Design, synthesis, anti-acetylcholinesterase evaluation and molecular modeling studies of novel coumarin-chalcone hybrids

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EXPERIMENTAL

Chemicals and Reagents

Reagents and solvents used in the research were commercially available 1,3-dibromopropane, 4-hydroxyacetophenone, 2-chlorobenzaldehyde, 4-bromobenzaldehyde, 3-bromobenzaldehyde, 2-bromobenzaldehyde, 4-methoxybenzaldehyde, 4-nitrobenzaldehyde, 3-nitrobenzaldehyde, and *p*-tolualdehyde were purchased from Sigma-Aldrich. While resorcinol, ethyl acetoacetate, benzaldehyde, and 1,4-dioxane were purchased from Merck. The other materials were purchased from Alfa Aesar, such as 4-chlorobenzaldehyde, 3-chlorobenzaldhyde, 3-methoxybenzaldehyde, and *o*-tolualdehyde. While the *m*-tolualdehyde was purchased from Acros Organics. Whereas sodium hydroxide pellets, chloroform, dichloromethane, ethyl acetate, methanol, ethanol, and *n*-hexane were bought from Qrec. Analytical grade (AR) solvents such as ethanol absolute AR (99.9%) were purchased from Fisher Scientific. The purity of these chemicals was 90-99.9% and they were used without further purification.

Instrumentations

Thin layer chromatography (TLC) was used to monitor the progress of reactions and to detect the formation of new spots in the reaction mixture. The TLC plates used were the thin aluminium plates from Merck pre-coated with silica gel F254 with a 0.2 mm thickness. The spots were visualised under UV light at 254 nm or 365 nm. Melting points (uncorrected) were determined using a Barnstead Electrothermal 9100 melting point. The infrared IR spectra were recorded using a Perkin-Elmer FTIR spectrometer. Samples were prepared as KBr discs. The 1H NMR (400 MHz) and 13C NMR (100 MHz) were recorded on the Bruker Avance II 400 MHz NMR Spectrometer using deuterated chloroform ($CDCl_3$, Sigma-Aldrich, 99.96%), acetone (CD_3COCD_3, Merck, 99.9%) or dimethyl sulfoxide (DMSO-d6, Sigma-Aldrich, 99.9%) as the solvent. Chemical shift values were given in δ (ppm) scales. The HRMS was recorded on Agilent Technologies' 6545 Q-TOF LC/MS.

Synthesis of 7-Hydroxy-4-methylcoumarin (3)

Concentrated H_2SO_4 (1 mL) was slowly added to an ice-cold solution of resorcinol (4.0 g, 36.37 mmol) in dioxane (20 mL) under 25ºC and followed by adding ethyl acetoacetate (6.0 g, 48.96 mmol). The reaction mixture was refluxed for 4 hours. After cooling to room temperature, the mixture was poured into crushed ice and stirred for 30 min. The resulting yellow precipitate was collected by filtration, washed several times with water and dried in the oven. The solid was recrystallized from methanol to give 7-hydroxy-4-methyl-2*H*-chromen-2-one **(3)** as a pale-yellow solid (6.32 g, 98.75%); R_f = 0.45 (hexane: EtOAc = 3:2); m.p 183.2-184.7ºC (lit. 180.0-182.0ºC [1]). IR (ATR) (υ_{max}/ cm^{-1}): 3435 (OH), 3124 (C-H sp^2), 2811 (C-H sp^3), 1672 (C=O lactone), 1594 and 1450 (C=C aromatic); ^{1}H NMR (400 MHz, acetone-d_6): δ 2.42 (3H, s, 4-CH_3), 6.09 (1H, s, H-3), 6.74 (1H, d, *J* = 2.4 Hz, H-8), 6.85 (1H, dd, *J* = 8.8 Hz, *J* = 2.4 Hz, H-6), 7.61 (1H, d, *J* = 8.8 Hz, H-5), 9.44 (1H, s, OH).

General Procedure of Synthesis of 4'-Hydroxychalcones (6a-n)

A mixture of 4'-hydroxyacetophenone (10 mmol) with various benzaldehyde substituents (12 mmol) was dissolved in a solution of absolute ethanol (25 mL) and 25% KOH (5 mL). The reaction mixture was stirred for 24 hours at room temperature. The solution was poured into cold water and acidified with concentrated HCl. The precipitate was collected, washed several times with water, and dried. The product was subjected to recrystallization from ethanol (96%) to afford 4'-hydroxychalcones **(6a-n)**.

(*E*)-1-(4-hydroxyphenyl)-3-phenylprop-2-en-1-one (6a)

Pale yellow powder; yield: (85.7%); R_f = 0.84 (hexane:EtOAc = 2:3); m.p 182.5-183.7ºC (lit. 179-181.2ºC [2]). IR (KBr) (υ_{max}/ cm^{-1}): 3125 (O-H), 1646 (C=O), 1605 (C=C olefinic), 1565 and 1442 (C=C aromatic), 1220 (C-O). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.83 (1H, s, OH), 6.96 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.43 (3H, m, H-3, H-4 and H-5), 7.55 (1H, d, *J* = 16.0 Hz, H-α), 7.65 (2H, d, *J* = 8.8 Hz, H-2 and H-6), 7.81 (1H, d, *J* = 16.0 Hz, H-β), 8.02 (2H, d, *J* = 8.8 Hz, H-2' and H-6').

(*E*)-3-(4-chlorophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one (6b)

Yellow powder; yield: (78.5%); R_f = 0.79 (hexane:EtOAc = 2:3); m.p 189.2-191.0ºC (lit. 187-189ºC [3]). IR (KBr) (υ_{max}/ cm^{-1}): 3094 (O-H), 1643 (C=O), 1599 (C=C olefinic), 1542 and 1488 (C=C aromatic), 1229 (C-O). ^{1}H NMR (400 MHz, acetone-d6): δ 6.98 (2H, d, *J* = 8.8 Hz, H-3'and H-5'), 7.48 (2H, d, *J* = 8.8 Hz, H-3 and H-5), 7.71 (1H, d, *J* = 15.6 Hz, H-α), 7.85 (2H, d, *J* = 8.8 Hz, H-2 and H-6), 7.89 (1H, d, *J* = 15.6 Hz, H-β), 8.10 (2H, d, *J* = 8.8 Hz, H-2' and H-6'), 9.38 (1H, s, OH).

(*E*)-3-(3-chlorophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one (6c)

Pale yellow powder; yield: (66.8%); R_f = 0.87 (hexane:EtOAc = 2:3); m.p 173.2-175.5ºC (lit. 176-178ºC [3]). IR (KBr) (υ_{max}/ cm^{-1}): 3263 (O-H), 1652 (C=O), 1599 (C=C olefinic), 1564 and 1476 (C=C aromatic), 1227 (C-O). ^{1}H NMR (400 MHz, acetone-d6): δ 6.98 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.45 (2H, m, H-4 and H-6), 7.70 (1H, d, *J* = 15.6 Hz, H-α), 7.76 (1H, dd, *J* = 2.8 Hz and *J* = 8.4 Hz, H-5), 7.93 (1H, d, *J* = 2.4 Hz, H-2), 7.95 (1H, d, *J* = 15.6 Hz, H-β), 8.12 (2H, d, *J* = 8.8 Hz, H-2' and H-6'), 9.40 (1H, s, OH).

(*E*)-3-(2-chlorophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one (6d)

Pale yellow powder; yield: (72.4%); R_f = 0.86 (hexane:EtOAc = 2:3); m.p 170.3-172.7ºC (lit. 168-169ºC [3]). IR (KBr) (υ_{max}/ cm^{-1}): 3232 (O-H), 1650 (C=O), 1611(C=C olefinic), 1562 and 1468 (C=C aromatic), 1225 (C-O). ^{1}H NMR (400 MHz, acetone-d6): δ 6.99 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.42 (2H, m, H-4 and H-5), 7.43 (1H, dd, *J* = 2.0 and 6.8 Hz, H-3), 7.88 (1H, d, *J* = 15.6 Hz, H-α), 8.09 (1H, dd, *J* = 2.8 and 8.0 Hz, H-6), 8.12 (2H, d, *J* = 8.8 Hz, H-2' and H-6'), 8.14 (1H, d, *J* = 15.6 Hz, H-β), 9.41 (H, s, OH).

(*E*)-3-(4-bromophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one (6e)

Yellow powder, yield: (87.3%); R_f = 0.91 (hexane:EtOAc = 2:3); m.p 197.2-199.0ºC (lit. 199-201ºC [3]). IR (KBr) (υ_{max}/ cm^{-1}): 3092 (O-H), 1642 (C=O), 1601(C=C olefinic), 1541 and 1484 (C=C aromatic), 1227 (C-O). ^{1}H NMR (400 MHz, acetone-d6): δ 6.98 (2H, d, *J* = 8.8 Hz, H-3'and H-5'), 7.63 (2H, d, *J* = 8.8 Hz, H-3 and H-5), 7.69 (1H, d, *J* = 16.0 Hz, H-α), 7.79 (2H, d, *J* = 8.8 Hz, H-2 and H-6), 7.91 (1H, d, *J* = 16.0 Hz, H-β), 8.10 (2H, d, *J* = 8.8 Hz, H-2' and H-6'), 9.35 (1H, s, OH).

(*E*)-3-(3-bromophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one (6f)
Pale yellow powder, yield: (78.2%); R_f = 0.67 (hexane:EtOAc = 2:3); m.p 168.4-169.7ºC (lit. 164-165ºC [4]). IR (KBr) (υ_{max}/ cm^{-1}): 3259 (O-H), 1651 (C=O), 1598 (C=C olefinic), 1563 and 1472 (C=C aromatic), 1225 (C-O). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.46 (1H, s, OH), 6.95 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.31 (1H, d, *J* = 7.6 Hz, H-5), 7.52 (3H, m, H-4, H-6 and H-α), 7.72 (1H, d, *J* = 16.0 Hz, H-β), 7.81 (1H, s, H-2) 8.02 (2H, d, *J* = 8.8 Hz, H-2' and H-6').

(*E*)-3-(2-bromophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one (6g)
Yellow powder, yield (83.3%); R_f = 0.64 (hexane:EtOAc = 2:3); m.p 166.7-168.4ºC (lit. 168-170ºC [5]). IR (KBr) (υ_{max}/ cm^{-1}): 3142 (O-H), 1642 (C=O), 1605 (C=C olefinic), 1590 and 1462 (C=C aromatic), 1224 (C-O). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.64 (1H, s, OH), 6.95 (2H, d, *J* = 8.0 Hz, H-3' and H-5'), 7.25 (1H, d, *J* = 8.0 Hz, H-4), 7.36 (1H, d, *J* = 8.0 Hz, H-5), 7.43 (1H, d, *J* = 16.0 Hz, H-α), 7.65 (1H, d, *J* = 8.0 Hz, H-6), 7.74 (1H, d, *J* = 8.0 Hz, H-3), 8.02 (2H, d, *J* = 8.0 Hz, H-2' and H-6'), 8.12 (1H, d, *J* = 16.0 Hz, H-β).

(*E*)-1-(4-hydroxyphenyl)-3-(4-nitrophenyl)prop-2-en-1-one (6h)
Yellow powder, yield (75.7%); R_f = 0.73 (hexane:EtOAc = 2:3); m.p 244.1-246.0ºC (lit. 247-249ºC [3]). IR (KBr) (υ_{max}/ cm^{-1}): 3383 (O-H), 1651(C=O), 1612 (C=C olefinic), 1590 and 1442 (C=C aromatic), 1223 (C-O). ^{1}H NMR (400 MHz, DMSO): δ 6.90 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.73 (1H, d, *J* = 16.0 Hz, H-α), 8.09 (2H, d, *J* = 8.8 Hz, H-2' and H-6'), 8.08 (1H, d, *J* = 16.0 Hz, H-β), 8.13 (2H, d, *J* = 8.0 Hz, H-2 and H-6), 8.27 (2H, d, *J* = 8.0 Hz, H-3 and H-5).

(*E*)-1-(4-hydroxyphenyl)-3-(3-nitrophenyl)prop-2-en-1-one (6i)
Pale yellow powder, yield (73.4%); R_f = 0.62 (hexane:EtOAc = 2:3); m.p 223.0-225.2ºC (lit. 222-223ºC [5]). IR (KBr) (υ_{max}/ cm^{-1}): 3153 (O-H), 1650 (C=O), 1606 (C=C olefinic), 1592 and 1482 (C=C aromatic), 1227 (C-O). ^{1}H NMR (400 MHz, DMSO): δ 6.90 (2H, d, *J* = 8.8 Hz, H-3'and H-5'), 7.72 (1H, d, *J* = 8.0 Hz, H-4), 7.76 (1H, d, *J* = 16.0 Hz, H-α), 8.10 (1H, d, *J* = 16.0 Hz, H-β), 8.11 (2H, d, *J* = 8.8 Hz, H-2' and H-6'), 8.24 (1H, dd, *J* = 2.0 Hz, and *J* = 8.4 Hz, H-5), 8.29 (1H, d, *J* = 7.6 Hz, H-6), 8.74 (1H, s, H-2).

(*E*)-1-(4-hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (6j)
Yellow powder, yield (71.8%); R_f = 0.54 (hexane:EtOAc = 2:3); m.p 167.5-168.3ºC (lit. 168-170ºC [6]). IR (KBr) (υ_{max}/ cm^{-1}): 3376 (O-H), 1641 (C=O), 1600 (C=C olefinic), 1572 and 1440 (C=C aromatic), 1223 (C-O). ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.88 (3H, s, OCH_3), 6.15 (1H, s, OH), 6.95 (4H, d, *J* = 8.8 Hz, H-3, H-5, H-3' and H-5'), 7.43 (1H, d, *J* = 16.0 Hz, H-α), 7.61 (2H, d, *J* = 8.8 Hz, H-2 and H-6), 7.79 (1H, d, *J* = 16.0 Hz, H-β), 8.00 (2H, d, *J* = 8.8 Hz, H-2' and H-6').

(*E*)-1-(4-hydroxyphenyl)-3-(3-methoxyphenyl)prop-2-en-1-one (6k)
Yellow powder, yield (63.4%); R_f = 0.68 (hexane:EtOAc = 2:3); m.p 162.5-164.1ºC (lit. 161-163ºC [7]). IR (KBr) (υ_{max}/ cm^{-1}): 3301 (O-H), 1652 (C=O), 1609 (C=C olefinic), 1584 and 1492 (C=C aromatic), 1257 (C-O). ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.88 (3H, s, OCH_3), 5.88 (1H, s, OH),6.95 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 6.99 (1H, d, *J* = 2.8 Hz, H-4), 7.17 (1H, s, H-2), 7.25 (1H, d, *J* = 8.0 Hz, H-6), 7.34 (1H, d, *J* = 8.0 Hz, H-5), 7.52 (1H, d, *J* = 16.0 Hz, H-α), 7.77 (1H, d, *J* = 16.0 Hz, H-β), 8.43 (2H, d, *J* = 8.8 Hz, H-2' and H-6').

(*E*)-1-(4-hydroxyphenyl)-3-(*p*-tolyl)prop-2-en-1-one (6l)

Pale yellow powder, yield (70.3%); R_f = 0.71 (hexane:EtOAc = 2:3); m.p 189.2-191.0ºC (lit. 190-192ºC [3]). IR (KBr) (υ $_{max}$/ cm^{-1}): 3121 (O-H), 1647 (C=O), 1605 (C=C olefinic), 1589 and 1554 (C=C aromatic), 1225 (C-O). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.41 (3H, s, CH_3), 7.00 (2H, d, *J* = 8.8 Hz, 3'-H, 5'-H,), 7.24 (2H, d, *J* = 8.8 Hz, H-3 and H-5), 7.51 (1H, d, *J* = 16.0 Hz, H-α), 7.61 (2H, d, *J* = 8.8 Hz, H-2 and H-6), 7.79 (1H, d, *J* = 16.0 Hz, H-β), 8.05 (2H, d, *J* = 8.8 Hz, H-2' and H-6').

(*E*)-1-(4-hydroxyphenyl)-3-(*m*-tolyl)prop-2-en-1-one (6m)
Yellow powder, yield (60.9%); R_f = 0.48 (hexane:EtOAc = 2:3); m.p 163.1-165.0ºC (lit. 161-162ºC [7]). IR (KBr) (υ $_{max}$/ cm^{-1}): 3182 (O-H), 1644 (C=O), 1603(C=C olefinic), 1566 and 1482 (C=C aromatic), 1240 (C-O). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.42 (3H, s, CH_3), 6.37 (1H, s, OH), 6.96 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.23 (1H, d, *J* = 7.6 Hz, H-2), 7.31 (1H, t, *J* = 8.0 Hz, H-5), 7.45 (2H, d, *J* = 6.8 Hz, H-4 and H-6), 7.53 (1H, d, *J* = 16.0 Hz, H-α), 7.79 (1H, d, *J* = 16.0 Hz, H-β), 8.02 (2H, d, *J* = 8.8 Hz, H-2' and H-6').

