

Regiospecific hydrogenation of bromochalcone by unconventional yeast strains

Mateusz Łużny¹, Dagmara Kaczanowska¹, Barbara Gawdzik², Alicja Wzorek², Aleksandra Pawlak³, Bożena Obmińska-Mrukowicz³, Monika Dymarska¹, Ewa Kozłowska¹, Edyta Kostrzewa-Susłow¹ and Tomasz Janeczko^{1,*}

¹Department of Food Chemistry and Biocatalysis, Wrocław University of Environmental and Life Sciences, Norwida 25, 50-375 Wrocław, Poland

²Institute of Chemistry, Jan Kochanowski University in Kielce, Uniwersytecka 7, 25-406 Kielce, Poland;

³Department of Pharmacology and Toxicology, Wrocław University of Environmental and Life Sciences, C.K. Norwida 31, 50-375 Wrocław, Poland

* Correspondence: janeczko13@interia.pl (T.J.); Tel.: +48-713-205-195 (T.J.)

e.a.kozłowska@gmail.com (E.K.), kaczanowskad@gmail.com (D.K.), b.gawdzik@ujk.edu.pl (B.G.), alicja.wzorek@ujk.edu.pl (A.W.), aleksandra.pawlak@upwr.edu.pl (A.P.), beatriz.hernandez-suarez@upwr.edu.pl (B.H.S.), monika.dymarska@upwr.edu.pl (M.D.), ewa.kozłowska1@upwr.edu.pl (E.K.), edyta.kostrzewa-suslow@upwr.edu.pl (E.K-S.)

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Figure S47. Preparative TLC plate showing the separation of the post-reaction mixture after biotransformation of 2'-hydroxy-2''-bromochalcone (**1**)

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Figure S51. Selected chromatograms showing the composition of the reaction mixtures during the biotransformation of the tested compounds:

- a) GC analysis obtained after 12 hours transformation of 2'-hydroxy-2''-bromochalcone (**1**)
- b) GC analysis obtained after 3 days transformation of 2'-hydroxy-2''-bromochalcone (**2**)
- c) GC analysis obtained after 3 hours transformation of 2'-hydroxy-5'-bromochalcone (**4**)
- d) GC analysis obtained after 10 days transformation of 2'-hydroxy-5'-bromochalcone (**4**)

Figure S1. ^1H NMR spectral of 1-(2'-hydroxyphenyl)-3-(2''-bromophenyl)-prop-2-en-1-one (**1**) (CDCl_3 , 600 MHz)

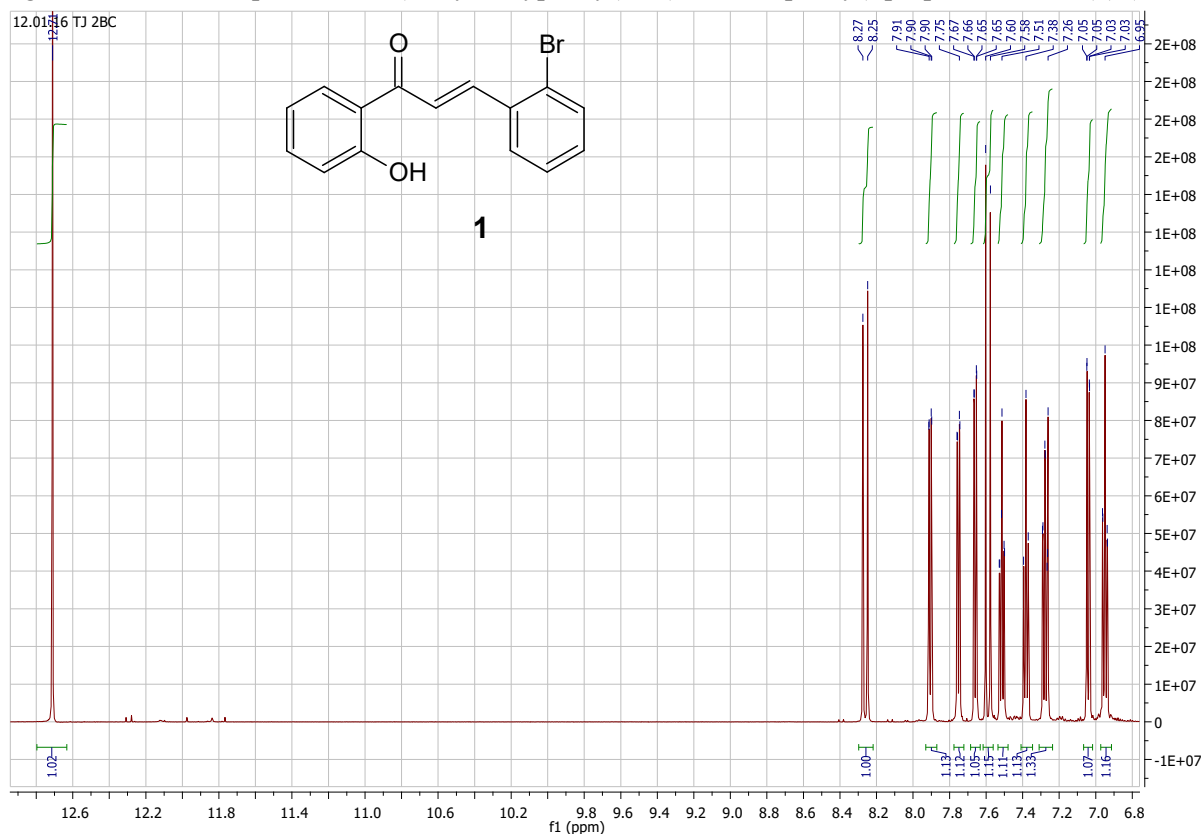


Figure S2. Part of the ^{13}C NMR spectral of 1-(2'-hydroxyphenyl)-3-(2''-bromophenyl)-prop-2-en-1-one (**1**) (CDCl_3 , 600 MHz)

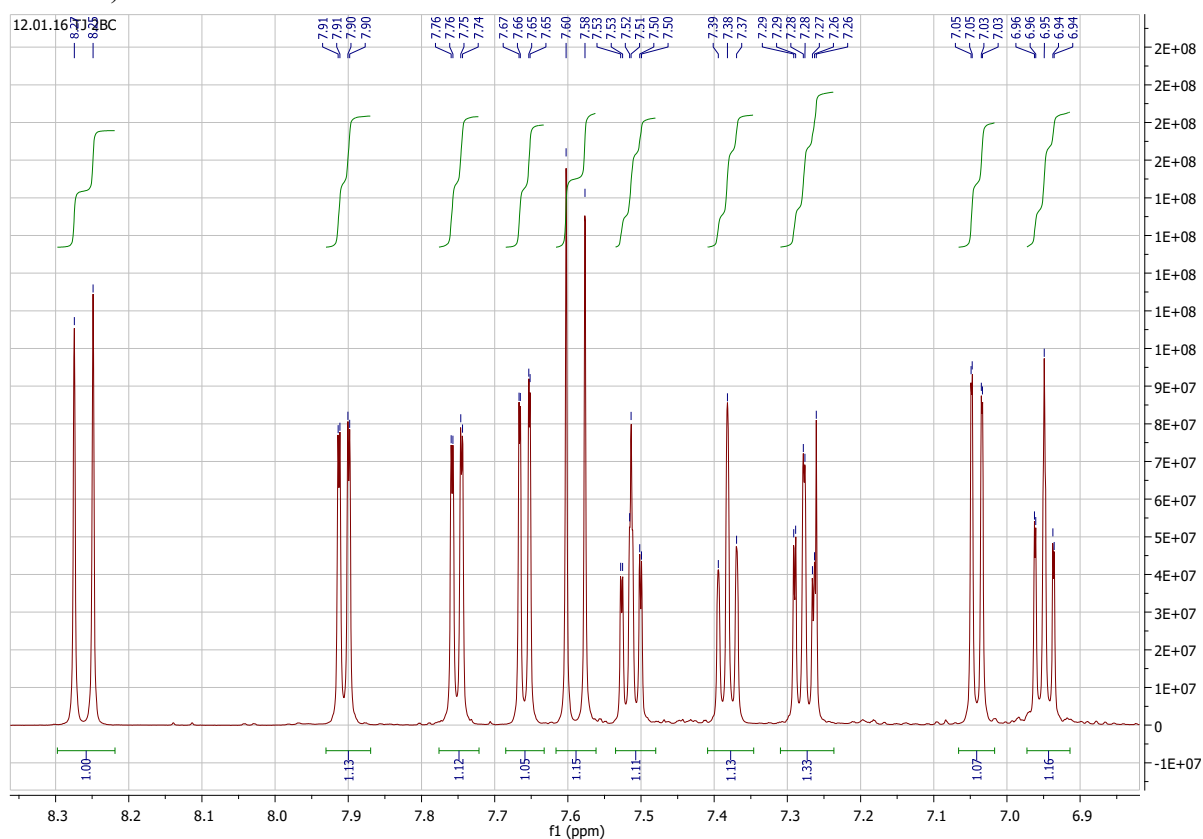


Figure S3. ^{13}C NMR spectral of 1-(2'-hydroxyphenyl)-3-(2''-bromophenyl)-prop-2-en-1-one (**1**) (CDCl_3 , 151 MHz)

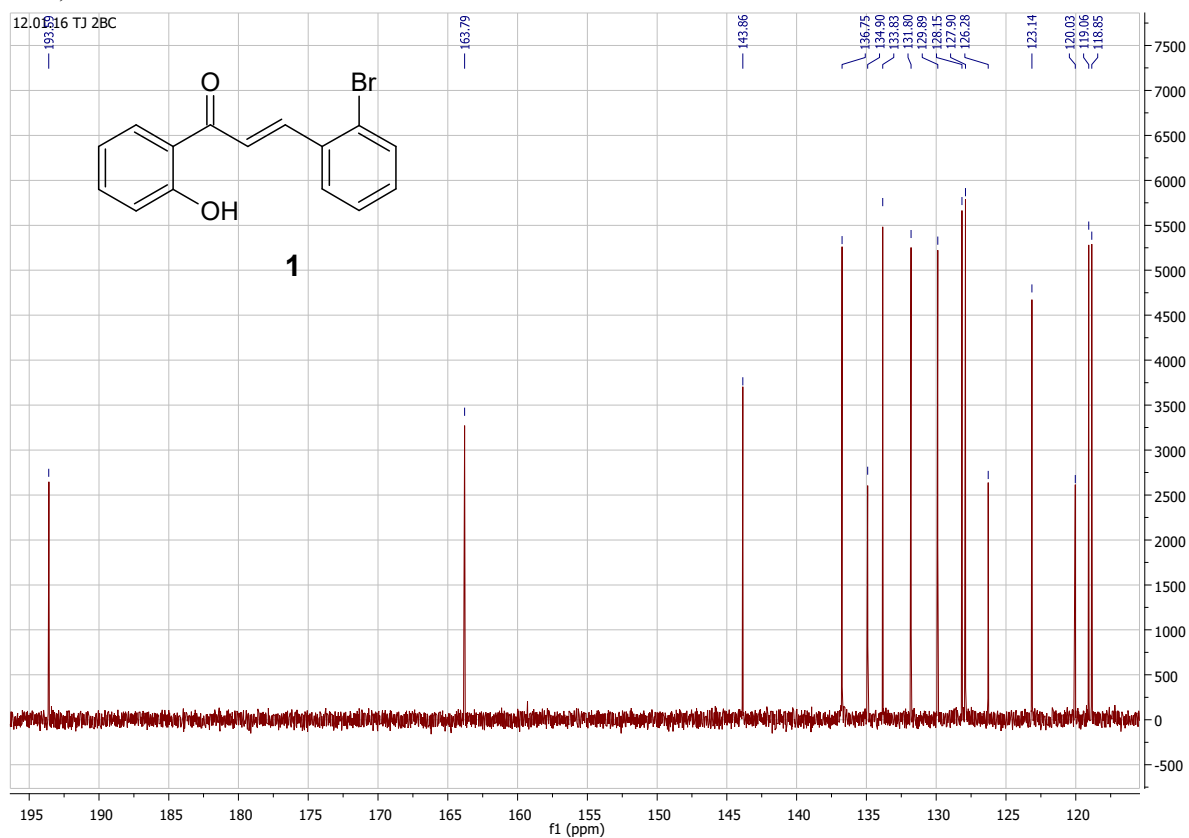


Figure S4. COSY spectral of 1-(2'-hydroxyphenyl)-3-(2''-bromophenyl)-prop-2-en-1-one (**1**) (CDCl_3 , 151 MHz)

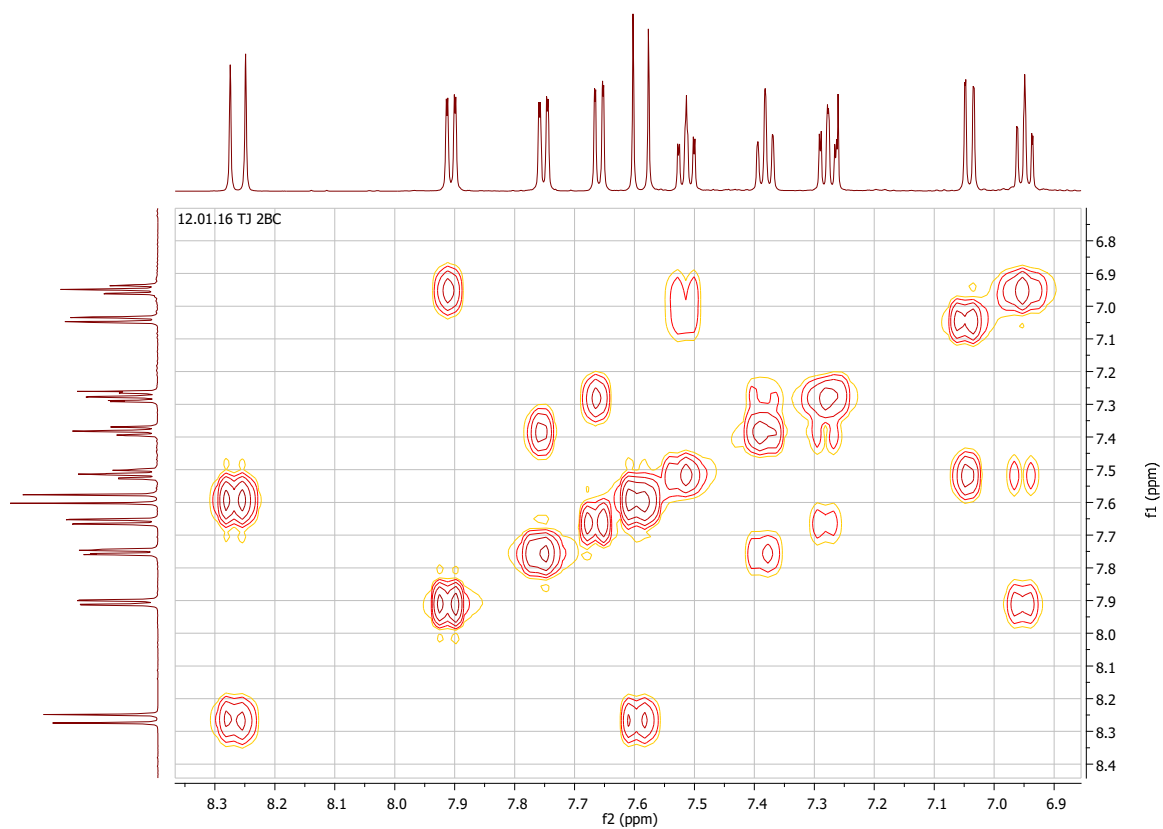


Figure S5. HSQC spectral of 1-(2'-hydroxyphenyl)-3-(2''-bromophenyl)-prop-2-en-1-one (**1**) (CDCl₃, 151 MHz)

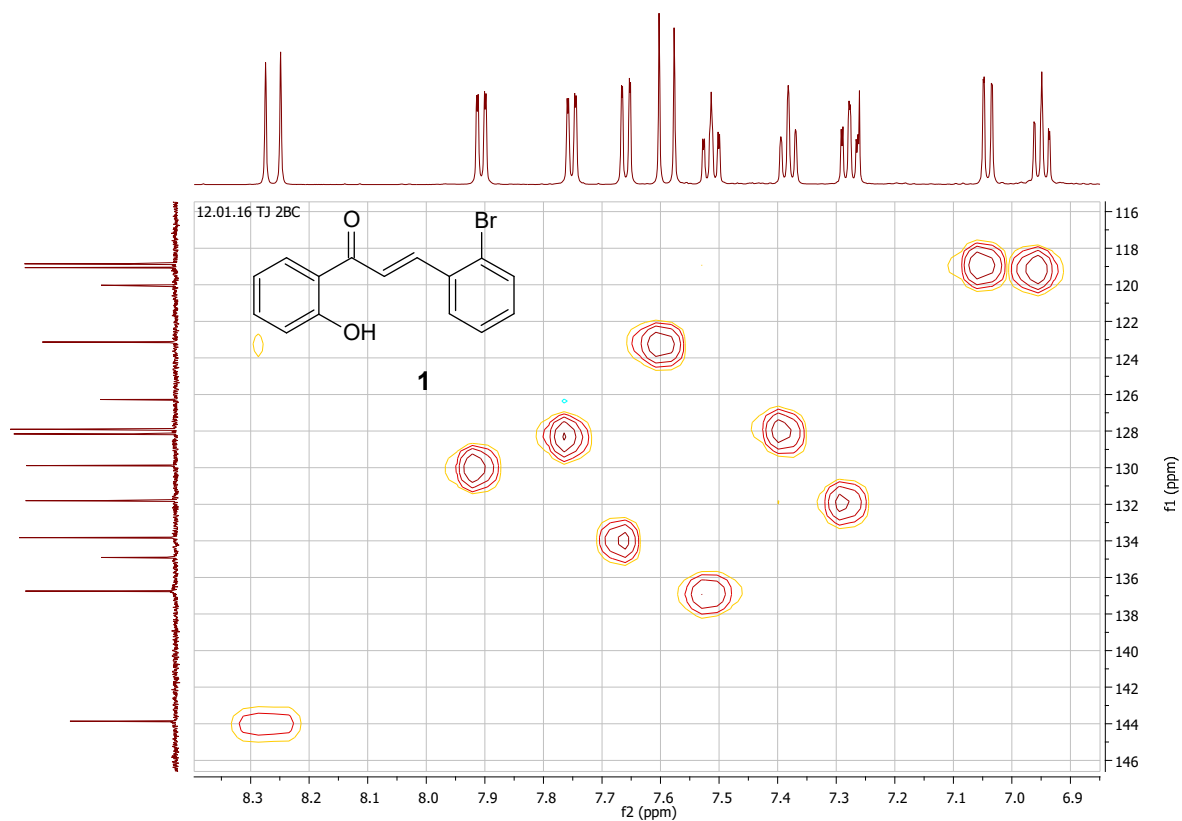


Figure S6. ¹H NMR spectral of 1-(2'-hydroxyphenyl)-3-(2''-bromophenyl)-propan-1-one (**5**) (CDCl₃, 600 MHz)

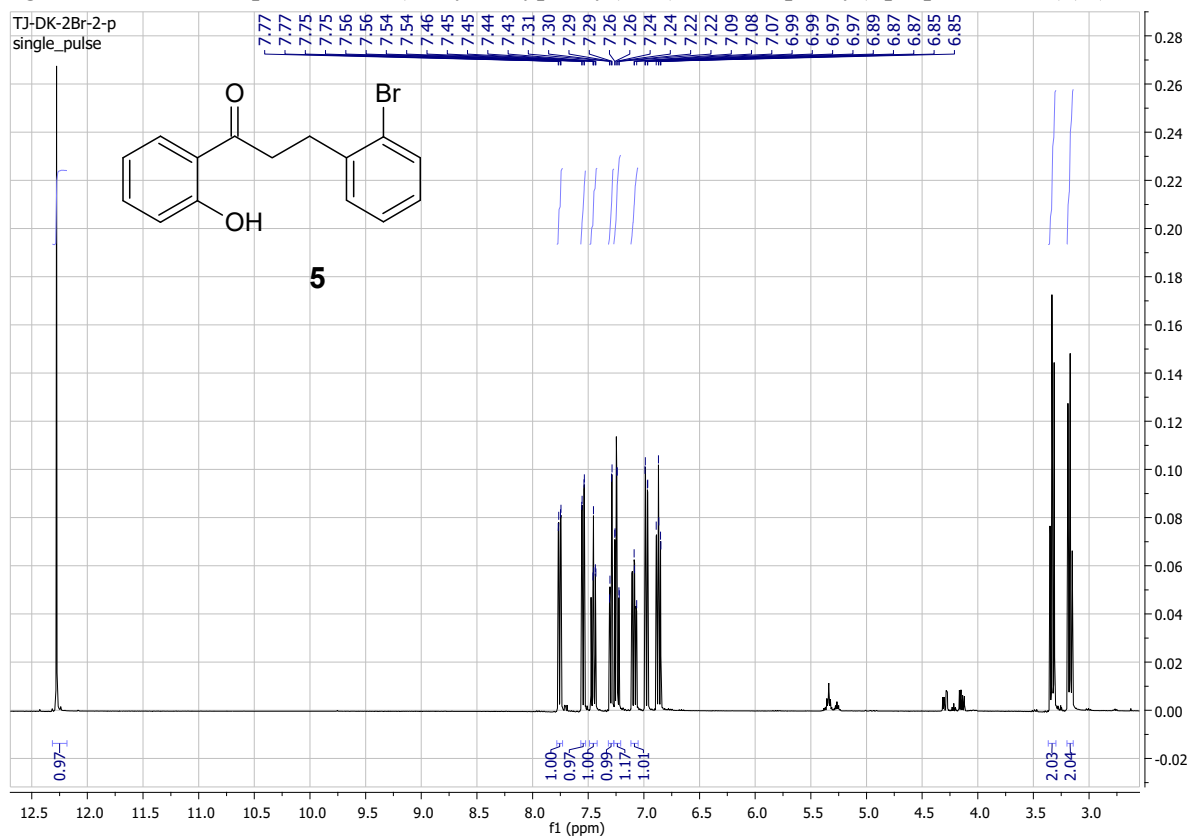


Figure S7. Part of the ^{13}C NMR spectral of 1-(2'-hydroxyphenyl)-3-(2''-bromophenyl)-propan-1-one (**5**) (CDCl_3 , 600 MHz)

