Supporting Information

For

Synthesis, characterization and photophysical studies of dual emissive base-modified fluorescent nucleosides

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Experimental Part and NMR Spectra

Table of Contents

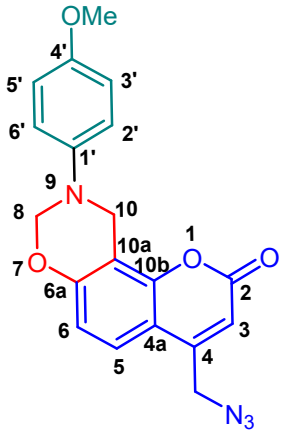
1. Experimental

All chemicals and solvents were purchased from Alfa-Aesar by Thermo Fischer Scientific, India Pvt. Limited, Sigma-Aldrich Chemicals Pvt. Limited India and from local commercial sources, and were used without any further purification unless otherwise specified. Solvents for column chromatography were dried and distilled prior to use. Solvents were removed under reduced pressure using rotary evaporator, followed by further removal of the residual solvent under high vacuum. Column chromatography was performed on silica gel (100-200 mesh). Melting points were determined on Buchi M-560 instrument and are uncorrected. HRMS analysis was carried out using Agilent G6530AA LC Q-TOF mass spectrometer using ESI method. The IR spectra of compounds were recorded on Perkin-Elmer model 2000 FT-IR spectrometer and are expressed as wavenumber (cm^{-1}). R_f values of compounds are reported from analytical TLC study using the specified solvents and 0.25 mm silica gel 60 F_{254} plates that were visualized by UV irradiation or by charring with 5% alcoholic sulfuric acid solution. The ^{1}H- and the ^{13}C- and other 2D NMR spectra were recorded on JEOL alpha-400 and Bruker-Avance Neo 400 FT-NMR spectrometers by using tetramethylsilane (TMS) as internal standard. The chemical shift values are on δ scale and the coupling constant (J) are in Hz. Absorption spectra were recorded between 200 nm and 600 nm using a Perkin-Elmer UV/Vis spectrometer Lambda 45 at scan speed 240 nm/min. All measurements were carried out in PEUV/ Vis Spectroscopy cells (1 cm). HPLC grade solvents were used for all solution preparation.

1.1. General method for the synthesis of 4-(azidomethyl)-N^9-(4'-aryl)-9,10-dihydro-2H,8H-chromeno[8,7-e][1,3]oxazin-2-one (6a-f)

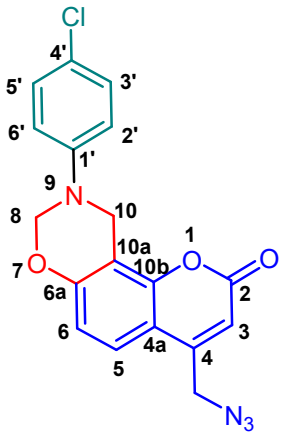
A solution of primary amine **5a-f** (1.1 mmol) in dioxane (5 mL) was treated with formalin solution (2.5 mmol). The resulting mixture was stirred at room temperature for 3-5 h. Subsequently, 7-hydroxy-4-azidomethylcoumarin **4** (1 mmol) and a catalytic amount of DMAP was added to the reaction mixture. The reaction was then stirred at 100˚C until the complete consumption of the reactant (the progress of the reaction was examined by thin layer chromatography). After completion of the reaction, the solvent was evaporated under reduced pressure and the crude product was purified by using silica gel column chromatography using ethyl acetate and hexane as the solvent system to attain the desired compounds **6a-f** in 72-86% yields.

1.1.1 4-(azidomethyl)-N⁹-(4'-methoxyphenyl)-9,10-dihydro-2H,8H-chromeno[8,7-e][1,3]oxazin-2-one (6a)



It was obtained as a yellow solid. Yield: 0.28 g (78%). R_f= 0.48 (30% ethyl acetate in petroleum ether); Melting Point = 140-142 ˚C; IR (KBr, cm^{-1}): 2116, 1732, 1517, 1412, 1298, 1143, 1057, 926, 781, 719; ^{1}H NMR ($CDCl_3$, 400MHz): δ 7.29 (d, J = 8.8 Hz, 1H, ArH), 7.10-7.07 (m, 2H, ArH), 6.82-6.79 (m, 3H, ArH), 6.33 (s, 1H, C-3H), 5.38 (s, 2H, CH_2), 4.73 (s, 2H, CH_2), 4.47 (d, J = 1.0 Hz, 2H, CH_2N_3), 3.74 (s, 3H, OCH_3); ^{13}C NMR ($CDCl_3$, 100MHz): δ 160.5 (C=O), 158.0 (ArC), 155.4 (ArC), 151.6 (ArC), 149.2 (ArC), 141.7 (ArC), 122.8 (ArC), 120.8 (ArC), 114.6 (ArC), 114.1 (ArC), 111.1 (ArC), 110.5 (C-3), 109.3 (ArC), 81.1 (CH_2), 55.6 (OCH_3), 50.8 (CH_2N_3), 46.9 (CH_2); HRMS (ESI): m/z calculated for $C_{19}H_{17}N_4O_4^+$ $[M+H]^+$: 365.1250, found: 365.1255.

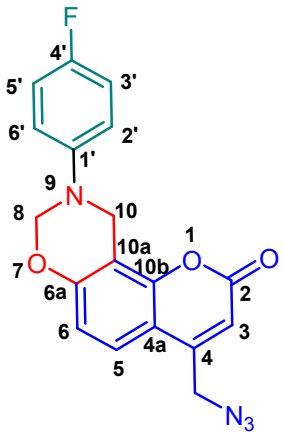
1.1.2. 4-(azidomethyl)-N⁹-(4'-chlorophenyl)-9,10-dihydro-2H,8H-chromeno[8,7-e][1,3]oxazin-2-one (6b)



It was obtained as a yellow solid. Yield: 0.28 g (75%). R_f= 0.52 (30% ethyl acetate in petroleum ether); Melting Point = 134-136 ˚C; IR (KBr, cm^{-1}): 2100, 1715, 1591, 1488, 1360, 1307, 1248, 1157, 1091, 916, 796, 713;^{1}H NMR ($CDCl_3$, 400MHz): δ 7.31 (d, J = 8.8 Hz, 1H, ArH), 7.22

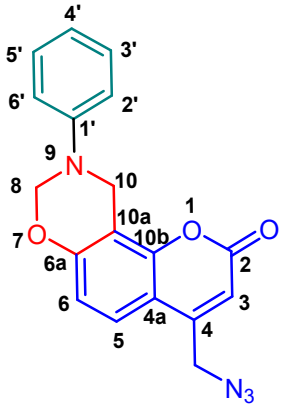
(d, J = 8.7 Hz, 2H, ArH), 7.06 (d, J = 8.7 Hz, 2H, ArH), 6.79 (d, J = 8.8 Hz, 1H, ArH), 6.35 (s, 1H, C-3H), 5.40 (s, 2H, CH_2), 4.78 (s, 2H, CH_2), 4.48 (d, J = 1.0 Hz, 2H, CH_2N_3); ^{13}C NMR ($CDCl_3$, 100MHz): δ 160.2 (C=O), 157.7 (ArC), 151.5 (ArC), 149.0 (ArC), 146.4 (ArC), 129.3 (ArC), 127.3 (ArC), 123.0 (ArC), 119.9 (ArC), 114.0 (ArC), 111.3 (ArC), 110.7 (C-3), 109.0 (ArC), 79.8 (CH_2), 50.8 (CH_2N_3), 46.5 (CH_2); HRMS (ESI): m/z calculated for $C_{18}H_{14}ClN_4O^+$ $[M+H]^+$: 369.0754, found: 369.0772.

1.1.3. 4-(azidomethyl)-N^9-(4'-fluorophenyl)-9,10-dihydro-2H,8H-chromeno[8,7-e][1,3]oxazin-2-one (6c)



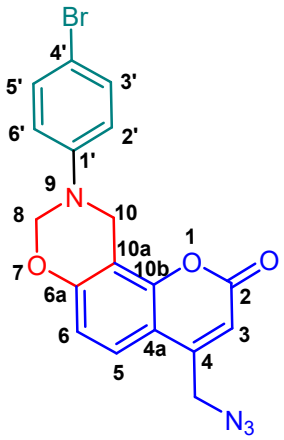
It was obtained as a yellow solid. Yield: 0.25 g (72%). R_f = 0.53 (30% ethyl acetate in petroleum ether); Melting Point = 124 ˚C; IR (KBr, cm^{-1}): 2118, 1711, 1556, 1414, 1336, 1222, 1154, 1071, 879, 743;^{1}H NMR ($CDCl_3$, 400MHz): δ 7.30 (d, J = 8.8 Hz, 1H, ArH), 7.08 (dd, J = 9.1 Hz, 4.6 Hz, 2H, ArH), 6.94-6.79 (m, 2H, ArH), 6.78 (d, J = 8.8 Hz, 1H, ArH), 6.33 (s, 1H, C-3H), 5.36 (s, 2H, CH_2), 4.74 (s, 2H, CH_2), 4.47 (s, 2H, CH_2N_3); ^{13}C NMR ($CDCl_3$, 100MHz): δ 160.4 (C=O), 159.7 (ArC), 157.9 (ArC), 157.3 (ArC), 151.5 (ArC), 149.2 (ArC), 144.3 (ArC), 144.3 (ArC), 123.0 (ArC), 120.7 (ArC), 120.6 (ArC), 116.1 (ArC), 115.9 (ArC), 114.1 (ArC), 111.3 (ArC), 110.7 (C-3), 109.1 (ArC), 80.6 (CH_2), 50.8 (CH_2N_3), 46.9 (CH_2); HRMS (ESI): m/z calculated for $C_{18}H_{14}FN_4O_3^+$ $[M+H]^+$: 353.1050, found: 353.1059.

1.1.4. 4-(azidomethyl)-N^9-phenyl-9,10-dihydro-2H,8H-chromeno[8,7-e][1,3]oxazin-2-one (6d)



It was obtained as a yellow solid in. Yield: 0.27 g (82%). R_f = 0.56 (30% ethyl acetate in petroleum ether); Melting Point = 129 ˚C; IR (KBr, cm^{-1}): 2110, 1709, 1595, 1495, 1388, 1296, 1242, 1205, 1158, 1037, 894, 840, 753, 685; ^{1}H NMR ($CDCl_3$, 400MHz): δ 7.30-7.26 (m, 3H, ArH), 7.15-7.12 (m, 2H, ArH), 6.98-6.94 (m, 1.0 Hz, 1H, ArH), 6.78 (d, J = 8.8 Hz, 1H, ArH), 6.34 (d, J = 1.0 Hz, 1H, C-3H), 5.44 (s, 2H, CH_2), 4.82 (s, 2H, CH_2), 4.47 (s, 2H, CH_2N_3); ^{13}C NMR ($CDCl_3$, 100MHz): δ 160.5 (C=O), 158.5 (ArC), 151.5 (ArC), 149.2 (ArC), 147.9 (ArC), 129.5 (ArC), 122.9 (ArC), 122.2 (ArC), 118.6 (ArC), 117.7 (ArC), 114.1 (ArC), 111.2 (C-3), 109.4 (ArC), 80.0 (CH_2), 50.8 (CH_2N_3), 46.4 (CH_2); HRMS (ESI): m/z calculated for $C_{18}H_{15}N_4O_3^+$ $[M+H]^+$: 335.1144, found: 335.1151.

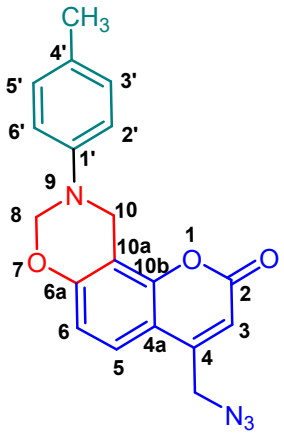
1.1.5. 4-(azidomethyl)-N^9-(4'-bromophenyl)-9,10-dihydro-2H,8H-chromeno[8,7-e][1,3]oxazin-2-one (6e)



It was obtained as a yellow solid. Yield: 0.36 g (86%). R_f = 0.54 (30% ethyl acetate in petroleum ether); Melting Point = 131-132 ˚C; IR (KBr, cm^{-1}): 2106, 1732, 1464, 1341, 1224, 1138, 1057, 923, 787, 707;^{1}H NMR ($CDCl_3$, 400MHz): δ 7.37-7.36 (m, 1H, ArH), 7.35-7.34 (m, 1H, ArH), 7.31 (d, J = 8.9 Hz, 1H, ArH), 7.02-7.01 (m, 1H, ArH), 7.00-6.99 (m, 1H, ArH), 6.78 (d, J = 8.8 Hz, 1H, ArH), 6.34 (s, 1H,C-3H), 5.39 (s, 2H, CH_2), 4.78 (s, 2H, CH_2), 4.47 (d, J = 0.9 Hz,

2H, CH_2N_3); ^{13}C NMR ($CDCl_3$, 100MHz): δ 160.3 (C=O), 157.8 (ArC), 151.5 (ArC), 149.1 (ArC), 147.0 (ArC), 132.4 (ArC), 123.0 (ArC), 120.3 (ArC), 114.8 (ArC), 114.1 (ArC), 111.4 (ArC), 110.7 (C-3), 109.1 (ArC), 79.7 (CH_2), 50.9 (CH_2N_3), 46.5 (CH_2); HRMS (ESI): m/z calculated for $C_{18}H_{14}BrN_4O_3^+$ $[M+H]^+$: 413.0249, found: 413.0266.

1.1.6. 4-(azidomethyl)-N⁹-(4'-methylphenyl)-9,10-dihydro-2H,8H-chromeno[8,7-e][1,3]oxazin-2-one (6f)



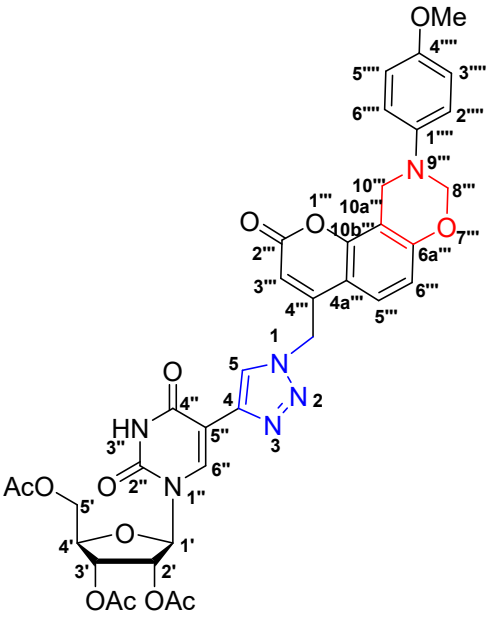
It was obtained as a yellow solid. Yield: 0.28 g (79%). R_f = 0.63 (30% ethyl acetate in petroleum ether); Melting Point = 118-120 ˚C; IR (KBr, cm^{-1}): 2103, 1726, 1550, 1478, 1336, 1317, 1231, 1129, 1064, 921, 771, 725;^1H NMR ($CDCl_3$, 400MHz): δ 7.20 (d, J = 8.8 Hz, 1H, ArH), 6.99-6.97 (m, 4H, ArH), 6.70 (d, J = 8.8 Hz, 1H, ArH), 6.25 (s, 1H, C-3H), 5.33 (s, 2H, CH_2), 4.70 (s, 2H, CH_2), 4.39 (d, J = 0.8 Hz, 2H, CH_2N_3), 2.18 (s, 3H, CH_3); ^{13}C NMR ($CDCl_3$, 100MHz): δ 160.2 (C=O), 157.7 (ArC), 151.5 (ArC), 149.0 (ArC), 146.4 (ArC), 129.3 (ArC), 127.3 (ArC), 123.0 (ArC), 119.9 (ArC), 114.0 (ArC), 111.3 (ArC), 110.7 (C-3), 109.0 (ArC), 79.8 (CH_2), 50.8 (CH_2N_3), 46.5 (CH_2), 20.6 (CH_3); HRMS (ESI): m/z calculated for $C_{19}H_{16}N_4NaO_3^+$ $[M+Na]^+$: 371.1120, found: 371.1104.

1.2. General procedure for the synthesis of N¹-(9'''-(4''''-substituted)-9''',10'''-dihydro-2'''H,8'''H-chromeno[8''',7'''-e][1''',3''']oxazin-2'''-one-4'''-methyl)-C⁴-(2',3',5'-tri-O-acetyl/3',5'-di-O-acetyl-β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole conjugates (12a-f and 13a-f)

A mixture of freshly synthesized dihydro[1,3]oxazines **6a-f** (1.2 mmol) and 5-ethynyl-2',3',5'-tri-*O*-acetyl/3',5'-di-*O*-acetyl-2'-deoxyuridine **11a-b** (1.0 mmol) was stirred at 80˚C in ^{t}BuOH (20 ml). Subsequently, a solution of sodium ascorbate (0.40 mmol) in H_2O was added followed by addition of $CuSO_4.5H_2O$ (0.20 mmol) solution in H_2O. The progress of the reaction was

monitored by TLC examination. After completion of the reaction (as observed by TLC), the solvent was evaporated under reduced pressure and the crude product was purified by using silica gel column chromatography using methanol in chloroform as the solvent system to attain the desired compounds **12a-f** and **13a-f** in 92-95% yields.

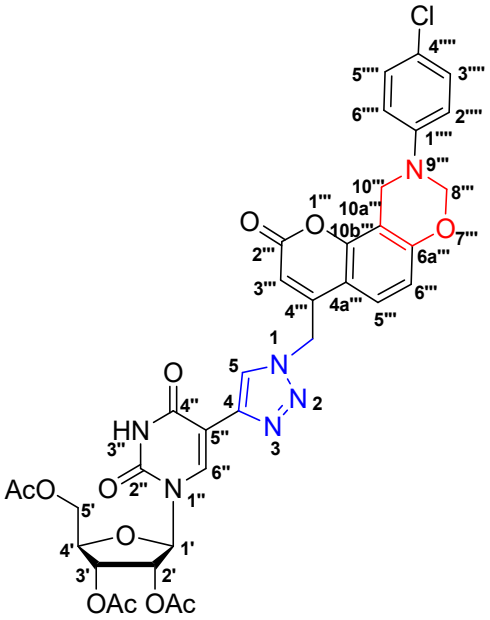
1.2.1. N^1-(9'''-(4''''-methoxy)-9''',10'''-dihydro-2'''H,8'''H-chromeno[8''',7'''-e][1''',3''']oxazin-2'''-one-4'''-methyl)-C^4-(2',3',5'-tri-O-acetyl-β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole (12a)



It was obtained as a bright yellow solid. Yield: 0.72 g (95%). R_f = 0.32 (5% methanol in chloroform); Melting Point = 252 ˚C; IR (KBr, cm^{-1}): 3318, 3074, 2937, 2840, 1680, 1602, 1514, 1465, 1377, 1217, 1102, 1043, 895, 826, 593; ^{1}H NMR (DMSO-d_6, 400MHz): δ 11.88 (s, 1H, N-3″H), 8.58 (s, 1H, C-5H), 8.47 (s, 1H, C-6″H), 7.66-7.63 (m, 1H, ArH), 7.11-7.06 (m, 2H, ArH), 6.86-6.79 (m, 3H, ArH), 6.11-6.08 (d, J = 5.3 Hz, 1H, C-1′H), 5.98 (s, 2H, CH_2), 5.68 (s, 1H, ArH), 5.52-5.49 (m, 1H, C-2′H), 5.49-5.48 (m, 2H, CH_2), 5.41-5.37 (m, 1H, C-3′H), 4.67 (s, 2H, CH_2), 4.39-4.36 (m, 1H, C-4′H), 4.32-4.29 (m, 2H, C-5′H), 3.66 (s, 3H, OCH_3), 2.14 (s, 3H, $OCOCH_3$), 2.11 (s, 3H, $OCOCH_3$), 2.06 (s, 3H, $OCOCH_3$); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 170.0 (C=O), 170.0 (C=O), 169.9 (C=O), 161.6 (ArC), 160.0 (ArC), 158.1 (ArC), 154.9 (ArC), 151.5 (ArC), 151.3 (ArC), 150.1 (ArC), 141.6 (ArC), 139.5 (C-4), 137.0 (C-6″), 124.2 (C-5), 124.2 (ArC), 120.4 (ArC), 115.0 (ArC), 113.8 (ArC), 110.6 (ArC), 110.5 (ArC), 109.2 (ArC), 106.2 (ArC), 88.2 (C-1′), 81.2 (CH_2), 80.0 (C-4′), 72.9 (C-2′), 70.5 (C-3′), 63.6 (C-5′), 55.7 (OCH_3), 49.7 (CH_2), 45.6 (CH_2), 21.1 ($OCOCH_3$), 20.9 ($OCOCH_3$),

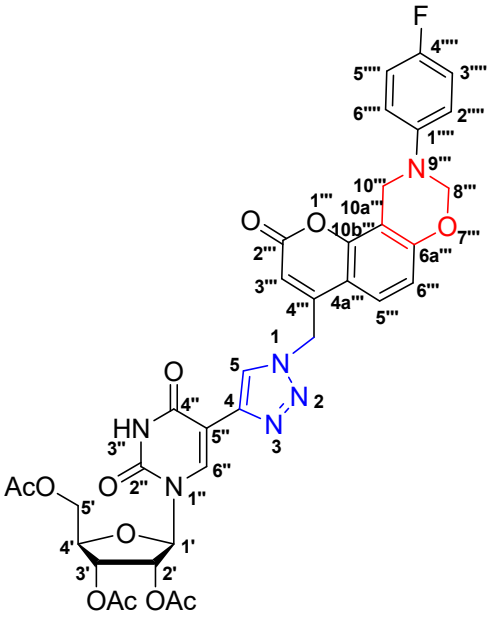
20.8 ($OCOCH_3$); HRMS (ESI): m/z calculated for $C_{36}H_{34}N_6O_{13}^+$ $[M]^+$: 758.2184, found: 758.2140.

1.2.2. N^1-(9'''-(4''''-chloro)-9''',10'''-dihydro-2'''H,8'''H-chromeno[8''',7'''-e][1''',3''']oxazin-2'''-one-4'''-methyl)-C^4-(2',3',5'-tri-O-acetyl-β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole (12b)



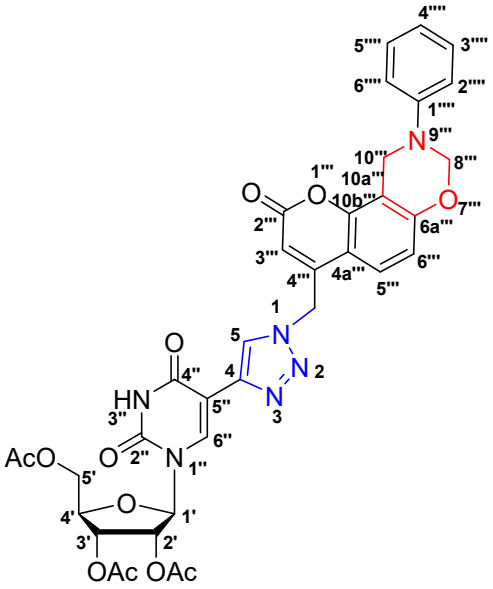
It was obtained as a yellowish white solid. Yield: 0.71 g (93%). R_f = 0.36 (5% methanol in chloroform); Melting Point = 214 ˚C; IR (KBr, cm^{-1}): 3037, 2833, 1747, 1711, 1692, 1604, 1496, 1363, 1267, 1225, 1218, 1100, 1059, 1047, 876, 817, 581; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.83 (s, 1H, N-3″H), 8.54 (s, 1H, C-5H), 8.43 (s, 1H, C-6″H), 7.63-7.59 (m, 1H, ArH), 7.25-7.21 (m, 2H, ArH), 7.17-7.13 (m, 2H, ArH), 6.83-6.79 (m, 1H, ArH), 6.07-6.04 (m, 1H, C-1′H), 5.93 (s, 2H, CH_2), 5.66 (s, 1H, ArH), 5.52 (s, 2H, CH_2), 5.48-5.44 (m, 1H, C-2′H), 5.37-5.33 (m, 1H, C-3′H), 4.71 (s, 2H, CH_2), 4.35-4.32 (m, 1H, C-4′H), 4.28-4.24 (m, 2H, C-5′H), 2.09 (s, 3H, $OCOCH_3$), 2.06 (s, 3H, $OCOCH_3$), 2.02 (s, 3H, $OCOCH_3$); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 170.7 (C=O), 170.0 (C=O), 170.0 (C=O), 161.6 (ArC), 160.0 (ArC), 157.9 (ArC), 151.2 (ArC), 151.2 (ArC), 150.1 (ArC), 146.9 (ArC), 139.5 (C-4), 137.0 (C-6″), 129.5 (C-5), 125.6 (ArC), 124.3 (ArC), 124.2 (ArC), 120.1 (ArC), 113.9 (ArC), 110.8 (ArC), 110.7 (ArC), 109.2 (ArC), 106.2 (ArC), 88.2 (C-1′), 80.0 (CH_2), 79.9 (C-4′), 72.9 (C-2′), 70.5 (C-3′), 63.6 (C-5′), 49.7 (CH_2), 45.1 (CH_2), 21.1 ($OCOCH_3$), 20.9 ($OCOCH_3$), 20.8 ($OCOCH_3$); HRMS (ESI): m/z calculated for $C_{35}H_{32}ClN_6O_{12}^+$ $[M+H]^+$: 763.1761, found: 763.1760.

1.2.3. N^1-(9'''-(4''''-fluoro)-9''',10'''-dihydro-2'''H,8'''H-chromeno[8''',7'''-e][1''',3''']oxazin-2'''-one-4'''-methyl)-C^4-(2',3',5'-tri-O-acetyl-β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole (12c)



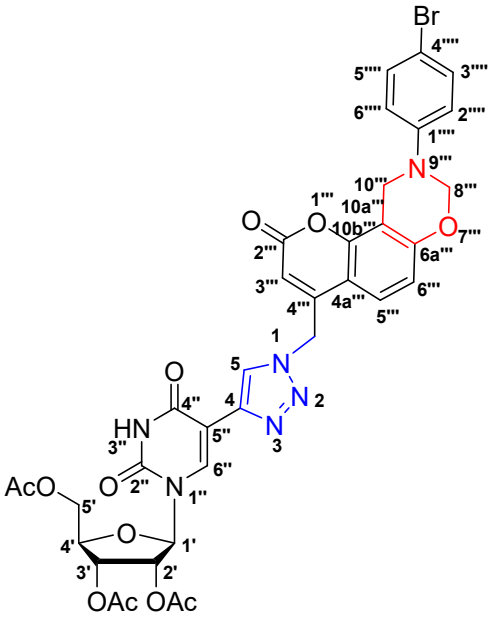
It was obtained as a yellow solid. Yield: 0.69 g (92%). R_f = 0.34 (5% methanol in chloroform); Melting Point = 222-226 ˚C; IR (KBr, cm^{-1}): 2982, 2918, 1693, 1596, 1504, 1454, 1368, 1221, 1045, 879, 811, 757, 581; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.89 (s, 1H, N-3″H), 8.60-8.58 (m, 1H, C-5H), 8.49-8.47 (m, 1H, C-6″H), 7.70-7.64 (m, 1H, ArH), 7.20-7.17 (m, 1H, ArH), 7.11-7.05 (m, 2H, ArH), 6.95-6.91 (m, 1H, ArH), 6.89-6.84 (m, 1H, ArH), 6.11-6.08 (m, 1H, C-1′H), 5.98 (s, 2H, CH_2), 5.70-5.65 (m, 1H, ArH), 5.55-5.51 (m, 2H, CH_2), 5.51-5.48 (m, 1H, C-2′H), 5.42-5.38 (m, 1H, C-3′H), 4.73 (s, 1H, C-4′H), 4.39-4.34 (m, 2H, CH_2), 4.33-4.29 (m, 2H, C-5′H), 2.14 (s, 3H, $OCOCH_3$), 2.11 (s, 3H, $OCOCH_3$), 2.06 (s, 3H, $OCOCH_3$); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 170.7 (C=O), 170.0 (C=O), 170.0 (C=O), 161.6 (ArC), 160.0 (ArC), 158.0 (ArC), 151.5 (ArC), 151.2 (ArC), 150.1 (ArC), 144.6 (ArC), 139.4 (C-4), 137.0 (C-6″), 124.3 (C-5), 124.2 (ArC), 120.5 (ArC), 120.4 (ArC), 116.3 (ArC), 116.1 (ArC), 113.8 (ArC), 110.7 (ArC), 110.6 (ArC), 109.1 (ArC), 106.2 (ArC), 88.2 (C-1′), 80.7 (CH_2), 80.0 (C-4′), 72.9 (C-2′), 70.5 (C-3′), 63.6 (C-5′), 49.7 (CH_2), 45.5 (CH_2), 21.1 ($OCOCH_3$), 20.9 ($OCOCH_3$), 20.8 ($OCOCH_3$); HRMS (ESI): m/z calculated for $C_{35}H_{32}FN_6O_{12}^+$ $[M+H]^+$: 747.2057, found: 747.2054.

1.2.4. N^1-(9‴,10‴-dihydro-2‴H,8‴H-chromeno[8‴,7‴-e][1‴,3‴]oxazin-2‴-one-4‴-methyl)-C^4-(2',3',5'-tri-O-acetyl-β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole (12d)



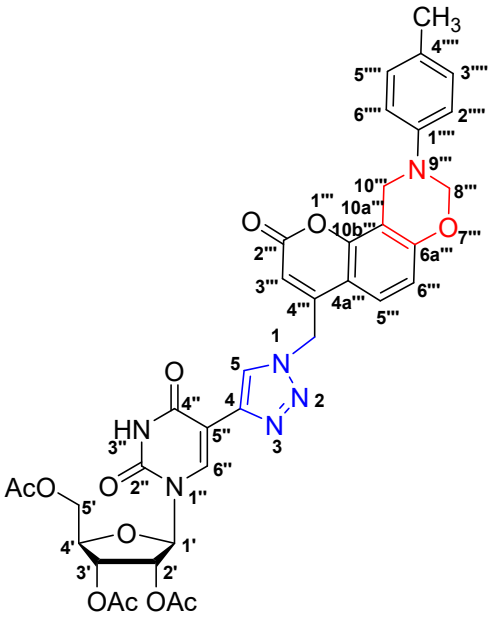
It was obtained as a yellow solid. Yield: 0.68 g (94%). R_f = 0.36 (5% methanol in chloroform); Melting Point = 238-240 ˚C; IR (KBr, cm^{-1}): 3082, 1686, 1598, 1506, 1447, 1364, 1214, 1103, 1049, 894, 820, 748, 691; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.84 (s, 1H, N-3″H), 8.54 (s, 1H, C-5H), 8.43 (s, 1H, C-6″H), 7.63-7.58 (m, 1H, ArH), 7.23-7.18 (m, 2H, ArH), 7.14-7.10 (m, 2H, ArH), 6.88-6.83 (m, 1H, ArH), 6.83-6.79 (m, 1H, ArH), 6.07-6.04 (m, 1H, C-1′H), 5.93 (s, 2H, CH_2), 5.64 (s, 1H, ArH), 5.53 (s, 2H, CH_2), 5.48-5.43 (m, 1H, C-2′H), 5.37-5.33 (m, 1H, C-3′H), 4.72 (s, 2H, CH_2), 4.35-4.31 (m, 1H, C-4′H), 4.28-4.24 (m, 2H, C-5′H), 2.09 (s, 3H, $OCOCH_3$), 2.06 (s, 3H, $OCOCH_3$), 2.02 (s, 3H, $OCOCH_3$); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 170.7 (C=O), 170.0 (C=O), 170.0 (C=O), 161.6 (ArC), 160.0 (ArC), 158.1 (ArC), 151.5 (ArC), 151.3 (ArC), 150.1 (ArC), 147.9 (ArC), 139.5 (C-4), 137.0 (C-6″), 129.8 (ArC), 124.2 (C-5, ArC), 121.8 (ArC), 118.4 (ArC), 113.9 (ArC), 110.7 (ArC), 110.5 (ArC), 109.3 (ArC), 106.2 (ArC), 88.2 (C-1′), 80.2 (CH_2), 80.0 (C-4′), 72.9 (C-2′), 70.5 (C-3′), 63.6 (C-5′), 49.7 (CH_2), 45.0 (CH_2), 21.1 ($OCOCH_3$), 20.9 ($OCOCH_3$), 20.8 ($OCOCH_3$); HRMS (ESI): m/z calculated for $C_{35}H_{33}N_6O_{12}^+$ $[M+H]^+$: 729.2151, found: 729.2129.

1.2.5. N^1-(9‴-(4''''-bromo)-9‴,10‴-dihydro-2‴H,8‴H-chromeno[8‴,7‴-e][1‴,3‴]oxazin-2‴-one-4‴-methyl)-C^4-(2',3',5'-tri-O-acetyl-β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole (12e)



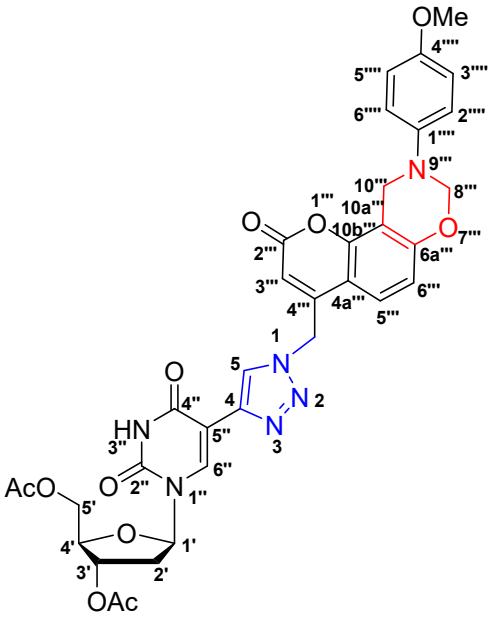
It was obtained as a yellowish white solid. Yield: 0.77 g (95%). R_f = 0.35 (5% methanol in chloroform); Melting Point = 275 ˚C; IR (KBr, cm^{-1}): 3156, 2993, 2829, 1692, 1603, 1479, 1454, 1366, 1215, 1103, 1058, 1006, 887, 812, 581; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.86 (s, 1H, N-3″H), 8.59-8.58 (m, 1H, C-5H), 8.49-8.46 (m, 1H, C-6″H), 7.69-7.64 (m, 1H, ArH), 7.42-7.37 (m, 2H, ArH), 7.17-7.13 (m, 2H, ArH), 6.89-6.84 (m, 1H, ArH), 6.12-6.08 (m, 1H, C-1′H), 5.98 (s, 2H, CH_2), 5.73-5.70 (m, 1H, ArH), 5.56 (s, 2H, CH_2), 5.53-5.49 (m, 1H, C-2′H), 5.42-5.38 (m, 1H, C-3′H), 4.76 (s, 2H, CH_2), 4.39-4.36 (m, 1H, C-4′H), 4.33-4.29 (m, 2H, C-5′H), 2.15-2.14 (m, 3H, $OCOCH_3$), 2.12-2.10 (m, 3H, $OCOCH_3$), 2.08-2.06 (m, 3H, $OCOCH_3$); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 170.7 (C=O), 170.0 (C=O), 169.9 (C=O), 161.6 (ArC), 160.0 (ArC), 157.9 (ArC), 151.5 (ArC), 151.2 (ArC), 150.1 (ArC), 147.3 (ArC), 139.5 (C-4), 137.0 (C-6″), 132.4 (ArC), 129.3 (C-5), 124.2 (ArC), 120.5 (ArC), 113.9 (ArC), 113.4 (ArC), 110.8 (ArC), 109.2 (ArC), 106.2 (ArC), 88.2 (C-1′), 80.0 (CH_2), 79.8 (C-4′), 72.9 (C-2′), 70.5 (C-3′), 63.6 (C-5′), 49.7 (CH_2), 45.1 (CH_2), 21.1 ($OCOCH_3$), 20.9 ($OCOCH_3$), 20.8 ($OCOCH_3$); HRMS (ESI): m/z calculated for $C_{35}H_{32}BrN_6O_{12}^+$ $[M+H]^+$: 807.1256, found: 807.1265.

1.2.6. N^1-(9‴-(4⁗-methyl)-9‴,10‴-dihydro-2‴H,8‴H-chromeno[8‴,7‴-e][1‴,3‴]oxazin-2‴-one-4‴-methyl)-C^4-(2′,3′,5′-tri-O-acetyl-β-D-ribofuranos-1′-(2″,4″-dioxo-3″,4″-dihydropyrimidin))-1,2,3-triazole (12f)



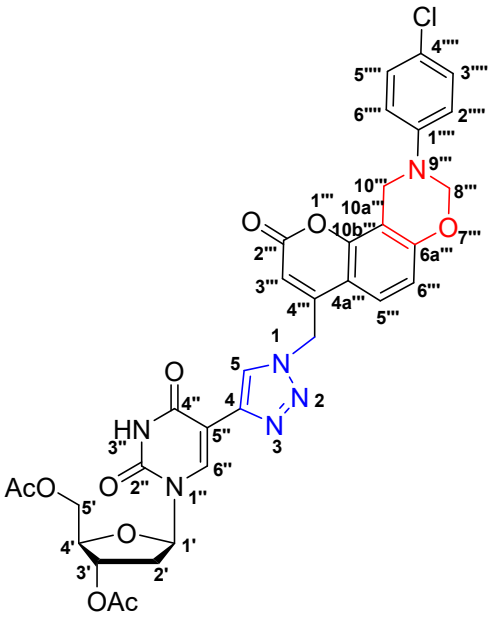
It was obtained as a yellow solid. Yield: 0.69 (93%). R_f = 0.38 (5% methanol in chloroform); Melting Point = 198 ˚C; IR (KBr, cm^{-1}): 3302, 2921, 1693, 1602, 1506, 1435, 1371, 1223, 1092, 1039, 878, 814, 760, 711; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.87 (brs, 1H, N-3″H), 8.58 (s, 1H, C-5H), 8.47 (s, 1H, C-6″H), 7.66-7.63 (m, 1H, ArH), 7.05-7.04 (m, 4H, ArH), 6.85-6.82 (m, 1H, ArH), 6.11-6.08 (m, 1H, C-1′H), 5.97 (s, 2H, CH_2), 5.69-5.68 (m, 1H, ArH), 5.53-5.51 (m, 2H, CH_2), 5.51-5.49 (m, 1H, C-2′H), 5.41-5.38 (m, 1H, C-3′H), 4.71 (s, 2H, CH_2), 4.39-4.36 (m, 1H, C-4′H), 4.33-4.29 (m, 2H, C-5′H), 2.18 (s, 3H, $OCOCH_3$), 2.14 (s, 3H, $OCOCH_3$), 2.11 (s, 3H, CH_3), 2.06 (m, 3H, $OCOCH_3$); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 170.7 (C=O), 170.0 (C=O), 169.9 (C=O), 161.6 (ArC), 160.0 (ArC), 158.1 (ArC), 151.5 (ArC), 151.2 (ArC), 150.1 (ArC), 145.6 (ArC), 139.5 (C-4), 137.0 (C-6″), 130.8 (C-5), 130.2 (ArC), 124.2 (ArC), 118.6 (ArC), 113.8 (ArC), 113.4 (ArC), 110.6 (ArC), 109.3 (ArC), 106.2 (ArC), 88.2 (C-1′), 80.6 (CH_2), 80.0 (C-4′), 72.9 (C-2′), 70.5 (C-3′), 63.6 (C-5′), 49.7 (CH_2), 45.2 (CH_2), 21.1 ($OCOCH_3$), 20.9 ($OCOCH_3$), 20.8 ($OCOCH_3$), 20.6 (CH_3); HRMS (ESI): m/z calculated for $C_{36}H_{35}N_6O_{12}^+$ $[M+H]^+$: 743.2307, found: 743.2295.

1.2.7. N^1-(9‴-(4⁗-methoxy)-9‴,10‴-dihydro-2‴H,8‴H-chromeno[8‴,7‴-e][1‴,3‴]oxazin-2‴-one-4‴-methyl)-C^4-(3′,5′-di-O-acetyl-β-D-ribofuranos-1′-(2″,4″-dioxo-3″,4″-dihydropyrimidin))-1,2,3-triazole (13a)



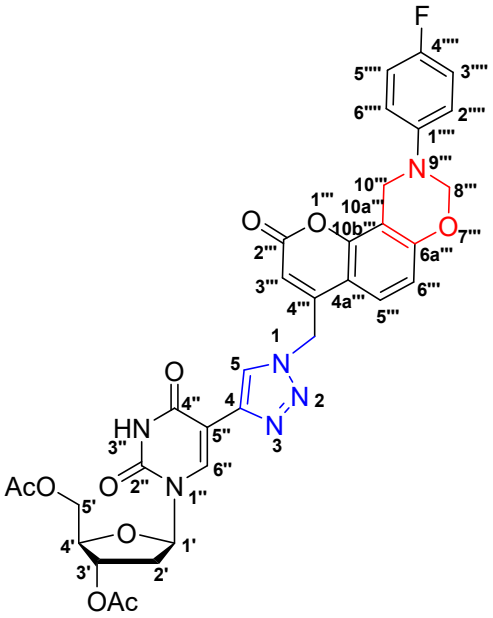
It was obtained as a yellow solid. Yield: 0.65 g (93%). R_f = 0.30 (5% methanol in chloroform); Melting Point = 226 ˚C; IR (KBr, cm^{-1}): 3414, 2927, 1683, 1586, 1511, 1414, 1226, 1097, 1034, 825, 760, 647; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.82 (brs, 1H, N-3″H), 8.61-8.56 (m, 1H, C-5H), 8.46-8.43 (m, 1H, C-6″H), 7.66-7.52 (m, 2H, ArH), 7.11-7.06 (m, 2H, ArH), 6.85-6.80 (m, 2H, ArH), 6.29-6.25 (m, 1H, C-1′H), 5.97 (s, 2H, CH_2), 5.68-5.63 (m, 1H, ArH), 5.49-5.47 (m, 1H, C-3′H), 5.27-5.24 (m, 1H, C-4′H), 4.67 (s, 2H, CH_2), 4.33-4.24 (m, 4H, CH_2, ArH), 3.66 (s, 3H, CH_3), 2.51-2.44 (m, 1H, C-2′H), 2.44-2.40 (m, 1H, C-2′H), 2.14 (s, 3H, $OCOCH_3$), 2.09 (s, 3H, $OCOCH_3$); ^{13}C NMR (DMSO-d_6,100 MHz) δ 170.9 (C=O), 170.6 (C=O), 161.6 (ArC), 160.0 (ArC), 158.1 (ArC), 154.9 (ArC), 151.5 (ArC), 151.3 (ArC), 150.1 (ArC), 141.6 (ArC), 139.7 (C-4), 136.1 (C-6″), 124.2 (C-5), 124.0 (ArC), 120.4 (ArC), 115.4 (ArC), 115.0 (ArC), 113.8 (ArC), 110.6 (ArC), 109.2 (ArC), 105.9 (ArC), 85.5 (C-1′), 82.2 (C-4′), 81.8 (CH_2), 74.7 (C-3′), 64.3 (C-5′), 55.7 (OCH_3), 49.7 (CH_2), 45.6 (CH_2), 37.3 (C-2′), 21.3 ($OCOCH_3$), 21.1 ($OCOCH_3$); HRMS (ESI): m/z calculated for $C_{34}H_{33}N_6O_{11}^+$ $[M+H]^+$: 701.2202, found: 701.2187.

1.2.8. N^1-(9'''-(4''''-chloro)-9''',10'''-dihydro-2'''H,8'''H-chromeno[8''',7'''-e][1''',3''']oxazin-2'''-one-4'''-methyl)-C^4-(3',5'-di-O-acetyl-β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole (13b)



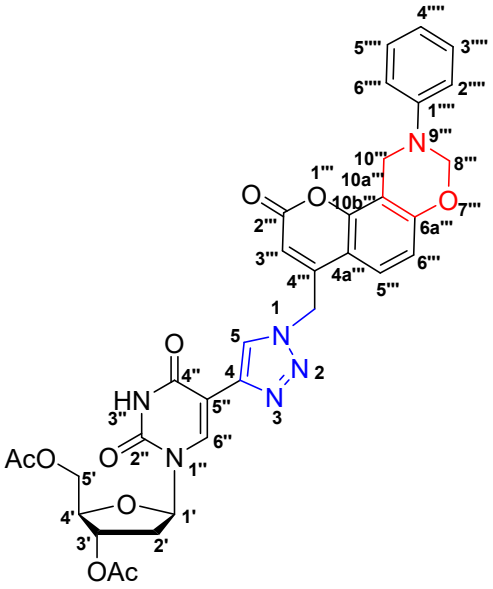
It was obtained as a yellowish white solid. Yield: 0.65 g (92%). R_f = 0.33 (5% methanol in chloroform); Melting Point = 210 ˚C; IR (KBr, cm^{-1}): 3350, 2933, 1611, 1571, 1441, 1360, 1232, 1108, 1049, 873, 754, 717; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.80 (brs, 1H, N-3″H), 8.61-8.55 (m, 1H, C-5H), 8.48-8.42 (m, 1H, C-6″H), 7.68-7.62 (m, 1H, ArH), 7.42-7.36 (m, 2H, ArH), 7.17-7.11 (m, 2H, ArH), 6.89-6.83 (m, 1H, ArH), 6.31-6.23 (m, 1H, C-1′H), 6.00-5.95 (s, 2H, CH_2), 5.71-5.66 (m, 1H, ArH), 5.55 (m, 2H, CH_2), 5.27-5.22 (m, 1H, C-3′H), 4.75 (s, 2H, CH_2), 4.32-4.28 (m, 1H, C-4′H), 4.28-4.23 (m, 2H, C-5′H), 2.46-2.37 (m, 2H, C-2′H), 2.13 (s, 3H, $OCOCH_3$), 2.08 (s, 3H, $OCOCH_3$); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 170.9 (C=O), 170.6 (C=O), 161.6 (ArC), 160.0 (ArC), 157.9 (ArC), 151.5 (ArC), 151.3 (ArC), 150.1 (ArC), 147.2 (ArC), 139.7 (C-4), 136.1 (C-6″), 132.4 (ArC), 124.3 (C-5), 124.0 (ArC), 120.5 (ArC), 113.9 (ArC), 113.4 (ArC), 110.6 (ArC), 109.2 (ArC), 105.9 (ArC), 85.5 (C-1′), 82.2 (C-4′), 79.8 (CH_2), 74.7 (C-3′), 64.3 (C-5′), 49.7 (CH_2), 45.0 (CH_2), 37.3 (C-2′), 21.3 ($OCOCH_3$), 21.1 ($OCOCH_3$); HRMS (ESI): m/z calculated for $C_{33}H_{30}ClN_6O_{10}^+$ $[M+H]^+$: 705.1706, found: 705.1728.

