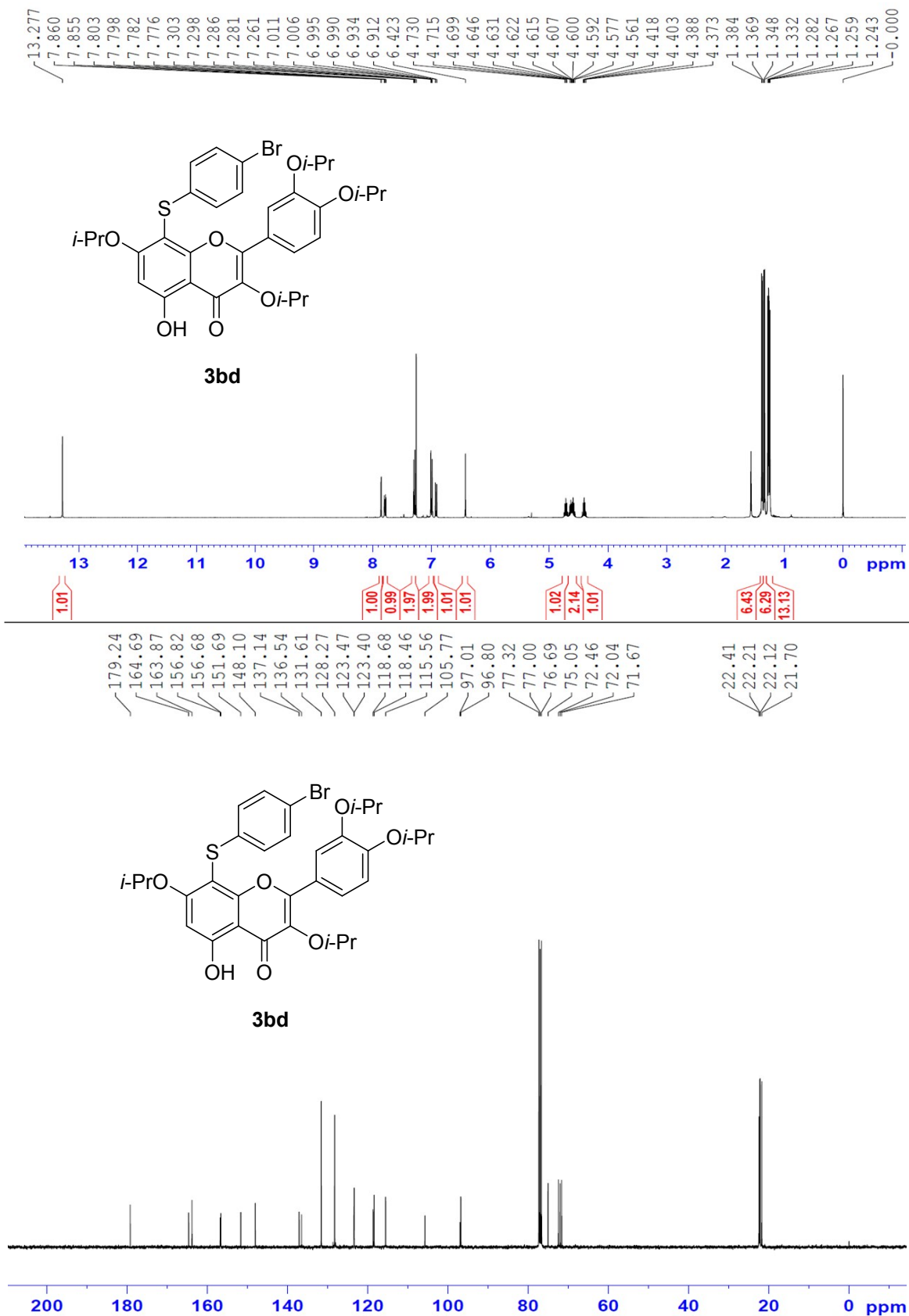
^1H and ^{13}C NMR spectra of 2-(3,4-diisopropoxyphenyl)-5-hydroxy-3,7-diisopropoxy-8-(phenylthio)-4H-chromen-4-one (**3bb**) in CDCl_3



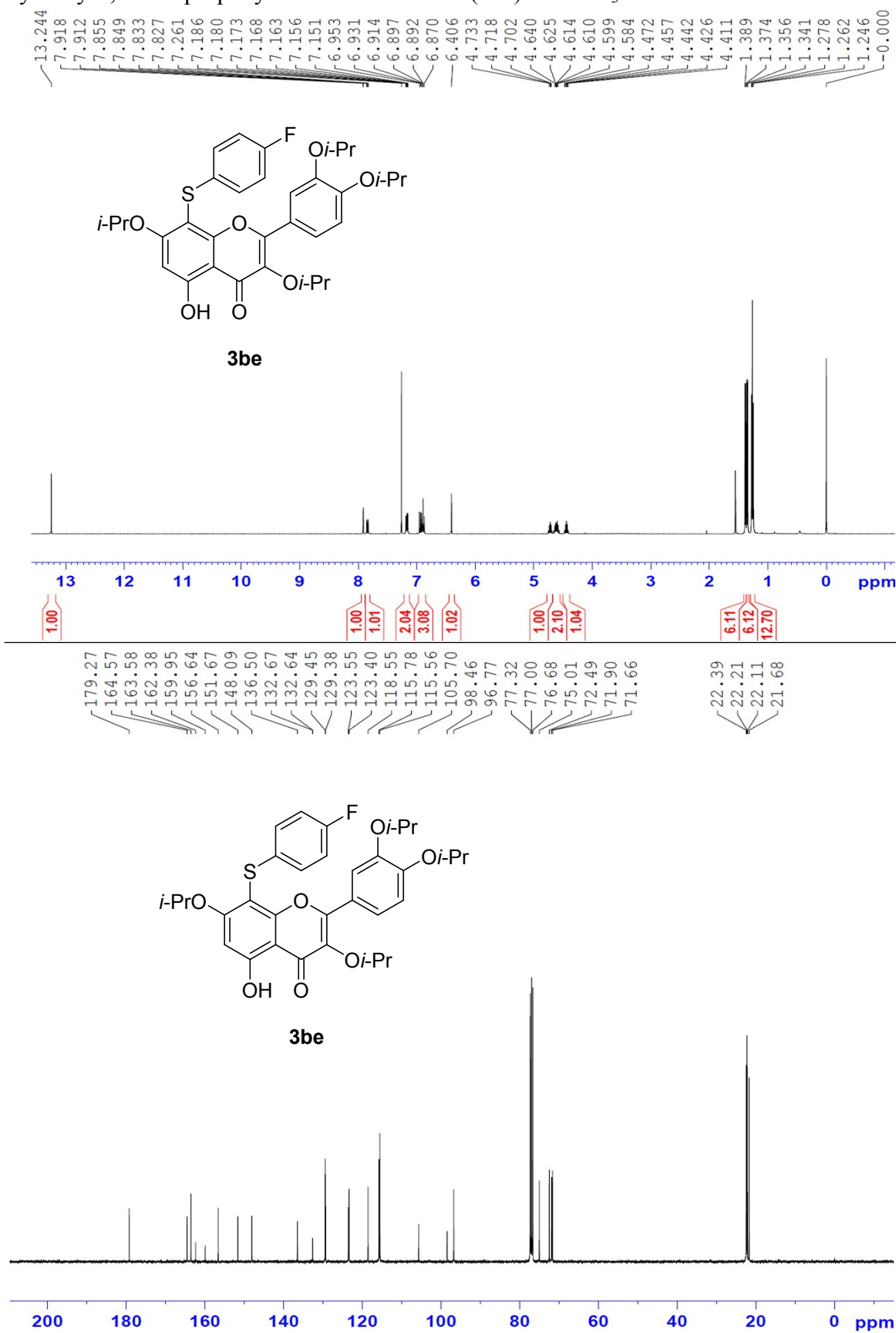
^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 2-(3,4-diisopropoxyphenyl)-5-hydroxy-3,7-diisopropoxy-8-((4-methoxyphenyl)thio)-4H-chromen-4-one (3bc) in CDCl_3



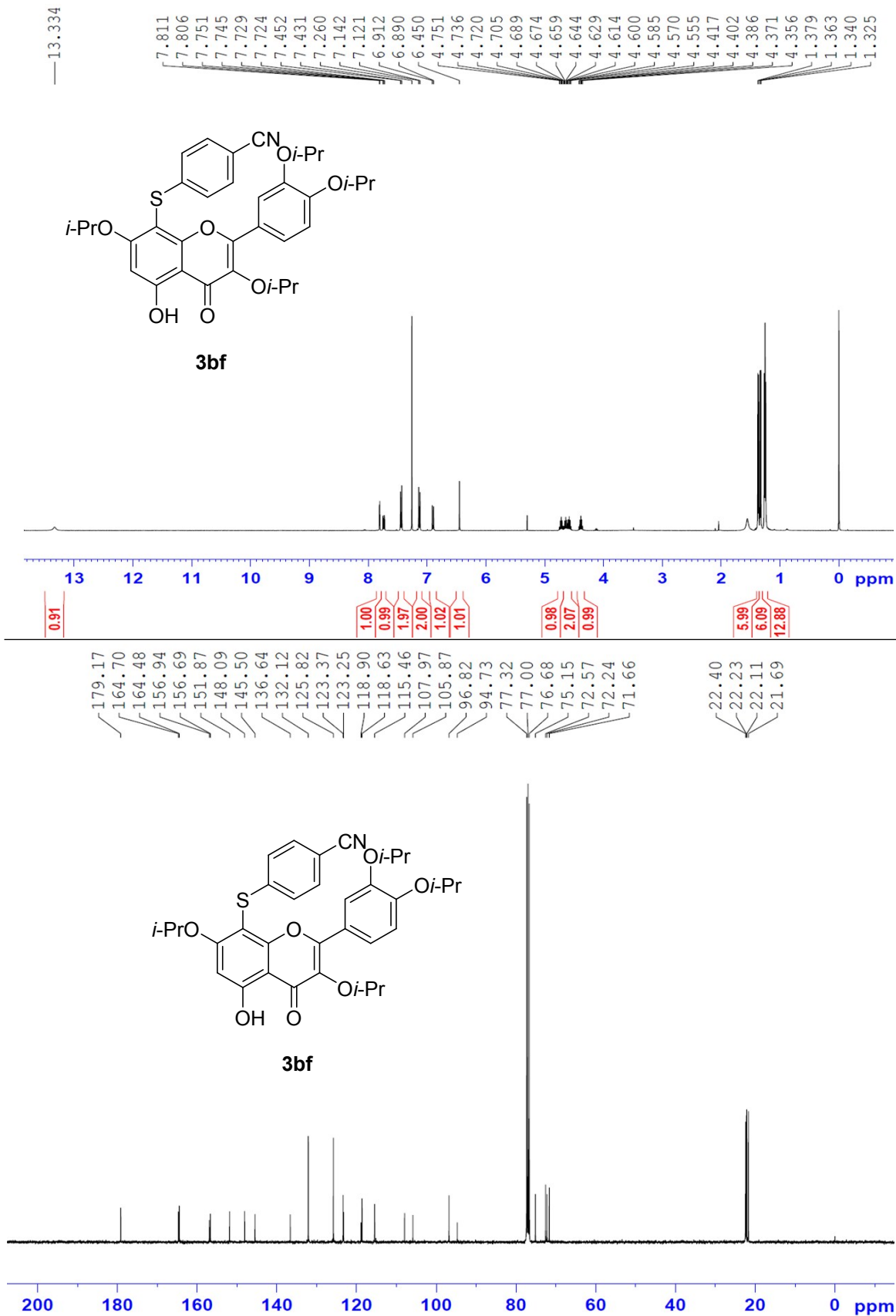
^1H and ^{13}C NMR spectra of 8-((4-bromophenyl)thio)-2-(3,4-diisopropoxyphenyl)-5-hydroxy-3,7-diisopropoxy-4H-chromen-4-one (3bd) in CDCl_3



