

Electronic Supplementary Information (ESI)

Switching of regioselectivity in base-mediated diastereoselective annulation of 2,3-epoxy tosylates and their *N*-tosylaziridine analogs with 2-mercaptobenzimidazole

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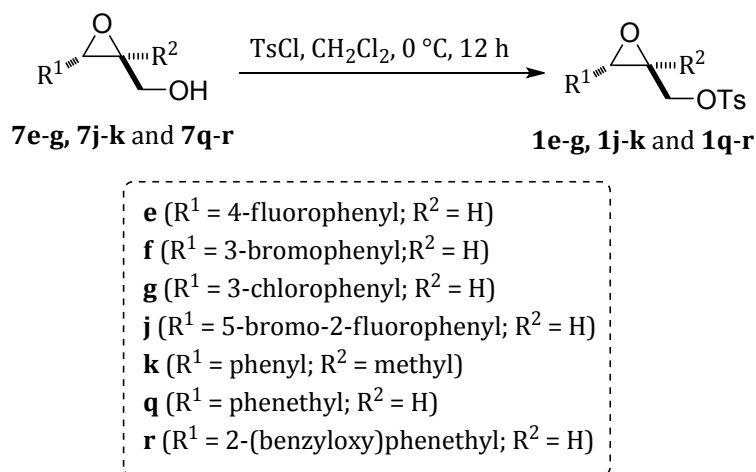
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1. General information:

All commercially available reagents were used without further purification. All dry reactions were carried out in oven-dried glassware and under nitrogen atmosphere. Solvents used in reactions were distilled over appropriate drying agents prior to use. Thin-layer chromatography (TLC) was performed on pre-coated Merck silica gel plates (60 F254). Compounds were visualized with UV light ($\lambda = 254$ nm). Column chromatography was performed using silica gel (60–120 mesh) procured from Merck using freshly distilled solvents. Melting points were determined with a Buchi-535 apparatus and are not corrected. Perkin Elmer 20 analyzer was utilized for elemental analysis of all compounds. ^1H NMR and ^{13}C NMR spectra were run on JEOL 400 MHz and Bruker Avance III 400 MHz spectrometers in CDCl_3 or $\text{DMSO}-d_6$ as solvent. Chemical shifts are expressed in δ ppm using residual solvent as the internal standard. Coupling constants (J) are reported in Hz. The following abbreviations were used to describe the NMR multiplicities: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, ddd = doublet of doublets of doublets, td = triplet of doublets, dt = doublet of triplets, tt = triplet of triplets, dq = doublet of quartets, qd = quartet of doublets, and m = multiplet. All spectra were recorded at 25 °C.

2. Synthesis of 2,3-epoxy tosylates:

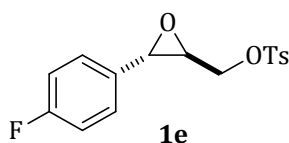
2,3-Epoxy tosylates **1a-d**,¹ **1h-i**,¹ **1l**,² **1p**³ and **1s**³ are known compounds and were prepared following the reported procedures. Scheme ESI-1 shows the preparation of the remaining starting epoxy tosylates **1e-g**, **1j-k** and **1q-r**.



Scheme ESI-1. Preparation of 2,3-epoxy tosylates **1e-g**, **1j-k** and **1q-r**.

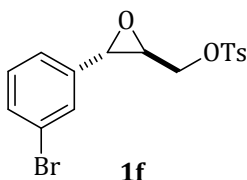
General procedure of tosylation: To a stirred solution of appropriate epoxy alcohol **7** (2.0 mmol) in CH₂Cl₂ (20 mL) at 0 °C was added triethylamine (0.5 mL, 3.5 mmol) followed by tosyl chloride (429 mg, 2.25 mmol) and kept in the refrigerator for 12 h. The reaction mixture was diluted with H₂O (20 mL), and extracted with CH₂Cl₂ (2 × 20 mL). The combined organic layers were washed with brine (40 mL) and dried over anhydrous Na₂SO₄. After filtration, the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography (5-10% EtOAc/hexanes) to afford epoxy tosylate **1**.

((2*S,3*S**)-3-(4-Fluorophenyl)oxiran-2-yl)methyl 4-methylbenzenesulfonate (**1e**):**



The title compound **1e** was prepared from epoxy alcohol **7e** (336 mg, 2.0 mmol) according to the general procedure. Colorless semi-solid. Yield: 85% (548 mg). ¹H NMR (CDCl₃, 400 MHz): δ 7.82 (dt, *J* = 8.2, 2.3 Hz, 2H), 7.36 (d, *J* = 8.2 Hz, 2H), 7.22-7.17 (m, 2H), 7.06-7.01 (m, 2H), 4.32 (dd, *J* = 11.5, 4.1 Hz, 1H), 4.16 (dd, *J* = 11.5, 5.0 Hz, 1H), 3.76 (d, *J* = 1.8 Hz, 1H), 3.23-3.20 (m, 1H), 2.46 (s, 3H). ¹³C NMR (CDCl₃, 100 MHz): δ 164.1, 161.6, 145.2, 132.5, 131.3, 129.9, 127.9, 115.4, 69.2, 58.4, 55.9, 21.6. Anal. calcd. for C₁₆H₁₅FO₄S: C, 59.62; H, 4.69; found: C, 59.78; H, 4.75.

((2*S,3*S**)-3-(3-Bromophenyl)oxiran-2-yl)methyl 4-methylbenzenesulfonate (**1f**):**

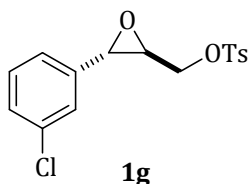


The title compound **1f** was prepared from epoxy alcohol **7f** (458 mg, 2.0 mmol) according to the general procedure. Colorless semi-solid. Yield: 82% (628 mg). ¹H NMR (CDCl₃, 400 MHz): δ 7.83 (dt, *J* = 8.2, 1.8 Hz, 2H), 7.46-7.43 (m, 1H), 7.38-7.33 (m, 3H), 7.21 (t, *J* = 7.8 Hz, 1H), 7.16 (dt, *J* = 7.8, 1.4 Hz, 1H), 4.31 (dd, *J* = 11.9, 3.7 Hz, 1H), 4.17 (dd, *J* = 11.5, 5.0 Hz, 1H), 3.73 (d, *J* = 2.3 Hz, 1H), 3.21-3.18 (m, 1H), 2.46 (s, 3H). ¹³C NMR (CDCl₃, 100 MHz): δ

145.3, 137.9, 132.6, 131.7, 130.0, 129.9, 128.6, 128.0, 124.4, 122.7, 68.9, 58.6, 55.7, 21.6.

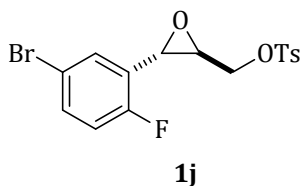
Anal. calcd. for C₁₆H₁₅BrO₄S: C, 50.14; H, 3.94; found: C, 50.31; H, 3.84.

((2*S,3*S**)-3-(3-Chlorophenyl)oxiran-2-yl)methyl 4-methylbenzenesulfonate (**1g**):**



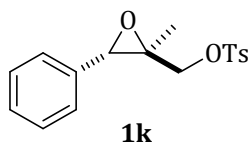
The title compound **1g** was prepared from epoxy alcohol **7g** (369 mg, 2.0 mmol) according to the general procedure. Colorless semi-solid. Yield: 86% (583 mg). ¹H NMR (CDCl₃, 400 MHz): δ 7.82 (dt, *J* = 8.2, 2.3 Hz, 2H), 7.37 (d, *J* = 0.9 Hz, 1H), 7.35 (s, 1H), 7.30-7.26 (m, 2H), 7.17 (t, *J* = 1.8 Hz, 1H), 7.10 (dt, *J* = 6.4, 1.8 Hz, 1H), 4.31 (dd, *J* = 11.9, 4.1 Hz, 1H), 4.16 (dd, *J* = 11.5, 5.5 Hz, 1H), 3.73 (d, *J* = 2.3 Hz, 1H), 3.20-3.17 (m, 1H), 2.45 (s, 3H). ¹³C NMR (CDCl₃, 100 MHz): δ 145.2, 137.7, 134.6, 132.6, 130.0, 129.9, 128.7, 127.9, 125.7, 123.9, 68.9, 58.6, 55.7, 21.7. Anal. calcd. for C₁₆H₁₅ClO₄S: C, 56.72; H, 4.46; found: C, 56.57; H, 4.41.

((2*S,3*S**)-3-(5-Bromo-2-fluorophenyl)oxiran-2-yl)methyl 4-methylbenzenesulfonate (**1j**):**



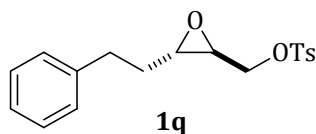
The title compound **1j** was prepared from epoxy alcohol **7j** (494 mg, 2.0 mmol) according to the general procedure. Colorless semi-solid. Yield: 80% (642 mg). ¹H NMR (CDCl₃, 400 MHz): δ 7.83 (d, *J* = 8.2 Hz, 2H), 7.41-7.36 (m, 3H), 7.24 (dd, *J* = 6.4, 2.7 Hz, 1H), 6.97-6.91 (m, 1H), 4.37 (dd, *J* = 11.4, 3.2 Hz, 1H), 4.13 (dd, *J* = 11.9, 6.0 Hz, 1H), 3.98 (d, *J* = 1.8 Hz, 1H), 3.24-3.21 (m, 1H), 2.46 (s, 3H). Anal. calcd. for C₁₆H₁₄BrFO₄S: C, 47.89; H, 3.52; found: C, 48.11; H, 3.57.

((2*S,2*S**)-2-Methyl-3-phenyloxiran-2-yl)methyl 4-methylbenzenesulfonate (**1k**):**



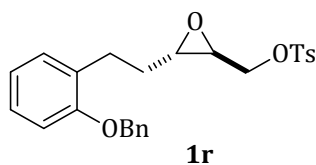
The title compound **1k** was prepared from epoxy alcohol **7k** (328 mg, 2.0 mmol) according to the general procedure. Colorless semi-solid. Yield: 84% (535 mg). ¹H NMR (CDCl₃, 400 MHz): δ 7.83 (d, *J* = 8.2 Hz, 2H), 7.38-7.32 (m, 4H), 7.31-7.29 (m, 1H), 7.26-7.24 (m, 2H), 4.12 (q, *J* = 8.9 Hz, 2H), 3.97 (s, 1H), 2.46 (s, 3H), 1.09 (s, 3H). ¹³C NMR (CDCl₃, 100 MHz): δ 145.1, 134.4, 132.6, 130.0, 129.9, 128.1, 128.0, 126.4, 73.6, 61.7, 60.5, 21.7, 13.3. Anal. calcd. For C₁₇H₁₈O₄S: C, 64.13; H, 5.70; found: C, 64.01; H, 5.75.

((2S*,3S*)-3phenethyloxiran-2-yl)methyl 4-methylbenzenesulfonate (1q):



The title compound **1q** was prepared from epoxy alcohol **7q** (356 mg, 2.0 mmol) according to the general procedure. Colorless semi-solid. Yield: 90% (598 mg). ¹H NMR (CDCl₃, 400 MHz): δ 7.79 (d, *J* = 8.2 Hz, 2H), 7.36 (d, *J* = 8.2 Hz, 2H), 7.31-7.27 (m, 2H), 7.22-7.16 (m, 3H), 4.13 (dd, *J* = 11.5, 3.7 Hz, 1H), 3.93 (dd, *J* = 11.0, 5.5 Hz, 1H), 2.92-2.89 (m, 1H), 2.84-2.66 (m, 3H), 2.46 (s, 3H), 1.92-1.79 (m, 2H). ¹³C NMR (CDCl₃, 100 MHz): δ 145.0, 140.7, 132.7, 129.9, 128.5, 128.3, 127.9, 126.2, 69.9, 56.0, 54.7, 33.0, 31.9, 21.7. Anal. calcd. for C₁₈H₂₀O₄S: C, 65.04; H, 6.06; found: C, 65.19; H, 6.03.

((2S*,3S*)-3phenethyloxiran-2-yl)methyl 4-methylbenzenesulfonate (1r):

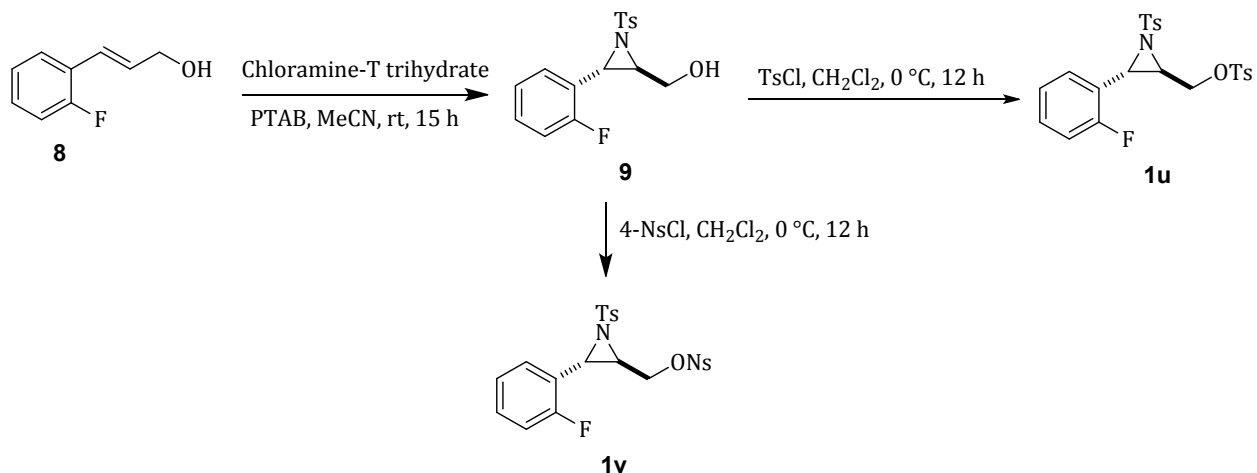


The title compound **1r** was prepared from epoxy alcohol **7r** (568 mg, 2.0 mmol) according to the general procedure. Colorless semi-solid. Yield: 87% (763 mg). ¹H NMR (400 MHz, CDCl₃): δ 7.84-7.74 (m, 2H), 7.44-7.11 (m, 9H), 6.93-6.87 (m, 2H), 5.07 (s, 2H), 4.15-4.08 (m, 1H), 3.86-3.81 (m, 1H), 2.87-2.74 (m, 3H), 2.44 (s, 3H), 1.93-1.77 (m, 2H). ¹³C NMR (100 MHz, CDCl₃): δ 156.3, 144.9, 137.0, 132.5, 129.9, 129.7, 129.2, 128.4, 127.7, 127.4, 127.0,

125.5, 120.6, 111.5, 70.1, 69.6, 56.0, 54.6, 31.3, 26.6, 21.5. Anal. calcd for C₂₅H₂₆O₅S: C, 68.47; H, 5.98, found: C, 68.39; H, 5.92.

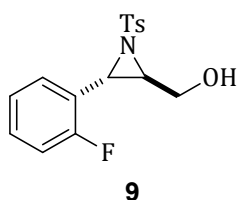
3. Synthesis of 2,3-(*N*-tosyl)aziridino tosylate **1u** and its nosylate analog **1v**

2,3-(*N*-tosyl)aziridino tosylates **1t**⁴ and **1w**⁵ are known compounds and were prepared following the reported procedures. Scheme ESI-2 shows the preparation of tosylate **1u** and nosylate **1v**.



Scheme ESI-2. Preparation of 2,3-(*N*-tosyl)aziridino tosylate **1u** and its nosylate analog **1v**.

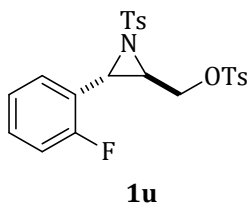
((2*R**,3*S**)-3-(2-Fluorophenyl)-1-tosylaziridin-2-yl)methanol (**9**)



To a stirred mixture of chloramine-T trihydrate (1.86 g, 6.6 mmol) and **8** (914 mg, 6.0 mmol) in CH₃CN (15 mL) was added phenyltrimethylammonium tribromide (228 mg, 0.6 mmol) at room temperature. The reaction was stirred vigorously for 15 h and then concentrated under reduced pressure. The resulting residue was dissolved in CH₂Cl₂ and filtered through a short column of silica gel (eluted with 30% EtOAc in hexanes). After removal of the solvent, the resultant crude product was subjected to further purification

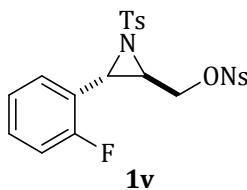
involving a silica gel column chromatography (5-20% EtOAc/hexanes) to furnish **9** as a colorless gum. Yield: 65% (1.25 g). ^1H NMR (400 MHz, CDCl_3): δ 7.86 (d, $J = 8.2$ Hz, 2H), 7.32 (d, $J = 8.2$ Hz, 2H), 7.24 (t, $J = 7.3$ Hz, 1H), 7.04-7.00 (m, 2H), 6.95 (t, $J = 6.9$ Hz, 1H), 4.38-4.31 (m, 1H), 4.24-4.18 (m, 2H), 3.25-3.21 (m, 1H), 3.10-3.06 (dd, $J = 10.1, 5.0$ Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$): δ 161.4 (d, $J_{\text{C-F}} = 248.2$ Hz), 144.5, 136.8, 129.3 (d, $J_{\text{C-F}} = 8.6$ Hz), 129.7, 127.3, 124.3 (d, $J_{\text{C-F}} = 3.8$ Hz), 121.9 (d, $J_{\text{C-F}} = 13.4$ Hz), 115.5, 115.2, 60.7, 53.4, 41.0, 21.6. Anal. calcd. for $\text{C}_{16}\text{H}_{16}\text{FNO}_3\text{S}$: C, 59.80; H, 5.02; N, 4.36; found: C, 59.63; H, 5.15; N, 4.27.

((2*R,3*S**)-3-(2-Fluorophenyl)-1-tosylaziridin-2-yl)methyl 4-methylbenzene sulfonate (**1u**)**



The title compound **1u** was prepared from **9** (643 mg, 2.0 mmol) following the general procedure described in ESI-1. Colorless semi-solid. Yield: 60% (571 mg). ^1H NMR (400 MHz, CDCl_3): δ 7.82-7.78 (m, 4H), 7.35-7.26 (m, 5H), 7.03-7.01 (m, 3H), 4.69 (dd, $J = 11.5, 6.0$ Hz, 1H), 4.59 (dd, $J = 11.5, 6.9$ Hz, 1H), 4.02 (d, $J = 4.1$ Hz, 1H), 3.27-3.23 (m, 1H), 2.44 (s, 3H), 2.42 (s, 3H). Anal. calcd. for $\text{C}_{23}\text{H}_{22}\text{FNO}_5\text{S}_2$: C, 58.09; H, 4.66; N, 2.95; found C, 58.32; H, 4.76; N, 2.83.

((2*R,3*S**)-3-(2-Fluorophenyl)-1-tosylaziridin-2-yl)methyl 4-nitrobenzene sulfonate (**1v**)**



The title compound **1v** was prepared from **9** (643 mg, 2.0 mmol) and 4-nitrobenzenesulphonyl chloride (499 mg, 2.25 mmol) following the general procedure

described in ESI-1. Colorless semi-solid. Yield: 54% (547 mg). $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.39 (d, $J = 9.2$ Hz, 2H), 8.15 (d, $J = 8.7$ Hz, 2H), 7.77 (d, $J = 8.2$ Hz, 2H), 7.31-7.23 (m, 3H), 7.03-6.98 (m, 2H), 6.95-6.91 (m, 1H), 4.80 (d, $J = 6.4$ Hz, 2H), 4.02 (d, $J = 3.7$ Hz, 1H), 3.27-3.23 (m, 1H), 2.42 (s, 3H). Anal. calcd. for $\text{C}_{22}\text{H}_{19}\text{FN}_2\text{O}_7\text{S}_2$: C, 52.17; H, 3.78; N, 5.53; found C, 52.35; H, 3.86; N, 5.44.

4. X-ray crystallography data

X-ray reflections were collected on a Bruker APEX-II, CCD diffractometer using Mo $\text{K}\alpha$ ($\lambda = 0.71073$ Å) radiation. Data reduction was performed using Bruker SAINT Software.⁶ Intensities for absorption were corrected using SADABS. Structures were solved and refined using SHELXL-2014 with anisotropic displacement parameters for non-H atoms. Hydrogen atom on O was experimentally located in the crystal structure. All C–H atoms were fixed geometrically using the HFIX command in SHELX-TL.⁷ A check of the final CIF file using PLATON did not show any missed symmetry.^{8,9} The crystallographic parameters for all structures are summarized in table ESI-1.

Table ESI-1: The crystallographic parameters for compound **5j**, **5p**, **6p** and **4t**

| Crystal Data | 5p | 6p | 5j | 4t |
|---|---|---|--|--|
| Formula unit | $\text{C}_{13}\text{H}_{16}\text{N}_2\text{OS}$ | $\text{C}_{13}\text{H}_{16}\text{N}_2\text{OS}$ | $\text{C}_{16}\text{H}_{12}\text{BrFN}_2\text{OS}$ | $\text{C}_{23}\text{H}_{21}\text{N}_3\text{O}_2\text{S}_2$ |
| Formula wt. | 248.34 | 248.34 | 379.25 | 435.55 |
| Crystal system | monoclinic | orthorhombic | monoclinic | monoclinic |
| T [K] | 296 | 100 | 296 | 296 |
| a [Å] | 6.3476 (3) | 9.914(3) | 21.440(8) | 12.881(3) |
| b [Å] | 13.4188 (6) | 12.666(5) | 6.442(2) | 19.724(4) |
| c [Å] | 15.2697(7) | 10.006(3) | 30.004(9) | 9.3055(19) |
| α [°] | 90 | 90 | 90 | 90 |
| β [°] | 96.662(3) | 90 | 132.808(18) | 101.12(3) |
| γ [°] | 90 | 90 | 90 | 90 |
| Volume [Å ³] | 1291.85(10) | 1256.5(7) | 3040.2(19) | 2319.7(8) |
| Space group | $P2_1/n$ | $Pna2_1$ | $P2_1/c$ | $P2_1/c$ |
| Z | 4 | 4 | 8 | 4 |
| D_{calc} [g cm ⁻³] | 1.277 | 1.313 | 1.657 | 1.230 |
| μ/mm^{-1} | 0.236 | 0.243 | 2.854 | 0.252 |

| | | | | |
|------------------------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| Reflns. Collected | 32562 | 36233 | 70108 | 72807 |
| Unique reflns. | 3304 | 3217 | 5363 | 5621 |
| Observed reflns. | 2238 | 1288 | 3505 | 2698 |
| R_1 [$I > 2\sigma(I)$], wR_2 | 0.0490, 0.1400 | 0.0627, 0.0970 | 0.0663, 0.1844 | 0.0974, 0.1191 |
| GOF | 0.909 | 1.055 | 0.755 | 1.087 |
| Instrument | Bruker APEX-II CCD | Bruker APEX-II CCD | Bruker APEX-II CCD | Bruker APEX-II CCD |
| X-ray | MoK α | MoK α | MoK α | MoK α |
| CCDC Reference No. | 1961866 | 1961865 | 1961867 | 1961868 |

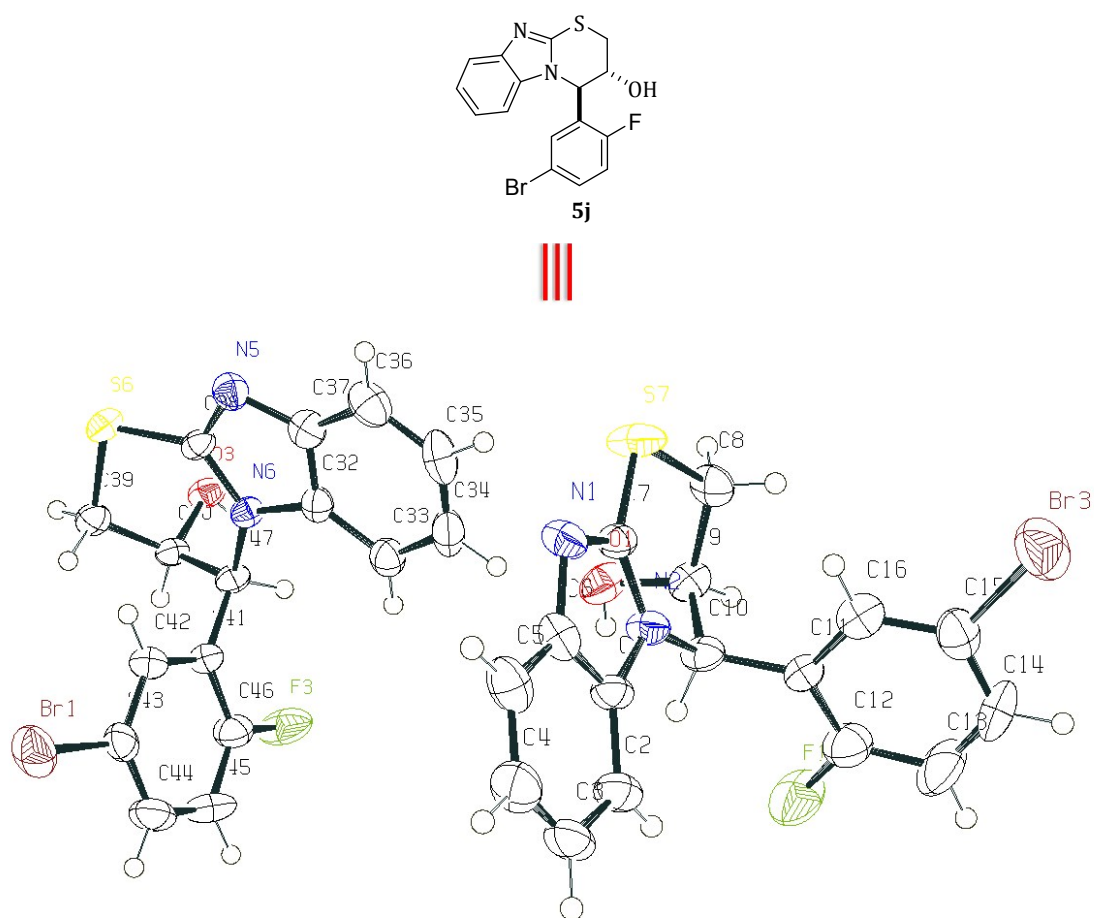


Figure ESI-1. ORTEP diagram of **5j** with 50% probability ellipsoid

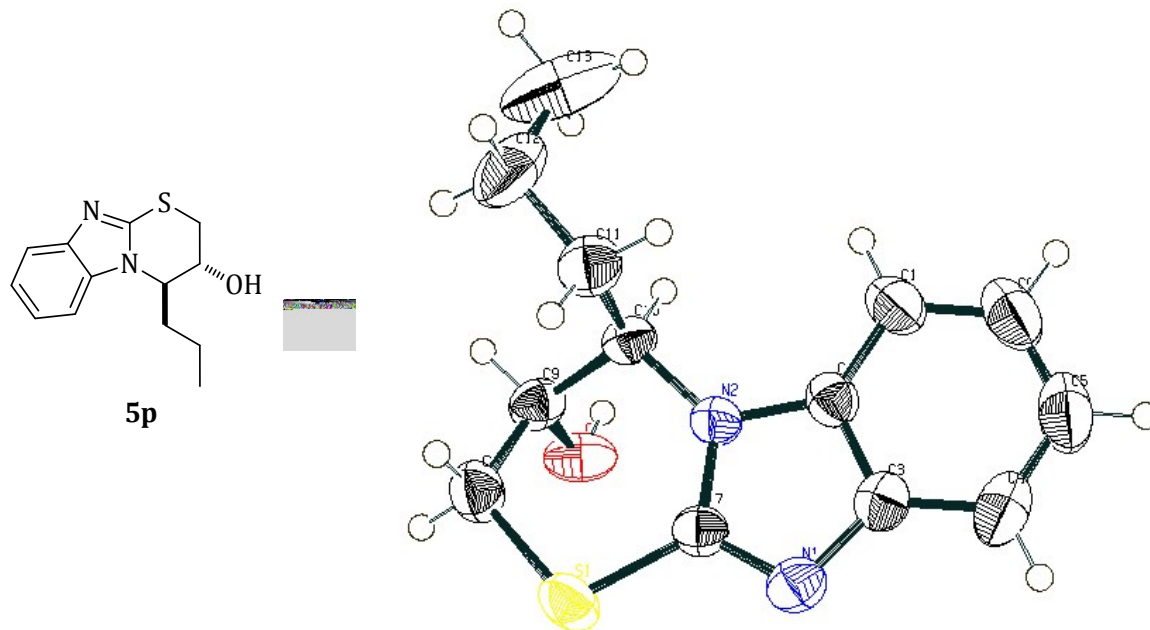


Figure ESI-2. ORTEP diagram of **5p** with 50% probability ellipsoid

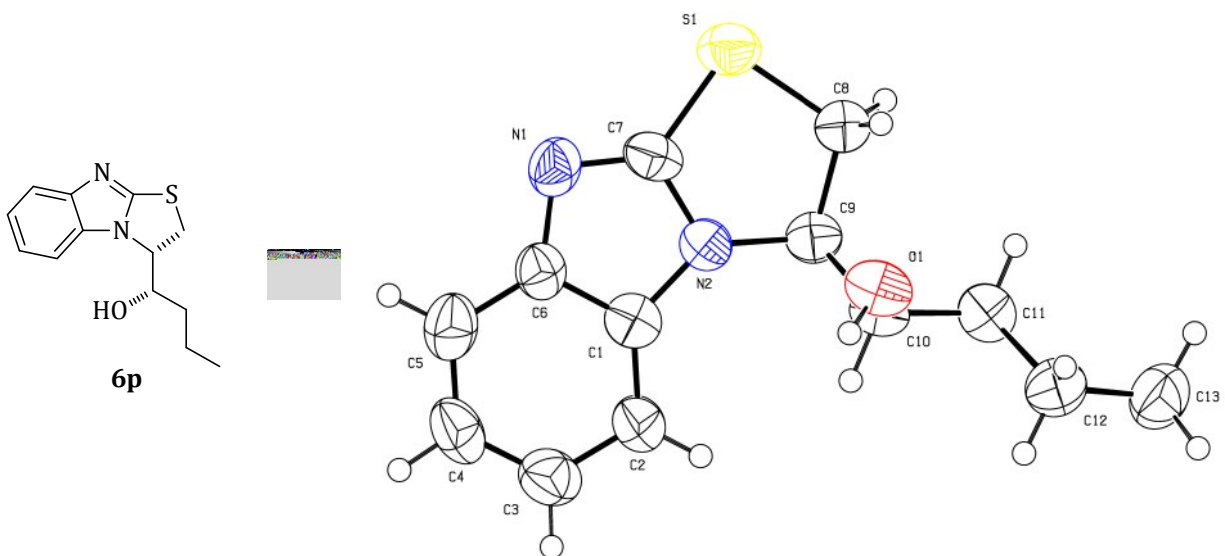


Figure ESI-3. ORTEP diagram of **6p** with 50% probability ellipsoid

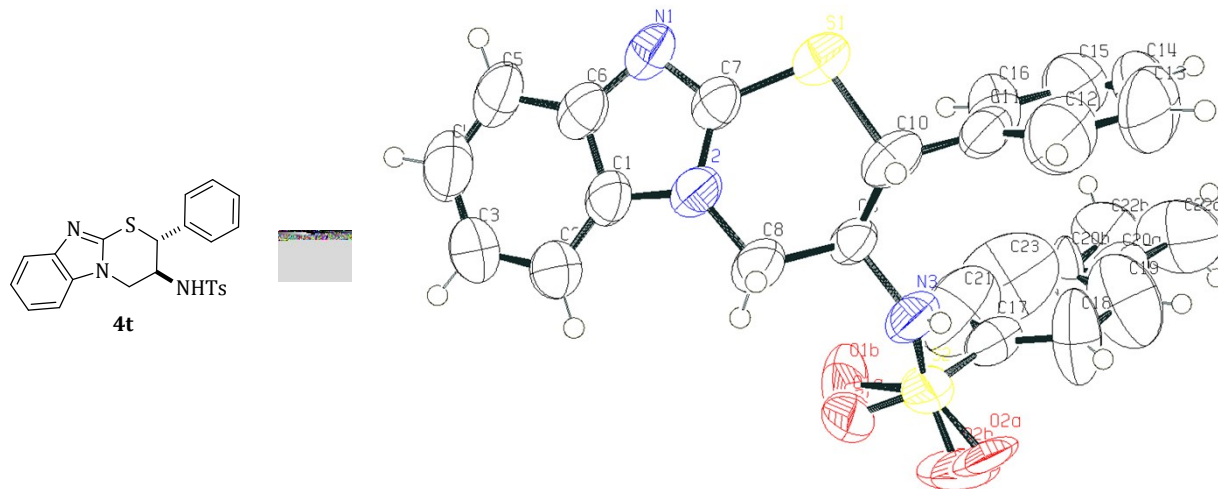


Figure ESI-4. ORTEP diagram of **4t** with 50% probability ellipsoid

6. NMR spectral analysis of compound **4w**

The ^1H NMR of **4w** shows two dd signals appearing at δ 4.12 and 4.00 assigned to the two diastereotopic 4-H (in structure **4w**, Figure ESI-5) or 2-H (in structure **4w'**, Figure ESI-5) protons. A correlated spectroscopy (COSY) correlation connected these two signals with the multiplet appearing at δ 3.86 which has another correlation connected to the multiplet at δ 3.38 (overlapped with DMSO water peak). A further network of COSY correlations of signal δ 3.38 with the two multiplets appearing at δ 1.75 and 1.36 (14-Hs) confirm that the multiplet at δ 3.86 is appearing for 3-H proton and multiplet at δ 3.38 is appearing for 2-H proton (in **4w**) or 4-H) proton (in **4w'**). The signal at δ 3.86 can also be assigned to 3-H proton from the COSY correlations with the N-H appearing at δ 8.39.

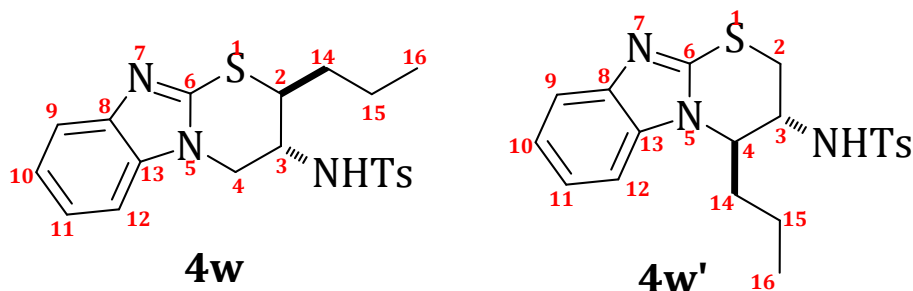
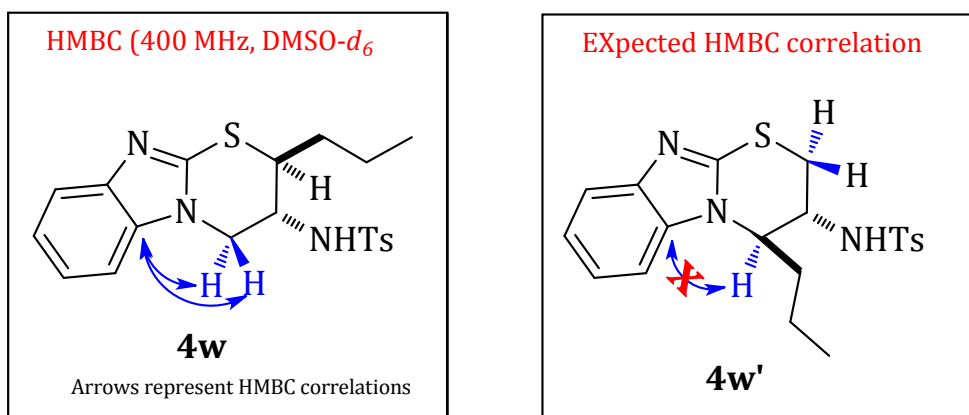
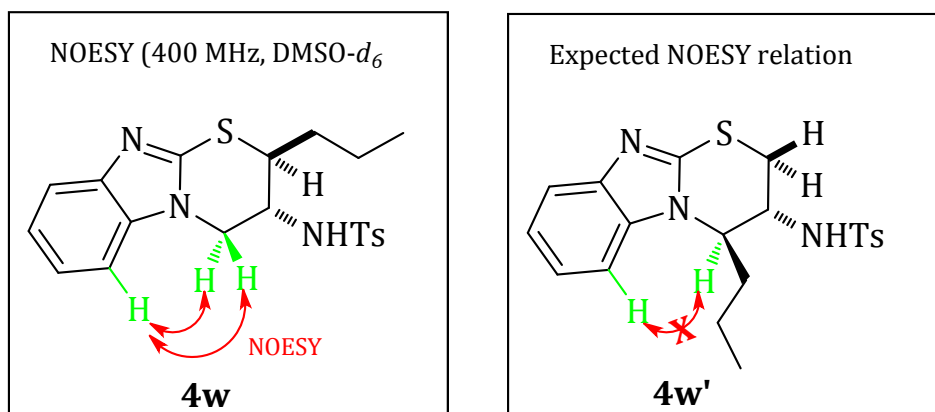


Figure ESI-5.