(*E*)-1-(4-hydroxyphenyl)-3-(*o*-tolyl)prop-2-en-1-one (6n)
Yellow powder, yield (66.9%); R_f = 0.44 (hexane:EtOAc = 2:3); m.p 186.7-187.9ºC (lit. 187.0ºC [7]). IR (KBr) (υ $_{max}$/ cm^{-1}): 3129 (O-H), 1648 (C=O), 1594 (C=C olefinic), 1558 and 1482 (C=C aromatic), 1221 (C-O). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.50 (3H, s, CH_3), 5.83 (1H, s, OH), 6.95 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.24 (2H, m, H-4 and H-5), 7.33 (1H, d, *J* = 6.4 Hz, H-3), 7.46 (1H, d, *J* = 16.0 Hz, H-α), 7.70 (1H, d, *J* = 7.2 Hz, H-6), 8.02 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 8.11 (1H, d, *J* = 16.0 Hz, H-β).

General Procedure of Synthesis of Intermediates (7a-n)

A mixture of chalcones (2 mmol), 1,3-dibromopropane (10 mmol), and anhydrous K_2CO_3 (450 mg) was dissolved in acetonitrile (50 mL). The reaction solution was refluxed for 7 hours. After that, the reaction mixture was poured into cold water (50 mL). The precipitate was immediately formed, filtered off, washed with cold water, and dried in the oven to afford the final compounds **(7a-n)**.

(*E*)-1-(4-(3-bromopropoxy)phenyl)-3-phenylprop-2-en-1-one (7a)
White powder, yield (58.3%); R_f =0.72 ($CHCl_3$:EtOAc =1:1); m.p 86.3-87.8ºC (lit. 84.0-86.0ºC [8]). IR (KBr) (υ $_{max}$/ cm^{-1}): 3061 (C-H sp^2), 2935 (C-H sp^3), 1655 (C=O), 1603 (C=C olefinic), 1592 and 1574 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.35-2.41 (2H, m, -CH_2-), 3.63 (2H, t, *J* = 6.0 Hz, CH_2Br), 4.21 (2H, t, *J* = 6.0 Hz, OCH_2), 7.00 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.43 (3H, m, H-3, H-4 and H-5), 7.55 (1H, d, *J* = 16.0 Hz, H-α), 7.66 (2H, d, *J* = 8.8 Hz, H-2 and H-6), 7.81 (1H, d, *J* = 16.0 Hz, H-β), 8.05 (2H, d, *J* = 8.8 Hz, H-2' and H-6').

(*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(4-chlorophenyl)prop-2-en-1-one (7b) [9]
White powder, yield (62.7%); R_f =0.67 ($CHCl_3$:EtOAc =1:1); m.p 115.2-116.7ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3069 (C-H sp^2), 2948 (C-H sp^3), 1659 (C=O), 1609 (C=C olefinic), 1591 and 1510 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.35 (2H, m, -CH_2-), 3.63 (2H, t, *J* = 7.2 Hz, CH_2Br), 4.21 (2H, t, *J* = 6.0 Hz, OCH_2), 7.00 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.40 (2H, d, *J* = 8.8 Hz, H-3 and H-5), 7.51 (1H, d, *J* = 16.0 Hz, H-α), 7.58 (2H, d, *J* = 8.8 Hz, H-2 and H-6), 7.75 (1H, d, *J* = 16.0 Hz, H-β), 8.04 (2H, d, *J* = 8.8 Hz, H-2' and H-6').

(*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(3-chlorophenyl)prop-2-en-1-one (7c)
White powder, yield (71.8%); R_f =0.60 ($CHCl_3$:EtOAc =1:1); m.p 110-111.5ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3054 (C-H sp^2), 2951 (C-H sp^3), 1658 (C=O), 1608 (C=C olefinic), 1593 and 1564 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.35 (2H, m, -CH_2-), 3.63 (2H, t, *J* = 7.2 Hz, CH_2Br), 4.21 (2H, t, *J* = 6.0 Hz, OCH_2), 7.00 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.37 (2H, m, H-4 and H-6), 7.51 (1H, d, *J* = 6.4 Hz, H-5), 7.54 (1H, d, *J* = 16.0 Hz, H-α), 7.65 (1H, s, H-2), 7.73 (1H, d, *J* = 16.0 Hz, H-β), 8.05 (2H, d,

J = 8.8 Hz, H-2' and H-6'). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.2 (C=O), 162.7 (C-4'), 142.2 (C-β), 136.9 (C-1), 134.9 (C-3), 131.0 (C-5), 130.9, (C-2' and C-6') 130.1 (C-1'), 130.1 (C-4), 127.8 (C-6), 126.7 (C-2), 123.1 (C-α), 114.4 (C-3' and C-5'), 65.6 (-OCH_2-), 32.1 ($BrCH_2$-), 29.6 (-CH_2-). HRMS (ESI): calcd. for $C_{18}H_{16}BrClO_2$ $[M + H]^+$ 378.0022, found 377.9969.

(*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(2-chlorophenyl)prop-2-en-1-one (7d)
White powder, yield (69.5%); R_f =0.69 ($CHCl_3$:EtOAc =1:1); m.p 115.4-117ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3069 (C-H sp^2), 2948 (C-H sp^3), 1659 (C=O), 1609 (C=C olefinic), 1591 and 1563 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.35 (2H, m, -CH_2-), 3.63 (2H, t, *J* = 7.2 Hz, CH_2Br), 4.21 (2H, t, *J* = 6.0 Hz, OCH_2), 7.00 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.33 (2H, m, H-4 and H-5), 7.45 (1H, d, *J* = 9.2 Hz, H-3), 7.49 (1H, d, *J* = 16.0 Hz, H-α), 7.76 (1H, d, *J* = 9.2 Hz, H-6), 8.04 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 8.16 (1H, d, *J* = 16.0 Hz, H-β). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.6 (C=O), 162.6 (C-4'), 139.8 (C-β), 135.4 (C-2), 133.5 (C-1), 130.9 (C-3, C-4, C-2' and C-6'), 130.2 (C-1'), 127.7 (C-6), 127.0 (C-5), 124.7 (C-α), 114.3 (C-3' and C-5'), 65.5 (-OCH_2-), 32.1 ($BrCH_2$-), 29.6 (-CH_2-). HRMS (ESI): calcd. for $C_{18}H_{16}BrClO_2$ $[M + H]^+$ 378.0022, found 377.9977.

(*E*)-3-(4-bromophenyl)-1-(4-(3-bromopropoxy)phenyl)prop-2-en-1-one (7e)
Yellow powder, yield (95.0%); R_f =0.75 ($CHCl_3$:EtOAc =1:1); m.p 117.6-119.5ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3071 (C-H sp^2), 2934 (C-H sp^3), 1656 (C=O), 1603 (C=C olefinic), 1589 and 1562 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.35 (2H, m, -CH_2-), 3.63 (2H, t, *J* = 6.0 Hz, CH_2Br), 4.21 (2H, t, *J* = 6.0 Hz, OCH_2), 7.00 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.51 (5H, m, H-2, H-3, H-5, H-6 and H-α), 7.73 (1H, d, *J* = 16.0 Hz, H-β), 8.04 (2H, d, *J* = 8.8 Hz, H-2' and H-6'). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.3 (C=O), 162.6 (C-4'), 142.5 (C-β), 134.0 (C-4), 132.1 (C-2' and C-6'), 131.1 (C-1), 130.8 (C-3 and C-5), 129.7 (C-2 and C-6), 124.5 (C-1'), 122.4 (C-α), 114.3 (C-3' and C-5'), 65.5 (-OCH_2-), 32.1 ($BrCH_2$-), 29.6 (-CH_2-). HRMS (ESI): calcd. for $C_{18}H_{16}Br_2O_2$ $[M + H]^+$ 421.9517, found 421.9465.

(*E*)-3-(3-bromophenyl)-1-(4-(3-bromopropoxy)phenyl)prop-2-en-1-one (7f)
Pale yellow powder, yield (60.4%); R_f =0.78 ($CHCl_3$:EtOAc =1:1); m.p 174.3-176.1ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3056 (C-H sp^2), 2930 (C-H sp^3), 1658 (C=O), 1607 (C=C olefinic), 1594 and 1558 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.36 (2H, m, -CH_2-), 3.64 (2H, t, *J* = 7.2 Hz, CH_2Br), 4.22 (2H, t, *J* = 6.0 Hz, OCH_2), 7.01 (2H, d, *J* = 8.8 Hz, H-3'-H and H-5'), 7.30 (1H, dd, *J* = 2.4 Hz and *J* = 7.6 Hz, H-5), 7.54 (3H, m, H-4, H-6 and H-α), 7.72 (1H, d, *J* = 16.0 Hz, H-β), 7.82 (1H, s, H-2), 8.06 (2H, d, *J* = 8.8 Hz, H-2' and H-6'). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.6 (C=O), 162.6 (C-4'), 142.4 (C-β), 135.3 (C-1), 133.5 (C-2), 131.1 (C-4), 131.0 (C-2' and C-6'), 127.8 (C-1' and C-5), 127.6 (C-6), 125.7 (C-3), 125.0 (C-α), 114.3 (C-3' and C-5'), 65.5 (-OCH_2-), 32.1 ($BrCH_2$-), 29.6 (-CH_2-). HRMS (ESI): calcd. for $C_{18}H_{16}Br_2O_2$ $[M + H]^+$ 421.9517, found 421.9464.

(*E*)-3-(2-bromophenyl)-1-(4-(3-bromopropoxy)phenyl)prop-2-en-1-one (7g)
Yellow powder, yield (82.1%); R_f =0.80 ($CHCl_3$:EtOAc =1:1); m.p 162.9-164.3ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3062 (C-H sp^2), 2946 (C-H sp^3), 1658 (C=O), 1609 (C=C olefinic), 1591 and 1509 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.37 (2H, m, -CH_2-), 3.63 (2H, t, *J* = 6.0 Hz, CH_2Br), 4.21 (2H, t, *J* = 6.0 Hz, OCH_2), 7.00 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.24 (1H, m, H-4), 7.36 (1H, m, H-5), 7.43 (1H, d, *J* = 16.0 Hz, H-α), 7.65 (1H, dd, *J* = 1.2 Hz and *J* = 8.0 Hz, H-6), 7.74 (1H, dd, *J* = 1.2 Hz and *J* = 8.0 Hz, H-3), 8.04 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 8.11 (1H, d, *J* = 16.0 Hz, H-β). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.6 (C=O), 162.6 (C-4'), 142.4 (C-β), 135.3 (C-1), 133.5 (C-3), 131.1 (C-2' and C-6'), 131.0 (C-1'), 127.8 (C-5 and C-6), 127.6 (C-4), 125.7 (C-2), 125.0 (C-α), 114.3 (C-3' and C-5'), 65.5 (-OCH_2-), 32.1 ($BrCH_2$-), 29.6 (-CH_2-). HRMS (ESI): calcd. for $C_{18}H_{16}Br_2O_2$ $[M + H]^+$ 421.9517, found 421.9467.

(*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(4-nitrophenyl)prop-2-en-1-one (7h)
Yellow powder, yield (89.7%); R_f =0.63 ($CHCl_3$:EtOAc =1:1); m.p 221.1-223.0ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3079 (C-H sp^2), 2927 (C-H sp^3), 1658 (C=O), 1599 (C=C olefinic), 1535 and 1510 (C=C aromatic).

^{1}H NMR (400 MHz, $CDCl_3$): δ 2.36 (2H, m, -CH_2-), 3.63 (2H, t, *J* = 7.7 Hz, CH_2Br), 4.22 (2H, t, *J* = 6.0 Hz, OCH_2), 7.02 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.65 (1H, d, *J* = 16.0 Hz, H-α), 7.79 (3H, m, H-β, H-3 and H-5), 8.06 (2H, d, *J* = 8.8 Hz, H-2 and H-6), 8.28 (2H, d, *J* = 8.8 Hz, H-2' and H-6').

(*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(3-nitrophenyl)prop-2-en-1-one (7i)
Yellow powder, yield (73.8%); R_f =0.65 ($CHCl_3$:EtOAc =1:1); m.p 230-231.6ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3078 (C-H *sp*^{2}), 2941 (C-H *sp*^{3}), 1662 (C=O), 1597 (C=C olefinic), 1526 and 1511 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.36 (2H, m, -CH_2-), 3.64 (2H, t, *J* = 7.2 Hz, -CH_2Br), 4.23 (2H, t, *J* = 6.0 Hz, OCH_2), 7.03 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.62 (1H, d, *J* = 8.0 Hz, H-4), 7.67 (1H, d, *J* = 15.6 Hz, H-α), 7.83 (1H, d, *J* = 15.6 Hz, H-β), 7.93 (1H, d, *J* = 7.6 Hz, H-6), 8.08 (2H, d, *J* = 8.8 Hz, H-2' and H-6'), 8.26 (1H, d, *J* = 7.6 Hz, H-5), 8.54 (1H, s, H-2). ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.7 (C=O), 162.9 (C-4'), 148.4 (C-3), 141.2 (C-β), 140.7 (C-1), 131.0 (C-2' and C-6'), 130.7 (C-6), 128.8 (C-1'), 125.6 (C-5), 124.2 (C-2 and C-4), 114.7 (C-α), 114.5 (C-3' and C-5'), 65.6 (-OCH_2-), 32.1 ($BrCH_2$-), 29.5 (-CH_2-). HRMS (ESI): calcd. for $C_{18}H_{16}BrNO_4$ $[M + H]^+$ 389.0263, found 389.0273.

(*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(4-methoxyphenyl) prop-2-en-1-one (7j)
Yellow powder, yield (73.7%); R_f =0.48 ($CHCl_3$:EtOAc =1:1); m.p 97.3-99.4ºC (lit. 100.0-102.0ºC [10]). IR (KBr) (υ $_{max}$/ cm^{-1}): 3073 (C-H *sp*^{2}), 2932 (C-H *sp*^{3}), 1654 (C=O), 1600 (C=C olefinic), 1570 and 1510 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.35 (2H, m, -CH_2-), 3.63 (2H, t, *J* = 7.2 Hz, CH_2Br), 3.87 (3H, s, OCH_3), 4.20 (2H, t, *J* = 6.0 Hz, OCH_2), 6.949 (2H, d, *J* = 8.8 Hz, H-3'and H-5'), 6.99 (2H, d, *J* = 8.8 Hz, H-3 and H-5), 7.43 (1H, d, *J* = 15.6 Hz, H-α), 7.61 (2H, d, *J* = 8.8 Hz, H-2 and H-6), 7.78 (1H, d, *J* = 15.6 Hz, H-β), 8.04 (2H, d, *J* = 8.8 Hz, H-2' and H-6').

(*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(3-methoxyphenyl) prop-2-en-1-one (7k)
Yellow powder, yield (84.0%); R_f =0.51 ($CHCl_3$:EtOAc =1:1); m.p 81.1-83.2ºC (lit. 80.0-82.0ºC [10]). IR (KBr) (υ $_{max}$/ cm^{-1}): 3085 (C-H *sp*^{2}), 2934 (C-H *sp*^{3}), 1657 (C=O), 1605 (C=C olefinic), 1593 and 1577 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.35 (2H, m, -CH_2-), 3.62 (2H, t, *J* = 7.2 Hz, CH_2Br), 3.88 (3H, s, OCH_3), 4.20 (2H, t, *J* = 6.0 Hz, OCH_2), 6.97 (3H, m, H-3', H-5' and H-4), 7.18 (1H, s, H-2), 7.25 (1H, d, *J* = 7.6 Hz, H-6), 7.34 (1H, t, *J* = 8 Hz, H-5), 7.52 (1H, d, *J* = 15.6 Hz, H-α), 7.77 (1H, d, *J* = 15.6 Hz, H-β), 8.02 (2H, d, *J* = 8.8 Hz, H-2' and H-6').

(*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(*p*-tolyl)prop-2-en-1-one (7l)
Yellow powder, yield (54.1%); R_f =0.49 ($CHCl_3$:EtOAc =1:1); m.p 116.5-118.2ºC (lit. 115.0-116.0ºC [10]). IR (KBr) (υ $_{max}$/ cm^{-1}): 3075 (C-H *sp*^{2}), 2923 (C-H *sp*^{3}), 1655 (C=O), 1598 (C=C olefinic), 1570 and 1510 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.35 (2H, m, -CH_2-), 2.42 (3H, s, CH_3), 3.63 (2H, t, *J* = 7.2 Hz, CH_2Br), 4.21 (2H, t, *J* = 6.0 Hz, OCH_2), 7.00 (2H, d, *J* = 8.8 Hz, H-3'and H-5'), 7.24 (2H, d, *J* = 8.0 Hz, H-3 and H-5), 7.51 (1H, d, *J* = 16.0 Hz, H-α), 7.56 (2H, d, *J* = 8.0 Hz, H-2 and H-6), 7.79 (1H, d, *J* = 16.0 Hz, H-β), 8.05 (2H, d, *J* = 8.8 Hz, H-2' and H-6').

