Supplementary Information

Figure S1. Analytical HPLC coupled to high resolution electrospray ionization mass spectrometer and diode array detector (HPLC/HRESI-MS-DAD) chromatograms for crude samples of dakaramine. The figure shows two peaks (**I** and **II**) with the same UV profile but separated by a column retention time of about 7 minutes. Solvents used for the gradient elution process were A (99.9% H_2O:0.1% HCOOH) and B (99.9% CH_3OH:0.1% HCOOH). The gradient is set to start at 100% A and 0% B at 0 minutes to 0% A and 100% B after 30 minutes at a flow rate of 1.0 mL/min in a Sunfire C18 column (4.6 × 150 mm, Waters).

Figure S2. HPLC/HRESI-MS-DAD shows peaks **I** and **II** to have the same $[M+H]^+$.

Figure S3. HPLC/HRESI- MS-DAD data shows peaks **I** and **II** with same fragmentation pattern.

Figure S4. Structures/substructures derived for some of the fragments in Figure S3 using ChemDraw Ultra.

Figure S5. Semi-preparative HPLC runs for crude dakaramine fractions shows it is possible for the two peaks **I** and **II** constantly seen in analytical mode (0.1% HCOOH) to separate out or combine to form one peak. Gradients of H_2O:MeOH (100% H_2O to 100% MeOH in 30 minutes and hold for 15 minutes) were used as eluents with flow rate set at 1.5 mL/min on a Sunfire prep C18 column (10 x 250 mm, Waters).

Figure S6. ^{1}H NMR spectrum of crude fraction containing dakaramine.

Figure S7. ^{13}C NMR spectrum of crude fraction containing dakaramine.

Figure S8. ^{1}H NMR spectrum of pure dakaramine (**1**).

Figure S9. ^{13}C NMR spectrum of pure dakaramine (**1**).

Figure S10. gHSQCAD NMR spectrum of pure dakaramine (**1**).

Figure S11. ^{1}H-^{1}H gCOSY NMR spectrum of pure dakaramine (**1**).

Figure S12. HMBCAD NMR spectrum of pure dakaramine (**1**).

Figure S13. ^{1}H NMR spectrum of pure 1-hydroxypropan-2-yl acetate (**2**).

Figure S14. ^{13}C NMR spectrum of pure 1-hydroxypropan-2-yl acetate (**2**).

Figure S15. gHSQCAD NMR spectrum of pure 1-hydroxypropan-2-yl acetate (**2**).

Figure S16. ^{1}H-^{1}H gCOSY NMR spectrum of pure 1-hydroxypropan-2-yl acetate (**2**).

Figure S17. HMBCAD NMR spectrum of pure 1-hydroxypropan-2-yl acetate (**2**).

Figure S1. Analytical HPLC coupled to high resolution electrospray ionization mass spectrometer and diode array detector (HPLC/HRESI-MS-DAD) chromatograms for crude samples of dakaramine. The figure shows two peaks (**I** and **II**) with the same UV profile but separated by a column retention time of about 7 minutes. Solvents used for the gradient elution process were A (99.9% H_2O:0.1% HCOOH) and B (99.9% CH_3OH:0.1% HCOOH). The gradient is set to start at 100% A and 0% B at 0 minutes to 0% A and 100% B after 30 minutes at a flow rate of 1.0 mL/min in a Sunfire C18 column (4.6 × 150 mm, Waters).

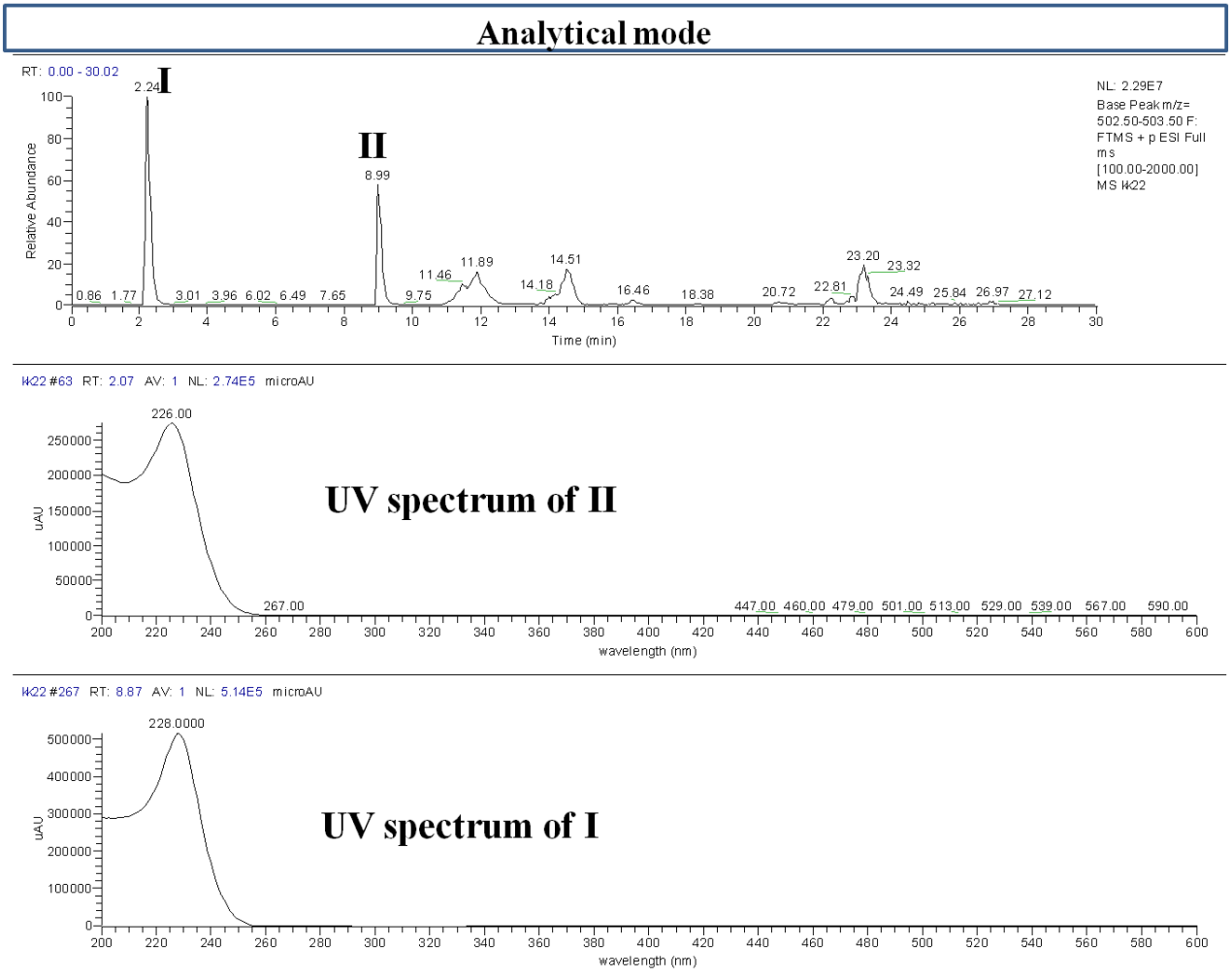


Figure S2. HPLC/HRESI-MS-DAD shows peaks **I** and **II** to have the same $[M+H]^+$.

