Supporting Information

for

A green bio-organic catalyst (Taurine) promoted one-pot synthesis of (R/S)-2-thioxo-3,4-dihydropyrimidine(TDHPM)-5-carboxanilides: Chiral investigations using circular dichroism and validates by computational approaches

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1. General Methods

1.1 Experimental techniques

The nomenclature of the synthesized molecules are done according to IUPAC. Also, the numbering in the carbon chain is based on the position of the carbon atom.

All the reactions are performed in an open-air atmosphere. The used glass devices (round bottomed flask) were heated with a temperature of 100 °C. All the solid and liquid reagents and needle are added to the RBF under the open-air atmosphere.

Percentages (%) refers to mass percentage.

The calculated yields refer to the limiting reagent component.

Silicone oil bath is used to record the melting points. The temperature is set and controlled by using an adjustable contact thermometer.

Reagents

All the reagents were purchased from TCI, Sigma-Aldrich, and Sisco Research Pvt. Ltd. and used without further purification. The reaction was performed using the conventional heating method.

Solvents

Solvents from the given companies were used with the corresponding quality grades and used without further purification. The following solvents were used in thin layer chromatography (TLC) and chiral High-performance liquid chromatography: ethyl acetate, n-hexane, methanol, ethanol, diethylamine, dichloromethane.

1.2 Analytical

Thin Layer Chromatography (TLC)

The progress of all chemical reactions was monitored by Thin-layer chromatography. For this purpose, TLC, on aluminium plates pre-coated with F252 silica gel 60 by Merck were used as the stationary phase. TLC plates were analyzed under Visible light (λ =400 nm to 750 nm).

Nuclear Magnetic Resonance (NMR) Spectroscopy

NMR Spectra ^{1}H NMR & ^{13}C NMR were recorded on the instruments *Brucker* Avance Neo 500 MHz FT-NMR and *JEOL* JNM-ECX500II (delta) spectrometer having proton noise decoupling mode with a standard 5 mm probe. The chemical shift values are given in δ (ppm) and the coupling constant (*J*) is provided in Hertz. For the solvent, deuterated DMSO-d_6, the signal of solvents was used in the ^{1}H NMR spectra (δ = 2.52 ppm) and ^{13}C NMR spectra (δ = 39 ppm) as an internal standard for calibration. The spectra were viewed by utilizing the MestReNova software. The following abbreviations were used for the clear assignment of the signals and for the spin multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, dd = double of doublet, td = triplet of doublet, m = multiplet.

Mass Spectrometry

Mass spectra were recorded using HRMS analysis.

Melting Points

Melting points of the synthesized solid products **4(a-w)** were recorded using open capillary method and are uncorrected.

Chiral HPLC

Normal-phase chiral HPLC analysis was performed on an Agilent 1260 Infinity II HPLC system, which equipped 1260 Quat pump VL pumps, 1260 Vial sampler automated sample injector, 1260 MCT column oven, 1260 DAD WR photodiode array (PDA) detector. Data were collected and processed by the Agilent Open Lab CDS Normal-phase chiral HPLC analysis was performed.

Circular Dichroism

Circular Dichroism spectra were recorded using Circular Dichroism Spectrometer instrument (model: J 815 (Jasco)). The wavelength (λ) was measured in the range of 190 nm to 400 nm. Dimethyl sulfoxide was used as an internal standard for the calibration of the instrument. The spectra were viewed using *Origin 2022 64Bit* software. The spectra of the individual isomer were obtained by direct subtraction from the calibrated spectra.

Crystallization

For the sample preparation, 50 mg of **4s** was dissolved in 60 ml of ethyl acetate: methanol (7:3) and heated until **4s** dissolved completely and the solution was reduced to half (30 ml), followed by 50 mg of activated charcoal was added to eradicate coloured impurities from the compound. After filtering out the content, the charcoal treatment solution was kept in a clean beaker covered with aluminium foil for a few days. When the ethyl acetate and methanol were evaporated, a single crystal of compound **4s** formed over the course of 10-15 days.

2. Materials and Methods

2.1 General Procedures for synthesis of 2-thio-3,4-DHPM-5-carboxanilides 4(a-w)

A mixture of diverse aryl aldehyde **1** (2 mmol), thiourea **2** (3 mmol), and diversely substituted acetoacetanilide **3** (2 mmol) in 1 mL ethanol were heated (charged) at 100 °C. After half an hour, yellowish-white solid falls out. Thereafter, 2 mL ethanol was further added to the reaction mixture and heating was continued up to 3 h. The progress of the reaction was monitored on TLC using ^{n}Hexane: ethyl acetate (7:3, V/V) as the mobile phase. As all the starting materials were consumed completely, the reaction mixture was cooled to room temperature and then 3 mL water was poured into it. The crude product **4(a-w)** was then filtered through the Büchner funnel and then dried. No further purification was required.

2.2 General Procedure for the separation of the racemic mixture of 4(a-w)

Accurately weighed 0.5 mg/mL of racemic mixture of sample. The product was not very soluble in n-Hexane/Ethanol and several precipitated in HPLC sample vials. Making a homogeneous sample solution is important for accurate determination of enantiomeric ratio. To a vial containing sample a minimal amount of DCM (30%) was added until the solution became homogeneous. Then Ethanol (70%) was added.

2.2.1 Isolation of enantiomers using Prep LC

1) **Racemic mixture of 4a:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (60:40:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 215 nm. The column temperature was Ambient.
2) **Racemic mixture of 4b:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (60:40:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 312 nm. The column temperature was Ambient.
3) **Racemic mixture of 4c:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (60:40:0.1%) under normal-phase conditions. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 312 nm. The column temperature was Ambient.
4) **Racemic mixture of 4d:** Enantiomers were separated on YMC Chiral ART Cellulose-SC (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3,5-dichlorophenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (70:30:0.1%) under normal-phase conditions. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 254 nm. The column temperature was Ambient.
5) **Racemic mixture of 4e:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (60:40:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 312 nm. The column temperature was Ambient.
6) **Racemic mixture of 4f:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: IPA: Diethylamine (70:30:0.1%) under normal-phase conditions. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 312 nm. The column temperature was Ambient.
7) **Racemic mixture of 4g:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (80:20:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 312 nm. The column temperature was Ambient.

8) **Racemic mixture of 4h:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (60:40:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 312 nm. The column temperature was Ambient.
9) **Racemic mixture of 4i:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separation were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (80:20:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 312 nm. The column temperature was Ambient.
10) **Racemic mixture of 4j:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethyl amine (60:40:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 312 nm. The column temperature was Ambient.
11) **Racemic mixture of 4k:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (80:20:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 312 nm. The column temperature was Ambient.
12) **Racemic mixture of 4l:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (80:20:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 342 nm. The column temperature was ambient.
13) **Racemic mixture of 4m:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (30:70:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength of 312 nm. The column temperature was Ambient.
14) **Racemic mixture of 4n:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (70:30:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength of 312 nm. The column temperature was Ambient.
15) **Racemic mixture of 4o:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate) under

normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (60:40:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 312 nm. The column temperature was Ambient.

16) **Racemic mixture of 4p:** Enantiomers were separated on YMC Chiral Art Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)]under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (60:40:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 312 nm. The column temperature was Ambient.
17) **Racemic mixture of 4q:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (60:40:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 312 nm. The column temperature was Ambient.
18) **Racemic mixture of 4r:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (80:20:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength of 312 nm. The column temperature was Ambient.
19) **Racemic mixture of 4s:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (80:20:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 312 nm. The column temperature was Ambient.
20) **Racemic mixture of 4t:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (80:20:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 312 nm. The column temperature was Ambient.
21) **Racemic mixture of 4u:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (80:20:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 312 nm. The column temperature was Ambient.
22) **Racemic mixture of 4v:** Enantiomers were separated on YMC Chiral ART Cellulose-SB (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3,5-dimethylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: Ethanol: Diethylamine (80:20:0.1%) under normal-phase

condition. In run, 10 µL of the sample was injected and the flow rate was 21.0 mL/min with the detection wavelength at 312 nm. The column temperature was Ambient.

23) **Racemic mixture of 4w:** Enantiomers were separated on YMC Chiral ART Cellulose-SZ (4.6×250 mm), 5.0 µm, [Cellulose-tris-(3-chloro-4-methylphenylcarbamate)] under normal-phase conditions. Separations were conducted using an isocratic elution with solvent mixture of n-Hexane: IPA: Diethylamine (70:30:0.1%) under normal-phase condition. In run, 10 µL of the sample was injected and the flow rate was 1.0 mL/min with the detection wavelength at 312 nm. The column temperature was Ambient.

2.3 General procedure for Electronic Circular Dichroism (ECD)

With respect to the concentration particulars, the primary stock solution was made by preparing a 500 µM solution of all the precisely weighed synthesized compounds **4(a-w)** in 4 mL of dimethyl sulfoxide (DMSO) in the prescribed Eppendorf. To calibrate the instrument, dimethyl sulphoxide (DMSO) was used as an internal standard. For the purpose of analysis from the aforementioned primary stock solution, 3 mL sample solution was added to the cuvette and then put it inside the CD spectrometer to measure the spectra. The calibrated solvent was subtracted from the spectra, which were measured in the range of 190 to 400 nm.

3 Analytical data of the synthesized 4 (a-w)

3.1 *N*-(2-chlorophenyl)-4(*R*/*S*)-(4-hydroxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxanilide (**4a**)

Off-White solid (0.344 mg, 92%); MP: 218-222 °C; TLC: R_f = 0.86 [(7:3)EtOAc: n-Hexane];
^{1}H NMR (500 MHz, DMSO-d_6) δ: 9.96 (s, 1H, NH), 9.43 (s, 1H, NH), 9.38 (s, 1H, NH), 9.13 (s, 1H, OH), 7.49 (dd, *J* = 5 Hz, 1H, Ar-H) , 7.44 (dd, *J* = 5Hz, 1H, Ar-H), 7.28 (dt, *J* = 5 Hz, 1H, Ar-H), 7.17 (dt, *J* = 5 Hz, 1H, Ar-H) , 7.13 (d, J = 10 Hz), 5.28 (s, 1H, Chiral H) , 2.18 (s, 3H, CH_3);
^{13}C NMR (126 MHz, DMSO-d_6) δ: 173.42 (C=S), 164.83 (C=O), 156.94 (=C-NH), 136.80 (C-OH), 134.76, 133.04 (C-NH), 129.21, 127.90, 127.42, 127.14, 126.50 (C-Cl) , 126.33, 115.08, 105.98 (-C=), 54.44 (Chiral-C), 16.50 (-CH_3);
HRMS (ESI-TOF) *m*/*z* found for $C_{18}H_{16}ClN_3O_2S$: 374.0767 $[M+H]^+$

3.2 *N*-(2-chlorophenyl)-4(*R*/*S*)-(4-hydroxy-3-methoxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4b**)

Light yellow solid (0.376 mg, 93%); MP: 174-176 °C; TLC: R_f = 0.83 [(7:3)EtOAc: n-Hexane];
^{1}H NMR (500 MHz, DMSO-d_6) δ: 9.58 (s, 1H, NH), 8.99 (s, 1H, OH), 8.91 (s, 1H, NH), 8.76 (s, 1H, NH), 8.73 (s, 1H, Ar-H), 7.09 (dt, 2.5 Hz and 12.5 Hz), 7.05 (t, J = 6 Hz, 1H, Ar-H), 6.90-6.84 (m, 1H, Ar-H), 6.80-6.72 (m, 1H, Ar-H), 6.47 (d, J = 17 Hz, 1H, Ar-H), 6.34 (t, J = 6 Hz, 1H, Ar-H), 4.90 (s, 1H, Chiral-H), 3.33 (s, 3H, CH_3), 1.78 (s, 3H, CH_3);
13C NMR (126 MHz,) δ: 174.00 (C=S), 166.77 (C=O), 165.37 (=C-NH), 147.80 (C-OH), 146.67, 135.27 (C-NH), 133.97, 129.74, 127.67, 127.00, 124.85, 119.41, 115.79, 111.58, 106.33, 81.51, 55.91 (-CH_3), 55.80 (Chiral-C), 17.00 (-CH_3).
HRMS (ESI-TOF) *m*/*z* found for $C_{19}H_{18}ClN_3O_3S$: 404.0845 $[M+H]^+$

3.3 *N*-(2-chlorophenyl)-4(*R*/*S*)-(3,4-dimethoxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4c**)

Light yellow solid (0.380 mg, 91%); MP: 166-168 °C; TLC: R_f = 0.84 [(7:3)EtOAc: n-Hexane];

^{1}H NMR (500 MHz, DMSO-d_6) δ 10.02 (s, 1H, NH), 9.43 (s, 1H, NH), 9.23 (s, 1H, NH), 7.49 (d, *J* = 5 Hz, 1H, Ar-H), 7.44 (d, *J* = 5 Hz, 1H, Ar-H)), 7.29 (t, *J* = 5 Hz, 1H, Ar-H)), 7.17 (t, *J* = 5 Hz, 1H, Ar-H)), 6.95 (d, *J* = 10 Hz, 1H, Ar-H), 6.92 (s, 1H, Ar-H), 6.85 (d, *J* = 10 Hz, 1H, Ar =H), 5.34 (s, 1H, Chiral H), 3.73 (s, 3H, CH_3), 3.72 (s. 3H, CH_3), 2.19 (s, 3H, CH_3);

^{13}C NMR (126 MHz, DMSO-d_6) δ: 173.90 (C=S), 165.07 (C=O), 148.69 (NH-C=), 148.52 (C-OMe), 137.17 (C-OMe), 135.20, 134.96 (C-NH), 129.46, 127.76, 127.38, 126.83 (C-Cl), 126.64, 118.72, 111.91, 110.75, 106.02 (-C=), 55.61 (-OMe), 55.47 (-OMe), 54.69 (Chiral-C), 16.72 (-CH_3);

HRMS (ESI-TOF) *m*/*z* found for $C_{20}H_{20}ClN_3O_3S$: 418.0996 $[M+H]^{+z}$

3.4 *N*-(2-chlorophenyl)-4(*R*/*S*)-(3,4-dihydroxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4d**)

Light brown solid (0.385 mg, 99%); MP: 134-136 °C; TLC: R_f = 0.74 [(7:3)EtOAc: n-Hexane];

^{1}H NMR (500 MHz, DMSO-d_6) δ 9.85 (s, 1H, NH), 9.28 (s, 1H, NH), 9.05 (s, 2H, OH), 8.80 (s, 1H, NH), 7.10 (m, 4H, Ar-H), 6.71 (s, 1H, Ar-H), 6.69 (m, 1H, Ar-H), 6.56(d, 1H, Ar-H), 5.23 (s, 1H, Chiral H), 2.11 (s, 3H, CH_3);

^{13}C NMR (126 MHz, DMSO-d_6) δ: 173.58 (C=S), 165.15 (C=O), 145.47 (NH-C=), 145.26 (C-OH), 136.48, 135.14, 134.35 (C-NH), 133.05, 130.39, 125.99 (C-Cl), 125.94, 125.61, 117.86, 115.44, 114.47, 107.30 (-C=), 55.31 (Chiral-C), 16.67 (-CH_3);

HRMS (ESI-TOF): *m*/*z* found for $C_{18}H_{16}ClN_3O_3S$: 390.0897 $[M+H]^+$

3.5 *N*-(4-chlorophenyl)-4(*R*/*S*)-(4-hydroxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4e**)

Light yellow solid (0.358 mg, 96%); MP: 224-226 °C; TLC: R_f = 0.77 [(7:3) EtOAc: n-Hexane];

^{1}H NMR (500 MHz, DMSO-d_6) δ: 9.93 (s, 1H, NH), 9.78 (s, 1H, NH), 9.42 (s, 1H, NH), 9.37 (s,1H, OH), 7.57 (d, *J* = 10 Hz, 2H, Ar-H), 7.30 (d, *J* = 5 Hz, 2H, Ar-H)), 7.04 (d, *J* = 2H, Ar-H), 6.71 (d, *J* = 10 Hz, 2H, Ar-H), 5.29 (s, Chiral H), 2.05 (s, 3H, CH_3);

^{13}C NMR (126 MHz, DMSO-d_6) δ 173.56 (C=S), 165.00 (C=O), 156.87 (NH-C=), 137.84 (C-OH), 135.47, 133.41 (C-NH), 128.33 (C-Cl), 127.60, 126.71, 120.99, 115.10, 107.09 (-C=), 54.45 (Chiral-C), 16.34 (-CH_3);

HRMS (ESI-TOF) *m*/*z* found for $C_{18}H_{16}ClN_3O_2S$: 374.0412 $[M+H]^+$

3.6 *N*-(4-chlorophenyl)-4(*R*/*S*)-(4-hydroxy-3-methoxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4f**)

Light orange solid (0.390 mg, 97%); MP: 194-196 °C; TLC: R_f = 0.72 [(7:3)EtOAc: n-Hexane];

^{1}H NMR (500 MHz, DMSO-d_6) δ: 9.94 (s, 1H, OH), 9.81 (s, 1H, NH), 9.37 (s, 1H, NH), 9.00 (s, 1H, NH), 7.58 (d, *J* = 5 Hz, 2H, Ar-H), 7.31 (d, *J* = 5 Hz, 2H, Ar-H), 6.79 (s, 1H, Ar-H),

6.72 (d, *J* = 10 Hz, 1H, Ar-H) , 6.67 (d, *J* = 10 Hz, 1H, Ar-H), 5.31 (s, Chiral H), 3.67 (s, 3H, CH_3), 2.05 (s, 3H, CH_3);
^{13}C NMR (126 MHz, DMSO-d_6) δ: 174.03 (C=S), 165.41 (C=O), 147.65 (NH-C=), 146.41 (C-OMe), 138.16 (C-OH), 135.81, 134.13 (C-NH), 128.79 (C-Cl), 127.05, 121.46, 118.88, 115.60, 111.05, 107.28 (-C=), 55.71 (-OMe), 54.78 (Chiral-C), 16.76 (-CH_3);
HRMS (ESI-TOF) *m*/*z* found for $C_{19}H_{18}ClN_3O_3S$: 404.0770 $[M+H]^+$

3.7 *N*-(4-chlorophenyl)-4(*R*/*S*)-(3,4-dimethoxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4g**)
Off-white solid (0.404 mg, 97%); MP: 204-206 °C; TLC: R_f = 0.80 [(7:3) EtOAc: n-Hexane];
^{1}H NMR (500 MHz, DMSO-d_6) δ: 9.99 (s, 1H, NH) 9.84 (s, 1H, NH), 9.41 (s, 1H, NH), 7.59 (d, *J* = 5 Hz, 2H, Ar-H)), 7.31 (dd, *J* = 10 Hz, 2H, Ar-H), 6.92 (d, *J* = 5 Hz, 1H, Ar-H), 6.84 (s, 1H, Ar-H), 6.77 (d, *J* = 5 Hz, 1H, Ar-H) , 5.36 (s, 1H, Chiral H), 3.71 (s, 3H, CH_3), 3.67 (s, 3H, CH_3), 2.06 (s, 3H, CH_3);
^{13}C NMR (126 MHz, DMSO-d_6) δ: 173.86 (C=S), 165.03 (C=O), 148.50 (NH-C=), 148.24 (C-OMe), 137.82 (C-OMe), 135.73, 135.23 (C-NH), 128.47 (C-Cl), 126.74, 121.11, 118.12, 111.66, 110.20, 106.80 (-C=), 55.23 (-OMe), 54.65 (-OMe), 54.35 (Chiral-C), 16.45 (-CH_3);
HRMS (ESI-TOF) found for $C_{20}H_{20}ClN_3O_3S$: 418.1005 $[M+H]^+$

3.8 4(*R*/*S*)-(4-hydroxyphenyl)-6-methyl-2-thioxo-*N*-(*o*-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4h**)
Off-white solid (0.332 mg, 94%); MP: 236-238 °C; TLC: R_f = 0.75 [(7:3) EtOAc: n-Hexane];
^{1}H NMR (500 MHz, DMSO-d_6) δ: 9.88 (s, 1H, NH), 9.43 (s, 1H, NH), 9.31 (s, 1H, NH), 9.10 (s, 1H, OH), 7.12 (m, 4H, Ar-H), 7.06 (m, 2H, Ar-H) ,6.75 (d, *J* = 10 Hz, 2H, Ar-H), 5.30 (s, 1H, Chiral-H), 2.13 (s, 3H, CH_3), 1.91 (s, 3H, CH_3);
13C NMR (126 MHz, DMSO-d_6) δ: 173.48 (C=S), 165.00 (C=O), 157.09 (NH-C=), 136.27 (C-OH), 135.16, 133.52 (C-NH), 132.96 (C-CH_3), 130.25, 128.13, 125.86, 125.81, 125.54, 115.20, 107.01 (-C=), 54.87 (Chiral-C), 17.90 (-CH_3), 16.55 (Ar-CH_3);
HRMS (ESI-TOF) found for $C_{19}H_{19}N_3O_2S$: 354.1288 $[M+H]^+$

3.9 4(*R*/*S*)-(4-hydroxy-3-methoxyphenyl)-6-methyl-2-thioxo-*N*-(*o*-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4i**)
Light brown solid (0.355 mg, 93%); MP: 182-184 °C; TLC: R_f = 0.70 [(7:3)EtOAc:n-Hexane];
^{1}H NMR (500 MHz, DMSO-d_6) δ: 9.89 (s, 1H, NH), 9.31 (s, 1H, OH), 9.11 (s, 1H, NH), 9.02 (s, 1H, NH), 7.09 (m, 4H, Ar-H), 6.87 (s, 1H, Ar-H), 6.74 (m, 2H, Ar-H), 5.31 (s, 1H, Ar-H), 3.73 (s, 3H, CH_3), 2.13 (s, 3H, CH_3), 1.93 (s, 3H, CH_3);
^{13}C NMR (126 MHz, DMSO-d_6) δ: 173.74 (C=S), 165.21 (C=O), 147.65 (NH-C=), 146.49 (C-OMe), 136.44 (C-OH), 135.47, 134.07 (C-NH), 133.08 (C-CH_3), 130.44, 126.03, 125.93, 125.70, 119.35, 115.58, 111.50, 107.00 (-C=), 55.80 (Chiral-C), 55.31 (-OMe), 18.02 (-CH_3), 16.74 (Ar-CH_3);
HRMS (ESI-TOF) found for $C_{20}H_{21}N_3O_3S$: 384.1385 $[M+H]^+$

3.10 4(*R*/*S*)-(3,4-dimethoxyphenyl)-6-methyl-2-thioxo-*N*-(*o*-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4j**)
Off-white solid (0.373 mg, 94%); MP: 200-202 °C; TLC: R_f = 0.75 [(7:3)EtOAc:n-Hexane)];

^{1}H NMR (500 MHz, DMSO-d_6) δ: 9.93 (s, 1H, NH), 9.35 (s, 1H, NH), 9.15 (s, 1H, NH), 7.11 (m, 4H, Ar-H), 6.95 (d, *J* = 10 Hz, 1H, Ar-H), 6.90 (s, 1H, Ar-H), 6.83 (d, *J* = 5 Hz, 1H, Ar-H), 5.35 (s, 1H, Chiral H), 3.73 (s, 3H, CH_3), 3.72 (s, 3H, CH_3), 2.14 (s, 3H, CH_3), 1.95 (s, 3H, CH_3);
^{13}C NMR (126 MHz, DMSO-d_6) δ: 173.60 (C=S), 164.84 (C=O), 148.51 (NH-C=), 148.34 (C-OMe), 136.09 (C-OMe), 135.30, 135.23 (C-NH), 132.75 (C-CH_3), 130.11, 125.71, 125.61, 125.39, 118.63, 111.70, 110.65, 106.59 (-C=), 55.47 (Chiral-C), 55.32 (-OMe), 54.80 (-OMe), 17.67 (-CH_3), 16.42 (Ar-CH_3);
HRMS (ESI-TOF) found for $C_{21}H_{23}N_3O_3S$: 398.1538 $[M+H]^+$

3.11 4(*R*/*S*)-(3,4-dihydroxyphenyl)-6-methyl-2-thioxo-*N*-(*o*-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4k**)
Light brown solid (0.343 mg, 93%); MP: 176-178 °C; TLC: R_f = 0.49 [(7:3)EtOAc: n-Hexane];
^{1}H NMR (500 MHz, DMSO-d_6) δ: 9.00 (s, 1H, NH), 8.79 (s, 1H, NH), 8.20 (s, 2H, OH), 8.12 (s, 1H, NH), 7.23 (d, *J* = 10 Hz, 1H, Ar-H) 7.17 (d, *J* = 5 Hz, 1H, Ar-H), 6.96 (t, *J* = , 1H, Ar-H), 6.83 (t, *J* =, 1H, Ar-H), 6.40 (s, 1H, Ar-H), 6.33 (d, *J* = 5 Hz, 1H, Ar-H), 6.23 (d, *J* = 10 Hz, 1H, Ar-H), 4.38 (d, 1H, Chiral H), 2.20 (s, 3H, CH_3), 1.22 (s, 3H, CH_3);
^{13}C NMR (126 MHz, DMSO-d_6) δ: 176.07 (C=S), 166.64 (C=O), 145.35 (NH-C=), 145.27 (C-OH), 134.64 (C-OH), 129.85, 129.49 (C-NH), 127.64 (C-CH_3), 126.10, 125.26, 124.79, 118.78, 115.32, 114.88, 106.86 (-C=), 81.35, 55.41, 21.55, 15.76;
HRMS (ESI-TOF) *m*/*z* found for $C_{19}H_{19}N_3O_3S$: 370.1280 $[M+H]^+$

3.12 4(*R*/*S*)-(4-hydroxyphenyl)-6-methyl-2-thioxo-*N*-(*p*-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4l**)
Off-white solid (0.306 mg, 87%); MP: 202-204 °C; TLC: R_f = 0.78 [(7:3)EtOAc: n-Hexane];
^{1}H NMR (500 MHz, DMSO-d_6) δ: 9.88 (s, 1H, NH), 9.57 (s, 1H, NH), 9.41 (s, 1H, NH), 9.32 (s, 1H, OH), 7.42 (d, *J* = 5 Hz, 2H, Ar-H), 7.06 (s, 2H, Ar-H), 7.05 (s, 2H, Ar-H), 6.71 (d, J = 10 Hz, 2H, Ar-H), 5.29 (s, Chiral H), 2.22 (s, 3H, CH_3), 2.05 (s, 3H, CH_3);
^{13}C NMR (126 MHz, DMSO-d_6) δ 173.52 (C=S), 164.71 (C=O), 156.84 (NH-C=), 136.37 (C-OH), 134.72 (C-CH_3), 133.47, 132.10 (C-NH), 128.79, 127.64, 119.53, 115.07, 107.49 (-C=), 54.56 (Chiral-C), 20.29 (Ar-CH_3), 16.29 (-CH_3);
HRMS (ESI-TOF) *m*/*z* found for $C_{19}H_{19}N_3O_2S$: 354.1270

3.13 4(*R*/*S*)-(4-hydroxy-3-methoxyphenyl)-6-methyl-2-thioxo-*N*-(*p*-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4m**)
Off-white solid (0.345 mg, 90%); MP: 180-182 °C; TLC: R_f = 0.79 [(7:3)EtOAc: n-Hexane];
1H NMR (500 MHz, DMSO-d_6) δ: 9.89 (s, 1H, OH), 9.60 (s, 1H, NH), 9.32 (s, 1H, NH), 8.98 (s, 1H, NH), 7.42 (d, *J* = 5 Hz, 2H, Ar-H), 7.06 (d, *J* = 10 Hz, 2H, Ar-H), 6.81 (s, 1H, Ar-H), 6.73 (d, *J* = 5 Hz, 1H, Ar-H), 6.66 (d, *J* = 10 Hz, 1H, Ar-H), 5.31 (s, Chiral H), 3.67 (s, 3H, CH_3), 2.22 (s, 3H, CH_3), 2.05 (s, 3H, CH_3);
^{13}C NMR (126 MHz, DMSO-d_6) δ: 173.83 (C=S), 164.96 (C=O), 147.48 (NH-C=), 146.21 (C-OMe), 136.50 (C-OH), 134.87, 134.02 (C-CH_3), 132.29 (C-NH), 128.96, 119.72, 118.75, 115.40, 110.91, 107.53 (-C=), 55.55 (-OCH_3), 54.83 (Chiral-C), 20.45 (Ar-CH_3), 16.44 (-CH_3);
HRMS (ESI-TOF) *m*/*z* found for $C_{20}H_{21}N_3O_3S$: 384.1042

3.14 4(*R*/*S*)-(3,4-dimethoxyphenyl)-6-methyl-2-thioxo-*N*-(*p*-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4n**)

Light yellow solid (0.322 mg, 81%); MP: 188-190 °C; TLC: R_f = 0.81 [(7: 3)EtOAc: n-Hexane];

^{1}H NMR (500 MHz, DMSO-d_6) δ 9.93 (s, 1H, NH), 9.63 (s, 1H, NH), 9.36 (s, 1H, NH), 7.44 (d, J = 5 Hz, 2H, Ar-H), 7.06 (d, 2H, J = 10 Hz), 6.92 (d, 1H, J = 10 Hz, Ar-H), 6.85 (s, 1H, Ar-H), 6.79 (d, 1H, J = 5 Hz, 1H, Ar-H), 5.35 (s, 1H, chiral H), 3.71 (s, 3H, CH_3), 3.67 (s, 3H, CH_3), 2.22 (s, 3H, CH_3), 2.05 (s, 3H, CH_3);

^{13}C NMR (126 MHz, DMSO-d_6) δ: 173.83 (C=S), 164.74 (C=O), 148.50 (NH-C=), 148.21 (C-OMe), 136.32 (C-OMe), 135.30 (C-CH_3), 134.93, 132.13 (C-NH), 128.79, 119.53, 118.17, 111.66, 110.24, 107.22 (-C=), 55.39 (-OMe), 55.23 (-OMe), 54.55 (Chiral-C), 20.27 (Ar-CH_3), 16.29 (-CH_3);

HRMS (ESI-TOF) *m*/*z* found for $C_{21}H_{23}N_3O_3S$: 398.1543 $[M+H]^+$

3.15 4(*R*/*S*)-(3,4-dihydroxyphenyl)-6-methyl-2-thioxo-*N*-(*p*-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4o**)

Light brown solid (0.336 mg, 91%); MP: 158-160 °C; TLC: R_f = 0.82 [(7:3)EtOAc: n-Hexane];

1H NMR (500 MHz, DMSO-d_6) δ: 9.84 (s, 1H, NH), 9.55 (s, 1H, NH), 9.52 (s, 2H, OH), 9.29 (s, 1H, NH), 7.43 (d, 2H, *J* = 5 Hz, 2H, Ar-H), 7.05 (d, *J* = 10 Hz, 2H, Ar-H), 6.65 (d, *J* = 10 Hz, 2H, Ar-H), 6.50 (s, 1H, Ar-H), 5.22 (s, 1H, Chiral H), 2.22 (s, 3H, CH_3), 2.04 (s, 3H, CH_3);

^{13}C NMR (126 MHz, DMSO-d_6) δ: 173.48 (C=S), 164.73 (C=O), 145.15 (NH-C=), 144.91 (C-OH), 136.42 (C-OH), 134.53, 134.19 (C-CH_3), 132.05 (C-NH), 128.72, 119.71, 119.43, 117.20, 115.17, 107.64 (-C=), 54.90 (Chiral-C), 20.35 (Ar-CH_3), 16.37 (-CH_3);

HRMS (ESI-TOF) *m*/*z* found for $C_{19}H_{19}N_3O_3S$: 370.1229 $[M+H]^+$

3.16 *N*-(2,4-dimethoxyphenyl)-4(*R*/*S*)-(4-hydroxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4p**)

Light brown solid (0.384 mg, 96%); MP: 156-158 °C; TLC: R_f = 0.78 [(7:3)EtOAc: n-Hexane];

1H NMR (500 MHz, DMSO-d_6) δ: 9.69(s, 1H, NH), 9.04 (s, 1H, NH), 8.90 (s, 1H, OH), 8.74 (s, 1H, NH), 7.81 (s, 1H, Ar-H), 7.53 (s, 1H, Ar-H), 6.68 (s, 1H, Ar-H), 6.38 (d, J = 5 Hz, 2H, Ar-H), 6.20 (m, 2H, Ar-H), 4.69 (s, 1H, Ar-H), 3.37 (s, 3H, CH_3), 3.28 (s, 3H, CH_3), 1.86 (s, 3H, CH_3);

^{13}NMR (126 MHz, DMSO-d_6) δ: 175.60 (C=S), 172.78 (C-OMe), 166.19 (C=O), 163.97 (NH-C=), 147.75 (C-OH), 145.35 (C-OMe), 145.26, 142.74, 139.35, 132.85 (C-NH), 126.83, 114.31, 105.48 (-C=), 104.65, 56.13 (Chiral-C), 55.97 (-OMe), 54.41 (O-Me), 16.59 (-CH_3);

HRMS (ESI-TOF) *m*/*z* found for $C_{20}H_{21}N_3O_4S$: 400.1253 $[M+H]^+$

3.17 *N*-(2,4-dimethoxyphenyl)-4(*R*/*S*)-(3,4-dimethoxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4q**)

Light yellow solid (0.359 mg, 81%); MP: 170-172 °C; TLC: R_f = 0.52 [(7:3)EtOAc: n-Hexane];

^{1}H NMR (500 MHz, DMSO-d_6) δ: 9.95 (s, 1H, NH), 9.33 (s, 1H, NH), 8.48 (s, 1H, NH), 7.49 (d, *J* = 10 Hz, 1H, Ar-H), 6.95 (d, *J* = 5 Hz, 1H, Ar-H), 6.91 (s, 1H, Ar-H), 6.84 (d, *J* = 10 Hz, 1H, Ar-H), 6.55 (s, 1H, Ar-H), 6.44 (d, *J* = 10 Hz, 1H, Ar-H), 5.25 (s, 1H, Chiral H), 3.74 (s, 3H, CH_3), 3.72 (s, 3H, CH_3), 3.71 (s, 3H, CH_3), 3.68 (s, 3H, CH_3), 2.15 (s, 3H, CH_3);
^{13}C NMR (126 MHz, DMSO-d_6) δ: 173.89 (C=S), 164.71 (C-OMe), 157.25 (C=O), 152.12 (NH-C=), 148.90 (C-OMe), 148.71 (C-OMe), 136.72 (C-OMe), 135.33, 120.21, 118.92, 112.06 (C-NH), 110.88, 106.57, 104.19 (-C=), 98.99, 98.90, 55.80 (Chiral-C), 55.63 (-OMe), 55.58 (-OMe), 55.50 (-OMe), 55.45 (-OMe), 16.78 (-CH_3);
HRMS (ESI-TOF) *m*/*z* found for $C_{22}H_{25}N_3O_5S$: 444.1603 $[M+H]^+$

3.18 4(*R*/*S*)-(3,4-dihydroxyphenyl)-*N*-(2,4-dimethoxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4r**)
Light brown solid (0.406 mg, 98%); MP: 168-170 °C; TLC: R_f = 0.47 [(7:3)EtOAc: n-Hexane];
^{1}H NMR (500 MHz, DMSO-d_6) δ: 9.92 (s, 1H, NH), 9.30 (s, 2H, OH), 8.82 (s, 1H, NH), 8.21 (s, 1H, NH), 7.60 (d, *J* = 5 Hz, 1H, Ar-H), 6.73 (s, 1H, Ar-H), 6.71 (s, 1H, Ar-H), 6.59 (d, *J* = 10 Hz, 1H, Ar-H), 6.54 (s, 1H, Ar-H), 6.54 (d, *J* = 5 Hz, 1H, Ar-H), 6.42 (d, *J* = 5 Hz, 1H, Ar-H), 5.07 (s, 1H, Chiral H), 3.71(s, 3H, CH_3), 3.67 (s, 3H, CH_3), 2.16 (s, 3H, CH_3);
^{13}C NMR (126 MHz, DMSO-d_6) δ: 173.10 (C=S), 164.11 (C-OMe), 156.59 (C=O), 151.13 (NH-C=), 145.29 (C-OMe), 145.23 (C-OH), 136.97 (C-OH), 133.50, 123.03, 120.19, 117.77 (C-NH), 115.33, 114.18, 106.05, 103.81 (-C=), 98.53, 55.45 (Chiral-C), 55.13(-OMe), 54.69 (-OMe), 16.40 (-CH_3);
HRMS (ESI-TOF) found for $C_{20}H_{21}N_3O_5S$: 416.1280 $[M+H]^+$

3.19 *N*-(4-chloro-2,5-dimethoxyphenyl)-4(*R*/*S*)-(4-hydroxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4s**)
Light orange solid (0.416 mg, 96%); MP: 132-134 °C; TLC: R_f = 0.86 [(7:3)EtOAc: n-Hexane];
^{1}H NMR (500 MHz, DMSO-d_6) δ: 10.05 (s, 1H, NH), 9.42 (s, 1H, NH), 9.27 (s, 1H, OH), 8.30 (s, 1H, NH), 7.84 (s, 1H, Ar-H), 7.14 (d, *J* = 5 Hz, 2H, Ar-H), 7.06 (s, 1H, Ar-H), 6.78 (d, *J* = 10 Hz, 2H, Ar-H), 5.16 (s, 1H, Chiral-H), 3.72 (s, 3H, CH_3), 3.66 (s, 3H, CH_3), 2.22 (s, 3H, CH_3);
^{13}C NMR (126 MHz, DMSO-d_6) δ: 173.43 (C=S), 164.52 (C=O), 157.66 (NH-C=), 148.25 (C-OH), 143.51 (C-OMe), 139.54 (C-OMe), 132.91, 128.62, 127.23 (C-NH), 115.69 (C-Cl), 115.02, 113.13, 106.33, 105.33 (-C=), 56.65 (Chiral-C), 56.51 (-OMe), 54.64 (-OMe), 17.02 (-CH_3);
HRMS (ESI-TOF) found for $C_{20}H_{20}ClN_3O_4S$: 434.0944 $[M+H]^+$

3.20 *N*-(4-chloro-2,5-dimethoxyphenyl)-4(*R*/*S*)-(3,4-dimethoxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4t**)
Yellow solid (0.467 mg, 98%); MP: 140-142 °C; TLC: R_f = 0.78 [(7:3)EtOAc: n-Hexane];
^{1}H NMR (500 MHz, DMSO-d_6) δ: 9.91 (s, 1H, NH), 9.27 (s, 1H, NH), 8.29 (s, 1H, NH), 7.64 (s, 1H, Ar-H), 6.92 (s, 1H, Ar-H), 6.81 (d, *J* = 5 Hz, 1H, Ar-H), 6.77 (s, 1H, Ar-H), 6.70 (d, *J* = 5 Hz, 1H, Ar-H), 5.09 (s, 1H, Chiral-H), 3.49 (s, 3H, 3H, -OCH_3, -OCH_3), 3.17 (s, 3H, -OCH_3), 2.34 (s, 3H, CH_3), 2.05 (s, 3H, CH_3);

^{13}C NMR (126 MHz, DMSO-d_6) δ: 173.71 (C=S), 164.64 (C=O), 148.99 (NH-C=), 148.91 (C-OMe), 148.23 (C-OMe), 143.76 (C-OMe), 139.15 (C-OMe), 134.89, 127.14 (C-NH), 119.14 (C-Cl), 115.21, 113.22, 112.14, 111.06, 106.68, 105.37 (-C=), 56.66 (Chiral-C), 56.50 (-OMe), 55.76 (-OMe), 55.62 (-OMe), 54.80 (-OMe), 16.96 (-CH_3);
HRMS (ESI-TOF) found for $C_{22}H_{24}ClN_3O_5S$: 478.1215 $[M+H]^+$

3.21 4(*R*/*S*)-(4-hydroxyphenyl)-6-methyl-2-thioxo-*N*-(3-(trifluoromethyl)phenyl)-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4u**)
Light yellow solid (0.379 mg, 93%); MP: 142-144 °C; TLC: R_f = 0.85 [(7:3)EtOAc: n-Hexane];
^{1}H NMR (500 MHz, DMSO-d_6) δ: 9.98 (s, 1H, NH), 9.97 (s, 1H, NH), 9.42 (s, 1H, NH), 9.33 (s, 1H, OH), 8.04 (s, 1H, Ar-H), 7.78 (d, *J* = 10 Hz, 1H, Ar-H), 7.50 (t, *J* = , 1H, Ar-H), 7.36 (d, *J* = 10 Hz, 1H, Ar-H), 7.05 (d, *J* = 5 Hz, 2H, Ar-H), 6.71 (d, *J* = 5 Hz, 2H, Ar-H), 5.32 (s, 1H, Chiral H), 2.09 (s, 3H, CH_3);
^{13}C NMR (126 MHz, DMSO-d_6) δ: 173.92 (C=S), 165.70 (C=O), 157.25 (NH-C=), 140.02 (C-OH), 136.52 (C-NH), 133.72, 130.02 (C-CF_3), 129.64, 127.96, 125.39, 123.27 (-CF_3), 119.76, 115.78, 115.47, 107.07 ((-C=), 54.69 (Chiral-C), 16.75 (-CH_3);
HRMS (ESI-TOF) found for $C_{19}H_{16}F_3N_3O_2S$: 408.1000 $[M+H]^+$

3.22 4(*R*/*S*)-(4-hydroxy-3-methoxyphenyl)-6-methyl-2-thioxo-*N*-(3-(trifluoromethyl)phenyl)-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4v**)
Light yellow solid (0.416 mg, 95%); MP: 128-130 °C; TLC: R_f = 0.80 [(7:3)EtOAc: n-Hexane];
^{1}H NMR (500 MHz, DMSO-d_6) δ: 9.98 (s, 1H, NH), 9.39 (s, 1H, OH), 9.38 (s, 1H, NH), 9.31 (s, 1H, NH), 8.52 (s, 1H, Ar-H), 7.49 (dt, J = 15.5Hz and 2.5 Hz, 2H, Ar-H), 7.45 (t, J = 5.5 Hz, 1H, Ar-H), 7.30-7.24 (m, 1H, Ar-H), 7.18-7.12 (m, 1H, Ar-H), 6.86 (d, 1H, Ar-H), 6.77-6.71 (m, 1H, Ar-H), 5.29 (s, 1H, Chiral-H), 3.73 (s, 3H, CH3), 2.18 (s, 3H, CH3);
^{13}C NMR (126 MHz, DMSO-d_6) δ: 174.03 (C=S), 165.77 (C=O), 147.68 (NH-C=), 146.48 (C-OMe), 140.00 (C-OH), 136.55 (C-NH), 134.12, 130.06 (C-CF_3), 129.64, 129.39, 123.32 (-CF_3), 119.79, 118.94, 115.79, 115.65, 111.10, 106.91 (-C=), 55.70 (Chiral-C), 54.85 (-OMe), 16.74 (-CH_3);
HRMS (ESI-TOF) found for $C_{20}H_{18}F_3N_3O_3S$: 438.0688 $[M+H]^+$

3.23 4(*R*/*S*)-(3,4-dimethoxyphenyl)-6-methyl-2-thioxo-*N*-(3-(trifluoromethyl)phenyl)-1,2,3,4-tetrahydropyrimidine-5-carboxanilide (**4w**)
Light yellow solid (0.415 mg, 92%); MP: 154-156 °C; TLC: R_f = 0.85 [(7:3)EtOAc: n-Hexane];
^{13}C NMR (126 MHz, DMSO-d_6) δ: 174.91 (C=S), 166.44 (C=O), 149.56 (NH-C=), 149.34 (-OMe), 140.71 (-OMe), 137.53 (C-NH), 136.26, 130.76 (C-CF_3), 130.36, 130.10, 124.02 (-CF_3), 120.51, 119.25, 116.51, 112.75, 111.31, 107.46 (-C=), 56.43 (Chiral-C), 56.25 (-OMe), 55.44 (-OMe), 17.47 (-CH_3);
HRMS (ESI-TOF) found for $C_{21}H_{20}F_3N_3O_3S$: 452.0815 $[M+H]^+$