1.2.9. N^1-(9‴-(4⁗-fluoro)-9‴,10‴-dihydro-2‴H,8‴H-chromeno[8‴,7‴-e][1‴,3‴]oxazin-2‴-one-4‴-methyl)-C^4-(3′,5′-di-O-acetyl-β-D-ribofuranos-1′-(2″,4″-dioxo-3″,4″-dihydropyrimidin))-1,2,3-triazole (13c)



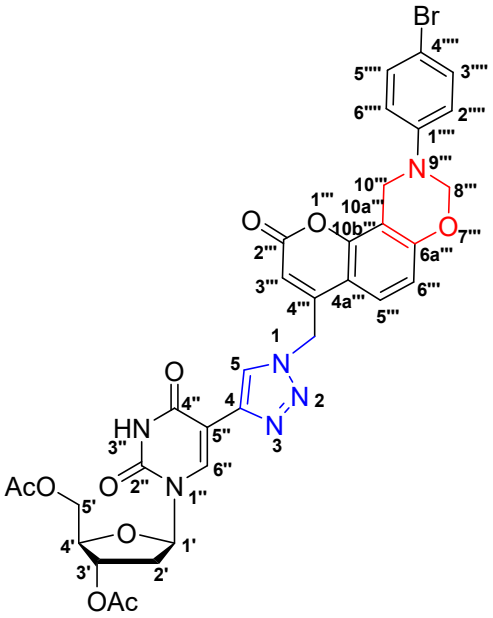
It was obtained as a yellowish brown solid. Yield: 0.63 g (92%). R_f = 0.32 (5% methanol in chloroform); Melting Point = 194-196 ˚C; IR (KBr, cm^{-1}): 3288, 1687, 1597, 1512, 1453, 1382, 1228, 1096, 1039, 817, 608, 552; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.82 (brs, 1H, N-3″H), 8.57-8.56 (m, 1H, C-5H), 8.44-8.43 (m, 1H, C-6″H), 7.67-7.64 (m, 1H, ArH), 7.21-7.16 (m, 2H, ArH), 7.10-7.05 (m, 2H, ArH), 6.87-6.84 (m, 1H, ArH), 6.28-6.25 (m, 1H, C-1′H), 5.97 (s, 2H, CH_2), 5.69-5.67 (m, 1H, ArH), 5.53 (m, 2H, CH_2), 5.26-5.24 (m, 1H, C-3′H), 4.73 (s, 2H, CH_2), 4.31-4.29 (m, 1H, C-4′H), 4.28-4.25 (m, 2H, C-5′H), 2.46-2.44 (m, 1H, C-2′H), 2.43-2.40 (m, 1H, C-2′H), 2.14 (s, 3H, $OCOCH_3$), 2.09 (s, 3H, $OCOCH_3$); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 170.9 (C=O), 170.6 (C=O), 161.6 (ArC), 160.0 (ArC), 158.0 (ArC), 151.5 (ArC), 151.3 (ArC), 150.1 (ArC), 144.6 (ArC), 139.7 (C-4), 136.1 (C-6″), 124.3 (C-5), 124.0 (ArC), 120.5 (ArC), 120.4 (ArC), 116.3 (ArC), 116.1 (ArC), 113.9 (ArC), 110.7 (ArC), 110.5 (ArC), 109.1 (ArC), 105.9 (ArC), 85.5 (C-1′), 82.2 (C-4′), 80.7 (CH_2), 74.7 (C-3′), 64.3 (C-5′), 49.7 (CH_2), 45.5 (CH_2), 37.3 (C-2′), 21.3 ($OCOCH_3$), 21.1 ($OCOCH_3$); HRMS (ESI): m/z calculated for $C_{33}H_{30}FN_6O_{10}^+$ $[M+H]^+$: 689.2002, found: 689.2041.

1.2.10. N^1-(9‴,10‴-dihydro-2‴H,8‴H-chromeno[8‴,7‴-e][1‴,3‴]oxazin-2‴-one-4‴-methyl)-C^4-(3',5'-di-O-acetyl-β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole (13d)



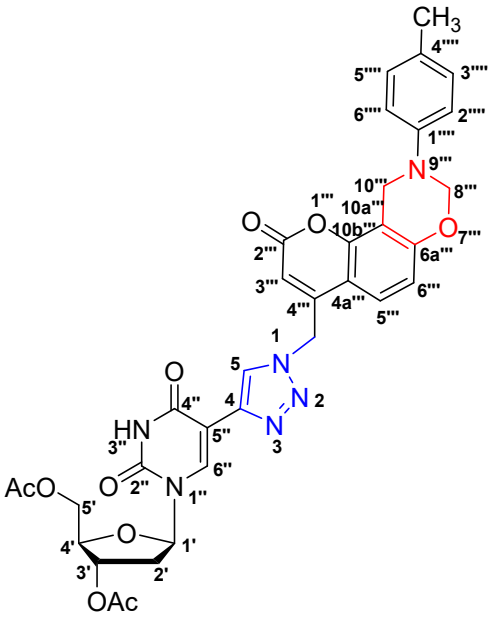
It was obtained as a yellow solid. Yield: 0.63 g (94%). R_f = 0.34 (5% methanol in chloroform); Melting Point = 246 ˚C; IR (KBr, cm^{-1}): 2889, 2106, 1720, 1585, 1495, 1359, 1302, 1251, 1162, 1097, 914, 797, 713; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.81 (brs, 1H, N-3″H), 8.57-8.55 (m, 1H, C-5H), 8.44-8.43 (m, 1H, C-6″H), 7.66-7.62 (m, 1H, ArH), 7.27-7.22 (m, 2H, ArH), 7.17-7.14 (m, 2H, ArH), 6.92-6.89 (m, 1H, ArH), 6.86-6.82 (m, 1H, ArH), 6.28-6.24 (m, 1H, C-1′H), 5.96 (s, 2H, CH_2), 5.67-5.64 (m, 1H, ArH), 5.57 (m, 2H, CH_2), 5.26-5.23 (m, 1H, C-3′H), 4.76 (s, 2H, CH_2), 4.30-4.29 (m, 1H, C-4′H), 4.27-4.25 (m, 2H, C-5′H), 2.46-2.43 (m, 1H, C-2′H), 2.43-2.41 (m, 1H, C-2′H), 2.13 (s, 3H, $OCOCH_3$), 2.08 (s, 3H, $OCOCH_3$); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 170.9 (C=O), 170.6 (C=O), 161.6 (ArC), 160.0 (ArC), 158.0 (ArC), 151.5 (ArC), 151.3 (ArC), 150.1 (ArC), 144.6 (ArC), 139.7 (C-4), 136.1 (C-6″), 124.3 (C-5), 124.0 (ArC), 120.5 (ArC), 120.4 (ArC), 116.3 (ArC), 116.1 (ArC), 113.9 (ArC), 110.7 (ArC), 110.5 (ArC), 109.1 (ArC), 105.9 (ArC), 85.5 (C-1′), 82.2 (C-4′), 80.7 (CH_2), 74.7 (C-3′), 64.3 (C-5′), 49.7 (CH_2), 45.5 (CH_2), 37.3 (C-2′), 21.3 ($OCOCH_3$), 21.1 ($OCOCH_3$); HRMS (ESI): m/z calculated for $C_{33}H_{31}N_6O_{10}^+$ $[M+H]^+$: 671.2096, found: 671.2111.

1.2.11. N^1-(9‴-(4⁗-bromo)-9‴,10‴-dihydro-2‴H,8‴H-chromeno[8‴,7‴-e][1‴,3‴]oxazin-2‴-one-4‴-methyl)-C^4-(3′,5′-di-O-acetyl-β-D-ribofuranos-1′-(2″,4″-dioxo-3″,4″-dihydropyrimidin))-1,2,3-triazole (13e)



It was obtained as a yellowish brown solid. Yield: 0.69 g (93%). R_f = 0.33 (5% methanol in chloroform); Melting Point = 249 ˚C; IR (KBr, cm^{-1}): 3054, 2811, 1707, 1687, 1599, 1492, 1228, 1052, 817, 602, 554; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.76 (brs, 1H, N-3″H), 8.57-8.50 (m, 1H, C-5H), 8.45-8.38 (m, 1H, C-6″H), 7.64-7.59 (m, 1H, ArH), 7.38-7.32 (m, 2H, ArH), 7.13-7.07 (m, 2H, ArH), 6.85-6.79 (m, 1H, ArH), 6.28-6.19 (m, 1H, C-1′H), 5.98-5.90 (m, 2H, CH_2), 5.69-5.63 (m, 1H, ArH), 5.52 (m, 2H, CH_2), 5.24-5.18 (m, 1H, C-3′H), 4.71 (s, 2H, CH_2), 4.28-4.24 (m, 1H, C-4′H), 4.23-4.19 (m, 2H, C-5′H), 2.43-2.40 (m, 1H, C-2′H), 2.39-2.36 (m, 1H, C-2′H), 2.10 (s, 3H, $OCOCH_3$), 2.04 (s, 3H, $OCOCH_3$); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 170.9 (C=O), 170.6 (C=O), 161.6 (ArC), 160.0 (ArC), 157.9 (ArC), 151.5 (ArC), 151.3 (ArC), 150.1 (ArC), 147.2 (ArC), 139.7 (C-4), 136.1 (C-6″), 132.4 (ArC), 124.3 (C-5), 124.0 (ArC), 120.5 (ArC), 113.9 (ArC), 110.8 (ArC), 110.6 (ArC), 109.2 (ArC), 105.9 (ArC), 85.5 (C-1′), 82.2 (C-4′), 79.8 (CH_2), 74.7 (C-3′), 64.3 (C-5′), 49.7 (CH_2), 45.0 (CH_2), 37.3 (C-2′), 21.3 ($OCOCH_3$), 21.1 ($OCOCH_3$); HRMS (ESI): m/z calculated for $C_{33}H_{30}BrN_6O_{10}^+$ $[M+H]^+$: 749.1201, found: 749.1179.

1.2.12. N^1-(9'''-(4''''-methyl)-9''',10'''-dihydro-2'''H,8'''H-chromeno[8''',7'''-e][1''',3''']oxazin-2'''-one-4'''-methyl)-C^4-(3',5'-di-O-acetyl-β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole (13f)



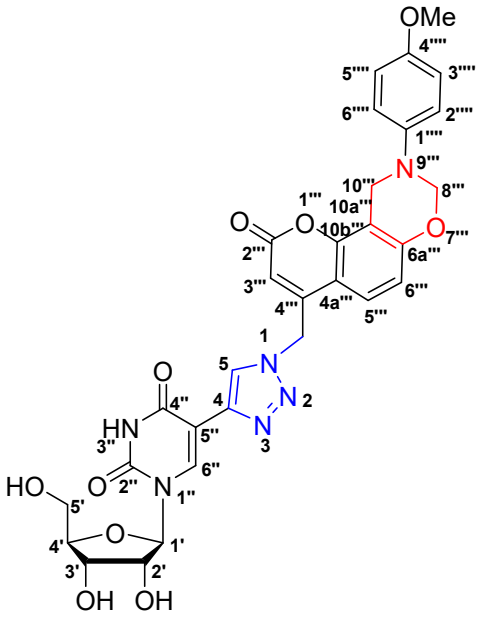
It was obtained as a yellow solid. Yield: 0.63 g (92%). R_f = 0.35 (5% methanol in chloroform); Melting Point = 217 ˚C; IR (KBr, cm^{-1}): 1689, 1597, 1509, 1444, 1361, 1226, 1103, 1045, 814; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.81 (brs, 1H, N-3″H), 8.59-8.55 (m, 1H, C-5H), 8.46-8.42 (m, 1H, C-6″H), 7.66-7.62 (m, 1H, ArH), 7.07-7.02 (m, 4H, ArH), 6.85-6.82 (m, 1H, ArH), 6.29-6.24 (m, 1H, C-1′H), 5.97 (m, 2H, CH_2), 5.67-5.61 (m, 1H, ArH), 5.53 (s, 2H, CH_2), 5.27-5.23 (m, 1H, C-3′H), 4.71 (s, 2H, CH_2), 4.33-4.29 (m, 1H, C-4′H), 4.27-4.25 (m, 2H, C-5′H), 2.48-2.39 (m, 2H, C-2′H), 2.18 (s, 3H, CH_3), 2.15 (s, 3H, $OCOCH_3$), 2.09 (s, 3H, $OCOCH_3$); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 170.9 (C=O), 170.6 (C=O), 161.6 (ArC), 160.0 (ArC), 158.1 (ArC), 151.5 (ArC), 151.3 (ArC), 150.1 (ArC), 145.6 (ArC), 139.7 (C-4), 136.1 (C-6″), 130.2 (ArC), 124.2 (C-5), 124.0 (ArC), 118.6 (ArC), 113.8 (ArC), 113.0 (ArC), 110.6 (ArC), 110.4 (ArC), 109.3 (ArC), 105.9 (ArC), 85.5 (C-1′), 82.2 (C-4′), 80.5 (CH_2), 74.7 (C-3′), 64.3 (C-5′), 49.7 (CH_2), 45.2 (CH_2), 37.3 (C-2′), 21.3 ($OCOCH_3$), 21.1 ($OCOCH_3$), 20.6 (CH_3); HRMS (ESI): m/z calculated for $C_{34}H_{33}N_6O_{10}^+$ $[M+H]^+$: 685.2253, found: 685.2280.

1.3. General procedure for the synthesis of N^1-(9‴-(4⁗-substituted)-9‴,10‴-dihydro-2‴H,8‴H-chromeno[8‴,7‴-e][1‴,3‴]oxazin-2‴-one-4‴-methyl)-C^4-(β-D-ribofuranos-/2'-deoxy-β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole conjugates (14a-f and 15a-f)

To a solution of N^1-(9‴-(4⁗-substituted)-9‴,10‴-dihydro-2‴H,8‴H-chromeno[8‴,7‴-e][1‴,3‴]oxazin-2‴-one-4‴-methyl)-C^4-(2',3',5'-tri-O-acetyl/3',5'-di-O-acetyl-β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole conjugates (**12a-f/13a-f**,

1.0 mmol) in methanol, NaOMe (2.2 mmol) was added. The reaction mixture was allowed to stir at 25˚C for 10-15 minutes. After completion of the reaction (as monitored by TLC), the reaction was neutralized with seralite (H^+) resin. The solution was filtered through a cotton plug and the solvent was evaporated under vaccum. The crude product thus obtained was purified by silica gel column chromatography using methanol in chloroform as the solvent system to afford the desired products **14a-f** and **15a-f** in quantitative yields.

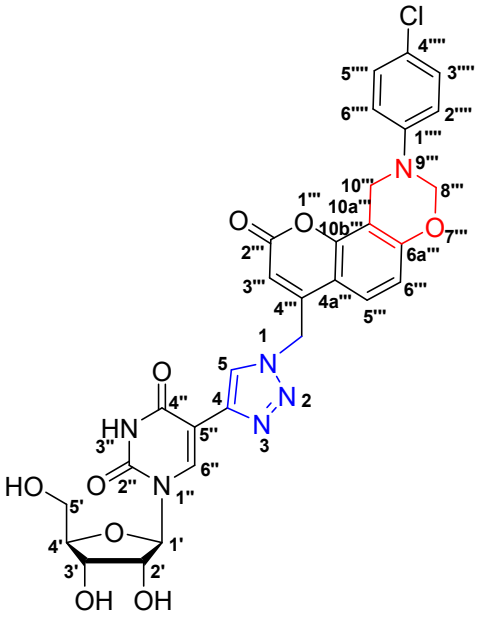
1.3.1. N^1-(9'''-(4''''-methoxy)-9''',10'''-dihydro-2'''H,8'''H-chromeno[8''',7'''-e][1''',3''']oxazin-2'''-one-4'''-methyl)-C^4-(β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole (14a)



It was obtained as a yellow solid. Yield: 0.61 g (97%). R_f = 0.24 (10% methanol in chloroform); Melting Point = 258 ˚C; IR (KBr, cm^{-1}): 3393, 1683, 1586, 1500, 1495, 1452, 1377, 1232, 1039, 818; ^{1}H NMR (DMSO-d_6,400 MHz) δ 11.75 (brs, 1H, N-3″H), 9.25-9.21 (m, 1H, C-6″H), 8.69-8.66 (m, 1H, C-5H), 8.60-8.55 (m, 1H, ArH), 7.94-7.87 (m, 1H, ArH), 7.57-7.52 (m, 2H, ArH), 7.08-7.03 (m, 2H, ArH), 6.99-6.95 (m, 1H, ArH), 6.04-6.00 (m, 1H, C-1′H), 5.93-5.88 (m, 2H, CH_2), 5.70 (brs, 1H, OH), 5.44 (brs, 1H, OH), 5.19-5.14 (m, 2H, CH_2), 4.18-4.14 (m, 1H, C-2′H), 4.04-4.00 (m, 1H, C-3′H), 3.93-3.89 (m, 1H, C-4′H), 3.81 (s, 3H, CH_3), 3.66-3.61 (m, 2H, C-5′H), 3.51 (m, 2H, CH_2); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 166.9 (ArC), 161.6 (ArC), 159.6 (ArC), 159.5 (ArC), 154.7 (ArC), 151.6 (ArC), 150.5 (ArC), 139.7 (C-4), 137.1 (C-6″), 129.9 (ArC), 124.3 (C-5), 124.0 (ArC) 123.2 (ArC), 115.3 (ArC) 109.6 (ArC), 108.6 (ArC), 106.8 (ArC), 105.6 (ArC), 88.4 (C-1′), 85.6 (C-4′), 74.3 (CH_2), 70.7 (C-3′), 70.2

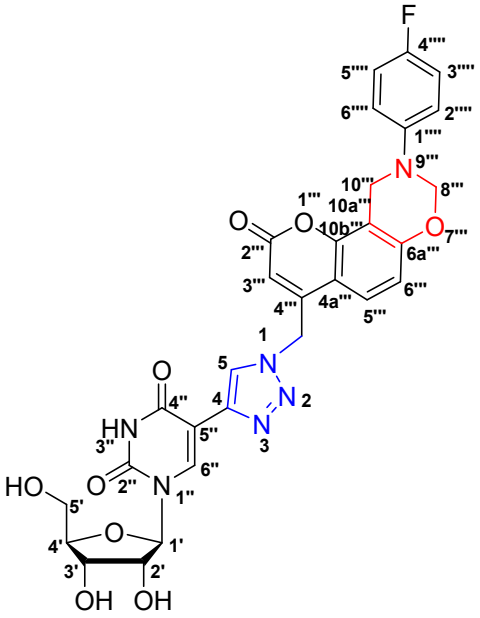
(C-2′), 61.5 (C-5′), 55.9 (CH_3), 49.7 (CH_2), 45.1 (CH_2); HRMS (ESI): m/z calculated for $C_{30}H_{29}N_6O_{10}^+$ $[M+H]^+$: 633.1940, found: 633.1944.

1.3.2. N^1-(9‴-(4⁗-chloro)-9‴,10‴-dihydro-2‴H,8‴H-chromeno[8‴,7‴-e][1‴,3‴]oxazin-2‴-one-4‴-methyl)-C^4-(β-D-ribofuranos-1′-(2″,4″-dioxo-3″,4″-dihydropyrimidin))-1,2,3-triazole (14b)



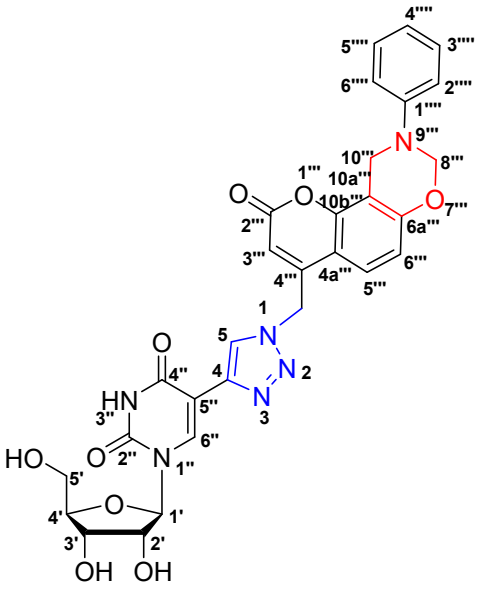
It was obtained as a yellow solid. Yield: 0.62 g (98%). R_f = 0.26 (10% methanol in chloroform); Melting Point = 262-264 ˚C; IR (KBr, cm^{-1}): 3307, 3153, 2928, 1686, 1591, 1495, 1459, 1400, 1317, 1257, 1044, 818; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.75 (brs, 1H, N-3″H), 8.69-8.67 (m, 1H, C-6″H), 8.58-8.55 (m, 1H, C-5H), 7.73-7.66 (m, 1H, ArH), 7.30-7.26 (m, 1H, ArH), 7.21-7.18 (m, 1H, ArH), 7.10-7.05 (m, 1H, ArH), 6.96-6.85 (m, 1H, ArH), 6.75-6.65 (m, 1H, ArH), 5.98-5.94 (m, 2H, CH_2), 5.93-5.90 (m, 1H, C-1′H), 5.74-5.69 (m, 1H, ArH), 5.62-5.48 (m, 2H, CH_2), 5.48-5.40 (brs, 1H, OH), 5.15 (brs, 2H, OH), 4.84-4.68 (m, 2H, CH_2), 4.18-4.14 (m, 1H, C-2′H), 4.03-4.01 (m, 1H, C-3′H), 3.93-3.91 (m, 1H, C-4′H), 3.66-3.59 (m, 2H, C-5′H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 161.6 (ArC), 159.9 (ArC), 157.8 (ArC), 154.1 (ArC), 151.5 (ArC), 150.5 (ArC), 148.2 (ArC), 146.8 (ArC), 139.7 (C-4), 137.1 (C-6″), 129.5 (ArC), 128.9 (ArC), 125.5 (ArC), 124.0 (C-5), 120.0 (ArC), 113.8 (ArC), 112.9 (ArC), 110.8 (ArC), 109.1 (ArC), 105.6 (ArC), 88.4 (C-1′), 85.6 (C-4′), 79.9 (CH_2), 74.3 (C-2′), 70.7 (C-3′), 61.5 (C-5′), 49.6 (CH_2), 45.1 (CH_2); HRMS (ESI): m/z calculated for $C_{29}H_{26}ClN_6O_9^+$ $[M+H]^+$: 637.1444, found: 637.1425.

1.3.3. N^1-(9'''-(4''''-fluoro)-9''',10'''-dihydro-2'''H,8'''H-chromeno[8''',7'''-e][1''',3''']oxazin-2'''-one-4'''-methyl)-C^4-(β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole (14c)



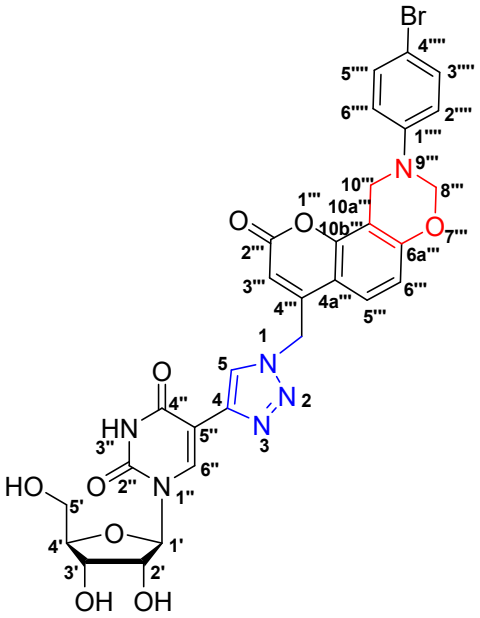
It was obtained as a yellow solid. Yield: 0.60 g (97%). R_f = 0.26 (10% methanol in chloroform); Melting Point = 241-243 ˚C; IR (KBr, cm^{-1}): 3314, 2718, 1684, 1596, 1512, 1455, 1396, 1338, 1269, 1211, 1103, 1054, 830, 644, 517; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.74 (brs, 1H, N-3″H), 8.69-8.66 (m, 1H, C-6″H), 8.58-8.55 (m, 1H, C-5H), 7.72-7.67 (m, 1H, ArH), 7.22-7.05 (m, 2H, ArH), 7.02-6.98 (m, 1H, ArH), 6.94-6.88 (m, 2H, ArH), 6.71-6.66 (m, 1H, ArH), 5.99-5.94 (m, 2H, CH_2), 5.93-5.89 (m, 1H, C-1′H), 5.73-5.66 (m, 1H, CH_2), 5.54-5.46 (m, 1H, CH_2), 5.16 (brs, 2H, OH), 4.25 (brs, 1H, OH), 4.18-4.14 (m, 1H, C-2′H), 4.04-4.01 (m, 1H, C-3′H), 3.93-3.90 (m, 1H, C-4′H), 3.67-3.58 (m, 4H, C-5′H, CH_2); ^{13}C NMR (DMSO-d_6,100 MHz) δ 161.6 (ArC), 160.7 (ArC), 160.4 (ArC), 154.0 (ArC), 153.7 (ArC), 151.4 (ArC), 150.5 (ArC), 146.0 (ArC), 139.7 (C-4), 137.1 (C-6″), 125.1 (ArC), 124.0 (C-5), 120.4 (ArC), 120.4 (ArC), 116.3 (ArC), 116.0 (ArC), 115.7 (ArC), 115.5 (ArC), 113.4 (ArC), 113.3 (ArC), 113.1 (ArC), 113.0 (ArC), 109.8 (ArC), 109.6 (ArC), 105.6 (ArC), 88.5 (C-1′), 85.6 (C-4′), 74.3 (CH_2), 70.7 (C-3′, C-2′), 61.5 (C-5′), 49.7 (CH_2), 36.4 (CH_2); HRMS (ESI): m/z calculated for $C_{29}H_{26}FN_6O_9^+$ $[M+H]^+$: 621.1740, found: 621.1716.

1.3.4. N^1-(9''',10'''-dihydro-2'''H,8'''H-chromeno[8''',7'''-e][1''',3''']oxazin-2'''-one-4'''-methyl)-C^4-(β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole (14d)



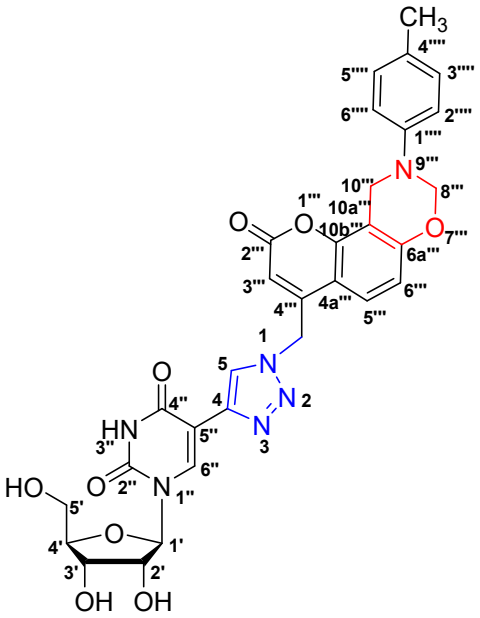
It was obtained as a yellow solid. Yield: 0.58 g (96%). R_f = 0.27 (10% methanol in chloroform); Melting Point = 216-220 ˚C; IR (KBr, cm^{-1}): 1686, 1591, 1511, 1451, 1359, 1226, 1104, 1045, 807; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.74 (brs, 1H, N-3″H), 8.69-8.65 (m, 1H, C-6″H), 8.57-8.53 (m, 1H, C-5H), 7.70-7.64 (m, 1H, ArH), 7.29-7.19 (m, 2H, ArH), 7.18-7.14 (m, 1H, ArH), 7.09-7.00 (m, 1H, ArH), 6.96-6.84 (m, 2H, ArH), 6.70-6.50 (m, 1H, ArH), 5.96 (m, 2H, CH_2), 5.92-5.88 (m, 1H, C-1′H), 5.72-5.66 (m, 1H, CH_2), 5.59-5.56 (m, 1H, CH_2), 5.14 (brs, 1H, OH), 4.76 (brs, 1H, OH), 4.28 (brs, 1H, OH), 4.17-4.13 (m, 1H, C-2′H), 4.03-3.99 (m, 1H, C-3′H), 3.93-3.89 (m, 1H, C-4′H), 3.69-3.54 (m, 4H, C-5′H, CH_2); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 161.6 (ArC), 160.0 (ArC), 158.0 (ArC), 151.5 (ArC), 151.2 (ArC), 150.5 (ArC), 149.3 (ArC), 147.9 (ArC), 139.7 (C-4), 137.1 (C-6″), 129.7 (ArC), 129.3 (ArC), 124.0 (C-5), 121.8 (ArC), 118.4 (ArC), 113.8 (ArC), 112.6 (ArC), 110.7 (ArC), 109.3 (ArC), 105.6 (ArC), 88.4 (C-1′), 85.6 (C-4′), 80.1 (CH_2), 74.3 (C-3′), 70.7 (C-2′), 61.5 (C-5′), 49.6 (CH_2), 45.0 (CH_2); HRMS (ESI): m/z calculated for $C_{29}H_{27}N_6O_9^+$ $[M+H]^+$: 603.1834, found: 603.1859.

1.3.5. N^1-(9‴-(4⁗-bromo)-9‴,10‴-dihydro-2‴H,8‴H-chromeno[8‴,7‴-e][1‴,3‴]oxazin-2‴-one-4‴-methyl)-C^4-(β-D-ribofuranos-1′-(2″,4″-dioxo-3″,4″-dihydropyrimidin))-1,2,3-triazole (14e)



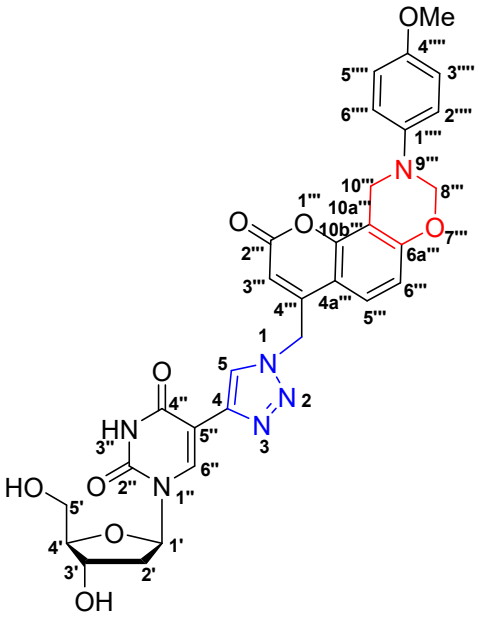
It was obtained as a yellow solid. Yield: 0.67 g (98%). R_f = 0.28 (10% methanol in chloroform); Melting Point = 254 ˚C; IR (KBr, cm^{-1}): 3324, 2741, 1644, 1531, 1415, 1367, 1332, 1258, 1123, 1035, 826, 643, 509; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.74 (brs, 1H, N-3″H), 8.67-8.66 (m, 1H, C-6″H), 8.56-8.54 (m, 1H, C-5H), 7.70-7.66 (m, 1H, ArH), 7.40-7.38 (m, 1H, ArH), 7.19-7.17 (m, 1H, ArH), 7.15-7.13 (m, 1H, ArH), 6.93-6.85 (m, 1H, ArH), 6.66-6.64 (m, 1H, ArH), 5.96-5.89 (m, 4H, CH_2, C-1′H, ArH), 5.72-5.66 (m, 1H, CH_2), 5.56-5.45 (m, 1H, CH_2), 5.13 (brs, 1H, OH), 4.75 (brs, 1H, OH), 4.24 (brs, 1H, OH), 4.16-4.13 (m, 1H, C-2′H), 4.01-3.99 (m, 1H, C-3′H), 3.91-3.89 (m, 1H, C-4′H), 3.66-3.56 (m, 4H, C-5′H, CH_2); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 161.6 (ArC), 160.4 (ArC), 154.1 (ArC), 150.5 (ArC), 148.6 (ArC), 147.2 (ArC), 139.7 (C-4), 137.1 (C-6″), 132.4 (ArC), 131.7 (ArC), 124.0 (C-5), 114.5 (ArC), 110.8 (ArC), 109.1 (ArC), 106.7 (ArC), 105.6 (ArC), 88.4 (C-1′), 85.6 (C-4′), 74.3 (CH_2), 70.7 (C-2′, C-3′), 61.5 (C-5′), 60.2 (CH_2), 49.6 (CH_2); HRMS (ESI): m/z calculated for $C_{29}H_{26}BrN_6O_9^+$ $[M+H]^+$: 681.0939, found: 681.1012.

1.3.6. N^1-(9'''-(4''''-methyl)-9''',10'''-dihydro-2'''H,8'''H-chromeno[8''',7'''-e][1''',3''']oxazin-2'''-one-4'''-methyl)-C^4-(β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole (14f)



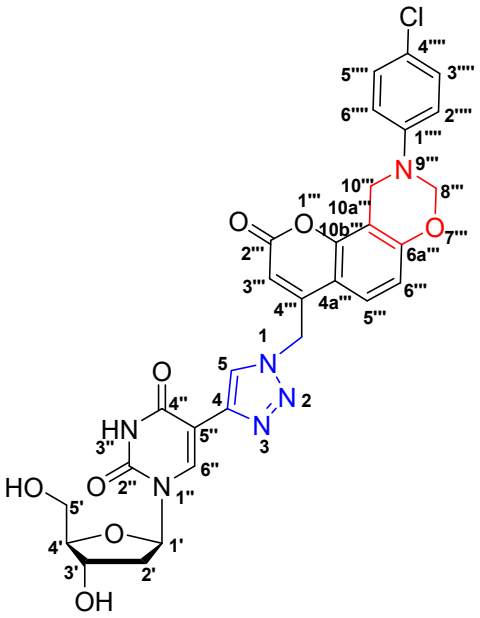
It was obtained as a yellow solid. Yield: 0.60 g (98%). R_f = 0.29 (10% methanol in chloroform); Melting Point = 235-237 ˚C; IR (KBr, cm^{-1}): 3309, 2722, 1676, 1545, 1501, 1452, 1337, 1242, 1112, 1067, 805, 663, 503;^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.71 (brs, 1H, N-3″H), 8.67-8.64 (m, 1H, C-6″H), 8.56-8.53 (m, 1H, C-5H), 7.68-7.63 (m, 1H, ArH), 7.40-7.33 (m, 1H, ArH), 7.04 (brs, 2H, ArH), 6.94-6.82 (m, 2H, ArH), 5.97-5.93 (m, 2H, CH_2), 5.91-5.88 (m, 1H, C-1′H), 5.73-5.70 (m, 1H, ArH), 5.56-5.50 (m, 2H, CH_2), 5.14 (brs, 2H, OH), 4.71 (brs, 1H, OH), 4.18-4.13 (m, 1H, C-2′H), 4.02-3.99 (m, 1H, C-3′H), 3.92-3.89 (m, 1H, C-4′H), 3.68-3.63 (m, 2H, C-5′H), 3.61-3.56 (m, 2H, CH_2), 2.18 (s, 3H, CH_3); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 161.6 (ArC), 160.0 (ArC), 158.0 (ArC), 154.0 (ArC), 151.5 (ArC), 150.5 (ArC), 147.0 (ArC), 145.5 (ArC), 139.7 (C-4), 137.1 (C-6″), 130.1 (ArC), 129.7 (ArC), 124.0 (C-5), 118.6 (ArC), 112.9 (ArC), 109.9 (ArC), 109.6 (ArC), 109.2 (ArC), 105.6 (ArC), 88.4 (C-1′), 85.6 (C-4′), 74.3 (CH_2), 70.7 (C-2′, C-3′), 61.5 (C-5′), 49.7 (CH_2), 45.1 (CH_2), 20.5 (CH_3) ; HRMS (ESI): m/z calculated for $C_{30}H_{29}N_6O_9^+$ $[M+H]^+$: 617.1991, found: 617.1997.

1.3.7. N^1-(9‴-(4⁗-methoxy)-9‴,10‴-dihydro-2‴H,8‴H-chromeno[8‴,7‴-e][1‴,3‴]oxazin-2‴-one-4‴-methyl)-C^4-(2'-deoxy-β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole (15a)



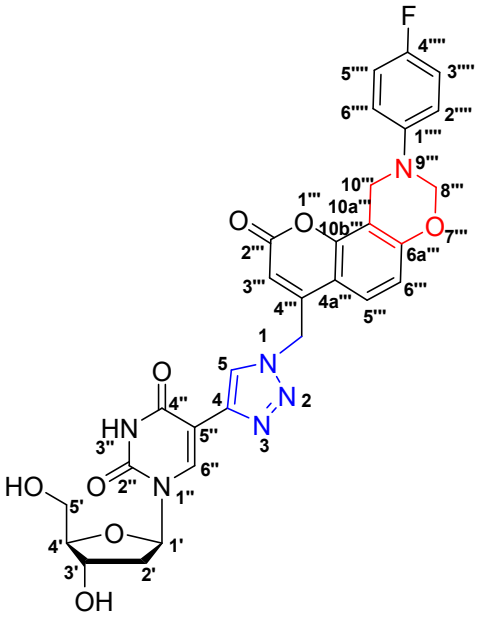
It was obtained as a yellow solid. Yield: 0.59 g (96%). R_f = 0.25 (10% methanol in chloroform); Melting Point = 266 ˚C; IR (KBr, cm^{-1}): 3275, 3071, 1672, 1586, 1489, 1446, 1254, 1174, 1040, 818; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.72 (brs, 1H, N-3′H), 8.66-8.60 (m, 1H, C-6′′H), 8.60-8.52 (m, 1H, C-5H), 7.66-7.54 (m, 1H, ArH), 7.12-6.62 (m, 5H, ArH), 6.28-6.21 (m, 1H, C-1′H), 6.03-5.89 (m, 2H, CH_2), 5.75-5.43 (m, 2H, CH_2), 5.32 (brs, 1H, OH), 5.10-5.02 (m, 1H, ArH), 4.67-4.50 (m, 1H, C-3′H), 4.32-4.25 (m, 1H, C-4′H), 3.90-3.78 (m, 2H, CH_2), 3.70-3.55 (m, 5H, C-5′H, CH_3), 2.23-2.16 (m, 2H,C-2′H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 161.6 (ArC), 160.0 (ArC), 159.6 (ArC), 158.0 (ArC), 154.8 (ArC), 151.5 (ArC), 150.1 (ArC), 141.6 (ArC), 139.8 (C-4), 136.8 (C-6′′), 123.2 (ArC), 120.3 (ArC), 115.3 (ArC), 114.9 (ArC), 113.8 (ArC), 110.6 (C-5), 109.1 (ArC), 105.4 (ArC), 88.1 (C-4′), 85.2 (C-1′), 55.9 (CH_2), 71.1 (C-3′), 61.8 (C-5′), 55.6 (CH_3), 55.6 (CH_2), 49.6 (CH_2), 45.6 (C-2′), 40.5(CH_2); HRMS (ESI): m/z calculated for $C_{30}H_{29}N_6O_9^+$ $[M+H]^+$: 617.1991, found: 617.1981.

1.3.8. N^1-(9'''-(4''''-chloro)-9''',10'''-dihydro-2'''H,8'''H-chromeno[8''',7'''-e][1''',3''']oxazin-2'''-one-4'''-methyl)-C^4-(2'-deoxy-β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole (15b)



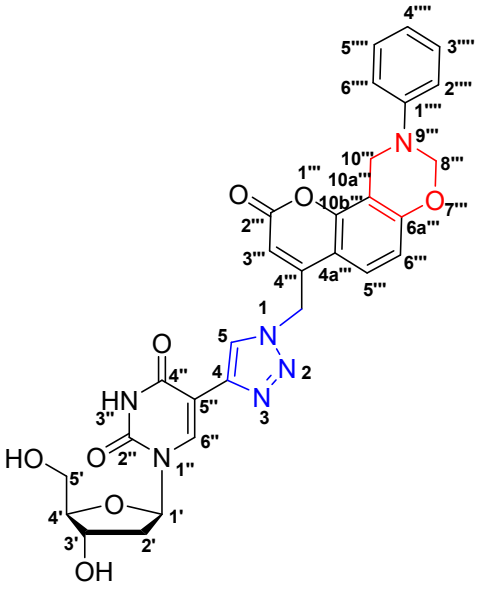
It was obtained as a yellow solid. Yield: 0.61 g (99%). R_f = 0.26 (10% methanol in chloroform); Melting Point = 259-260 ˚C; IR (KBr, cm^{-1}): 3186, 3004, 1659, 1581, 1440, 1387, 1257, 1048, 834; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 8.62-8.61 (m, 1H, C-6″H), 8.54-8.53 (m, 1H, C-5H), 7.67-7.61 (m, 1H, ArH), 7.40-7.38 (m, 1H, ArH), 7.17-7.15 (m, 1H, ArH), 7.14-7.12 (m, 1H, ArH), 6.88-6.84 (m, 1H, ArH), 6.67-6.64 (m, 1H, ArH), 6.25-6.22 (m, 1H, C-1′H), 5.96-5.94 (m, 1H, CH_2), 5.92-5.90 (m, 1H, CH_2), 5.56-5.53 (m, 2H, CH_2), 4.75-4.74 (m, 1H, ArH), 4.29-4.22 (m, 3H, C-3′H, CH_2), 3.86-3.84 (m, 1H, C-4′H), 3.60-3.59 (m, 2H, C-5′H), 2.20-2.17 (m, 2H, C-2′H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 161.2 (ArC), 160.2 (ArC), 159.5 (ArC), 157.4 (ArC), 151.0 (ArC), 150.7 (ArC), 149.7 (ArC), 146.7 (ArC), 139.4 (C-4), 136.4 (C-6″), 131.9 (ArC), 131.2 (ArC), 123.4 (ArC), 120.0 (ArC), 114.1 (ArC), 112.9 (ArC), 110.3 (ArC), 108.7 (C-5), 106.2 (ArC), 105.0 (ArC), 87.7 (C-4′), 84.8 (C-1′), 79.3 (CH_2), 70.7 (C-3′), 61.4 (C-5′), 49.1 (CH_2), 44.5 (C-2′), 35.6 (CH_2); HRMS (ESI): m/z calculated for $C_{29}H_{26}ClN_6O_8^+$ $[M+H]^+$: 621.1495, found: 621.1491.

1.3.9. N^1-(9‴-(4⁗-fluoro)-9‴,10‴-dihydro-2‴H,8‴H-chromeno[8‴,7‴-e][1‴,3‴]oxazin-2‴-one-4‴-methyl)-C^4-(2'-deoxy-β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole (15c)



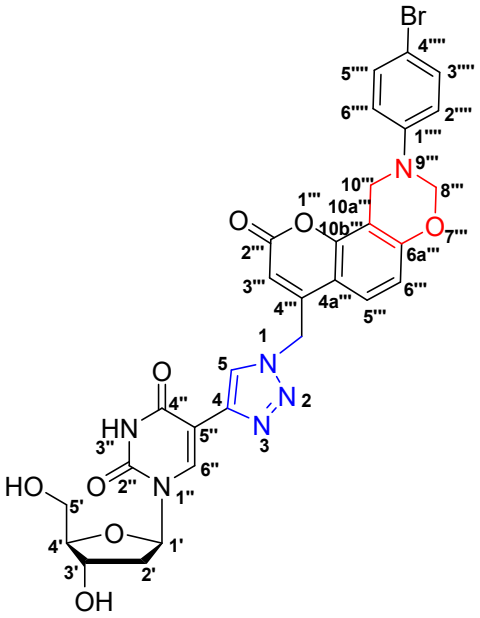
It was obtained as a yellow solid. Yield: 0.59 g (98%). R_f = 0.26 (10% methanol in chloroform); Melting Point = 208-210 ˚C; IR (KBr, cm^{-1}): 3363, 3280, 2924, 1678, 1583, 1512, 1453, 1405, 1275, 1215, 1097, 1037, 824; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.71 (brs, 1H, NH), 8.63-8.62 (m, 1H, C-6″H), 8.56-8.54 (m, 1H, C-5H), 7.70-7.66 (m, 1H, ArH), 7.19-7.16 (m, 1H, ArH), 7.01-6.97 (m, 1H, ArH), 6.93-6.87 (m, 2H, ArH), 6.69-6.67 (m, 1H, ArH), 6.26-6.23 (m, 1H, C-1′H), 5.97-5.94 (m, 2H, CH_2), 5.72-5.66 (m, 1H, CH_2), 5.57-5.48 (m, 1H, CH_2), 5.34 (brs, 1H, OH), 5.07 (brs, 1H, OH), 4.76-4.69 (m, 1H, ArH), 4.30-4.28 (m, 1H, C-3′H), 4.26-4.22 (m, 2H, CH_2), 3.87-3.85 (m, 1H, C-4′H), 3.62-3.59 (m, 2H, C-5′H), 2.21-2.18 (m, 2H, C-2′H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 161.7 (ArC), 160.8 (ArC), 160.4 (ArC), 155.9 (ArC), 154.0 (ArC), 151.4 (ArC), 150.1 (ArC), 146.0 (ArC), 139.8 (C-4), 136.8 (C-6″), 125.1 (ArC), 123.9 (ArC), 120.5 (ArC), 120.4 (ArC), 116.3 (ArC), 116.0 (ArC), 115.7 (ArC), 115.5 (ArC), 113.4 (ArC), 113.3 (ArC), 113.1 (ArC), 109.7 (C-5), 109.5 (ArC), 105.4 (ArC), 88.1 (C-4′), 85.2 (C-1′), 80.6 (CH_2), 71.1 (C-3′), 61.8 (C-5′), 49.7 (CH_2), 45.5 (C-2′), 36.4 (CH_2); HRMS (ESI): m/z calculated for $C_{29}H_{26}FN_6O_8^+$ $[M+H]^+$: 605.1718, found: 605.1787.