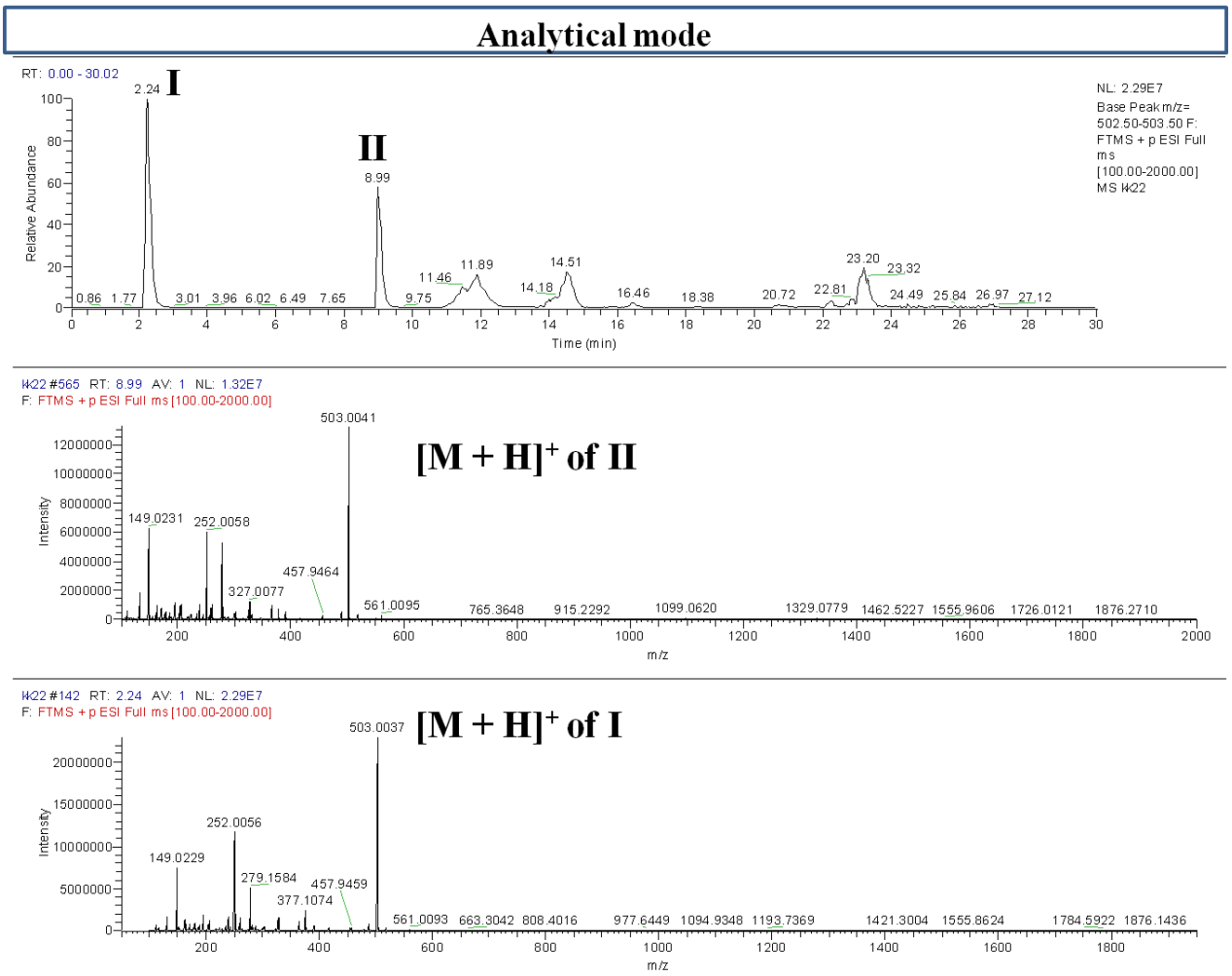


Figure S3. HPLC/HRESI-MS-DAD data shows peaks **I** and **II** with same fragmentation pattern.

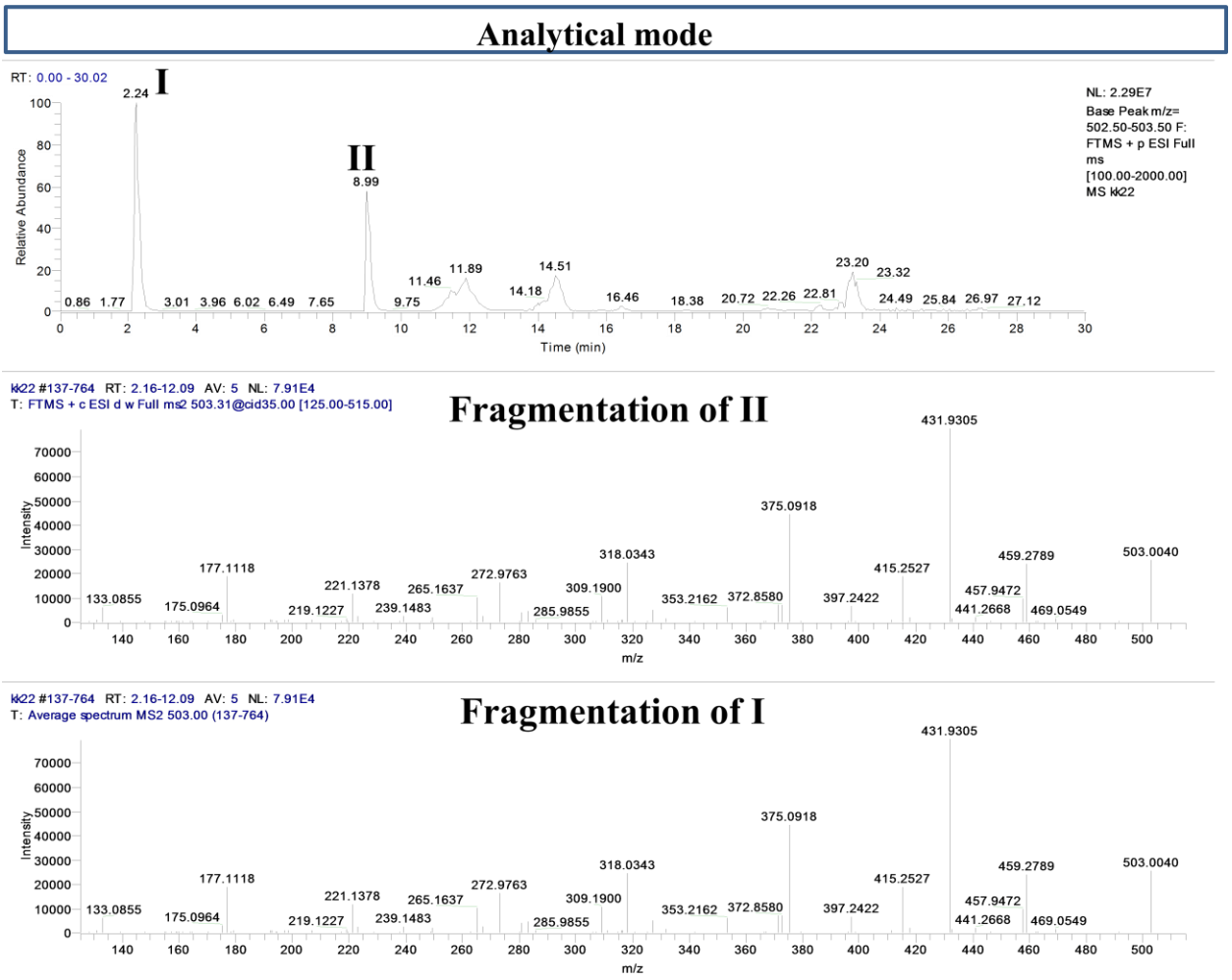
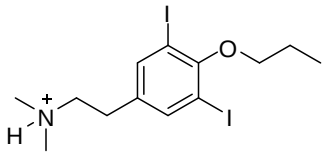
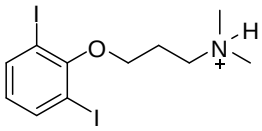


Figure S4. Structures/sub-structures derived for some of the fragments in Figure S3 using ChemDraw Ultra.