(*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(*m*-tolyl)prop-2-en-1-one (7m)
Pale yellow powder, yield (68.7%); R_f =0.47 ($CHCl_3$:EtOAc =1:1); m.p 111.3-112.7ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3074 (C-H *sp*^{2}), 2963 (C-H *sp*^{3}), 1655 (C=O), 1600 (C=C olefinic), 1573 and 1509 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.35 (2H, m, -CH_2-), 2.42 (3H, s, CH_3), 3.63 (2H, t, *J* = 7.2 Hz, CH_2Br), 4.20 (2H, t, *J* = 6.0 Hz, OCH_2), 7.00 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.23 (1H, d, *J* = 7.6 Hz, H-2), 7.31 (1H, t, *J* = 7.8 Hz, H-5), 7.46 (2H, d, *J* = 6.8 Hz, H-4 and H-6), 7.54 (1H, d, *J* = 15.6 Hz, H-α), 7.78 (1H, d, *J* = 15.6 Hz, H-β), 8.06 (2H, d, *J* = 9.2 Hz, H-2' and H-6'). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.7 (C=O), 162.4 (C-4'), 144.2 (C-β), 138.5 (C-3), 135.0 (C-1), 131.4 (C-1'), 131.2 (C-5), 130.8 (C-2' and C-6'), 128.9 (C-4), 128.8 (C-2), 125.6 (C-6), 121.7 (C-α), 114.3 (C-3' and C-5'), 65.5 (-OCH_2-), 32.1 ($BrCH_2$-), 29.6 (-CH_2-), 21.3 (3-CH_3). HRMS (ESI): calcd. for $C_{19}H_{19}BrO_2$ $[M + H]^+$ 358.0568, found 358.0535.

(*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(*o*-tolyl)prop-2-en-1-one (7n)

Pale yellow powder, yield (42.7%); R_f =0.53 ($CHCl_3$:EtOAc =1:1); m.p 114.8-160.3ºC. IR (KBr) (υ_{max}/ cm^{-1}): 3072 (C-H *sp*^{2}), 2949 (C-H *sp*^{3}), 1657 (C=O), 1609 (C=C olefinic), 1594 and 1510 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.35 (2H, m, -CH_2-), 2.50 (3H, s, CH_3), 3.63 (2H, t, *J* = 6.0 Hz, CH_2Br), 4.21 (2H, t, *J* = 6.0 Hz, OCH_2), 7.00 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.24 (1H, d, *J* = 8.0 Hz, H-3), 7.30 (2H, m, H-4 and H-5), 7.47 (1H, d, *J* = 15.6 Hz, H-α), 7.71 (1H, d, *J* = 7.6 Hz, H-6), 8.06 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 8.11 (1H, d, *J* = 15.6 Hz, H-β). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.7 (C=O), 162.5 (C-4'), 141.7 (C-β), 138.2 (C-1), 134.1 (C-2), 132.5 (C-1'), 131.4 (C-2' and C-6'), 130.8 (C-4), 130.0 (C-3), 126.3 (C-6), 126.3 (C-5), 123.0 (C-α), 114.3 (C-3' and C-5'), 65.5 (-OCH_2-), 32.1 (BrCH_2-), 29.6 (-CH_2-), 19.8 (2-CH_3). HRMS (ESI): calcd. for $C_{19}H_{19}BrO_2$ $[M + H]^+$ 358.0568, found 358.0526.

General Procedure of Synthesis of Coumarin-Chalcone Hybrids (8a-n)

Anhydrous potassium carbonate (0.2 g) was added to the solution of coumarin (**3**) (1 mmol) and derivatives (**7a-n**) (1 mmol) in acetonitrile (30 mL). The mixture was refluxed for 22 hours and then the reaction solution was poured into ice-water (25 mL). The precipitate was immediately formed, filtered off, washed several times with cold water, and dried to give hybrids **(8a-n)**.

7-(3-(4-cinnamoylphenoxy)propoxy)-4-methyl-2*H*-chromen-2-one (8a)
White powder, yield (57.8%); R_f = 0.35 in hexane:CH_2Cl_2 (1:1); m.p 168.3-170.5ºC. IR (KBr) (υ_{max}/ cm^{-1}): 3057(C-H *sp*^{2}), 2923 (C-H *sp*^{3}), 1717 (C=O lactone), 1658 (C=O ketone), 1607 (C=C olefinic), 1571 and 1509 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.37 (2H, m, -CH_2-), 2.42 (3H, s, 4"-CH_3), 4.25 (4H, m, 2xOCH_2), 6.16 (1H, s, H-3"), 6.86 (2H, m, H-6" and H-8"), 7.01 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.43 (3H, m, H-3, H-4 and H-5"), 7.50 (1H, d, *J* = 8.8 Hz, H-5), 7.54 (1H, d, *J* = 15.6 Hz, H-α), 7.65 (2H, m, H-2 and H-6), 7.80 (1H, d, *J* = 15.6Hz, H-β), 8.05 (2H, d, *J* = 8.8 Hz, H-2' and H-6'). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.7 (C=O ketone), 162.5 (C-4'), 161.8 (C=O lactone), 161.2 (C-7"), 155.2 (C-8a"), 152.4 (C-4"), 144.0 (C-β), 135.0 (C-1), 131.2 (C-1'), 130.8 (C-2' and C-6'), 130.3 (C-4), 128.9 (C-3 and C-5), 128.3 (C-2 and C-6), 125.5 (C-5"), 121.9 (C-α), 114.5 (C-3'and C-5'), 114.3 (C-3"), 113.7 (C-4a"), 112.4 (C-6"), 101.5 (C-8"), 64.8 (-OCH_2-), 64.4 (-OCH_2-), 28.9 (-CH_2-), 18.6 (4"-CH_3). HRMS (ESI): calcd. for $C_{28}H_{24}O_5$ $[M + H]^+$ 440.1624, found 440.1583.

(*E*)-7-(3-(4-(3-(4-chlorophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one (8b)
White powder, yield (67.2%); R_f = 0.38 in hexane:CH_2Cl_2 (1:1); m.p 178.8-180.4ºC. IR (KBr) (υ_{max}/ cm^{-1}): 3065 (C-H *sp*^{2}), 2927 (C-H *sp*^{3}), 1719 (C=O lactone), 1659 (C=O ketone), 1608 (C=C olefinic), 1568 and 1510 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.35 (2H, t, *J* = 6.0 Hz, -CH_2-), 2.41 (3H, s, 4"-CH_3), 4.24 (4H, m, 2xOCH_2), 6.15 (1H, s, H-3"), 6.85 (2H, m, H-6" and H-8"), 7.01 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.39 (2H, d, *J* = 8.4 Hz, H-3 and H-5), 7.50 (1H, d, *J* = 7.6 Hz, H-5"), 7.51 (1H, d, *J* = 15.6 Hz, H-α), 7.58 (2H, d, *J* = 8.4 Hz, H-2 and H-6), 7.74 (1H, d, *J* = 15.6 Hz, H-β), 8.03 (2H, d, *J* = 8.8 Hz, H-2' and H-6'). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.3 (C=O ketone), 162.7 (C-4'), 161.7 (C=O lactone), 161.2 (C-7"), 155.2 (C-8a"), 152.4 (C-4"), 142.5 (C-β), 136.2 (C-4), 133.5 (C-1), 131.1 (C-1'), 130.8 (C-2' and C-6'), 129.4 (C-3 and C-5), 129.2 (C-2 and C-6), 125.5 (C-5"), 122.3 (C-α), 114.3 (C-3'and C-5'), 113.7 (C-3"), 112.4 (C-4a"), 112.1 (C-6"), 101.5 (C-8"), 64.8 (-OCH_2-), 64.4 (-OCH_2), 28.9 (-CH_2-), 18.6 (4"-CH_3). HRMS (ESI): calcd. for $C_{28}H_{23}ClO_5$ $[M + H]^+$ 474.1234, found 474.1180.

(*E*)-7-(3-(4-(3-(3-chlorophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one (8c)
White powder, yield (72.9%); R_f = 0.49 in hexane:CH_2Cl_2 (1:1); m.p 187.2-188.5ºC. IR (KBr) (υ_{max}/ cm^{-1}): 3069 (C-H *sp*^{2}), 2824 (C-H *sp*^{3}), 1716 (C=O lactone), 1659 (C=O ketone), 1608 (C=C olefinic), 1571 and 1509 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.34 (2H, q, *J* = 6.0 Hz, -CH_2-), 2.41 (3H, s, 4"-CH_3), 4.25 (4H, m, 2xOCH_2), 6.16 (1H, s, H-3"), 6.86 (2H, m, H-6" and H-8"), 7.01 (2H, d, *J*

= 8.4 Hz, H-3' and H-5'), 7.35 (2H, m, H-4 and H-6), 7.50 (2H, m, H-5 and H-5"), 7.53 (1H, d, *J* = 15.6 Hz, H-α), 7.65 (1H, s, H-2), 7.72 (1H, d, *J* = 15.6 Hz, H-β), 8.05 (2H, d, *J* = 8.4 Hz, H-2' and H-6'). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.2 (C=O ketone), 162.7 (C-4'), 161.8 (C=O lactone), 161.2 (C-7"), 155.2 (C-8a"), 152.4 (C-4"), 142.2 (C-β), 136.9 (C-1), 134.9 (C-3), 130.9 (C-2'and C-6'), 130.1 (C-2 and C-6), 127.7 (C-1' and C-5), 126.7 (C-4), 125.5 (C-5"), 123.1 (C-α), 114.4 (C-3'and C-5'), 113.7 (C-3"), 112.4 (C-4a"), 112.1 (C-6"), 101.5 (C-8"), 64.7 (-OCH_2-), 64.4 (-OCH_2-), 28.9 (-CH_2-), 18.6 (4"-CH_3). HRMS (ESI): calcd. for $C_{28}H_{23}ClO_5$ $[M + H]^+$ 474.1234, found 474.1193.

(*E*)-7-(3-(4-(3-(2-chlorophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one (8d)
White powder, yield (68.3%); R_f = 0.45 in hexane:CH_2Cl_2 (1:1); m.p 169.0-170.7ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3066 (C-H *sp*^{2}), 2953 (C-H *sp*^{3}), 1717 (C=O lactone), 1658 (C=O ketone), 1607 (C=C olefinic), 1571 and 1509 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.35 (2H, t, *J* = 6.0 Hz, -CH_2-), 2.41 (3H, s, 4"-CH_3), 4.25 (4H, m, 2xOCH_2), 6.15 (1H, s, H-3"), 6.86 (2H, m, H-6" and H-8"), 7.01 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.33 (2H, m, H-4 and H-5), 7.45 (3H, m, H-3, H-α and H-5"), 7.75 (1H, dd, *J* = 2.8 Hz and *J* = 5.6 Hz, H-6), 8.04 (2H, d, *J* = 8.8 Hz, H-2' and H-6'), 8.16 (1H, d, *J* = 15.6 Hz, H-β). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.6 (C=O ketone), 162.7 (C-4'), 161.8 (C=O lactone), 161.2 (C-7"), 155.2 (C-8a"), 152.4 (C-4"), 139.8 (C-β), 135.3 (C-2), 133.4 (C-1), 130.9 (C-3, C-4, C-2'and C-6'), 130.2 (C-1'), 127.7 (C-6), 127.0 (C-5), 125.5 (C-5"), 124.7 (C-α), 114.3 (C-3'and C-5'), 113.7 (C-3"), 112.4 (4a"), 112.0 (C-6"), 101.5 (C-8"), 64.8 (-OCH_2-), 64.4 (-OCH_2-), 28.9 (-CH_2-), 18.6 (4"-CH_3). HRMS (ESI): calcd. for $C_{28}H_{23}ClO_5$ $[M + H]^+$ 474.1234, found 474.1190.

(*E*)-7-(3-(4-(3-(4-bromophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one (8e)
Yellow powder, yield (86.6%); R_f = 0.44 in hexane:CH_2Cl_2 (1:1); m.p 185.6-187.3ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3062(C-H *sp*^{2}), 2923 (C-H *sp*^{3}), 1718 (C=O lactone), 1658 (C=O ketone), 1607(C=C olefinic), 1589 and 1510 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.34 (2H, m, -CH_2-), 2.41 (3H, s, 4"-CH_3), 4.25 (4H, q, *J* = 6.6 Hz, 2xOCH_2), 6.16 (1H, s, H-3''), 6.86 (2H, m, H-6'' and H-8''), 7.01 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.50 (6H, m, H-2, H-3, H-5, H-5'', H-6 and H-α), 7.73 (1H, d, *J* = 15.6 Hz, H-β), 8.04 (2H, d, *J* = 8.8 Hz, H-2' and H-6'). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.3 (C=O ketone), 162.7 (C-4'), 161.7 (C=O lactone), 161.2 (C-7"), 155.2 (C-8a"), 152.4 (C-4"), 142.5 (C-β), 134.0 (C-4), 132.1 (C-2'and C-6'), 131.1 (C-1), 130.8 (C-3 and C-5), 129.7 (C-2 and C-6), 125.5 (C-5"), 124.5 (C-1'), 122.3 (C-α), 114.3 (C-3'and C-5'), 113.7 (C-3"), 112.4 (C-4a"), 112.1 (C-6"), 101.5 (C-8"), 64.7 (-OCH_2-), 64.4 (-OCH_2-), 28.9 (-CH_2-), 18.6 (4"-CH_3). HRMS (ESI): calcd. for $C_{28}H_{23}BrO_5$ $[M + H]^+$ 518.0729, found 518.0664.

(*E*)-7-(3-(4-(3-(3-bromophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one (8f)
Yellow powder, yield (84.0%); R_f = 0.48 in hexane:CH_2Cl_2 (1:1); m.p 180.9-182.1ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3060 (C-H *sp*^{2}), 2924 (C-H *sp*^{3}), 1720 (C=O lactone), 1660 (C=O ketone), 1608 (C=C olefinic), 1510 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.37 (2H, t, *J* = 6.0 Hz, -CH_2-), 2.41 (3H, s, 4"-CH_3), 4.25 (4H, m, 2xOCH_2), 6.16 (1H, s, H-3''), 6.86 (2H, m, H-6'' and H-8''), 7.01 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.29 (1H, t, *J* = 7.8 Hz, H-5), 7.50 (4H, m, H-4, H-5'', H-6 and H-α), 7.71 (1H, d, *J* = 15.6 Hz, H-β), 7.81 (1H, s, H-2), 8.04 (2H, d, *J* = 8.8 Hz, H-2' and H-6'). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.1 (C=O ketone), 162.7 (C-4'), 161.7 (C=O lactone), 161.2 (C-7"), 155.2 (C-8a"), 152.4 (C-4"), 142.1 (C-β), 137.2 (C-1), 133.0 (C-2), 130.9 (C-2', C-5 and C-6'), 130.7 (C-4), 130.4 (C-1'), 127.1 (C-6), 125.5 (C-5"), 123.1 (C-3 and C-α), 114.4 (C-3'and C-5'), 113.7 (C-3"), 112.4 (C-4a"), 112.1 (C-6"), 101.5 (C-8"), 64.7 (-OCH_2-), 64.4 (-OCH_2-), 28.9 (-CH_2-), 18.6 (4"-CH_3). HRMS (ESI): calcd. for $C_{28}H_{23}BrO_5$ $[M + H]^+$ 518.0729, found 518.0680.

(*E*)-7-(3-(4-(3-(2-bromophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one (8g)
Yellow powder, yield (73.3%); R_f = 0.55 in hexane:CH_2Cl_2 (1:1); m.p 177.3-187.3ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3063 (C-H *sp*^{2}), 2952 (C-H *sp*^{3}), 1719 (C=O lactone), 1659 (C=O ketone), 1605 (C=C olefinic), 1572 and 1509 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.35 (2H, m, -CH_2-), 2.41 (3H, s, 4"-CH_3), 4.25 (4H, m, 2xOCH_2), 6.16 (1H, s, H-3''), 6.86 (2H, m, H-6'' and H-8''), 7.01 (2H, d, *J* = 8.8

Hz, H-3' and H-5'), 7.24 (1H, dd, *J* = 1.2 Hz and *J* = 8.0 Hz, H-4), 7.36 (1H, t, *J* = 7.6 Hz, H-5), 7.43 (1H, d, *J* = 16.0 Hz, H-α), 7.50 (1H, d, *J* = 8.8 Hz, H-5''), 7.65 (1H, d, *J* = 8.0 Hz, H-6), 7.74 (1H, dd, *J* = 1.6 Hz and *J* = 8.0 Hz, H-3), 8.04 (2H, d, *J* = 8.8 Hz, H-2' and H-6'), 8.11 (1H, d, *J* = 16.0 Hz, H-β). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.6 (C=O ketone), 162.7 (C-4'), 161.8 (C=O lactone), 161.2 (C-7"), 155.3 (C-8a"), 152.4 (C-4"), 139.8 (C-β), 135.4 (C-2), 133.5 (C-1), 131.0 (C-3, C-4, C-2'and C-6'), 130.3 (C-1'), 127.8 (C-6), 127.0 (C-5), 125.6 (C-5"), 124.7 (C-α), 114.4 (C-3'and C-5'), 113.7 (C-3"), 112.5 (C-4a"), 112.1 (C-6"), 101.5 (C-8"), 64.8 (-OCH_2-), 64.4 (-OCH_2-), 28.9 (-CH_2-), 18.6 (4''-CH_3). HRMS (ESI): calcd. for $C_{28}H_{23}BrO_5$ $[M + H]^+$ 518.0729, found 518.0740.