Based on the correlations observed in HSQC spectrum, the signals arising at δ 49.4, 45.0, 44.1 can be assigned to C-3, C-2 (or C-4 in **4w'**), and C-4 (or C-2 in **4w'**) of structure **4w**, respectively. In the aromatic region C-6 being the highly deshielded carbon atom can be assigned to signal appearing at δ 145.4, which does not show any correlation in HSQC spectrum but shows very good correlations with 2-H and 4-H protons in HMBC. Similarly, signal at δ 135.6 appears due to C-13 which gives good correlation with the two 4-Hs. However, had the structure been **4w'** instead of **4w**, only the multiplet of single 4-H would have shown correlation with C-13.



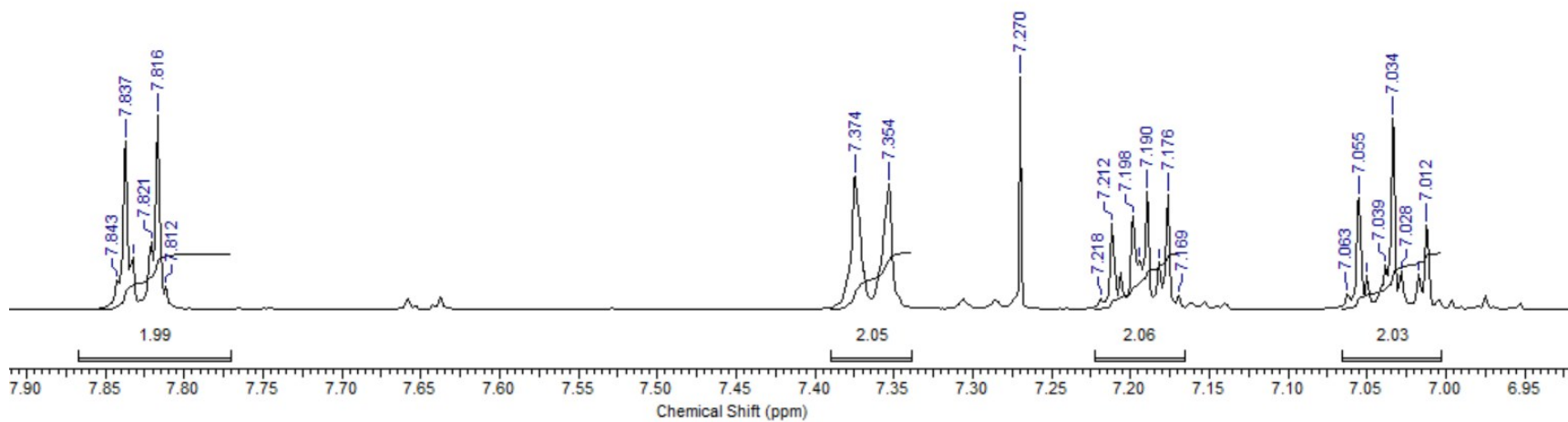
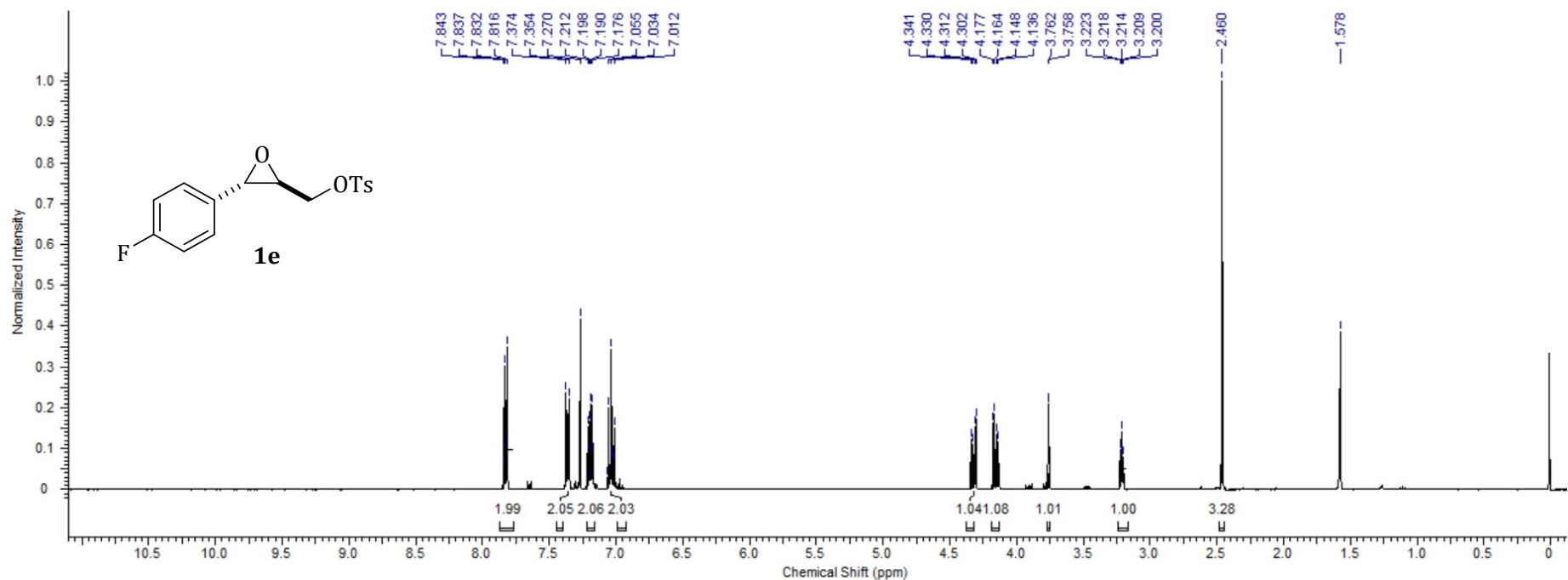
Similarly, in the NOESY spectrum, two doublet of doublets appearing at δ 4.12 and 4.00 shows very good correlations with the aromatic H appearing as doublet at δ 7.21 which can be assigned to 12-H from COSY spectrum. This NOE relation also further confirms the formation of product **4w**.



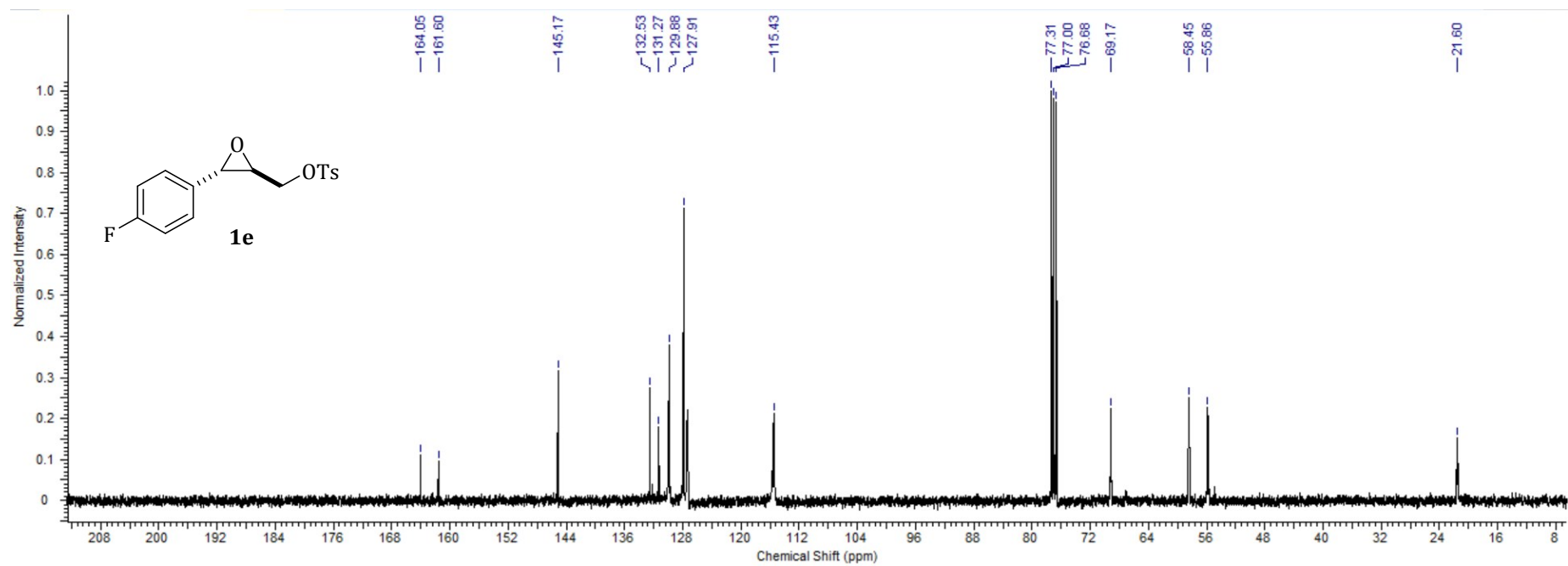
7. References

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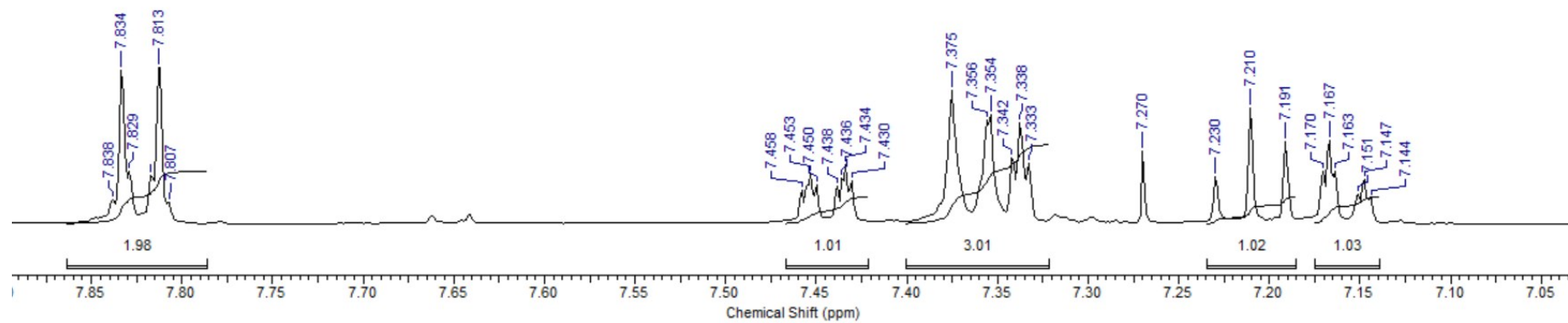
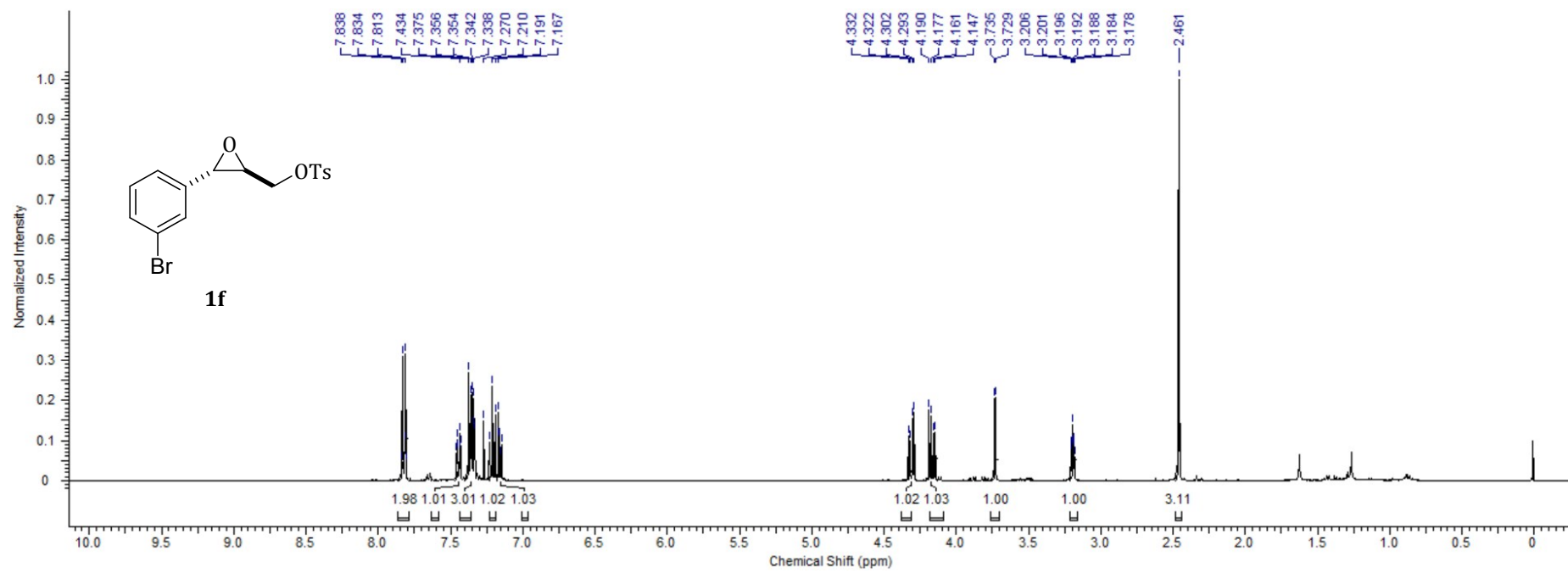
8. Copies of ^1H and ^{13}C NMR



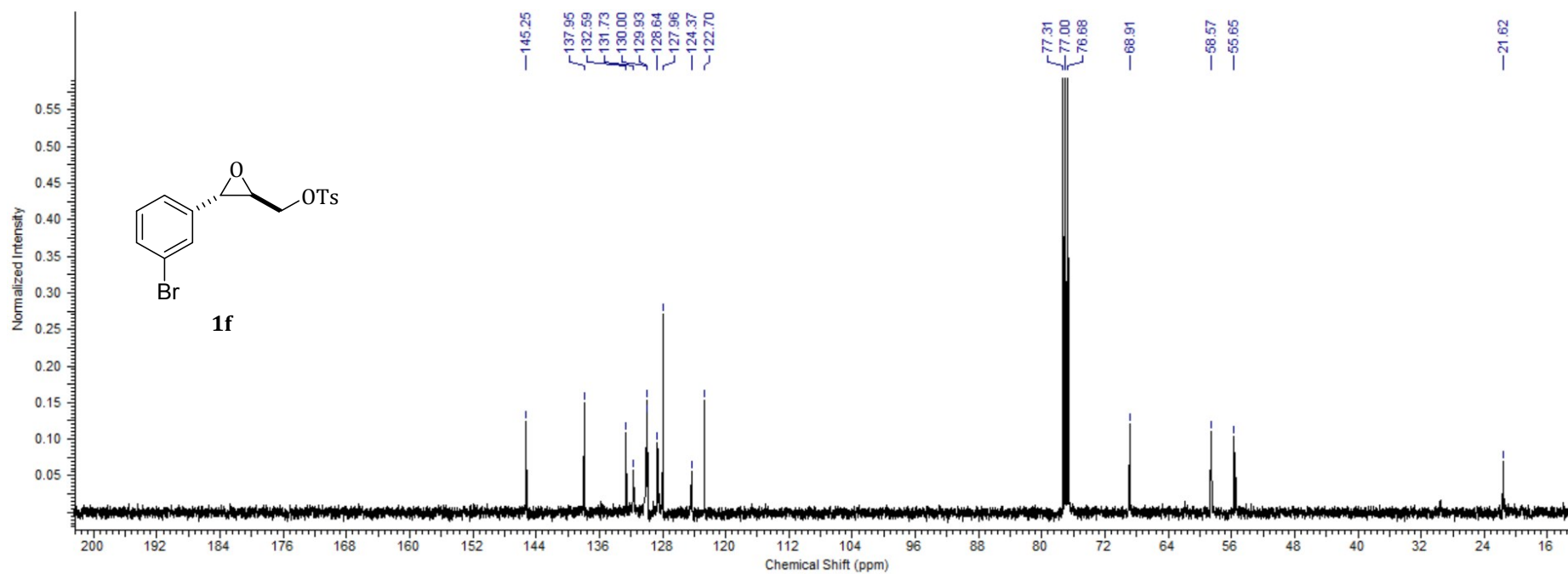
¹H NMR spectrum (400 MHz, CDCl₃) of 1e



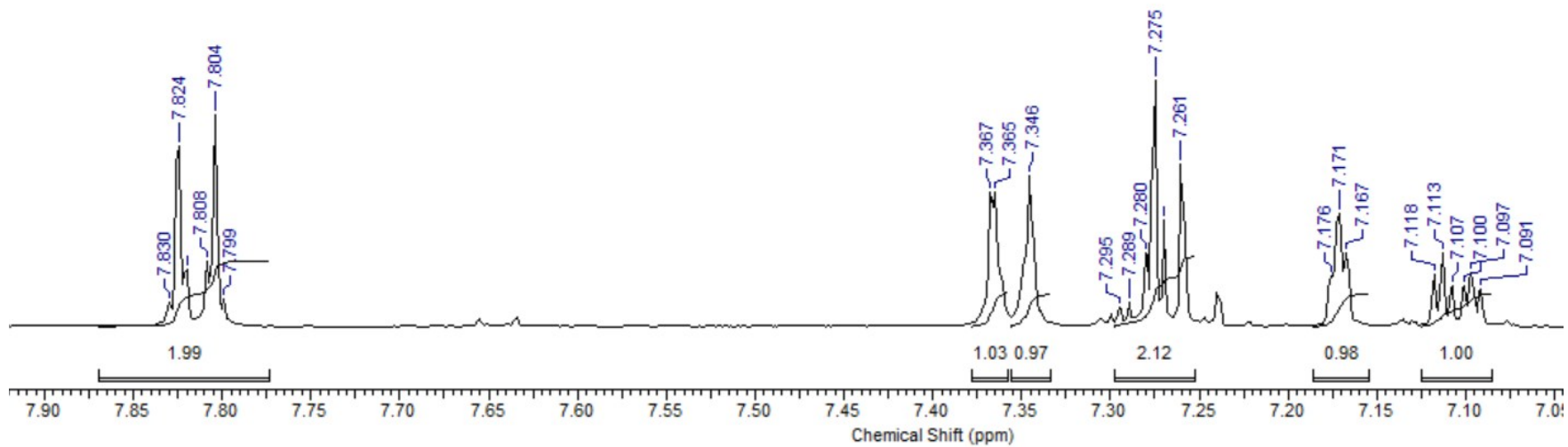
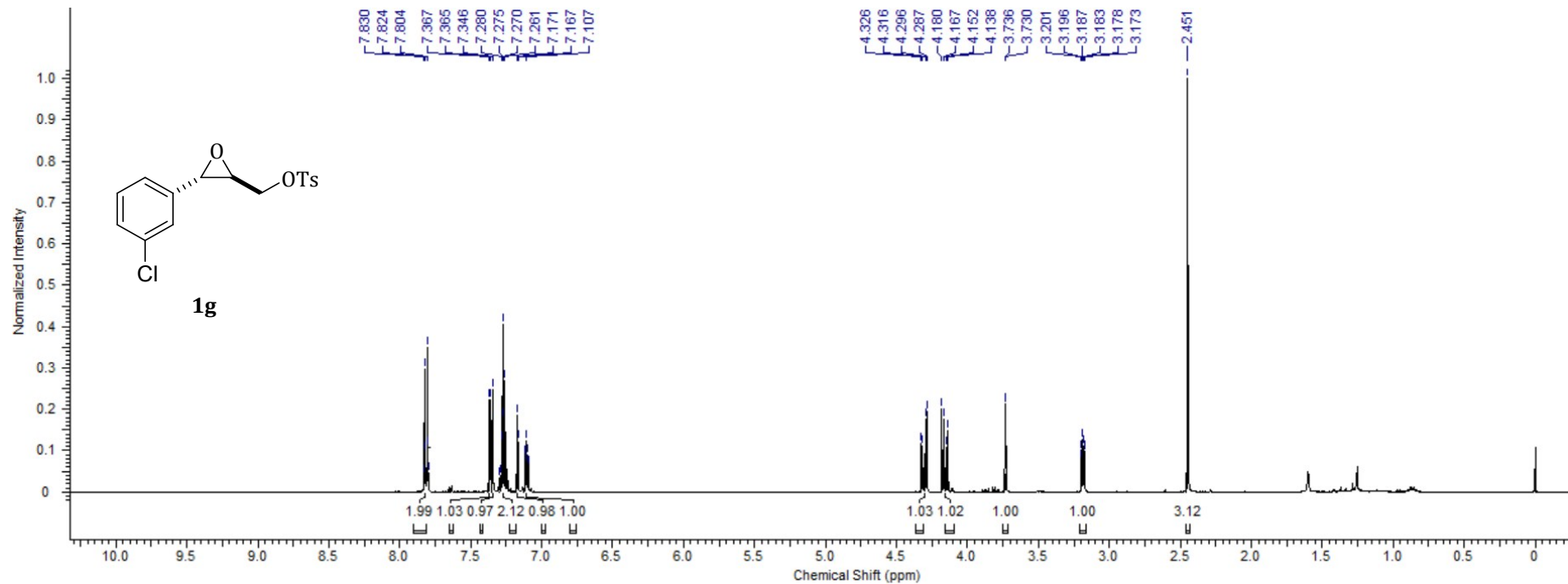
^{13}C NMR spectrum (100 MHz, CDCl_3) of **1e**



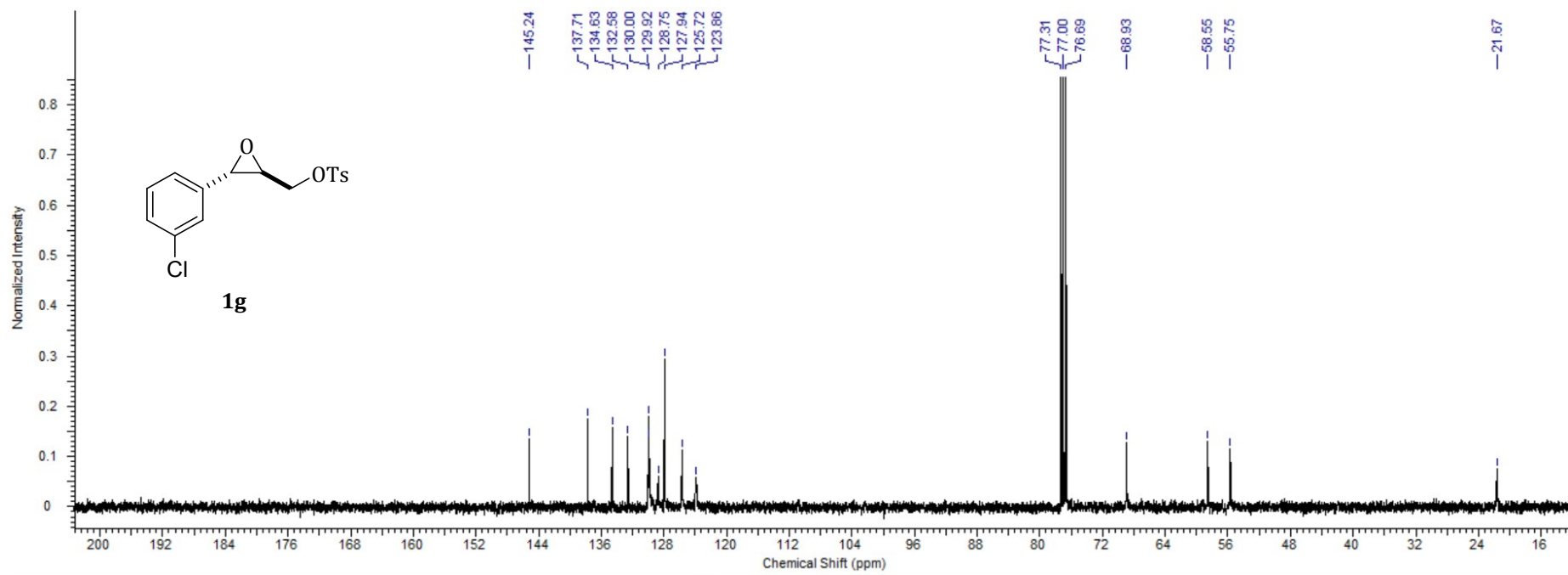
¹H NMR spectrum (400 MHz, CDCl₃) of 1f



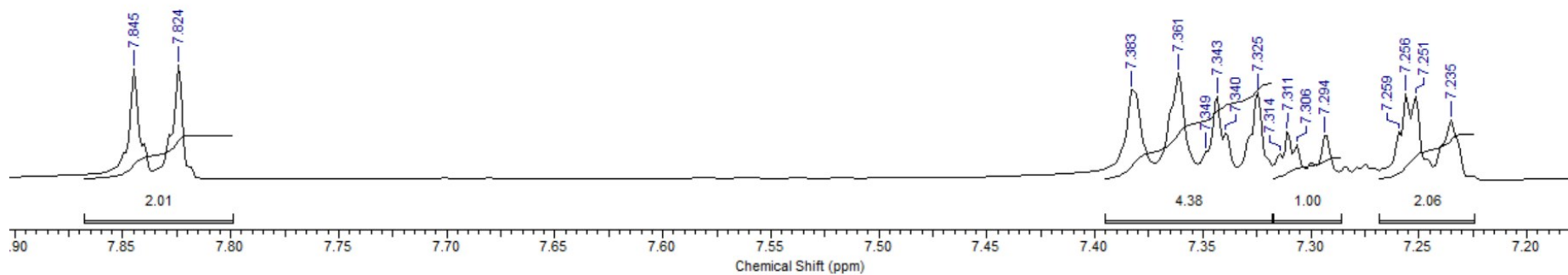
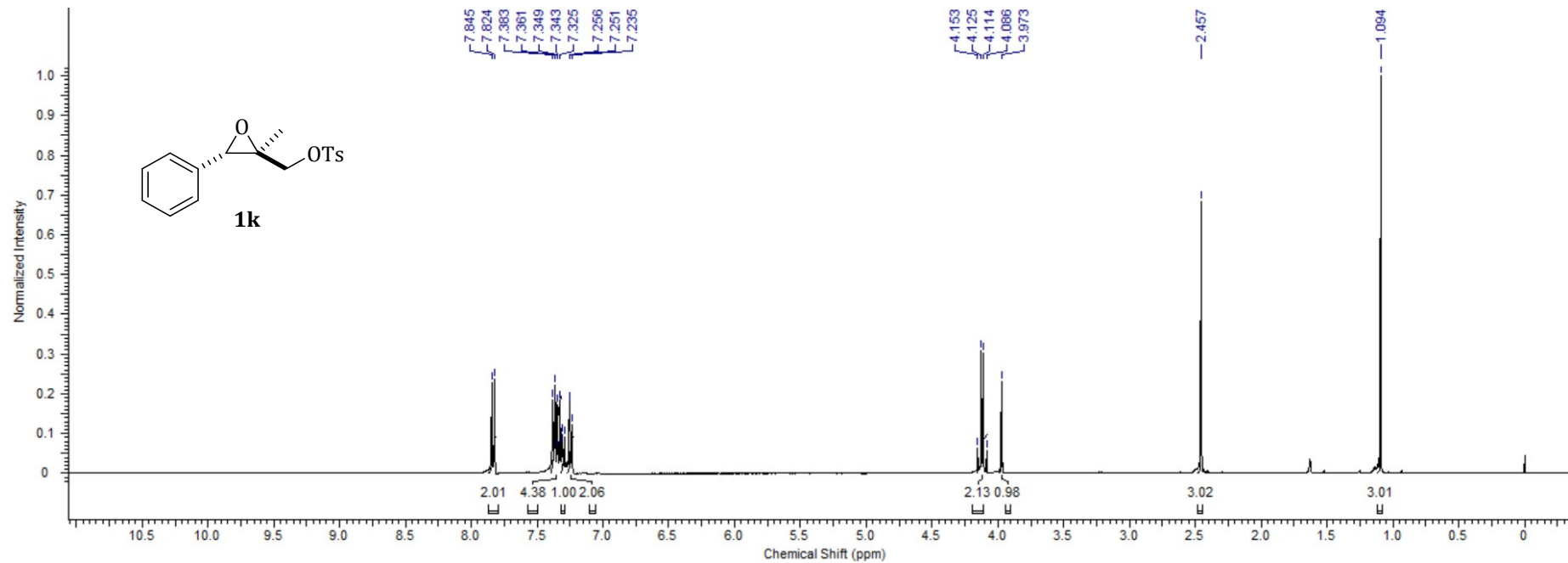
¹³C NMR spectrum (100 MHz, CDCl₃) of 1f



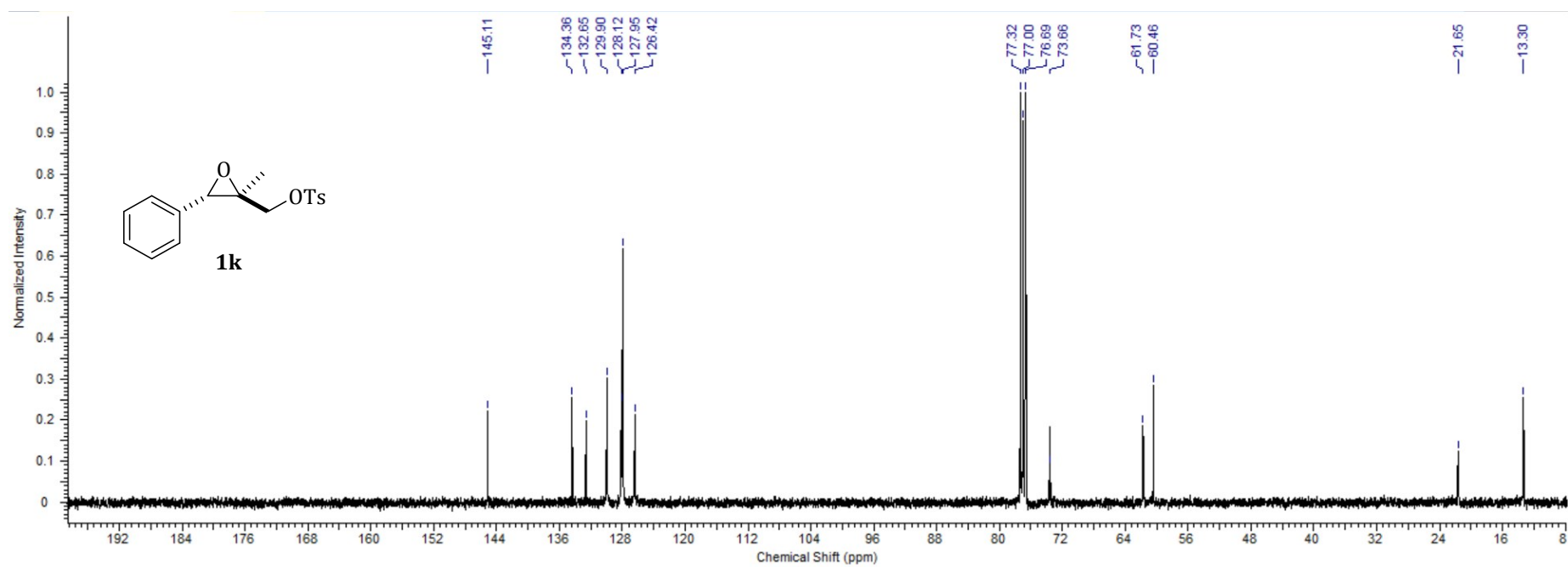
¹H NMR spectrum (400 MHz, CDCl₃) of 1g



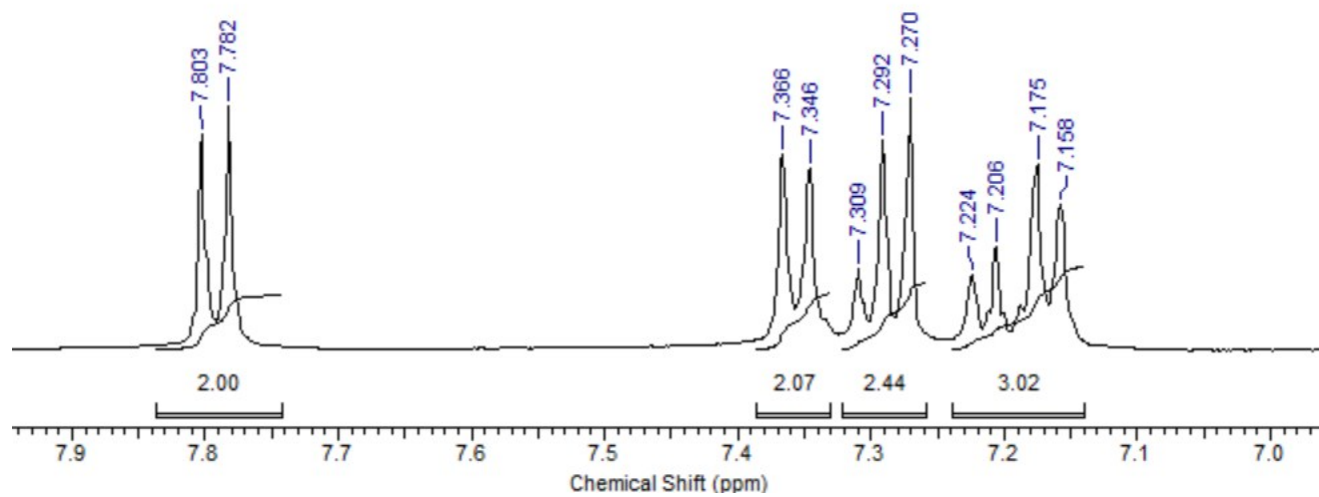
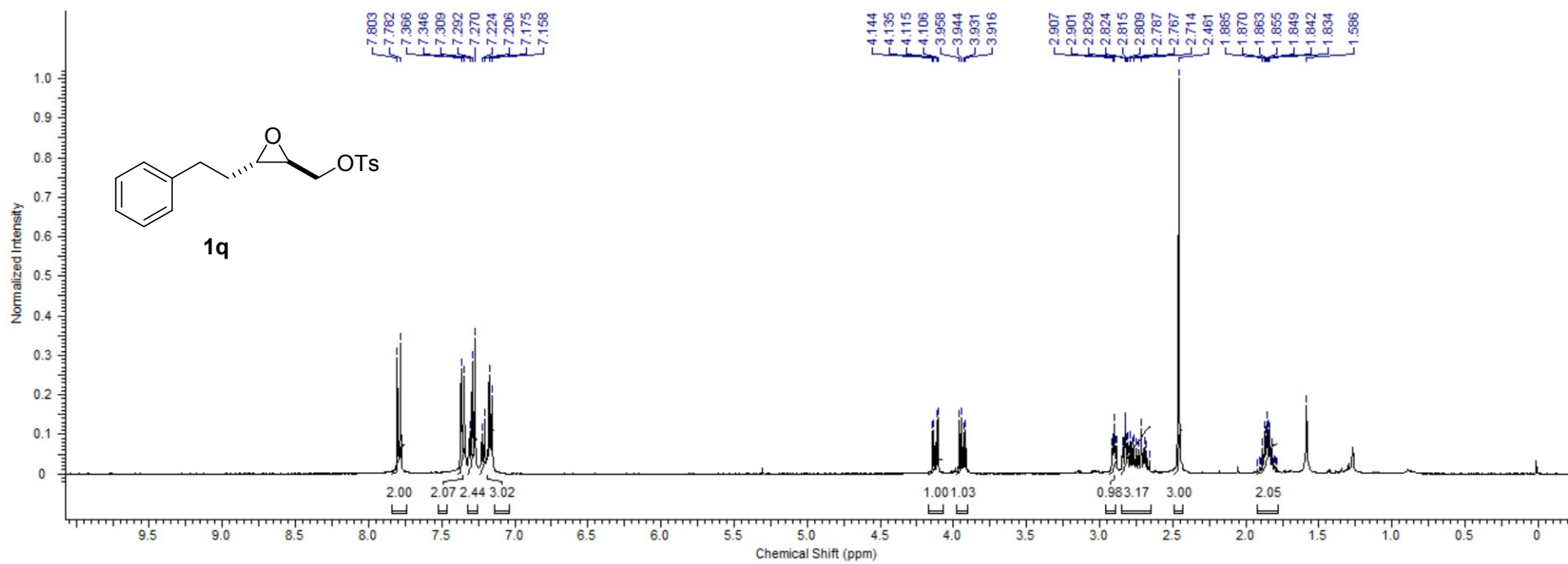
^{13}C NMR spectrum (100 MHz, CDCl_3) of **1g**