1.3.10. N^1-(9‴,10‴-dihydro-2‴H,8‴H-chromeno[8‴,7‴-e][1‴,3‴]oxazin-2‴-one-4‴-methyl)-C^4-(2′-deoxy-β-D-ribofuranos-1′-(2″,4″-dioxo-3″,4″-dihydropyrimidin))-1,2,3-triazole (15d)



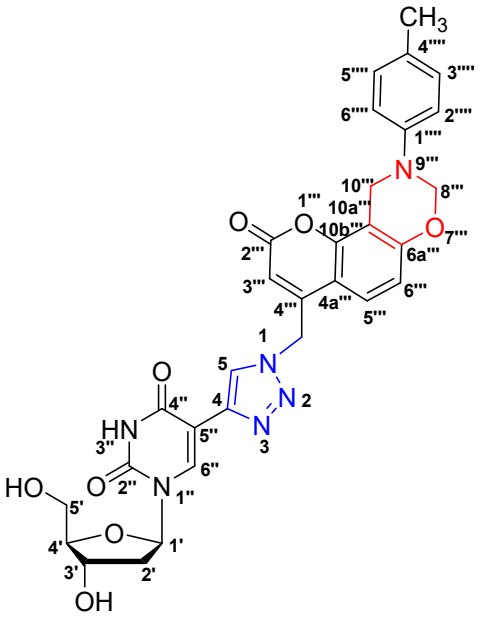
It was obtained as a yellow solid. Yield: 0.57 g (98%). R_f = 0.27 (10% methanol in chloroform); Melting Point = 242 ˚C; IR (KBr, cm^{-1}): 3276, 2946, 1648, 1565, 1417, 1405, 1266, 1043, 811, 524; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 8.64-8.62 (m, 1H, C-6″H), 8.56-8.55 (m, 1H, C-5H), 7.71-7.65 (m, 1H, ArH), 7.27-7.16 (m, 2H, ArH), 7.07-7.00 (m, 2H, ArH), 6.91-6.85 (m, 1H, ArH), 6.72-6.68 (m, 1H, ArH), 6.56-6.48 (m, 1H, C-1′H), 6.26-6.23 (m, 1H, CH_2), 5.97-5.93 (m, 2H, CH_2), 5.59-5.56 (m, 1H, CH_2), 4.80-4.73 (m, 1H, ArH), 4.32-4.23 (m, 3H, C-3′H, CH_2), 3.88-3.85 (m, 1H, C-4′H), 3.62-3.60 (m, 2H, C-5′H), 2.22-2.18 (m, 2H, C-2′H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 161.7 (ArC), 160.7 (ArC), 160.0 (ArC), 158.0 (ArC), 155.7 (ArC), 154.2 (ArC), 150.1 (ArC), 149.4 (ArC), 139.8 (C-4), 136.8 (C-6″), 129.7 (ArC), 129.2 (ArC), 123.9 (ArC), 118.4 (ArC), 116.1 (ArC), 113.1 (C-5), 113.2 (ArC), 112.7 (ArC), 105.4 (ArC), 88.1 (C-4′), 85.2 (C-1′), 80.1 (CH_2), 71.1 (C-3′), 61.8 (C-5′), 49.1 (C-2′, CH_2), 36.0 (CH_2); HRMS (ESI): m/z calculated for $C_{29}H_{27}N_6O_8^+$ $[M+H]^+$: 587.1885, found: 587.1869.

1.3.11. N^1-(9‴-(4⁗-bromo)-9‴,10‴-dihydro-2‴H,8‴H-chromeno[8‴,7‴-e][1‴,3‴]oxazin-2‴-one-4‴-methyl)-C^4-(2′-deoxy-β-D-ribofuranos-1′-(2″,4″-dioxo-3″,4″-dihydropyrimidin))-1,2,3-triazole (15e)



It was obtained as a yellow solid. Yield: 0.64 g (97%). R_f = 0.27 (10% methanol in chloroform); Melting Point = 229 ˚C; IR (KBr, cm^{-1}): 3325, 3224, 2814, 1708, 1683, 1658, 1583, 1557, 1516, 1457, 1306, 1222, 1047, 820, 644, 517; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 8.63-8.62 (m, 1H, C-6″H), 8.56-8.54 (m, 1H, C-5H), 7.69-7.61 (m, 1H, ArH), 7.42-7.38 (m, 1H, ArH), 7.19-7.15 (m, 1H, ArH), 7.15-7.13 (m, 1H, ArH), 6.89-6.85 (m, 1H, ArH), 6.68-6.65 (m, 1H, ArH), 6.26-6.23 (m, 1H, C-1′H), 5.97-5.95 (m, 1H, CH_2), 5.94-5.91 (m, 1H, CH_2), 5.59-5.52 (m, 2H, CH_2), 4.76-4.74 (m, 1H, ArH), 4.30-4.21 (m, 3H, C-3′H, CH_2), 3.87-3.85 (m, 1H, C-4′H), 3.62-3.59 (m, 2H, C-5′H), 2.21-2.18 (m, 2H, C-2′H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 161.7 (ArC), 160.7 (ArC), 159.9 (ArC), 157.8 (ArC), 151.5 (ArC), 151.2 (ArC), 150.1 (ArC), 147.2 (ArC), 139.8 (C-4), 136.8 (C-6″), 132.3 (ArC), 131.7 (ArC), 123.9 (ArC), 120.4 (ArC), 114.5 (ArC), 113.3 (ArC), 110.8 (ArC), 109.1 (C-5), 106.6 (ArC), 105.4 (ArC), 88.1 (C-4′), 85.2 (C-1′), 79.7 (CH_2), 71.1 (C-3′), 61.8 (C-5′), 49.5 (CH_2), 45.0 (CH_2), 40.5 (C-2′), 36.0 (CH_2); HRMS (ESI): m/z calculated for $C_{29}H_{26}BrN_6O_8^+$ $[M+H]^+$: 665.0990, found: 665.1005.

1.3.12. N^1-(9'''-(4''''-methyl)-9''',10'''-dihydro-2'''H,8'''H-chromeno[8''',7'''-e][1''',3''']oxazin-2'''-one-4'''-methyl)-C^4-(2'-deoxy-β-D-ribofuranos-1'-(2'',4''-dioxo-3'',4''-dihydropyrimidin))-1,2,3-triazole (15f)



It was obtained as a yellow solid. Yield: 0.58 g (97%). R_f = 0.28 (10% methanol in chloroform); Melting Point = 202 ˚C; IR (KBr, cm^{-1}): 3296, 2932, 1672, 1589, 1506, 1446, 1399, 1268, 1043, 817;^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.72 (brs, 1H, NH), 8.63-8.62 (m, 1H, C-6″H), 8.56-8.54 (m, 1H, C-5H), 7.70-7.62 (m, 1H, ArH), 7.05-7.02 (m, 2H, ArH), 6.93-6.83 (m, 2H, ArH), 6.64-6.56 (m, 1H, ArH), 6.26-6.23 (m, 1H, C-1′H), 5.97-5.92 (m, 2H, CH_2), 5.73-5.64 (m, 1H, CH_2), 5.55-5.52 (m, 1H, CH_2), 5.34-5.32 (m, 1H, ArH), 5.08-5.05 (m, 1H, C-3′H), 4.71 (brs, 1H, OH), 4.31-4.25 (m, 2H, CH_2), 3.88-3.85 (m, 1H, C-4′H), 3.63-3.59 (m, 2H, C-5′H), 2.22-2.17 (m, 4H, C-2′H, CH_3), 2.14-2.13 (m, 1H, C-2′H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 161.6 (ArC), 160.5 (ArC), 160.0 (ArC), 158.0 (ArC), 154.0 (ArC), 150.1 (ArC), 145.5 (ArC), 139.8 (C-4), 136.8 (C-6″), 130.8 (ArC), 130.1 (ArC), 129.7 (ArC), 123.9 (ArC), 118.6 (ArC), 112.9 (ArC), 110.6 (C-5), 109.2 (ArC), 105.4 (ArC), 88.1 (C-4′), 85.2 (C-1′), 80.5 (CH_2), 71.1 (C-3′), 61.8 (C-5′), 49.7 (CH_2), 45.1 (C-2′), 36.3 (CH_2), 20.5 (CH_3); HRMS (ESI): m/z calculated for $C_{30}H_{29}N_6O_8^+$ $[M+H]^+$: 601.2041, found: 601.2064.

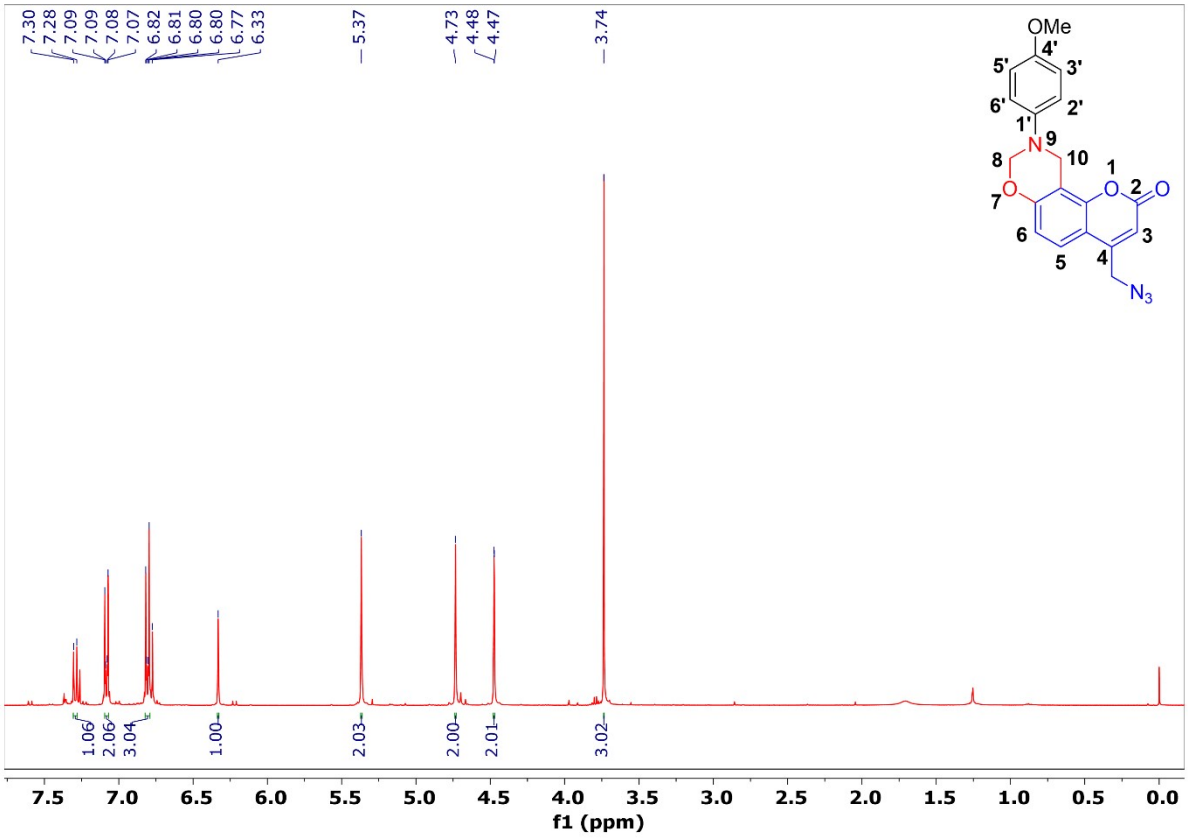


Figure S1: ^{1}H NMR spectrum of compound **6a** (400 MHz, $CDCl_3$).

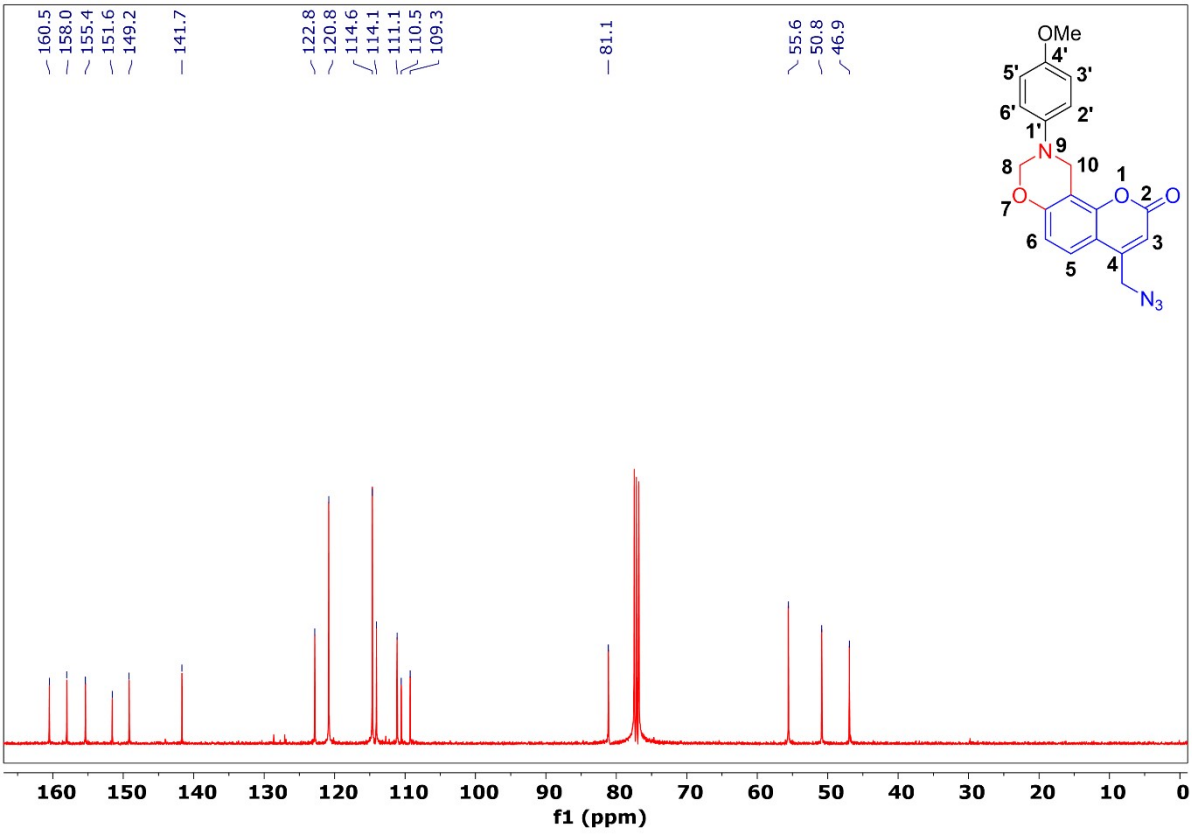


Figure S2: ^{13}C NMR spectrum of compound **6a** (100 MHz, $CDCl_3$).

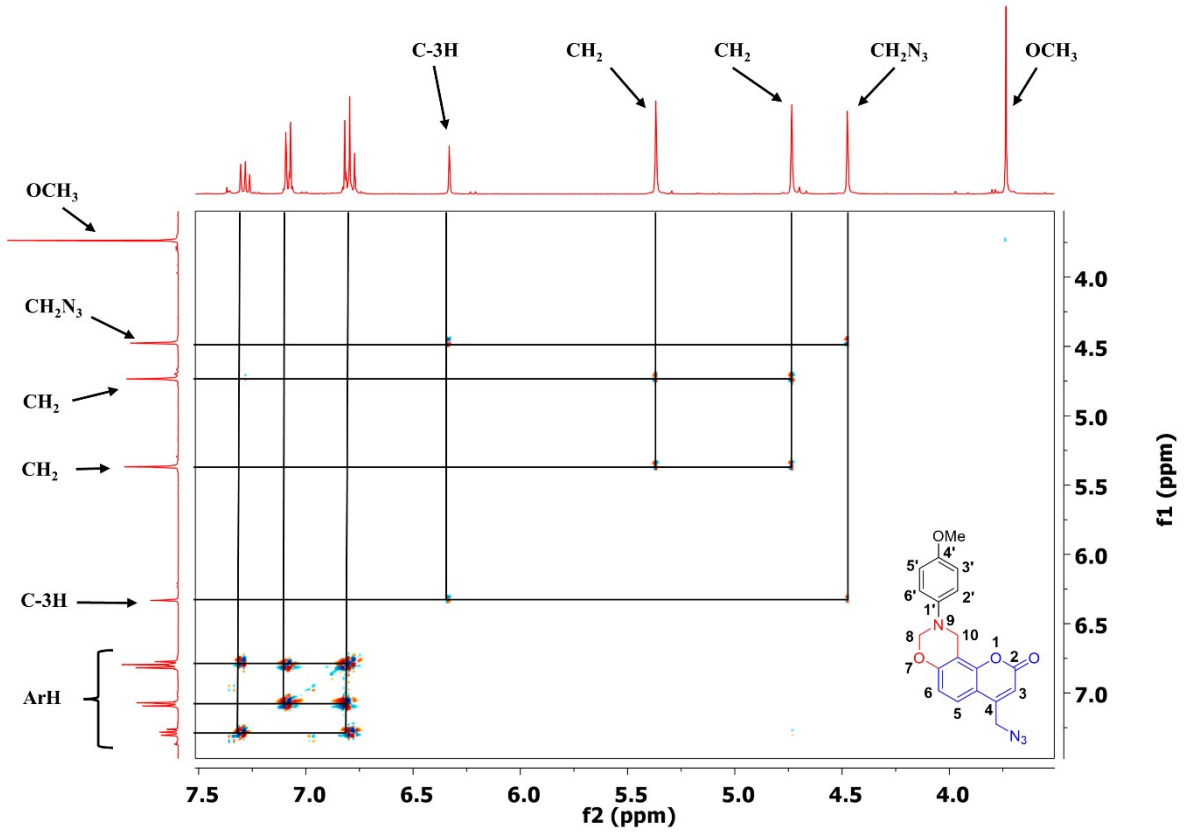


Figure S3: ^{1}H-^{1}H COSY NMR spectrum of compound **6a** (400 MHz, $CDCl_3$).

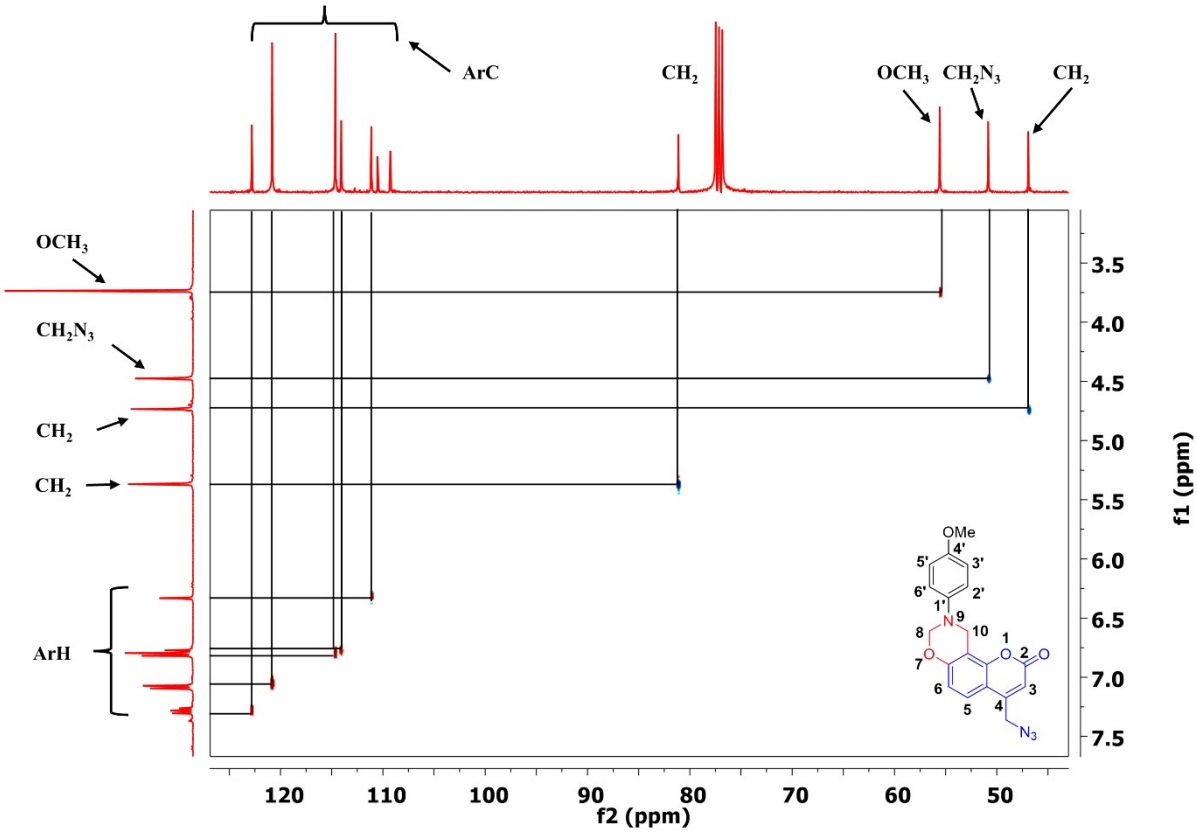


Figure S4: ^{1}H-^{13}C HETCOR NMR spectrum of compound **6a** (100 MHz, $CDCl_3$).

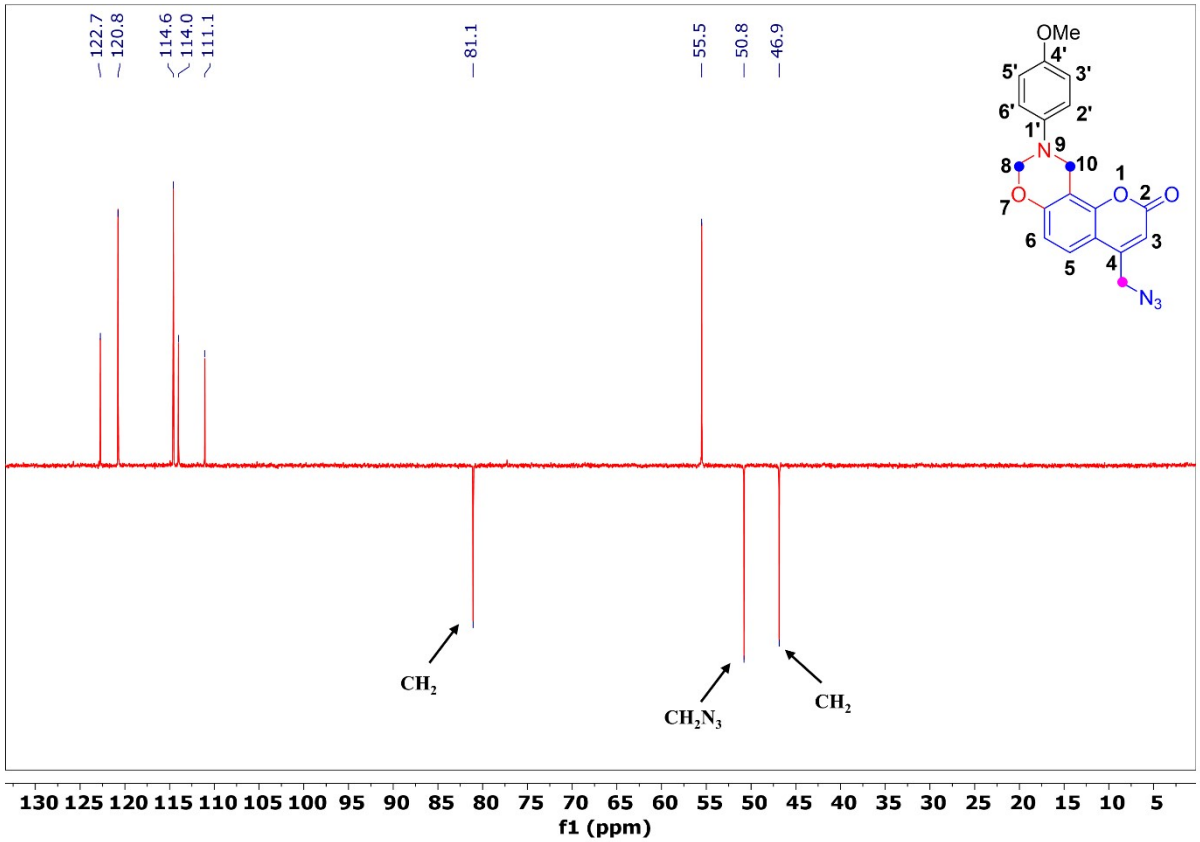


Figure S5: DEPT-135 NMR spectrum of compound **6a** (100 MHz, $CDCl_3$).

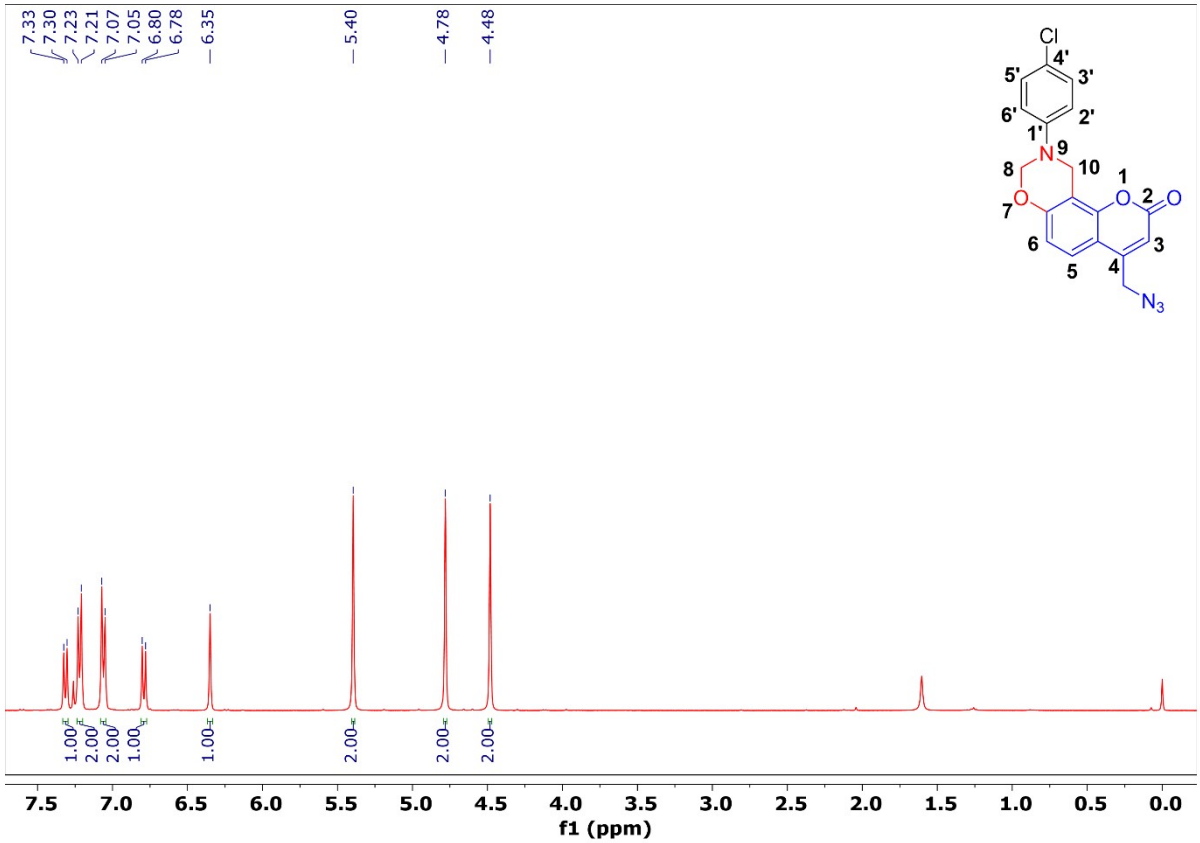


Figure S6: ^{1}H NMR spectrum of compound **6b** (400 MHz, $CDCl_3$).

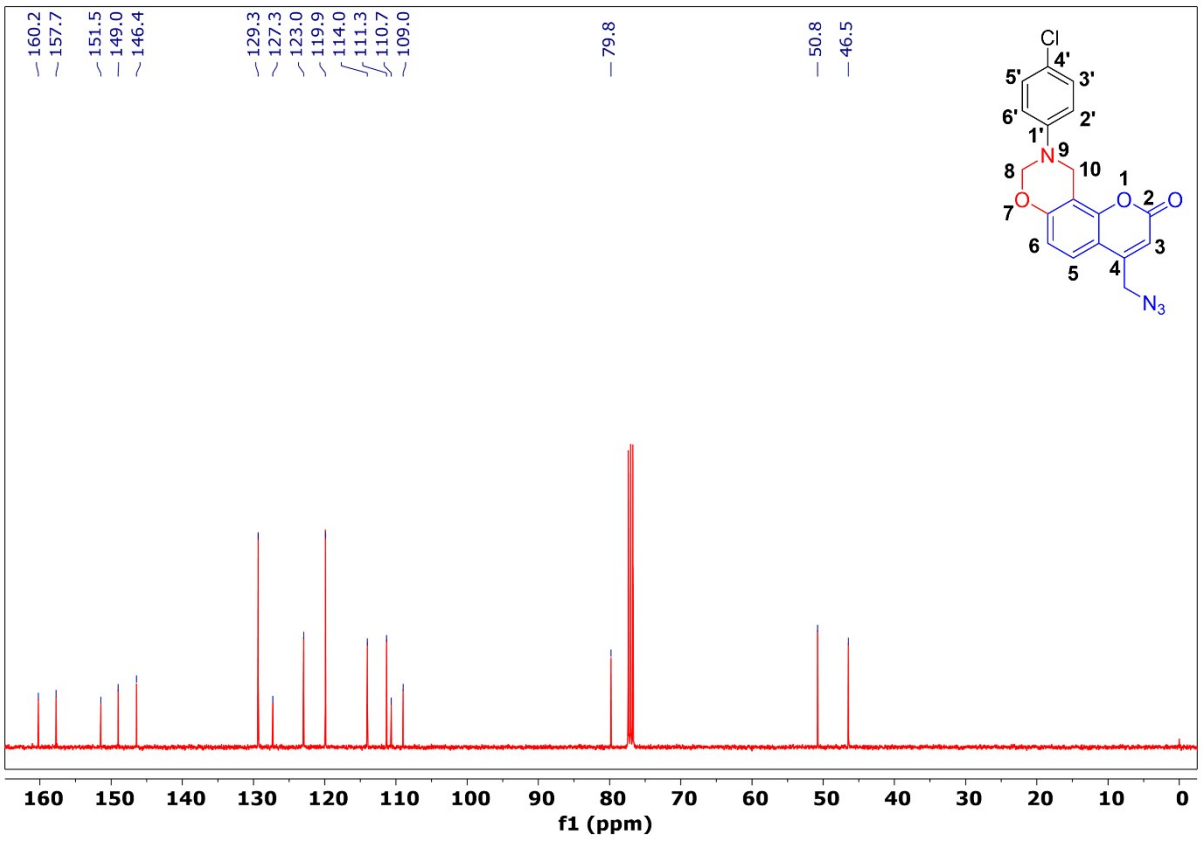


Figure S7: ^{13}C NMR spectrum of compound **6b** (100 MHz, $CDCl_3$).

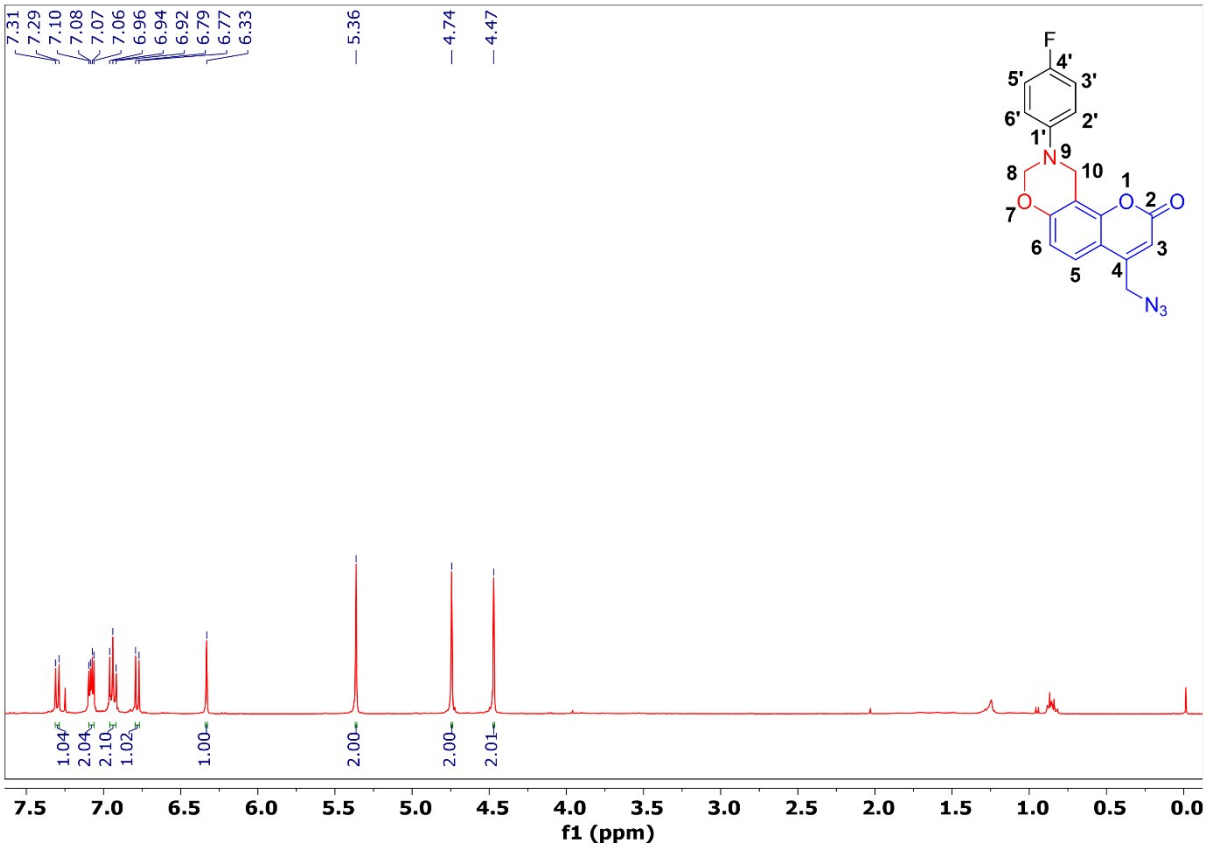


Figure S8: ^{1}H NMR spectrum of compound **6c** (400 MHz, $CDCl_3$).

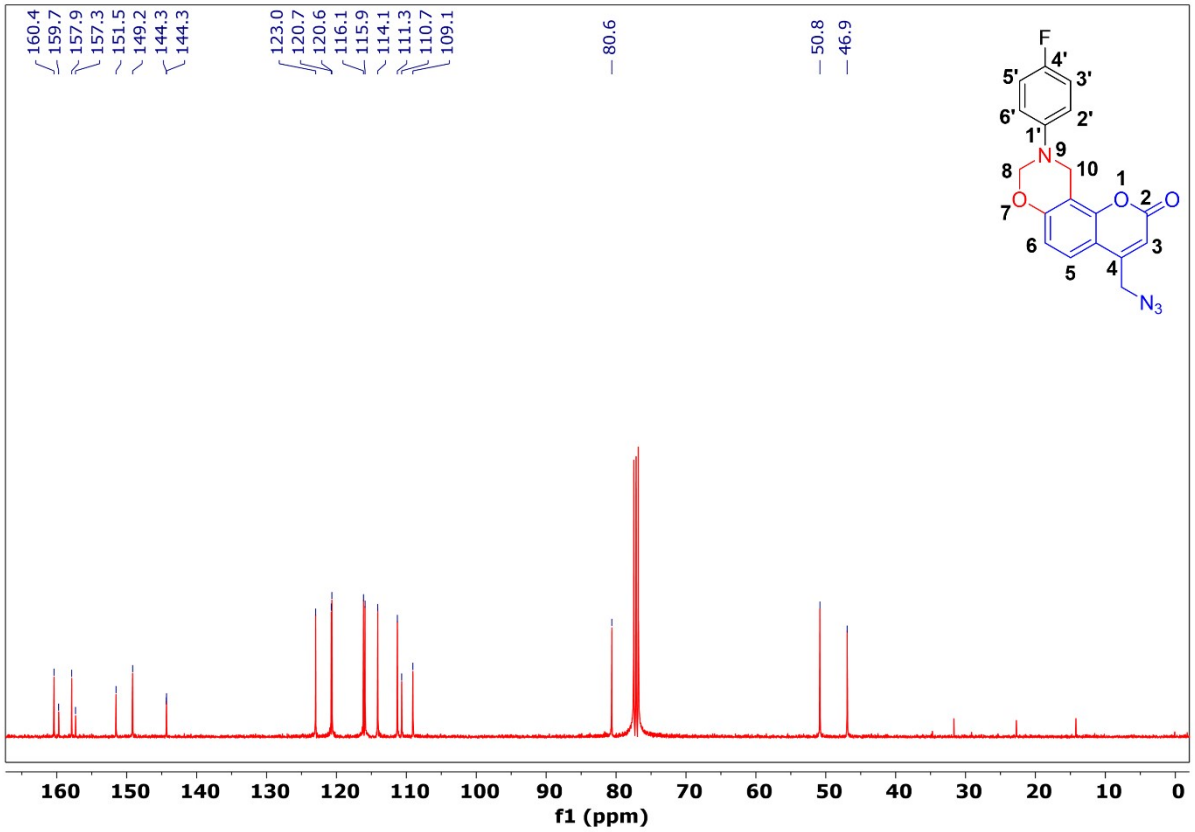


Figure S9: ^{13}C NMR spectrum of compound **6c** (100 MHz, $CDCl_3$).

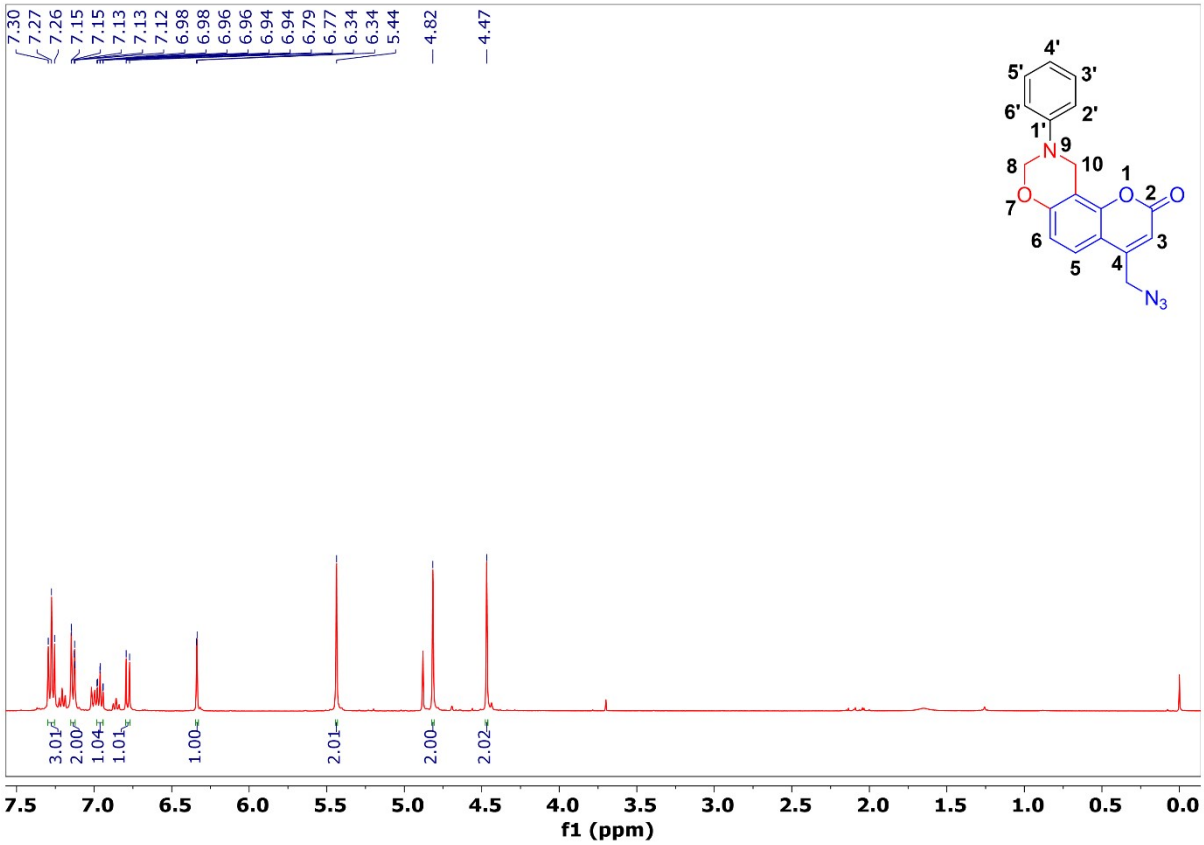


Figure S10: ^{1}H NMR spectrum of compound **6d** (400 MHz, $CDCl_3$).

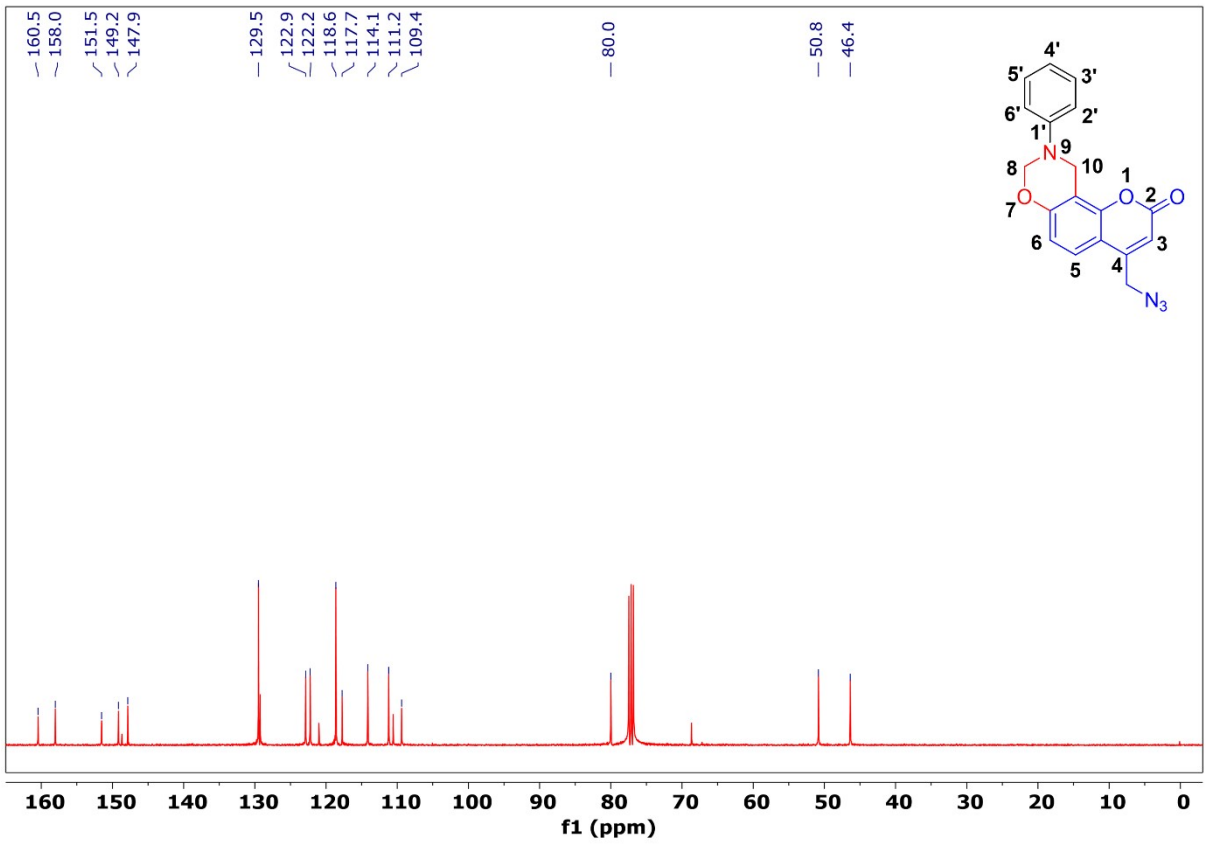


Figure S11: ^{13}C NMR spectrum of compound **6d** (100 MHz, $CDCl_3$).

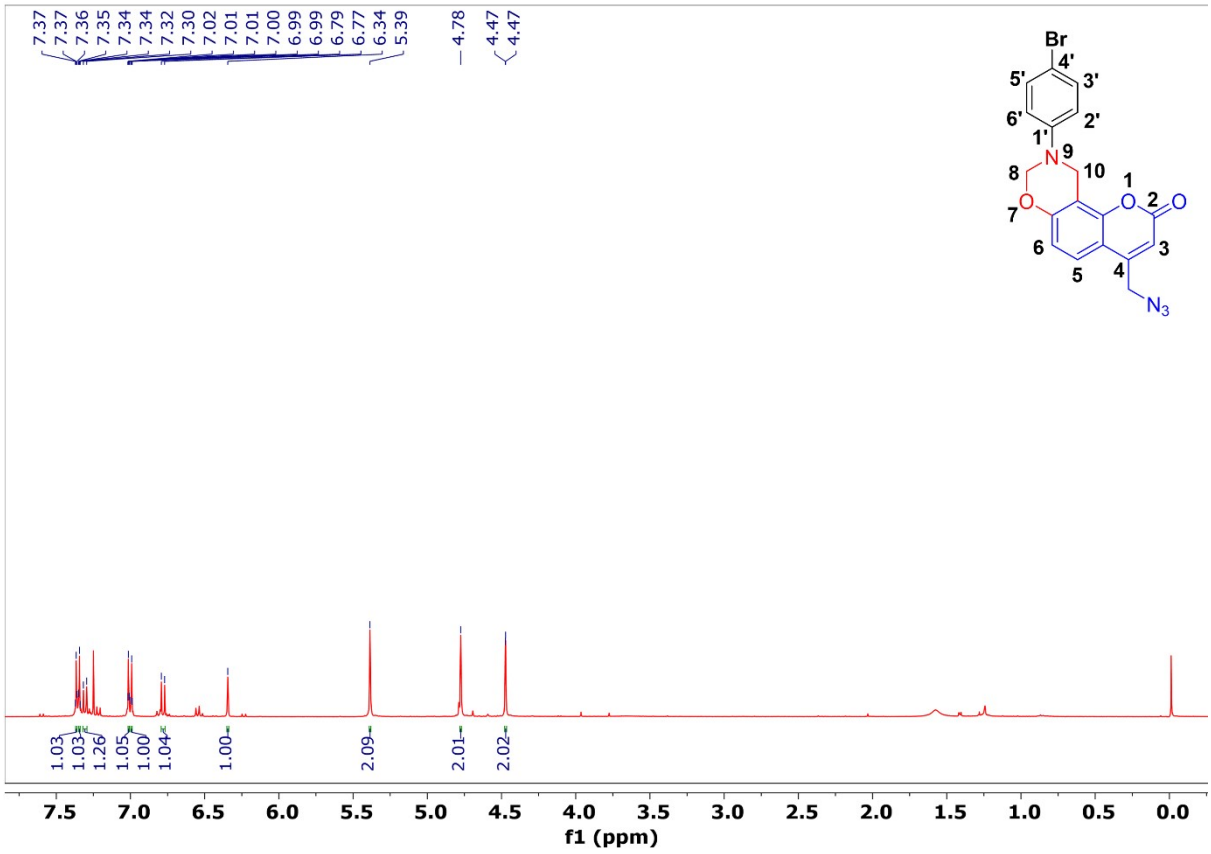


Figure S12: ^{1}H NMR spectrum of compound **6e** (400 MHz, $CDCl_3$).