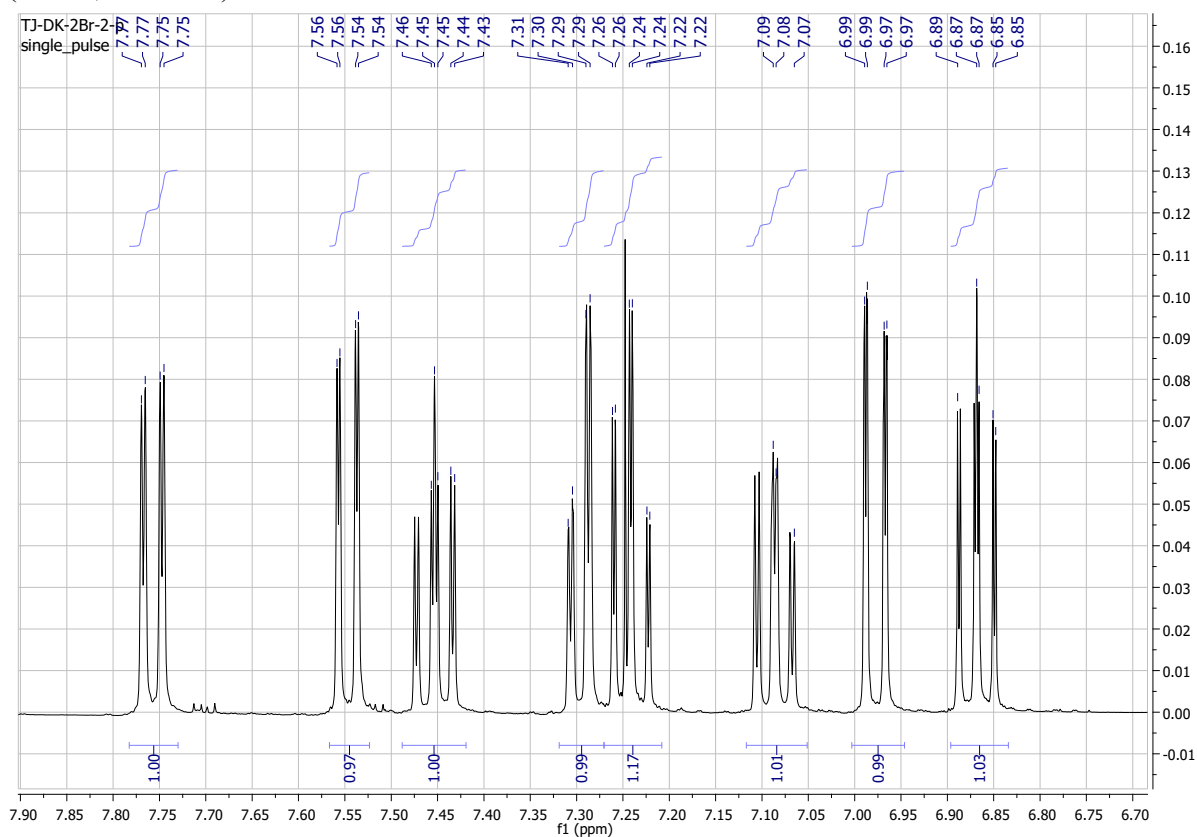


Figure S8. ^{13}C NMR spectral of 1-(2'-hydroxyphenyl)-3-(2''-bromophenyl)-propan-1-one (**5**) (CDCl_3 , 151 MHz)

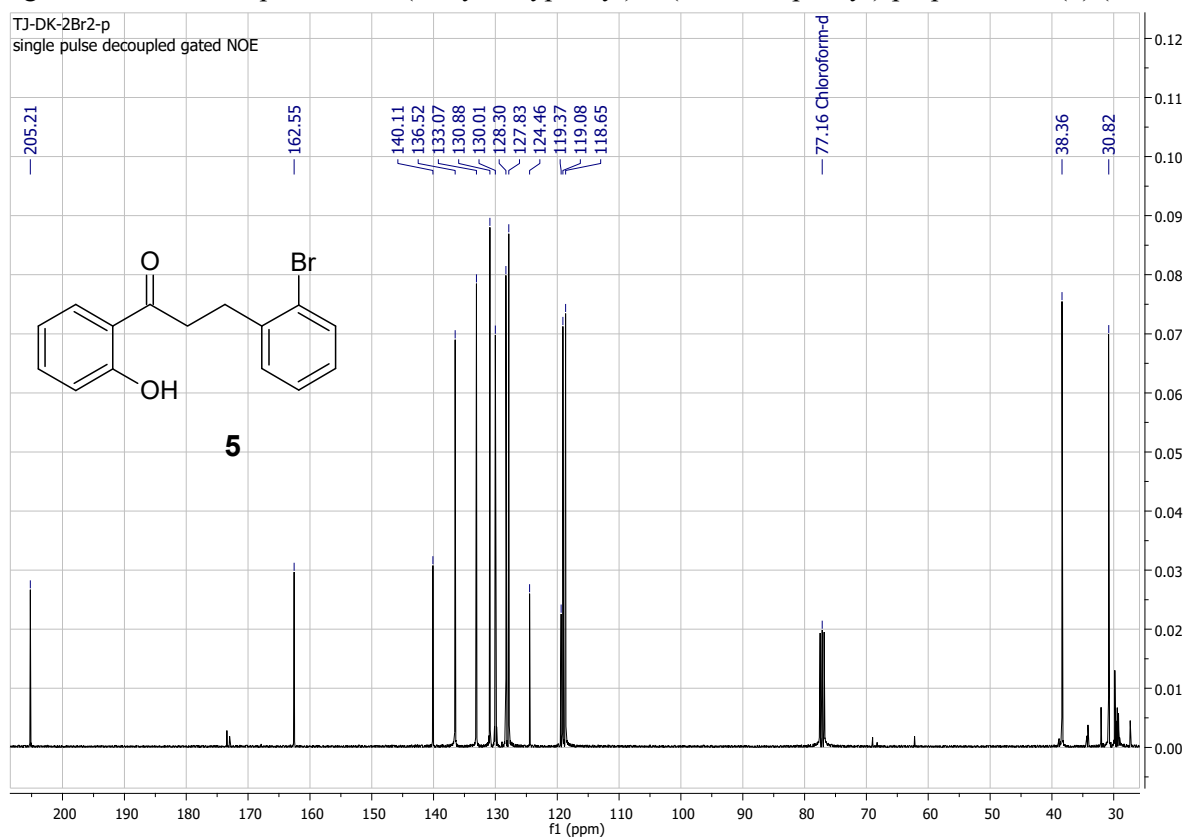


Figure S9. Part of the ^{13}C NMR spectral of 1-(2'-hydroxyphenyl)-3-(2''-bromophenyl)-propan-1-one (**5**) (CDCl_3 , 151 MHz)

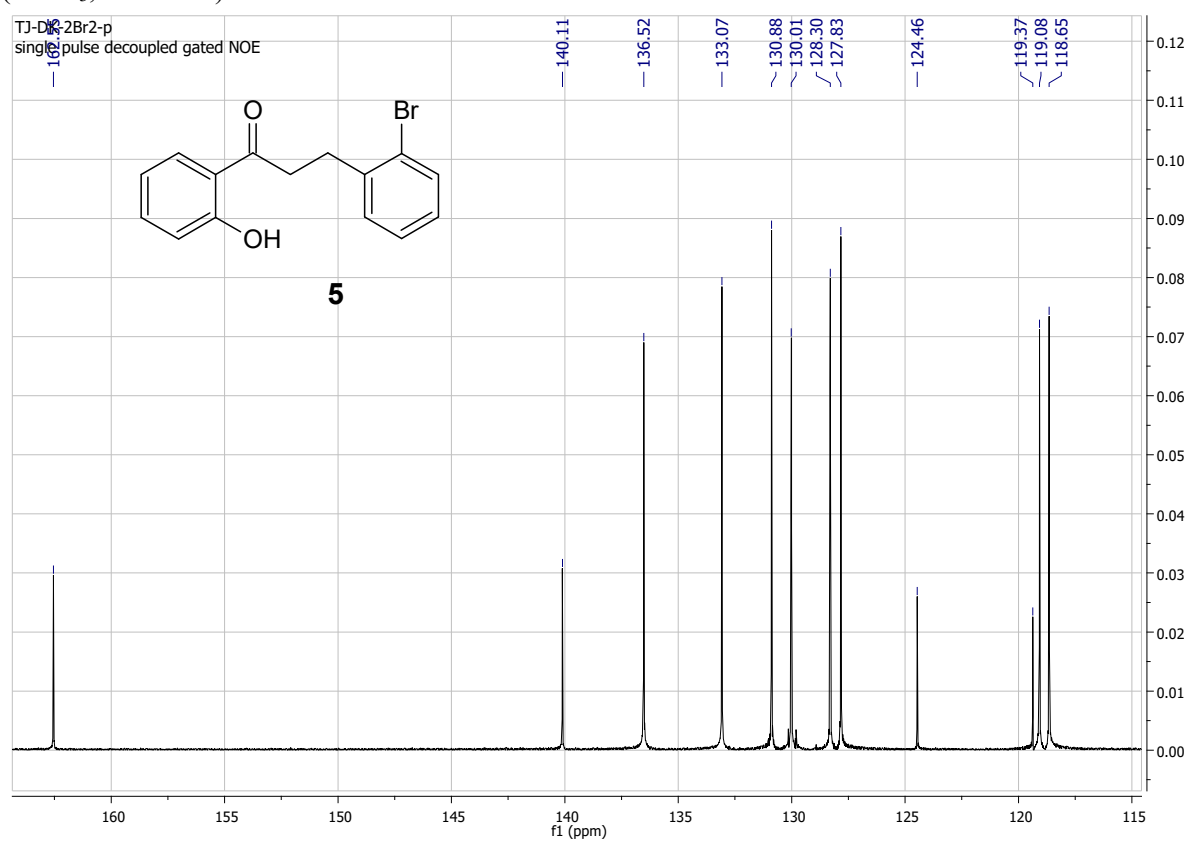


Figure S10. COSY spectral of 1-(2'-hydroxyphenyl)-3-(2''-bromophenyl)-propan-1-one (**5**) (CDCl_3 , 151 MHz)

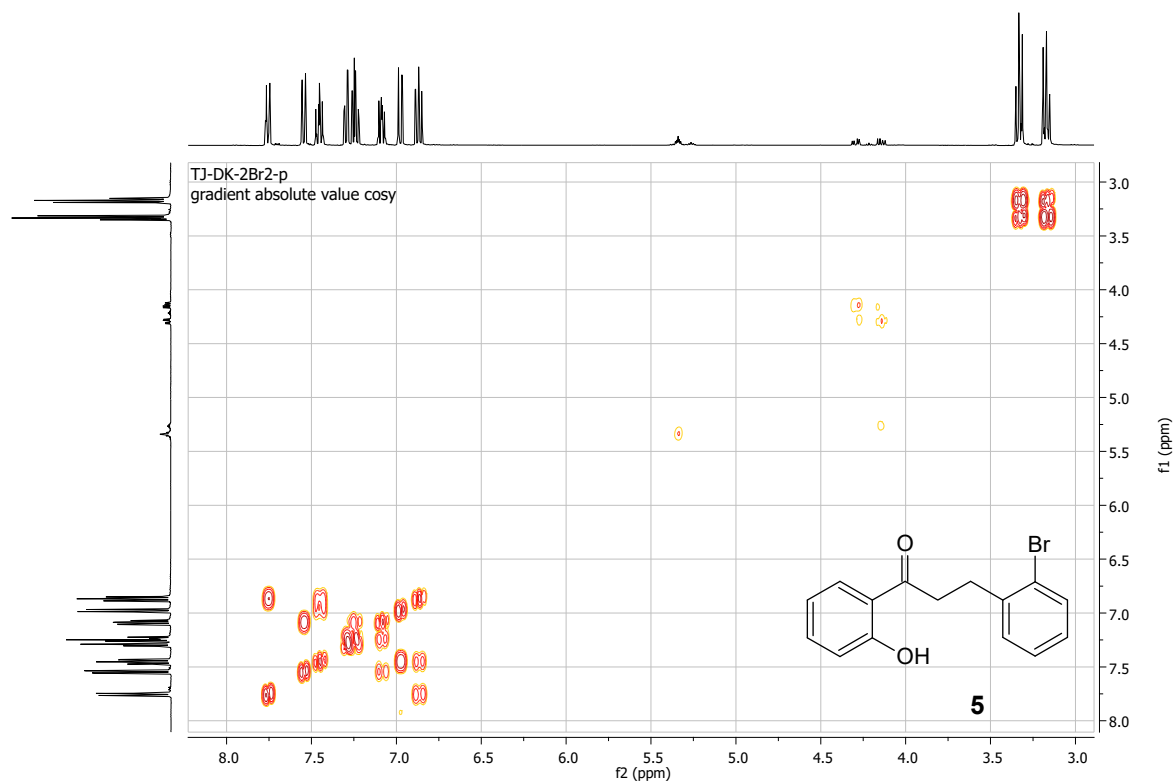


Figure S11. Part of the COSY spectral of 1-(2'-hydroxyphenyl)-3-(2''-bromophenyl)-propan-1-one (**5**) (CDCl₃, 151 MHz)

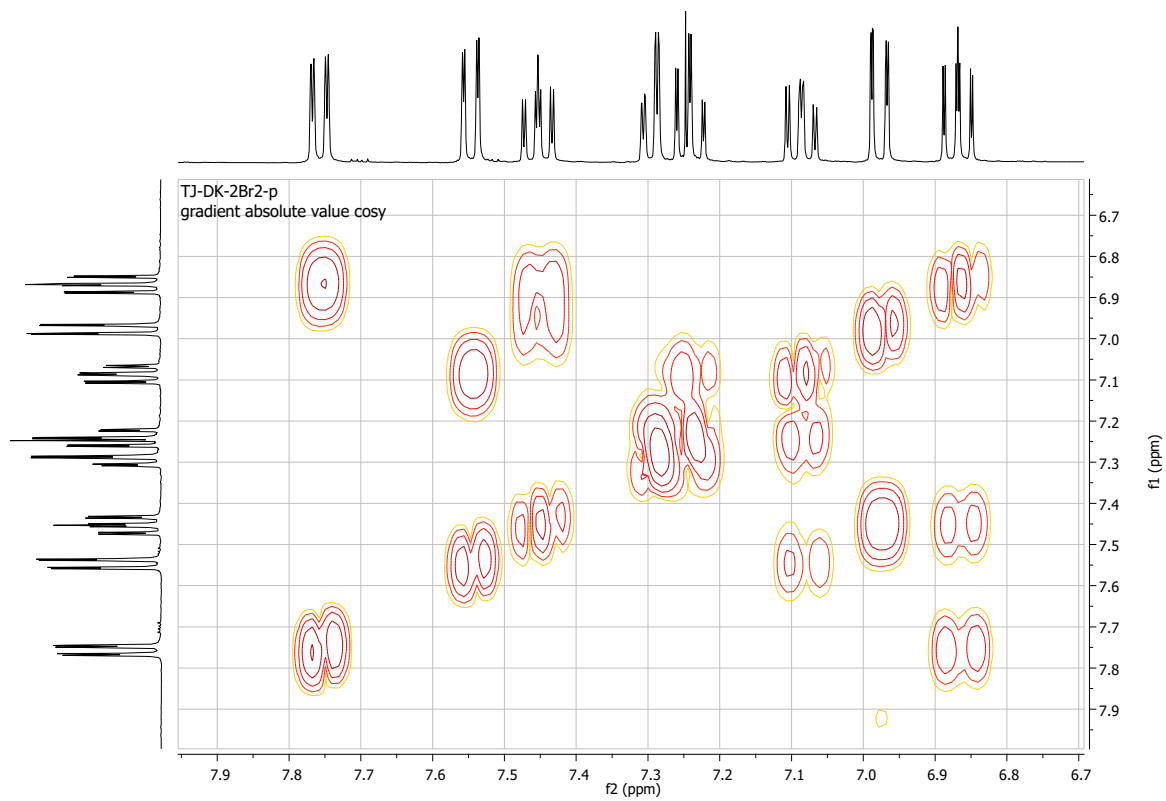


Figure S12. HSQC spectral of 1-(2'-hydroxyphenyl)-3-(2''-bromophenyl)-propan-1-one (**5**) (CDCl₃, 151 MHz)

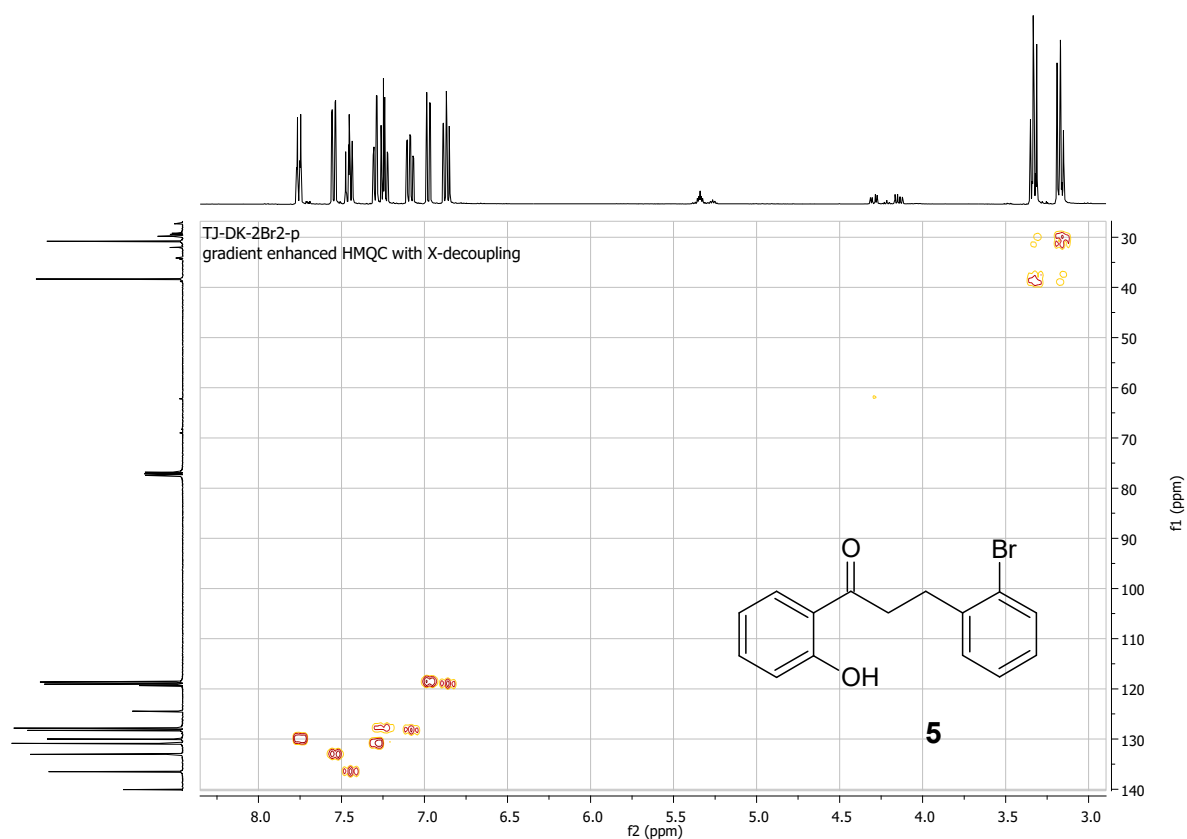


Figure S13. HMBC spectral of 1-(2'-hydroxyphenyl)-3-(2''-bromophenyl)-propan-1-one (**5**) (CDCl₃, 151 MHz)

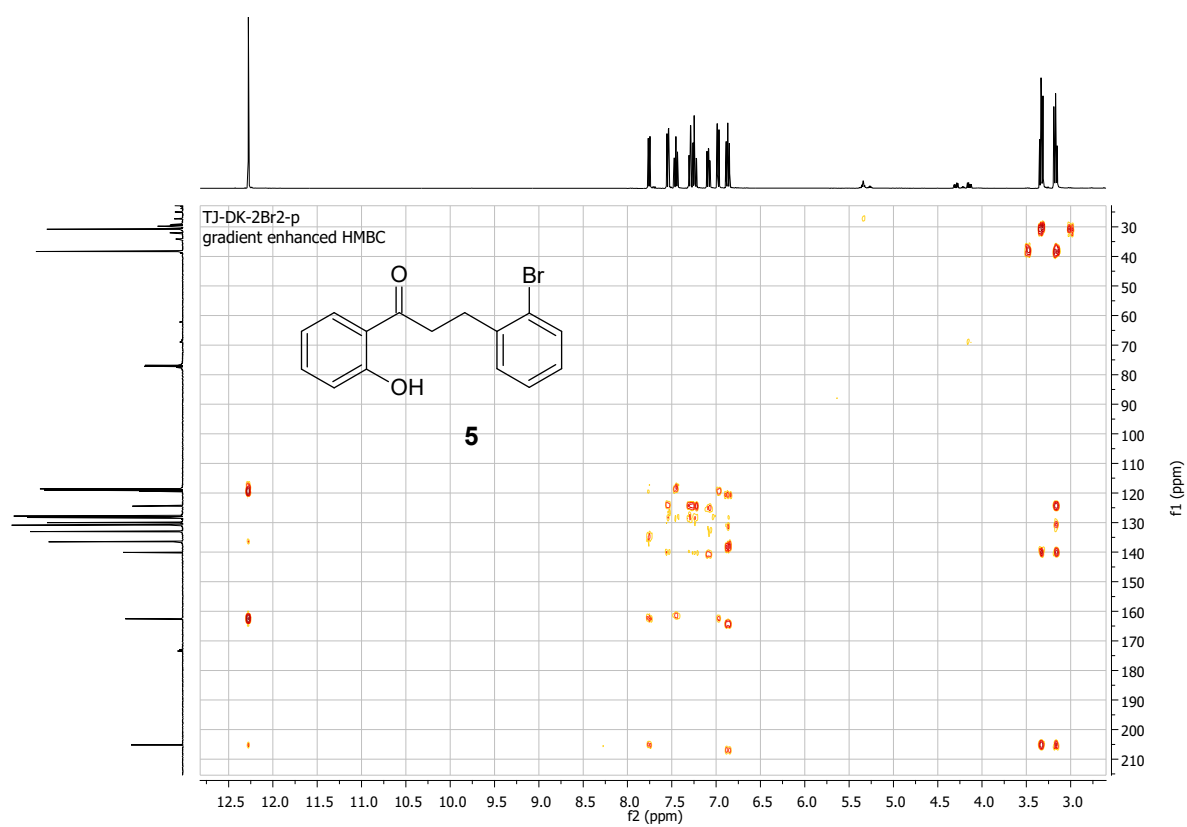


Figure S14. ¹H NMR spectral of 1-(2'-hydroxyphenyl)-3-(3''-bromophenyl)-prop-2-en-1-one (**2**) (CDCl₃, 600 MHz)