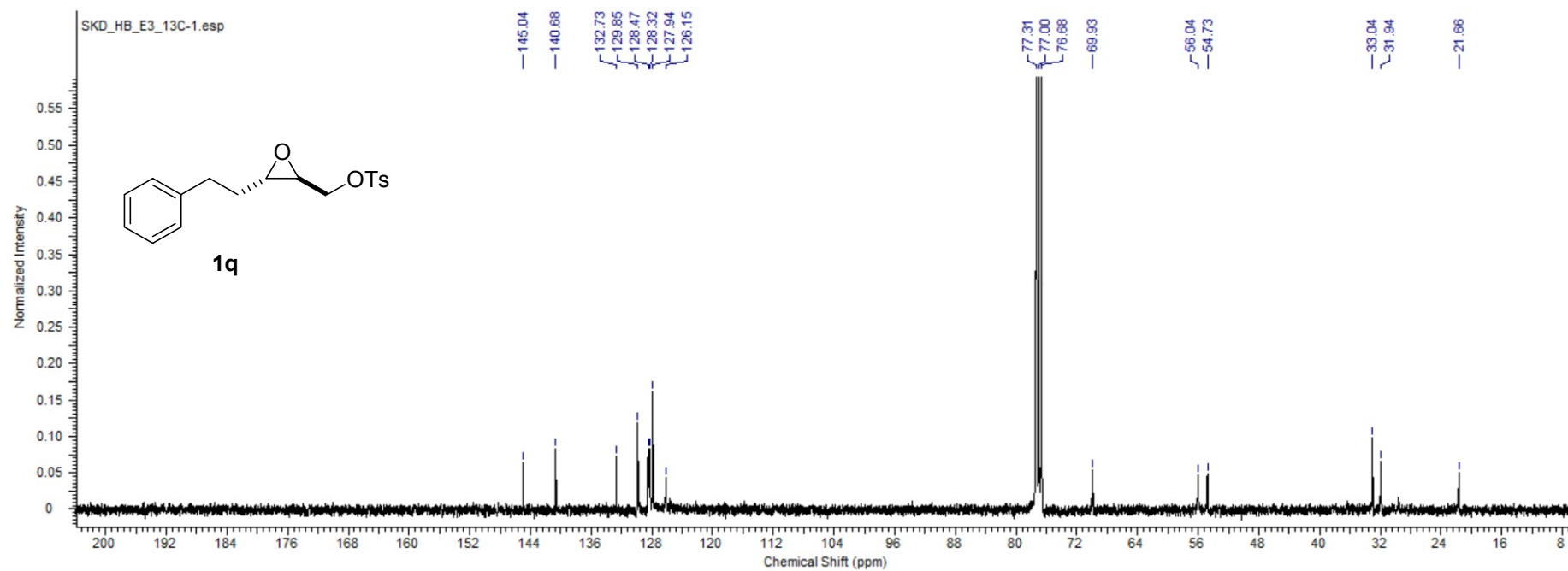
¹H NMR spectrum (400 MHz, CDCl₃) of 1k



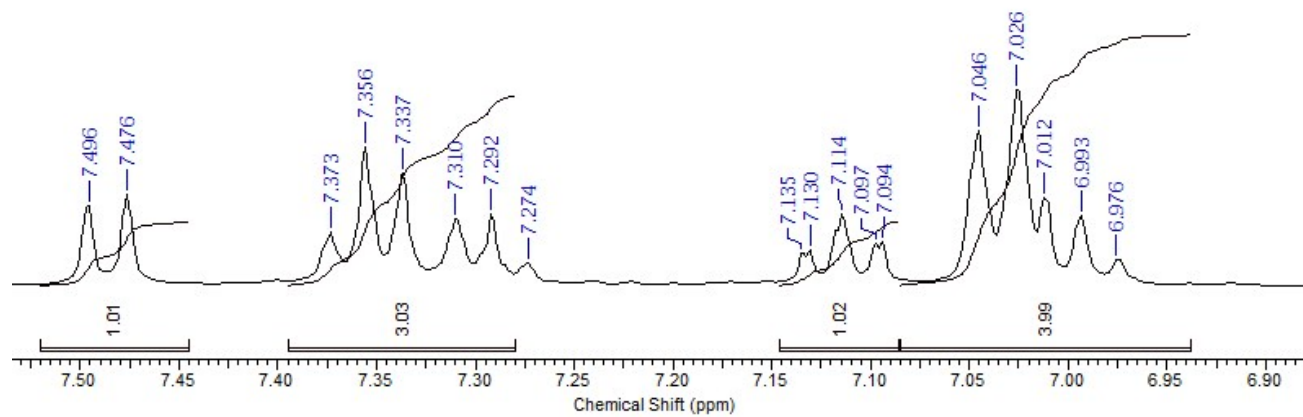
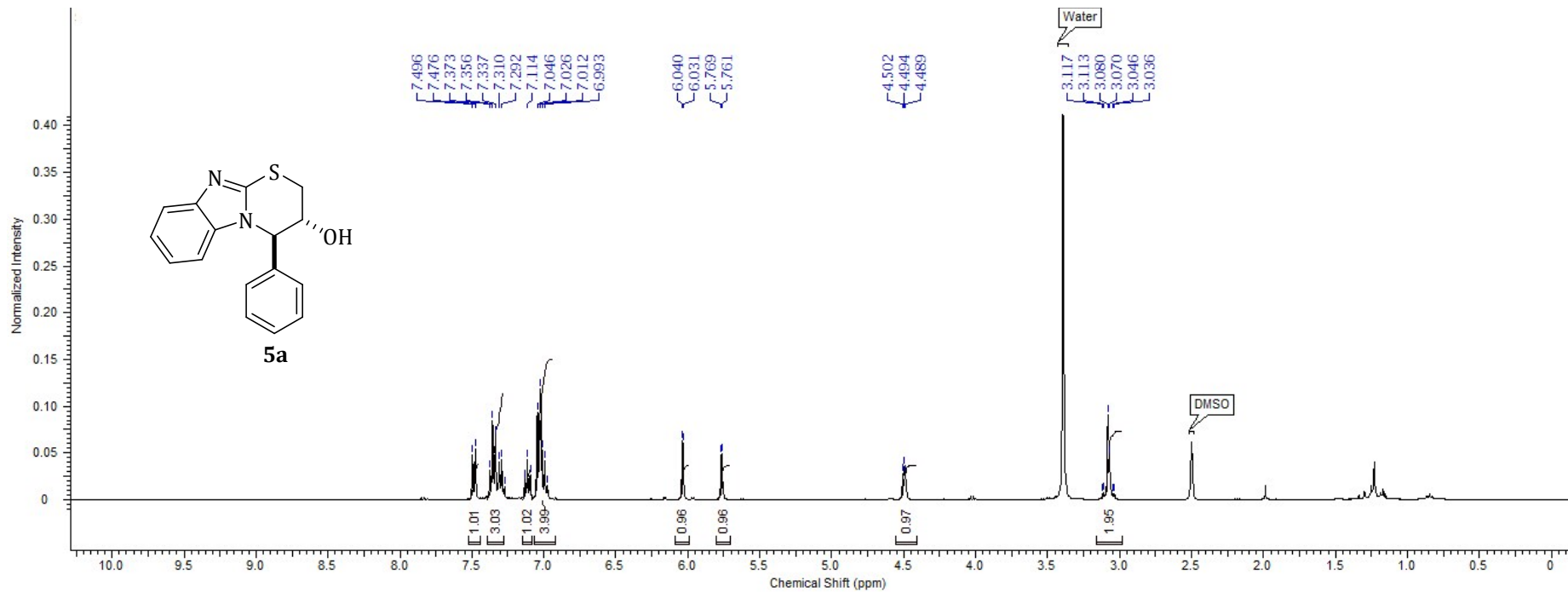
^{13}C NMR spectrum (100 MHz, CDCl_3) of **1k**



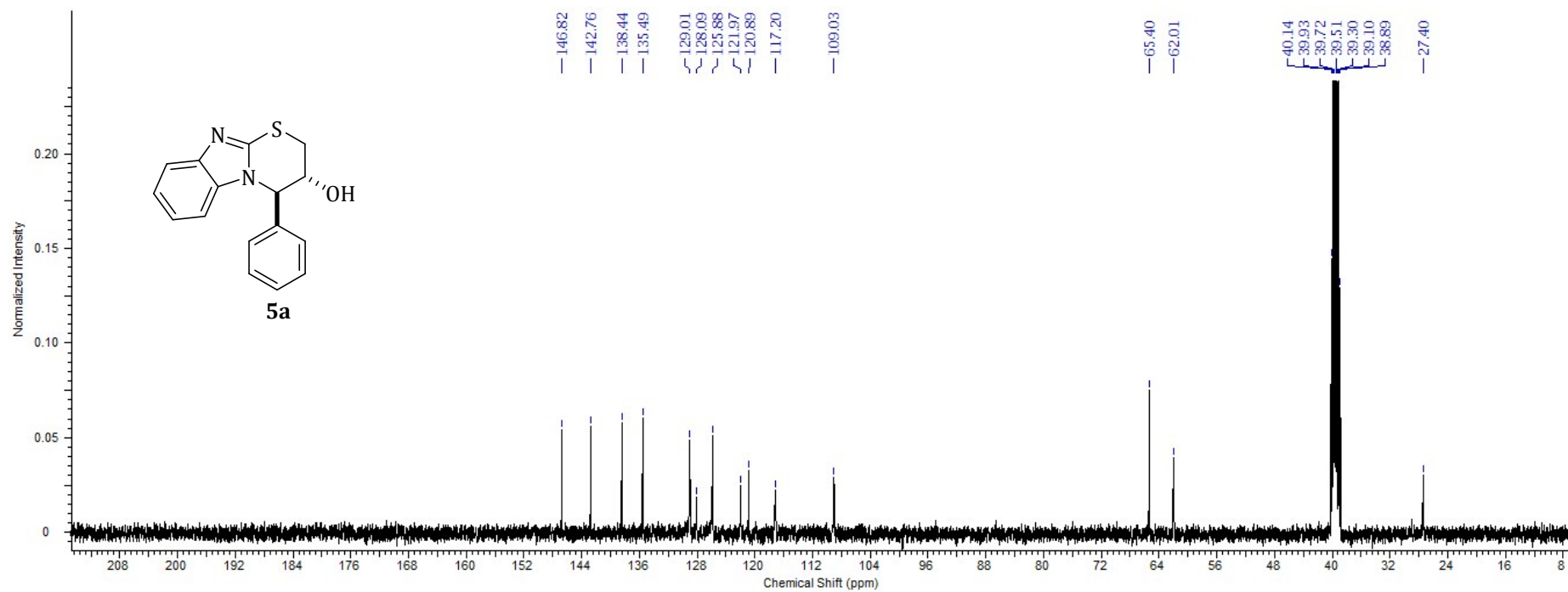
¹H NMR spectrum (400 MHz, CDCl₃) of 1q



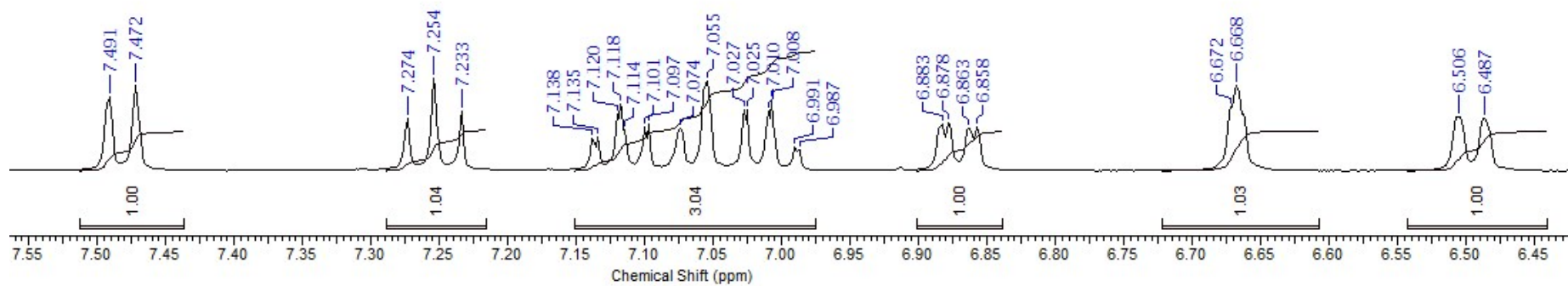
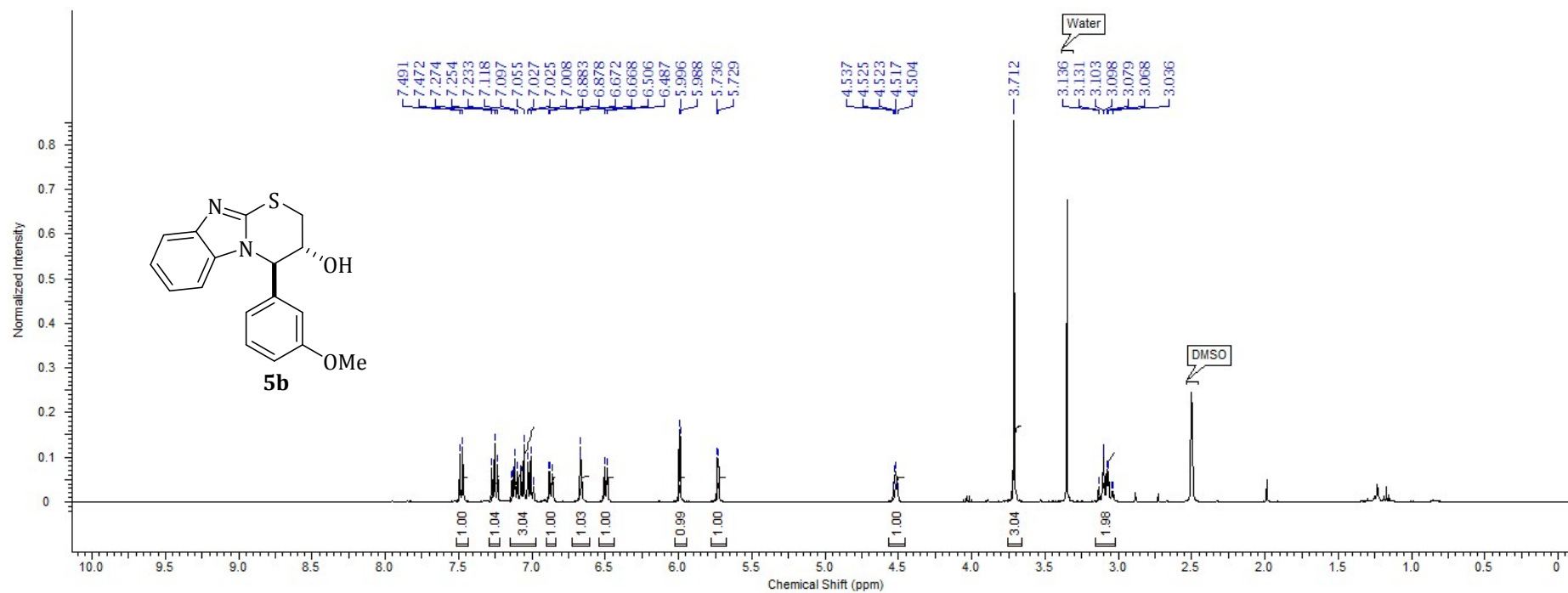
^{13}C NMR spectrum (100 MHz, CDCl_3) of **1q**



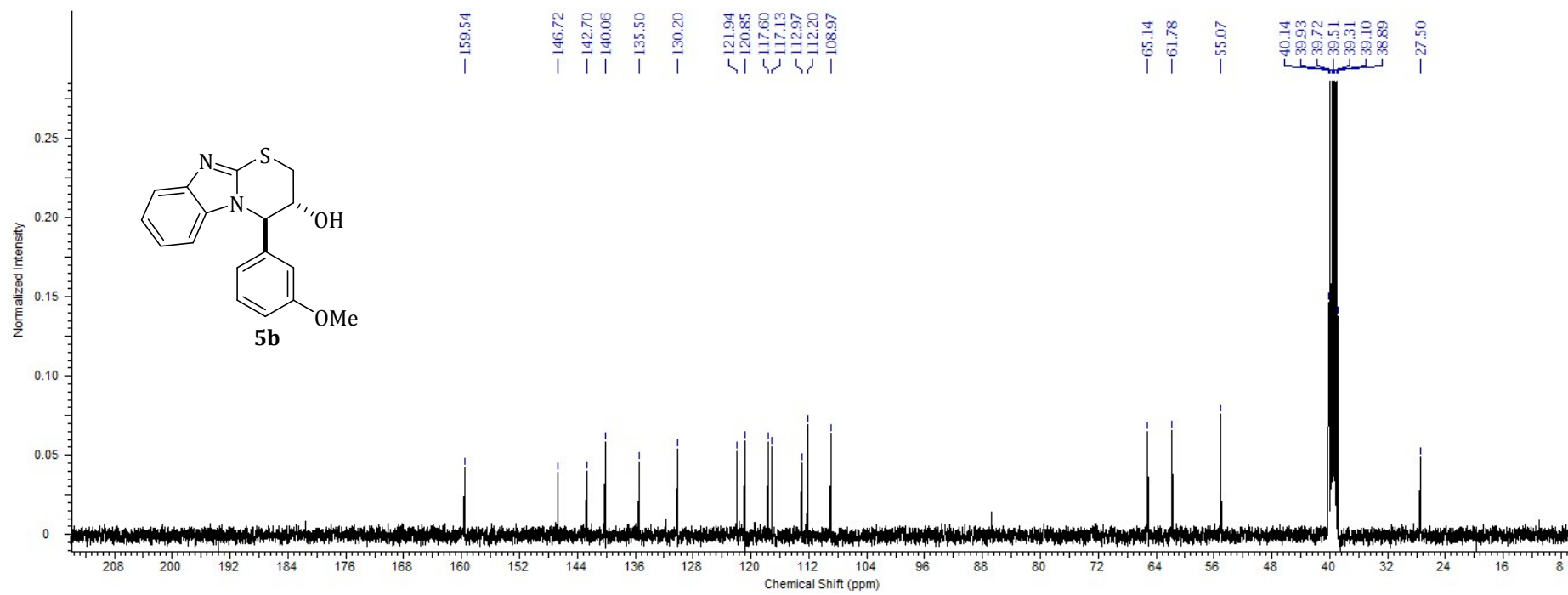
¹H NMR spectrum (400 MHz, DMSO-*d*₆) of 5a



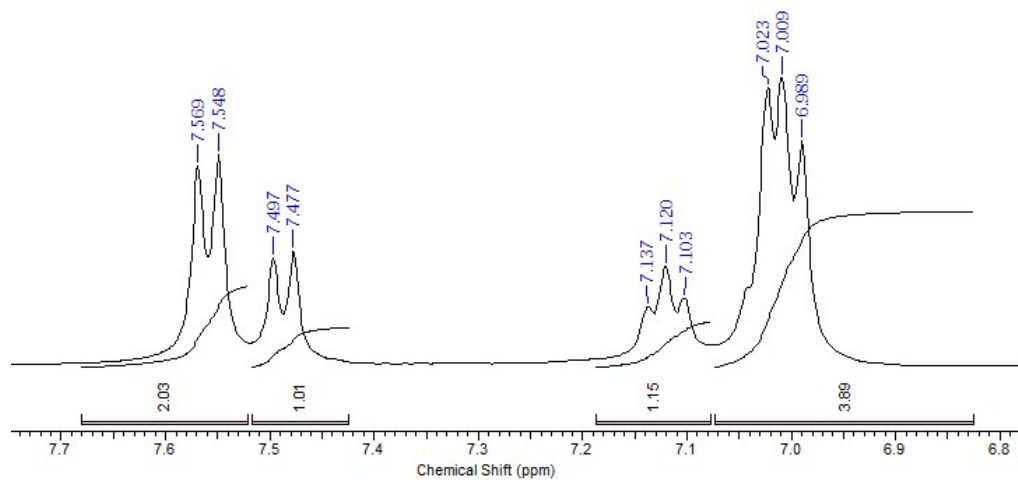
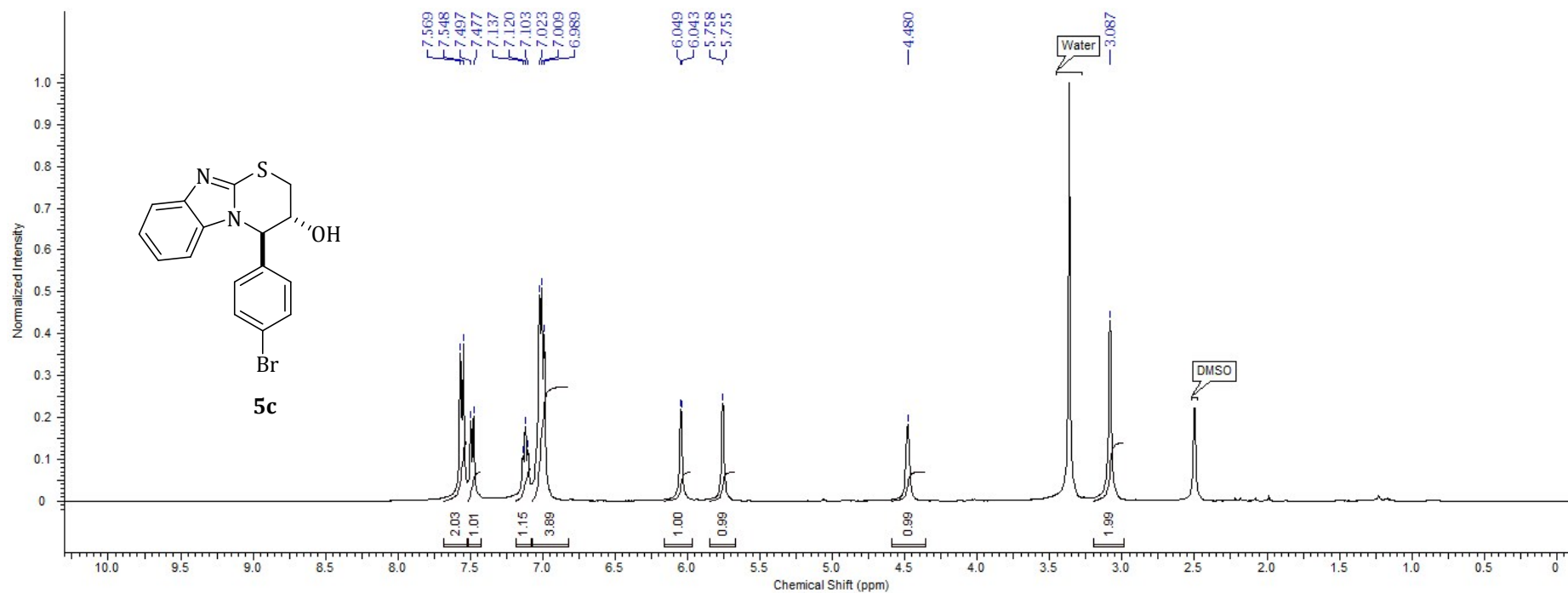
¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of 5a



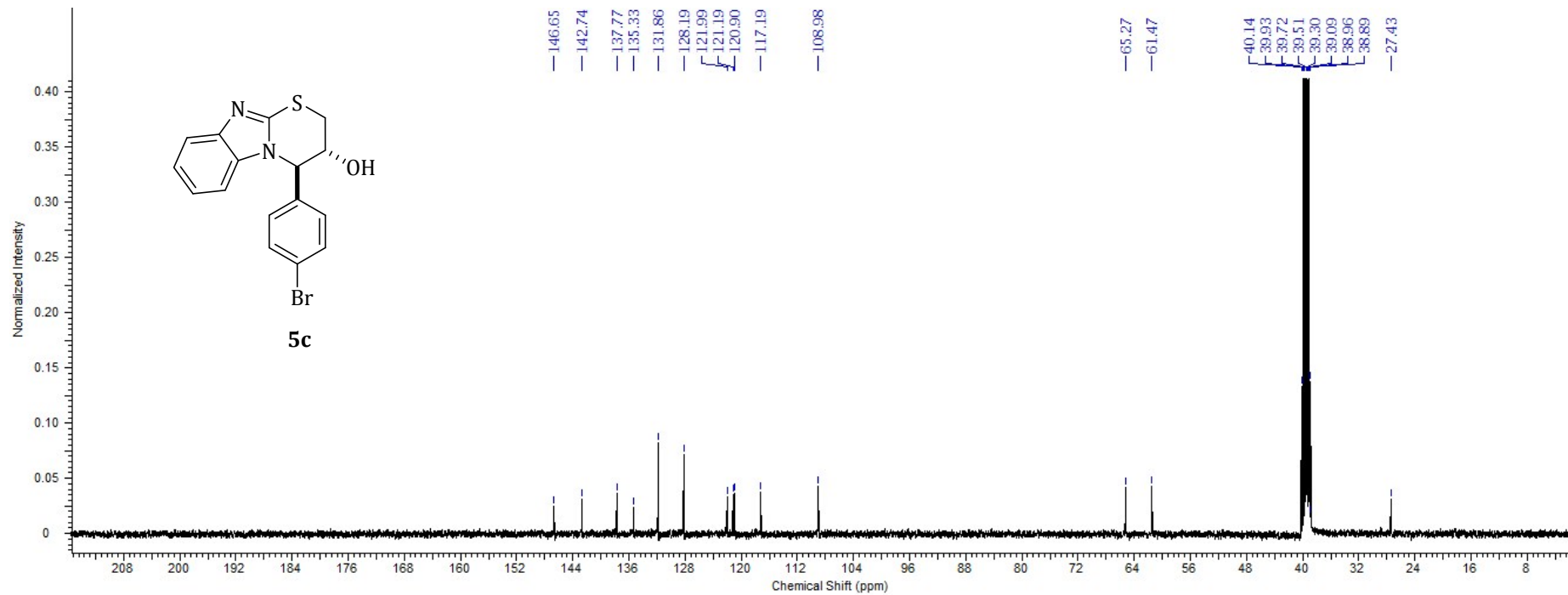
¹H NMR spectrum (400 MHz, DMSO-*d*₆) of **5b**



