Supporting Information

Fluorescent chemodosimeter based on spirobenzopyran in NIR for organophosphorus nerve agent mimics (DCP)

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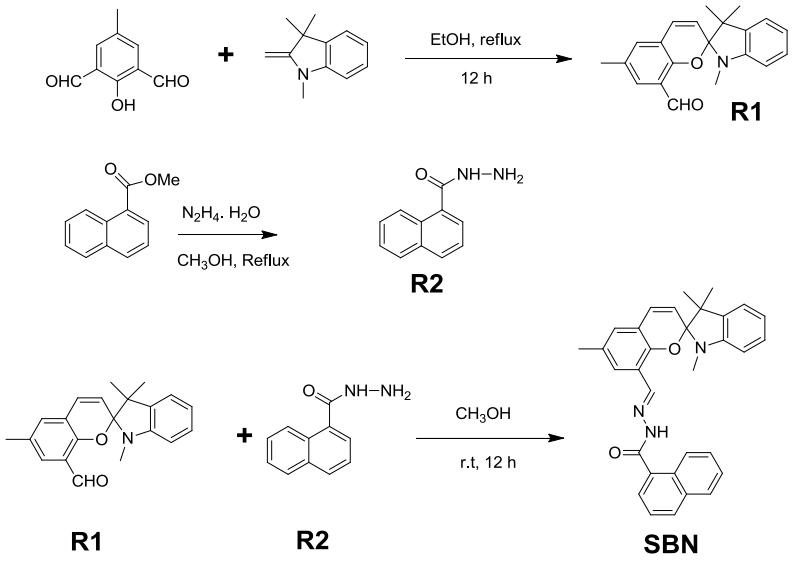
1. Synthetic scheme for the preparation of the probe (SBN):



Scheme 1: Synthetic strategy of SBN

2. Time dependent fluorescence change of SBN upon addition of DCP and reaction kinetics:

The time vs. emission I_{675} plots was obtained by using first order rate equation. We get the rate constant = k = slope×2.303 = 0.55×10^{-2} Sec^{-1}.