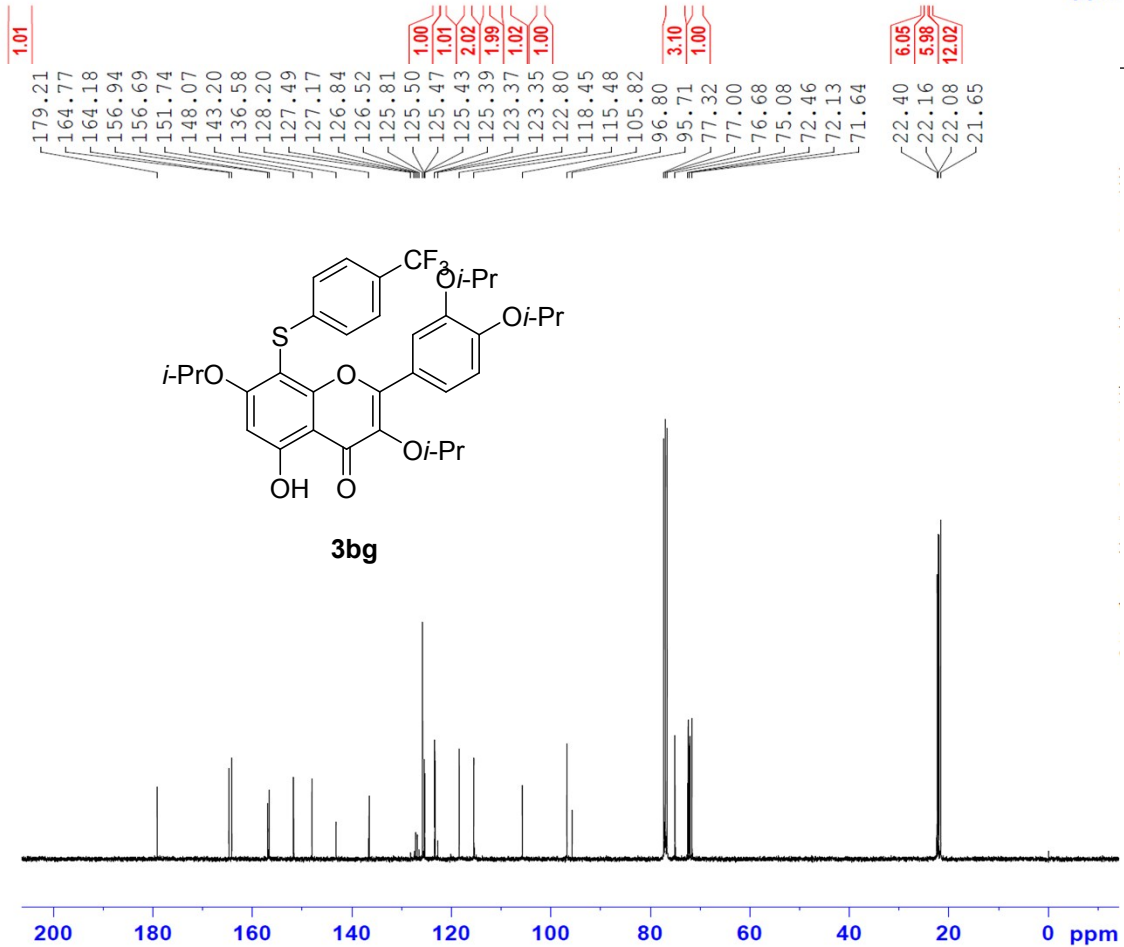
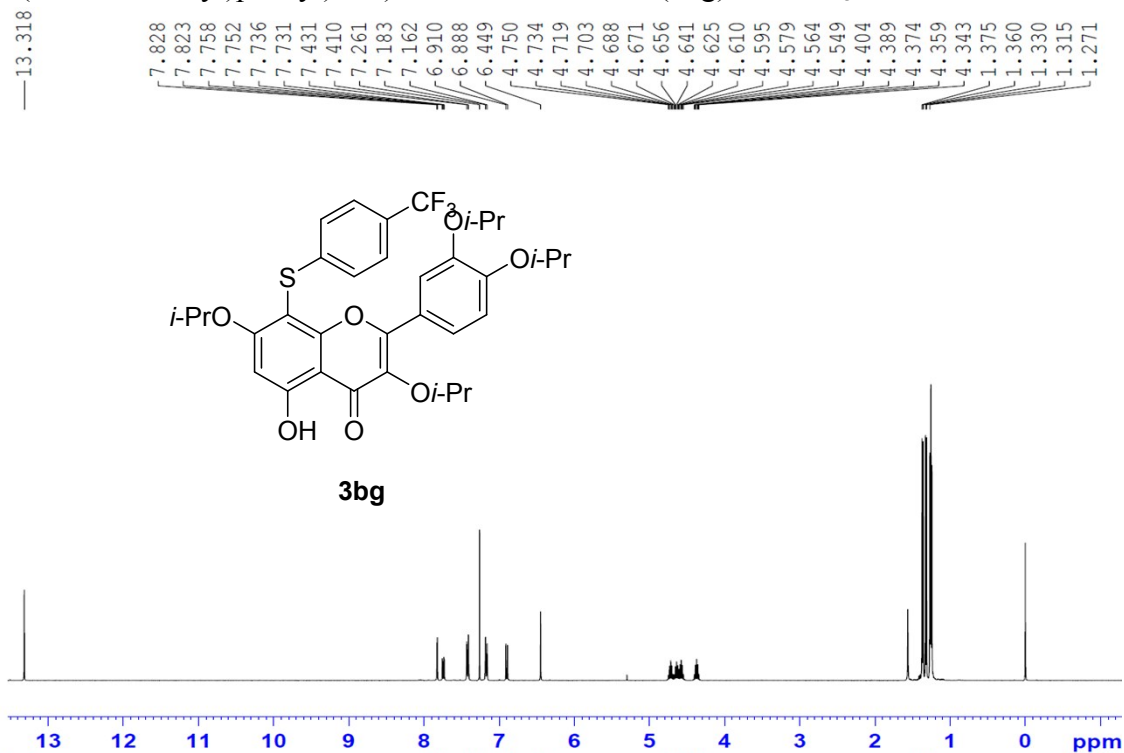
^1H and ^{13}C NMR spectra of 2-(3,4-diisopropoxyphenyl)-8-((4-fluorophenyl)thio)-5-hydroxy-3,7-diisopropoxy-4H-chromen-4-one (3be) in CDCl_3



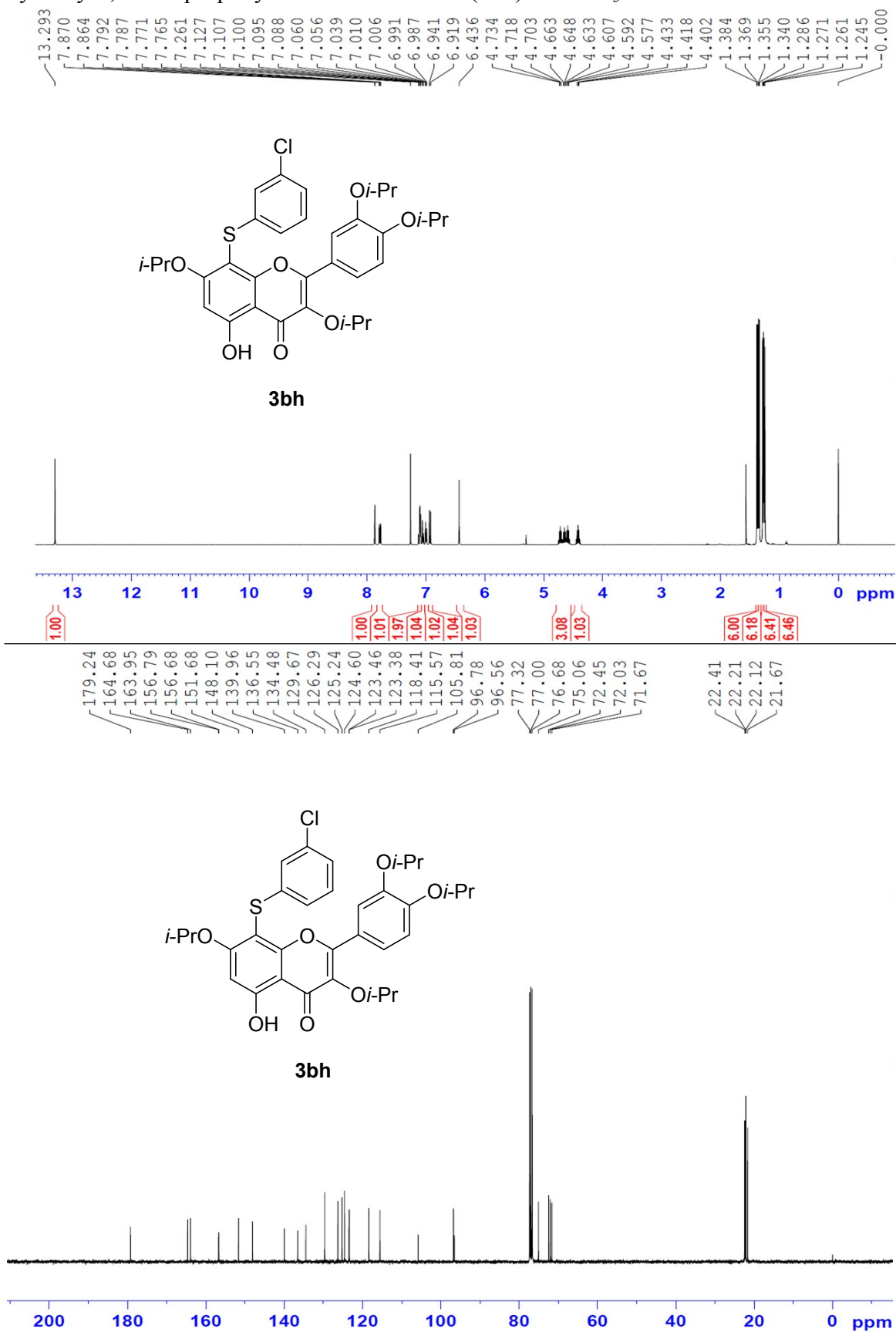
^1H and ^{13}C NMR spectra of 4-((2-(3,4-diisopropoxyphenyl)-5-hydroxy-3,7-diisopropoxy-4-oxo-4H-chromen-8-yl)thio)benzonitrile (**3bf**) in CDCl_3



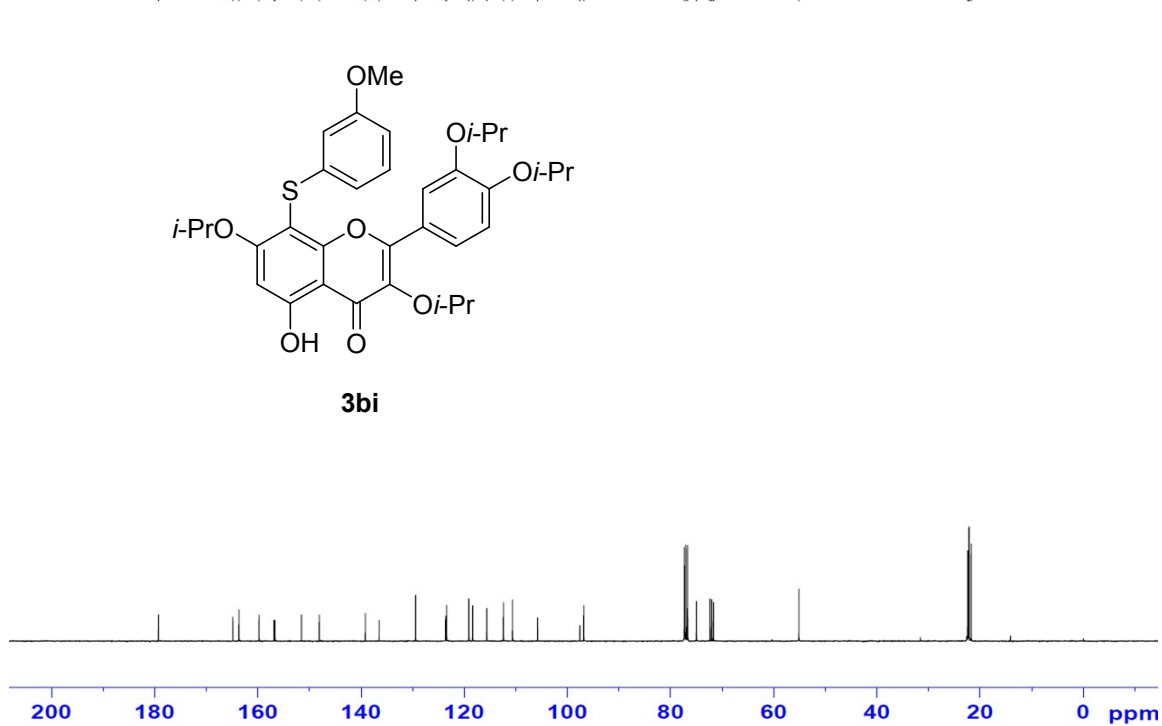
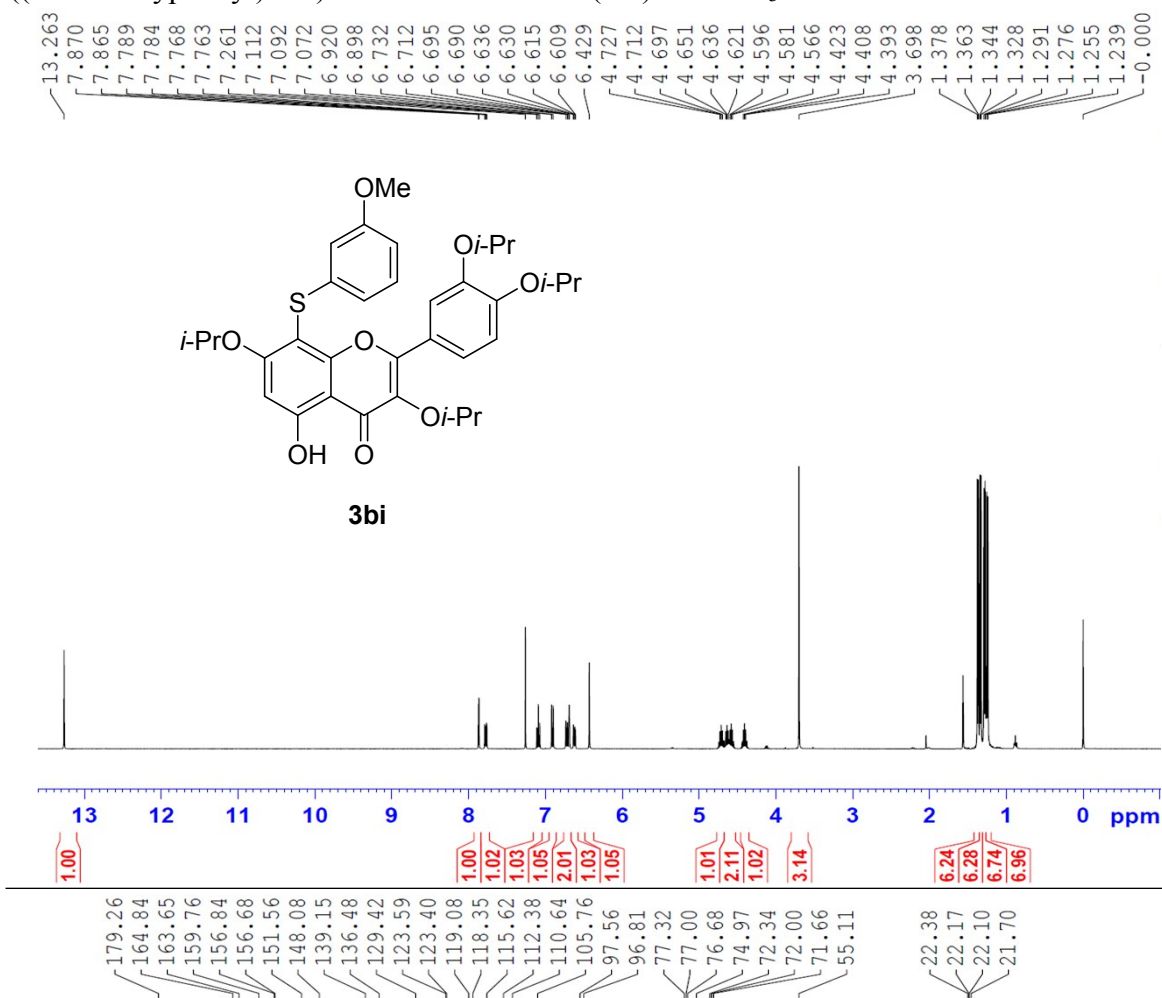
^1H and ^{13}C NMR spectra of 2-(3,4-diisopropoxyphenyl)-5-hydroxy-3,7-diisopropoxy-8-((4-(trifluoromethyl)phenyl)thio)-4H-chromen-4-one (3bg) in CDCl_3