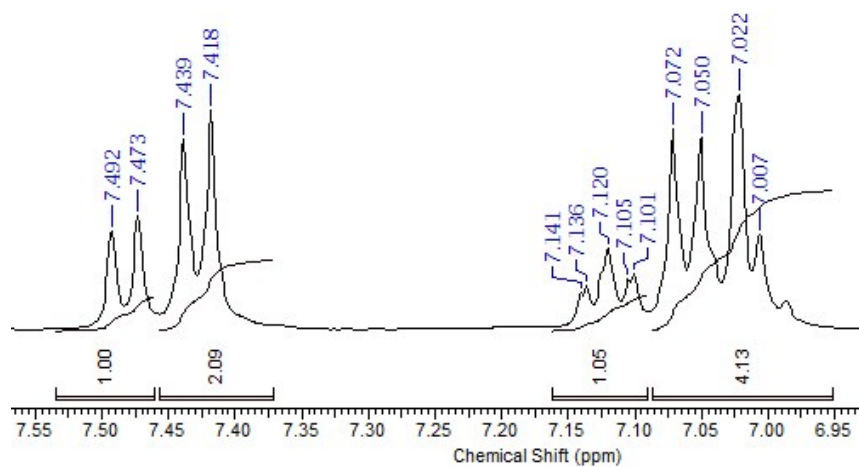
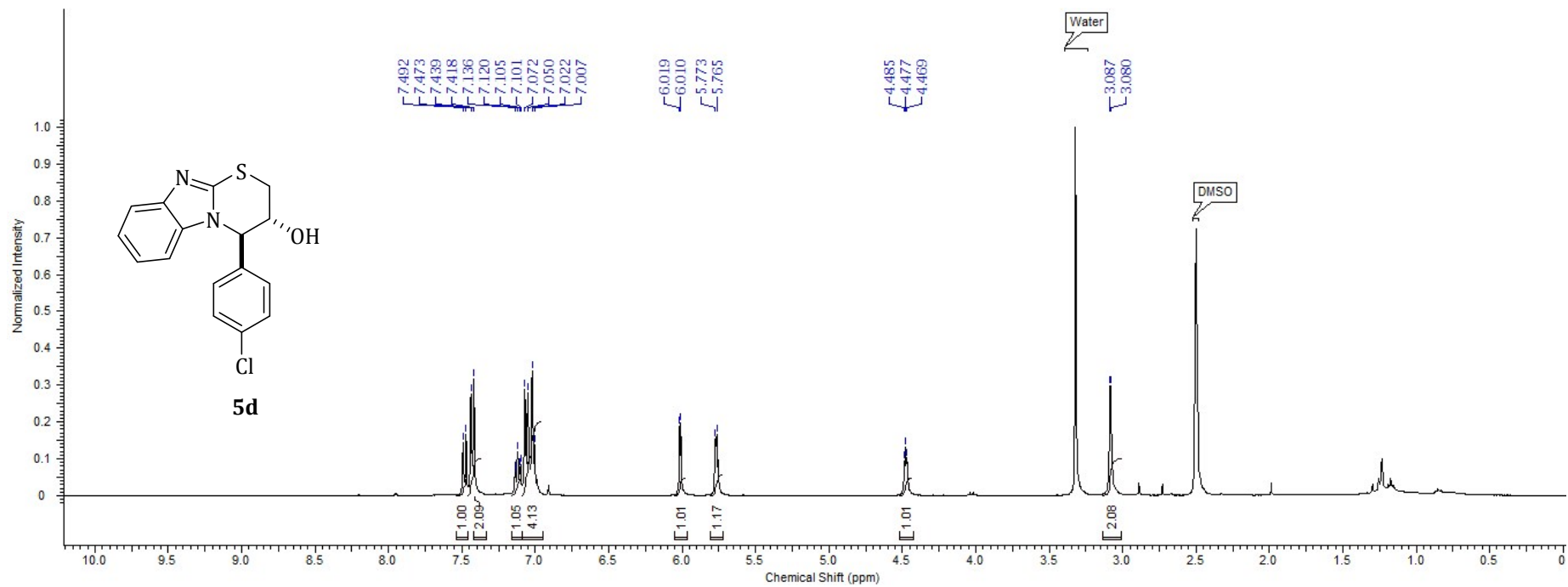
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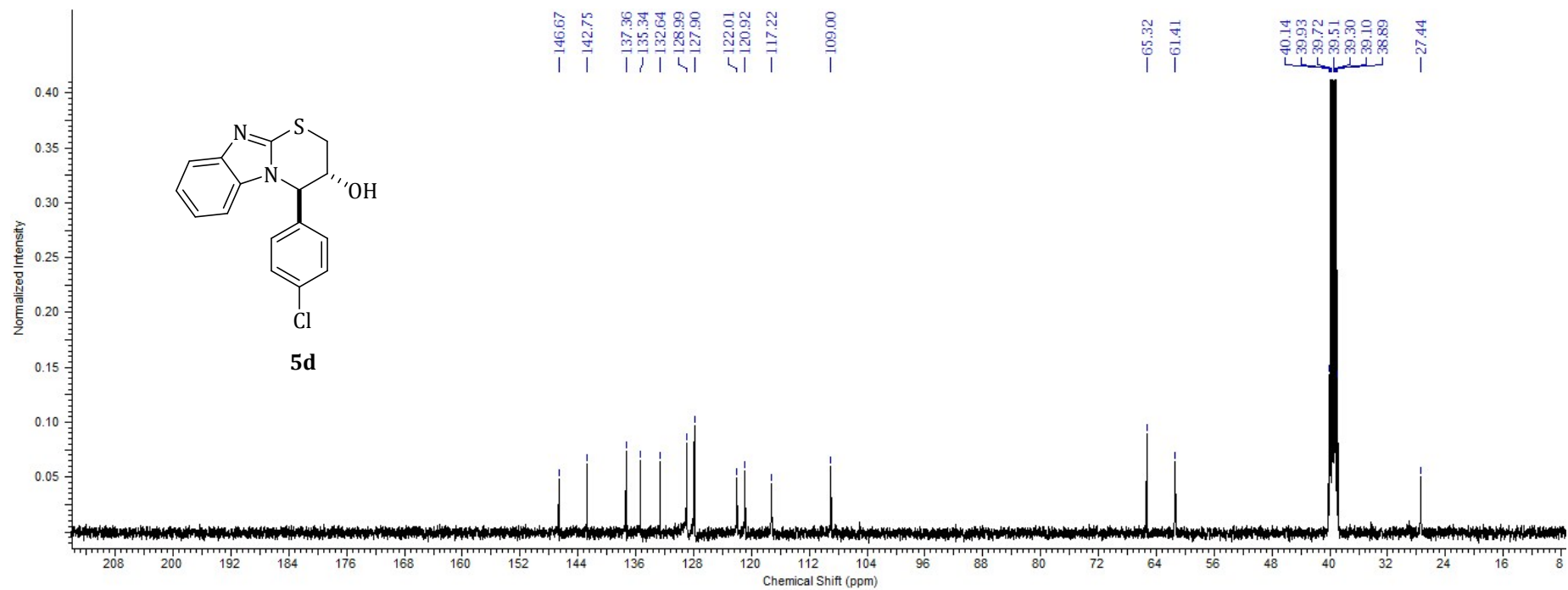
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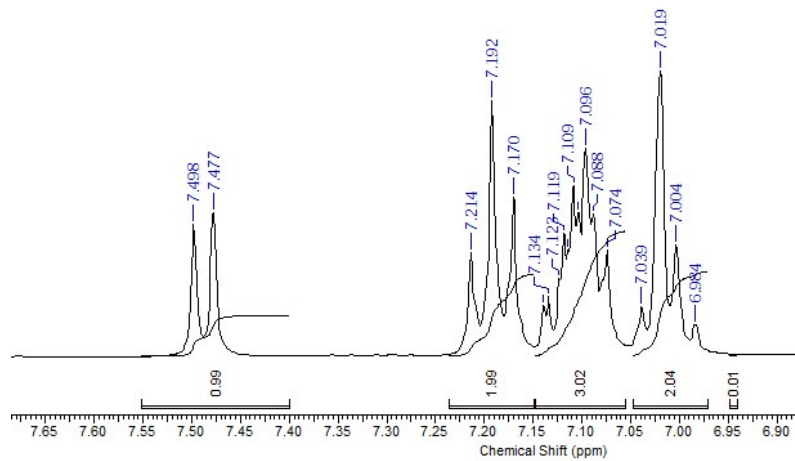
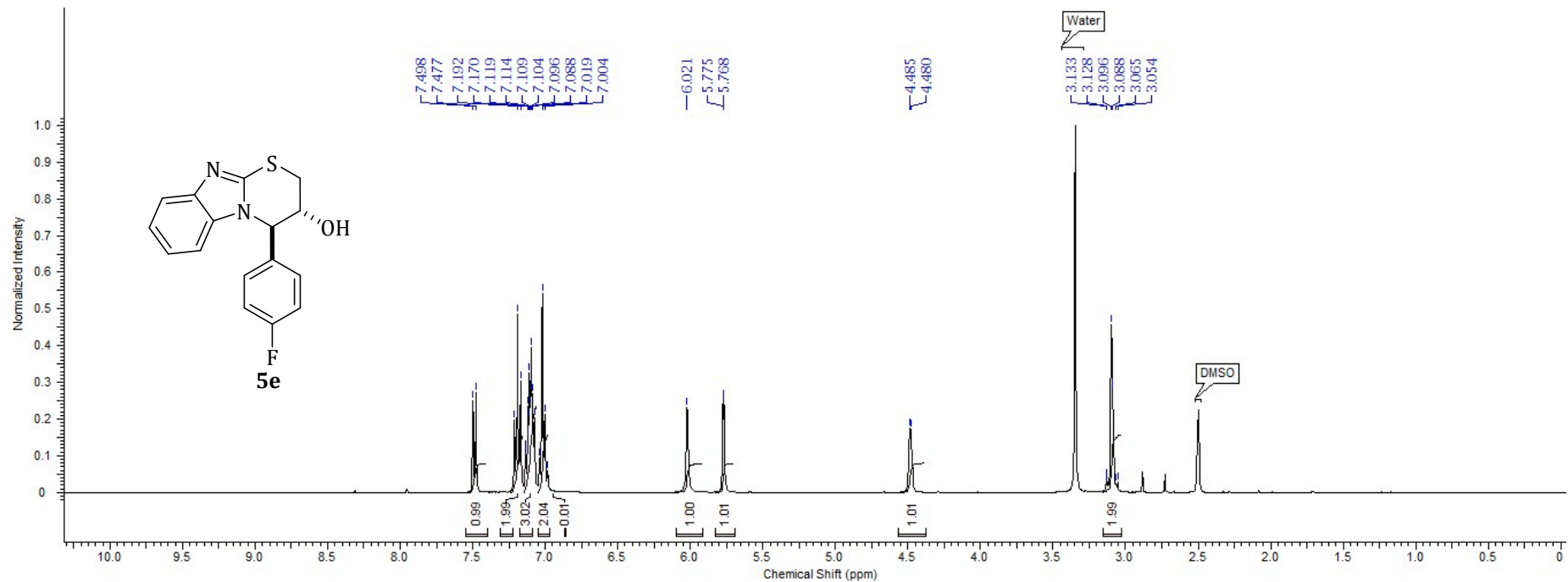
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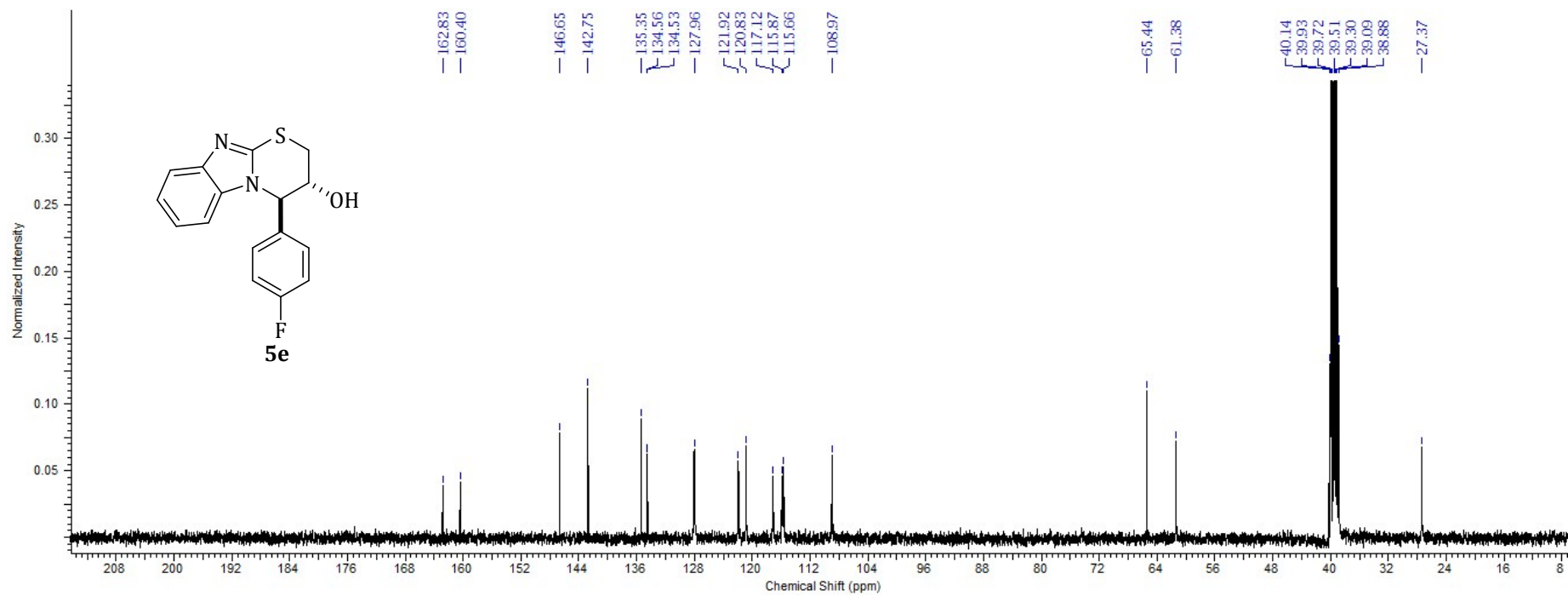
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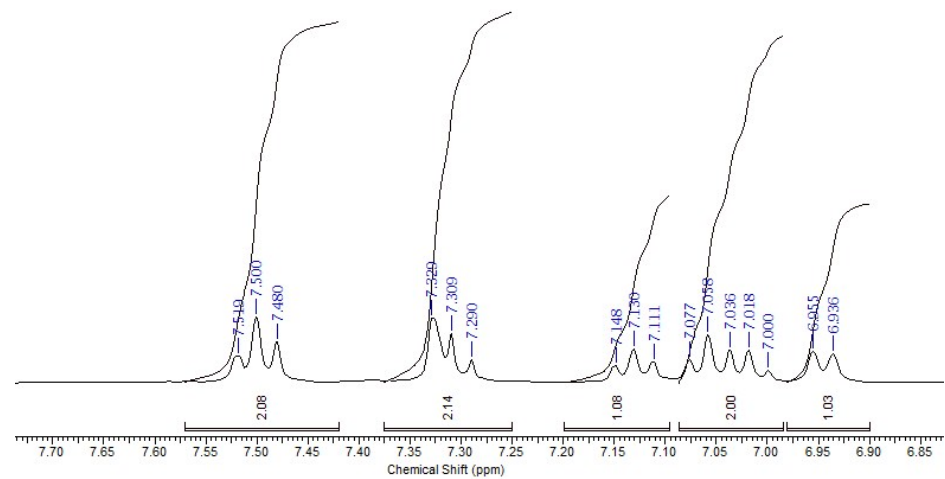
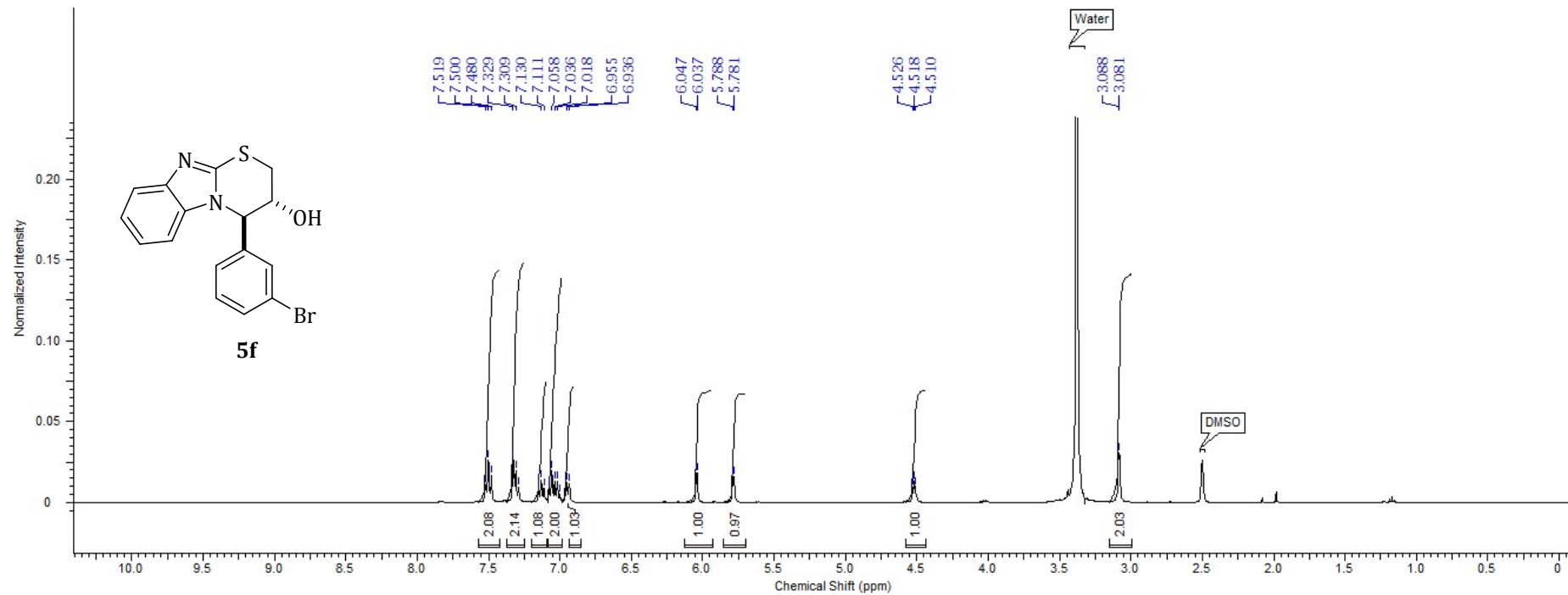
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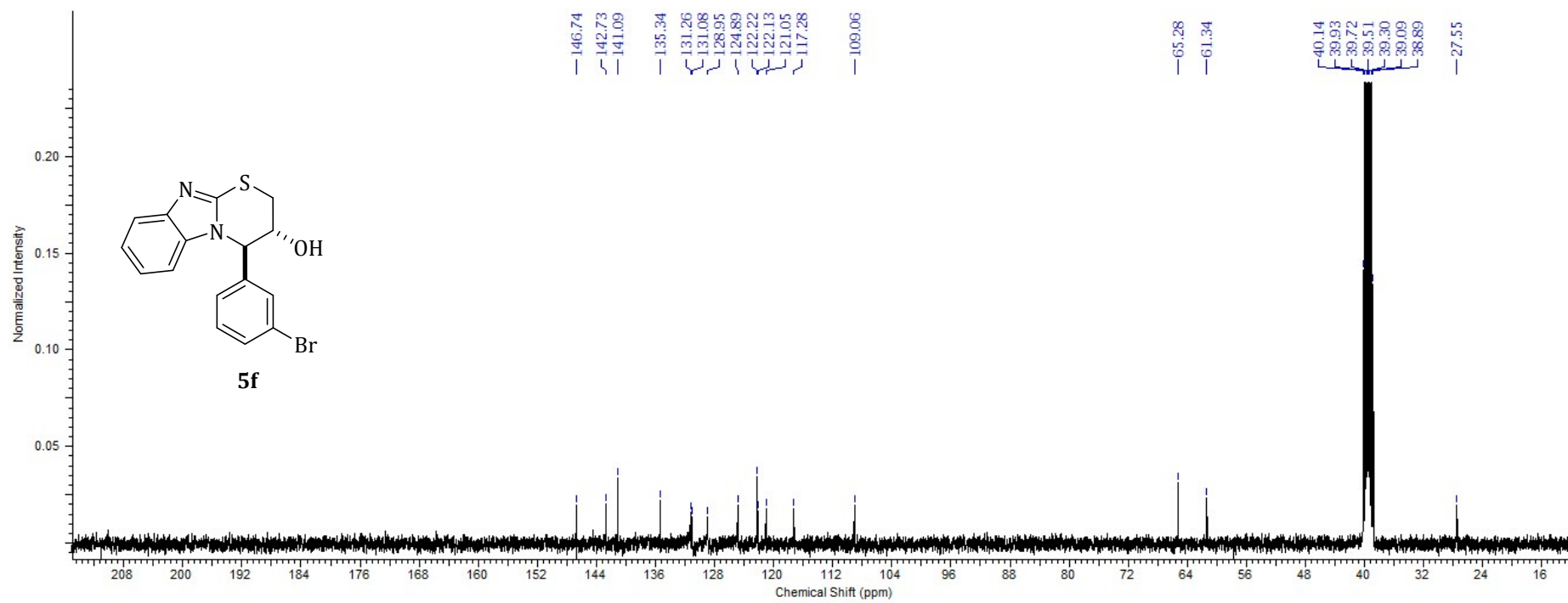
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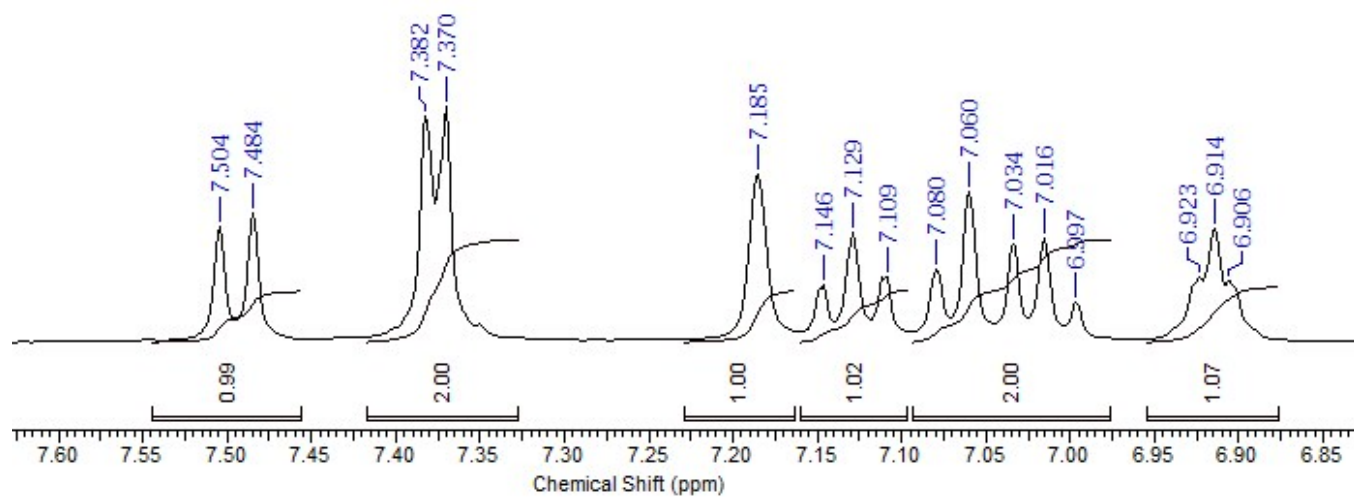
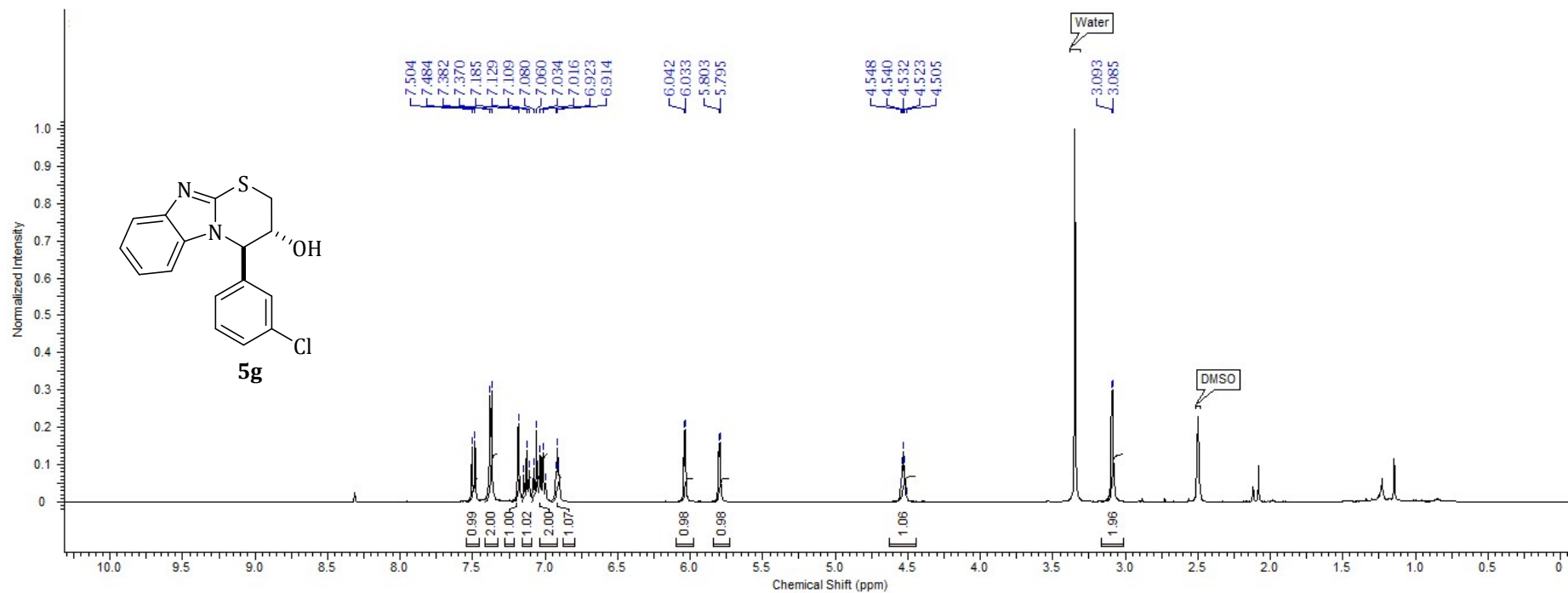
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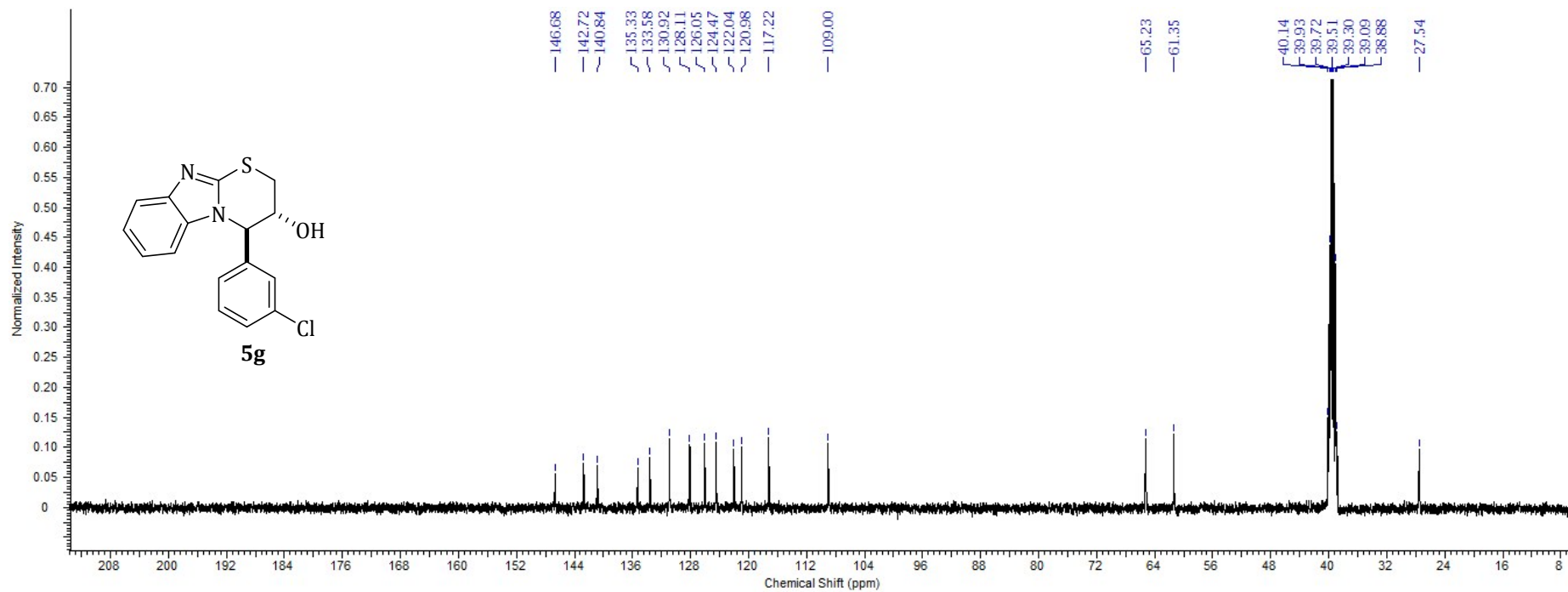
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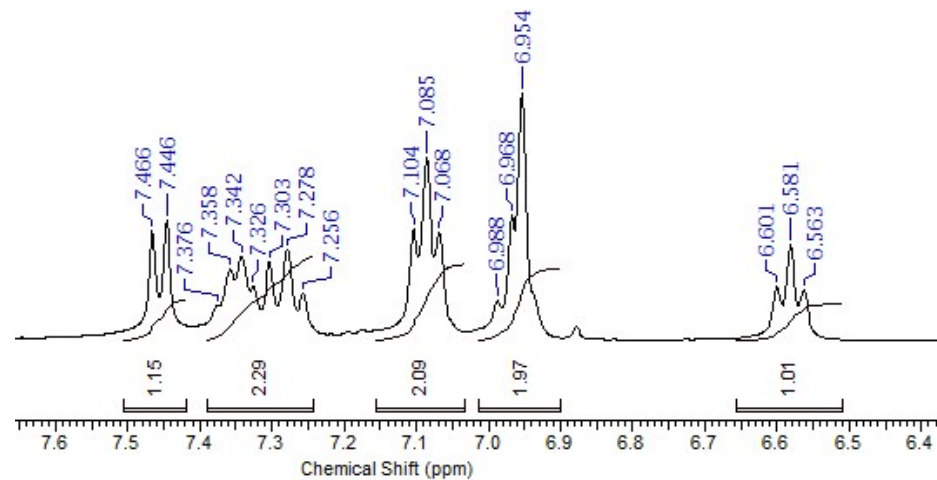
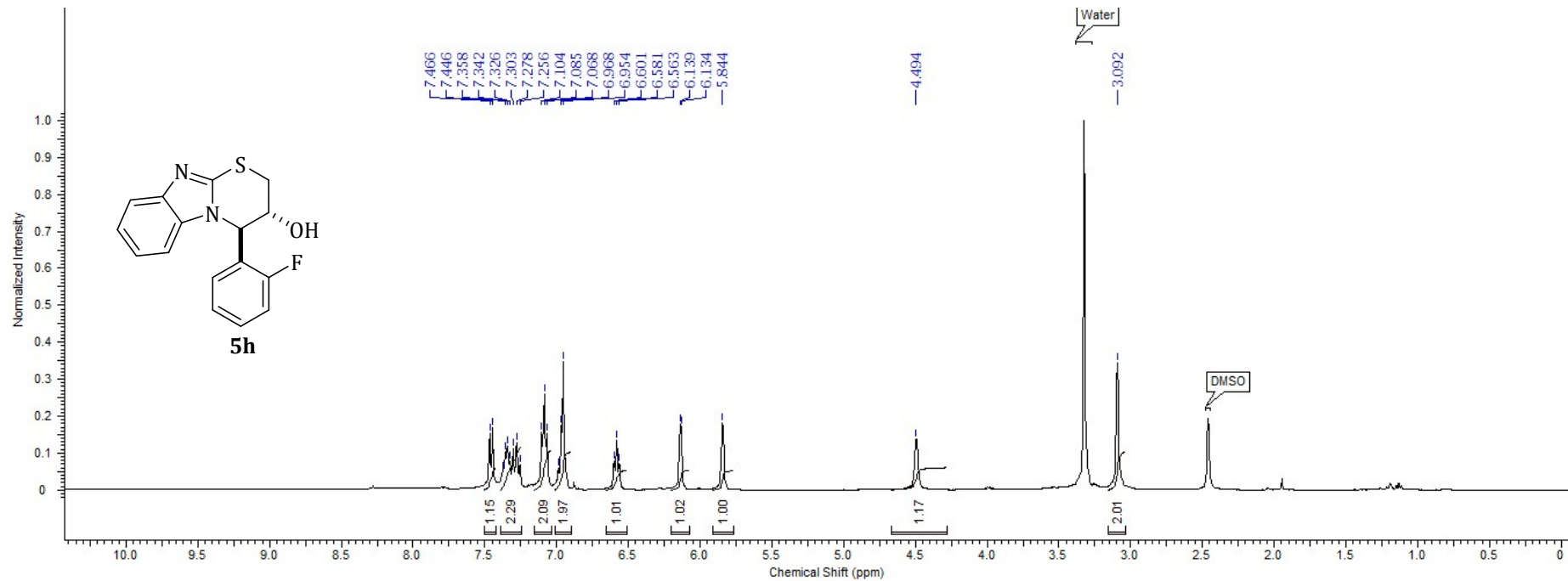
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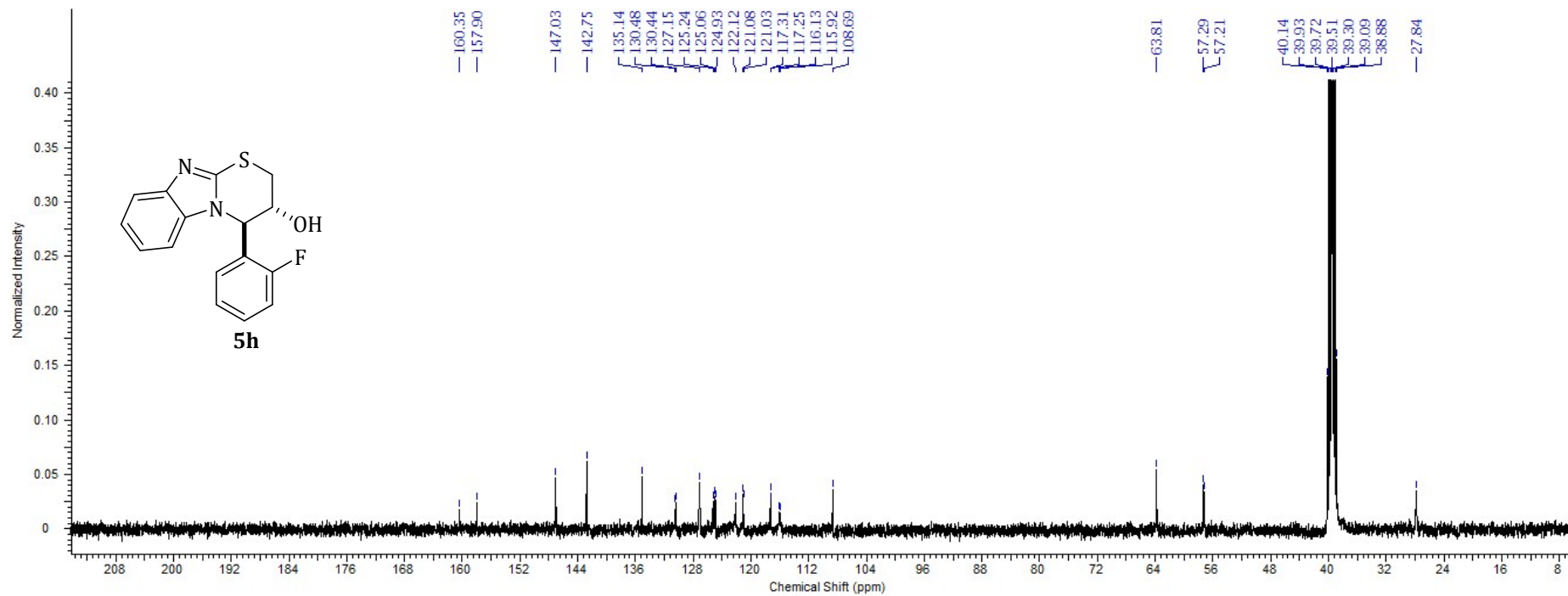
¹H NMR spectrum (400 MHz, DMSO-*d*₆) of 5g



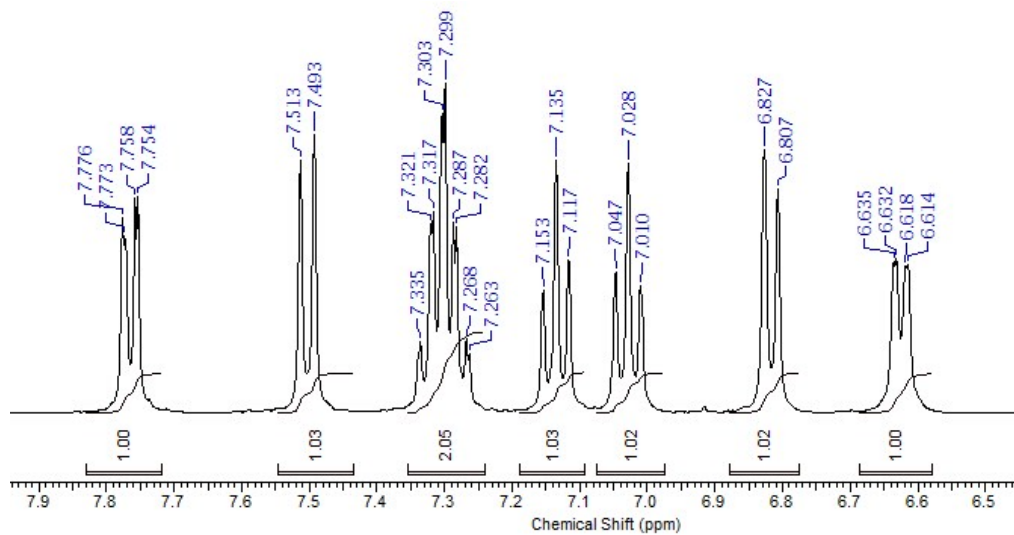
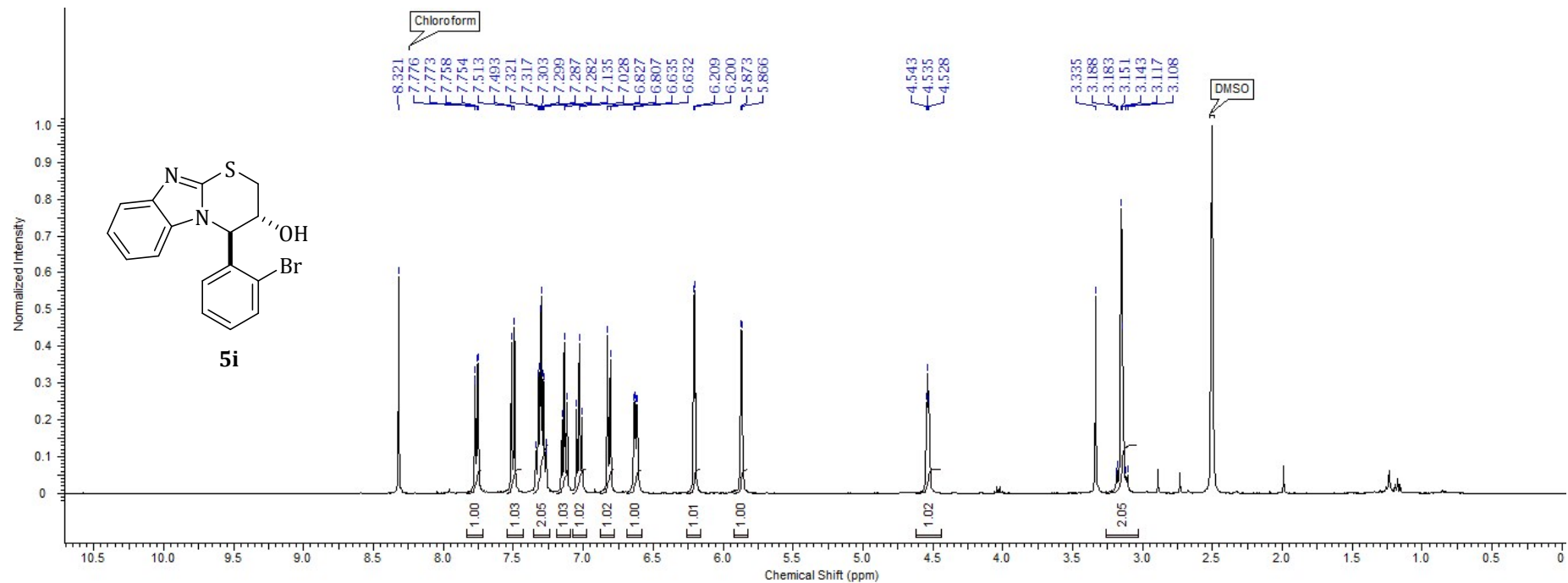
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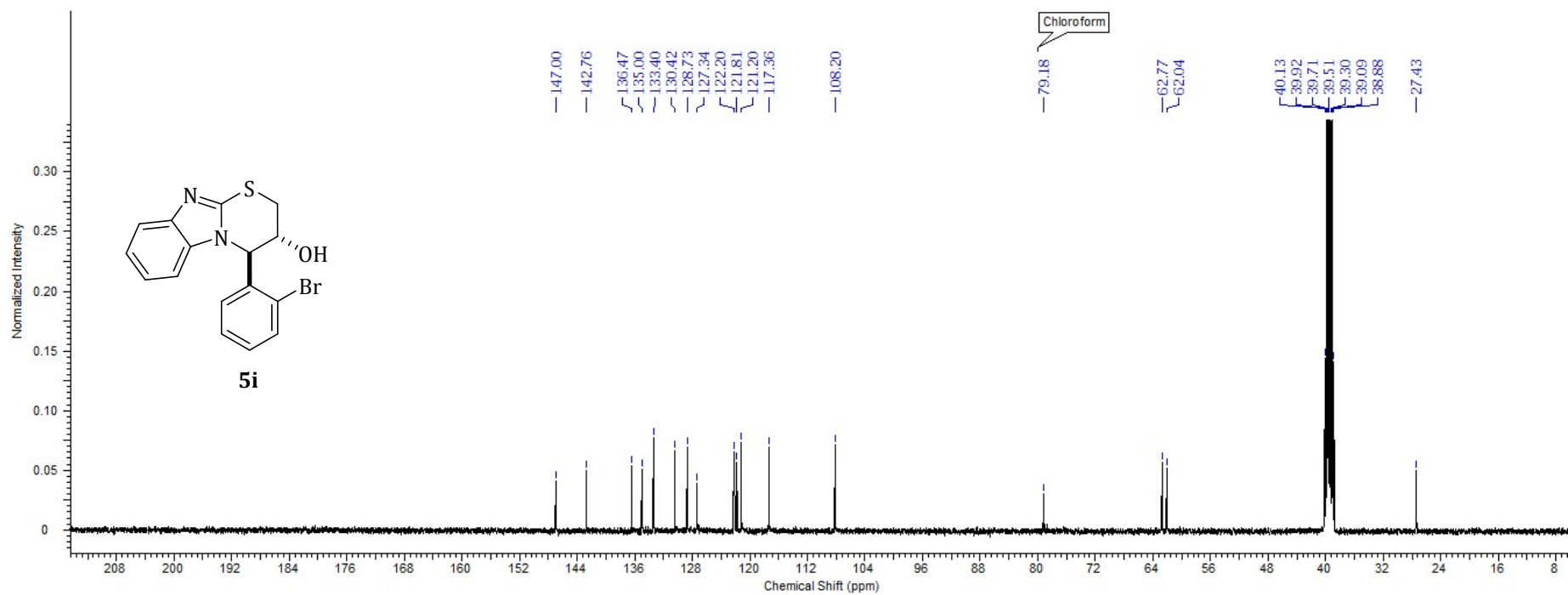
¹H NMR spectrum (400 MHz, DMSO-*d*₆) of 5h



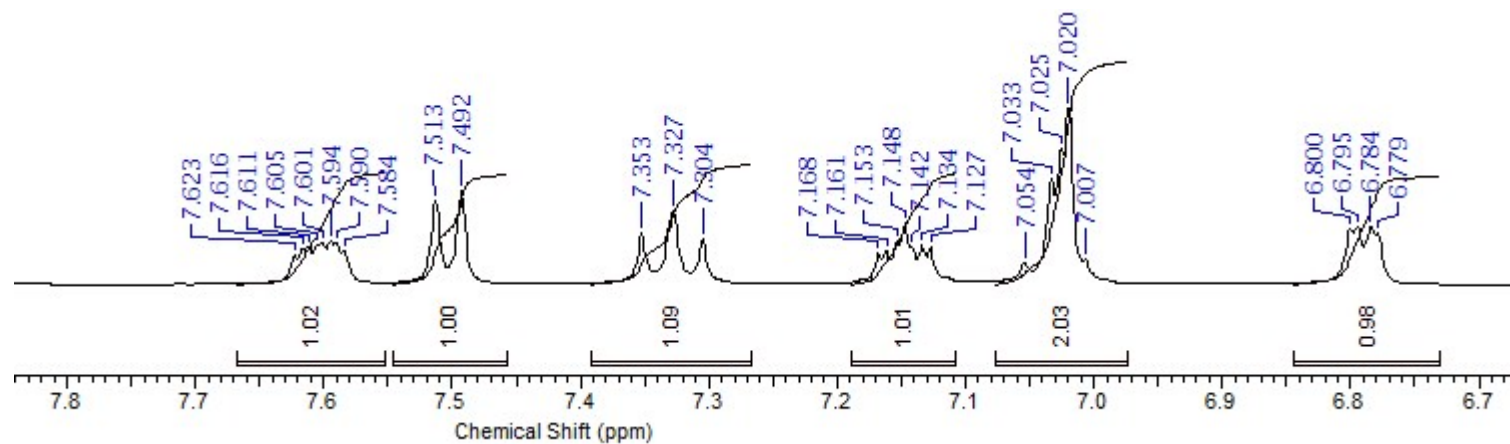
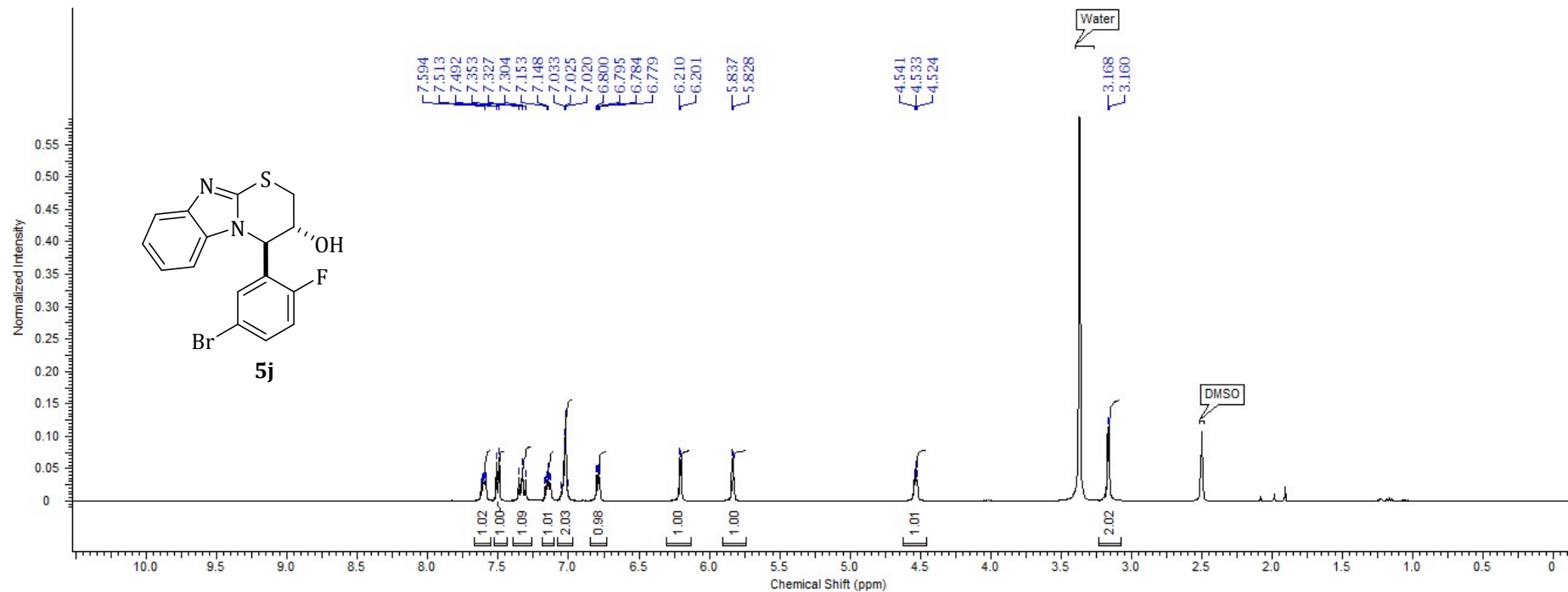
^{13}C NMR spectrum (100 MHz, $\text{DMSO-}d_6$) of 5h