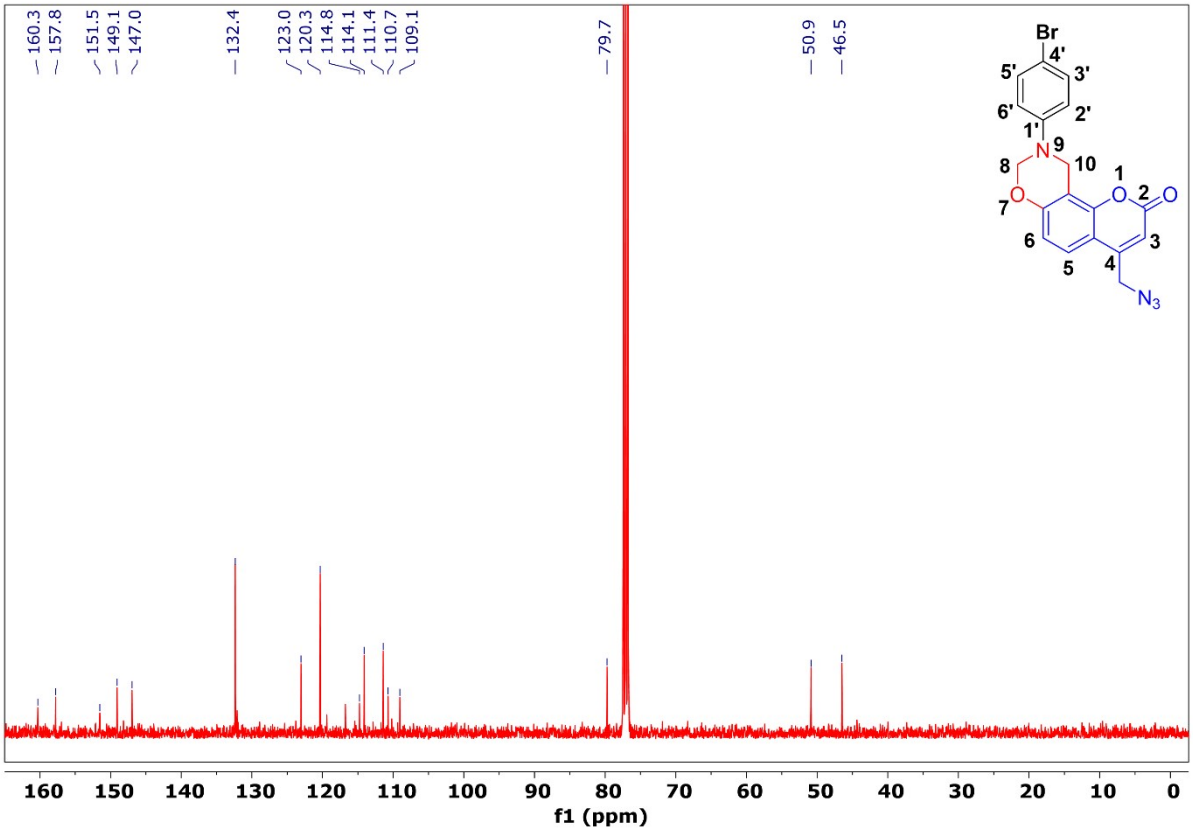


Figure S13: ^{13}C NMR spectrum of compound **6e** (100 MHz, $CDCl_3$).

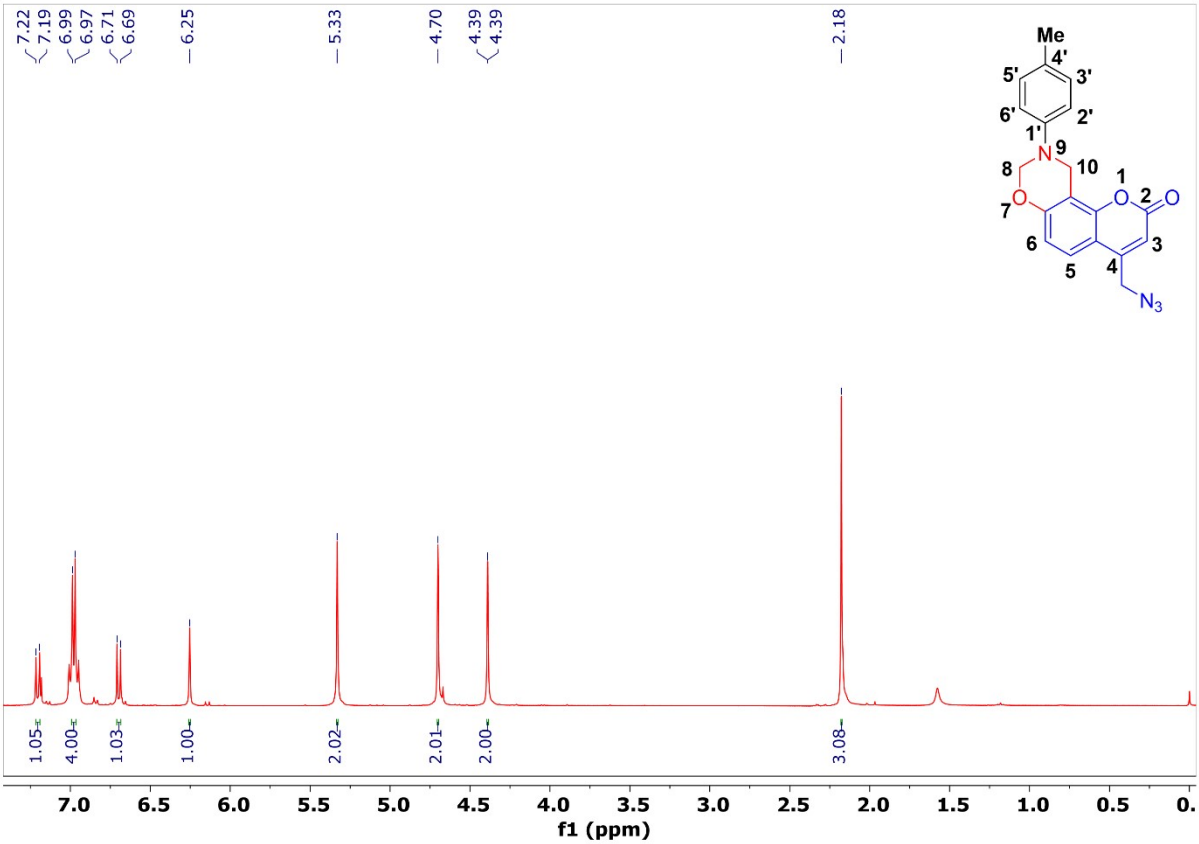


Figure S14: ^{1}H NMR spectrum of compound **6f** (400 MHz, $CDCl_3$).

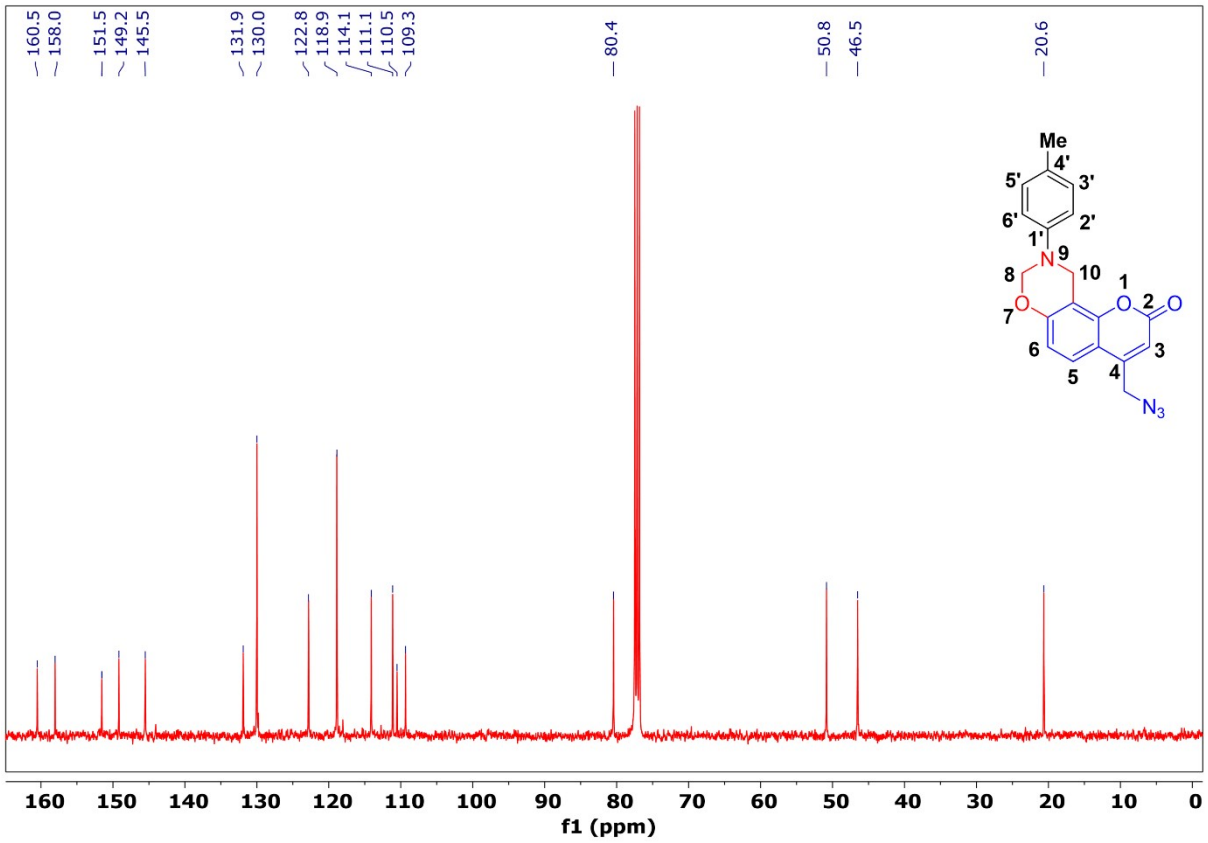


Figure S15: ^{13}C NMR spectrum of compound **6f** (100 MHz, $CDCl_3$).

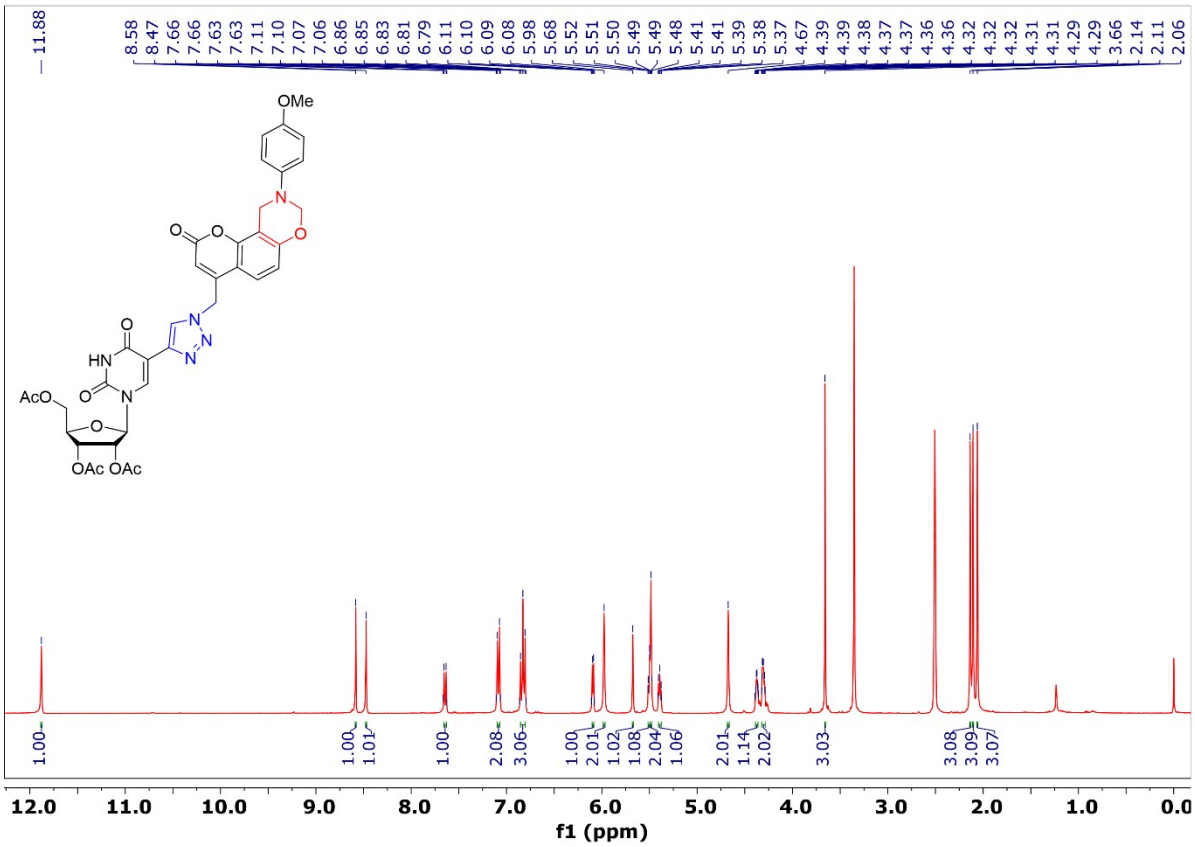


Figure S16: ^{1}H NMR spectrum of compound **12a** (400 MHz, DMSO-d_6).

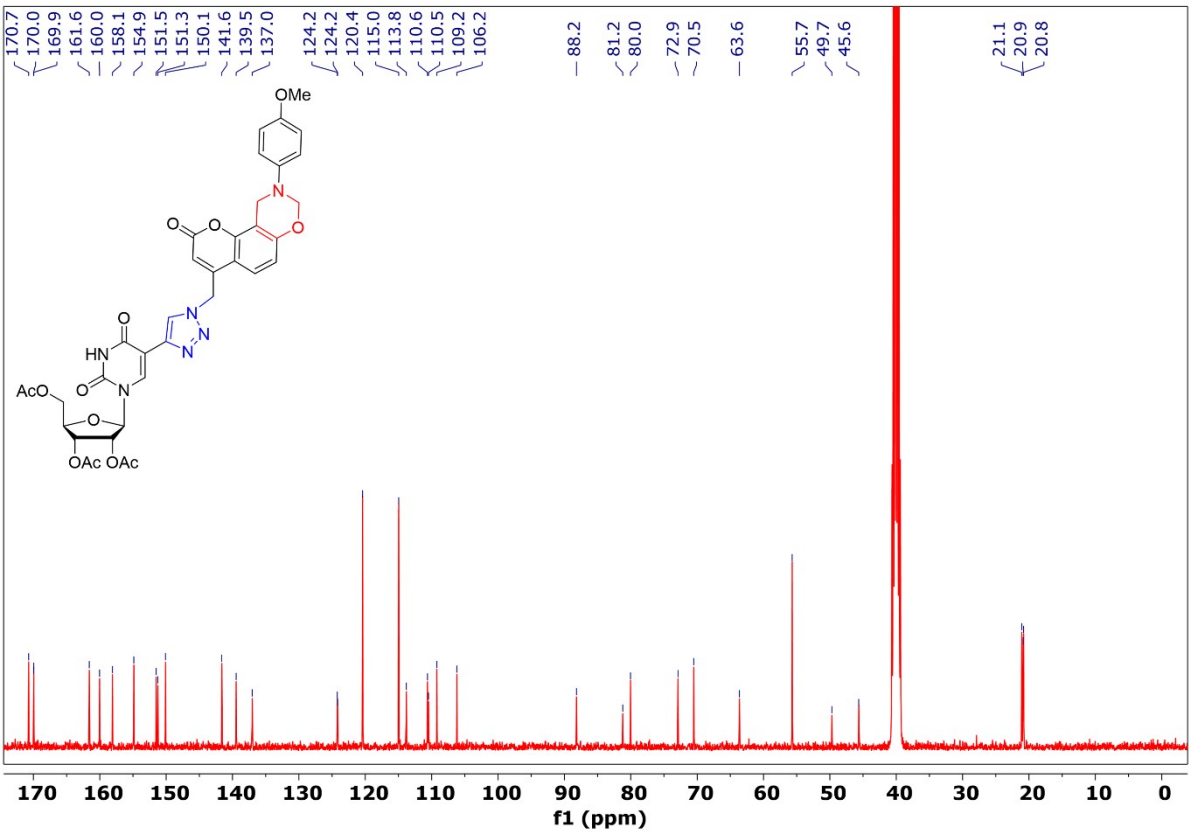


Figure S17: ^{13}C NMR spectrum of compound **12a** (100 MHz, DMSO-d_6).

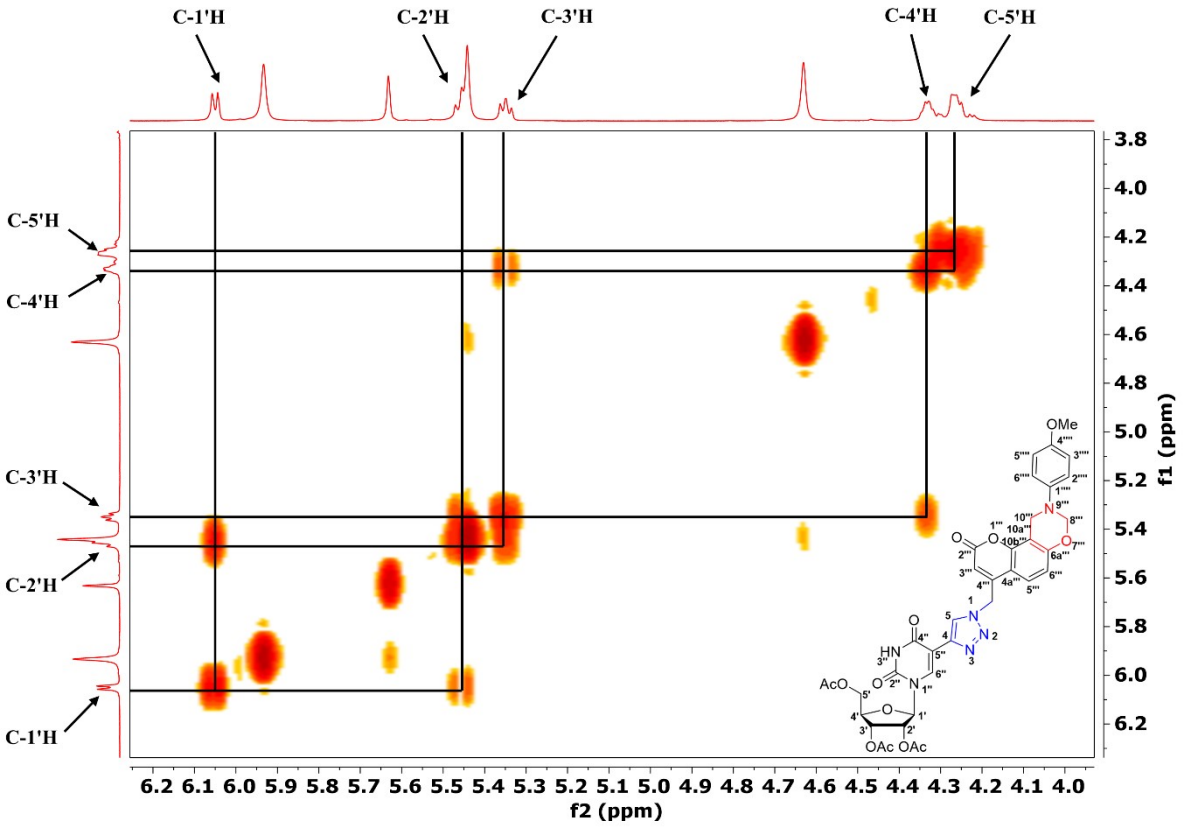


Figure S18: ^{1}H-^{1}H COSY NMR spectrum of compound **12a** (400 MHz, DMSO-d_6).

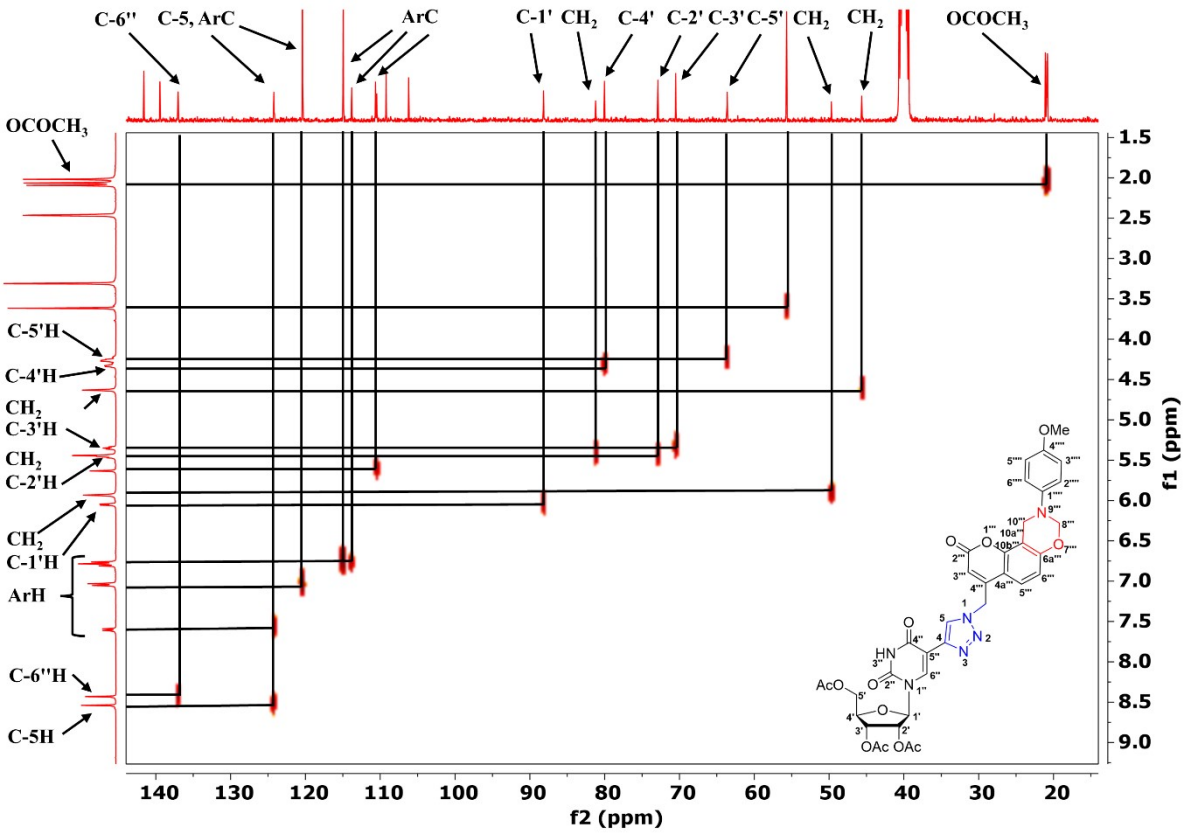


Figure S19: ^{1}H-^{13}C HETCOR NMR spectrum of compound **12a** (100 MHz, DMSO-d_6).

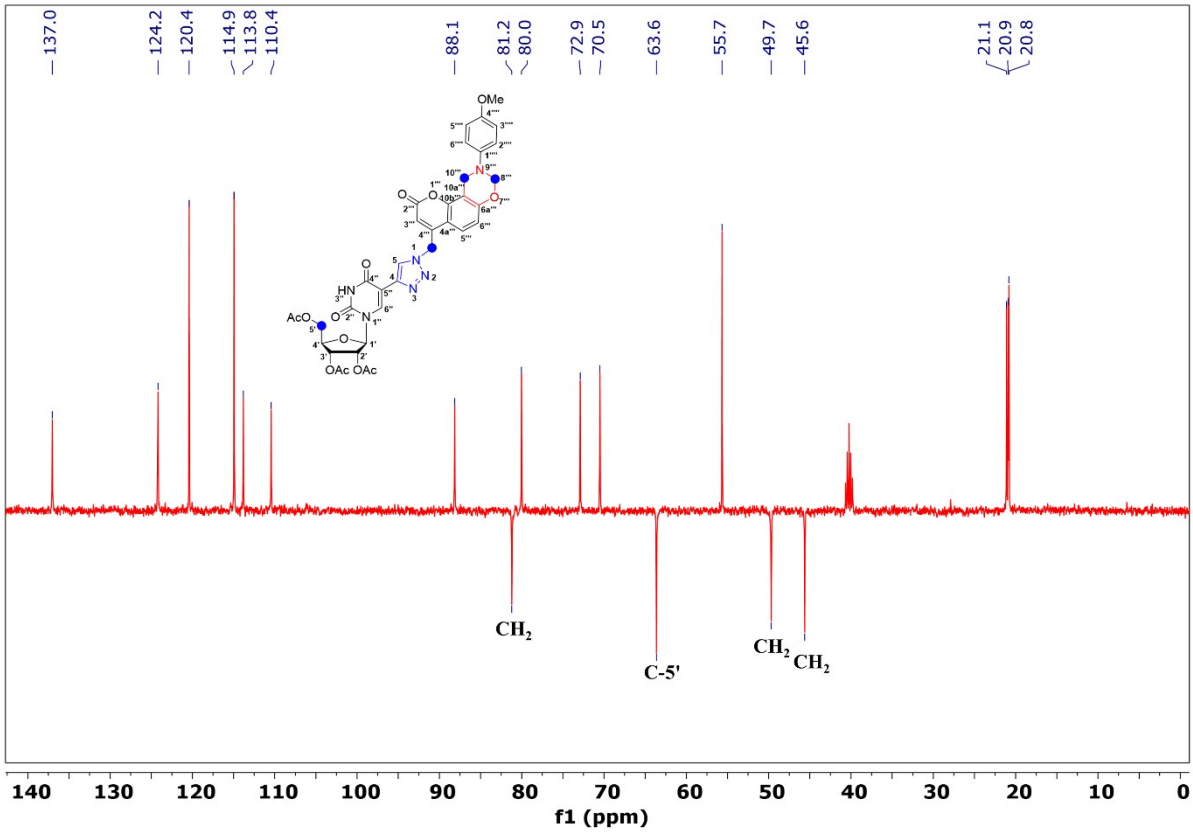


Figure S20: DEPT-135 NMR spectrum of compound **12a** (100 MHz, DMSO-d_6).

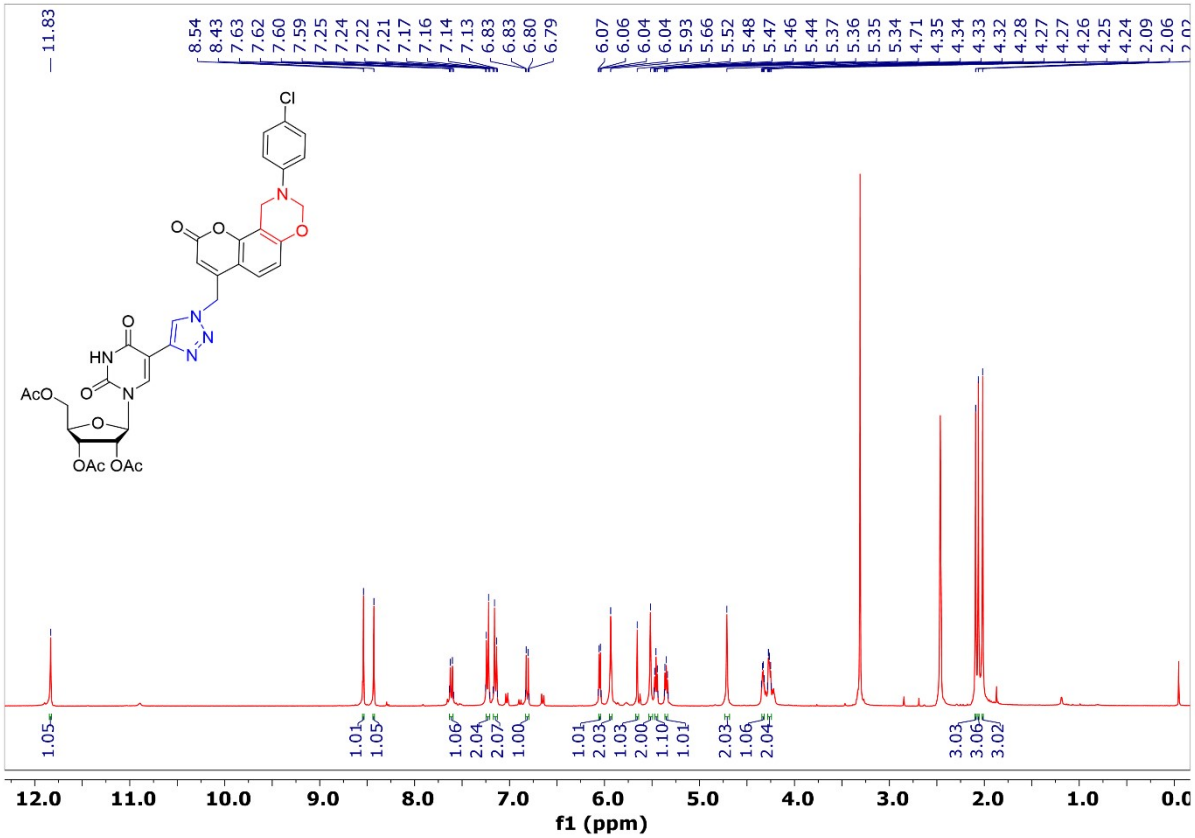


Figure S21: ^{1}H NMR spectrum of compound **12b** (400 MHz, DMSO-d_6).

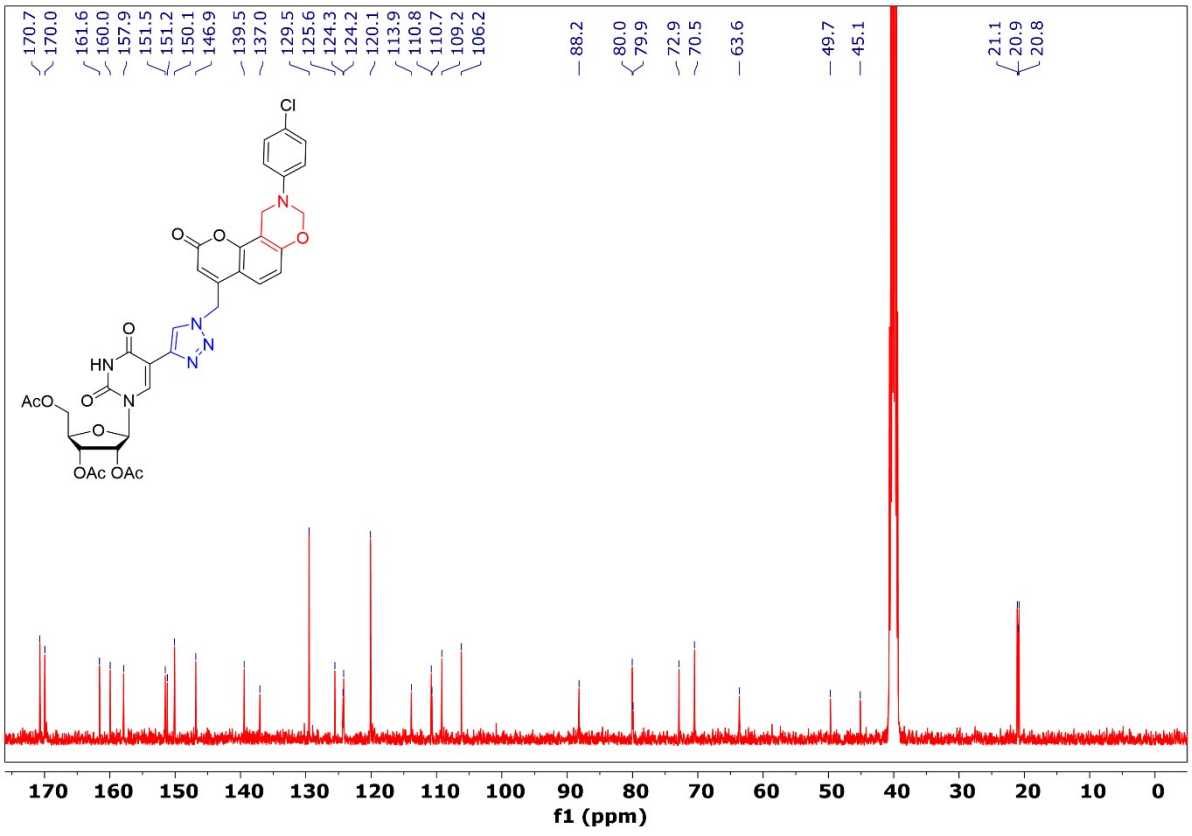


Figure S22: ^{13}C NMR spectrum of compound **12b** (100 MHz, DMSO-d_6).

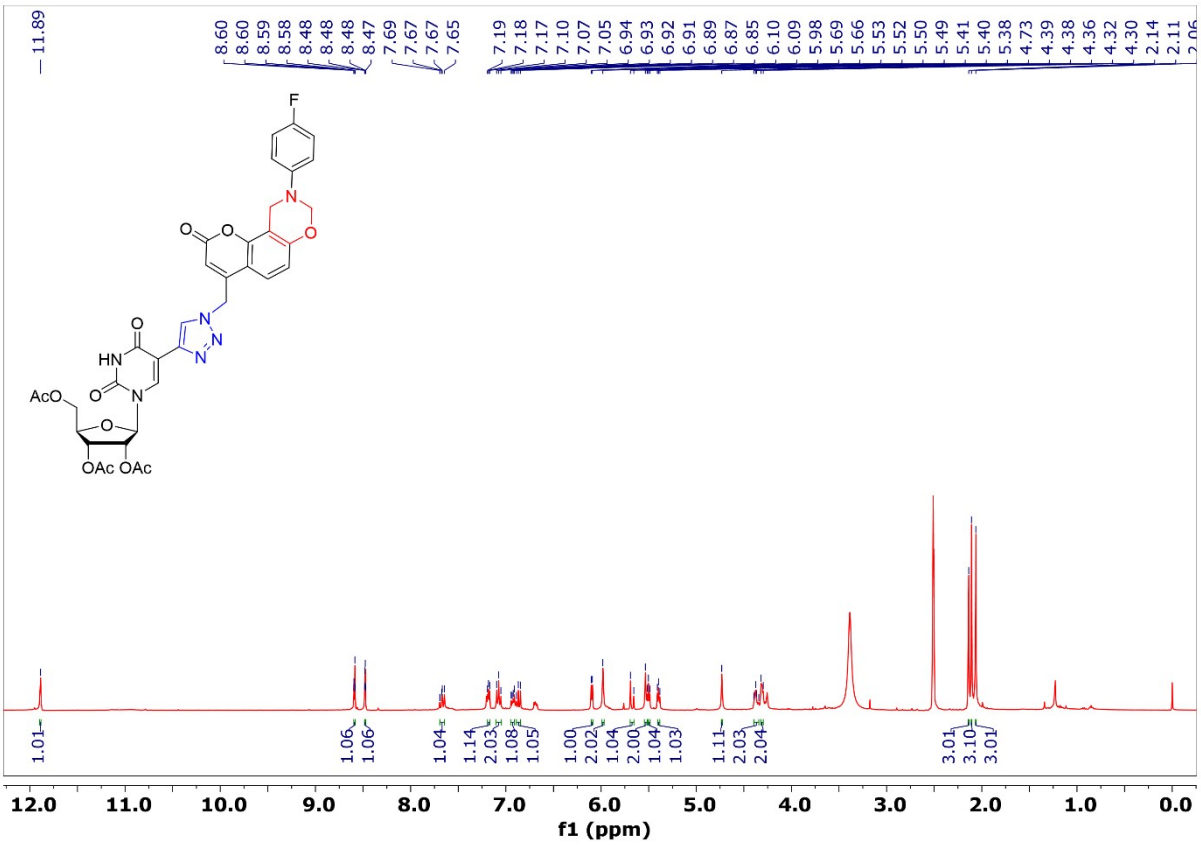


Figure S23: ^{1}H NMR spectrum of compound **12c** (400 MHz, DMSO-d_6).

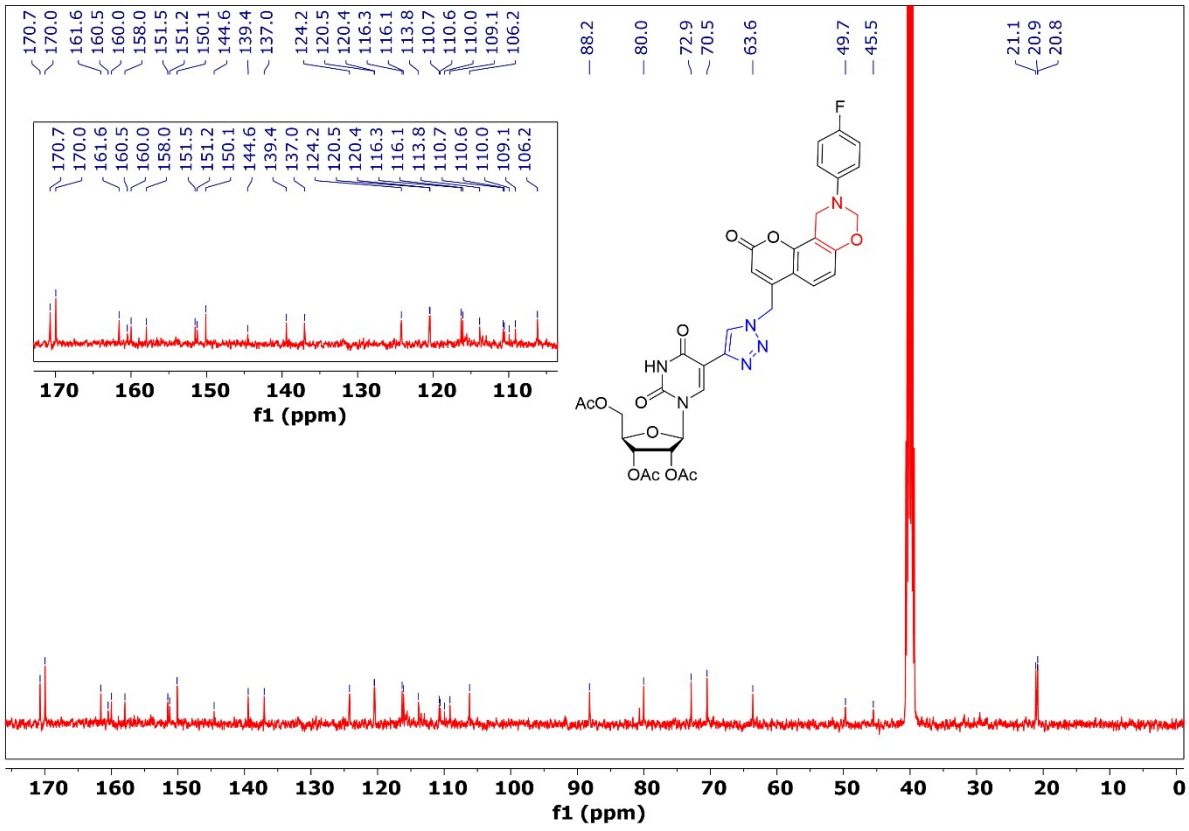


Figure S24: ^{13}C NMR spectrum of compound **12c** (100 MHz, DMSO-d_6).

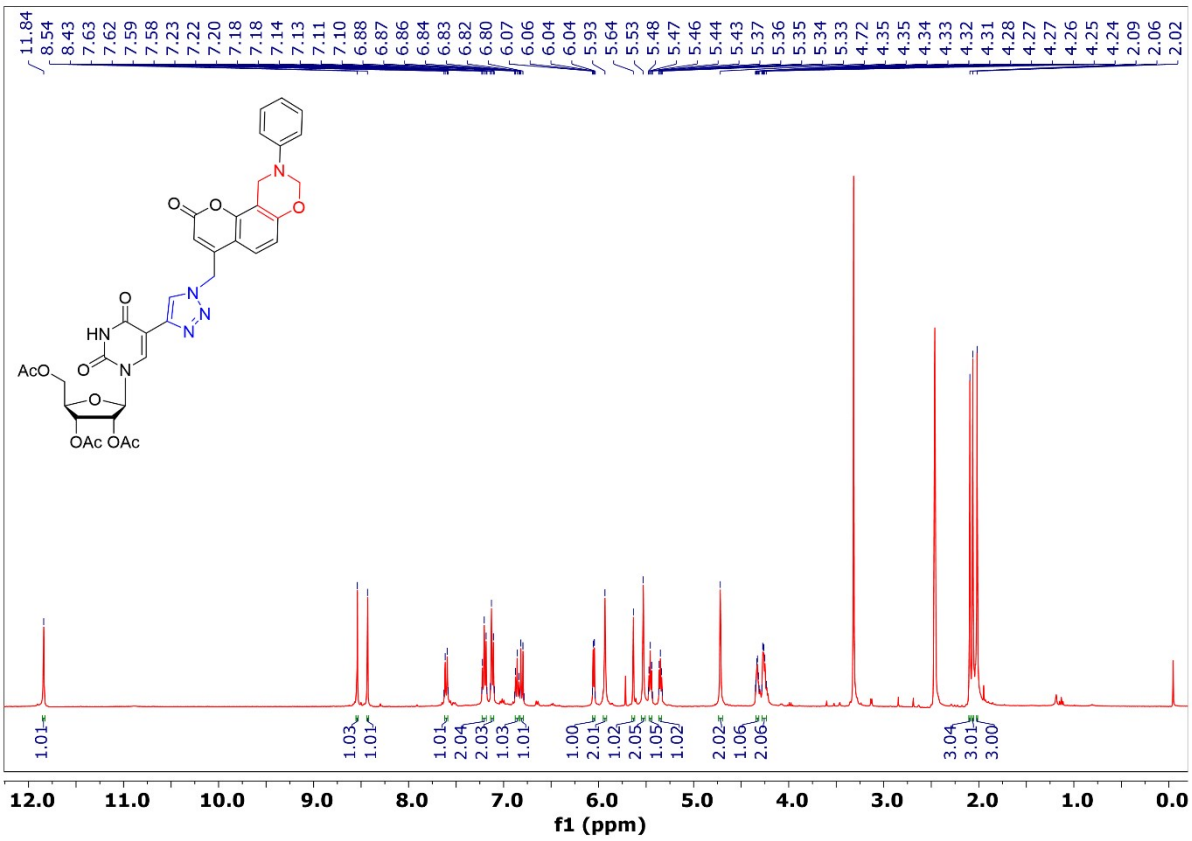


Figure S25: ^{1}H NMR spectrum of compound **12d** (400 MHz, DMSO-d_6).

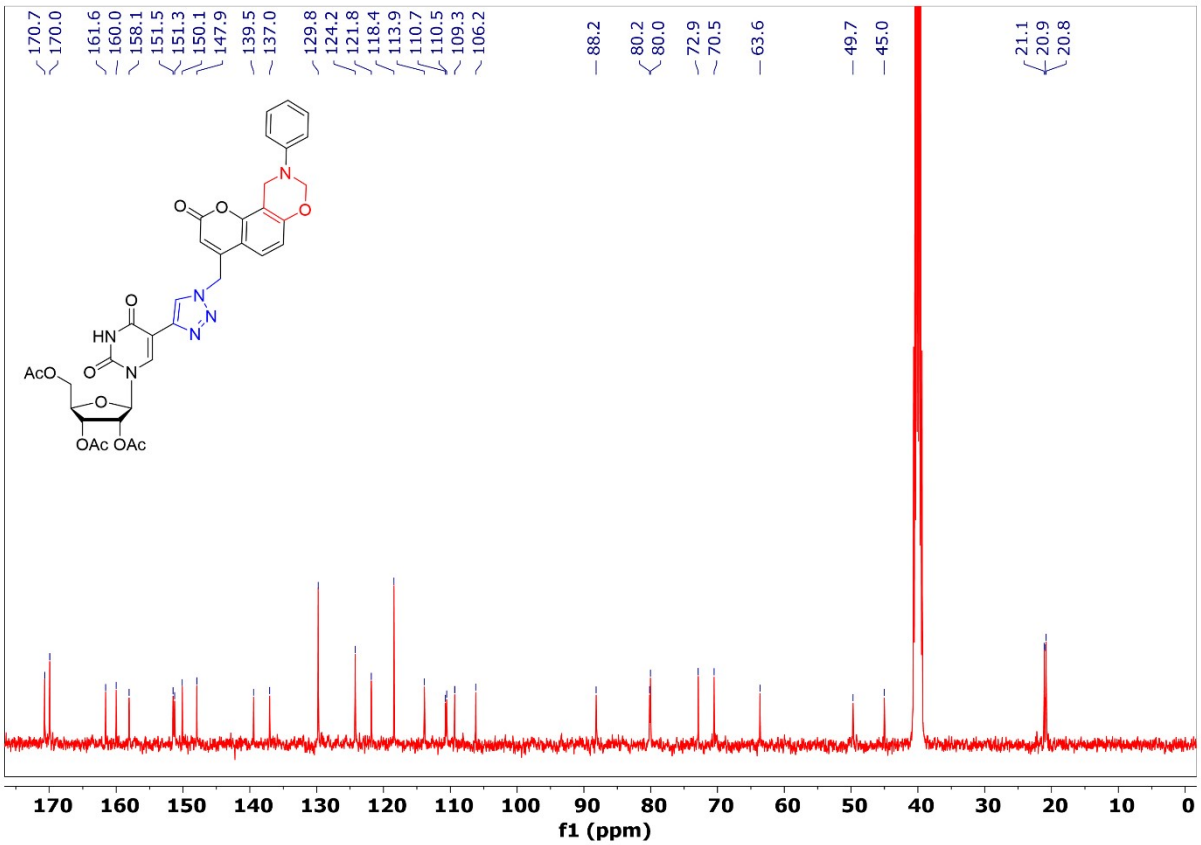


Figure S26: ^{13}C NMR spectrum of compound **12d** (100 MHz, DMSO-d_6).