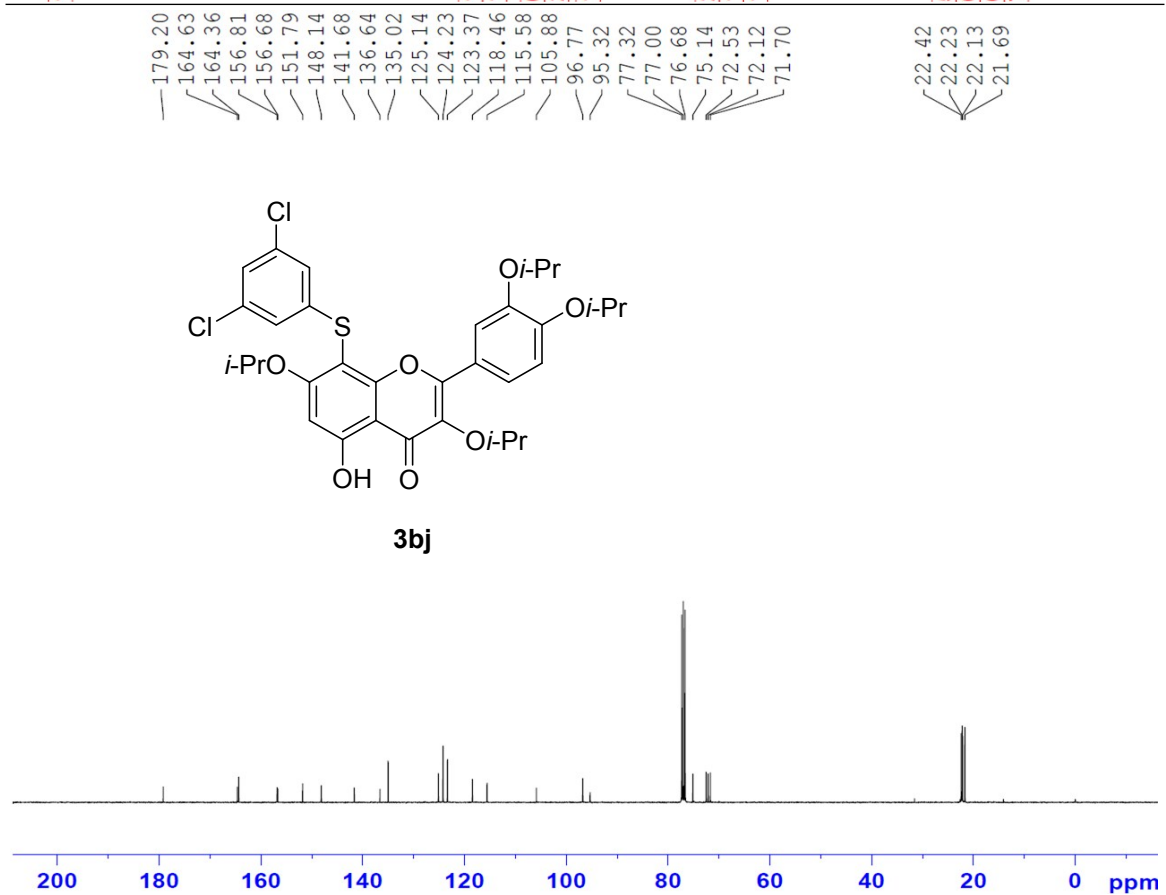
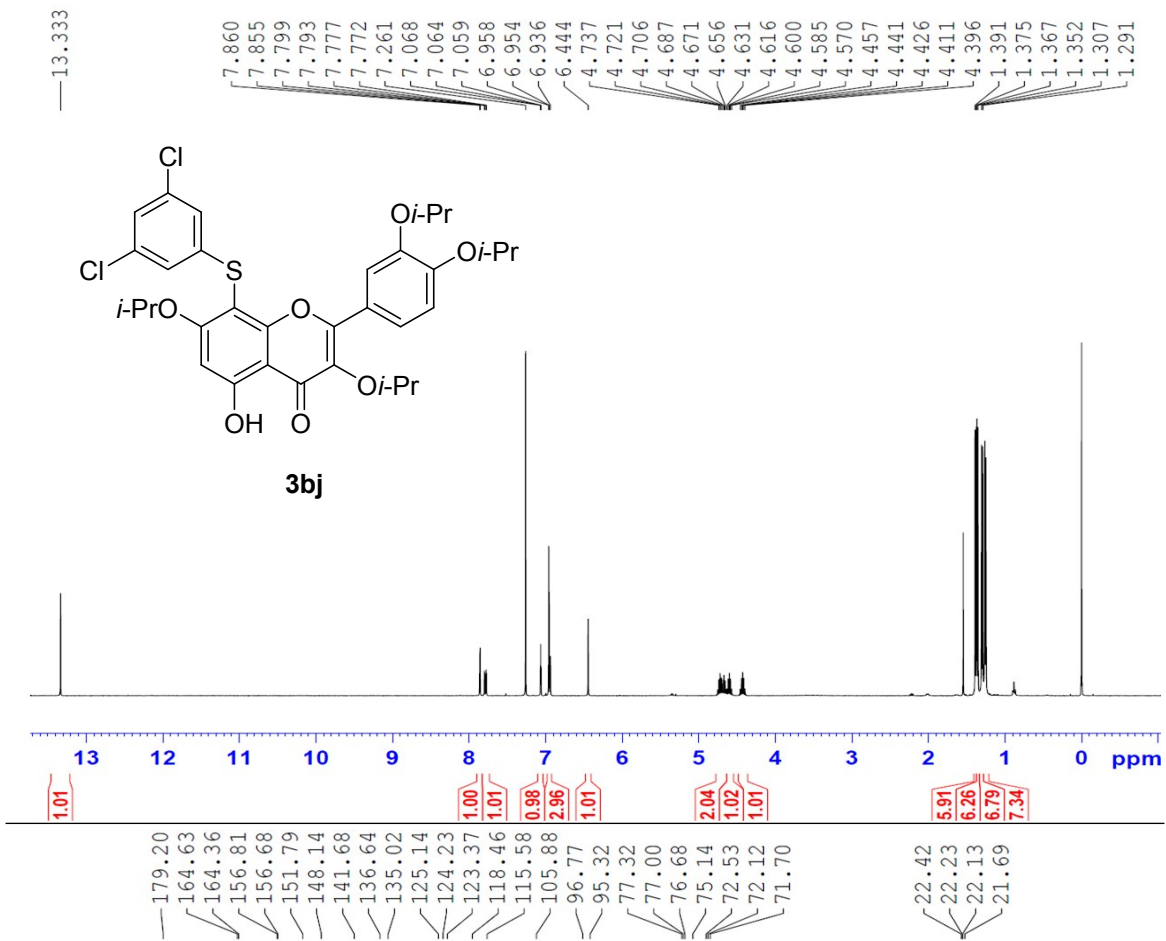
¹H and ¹³C NMR spectra of 8-((3-chlorophenyl)thio)-2-(3,4-diisopropoxyphenyl)-5-hydroxy-3,7-diisopropoxy-4H-chromen-4-one (3bh) in CDCl₃



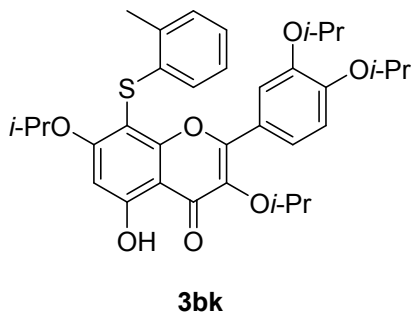
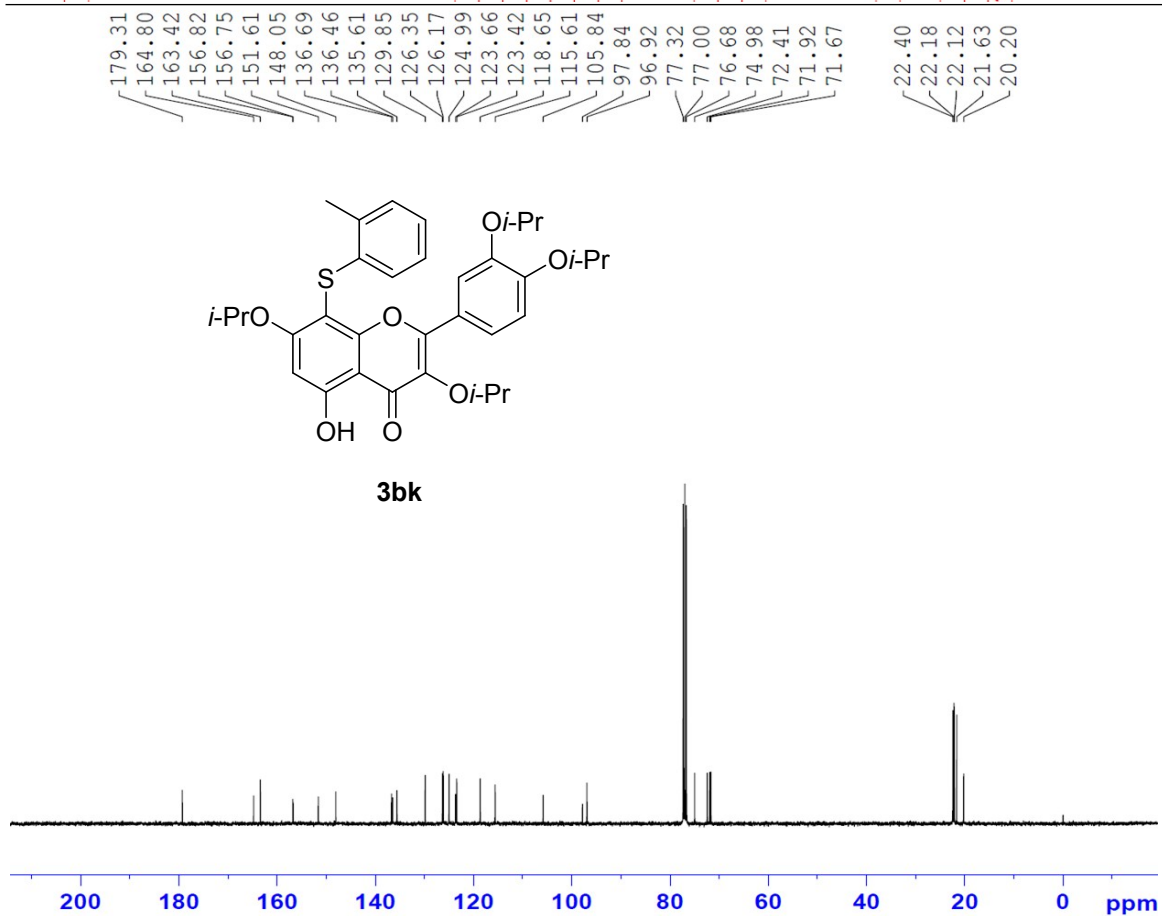
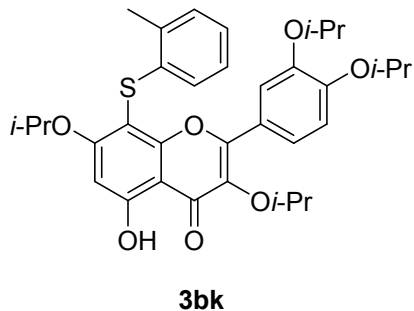
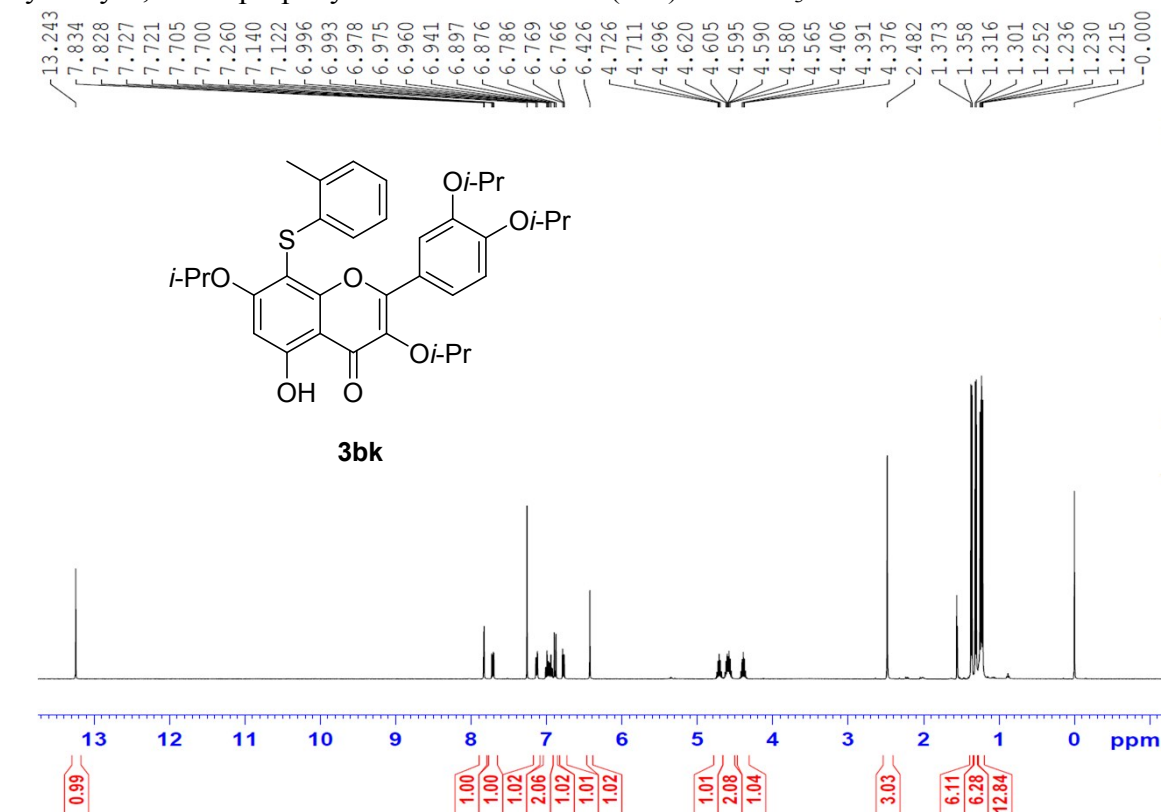
^1H and ^{13}C NMR spectra of 2-(3,4-diisopropoxyphenyl)-5-hydroxy-3,7-diisopropoxy-8-((3-methoxyphenyl)thio)-4H-chromen-4-one (3bi) in CDCl_3