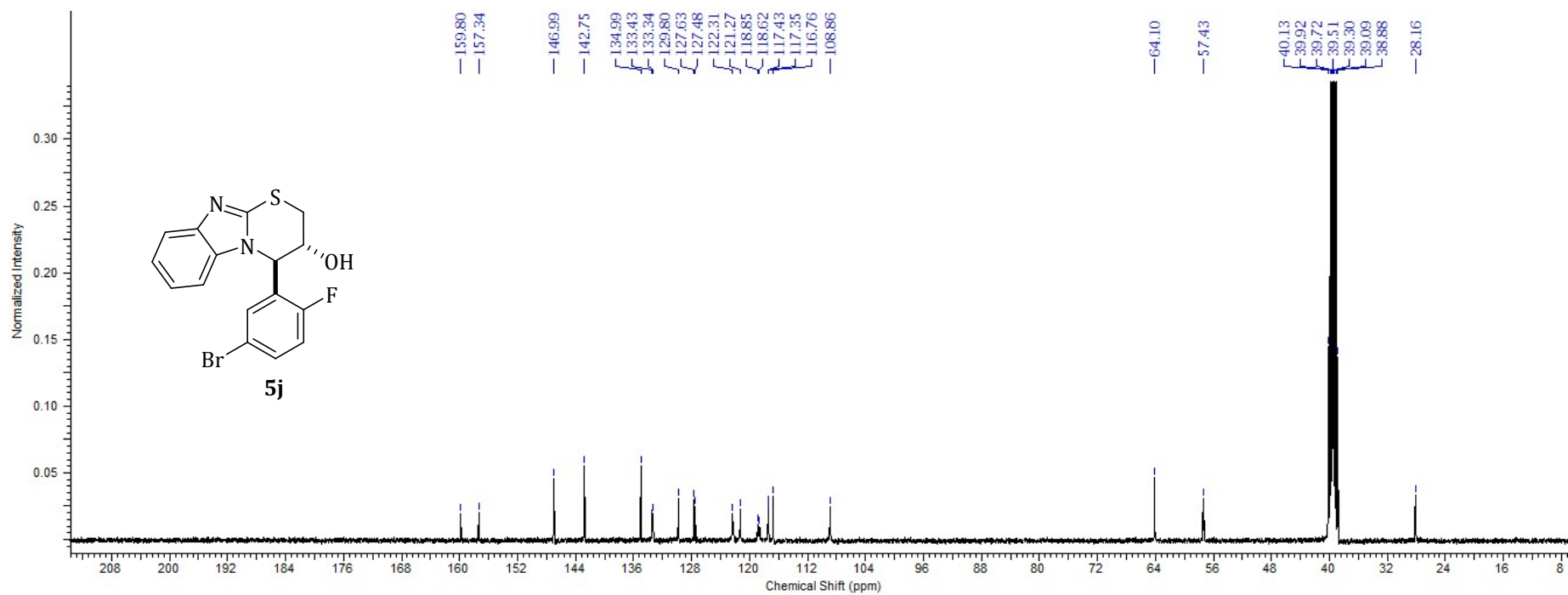
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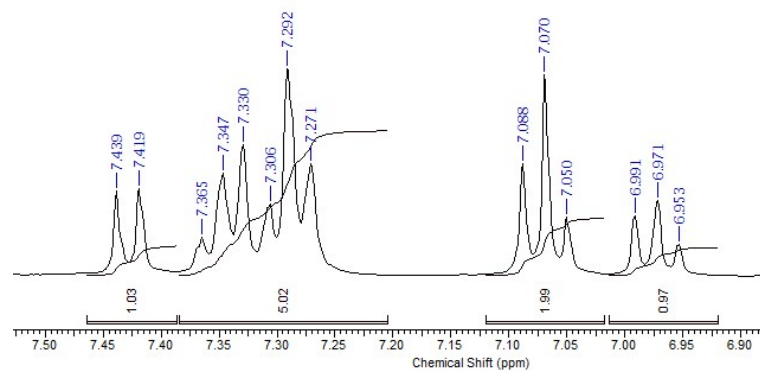
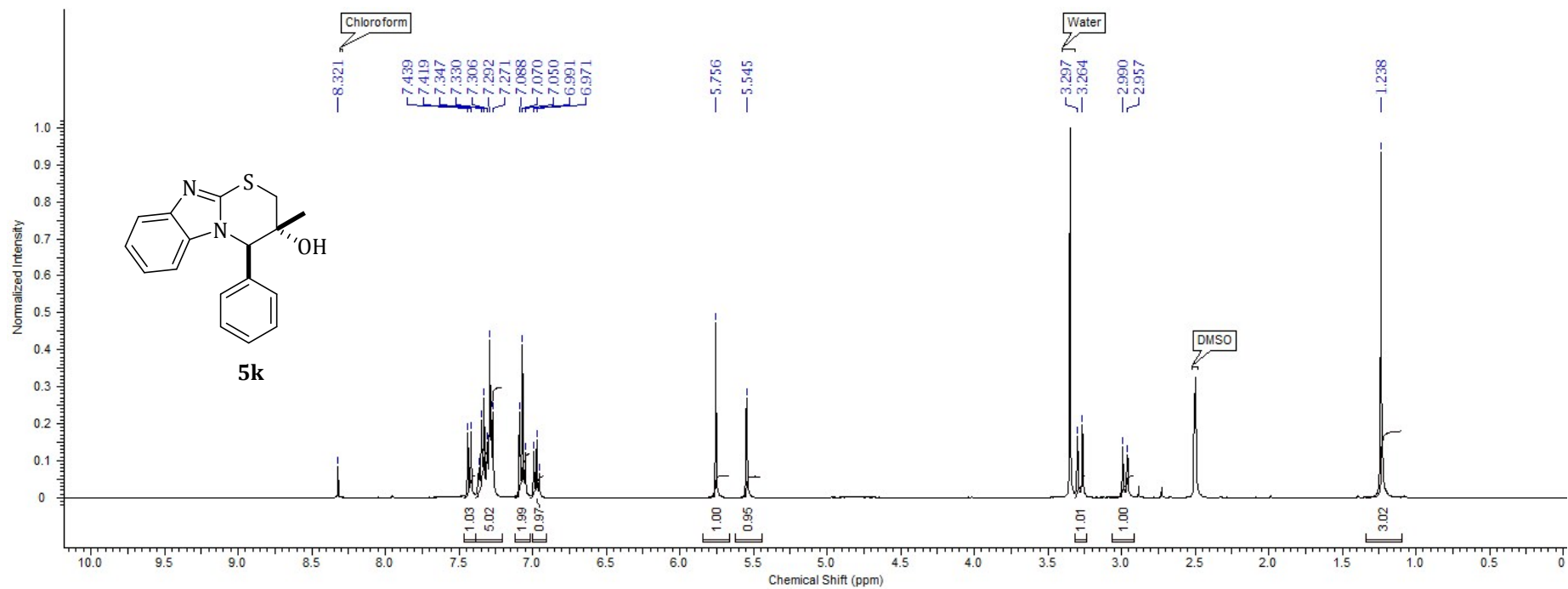
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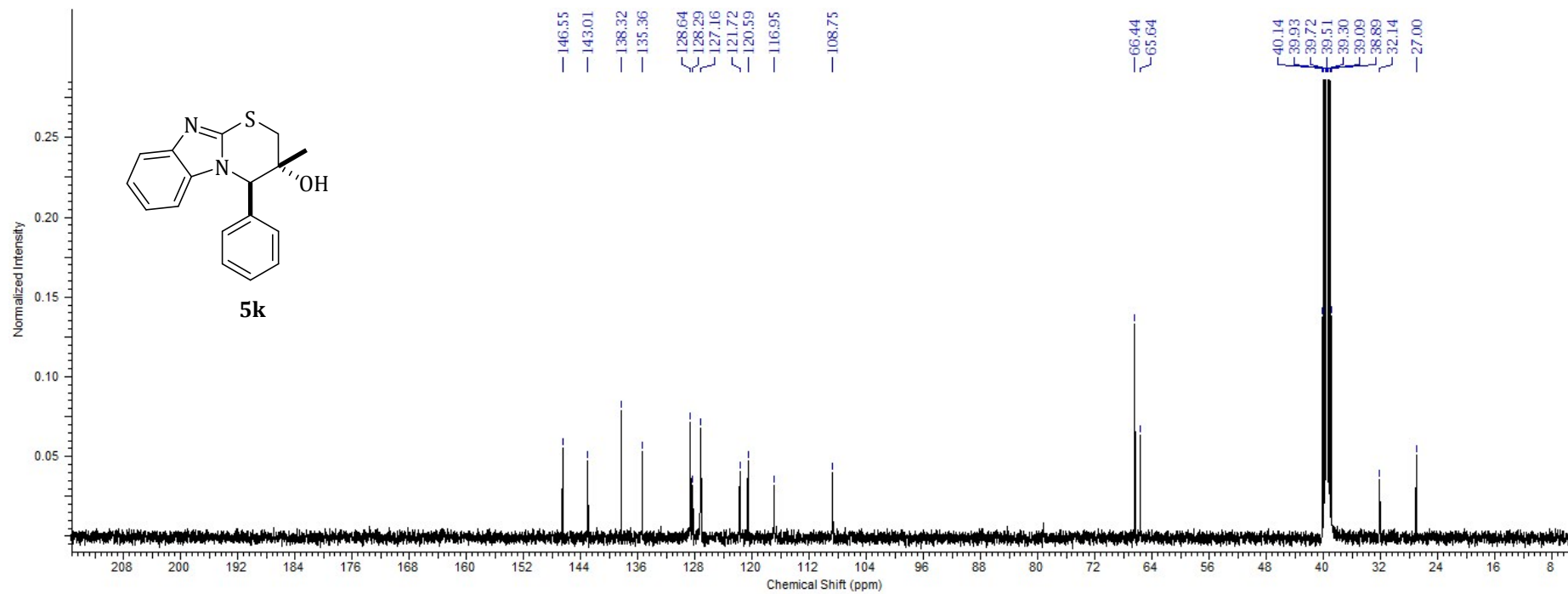
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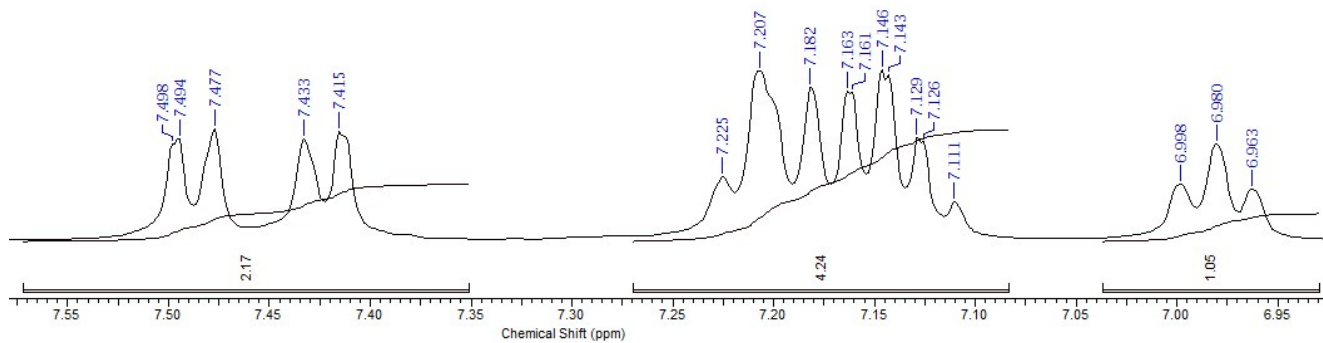
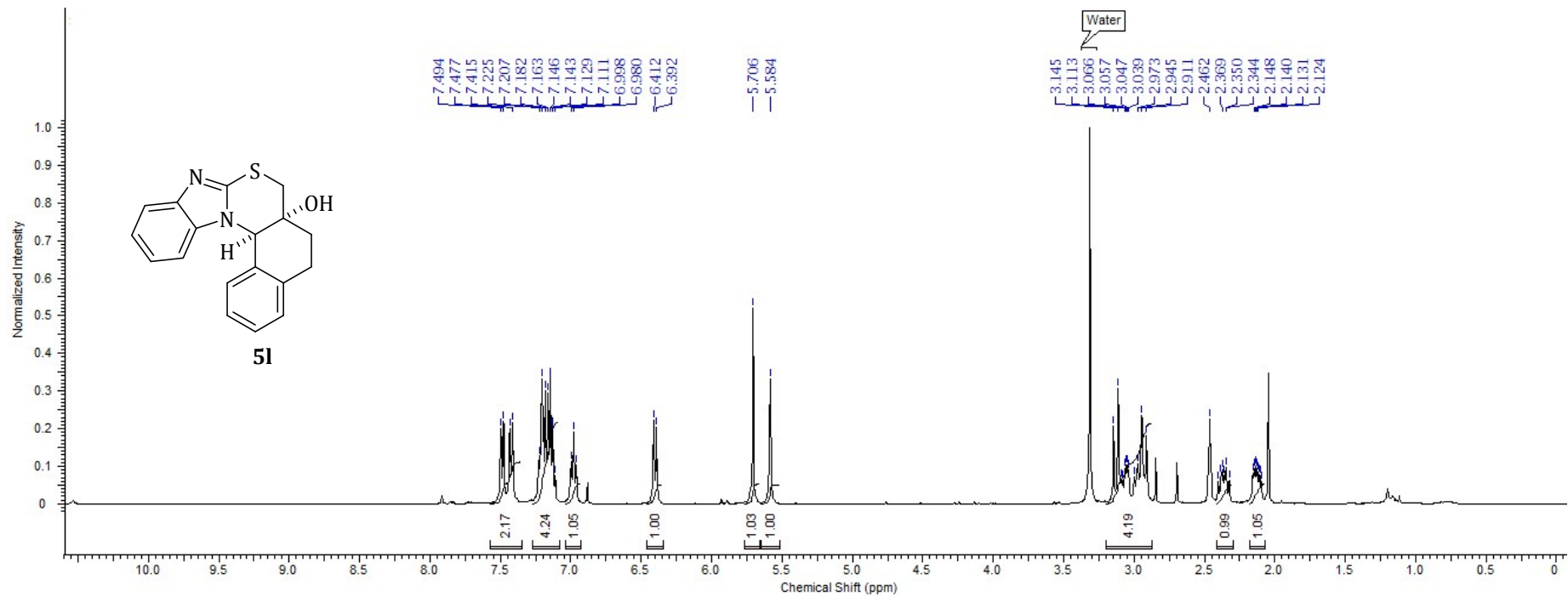
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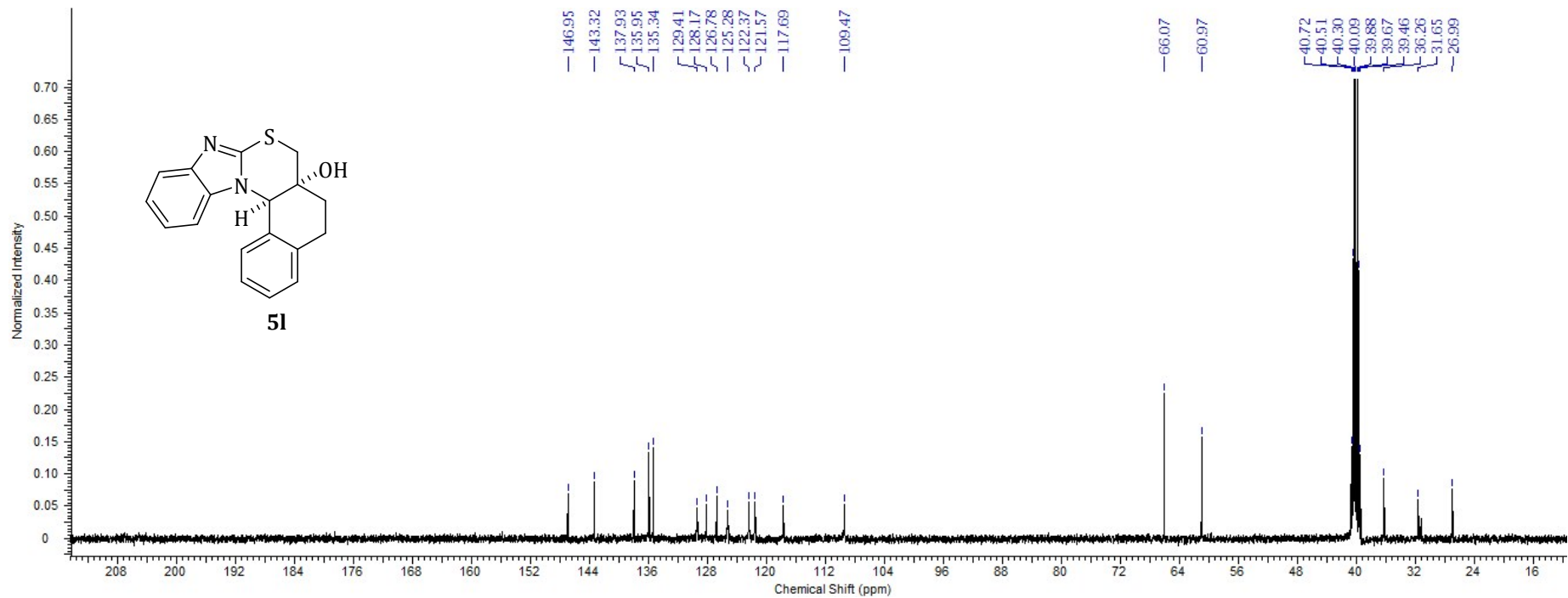
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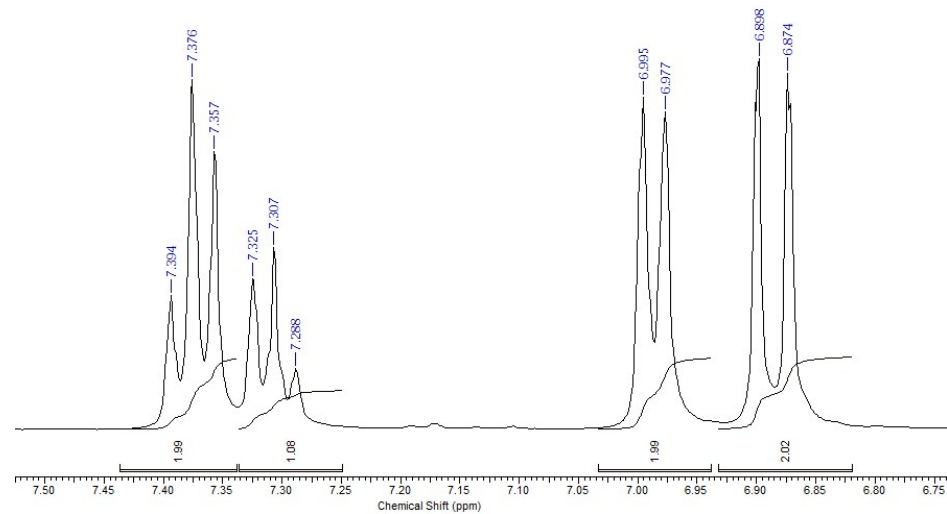
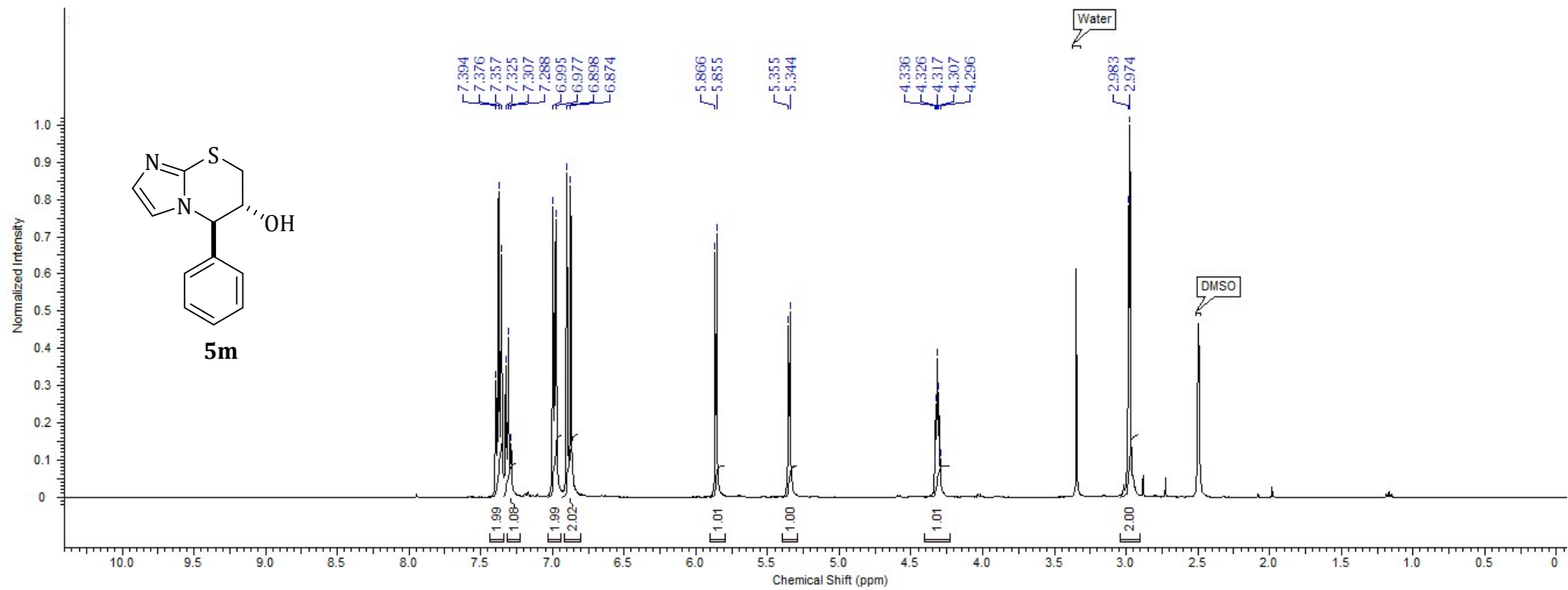
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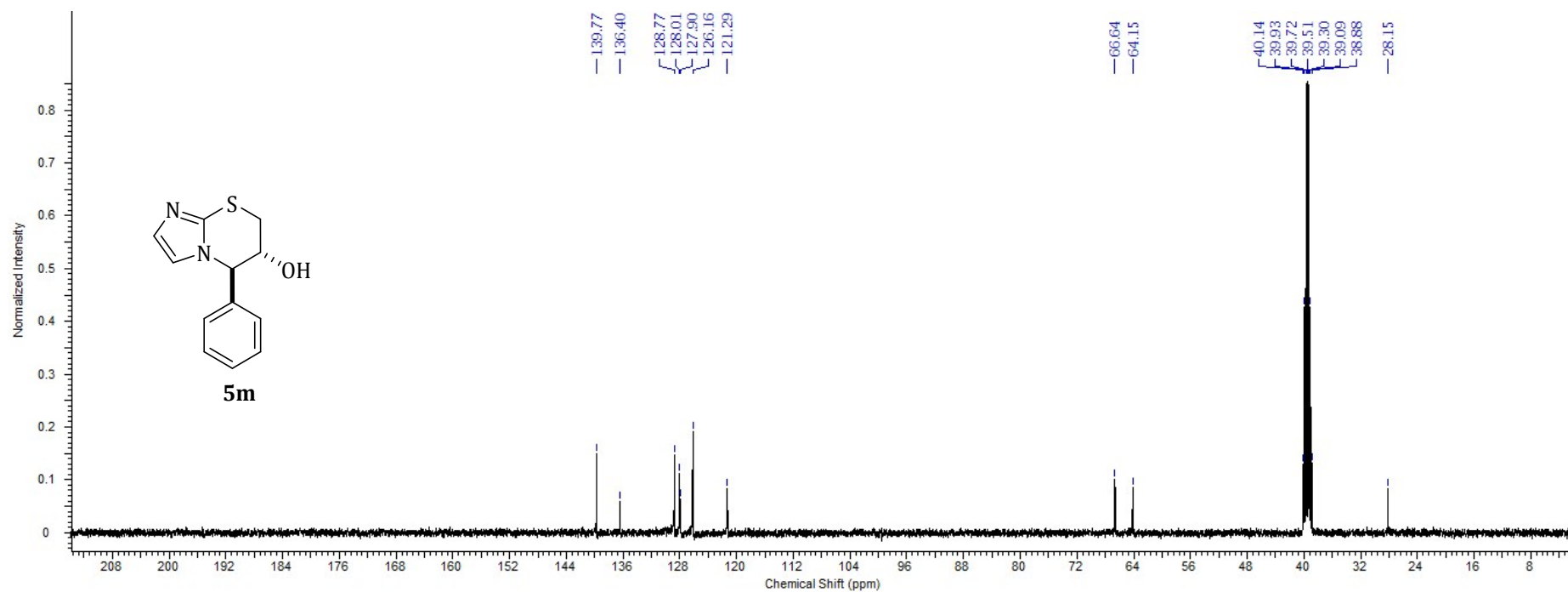
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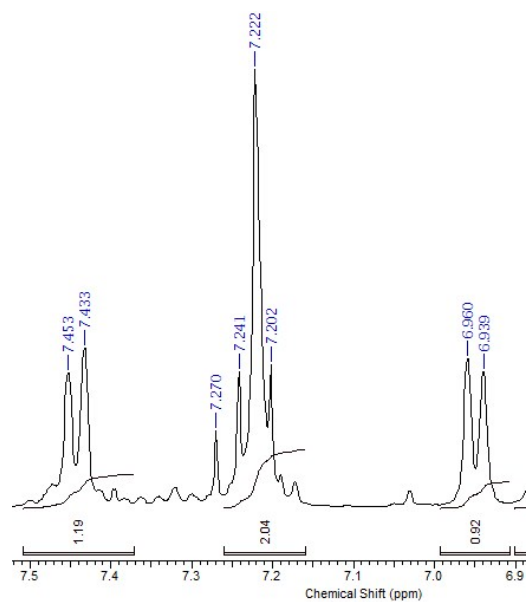
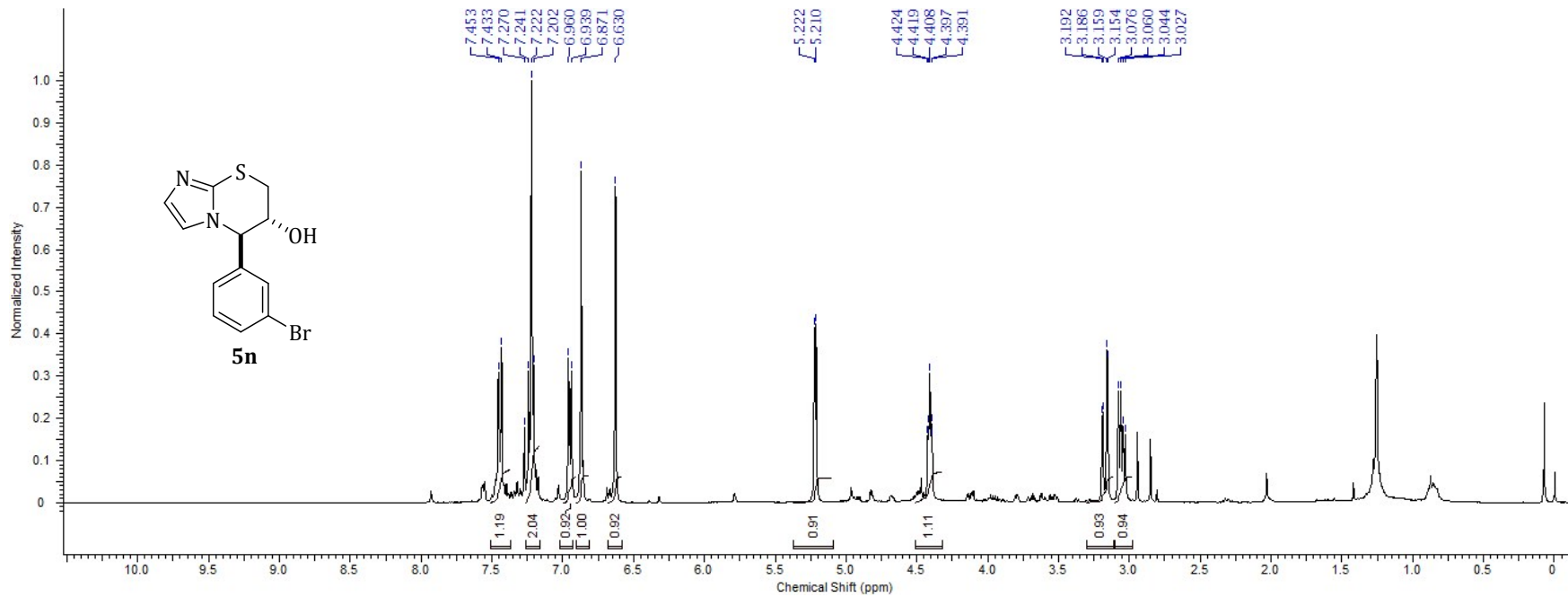
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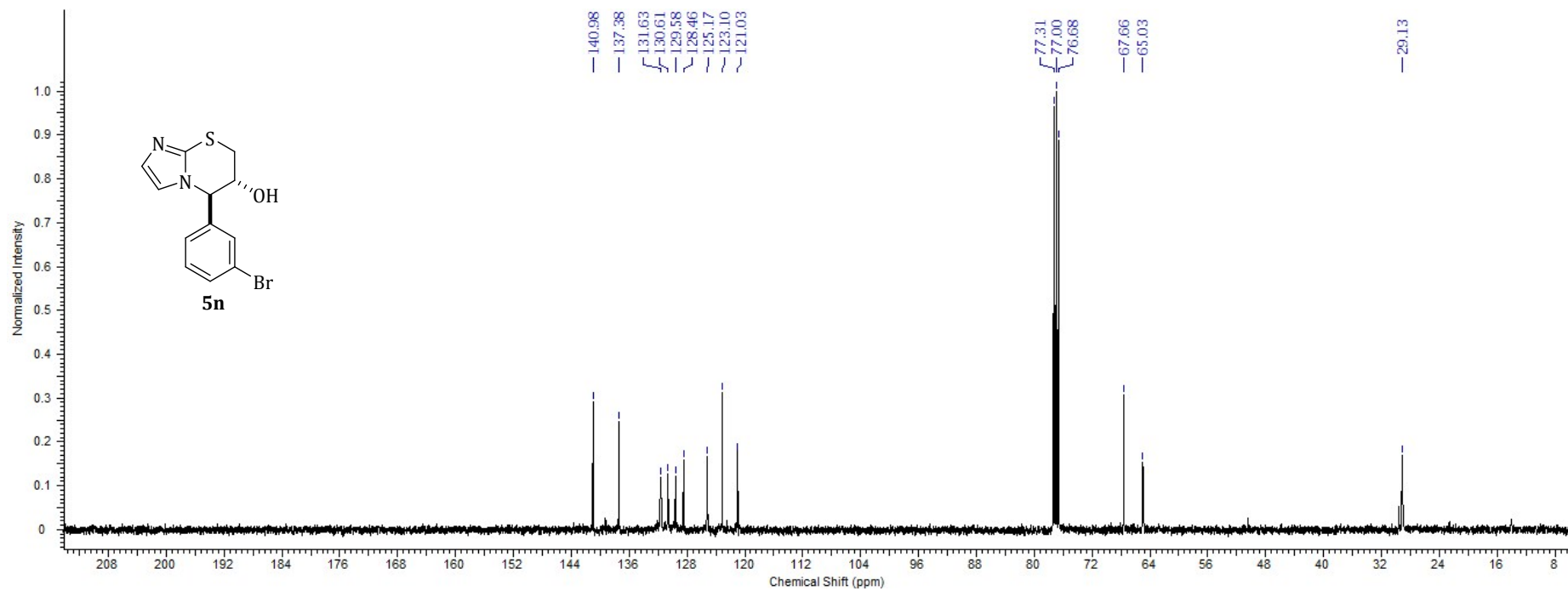
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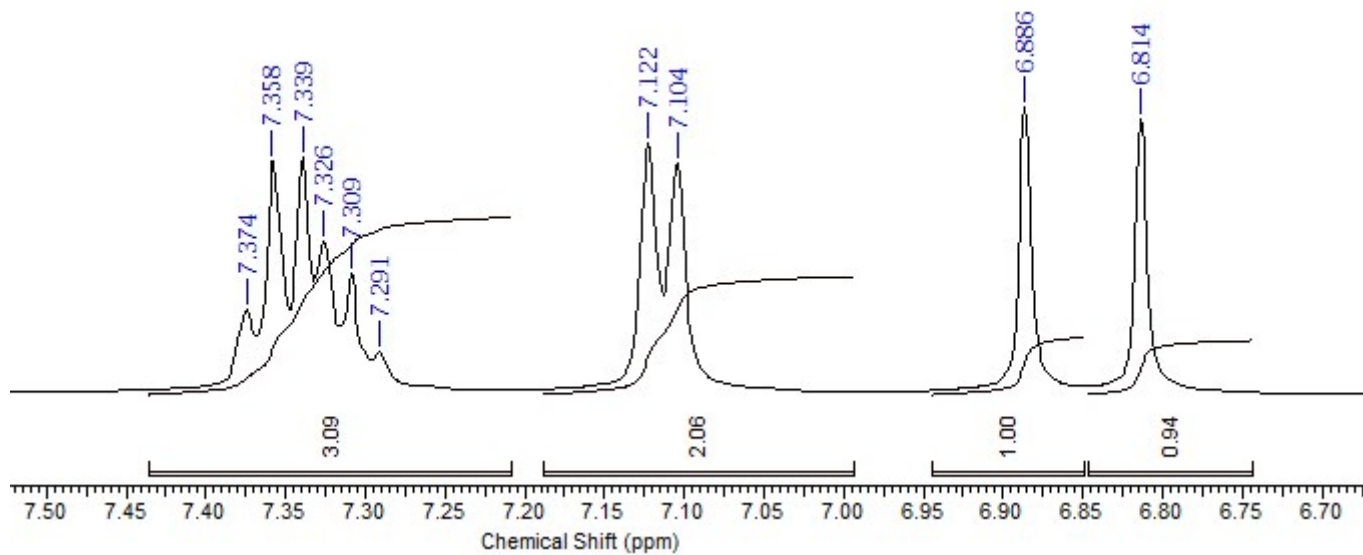
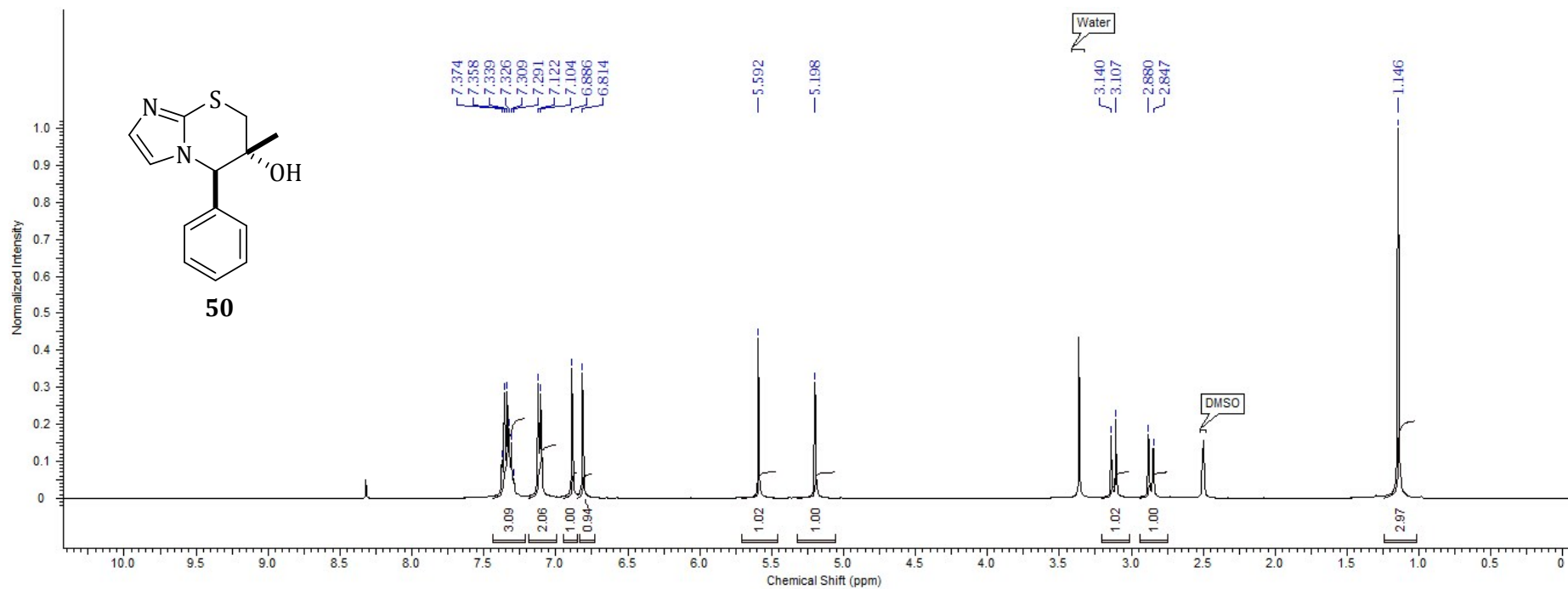