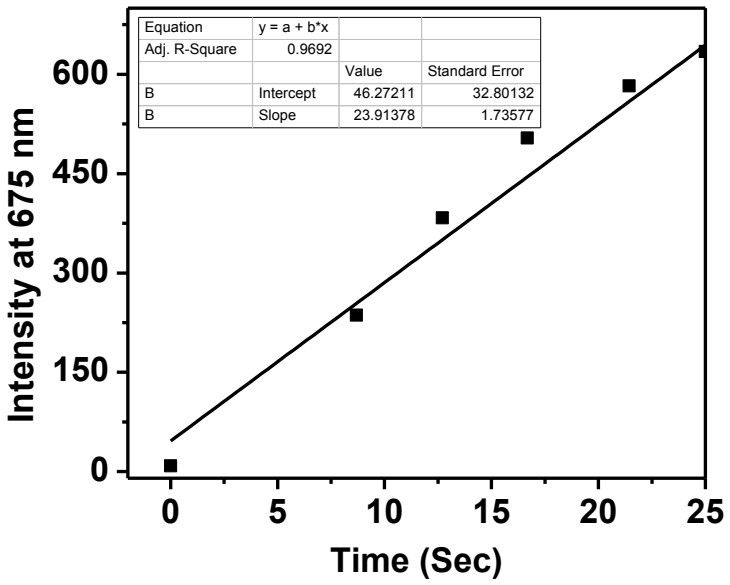


Figure S1: Time (Sec) vs. emission (I_{675}) plot

3. Comparison of absorbance and fluorescence study of SBN after addition of DCP and other analytes.

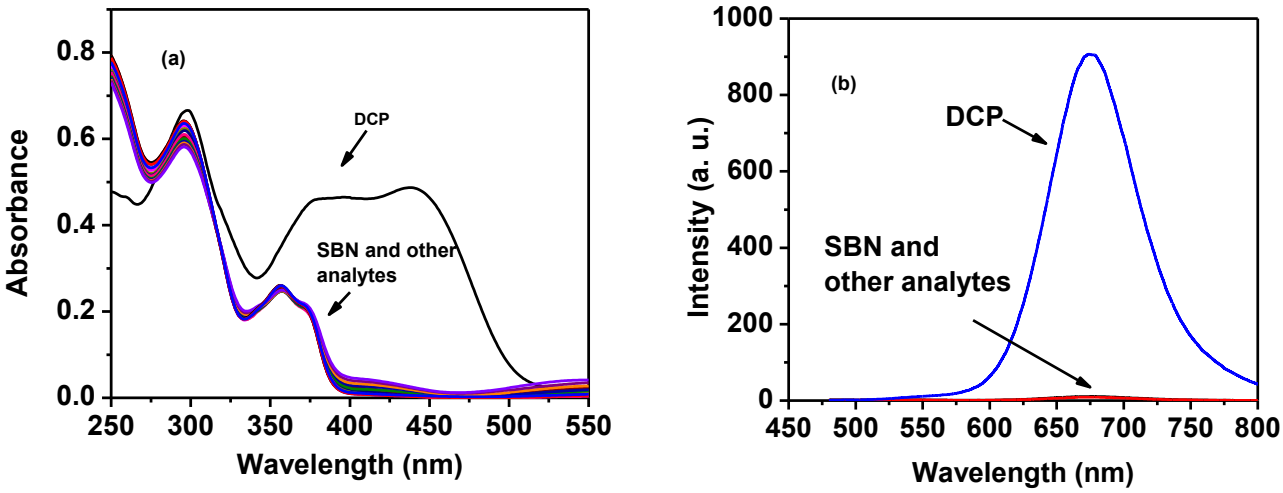


Figure S2. (a) Absorbance and (b) fluorescence spectra of SBN (10 μM) upon addition of different analytes (5 equivalents) in aqueous-CH_3CN solution.

4. Determination of detection limit

The detection limit was calculated based on the fluorescence titration. To determine the S/N ratio, the emission intensity of **SBN** without DCP was measured by 10 times and the standard deviation of blank measurements was determined.

The detection limit (DL) of **SBN** for DCP was determined from the following equation: $DL = K \times Sb_1/S$, Where K = 2 or 3 (we take 3 in this case); Sb_1 is the standard deviation of the blank solution; S is the slope of the calibration curve.

From the graph we get slope = 7.58×10^7, and Sb_1 value is 0.54

Thus using the formula we get the Detection Limit = 2.1×10^{-8} M i.e. SBN can detect DCP in this minimum concentration by fluorescence techniques

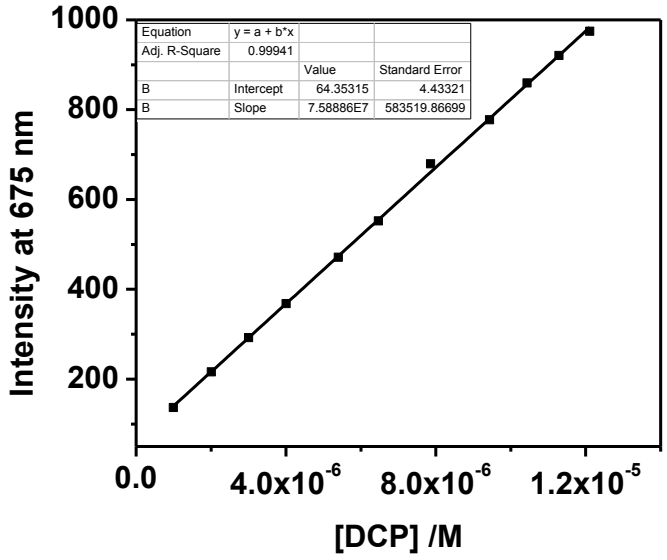


Figure S3: The linear response curve of emission at 675 nm of SBN depending on DCP concentration

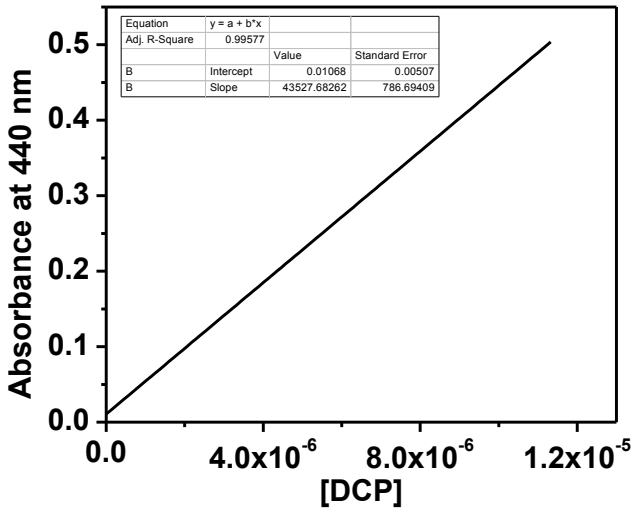


Figure S4: The linear response curve of absorbance at 440 nm of SBN depending on DCP concentration