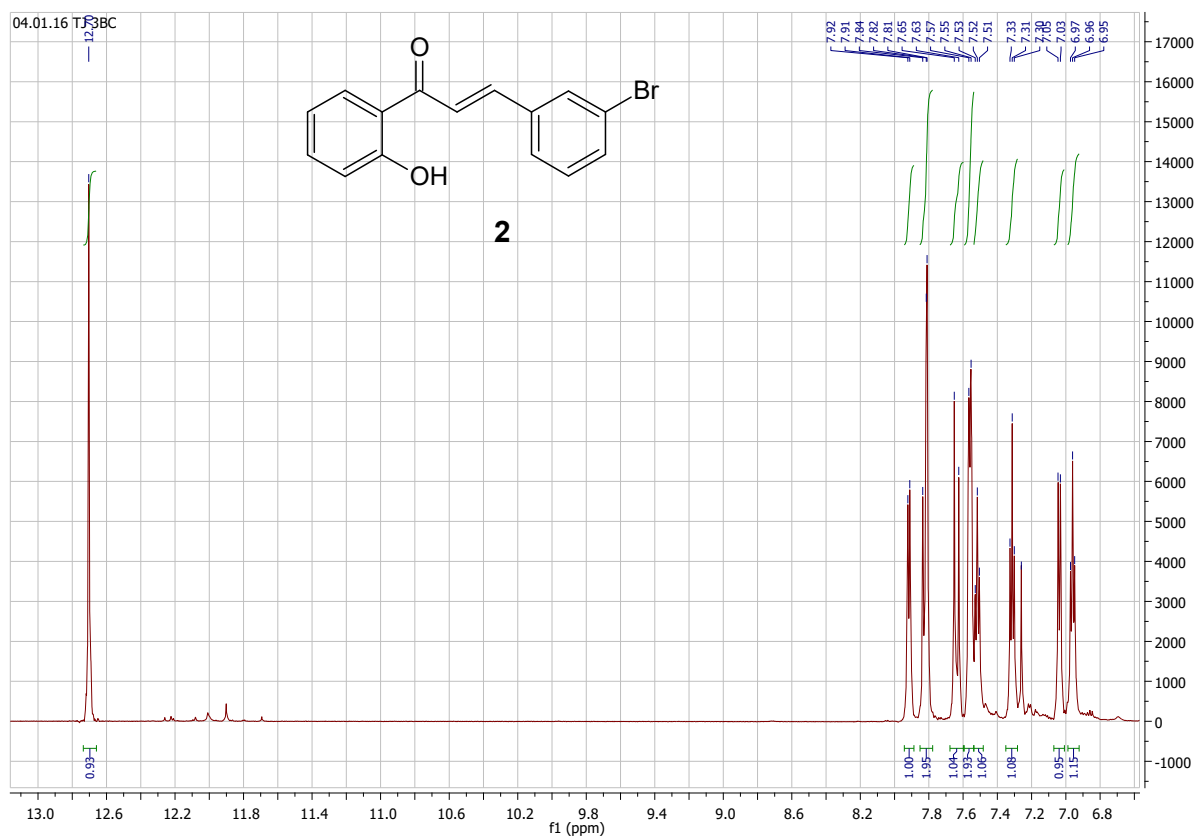


Figure S15. Part of the ¹³C NMR spectral of 1-(2'-hydroxyphenyl)-3-(3''-bromophenyl)-prop-2-en-1-one (**2**) (CDCl₃, 600 MHz)

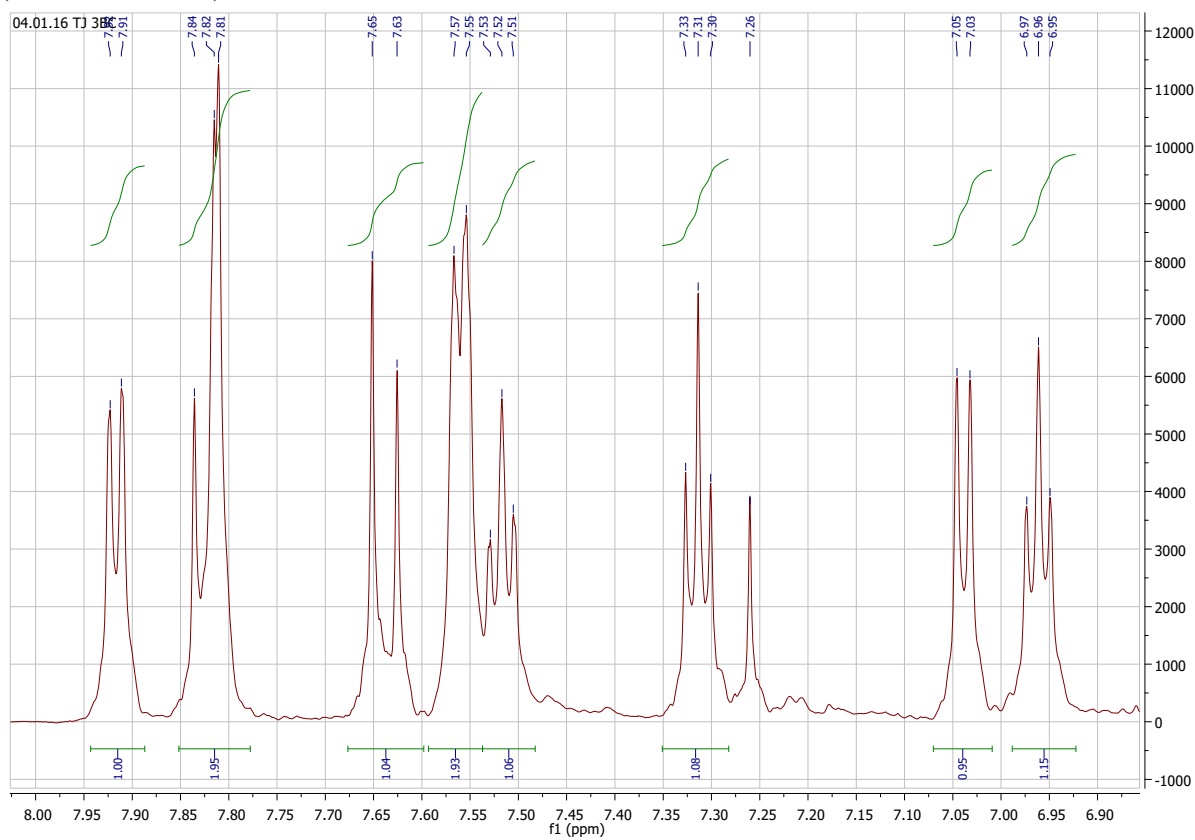


Figure S16. ¹³C NMR spectral of 1-(2'-hydroxyphenyl)-3-(3''-bromophenyl)-prop-2-en-1-one (**2**) (CDCl₃, 151 MHz)

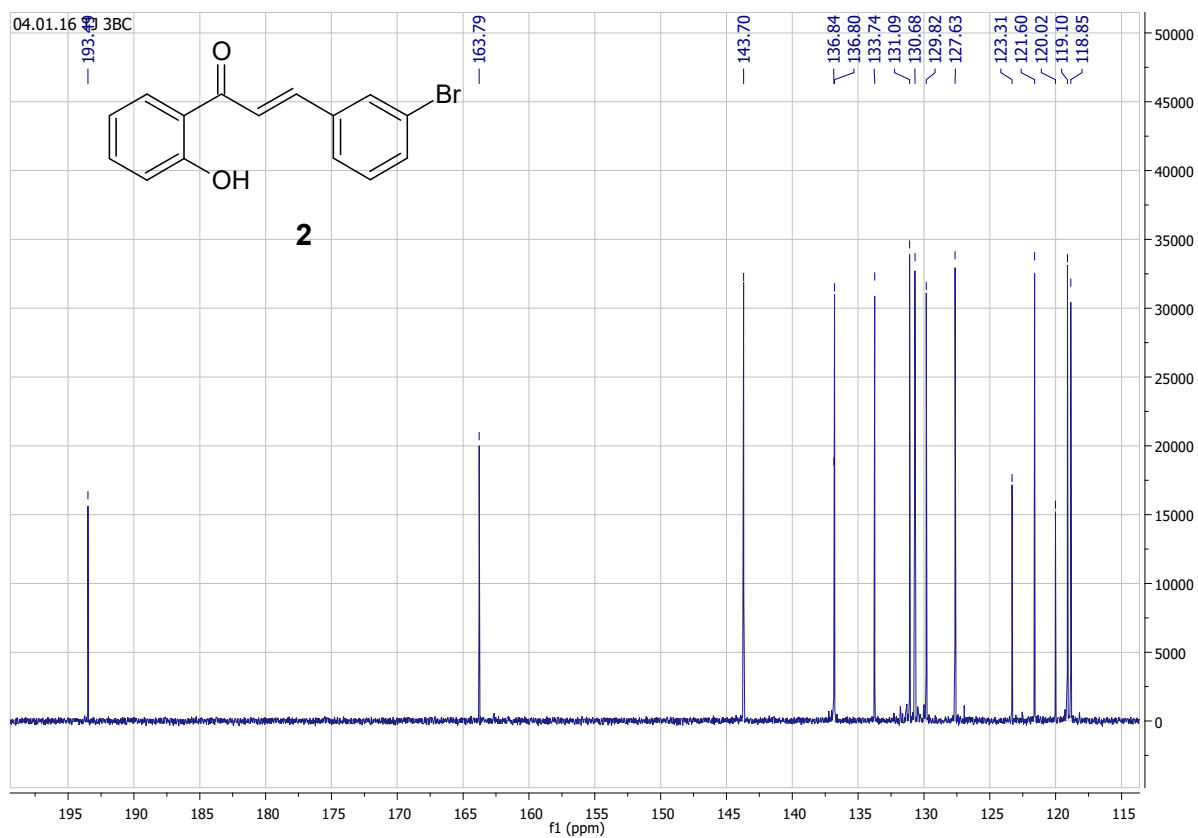


Figure S17. COSY spectral of 1-(2'-hydroxyphenyl)-3-(3''-bromophenyl)-prop-2-en-1-one (**2**) (CDCl₃, 151 MHz)

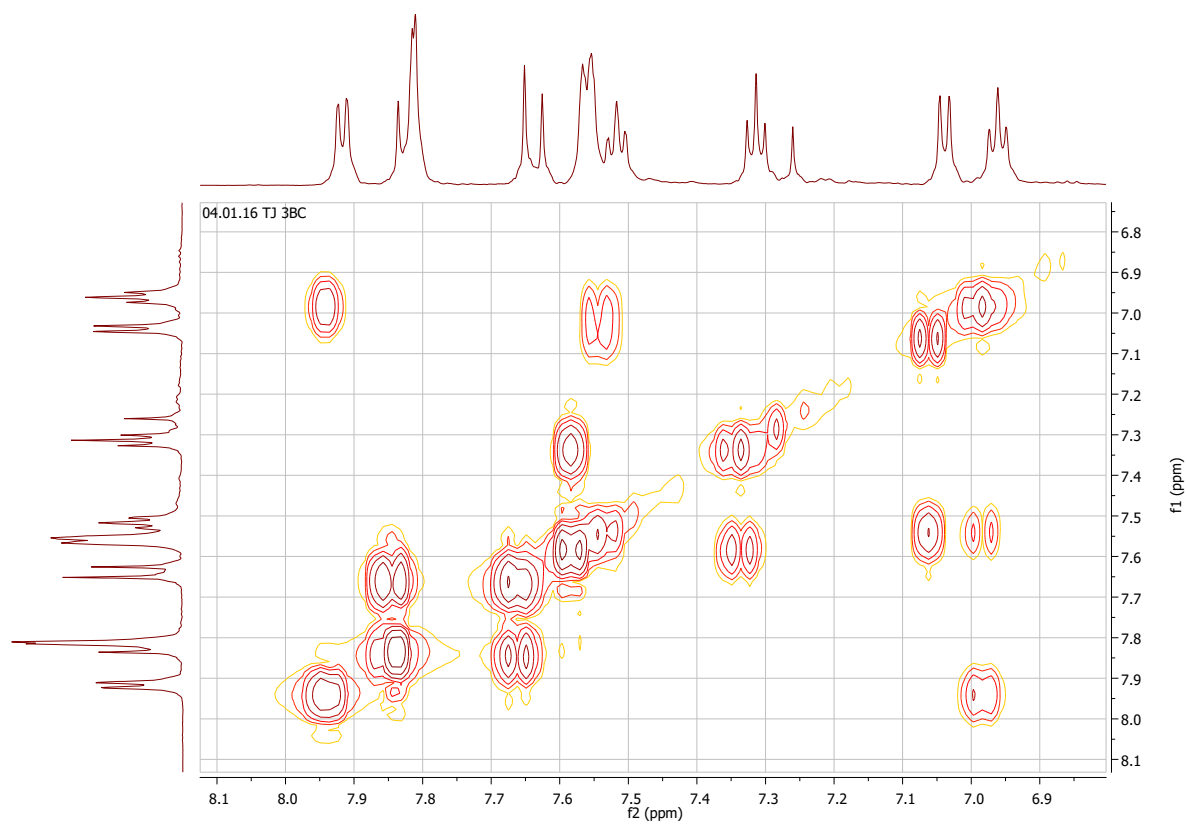


Figure S18. HSQC spectral of 1-(2'-hydroxyphenyl)-3-(3''-bromophenyl)-prop-2-en-1-one (**2**) (CDCl₃, 151 MHz)

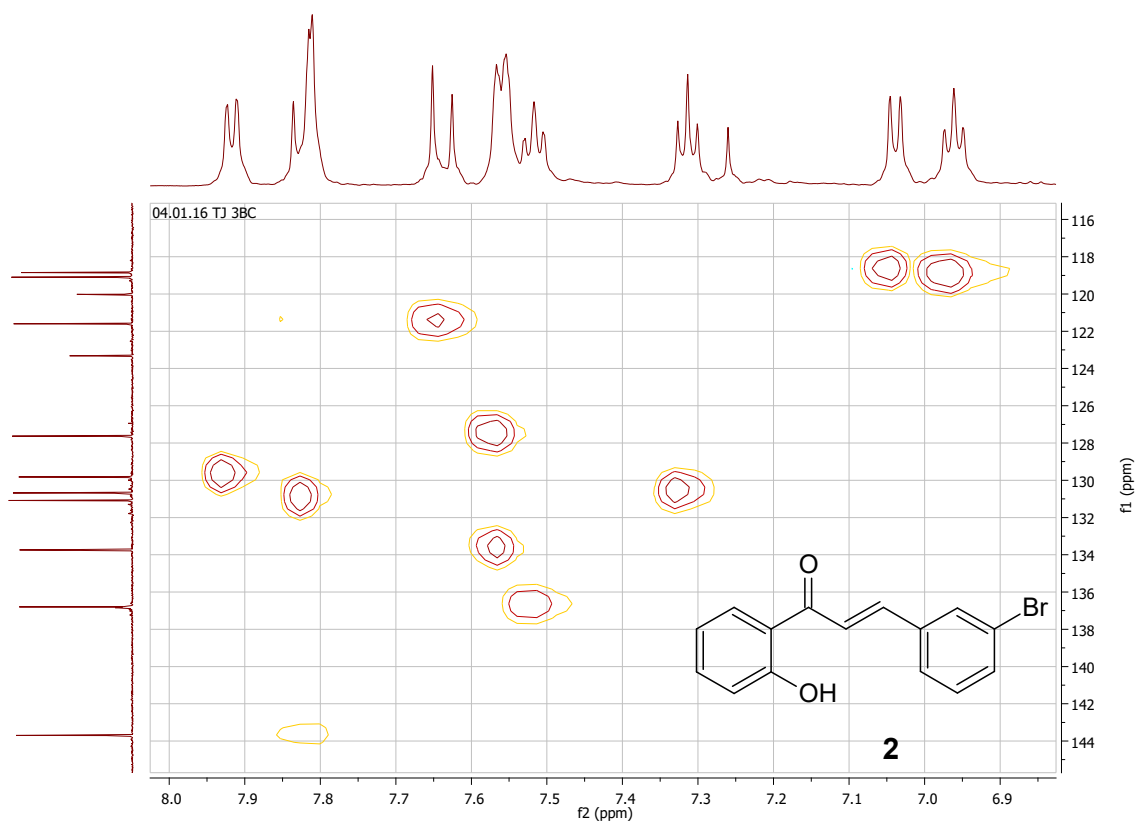


Figure S19. ^1H NMR spectral of 1-(2'-hydroxyphenyl)-3-(3''-bromophenyl)propan-1-one (**6**) (CDCl_3 , 600 MHz)

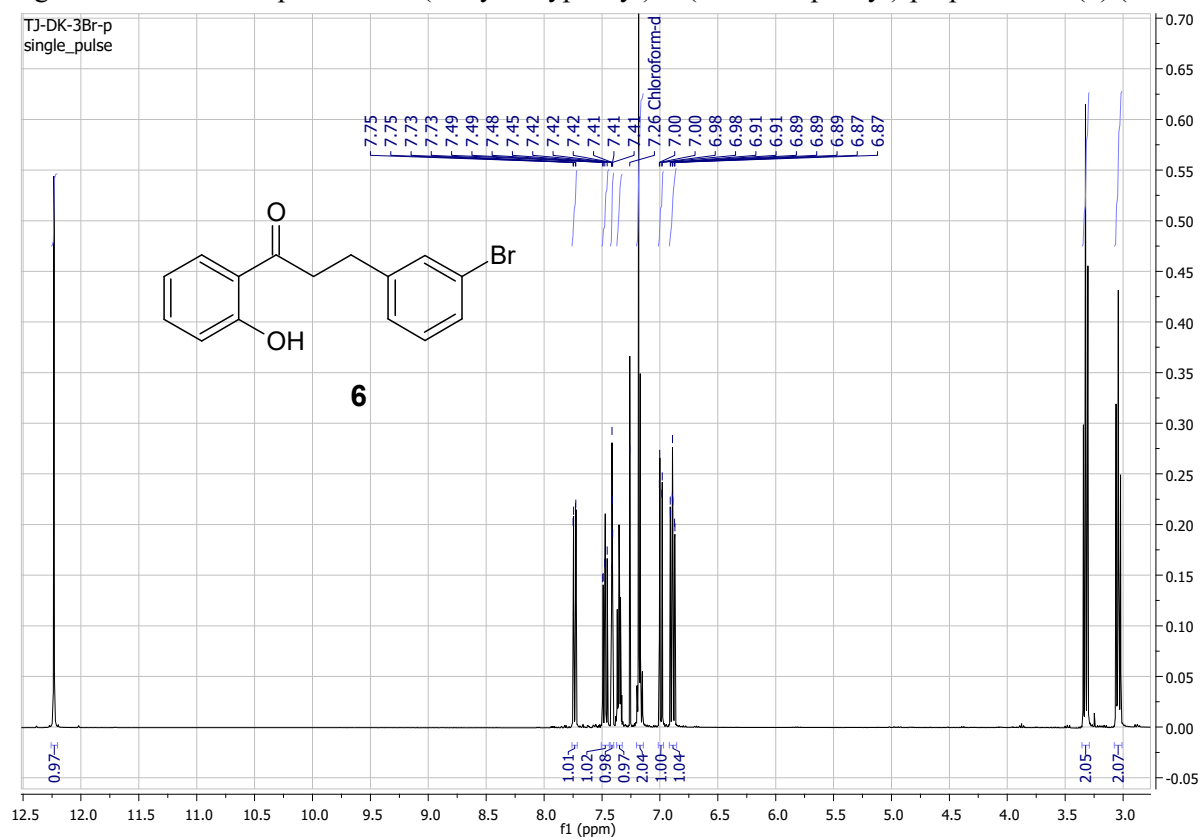


Figure S20. Part of the ^{13}C NMR spectral of 1-(2'-hydroxyphenyl)-3-(3''-bromophenyl)-propan-1-one (**6**) (CDCl_3 , 600 MHz)