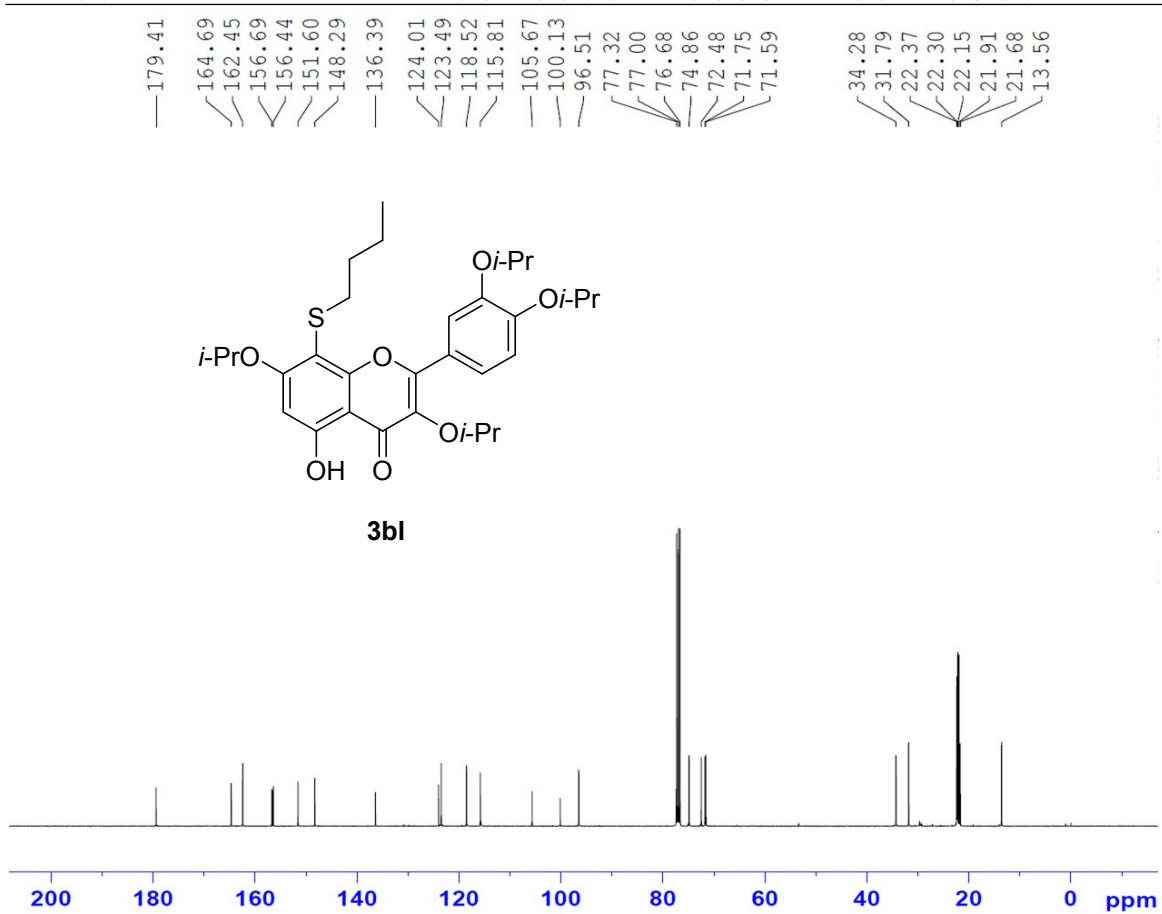
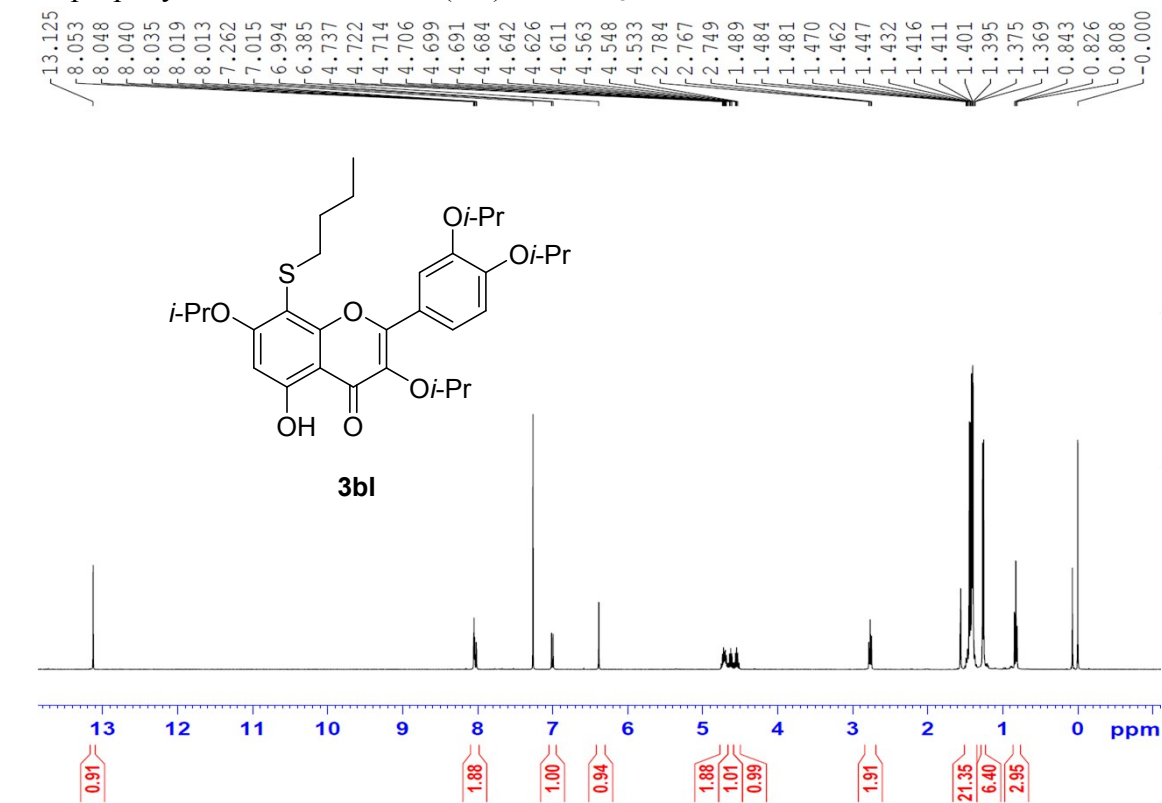
¹H and ¹³C NMR spectra of 8-((3,5-dichlorophenyl)thio)-2-(3,4-diisopropoxyphenyl)-5-hydroxy-3,7-diisopropoxy-4H-chromen-4-one (3bj) in CDCl₃