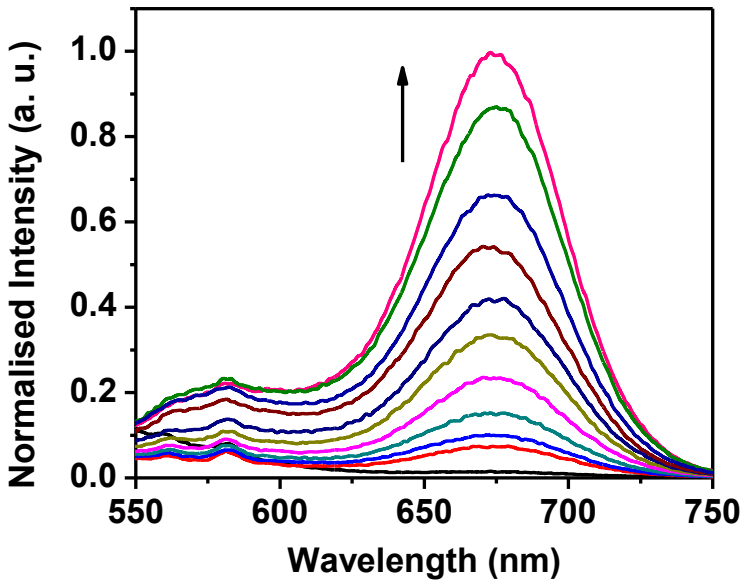


Figure S5: Change of emission intensity of SBN (10 μM) upon addition of DCP (1×10^{-4} M) in DCM