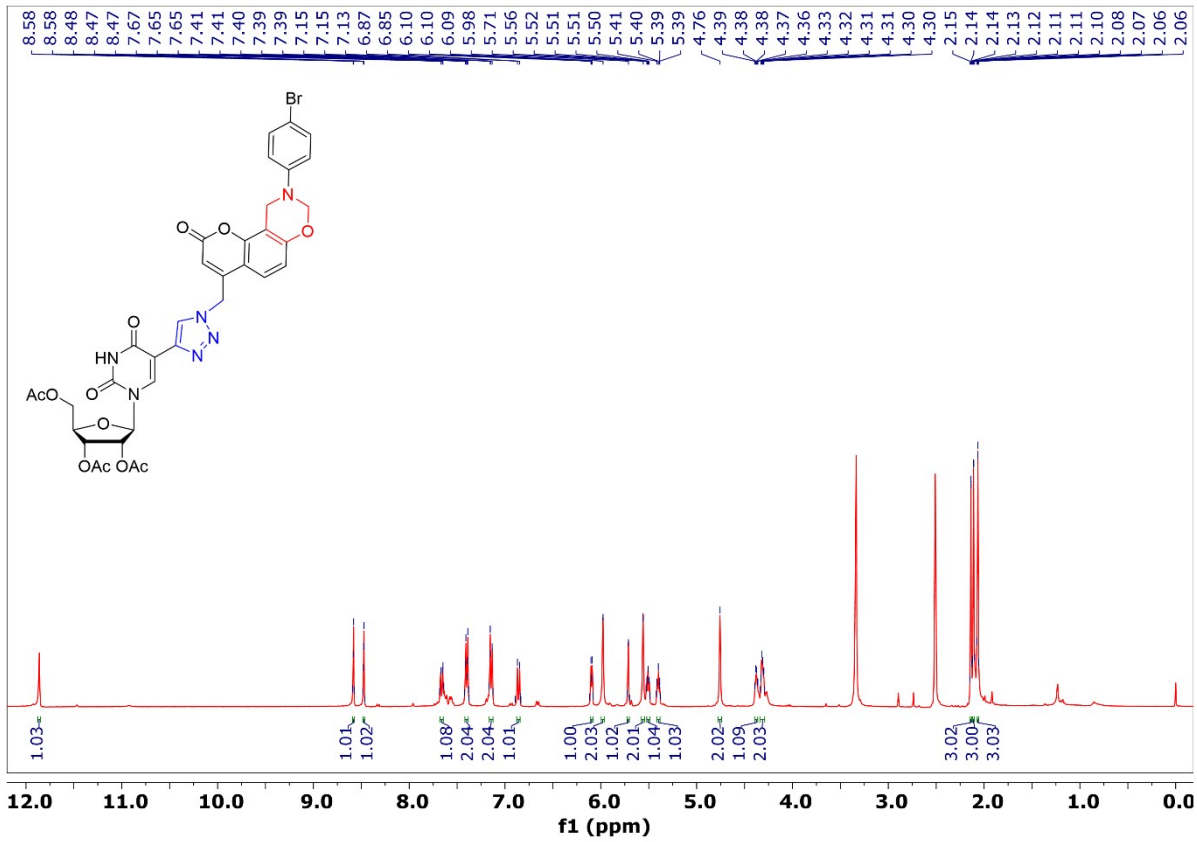


Figure S27: ^{1}H NMR spectrum of compound **12e** (400 MHz, DMSO-d_6).

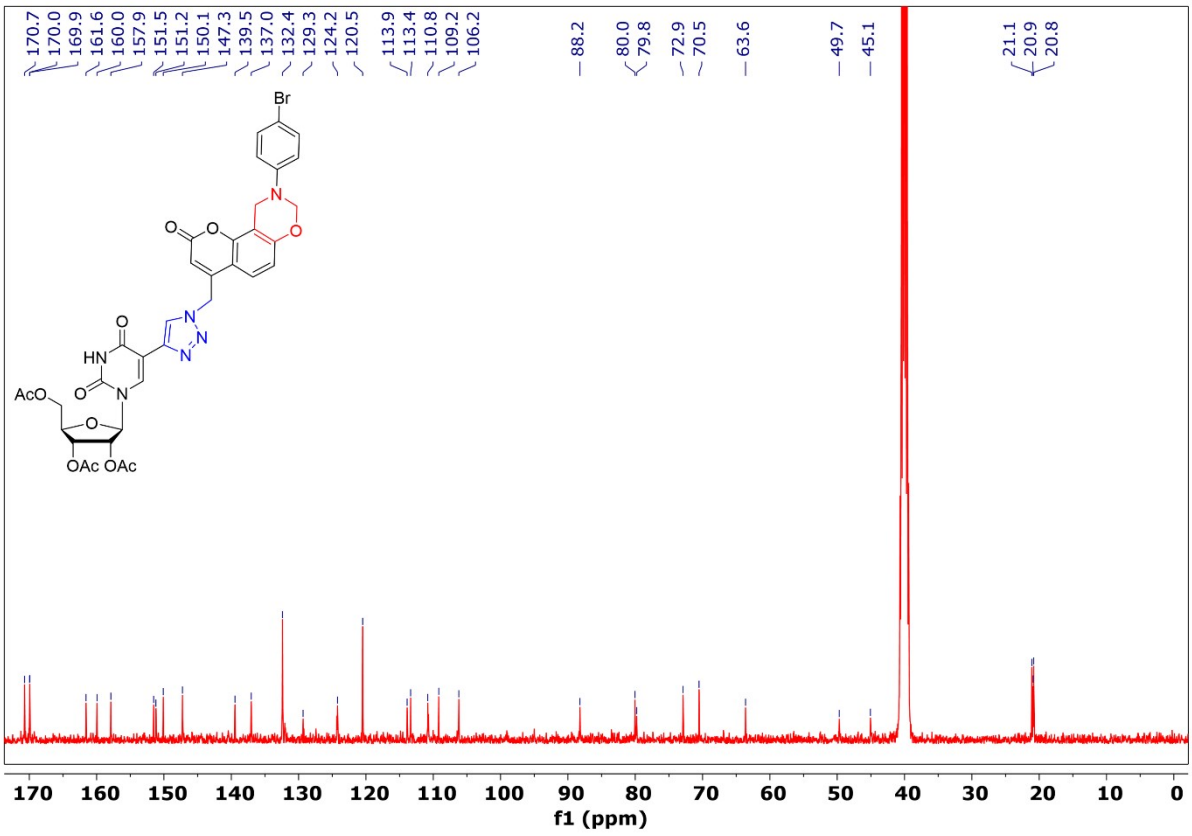


Figure S28: ^{13}C NMR spectrum of compound **12e** (100 MHz, DMSO-d_6).

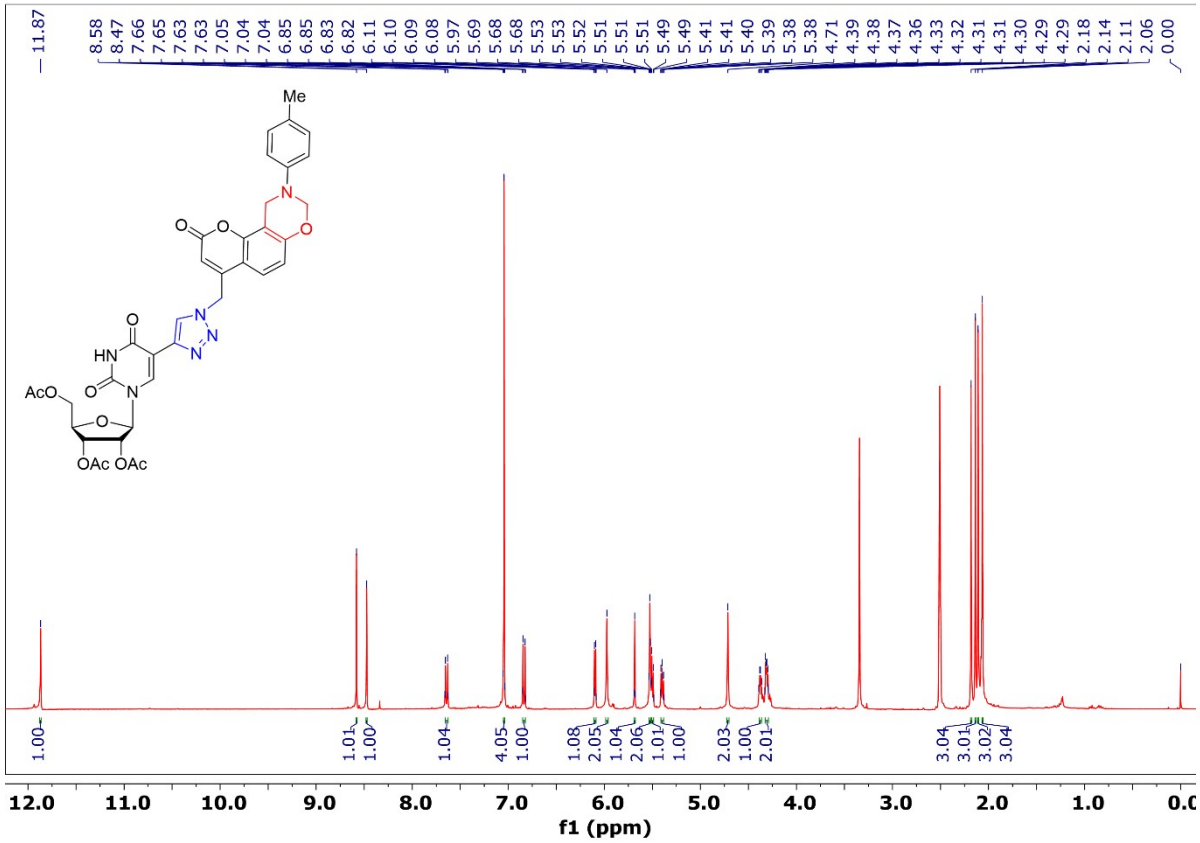


Figure S29: ^{1}H NMR spectrum of compound **12f** (400 MHz, DMSO-d_6).

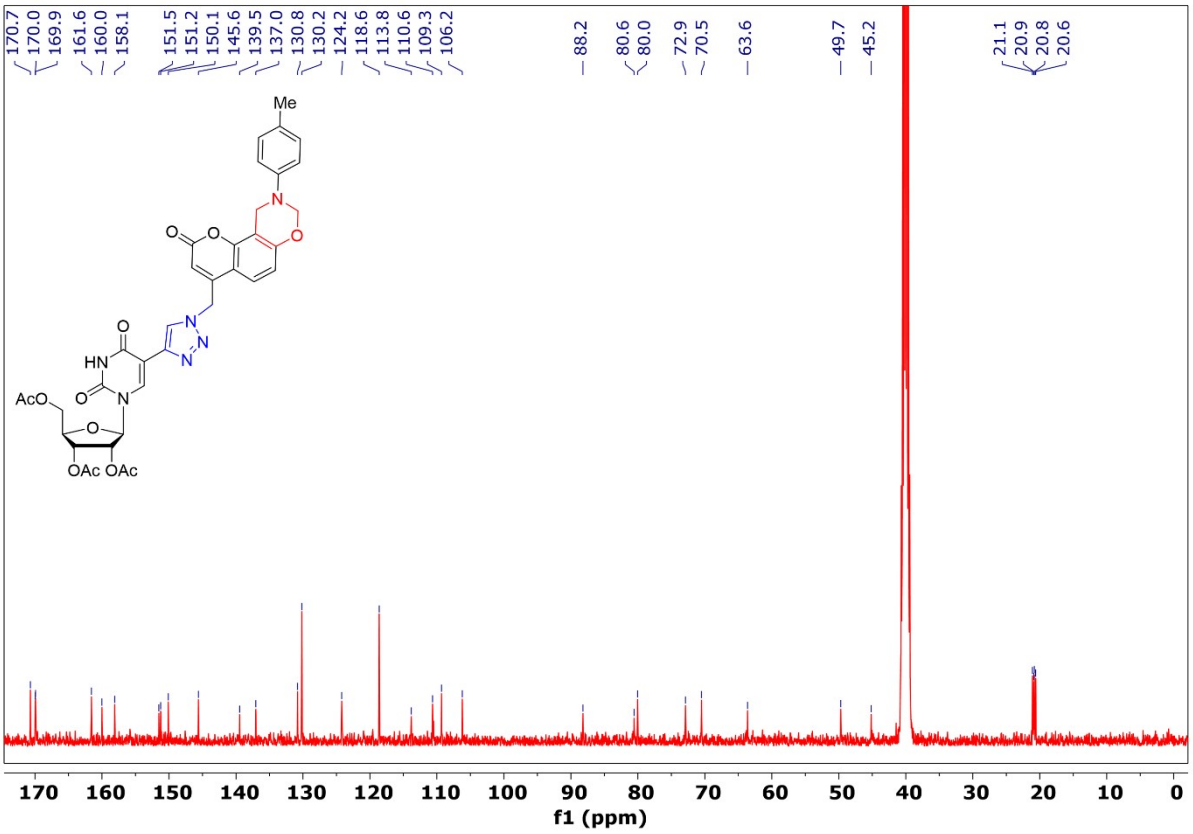


Figure S30: ^{13}C NMR spectrum of compound **12f** (100 MHz, DMSO-d_6).

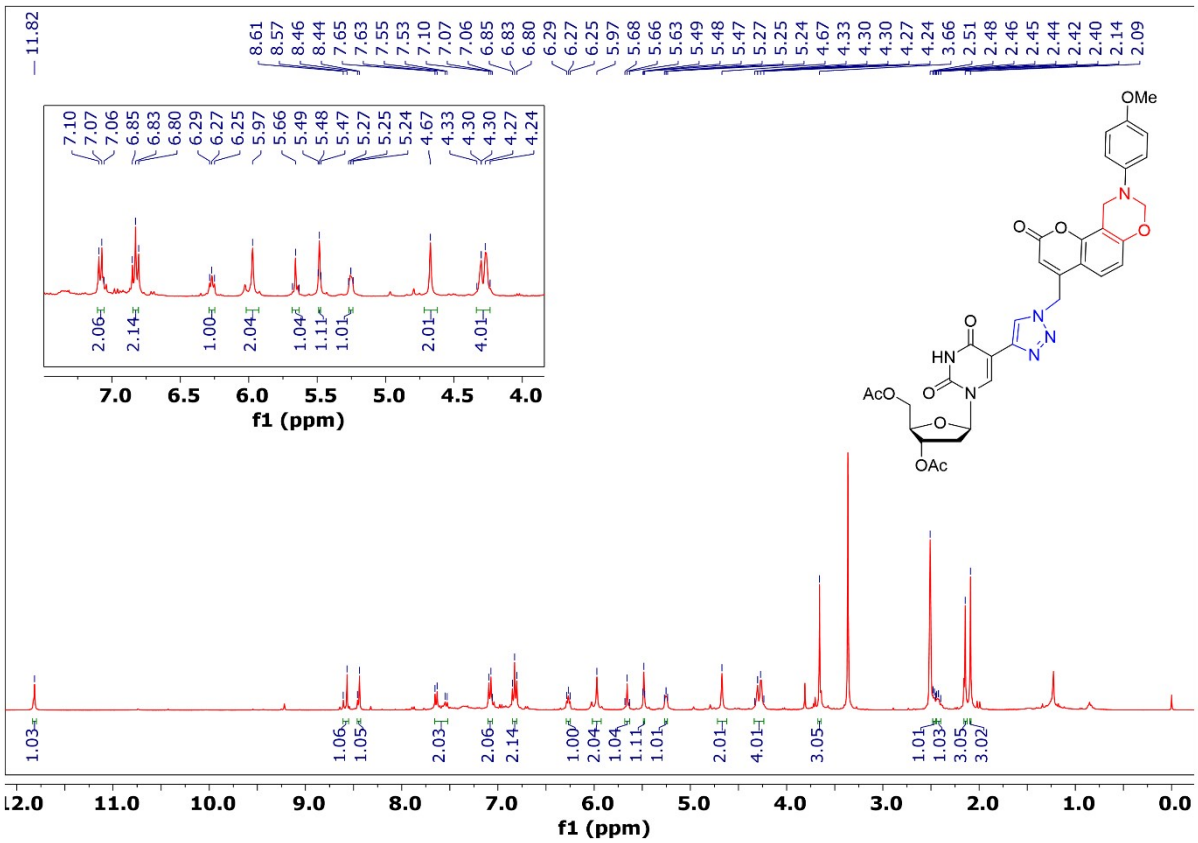


Figure S31: ^{1}H NMR spectrum of compound **13a** (400 MHz, DMSO-d_6).

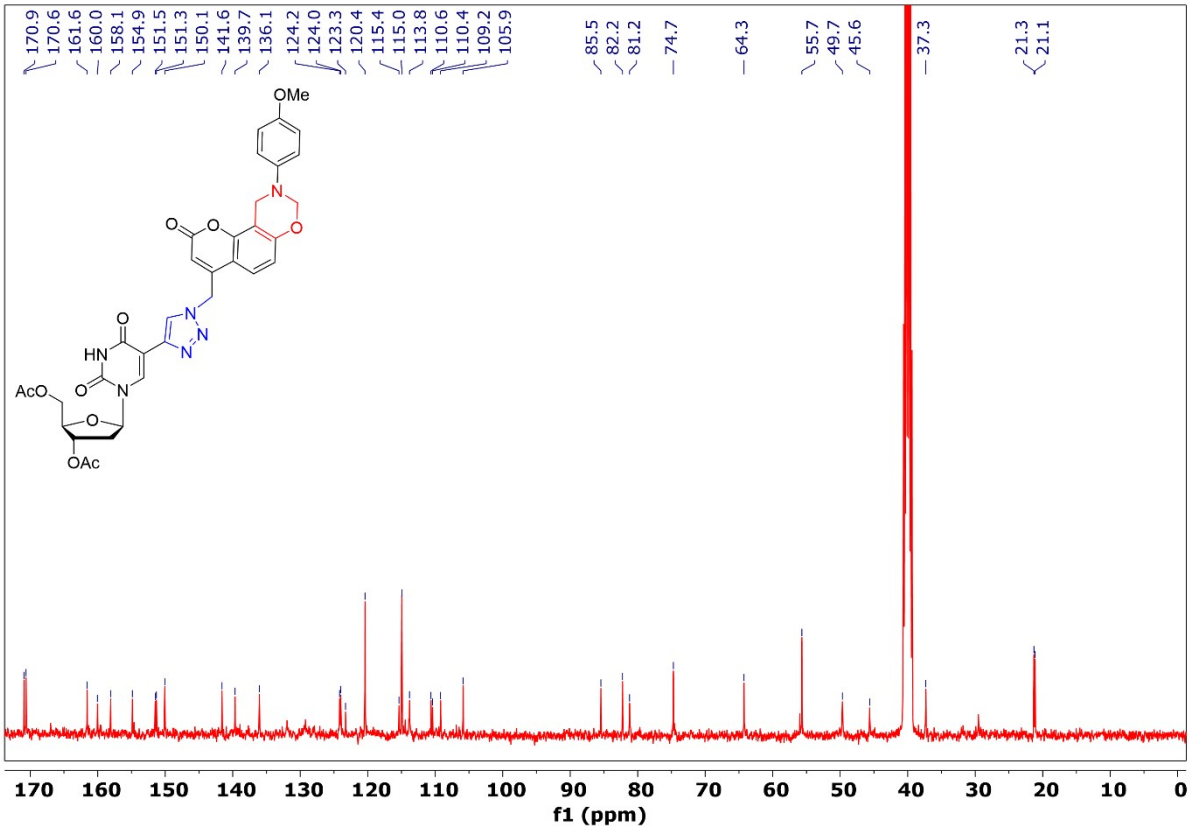


Figure S32: ^{13}C NMR spectrum of compound **13a** (100 MHz, DMSO-d_6).

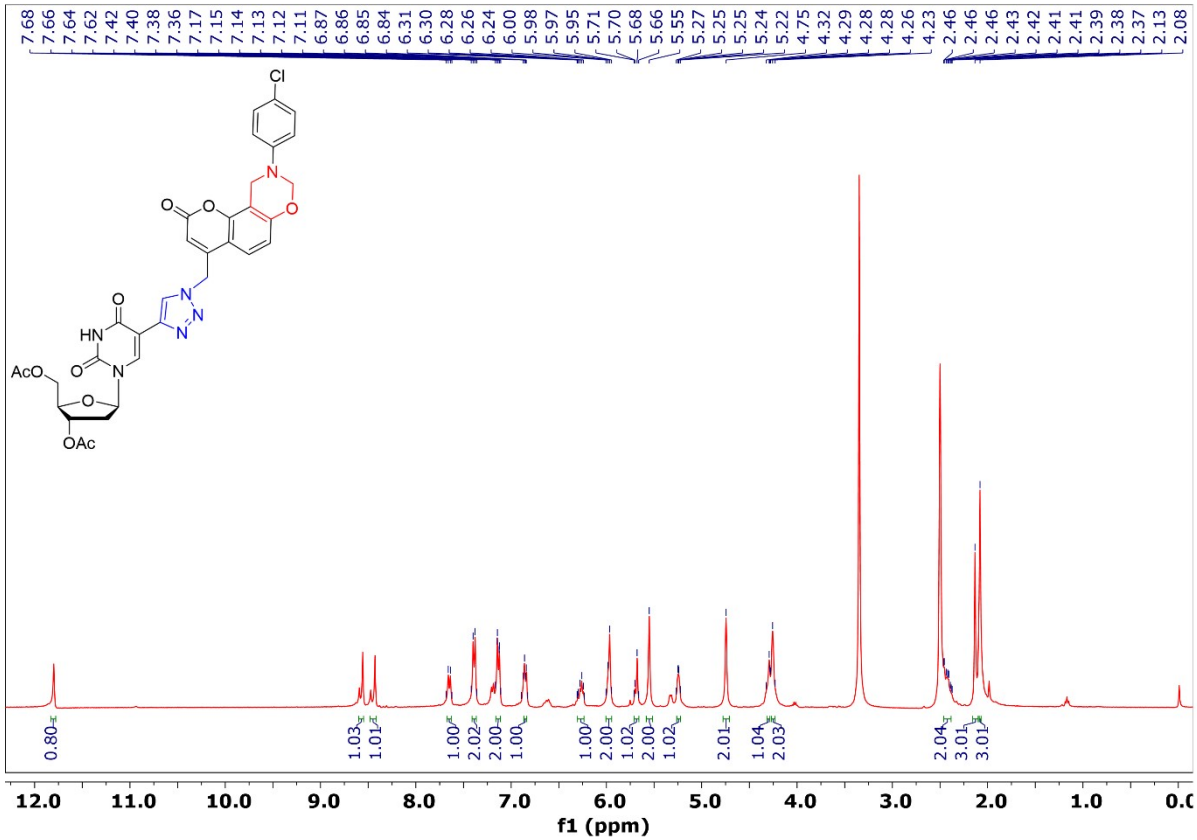


Figure S33: ^{1}H NMR spectrum of compound **13b** (400 MHz, DMSO-d_6).

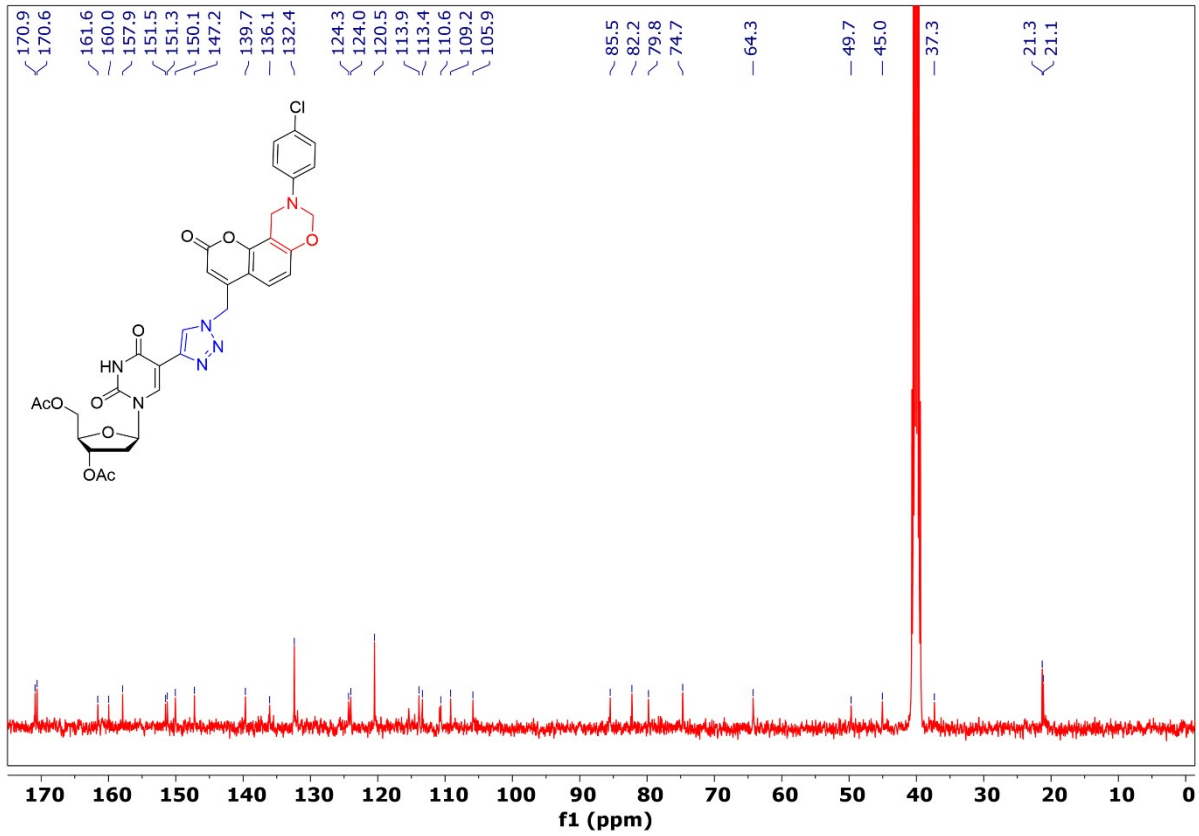


Figure S34: ^{13}C NMR spectrum of compound **13b** (100 MHz, DMSO-d_6).

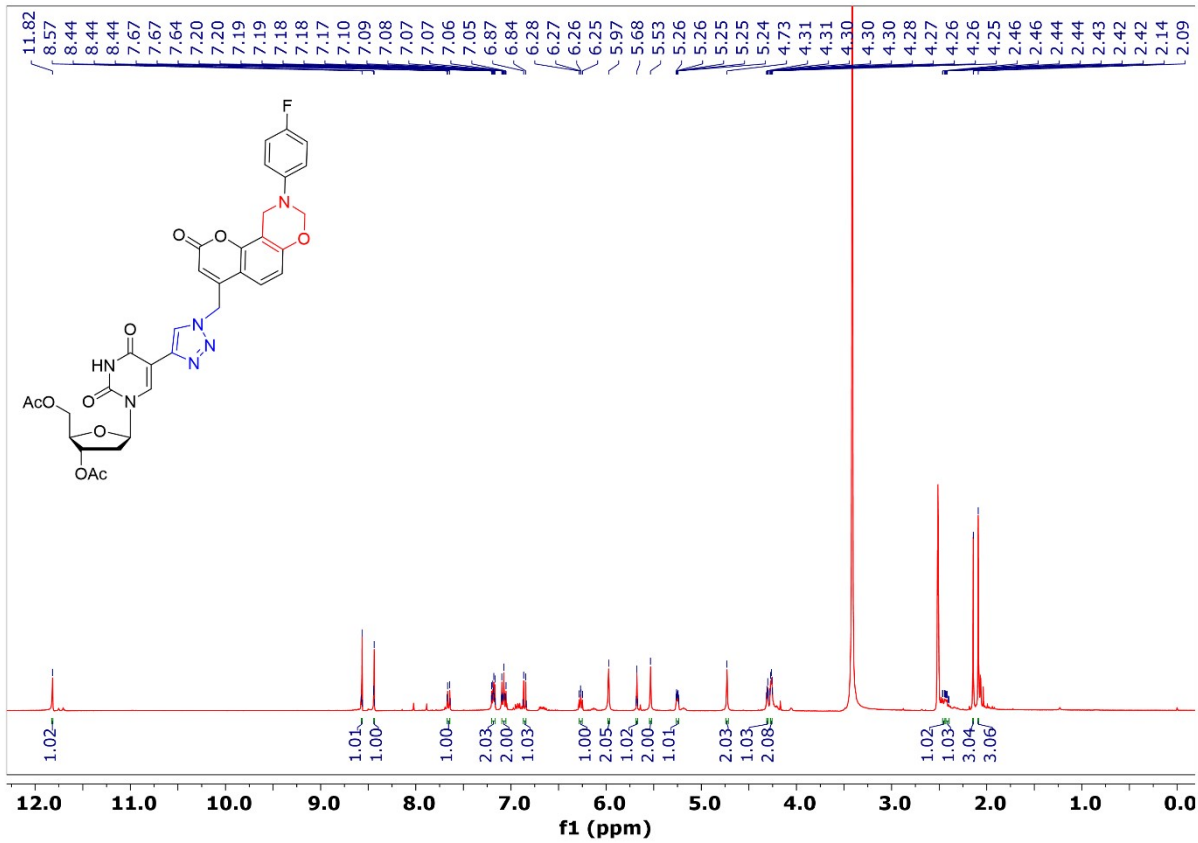


Figure S35: ^{1}H NMR spectrum of compound **13c** (400 MHz, DMSO-d_6).

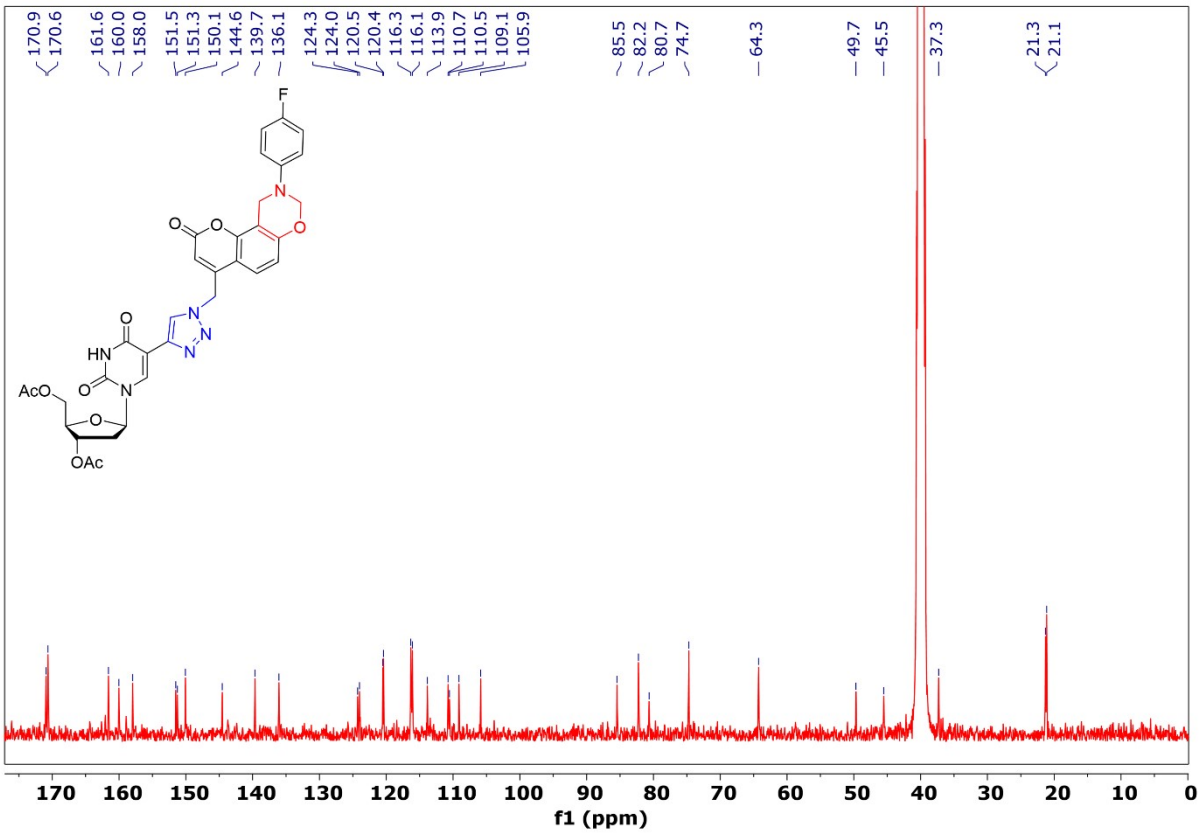


Figure S36: ^{13}C NMR spectrum of compound **13c** (100 MHz, DMSO-d_6).

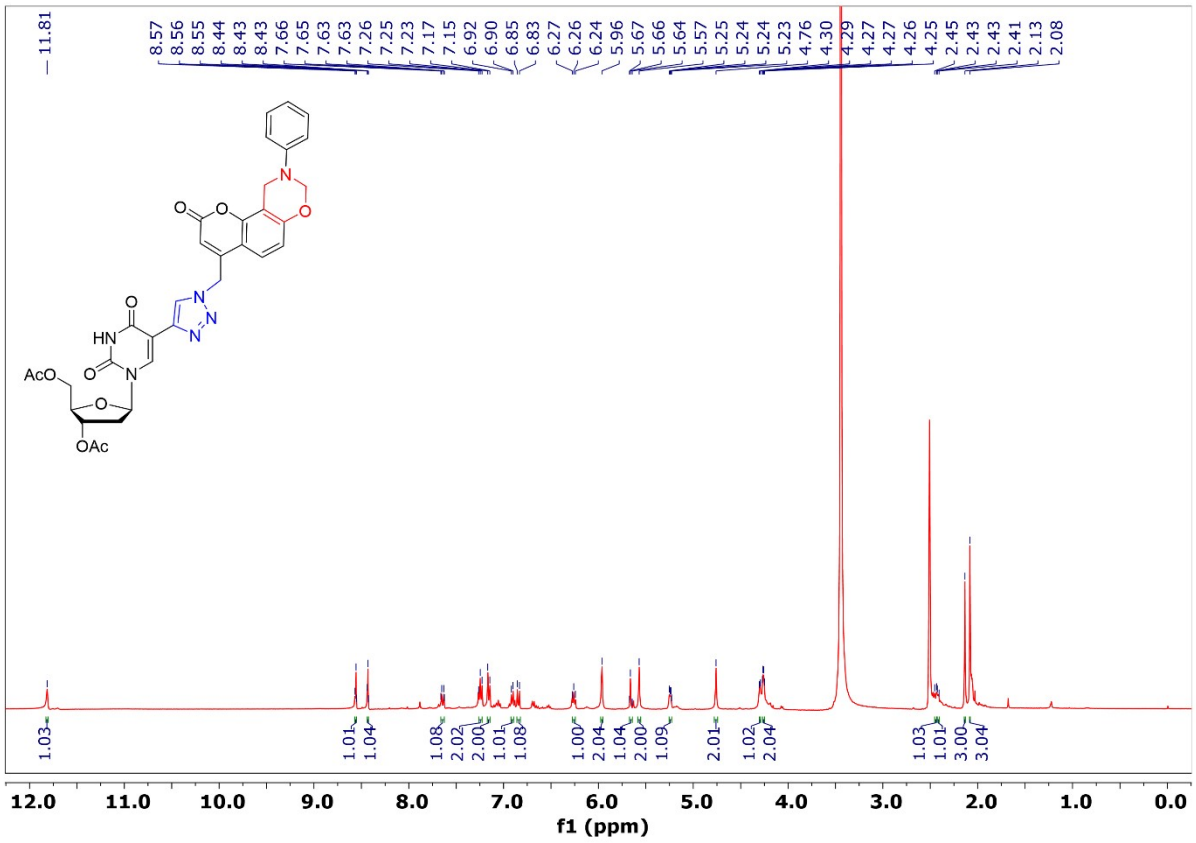


Figure S37: ^{1}H NMR spectrum of compound **13d** (400 MHz, DMSO-d_6).

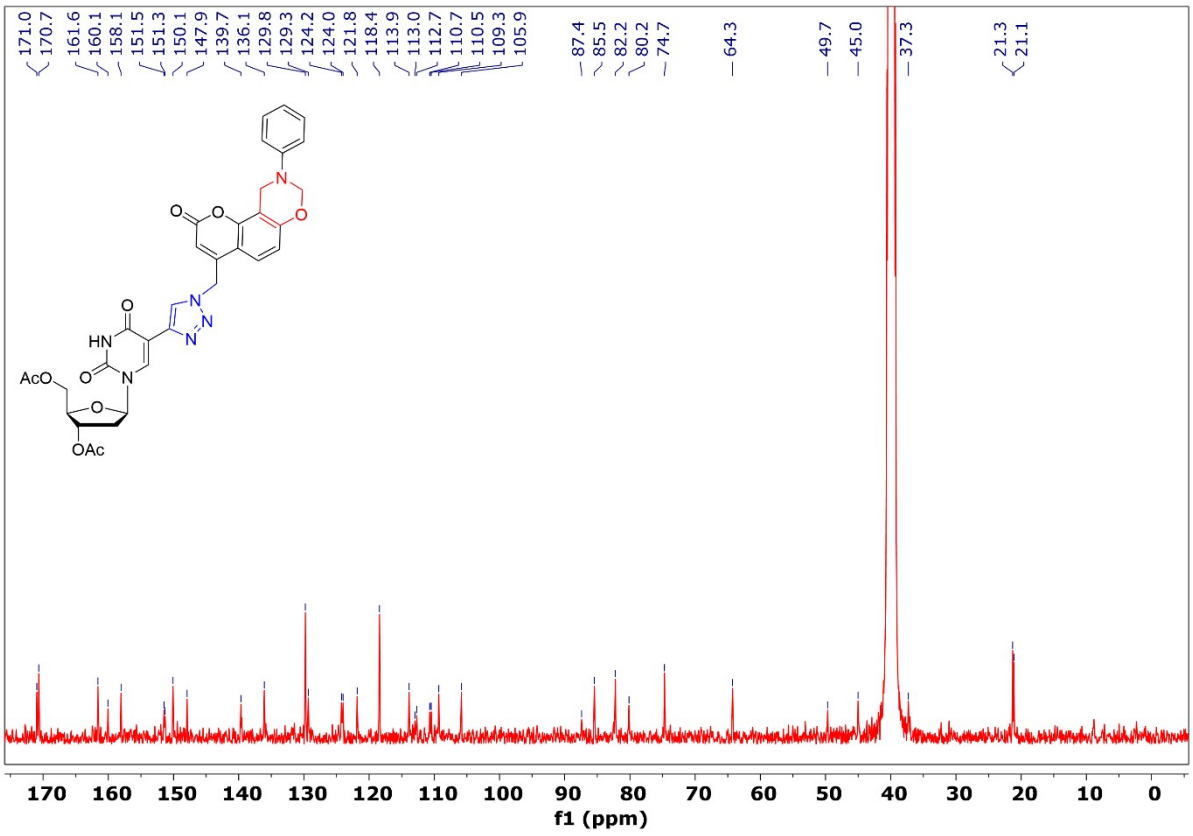


Figure S38: ^{13}C NMR spectrum of compound **13d** (100 MHz, DMSO-d_6).

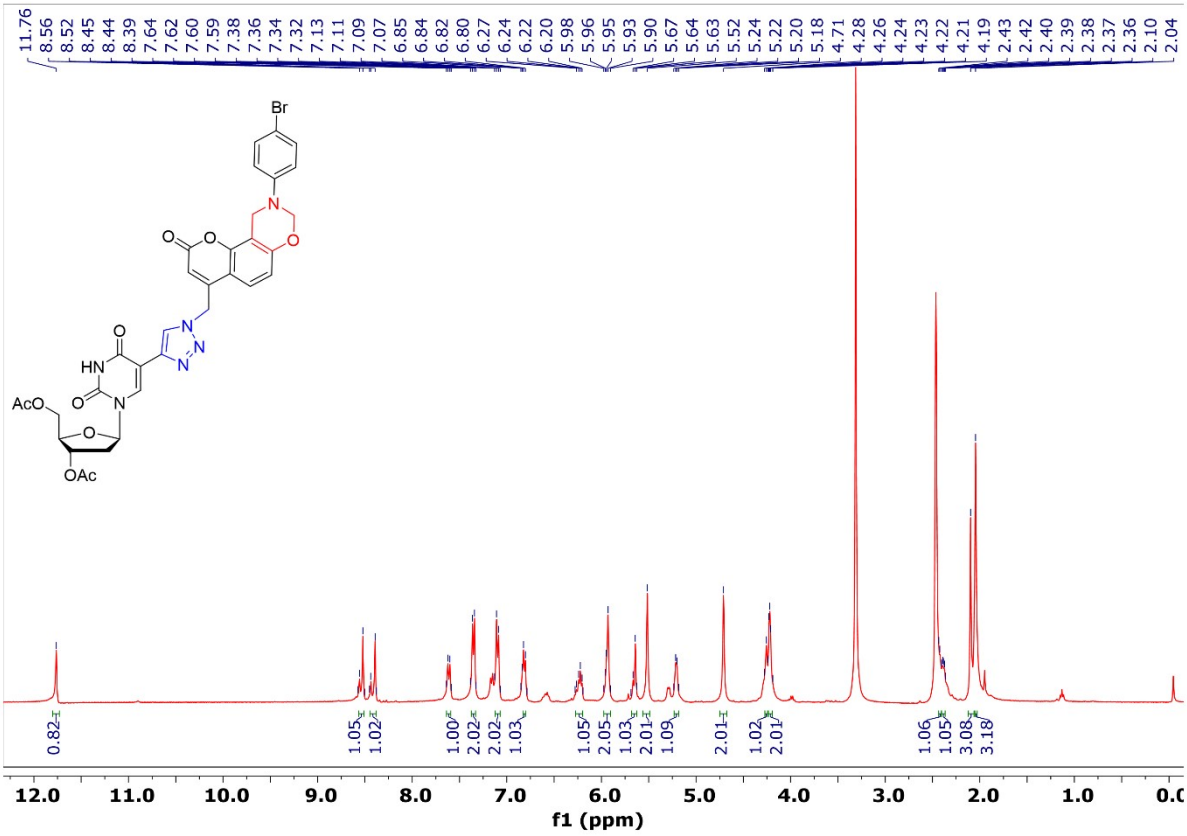


Figure S39: ^{1}H NMR spectrum of compound **13e** (400 MHz, DMSO-d_6).

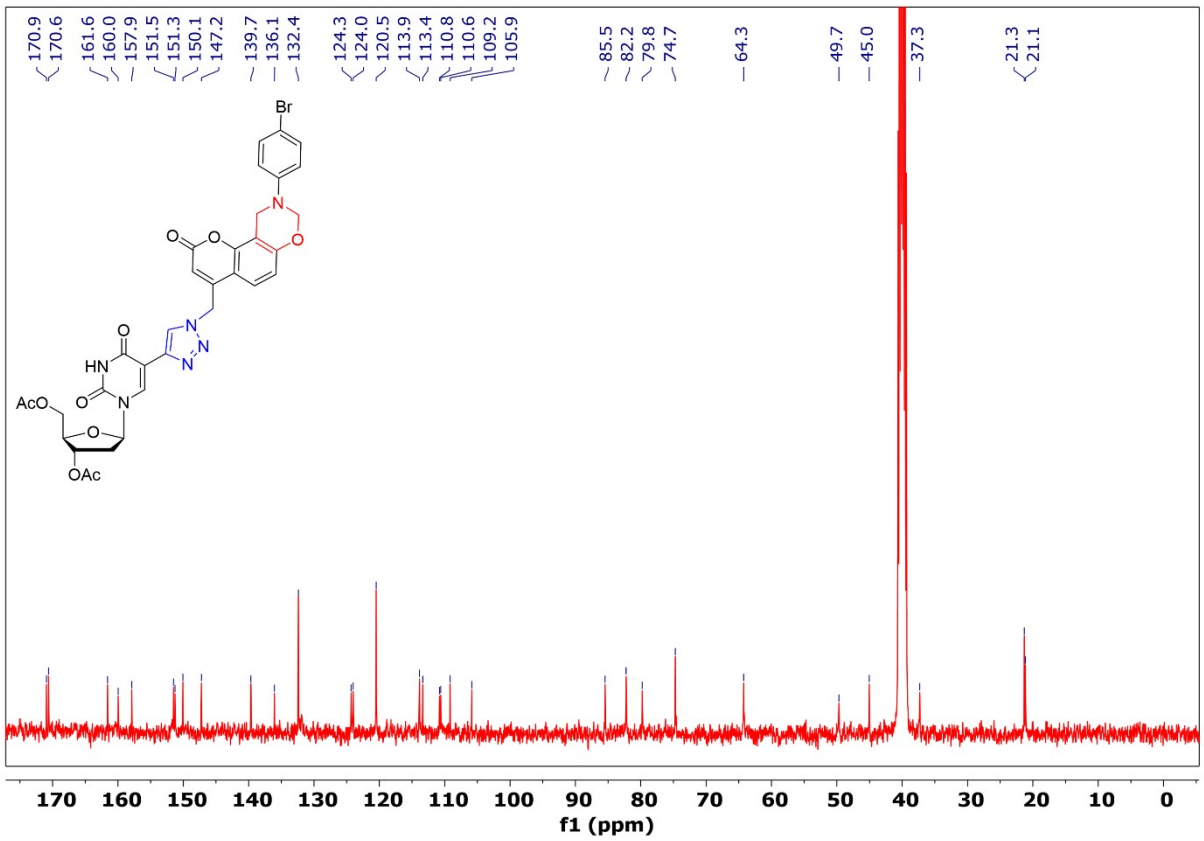


Figure S40: ^{13}C NMR spectrum of compound **13e** (100 MHz, DMSO-d_6).

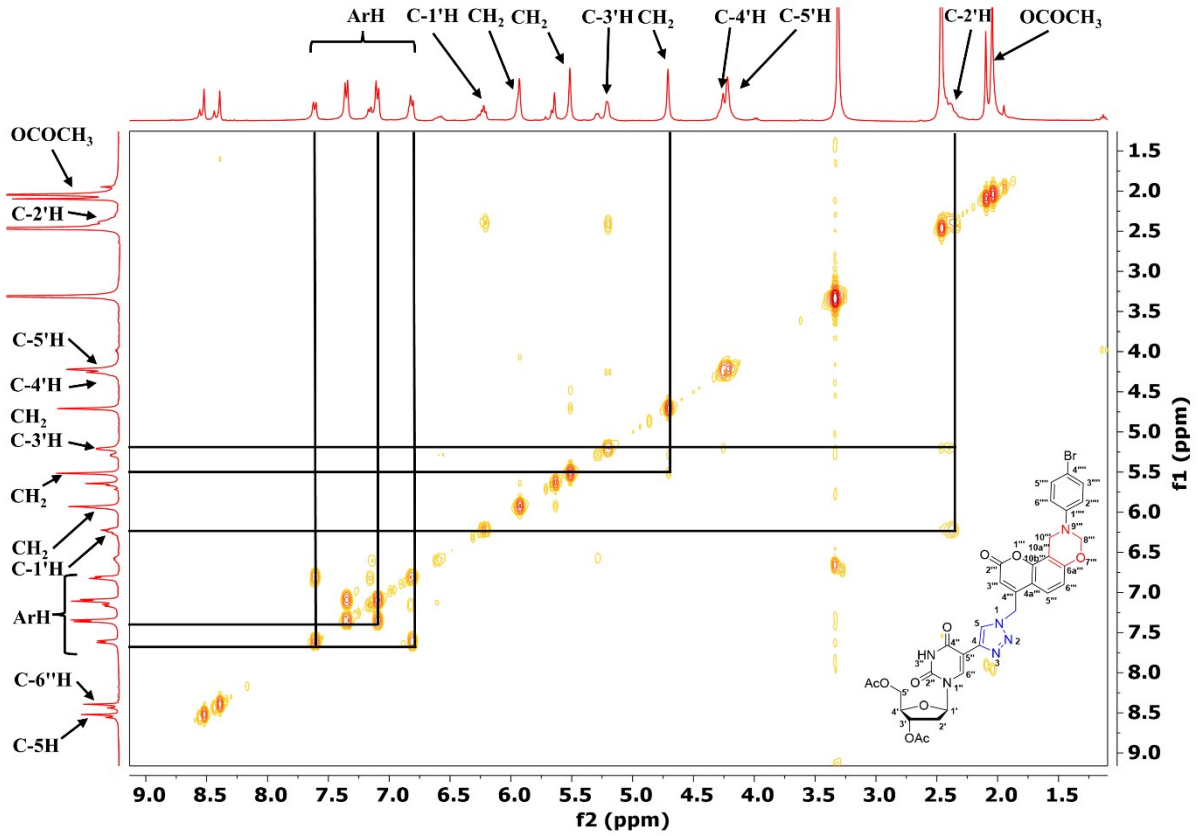


Figure S41: ^{1}H-^{1}H COSY NMR spectrum of compound **13e** (400 MHz, DMSO-d_6).