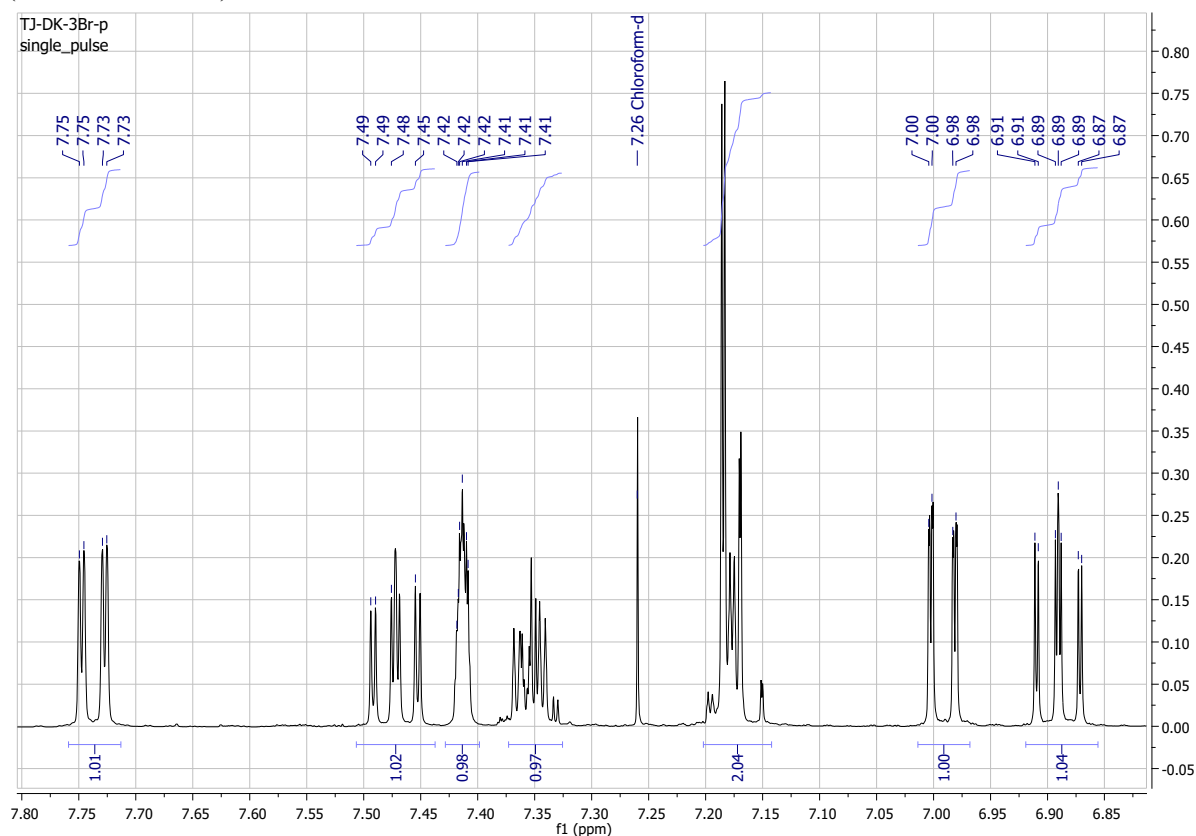


Figure S21. ^{13}C NMR spectral of 1-(2'-hydroxyphenyl)-3-(3''-bromophenyl)-propan-1-one (**6**) (CDCl_3 , 151 MHz)

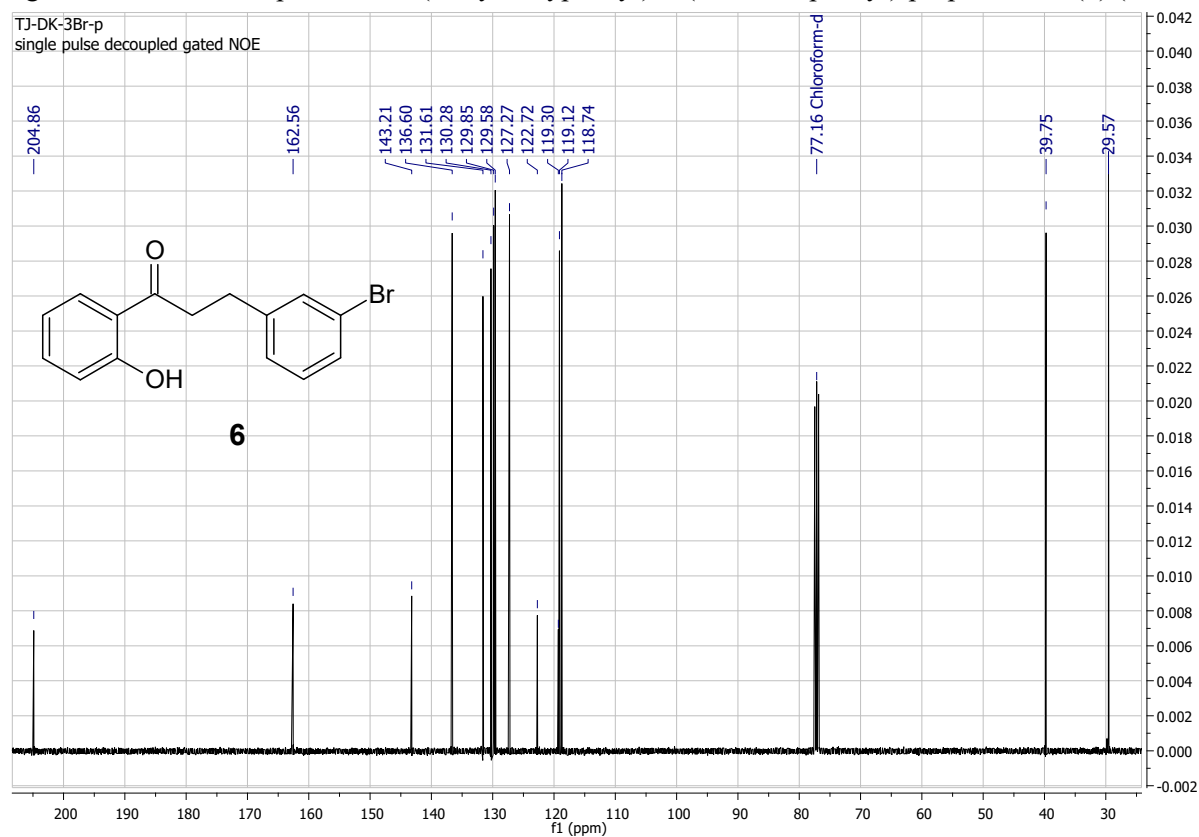


Figure S22. COSY spectral of 1-(2'-hydroxyphenyl)-3-(3''-bromophenyl)-propan-1-one (**6**) (CDCl₃, 151 MHz)

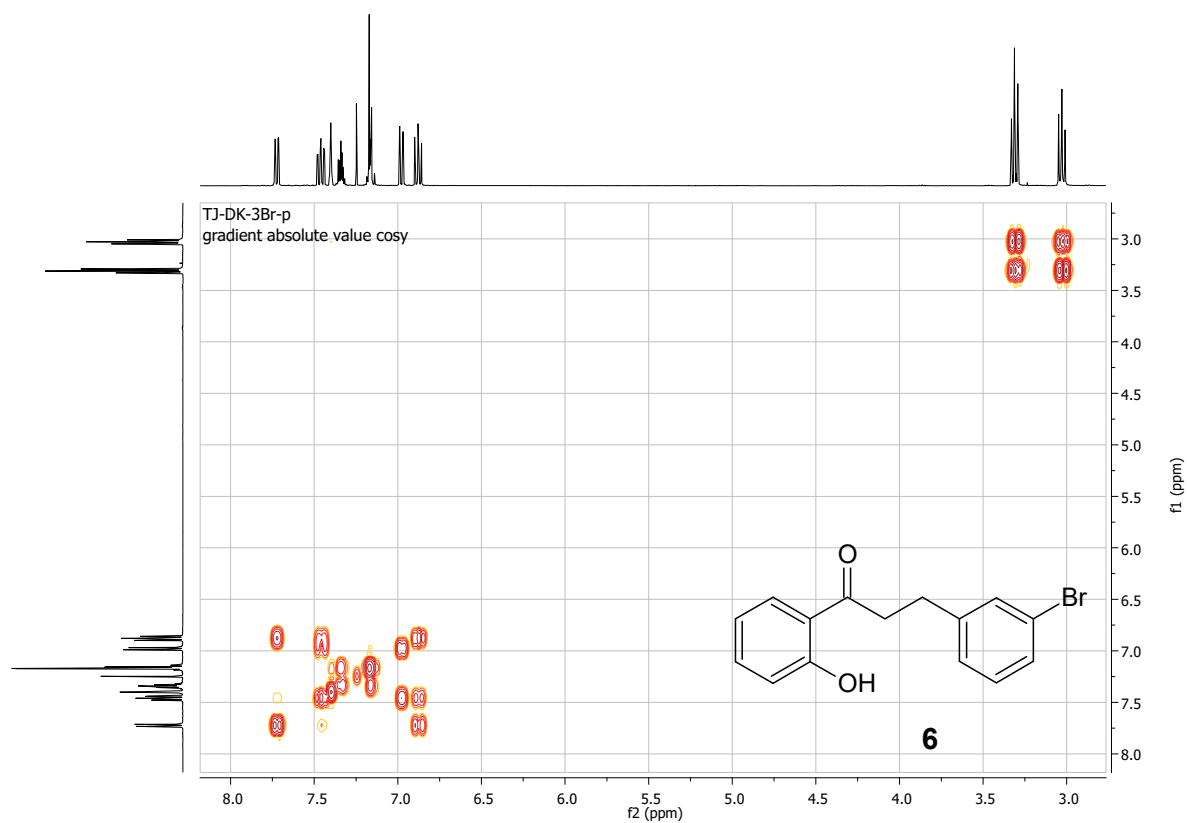


Figure S23. HSQC spectral of 1-(2'-hydroxyphenyl)-3-(3''-bromophenyl)-propan-1-one (**6**) (CDCl₃, 151 MHz)

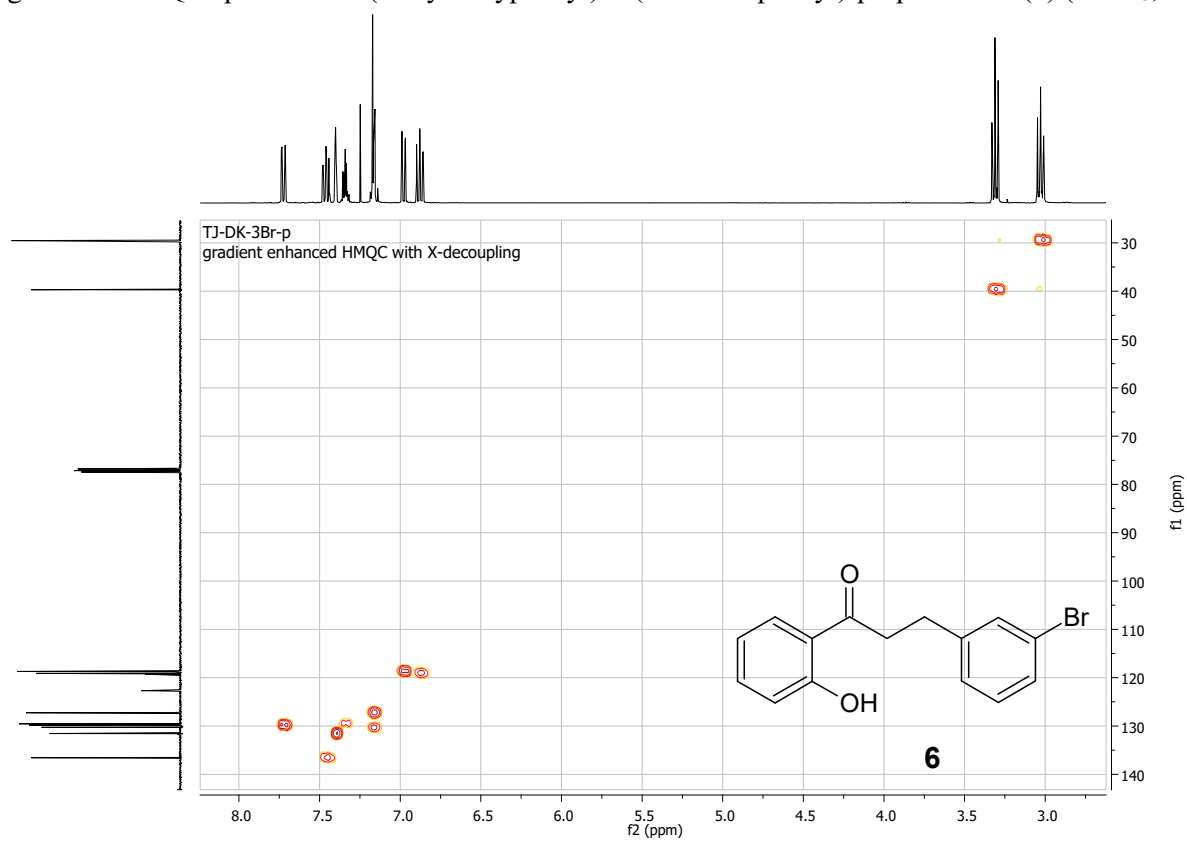


Figure S24. HMBC spectral of 1-(2'-hydroxyphenyl)-3-(3''-bromophenyl)-propan-1-one (**6**) (CDCl₃, 151 MHz)

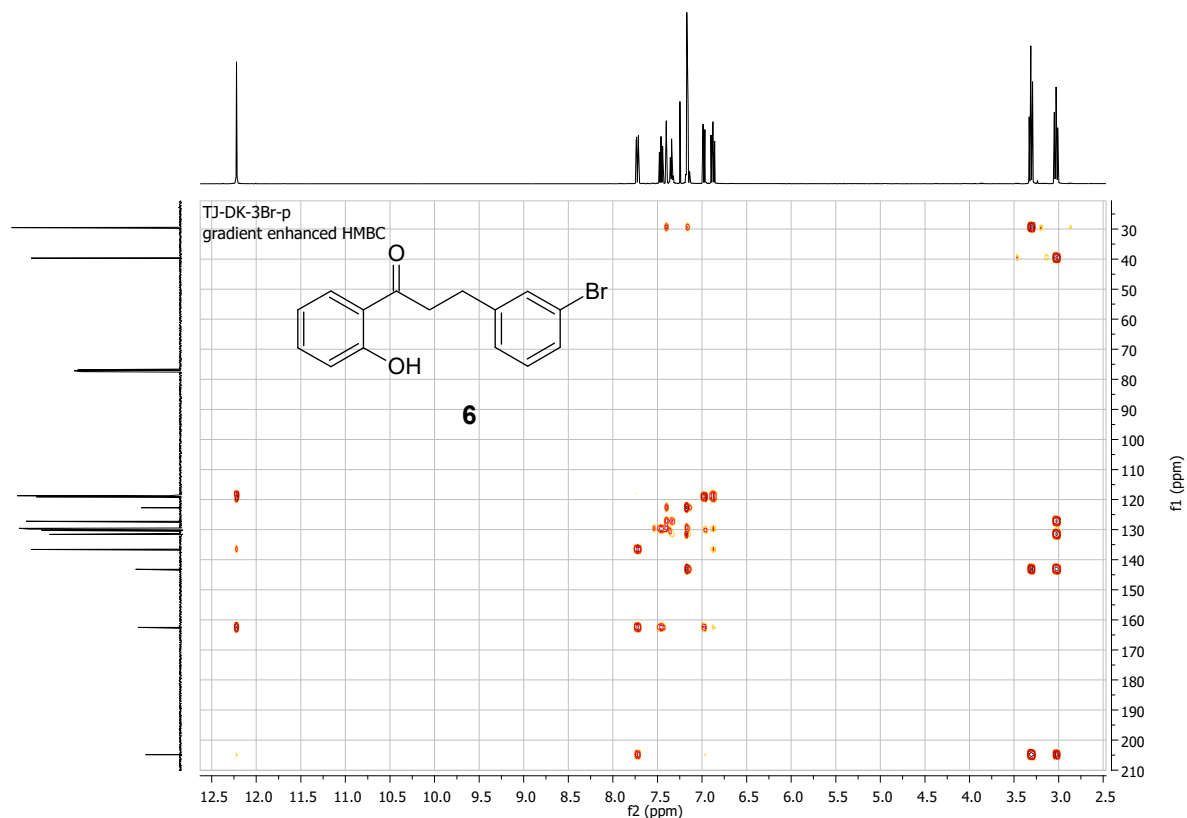


Figure S25. ¹H NMR spectral of 1-(2'-hydroxyphenyl)-3-(4''-bromophenyl)-prop-2-en-1-one (**3**) (CDCl₃, 600 MHz)

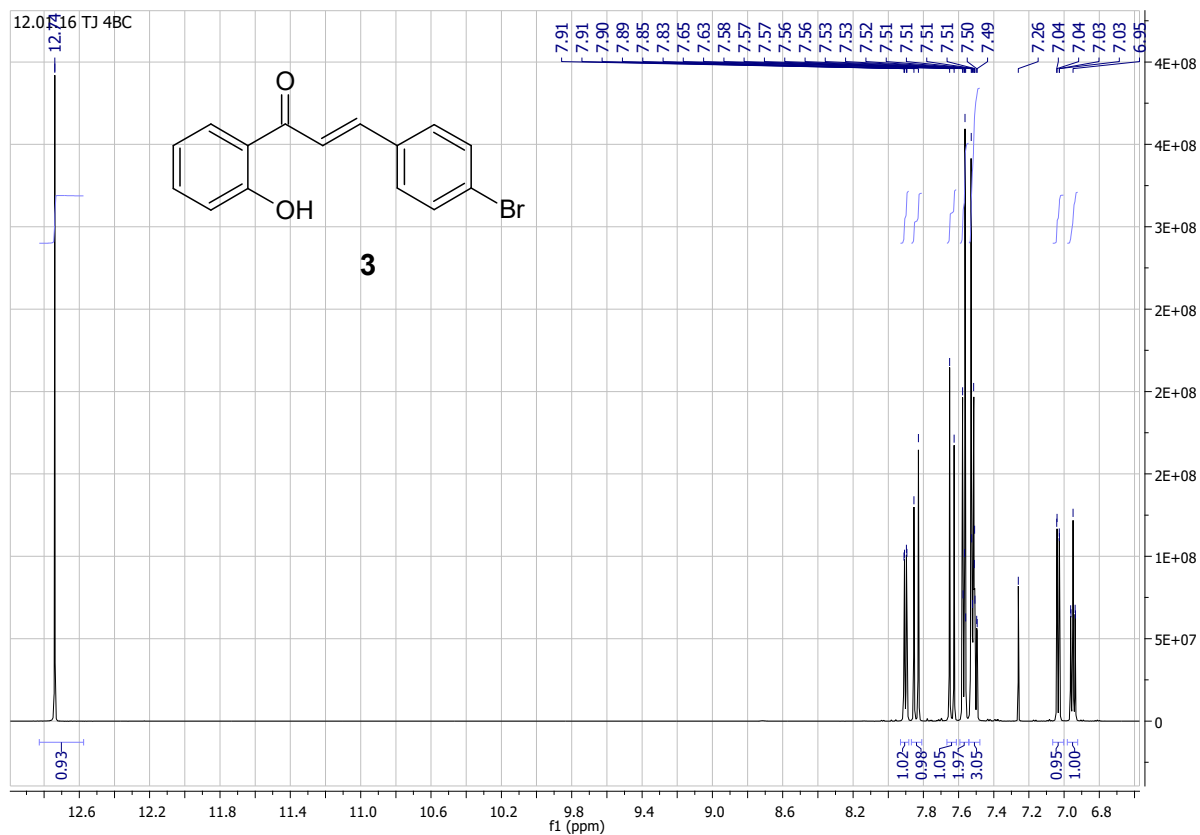


Figure S26. Part of the ^1H NMR spectral of 1-(2'-hydroxyphenyl)-3-(4''-bromophenyl)-prop-2-en-1-one (**3**) (CDCl_3 , 600 MHz)

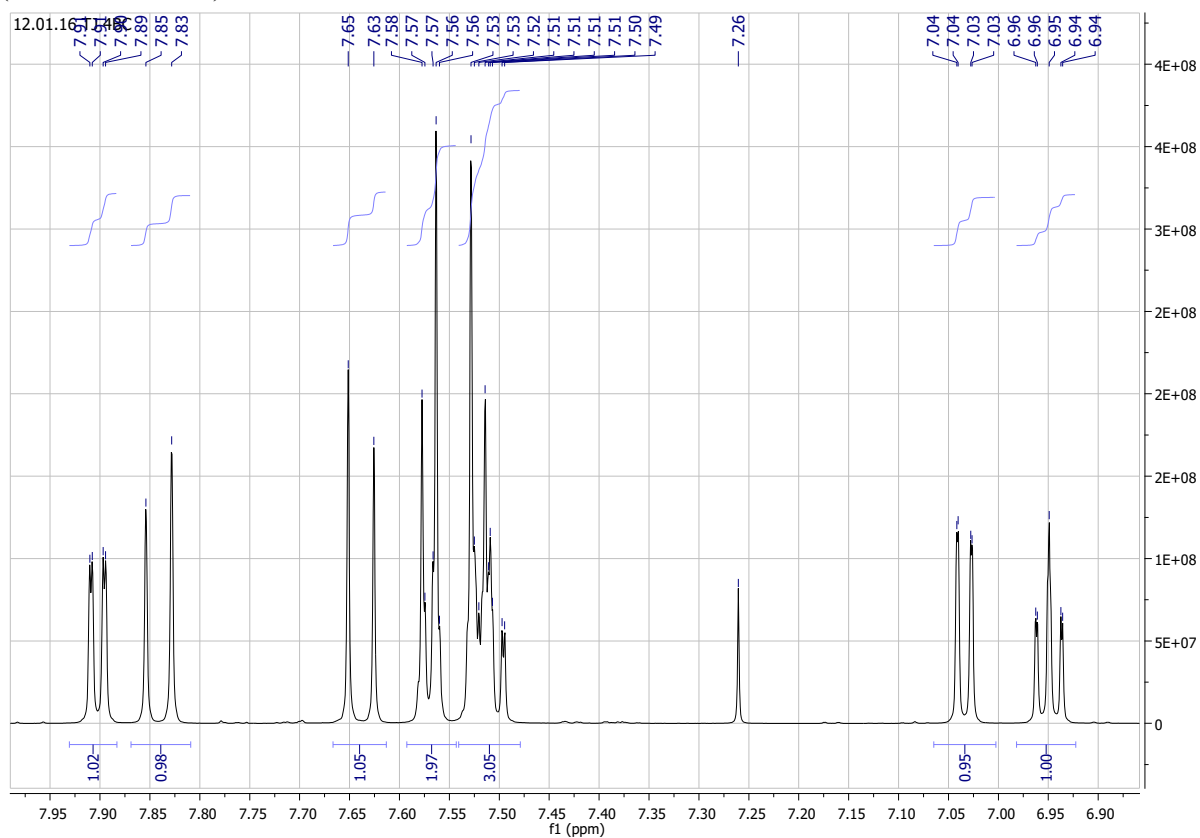


Figure S27. ^{13}C NMR spectral of 1-(2'-hydroxyphenyl)-3-(4''-bromophenyl)-prop-2-en-1-one (**3**) (CDCl_3 , 151 MHz)

