

***tert*-Butylphenolic Derivatives from *Paenibacillus odorifer*—A Case of Bioconversion**

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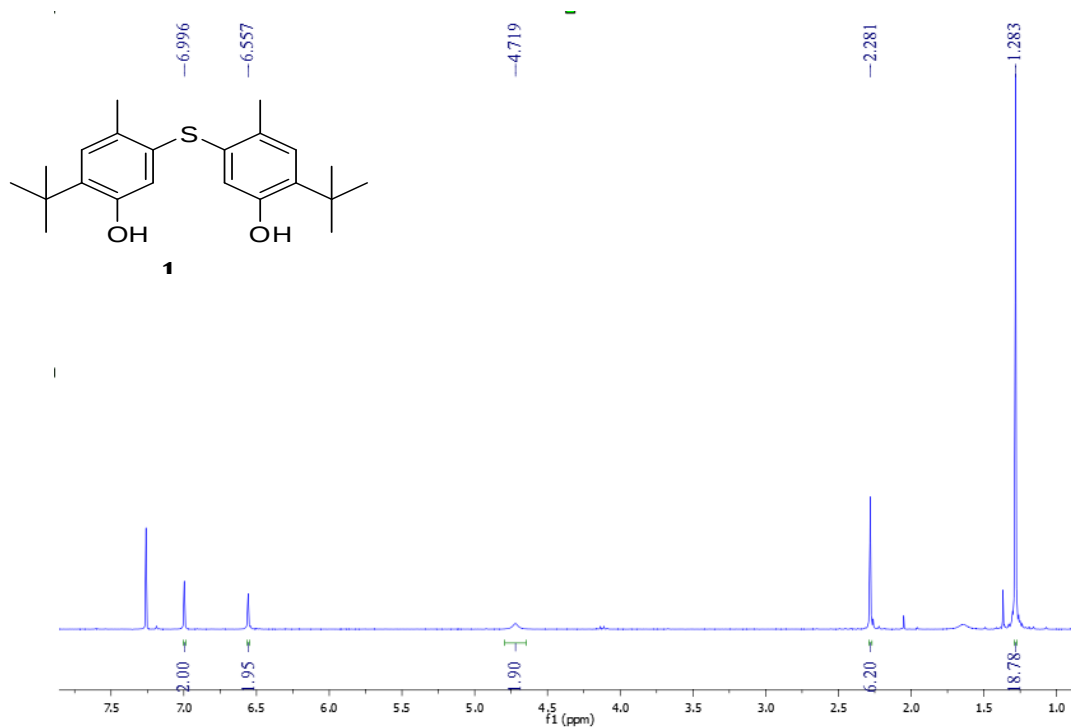
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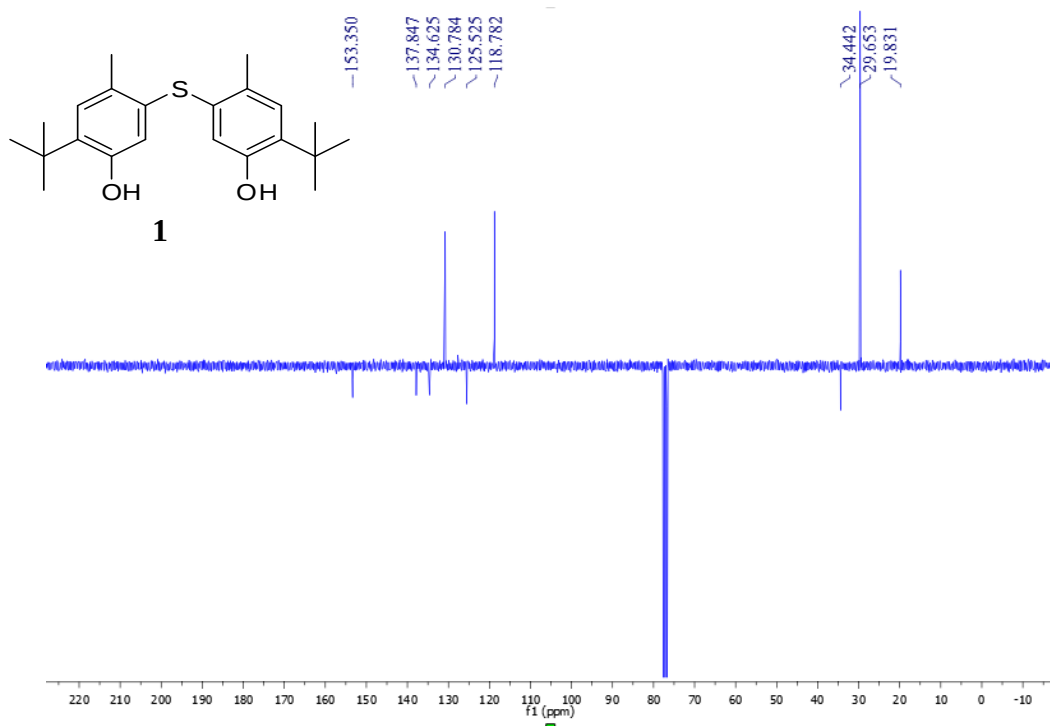
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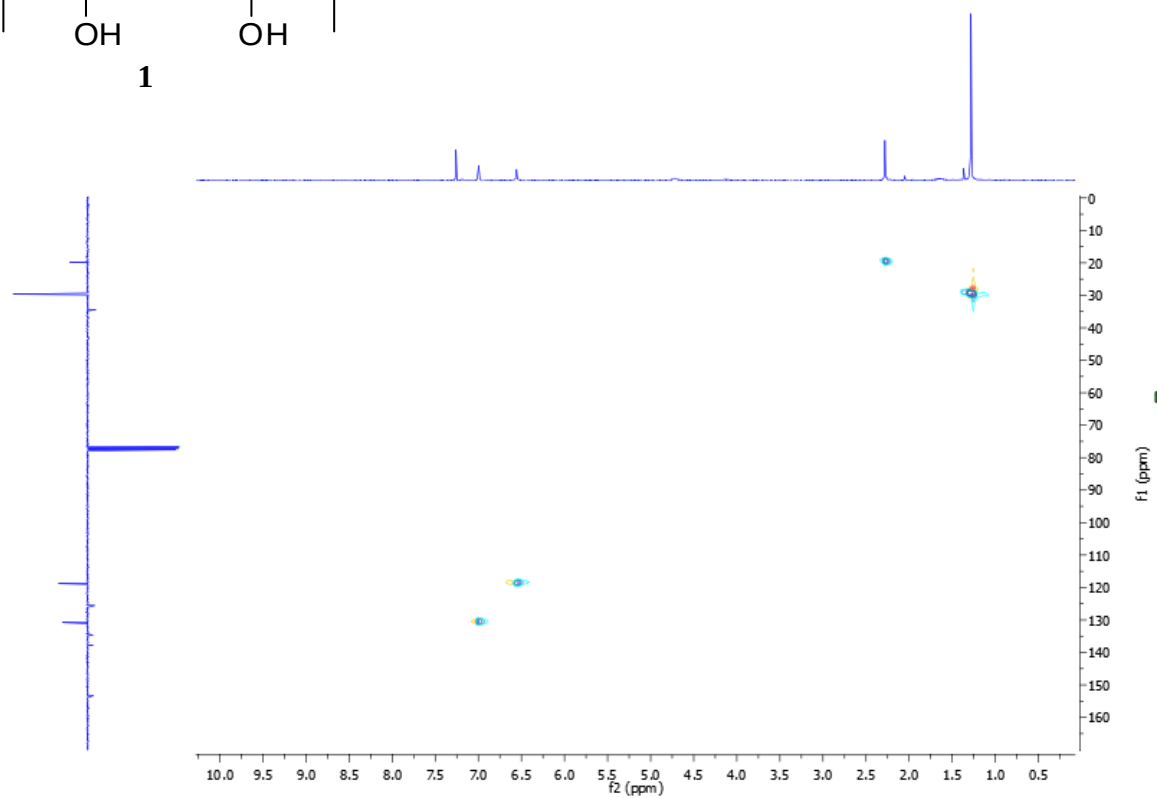
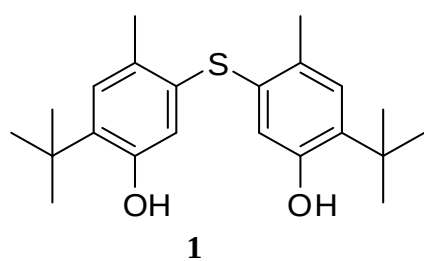
Table of contents	Page
S1. ^1H -NMR spectrum of compound 1 in CDCl_3 (300 MHz)	3
S2. Jmod spectrum of compound 1 in CDCl_3 (75 MHz)	3
S3. 2D-NMR HSQCedit spectrum of compound 1 in CDCl_3 (300 MHz)	4
S4. 2D-NMR HMBC spectrum of compound 1 in CDCl_3 (300 MHz)	5
S5. 2D-NMR COSY spectrum of compound 1 in CDCl_3 (300 MHz)	5
S6. 2D-NMR NOESY spectrum of compound 1 in CDCl_3 (300 MHz)	6
S7. ^1H -NMR spectrum of Santonox in CDCl_3 (300 MHz)	7
S8. Jmod spectrum of Santonox in CDCl_3 (75 MHz)	7
S9. 2D-NMR HSQCedit spectrum of Santonox in CDCl_3 (300 MHz)	8
S10. 2D-NMR HSQCedit spectrum of Santonox in CDCl_3 (300 MHz)	8
S11. 2D-NMR COSY spectrum of Santonox in CDCl_3 (300 MHz)	9
S12. 2D-NMR NOESY spectrum of Santonox in CDCl_3 (300 MHz)	9
S13. NOESY spectrum of fraction 1' from the extract of the culture supplemented with BHA in Erlenmeyer flask	10
S14. ^1H – NMR spectra of fraction 1' (mixture of compound 1 and BHA) (a); compound 1 (b) and BHA (c)	10
S15. ^1H -NMR spectrum of compound 2 in CDCl_3 (300 MHz)	11
S16. Jmod spectrum of compound 2 in CDCl_3 (75 MHz)	11
S17. 2D-NMR HSQCedit spectrum of compound 2 in CDCl_3 (300 MHz)	12
S18. 2D-NMR HMBC spectrum of compound 2 in CDCl_3 (300 MHz)	12
S19. 2D-NMR COSY spectrum of compound 2 in CDCl_3 (300 MHz)	13
Table 1 and S20. Major conformers for the compound 1 (0.34) and santonox (0.46) extracted from the molecular dynamics simulations performed in chloroform	14