5. NMR and HRMS of SBN

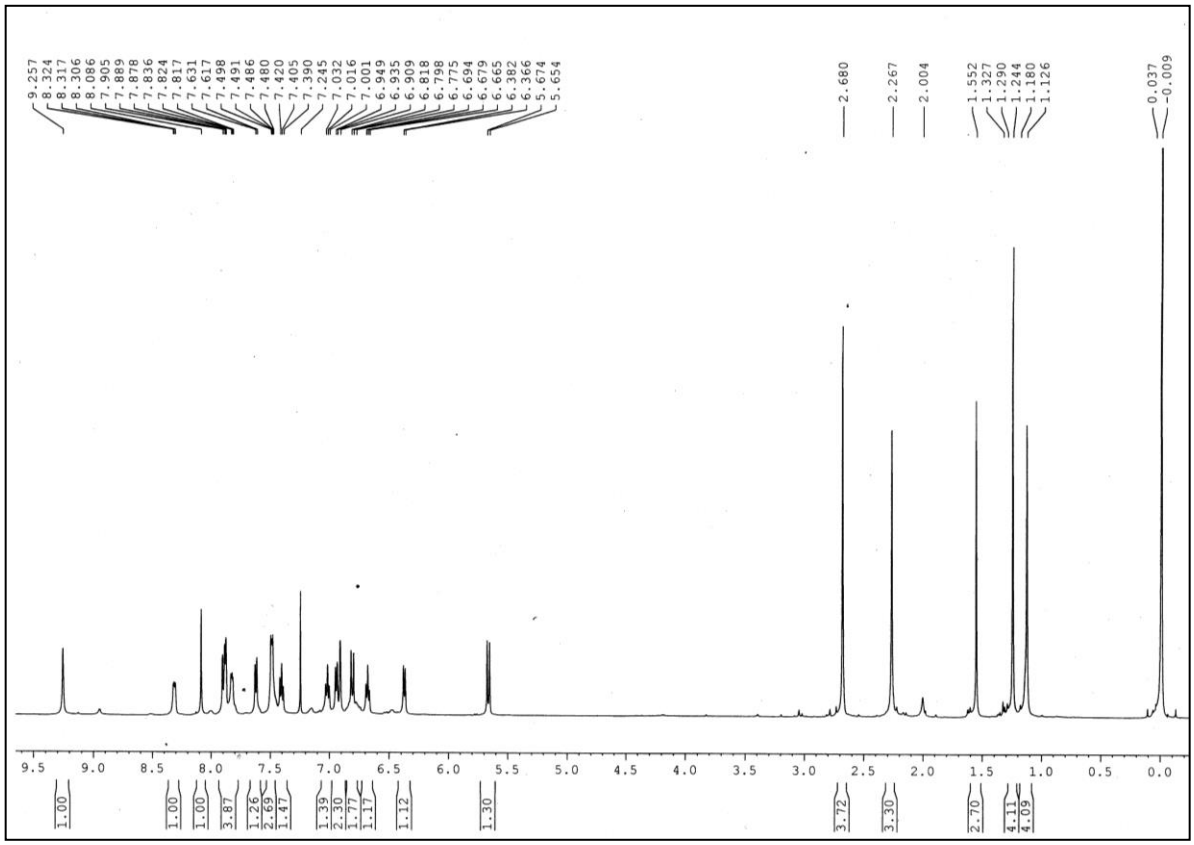


Figure S6: ^{1}H NMR (400 MHz) spectra of compound SBN in $CDCl_3$

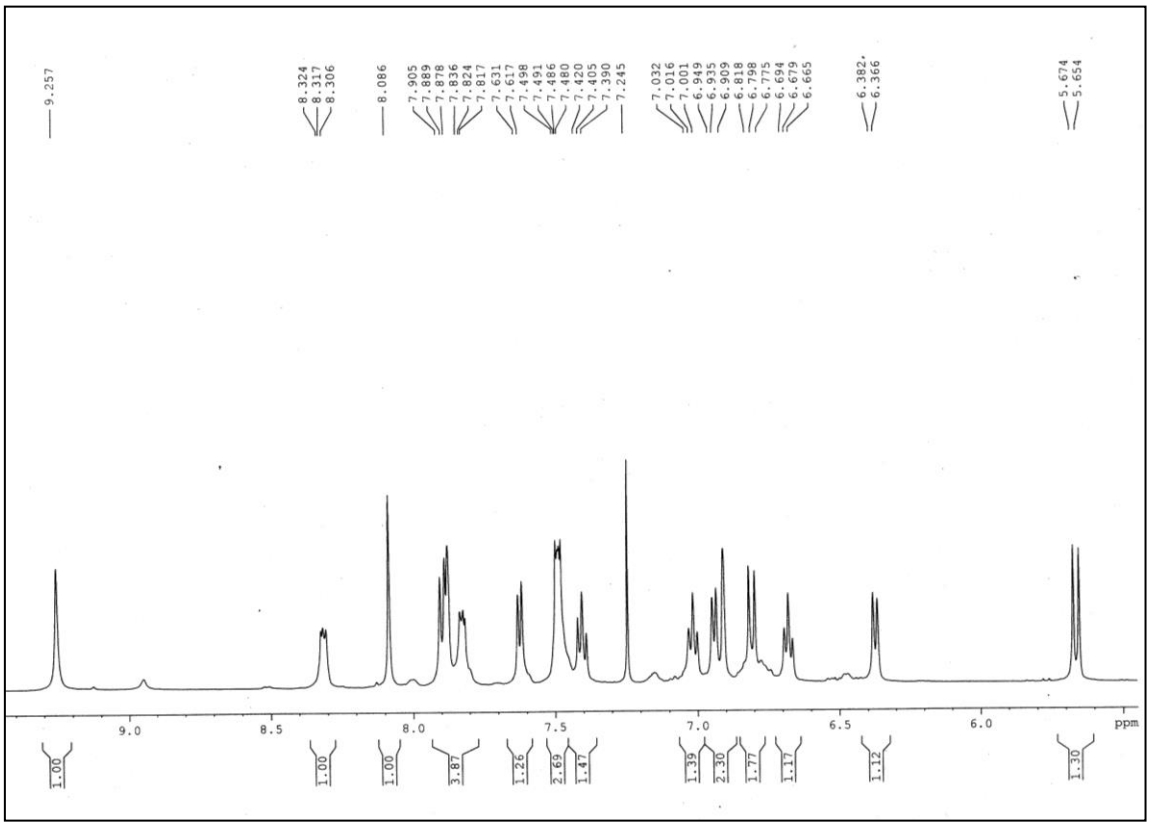


Figure S7: ^{1}H NMR (expansion) spectra of compound SBN in $CDCl_3$.

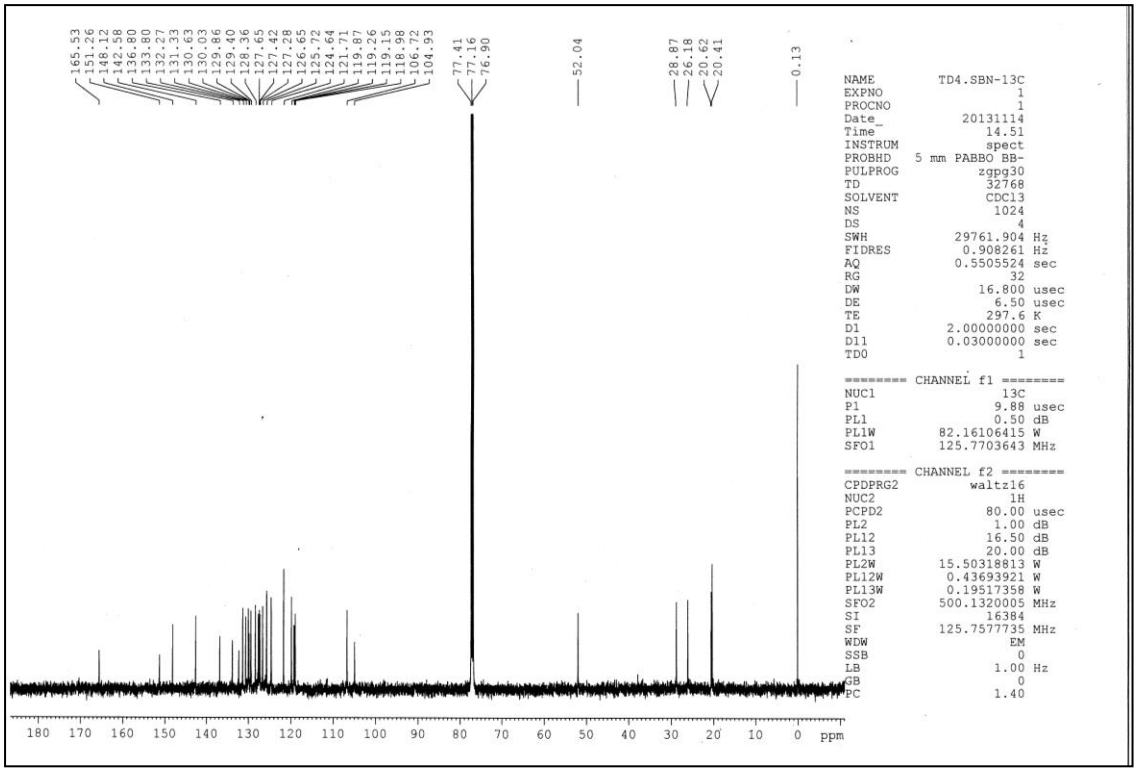


Figure S8: ^{13}C NMR (125 MHz) spectra of compound SBN in $CDCl_3$.