4 NMR Spectra of 4(a-w)

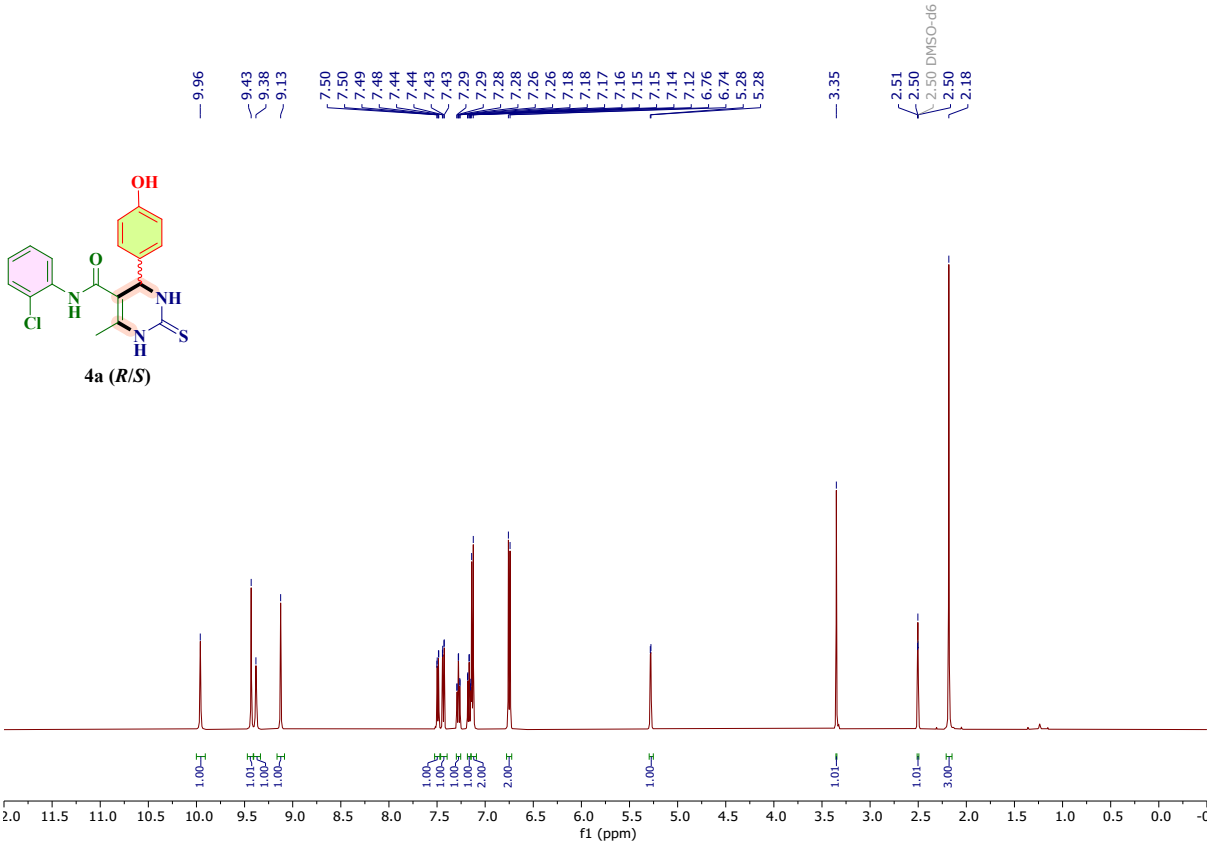


Figure S1: ^{1}H NMR spectra of **4a (*R*/*S*)** (500MHz, DMSO-d_6)

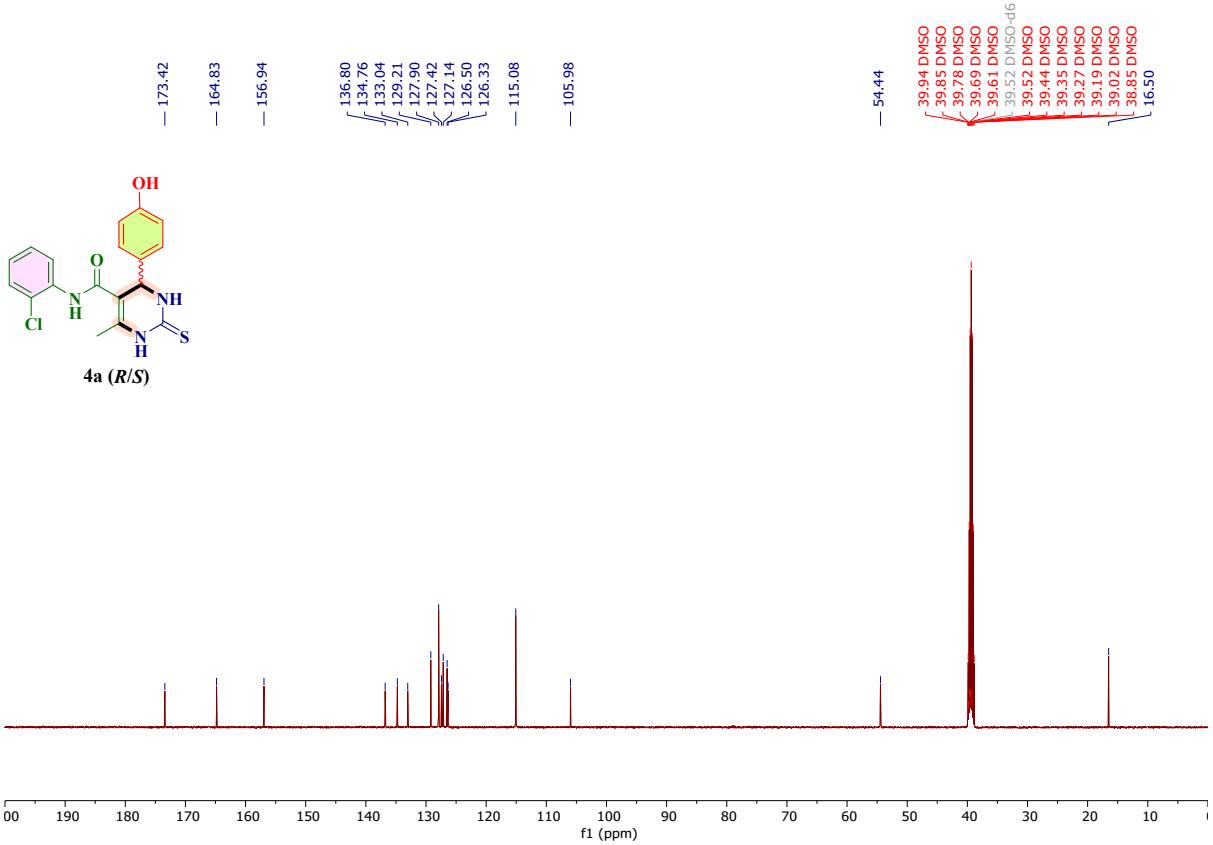


Figure S2: ^{13}C NMR of **4a** (***R*/*S***) (126 MHz, DMSO-d_6)

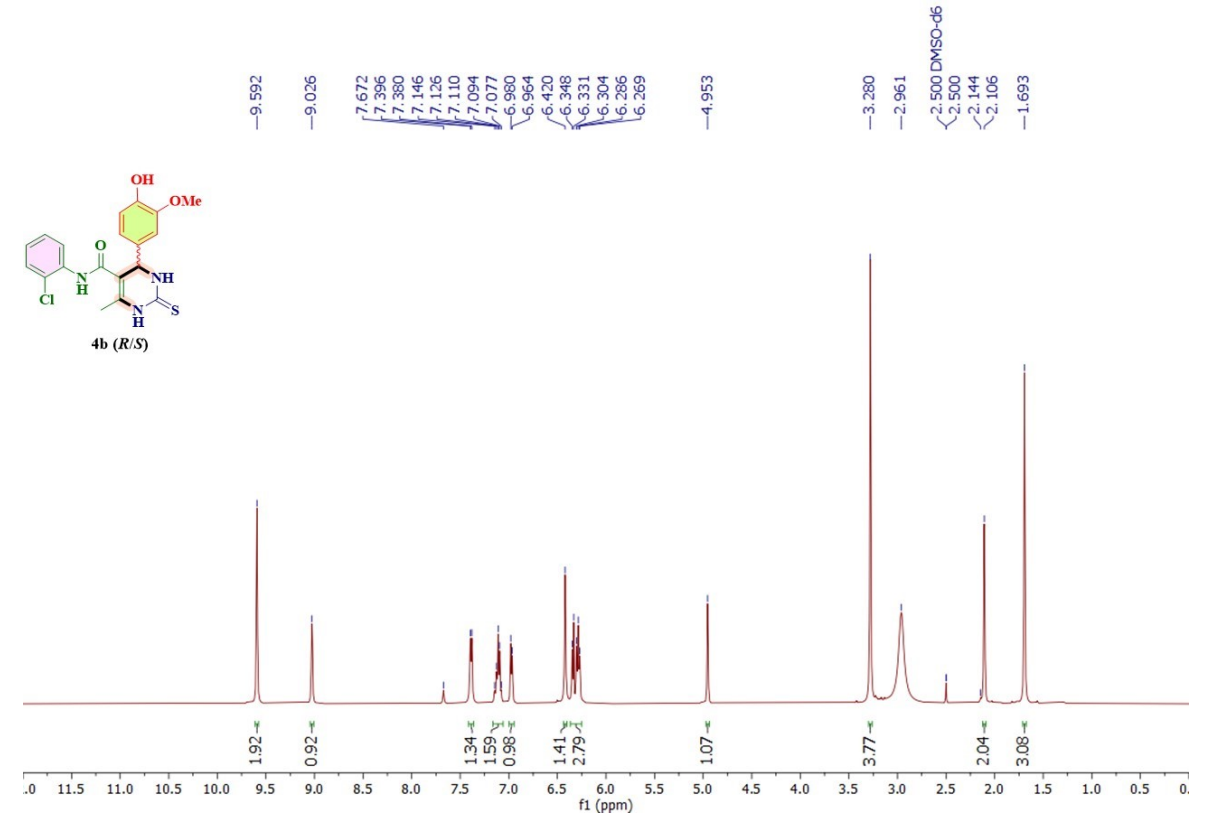


Figure S3: ^{1}H NMR spectra of **4b (*R*/*S*)** (500MHz, DMSO-d_6)

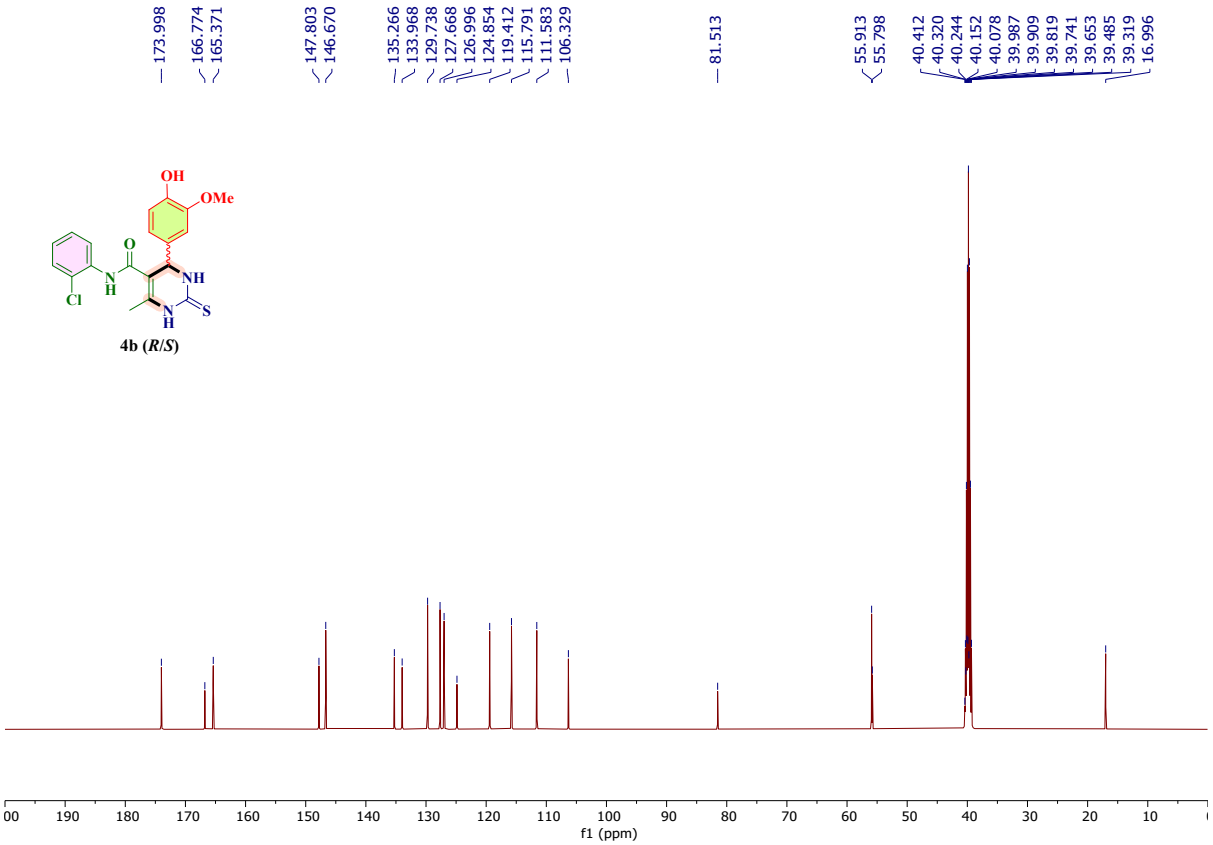


Figure S4: ^{13}C NMR of **4b** (***R*/*S***) (126 MHz, DMSO-d_6)

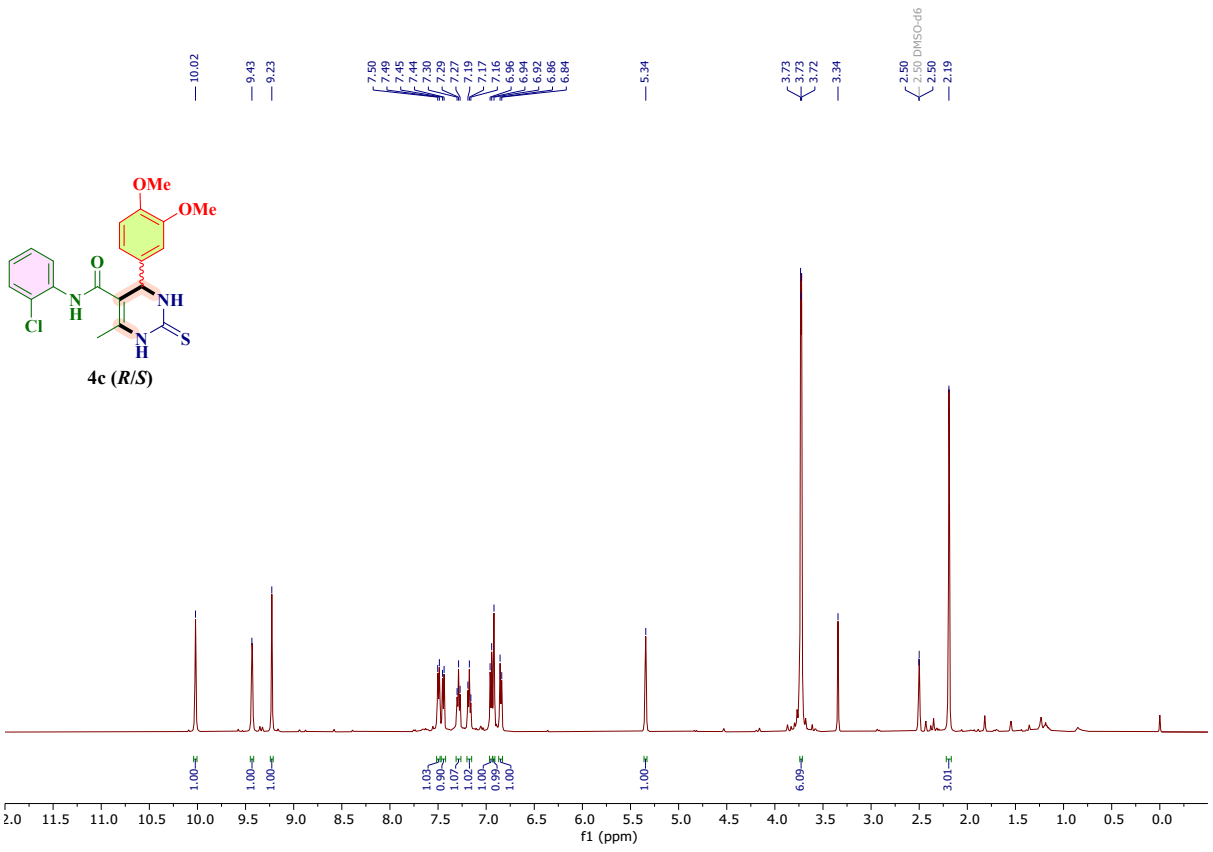


Figure S5: ^{1}H NMR spectra of **4c** (***R*/*S***) (500MHz, DMSO-d_6)

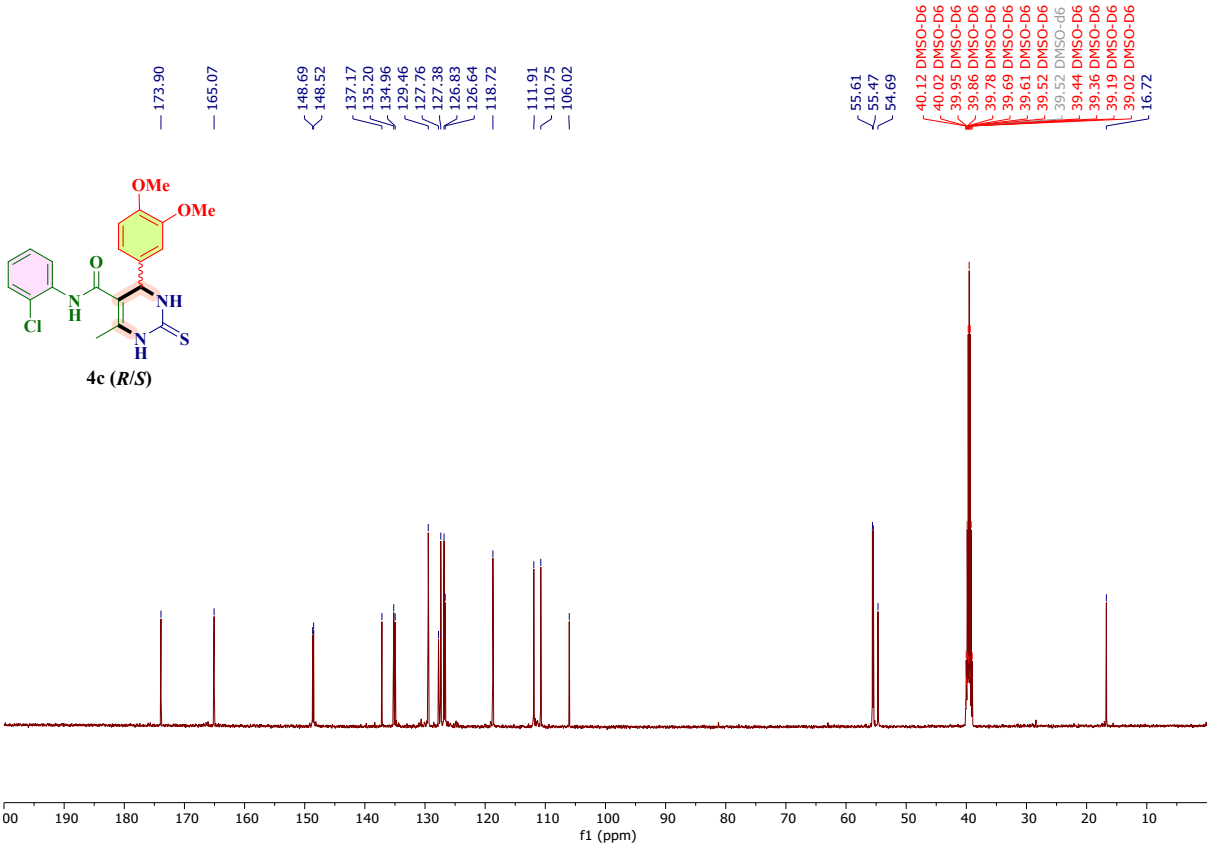


Figure S6: ^{13}C NMR of **4c** (***R*/*S***) (126 MHz, DMSO-d_6)

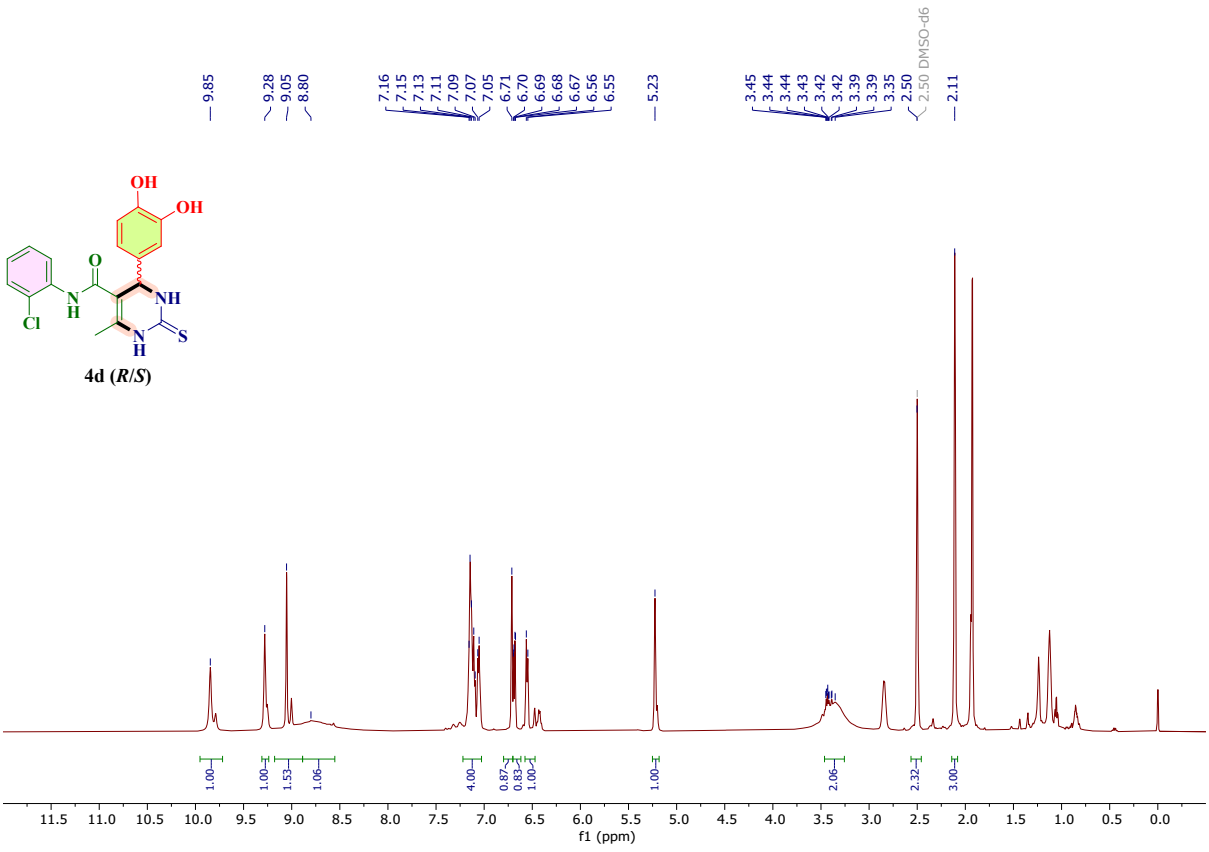


Figure S7: ^{1}H NMR spectra of **4d** (***R*/*S***) (500MHz, DMSO-d_6)

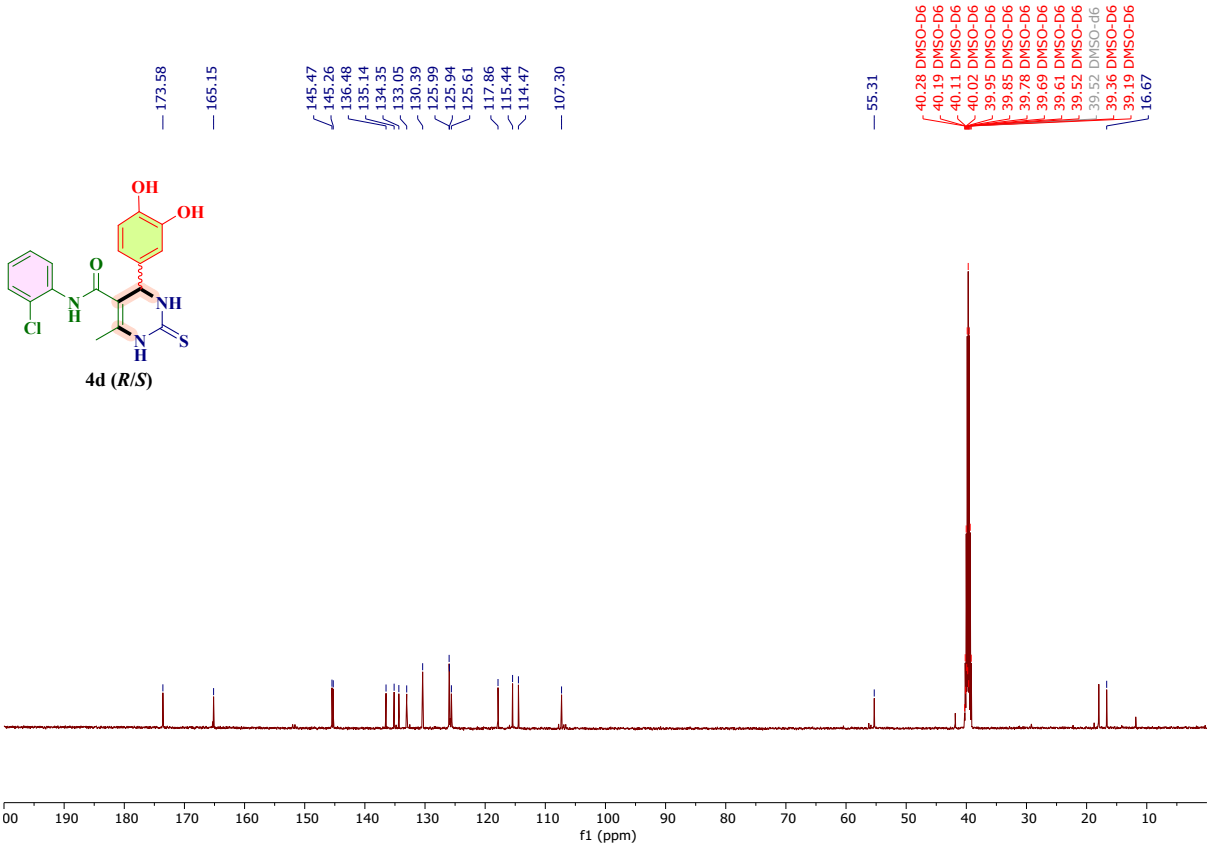


Figure S8: ^{13}C NMR of **4d** (***R*/*S***) (126 MHz, DMSO-d_6)

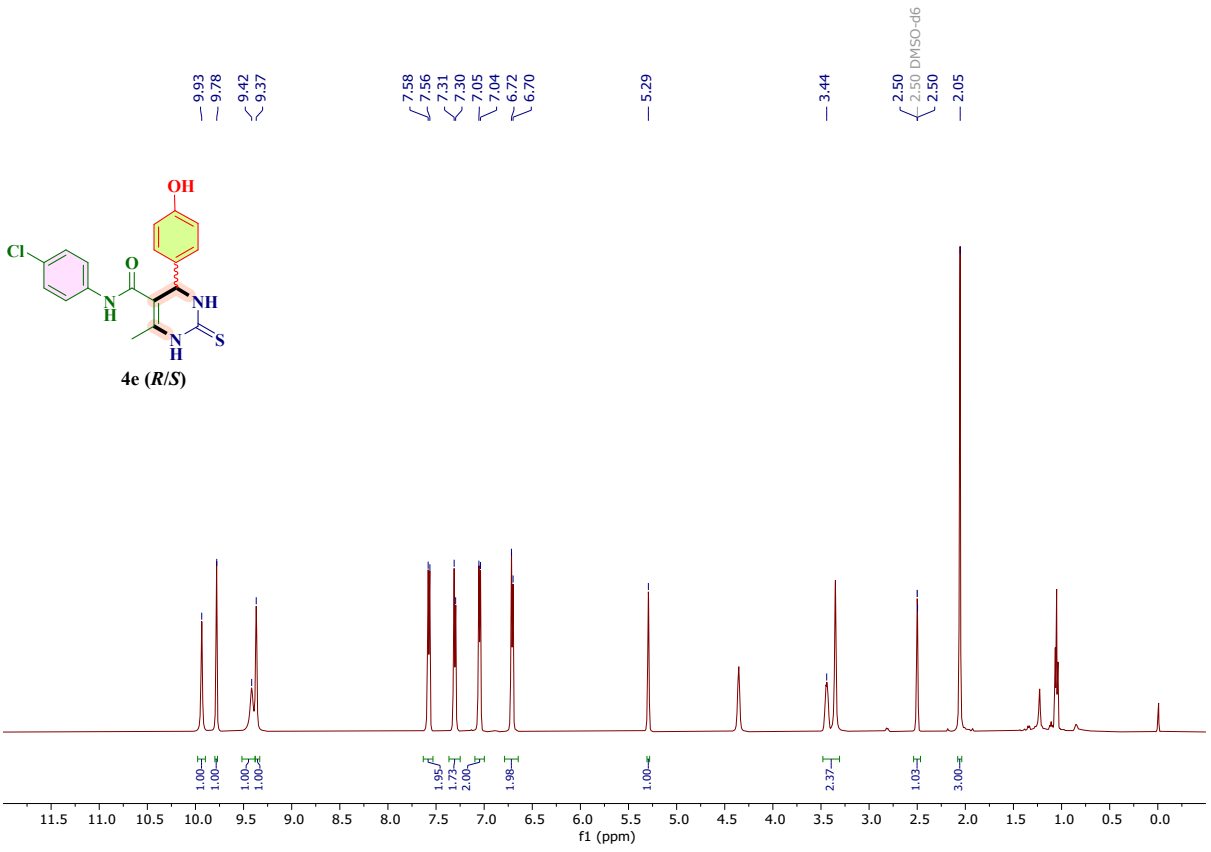


Figure S9: ^{1}H NMR spectra of **4e (*R*/*S*)** (500MHz, DMSO-d_6)

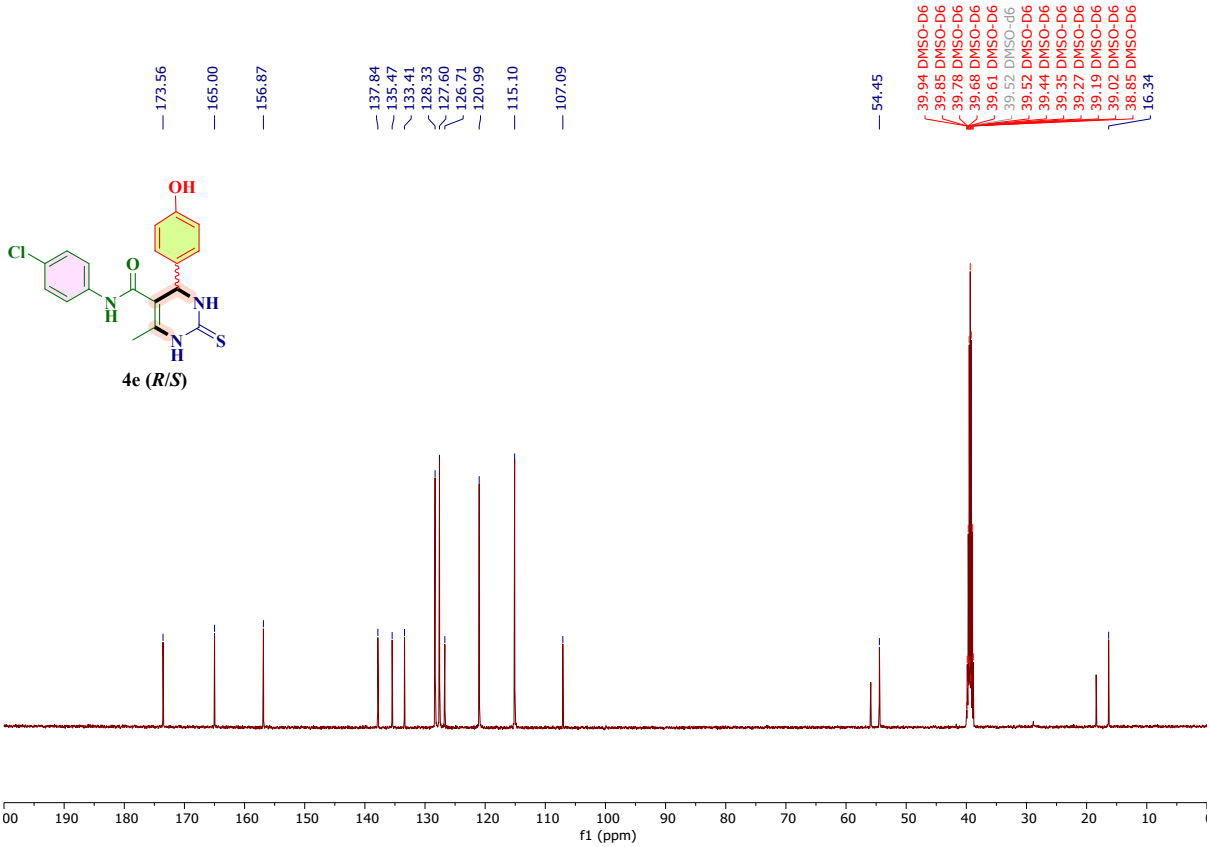


Figure S10: ^{13}C NMR of **4e** (***R*/*S***)(126 MHz, DMSO-d_6)

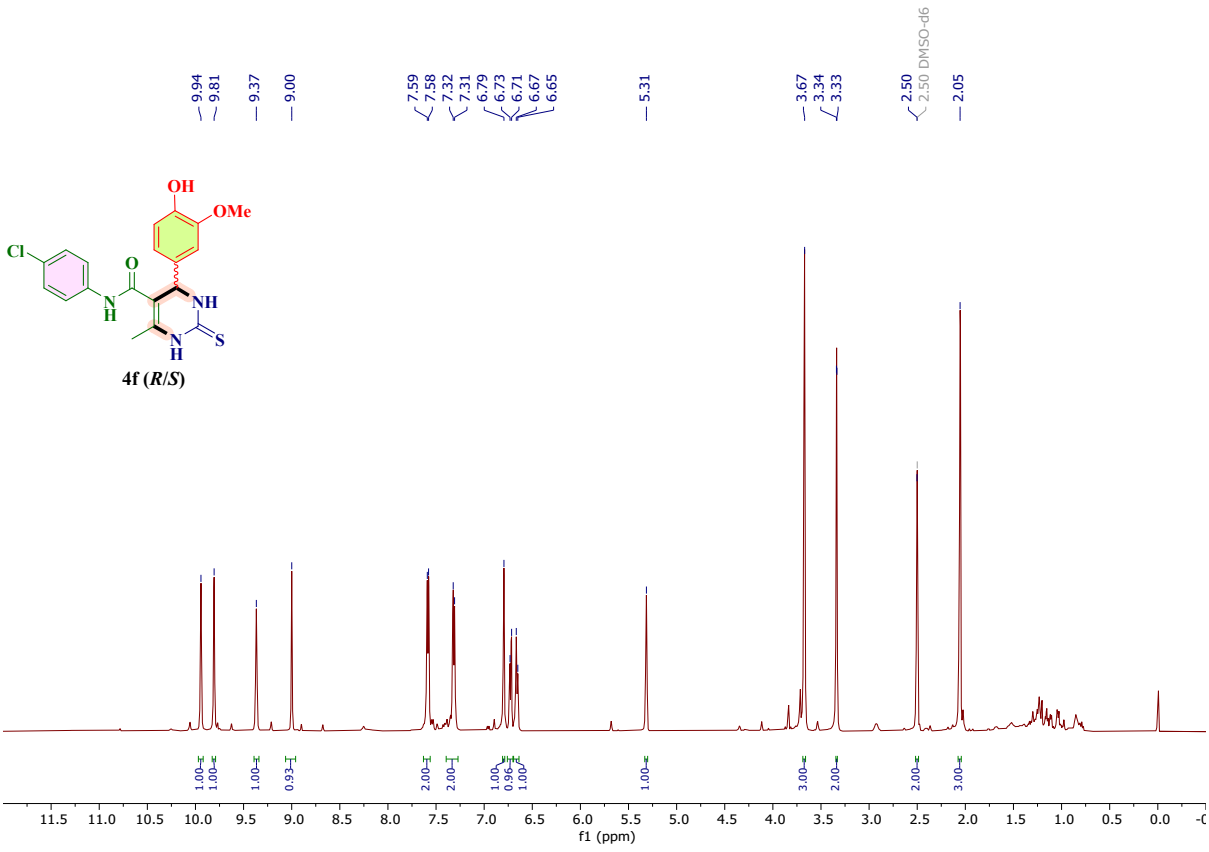


Figure S11: ^{1}H NMR spectra of **4f (*R*/*S*)** (500MHz, DMSO-d_6)

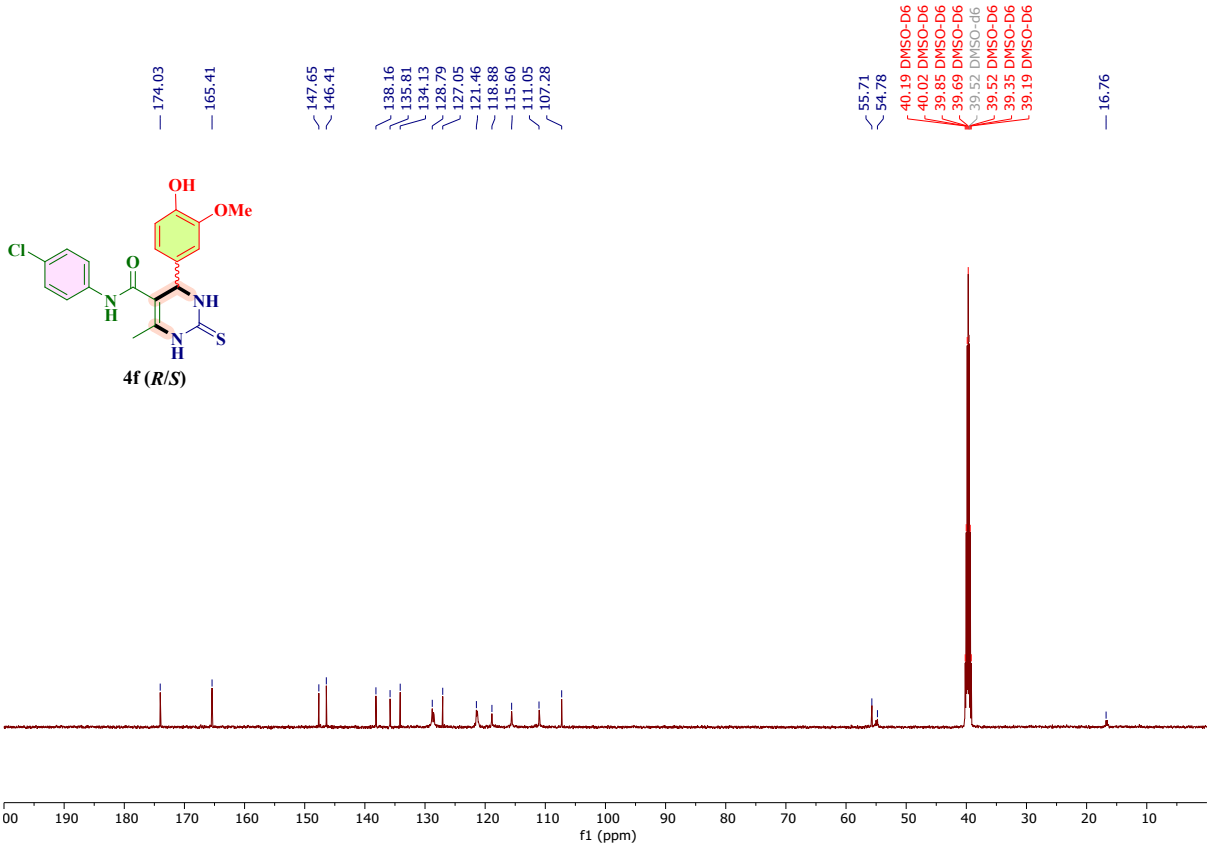


Figure S12: ^{13}C NMR of **4f** (***R*/*S***) (126 MHz, DMSO-d_6)

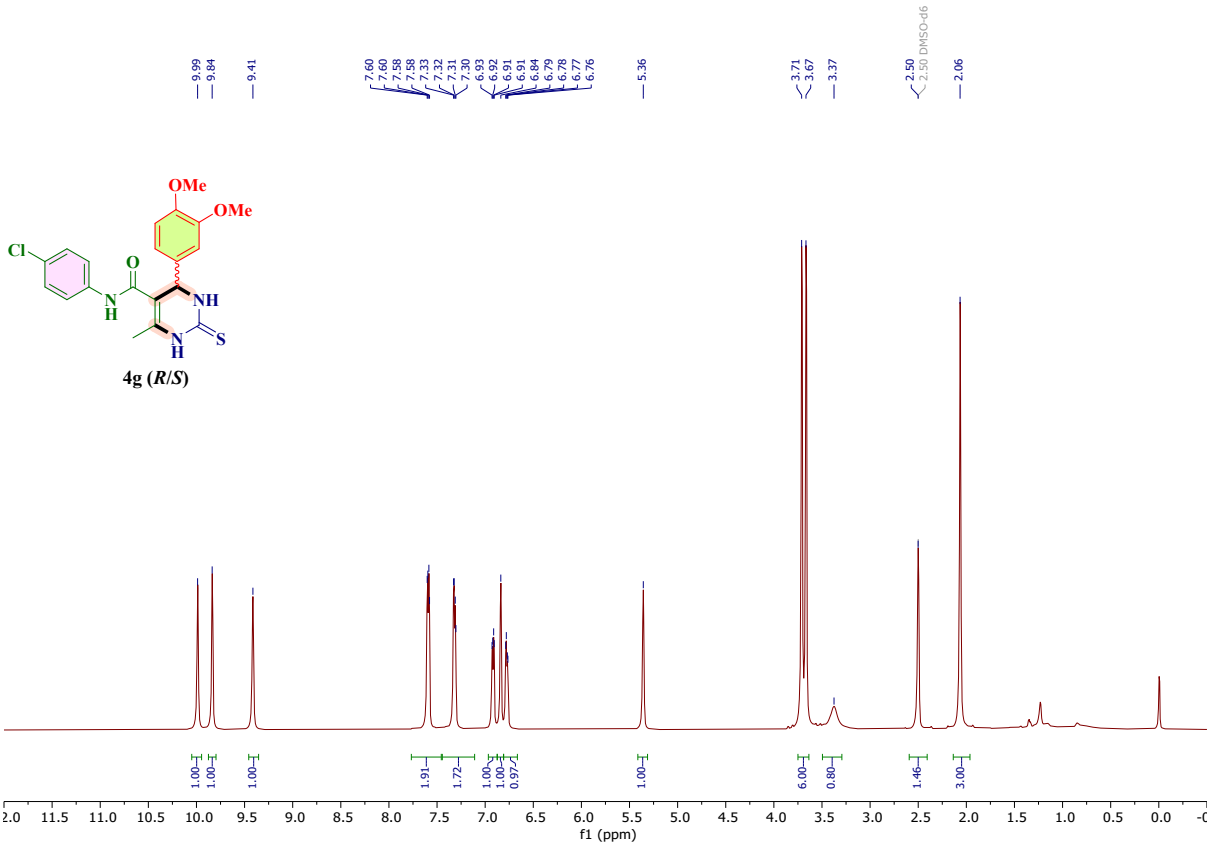


Figure S13: ^{1}H NMR spectra of **4g (*R*/*S*)** (500MHz, DMSO-d_6)