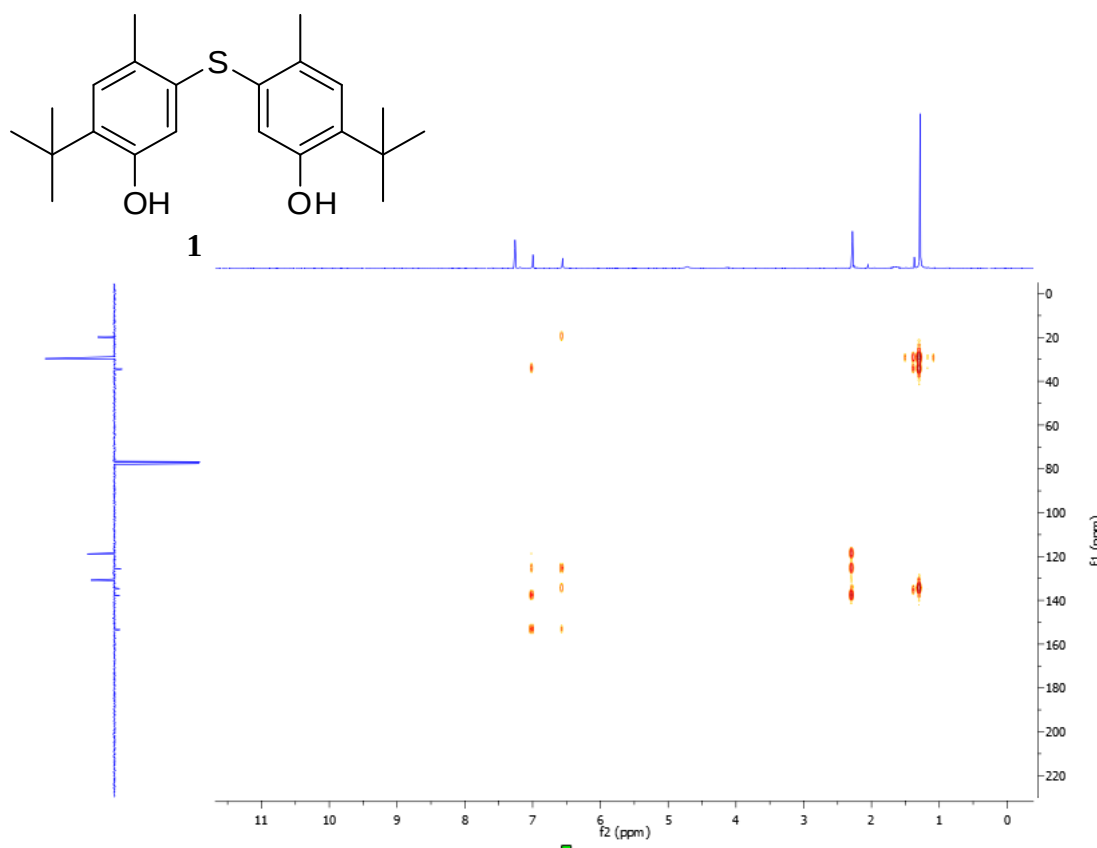
S1. $^1\text{H-NMR}$ spectrum of compound **1** in CDCl_3 (300 MHz)



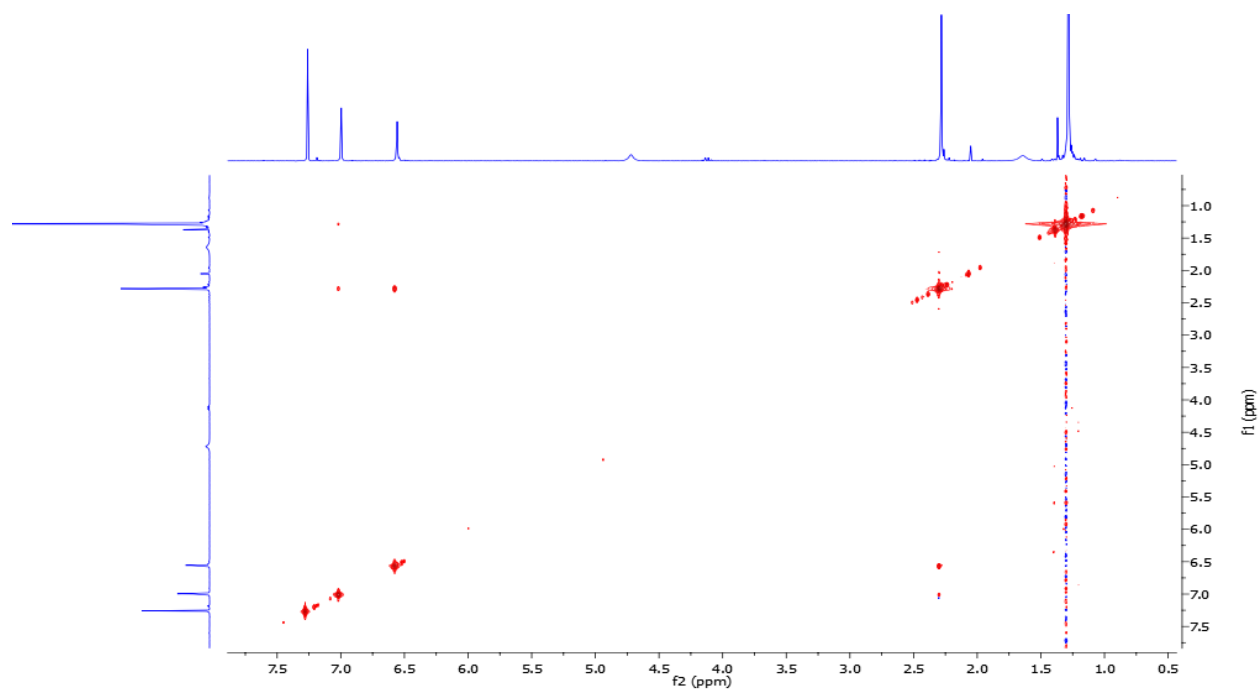
S2. $^{13}\text{C-NMR}$ spectrum of compound **1** in CDCl_3 (75 MHz)