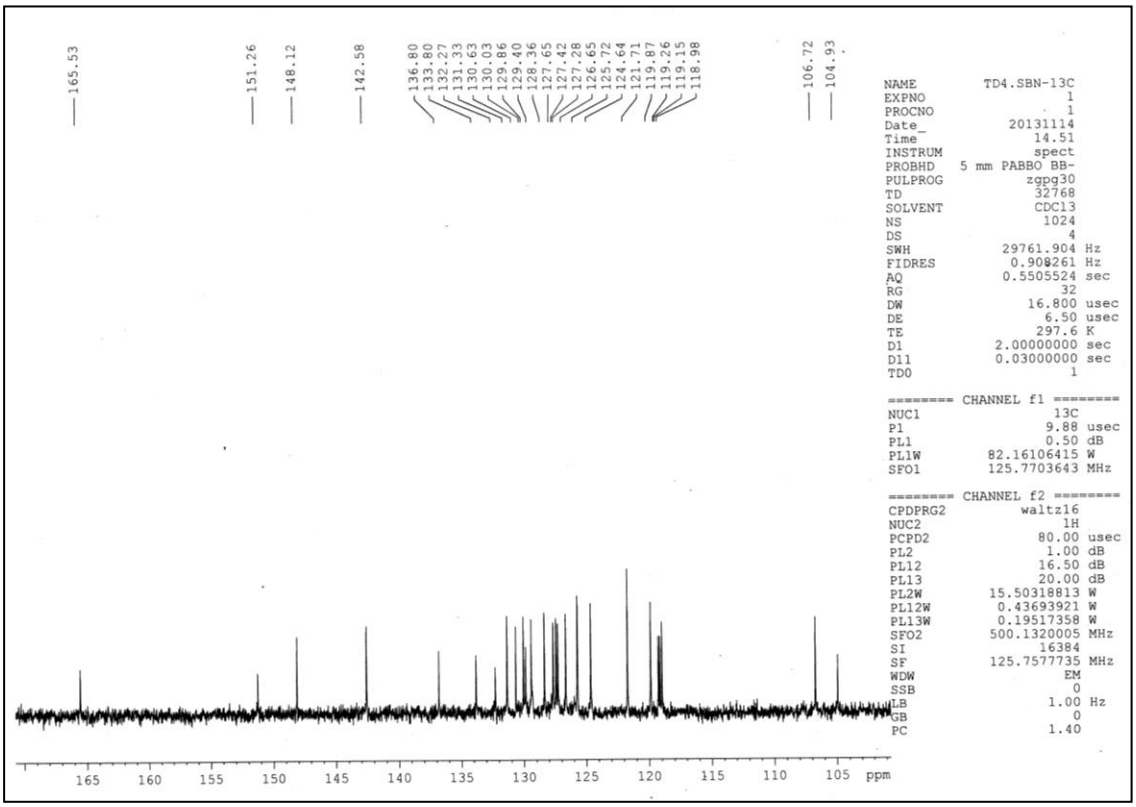


Figure S9: ^{13}C NMR (expansion) spectra of compound SBN in $CDCl_3$.