Chemical Formula: $C_{13}H_{20}I_2NO^+$
Exact Mass: 459.9629



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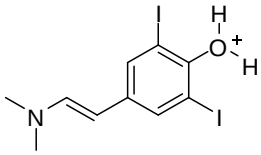

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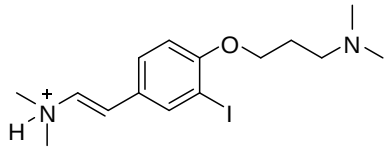

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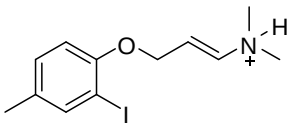
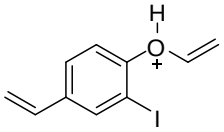


Chemical Formula: $C_{12}H_{17}INO^+$
Exact Mass: 318.0349



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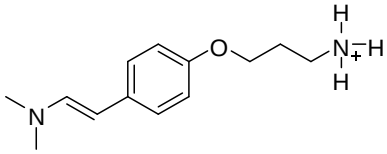
Exact Mass: 272.9771



Chemical Formula: $C_{13}H_{21}N_2O^+$
Exact Mass: 221.1648

Figure S5. Semi-preparative HPLC runs for crude dakaramine fractions shows it is possible for the two peaks **I** and **II** constantly seen in analytical mode (0.1% HCOOH) to separate out or combine to form one peak. Gradients of H_2O:MeOH (100% H_2O to 100% MeOH in 30 minutes and hold for 15 minutes) were used as eluents with flow rate set at 1.5 mL/min on a Sunfire prep C18 column (10 x 250 mm, Waters).

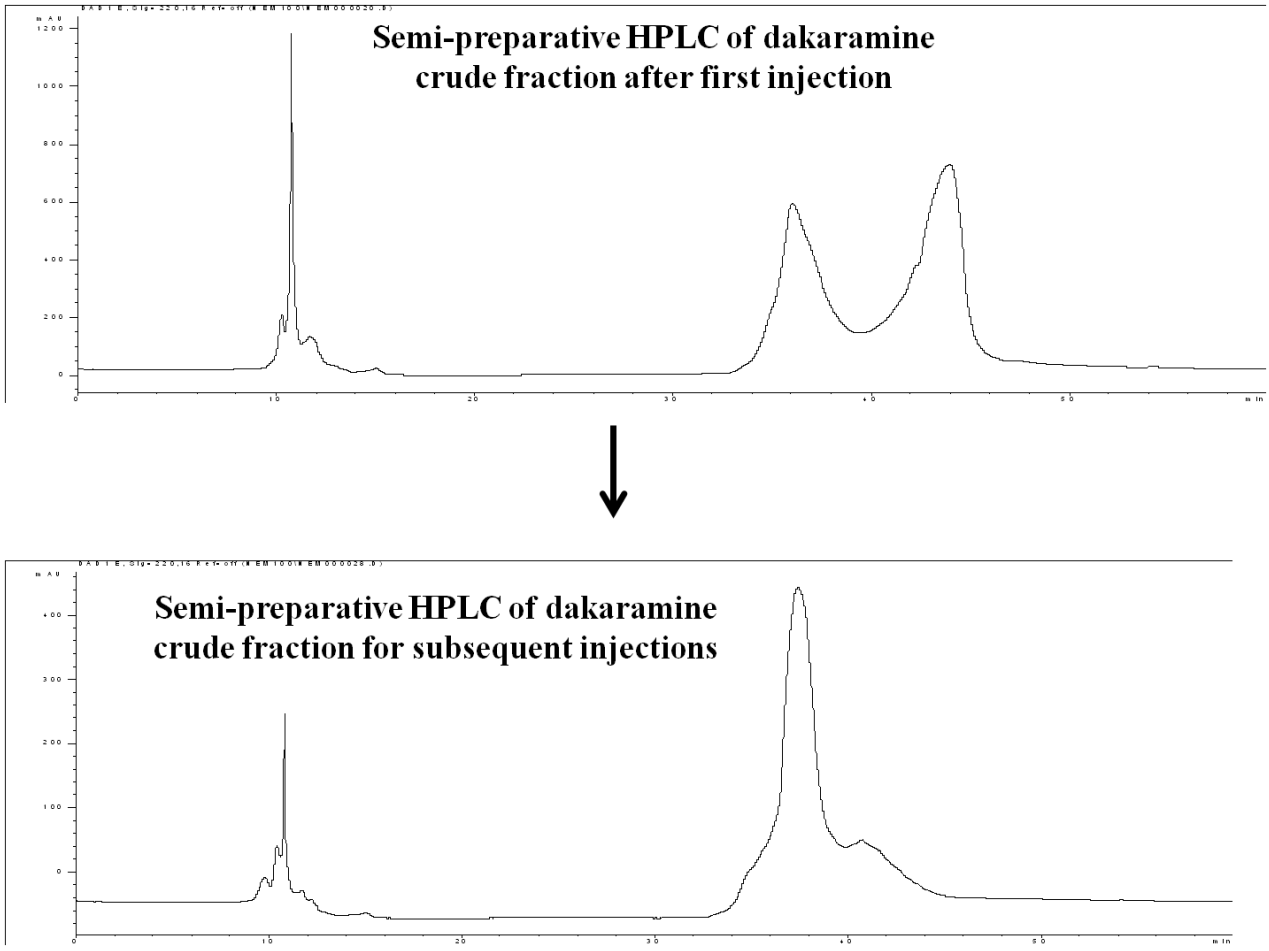


Figure S6. ^{1}H NMR spectrum of crude fraction containing dakaramine.

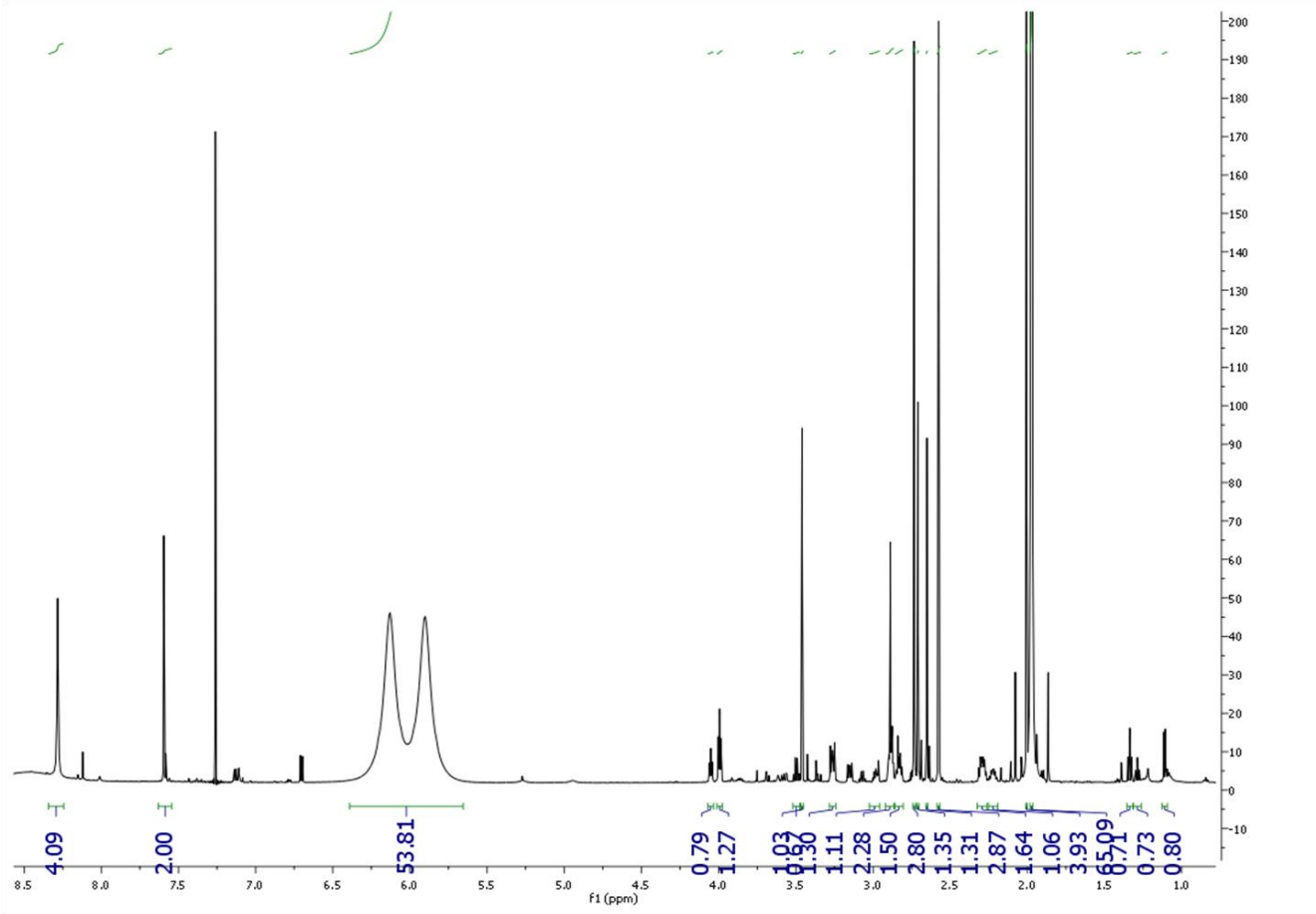


Figure S7. ^{13}C NMR spectrum of crude fraction containing dakaramine.