(*E*)-4-methyl-7-(3-(4-(3-(4-nitrophenyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one (8h)
Pale yellow powder, yield (72.1%); R_f = 0. 58 in hexane:CH_2Cl_2 (1:1); m.p 243.4-244.8ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3076 (C-H *sp*^{2}), 2946 (C-H *sp*^{3}), 1713 (C=O lactone), 1660 (C=O ketone), 1610 (C=C olefinic), 1601 and1512 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.34 (2H, q, *J* = 6.0 Hz, -CH_2-), 2.41 (3H, s, 4"-CH_3),4.25 (4H, m, 2xOCH_2), 6.16 (1H, s, H-3''), 6.86 (1H, d, *J* = 7.6 Hz, H-8''), 6.88 (1H, dd, *J* = 2.4 and 8.8 Hz, H-6''), 7.03 (2H, d, *J* = 8.4 Hz, H-3'-H and H-5'), 7.50 (1H, d, *J* = 8.8 Hz, H-5''), 7.65 (1H, d, *J* = 16.0 Hz, H-α), 7.79 (3H, m, H-β, H-3 and H-5), 8.06 (2H, d, *J* = 8.4 Hz, H-2 and H-6), 8.28 (2H, d, *J* = 8.4 Hz, H-2' and H-6'). ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.7 (C=O ketone), 163.0 (C-4'), 161.7 (C=O lactone), 161.2 (C-7"), 155.3 (C-8a"), 152.4 (C-4"), 148.5 (C-4), 141.3 (C-β), 140.7 (C-1), 131.0 (C-2' and C-6'), 130.6 (C-1'), 128.8 (C-2 and C-6), 125.6 (C-5"), 125.6 (C-α), 124.2 (C-3 and C-5), 114.5 (C-3' and C-5'), 113.7 (C-3"), 112.5 (C-4a"), 112.1 (C-6"), 101.5 (C-8"), 64.7 (-OCH_2-), 64.5 (-OCH_2-), 28.9 (-CH_2-), 18.6 (4''-CH_3). HRMS (ESI): calcd. for $C_{28}H_{23}NO_7$ $[M + H]^+$ 485.1475, found 485.1419.

(*E*)-4-methyl-7-(3-(4-(3-(3-nitrophenyl)acryloyl)phenoxy) propoxy)-2*H*-chromen-2-one (8i)
Pale yellow powder, yield (83.3%); R_f = 0.62 in hexane:CH_2Cl_2 (1:1); m.p 256.2-257.8ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3079 (C-H *sp*^{2}), 2951 (C-H *sp*^{3}), 1713 (C=O lactone), 1660 (C=O ketone), 1609 (C=C olefinic), 1573and 1511 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.36 (2H, q, *J* = 6.0 Hz , -CH_2-), 2.42 (3H, s, 4"-CH_3), 4.26 (4H, m, 2xOCH_2), 6.16 (1H, s, H-3''), 6.86 (2H, m, H-6'' and H-8''), 7.04 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.51 (1H, d, *J* = 8.8 Hz, H-5''), 7.62 (1H, d, *J* = 8.0 Hz, H-4), 7.66 (1H, d, *J* = 15.6 Hz, H-α), 7.82 (1H, d, *J* = 15.6 Hz, H-β), 7.92 (1H, d, *J* = 7.6 Hz, H-6), 8.07 (2H, d, *J* = 8.8 Hz, H-2' and H-6'), 8.26 (1H, d, *J* = 8.4 Hz, H-5), 8.54 (1H, s, H-2). ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.7 (C=O ketone), 162.9 (C-4'), 161.7 (C=O lactone), 161.2 (C-7"), 155.2 (C-8a"), 152.4 (C-4"), 148.7 (C-3), 140.8 (C-β), 136.8 (C-1), 134.3 (C-6), 131.0 (C-2' and C-6'), 130.7 (C-1'), 130.0 (C-5), 125.5 (C-5"), 124.5 (C-4), 124.4 (C-2), 122.1 (C-α), 114.5 (C-3' and C-5'), 113.7 (C-3"), 112.4 (C-4a"), 112.1 (C-6"), 101.5 (C-8"), 64.7 (-OCH_2-), 64.4 (-OCH_2-), 28.9 (-CH_2-), 18.6 (4''-CH_3). HRMS (ESI): calcd. for $C_{28}H_{23}NO_7$ $[M + H]^+$ 485.1475, found 485.1414.

(*E*)-7-(3-(4-(3-(4-methoxyphenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one (8j)
Yellow powder, yield (73.7%); R_f = 0.55 in hexane:CH_2Cl_2 (1:1); m.p 192.9-194.4ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3070 (C-H *sp*^{2}), 2956 (C-H *sp*^{3}), 1724 (C=O lactone), 1654 (C=O ketone), 1601 (C=C olefinic), 1570 and 1510 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.35-2.38 (2H, t, *J* = 6.0 Hz, -CH_2-), 2.42 (3H, s, 4"-CH_3), 3.88 (3H, s, OCH_3), 4.25 (4H, m, 2xOCH_2), 6.16 (1H, s, H-3''), 6.86 (1H, d, *J* = 2.4 Hz, H-8''), 6.88 (1H, dd, *J* = 2.4 and 8.8 Hz, H-6''), 6.95 (2H, d, *J* = 8.8 Hz, H-3' and H-5'), 7.01 (2H, d, *J* = 8.8 Hz, H-3 and H-5), 7.43 (1H, d, *J* = 15.6 Hz, H-α), 7.50 (1H, d, *J* = 8.8 Hz, H-5''), 7.61 (2H, d, *J* = 8.8 Hz, H-2 and H-6), 7.78 (1H, d, *J* = 15.6 Hz, H-β), 8.04 (2H, d, *J* = 8.8 Hz, H-2' and H-6'). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.7 (C=O ketone), 162.4 (C-4'), 161.8 (C=O lactone), 161.5 (C-7"), 161.2 (C-8a"), 155.2 (C-4"), 152.4 (C-4), 143.8 (C-β), 131.5 (C-1), 130.7 (C-2 and C-6), 130.0 (C-2' and C-6'), 127.8 (C-1'), 125.5 (C-5"), 119.5 (C-α), 114.4 (C-3' and C-5'), 114.2 (C-3 and C-5), 113.7 (C-3"), 112.4 (C-4a"), 112.0 (C-6"), 101.5 (C-8"), 64.8 (-OCH_2-), 64.3 (-OCH_2-), 55.4 (4-OCH_3), 28.9 (-CH_2-), 18.6 (4''-CH_3). HRMS (ESI): calcd. for $C_{29}H_{26}O_6$ $[M + H]^+$ 470.1729, found 470.1688.

(*E*)-7-(3-(4-(3-(3-methoxyphenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one (8k)

Pale yellow powder, yield (84.1%); R_f = 0.58 in hexane:CH_2Cl_2 (1:1); m.p 197.1-199.2ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3069 (C-H sp^2), 2960 (C-H sp^3), 1724 (C=O lactone), 1658 (C=O ketone), 1607 (C=C olefinic), 1510 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.37 (2H, t, *J* = 6.0 Hz, -CH_2-), 2.42 (3H, s, 4”-CH_3), 3.88 (3H, s, OCH_3), 4.25 (2H, t, *J* = 6.0 Hz 2xOCH_2), 6.16 (1H, s, H-3’’), 6.88 (2H, m, H-6’’ and H-8’’), 6.97 (3H, m, H-3’, H-5’ and H-4), 7.17 (1H, s, H-2), 7.25 (1H, d, *J* = 7.6 Hz, H-6), 7.34 (1H, t, *J* = 8.0 Hz, H-5), 7.50 (1H, d, *J* = 8.8 Hz, H-5’’), 7.52 (1H, d, *J* = 15.6 Hz, H-α), 7.76 (1H, d, *J* = 15.6 Hz, H-β), 8.04 (2H, d, *J* = 8.8 Hz, H-2’ and H-6’). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.7 (C=O ketone), 162.4 (C-4’), 161.8 (C=O lactone), 161.5 (C-3), 161.2 (C-7”), 155.3 (C-8a”), 152.4 (C-4”), 143.9 (C-β), 131.5 (C-1), 130.7 (C-2’ and C-6’), 130.1 (C-1’ and C-5), 127.8 (C-6), 125.5 (C-5”), 119.6 (C-α), 114.4 (C-3’ and C-5’), 114.3 (C-2 and C-4), 113.7 (C-3”), 112.5 (C-4a”), 112.1 (C-6”), 101.6 (C-8”), 64.8 (-OCH_2-), 64.4 (-OCH_2-), 55.4 (3-OCH_3), 29.0 (-CH_2-), 18.6 (4’’-CH_3). HRMS (ESI): calcd. for $C_{29}H_{26}O_6$ $[M + H]^+$ 470.1729, found 470.1688.

(*E*)-4-methyl-7-(3-(4-(3-(*p*-tolyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one (8l)
Yellow powder, yield (52.2%); R_f = 0.66 in hexane:CH_2Cl_2 (1:1); m.p 180.4-182.7ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3068 (C-H sp^2), 2922 (C-H sp^3), 1724 (C=O lactone), 1657 (C=O ketone), 1605 (C=C olefinic), 1569 and 1509 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.34 (2H, q, *J* = 6.0 Hz, -CH_2-), 2.41 (6H, s, 4-CH_3 and 4”-CH_3), 4.25 (4H, m, 2xOCH_2), 6.16 (1H, s, H-3”), 6.88 (2H, m, H-6” and H-8”), 7.01 (2H, d, *J* = 8.8 Hz, H-3’and H-5’), 7.23 (2H, d, *J* = 8.0 Hz, H-3 and H-5), 7.50 (d, 1H, *J* = 8.8 Hz, H-5”), 7.50 (1H, d, *J* = 15.6 Hz, H-α), 7.55 (2H, d, *J* = 8.0 Hz, H-2 and H-6), 7.79 (1H, d, *J* = 15.6 Hz, H-β), 8.04 (2H, d, *J* = 8.8 Hz, H-2’ and H-6’). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.8 (C=O ketone), 162.5 (C-4’), 161.8 (C=O lactone), 161.2 (C-7”), 155.3 (C-8a”), 152.4 (C-4”), 144.1 (C-β), 140.8 (C-4), 132.3 (C-1), 131.4 (C-1’), 130.7 (C-2’ and C-6’), 129.6 (C-3 and C-5), 128.3 (C-2 and C-6), 125.5 (C-5”), 120.8 (C-α), 114.3 (C-3’ and C-5’), 113.7 (C-3”), 112.4 (C-4a”), 112.1 (C-6”), 101.5 (C-8”), 64.8 (-OCH_2-), 64.3 (-OCH_2-), 28.9 (-CH_2-), 21.5 (4-CH_3), 18.6 (4’’-CH_3). HRMS (ESI): calcd. for $C_{29}H_{26}O_5$ $[M + H]^+$ 454.1780, found 454.1729.

(*E*)-4-methyl-7-(3-(4-(3-(*m*-tolyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one (8m)
White powder, yield (38.5%); R_f = 0.75 in hexane:CH_2Cl_2 (1:1); m.p 172.3-173.5ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3069 (C-H sp^2), 2922 (C-H sp^3), 1736 (C=O lactone), 1658 (C=O ketone), 1607 (C=C olefinic), 1571 and 1509 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.35 (2H, m, -CH_2-), 2.42 (6H, s, 3-CH_3 and 4”-CH_3), 4.25 (4H, m, 2xOCH_2), 6.16 (1H, s, H-3”), 6.88 (2H, m, H-6” and H-8”), 7.01 (2H, d, *J* = 8.8 Hz, H-3’ and H-5’), 7.23 (1H, d, *J* = 7.6 Hz, H-2), 7.31 (1H, t, *J* = 7.8 Hz, H-5), 7.46 (2H, d, *J* = 6.8 Hz, H-4 and H-6), 7.50 (d, 1H, *J* = 8.8 Hz, H-5”), 7.53 (1H, d, *J* = 15.6 Hz, H-α), 7.78 (1H, d, *J* = 15.6 Hz, H-β), 8.05 (2H, d, *J* = 8.8 Hz, H-2’ and H-6’). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.6 (C=O ketone), 162.5 (C-4’), 161.7 (C=O lactone), 161.2 (C-7”), 155.2 (C-8a”), 152.4 (C-4”), 141.7 (C-β), 138.2 (C-3), 134.1 (C-1), 131.3 (C-1’), 131.0 (C-5), 130.8 (C-2’and C-6’), 130.0 (C-4), 126.3 (C-2), 126.2 (C-6), 125.5 (C-5”), 122.9 (C-α), 114.3 (C-3’and C-5’), 113.7 (C-3”), 112.4 (C-4a”), 112.0 (C-6”), 101.5 (C-8”), 64.7 (-OCH_2-), 64.3 (-OCH_2-), 28.9 (-CH_2-), 19.8 (3-CH_3), 18.6 (4’’-CH_3). HRMS (ESI): calcd. for $C_{29}H_{26}O_5$ $[M + H]^+$ 454.1780, found 454.1725.

(*E*)-4-methyl-7-(3-(4-(3-(*o*-tolyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one (8n)
White powder, yield (41.6%); R_f = 0.69 in hexane:CH_2Cl_2 (1:1); m.p 162.7-164.5ºC. IR (KBr) (υ $_{max}$/ cm^{-1}): 3067 (C-H sp^2), 2952 (C-H sp^3), 1722 (C=O lactone), 1656 (C=O ketone), 1603 (C=C olefinic), 1570 and 1510 (C=C aromatic). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.36 (2H, t, *J* = 6.0 Hz, -CH_2-), 2.41(3H, s, 4”-CH_3), 2.50 (3H, s, 2-CH_3), 4.25 (4H, m, 2xOCH_2), 6.15 (1H, s, H-3”), 6.86 (2H, m, H-6” and H-8”), 7.01 (2H, d, *J* = 8.8 Hz, H-3’ and H-5’), 7.24 (1H, d, *J* = 7.6 Hz, H-3), 7.30 (2H, m, H-4 and H-5), 7.46 (2H, m, H-α and H-5”), 7.70 (1H, d, *J* = 7.6 Hz, H-6), 8.05 (2H, d, *J* = 8.8 Hz, H-3’ and H-5’), 8.10 (1H, d, *J* = 15.6 Hz, H-β). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.6 (C=O ketone), 162.5 (C-4’), 161.8 (C=O lactone), 161.2 (C-7”), 155.2 (C-8a”), 152.4 (C-4”), 141.7 (C-β), 138.2 (C-1), 134.1 (C-2), 131.3 (C-1’), 130.8 (C-2’and C-6’), 130.0 (C-3 and C-4), 126.3 (C-6), 126.3 (C-5), 125.5 (C-5”), 123.0 (C-α), 114.3 (C-3’and C-5’), 113.7 (C-3”), 112.4 (C-4a”), 112.1 (C-6”), 101.5 (C-8”), 64.8 (-OCH_2-),

64.4 (-OCH_2-), 28.9 (-CH_2-), 19.8 (2-CH_3), 18.6 (4''-CH_3). HRMS (ESI): calcd. for $C_{29}H_{26}O_5$ $[M + H]^+$ 454.1780, found 454.1727.

ADMET profile

Prediction of physicochemical and ADMET properties of the synthesised compounds was carried out in silico with a combination of several web servers such as SwissADME, pkCSM, and ProTox-II, with the procedure as reported in our previous study [11]. Several critical parameters were predicted, including molecular weight (Mol Wt), topological polar surface area (TPSA), number of hydrogen bond donors (HBD), number of hydrogen bond acceptors (HBA), octanol/water partition coefficient (log P), aqueous solubility (log S), Caco-2 permeability (Caco2), brain/blood partition coefficient (log BB), number of rotatable bonds (Rot), acute toxicity (Acute tox.), predicted LD50 (pLD50), and Ames mutagenicity (Ames).