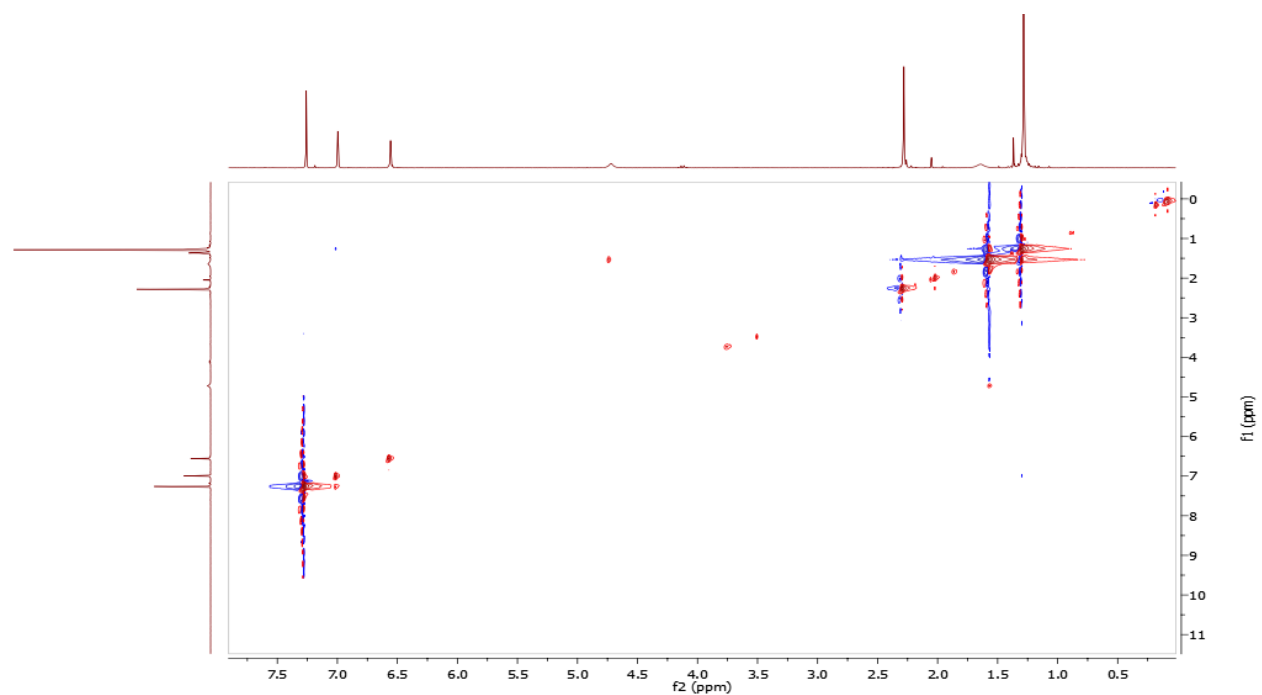
S3. 2D-NMR HSQCedit spectrum of compound **1** in CDCl_3 (300 MHz)



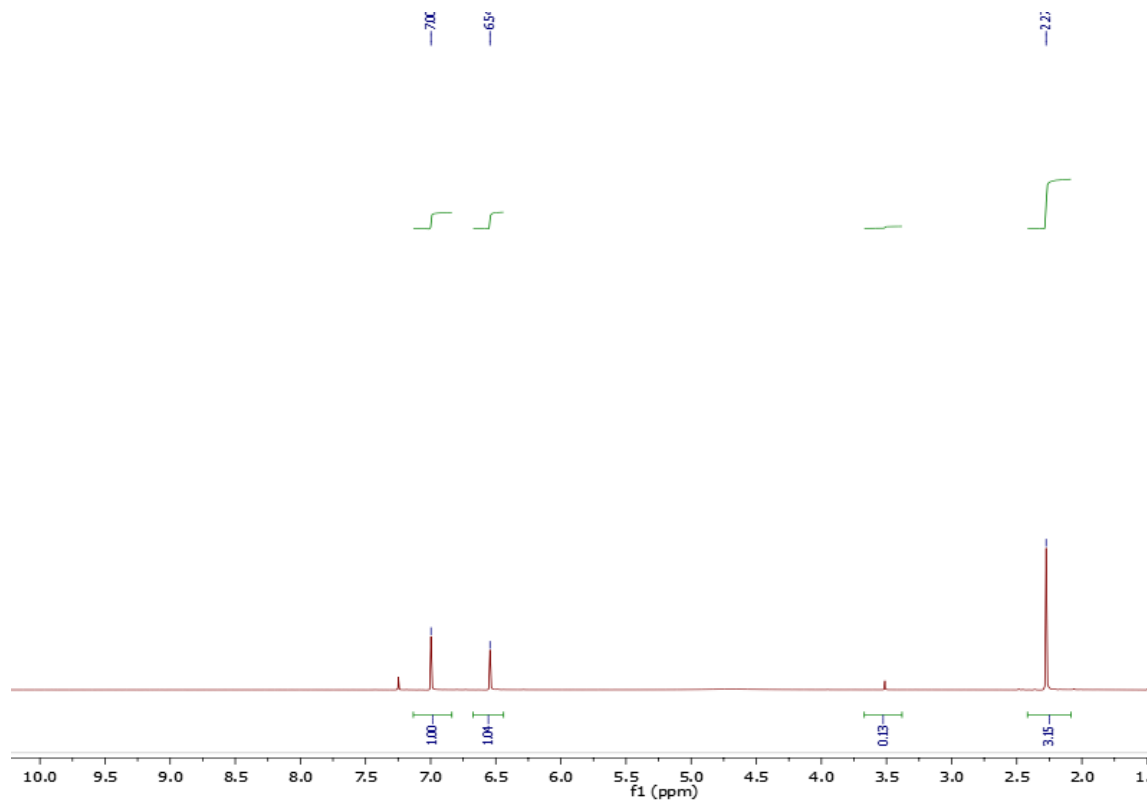
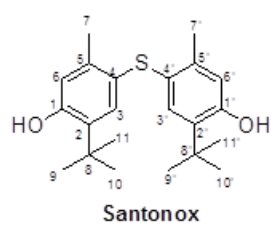
S4. 2D-NMR HMBC spectrum of compound **1** in CDCl_3 (300 MHz)