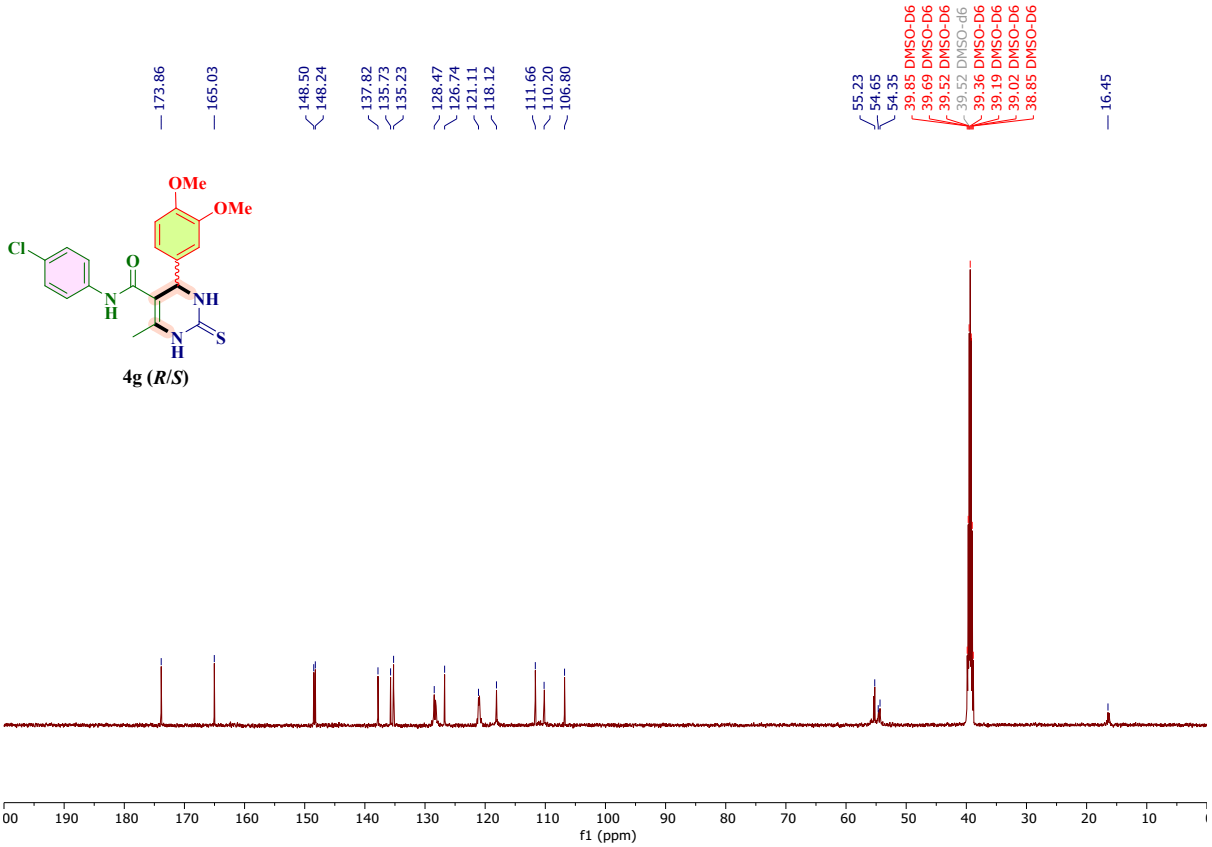


Figure S14: ^{13}C NMR of **4g** (***R*/*S***) (126 MHz, DMSO-d_6)

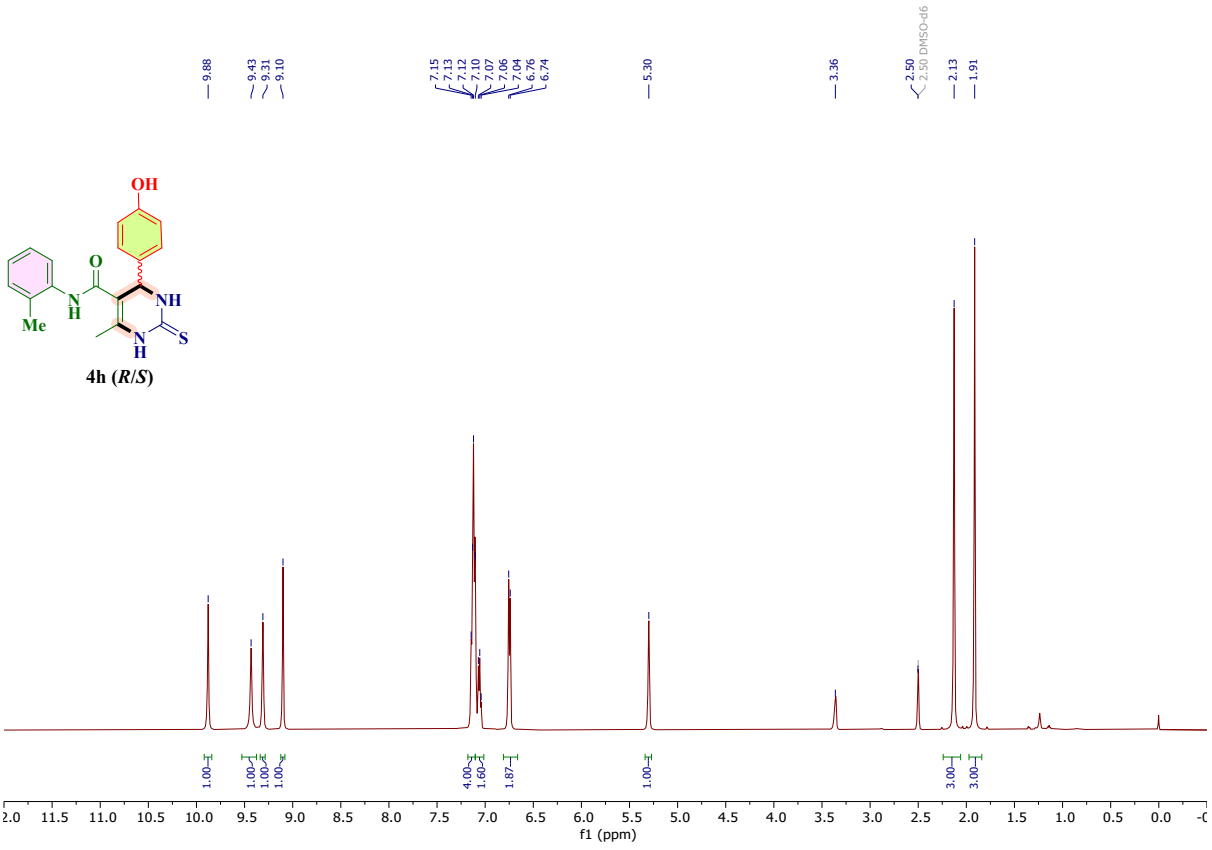


Figure S15: ^{1}H NMR spectra of **4h (*R*/*S*)** (500MHz, DMSO-d_6)

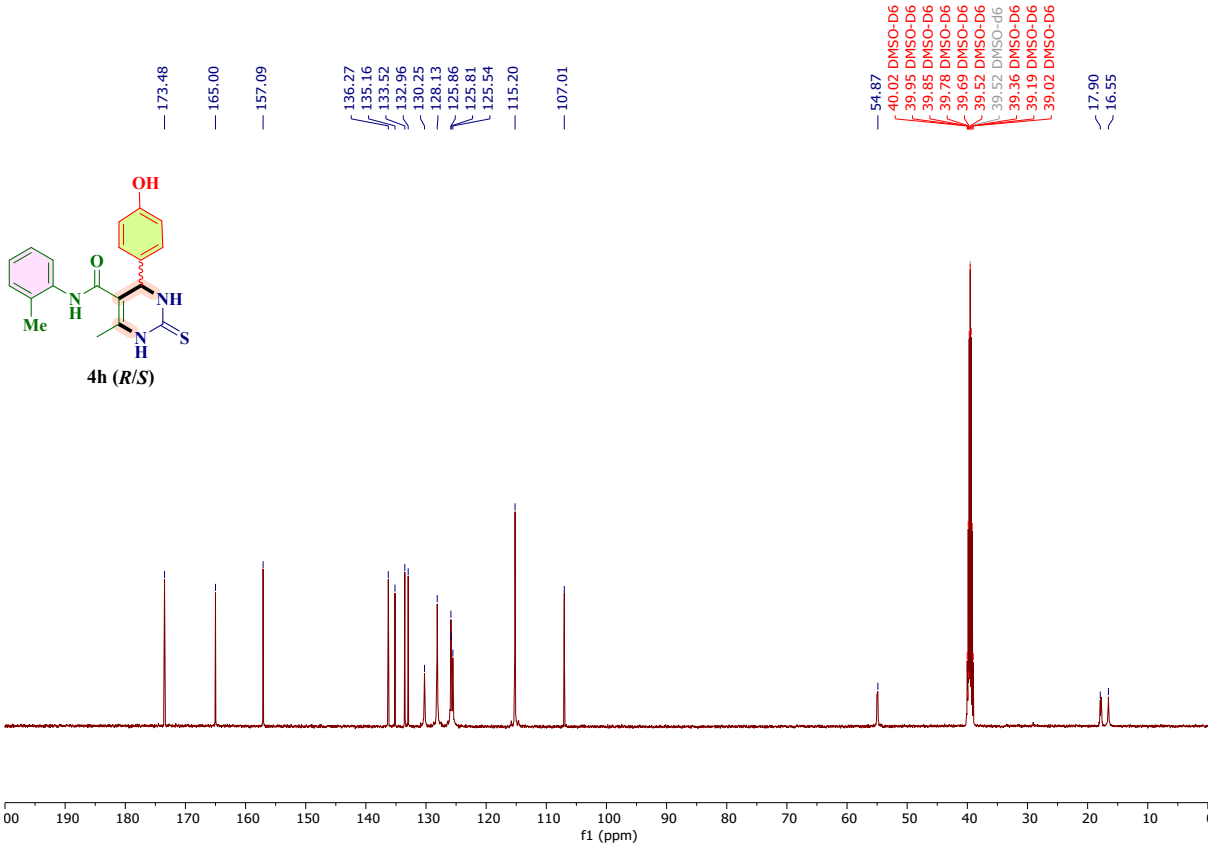


Figure S16: ^{13}C NMR of **4h** (***R*/*S***) (126 MHz, DMSO-d_6)

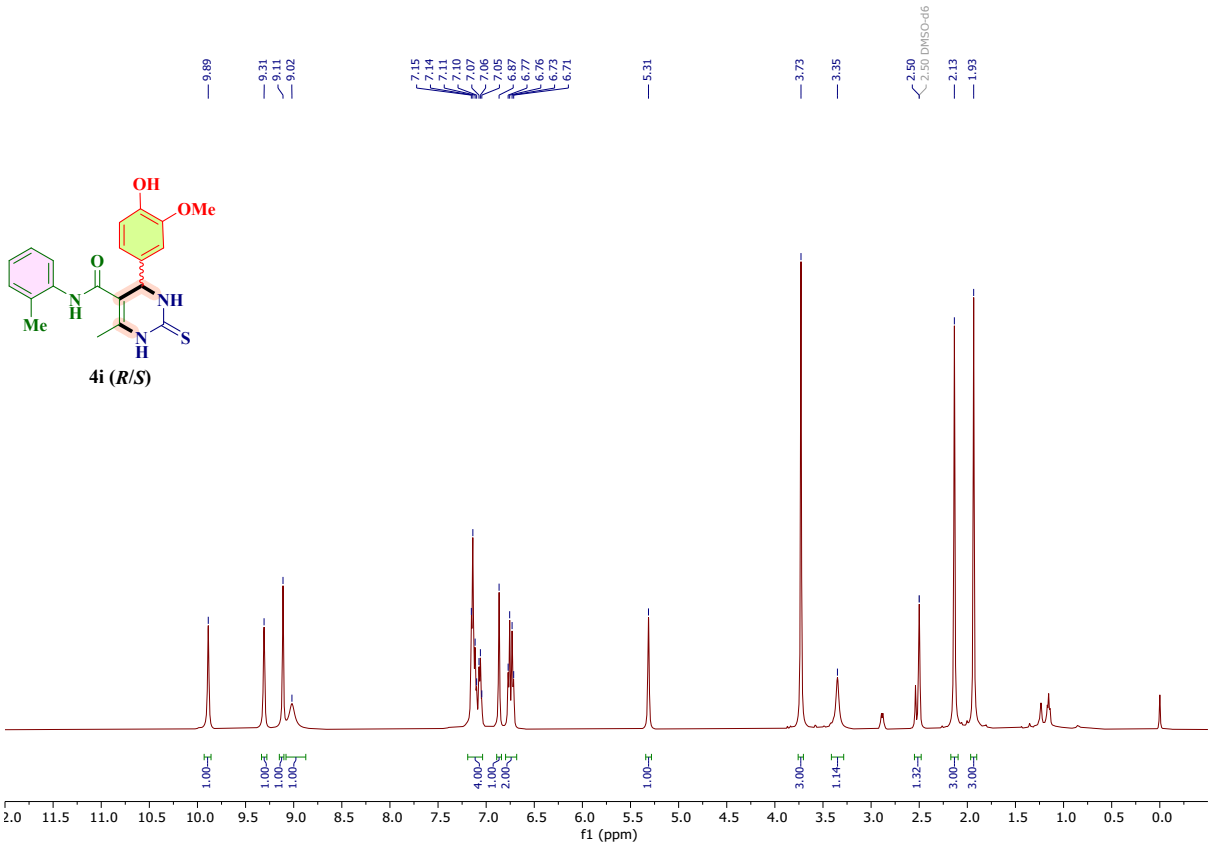


Figure S17: ^{1}H NMR spectra of **4i (*R*/*S*)** (500MHz, DMSO-d_6)

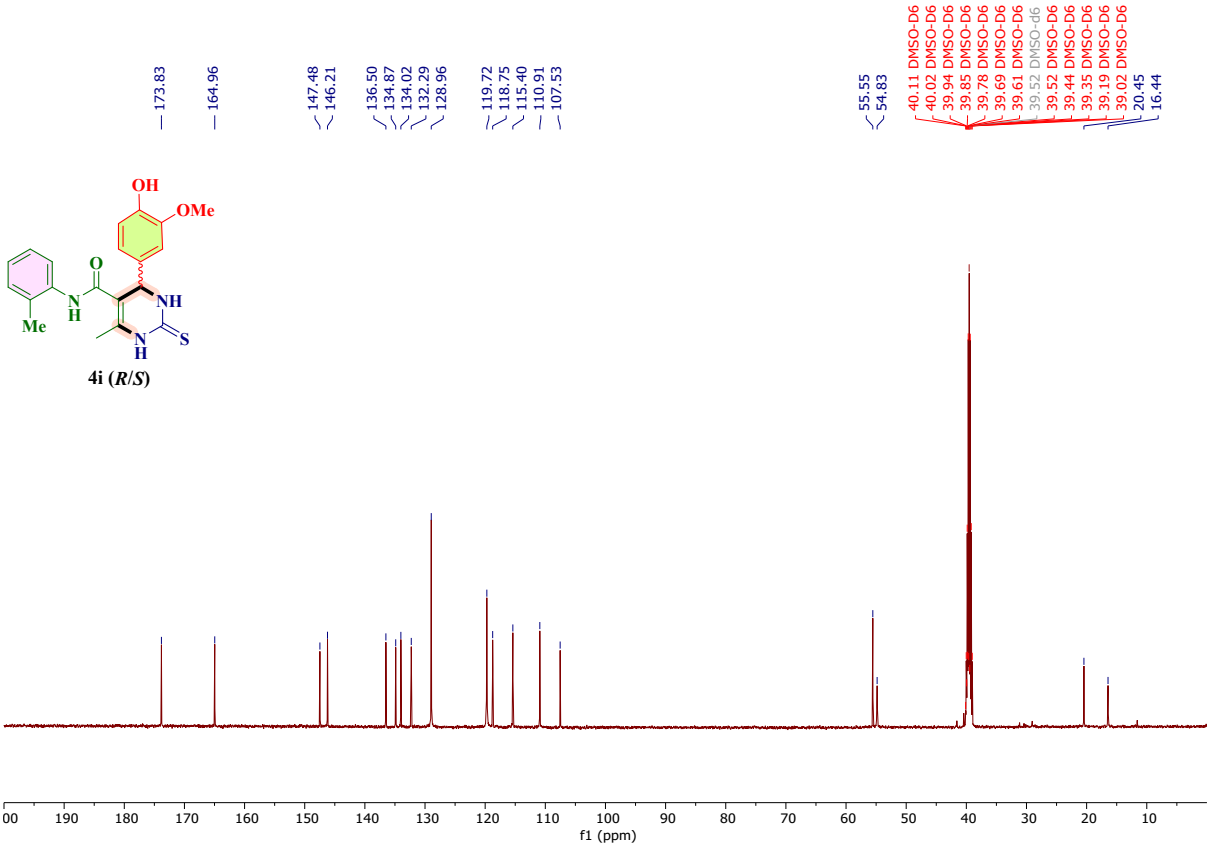


Figure S18: 13C NMR of **4i** (***R*/*S***) (126 MHz, DMSO-d_6)

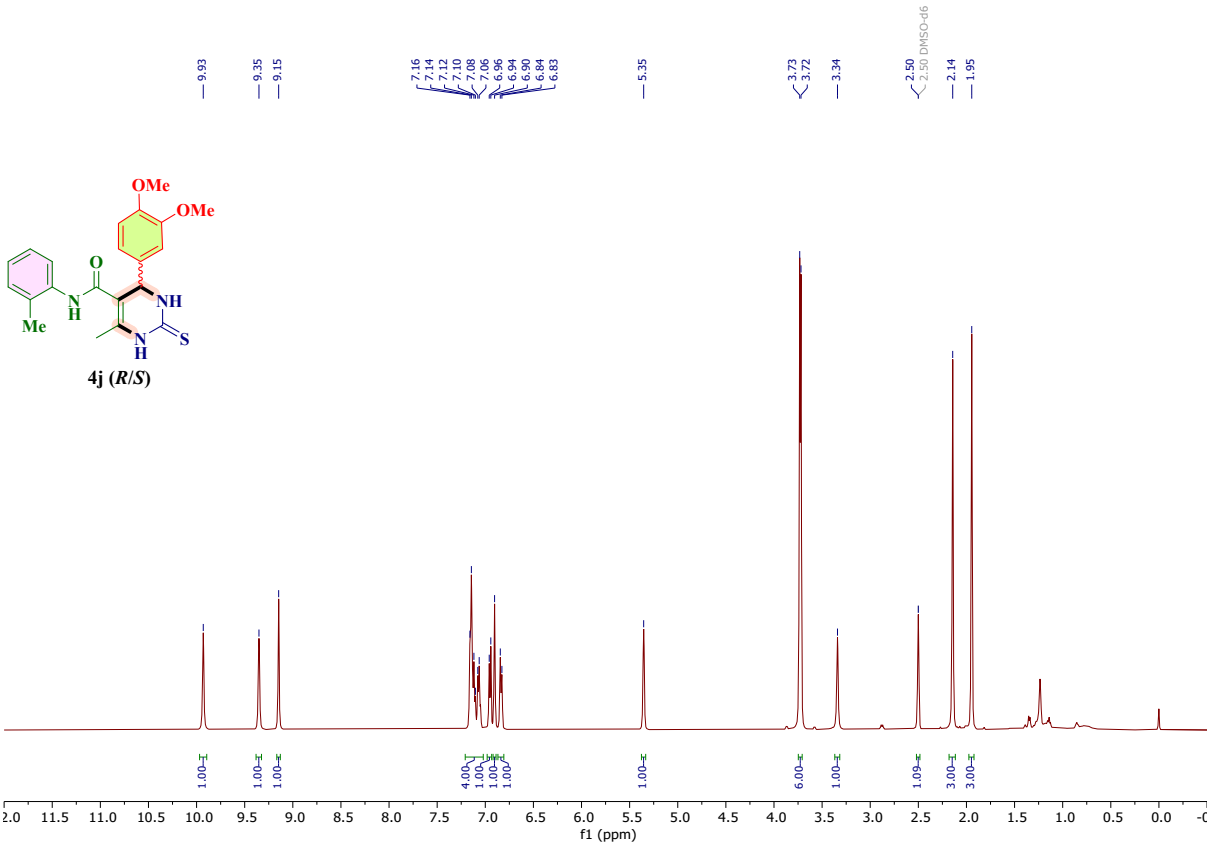


Figure S19: [1]H NMR spectra of **4j (*R*/*S*)** (500MHz, DMSO-d_6)

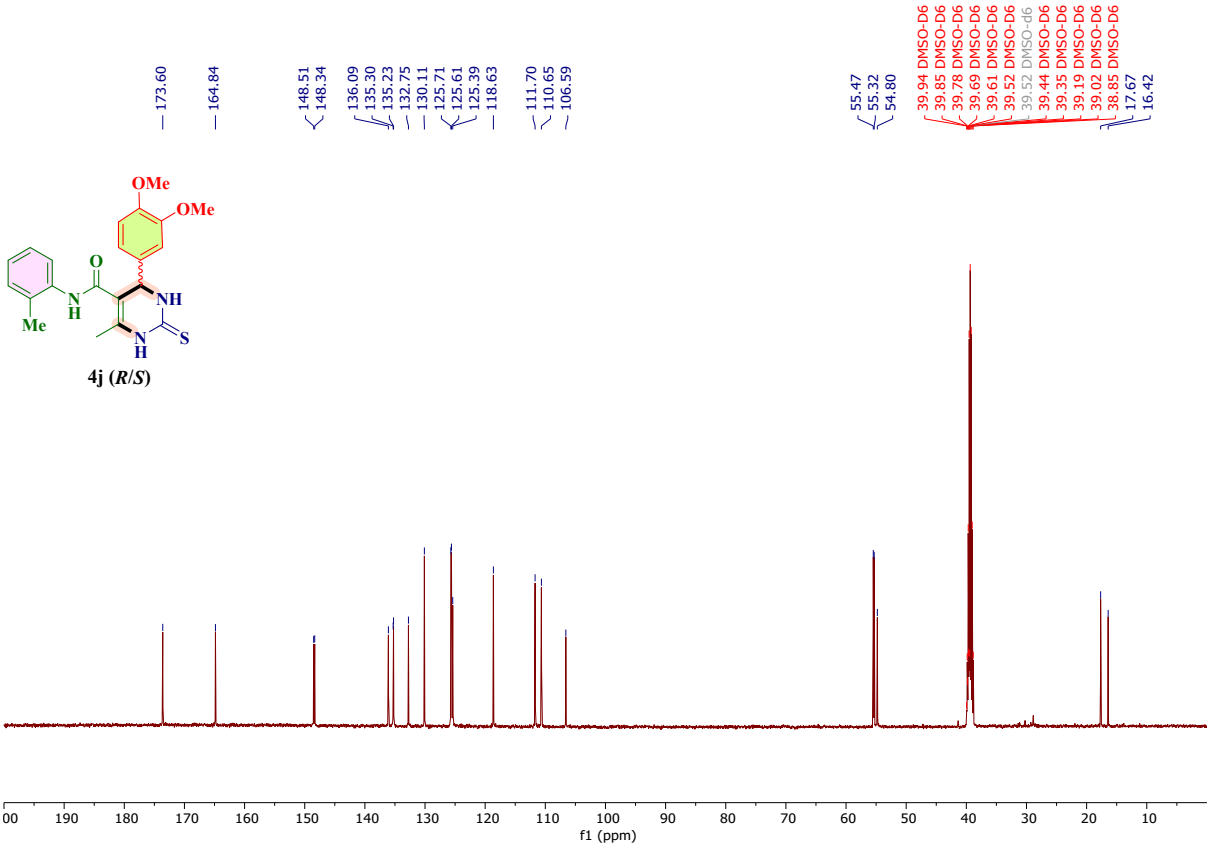


Figure S20: 13C NMR of **4j** (***R*/*S***) (126 MHz, DMSO-d_6)

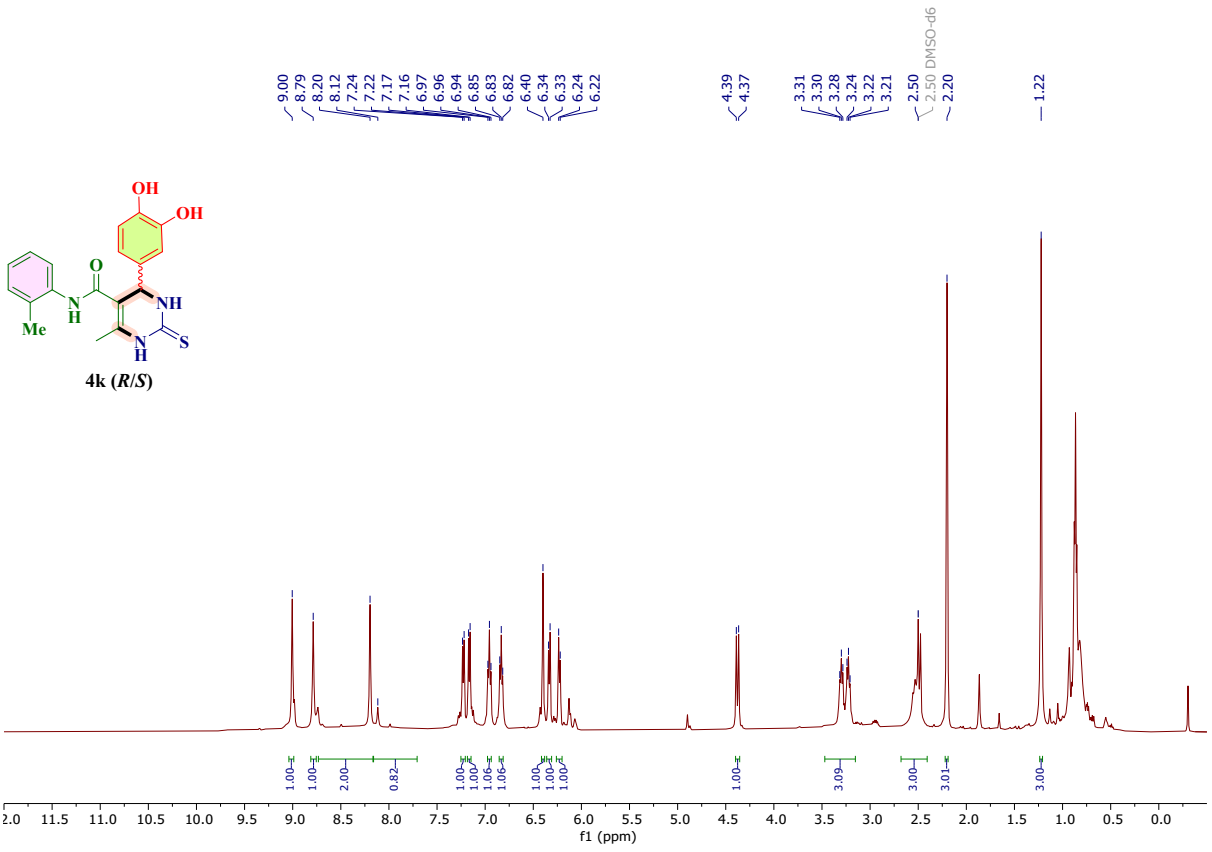


Figure S21: ^{1}H NMR spectra of **4k (*R*/*S*)** (500MHz, DMSO-d_6)

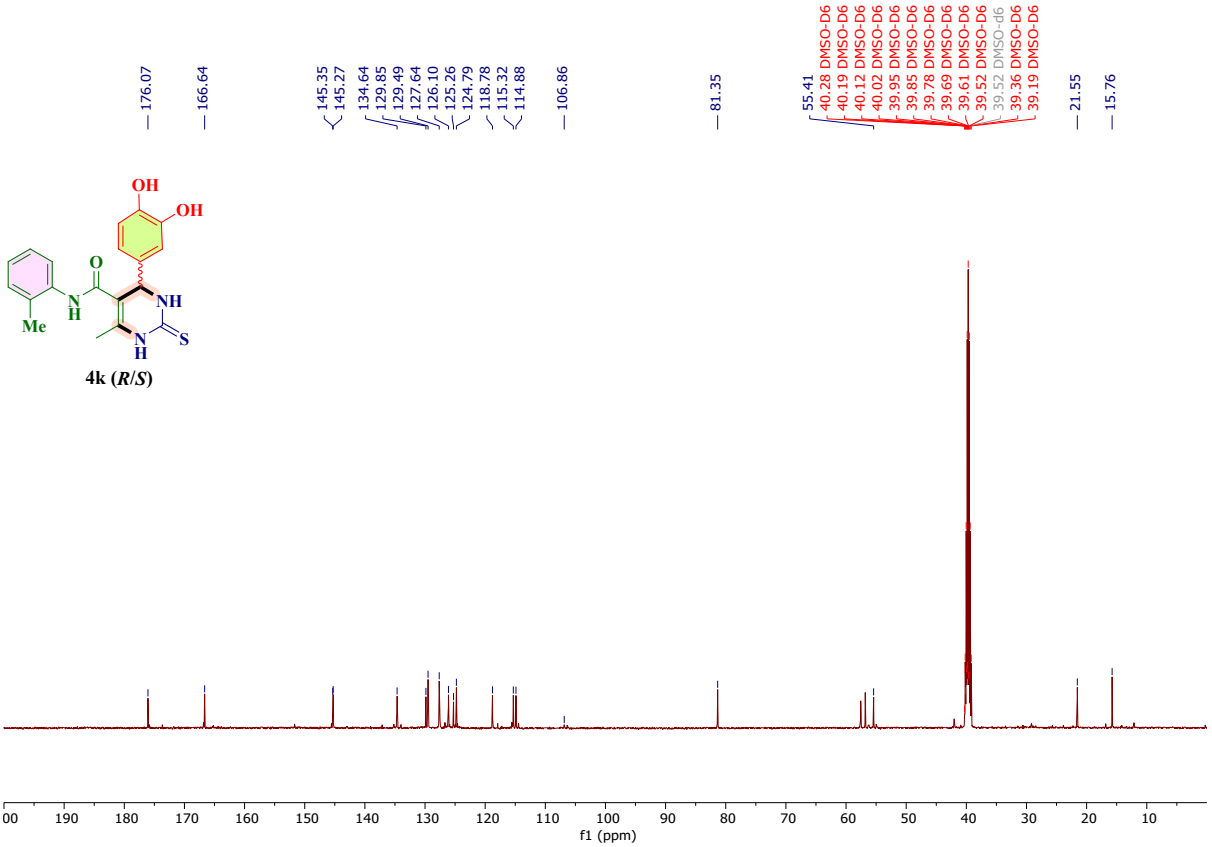


Figure S22: 13C NMR of **4k** (***R***/***S***) (126 MHz, DMSO-d_6)

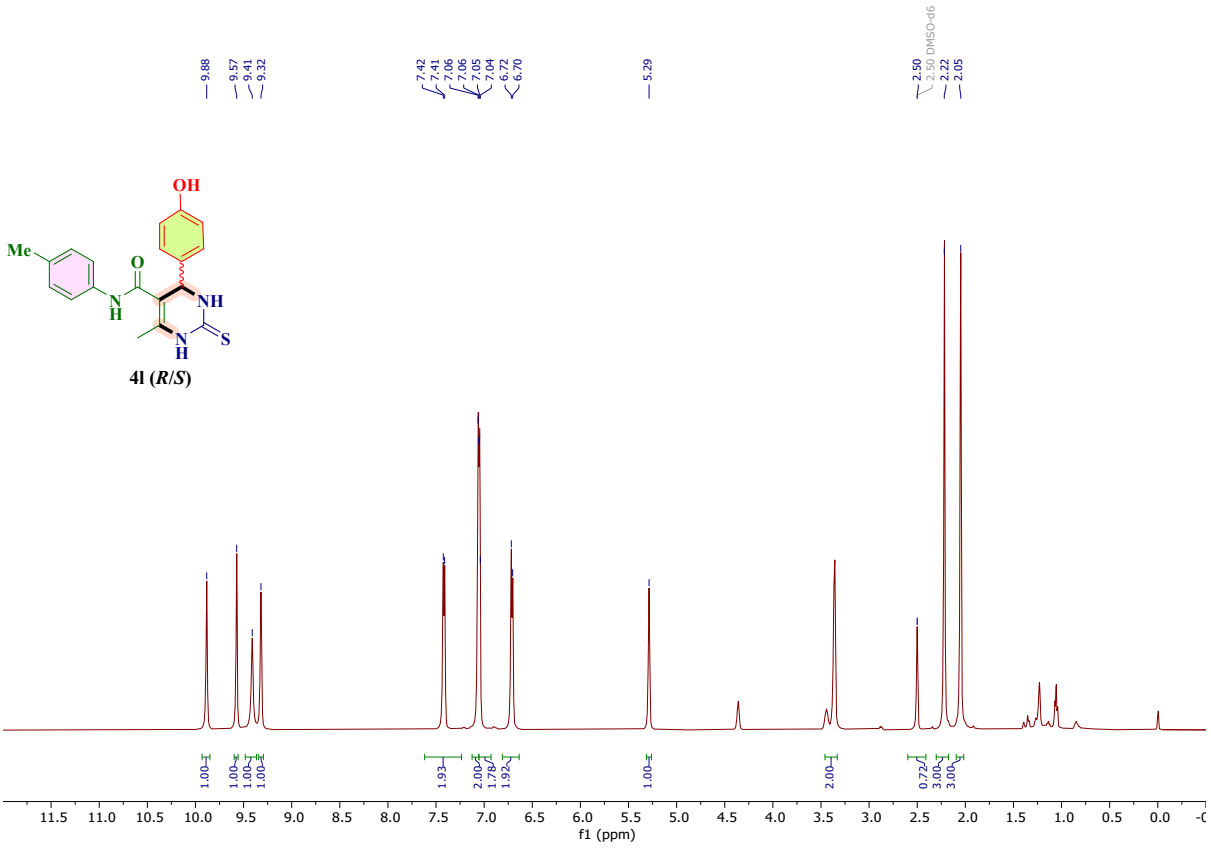


Figure S23: ^{1}H NMR spectra of **4l (*R*/*S*)** (500MHz, DMSO-d_6)

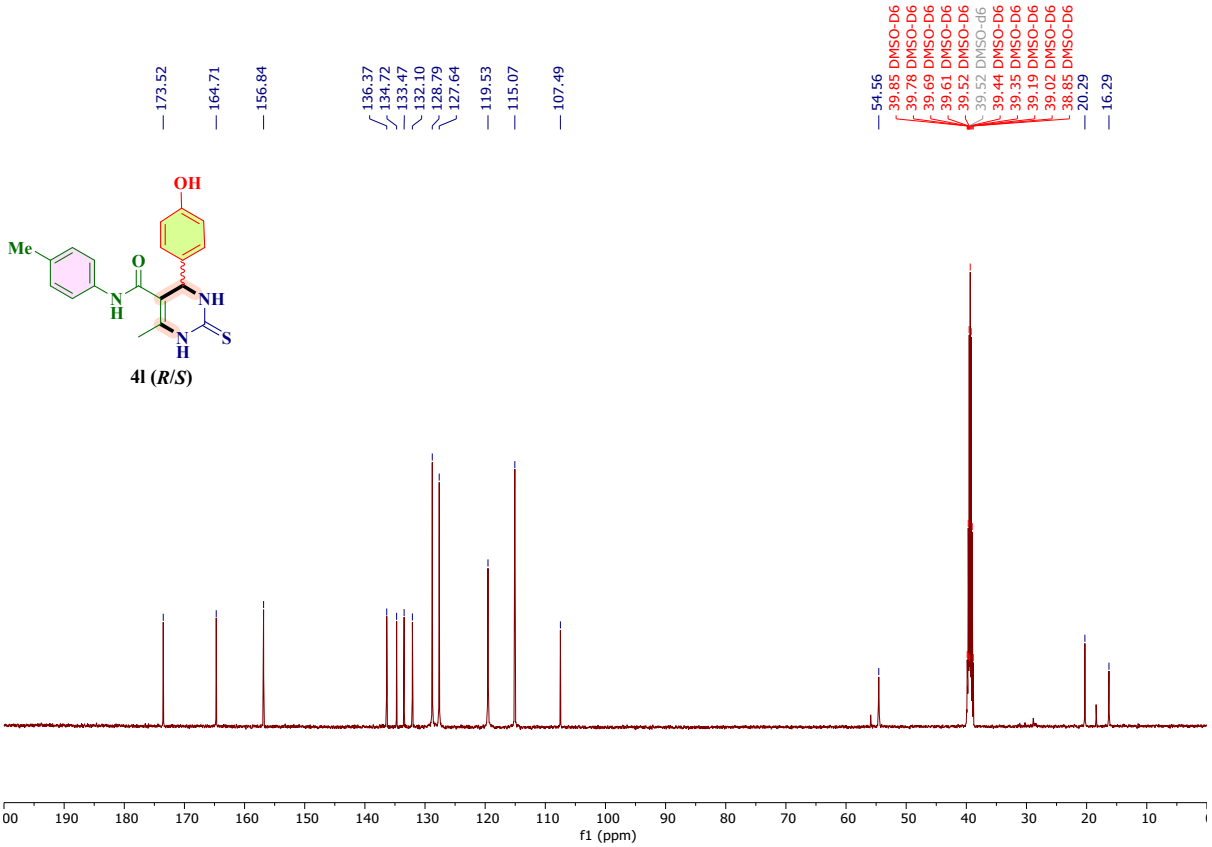


Figure S24: ^{13}C NMR of **4l** (***R*/*S***) (126 MHz, DMSO-d_6)

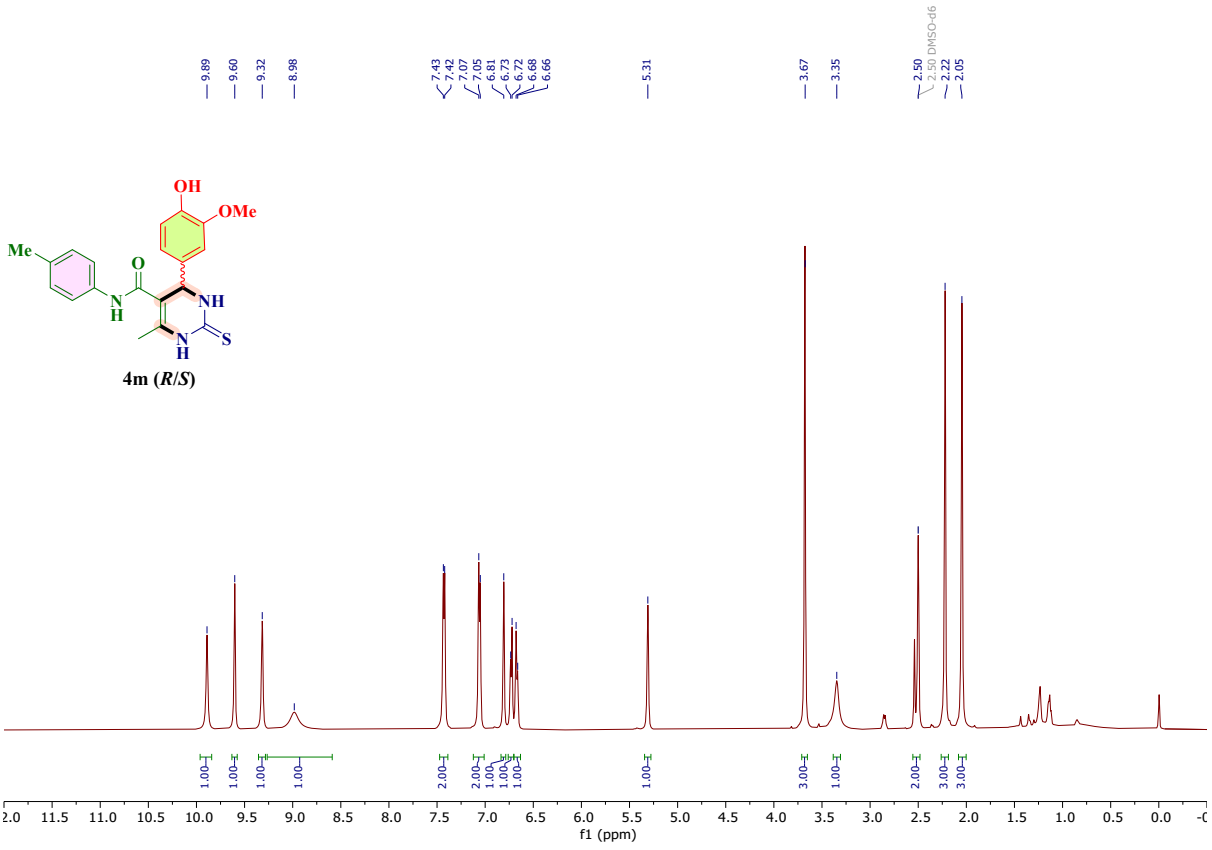


Figure S25: ^{1}H NMR spectra of **4m (*R*/*S*)** (500MHz, DMSO-d_6)

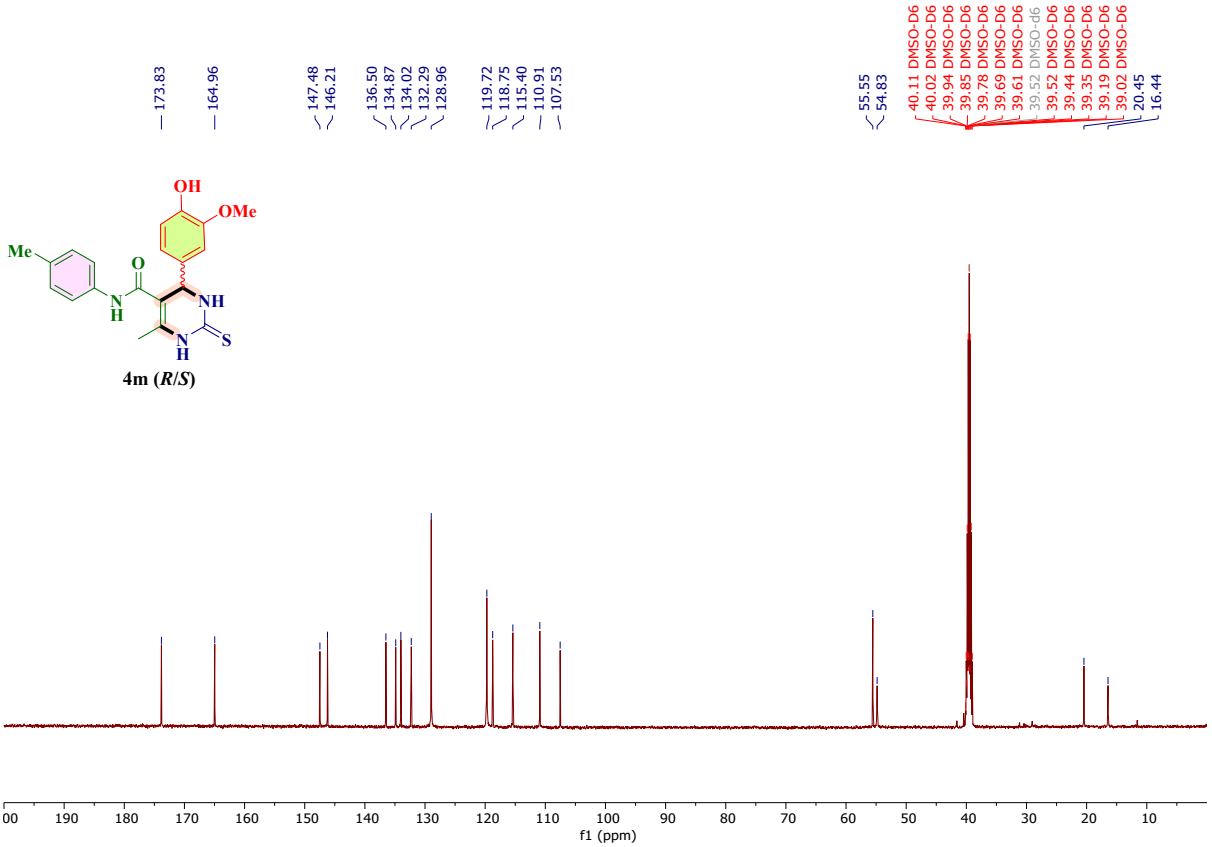


Figure S26: ^{13}C NMR of **4m** (***R*/*S***) (126 MHz, DMSO-d_6)