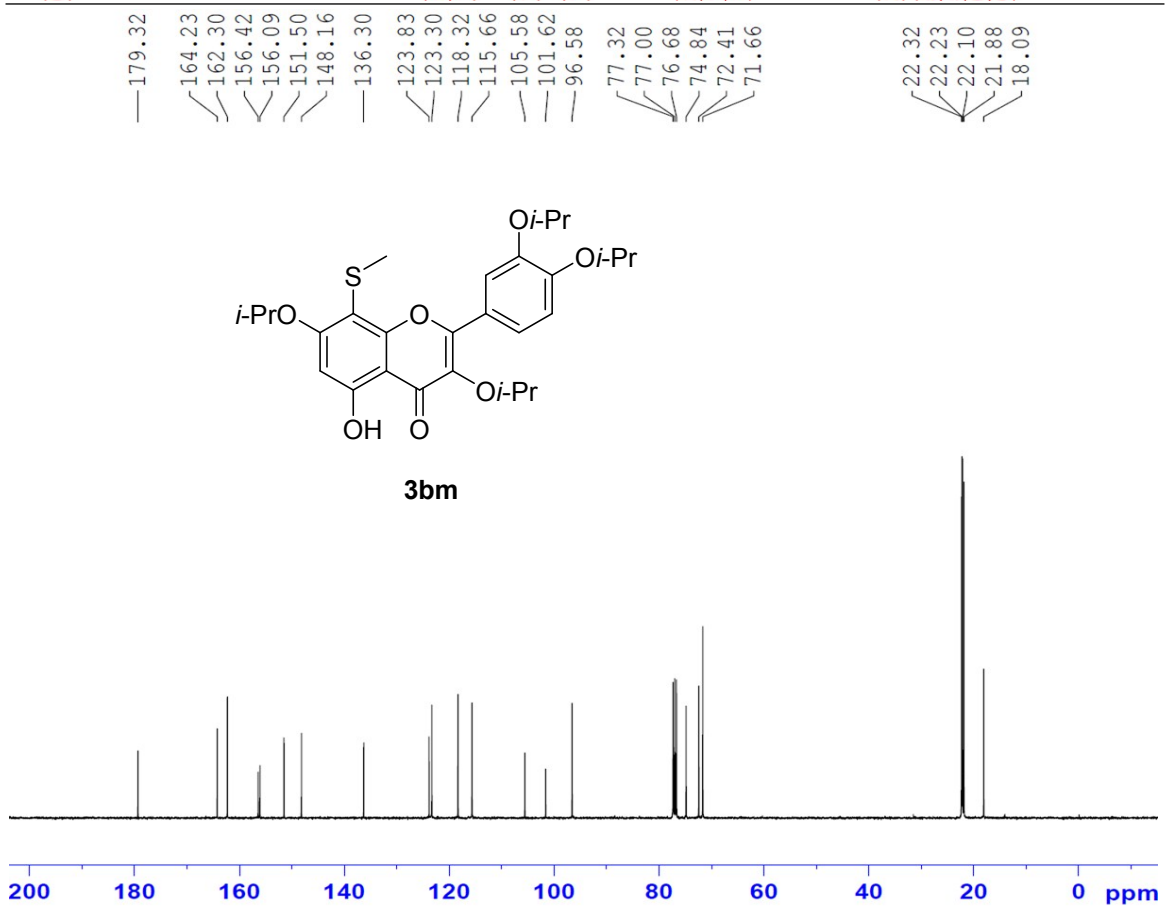
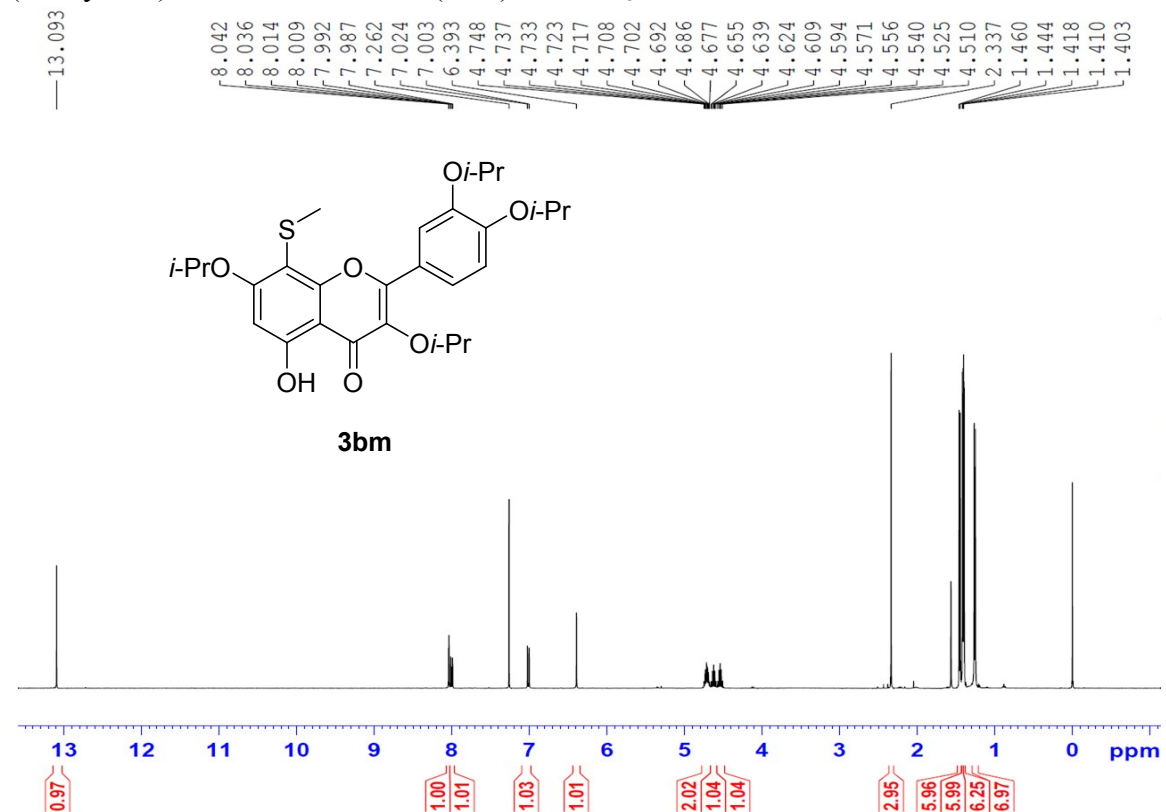
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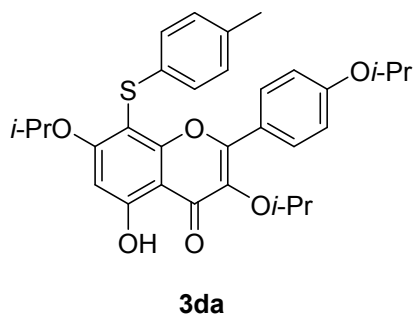
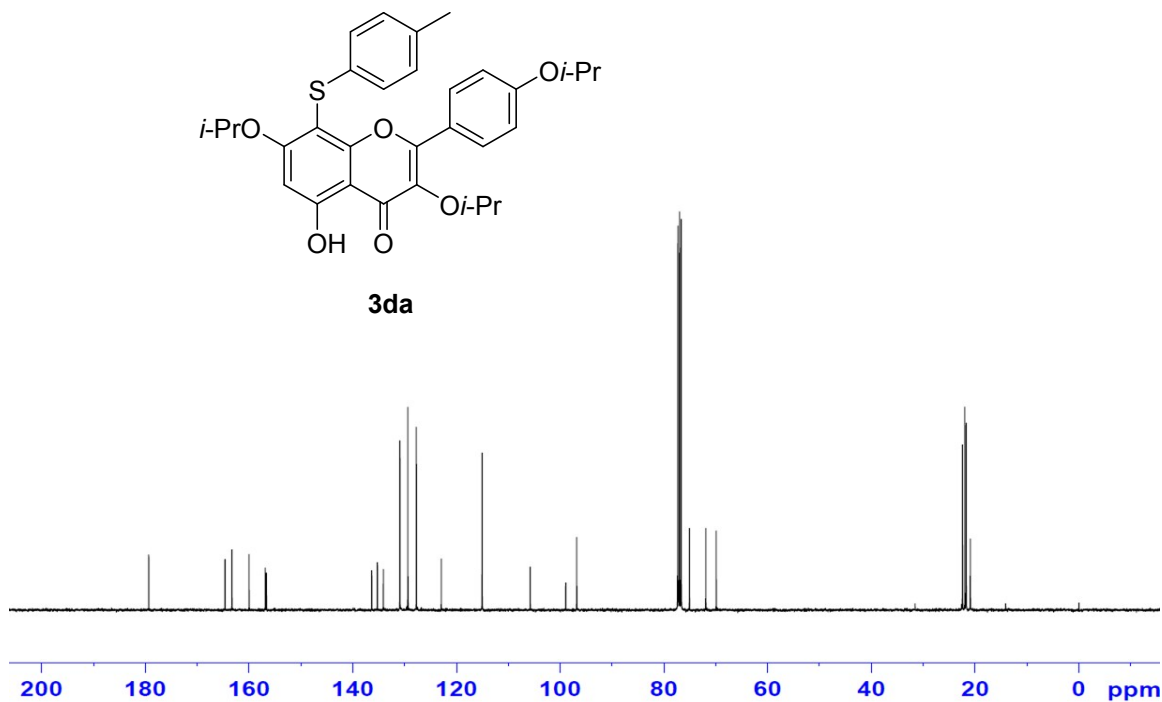
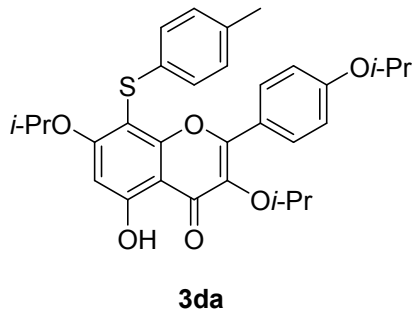
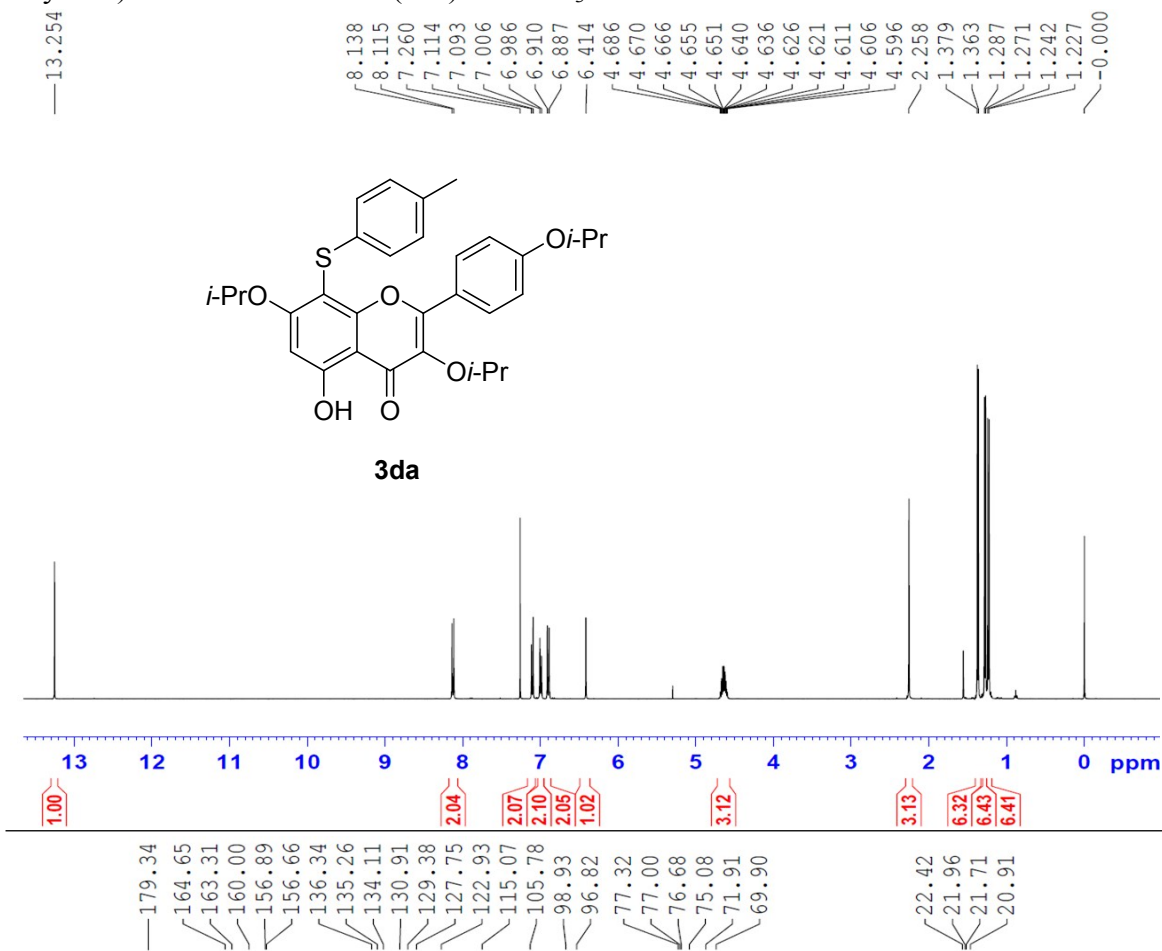
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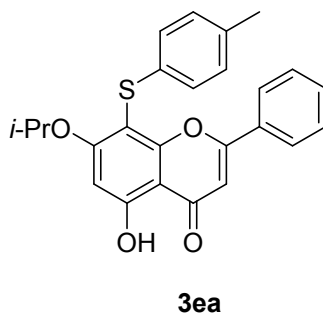
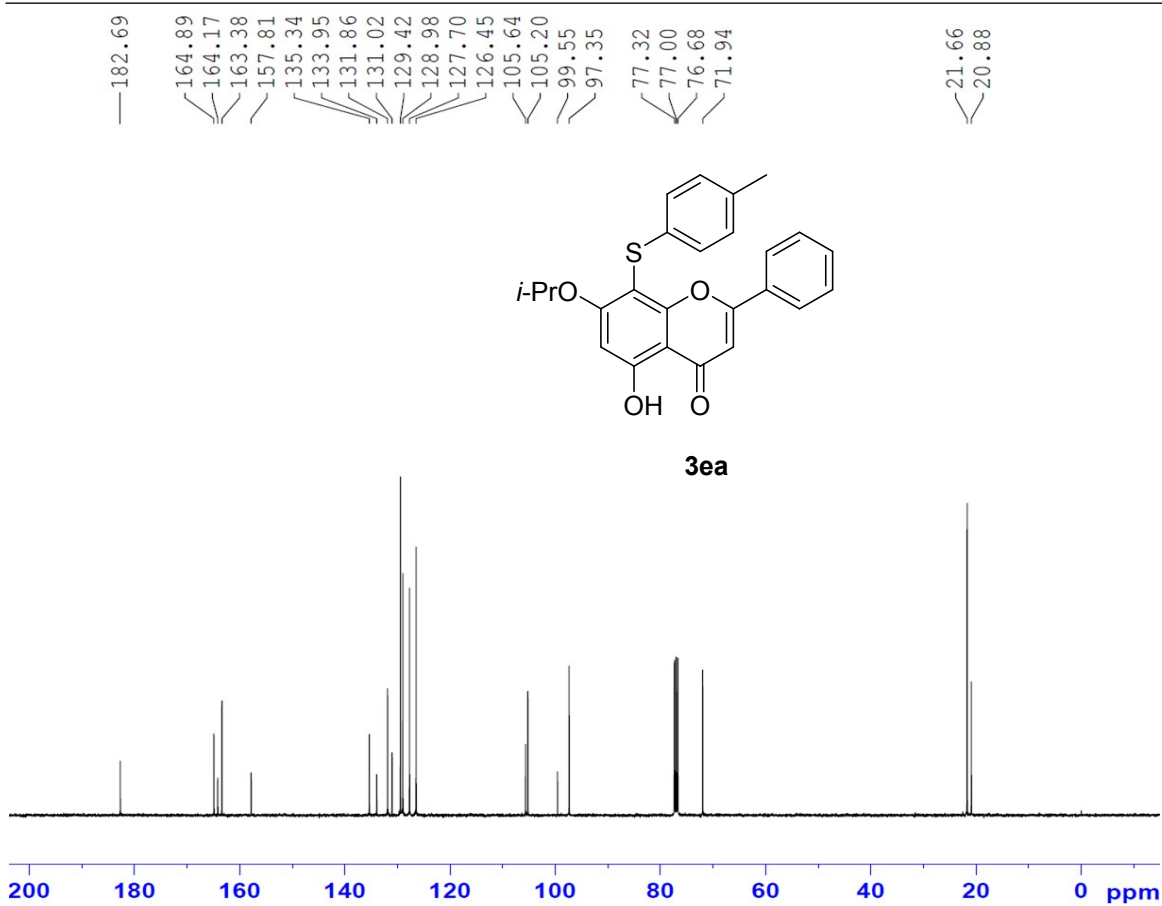
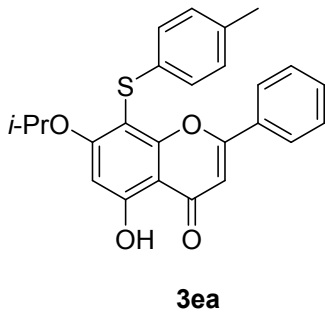
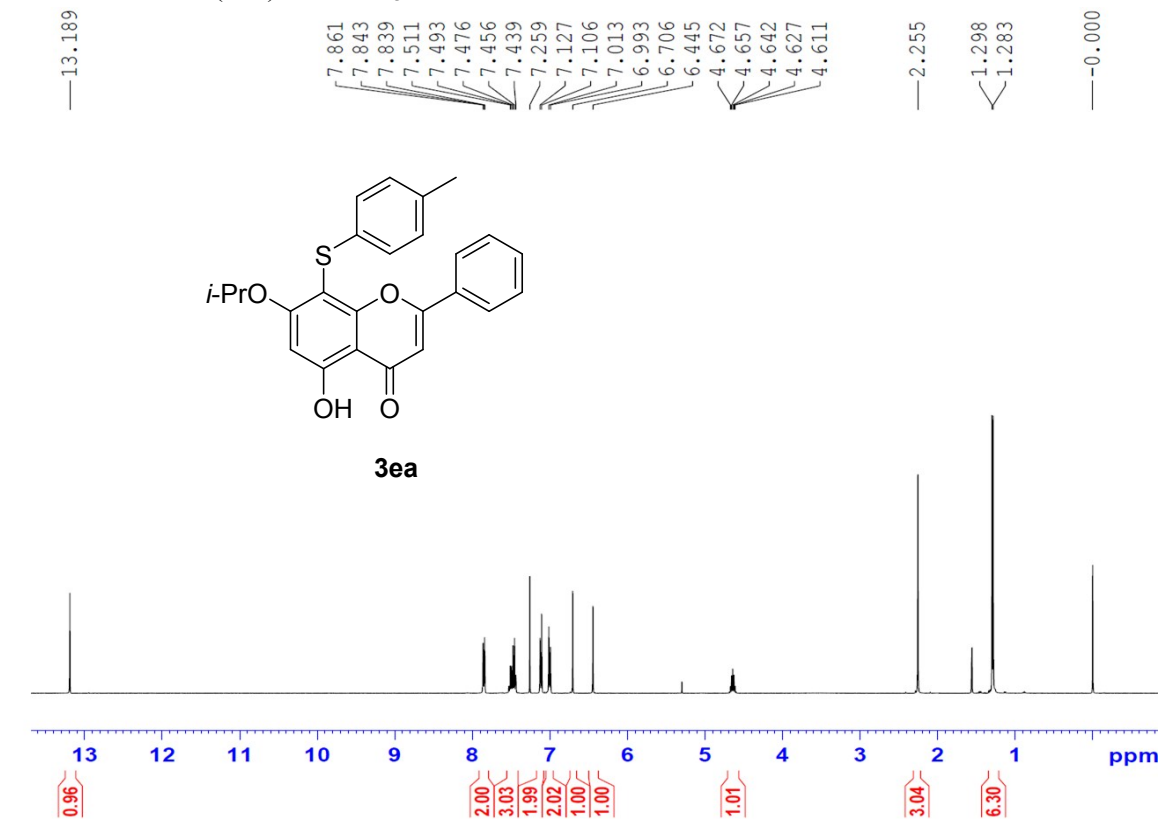
^1H and ^{13}C NMR spectra of 2-(3,4-diisopropoxyphenyl)-5-hydroxy-3,7-diisopropoxy-8-(methylthio)-4H-chromen-4-one (**3bm**) in CDCl_3