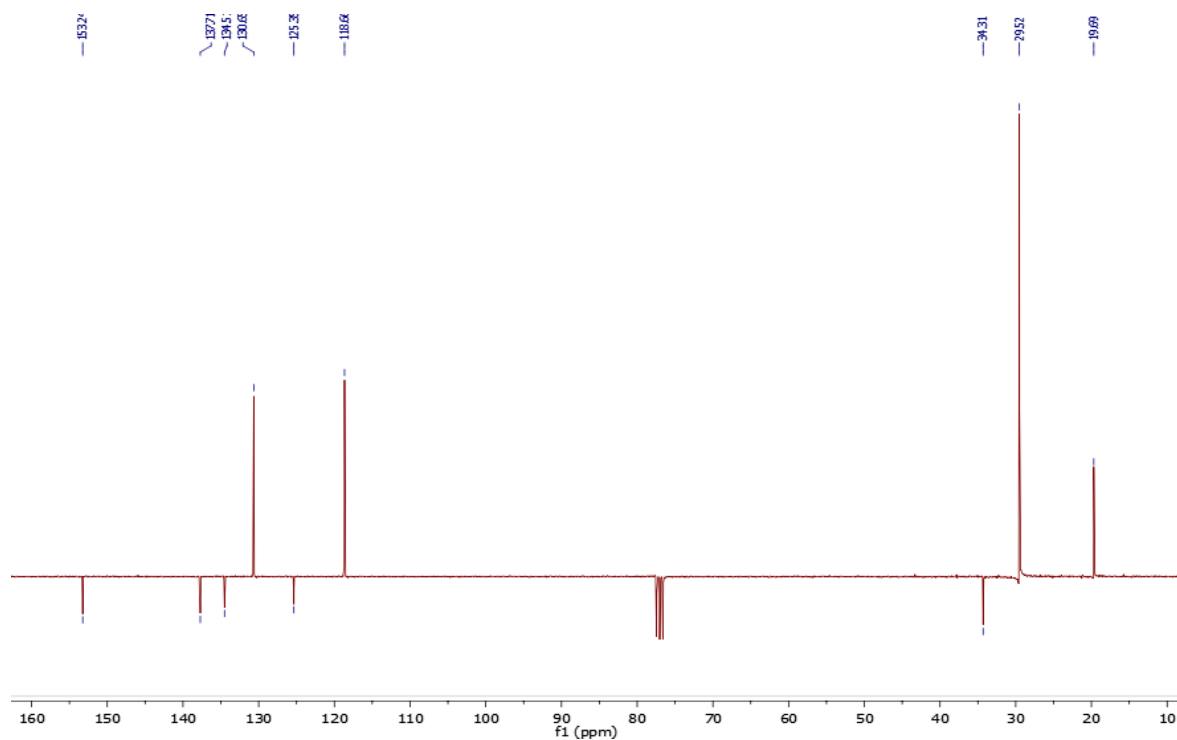
S5. 2D-NMR COSY spectrum of compound **1** in CDCl_3 (300 MHz)



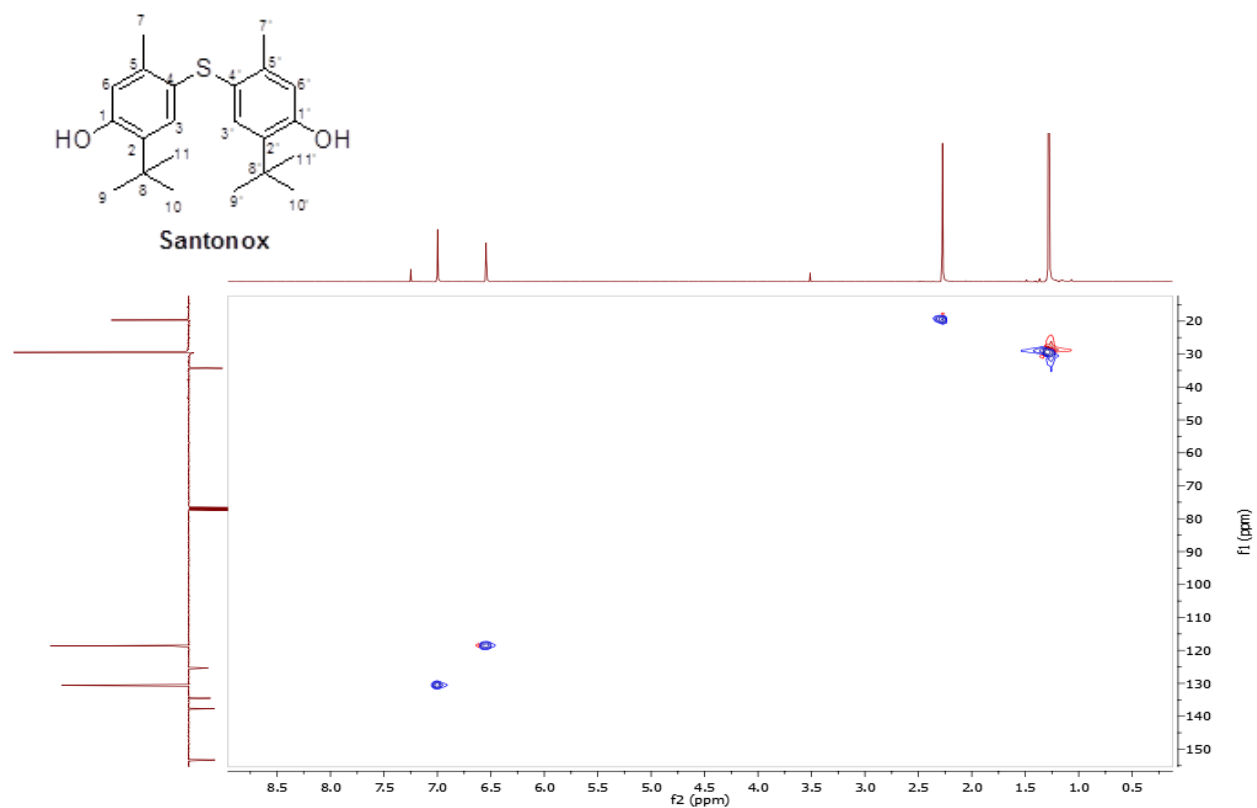
S6. 2D-NMR NOESY spectrum of compound **1** in CDCl_3 (300 MHz)



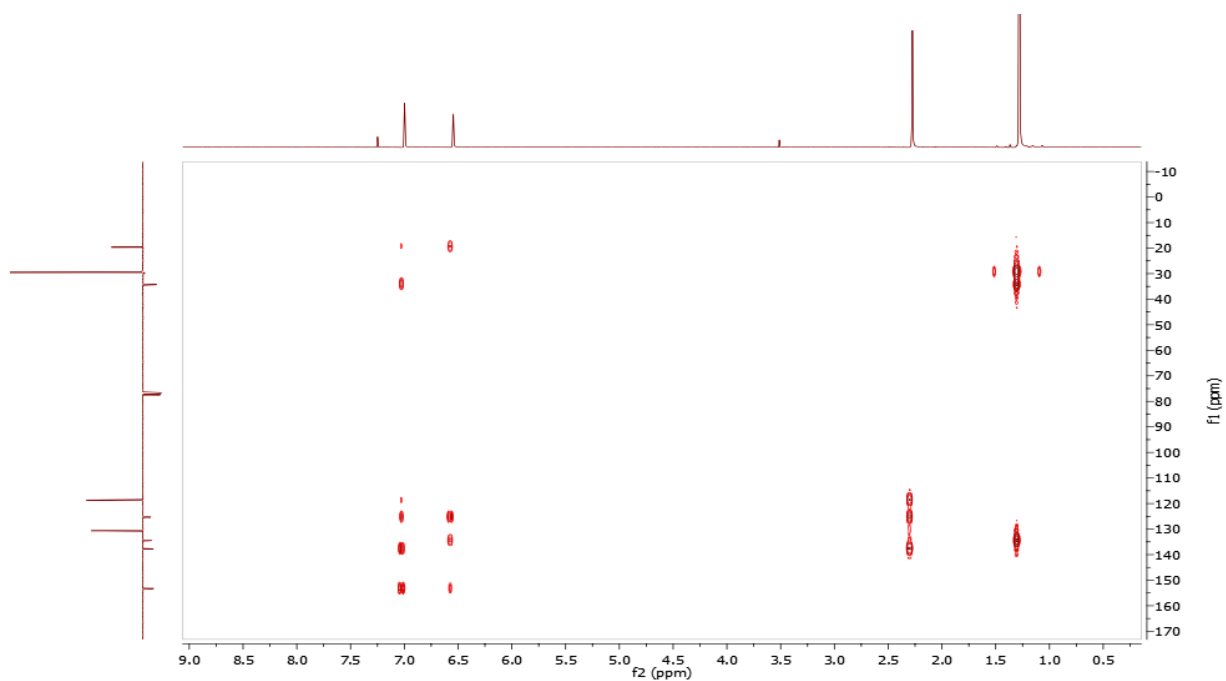
S7. ^1H -NMR spectrum of compound Santonox in CDCl_3 (300 MHz)