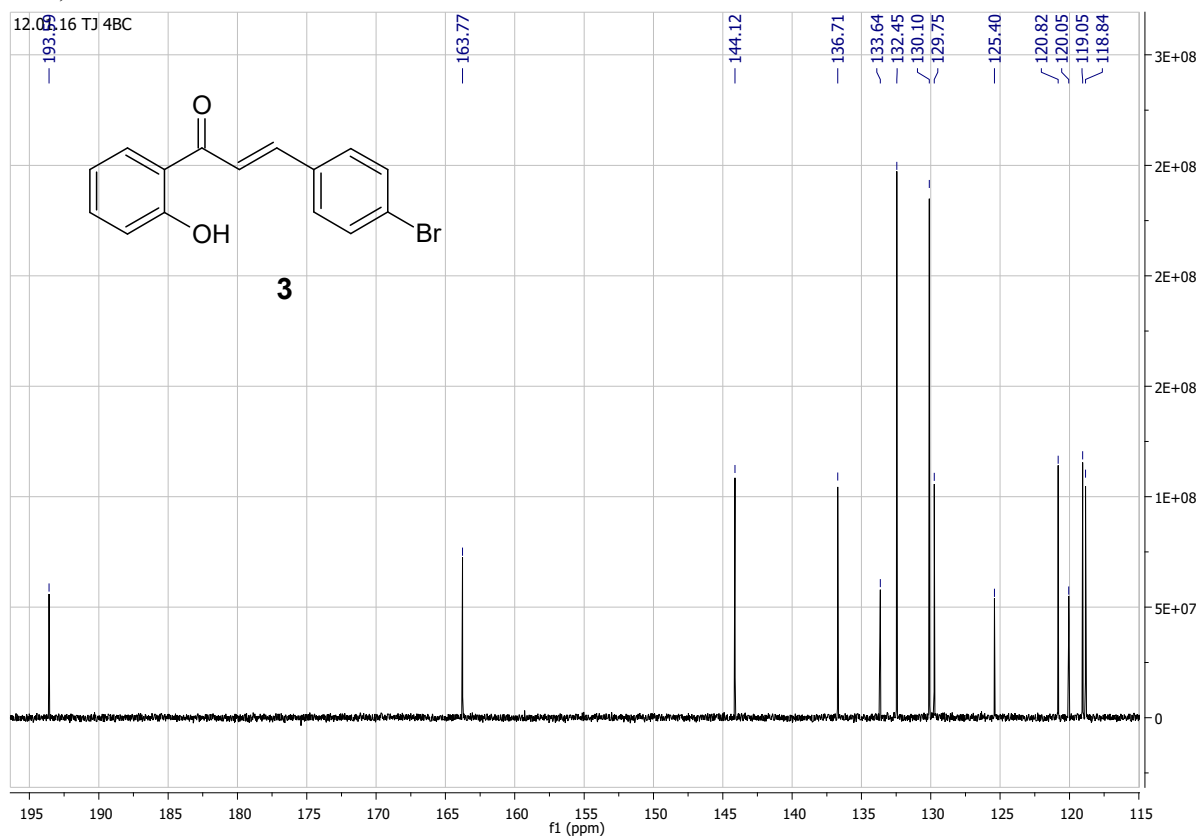


Figure S28. COSY spectral of 1-(2'-hydroxyphenyl)-3-(4''-bromophenyl)-prop-2-en-1-one (**3**) (CDCl₃, 151 MHz)

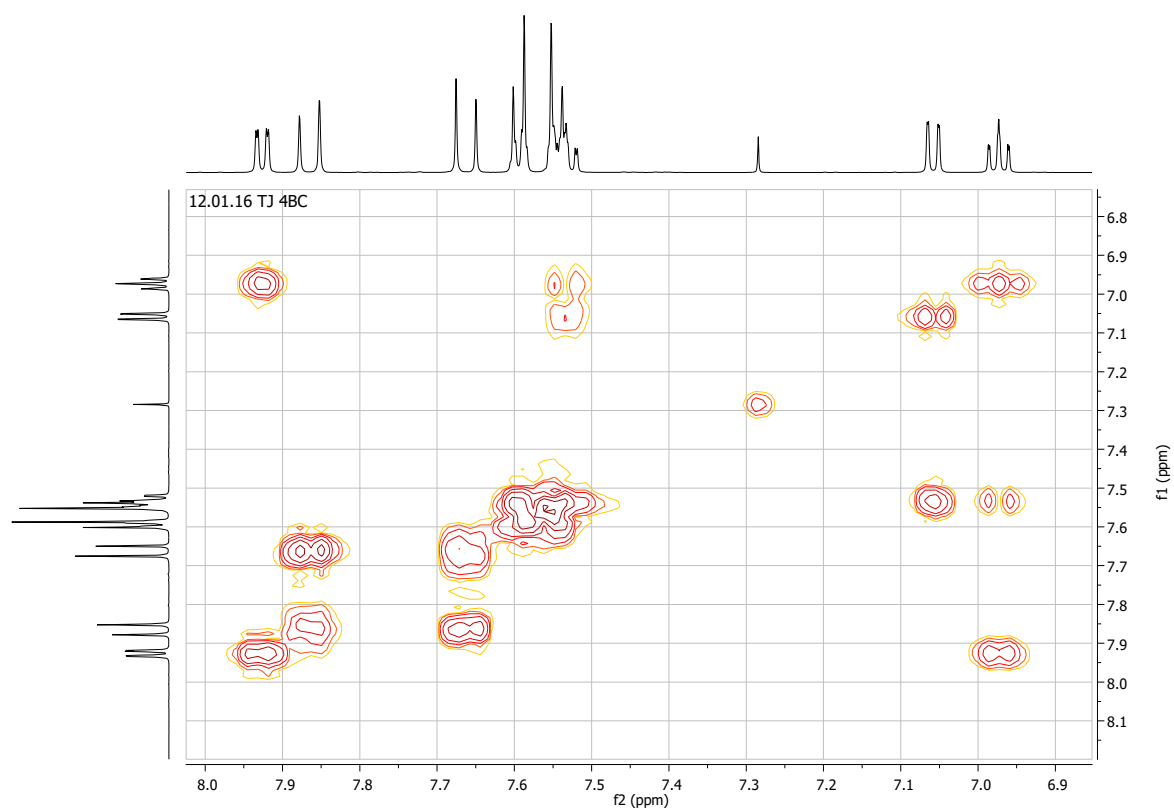


Figure S29. HSQC spectral of 1-(2'-hydroxyphenyl)-3-(4''-bromophenyl)-prop-2-en-1-one (**3**) (CDCl₃, 151 MHz)

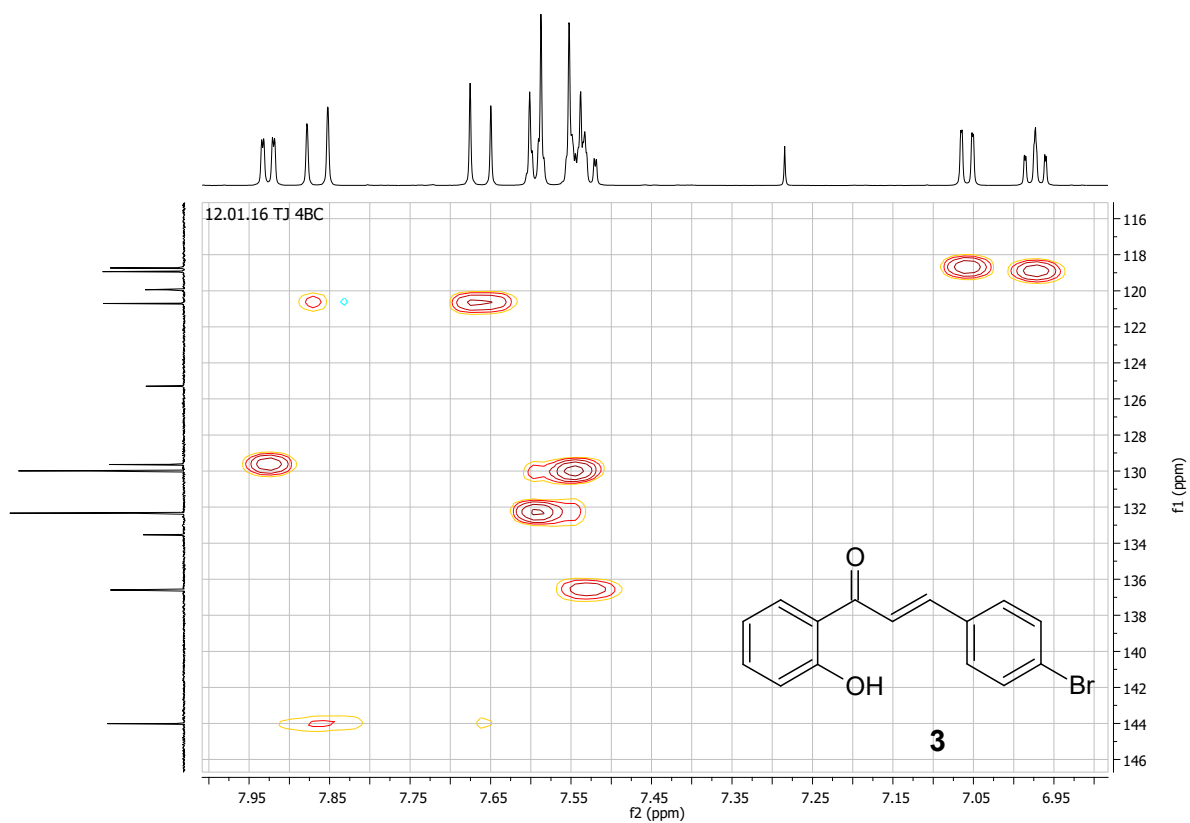


Figure S30. ^1H NMR spectral of 1-(2'-hydroxyphenyl)-3-(4''-bromophenyl)-propan-1-one (**7**) (CDCl_3 , 600 MHz)

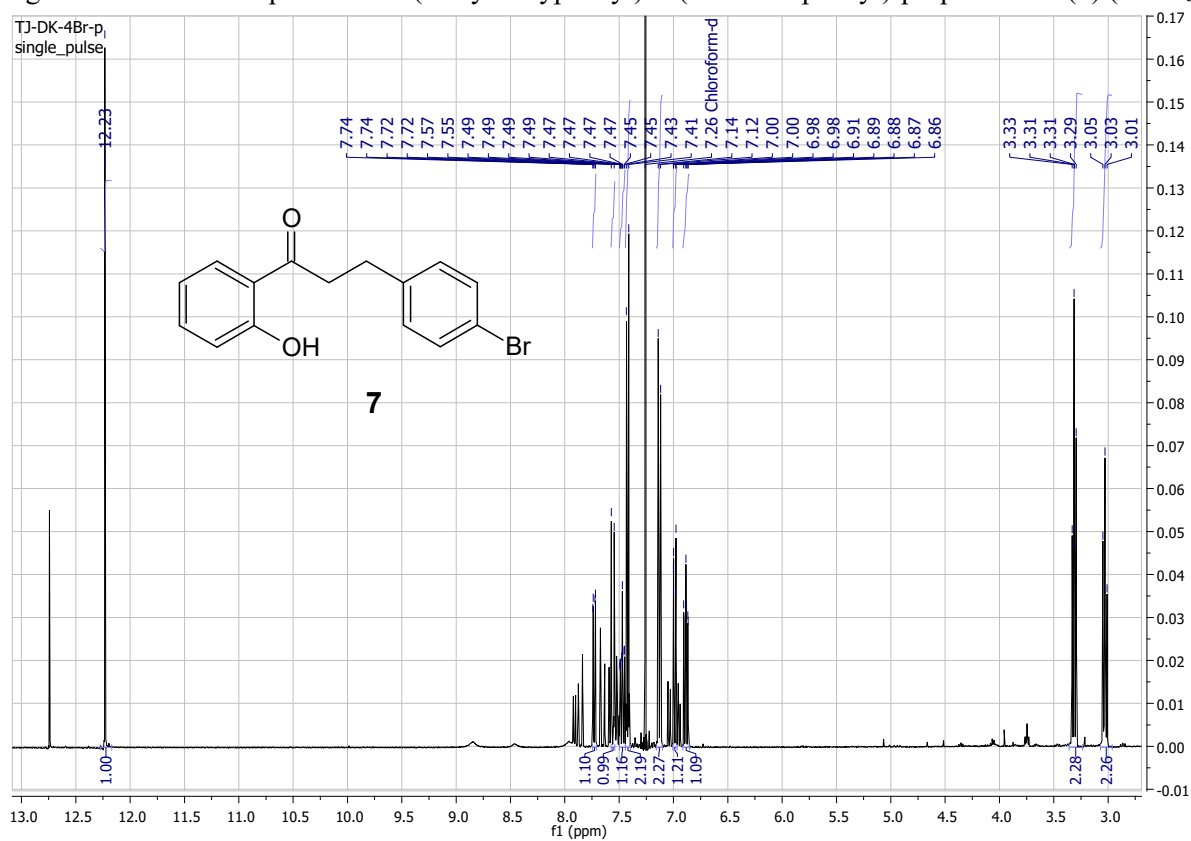


Figure S31. Part of the ^{13}C NMR spectral of 1-(2'-hydroxyphenyl)-3-(4''-bromophenyl)-propan-1-one (**7**) (CDCl_3 , 600 MHz)

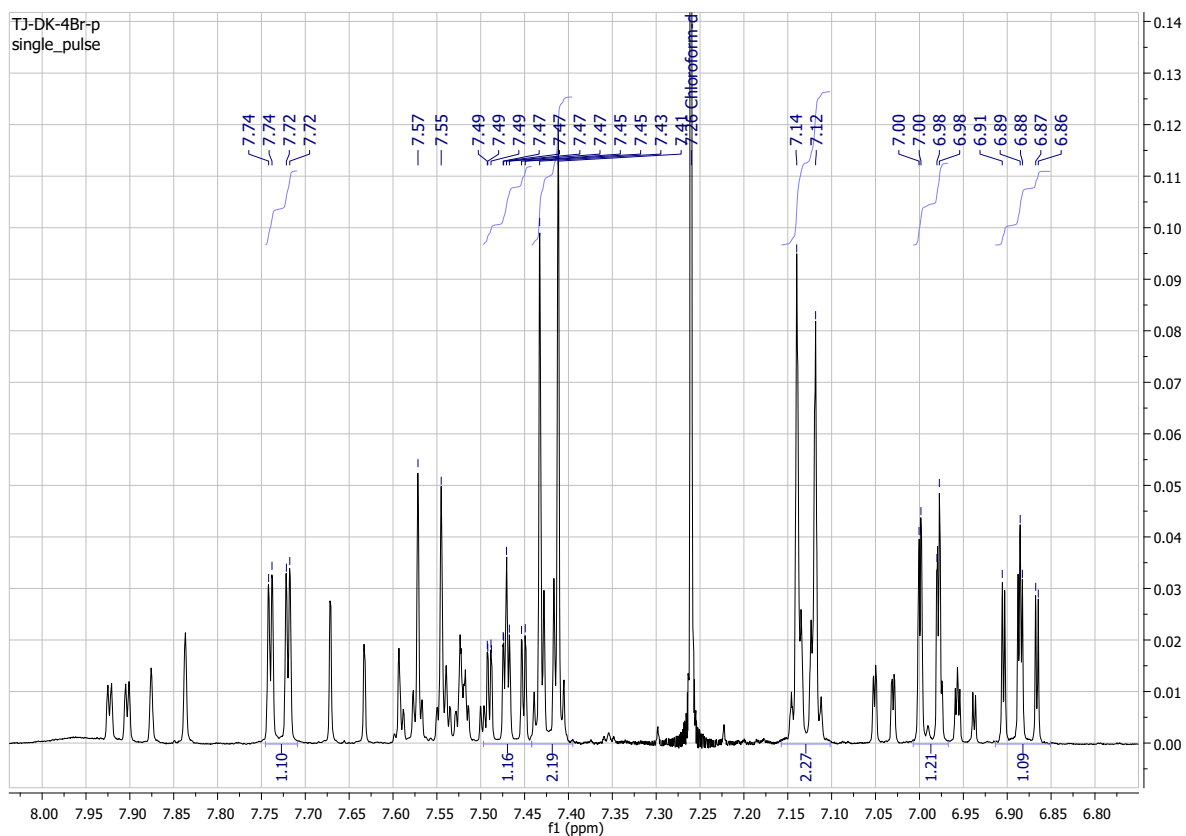


Figure S32. ^{13}C NMR spectral of 1-(2'-hydroxyphenyl)-3-(4''-bromophenyl)propan-1-one (**7**) (CDCl_3 , 151 MHz)

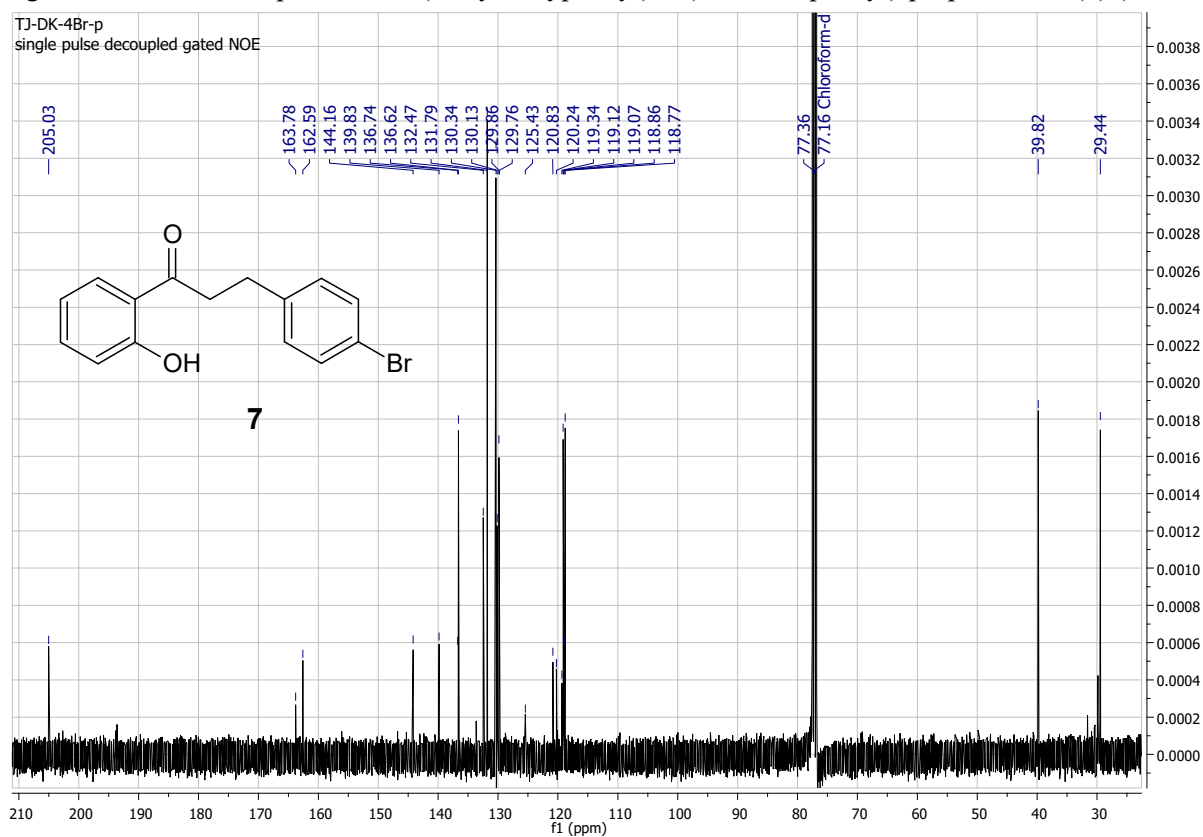


Figure S33. COSY spectral of 1-(2'-hydroxyphenyl)-3-(4''-bromophenyl)propan-1-one (**7**) (CDCl_3 , 151 MHz)