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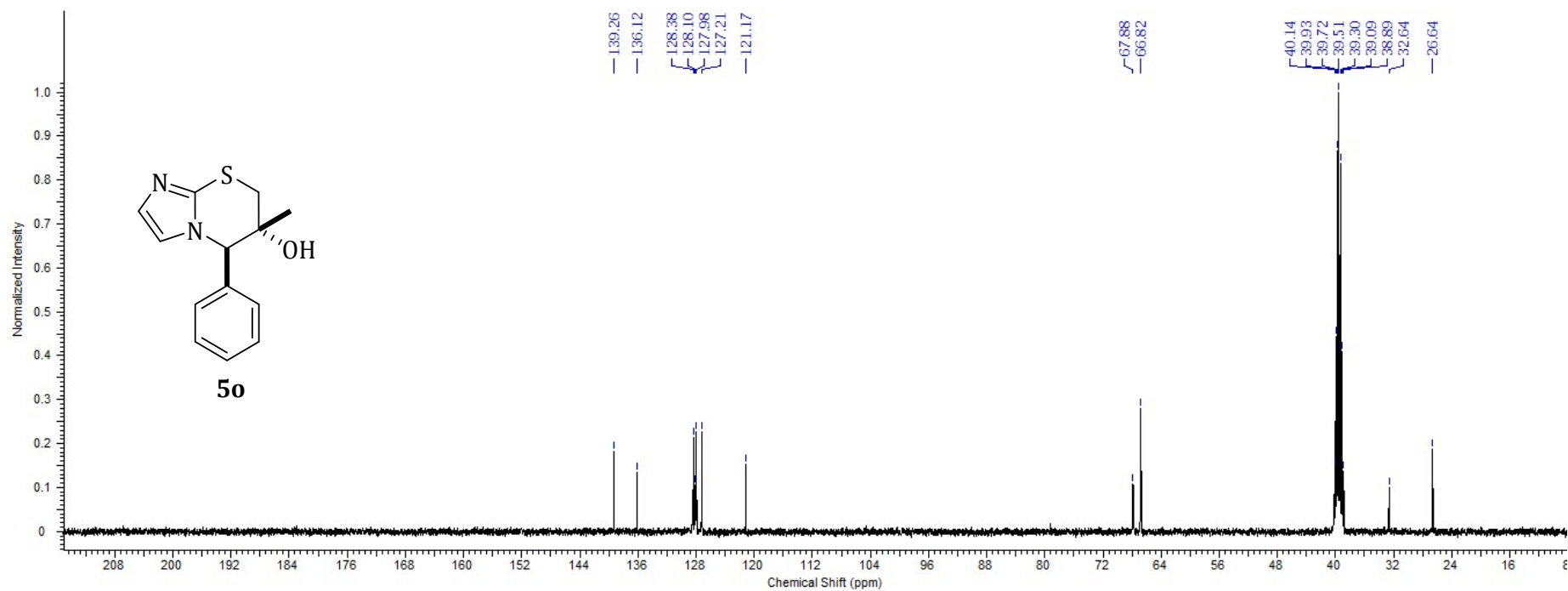


¹H NMR spectrum (400 MHz, CDCl₃) of 5n

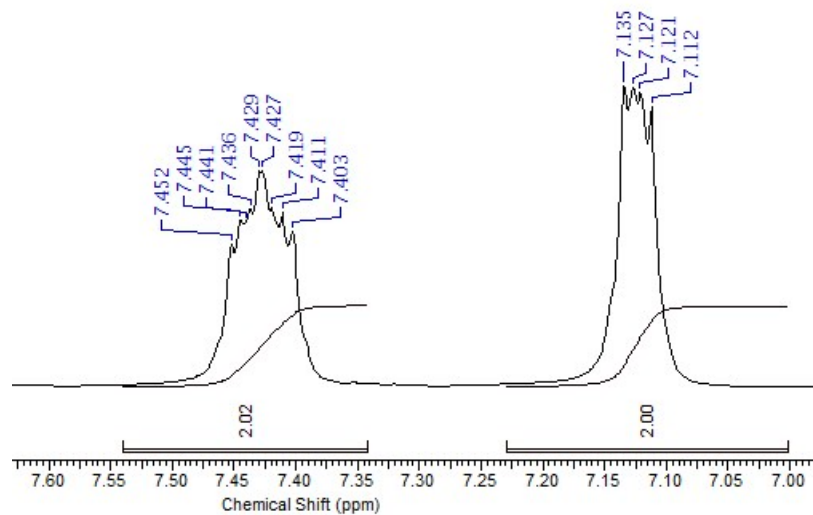
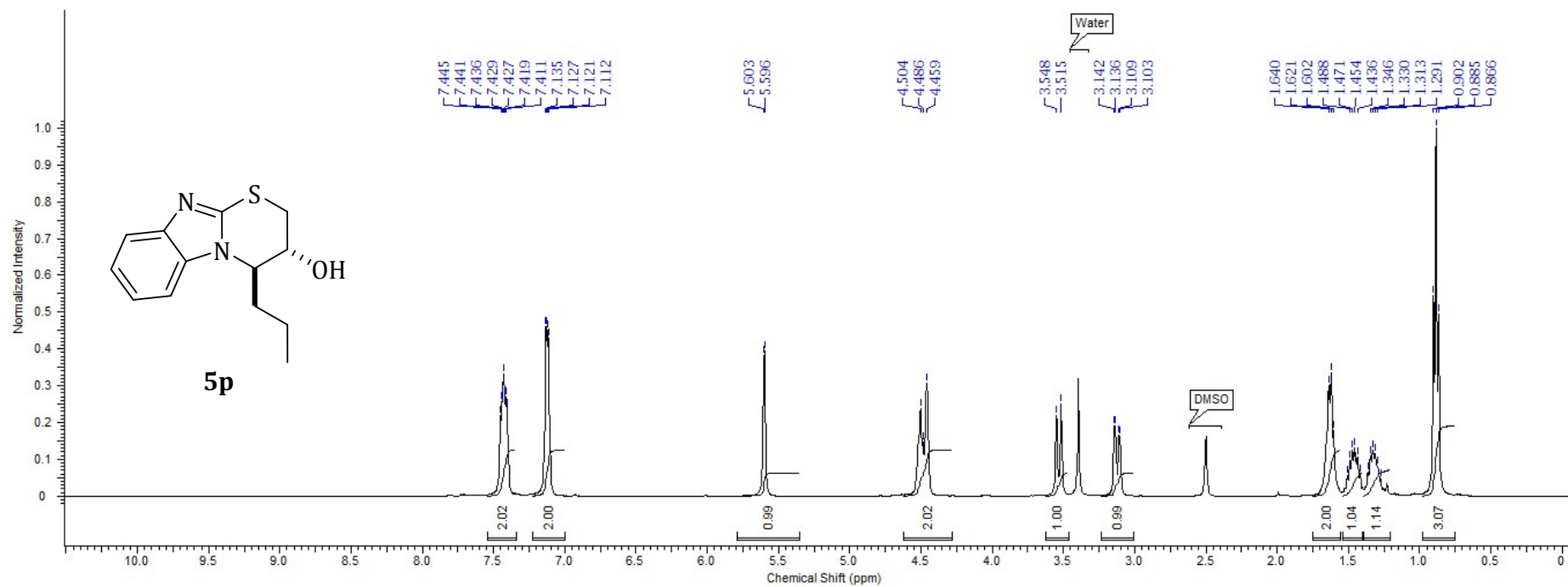




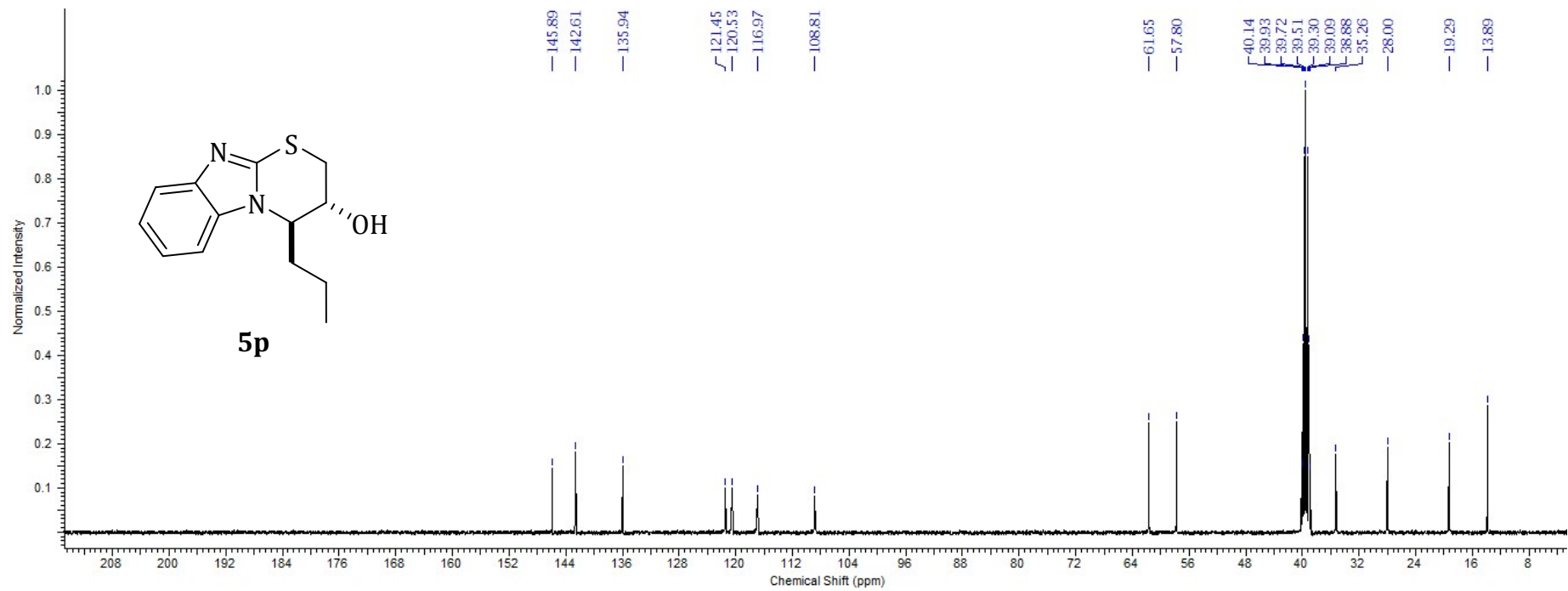
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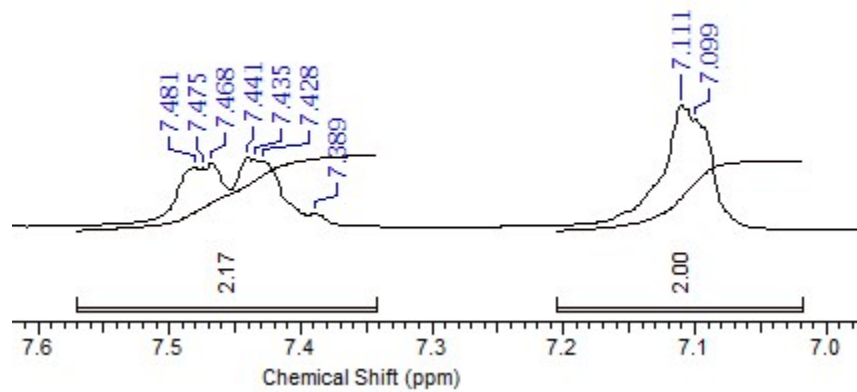
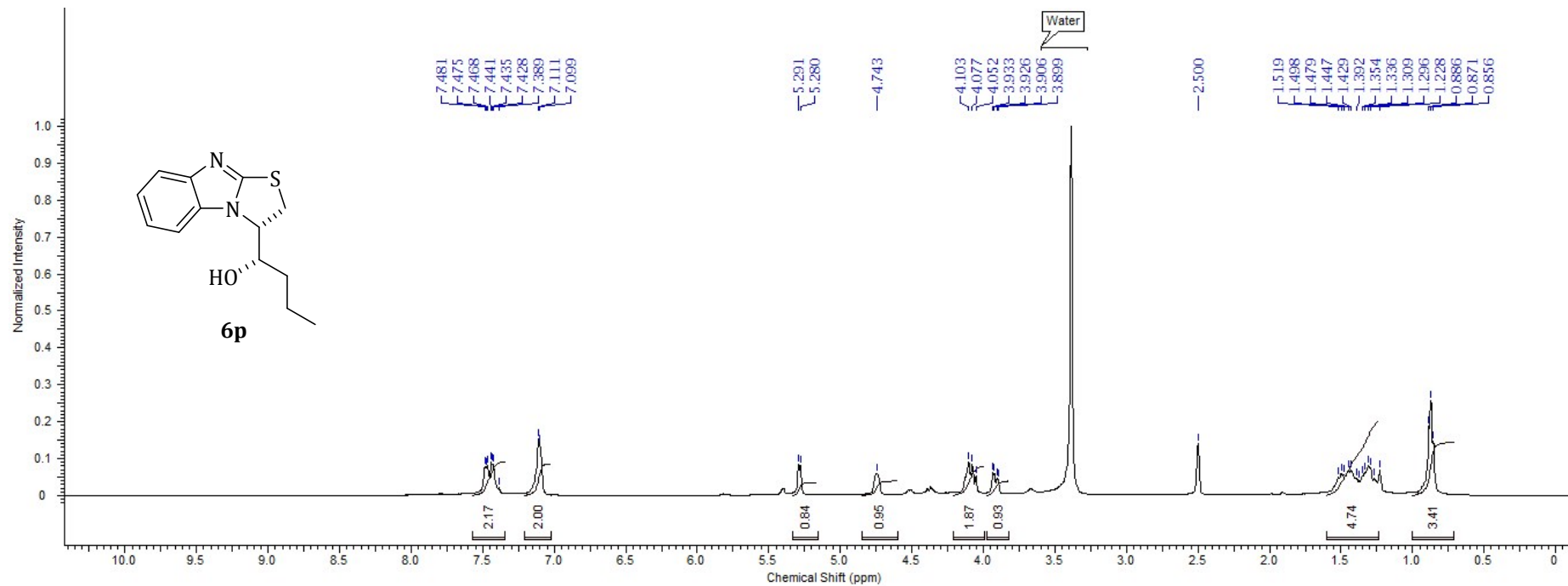
^{13}C NMR spectrum (100 MHz, $\text{DMSO-}d_6$) of 5o



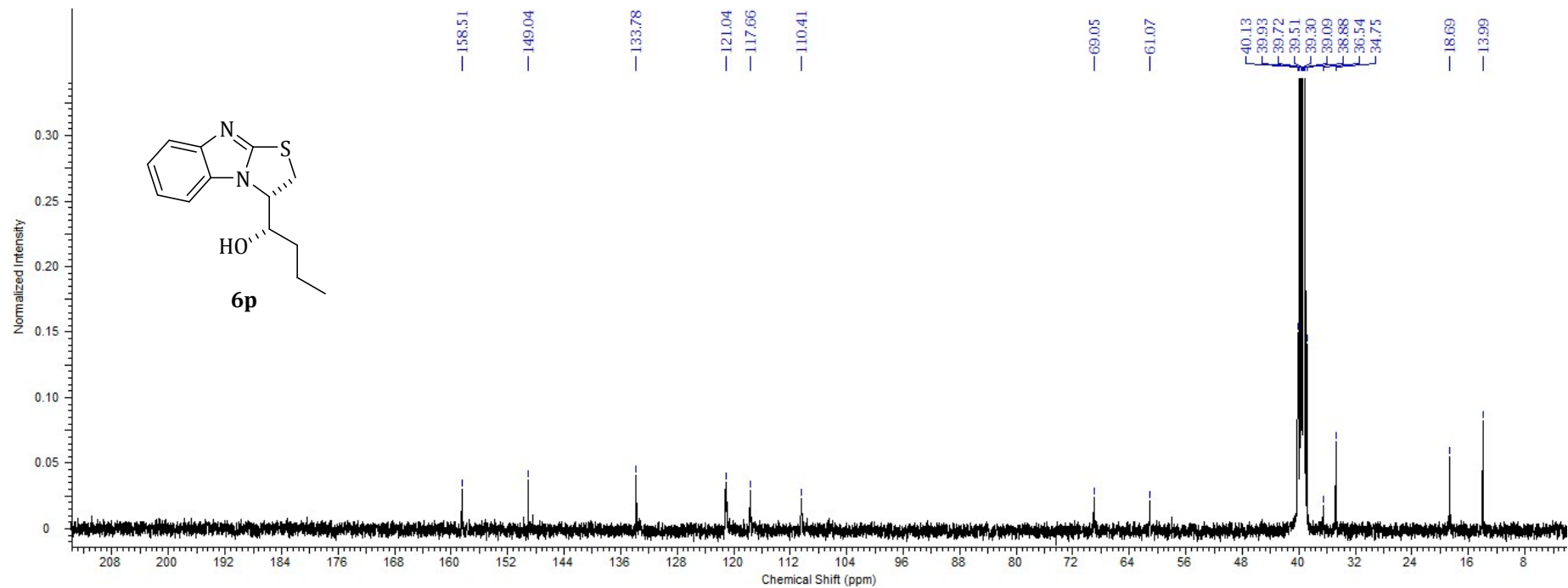
¹H NMR spectrum (400 MHz, DMSO-*d*₆) of 5p



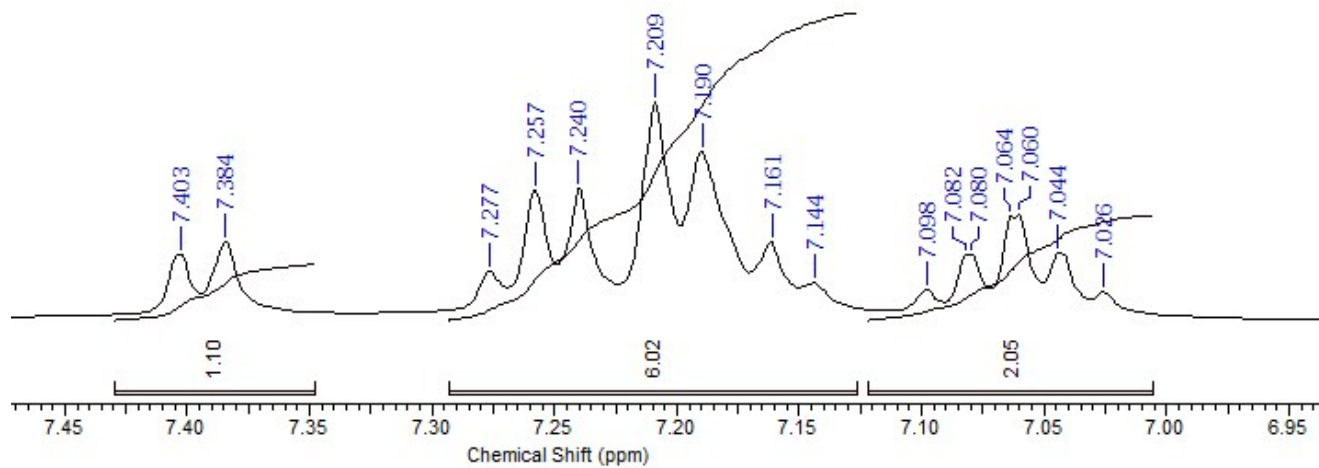
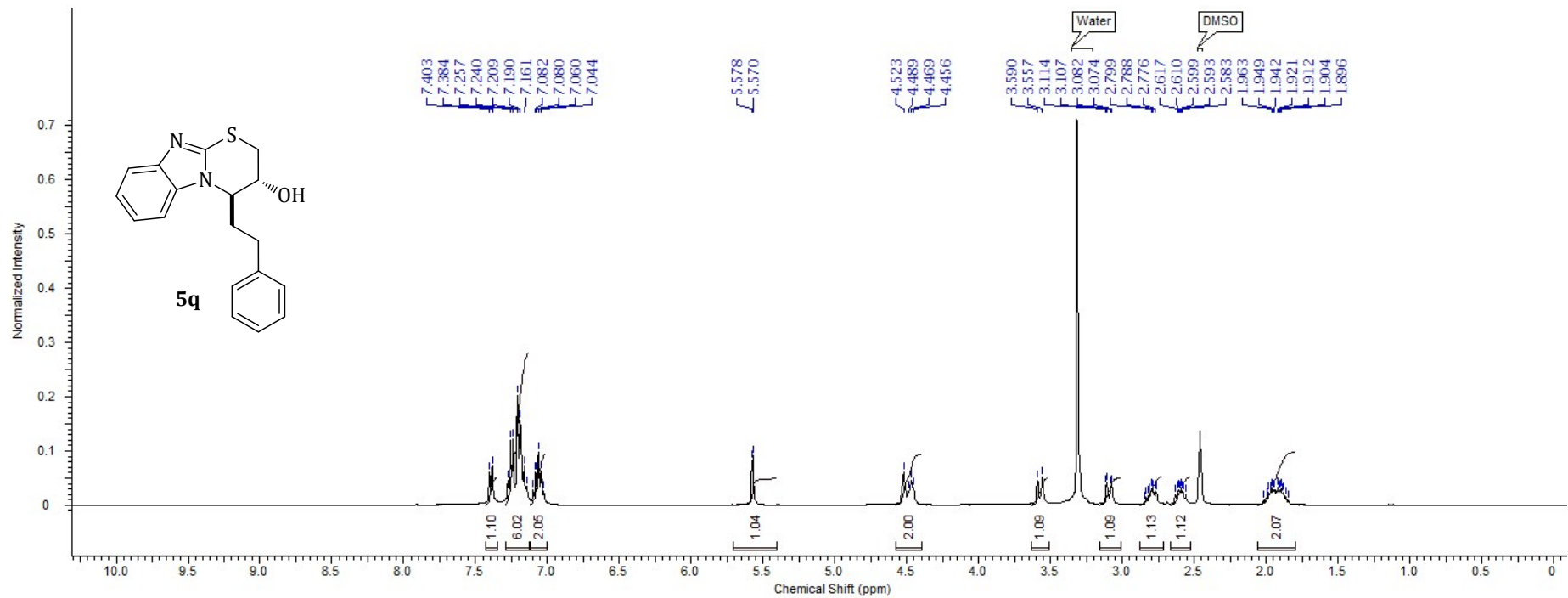
^{13}C NMR spectrum (100 MHz, $\text{DMSO-}d_6$) of 5p



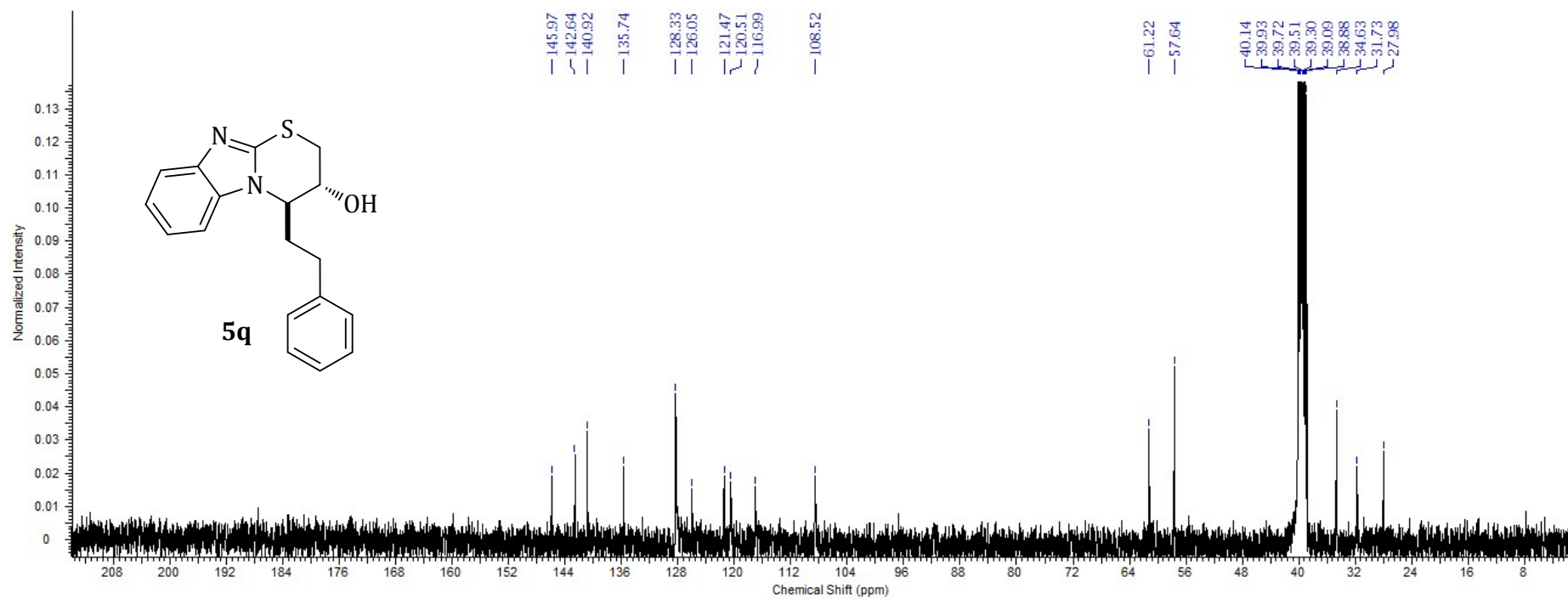
¹H NMR spectrum (400 MHz, DMSO-*d*₆) of 6p



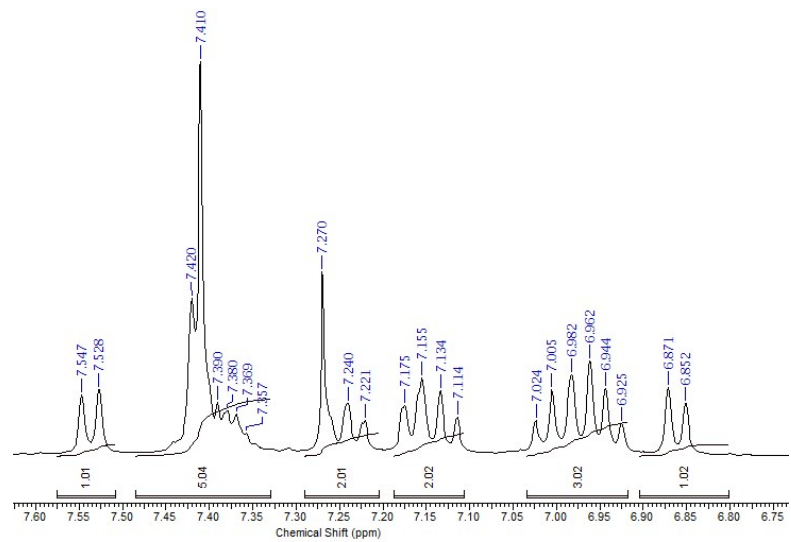
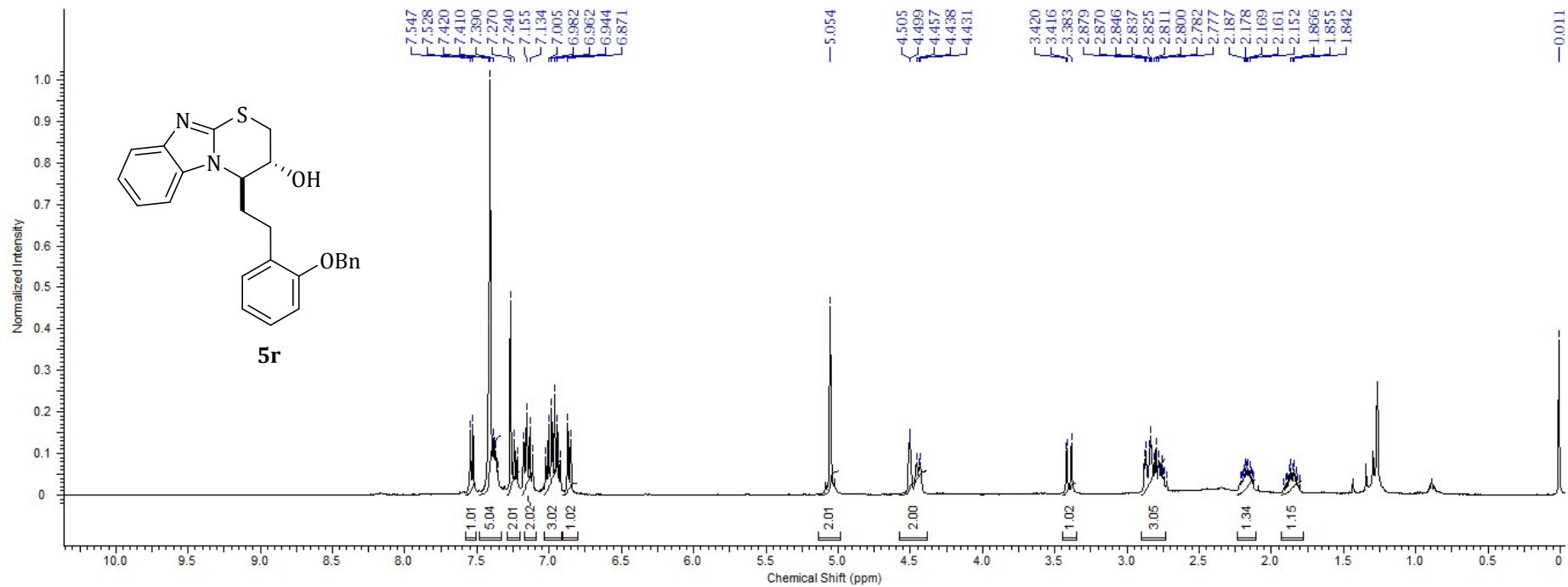
^{13}C NMR spectrum (100 MHz, $\text{DMSO-}d_6$) of 6p