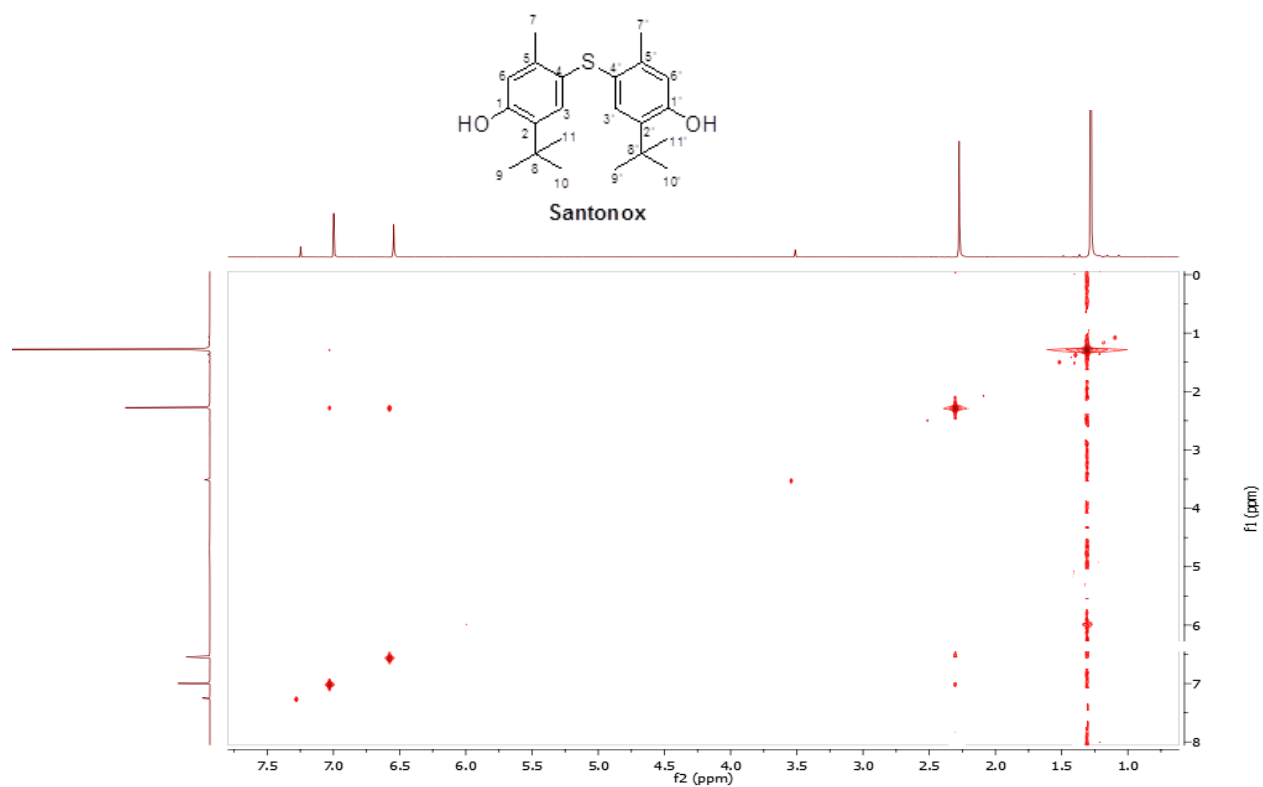
S8. Jmod-spectrum of compound Santonox in CDCl_3 (75 MHz)



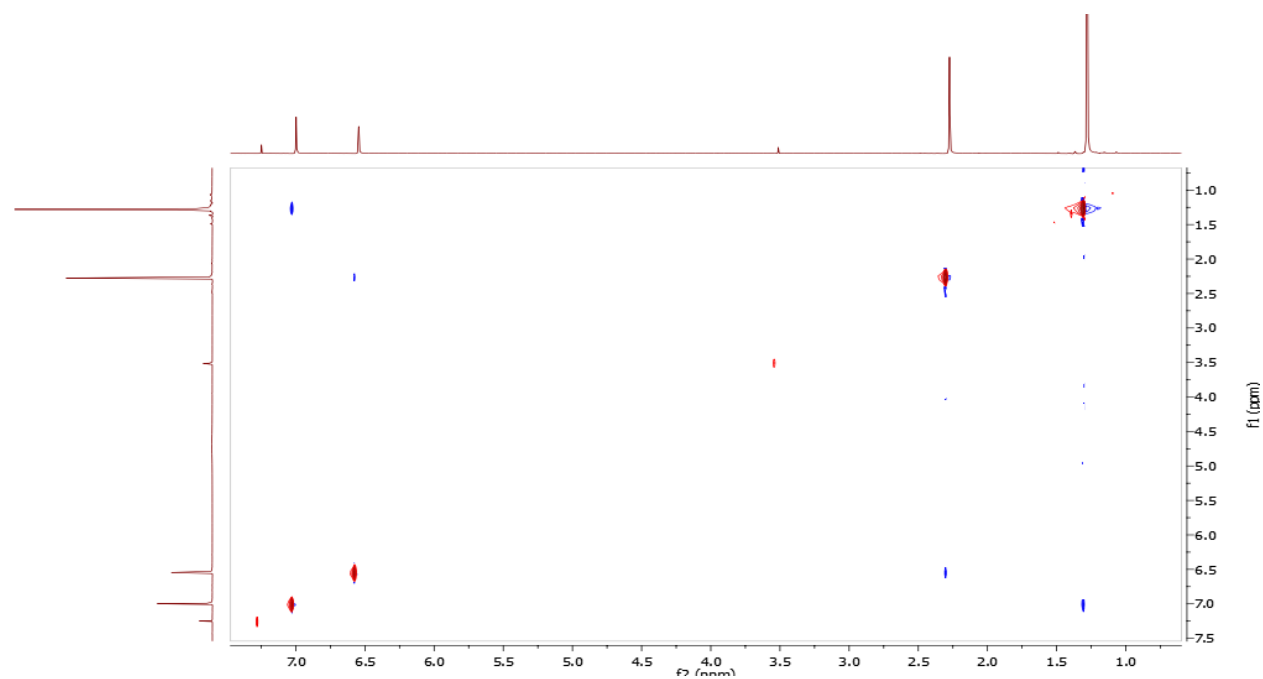
S9. 2D-NMR HSQC spectrum of Santonox in CDCl₃ (300 MHz)