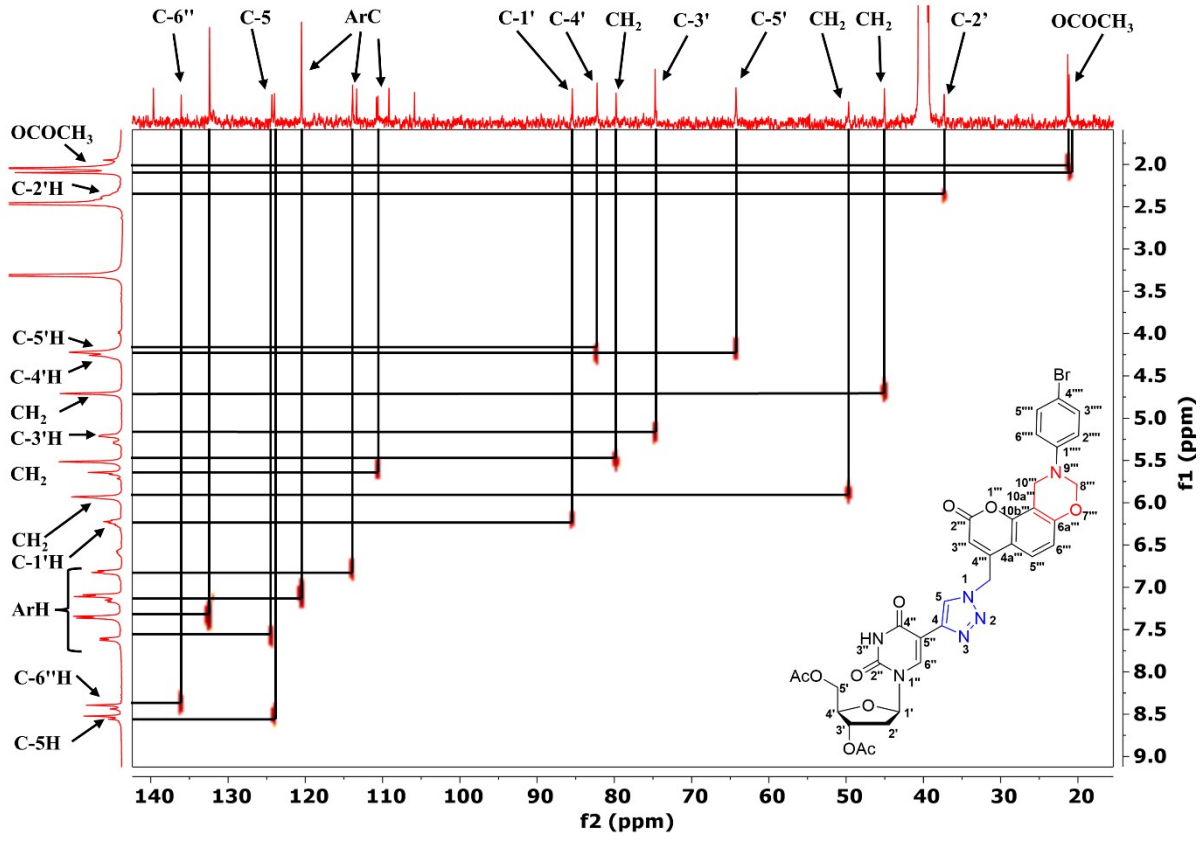


Figure S42: ^{1}H-^{13}C HETCOR NMR spectrum of compound **13e** (100 MHz, DMSO-d_6).

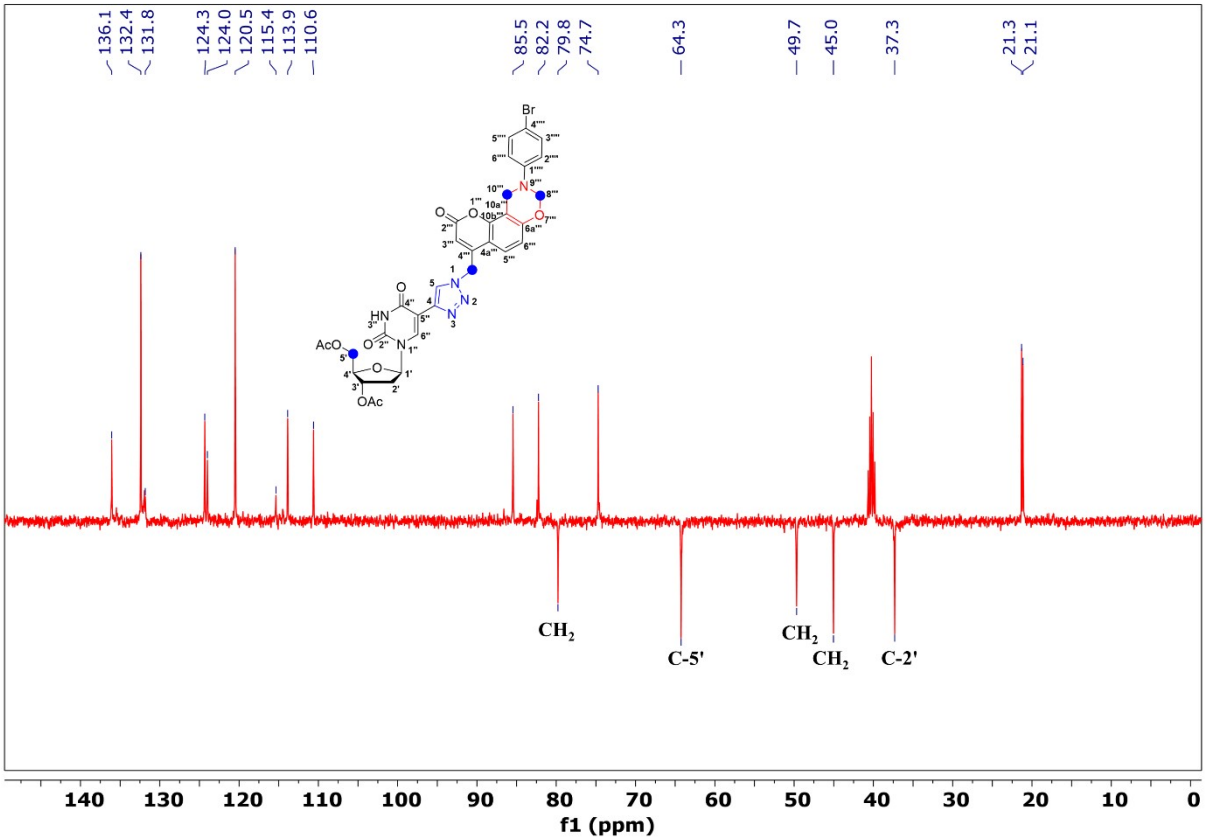


Figure S43: DEPT-135 NMR spectrum of compound **13e** (100 MHz, DMSO-d_6).

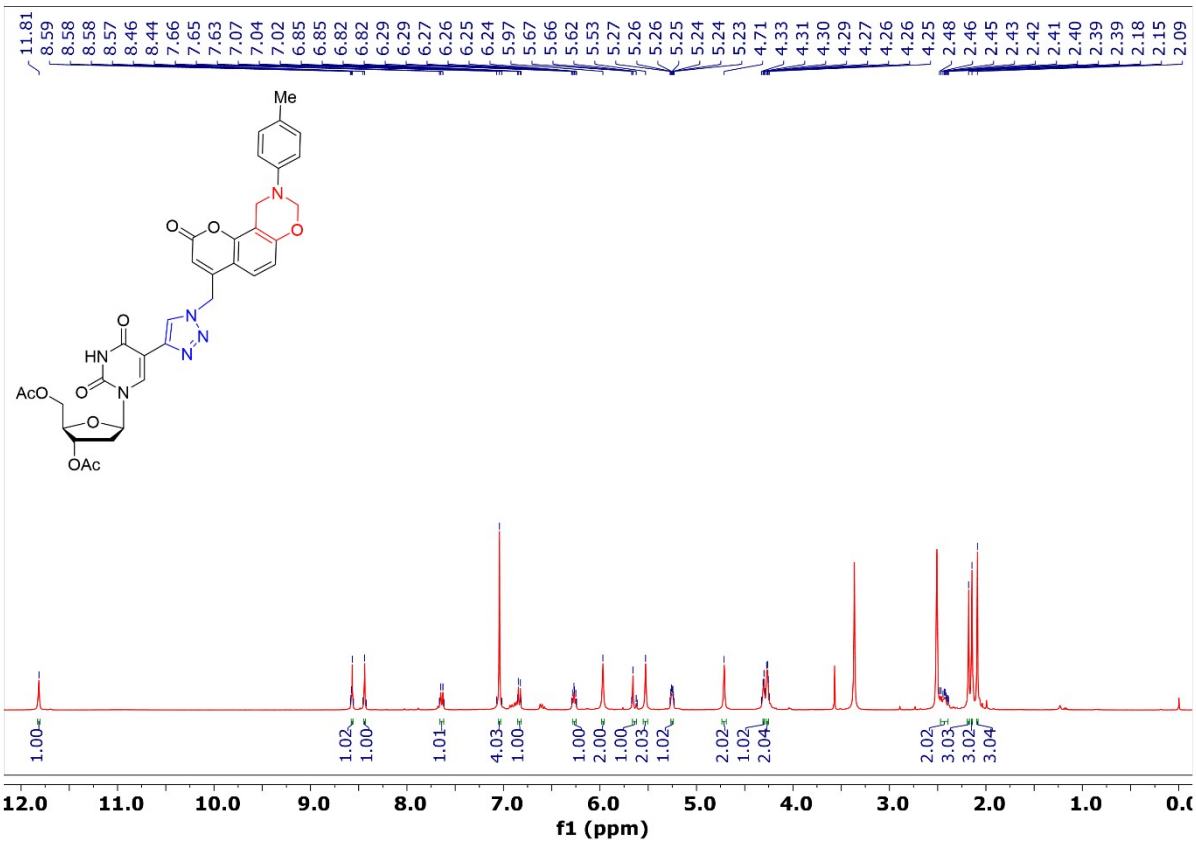


Figure S44: ^{1}H NMR spectrum of compound **13f** (400 MHz, DMSO-d_6).

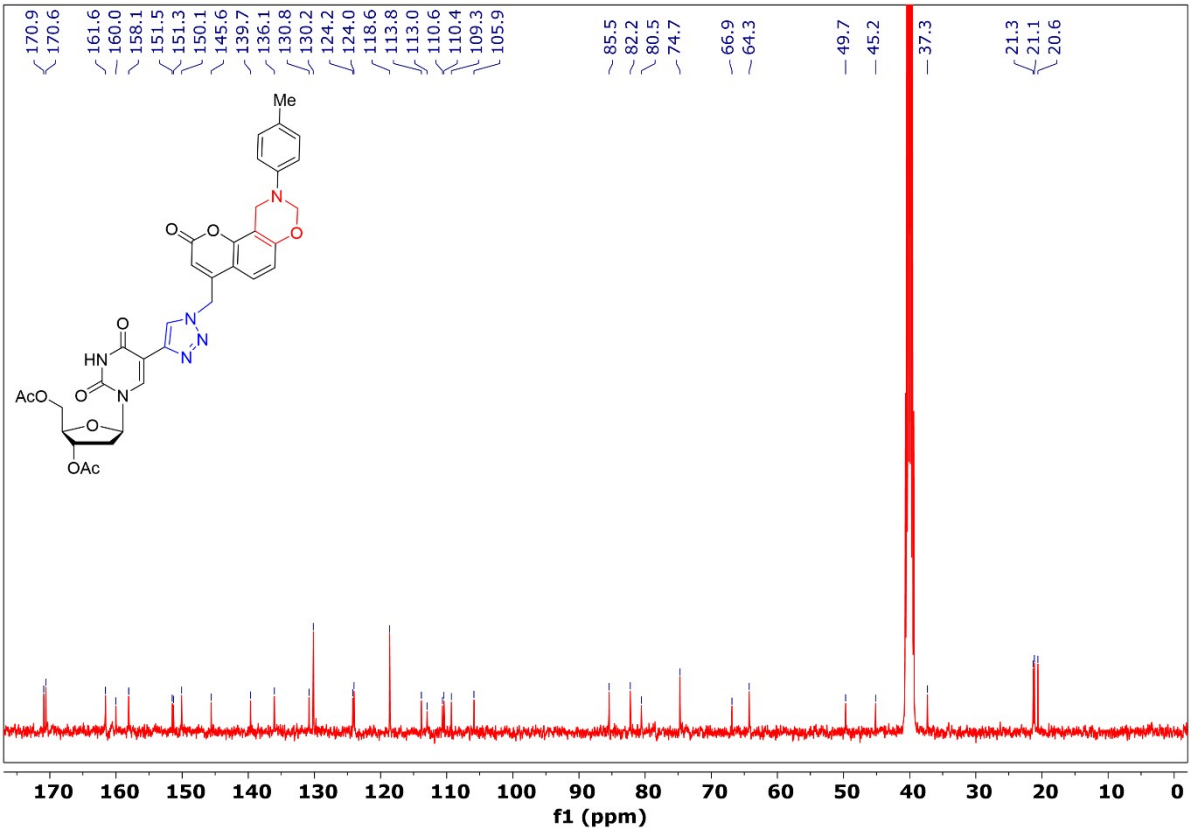


Figure S45: ^{13}C NMR spectrum of compound **13f** (100 MHz, DMSO-d_6).

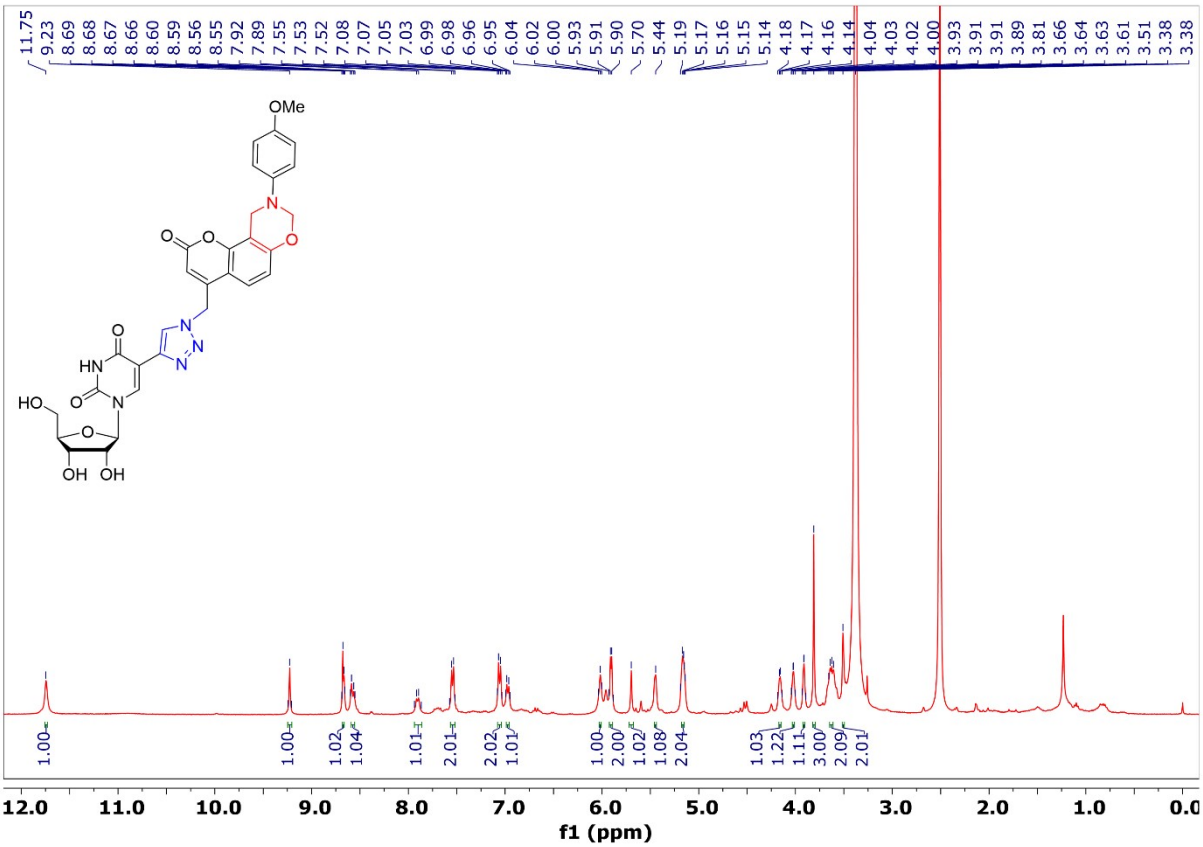


Figure S46: ^{1}H NMR spectrum of compound **14a** (400 MHz, DMSO-d_6).

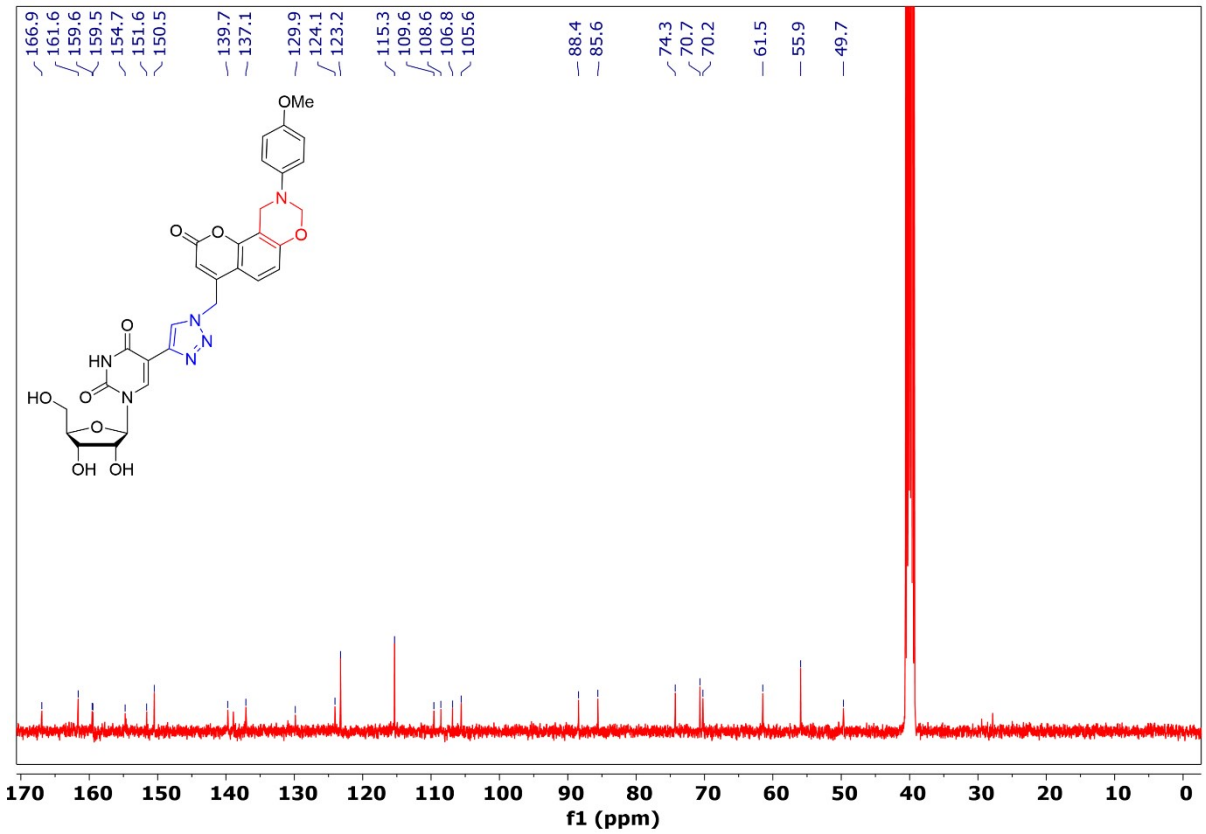


Figure S47: ^{13}C NMR spectrum of compound **14a** (100 MHz, DMSO-d_6).

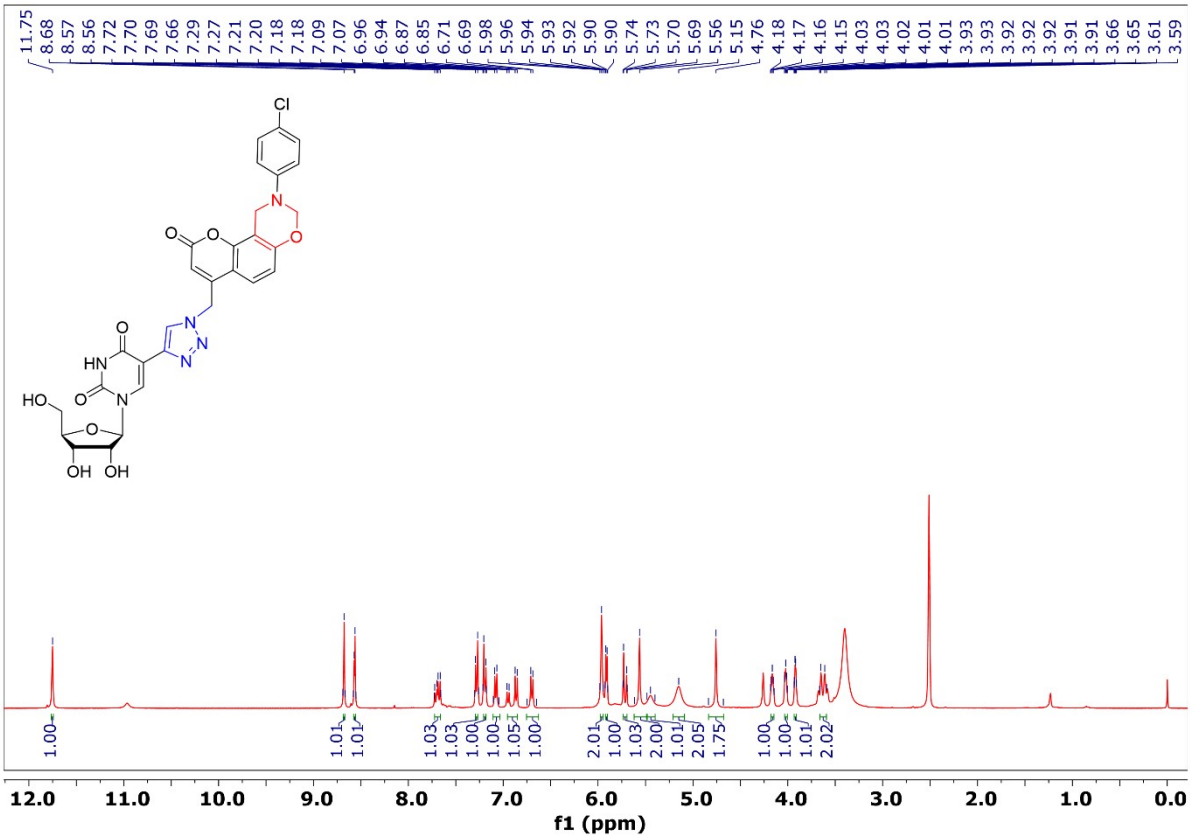


Figure S48: ^{1}H NMR spectrum of compound **14b** (400 MHz, DMSO-d_6).

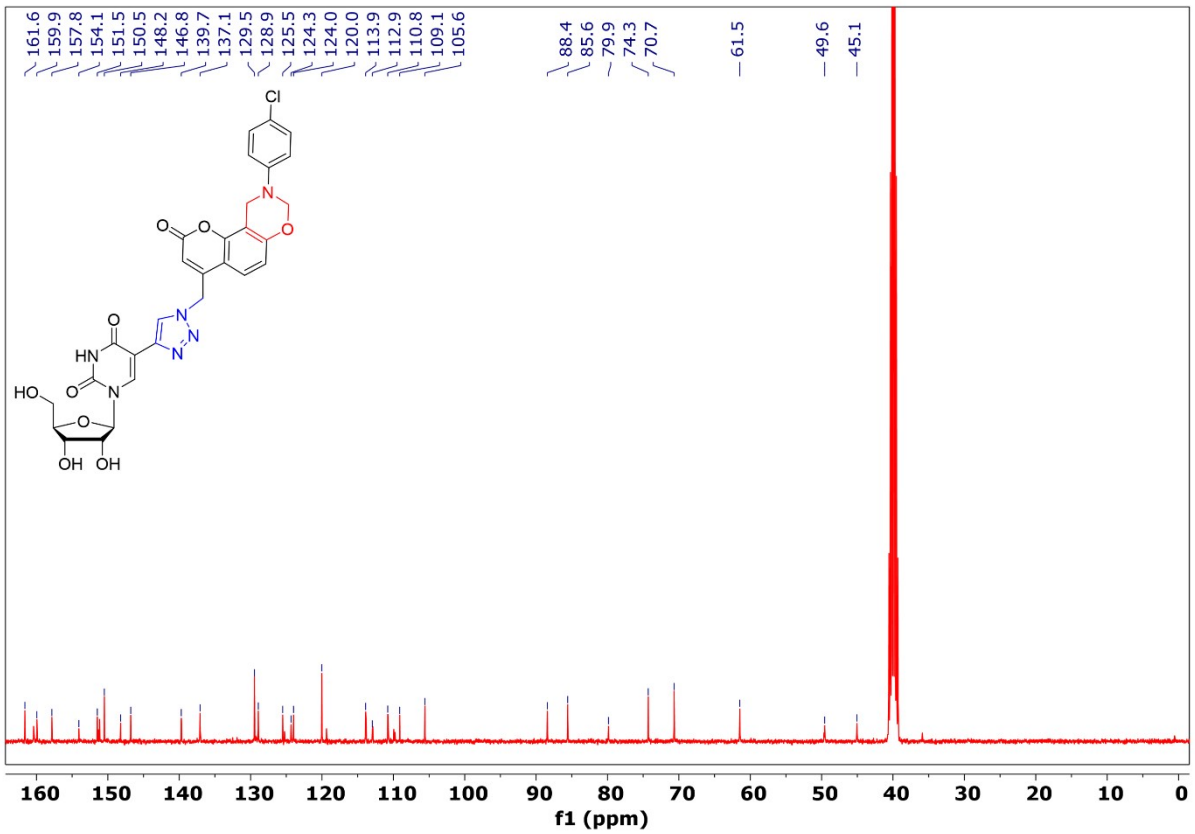


Figure S49: ^{13}C NMR spectrum of compound **14b** (100 MHz, DMSO-d_6).

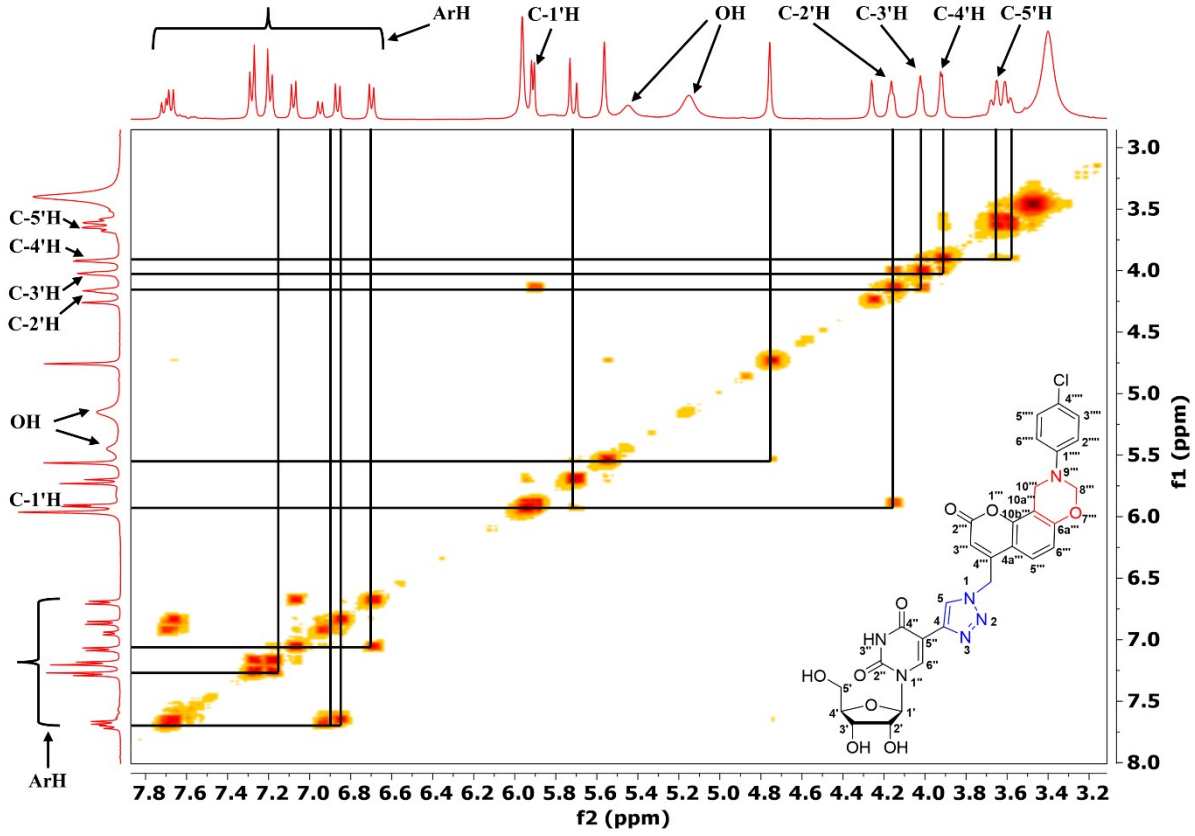


Figure S50: ^{1}H-^{1}H COSY NMR spectrum of compound **14b** (400 MHz, DMSO-d_6).

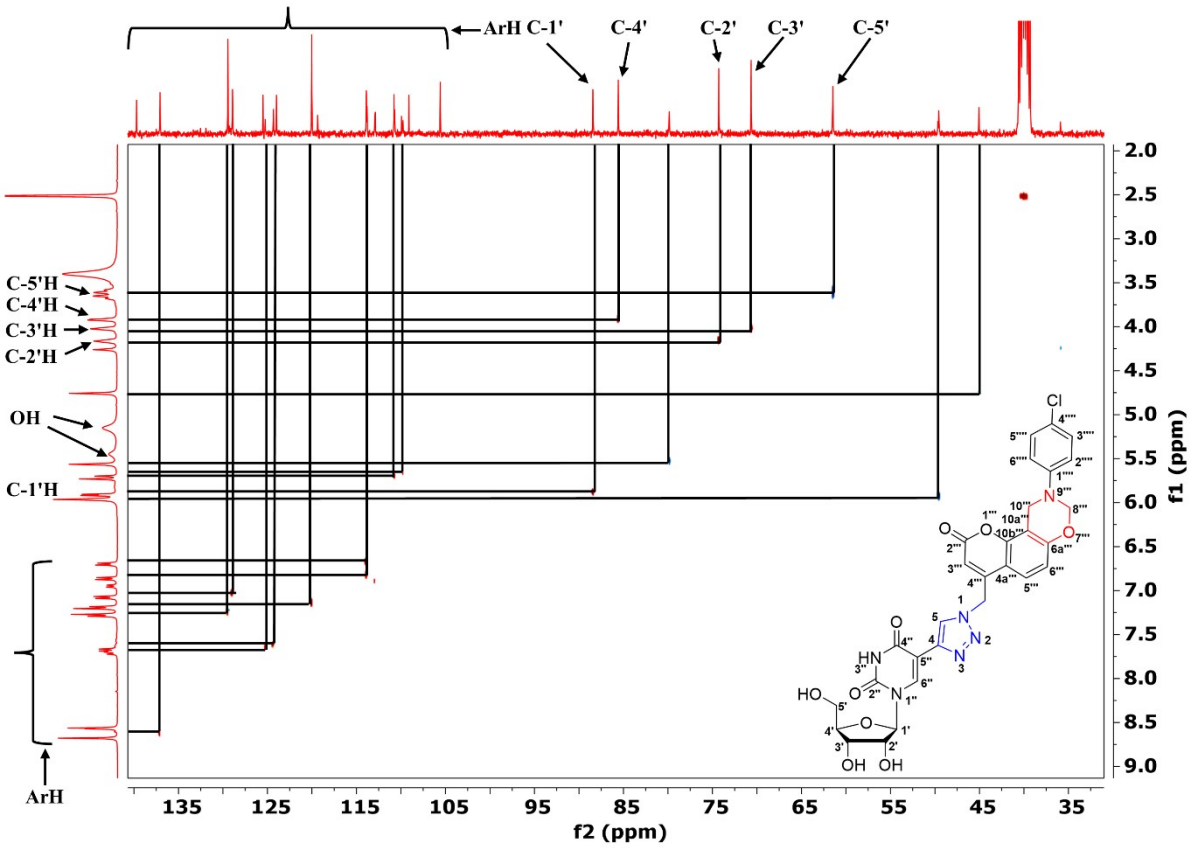


Figure S51: ^{1}H-^{13}C HETCOR NMR spectrum of compound **14b** (100 MHz, DMSO-d_6).

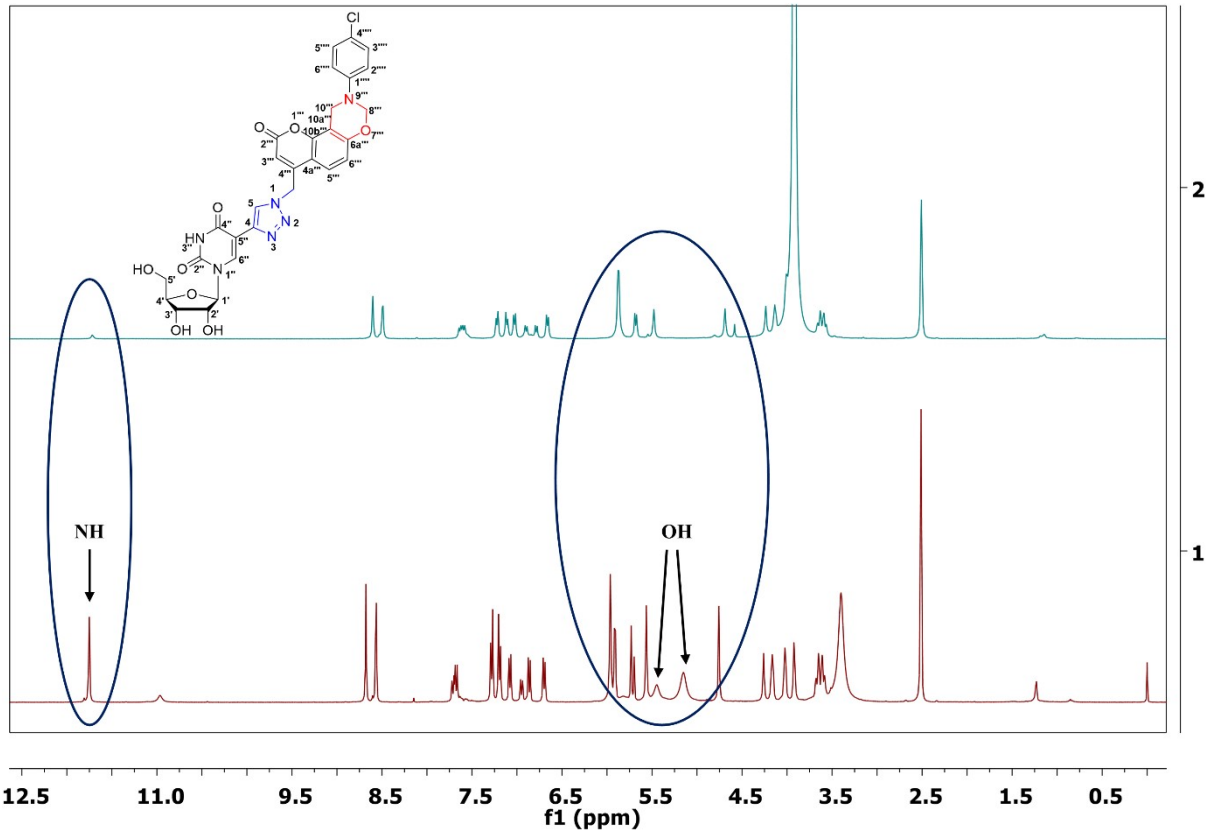


Figure S52: D_2O Exchange NMR spectrum of compound **14b** (DMSO-d_6 + 2 drops of D_2O).

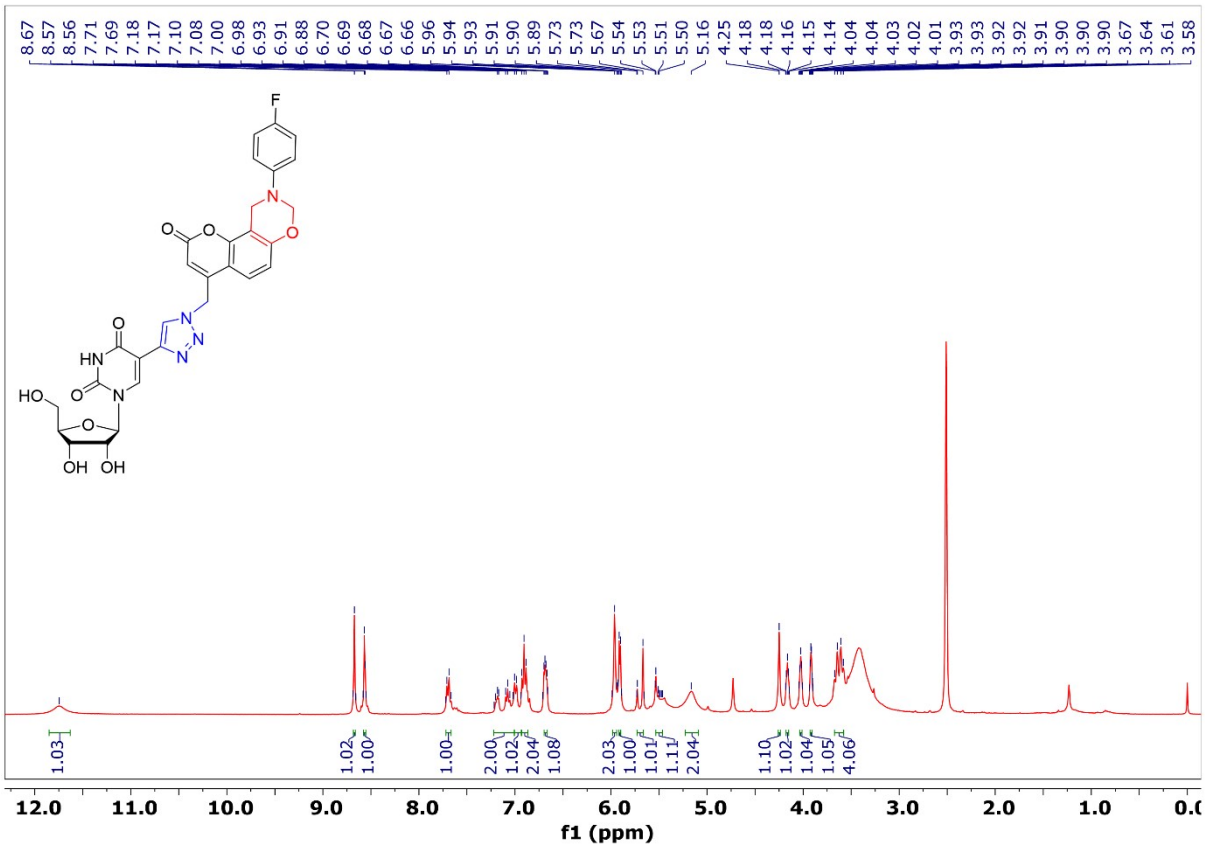


Figure S53: ^{1}H NMR spectrum of compound **14c** (400 MHz, DMSO-d_6).

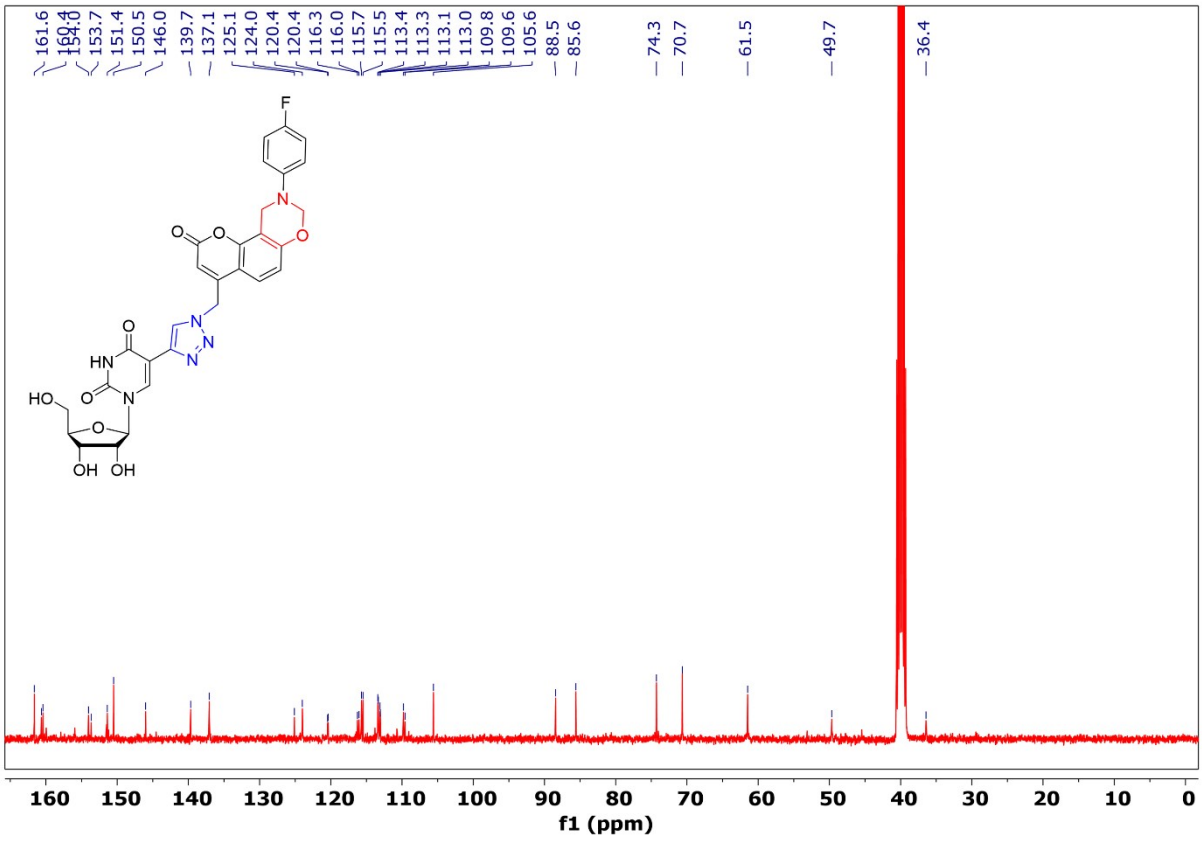


Figure S54: ^{13}C NMR spectrum of compound **14c** (100 MHz, DMSO-d_6).

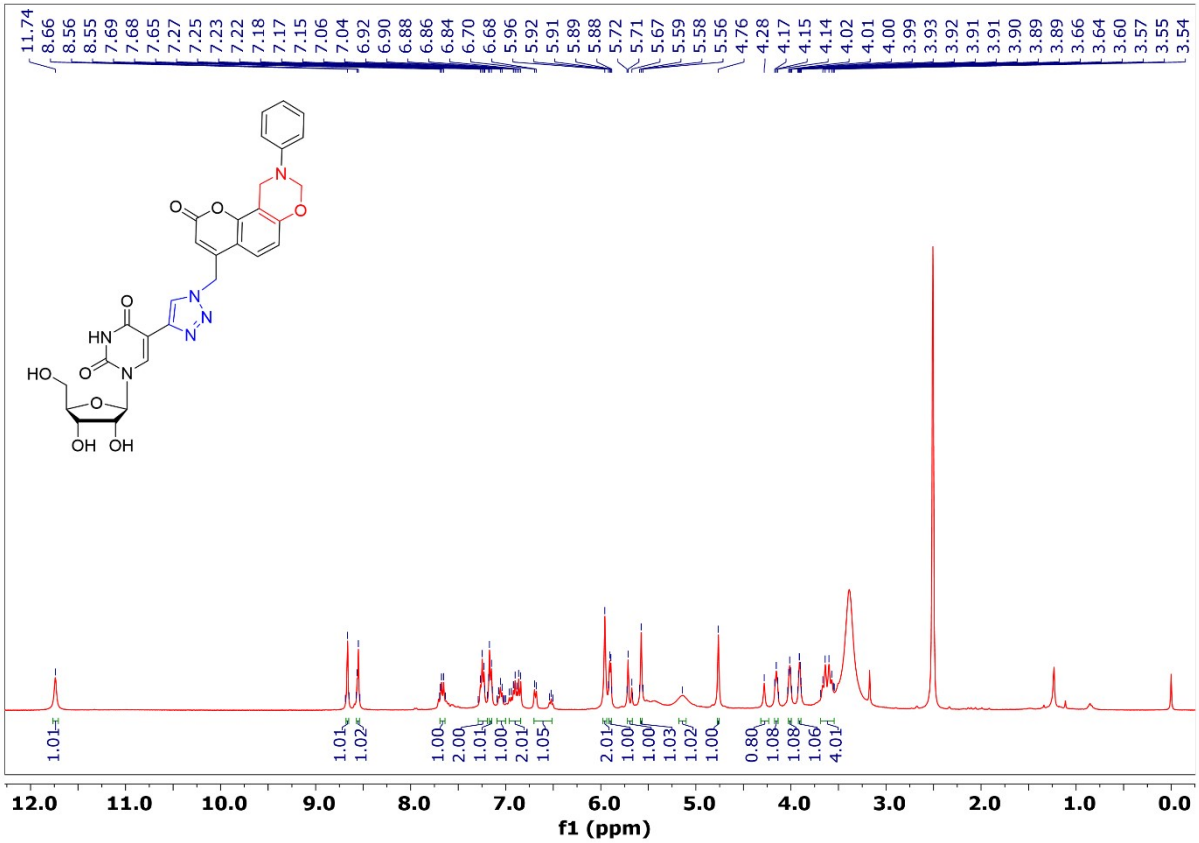


Figure S55: ^{1}H NMR spectrum of compound **14d** (400 MHz, DMSO-d_6).