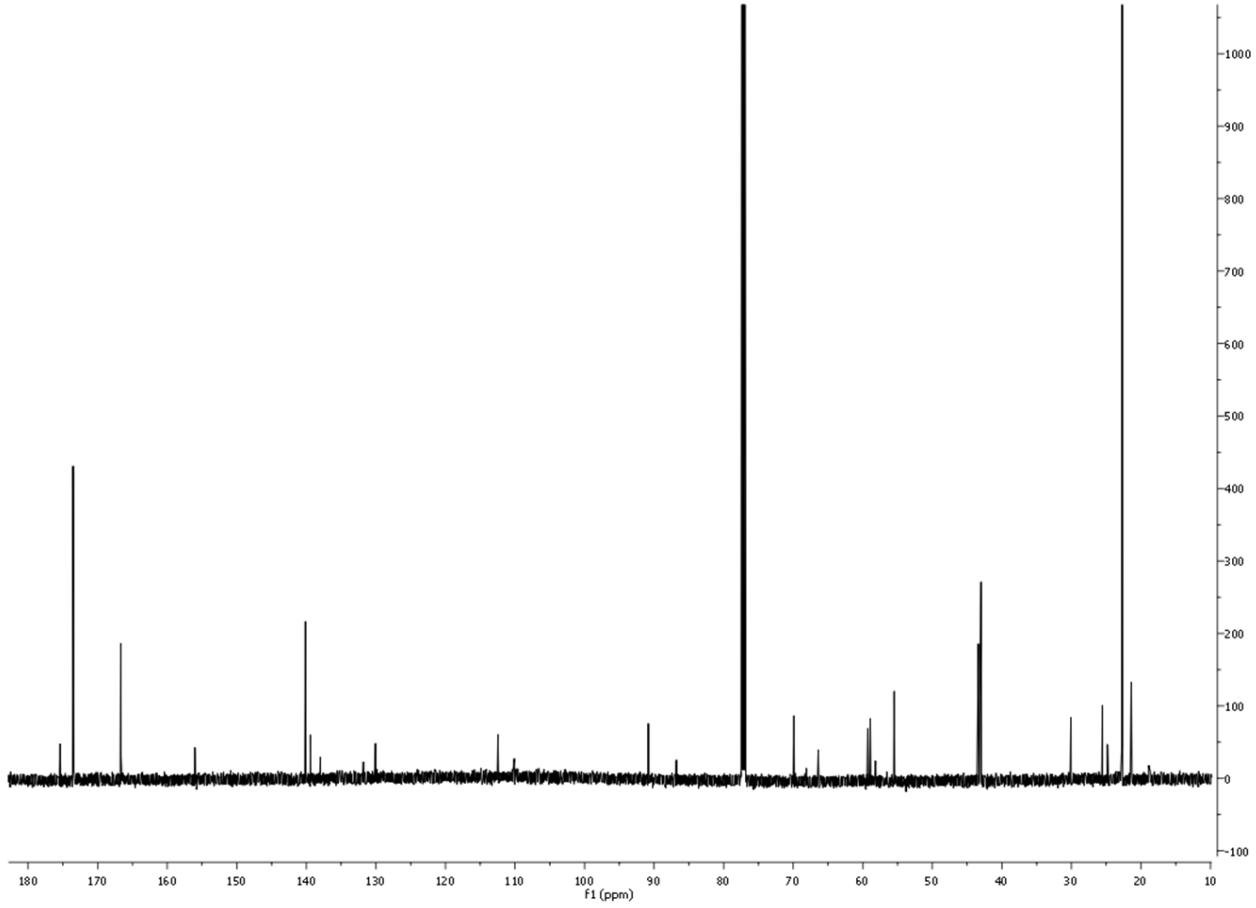


Figure S8. ^{1}H NMR spectrum of pure dakaramine (**1**).

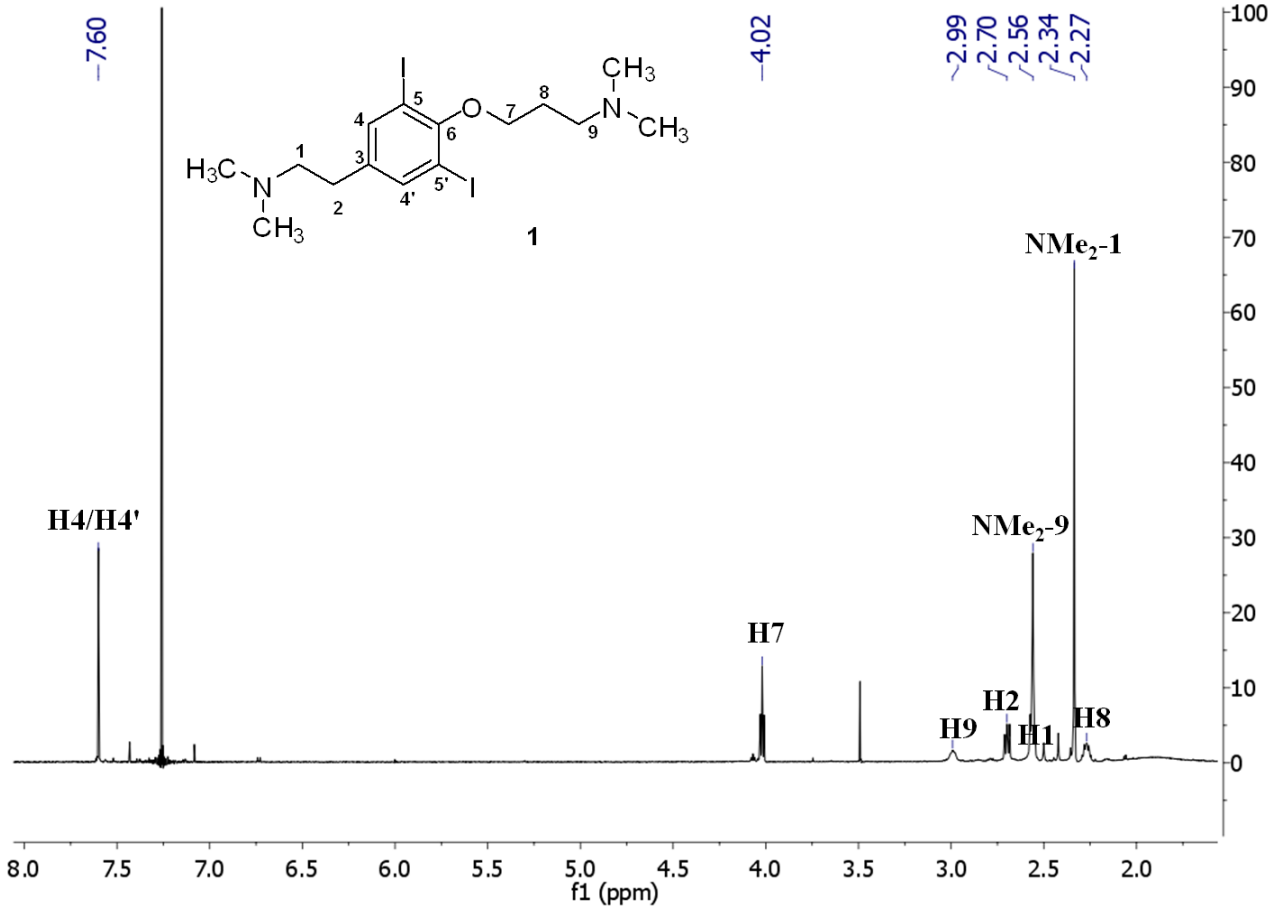


Figure S9. ^{13}C NMR spectrum of pure dakaramine (**1**).