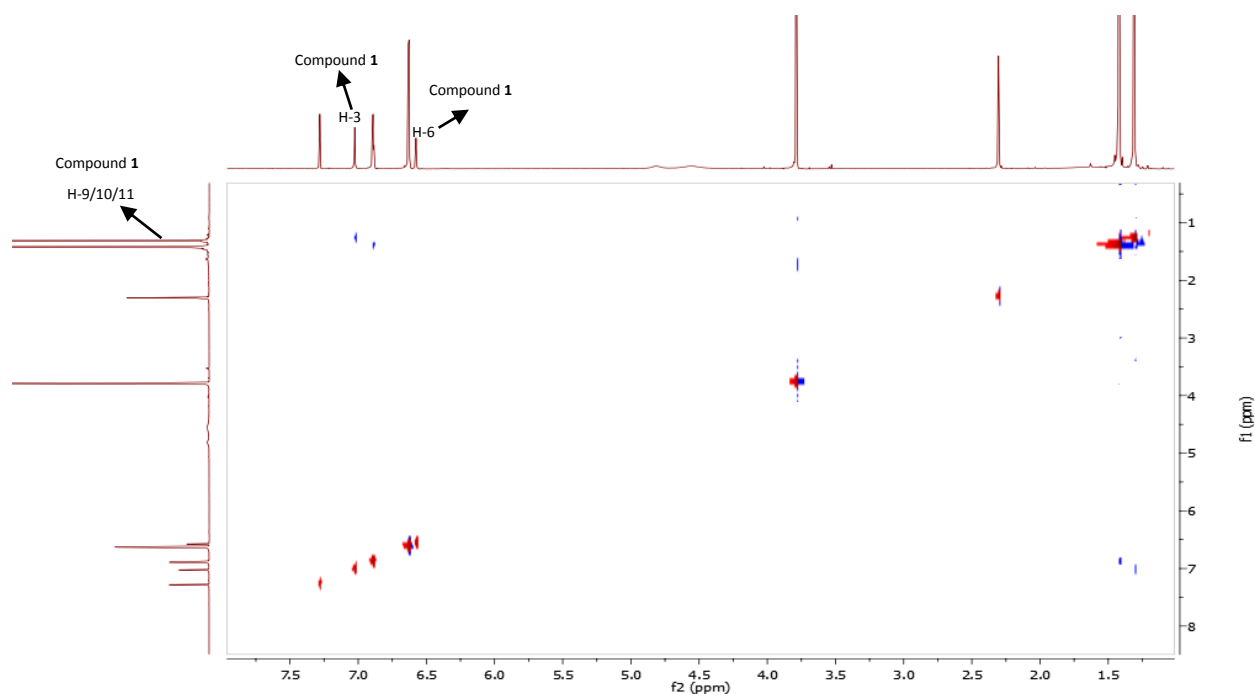
S10. 2D-NMR HMBC spectrum of Santonox in CDCl₃ (300 MHz)



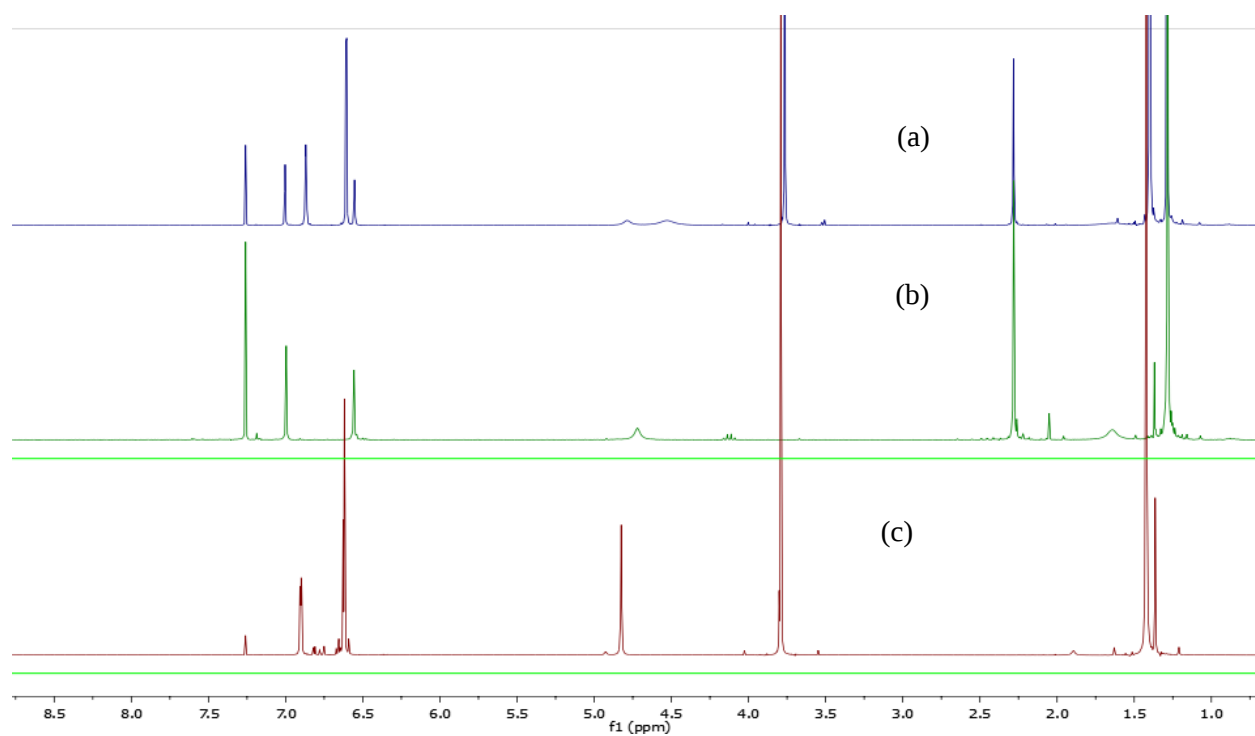
S11. 2D-NMR COSY spectrum of Santonox in CDCl_3 (300 MHz)



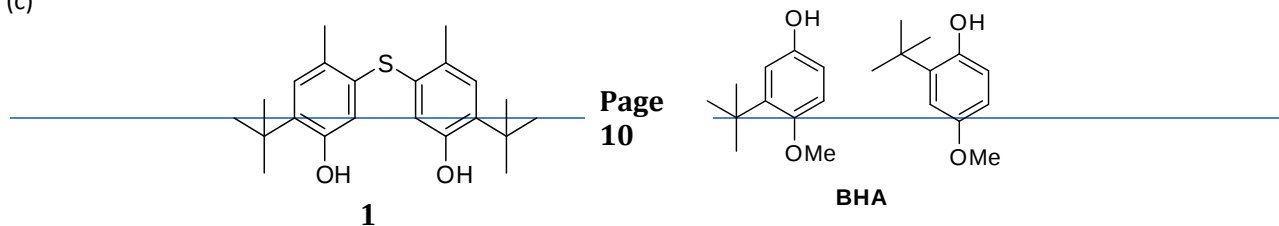
S12. 2D-NMR NOESY spectrum of Santonox in CDCl_3 (300 MHz)

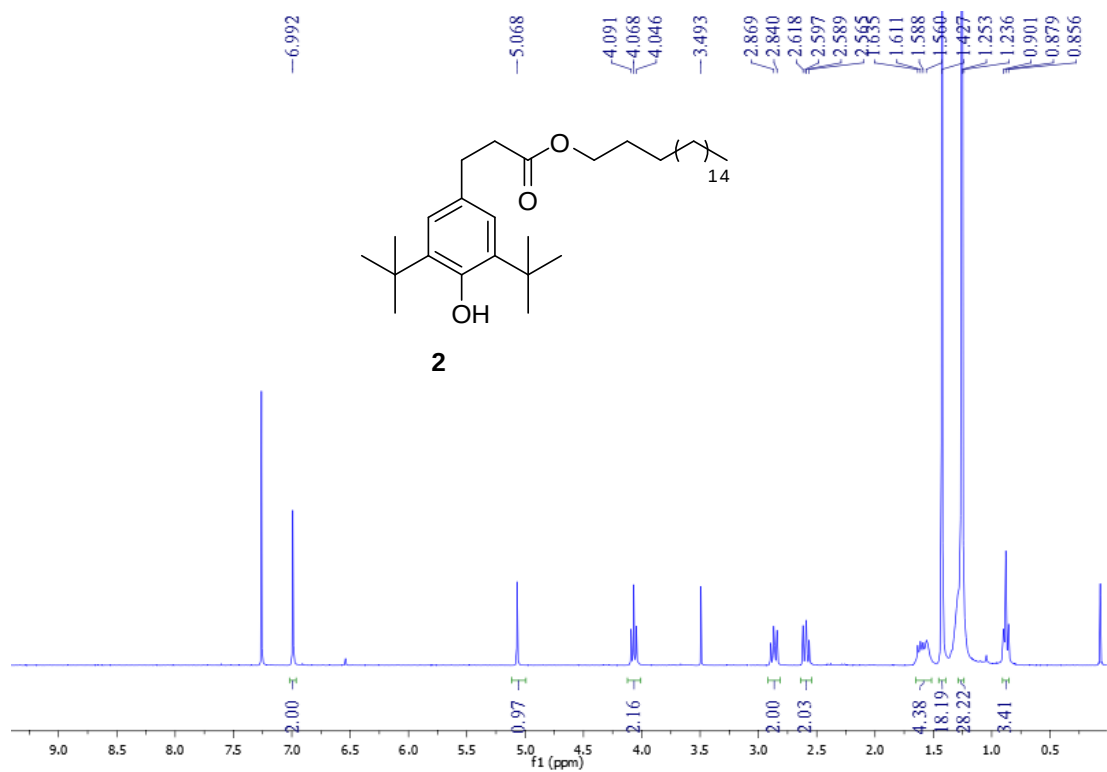


S13: NOESY spectrum of fraction **1'** (mixture of non-separable BHA and compound **1**) from the extract of the culture supplemented with BHA in Erlenmeyer flask