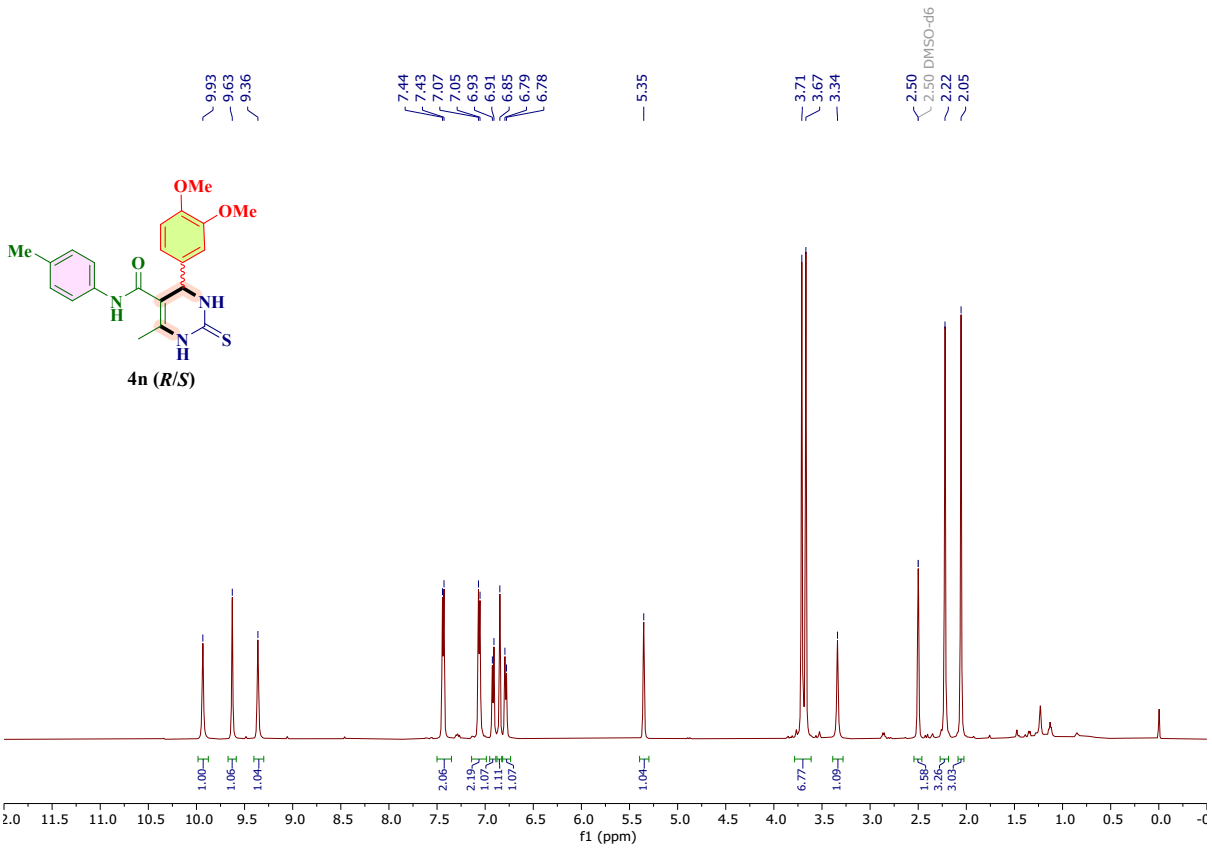


Figure S27: ^{1}H NMR spectra of **4n (*R*/*S*)** (500MHz, DMSO-d_6)

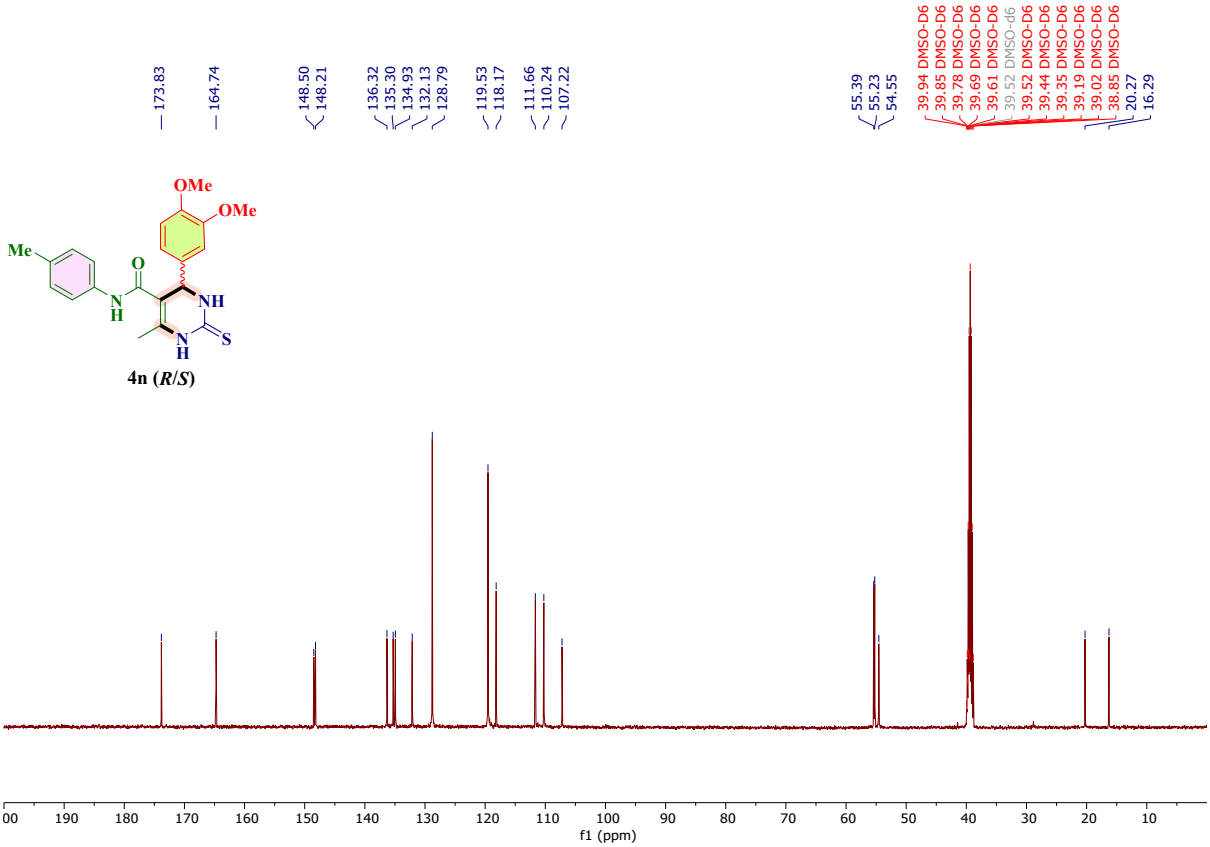


Figure S28: ^{13}C NMR of **4n** (***R*/*S***) (126 MHz, DMSO-d_6)

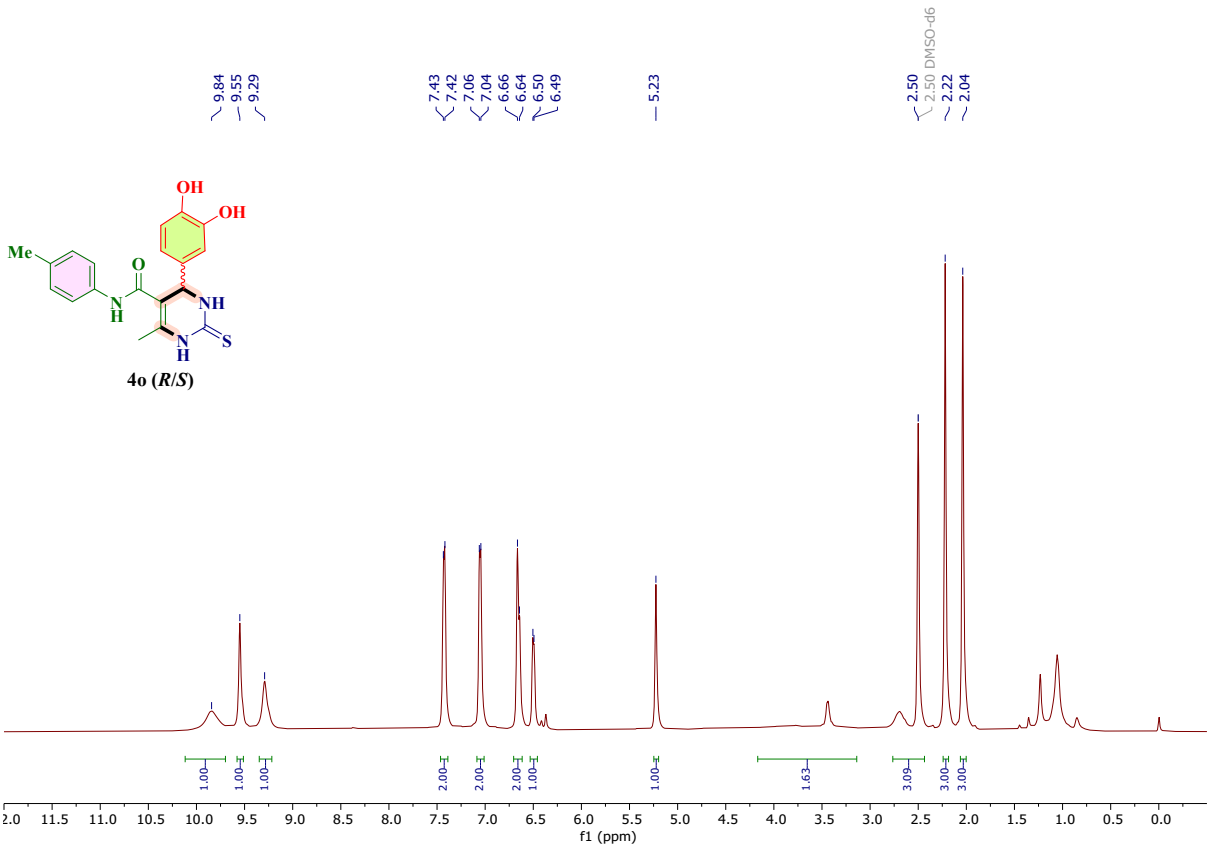


Figure S29: ^{1}H NMR spectra of **4o (*R*/*S*)** (500MHz, DMSO-d_6)

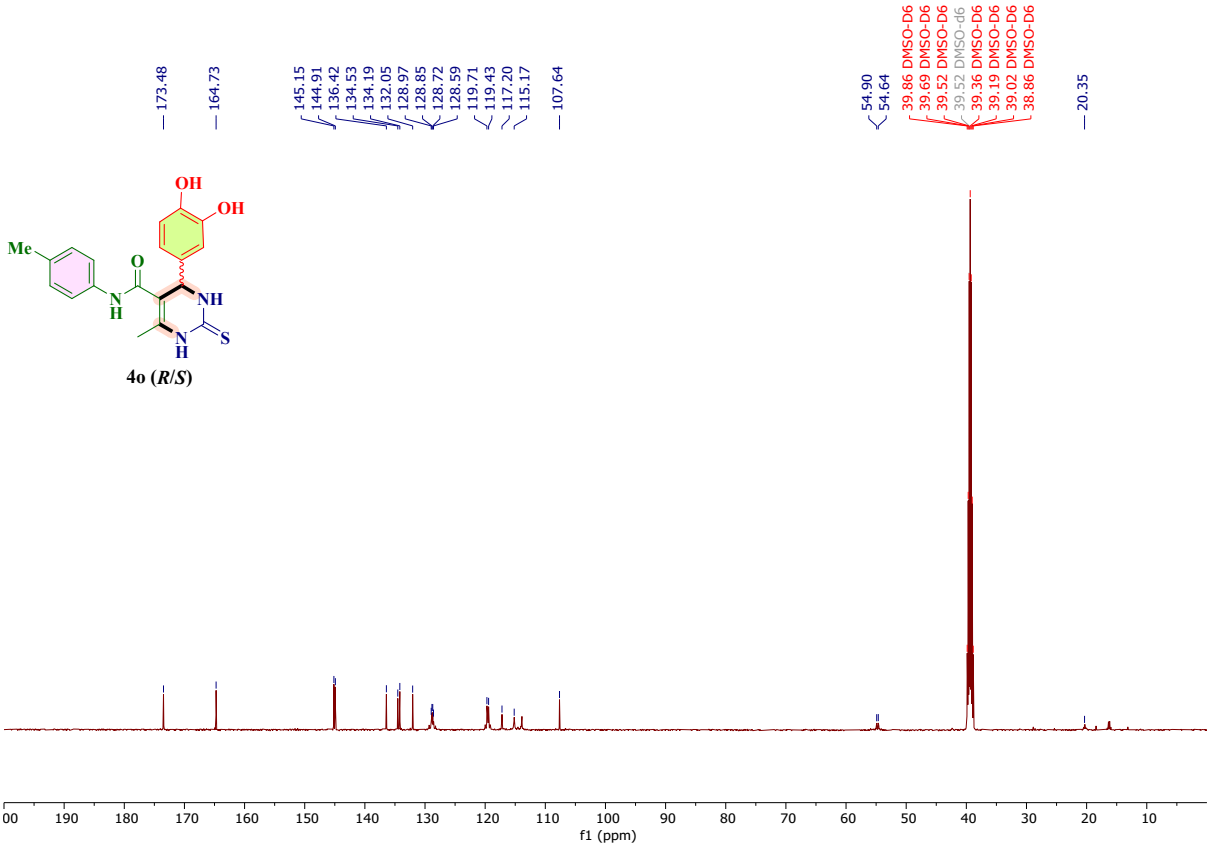


Figure S30: ^{13}C NMR of **4o** (***R***/***S***) (126 MHz, DMSO-d_6)

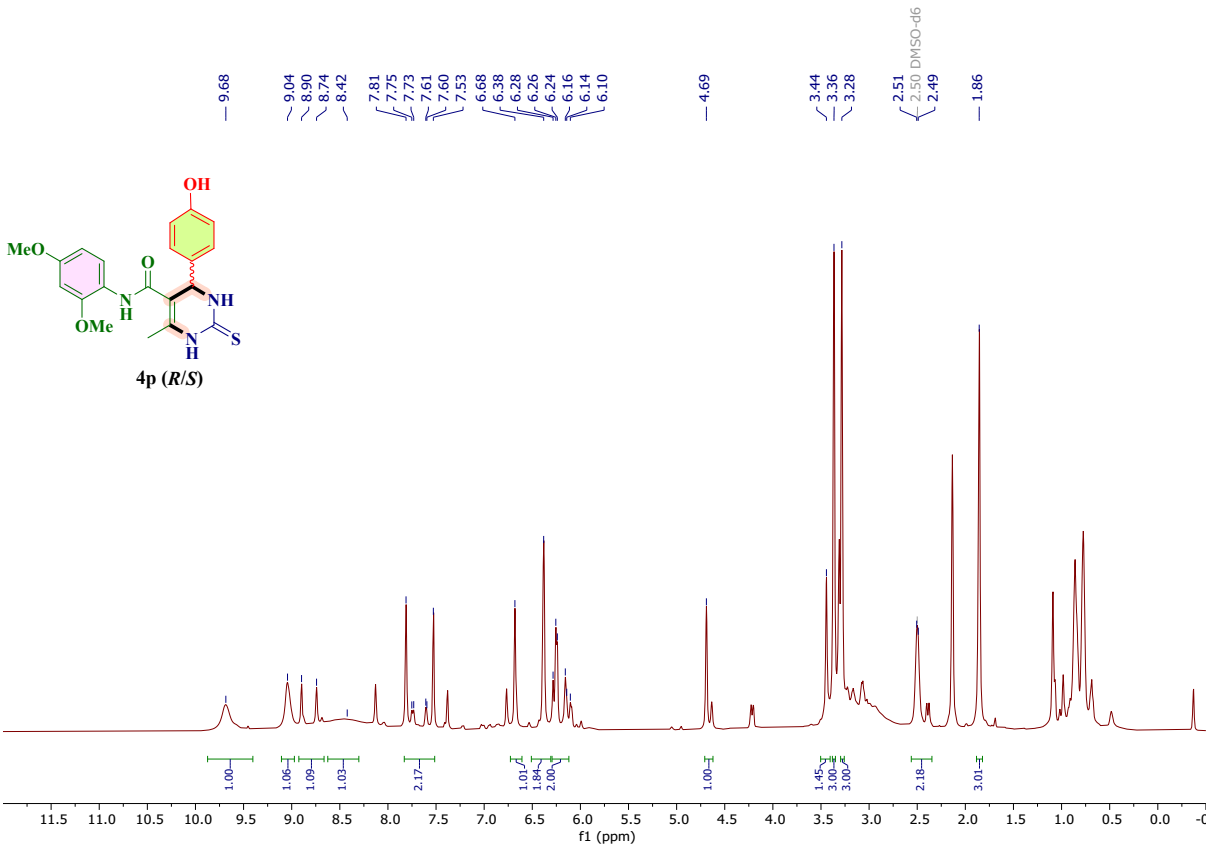


Figure S31: ^{1}H NMR spectra of **4p (*R*/*S*)** (500MHz, DMSO-d_6)

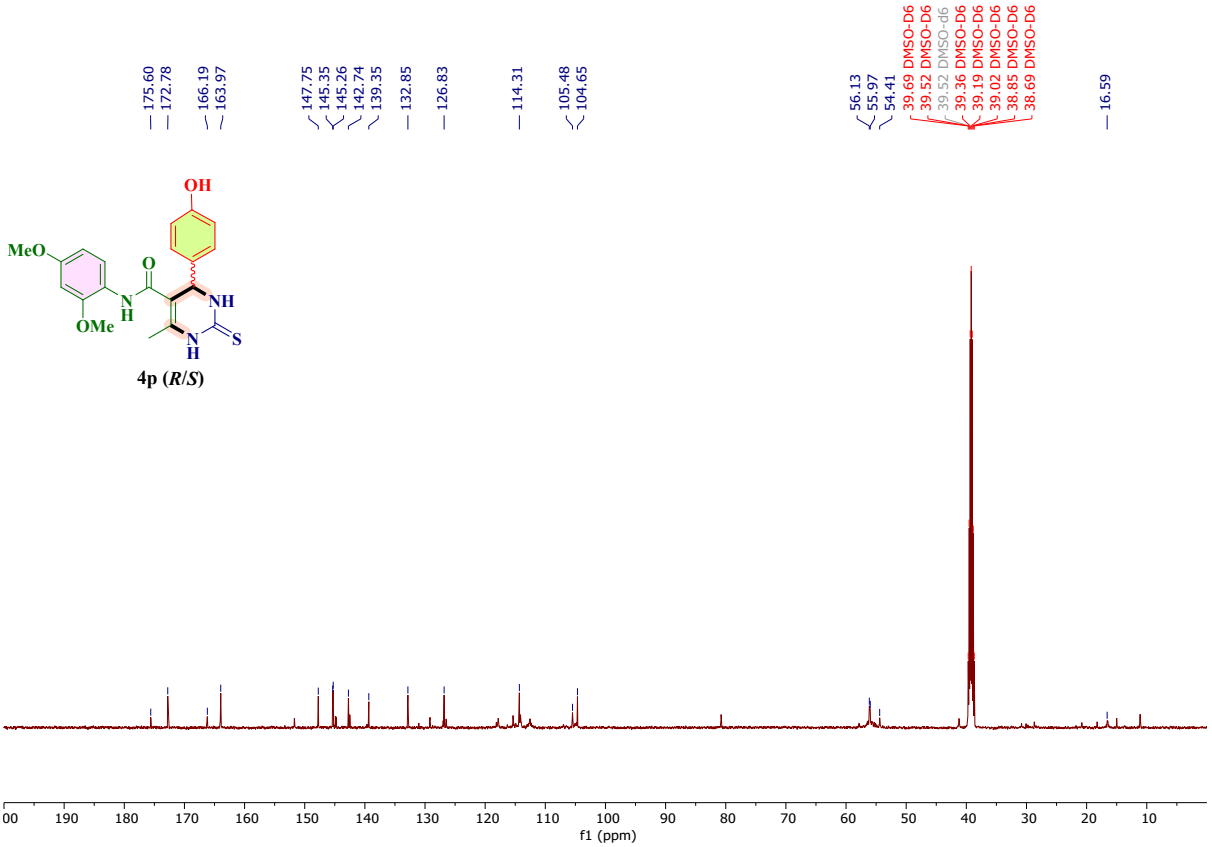


Figure S32: ^{13}C NMR of **4p** (***R*/*S***) (126 MHz, DMSO-d_6)

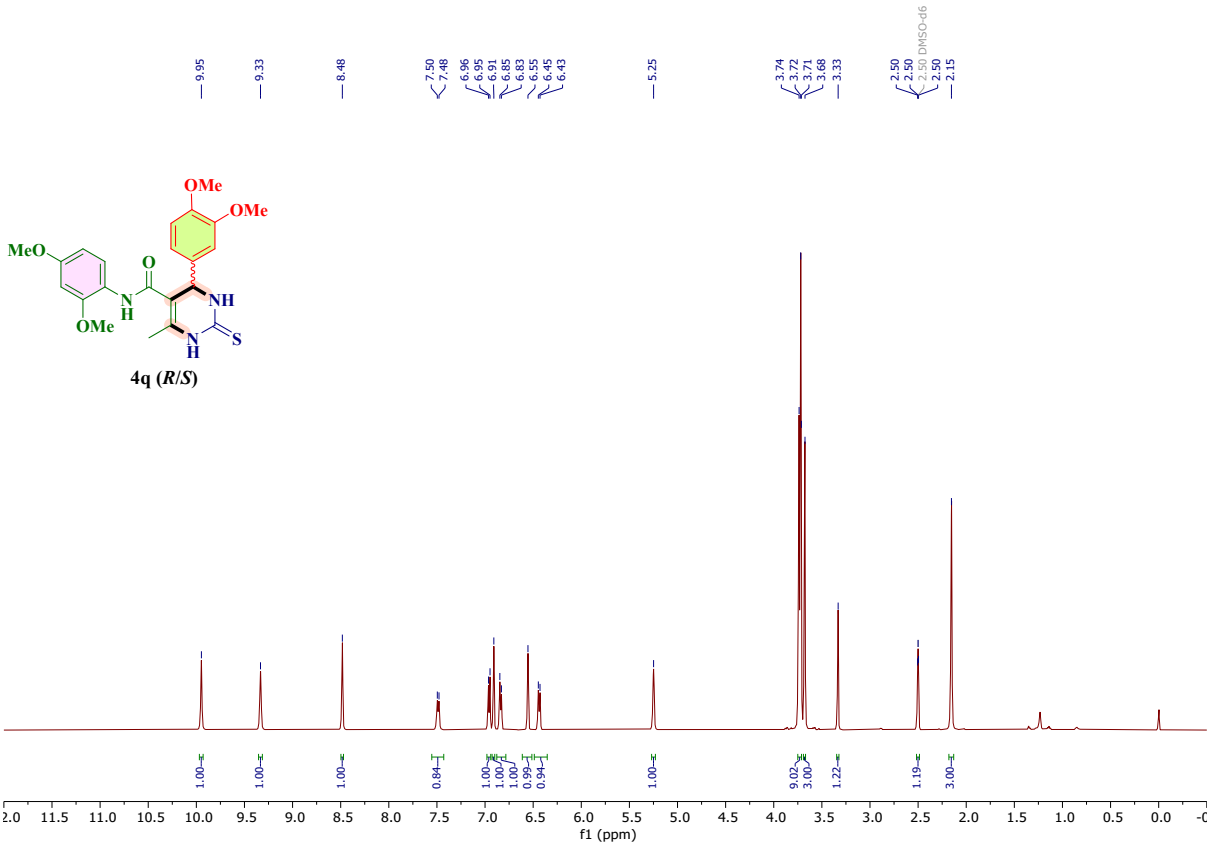


Figure S33: ^{1}H NMR spectra of **4q (*R*/*S*)** (500MHz, DMSO-d_6)

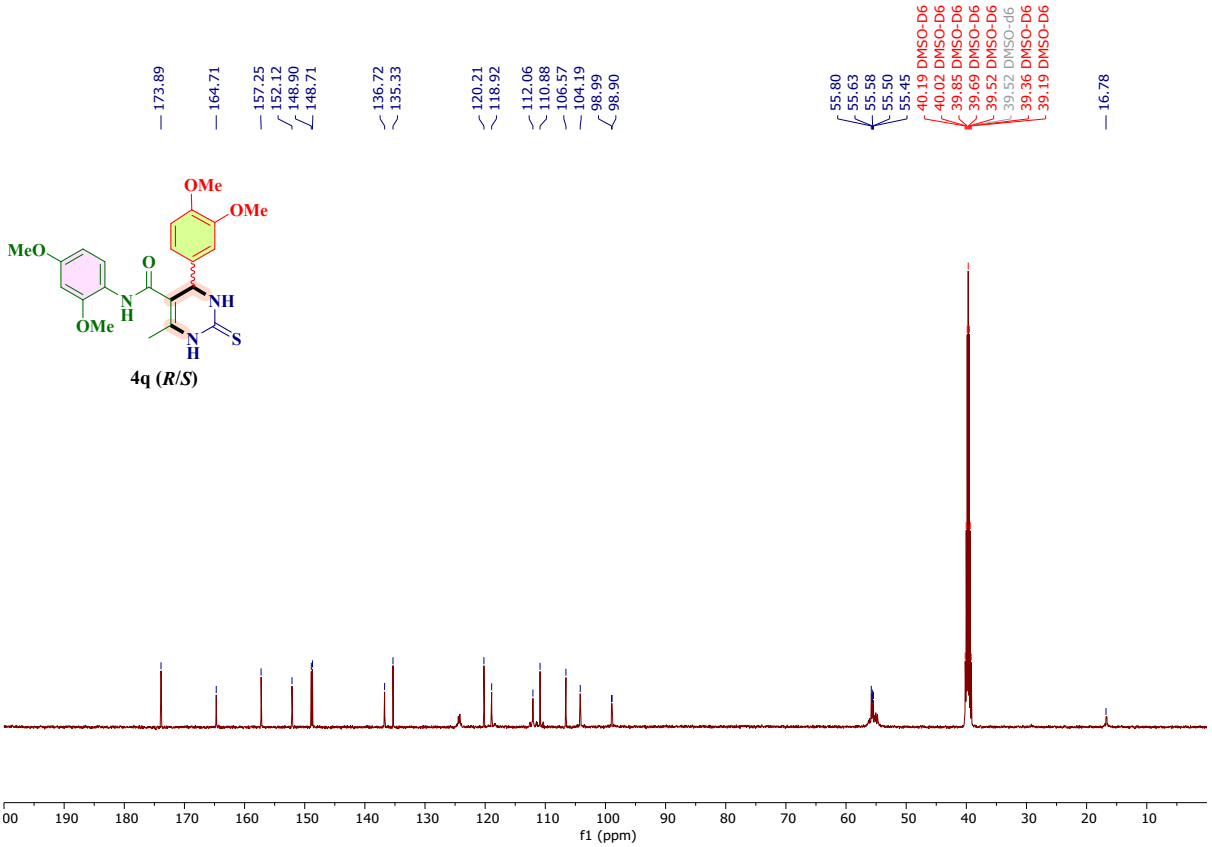


Figure S34: ^{13}C NMR of **4q** (***R*/*S***) (126 MHz, DMSO-d_6)

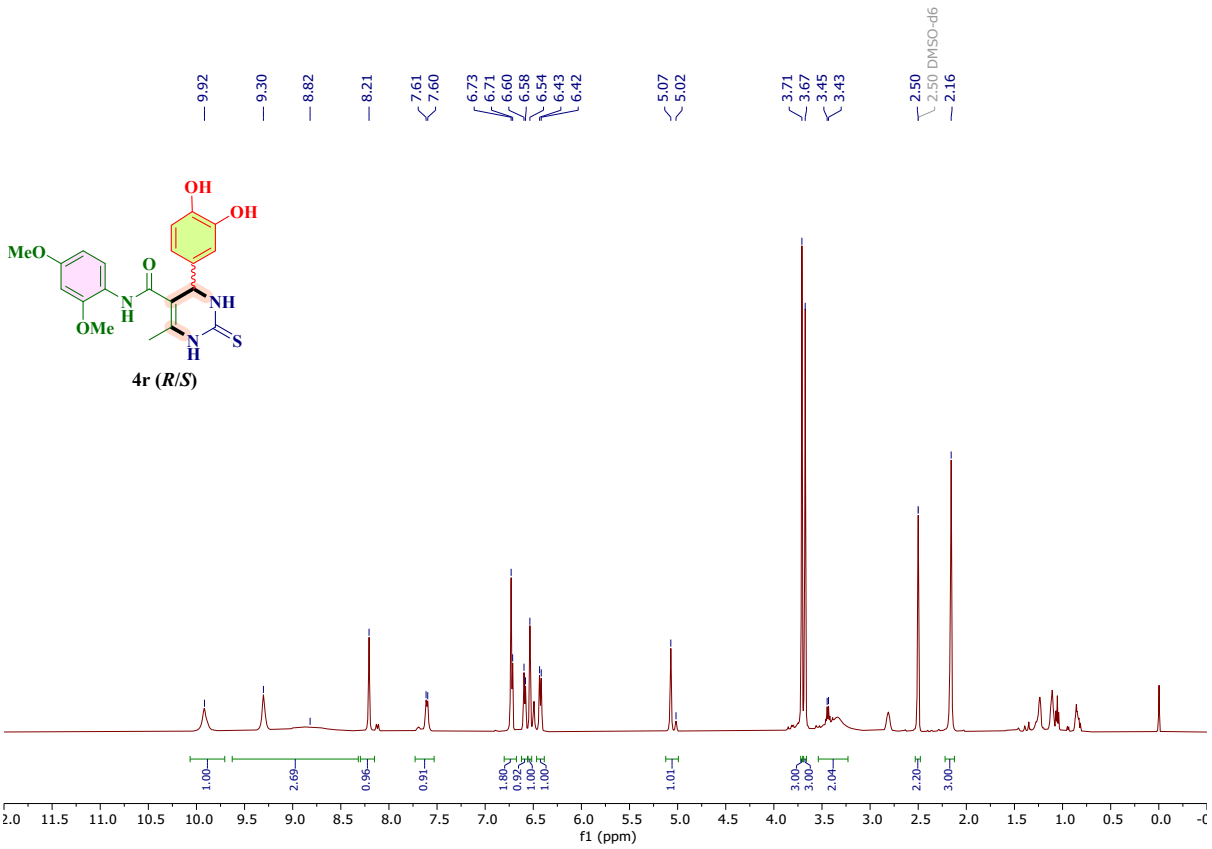


Figure S35: ^{1}H NMR spectra of **4r (*R*/*S*)** (500MHz, DMSO-d_6)

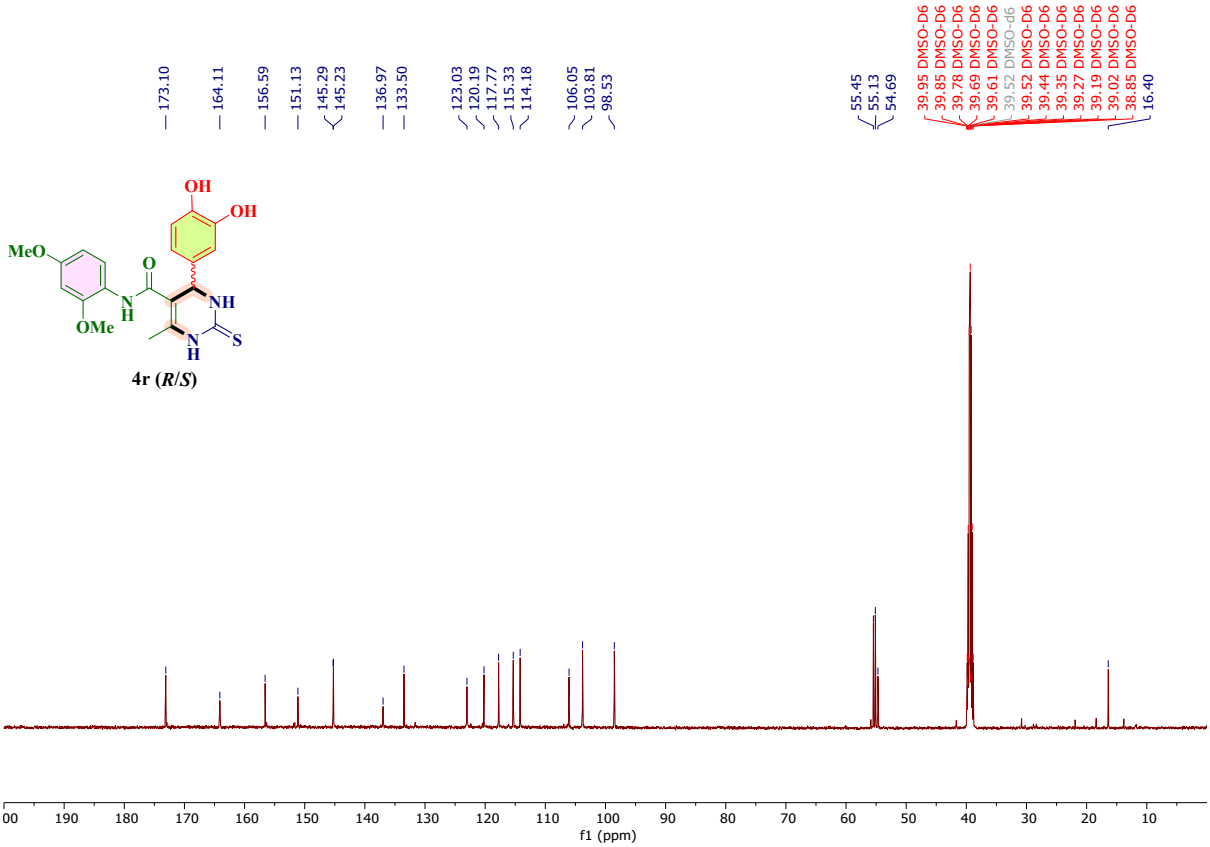


Figure S36: ^{13}C NMR of **4r** (***R*/*S***) (126 MHz, DMSO-d_6)

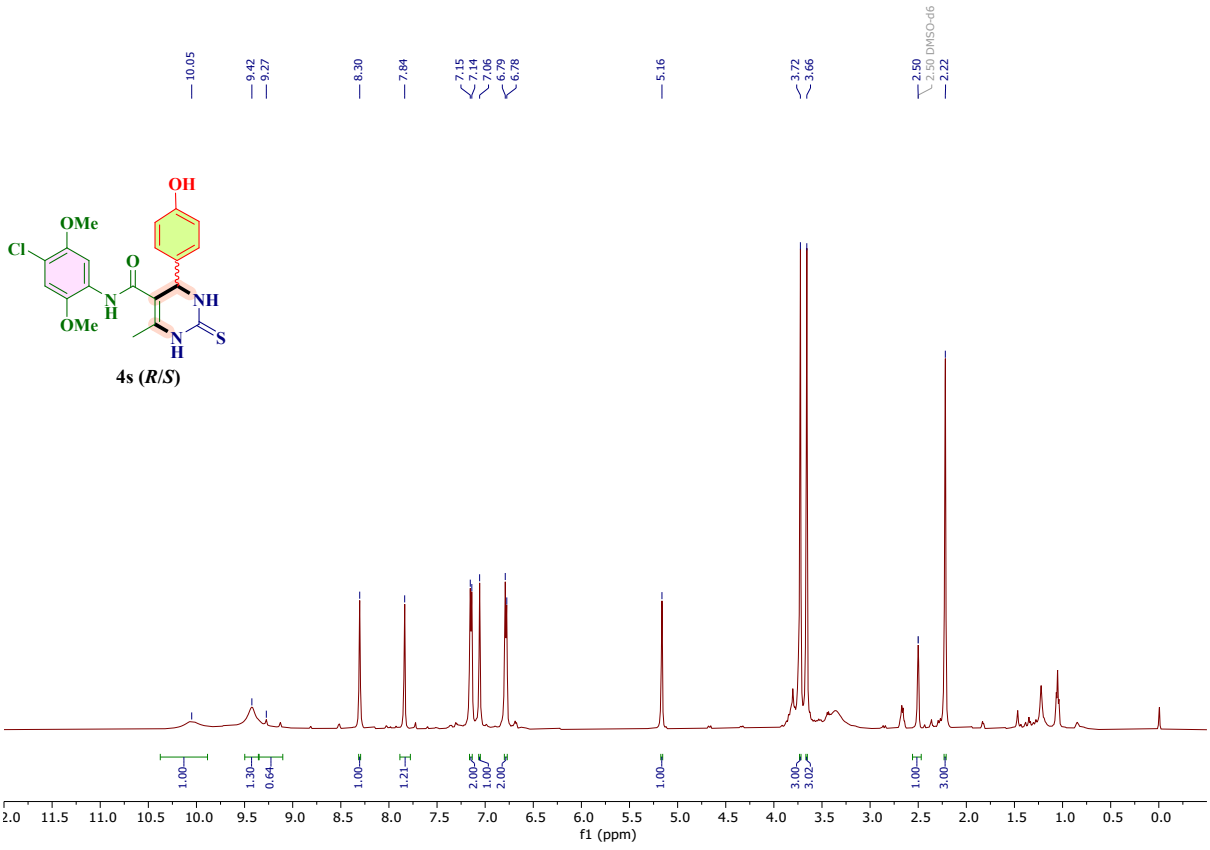


Figure S37: ^{1}H NMR spectra of **4s (*R*/*S*)** (500MHz, DMSO-d_6)

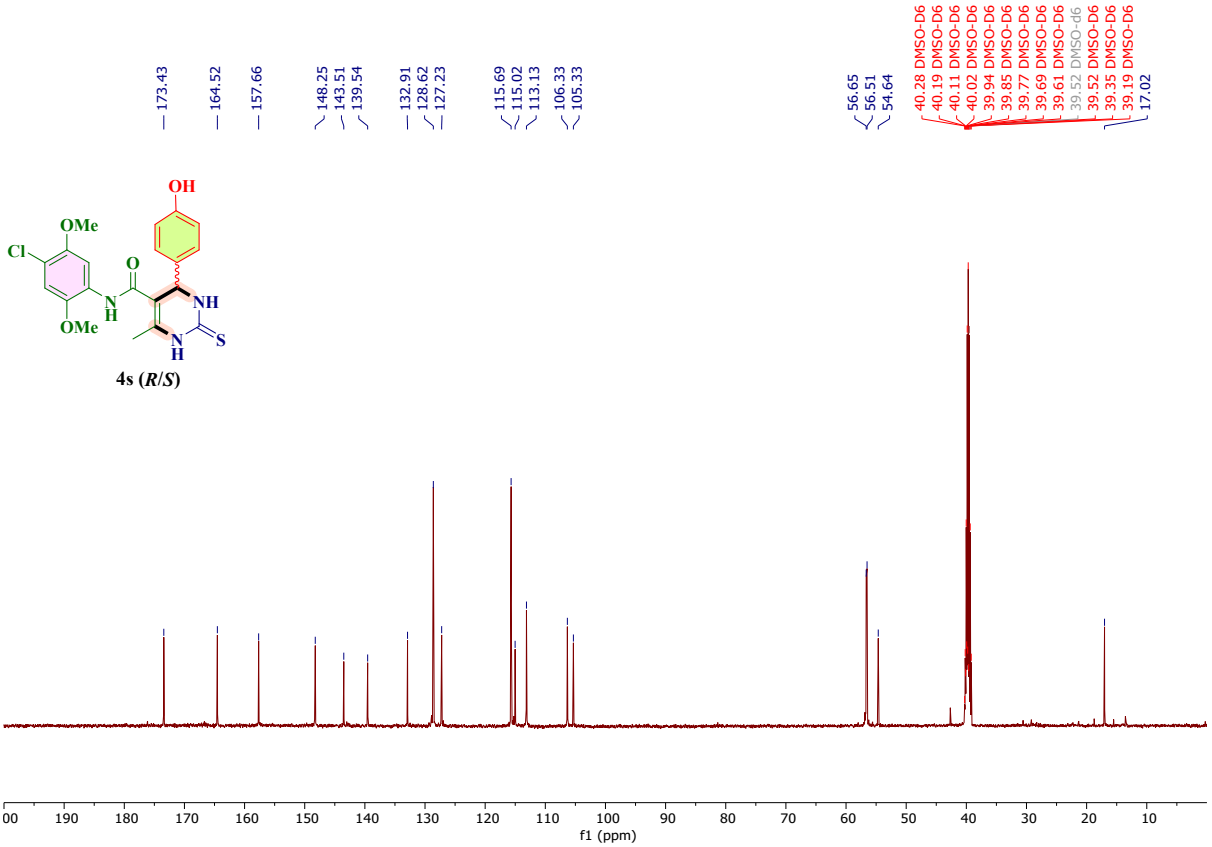


Figure S38: ^{13}C NMR of **4s** (***R*/*S***) (126 MHz, DMSO-d_6)