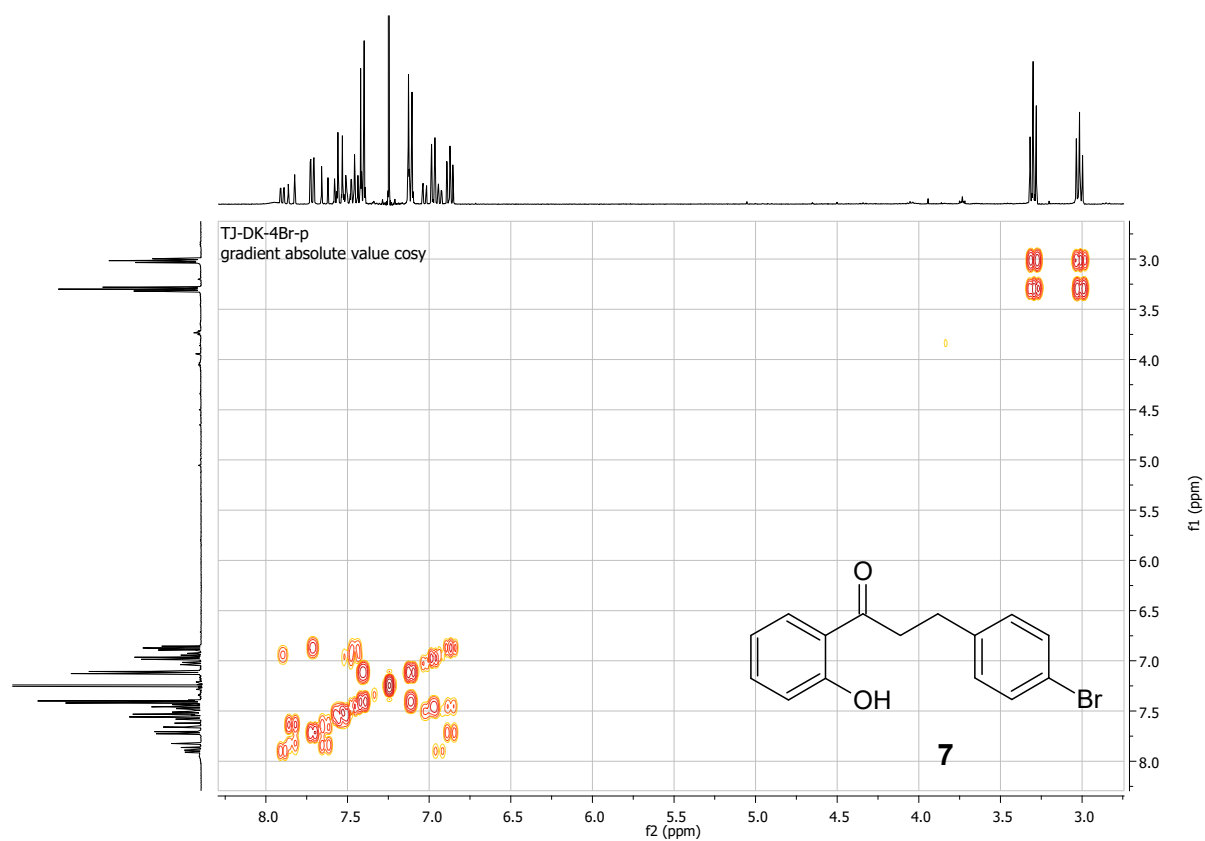


Figure S34. HSQC spectral of 1-(2'-hydroxyphenyl)-3-(4''-bromophenyl)-propan-1-one (**7**) (CDCl₃, 151 MHz)

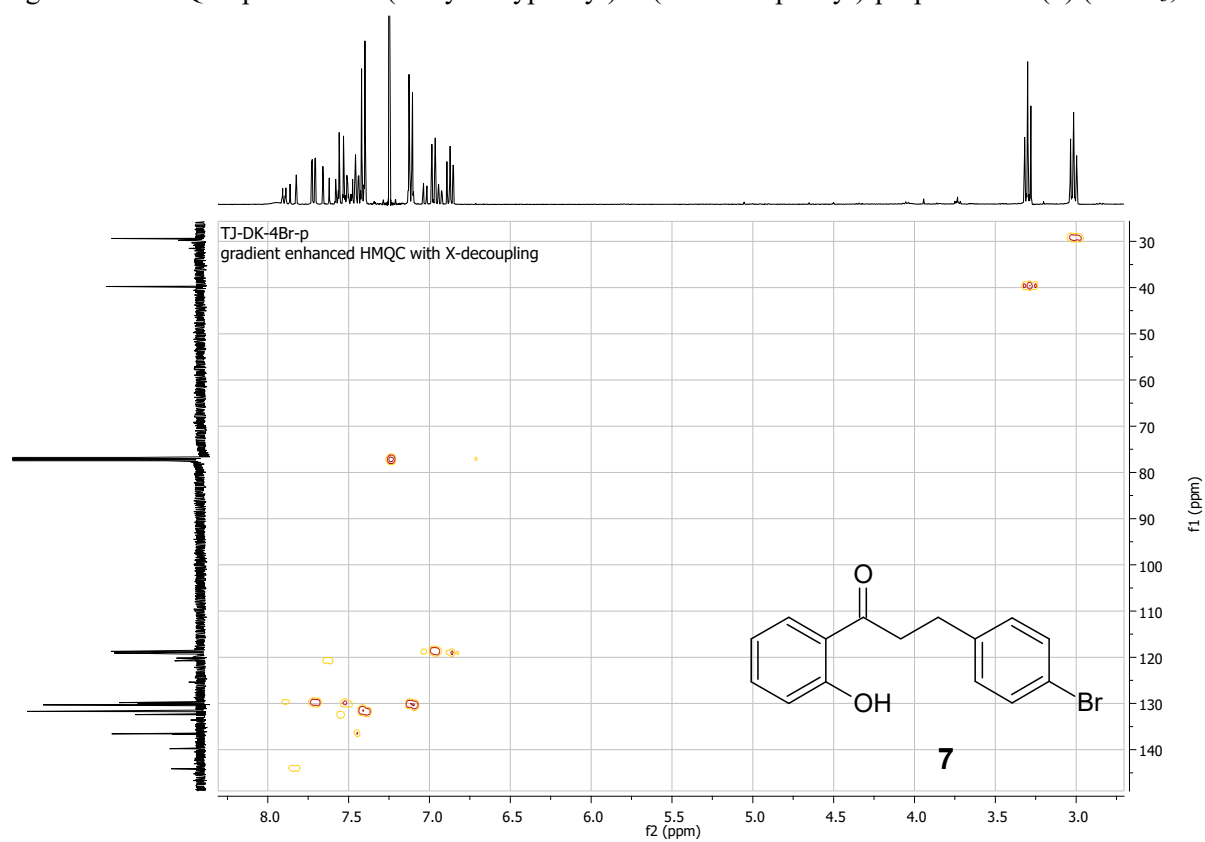


Figure S35. HMBC spectral of 1-(2'-hydroxyphenyl)-3-(4''-bromophenyl)-propan-1-one (**7**) (CDCl₃, 151 MHz)

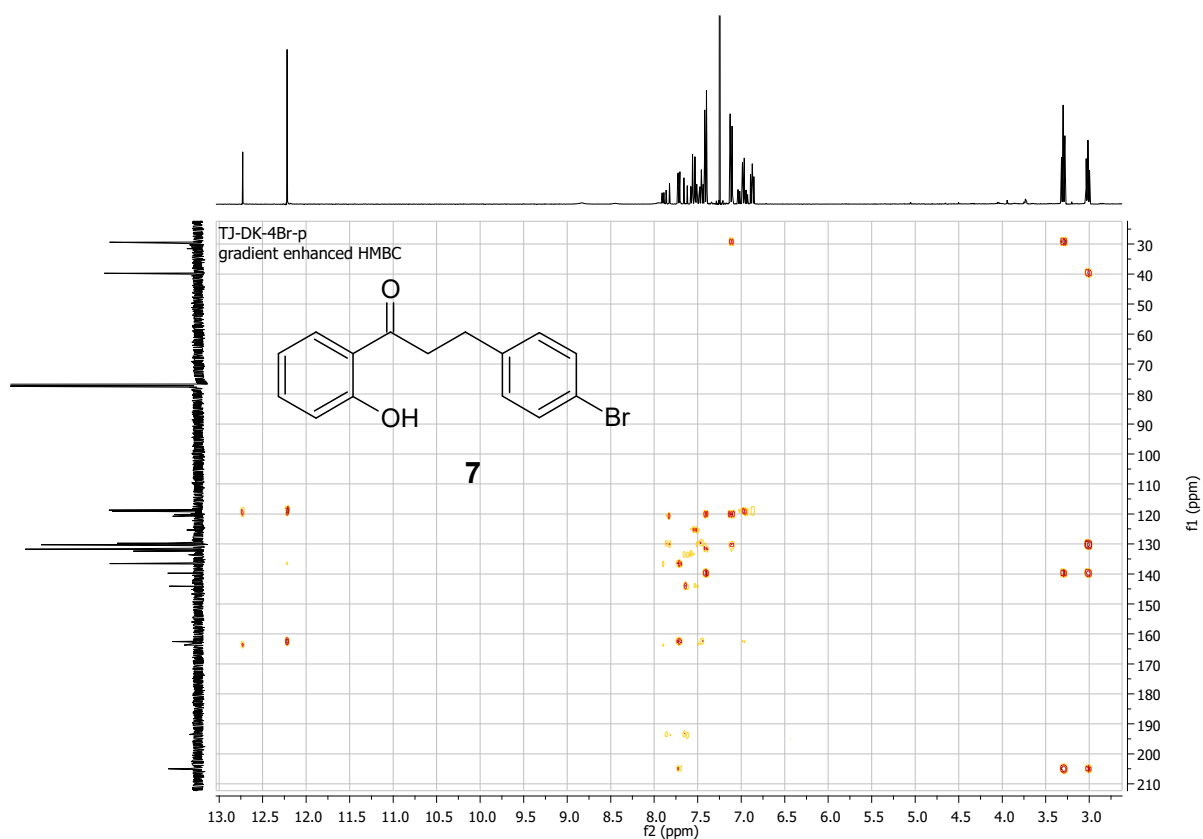


Figure S36. ^1H NMR spectral of 1-(5'-bromo-2'-hydroxyphenyl)-3-phenyl-propan-1-one (**4**) (CDCl_3 , 600 MHz)

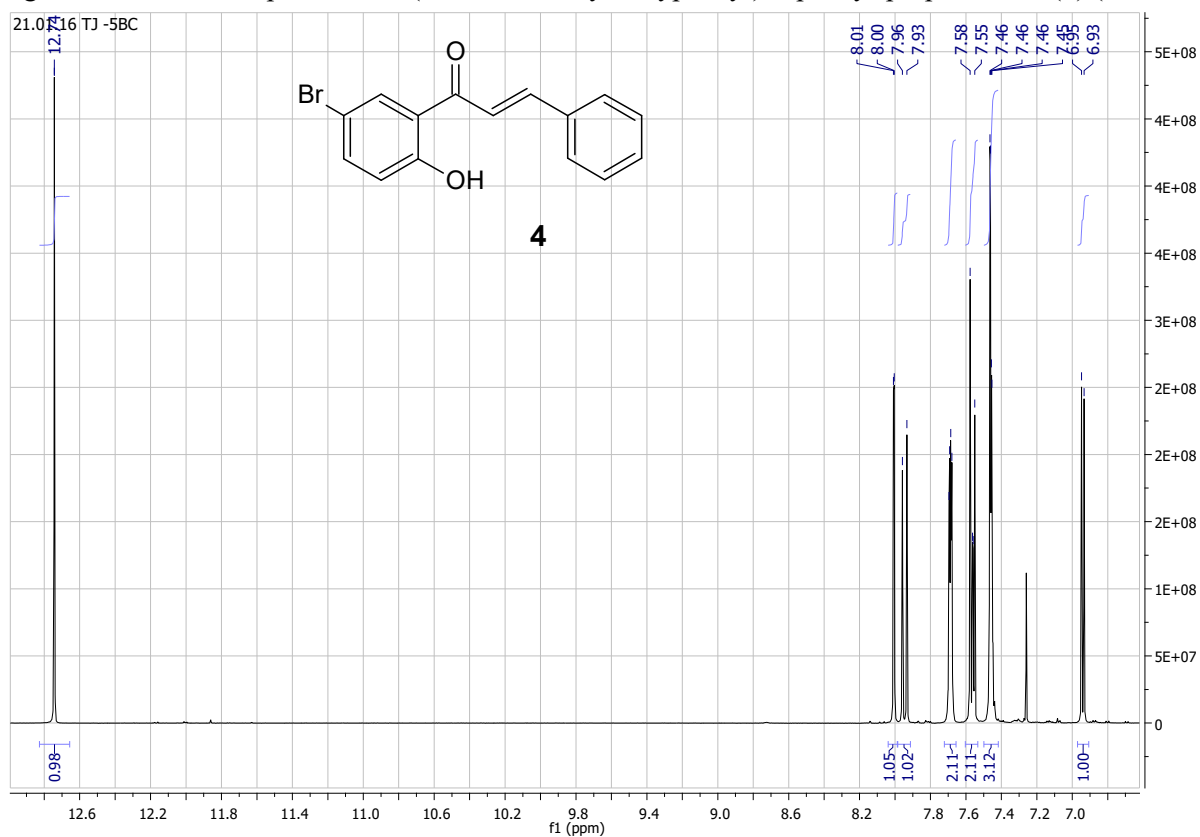


Figure S37. Part of the ^1H NMR spectral of 1-(5'-bromo-2'-hydroxyphenyl)-3-phenyl-propan-1-one (**4**)

(CDCl₃, 600 MHz)

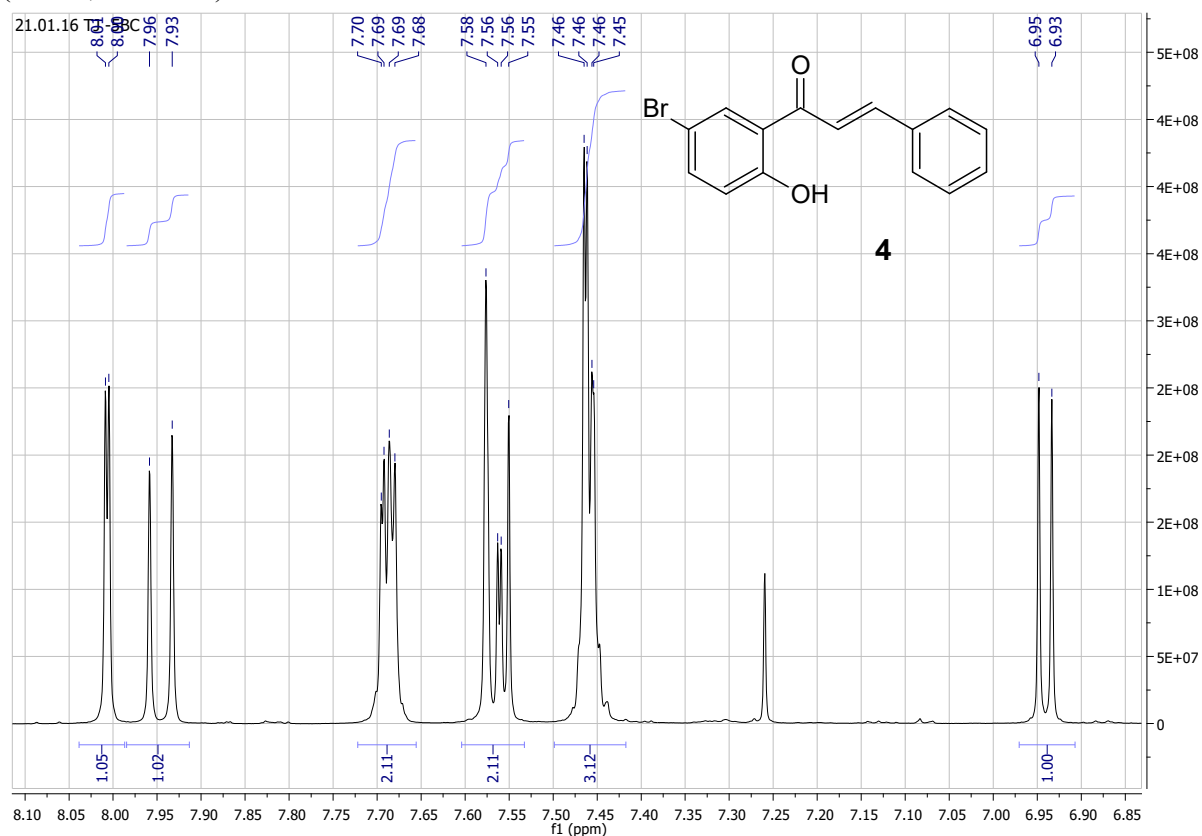


Figure S38. ¹³C NMR spectral of 1-(5'-bromo-2'-hydroxyphenyl)-3-phenyl-propan-1-one (**4**) (CDCl₃, 151 MHz)

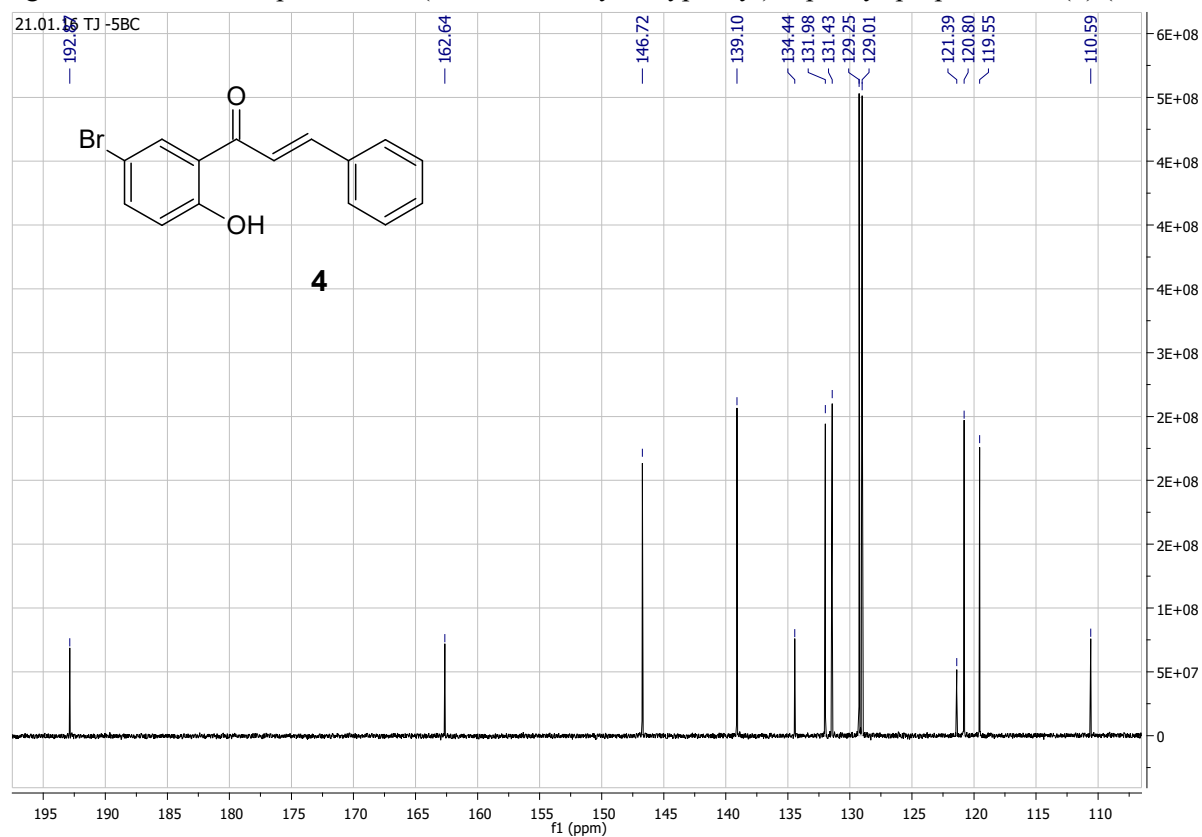


Figure S39. COSY spectral of 1-(5'-bromo-2'-hydroxyphenyl)-3-phenyl-propan-1-one (**4**) (CDCl₃, 151 MHz)

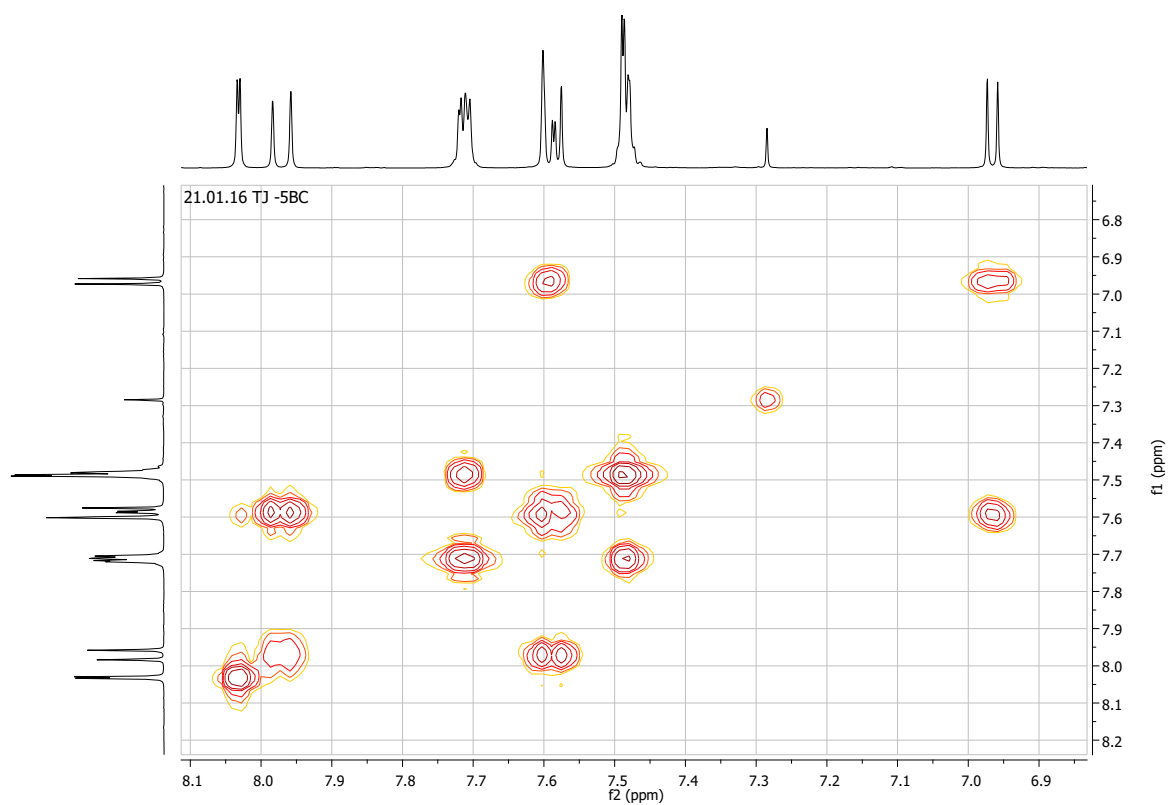


Figure S40. HSQC spectral of 1-(5'-bromo-2'-hydroxyphenyl)-3-phenyl-propan-1-one (**4**) (CDCl₃, 151 MHz)