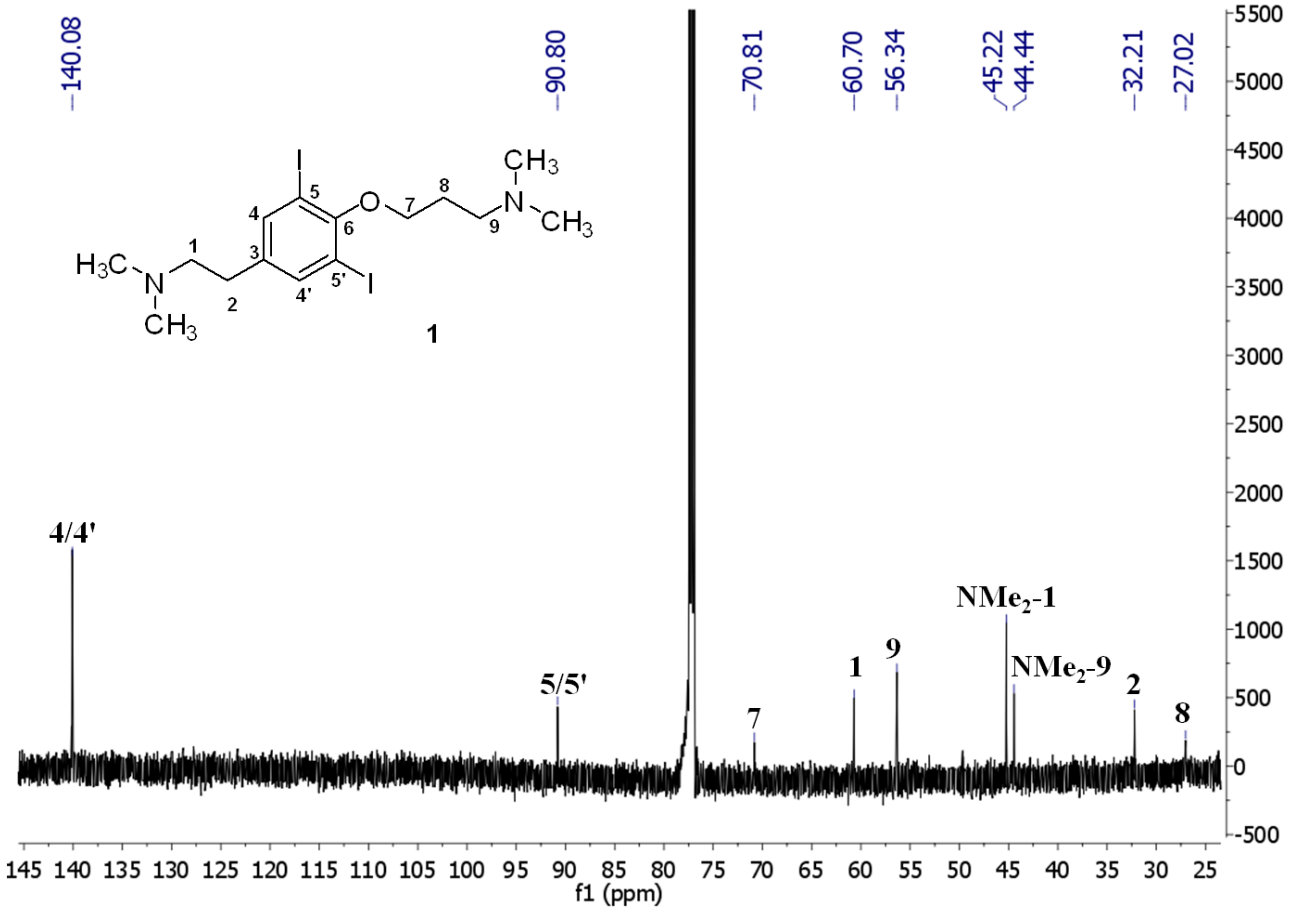


Figure S10. gHSQCAD NMR spectrum of pure dakaramine (**1**).

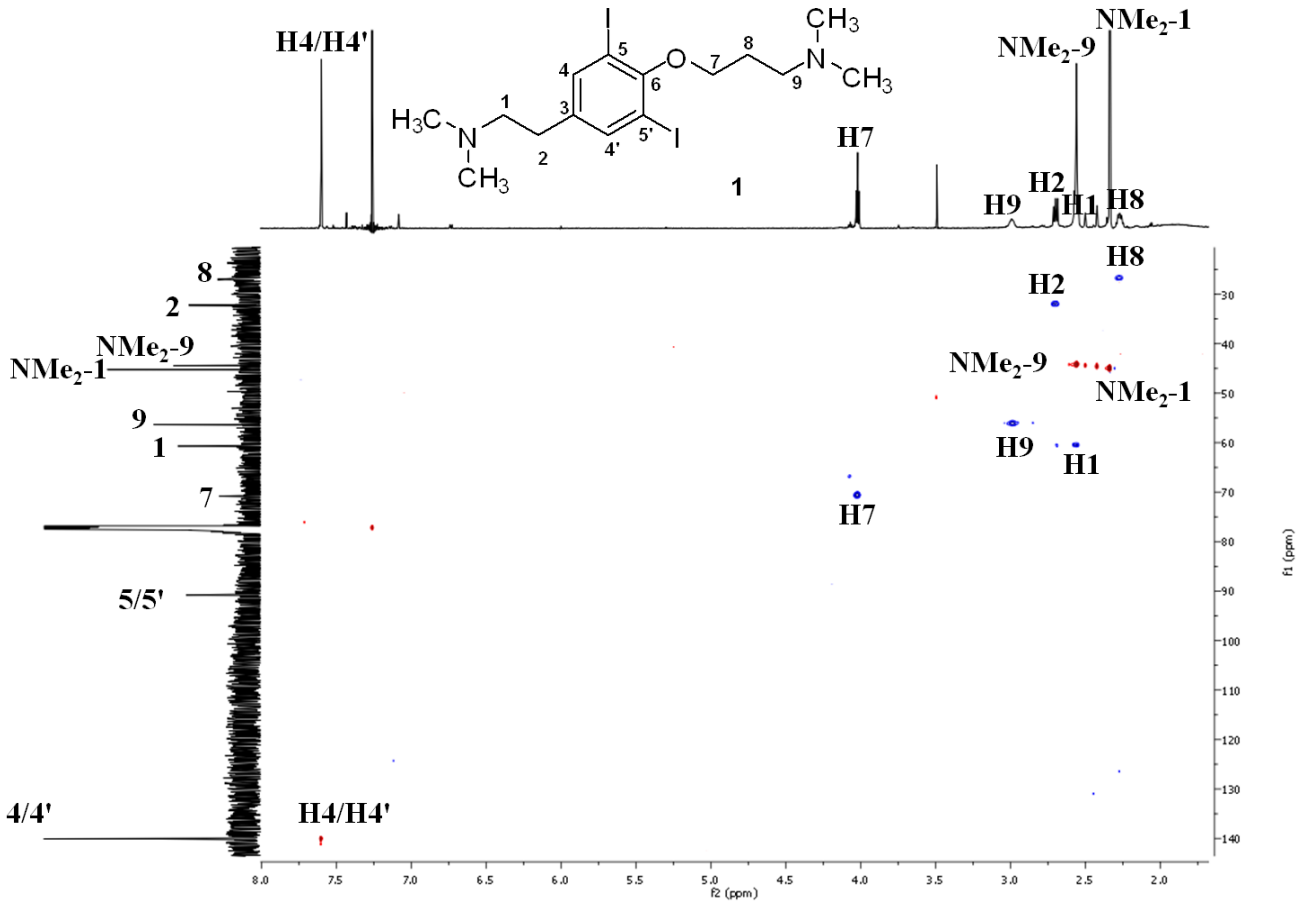


Figure S11. ^{1}H-^{1}H gCOSY NMR spectrum of pure dakaramine (**1**).