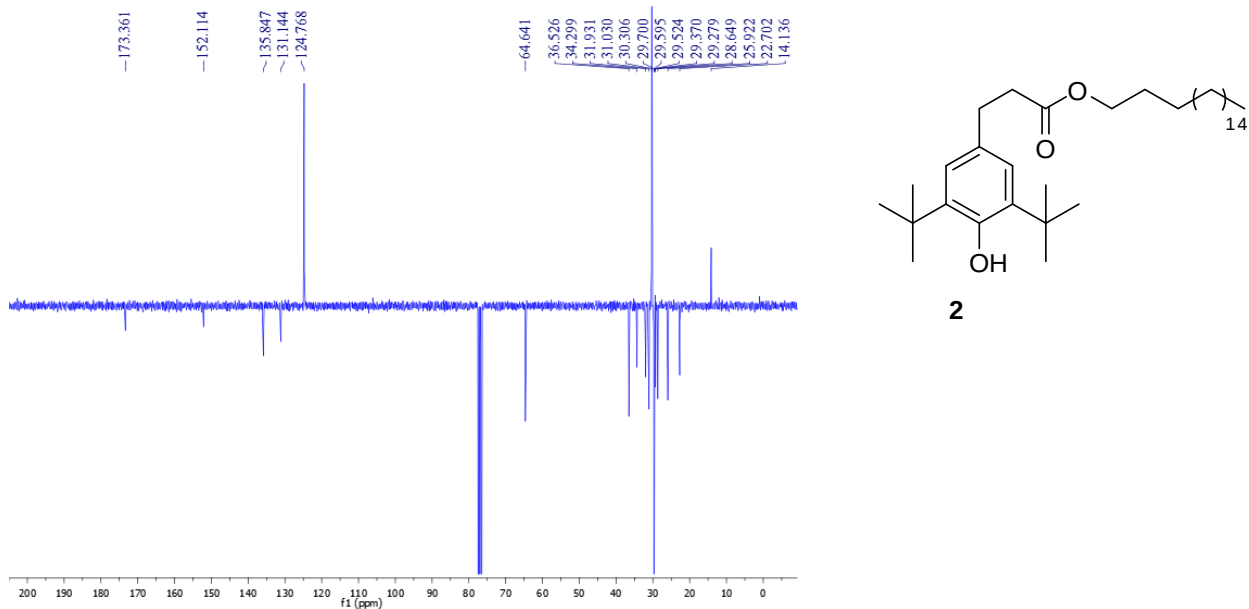


S14: ¹H – NMR spectra of fraction **1'** (mixture of non-separable compound **1** and BHA) (a); compound **1** (b) and BHA (c)

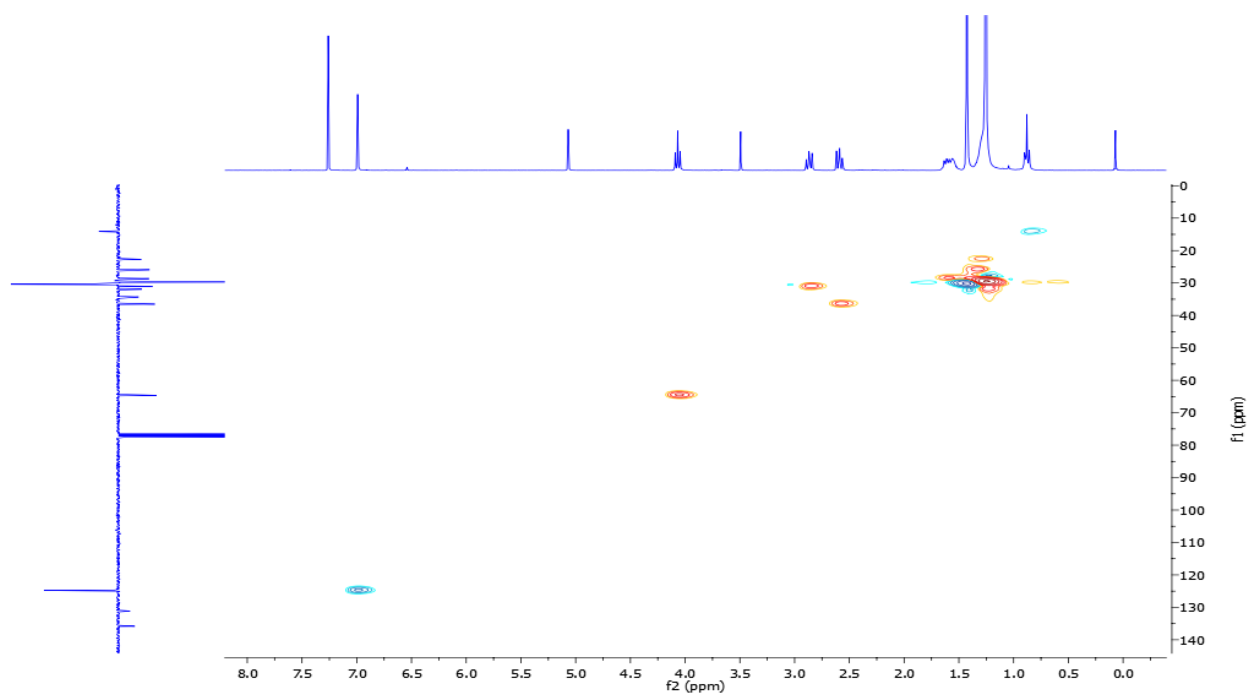




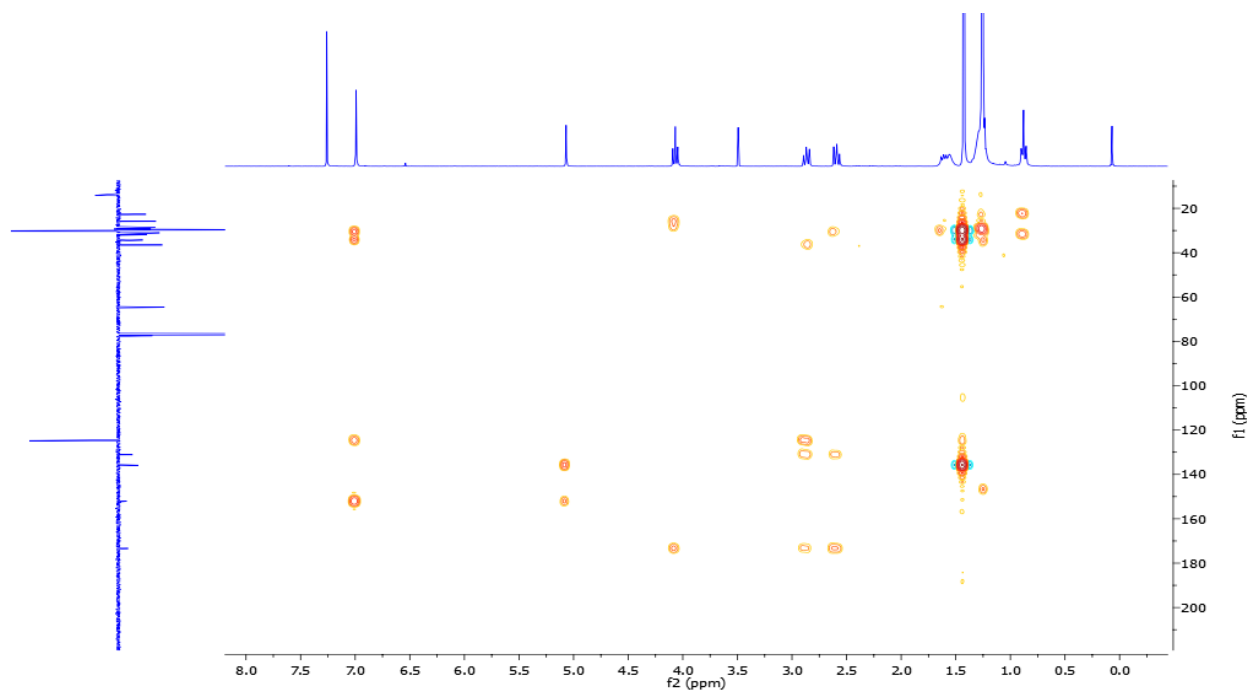
S15. ¹H-NMR spectrum of compound **2** in CDCl₃ (300 MHz)