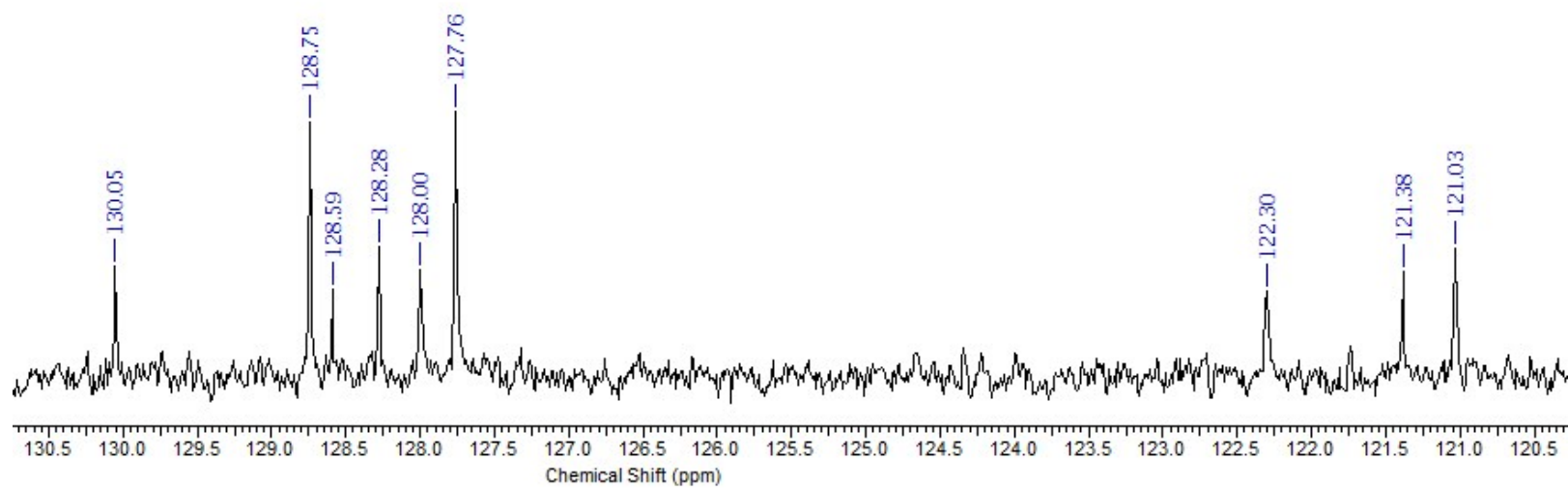
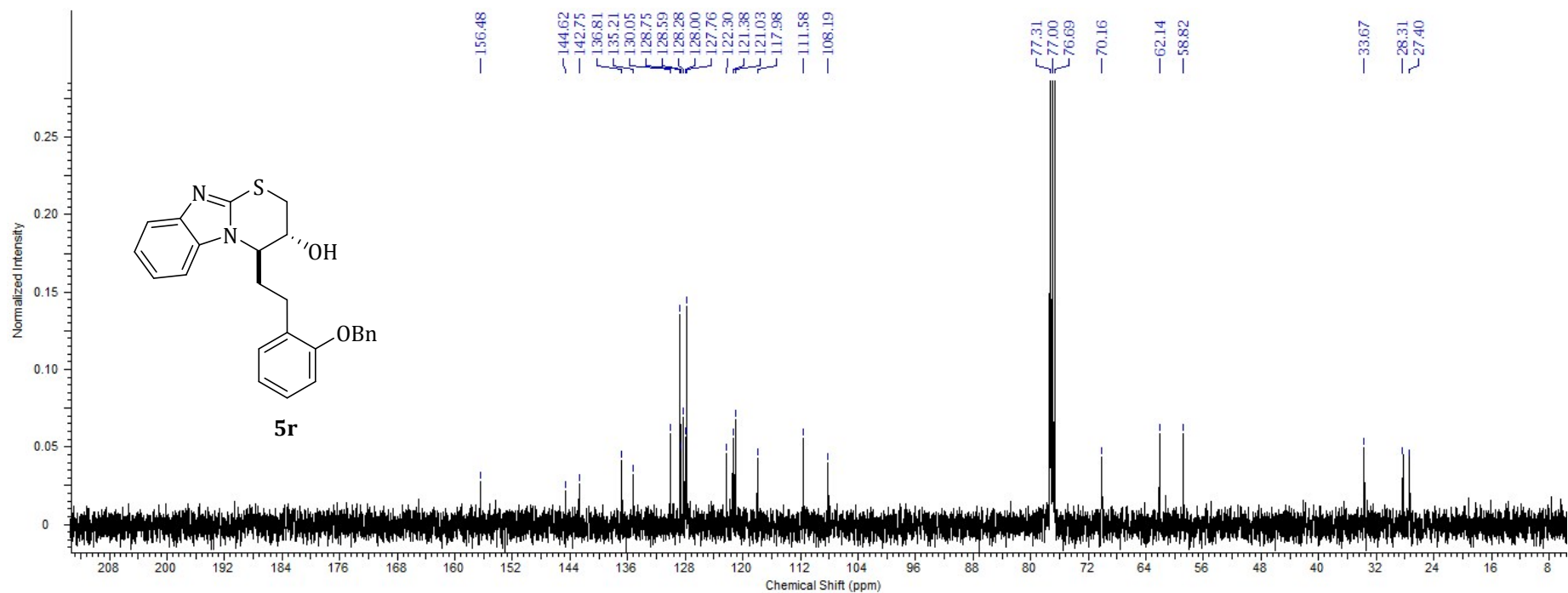
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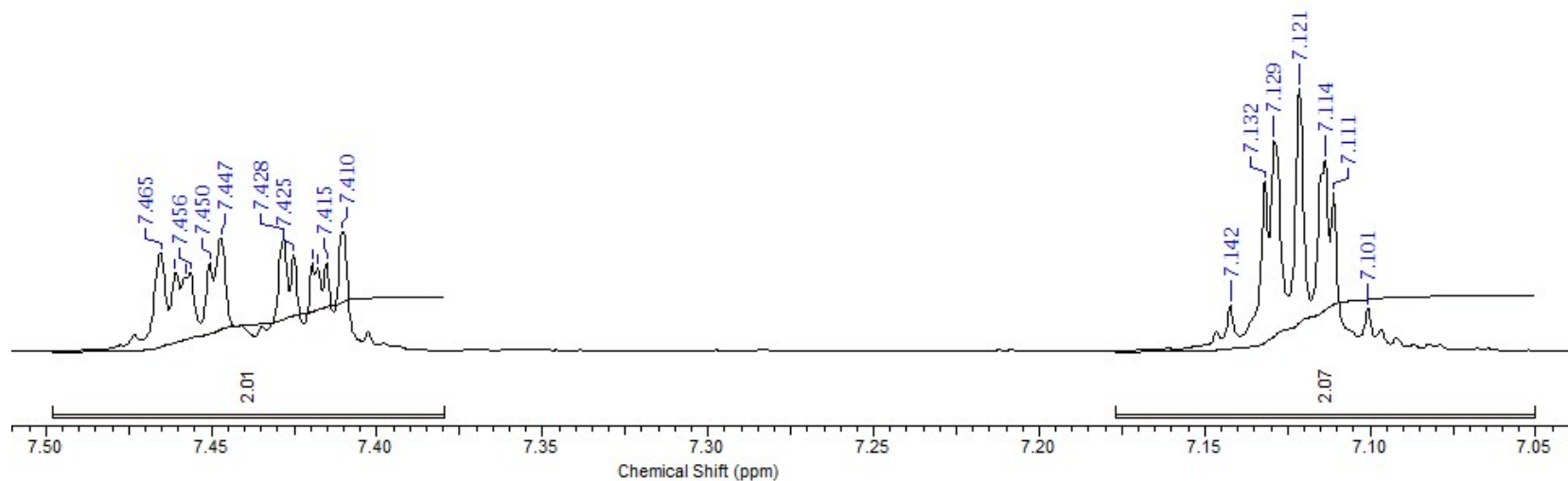
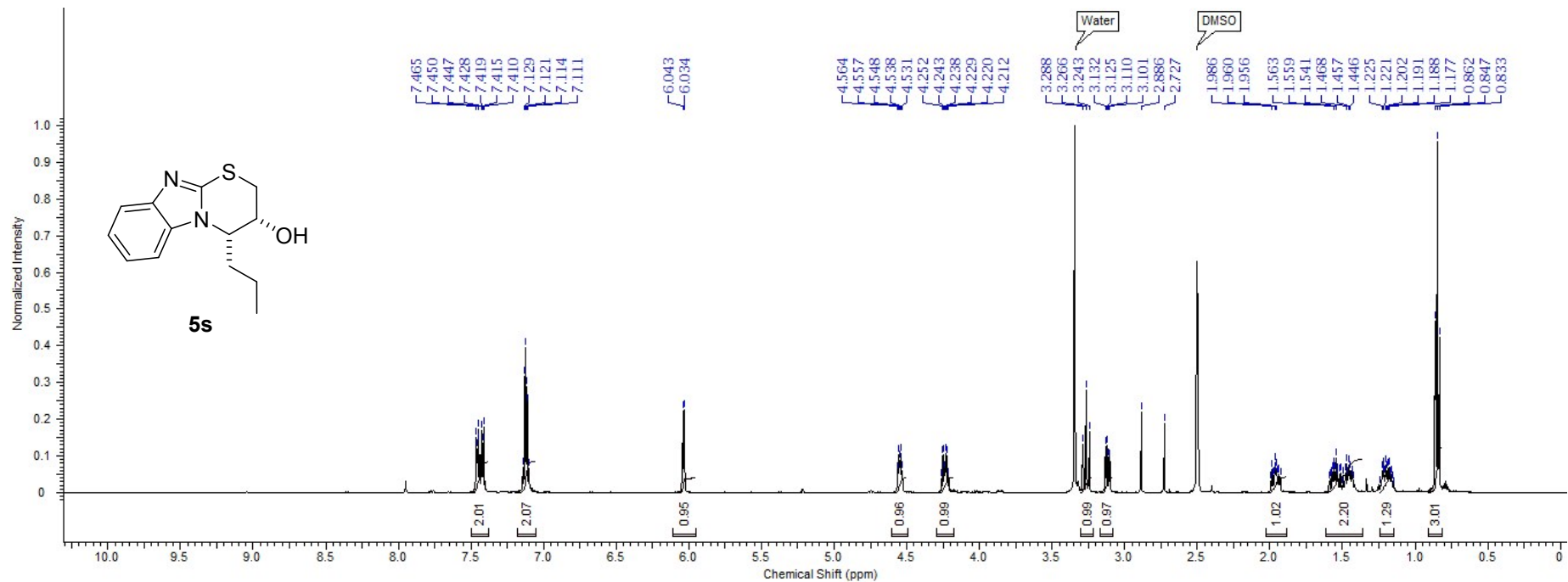
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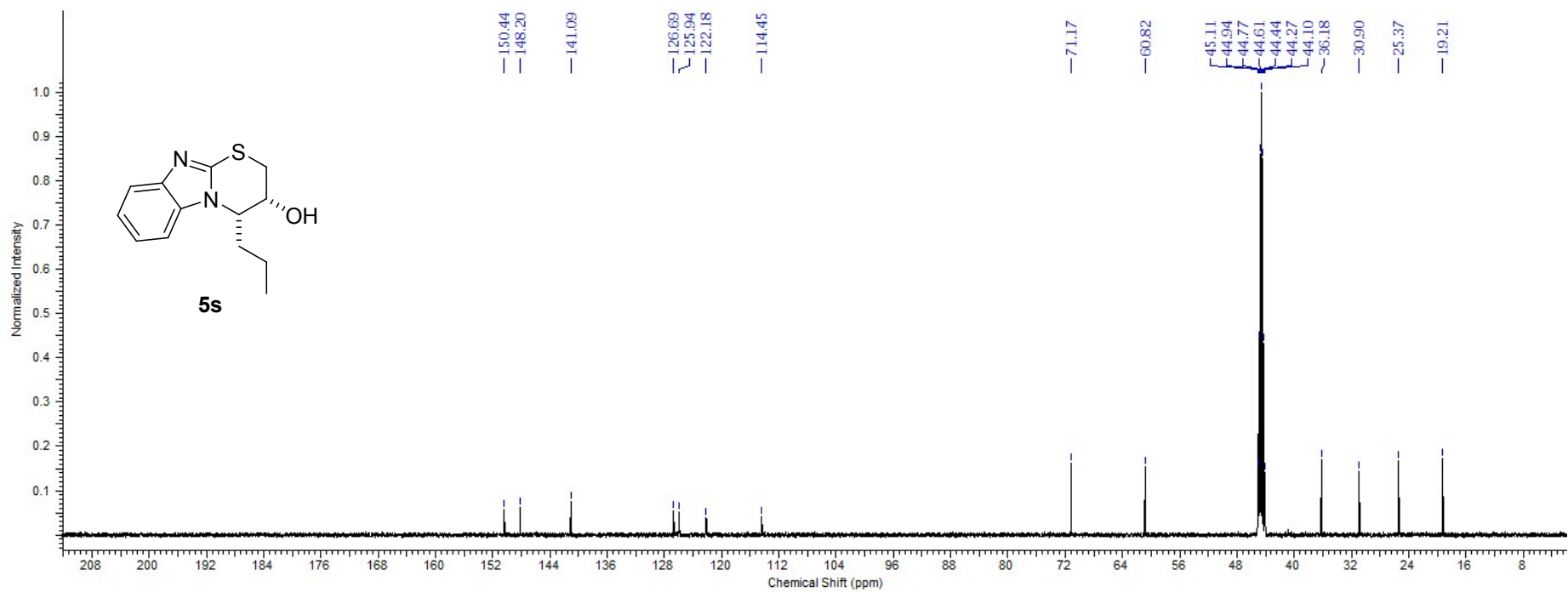
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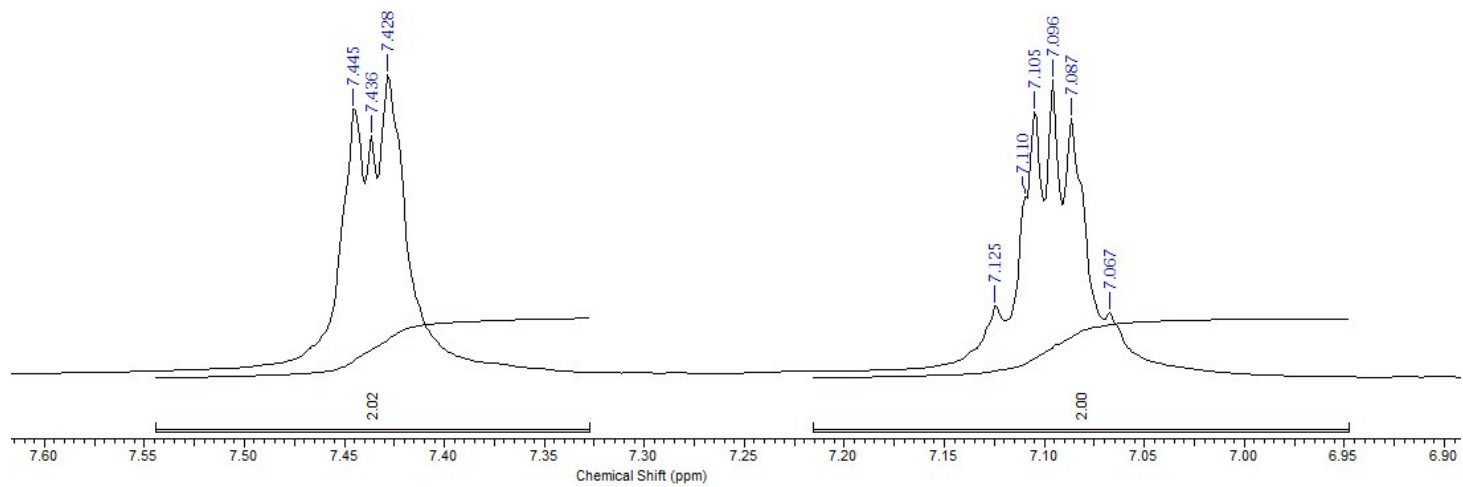
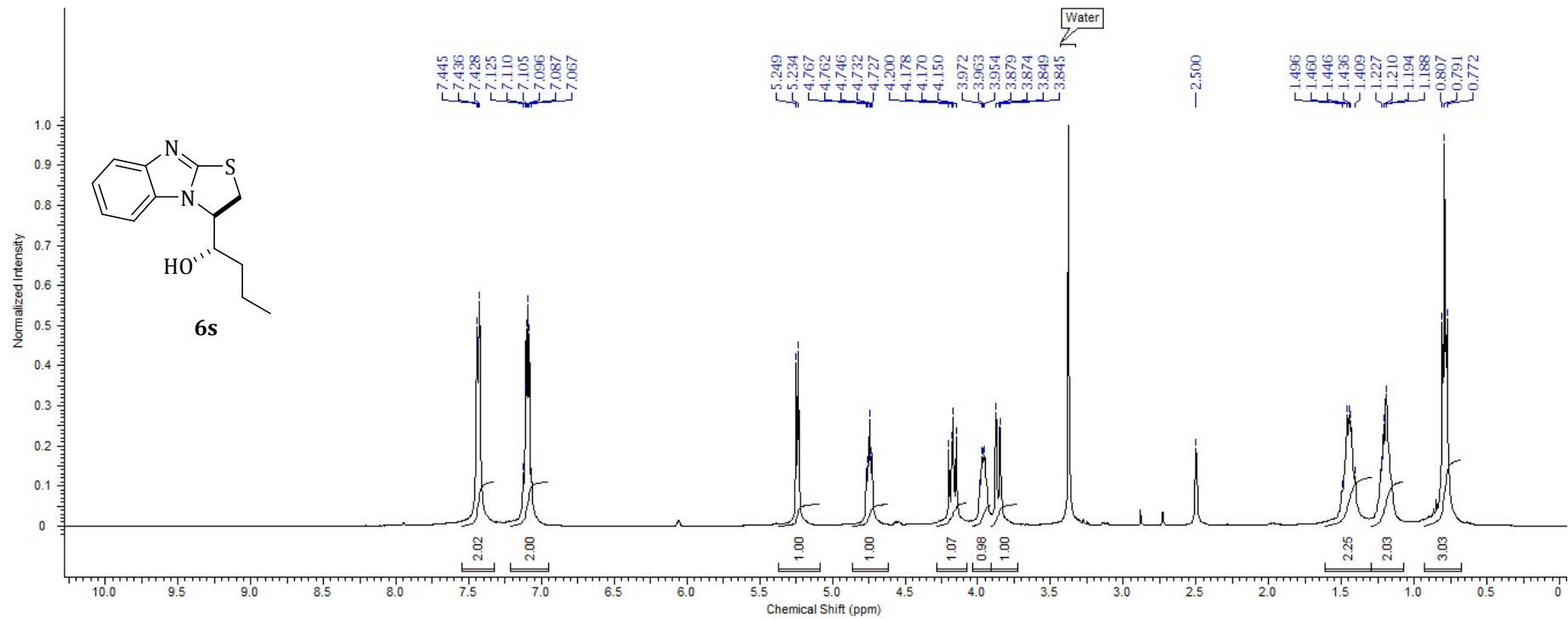
¹³C NMR spectrum (100 MHz, CDCl₃) of 5r



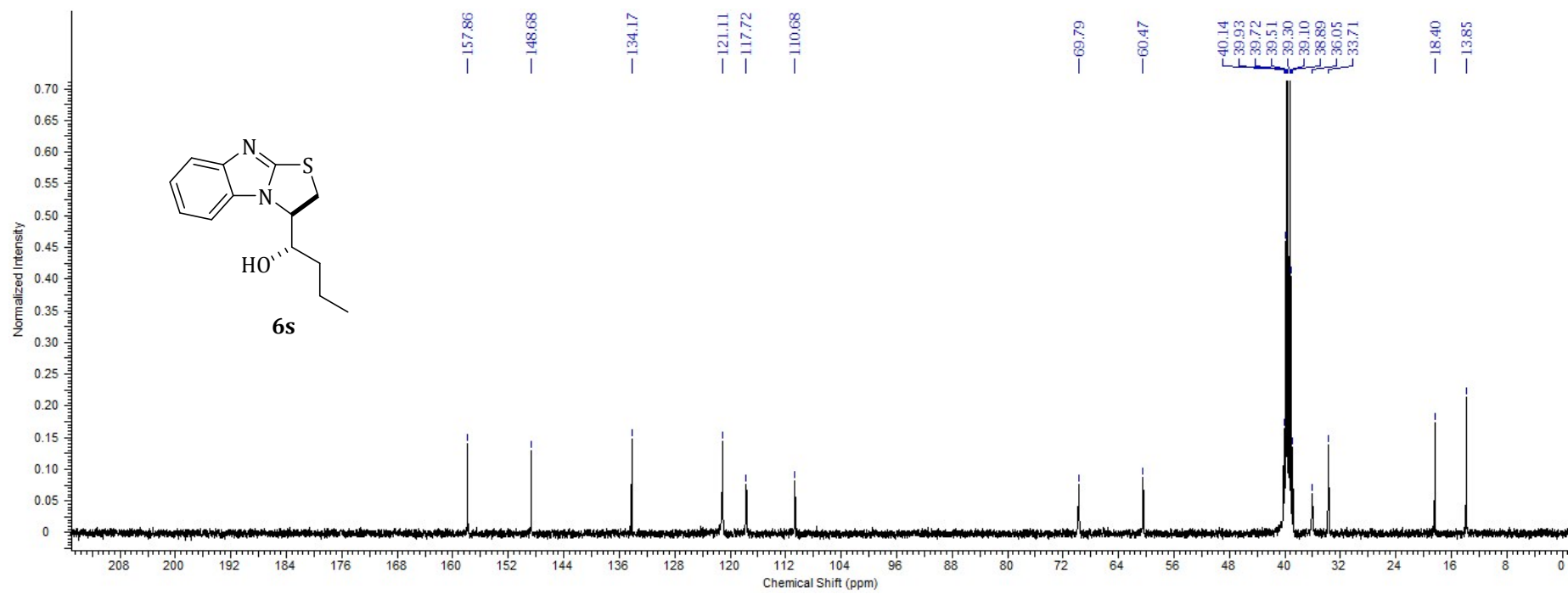
¹H NMR spectrum (400 MHz, DMSO-*d*₆) of 5s

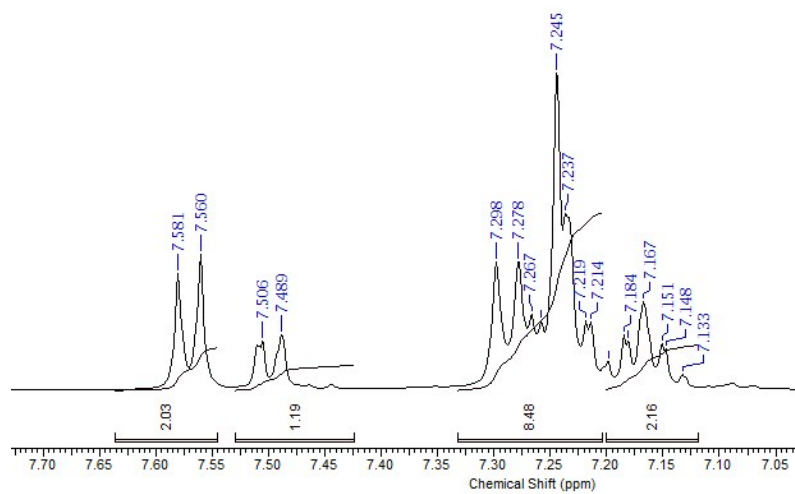
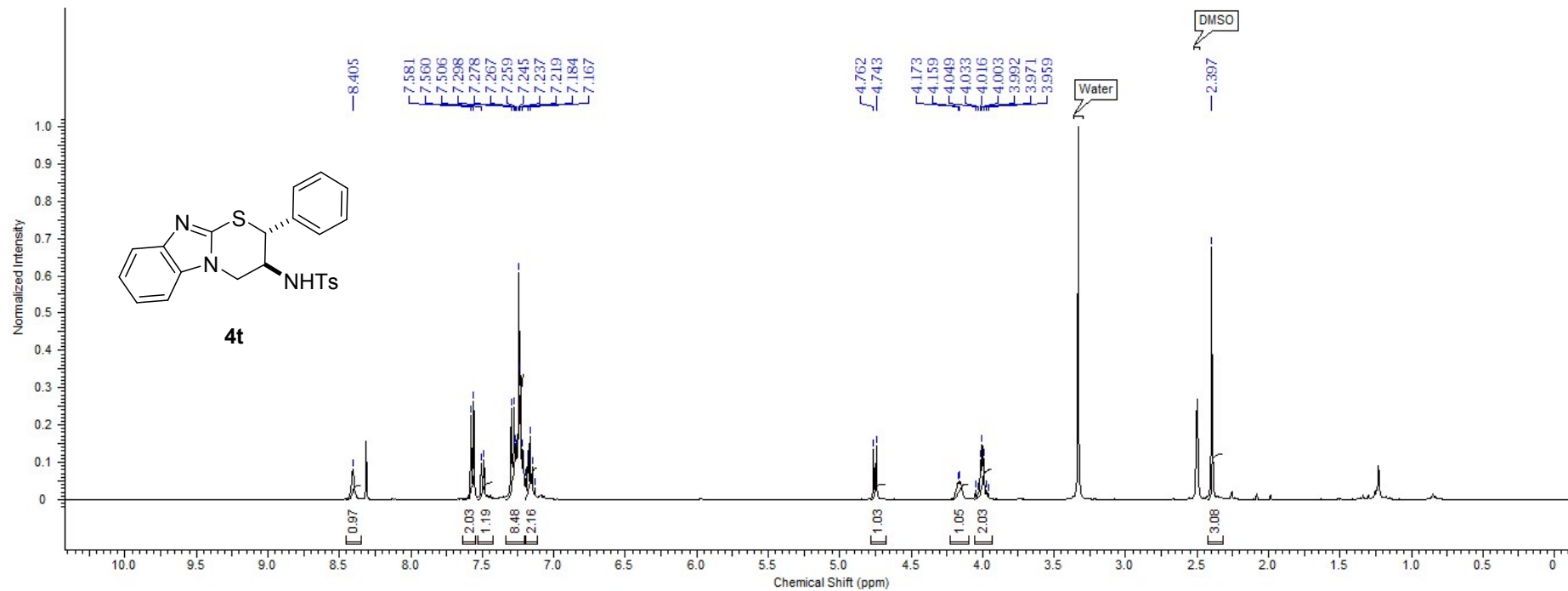


¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of 5s

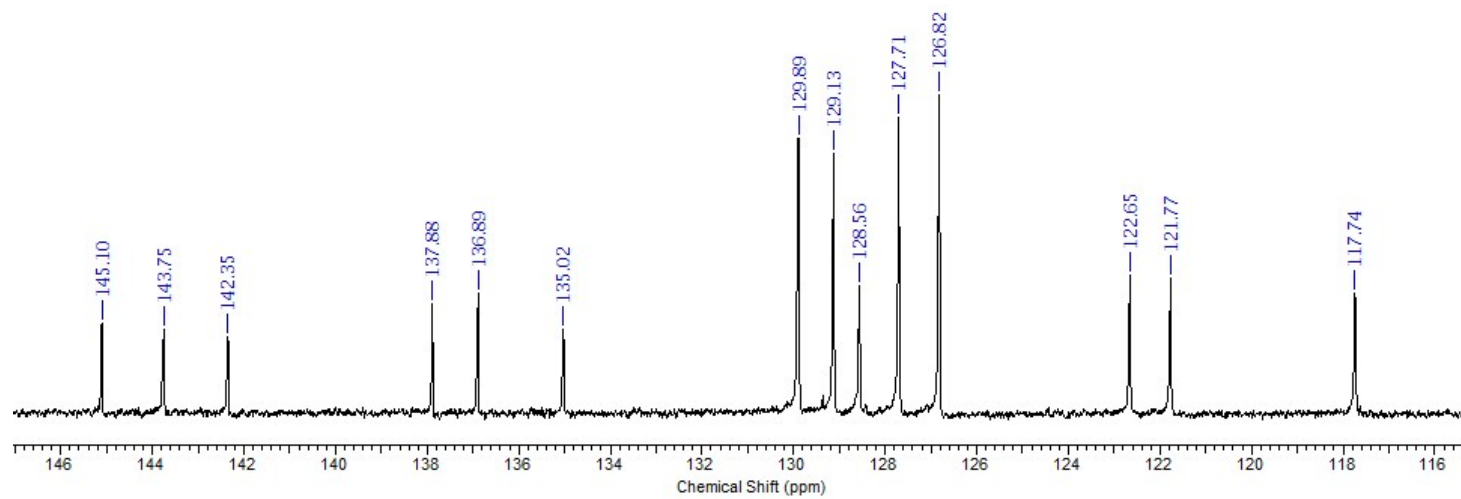
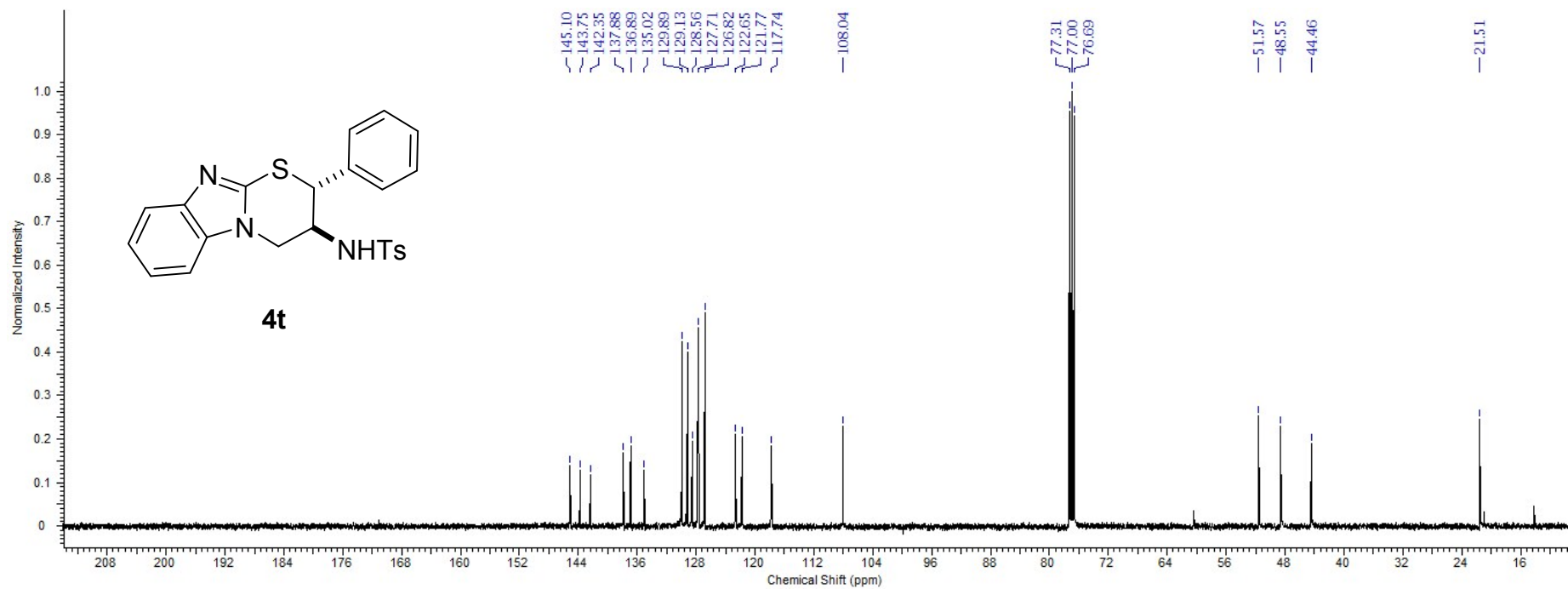


^1H NMR spectrum (400 MHz, $\text{DMSO-}d_6$) of 6s

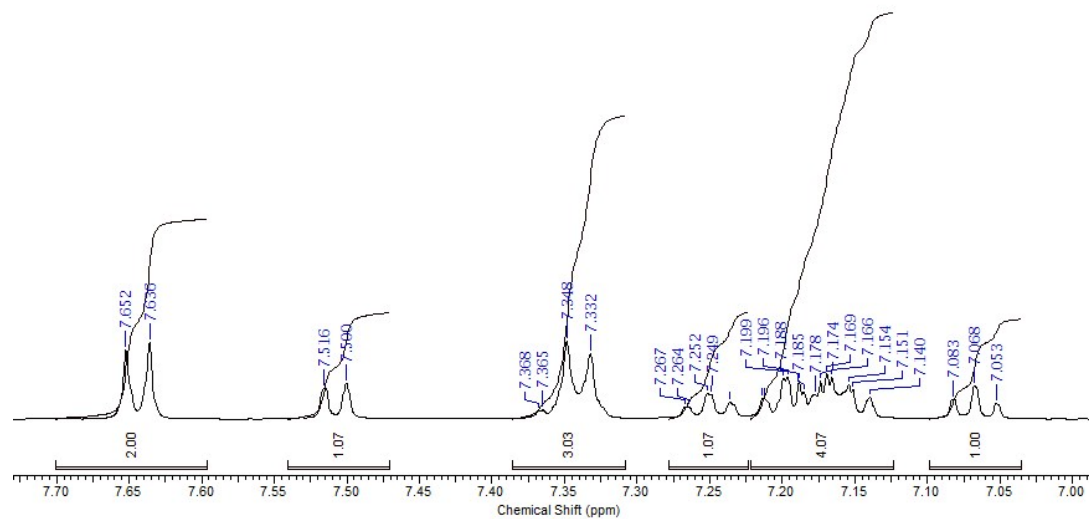
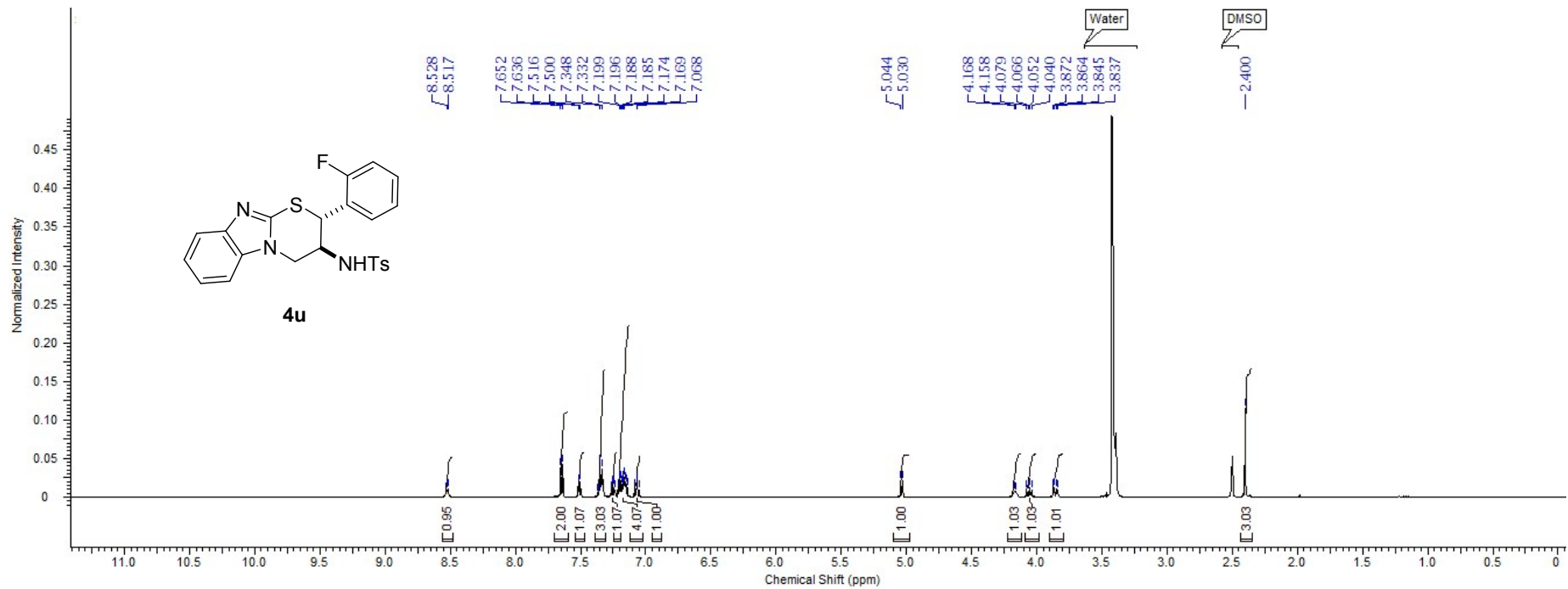




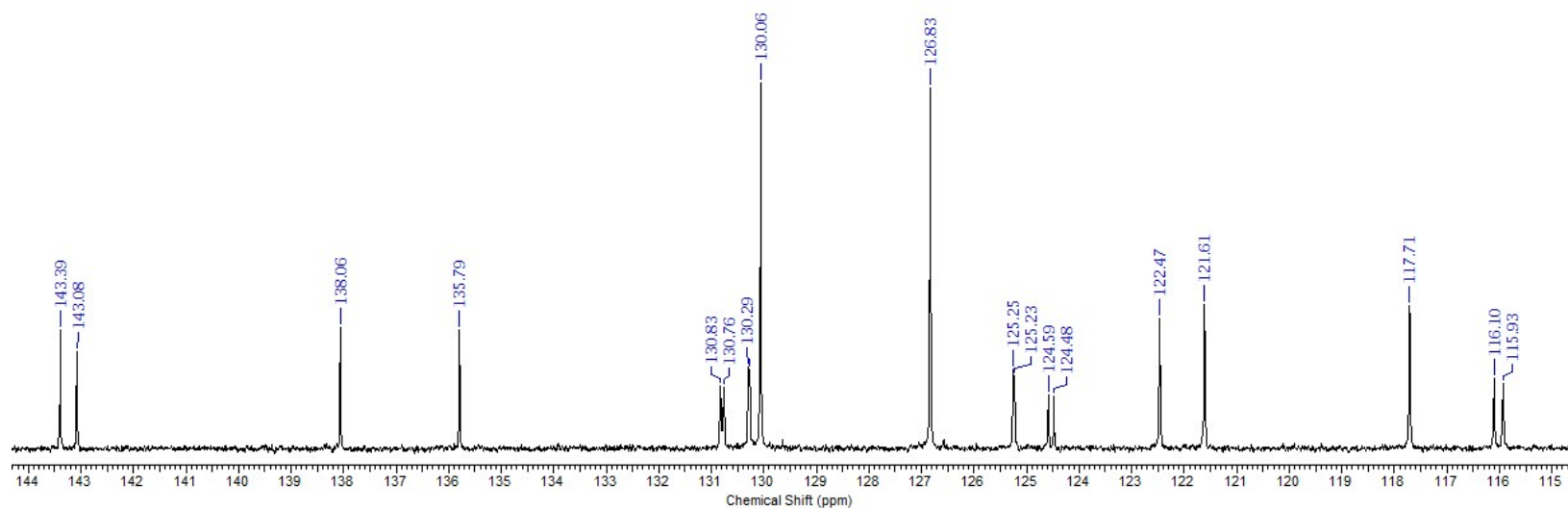
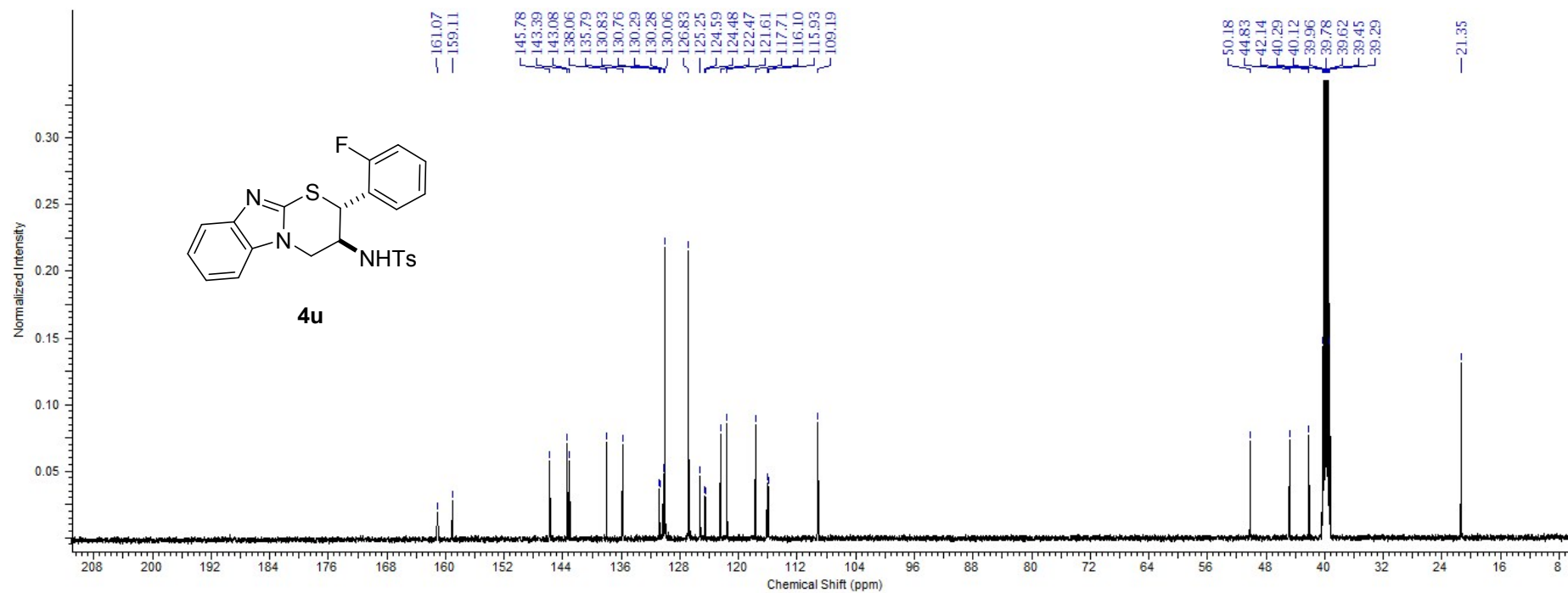
¹H NMR spectrum (400 MHz, DMSO-*d*₆) of 4t