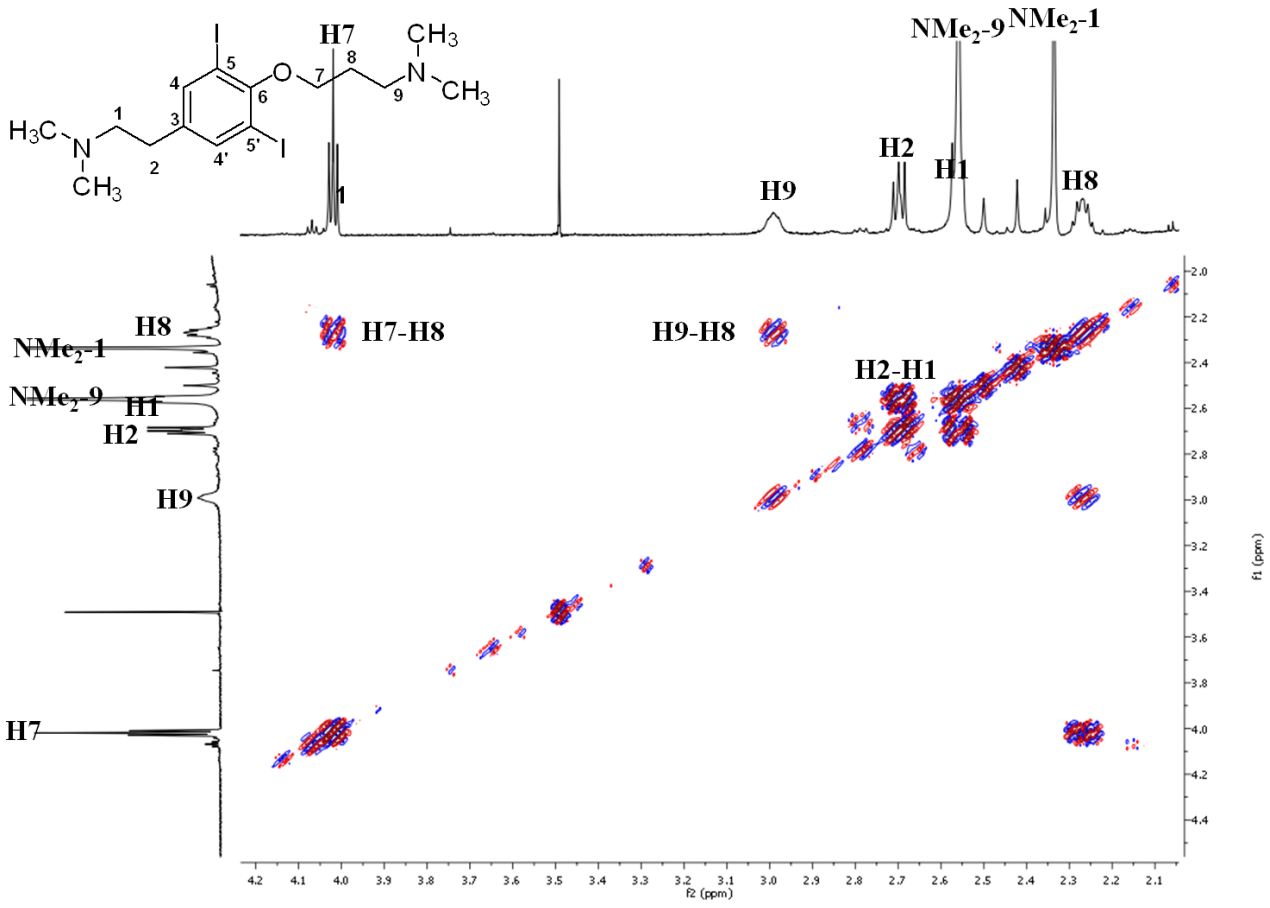


Figure S12. HMBCAD NMR spectrum of pure dakaramine (**1**).

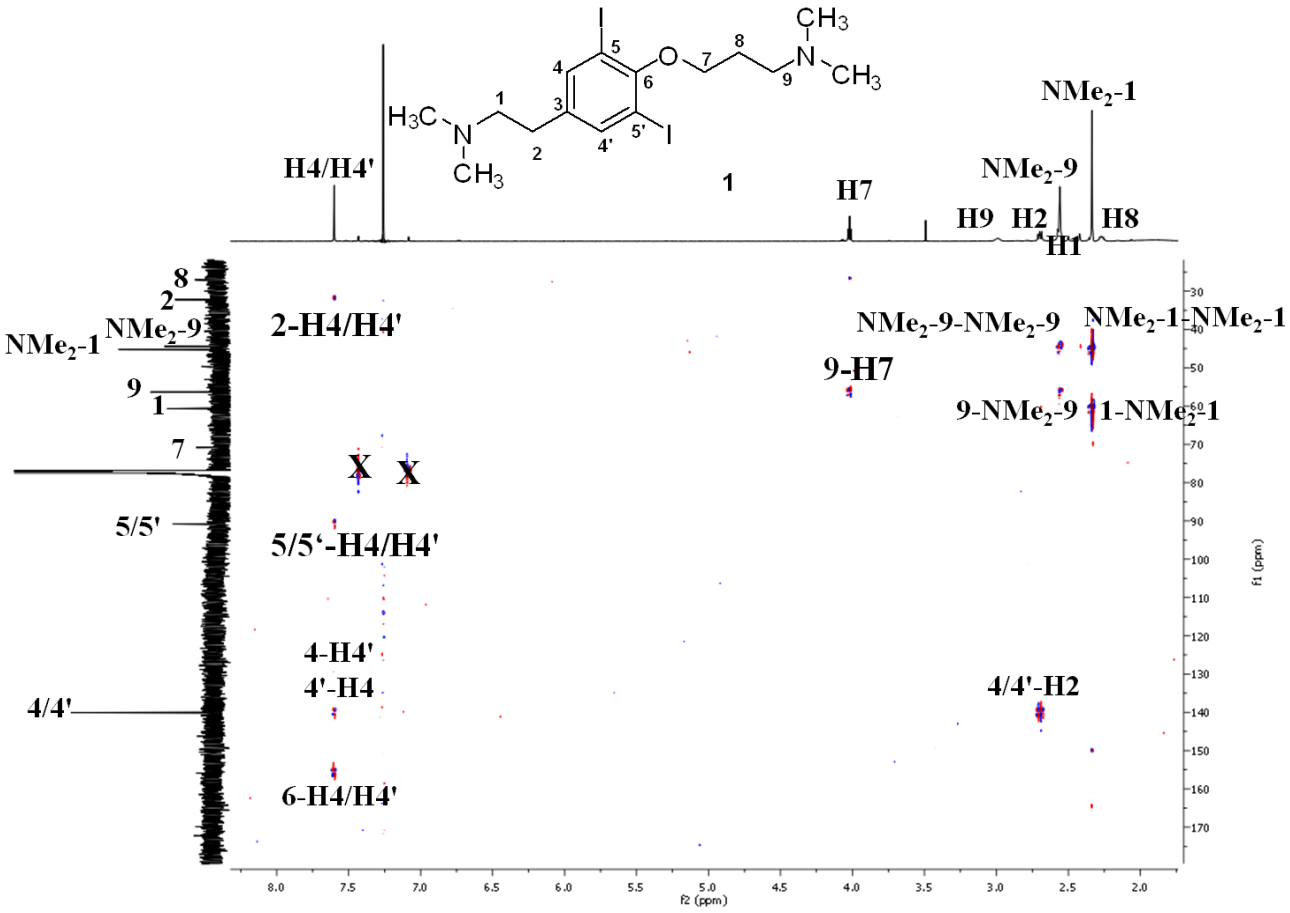


Figure S13. ^{1}H NMR spectrum of pure 1-hydroxypropan-2-yl acetate (**2**).