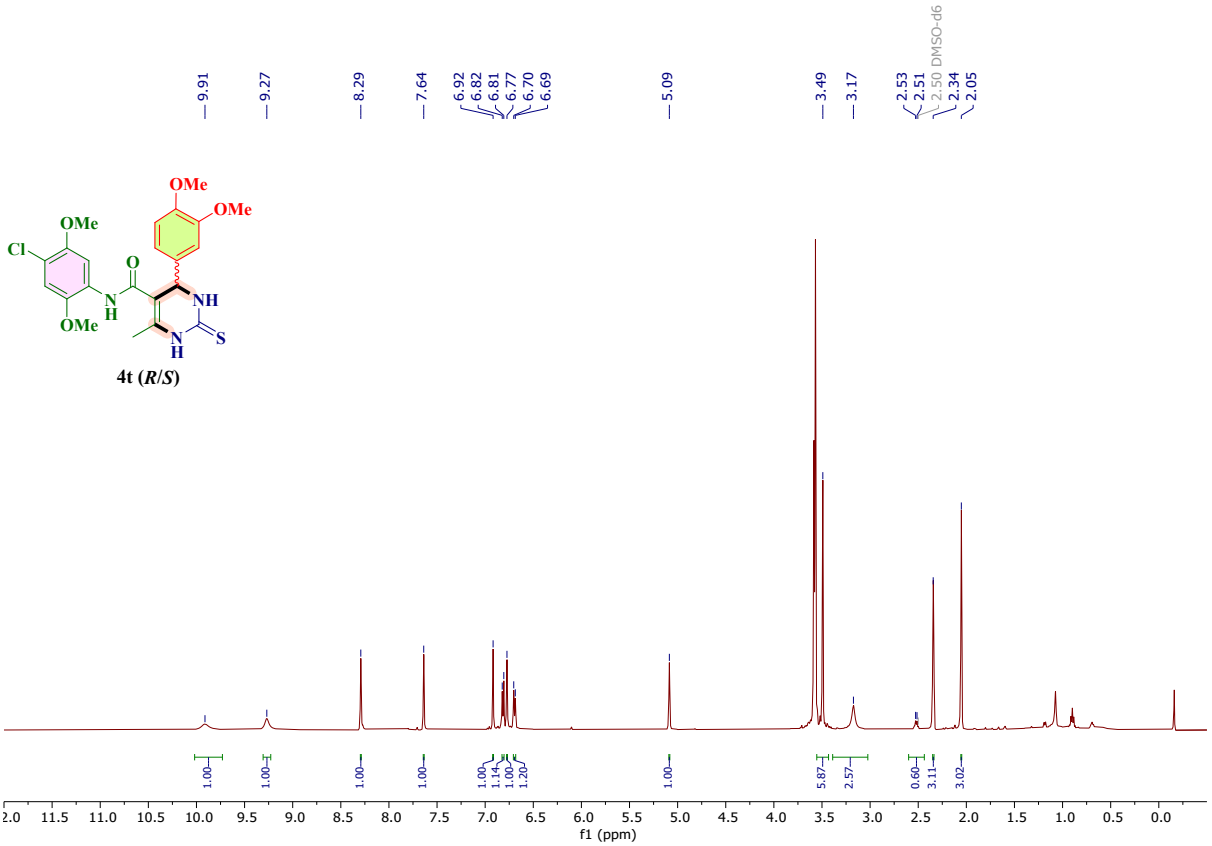


Figure S39: ^{1}H NMR spectra of **4t (*R*/*S*)** (500MHz, DMSO-d_6)

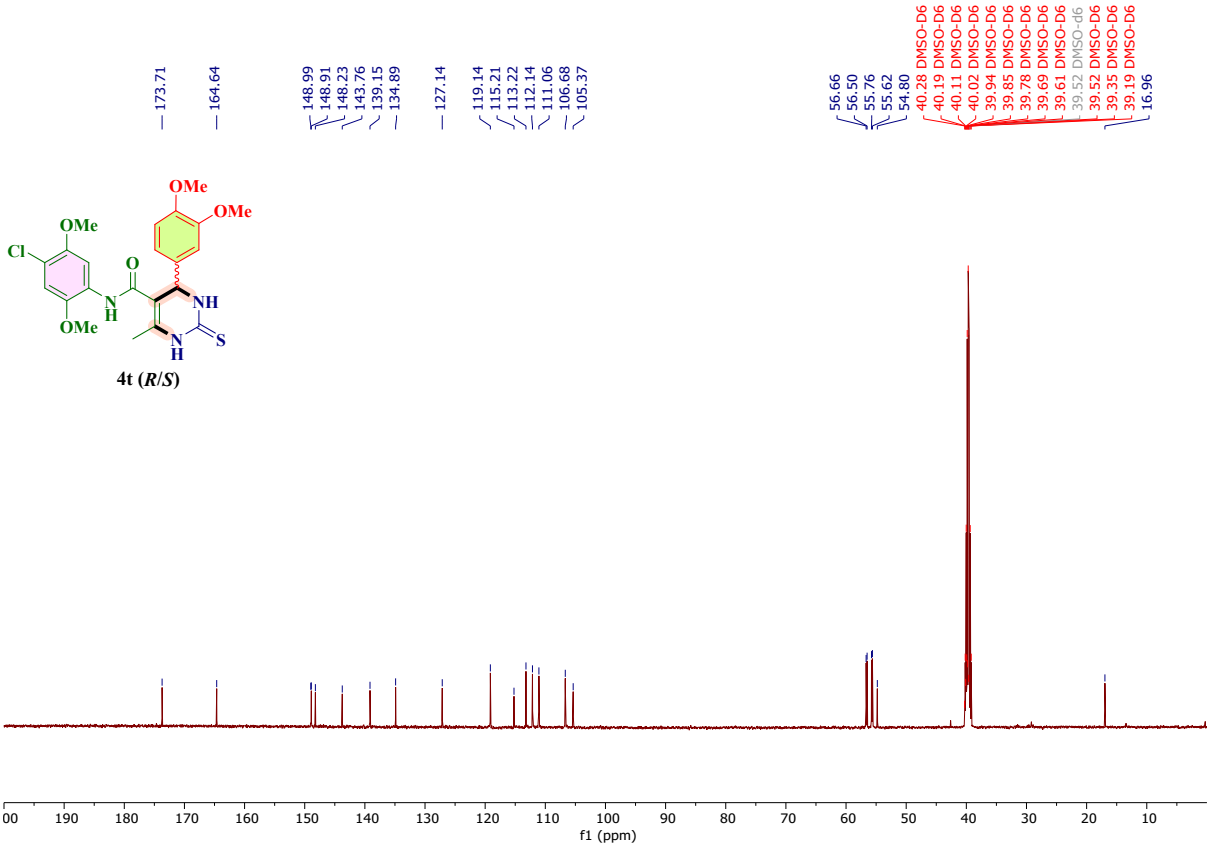


Figure S40: ^{13}C NMR of **4t** (***R*/*S***) (126 MHz, DMSO-d_6)

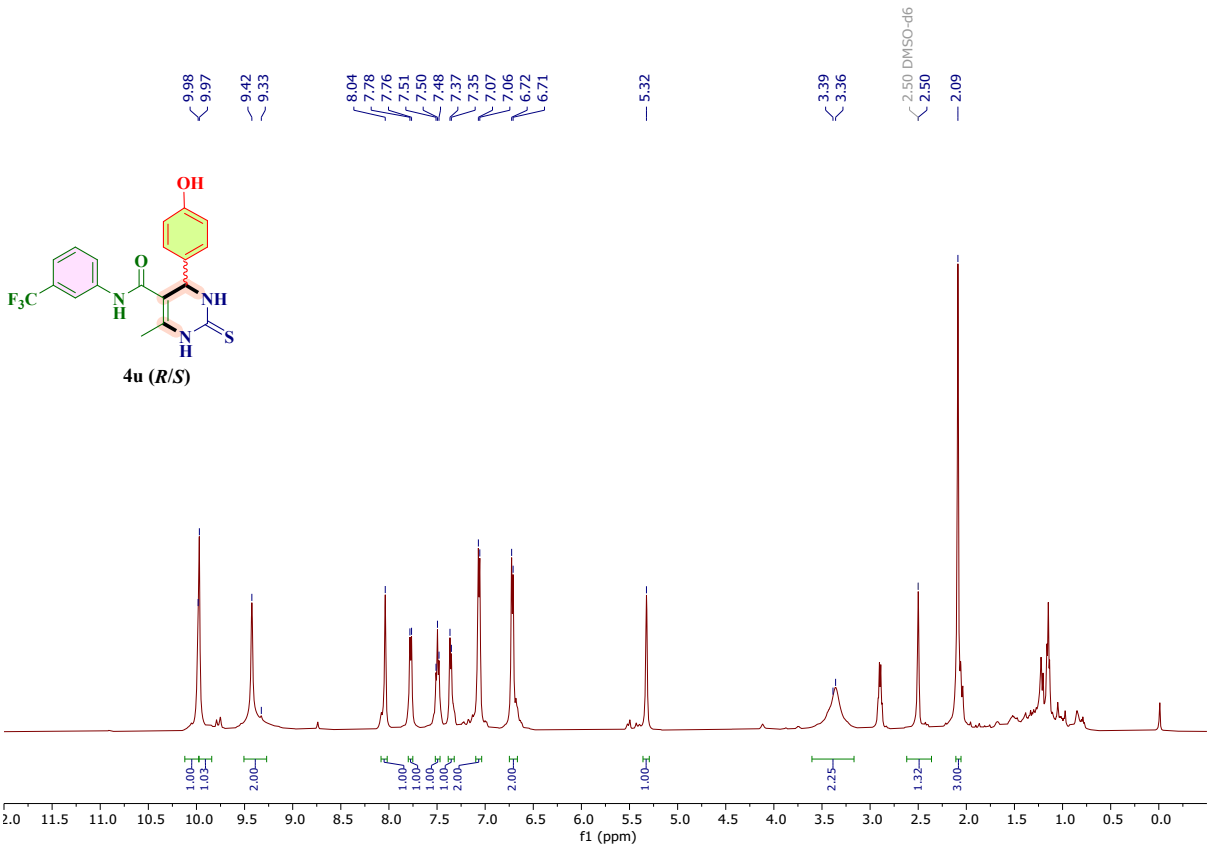


Figure S41: ^{1}H NMR spectra of **4u (*R*/*S*)** (500MHz, DMSO-d_6)

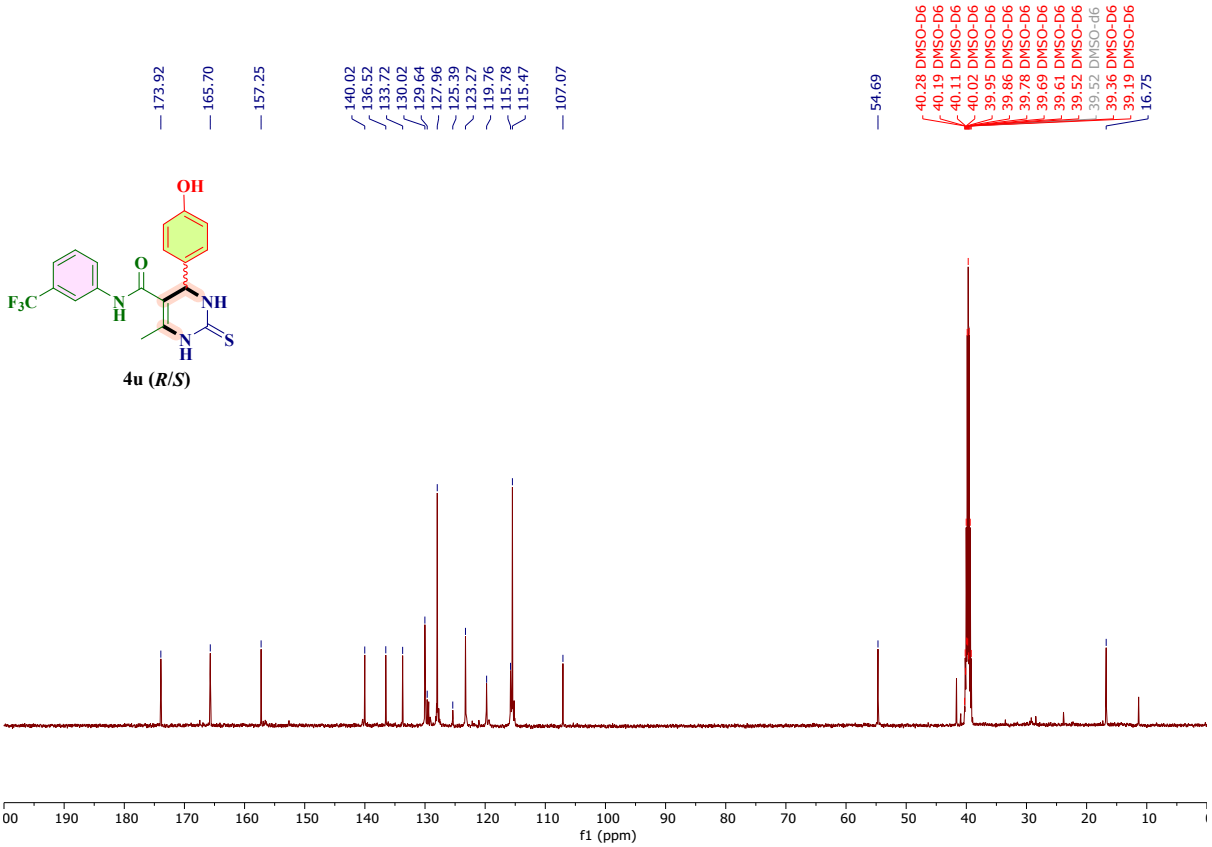


Figure S42: ^{13}C NMR of **4u** (***R*/*S***) (126 MHz, DMSO-d_6)

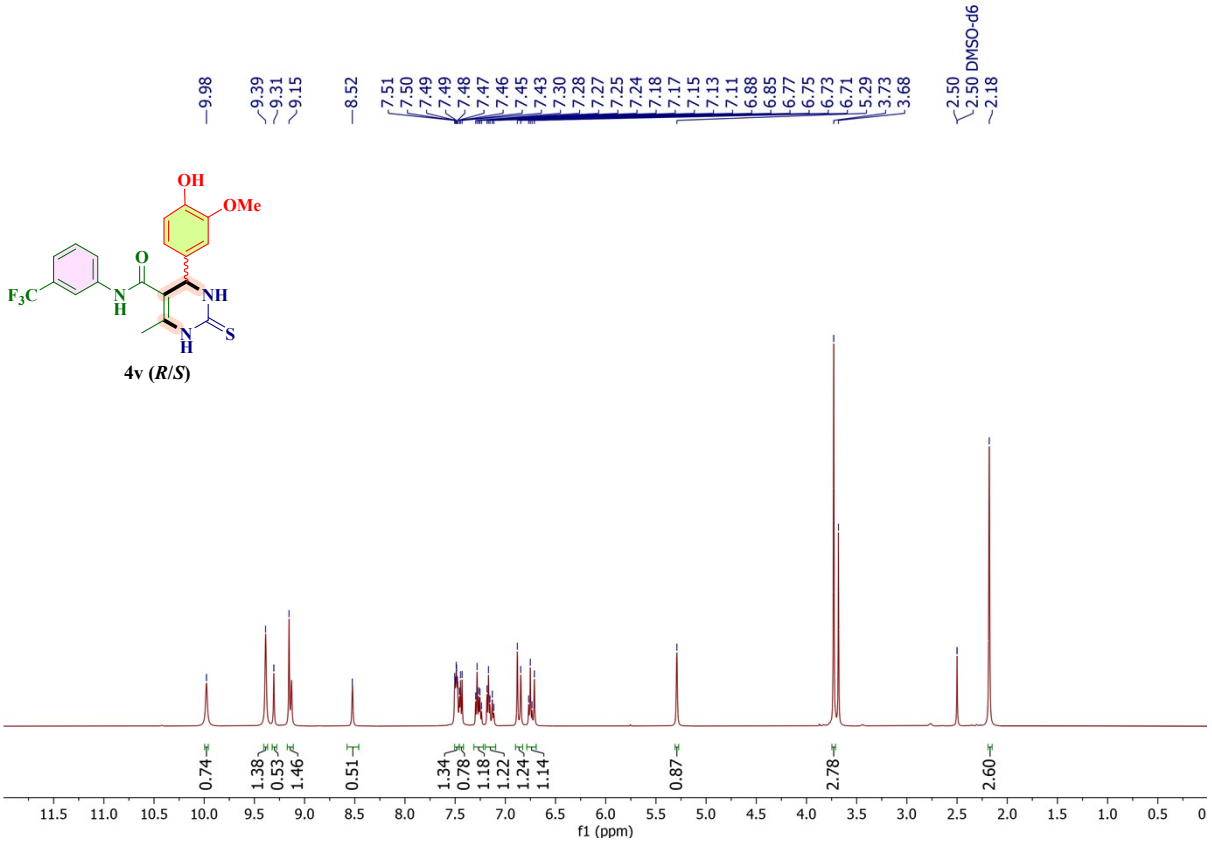


Figure S43: ^{1}H NMR spectra of **4v (*R*/*S*)** (500MHz, DMSO-d_6)

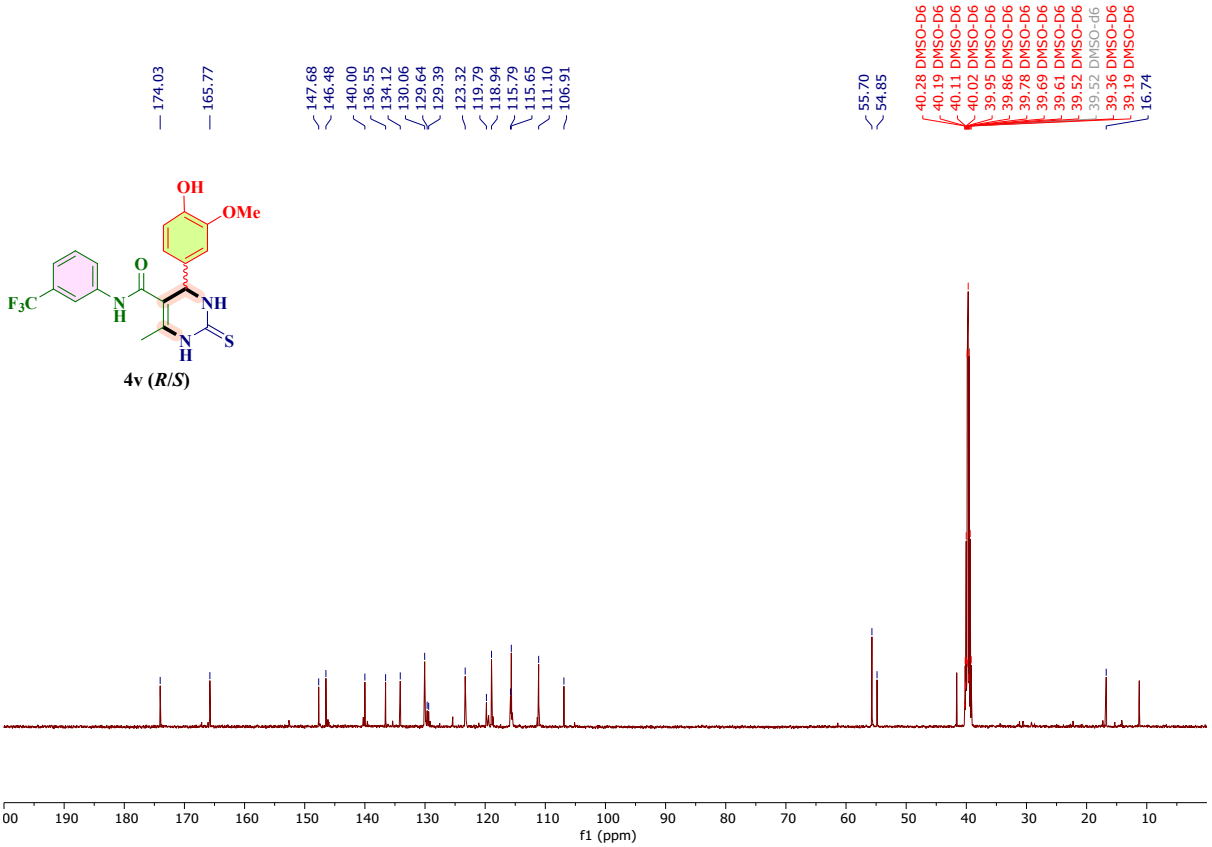


Figure S44: ^{13}C NMR of **4v** (***R***/***S***) (126 MHz, DMSO-d_6)

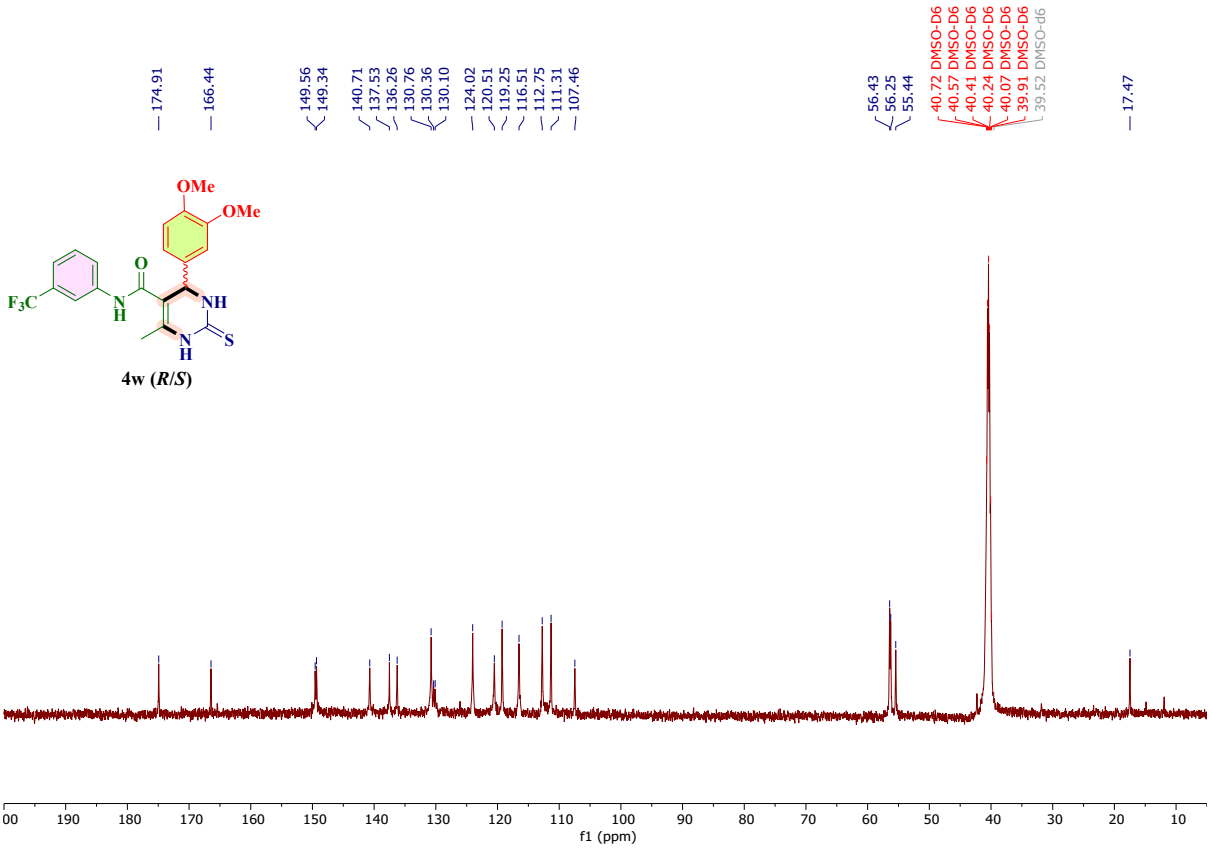


Figure S45: ^{13}C NMR of **4w** (***R***/***S***) (126 MHz, DMSO-d_6)

6 Determination of the absolute configuration

6.1 Chiral HPLC data

HPLC Images

HPLC image of Compound **4b**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:DEA (60:40: 0.1% v/v/v) at 30mL/min, λ = 215 nm, t_{major} = 5.72 min, t_{minor} = 8.36 min.

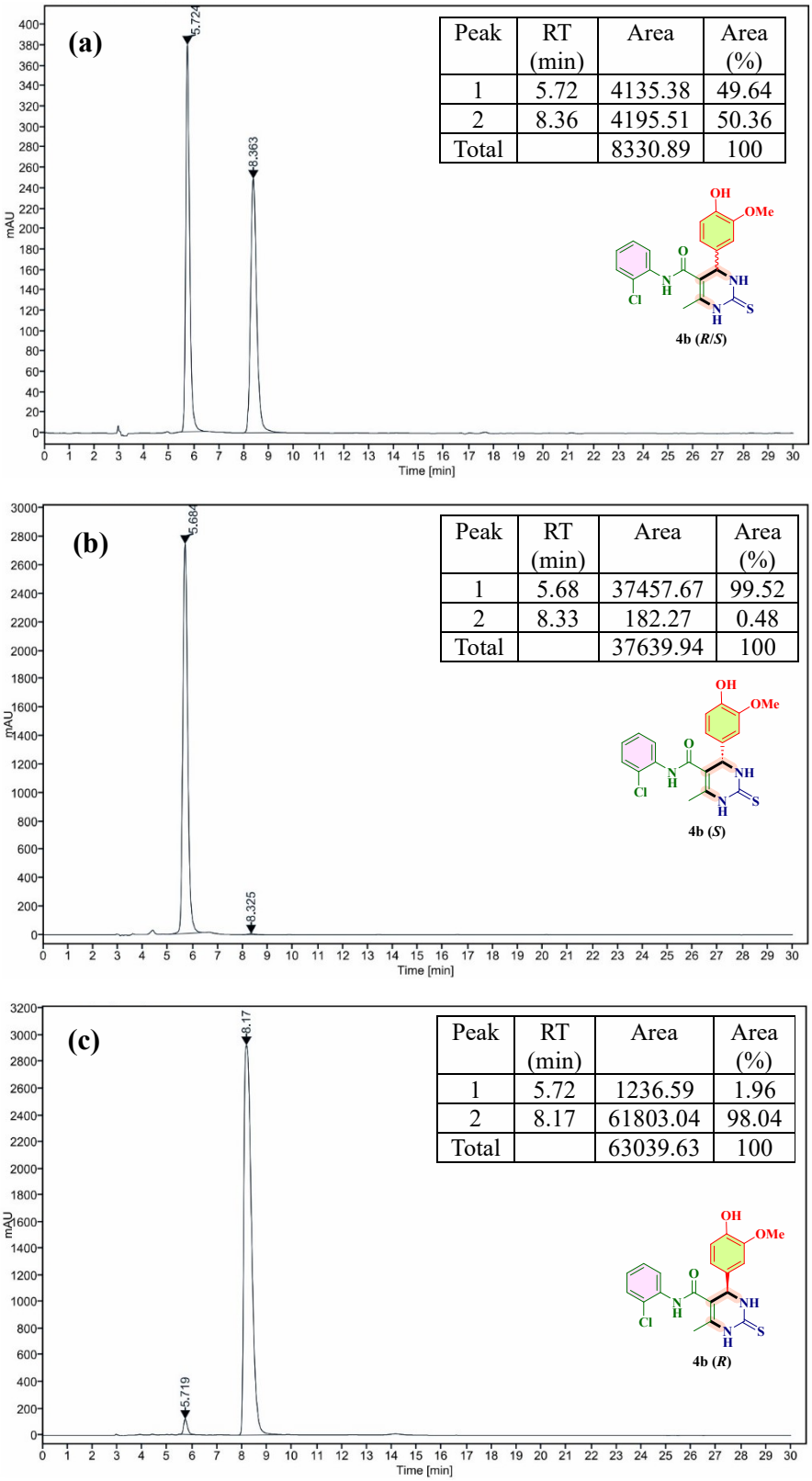
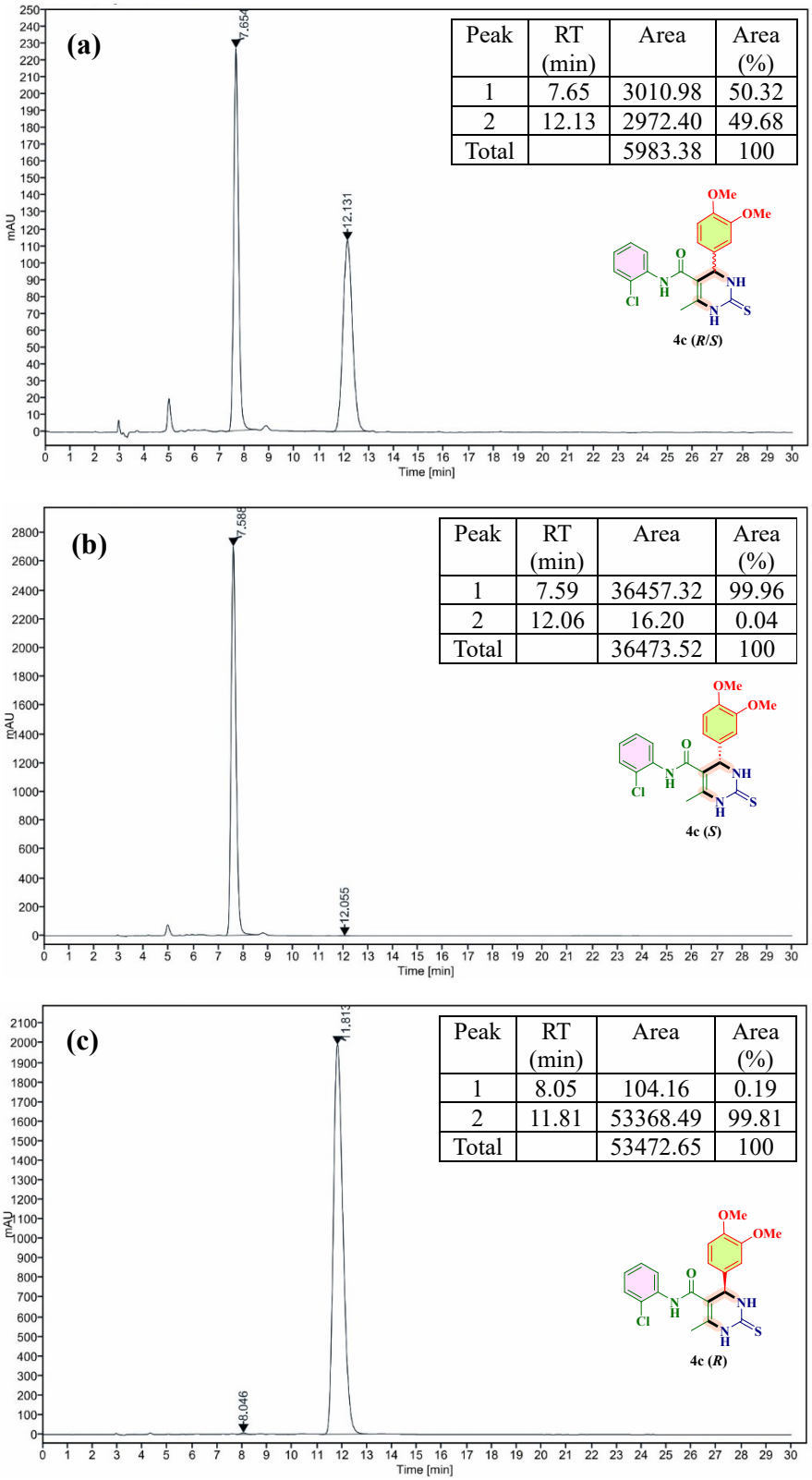


Figure S46. HPLC images of **4b**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4b** and **(c)** resolved (4*R*)(+)-**4b**.

HPLC Image of Compound **4c**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:DEA (60:40: 0.1% v/v/v) at 30mL/min, λ = 215 nm, t_{major} = 7.65 min, t_{minor} = 12.13 min.



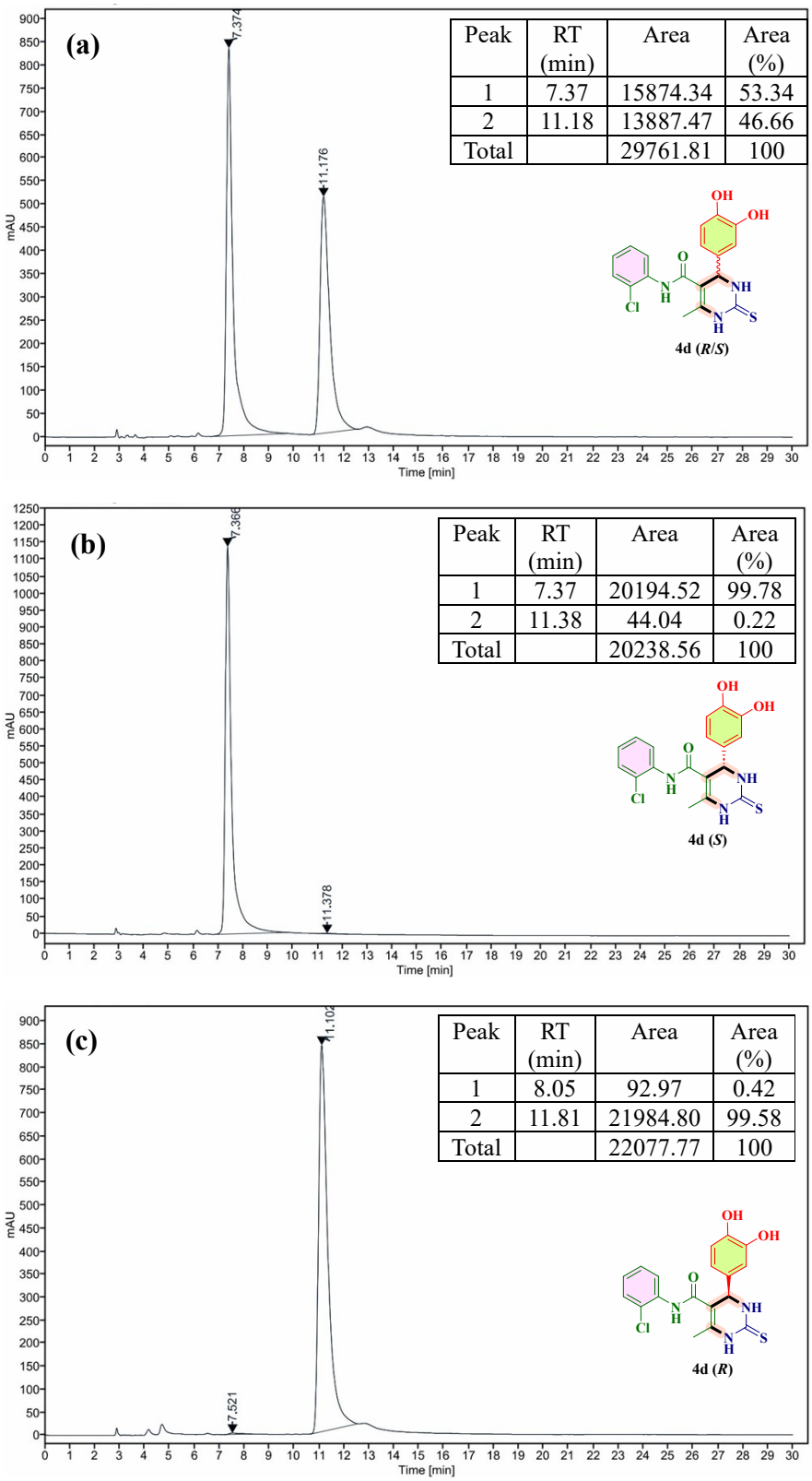
Peak	RT (min)	Area	Area (%)
1	7.65	3010.98	50.32
2	12.13	2972.40	49.68
Total		5983.38	100

Peak	RT (min)	Area	Area (%)
1	7.59	36457.32	99.96
2	12.06	16.20	0.04
Total		36473.52	100

Peak	RT (min)	Area	Area (%)
1	8.05	104.16	0.19
2	11.81	53368.49	99.81
Total		53472.65	100

Figure S47. HPLC images of **4c**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4c** and **(c)** resolved (4*R*)(+)-**4c**.

HPLC Image of Compound **4d**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:IPA:DEA (70:0.0:30:0.1% v/v/v/v) at 30mL/min, λ = 254 nm and 312 nm, t_{major} = 7.37 min, t_{minor} = 11.18 min.



Peak	RT (min)	Area	Area (%)
1	7.37	15874.34	53.34
2	11.18	13887.47	46.66
Total		29761.81	100

Peak	RT (min)	Area	Area (%)
1	7.37	20194.52	99.78
2	11.38	44.04	0.22
Total		20238.56	100

Peak	RT (min)	Area	Area (%)
1	8.05	92.97	0.42
2	11.81	21984.80	99.58
Total		22077.77	100

Figure S48. HPLC images of **4d**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4d** and **(c)** resolved (4*R*)(+)-**4d**.

HPLC Image of Compound **4e**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:DEA (60:40: 0.1% v/v/v) at 30mL/min, λ = 215 nm, t_{major} = 4.15 min, t_{minor} = 5.58 min.

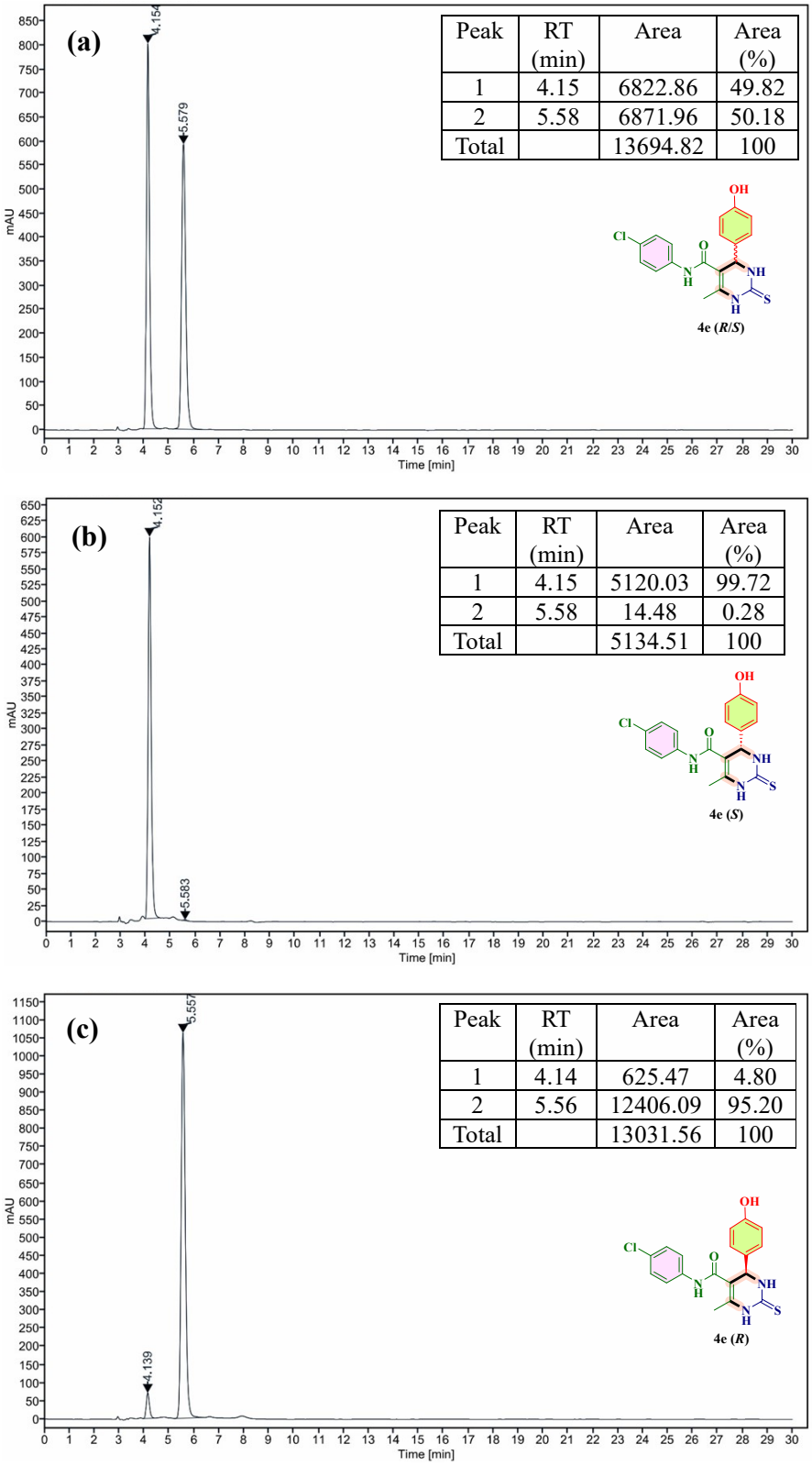
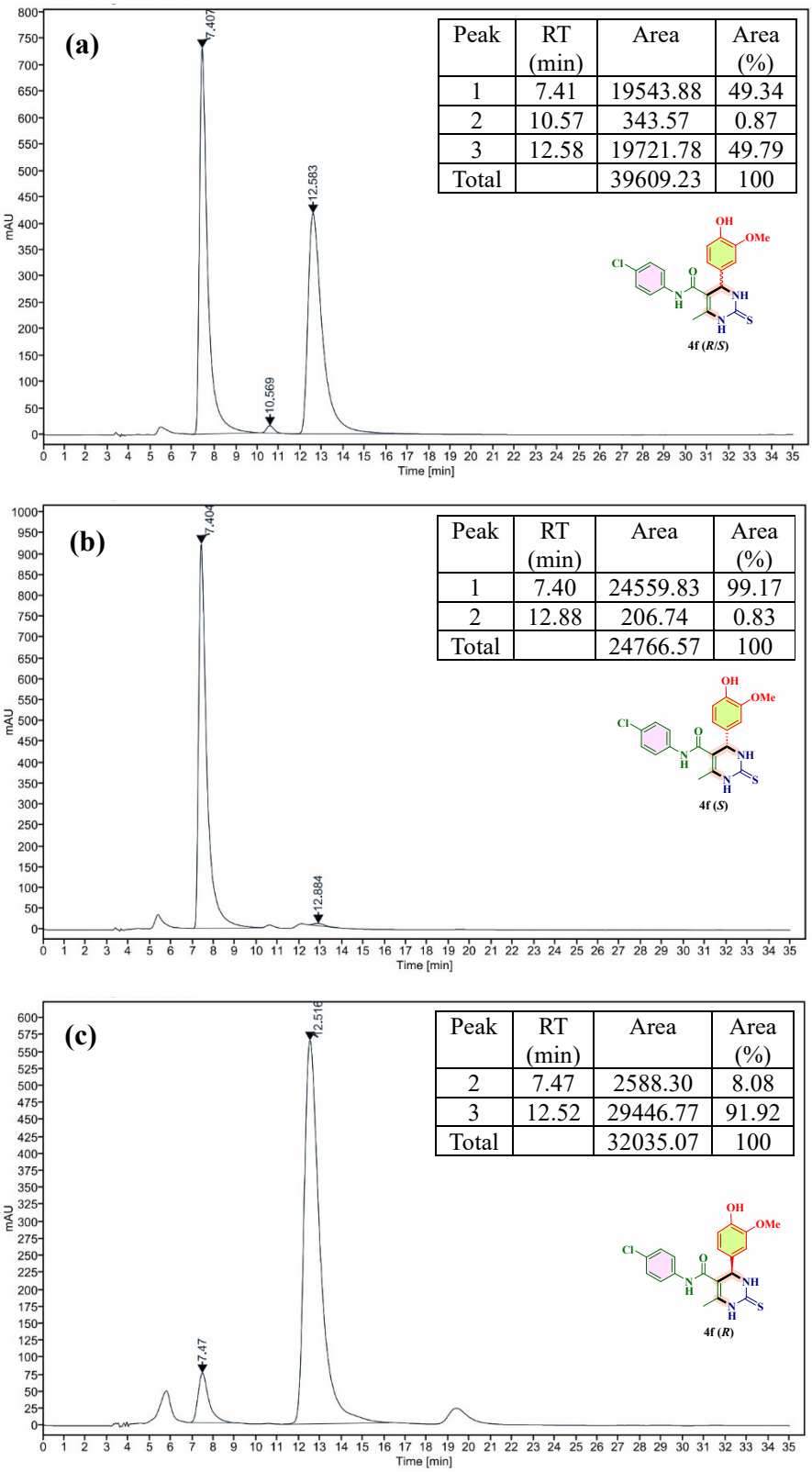


Figure S49. HPLC images of **4e**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4e** and **(c)** resolved (4*R*)(+)-**4e**.

HPLC images of Compound **4f**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:IPA:DEA (60:00:40:0.1 % v/v/v/v) at 30mL/min, λ = 254 nm and 312 nm, t_{major} = 7.41 min, t_{minor} = 12.58 min.



Peak	RT (min)	Area	Area (%)
1	7.41	19543.88	49.34
2	10.57	343.57	0.87
3	12.58	19721.78	49.79
Total		39609.23	100

Peak	RT (min)	Area	Area (%)
1	7.40	24559.83	99.17
2	12.88	206.74	0.83
Total		24766.57	100

Peak	RT (min)	Area	Area (%)
2	7.47	2588.30	8.08
3	12.52	29446.77	91.92
Total		32035.07	100

Figure S50. HPLC images of **4f**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4f** and **(c)** resolved (4*R*)(+)-**4f**.