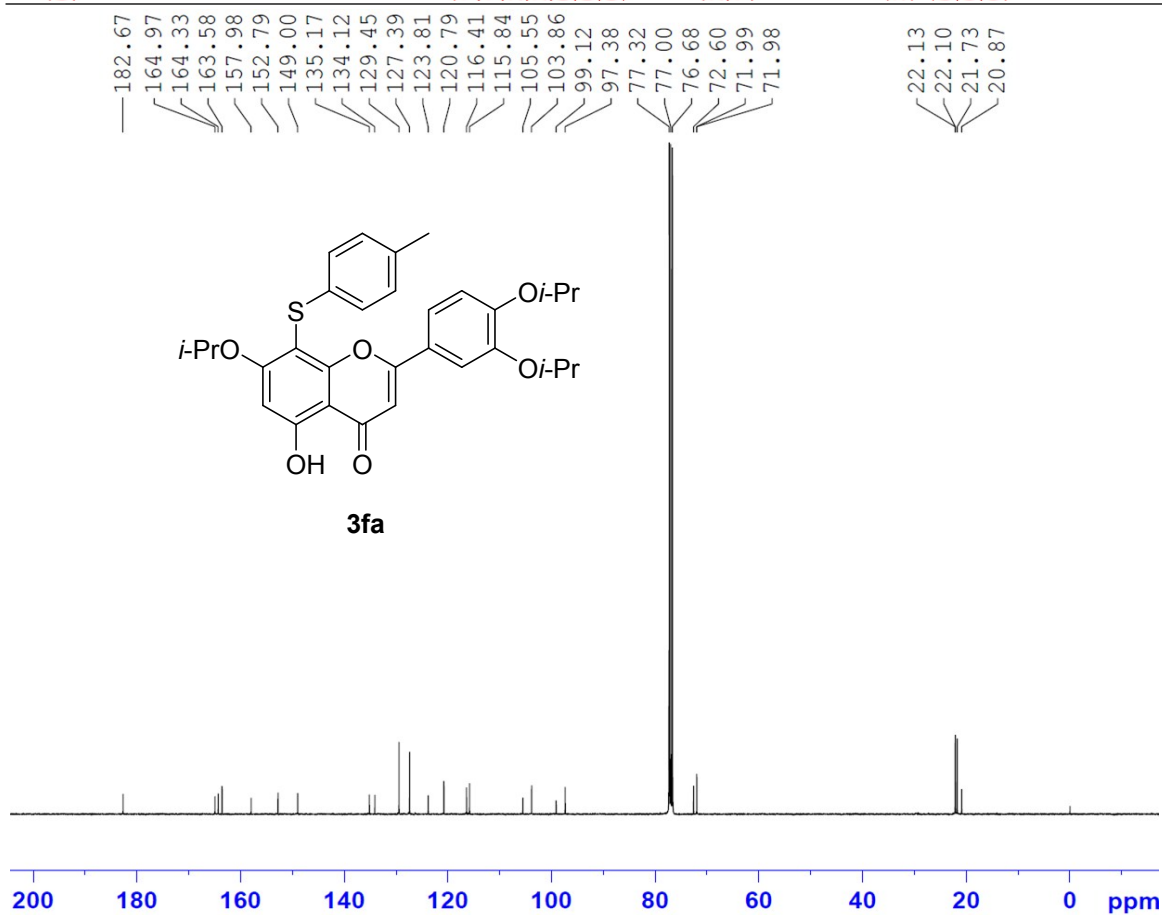
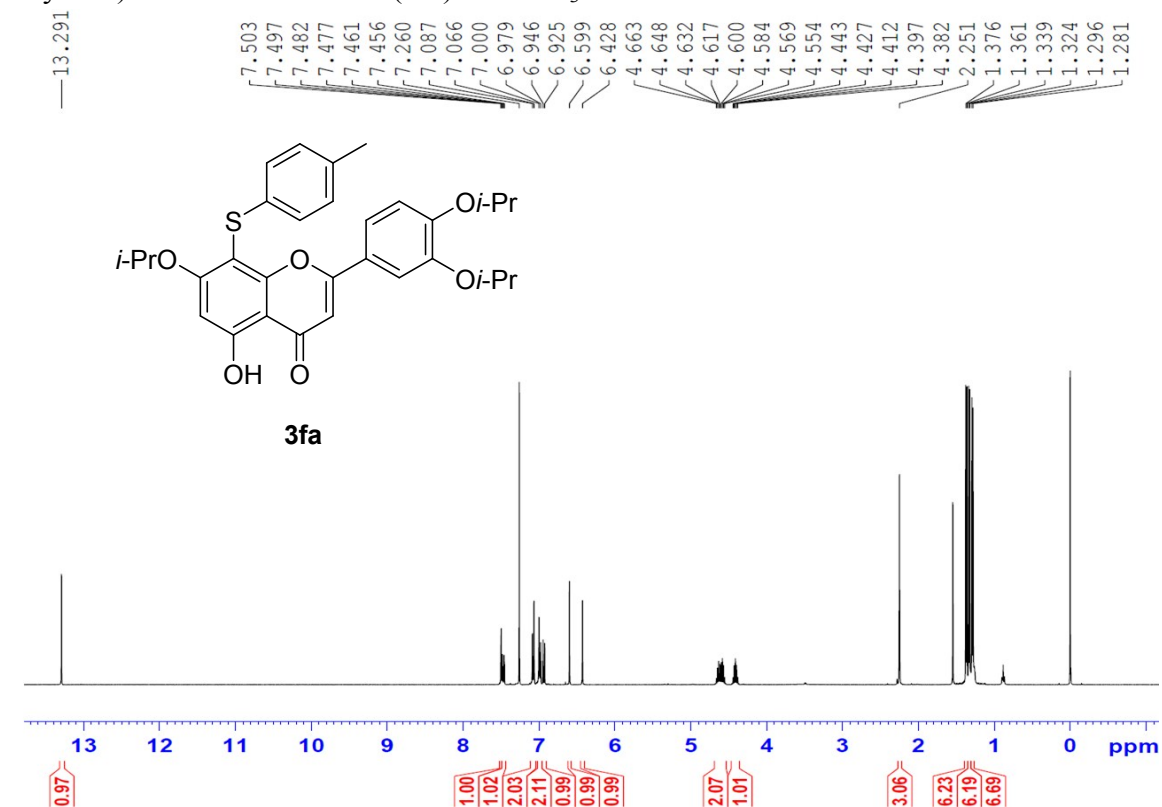
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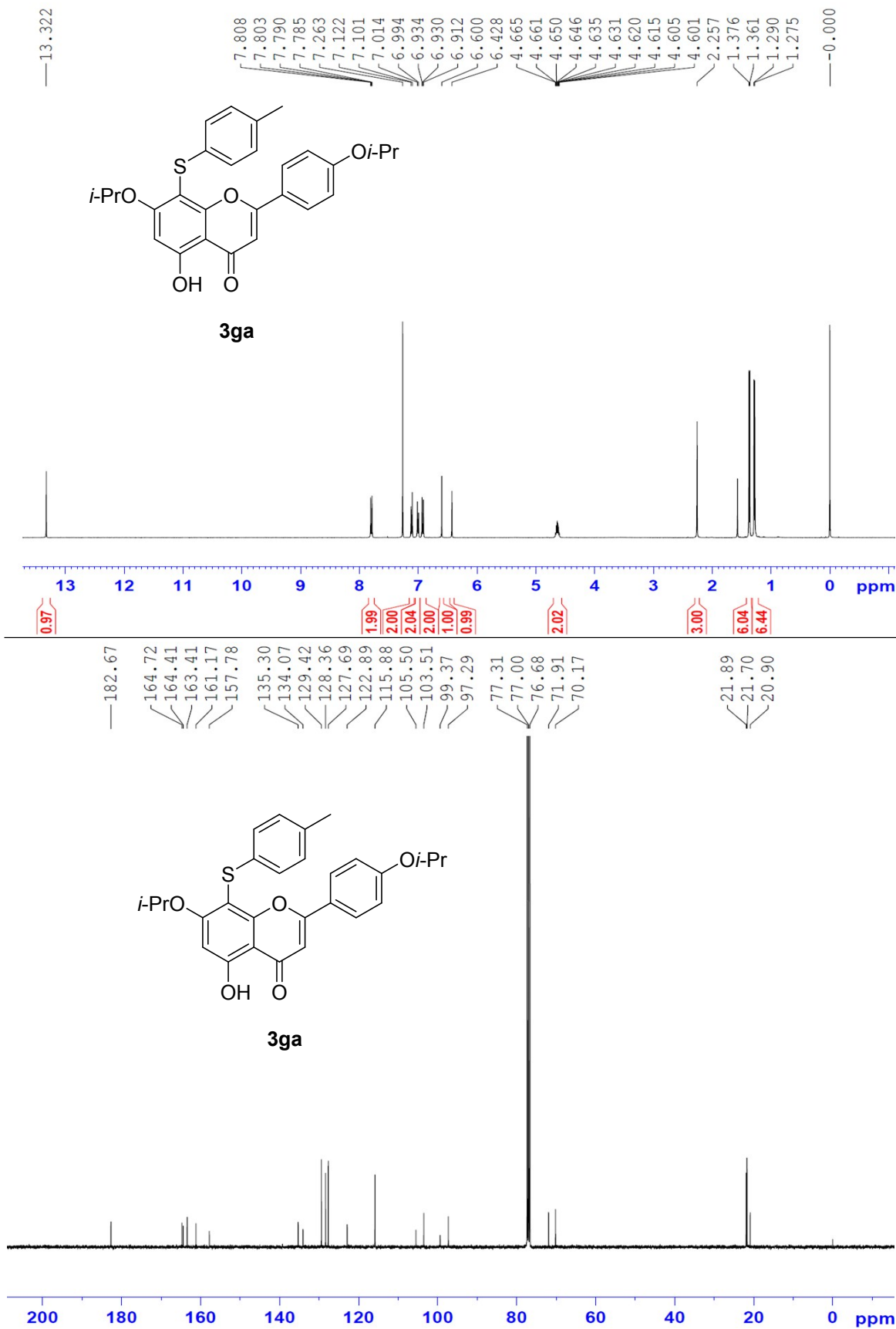
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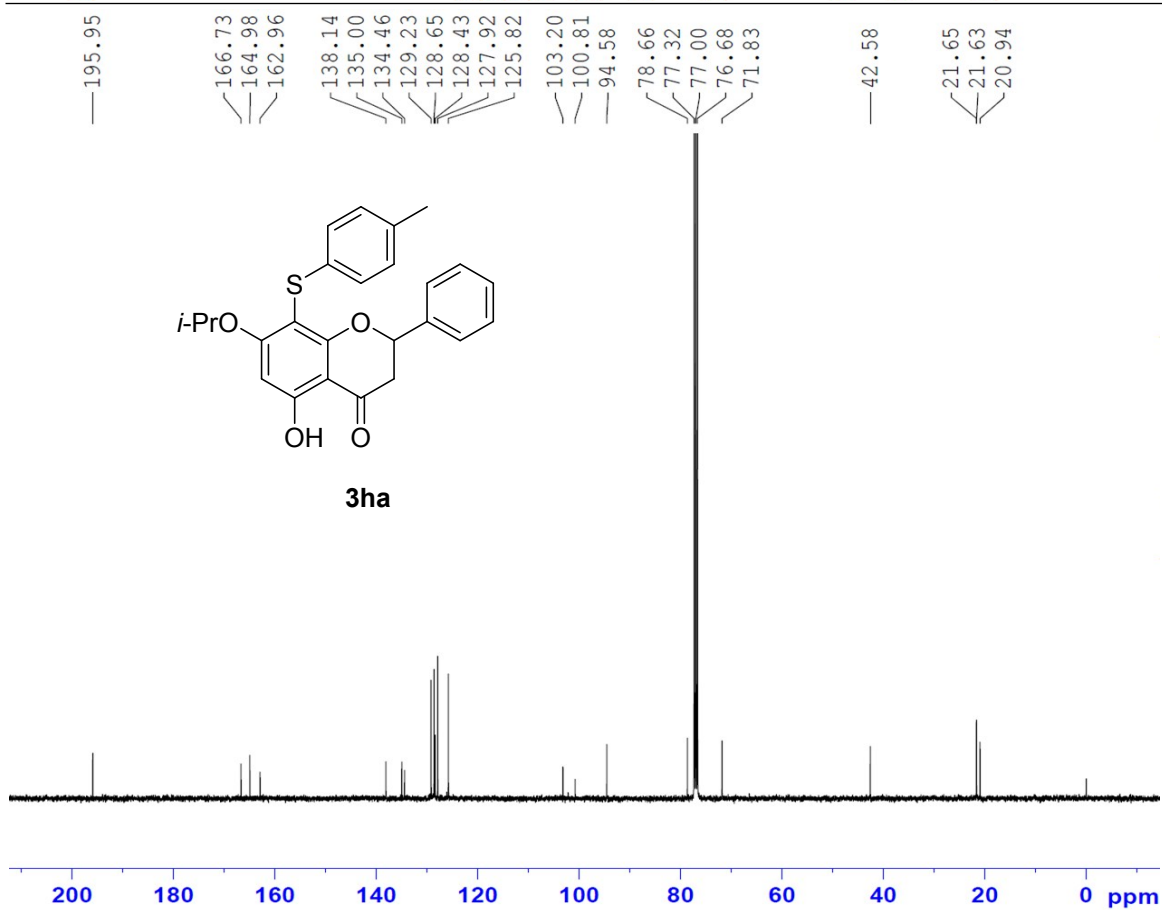
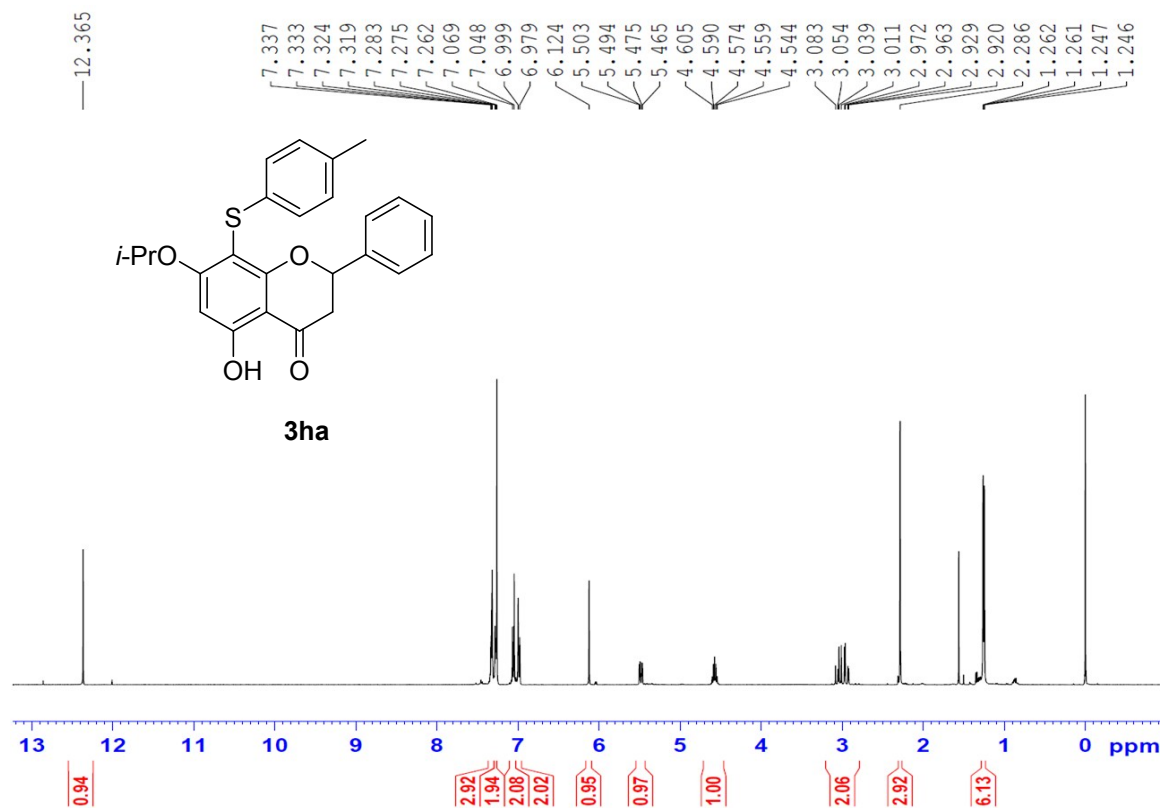
¹H and ¹³C NMR spectra of 2-(3,4-diisopropoxyphenyl)-5-hydroxy-7-isopropoxy-8-(p-tolylthio)-4H-chromen-4-one (3fa) in CDCl₃