***In vitro* inhibition study on AChE**

The assay for AChE inhibitory activity was done based on a modified protocol reported by Yang *et al*. [12]. Acetylcholinesterase (Type VI-S, from Electrophorus electricus), 5,5′-dithiobis-2-nitrobenzoic acid (Ellman's reagent, DTNB) and acetylthiocholine chloride (ATCI) were purchased from Sigma Aldrich. Enzyme solutions were prepared to give 0.28 units/mL aliquots. Stock Solutions were prepared by dissolving 1 mg of tested compounds in 1 mL of DMSO and diluted to a final concentration of 1000, 800, 600, 400, 200, 100, and 50 µg/mL. The assay buffer solution (pH = 8.0) was prepared by taking 93.2 mL of solution (6 g of sodium dihydrogen phosphate was dissolved in 500 mL of deionized water and mixed with 6.8 mL of solution (7 g of sodium hydrogen phosphate was dissolved in 500 mL of deionized water) and adjusted. Otherwise, 57.7 mL of sodium dihydrogen phosphate and 42.3 mL of sodium hydrogen phosphate were mixed and adjusted to prepare buffer (pH = 7.0). Furthermore, freshly solutions of 0.01 M DTNB (0.396 g of DTNB and 15 mg $NaHCO_3$ were dissolved in 100 mL of buffer pH 7.0) in dark place, and 0.075 M ATCI (0.2048 g of ATCI was dissolved in 10 mL of deionized water), were prepared. In 96-well plates, 20 µL of the test compounds, 10 µL of DTNB, 15 µL of enzyme (AChE) and 140 µL of buffer solution (pH = 8.0), were added in dark conditions and incubated for 15 min, followed by the addition of ATCI (10 µL) and incubated again for the same period. The activity was measured by reading the absorbance of the solution at 412 nm. Blanks containing all the components except the enzyme were carried out. IC_{50} values were calculated as the concentration of a compound that produces 50% enzyme activity inhibition, using the GraphPad Prism 8 programme package. Results are expressed as the mean ± SD of at least three different experiments performed in triplicate.

Cytotoxicity Studies

Norman human liver cells, THLE-2 were a kind gift from Dr. Biswas, AIMMSCR, Amity University and were cultured in DMEM-F12 (HiMedia) media supplemented with 10% FBS (HiMedia), 70ng/mL of phosphoethanolamine (TCI Chemicals), 5ng/mL of epidermal growth factor (Gibco), Insulin Transferrin Selenium (ThermoScientific, diluted to 1X), Penicillin-Streptomycin solution, 100µg/mL (HiMedia), at 5%CO2 in a CO2 incubator. Experiments were carried out when cells were 70-80% confluent. To perform the cell viability assay, a 96-well plate (SPL) was coated with collagen peptide and incubated for 2-3 hours prior to cell seeding. $5x10^3$ of THLE-2 cells were resuspended in complete medium as described above and seeded in each well. After 24 hours, the media was carefully aspirated from the wells. Stock solution of synthesised compounds were prepared in DMSO. Cells were treated with the respective compounds dissolved in complete culture medium at different concentrations for 12 hours. MTT reagent (HiMedia) with a final concentration of 0.5 mg/mL was added to each well and further incubated for 4 hours. An equal volume of DMSO (SRL) was added to each well to solubilize the formazan crystals with a final incubation of 15-20 minutes. Absorbance was measured

using a Multiskan Microplate Reader (ThermoScientific) at 570 nm wavelength. All experiments were performed in triplicates.

Table S1. Optimum range of physicochemical and ADMET parameters

Molecular descriptor	**Optimum range** Error! Reference source not found.
Molecular weight (Mol wt) in g/mol	130-725
Topological polar surface area in Å²	90-140
No. of hydrogen bond donor groups (HBD)	0-6
No. of hydrogen bond acceptor groups (HBA)	2-20
Octanol/water partition coefficient (log P)	-2 to 6.5
Aqueous solubility (log S) in mol/L	-6.5 to 0.5
Apparent Caco-2 cell permeability (PCaco) in 10^{-6} cm/s	<0.25 poor; >5 great
Brain/blood partition coefficient (log BB)	-0.3 to 1.2
No. of rotatable bonds (Rot)	0-15

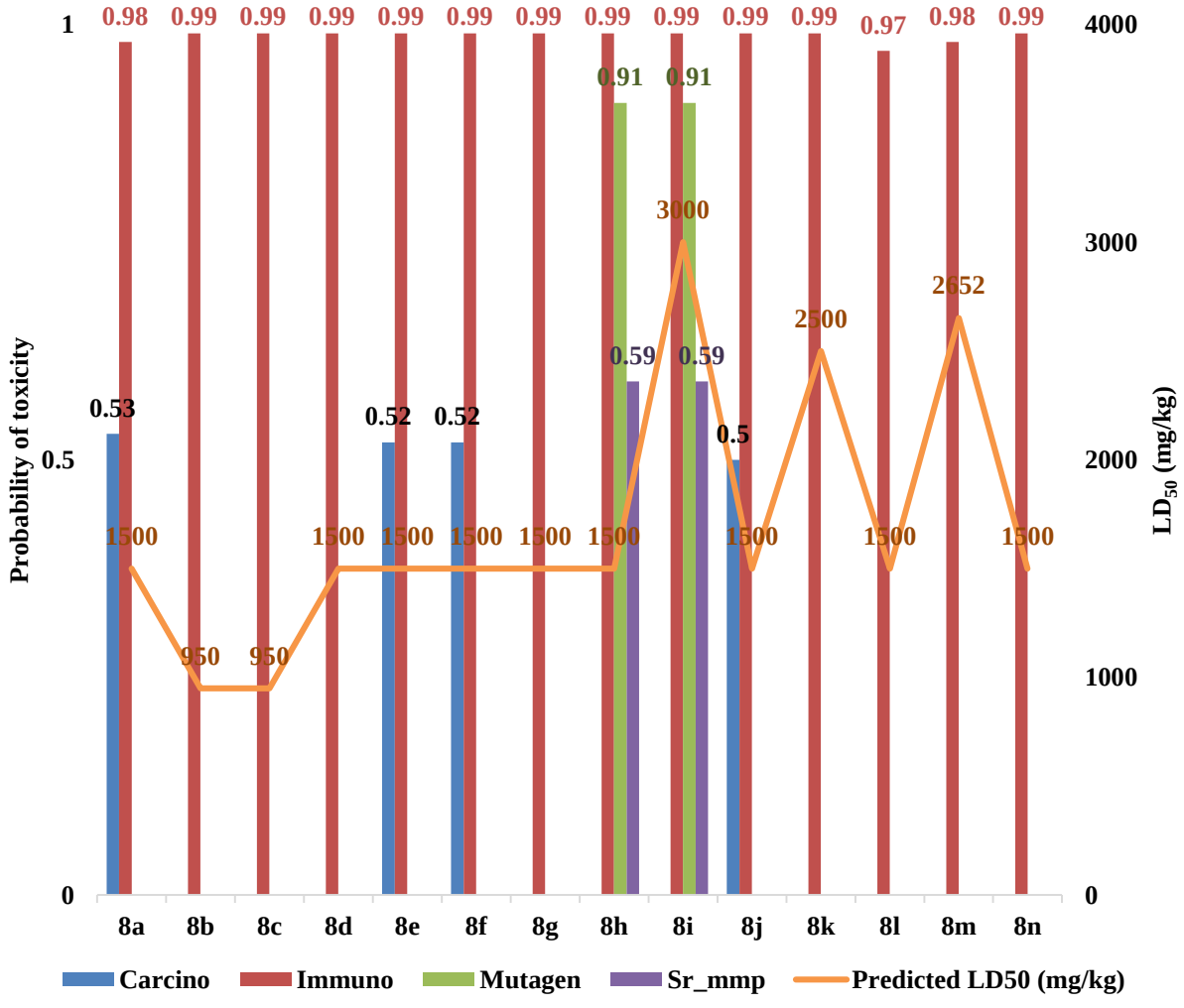


Figure S1. Prediction of toxicity parameters with ProTox-II

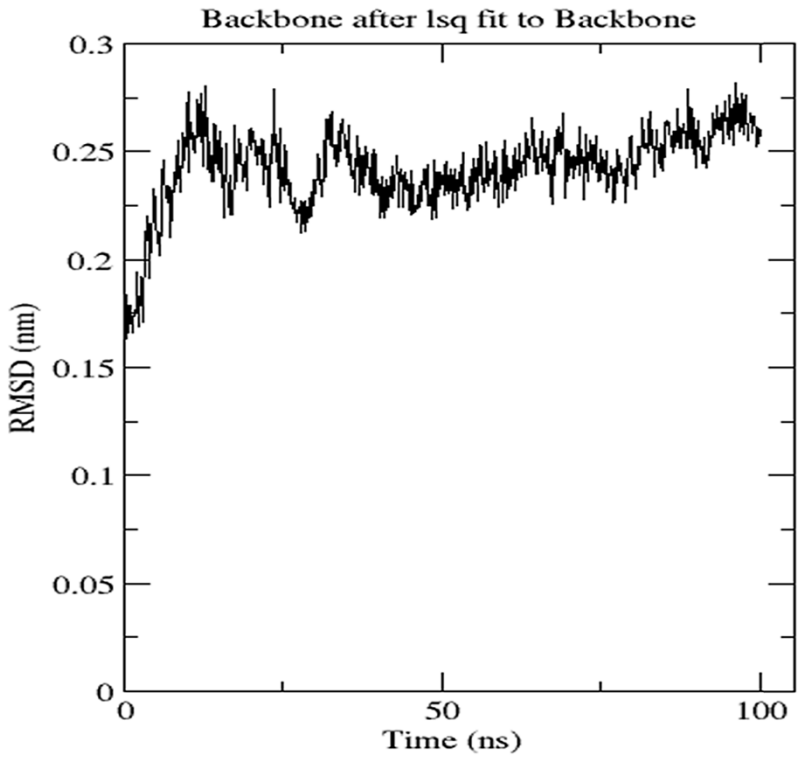


Figure S2. The root mean square deviation (RMSD) of solvated protein backbone and ligand complex during 100 ns MD simulation

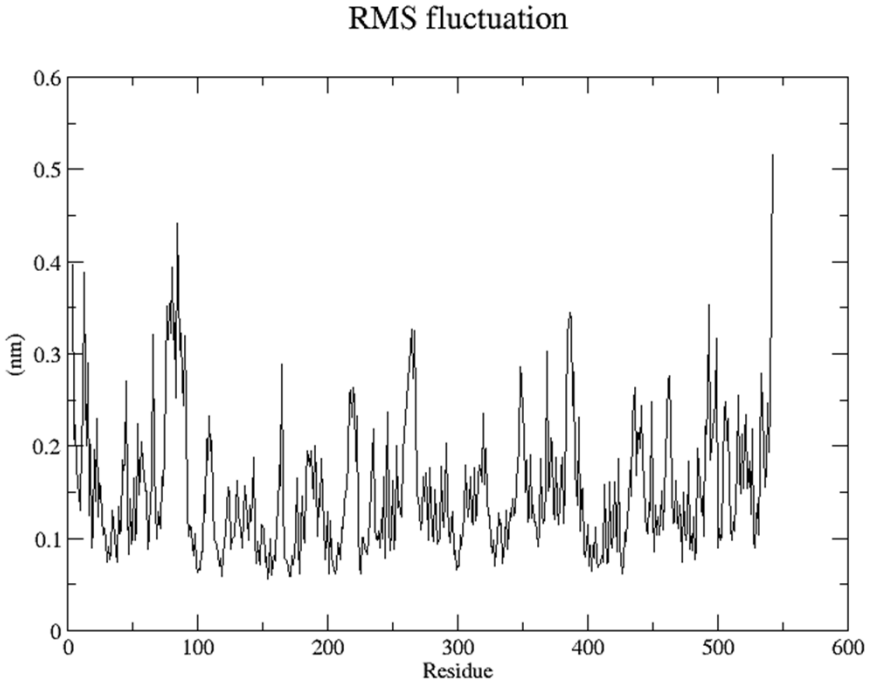


Figure S3. The root mean square fluctuation (RMSF) values of solvated protein-ligand complex plotted against residue numbers

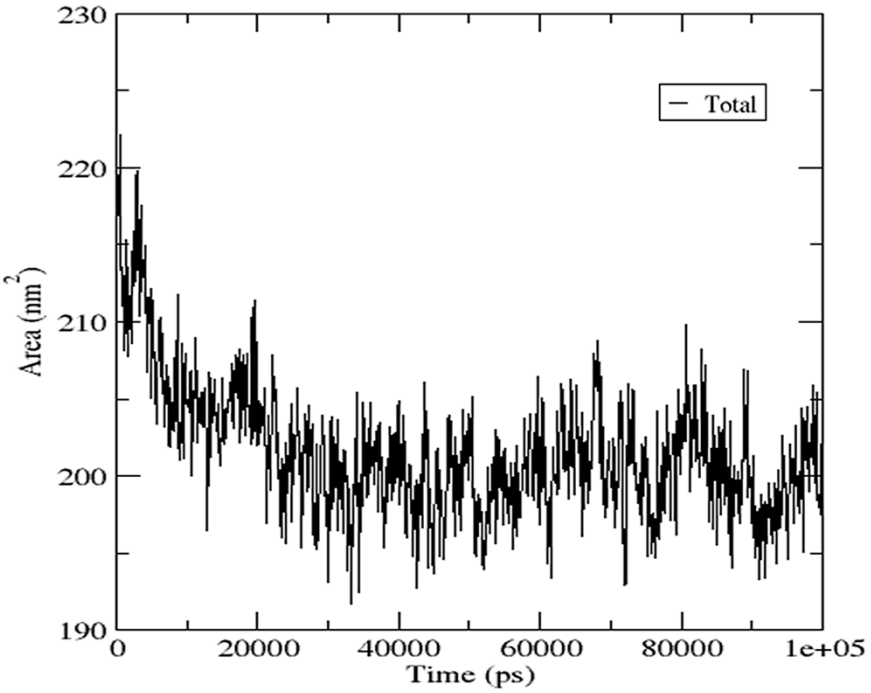


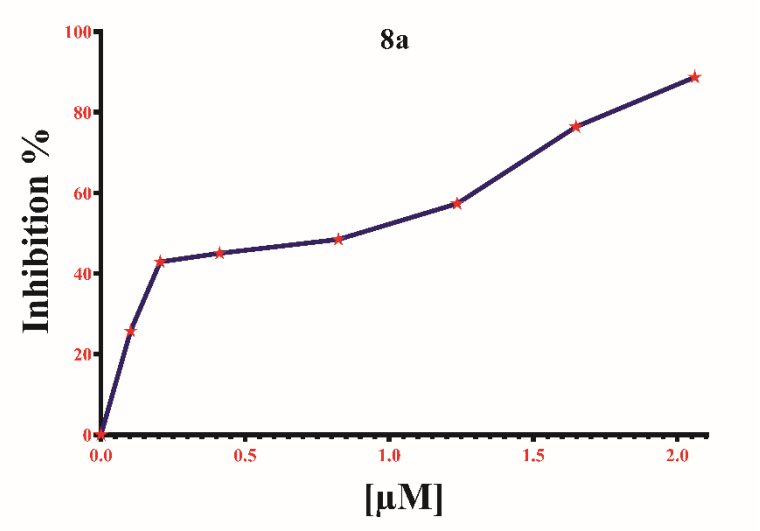
Figure S4. Solvent accessible surface area (SASA) analysis for protein-ligand complex during 100 ns simulation time

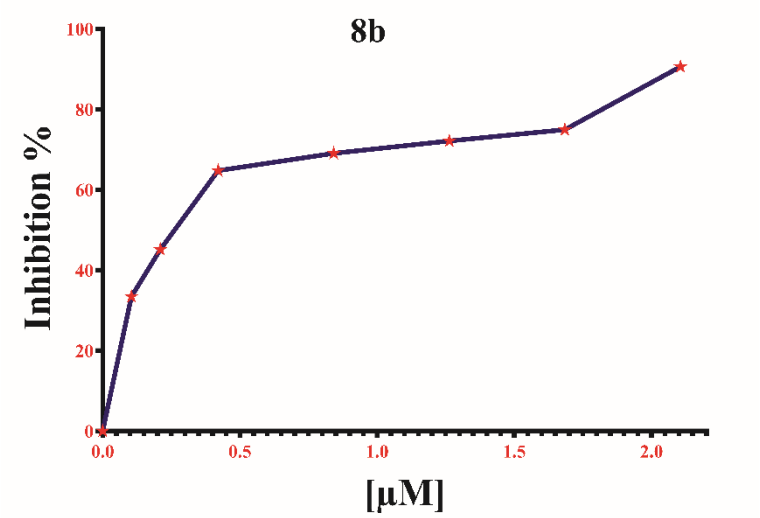
IC_{50} Calculations

Percentage inhibition was calculated by this formula:

$$\%\ (\text{Inhibition}) = \frac{B - A}{B} X\ 100$$

- A= absorbance of the enzyme with test sample;
- B = absorbance of enzyme without test sample.
- Each experiment was repeated thrice.
- Concentrations were converted from µg/mL to µM.
- IC_{50} value was calculated by GraphPad Prism.
- Galantamine was used as reference compound.