HPLC Image of Compound **4g**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:DEA (60:40: 0.1% v/v/v) at 30mL/min, λ = 215 nm, t_{major} = 11.60 min, t_{minor} = 17.20 min.

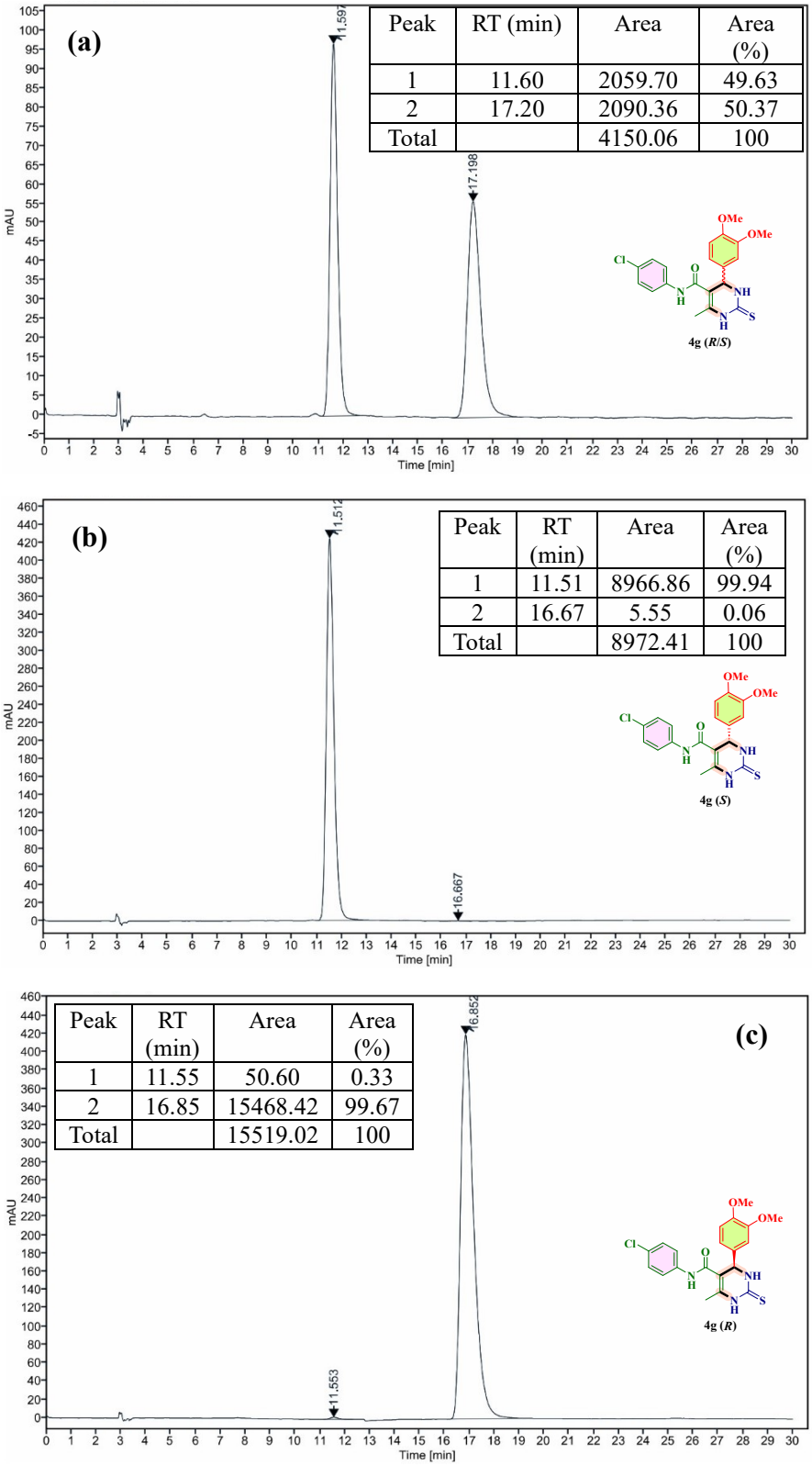


Figure S51. HPLC images of **4g**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4g** and **(c)** resolved (4*R*)(+)-**4g**

HPLC Image of Compound **4h**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:DEA (60:40: 0.1% v/v/v) at 30mL/min, λ = 215 nm, t_{major} = 4.97 min, t_{minor} = 7.19 min.

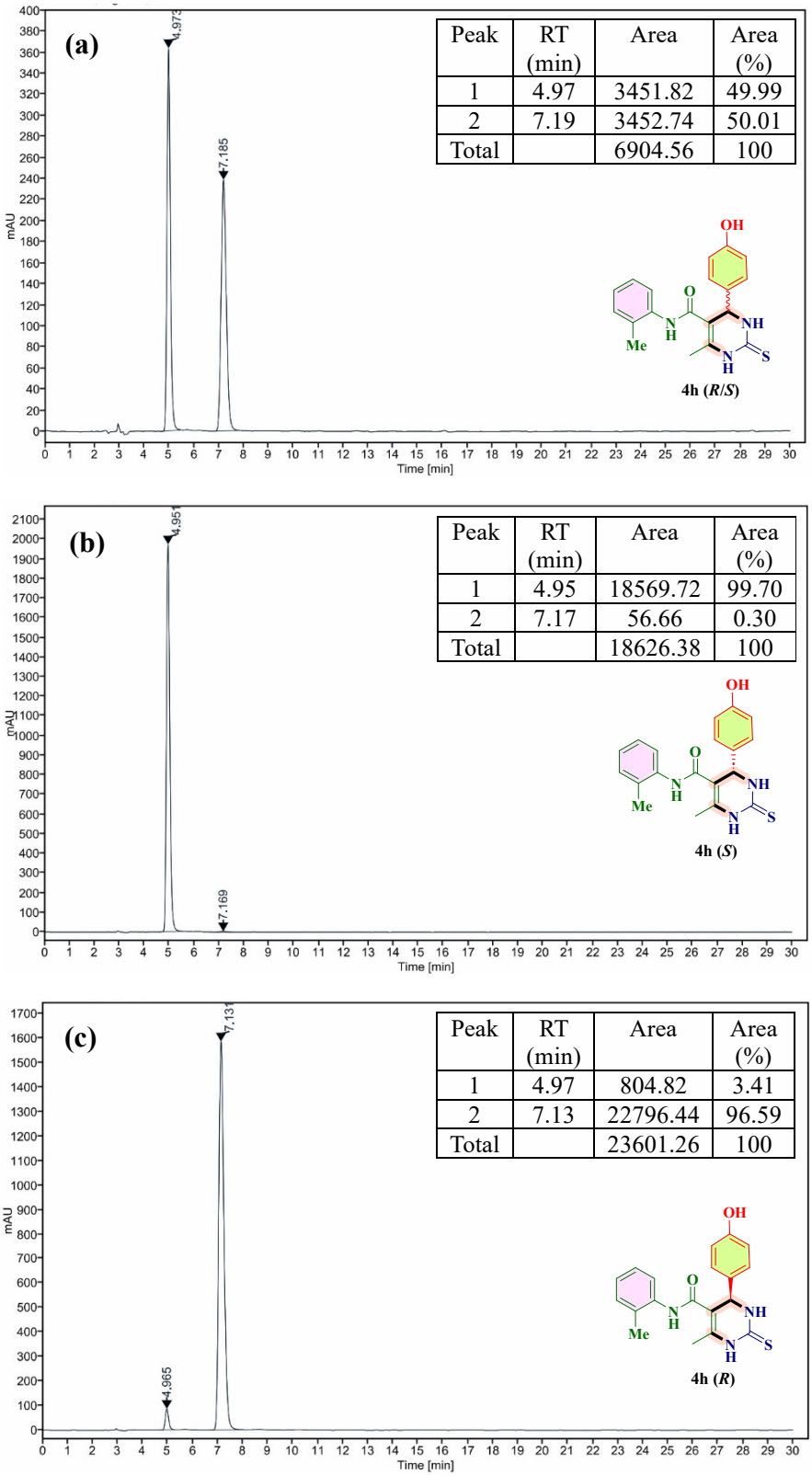


Figure S52. HPLC images of **4h**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4h** and **(c)** resolved (4*R*)(+)-**4h**

HPLC Image of Compound **4i**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:DEA (60:40: 0.1% v/v/v) at 30mL/min, λ = 215 nm, t_{major} = 5.94 min, t_{minor} = 7.12 min.

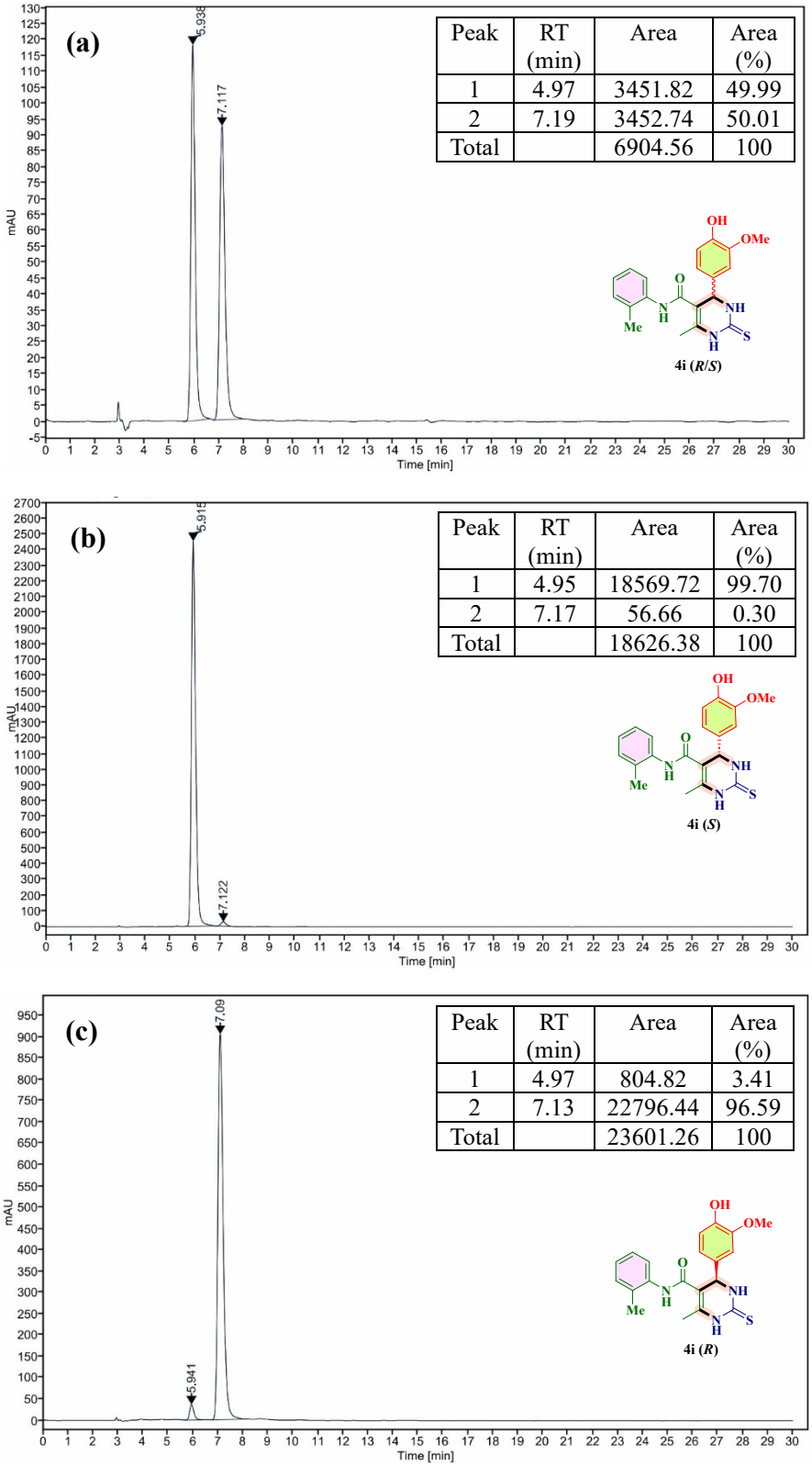


Figure S53. HPLC images of **4i**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4i** and **(c)** resolved (4*R*)(+)-**4i**

HPLC Image of Compound **4j**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:DEA (60:40: 0.1% v/v/v) at 30mL/min, λ = 215 nm, t_{major} = 20.56 min, t_{minor} = 27.96 min.

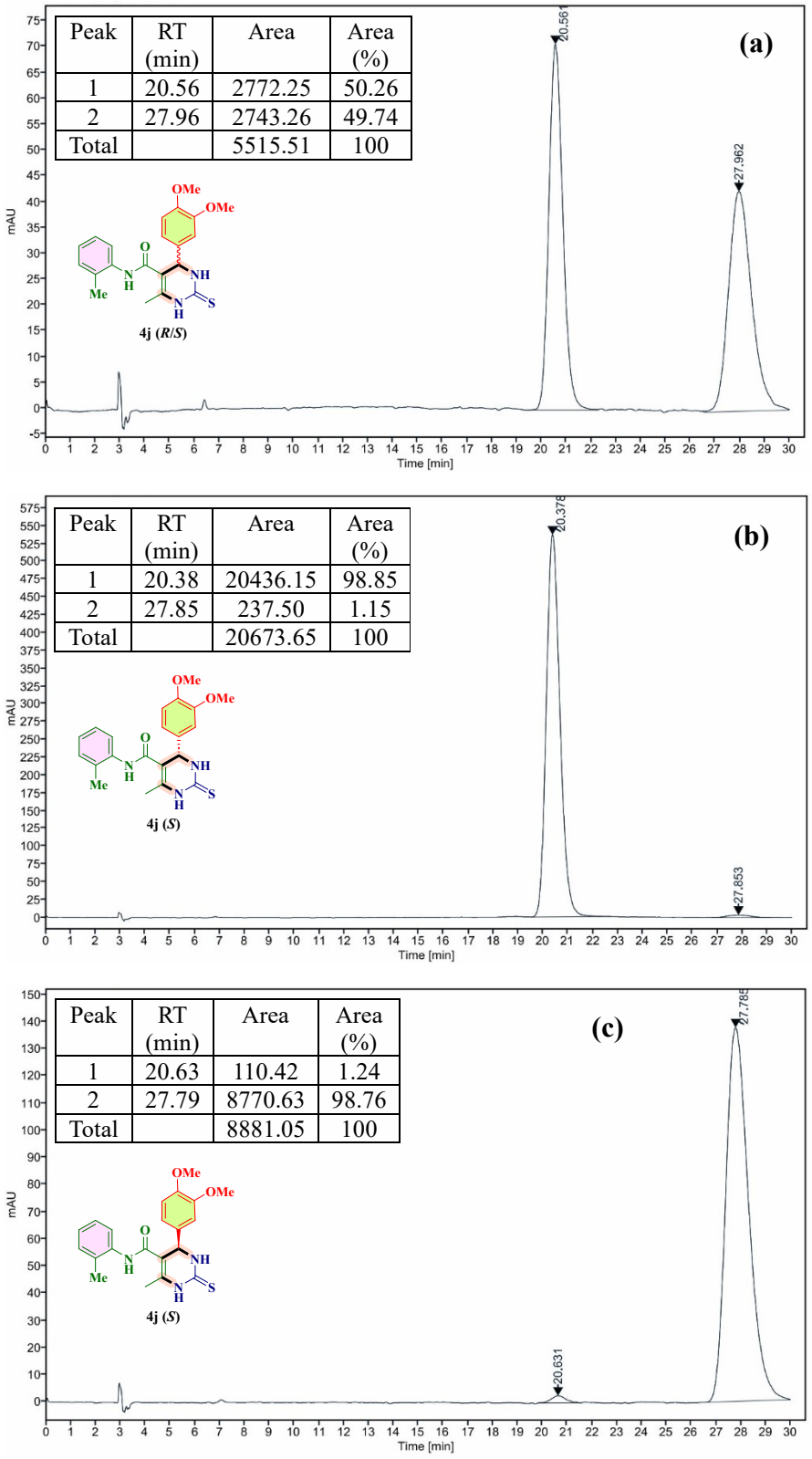
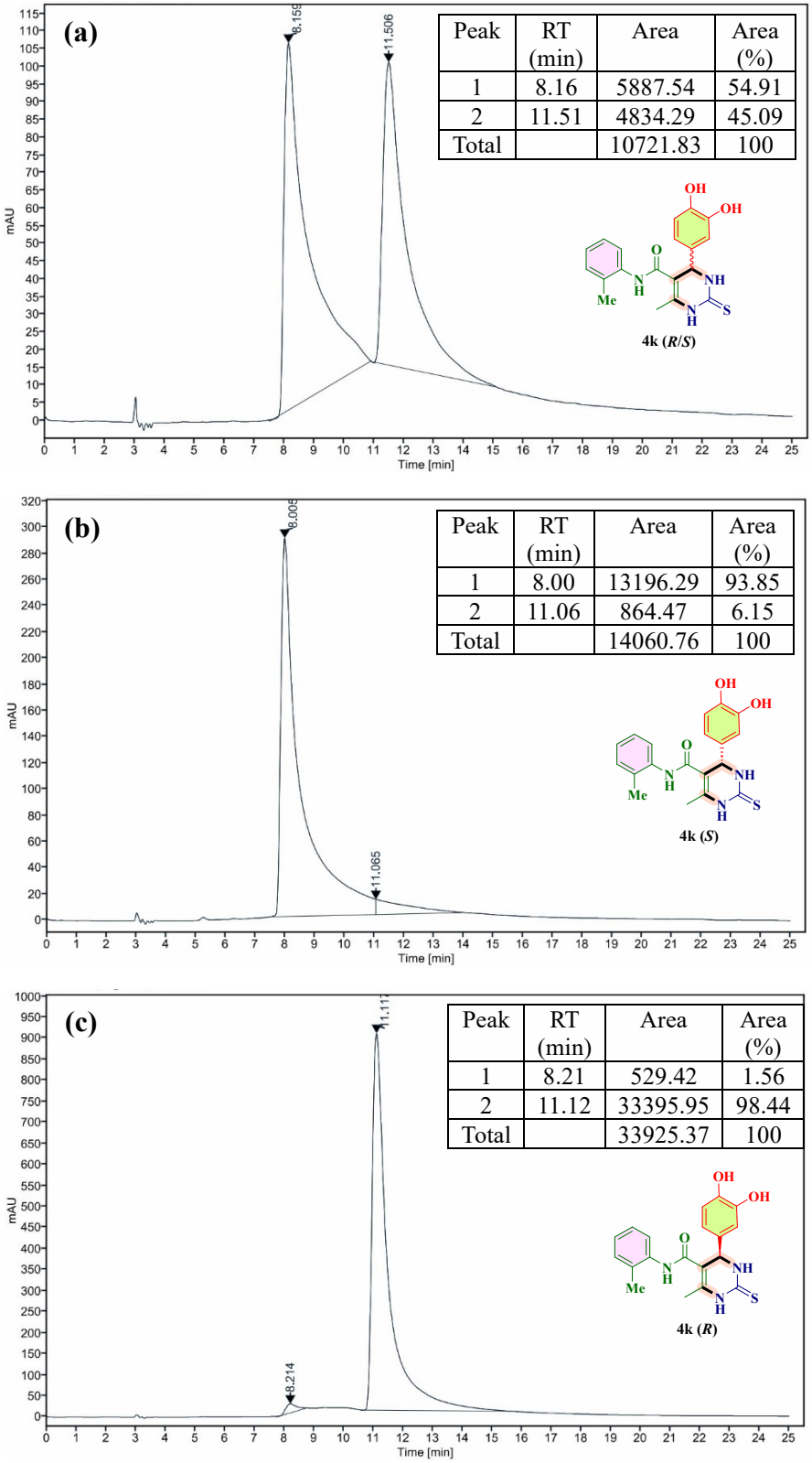


Figure S54. HPLC images of **4j**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4j** and **(c)** resolved (4*R*)(+)-**4j**

HPLC Image of Compound **4k**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:IPA:DEA (80:20:0.0:0.1% v/v/v/v) at 30mL/min, λ = 254 nm and 312 nm, t_{major} = 8.16 min, t_{minor} = 11.51 min.



Peak	RT (min)	Area	Area (%)
1	8.16	5887.54	54.91
2	11.51	4834.29	45.09
Total		10721.83	100

Peak	RT (min)	Area	Area (%)
1	8.00	13196.29	93.85
2	11.06	864.47	6.15
Total		14060.76	100

Peak	RT (min)	Area	Area (%)
1	8.21	529.42	1.56
2	11.12	33395.95	98.44
Total		33925.37	100

Figure S55. HPLC images of **4k**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4k** and **(c)** resolved (4*R*)(+)-**4k**.

HPLC Image of Compound **4l**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:DEA (60:40: 0.1% v/v/v) at 30mL/min, λ = 215 nm, t_{major} = 9.30 min, t_{minor} = 18.96 min.

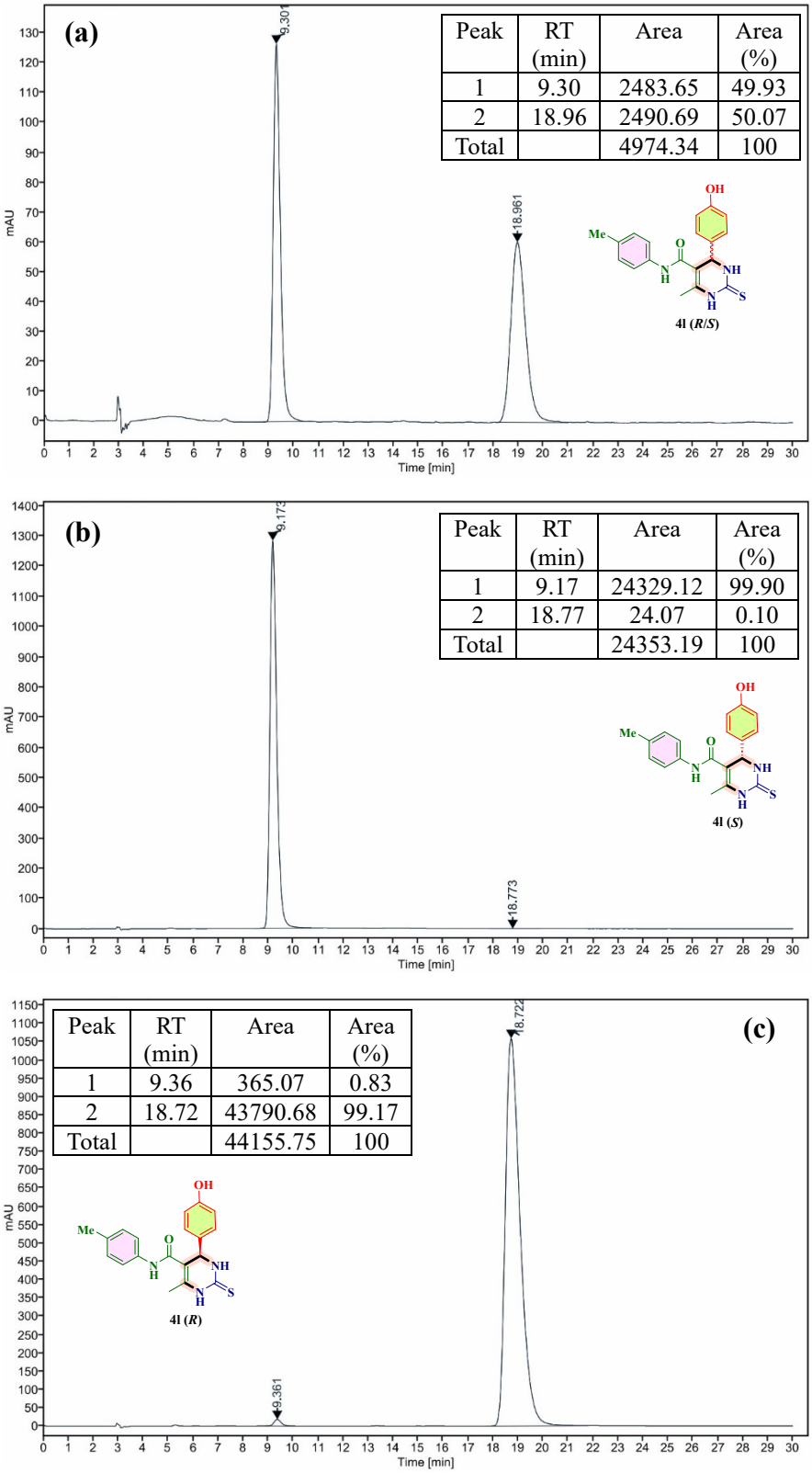


Figure S56. HPLC images of **4l**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4l** and **(c)** resolved (4*R*)(+)-**4l**.

HPLC Image of Compound **4m**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:DEA (60:40: 0.1% v/v/v) at 30mL/min, λ = 215 nm, t_{major} = 11.93 min, t_{minor} = 18.47 min.

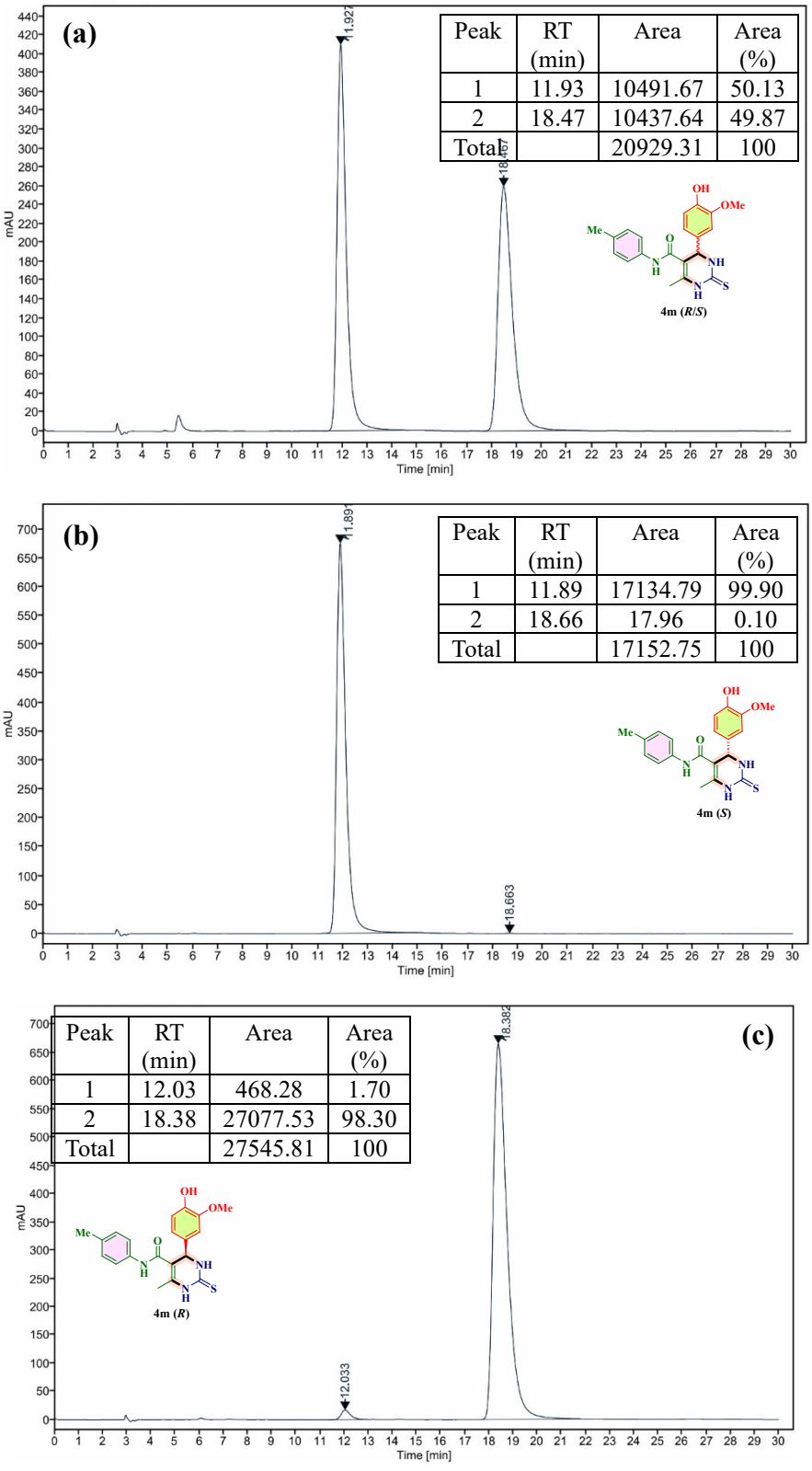
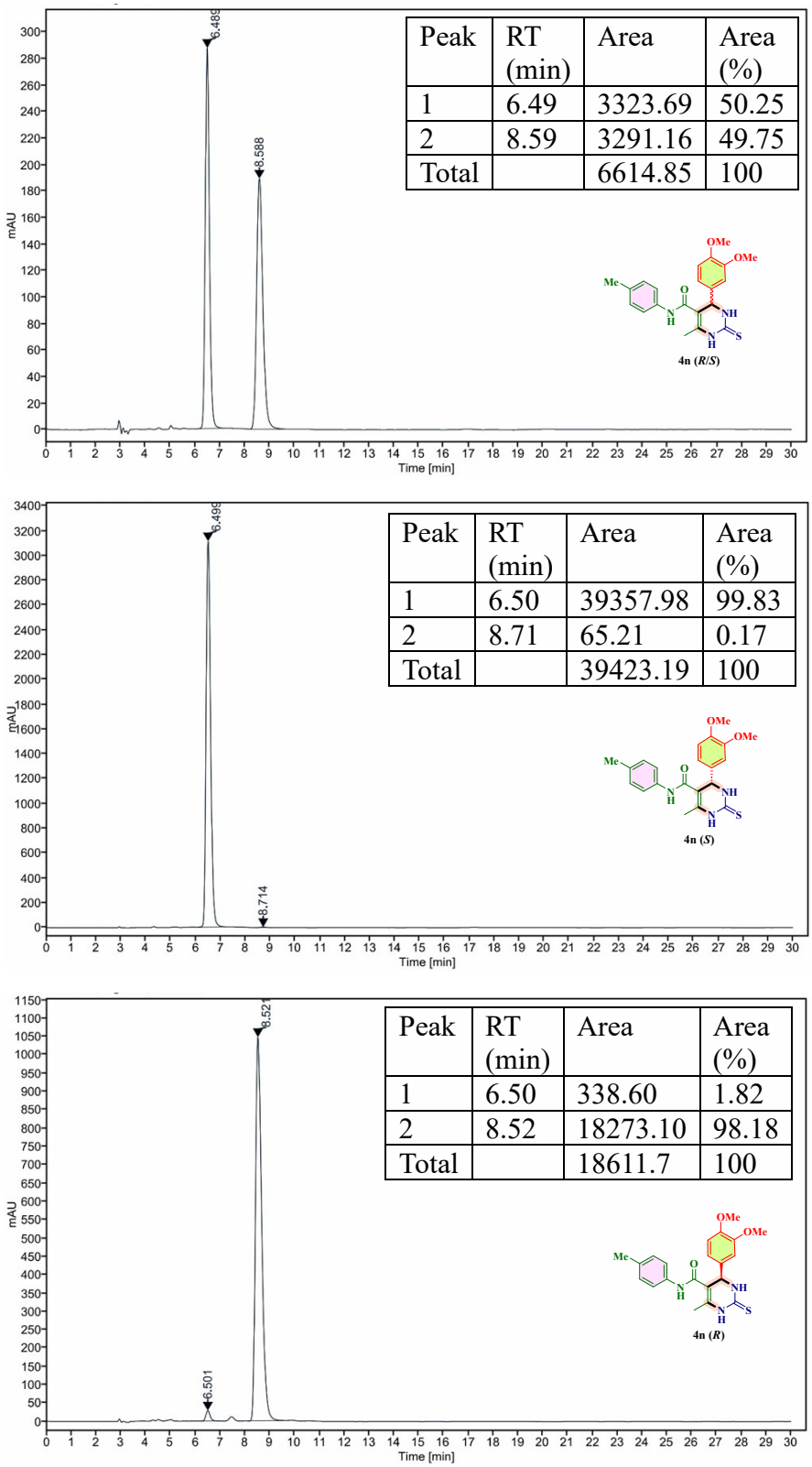


Figure S57. HPLC images of **4m**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4m** and **(c)** resolved (4*R*)(+)-**4m**.

HPLC Image of Compound **4n**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:DEA (60:40: 0.1% v/v/v) at 30mL/min, λ = 215 nm, t_{major} = 6.49 min, t_{minor} = 8.59 min.



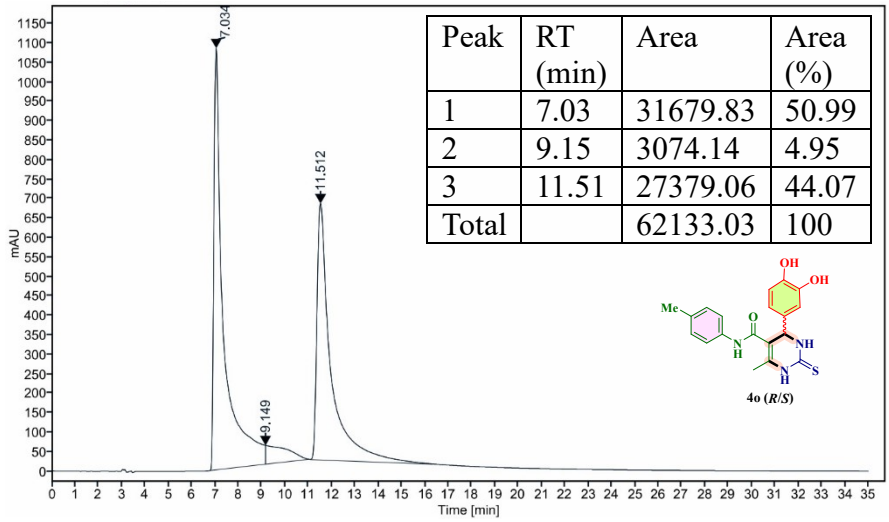
Peak	RT (min)	Area	Area (%)
1	6.49	3323.69	50.25
2	8.59	3291.16	49.75
Total		6614.85	100

Peak	RT (min)	Area	Area (%)
1	6.50	39357.98	99.83
2	8.71	65.21	0.17
Total		39423.19	100

Peak	RT (min)	Area	Area (%)
1	6.50	338.60	1.82
2	8.52	18273.10	98.18
Total		18611.7	100

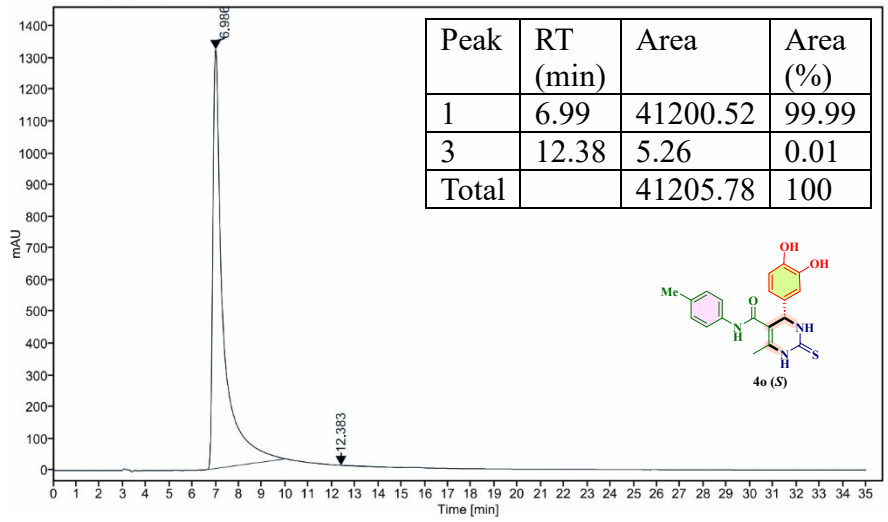
Figure S58. HPLC images of **4n**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4n** and **(c)** resolved (4*R*)(+)-**4n**.

HPLC Image of Compound **4o**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:IPA:DEA (80:20:0.0:0.1 % v/v/v/v) at 30mL/min, λ = 254 nm and 312 nm, t_{major} = 7.03 min, t_{minor} = 11.51 min.



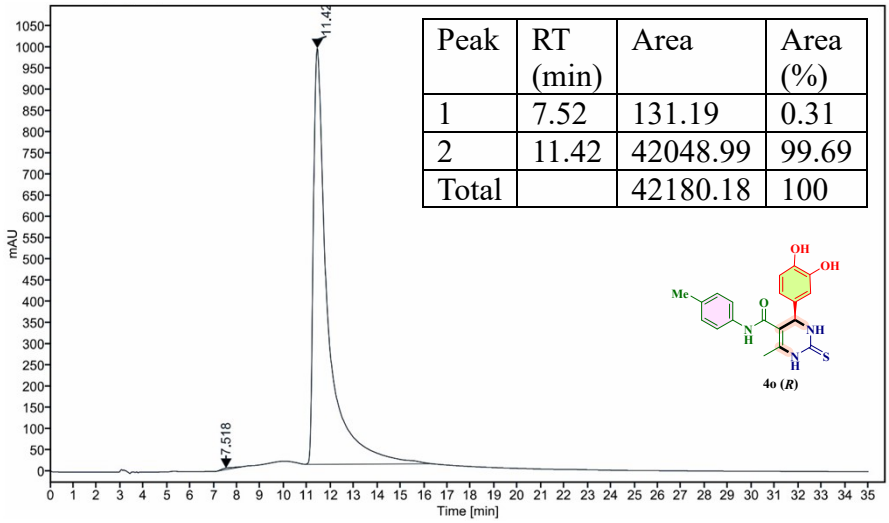
Peak	RT (min)	Area	Area (%)
1	7.03	31679.83	50.99
2	9.15	3074.14	4.95
3	11.51	27379.06	44.07
Total		62133.03	100

4o (*R*/*S*)



Peak	RT (min)	Area	Area (%)
1	6.99	41200.52	99.99
3	12.38	5.26	0.01
Total		41205.78	100

4o (*S*)

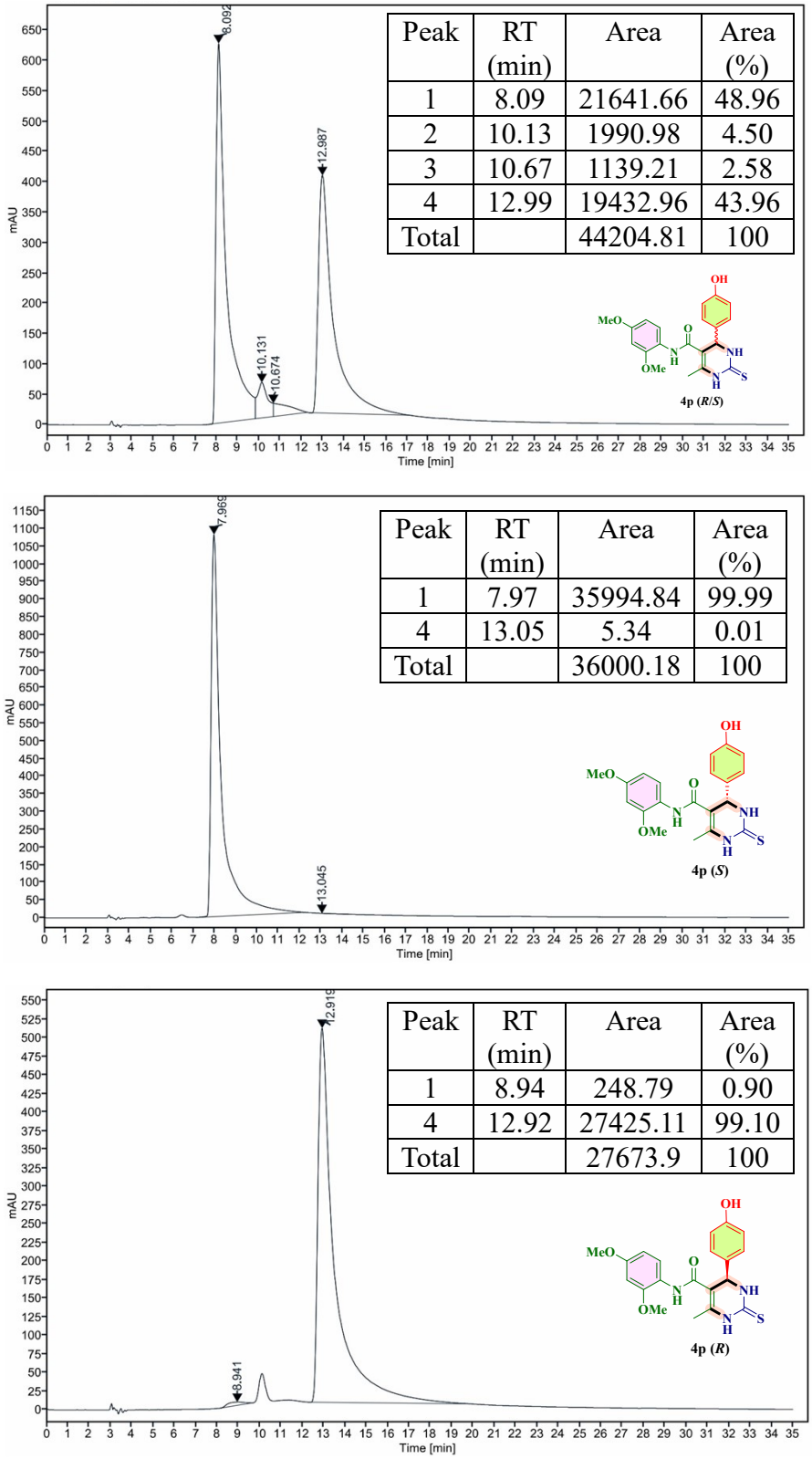


Peak	RT (min)	Area	Area (%)
1	7.52	131.19	0.31
2	11.42	42048.99	99.69
Total		42180.18	100

4o (*R*)

Figure S59. HPLC images of **4o**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4o** and **(c)** resolved (4*R*)(+)-**4o**.

HPLC Image of Compound **4p**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:IPA:DEA (80:20:0.0:0.1% v/v/v/v) at 30mL/min, λ = 254 nm and 312 nm, t_{major} = 8.09 min, t_{minor} = 12.99 min.



Peak	RT (min)	Area	Area (%)
1	8.09	21641.66	48.96
2	10.13	1990.98	4.50
3	10.67	1139.21	2.58
4	12.99	19432.96	43.96
Total		44204.81	100

Peak	RT (min)	Area	Area (%)
1	7.97	35994.84	99.99
4	13.05	5.34	0.01
Total		36000.18	100

Peak	RT (min)	Area	Area (%)
1	8.94	248.79	0.90
4	12.92	27425.11	99.10
Total		27673.9	100

Figure S60. HPLC images of **4p**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4p** and **(c)** resolved (4*R*)(+)-**4p**.

HPLC image of Compound **4q**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:IPA:DEA (30:70:0.0:0.1% v/v/v/v) at 30mL/min, λ = 254 nm and 312 nm, t_{major} = 5.80 min, t_{minor} = 13.91 min.