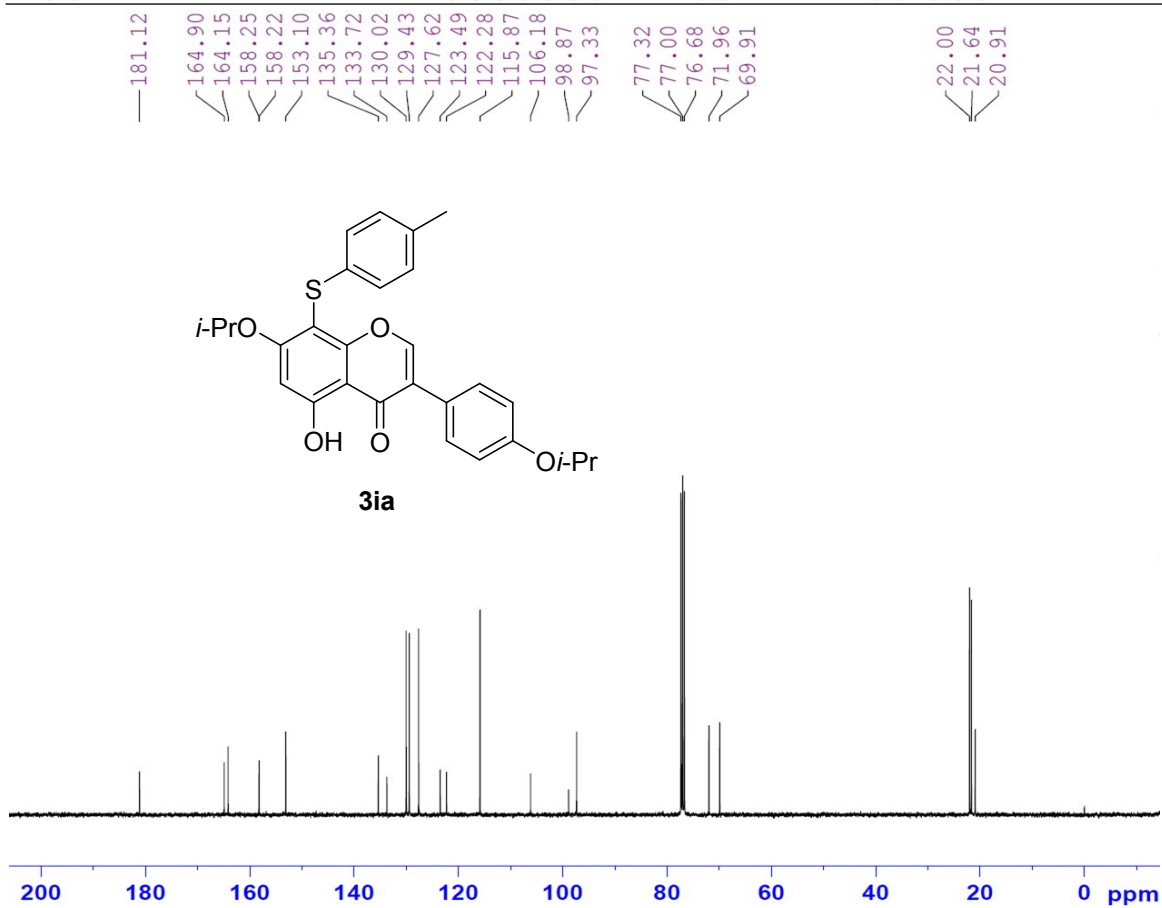
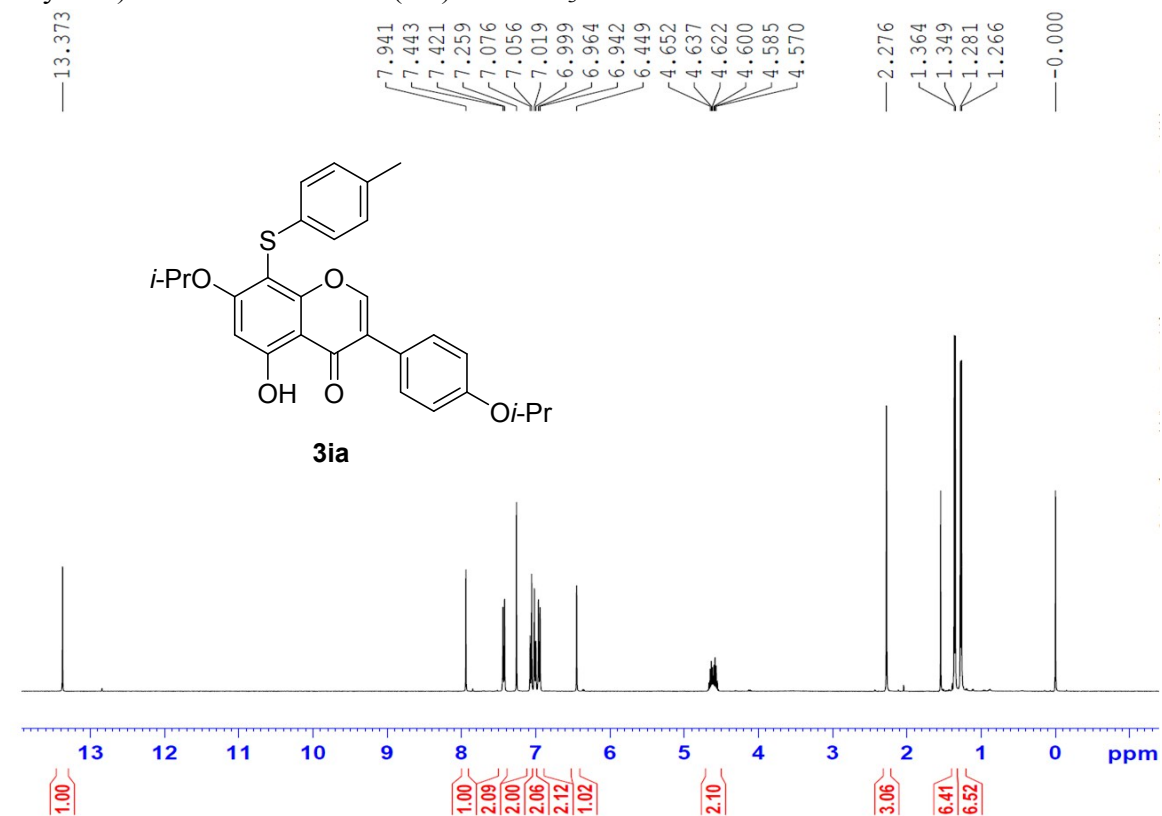
^1H and ^{13}C NMR spectra of 5-hydroxy-7-isopropoxy-2-(4-isopropoxyphenyl)-8-(p-tolylthio)-4H-chromen-4-one (3ga) in CDCl_3