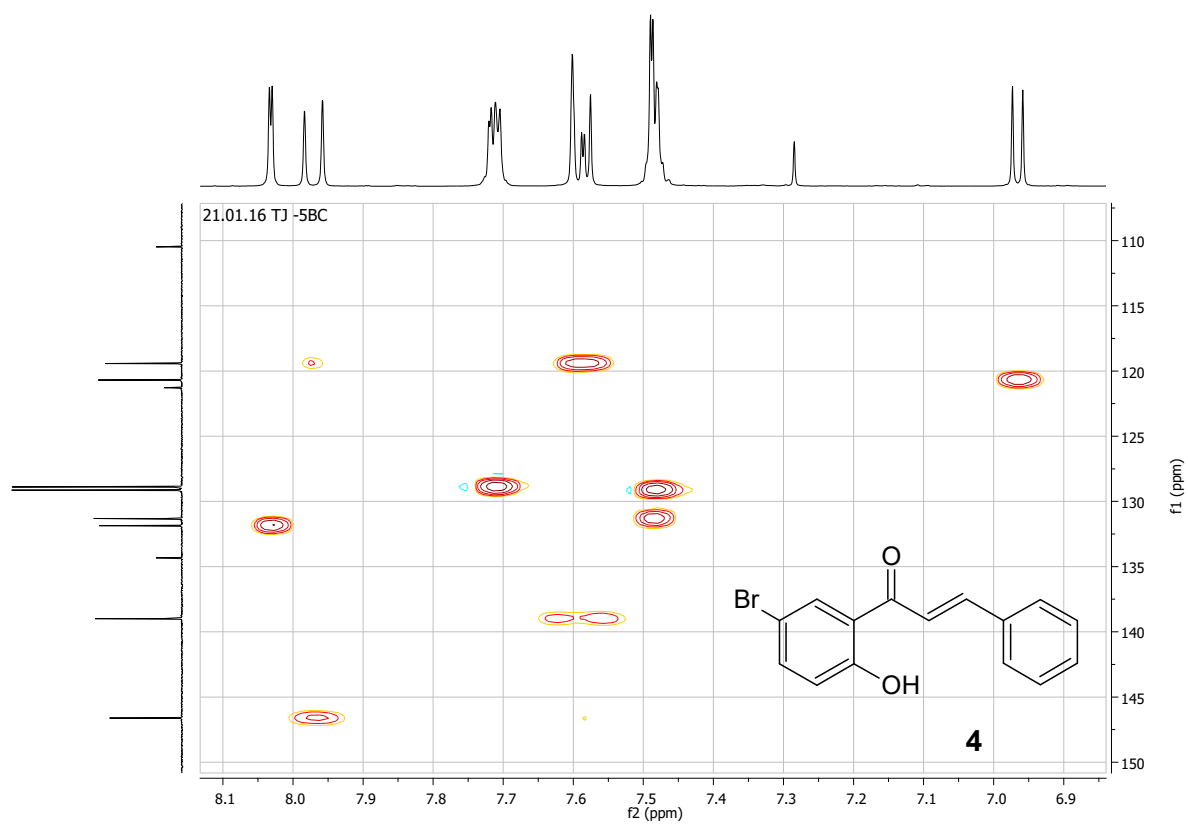


Figure S41. ¹H NMR spectral of 1-(5'-bromo-2'-hydroxyphenyl)-3-phenyl-prop-2-en-1-one (**8**) (CDCl₃, 600 MHz)

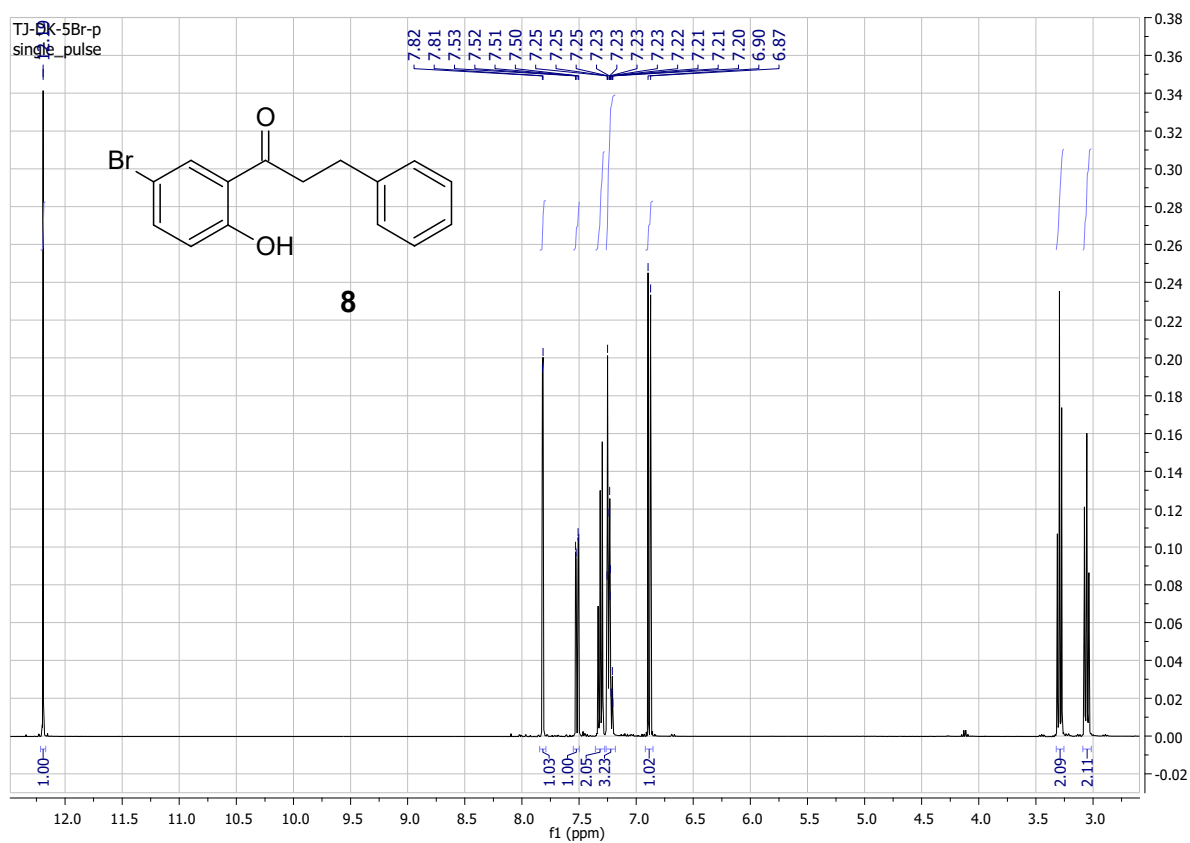


Figure S42. Part of the ¹³C NMR spectral of 1-(5'-bromo-2'-hydroxyphenyl)-3-phenyl-prop-2-en-1-one (**8**) (CDCl₃, 600 MHz)

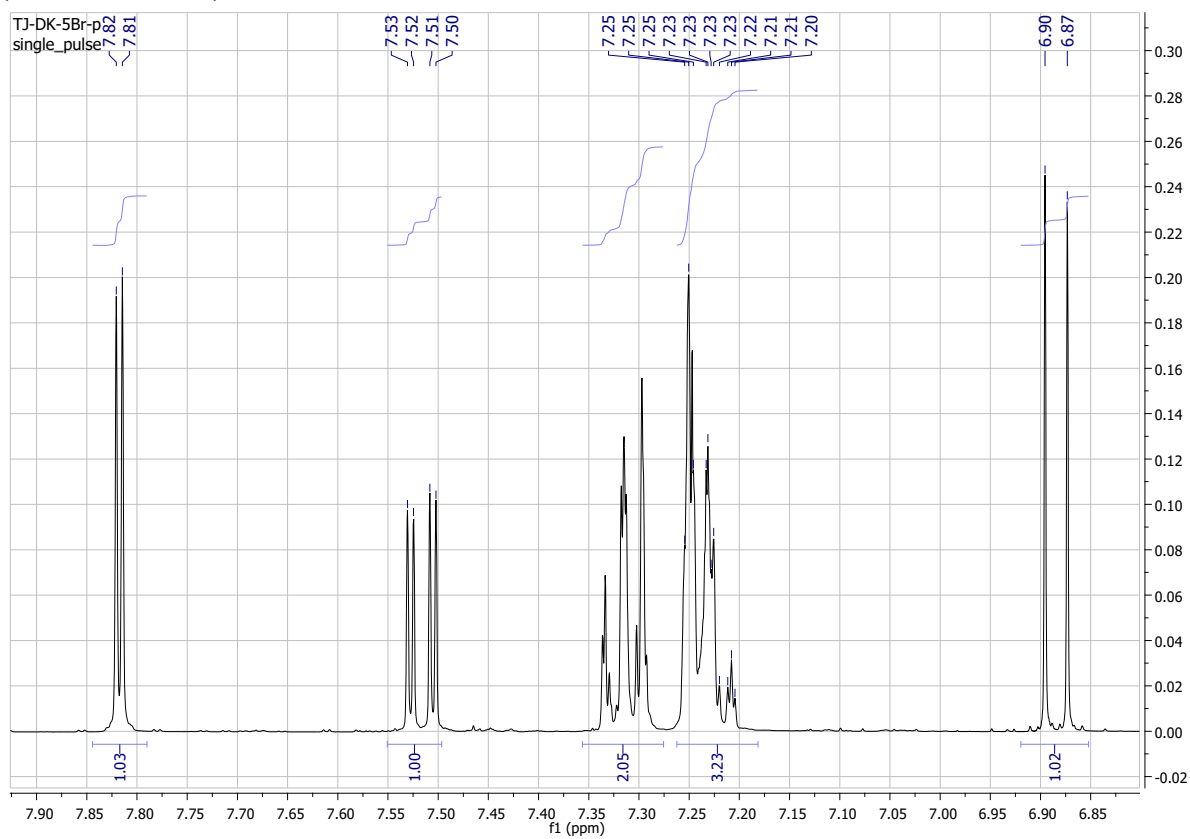


Figure S43. ^{13}C NMR spectral of 1-(5'-bromo-2'-hydroxyphenyl)-3-phenyl-prop-2-en-1-one (**8**) (CDCl_3 , 151 MHz)

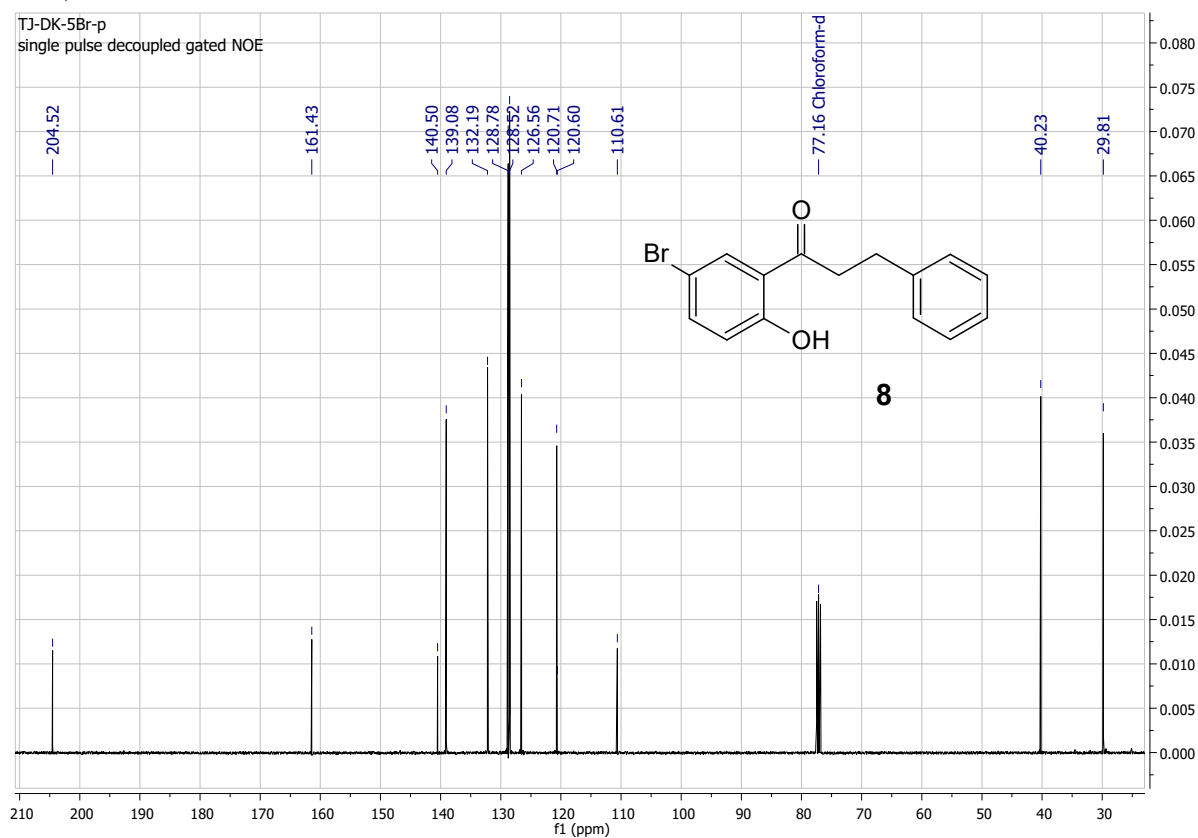


Figure S44. COSY spectral of 1-(5'-bromo-2'-hydroxyphenyl)-3-phenyl-prop-2-en-1-one (**8**) (CDCl_3 , 151 MHz)

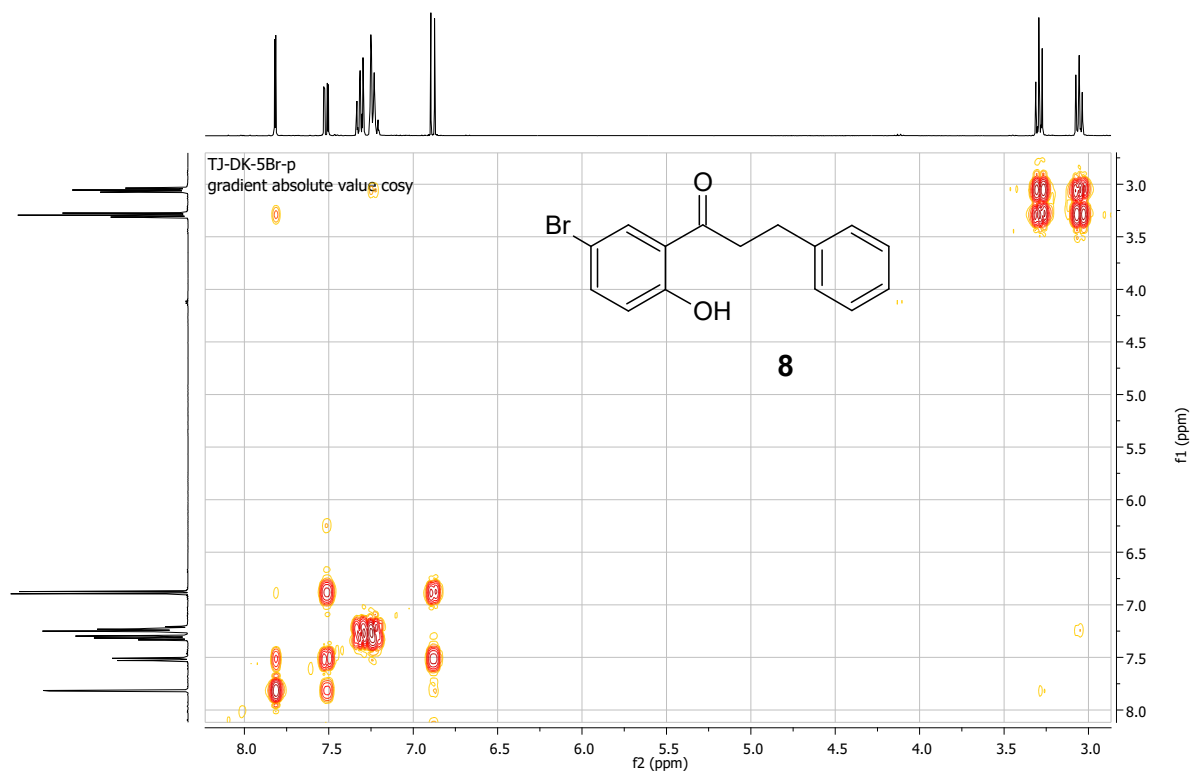


Figure S45. HSQC spectral of 1-(5'-bromo-2'-hydroxyphenyl)-3-phenyl-prop-2-en-1-one (**8**) (CDCl₃, 151 MHz)

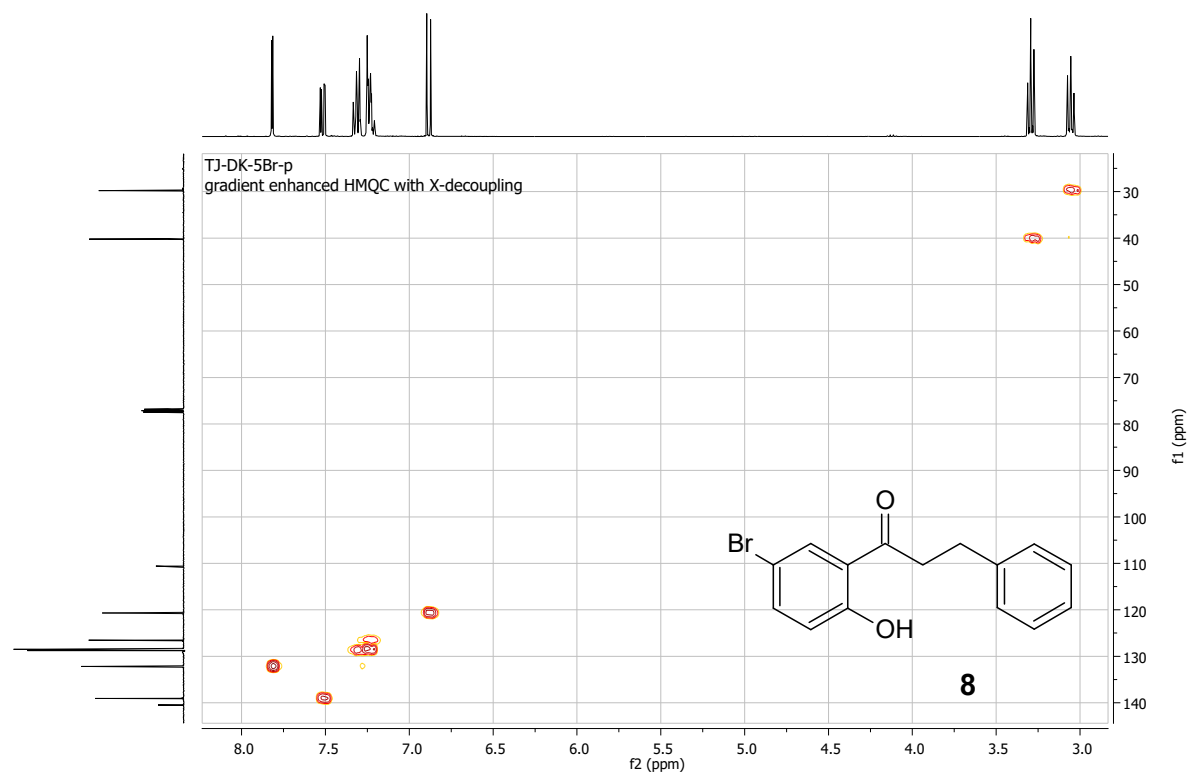


Figure S46. HMBC spectral of 1-(5'-bromo-2'-hydroxyphenyl)-3-phenyl-prop-2-en-1-one (**8**) (CDCl₃, 151 MHz)