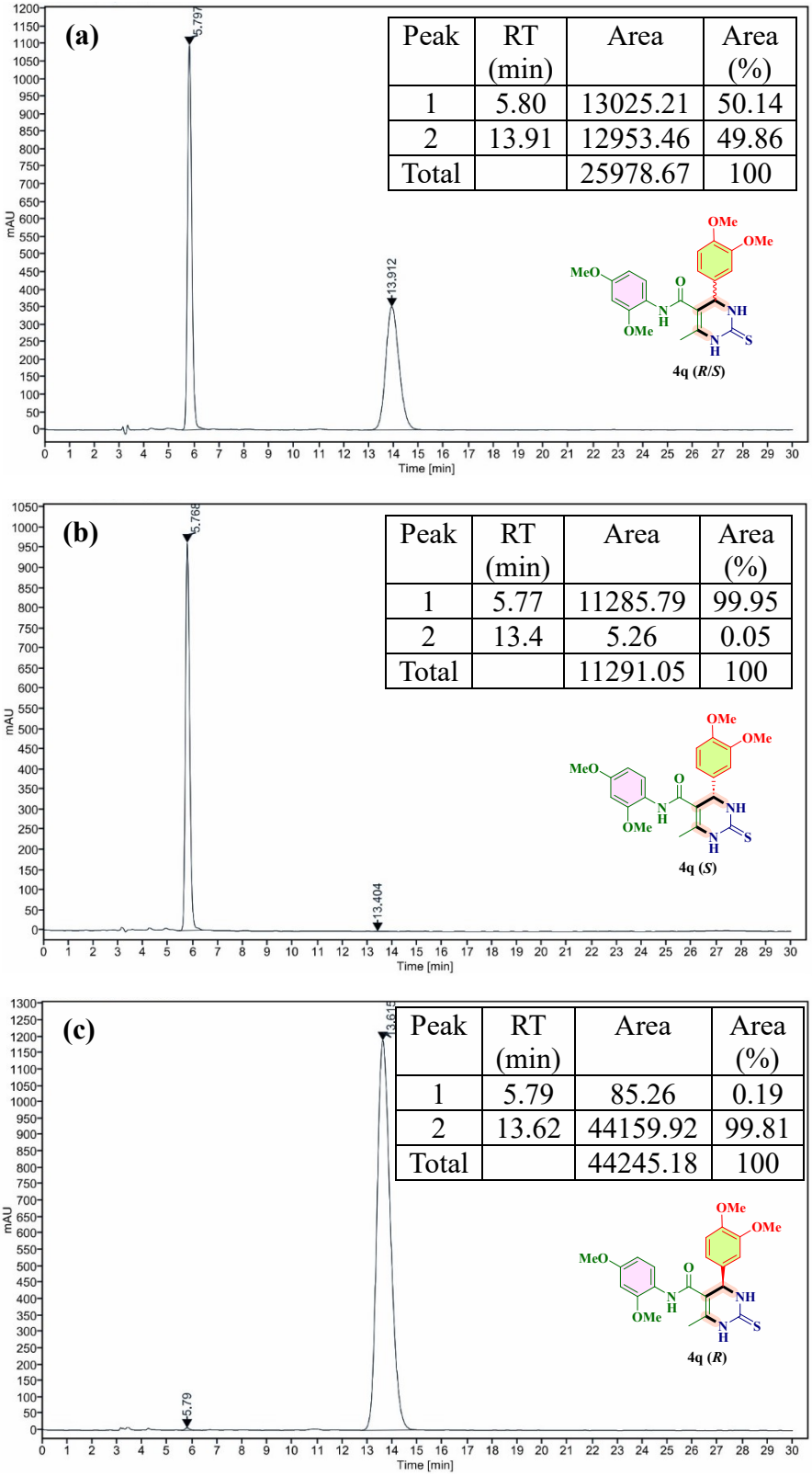


Figure S61. HPLC images of **4q**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4q** and **(c)** resolved (4*R*)(+)-**4q**.

HPLC Image of Compound **4r**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:IPA:DEA (60:40:0.0:0.1 % v/v/v/v) at 30mL/min, λ = 254 nm and 312 nm, t_{major} = 5.85 min, t_{minor} = 17.50 min.

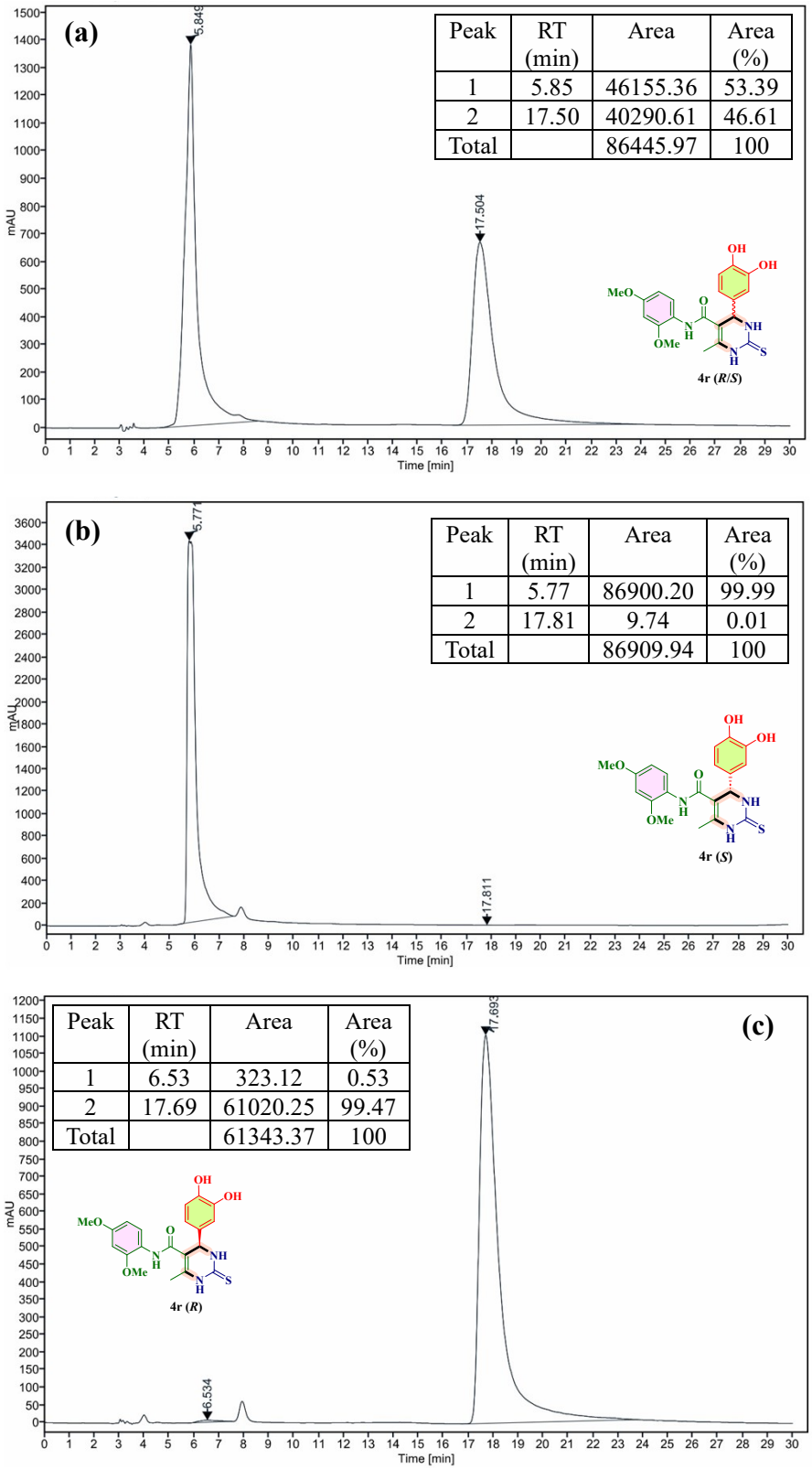
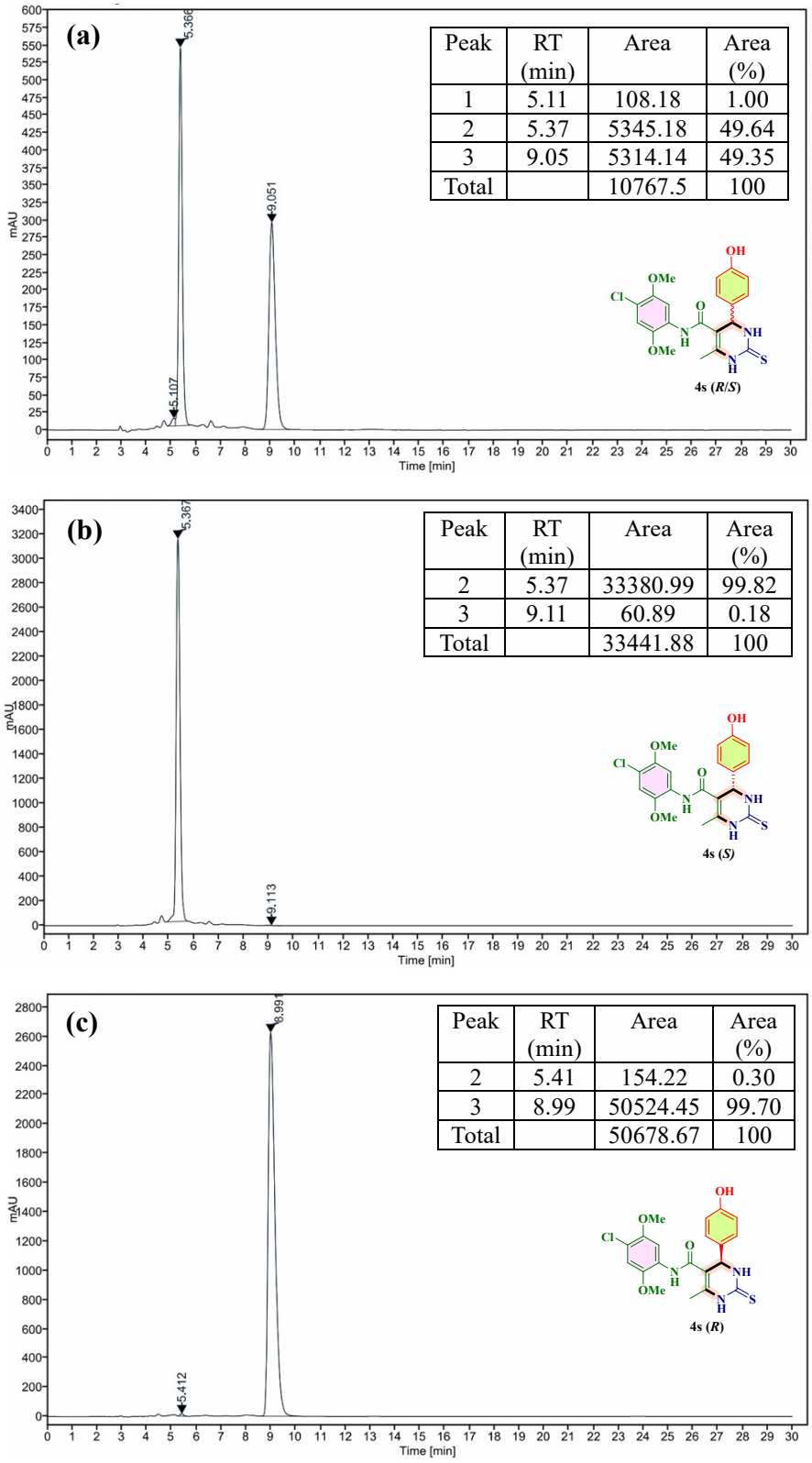


Figure S62. HPLC images of **4r**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4r** and **(c)** resolved (4*R*)(+)-**4r**.

HPLC Image of Compound **4s**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:DEA (60:40: 0.1% v/v/v) at 30mL/min, λ = 215 nm, t_{major} = 5.11 min, t_{minor} = 9.05 min.



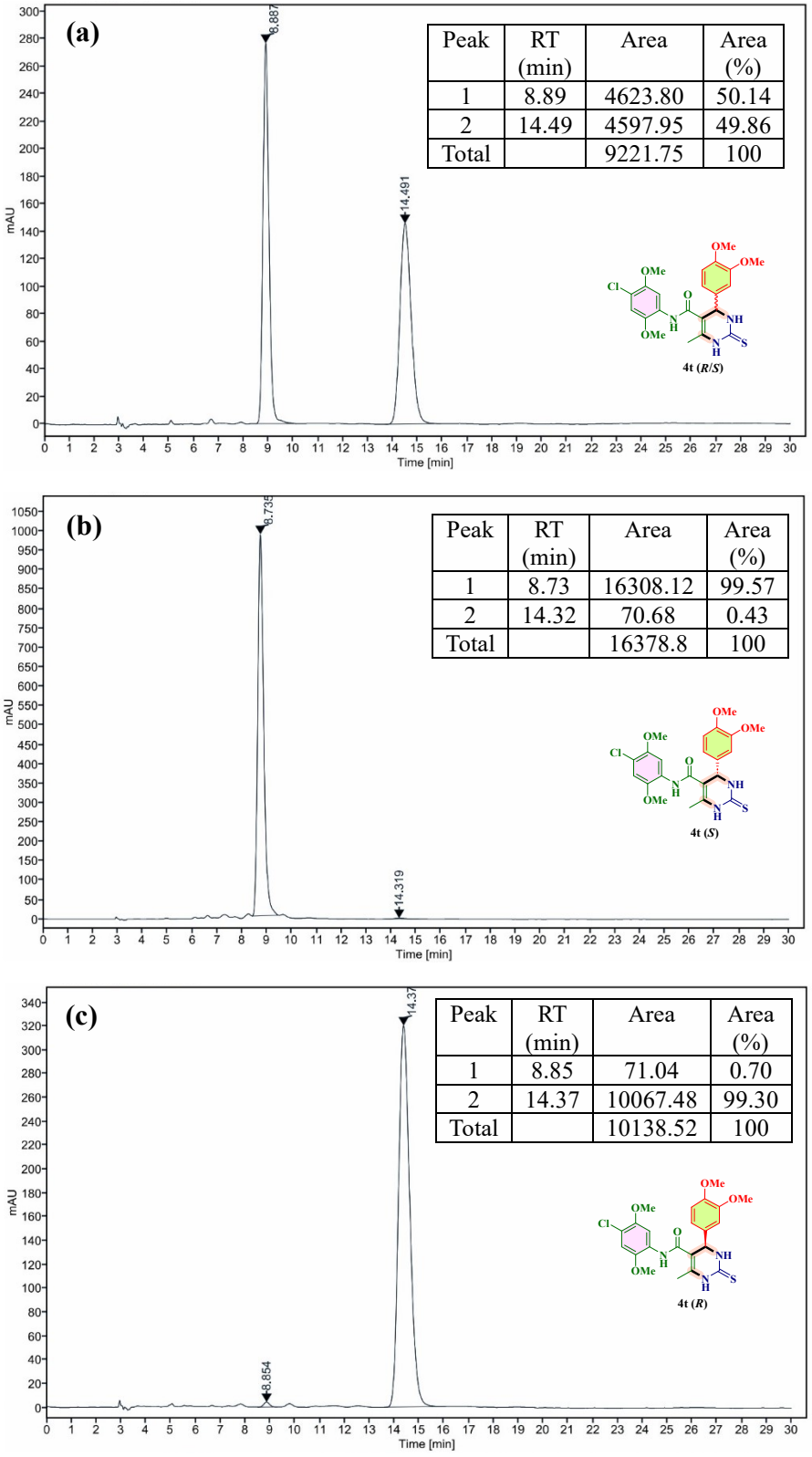
Peak	RT (min)	Area	Area (%)
1	5.11	108.18	1.00
2	5.37	5345.18	49.64
3	9.05	5314.14	49.35
Total		10767.5	100

Peak	RT (min)	Area	Area (%)
2	5.37	33380.99	99.82
3	9.11	60.89	0.18
Total		33441.88	100

Peak	RT (min)	Area	Area (%)
2	5.41	154.22	0.30
3	8.99	50524.45	99.70
Total		50678.67	100

Figure S63. HPLC images of **4s**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4s** and **(c)** resolved (4*R*)(+)-**4s**.

HPLC Image of Compound **4t**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:DEA (60:40: 0.1% v/v/v) at 30mL/min, λ = 215 nm, t_{major} = 8.89 min, t_{minor} = 14.49 min.



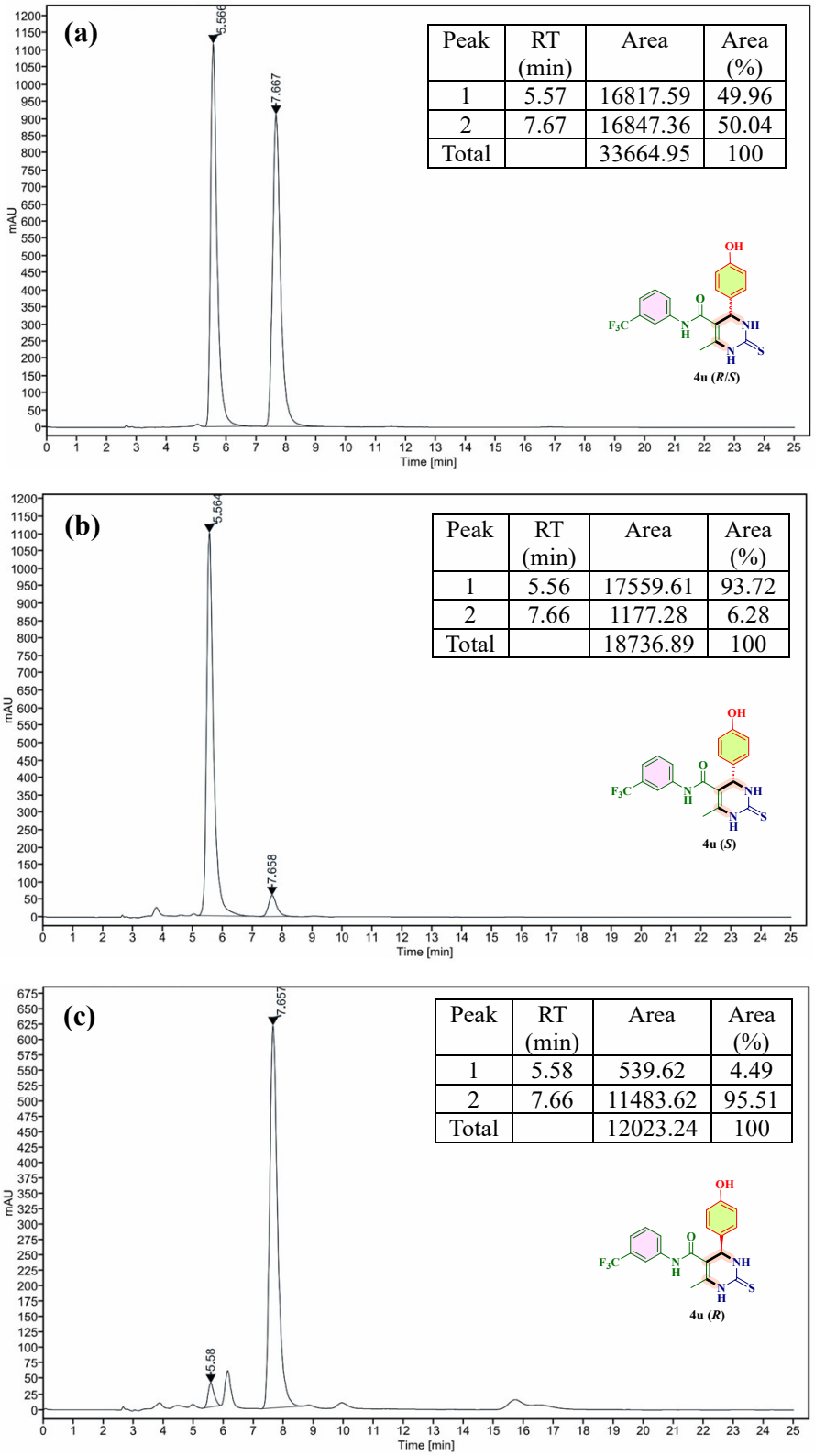
Peak	RT (min)	Area	Area (%)
1	8.89	4623.80	50.14
2	14.49	4597.95	49.86
Total		9221.75	100

Peak	RT (min)	Area	Area (%)
1	8.73	16308.12	99.57
2	14.32	70.68	0.43
Total		16378.8	100

Peak	RT (min)	Area	Area (%)
1	8.85	71.04	0.70
2	14.37	10067.48	99.30
Total		10138.52	100

Figure S64. HPLC images of **4t**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4t** and **(c)** resolved (4*R*)(+)-**4t**.

HPLC Image of Compound **4u**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:IPA:DEA (80:20:0.0:0.1% v/v/v/v) at 20mL/min, λ = 254 nm and 312 nm, t_{major} = 5.57 min, t_{minor} = 7.67 min.



Peak	RT (min)	Area	Area (%)
1	5.57	16817.59	49.96
2	7.67	16847.36	50.04
Total		33664.95	100

Peak	RT (min)	Area	Area (%)
1	5.56	17559.61	93.72
2	7.66	1177.28	6.28
Total		18736.89	100

Peak	RT (min)	Area	Area (%)
1	5.58	539.62	4.49
2	7.66	11483.62	95.51
Total		12023.24	100

Figure S65. HPLC images of **4u**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4u** and **(c)** resolved (4*R*)(+)-**4u**.

HPLC Image of Compound **4v**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:IPA:DEA (80:20:0.0:0.1% v/v/v/v) at 20mL/min, λ = 254 nm and 312 nm, t_{major} = 6.46 min, t_{minor} = 8.26 min.

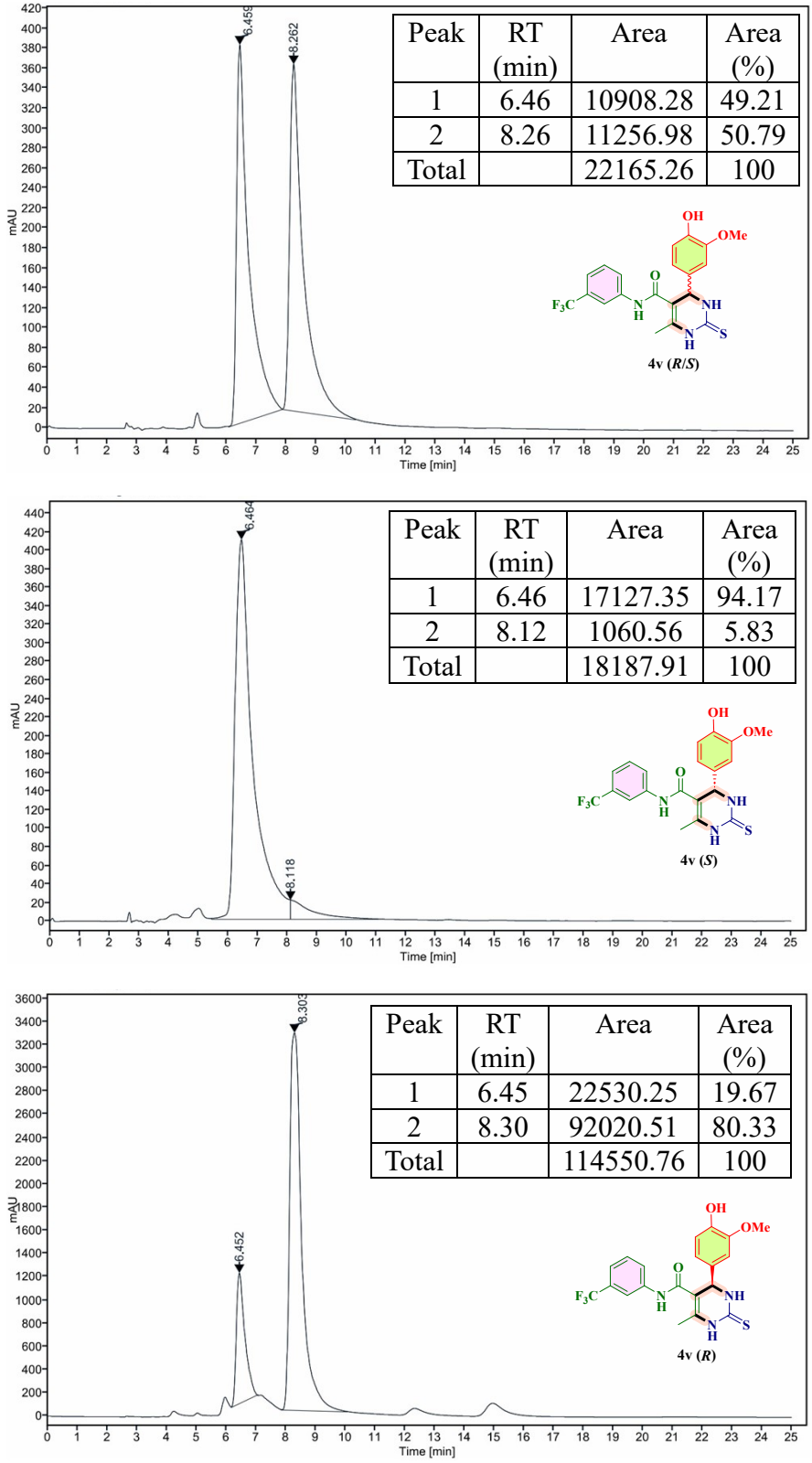
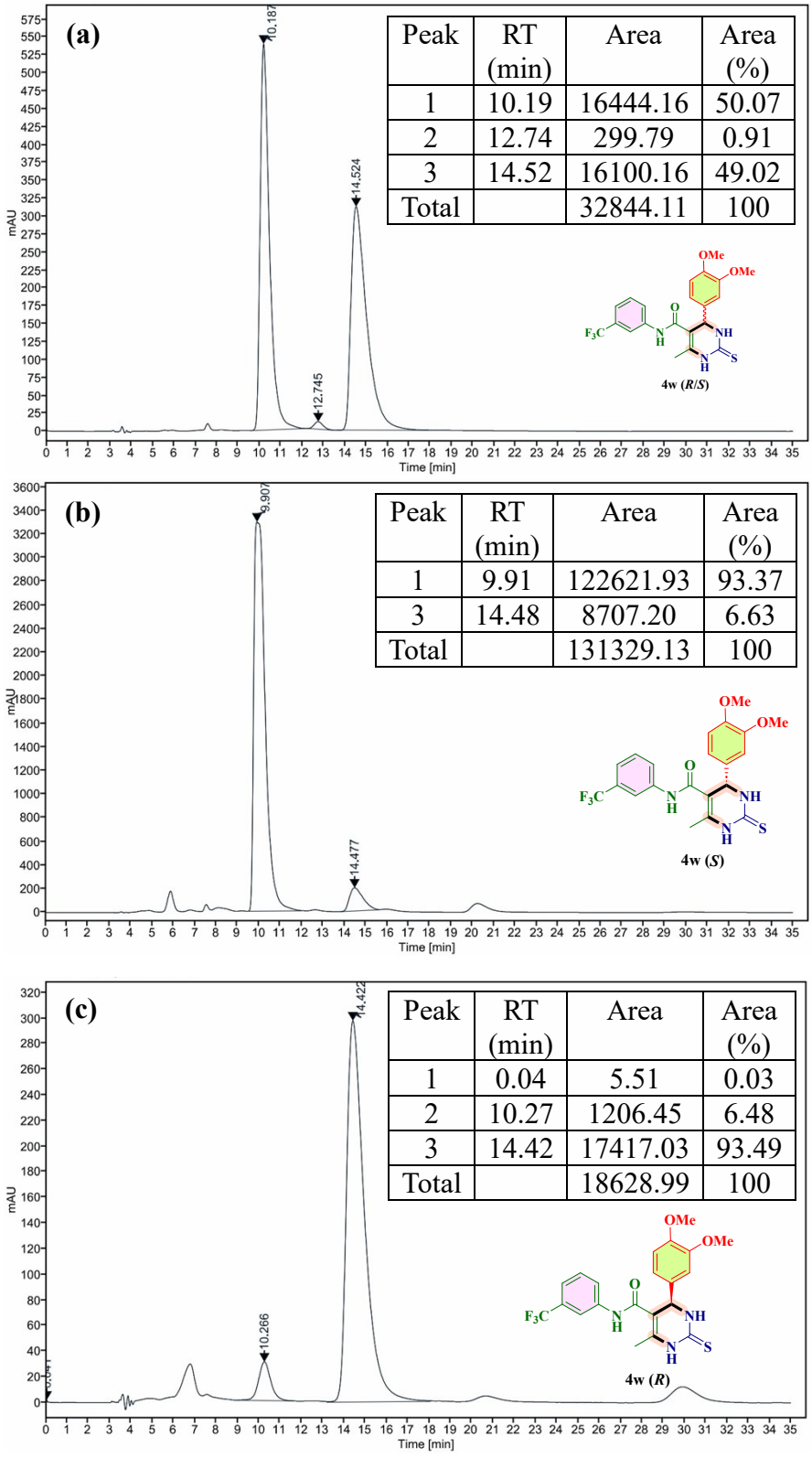


Figure S66. HPLC images of **4v**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4v** and **(c)** resolved (4*R*)(+)-**4v**.

HPLC Image of Compound **4w**. YMC Chiral ART Cellulose SZ (250 x 30 mm) 5 mic column, Hexane:Ethanol:IPA:DEA (80:0.0:20:0.1% v/v/v/v) at 30mL/min, λ = 254 nm and 312 nm, t_{major} = 10.19 min, t_{minor} = 14.52 min.



Peak	RT (min)	Area	Area (%)
1	10.19	16444.16	50.07
2	12.74	299.79	0.91
3	14.52	16100.16	49.02
Total		32844.11	100

Peak	RT (min)	Area	Area (%)
1	9.91	122621.93	93.37
3	14.48	8707.20	6.63
Total		131329.13	100

Peak	RT (min)	Area	Area (%)
1	0.04	5.51	0.03
2	10.27	1206.45	6.48
3	14.42	17417.03	93.49
Total		18628.99	100

Figure S67. HPLC images of **4w**; **(a)** racemic mixture, **(b)** resolved (4*S*)(-)-**4w** and **(c)** resolved (4*R*)(+)-**4w**.

6 Stereochemical assignment of 4(a-w)

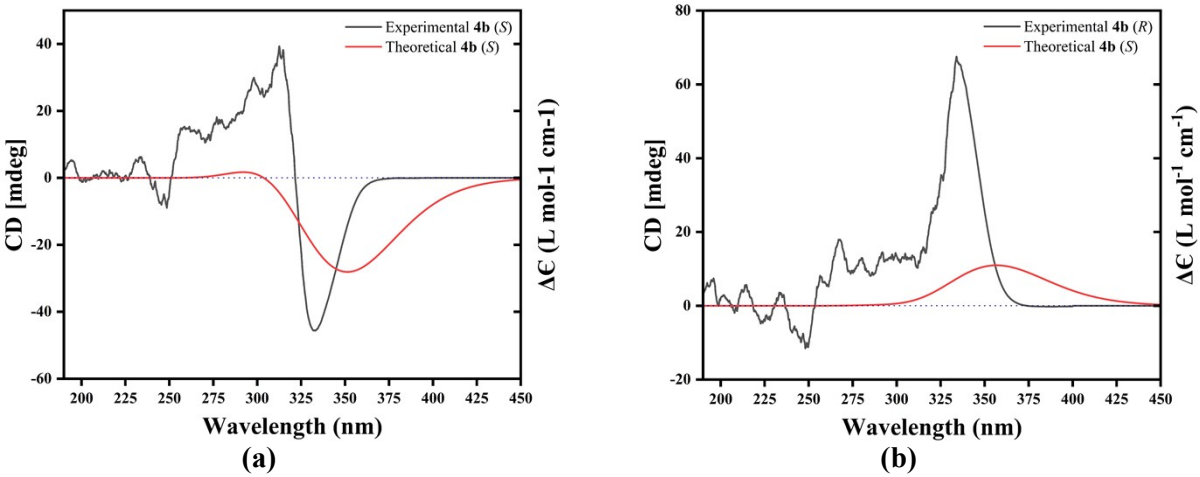


Figure S68: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4b** and (4*R*)(+)-**4b** respectively.

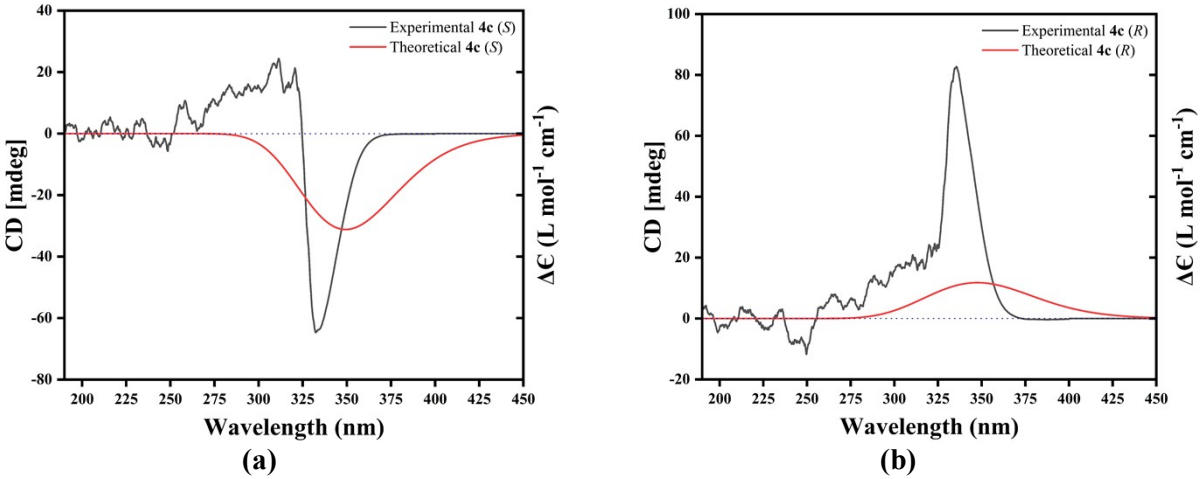


Figure S69: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4c** and (4*R*)(+)-**4c** respectively.

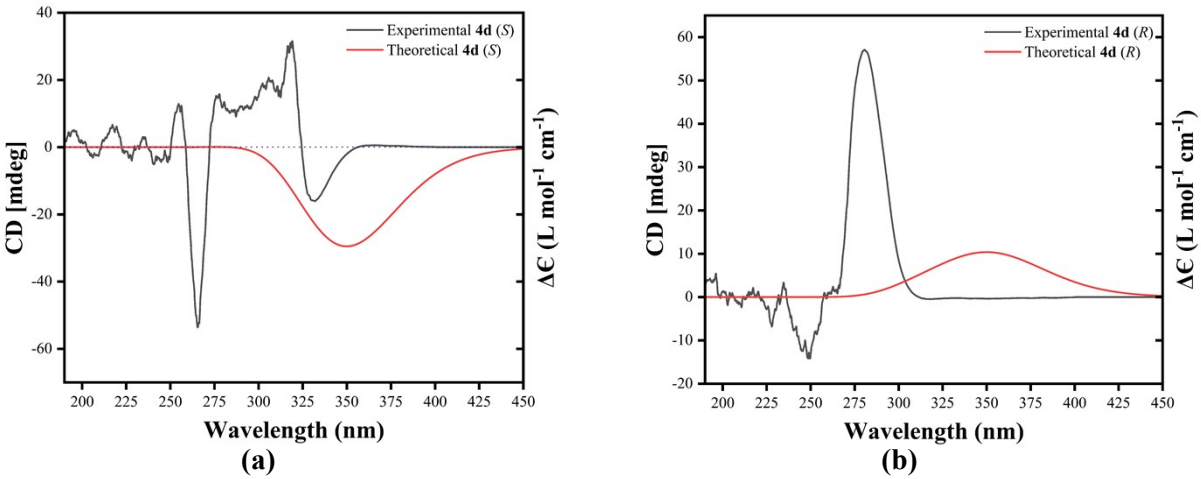


Figure S70: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4d** and (4*R*)(+)-**4d** respectively.

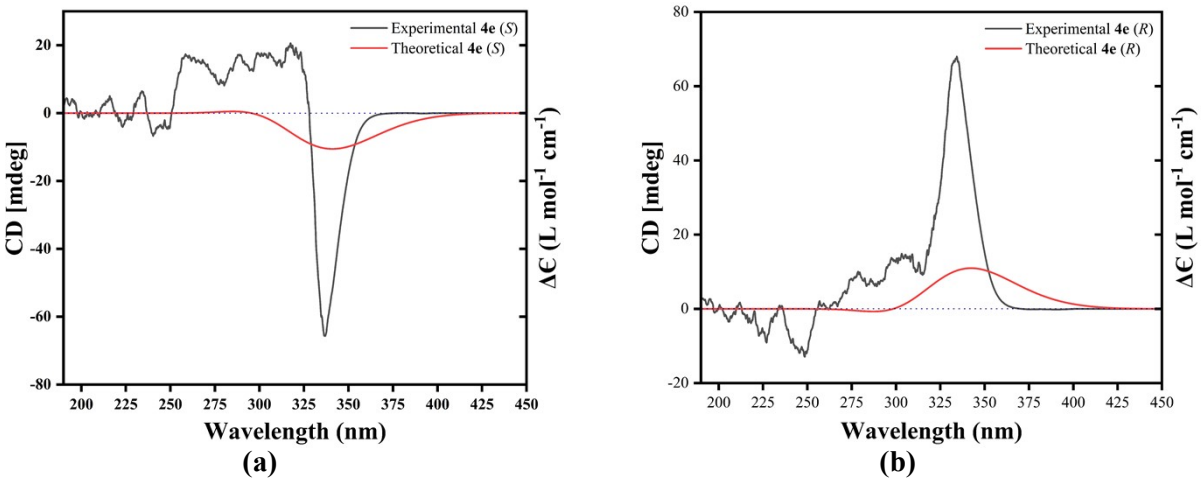


Figure S71: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4e** and (4*R*)(+)-**4e** respectively.

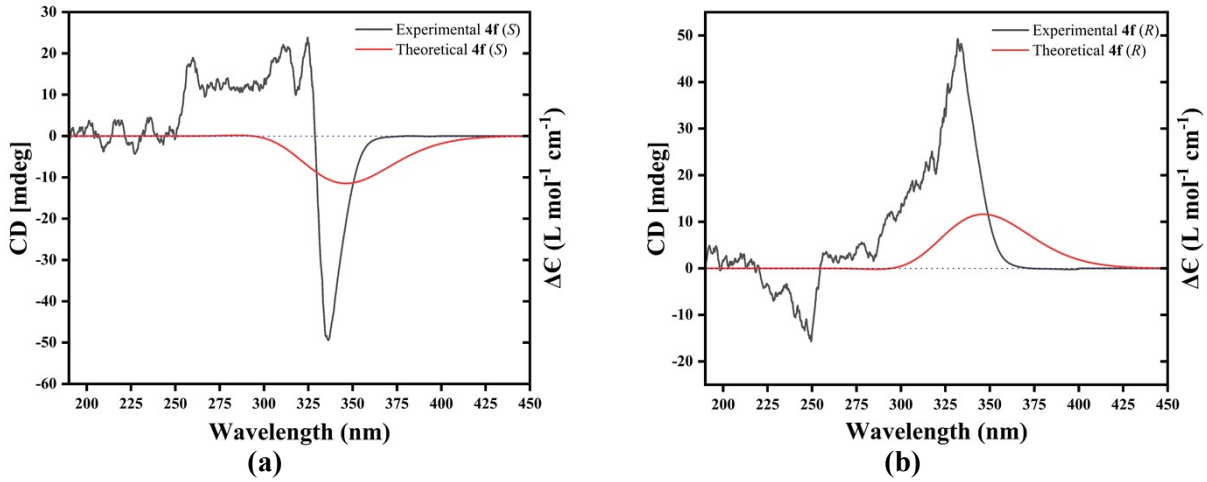


Figure S72: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4f** and (4*R*)(+)-**4f** respectively.

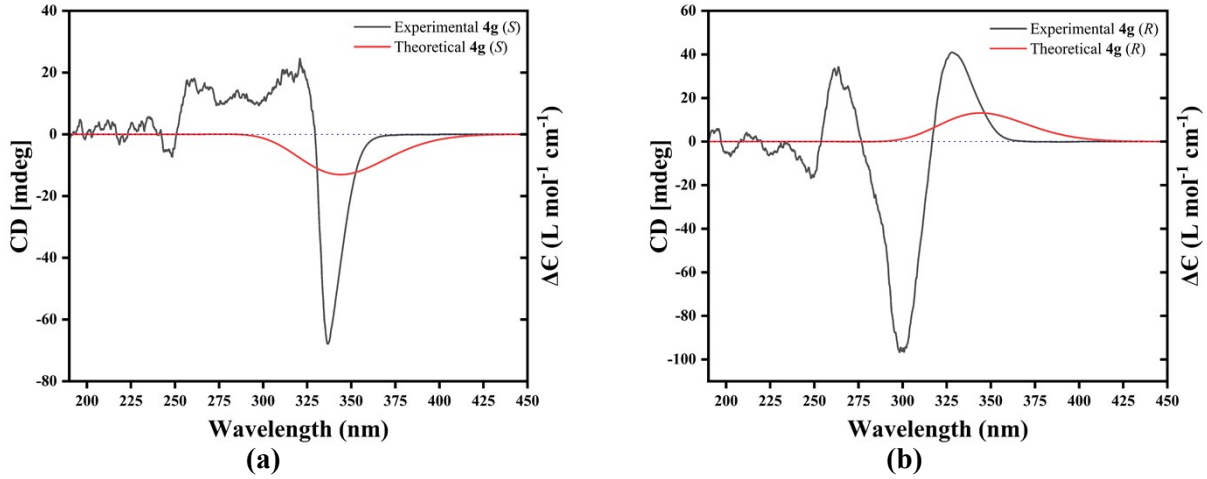


Figure S73: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4g** and (4*R*)(+)-**4g** respectively.

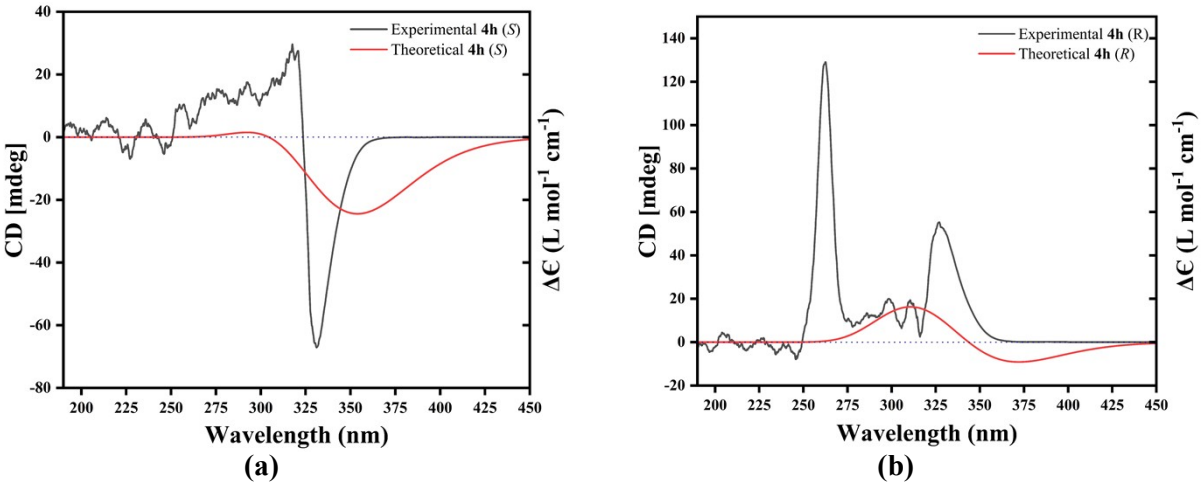


Figure S74: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4h** and (4*R*)(+)-**4h** respectively.