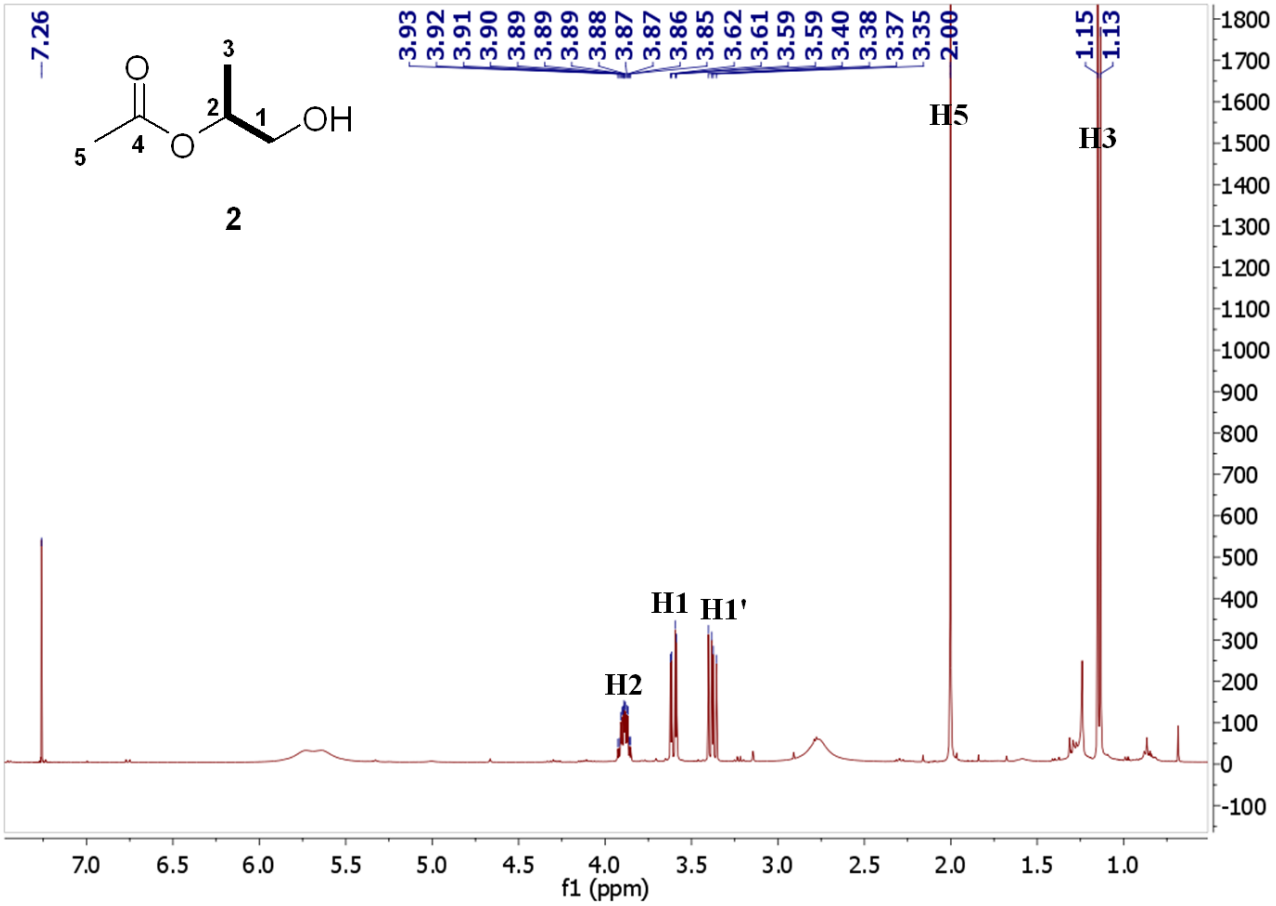


Figure S14. ^{13}C NMR spectrum of pure 1-hydroxypropan-2-yl acetate (**2**).

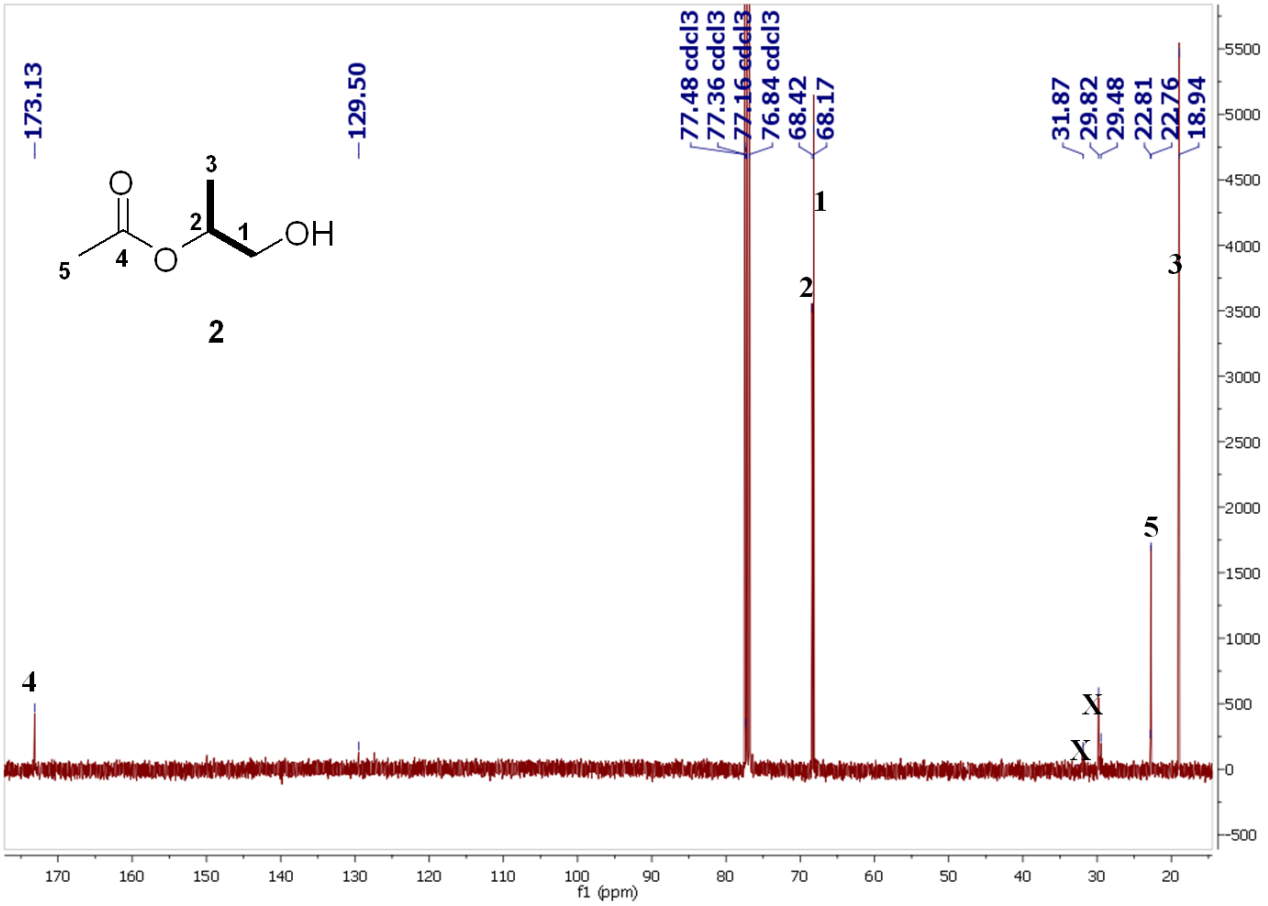


Figure S15. gHSQCAD NMR spectrum of pure 1-hydroxypropan-2-yl acetate (**2**).