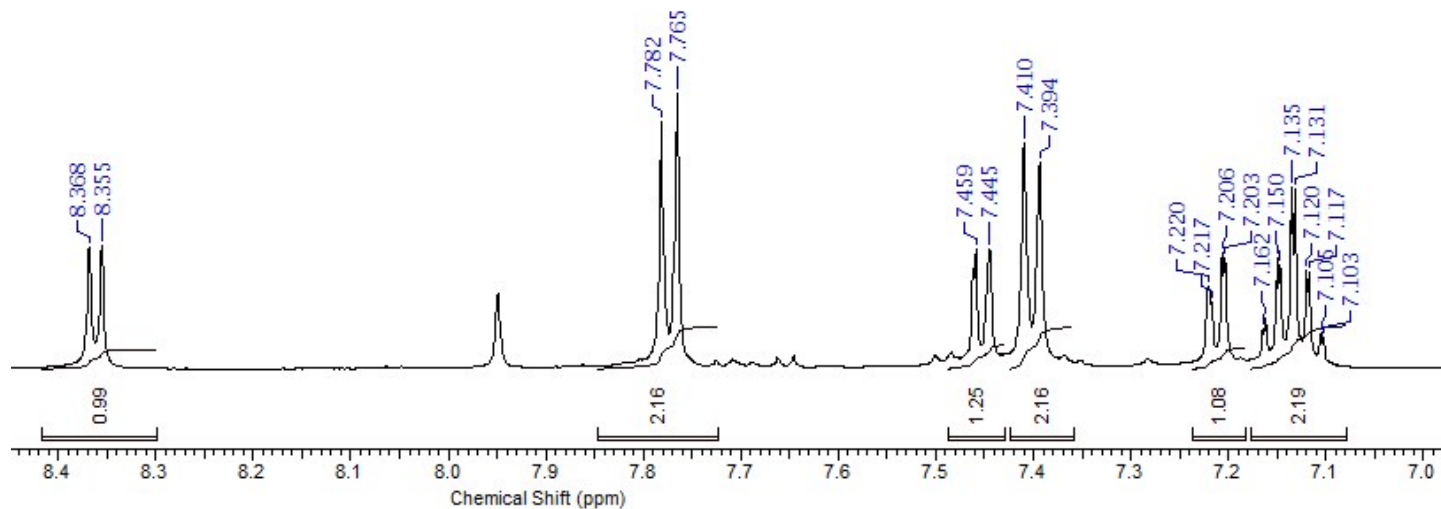
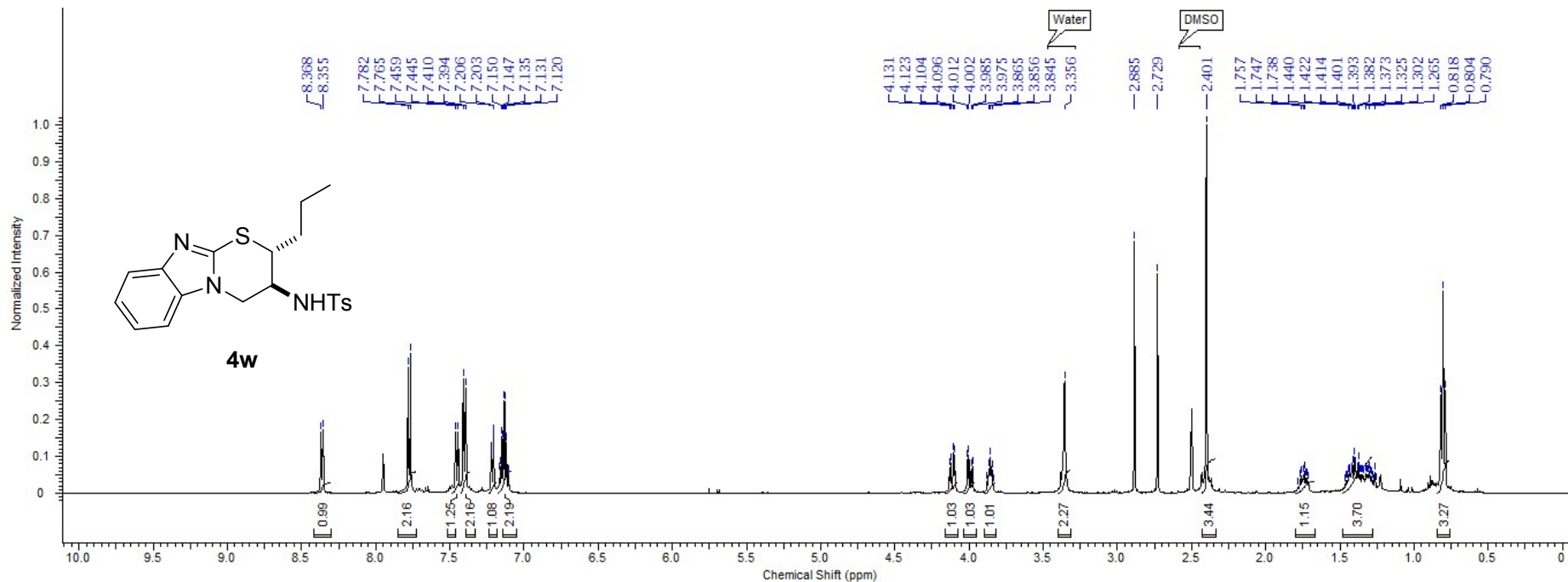
¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of 4t



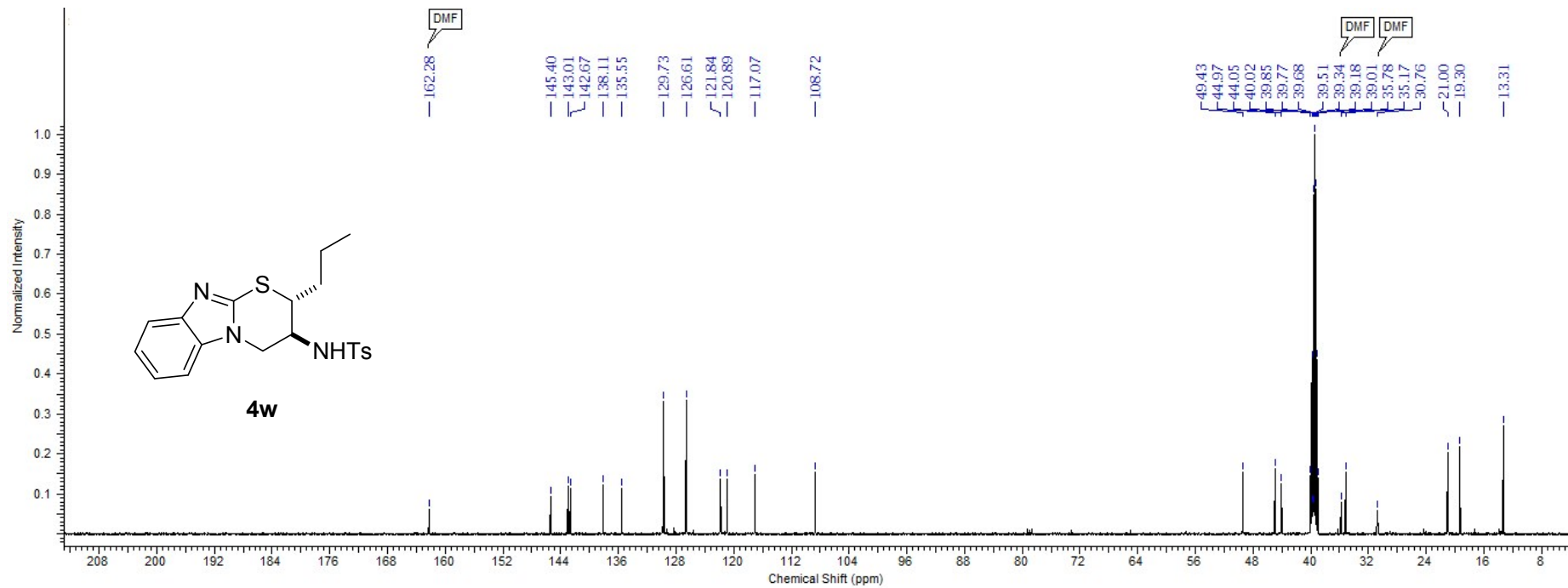
¹H NMR spectrum (400 MHz, DMSO-*d*₆) of 4u



¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of 4u

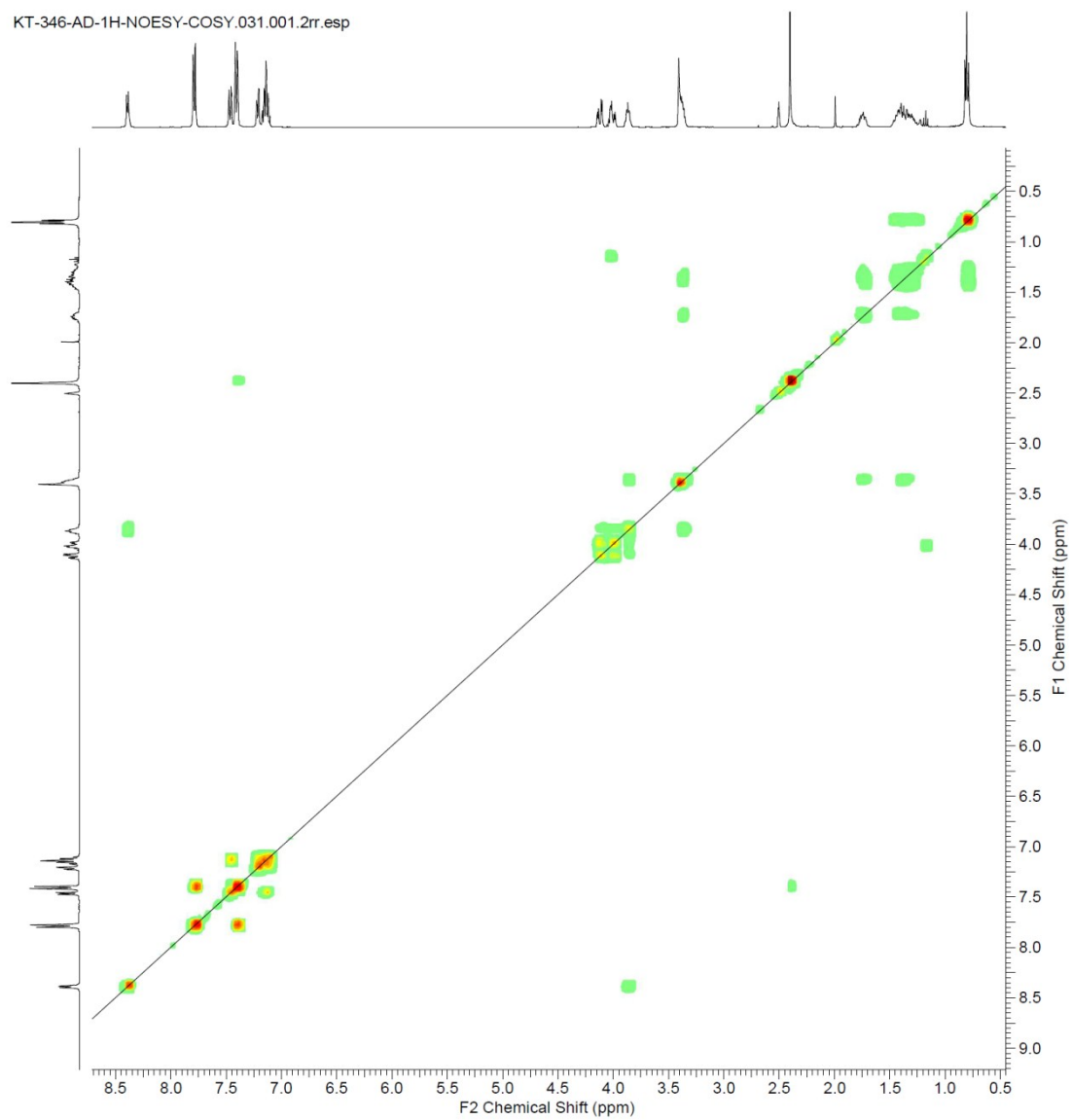


¹H NMR spectrum (400 MHz, DMSO-*d*₆) of 4w



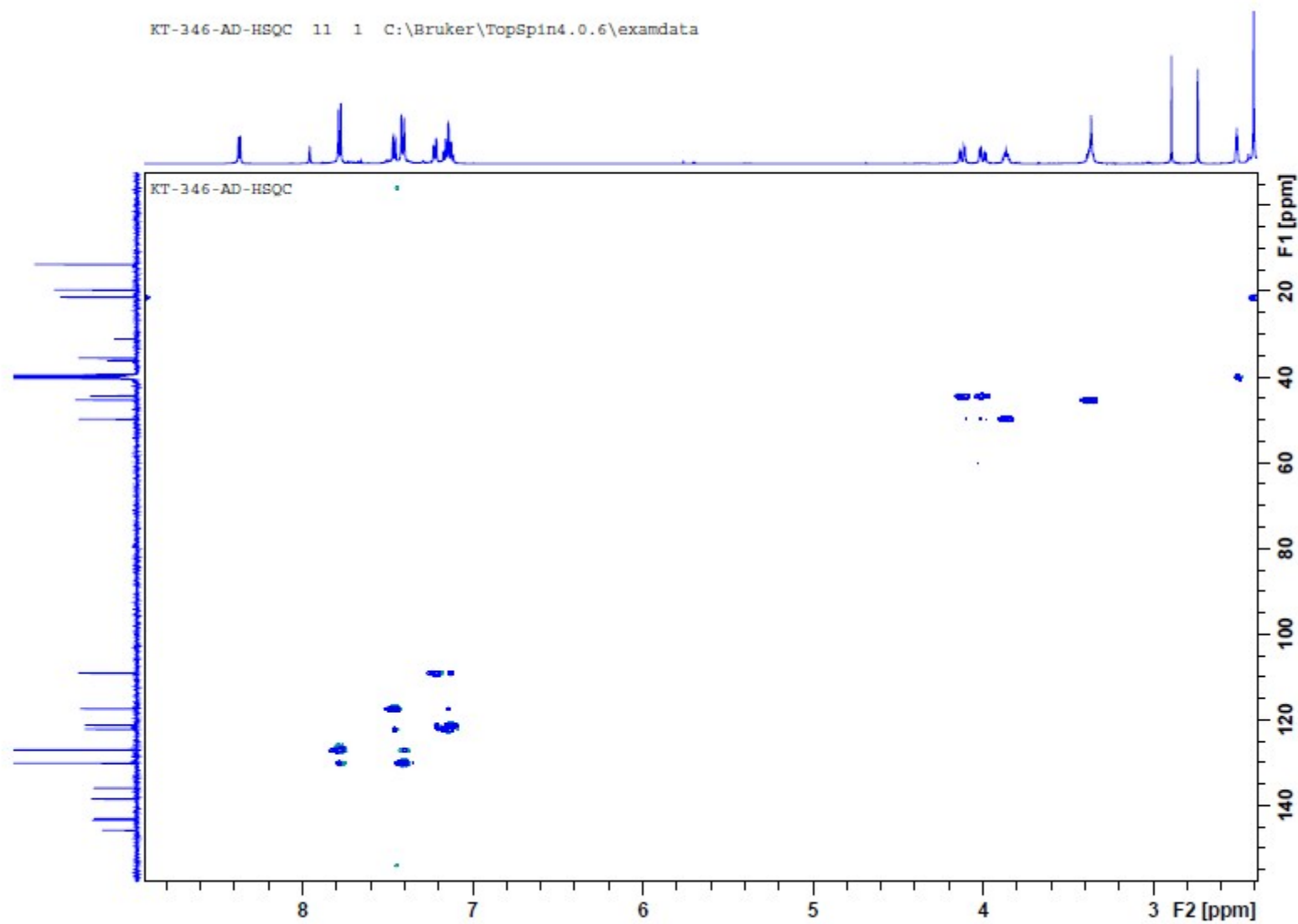
¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of 4w

KT-346-AD-1H-NOESY-COSY.031.001.2rr.esp



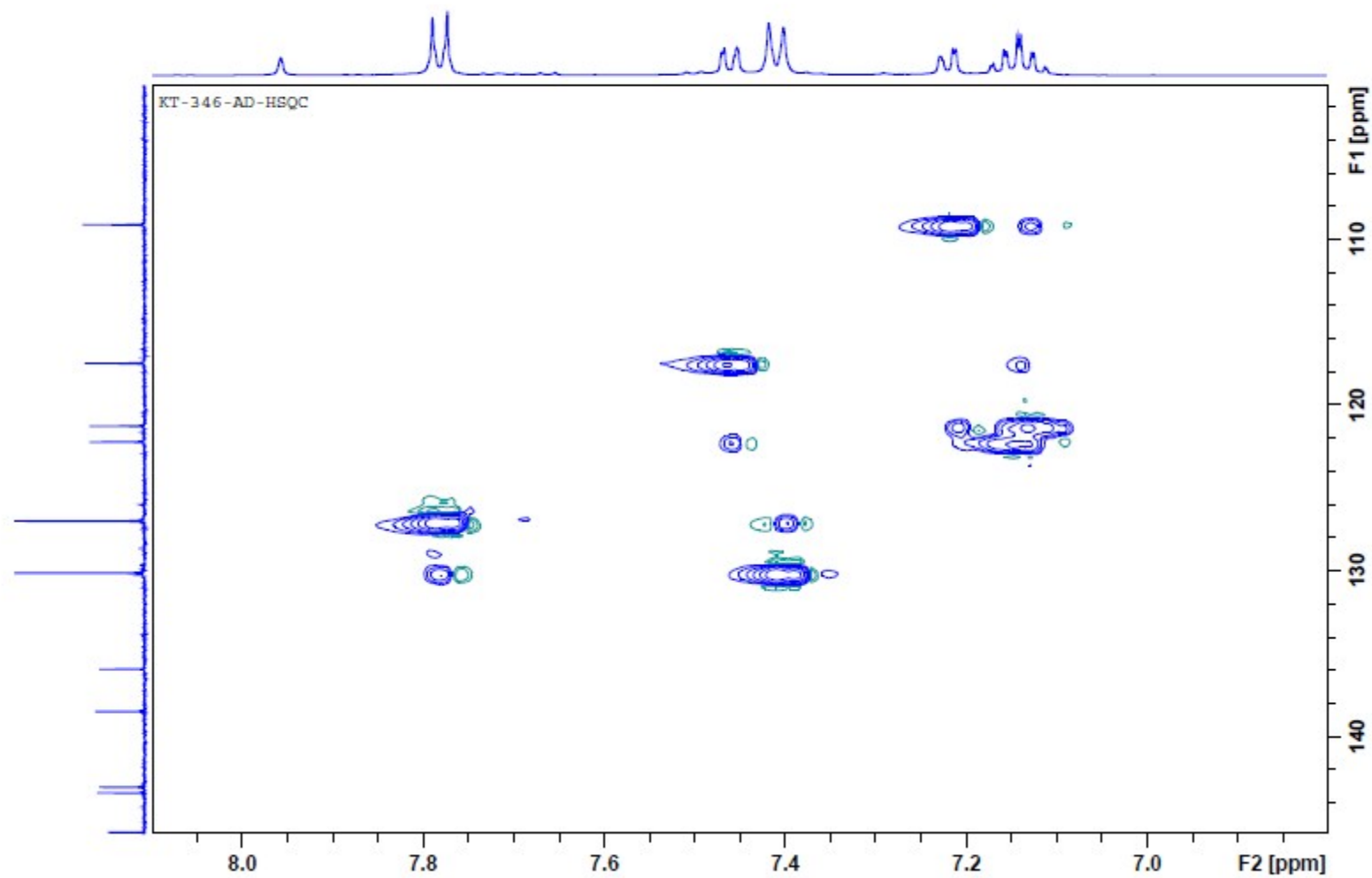
^1H - ^1H COSY spectrum (400 MHz, $\text{DMSO-}d_6$) of 4w

KT-346-AD-HSQC 11 1 C:\Bruker\TopSpin4.0.6\examdata



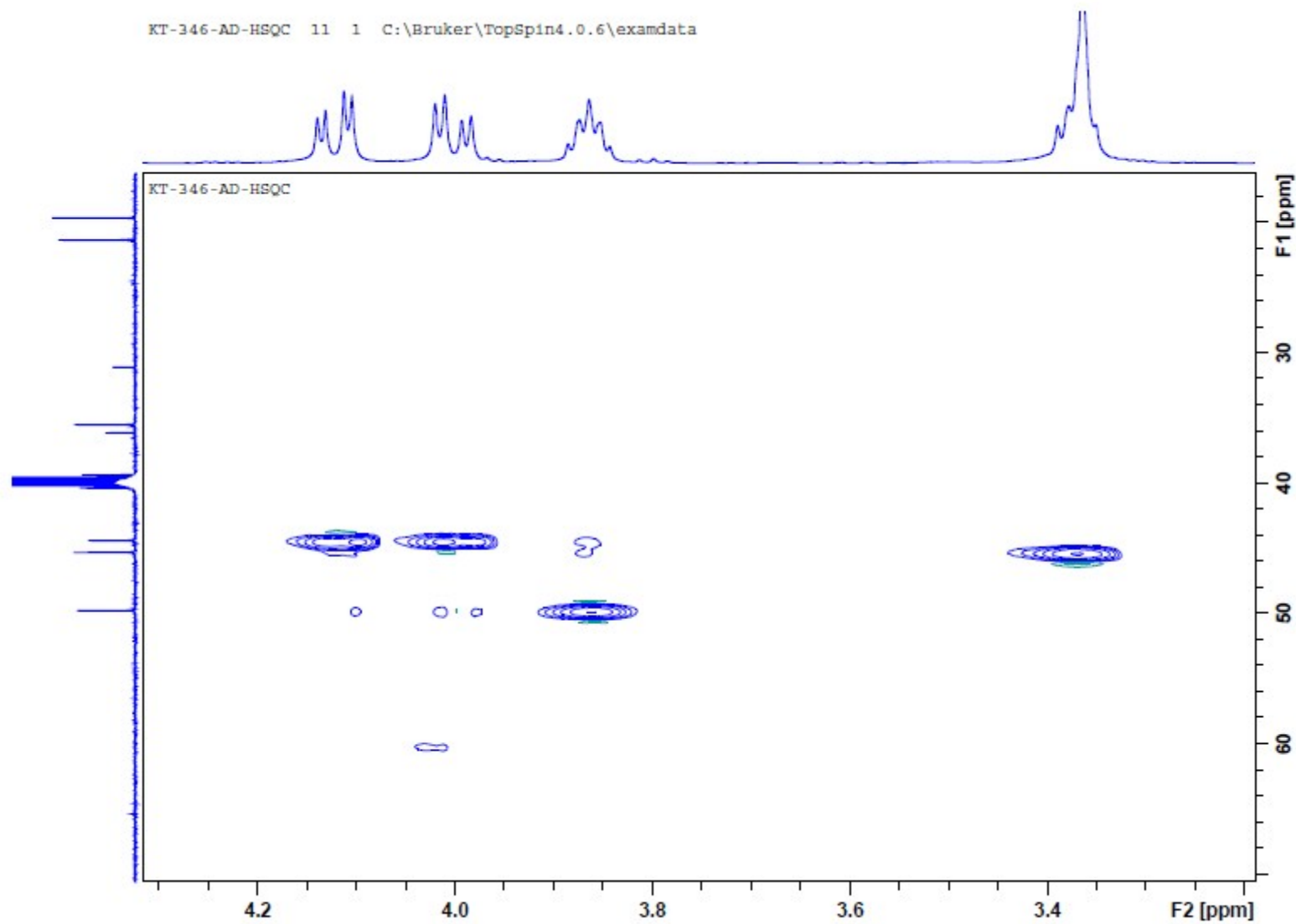
HSQC spectrum (400 MHz, DMSO- d_6) of 4w

KT-346-AD-HSQC 11 1 C:\Bruker\TopSpin4.0.6\examdata

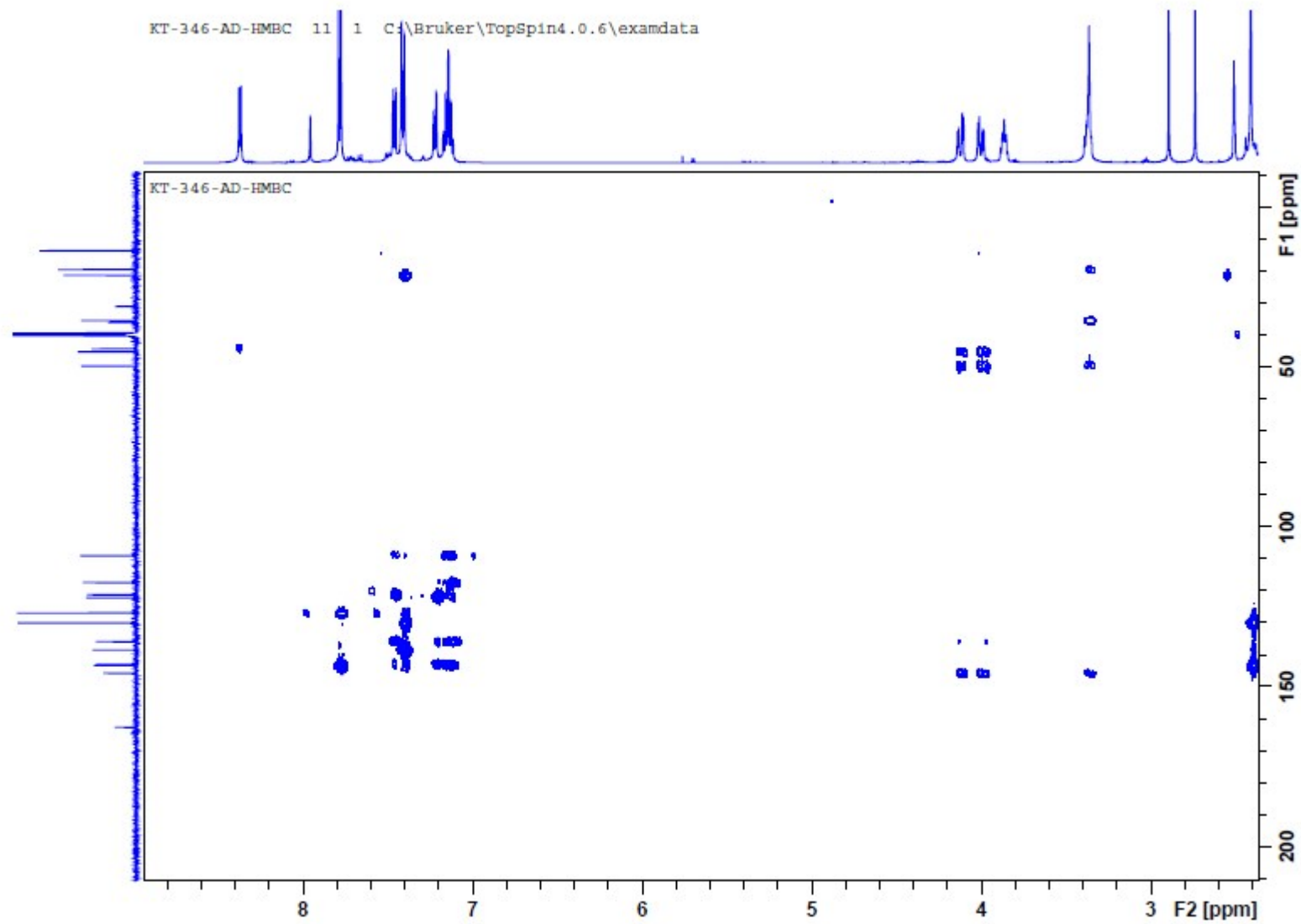


Partial (expanded) HSQC spectrum (400 MHz, DMSO- d_6) of 4w

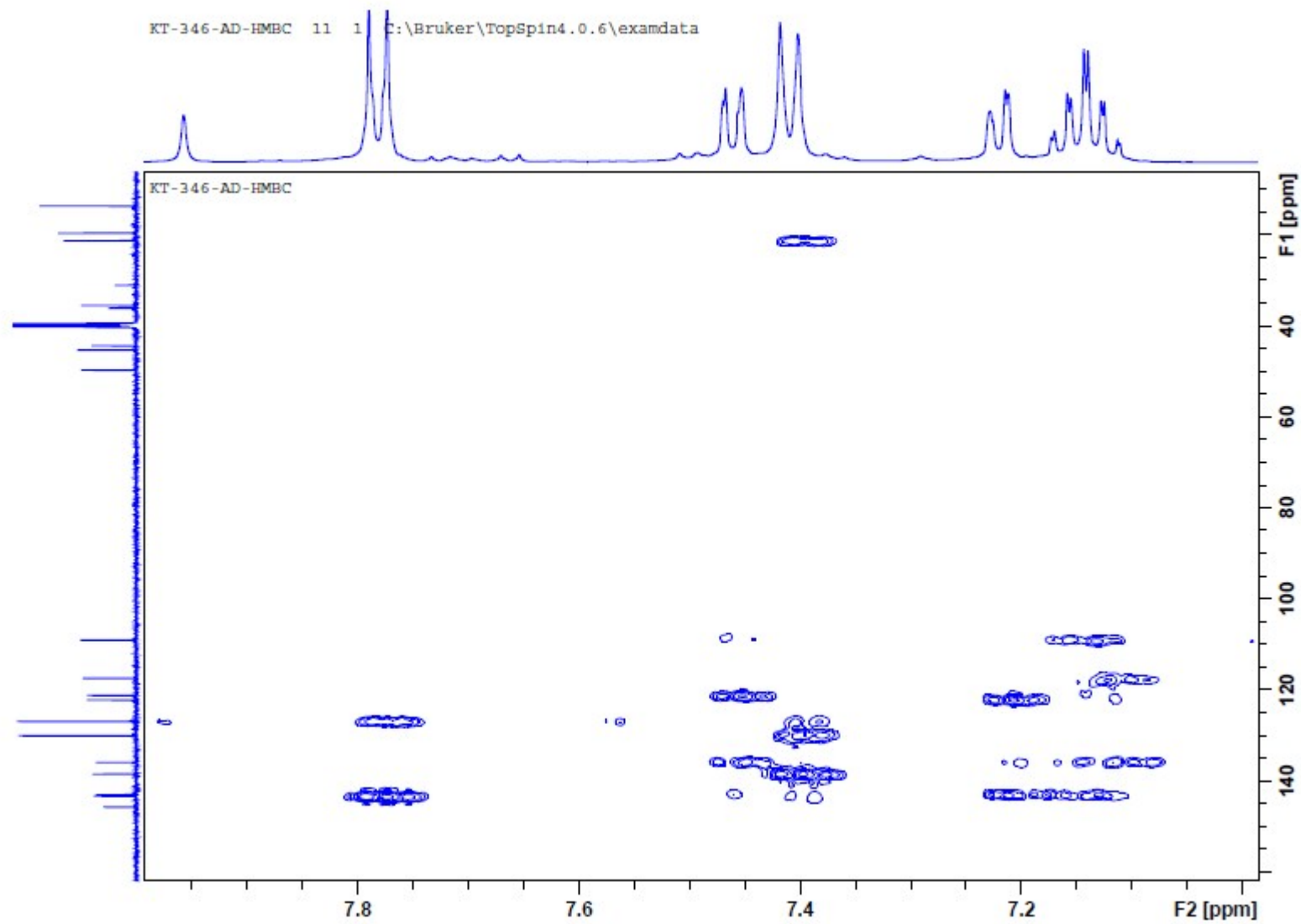
KT-346-AD-HSQC 11 1 C:\Bruker\TopSpin4.0.6\examdata



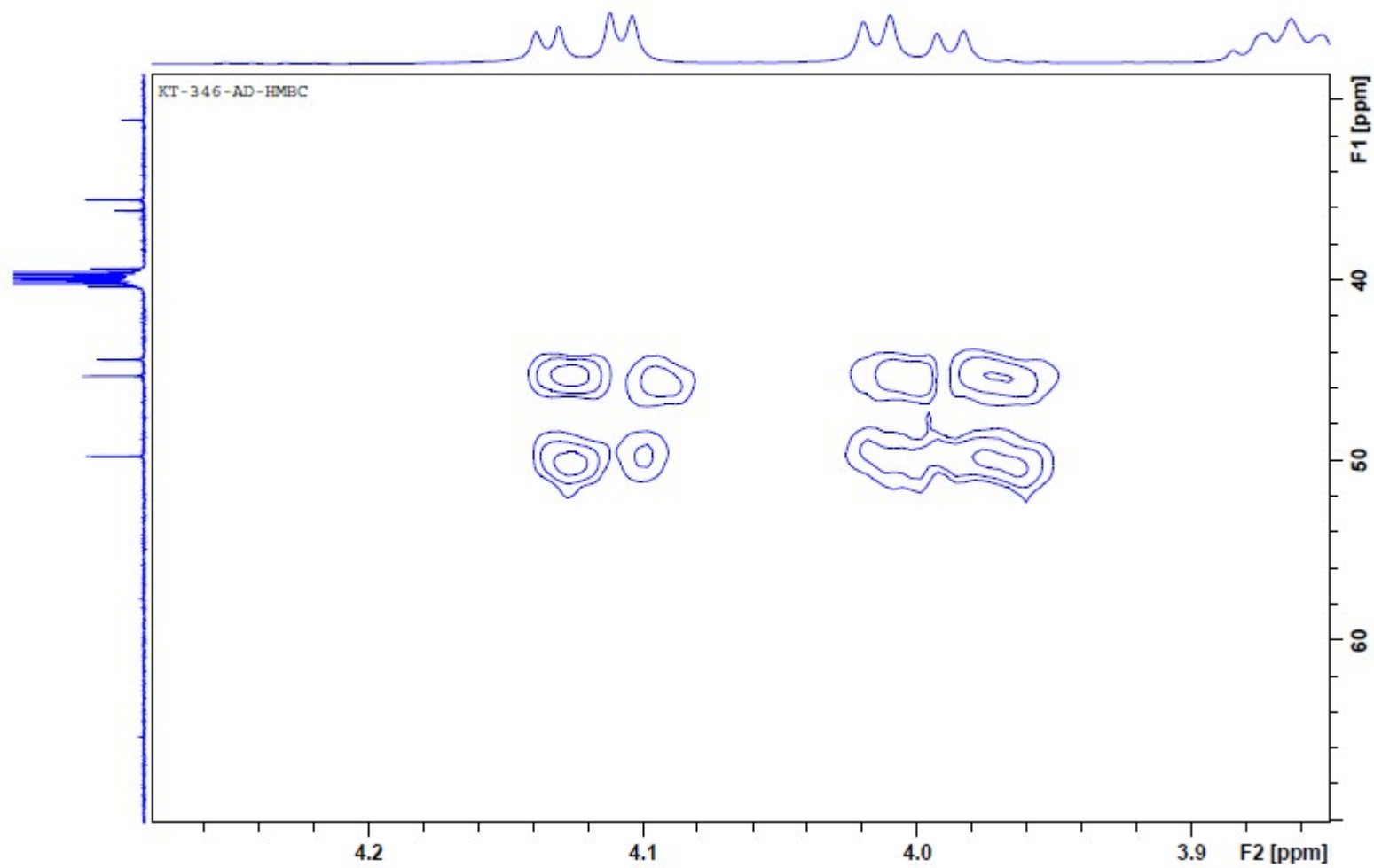
Partial (expanded) HSQC spectrum (400 MHz, DMSO- d_6) of 4w



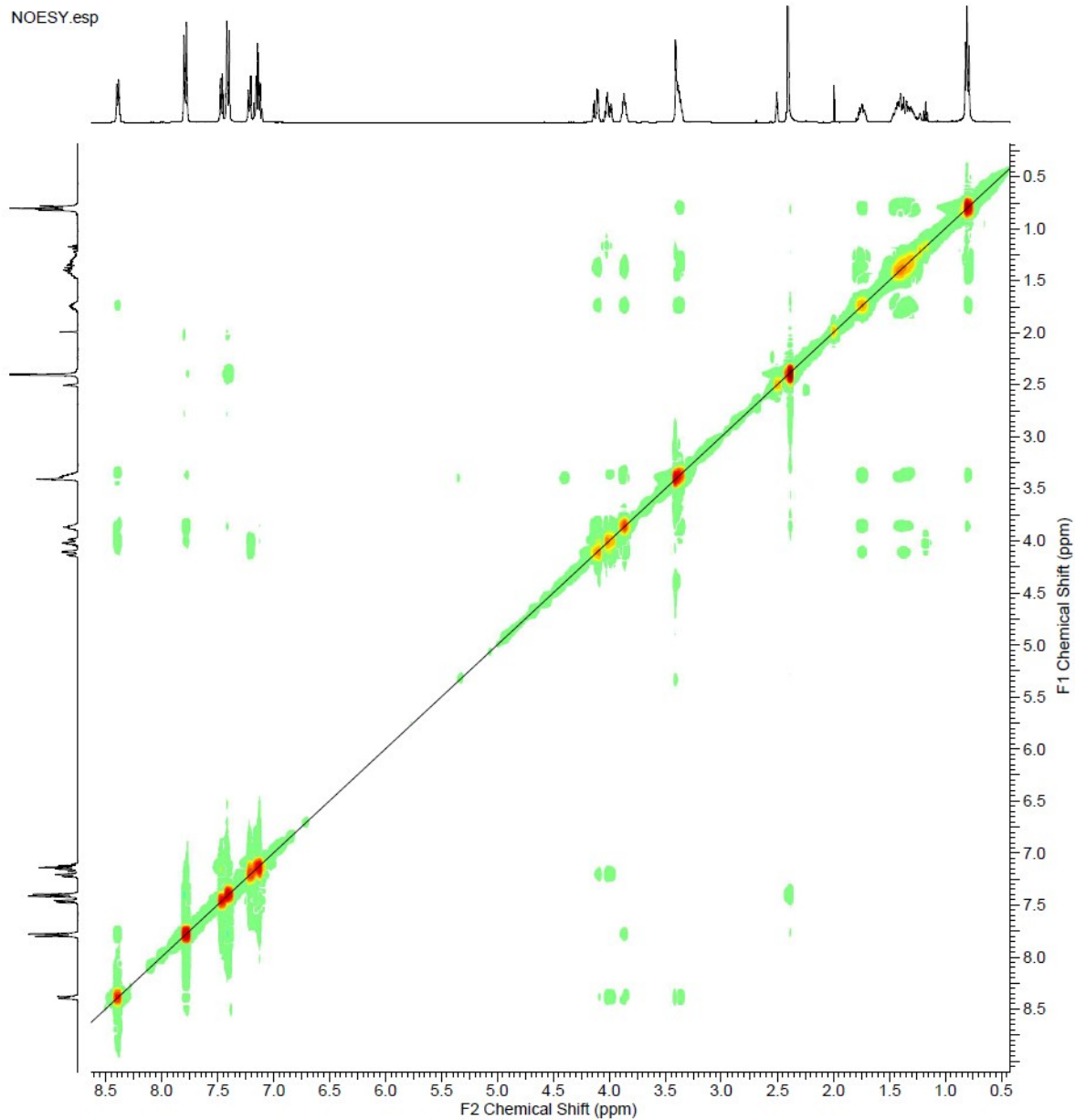
HMBC spectrum (400 MHz, DMSO- d_6) of 4w



Partial (expanded) HMBC spectrum (400 MHz, DMSO- d_6) of 4w



Partial (expanded) HMBC spectrum (400 MHz, DMSO-*d*₆) of 4w



NOESY spectrum (400 MHz, DMSO-*d*₆) of 4w