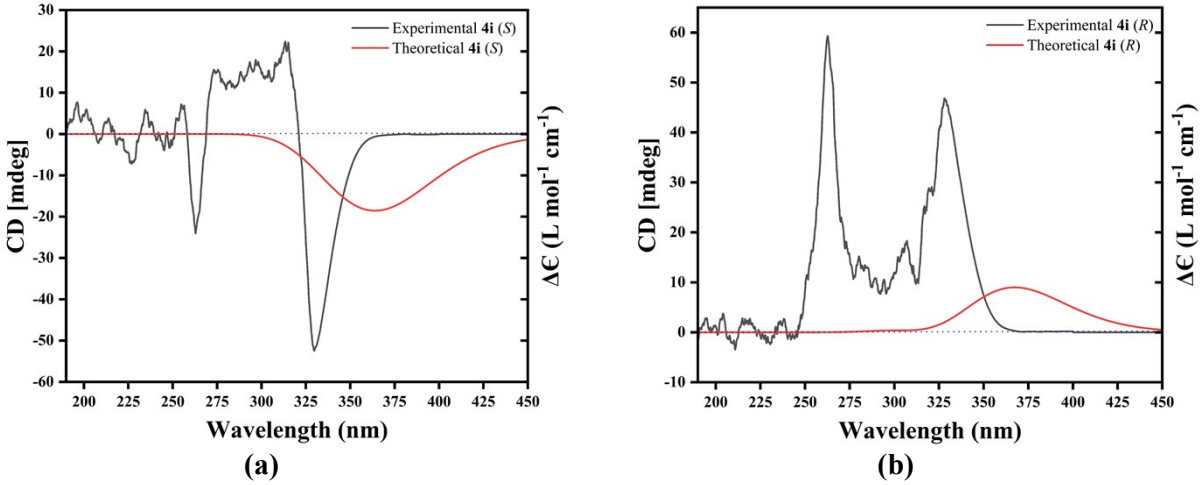


Figure S75: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4i** and (4*R*)(+)-**4i** respectively.

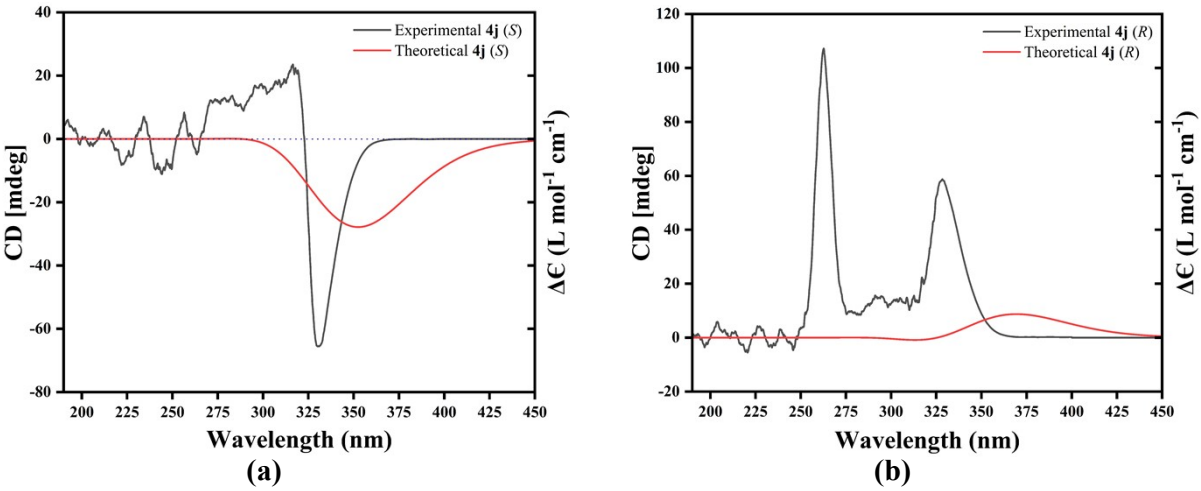


Figure S76: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4j** and (4*R*)(+)-**4j** respectively.

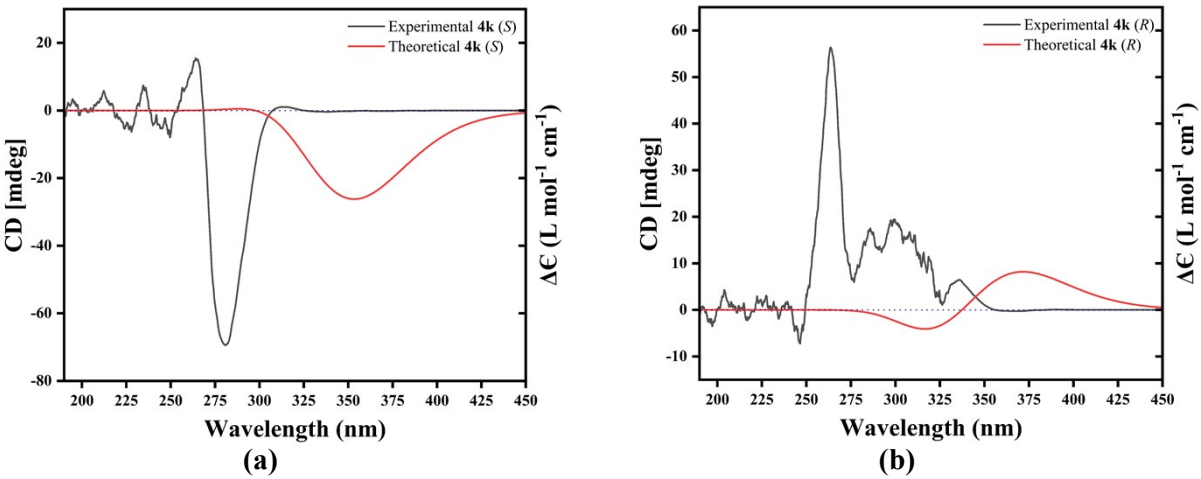


Figure S77: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4k** and (4*R*)(+)-**4k** respectively.

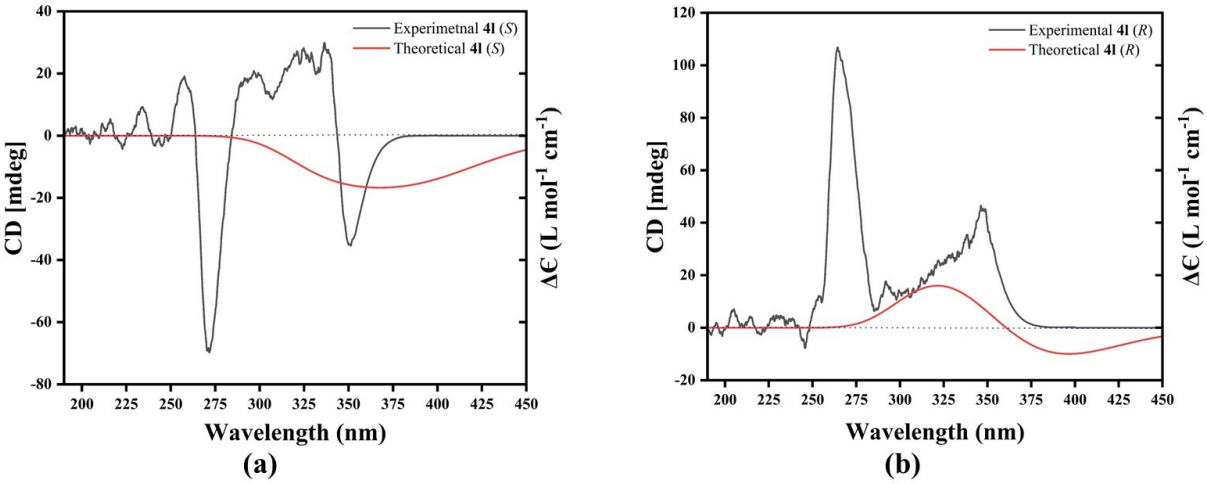


Figure S78: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4l** and (4*R*)(+)-**4l** respectively.

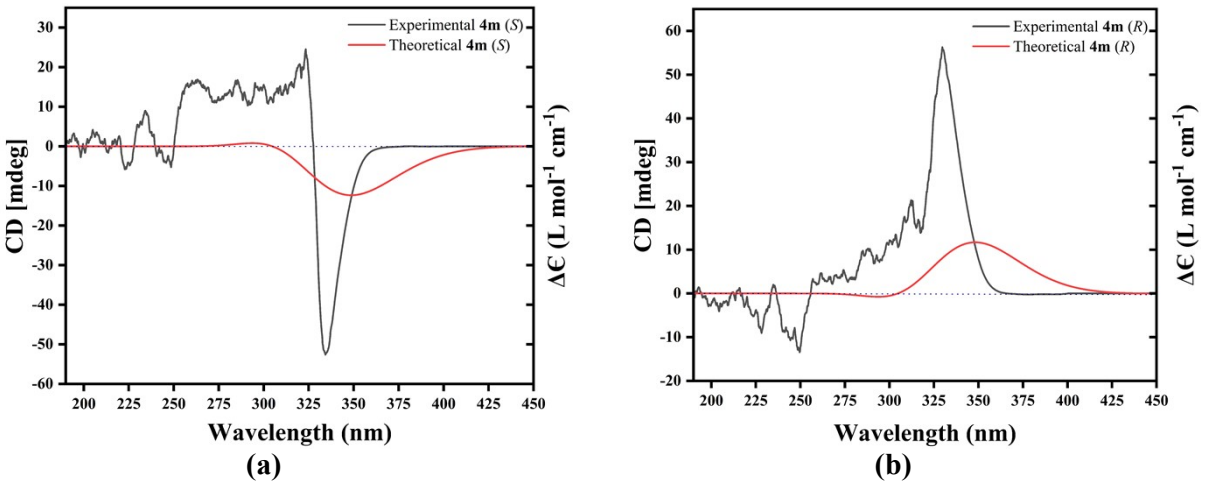


Figure S79: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4m** and (4*R*)(+)-**4m** respectively.

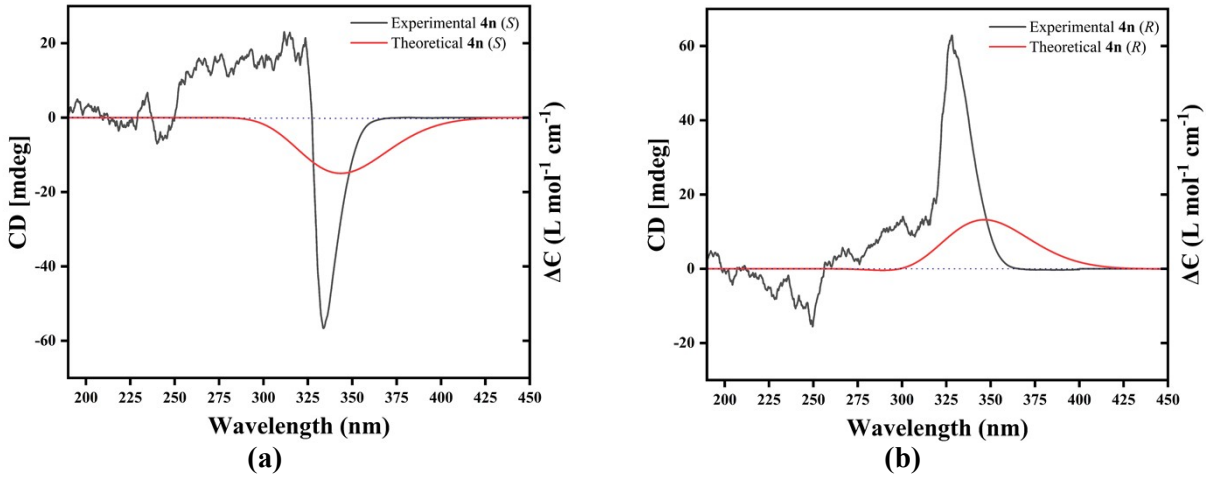


Figure S80: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4n** and (4*R*)(+)-**4n** respectively.

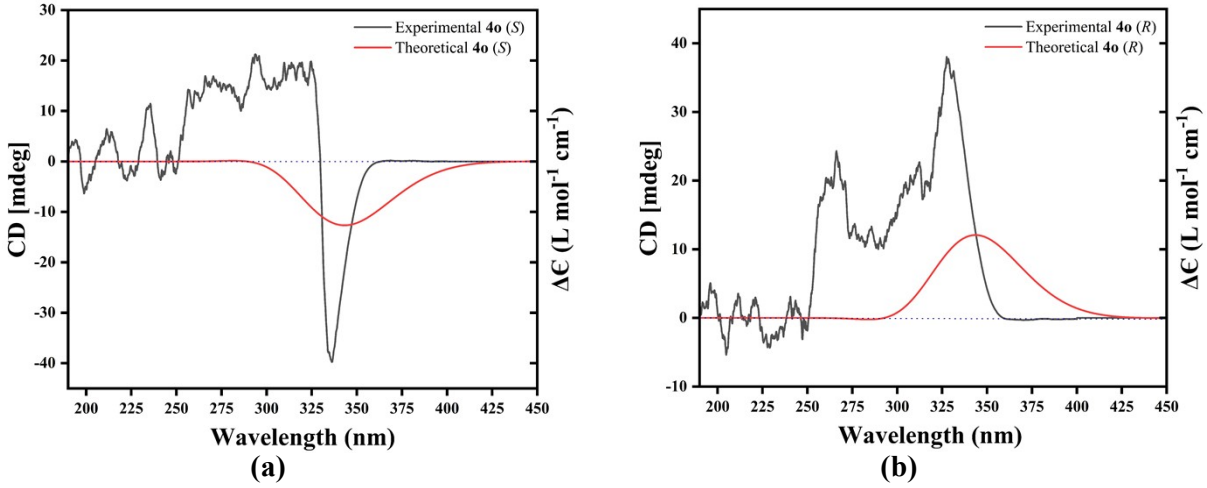


Figure S81: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4o** and (4*R*)(+)-**4o** respectively.

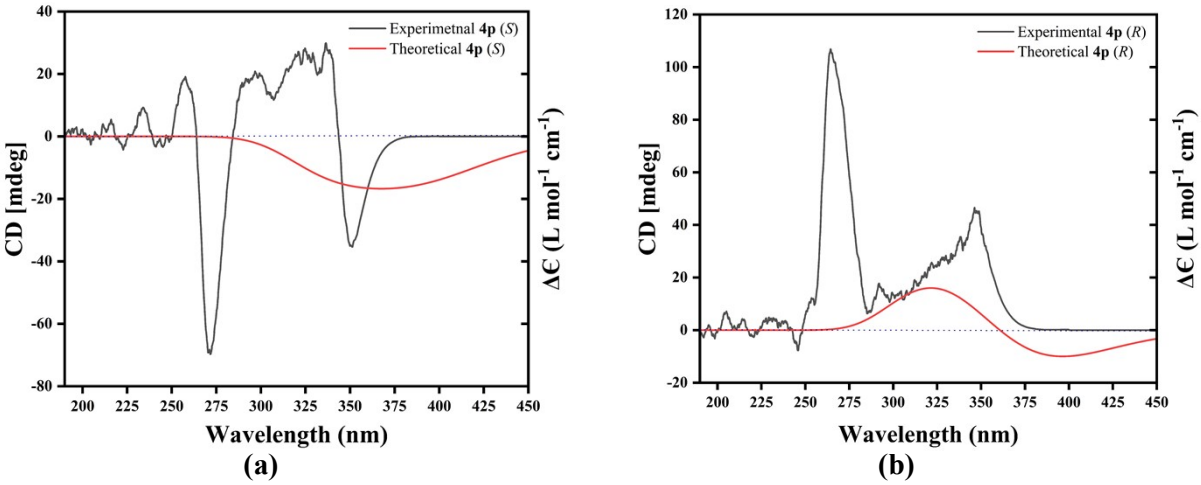


Figure S82: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4p** and (4*R*)(+)-**4p** respectively.

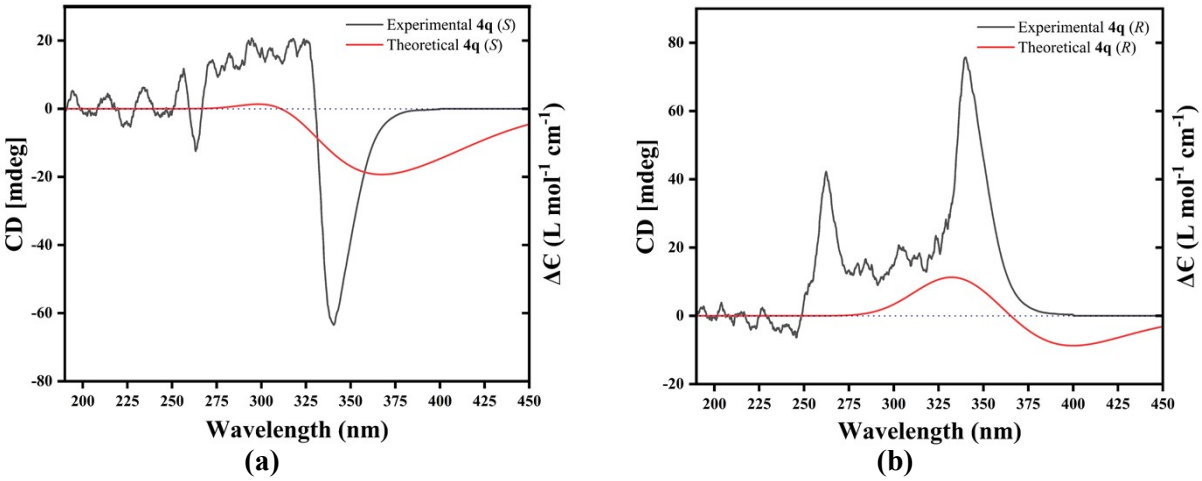


Figure S83: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4q** and (4*R*)(+)-**4q** respectively.

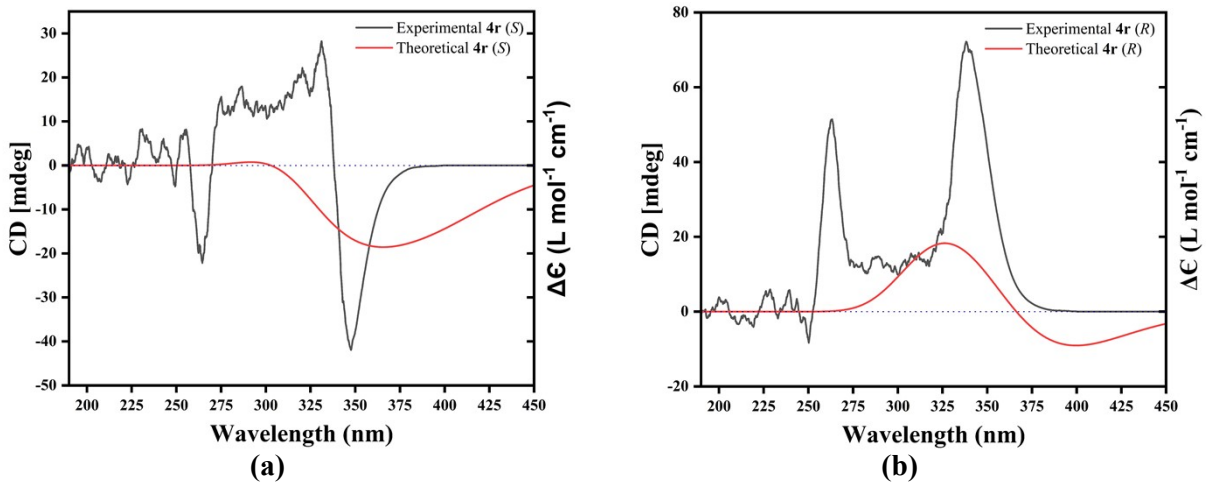


Figure S84: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4r** and (4*R*)(+)-**4r** respectively.

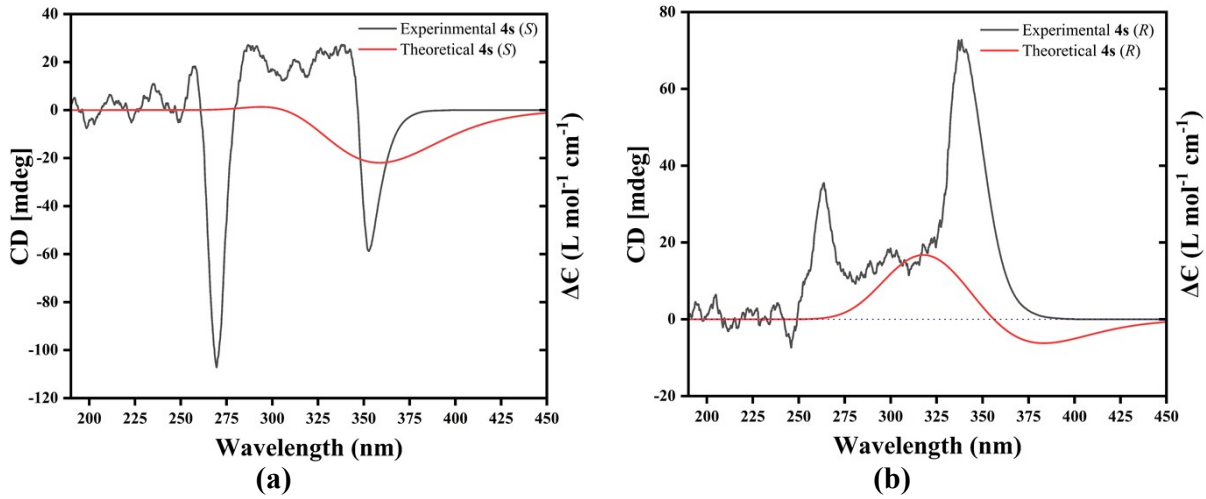


Figure S85: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4s** and (4*R*)(+)-**4s** respectively.

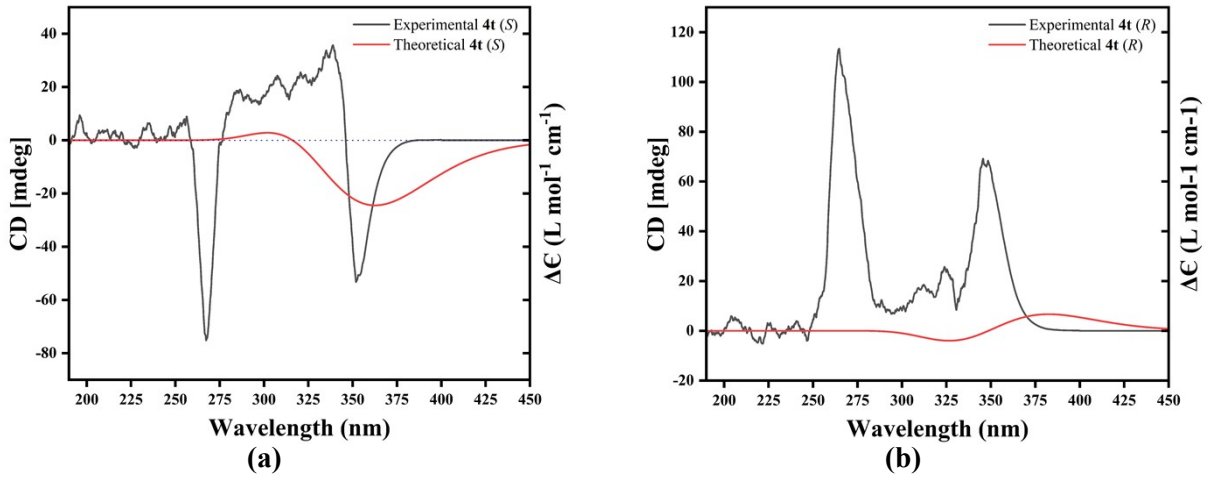


Figure S86: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4t** and (4*R*)(+)-**4t** respectively.

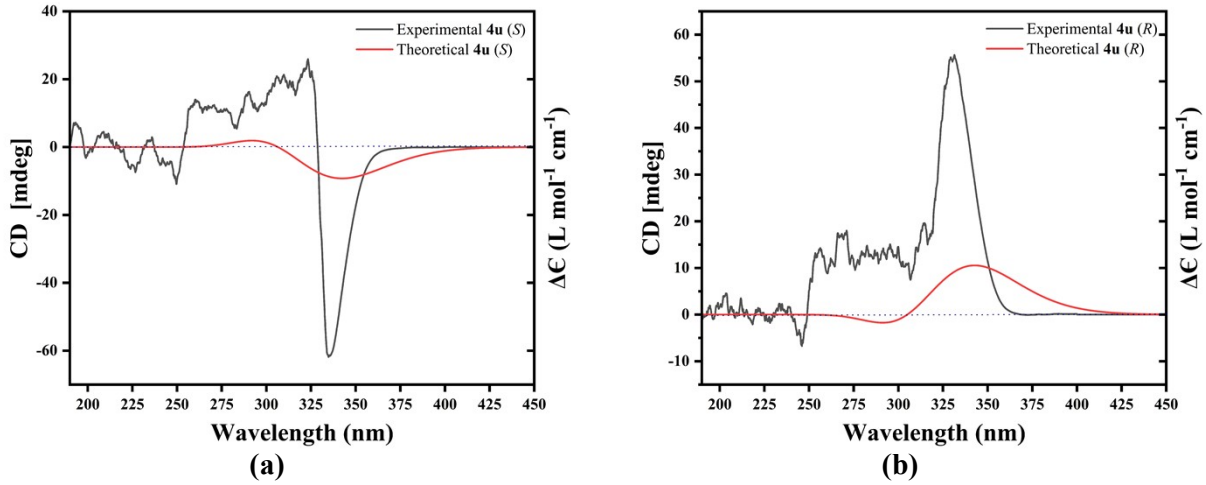


Figure S87: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4u** and (4*R*)(+)-**4u** respectively.

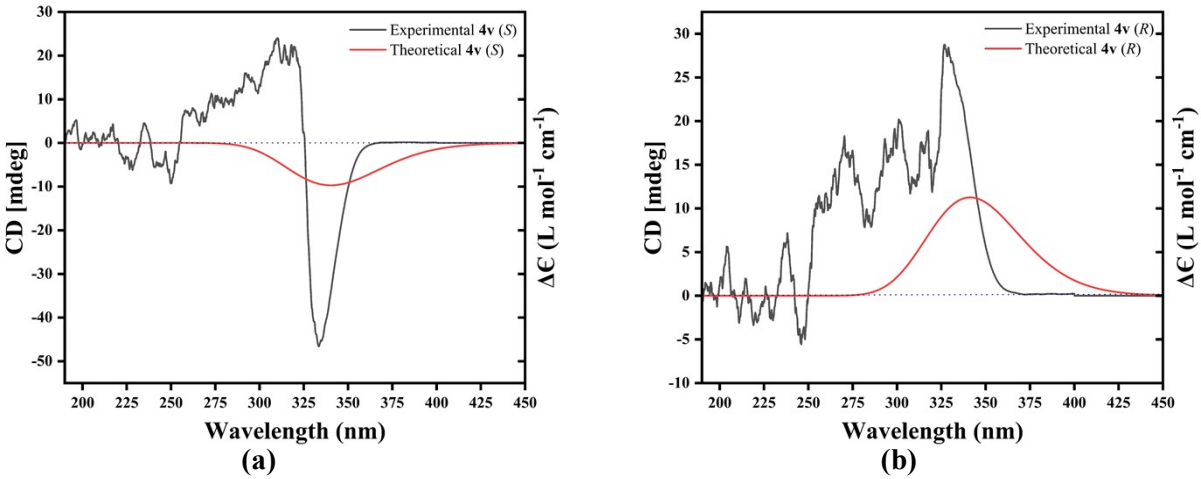


Figure S88: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4v** and (4*R*)(+)-**4v** respectively.

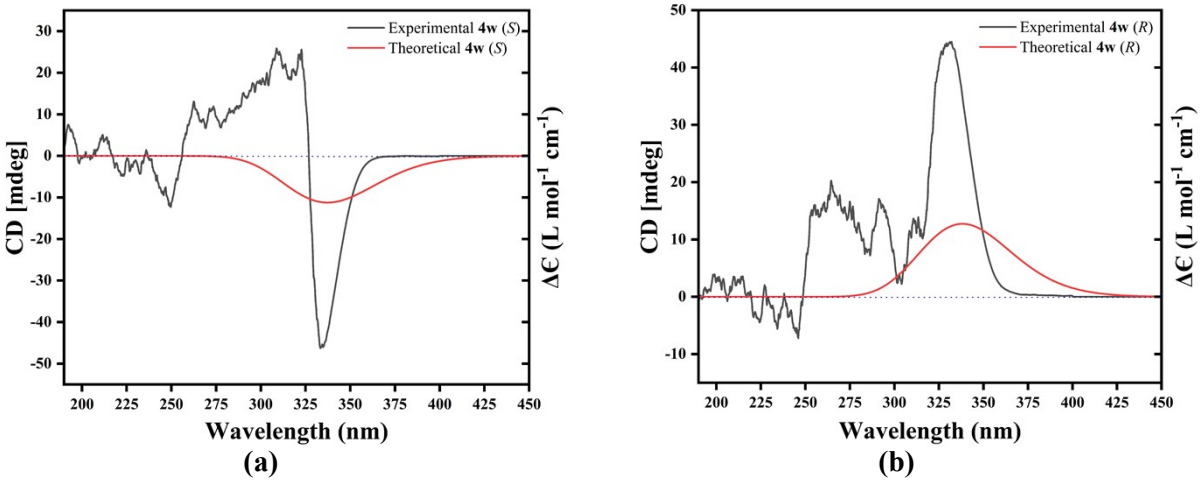


Figure S89: (a) and (b) represents the Comparison of experimental (Black) and calculated ECD (Red) spectra [Using TD-DFT method with B3LYP/6-311++G(d,p) as basis set] level in gas phase of (4*S*)(-)-**4w** and (4*R*)(+)-**4w** respectively.

7 Green Metrics Calculations

The following formulae were used for calculating Atom Economy (AE), Atom Efficiency (AEf), Carbon Efficiency (CE), Reaction Mass Efficiency (RME), Optimum Efficiency (OE), Mass Productivity (MP), Mass Intensity (MI) and Process Mass Intensity (PMI), E-factor, Solvent and Water Intensity (SI and WI).

$$AE = \frac{Molecular\ weight\ of\ product}{Total\ molecular\ weight\ of\ reactants} \times 100$$

$$AEf = AE \times \%yield$$

$$CE = \frac{Amount\ of\ carbon\ in\ the\ product}{Total\ carbon\ present\ in\ the\ reactant} \times 100$$

$$RME = \frac{Mass\ of\ isolated\ product}{Total\ mass\ of\ reactant} \times 100$$

$$OE = \frac{RME}{AE} \times 100$$

$$PMI = \frac{Total\ mass\ of\ input\ material\ in\ the\ whole\ process}{Mass\ of\ product}$$

$$MP = \frac{1}{PMI} \times 100$$

$$E\ Factor = PMI - 1$$

$$SI = \frac{Total\ mass\ of\ solvents\ excluding\ water\ in\ the\ whole\ process}{Mass\ of\ product}$$

$$WI = \frac{Total\ mass\ of\ water\ in\ the\ whole\ process}{Mass\ of\ product}$$

7.1 Green Metrics Analysis for Process A:

Materials used for metrics calculations: 4-hydroxybenzaldehyde **1a** (122.12 mg, 1 mmol), thiourea **2** (114.18 mg, 1.5 mmol), 2-chloroacetoacetanilide **3a** (211.64 mg, 1 mmol), Product **4a** (108 mg, 0.29 mmol), Taurine (18 mg, 15 mol %), t-butyl alcohol (3.875 g, 5 mL), water (3 g, 3 mL).

$$AE = \frac{373.86}{122.12 + 114.18 + 211.64} \times 100 = \frac{370.11}{447.94} \times 100 = 82.62$$

$$AEf = 82.62 \times 28.95\ \% = 23.91$$

$$CE = \frac{18 \times 108}{7 \times 122.12 + 1 \times 76.12 + 10 \times 211.64} \times 100 = \frac{1944}{3047.36} \times 100 = 63.79$$

$$RME = \frac{108}{447.94} \times 100 = 24.11$$

$$OE = \frac{24.11}{82.62} \times 100 = 29.18$$

$$PMI = \frac{0.12212 + 0.11418 + 0.21164 + 3.1 + 3}{0.108} = \frac{6.54794}{0.108} = 60.63$$

$$MP = \frac{1}{60.63} \times 100 = 1.65$$

$$E\ Factor = 60.63 - 1 = 59.63$$

$$SI = \frac{3.875}{0.108} = 35.88$$

$$WI = \frac{3}{0.108} = 27.78$$

7.2 Green Metrics Analysis for Process B:

Materials used for metrics calculations: 4-hydroxybenzaldehyde **1a** (122.12 mg, 1 mmol), thiourea **2** (114.18 mg, 1.5 mmol), 2-chloroacetoacetanilide **3a** (211.64 mg, 1 mmol), Product **4a** (157 mg, 0.42 mmol), Taurine (18 mg, 15 mol %), Methanol (3.956 g, 5 mL), water (3 g, 3 mL).

$$AE = \frac{373.86}{122.12 + 114.18 + 211.64} \times 100 = \frac{370.11}{447.94} \times 100 = 82.62$$

$$AEf = 82.62 \times 42.09\ \% = 34.77$$

$$CE = \frac{18 \times 157}{7 \times 122.12 + 1 \times 76.12 + 10 \times 211.64} \times 100 = \frac{2826}{3047.36} \times 100 = 92.74$$

$$RME = \frac{157}{447.94} \times 100 = 35.05$$

$$OE = \frac{35.05}{82.62} \times 100 = 42.42$$

$$PMI = \frac{0.12212 + 0.11418 + 0.21164 + 3.1 + 3}{0.157} = \frac{6.54794}{0.157} = 41.71$$

$$MP = \frac{1}{41.71} \times 100 = 2.40$$

$$E\ Factor = 41.71 - 1 = 40.71$$

$$SI = \frac{3.956}{0.157} = 25.19$$

$$WI = \frac{3}{0.157} = 19.11$$

7.3 Green Metrics Analysis for Process C:

Materials used for metrics calculations: 4-hydroxybenzaldehyde **1a** (122.12 mg, 1 mmol), thiourea **2** (114.18 mg, 1.5 mmol), 2-chloroacetoacetanilide **3a** (211.64 mg, 1 mmol), Product **4a** (160 mg, 0.428 mmol), Taurine (18 mg, 15 mol %), i-propyl alcohol (3.925 g, 5 mL), water (3 g, 3 mL).

$$AE = \frac{373.86}{122.12 + 114.18 + 211.64} \times 100 = \frac{370.11}{447.94} \times 100 = 82.62$$

$$AEf = 82.62 \times 28.95\ \% = 23.91$$

$$CE = \frac{18 \times 160}{7 \times 122.12 + 1 \times 76.12 + 10 \times 211.64} \times 100 = \frac{2880}{3047.36} \times 100 = 94.51$$

$$RME = \frac{160}{447.94} \times 100 = 35.72$$

$$OE = \frac{35.72}{82.62} \times 100 = 43.23$$

$$PMI = \frac{0.12212 + 0.11418 + 0.21164 + 3.1 + 3}{0.160} = \frac{6.54794}{0.160} = 40.92$$

$$MP = \frac{1}{40.92} \times 100 = 2.44$$

$$E\ Factor = 40.92 - 1 = 39.92$$

$$SI = \frac{3.925}{0.160} = 24.53$$

$$WI = \frac{3}{0.160} = 18.75$$

7.4 Green Metrics Analysis for Process D:

Materials used for metrics calculations: 4-hydroxybenzaldehyde **1a** (122.12 mg, 1 mmol), thiourea **2** (114.18 mg, 1.5 mmol), 2-chloroacetoacetanilide **3a** (211.64 mg, 1 mmol), Product **4a** (173 mg, 0.463 mmol), Taurine (18 mg, 15 mol %), Acetonitrile (3.883 g, 5 mL), water (3 g, 3 mL).

$$AE = \frac{373.86}{122.12 + 114.18 + 211.64} \times 100 = \frac{370.11}{447.94} \times 100 = 82.62$$

$$AEf = 82.62 \times 46.38\,\% = 38.31$$

$$CE = \frac{18 \times 173}{7 \times 122.12 + 1 \times 76.12 + 10 \times 211.64} \times 100 = \frac{3114}{3047.36} \times 100 = 102.19$$

$$RME = \frac{173}{447.94} \times 100 = 38.62$$

$$OE = \frac{38.62}{82.62} \times 100 = 46.74$$

$$PMI = \frac{0.12212 + 0.11418 + 0.21164 + 3.1 + 3}{0.173} = \frac{6.54794}{0.173} = 37.85$$

$$MP = \frac{1}{37.85} \times 100 = 2.64$$

$$E\,Factor = 37.85 - 1 = 36.85$$

$$SI = \frac{3.883}{0.173} = 22.44$$

$$WI = \frac{3}{0.173} = 17.34$$

7.5 Green Metrics Analysis for Process E:

Materials used for metrics calculations: 4-hydroxybenzaldehyde **1a** (122.12 mg, 1 mmol), thiourea **2** (114.18 mg, 1.5 mmol), 2-chloroacetoacetanilide **3a** (211.64 mg, 1 mmol), Product **4a** (224 mg, 0.744 mmol), Taurine (18 mg, 15 mol %), Water (4.985 g, 5 mL), water (3 g, 3 mL).

$$AE = \frac{373.86}{122.12 + 114.18 + 211.64} \times 100 = \frac{370.11}{447.94} \times 100 = 82.62$$

$$AEf = 82.62 \times 59.92\ \% = 49.51$$

$$CE = \frac{18 \times 224}{7 \times 122.12 + 1 \times 76.12 + 10 \times 211.64} \times 100 = \frac{4032}{3047.36} \times 100 = 132.31$$

$$RME = \frac{224}{447.94} \times 100 = 50.01$$

$$OE = \frac{50.01}{82.62} \times 100 = 60.53$$

$$PMI = \frac{0.12212 + 0.11418 + 0.21164 + 3.1 + 3}{0.224} = \frac{6.54794}{0.224} = 29.23$$

$$MP = \frac{1}{29.23} \times 100 = 3.42$$

$$E\ Factor = 29.23 - 1 = 28.23$$

$$SI = \frac{4.985}{0.224} = 22.25$$

$$WI = \frac{3}{0.224} = 13.39$$

7.6 Green Metrics Analysis for Process F:

Materials used for metrics calculations: 4-hydroxybenzaldehyde **1a** (122.12 mg, 1 mmol), thiourea **2** (114.18 mg, 1.5 mmol), 2-chloroacetoacetanilide **3a** (211.64 mg, 1 mmol), Product **4a** (278 mg, 0.744 mmol), Taurine (18 mg, 15 mol %), Acetic acid (5.245 g, 5 mL), water (3 g, 3 mL).

$$AE = \frac{373.86}{122.12 + 114.18 + 211.64} \times 100 = \frac{370.11}{447.94} \times 100 = 82.62$$

$$AEf = 82.62 \times 74.53\ \% = 61.58$$

$$CE = \frac{18 \times 278}{7 \times 122.12 + 1 \times 76.12 + 10 \times 211.64} \times 100 = \frac{5004}{3047.36} \times 100 = 164.21$$

$$RME = \frac{278}{447.94} \times 100 = 62.06$$

$$OE = \frac{62.06}{82.62} \times 100 = 75.12$$

$$PMI = \frac{0.12212 + 0.11418 + 0.21164 + 3.1 + 3}{0.278} = \frac{6.54794}{0.278} = 23.55$$

$$MP = \frac{1}{23.55} \times 100 = 4.25$$

$$E\ Factor = 23.55 - 1 = 22.55$$

$$SI = \frac{5.245}{0.278} = 18.87$$

$$WI = \frac{3}{0.278} = 10.79$$

7.7 Green Metrics Analysis for Process G:

Materials used for metrics calculations: 4-hydroxybenzaldehyde **1a** (122.12 mg, 1 mmol), thiourea **2** (114.18 mg, 1.5 mmol), 2-chloroacetoacetanilide **3a** (211.64 mg, 1 mmol), Product **4a** (298 mg, 0.744 mmol), Taurine (18 mg, 15 mol %), (1:1) aq. EtOH (4.4728 g, 5 mL), water (3 g, 3 mL).

$$AE = \frac{373.86}{122.12 + 114.18 + 211.64} \times 100 = \frac{370.11}{447.94} \times 100 = 82.62$$

$$AEf = 82.62 \times 79.71\ \% = 65.86$$

$$CE = \frac{18 \times 298}{7 \times 122.12 + 1 \times 76.12 + 10 \times 211.64} \times 100 = \frac{5364}{3047.36} \times 100 = 176.02$$

$$RME = \frac{298}{447.94} \times 100 = 66.53$$

$$OE = \frac{66.53}{82.62} \times 100 = 80.52$$

$$PMI = \frac{0.12212 + 0.11418 + 0.21164 + 3.1 + 3}{0.298} = \frac{6.54794}{0.298} = 21.97$$

$$MP = \frac{1}{21.97} \times 100 = 4.55$$

$$E\ Factor = 21.97 - 1 = 20.97$$

$$SI = \frac{4.4728}{0.298} = 15.01$$

$$WI = \frac{3}{0.298} = 10.06$$

7.8 Green Metrics Analysis for Process H:

Materials used for metrics calculations: 4-hydroxybenzaldehyde **1a** (122.12 mg, 1 mmol), thiourea **2** (114.18 mg, 1.5 mmol), 2-chloroacetoacetanilide **3a** (211.64 mg, 1 mmol), Product **4a** (308 mg, 0.825 mmol), Taurine (18 mg, 15 mol %), Acetone (3.922 g, 5 mL), water (3 g, 3 mL).

$$AE = \frac{373.86}{122.12 + 114.18 + 211.64} \times 100 = \frac{370.11}{447.94} \times 100 = 82.62$$

$$AEf = 82.62 \times 82.57\ \% = 68.22$$

$$CE = \frac{18 \times 308}{7 \times 122.12 + 1 \times 76.12 + 10 \times 211.64} \times 100 = \frac{5544}{3047.36} \times 100 = 181.93$$

$$RME = \frac{308}{447.94} \times 100 = 68.76$$

$$OE = \frac{68.76}{82.62} \times 100 = 83.22$$

$$PMI = \frac{0.12212 + 0.11418 + 0.21164 + 3.1 + 3}{0.308} = \frac{6.54794}{0.308} = 21.26$$

$$MP = \frac{1}{21.26} \times 100 = 4.70$$

$$E\ Factor = 21.26 - 1 = 20.26$$

$$SI = \frac{3.922}{0.308} = 12.73$$

$$WI = \frac{3}{0.308} = 9.74$$

7.9 Green Chemistry metrics analysis for Process I:

Materials used for metrics calculations: 4-hydroxybenzaldehyde **1a** (122.12 mg, 1 mmol), thiourea **2** (114.18 mg, 1.5 mmol), 2-chloroacetoacetanilide **3a** (211.64 mg, 1 mmol), Product **4a** (344 mg, 0.891 mmol), Taurine (18 mg, 15 mol %), Ethanol (3.16 g, 4 mL), water (3 g, 3 mL).

$$AE = \frac{373.86}{122.12 + 114.18 + 211.64} \times 100 = \frac{370.11}{447.94} \times 100 = 82.62$$

$$AEf = 82.62 \times 92\ \% = 76.01$$

$$CE = \frac{18 \times 344}{7 \times 122.12 + 1 \times 76.12 + 10 \times 211.64} \times 100 = \frac{6192}{3047.36} \times 100 = 203.192$$

$$RME = \frac{344}{447.94} \times 100 = 76.80$$

$$OE = \frac{76.80}{82.62} \times 100 = 92.96$$

$$PMI = \frac{0.12212 + 0.11418 + 0.21164 + 3.1 + 3}{0.344} = \frac{6.54794}{0.344} = 19.04$$

$$MP = \frac{1}{19.04} \times 100 = 5.25$$

$$E\ Factor = 19.04 - 1 = 18.04$$

$$SI = \frac{3.16}{0.344} = 9.18$$

$$WI = \frac{3}{0.344} = 8.72$$