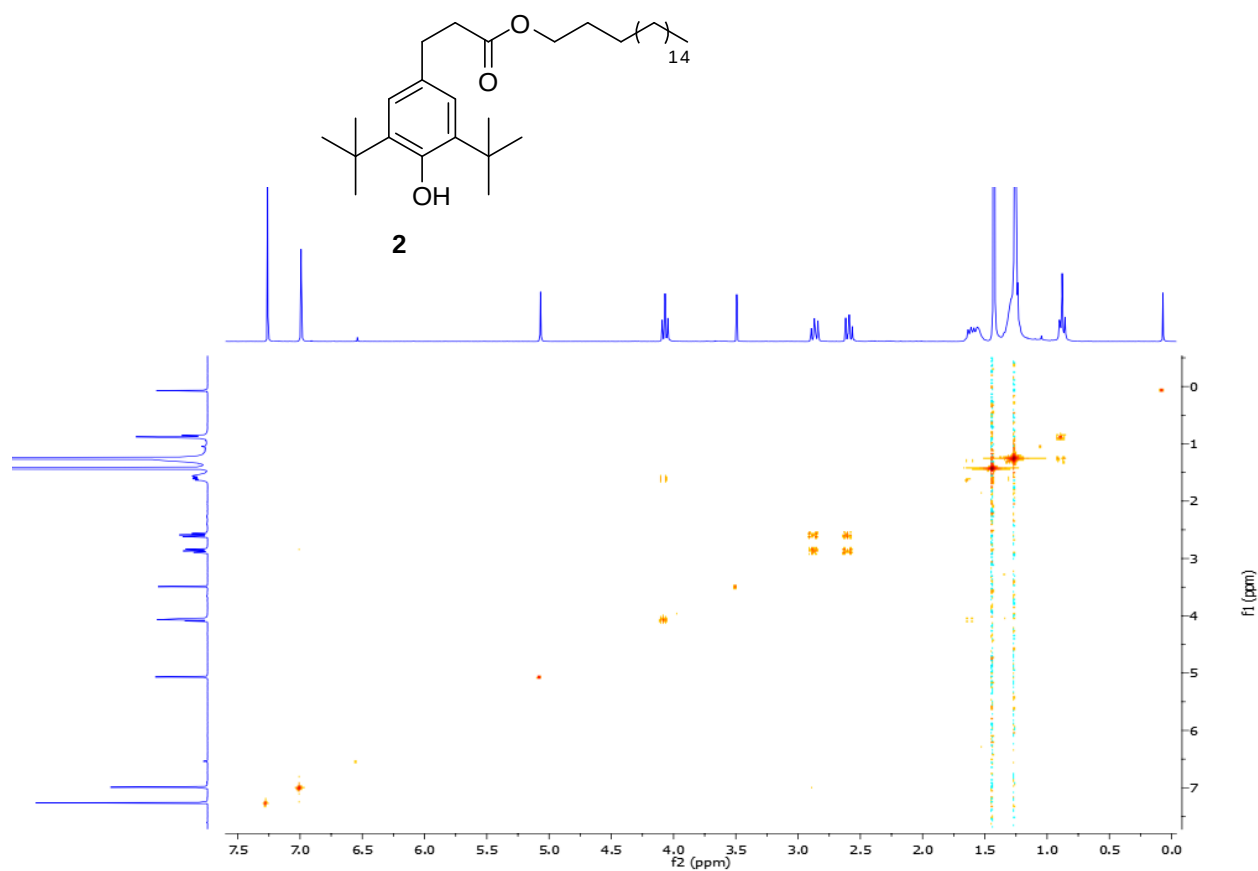
S16. Jmod-NMR spectrum of compound **2** in CDCl₃ (75 MHz)



S17. 2D-NMR HSQCedit spectrum of compound **2** in CDCl₃ (300 MHz)

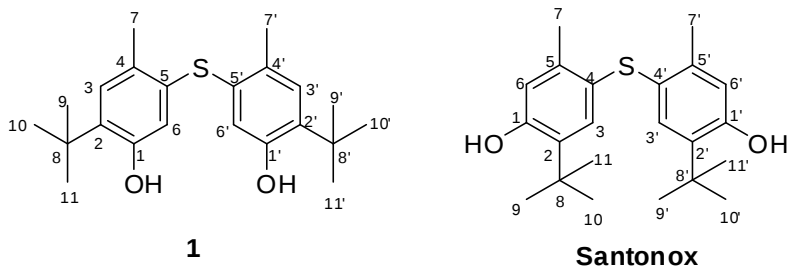


S18. 2D-NMR HMBC spectrum of compound **2** in CDCl₃ (300 MHz)

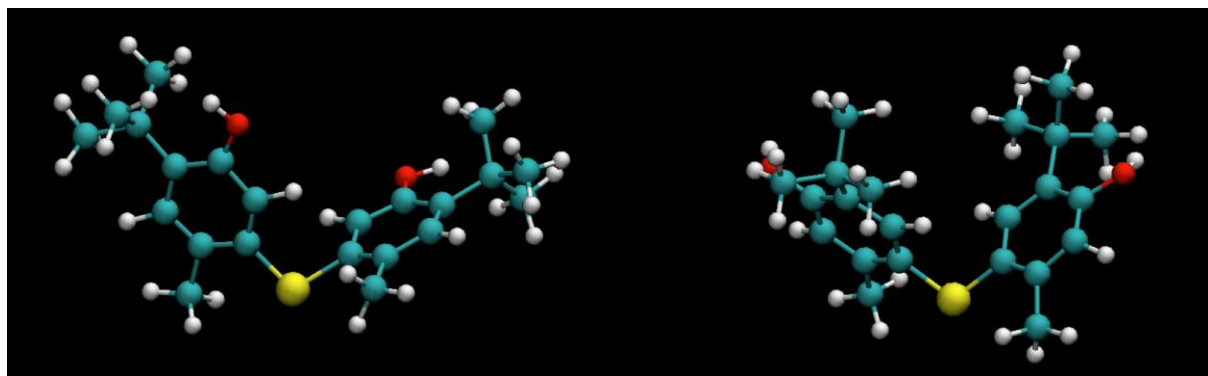


S19. 2D-NMR COSY of compound **2** in CDCl₃ (300 MHz)

Table S1: Predicted inter-protons distances on the base of molecular models corresponding to the major conformers of compound **1** and santonox extracted from the molecular dynamics simulation (see S20)



Compound 1		Santonox	
H3-tBut	3.87	H3-tBut	3.58
H6-tBut	5.66	H6-tBut	5.83



S20: Major conformers for the compound **1** (0.34) and santonox (0.46) extracted from the molecular dynamics simulations performed in chloroform.