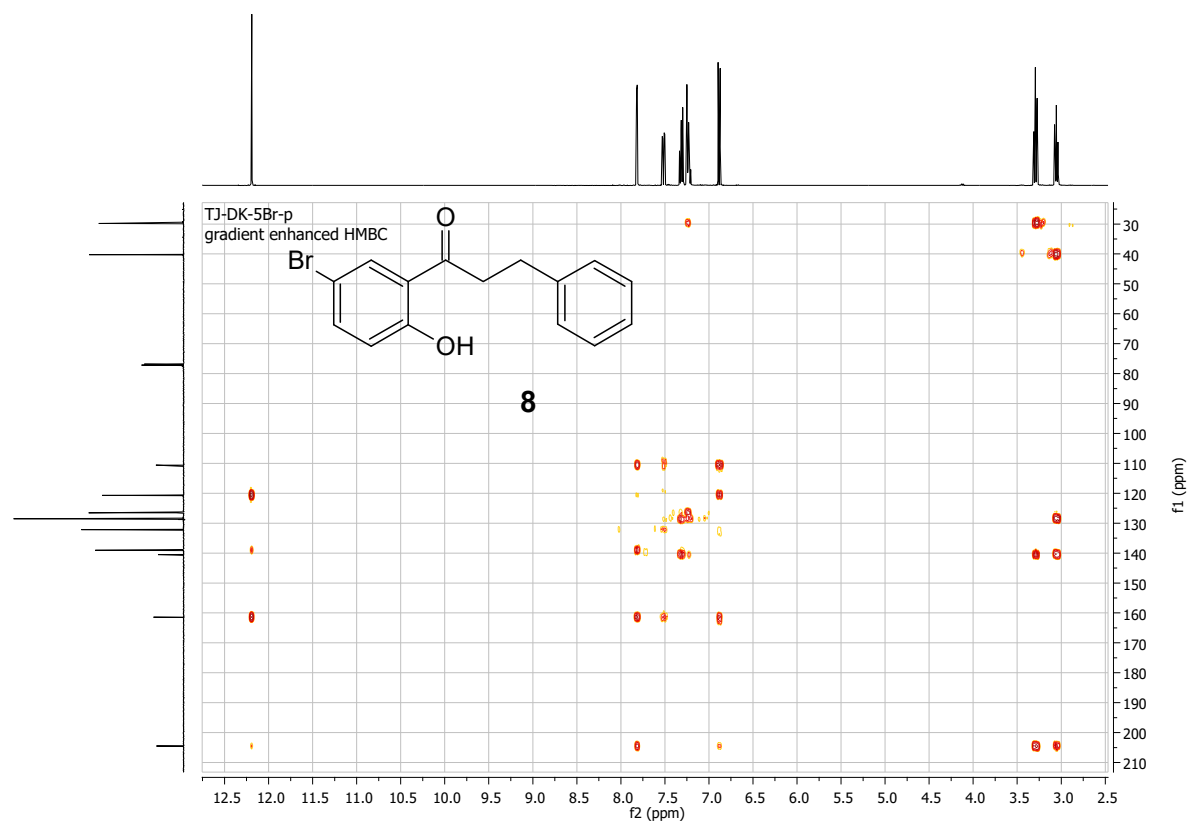


Figure S47. Preparative TLC plate showing the separation of the post-reaction mixture after biotransformation of 2'-hydroxy-2"-bromochalcone (**1**)

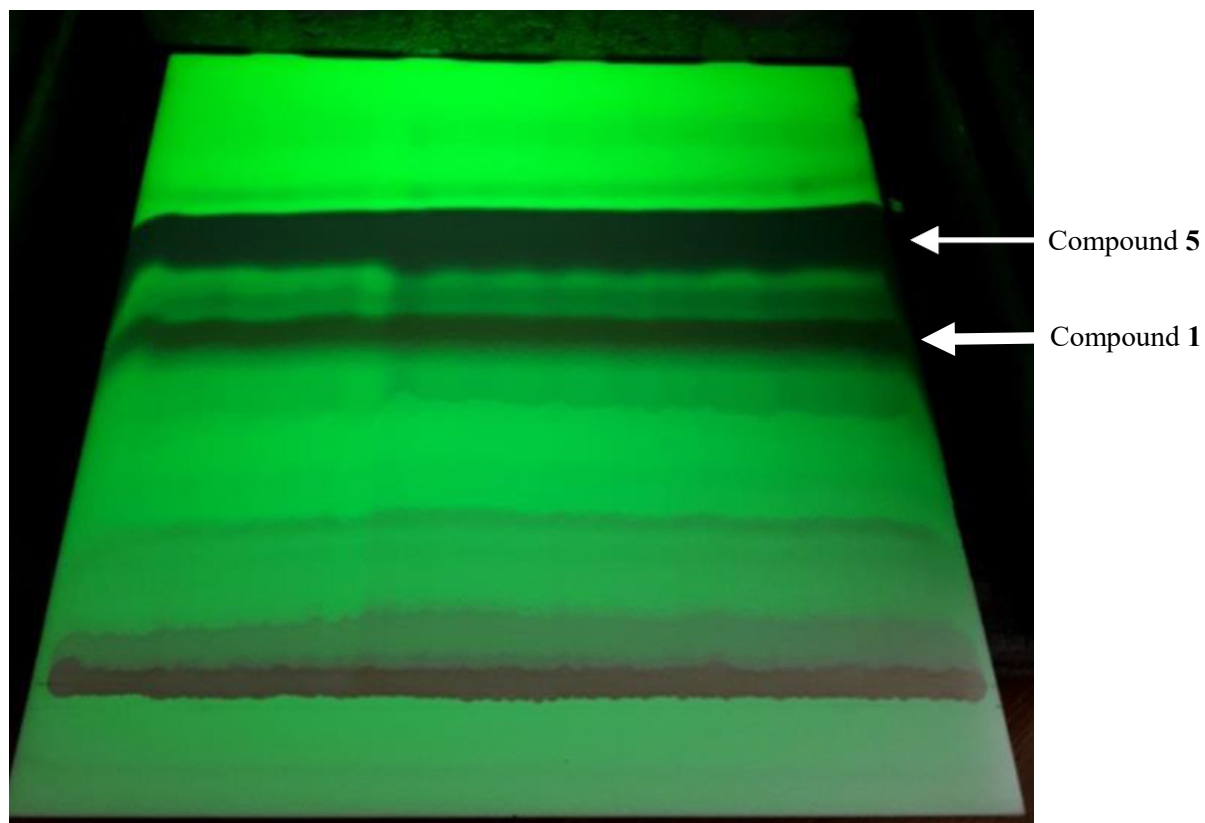


Figure S48. Preparative TLC plate showing the separation of the post-reaction mixture after biotransformation of 2'-hydroxy-3"-bromochalcone (**2**)

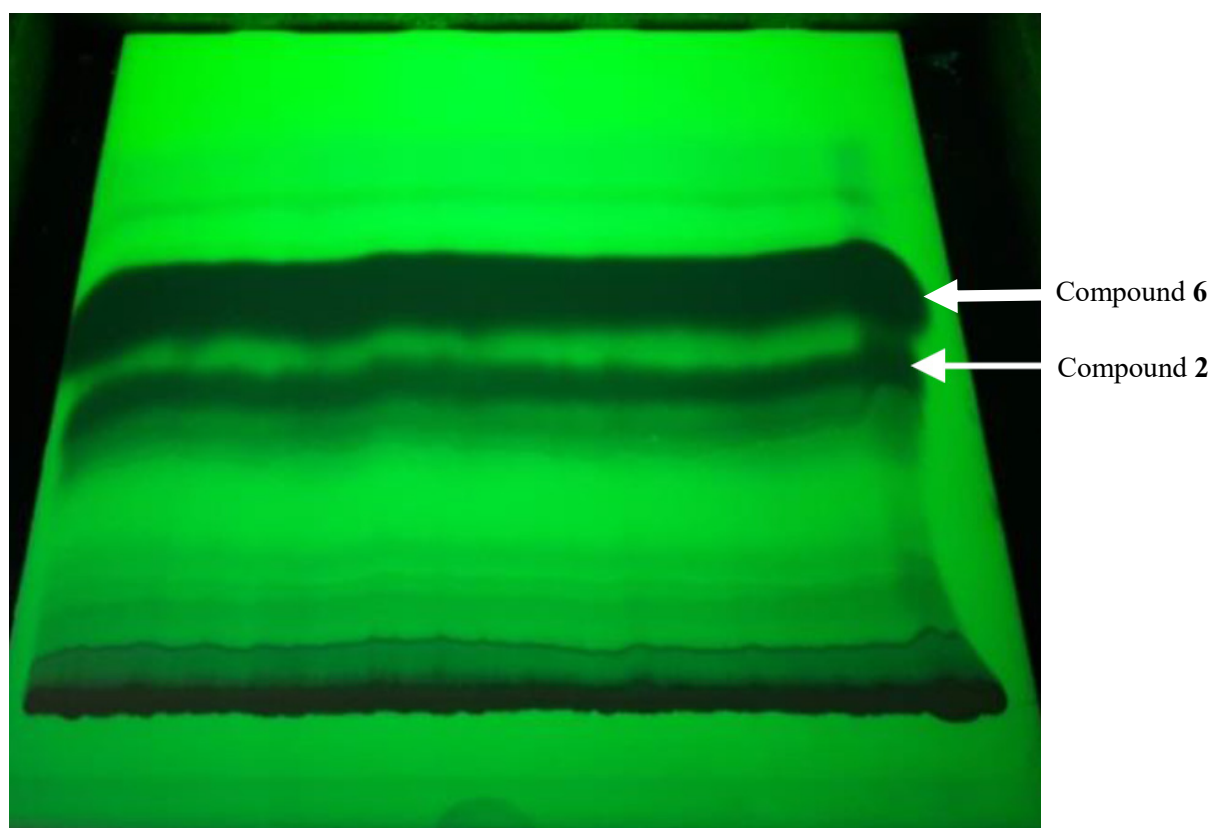


Figure S49. Preparative TLC plate showing the separation of the post-reaction mixture after biotransformation of 2'-hydroxy-4''-bromochalcone (**3**)

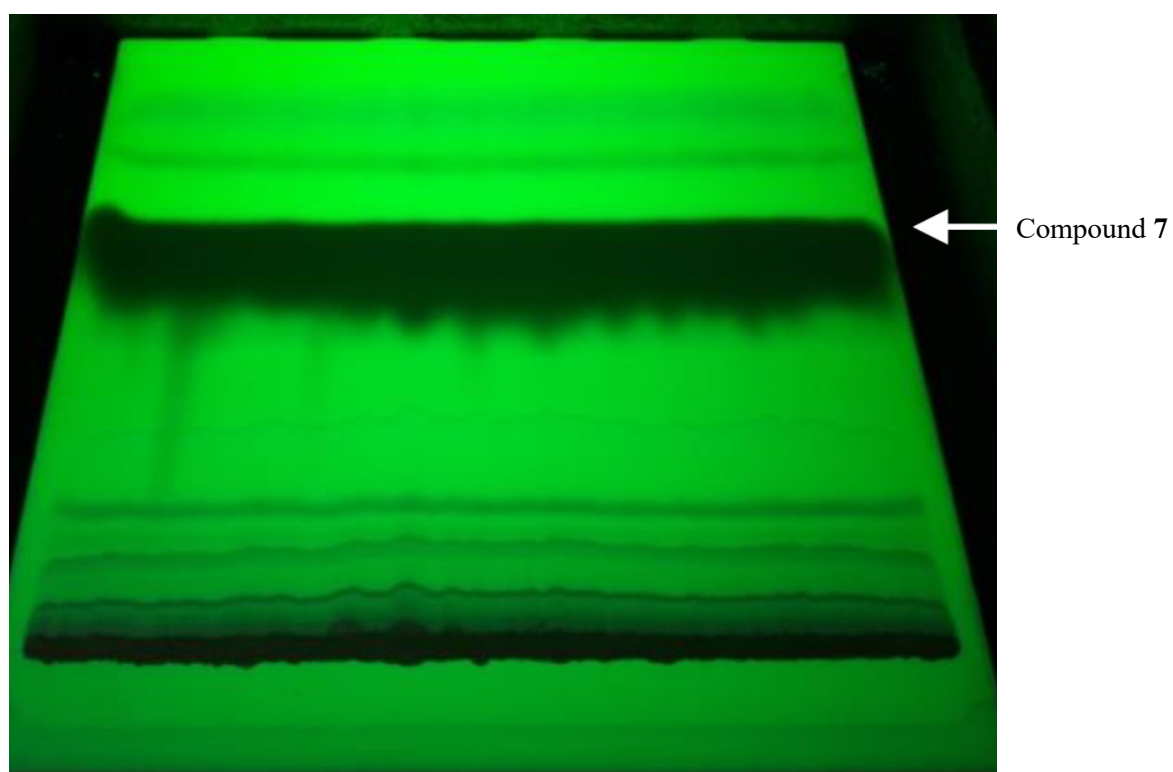


Figure S50. Preparative TLC plate showing the separation of the post-reaction mixture after biotransformation of 2'-hydroxy-5'-bromochalcone (**4**)

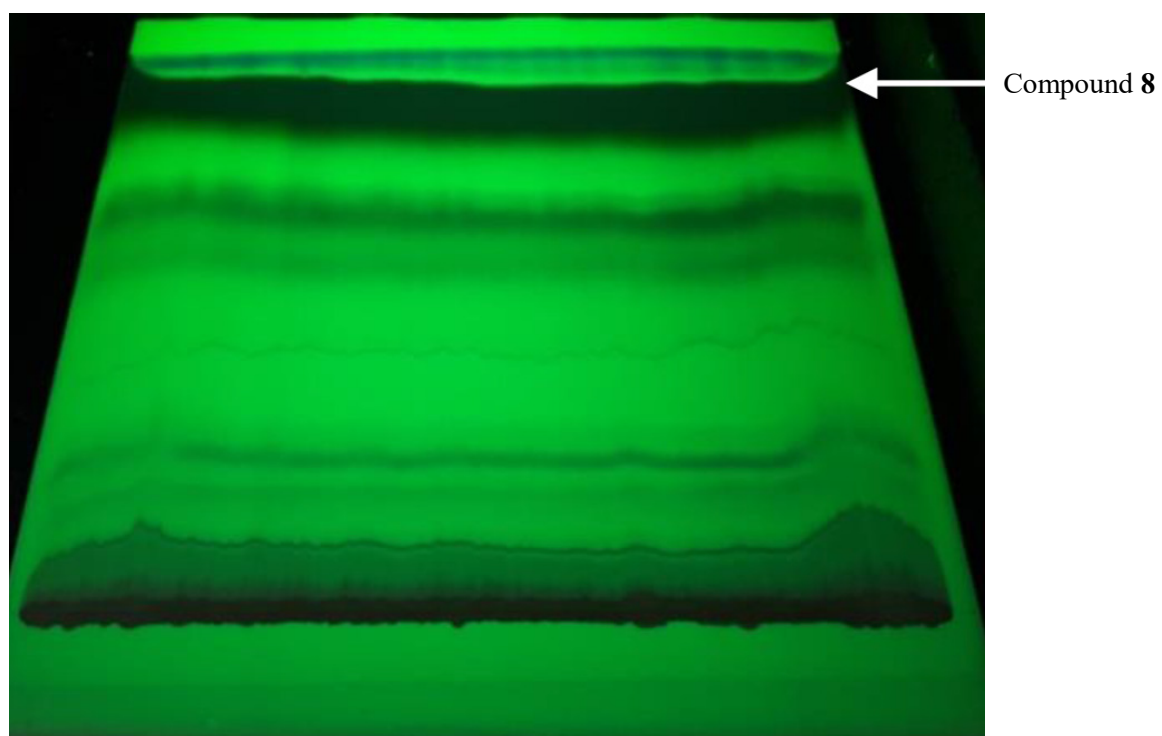
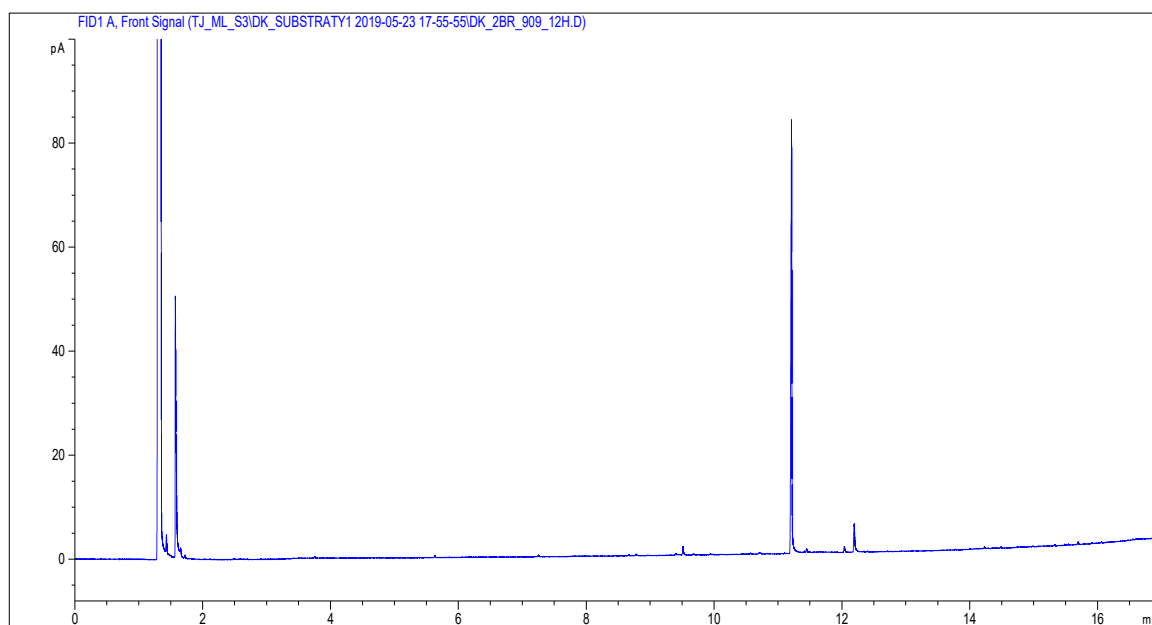
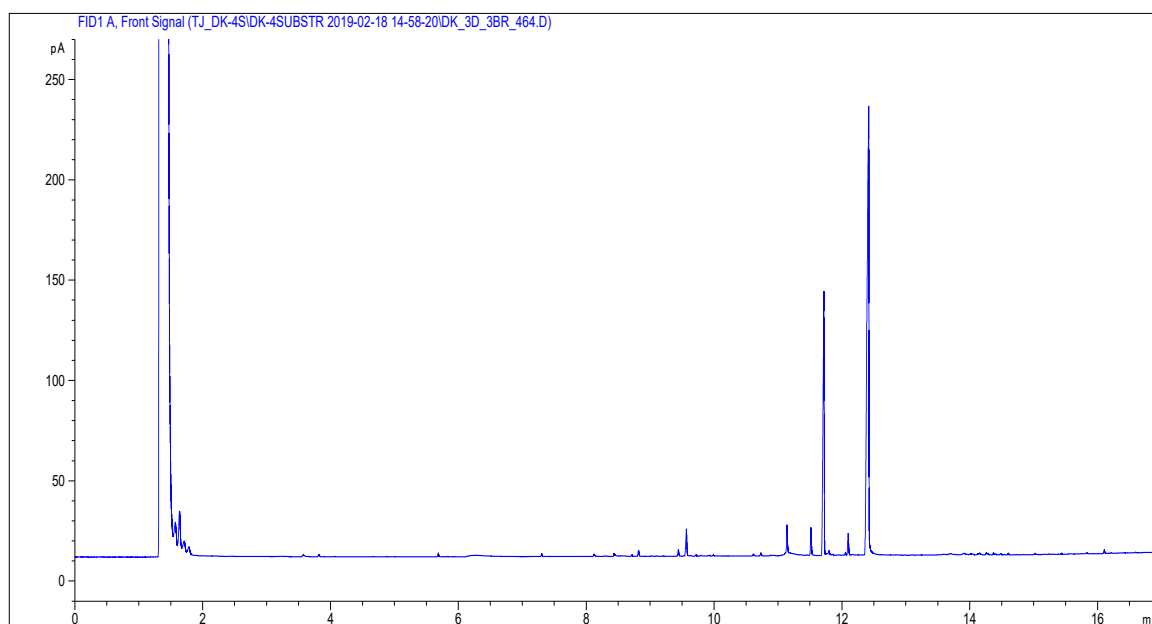


Figure S51. Selected chromatograms showing the composition of the reaction mixtures during the biotransformation of the tested compounds:

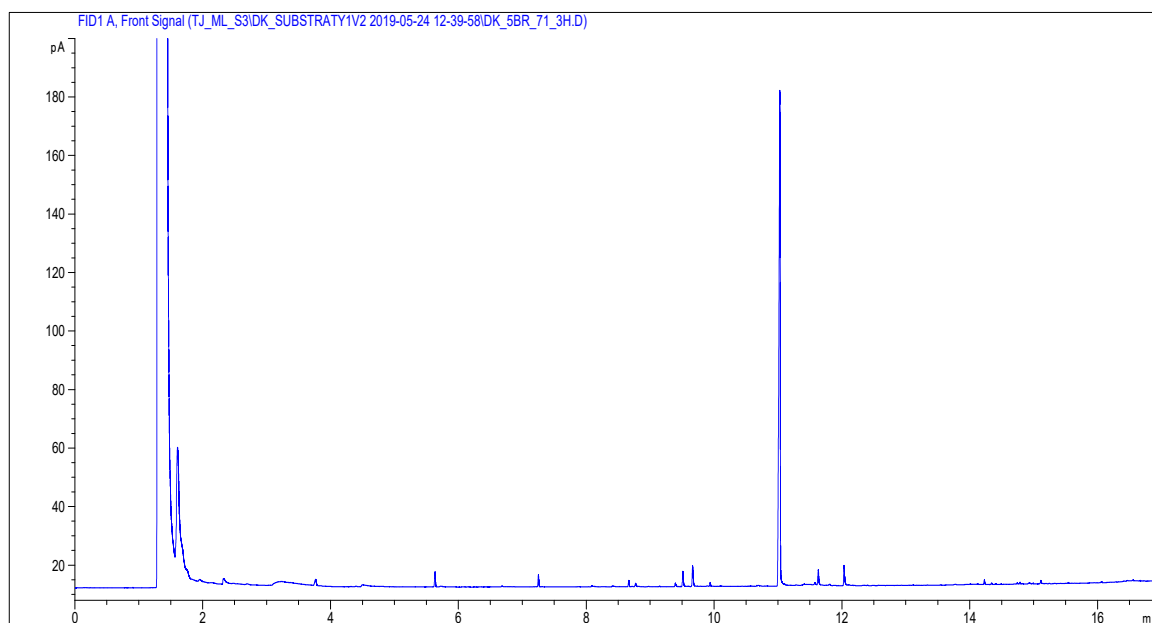
a) GC analysis obtained after 12 hours transformation of 2'-hydroxy-2"-bromochalcone (**1**)



b) GC analysis obtained after 3 days transformation of 2'-hydroxy-2"-bromochalcone (**2**)



c) GC analysis obtained after 3 hours transformation of 2'-hydroxy-5'-bromochalcone (**4**)



d) GC analysis obtained after 10 days transformation of 2'-hydroxy-5'-bromochalcone (**4**)