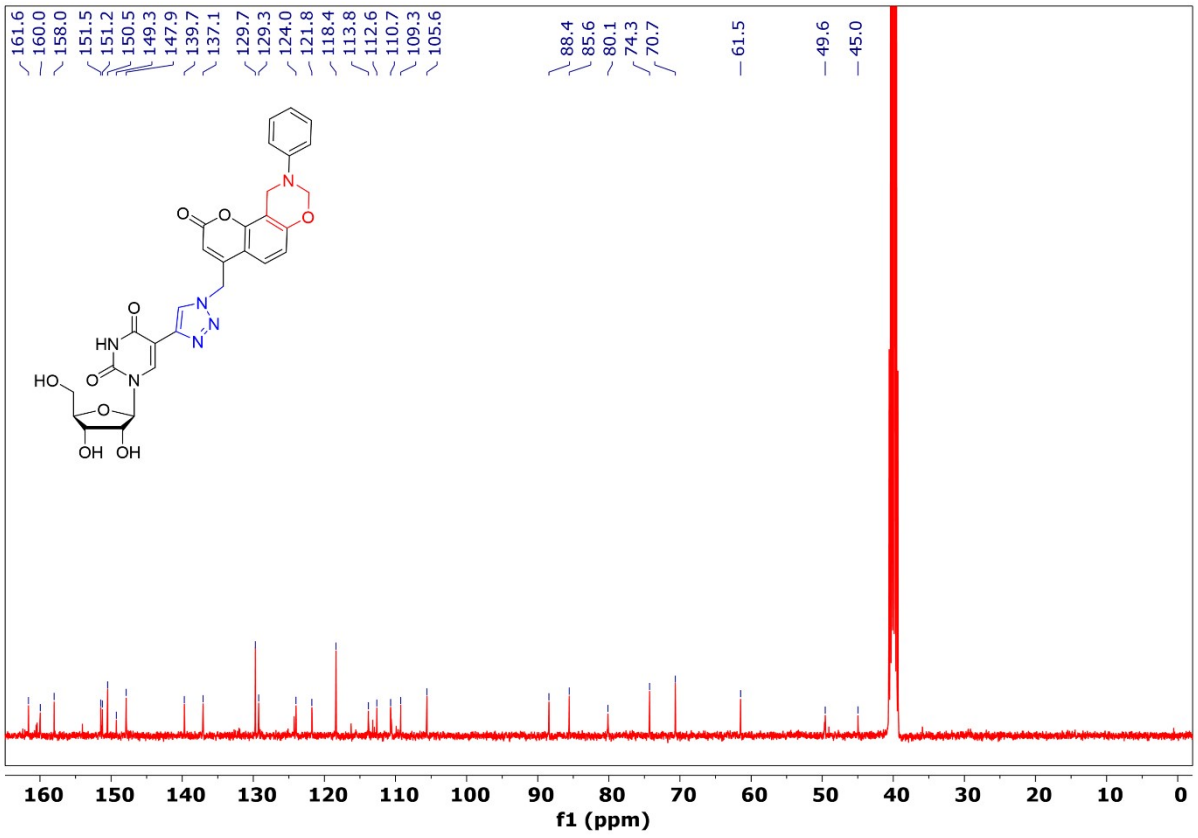


Figure S56: ^{13}C NMR spectrum of compound **14d** (100 MHz, DMSO-d_6).

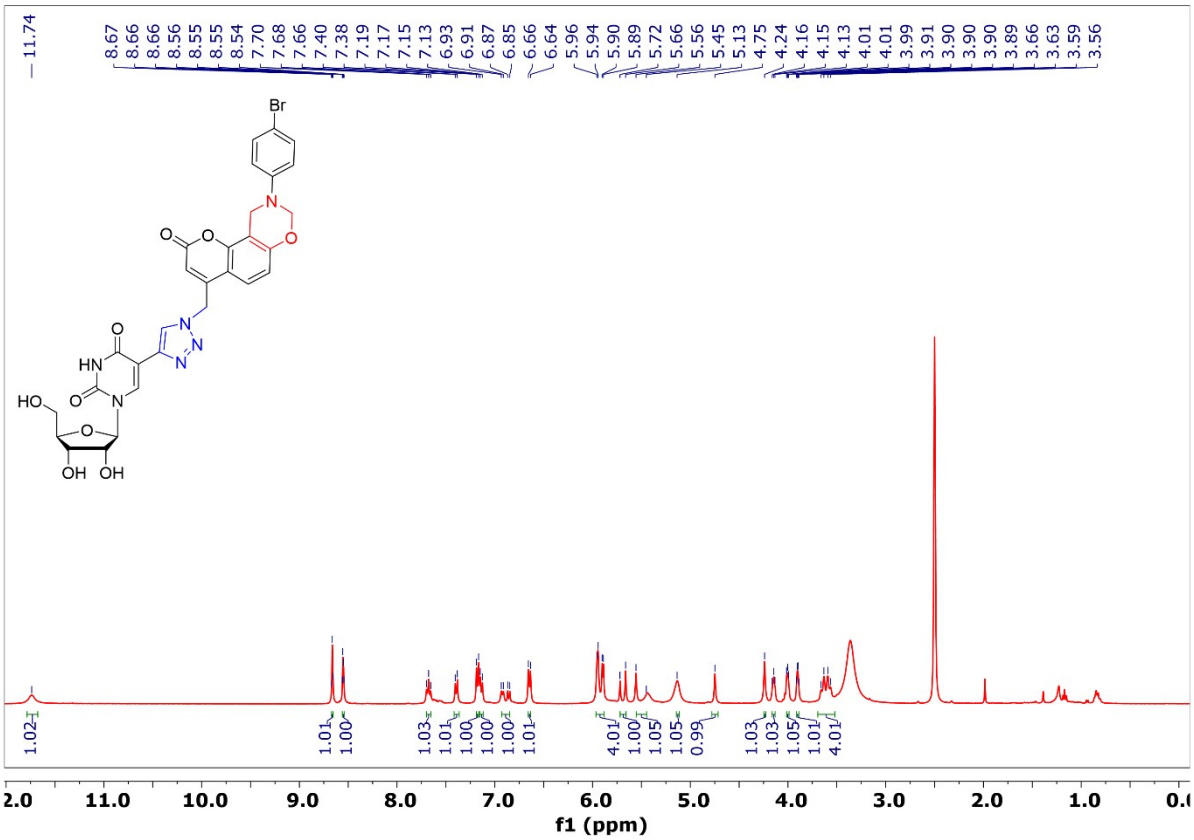


Figure S57: ^{1}H NMR spectrum of compound **14e** (400 MHz, DMSO-d_6).

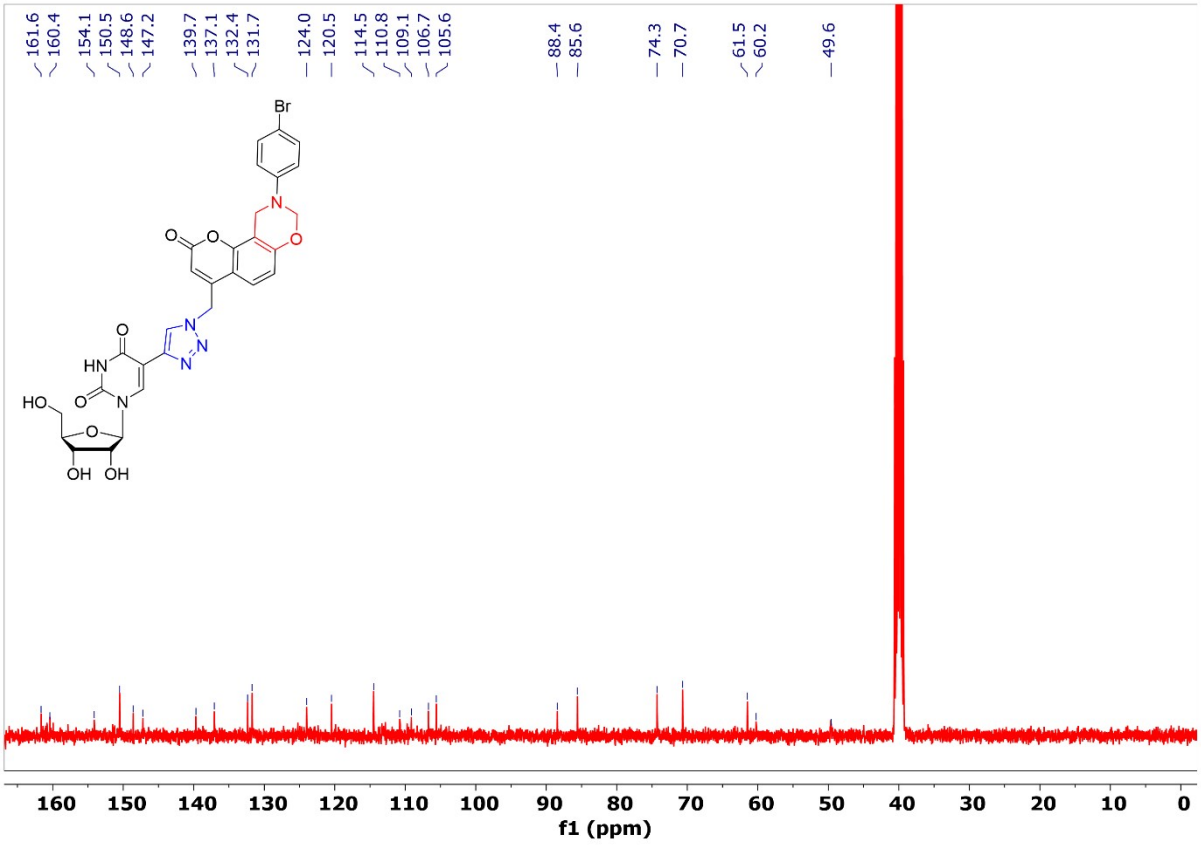


Figure S58: ^{13}C NMR spectrum of compound **14e** (100 MHz, DMSO-d_6).

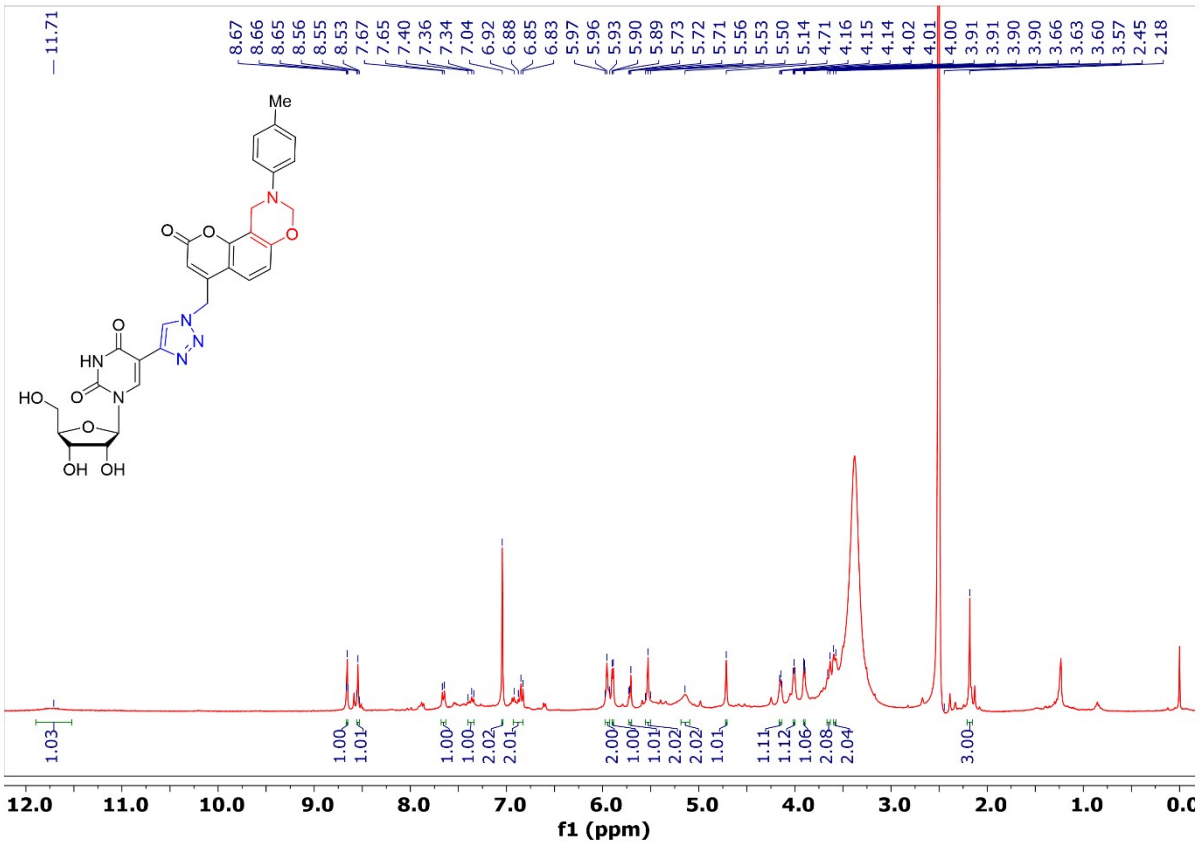


Figure S59: ^{1}H NMR spectrum of compound **14f** (400 MHz, DMSO-d_6).

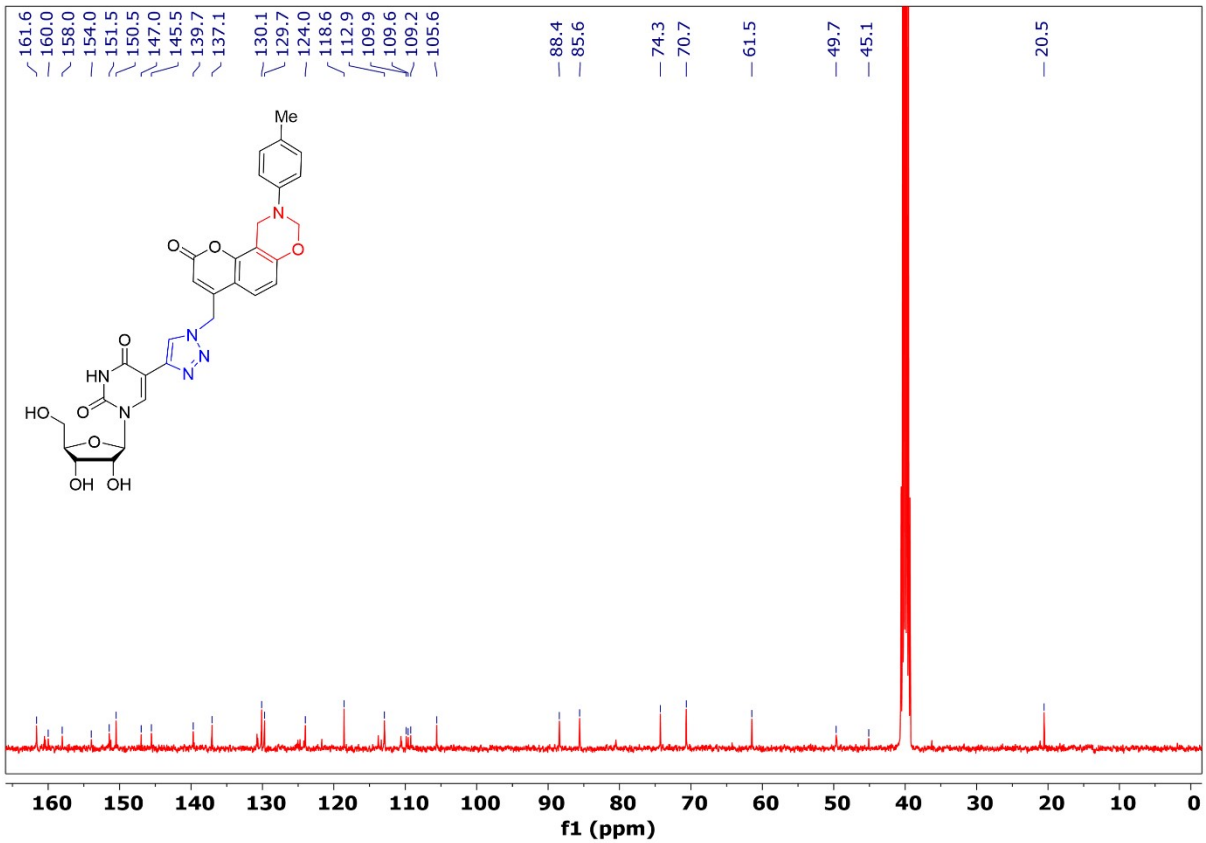


Figure S60: ^{13}C NMR spectrum of compound **14f** (100 MHz, DMSO-d_6).

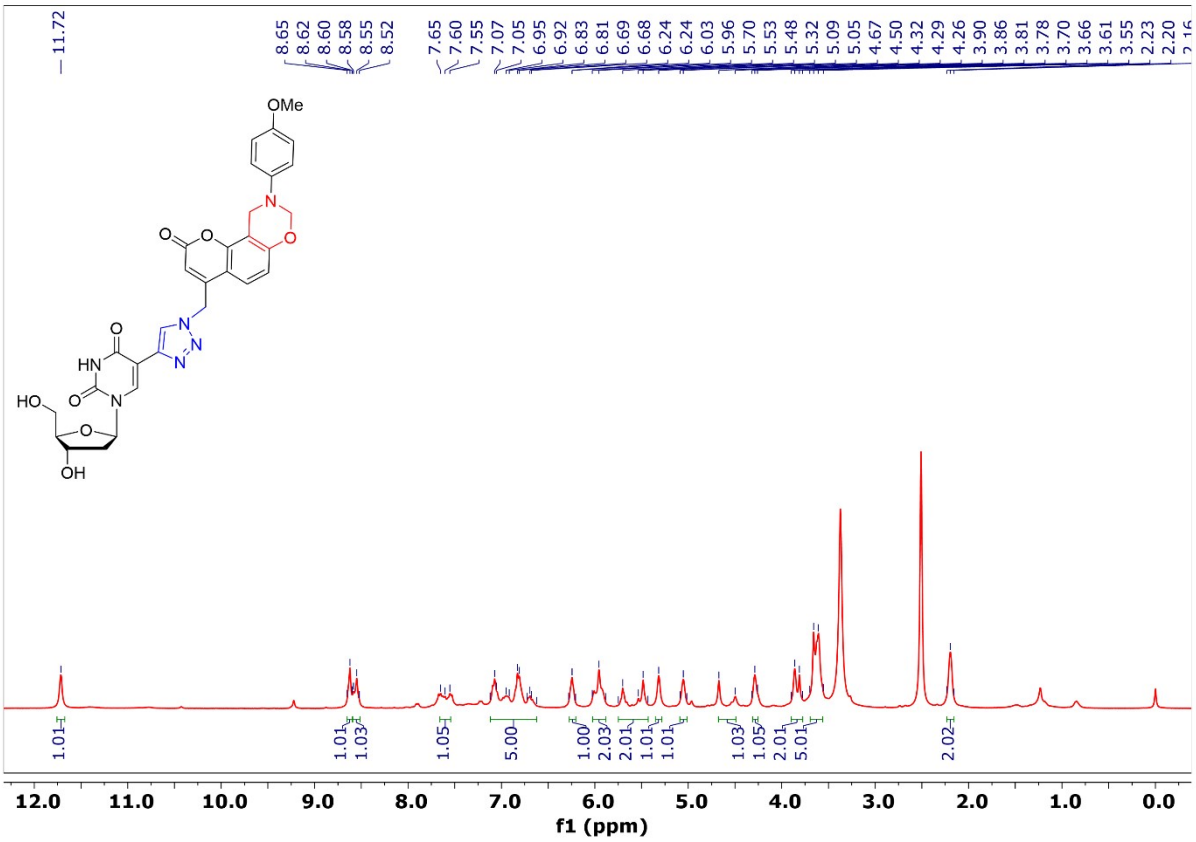


Figure S61: ^{1}H NMR spectrum of compound **15a** (400 MHz, DMSO-d_6).

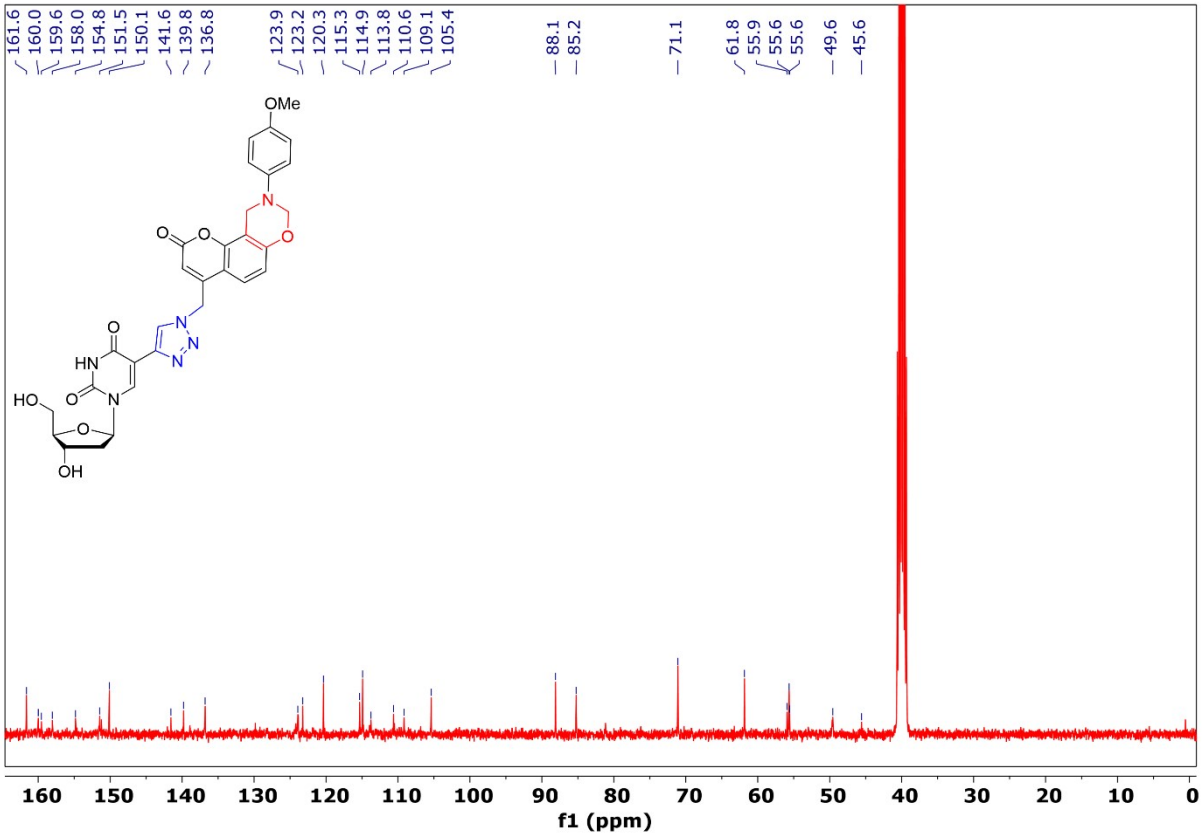


Figure S62: ^{13}C NMR spectrum of compound **15a** (100 MHz, DMSO-d_6).

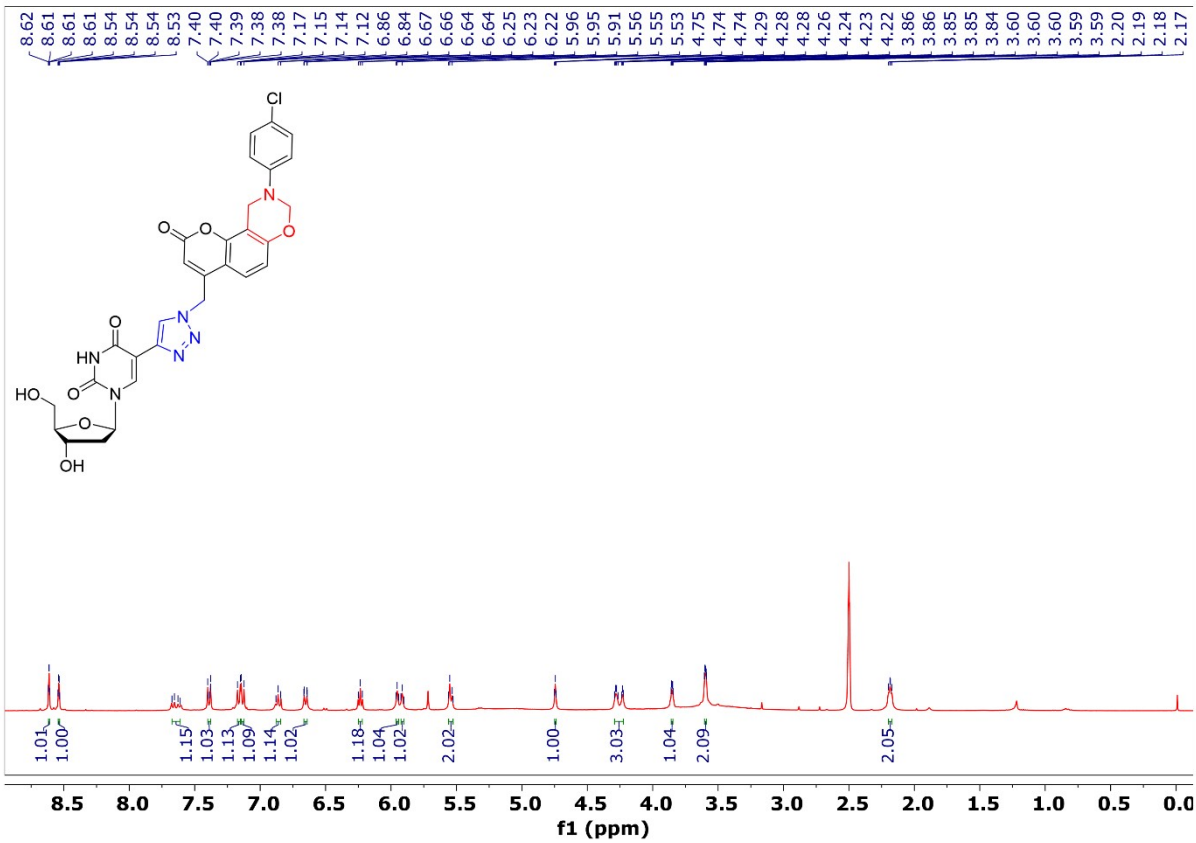


Figure S63: ^{1}H NMR spectrum of compound **15b** (400 MHz, DMSO-d_6).

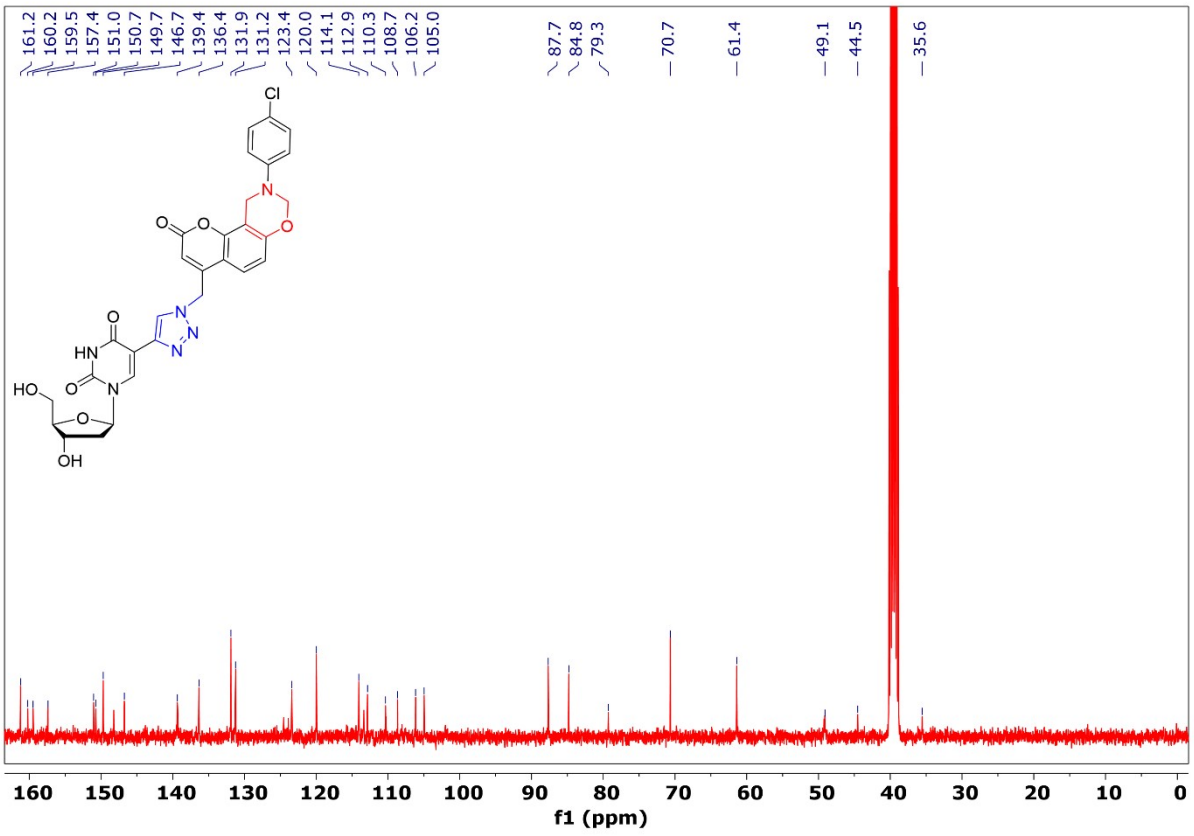


Figure S64: ^{13}C NMR spectrum of compound **15b** (100 MHz, DMSO-d_6).

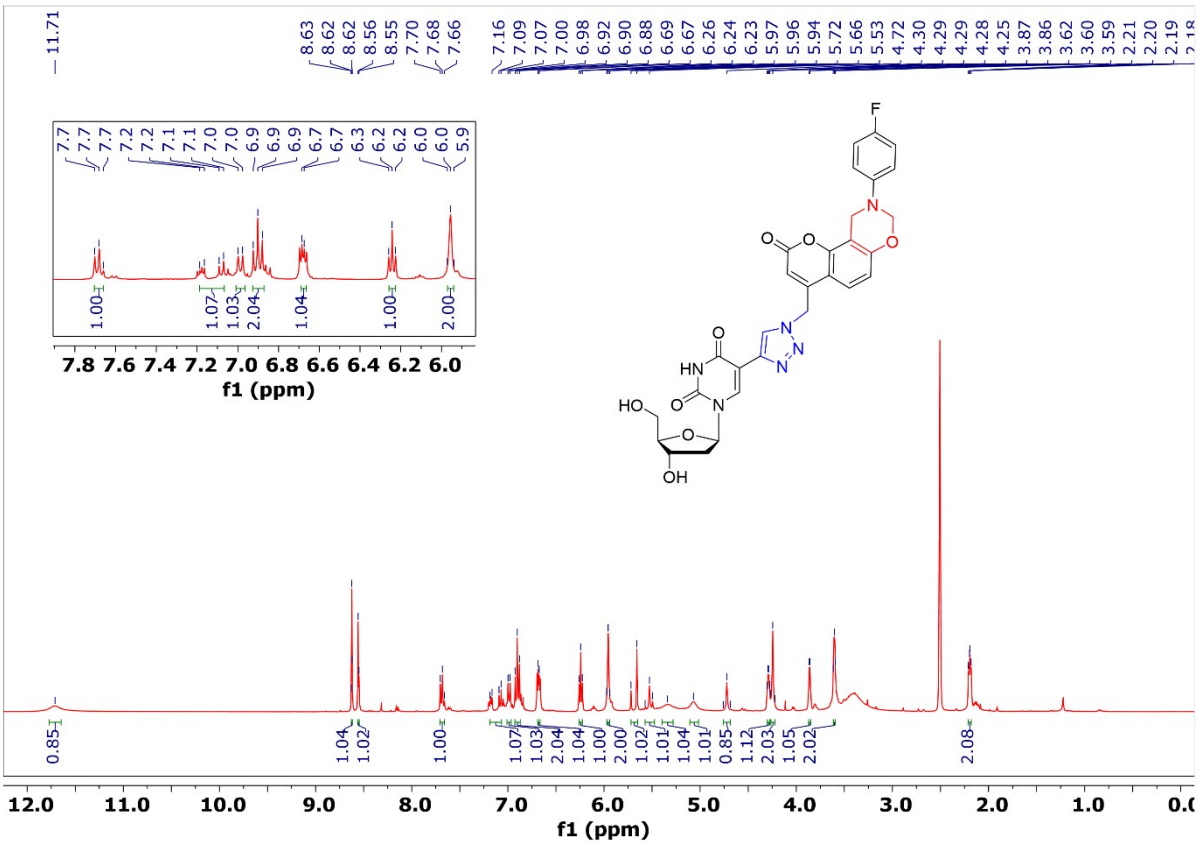


Figure S65: ^{1}H NMR spectrum of compound **15c** (400 MHz, DMSO-d_6).

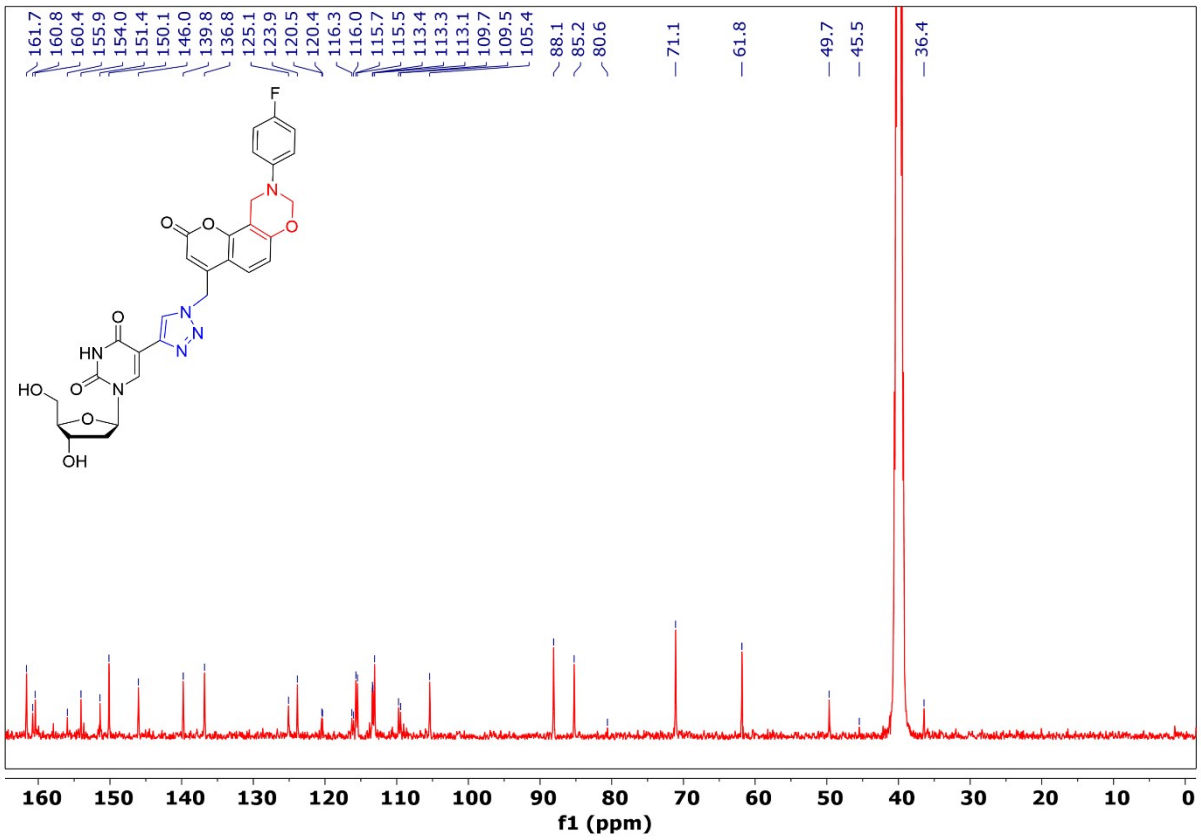


Figure S66: ^{13}C NMR spectrum of compound **15c** (100 MHz, DMSO-d_6).

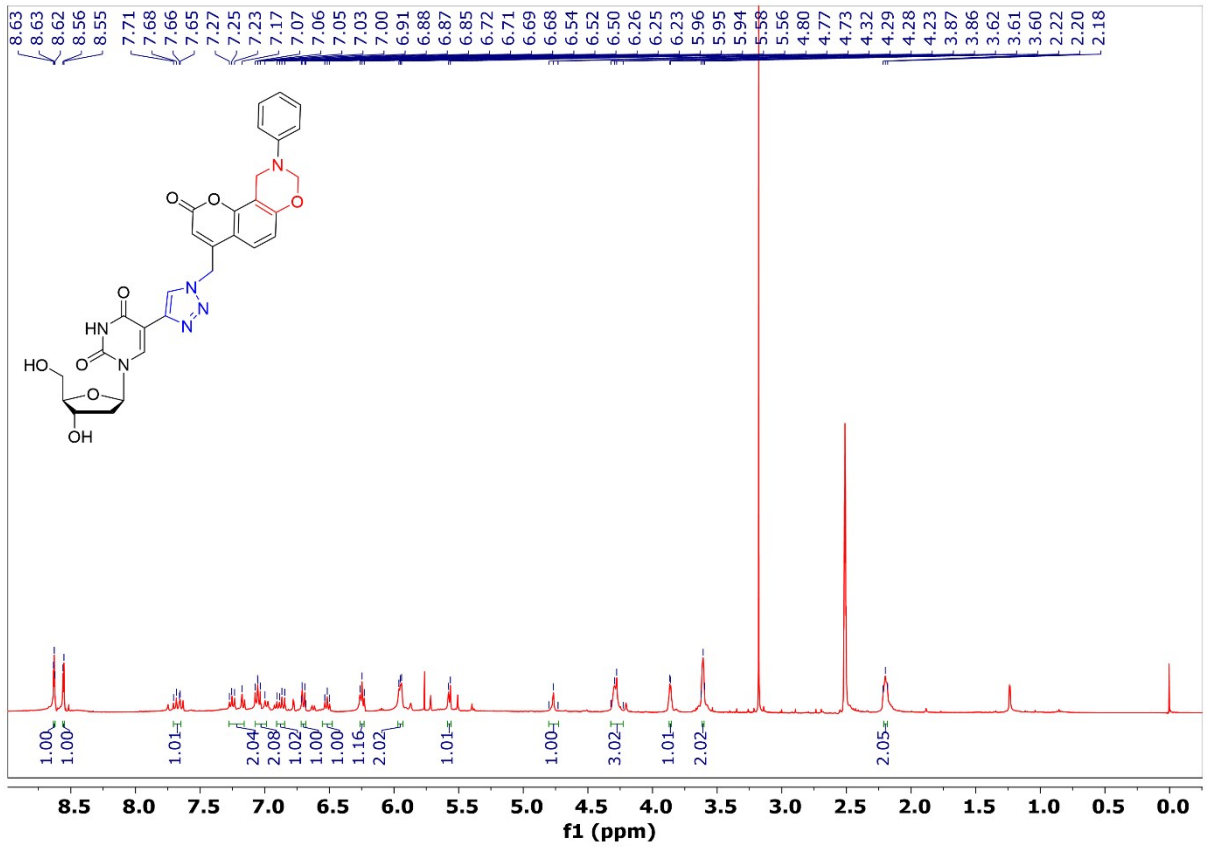


Figure S67: ^{1}H NMR spectrum of compound **15d** (400 MHz, DMSO-d_6).

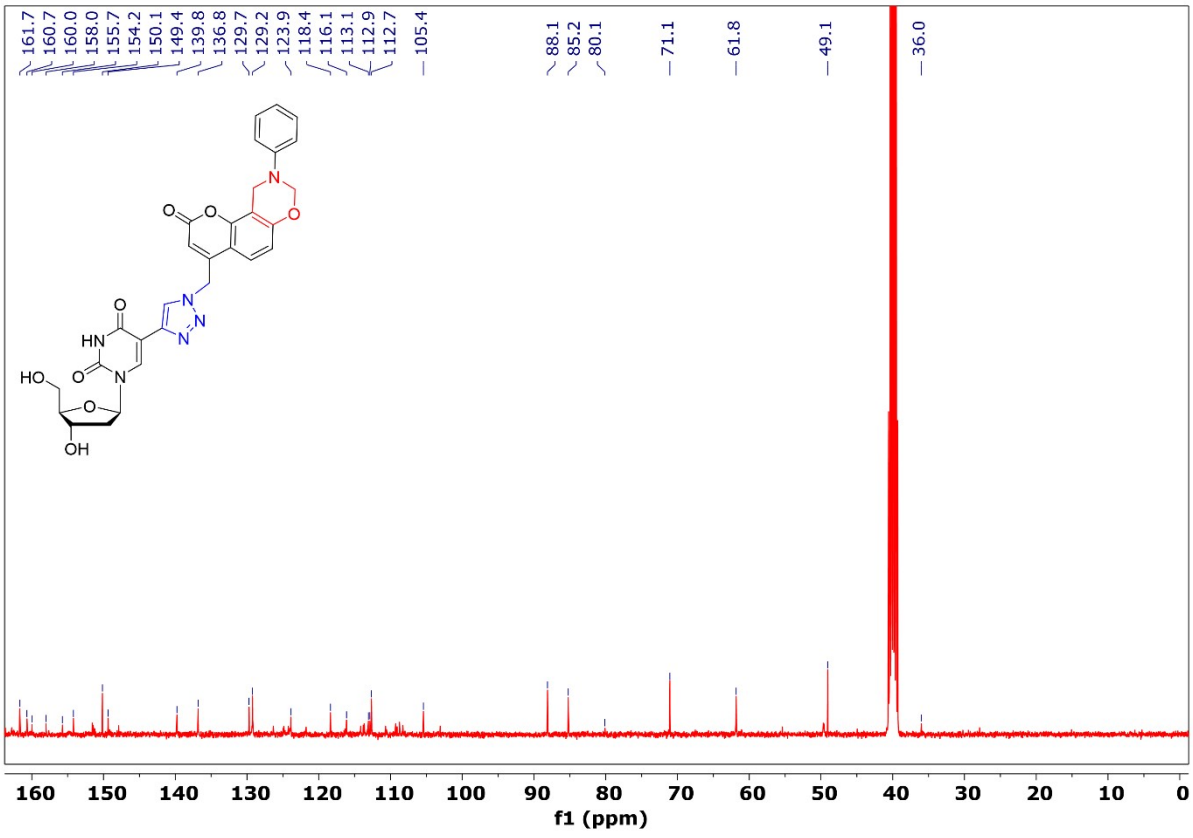


Figure S68: ^{13}C NMR spectrum of compound **15d** (100 MHz, DMSO-d_6).

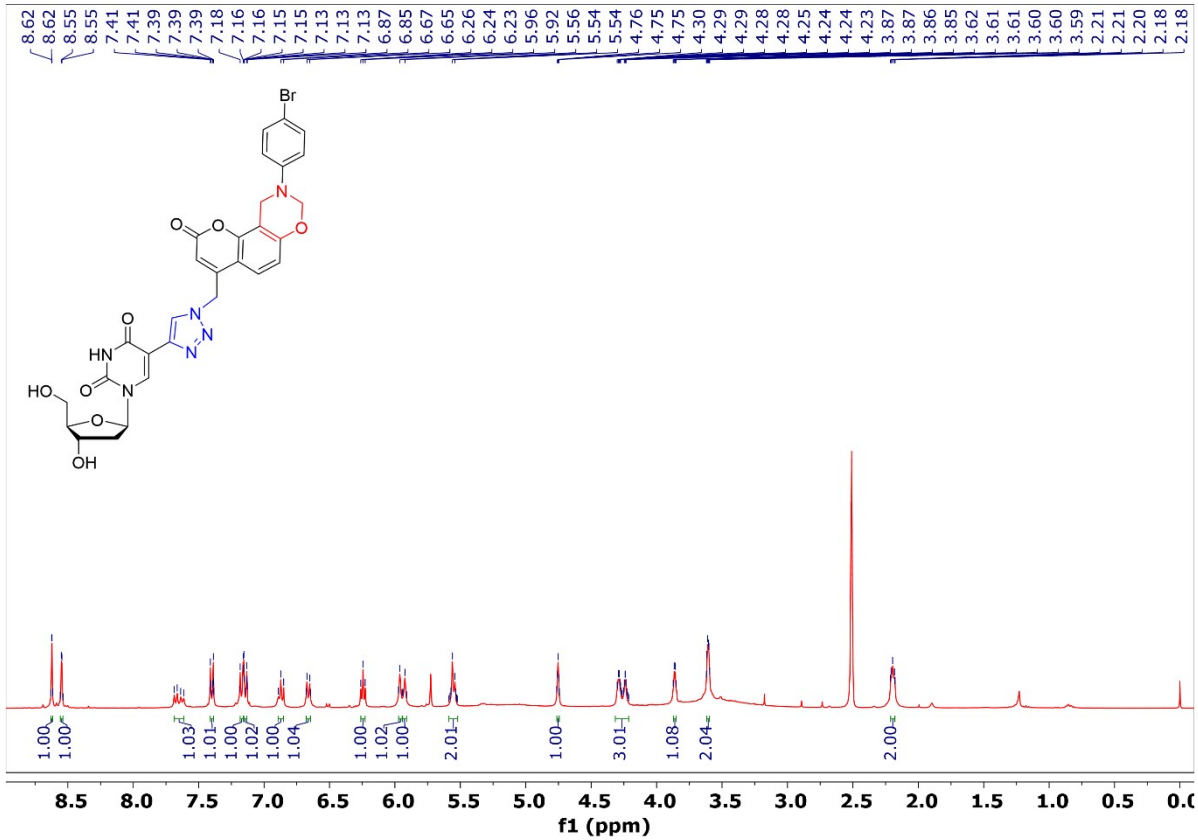


Figure S69: ^{1}H NMR spectrum of compound **15e** (400 MHz, DMSO-d_6).