8a
Inhibition %
100
80
60
40
20
0
0.0
0.5
1.0
1.5
2.0
[µM]


8b
Inhibition %
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40
20
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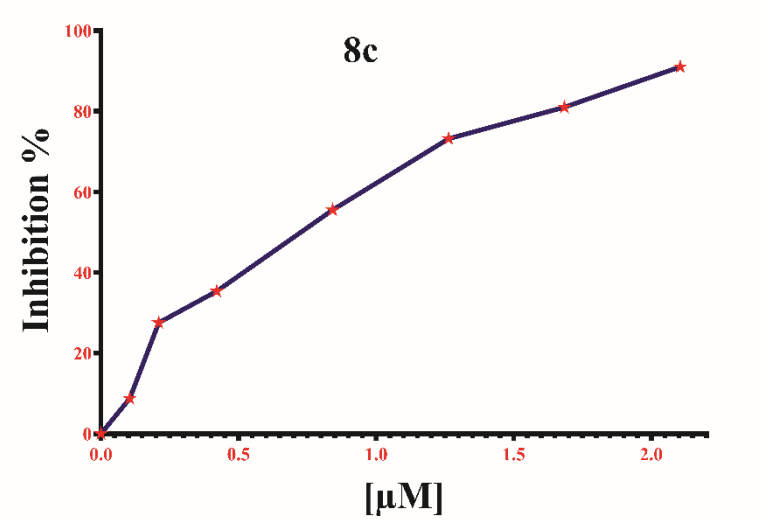
0.0
0.5
1.0
1.5
2.0
[µM]


8c
Inhibition %
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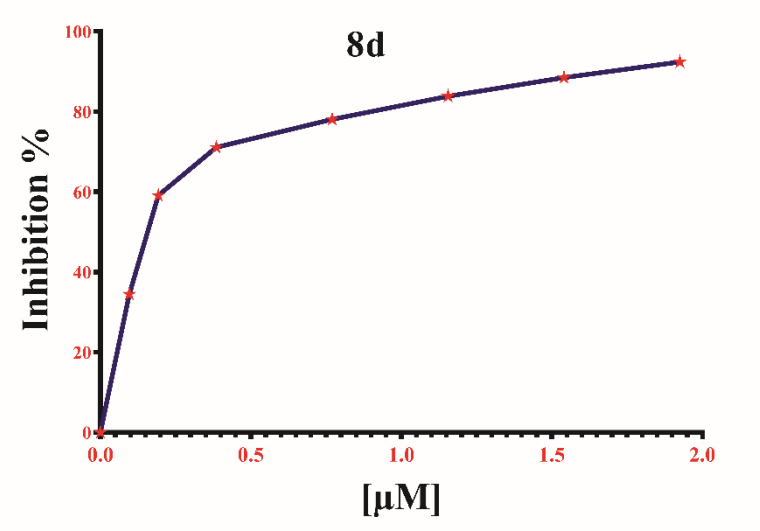
40
20
0
0.0
0.5
1.0
1.5
2.0
[µM]


8d
Inhibition %
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80
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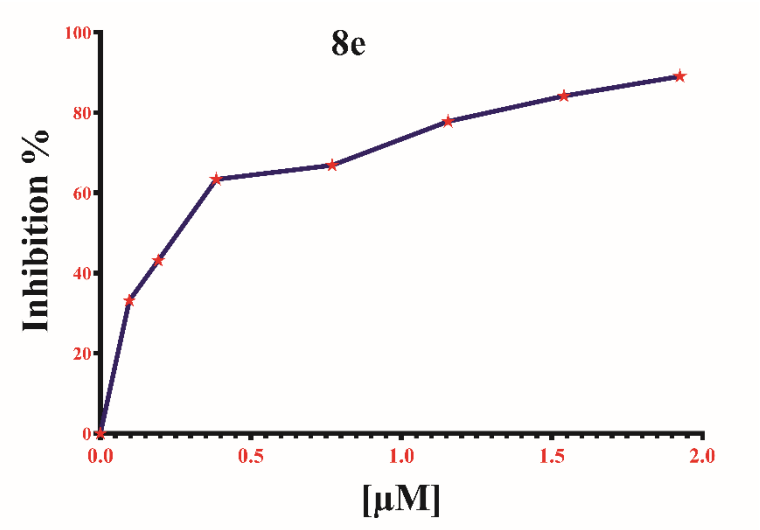
40
20
0
0.0
0.5
1.0
1.5
2.0
[μM]


8e
Inhibition %
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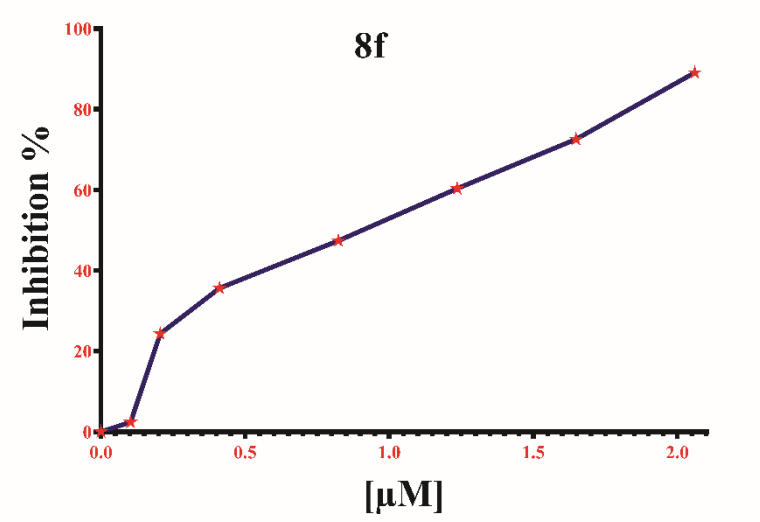
80
60
40
20
0
0.0
0.5
1.0
1.5
2.0
[μM]


8f
Inhibition %
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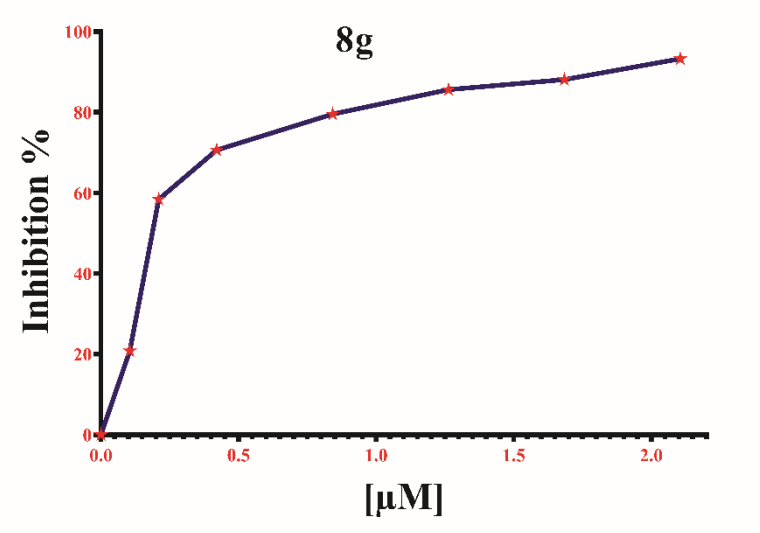
40
20
0
0.0
0.5
1.0
1.5
2.0
[μM]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Inhibition %
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0
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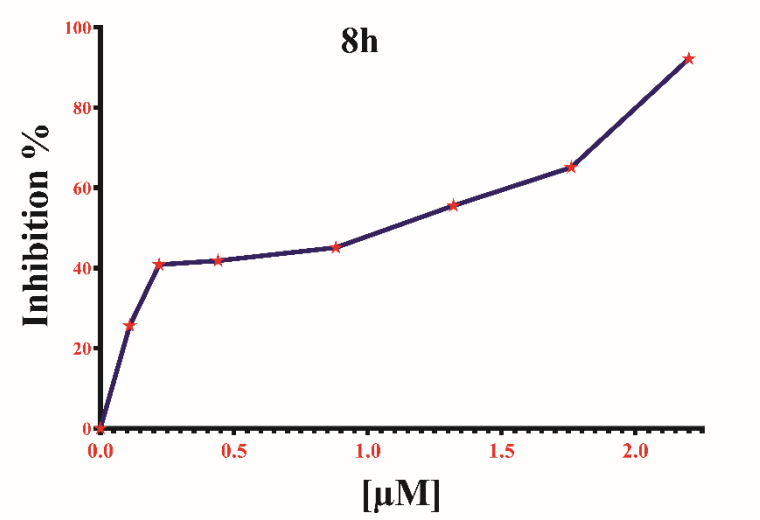
0.5
1.0
1.5
2.0
[μM]


8h
Inhibition %
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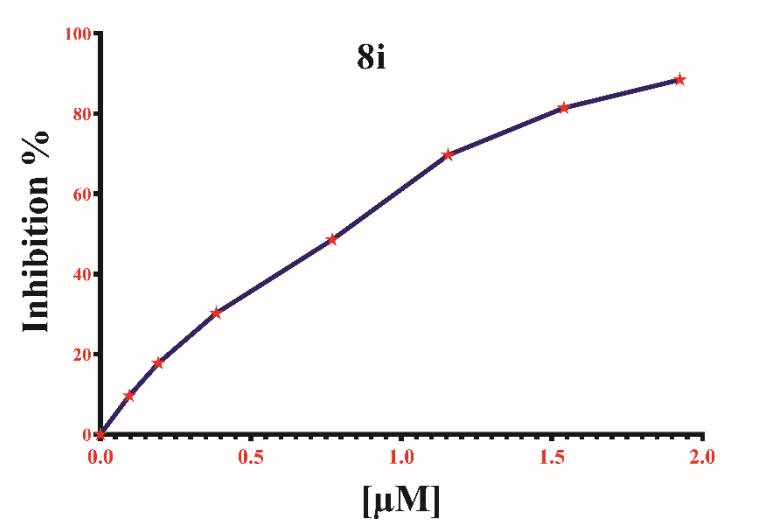
40
20
0
0.0
0.5
1.0
1.5
2.0
[μM]


8i
Inhibition %
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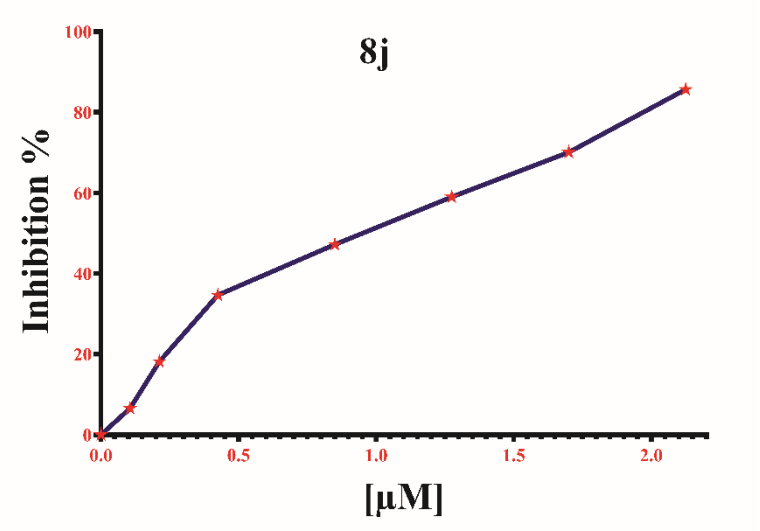
20
0
0.0
0.5
1.0
1.5
2.0
[μM]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Inhibition %
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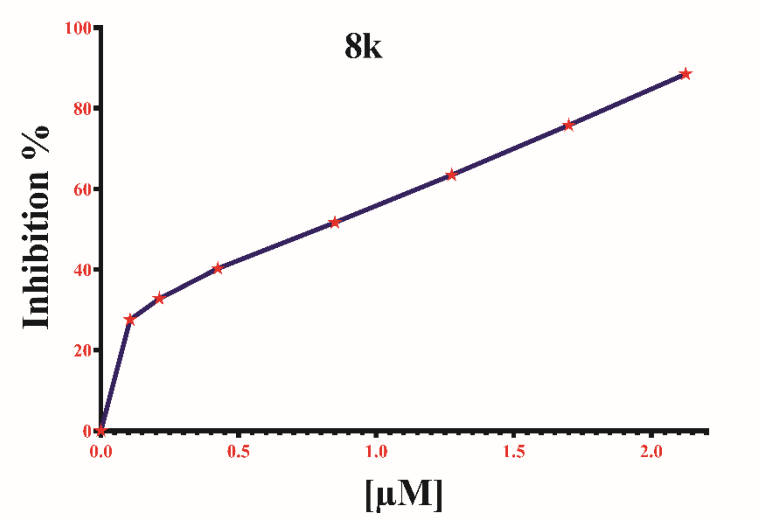
0.5
1.0
1.5
2.0
[μM]


8k
Inhibition %
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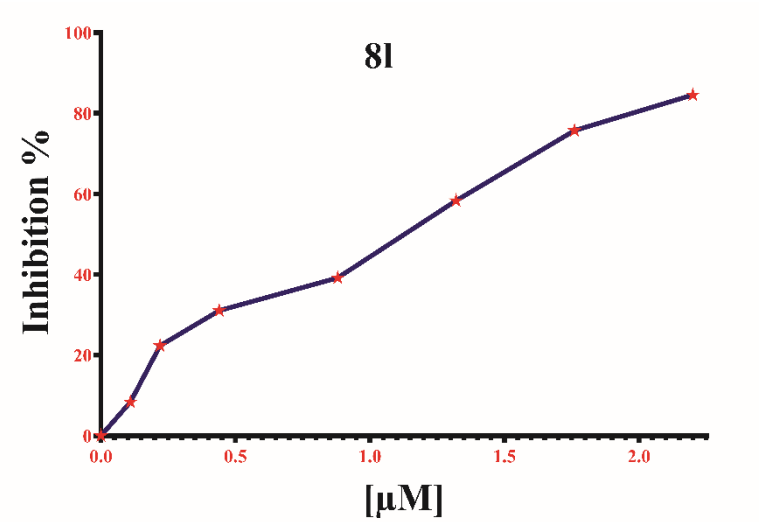
40
20
0
0.0
0.5
1.0
1.5
2.0
[μM]


8l
Inhibition %
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80
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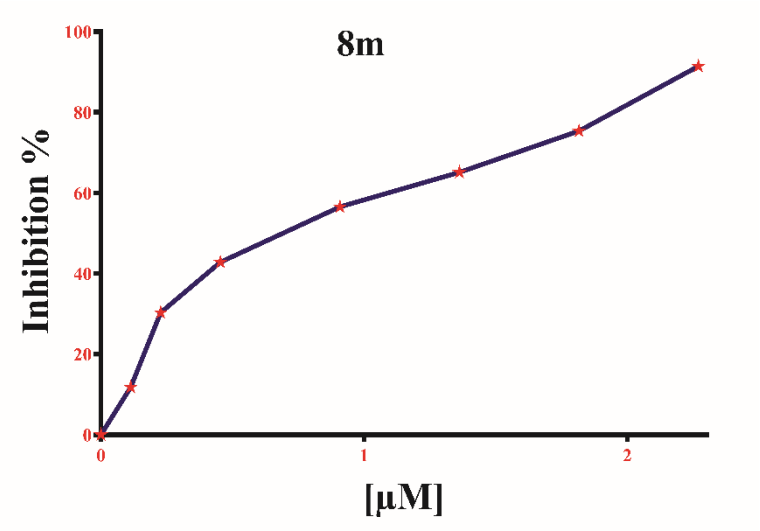
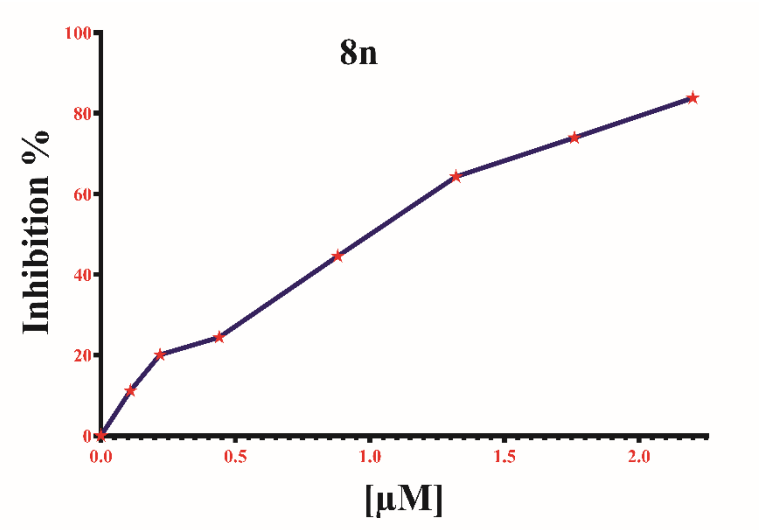
40
20
0
0.0
0.5
1.0
1.5
2.0
[μM]