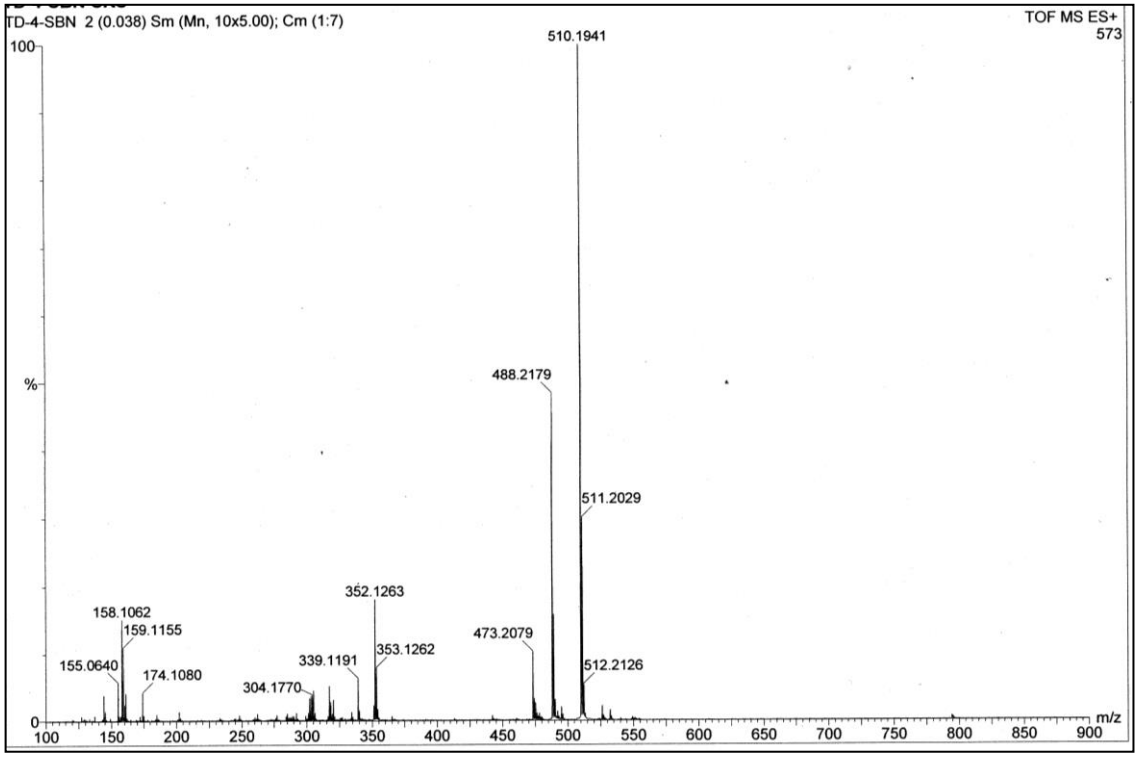


Figure S10: HRMS of the receptor (SBN).

6. ^{1}H and ^{13}C NMR of reaction product:

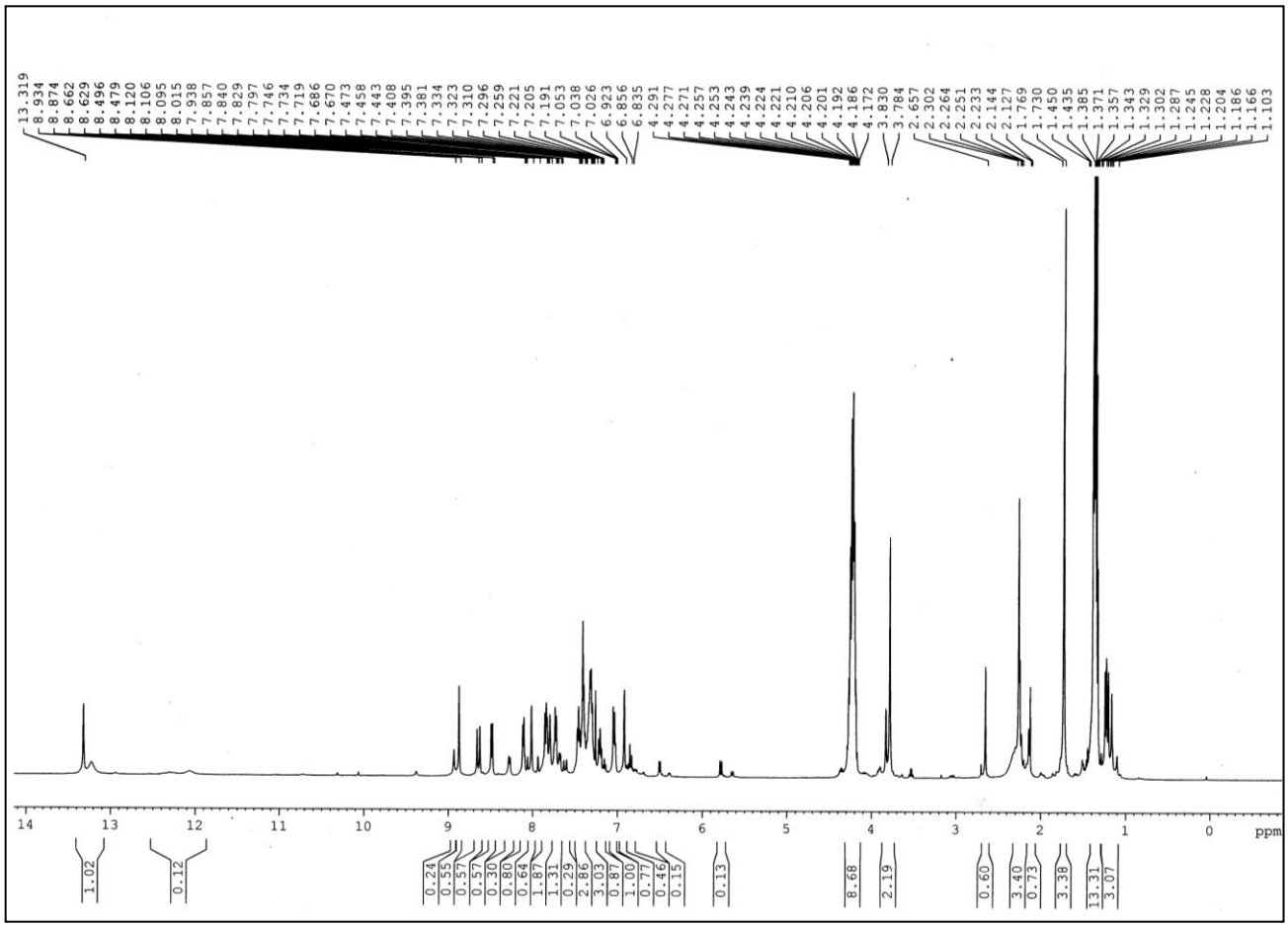


Figure S11: ^{1}H NMR (400 MHz) of the reaction product after hydrolysis.

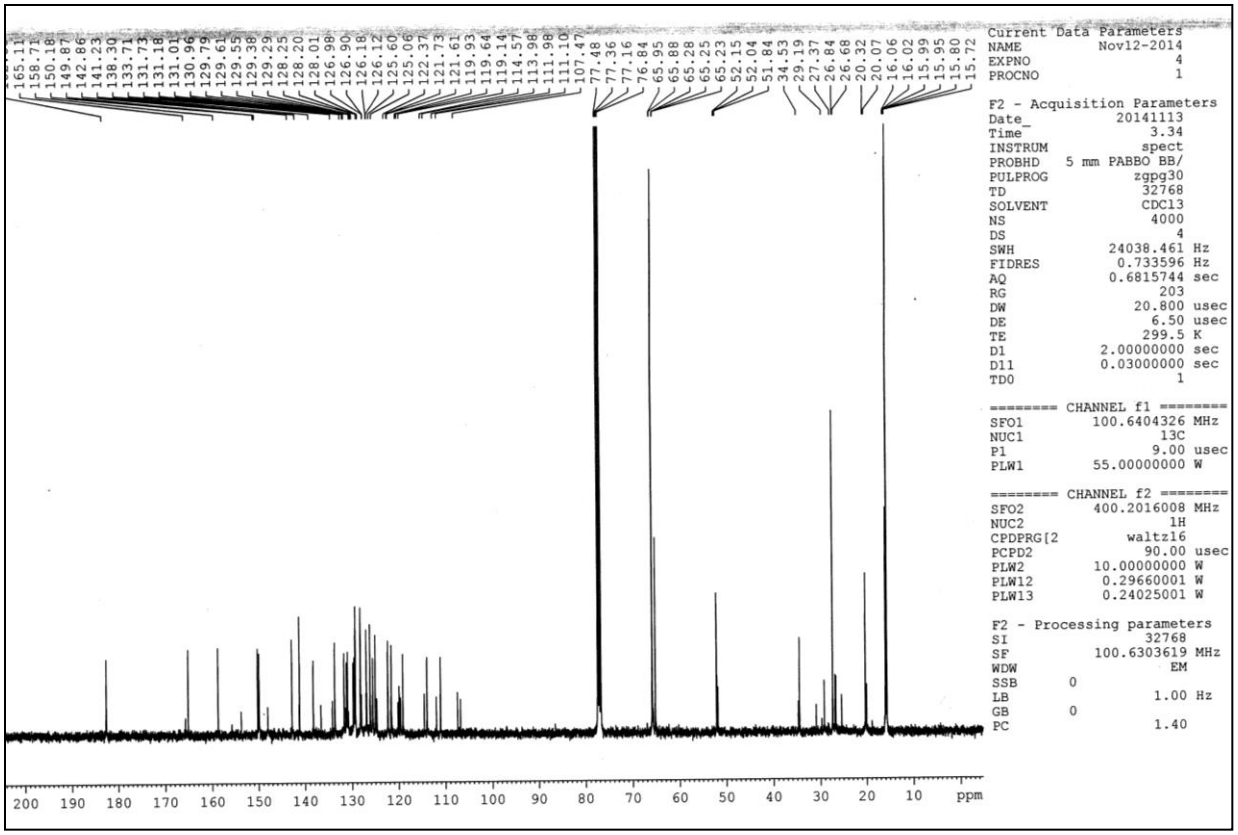


Figure S12: ^{13}C NMR (100 MHz) of the reaction product after hydrolysis.