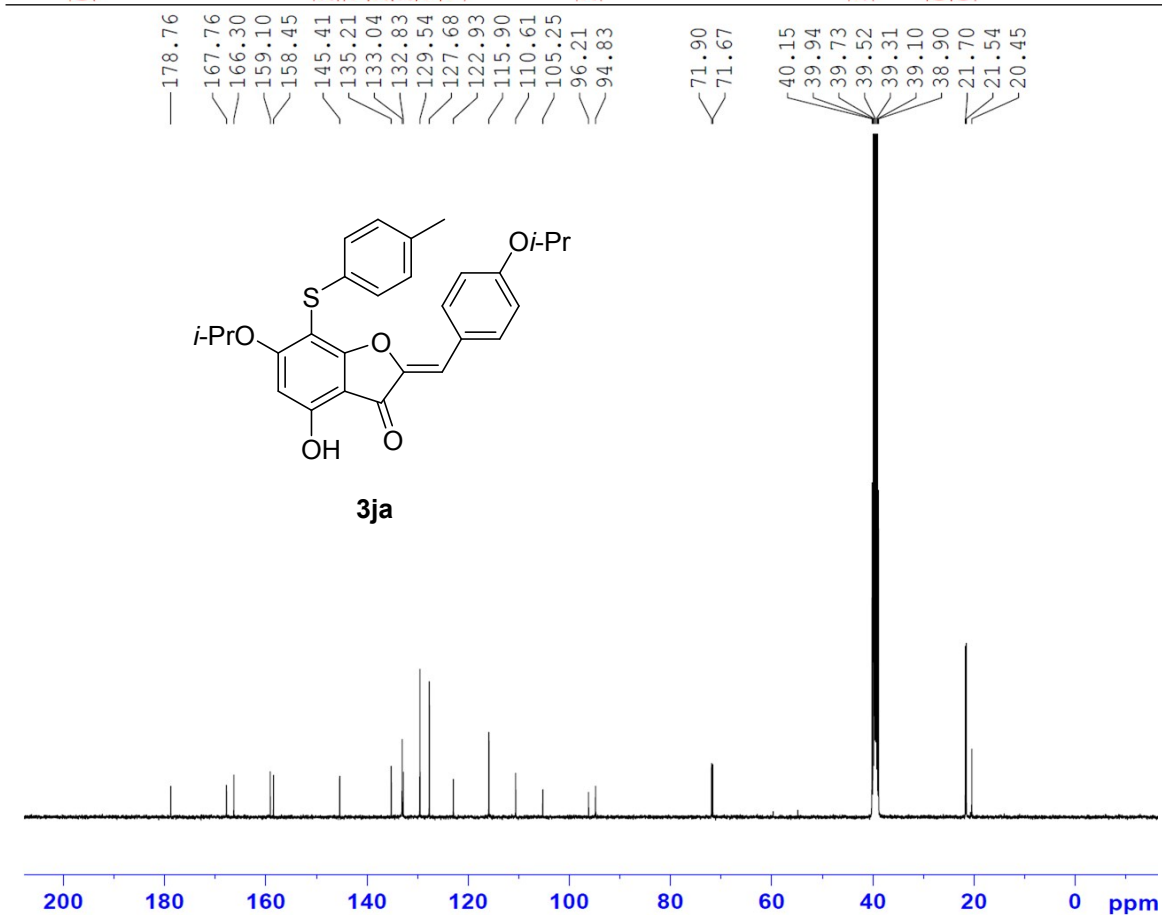
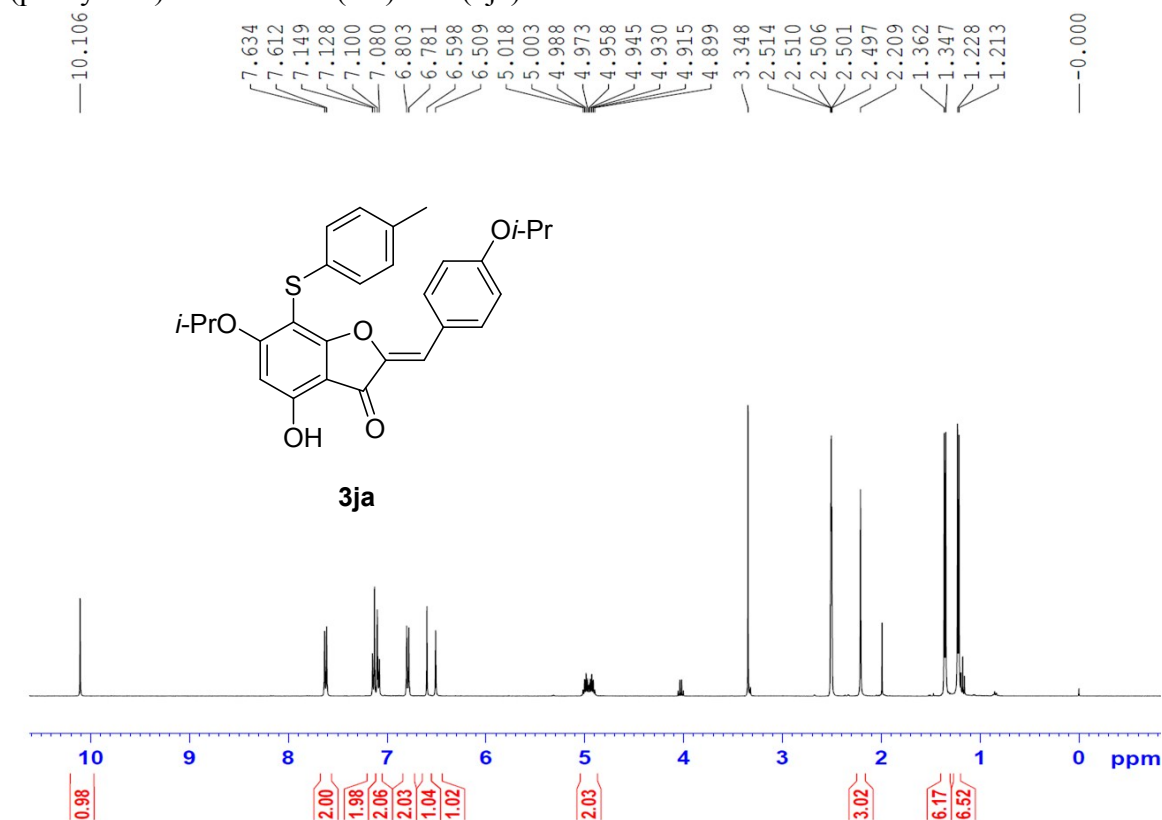
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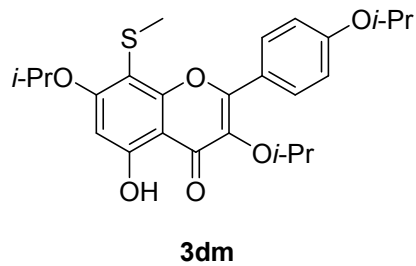
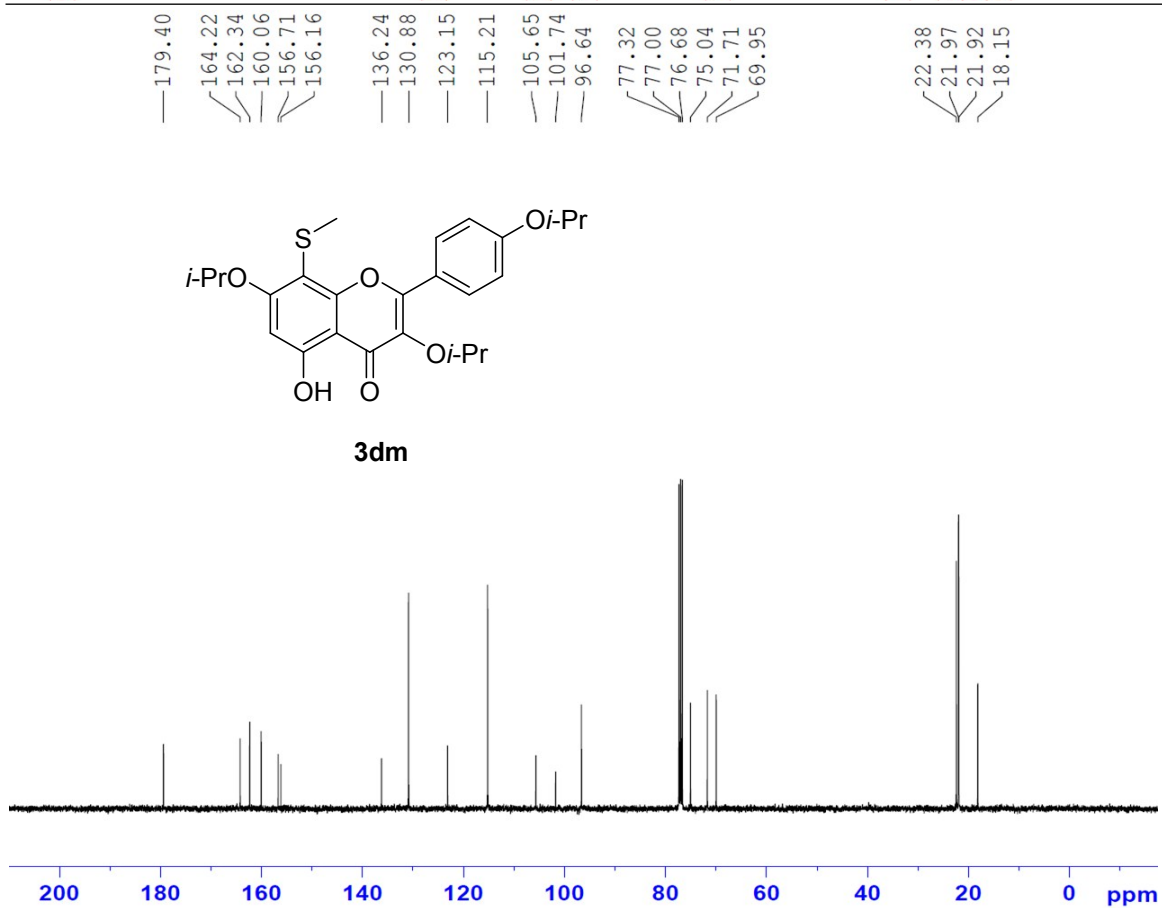
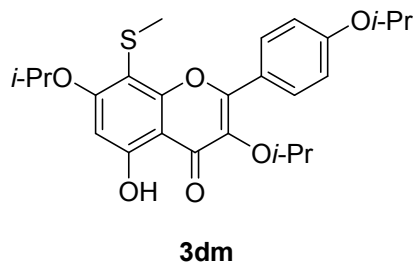
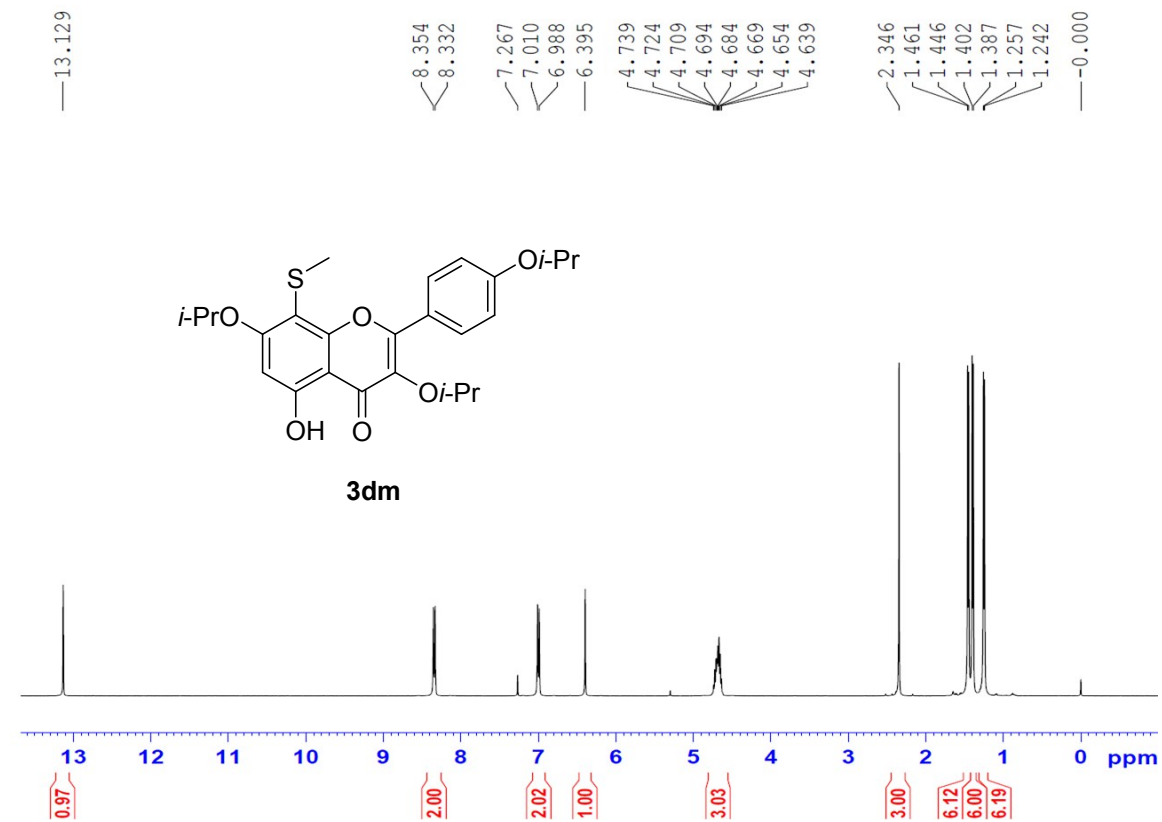
^1H and ^{13}C NMR spectra of 5-hydroxy-7-isopropoxy-3-(4-isopropoxyphenyl)-8-(p-tolylthio)-4H-chromen-4-one (3ia) in CDCl_3



¹H and ¹³C NMR spectra of (Z)-4-hydroxy-6-isopropoxy-2-(4-isopropoxybenzylidene)-7-(p-tolylthio)benzofuran-3(2H)-one (3ja) in DMSO^{d6}



^1H and ^{13}C NMR spectra of 5-hydroxy-3,7-diisopropoxy-2-(4-isopropoxyphenyl)-8-(methylthio)-4H-chromen-4-one (3dm) in CDCl_3



¹H and ¹³C NMR spectra of 5-hydroxy-7-isopropoxy-3-(4-isopropoxyphenyl)-8-(methylthio)-4H-chromen-4-one (3im) in CDCl₃