8m
Inhibition %
100
80
60
40
20
0
0
1
2
[μM]


8n
Inhibition %
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80
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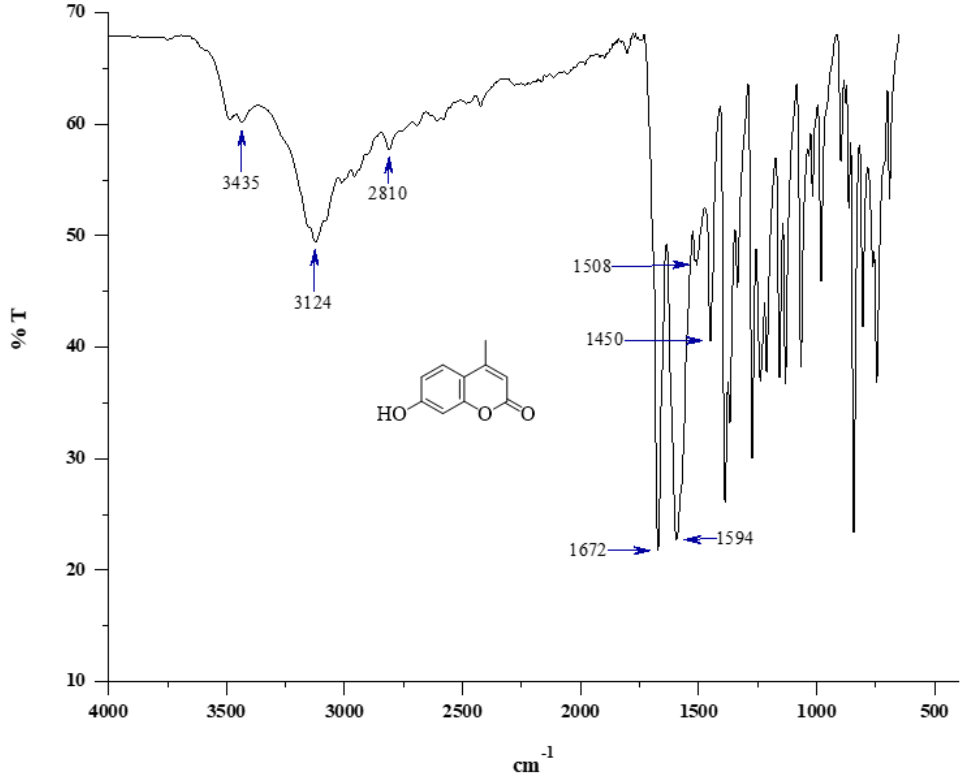
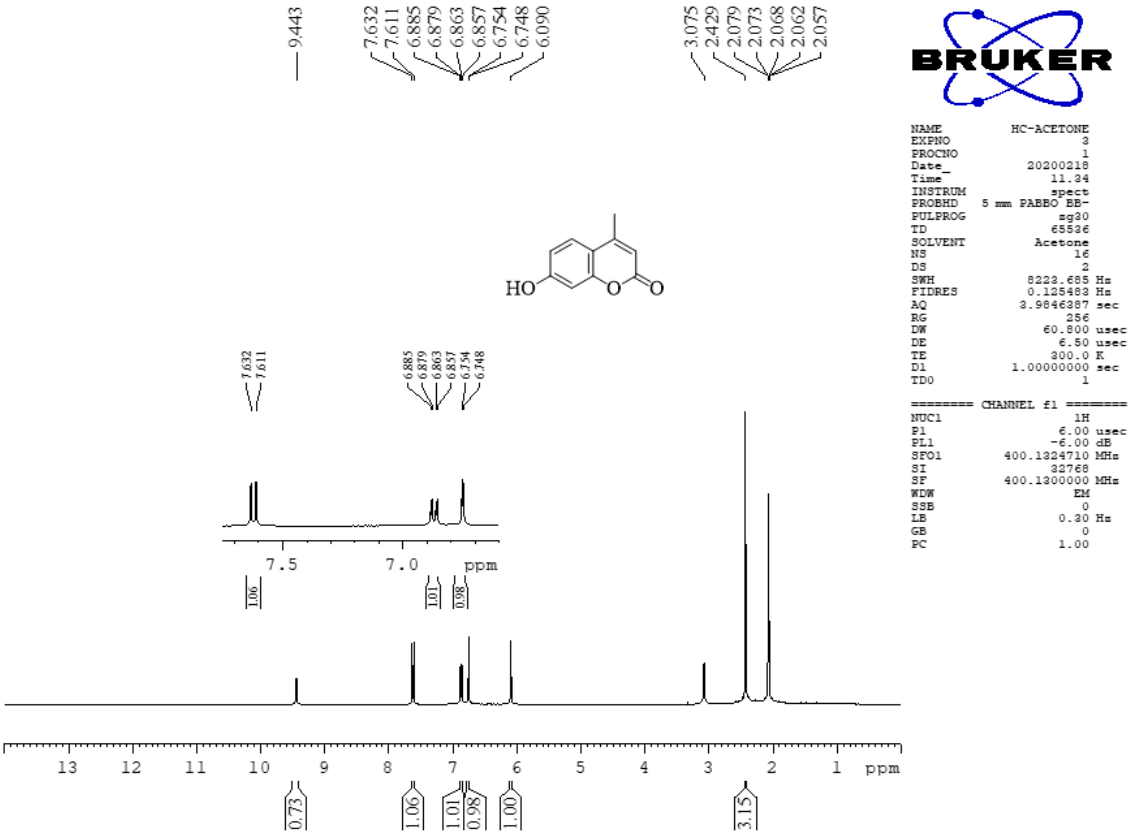
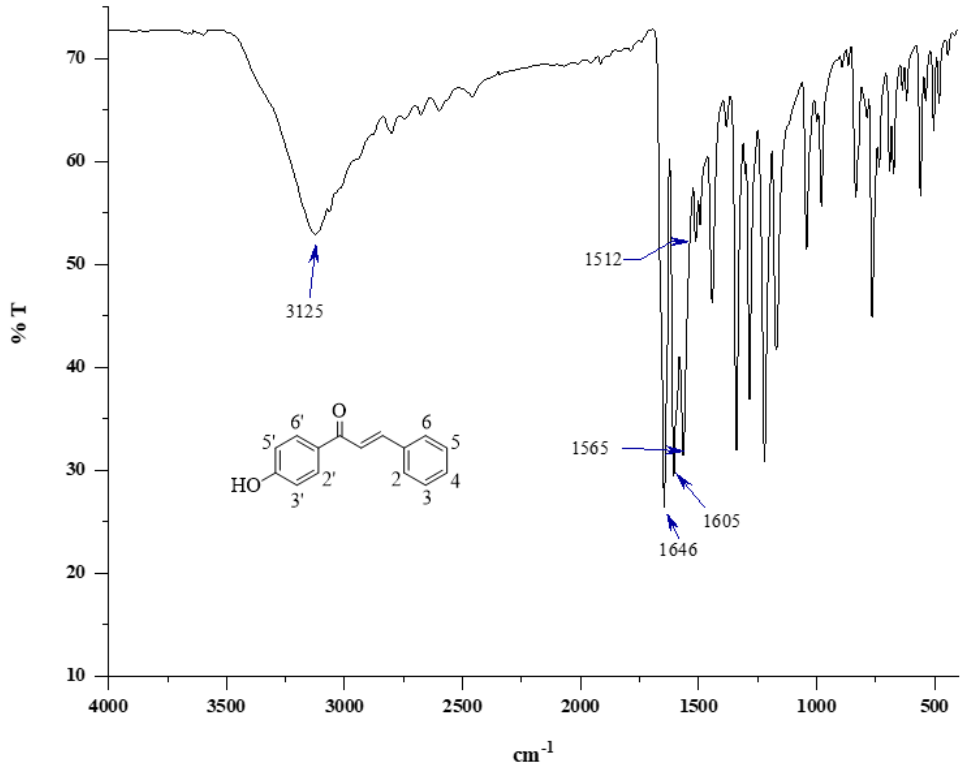
40
20
0
0.0
0.5
1.0
1.5
2.0
[μM]



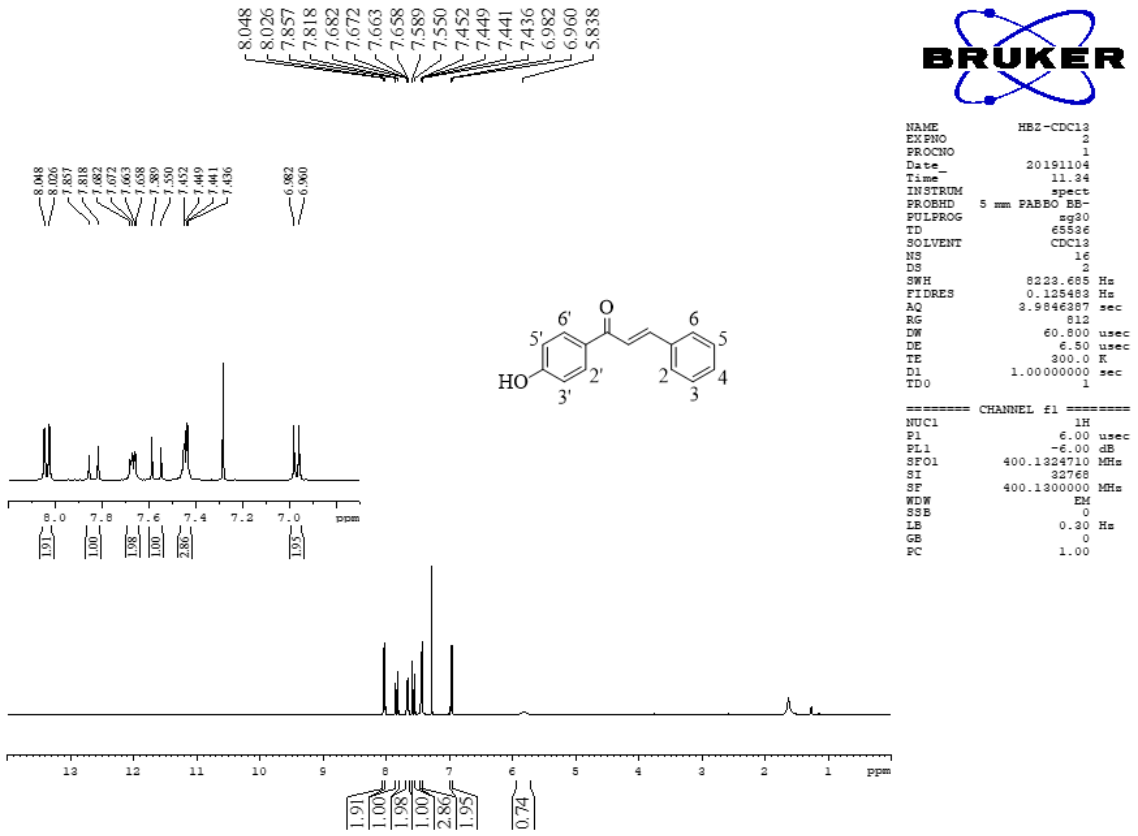
IR spectrum of 7-Hydroxy-4-methylcoumarin **(3)**



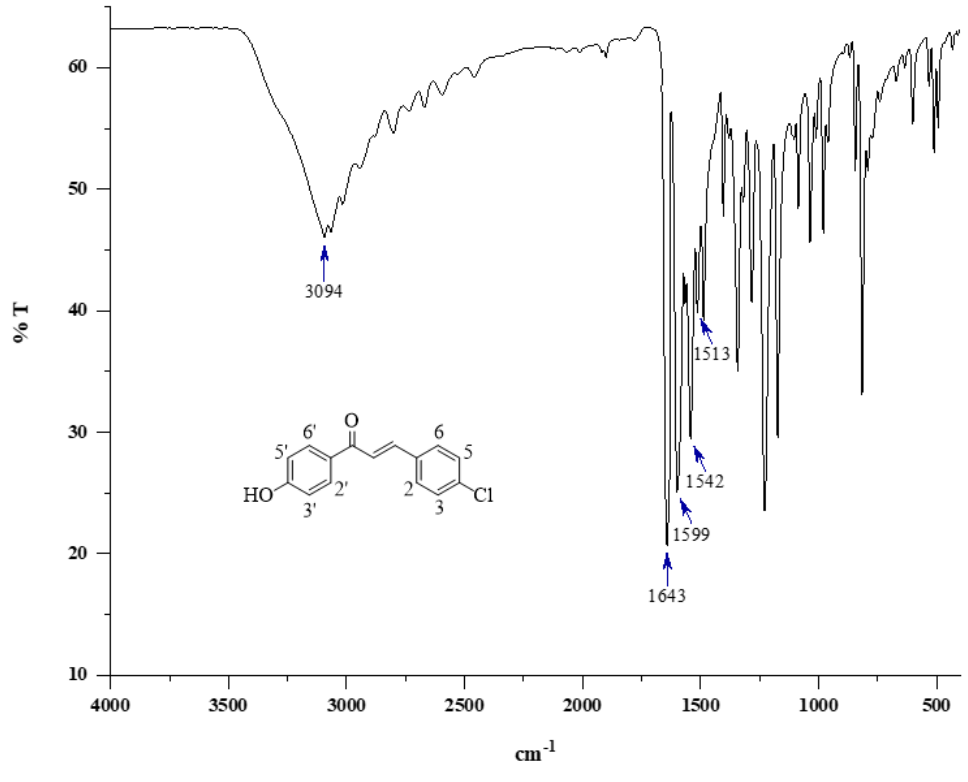
^{1}H NMR spectrum of 7-Hydroxy-4-methylcoumarin **(3)**



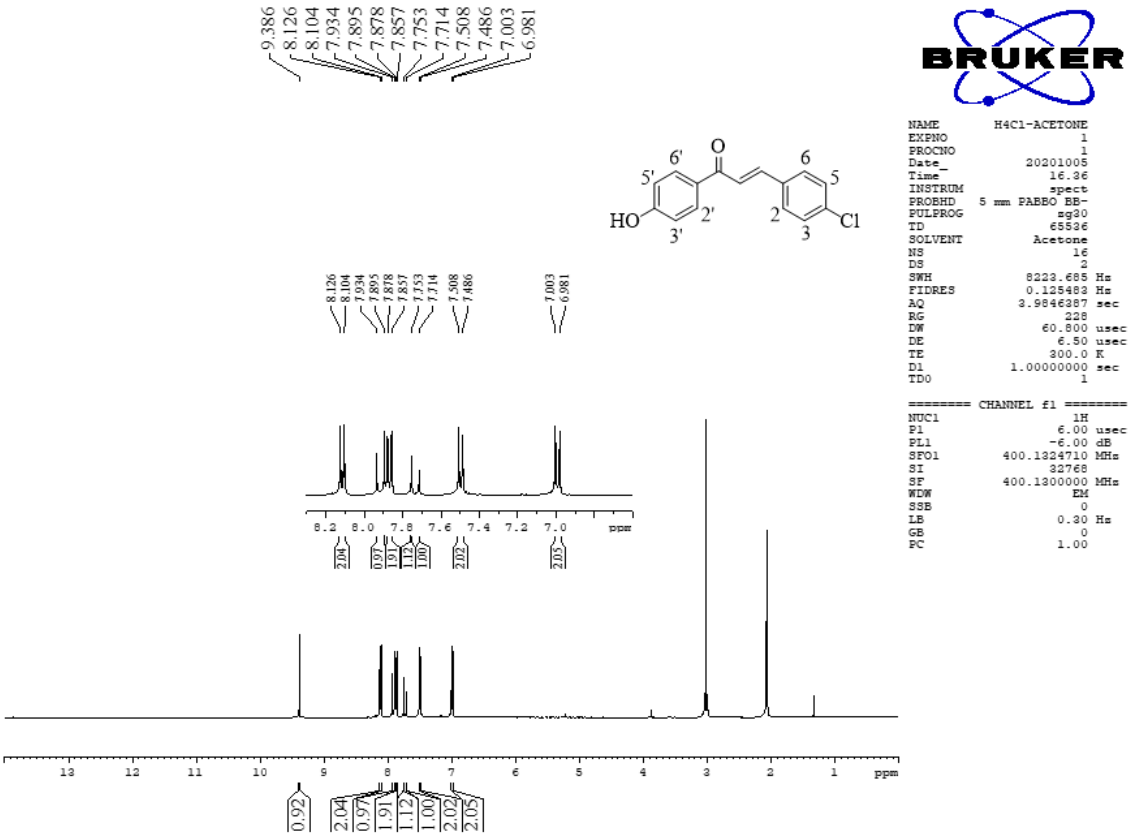
IR spectrum of (*E*)-1-(4-hydroxyphenyl)-3-phenylprop-2-en-1-one **(5a)**