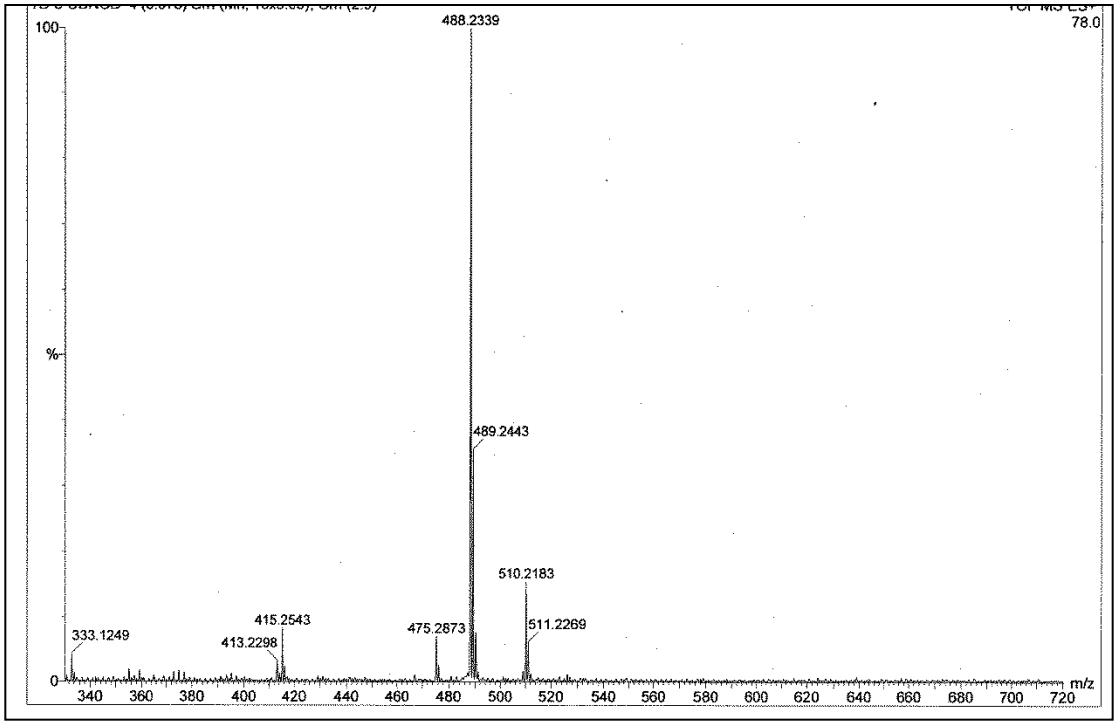


Figure S13: HRMS of the reaction product after hydrolysis.

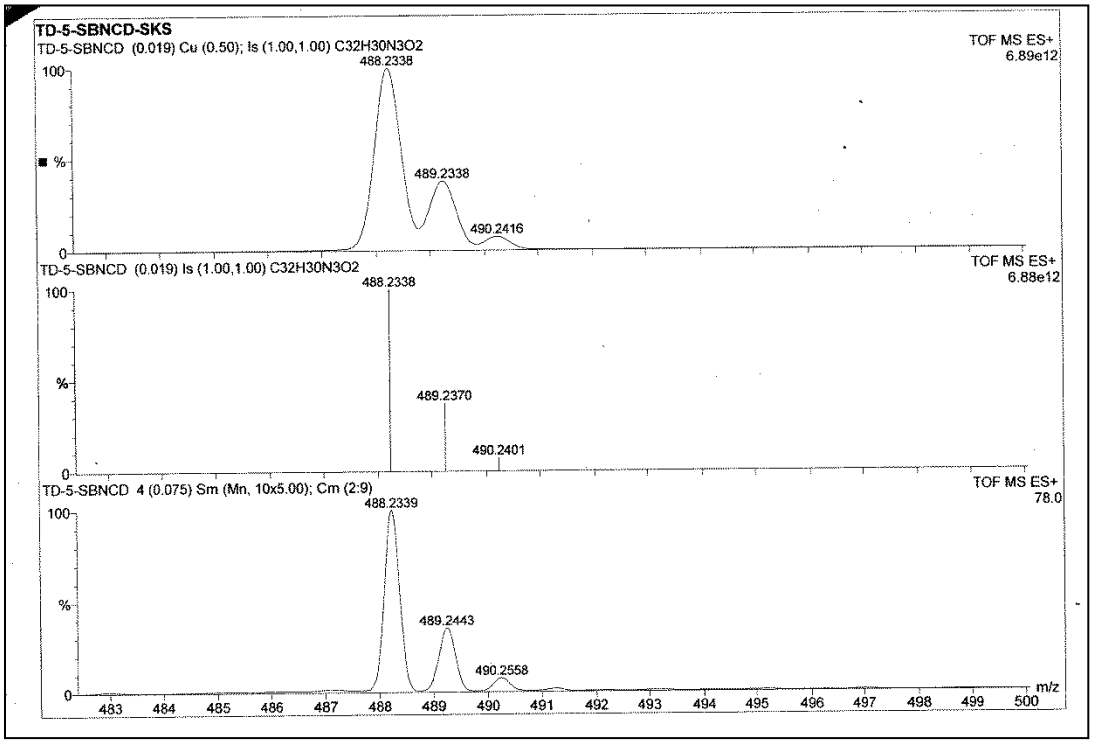


Figure S14: HRMS (expansion) of the reaction product after hydrolysis.