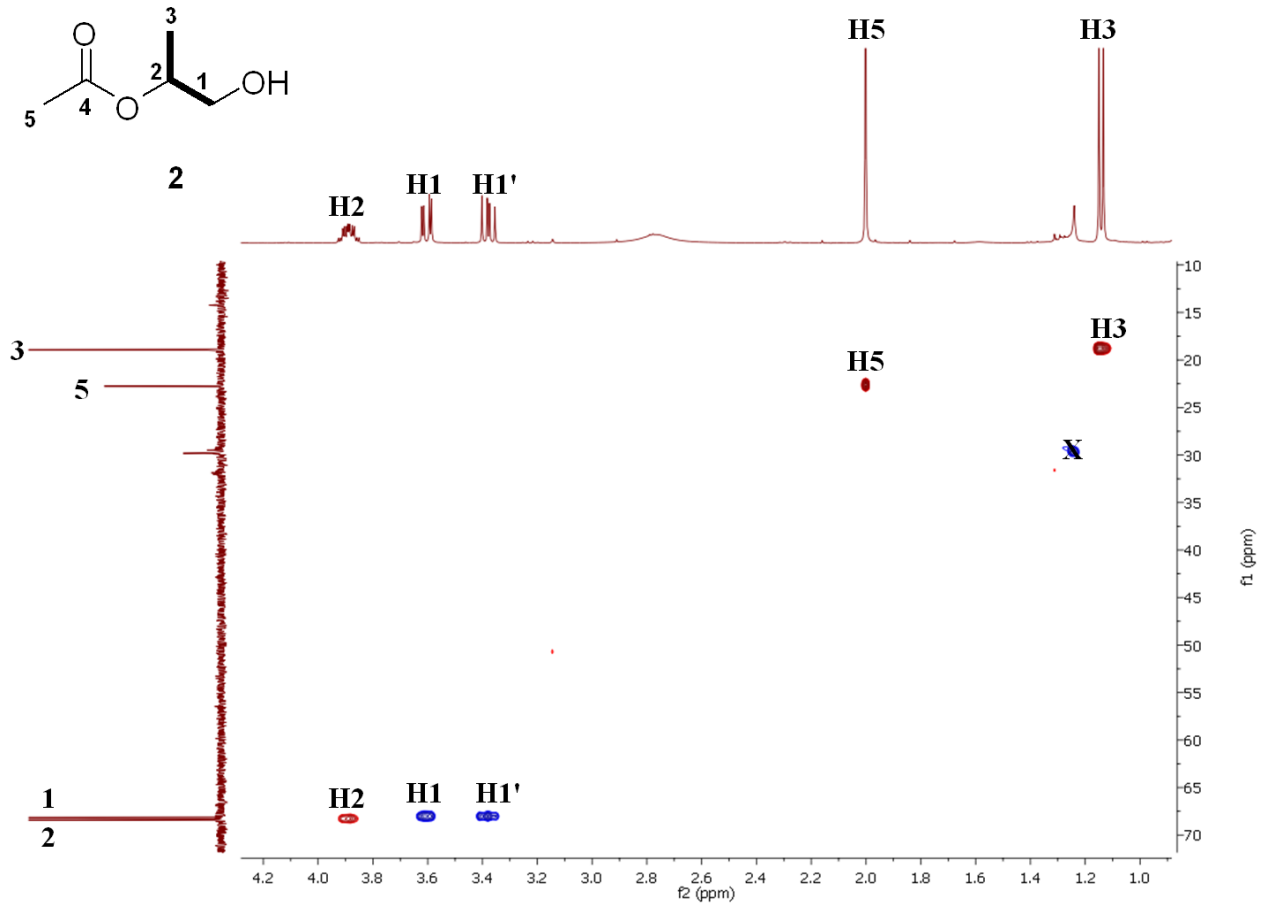


Figure S16. ^{1}H-^{1}H gCOSY NMR spectrum of pure 1-hydroxypropan-2-yl acetate (**2**).

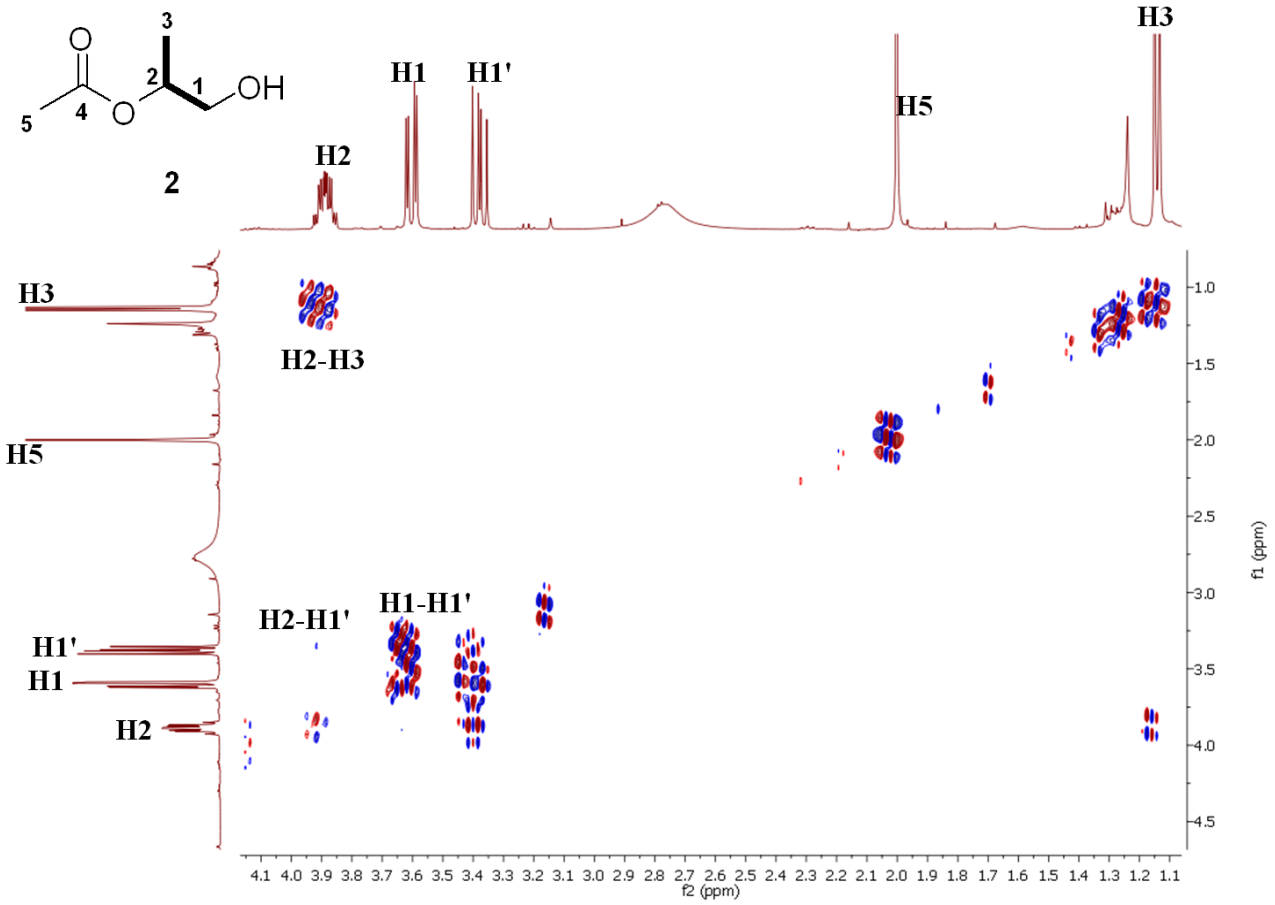


Figure S17. HMBCAD NMR spectrum of pure 1-hydroxypropan-2-yl acetate (**2**).