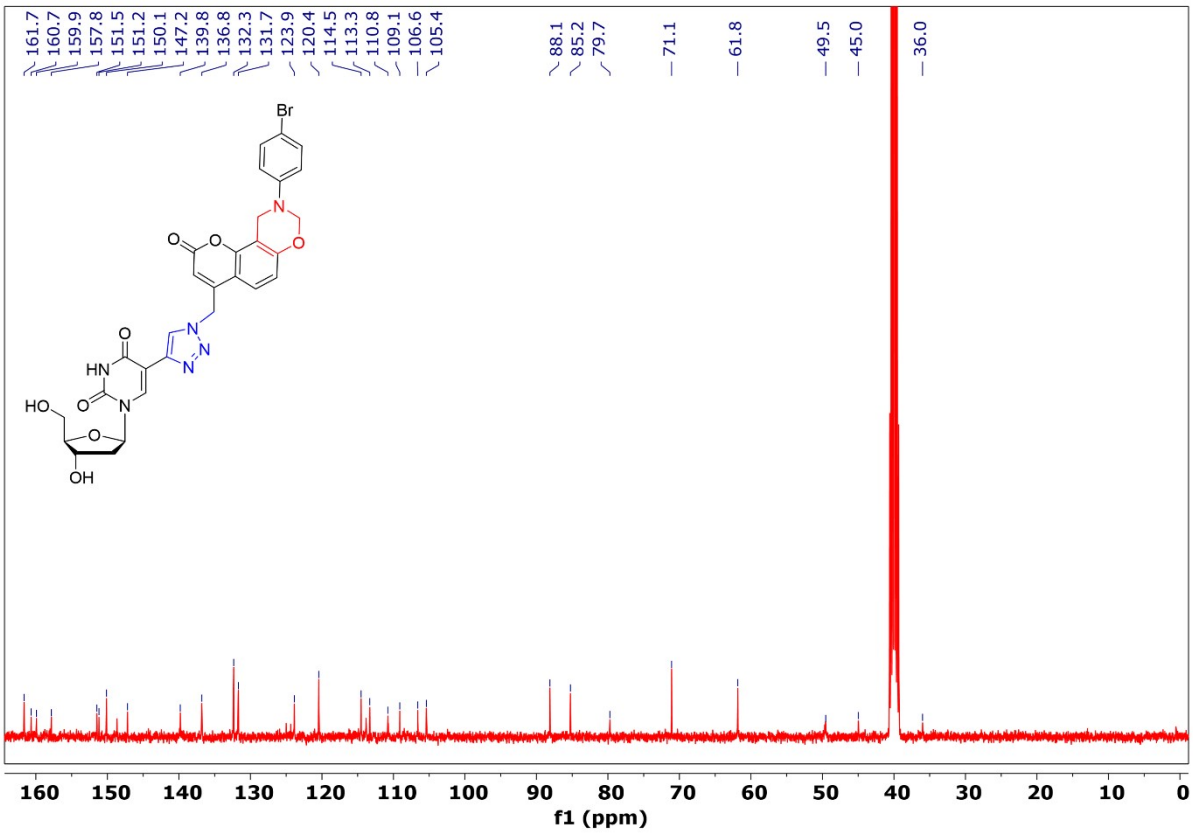


Figure S70: ^{13}C NMR spectrum of compound **15e** (100 MHz, DMSO-d_6).

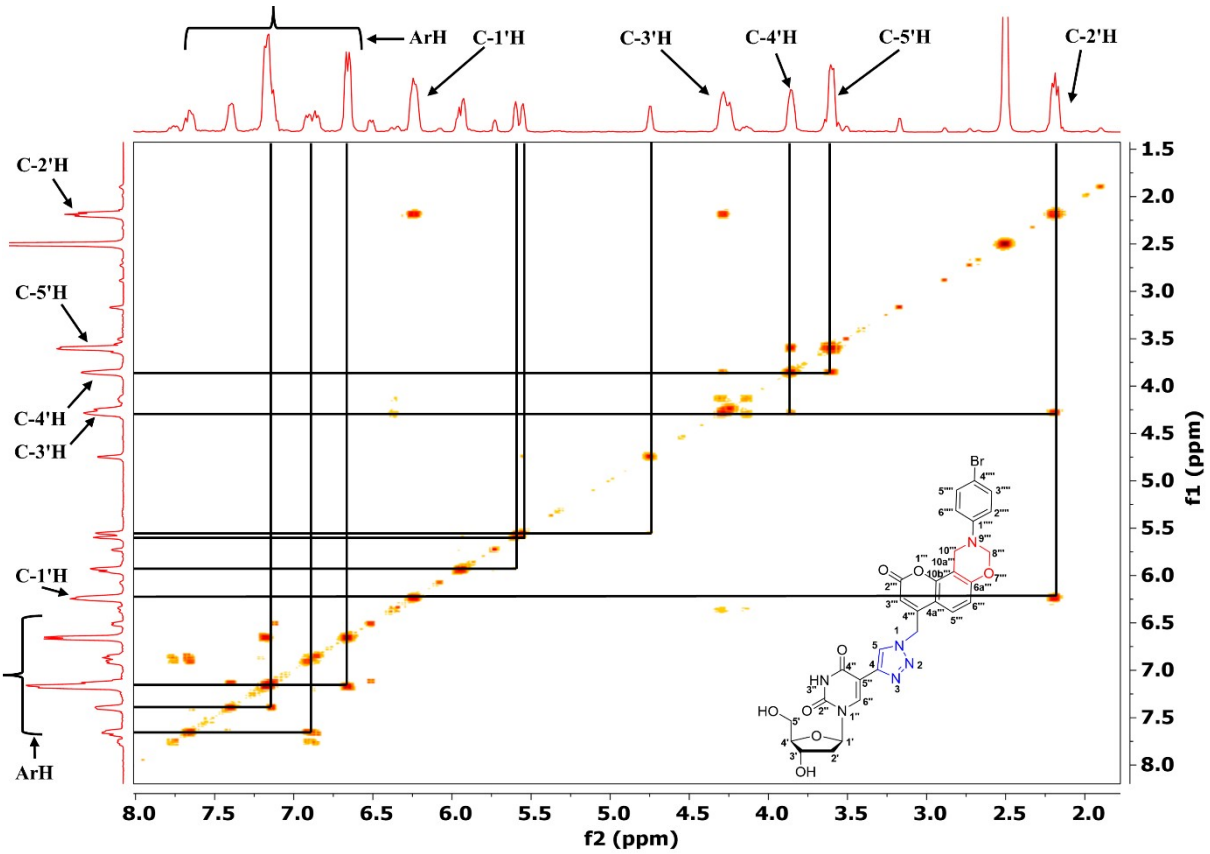


Figure S71: ^{1}H-^{1}H COSY NMR spectrum of compound **15e** (400 MHz, DMSO-d_6).

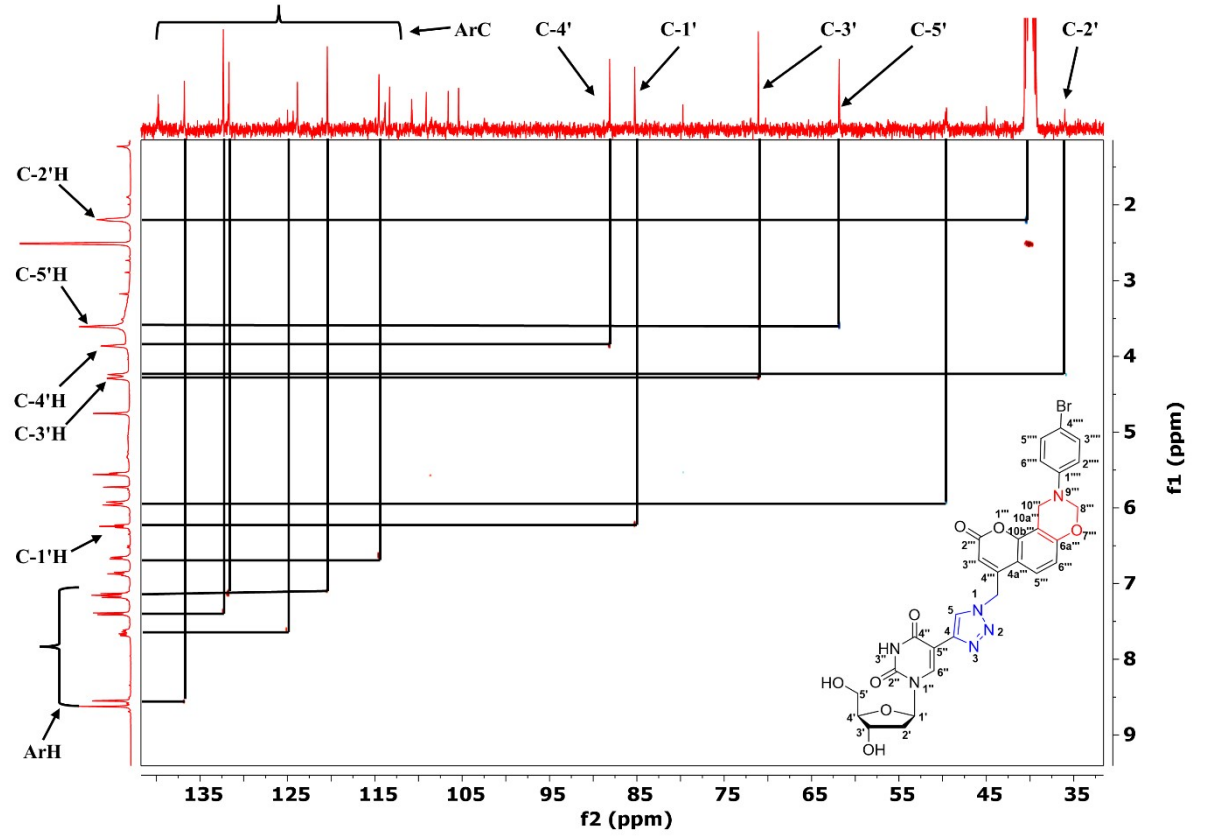


Figure S72: ^{1}H-^{13}C HETCOR NMR spectrum of compound **15e** (100 MHz, DMSO-d_6).

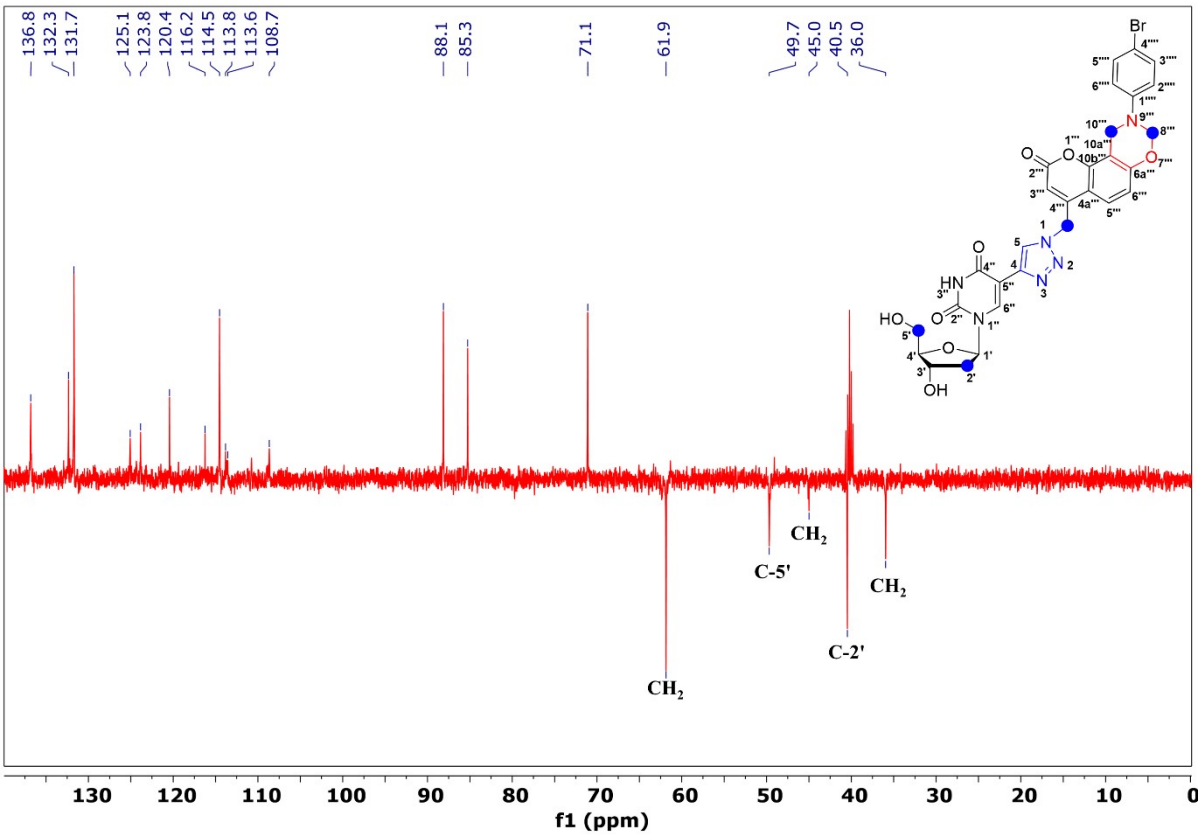


Figure S73: DEPT-135 NMR spectrum of compound **15e** (100 MHz, DMSO-d_6).

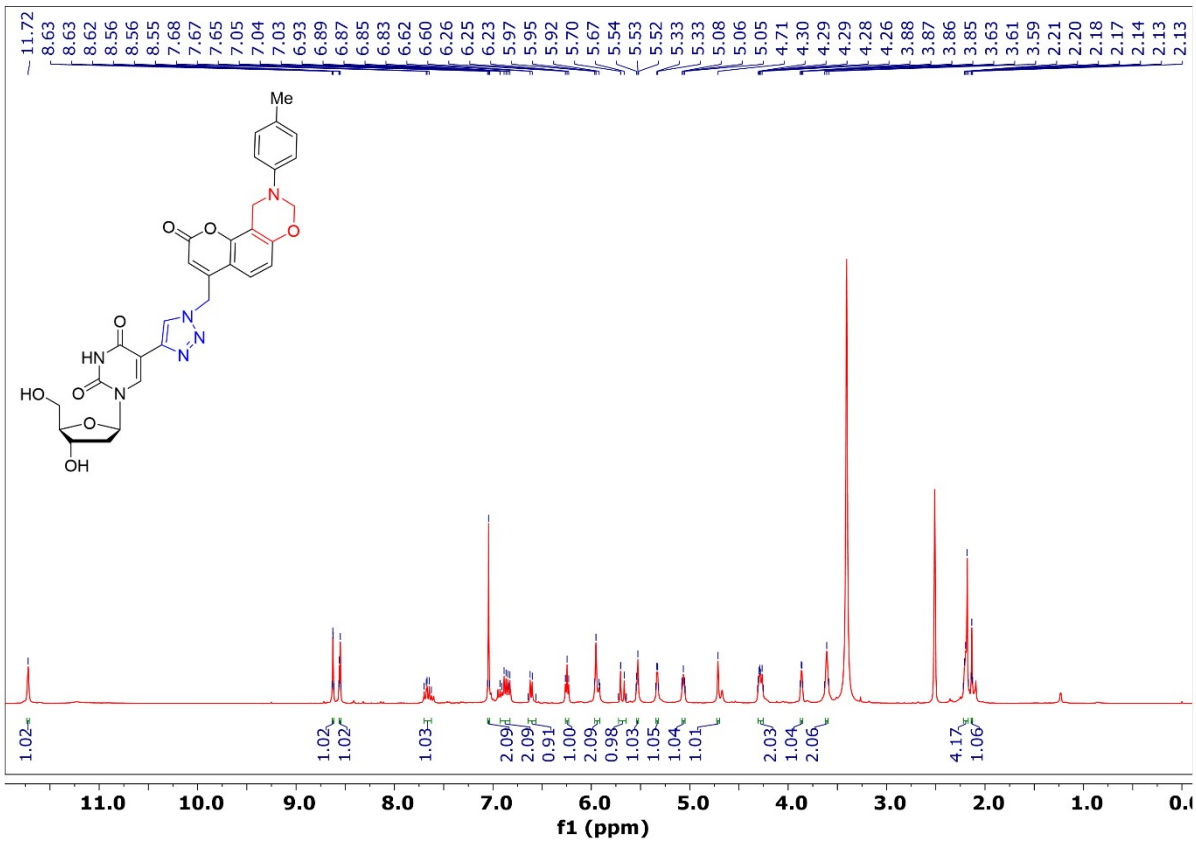


Figure S74: ^{1}H NMR spectrum of compound **15f** (400 MHz, DMSO-d_6).

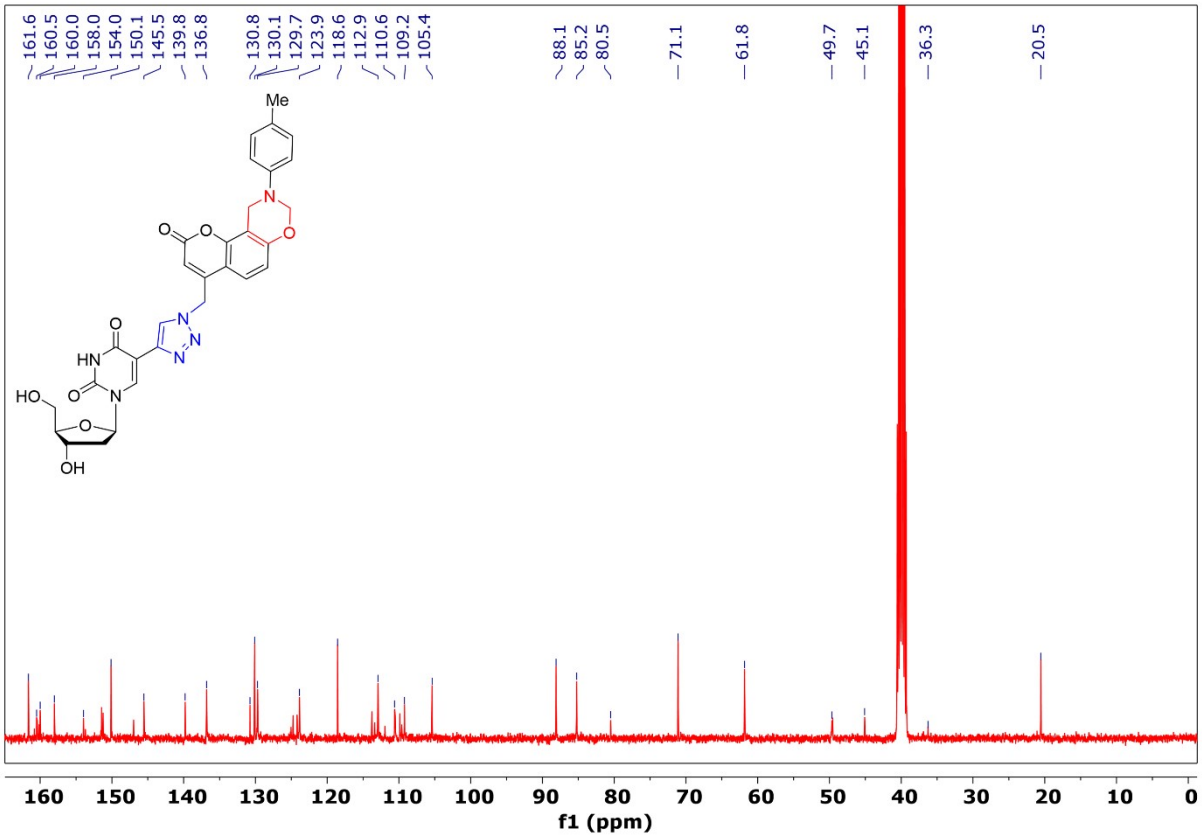


Figure S75: ^{13}C NMR spectrum of compound **15f** (100 MHz, DMSO-d_6).

2. Absorption and Emission Spectra of Compounds 14a-f and 15a-f.

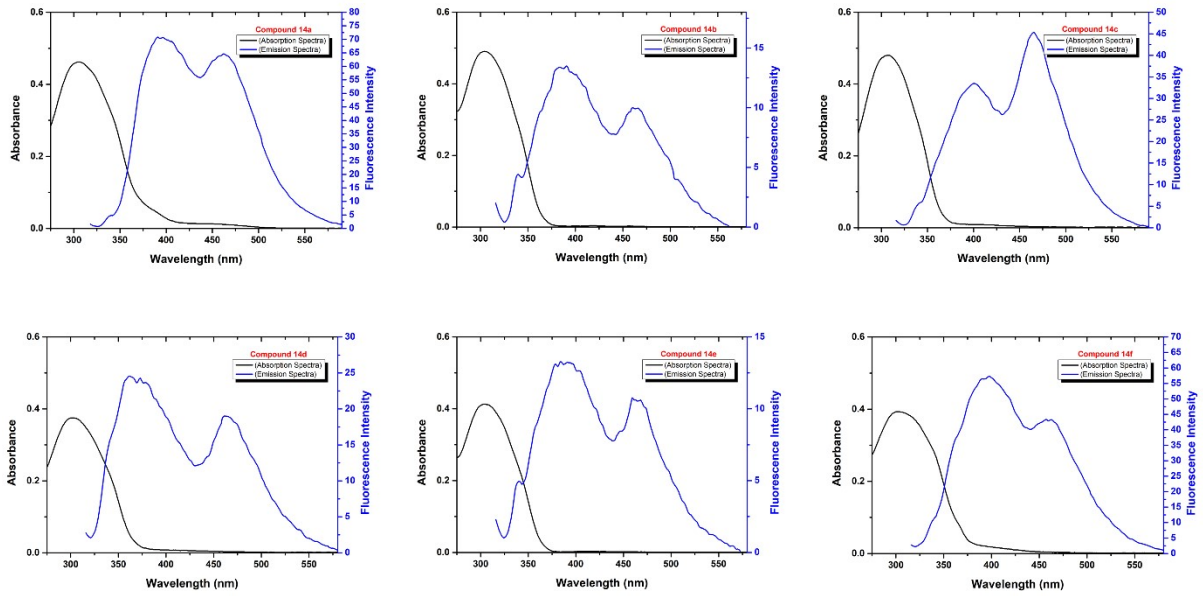


Figure S76: Absorption and Emission Spectra for compounds **14a-f**.

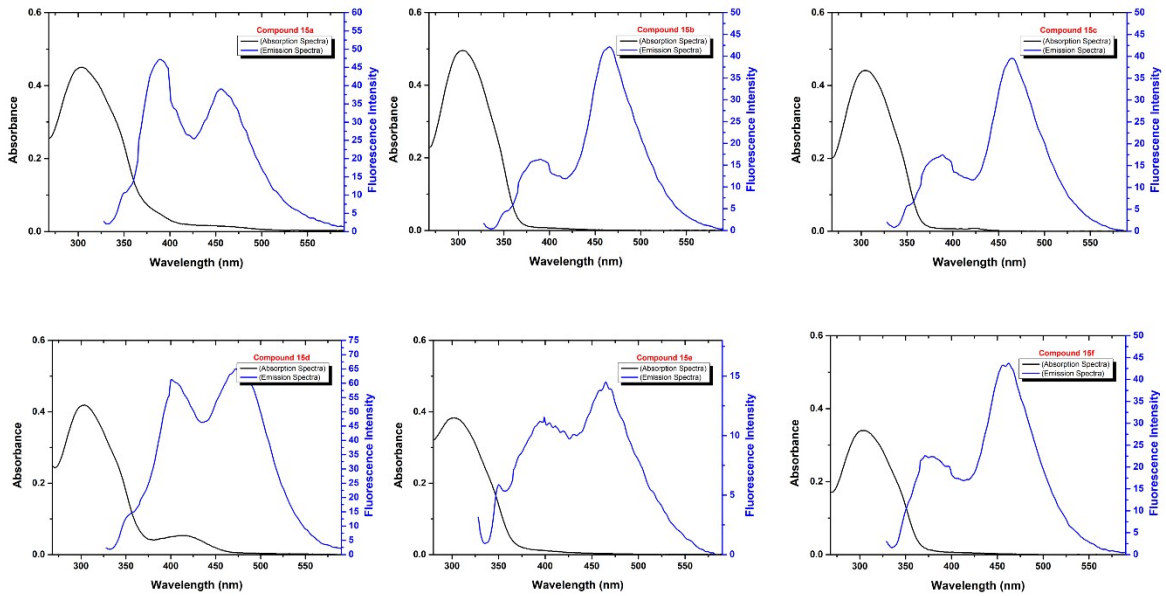
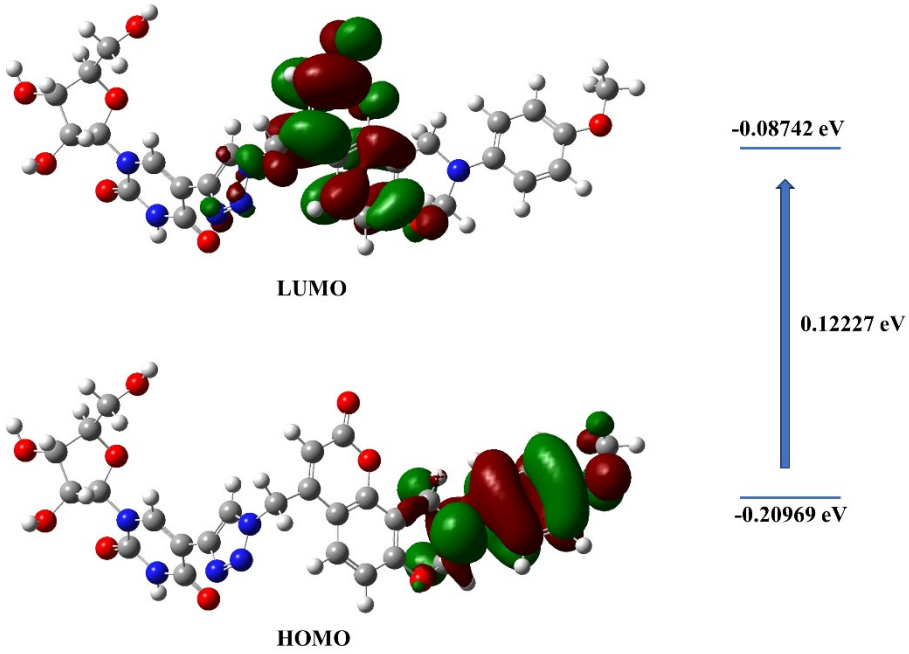
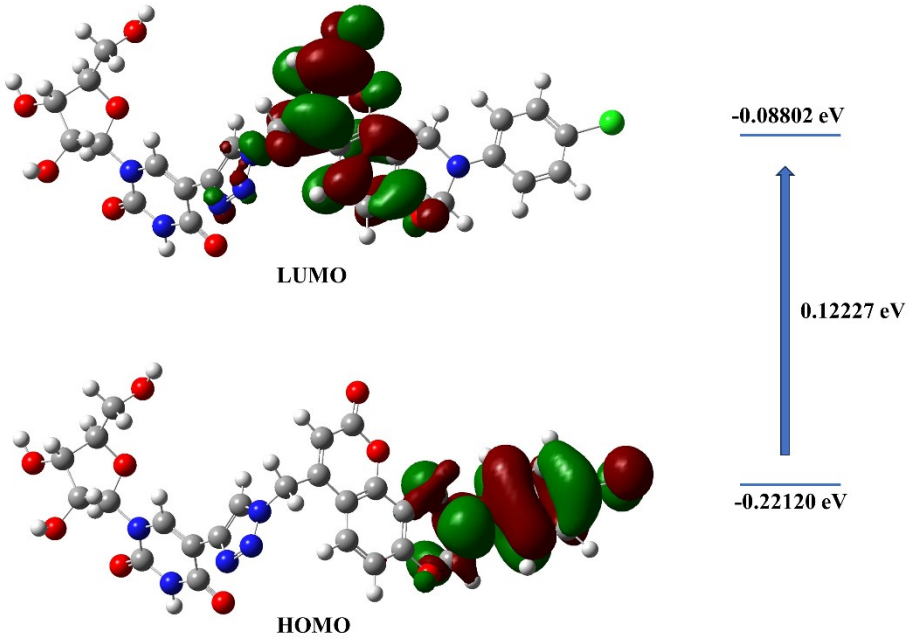


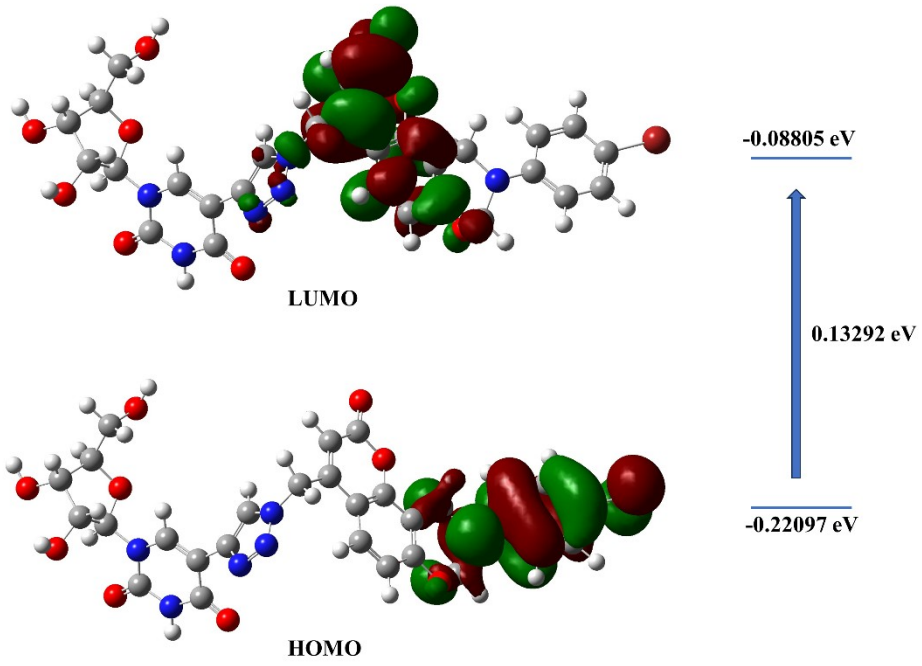
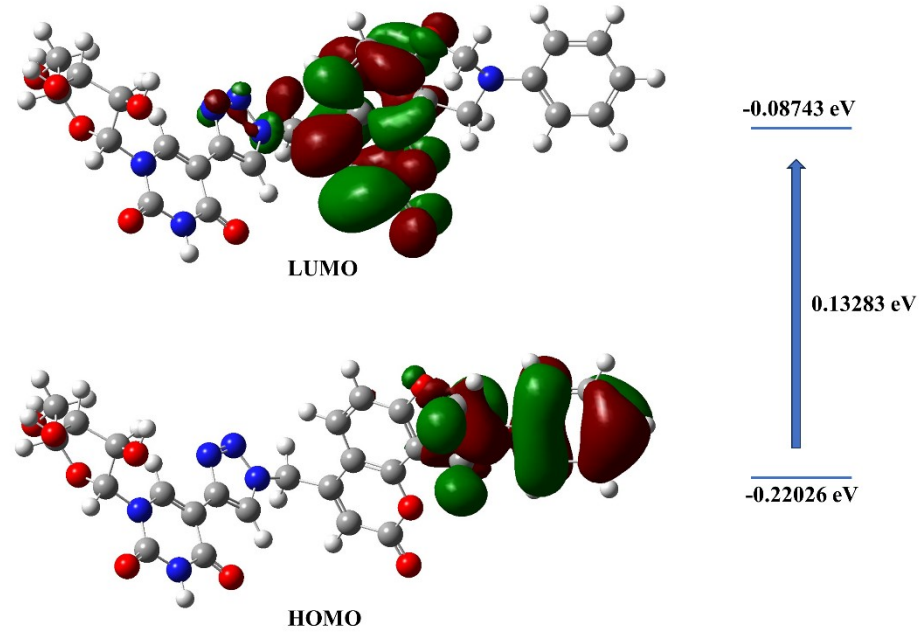
Figure S77: Absorption and Emission Spectra for compounds **15a-f**.

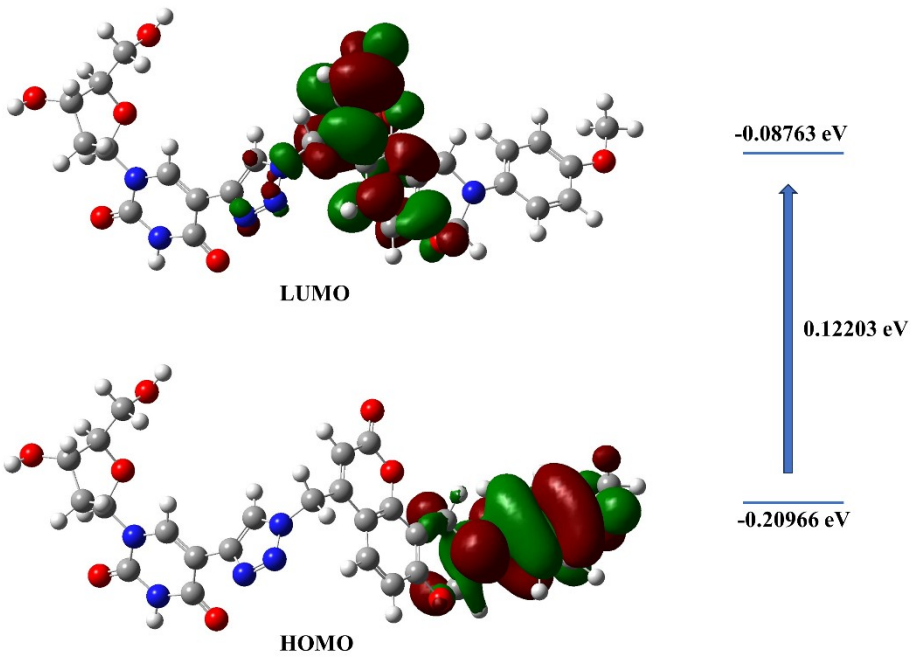
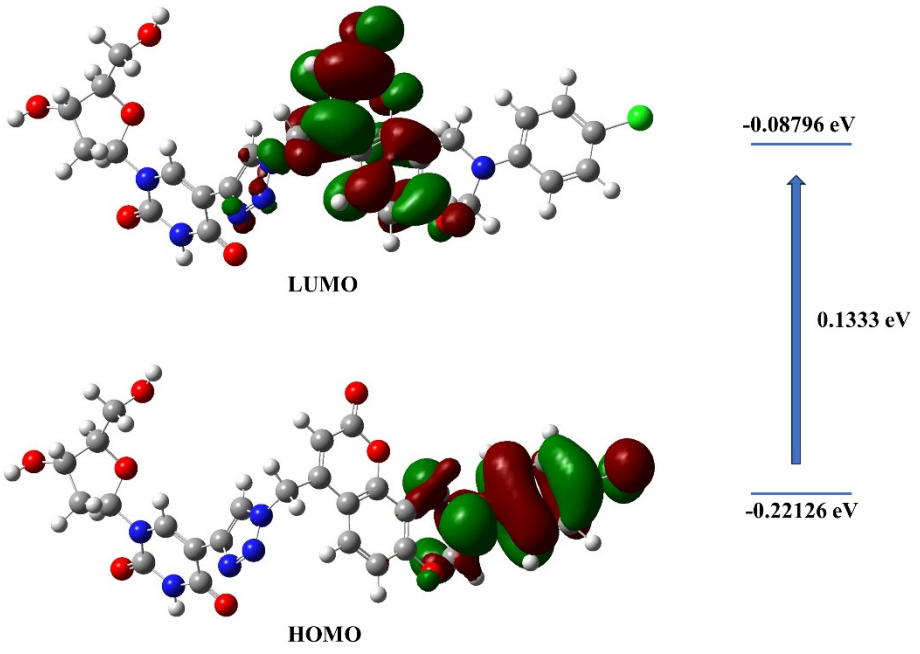
3. DFT Calculations

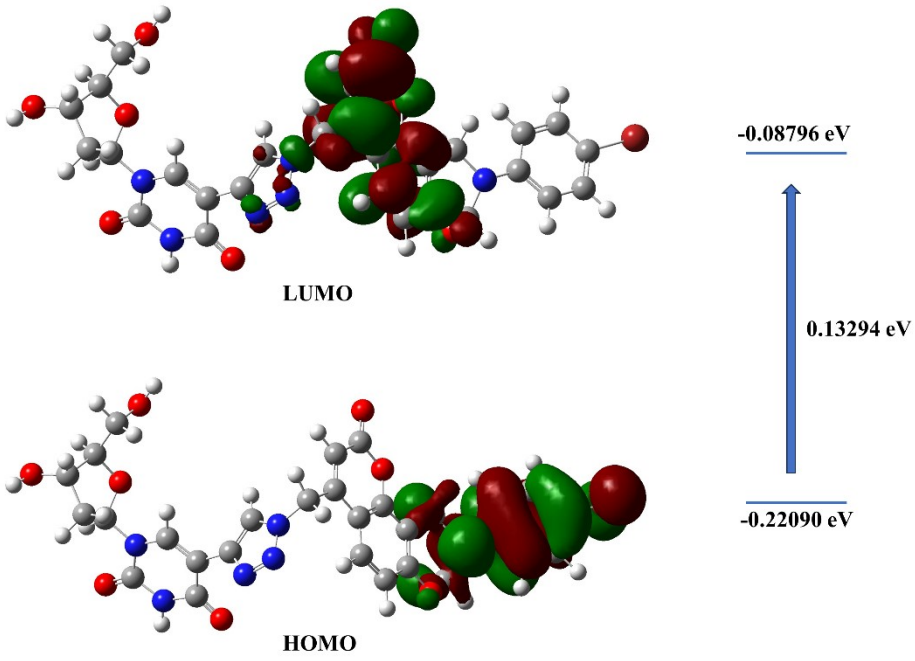
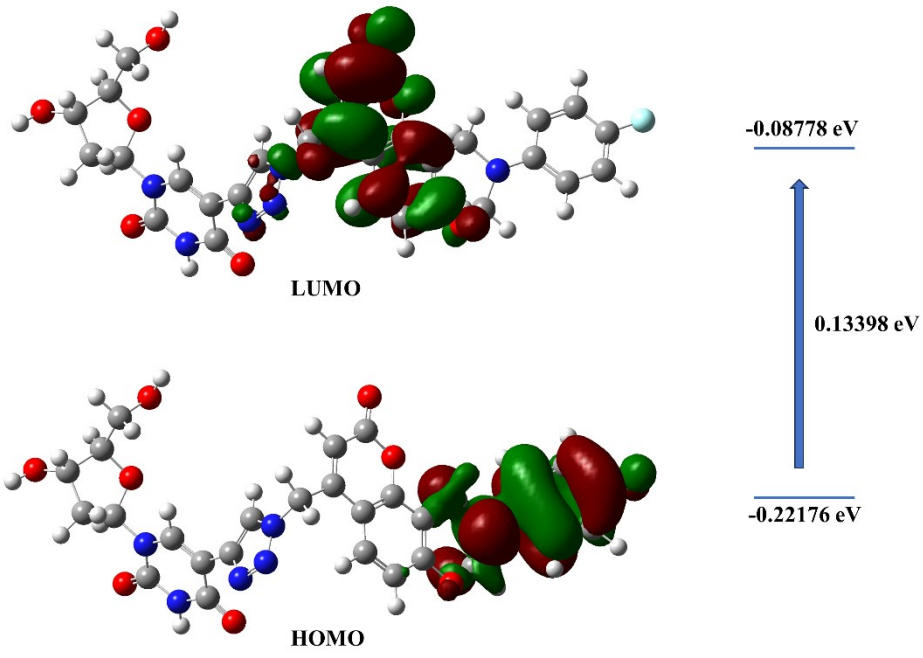
The quantum mechanical calculations of the synthesized molecules for better understanding of their electronic structures using the Gaussian 09 program.[1] The GaussView program[2] was used to visualize the molecular structures. The DFT computations employed the B3LYP functional with Becke's gradient-exchange correction[3] along with the Lee-Yang-Parr correlation functional.[4] The geometry optimizations utilized the B3LYP/6-311++G(d,p) basis set.[5] The HOMO and LUMO for some of the compounds of series **14a-f** and **15a-f** are depicted in **Table S1.**

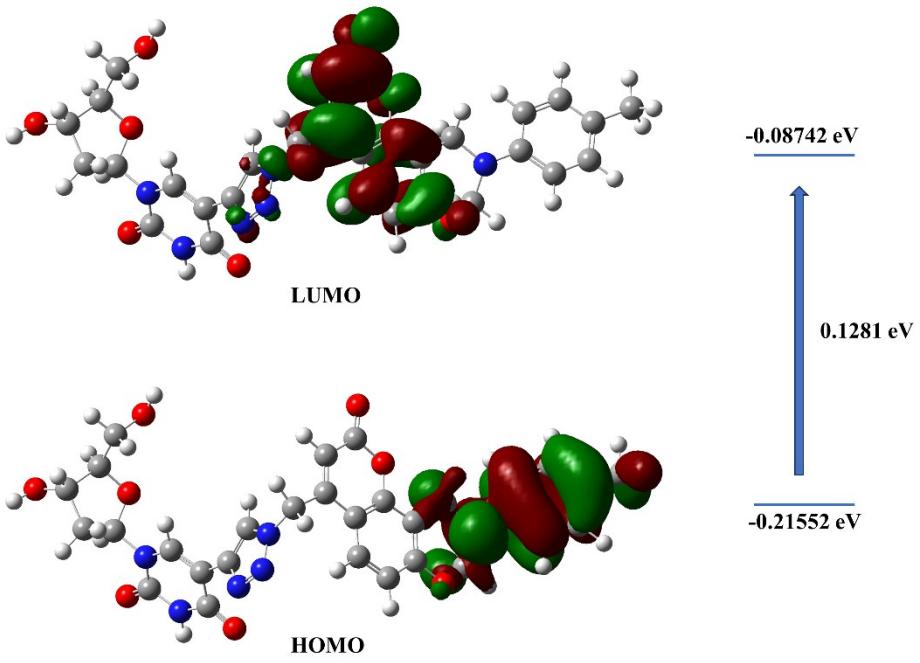
Table S1. HOMO-LUMO orbitals of compounds **14a-c**, **14f**, **15a-e**.

S.No.	Entry	HOMO-LUMO with their energy and band gaps (eV)
1.	**14a**	
2.	**14b**	

3.	**14c**	 LUMO HOMO -0.08805 eV 0.13292 eV -0.22097 eV
4.	**14f**	 LUMO HOMO -0.08743 eV 0.13283 eV -0.22026 eV

5.	**15a**	 LUMO HOMO -0.08763 eV 0.12203 eV -0.20966 eV
6.	**15b**	 LUMO HOMO -0.08796 eV 0.1333 eV -0.22126 eV

7.	**15c**	 LUMO HOMO -0.08796 eV 0.13294 eV -0.22090 eV
8.	**15d**	 LUMO HOMO -0.08778 eV 0.13398 eV -0.22176 eV

9.	**15e**	

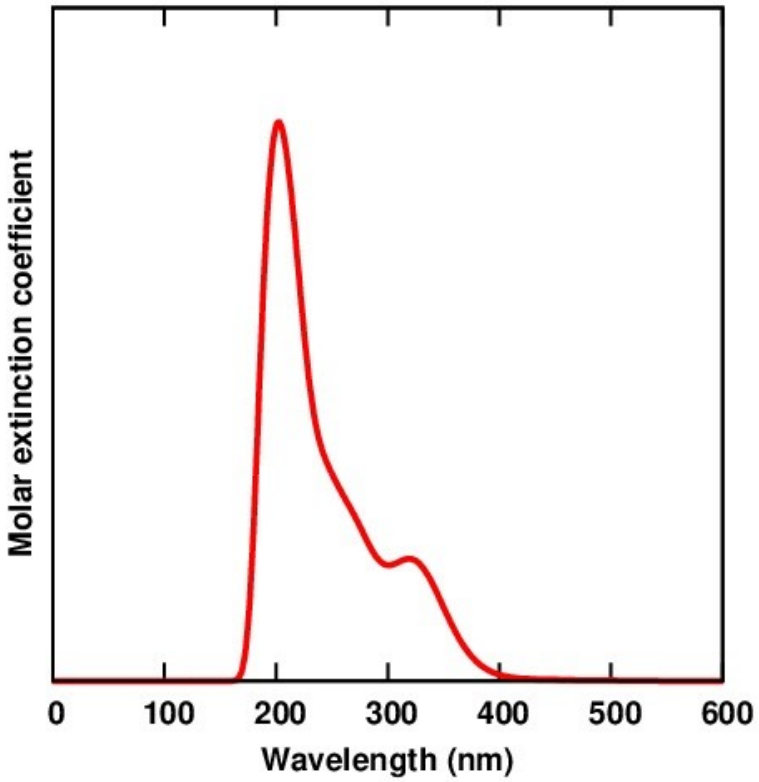


Figure S78: UV-Visible absorption spectra of compound **14a**.

4. Single crystal X-ray diffraction analysis of compound 6f

Table S2: Single crystal X-ray diffraction analysis of compound **6f**.

Identification code	AKP-A-6171_auto	
Empirical formula	$C_{18}H_{14}N_4O_3$	
Formula weight	334.33	
Temperature/K	293(2)	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions/Å	a = 13.1867(6)	a = 90˚
	b = 14.9870(6)	b = 98.777(4)˚
	c = 8.0323(4)	γ = 90 ˚
Volume/$Å^3$	1568.83(12)	
Z	4	
Density (calculated)/g/cm^3	1.416	
Absorption coefficient/mm^{-1}	0.100	
F(000)	696.0	
Crystal size/mm^3	0.2 x 0.1 x 0.1	
Theta range for data collection/˚	6.272 to 62.092	
Index ranges	$-18 \leq h \leq 19, -19 \leq k \leq 21, -11 \leq l \leq 10$	
Reflections collected	18230	
Independent reflections	4134 [R_{int} = 0.0372, R_{sigma} = 0.0321]	
Max. and min. transmission	1.000 and 0.448	
Data /restraints /parameters	4134/0/226	
Goodness-of-fit on F^2	1.073	
Final R indices [I>=2σ (I)]	R_1 = 0.0457, wR_2 = 0.1123	
R indices (all data)	R_1 = 0.0715, wR_2 = 0.1229	
Largest diff. peak and hole/$e.Å^{-3}$	0.21/-0.21	

References

1. Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G.A.; Nakatsuji, H. Gaussian 09. Wallingford, CT: Gaussian Inc, **2009**.

2. Dennington, R.; Keith, T.; Millam, J. Gauss View 5.0. Shawnee, KS: Semichem Inc, **2009**.

3. Becke, A.D. *Phys. Rev. A*, **1988**, *38*, 3098-3100.

4. Lee, C.; Yang, W.; Parr, R.G. *Phy. Rev. B Condens. Matter* **1988**, *37*, 785-789.

5. Daga, L.E.; Civalleri, B.; Maschio, L. *J. Chem. Theory Comput.* **2020**, *16*, 2192-2201.