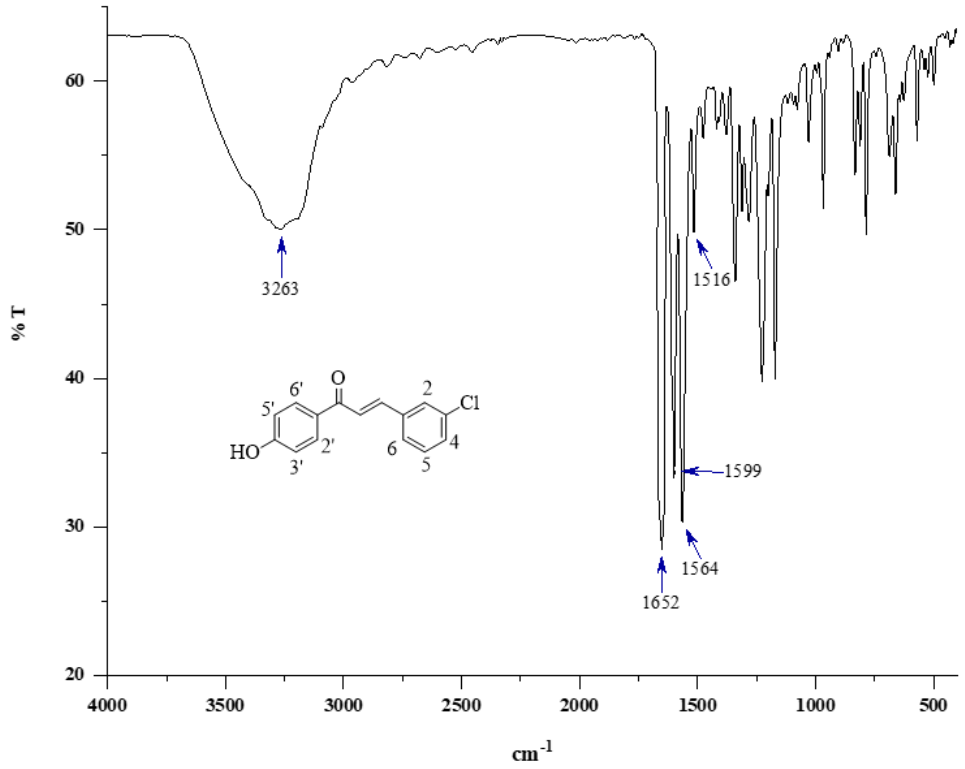
^{1}H NMR spectrum of (*E*)-1-(4-hydroxyphenyl)-3-phenylprop-2-en-1-one **(5a)**



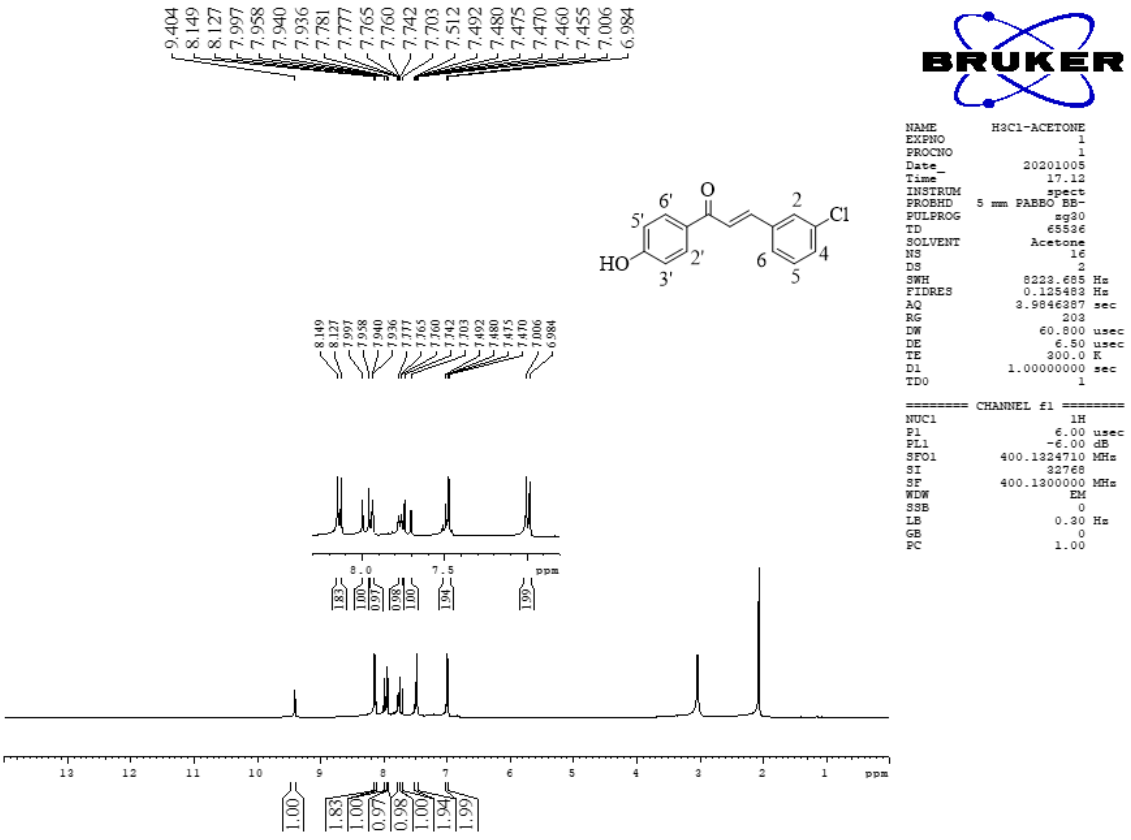
IR spectrum of (*E*)-3-(4-chlorophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one **(5b)**



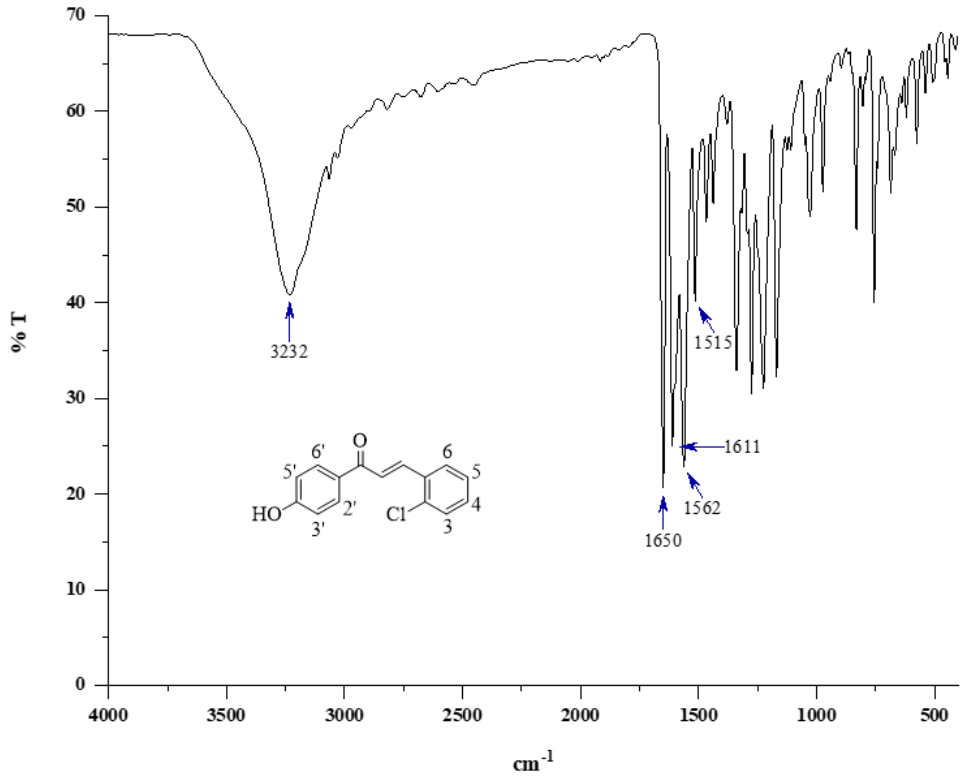
^{1}H NMR spectrum of (*E*)-3-(4-chlorophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one **(5b)**



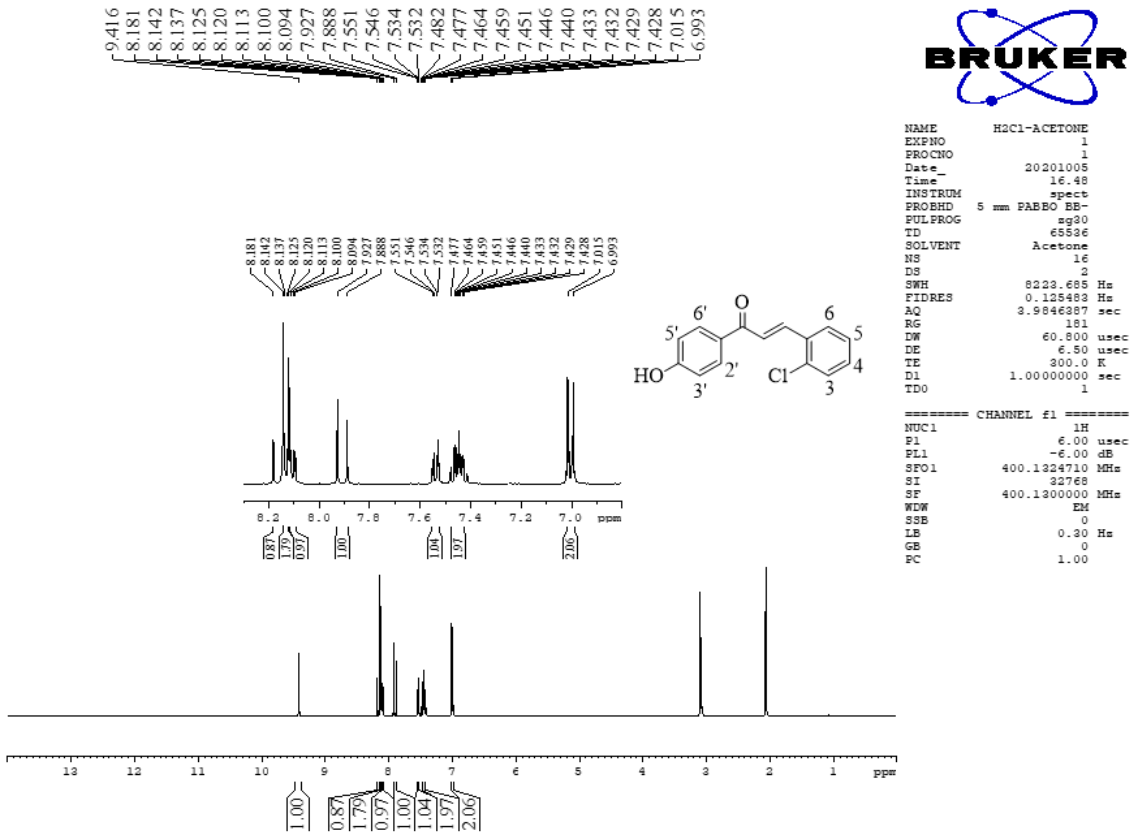
IR spectrum of (*E*)-3-(3-chlorophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one **(5c)**



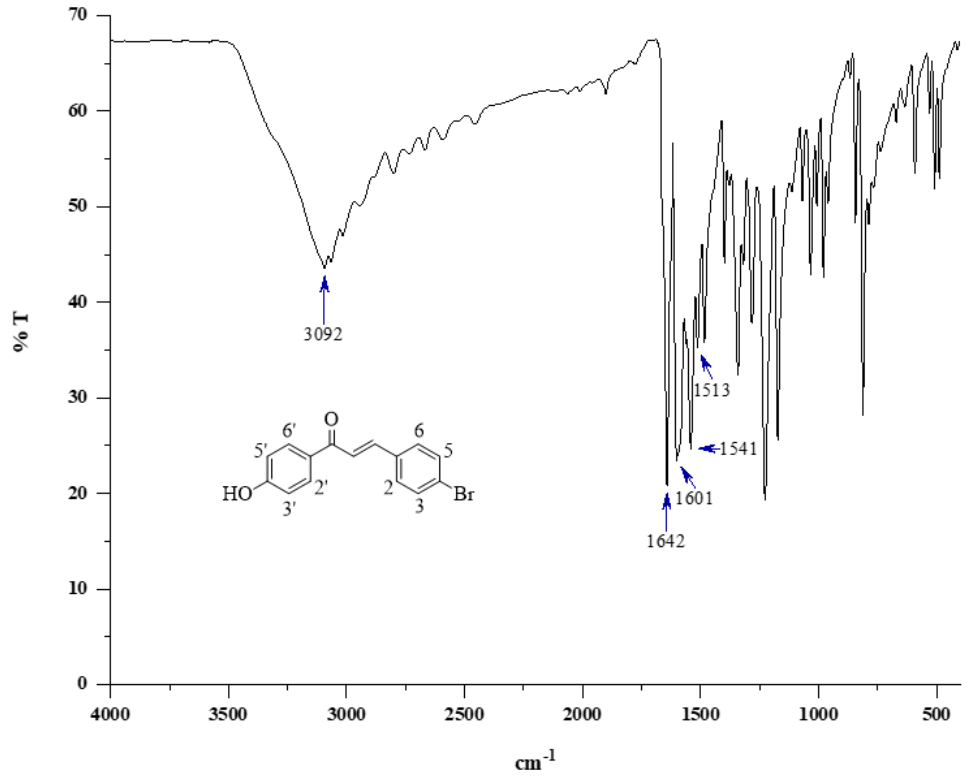
^{1}H NMR spectrum of (*E*)-3-(3-chlorophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one **(5c)**



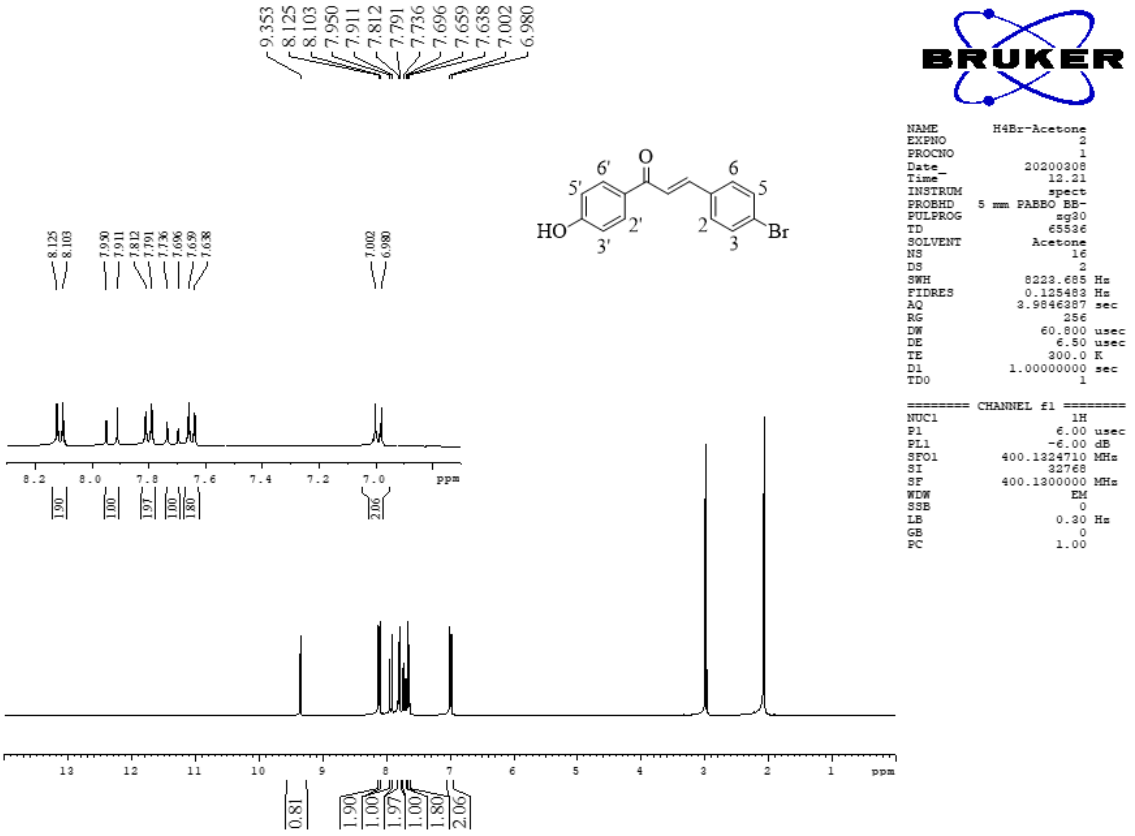
IR spectrum of (*E*)-3-(2-chlorophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one **(5d)**



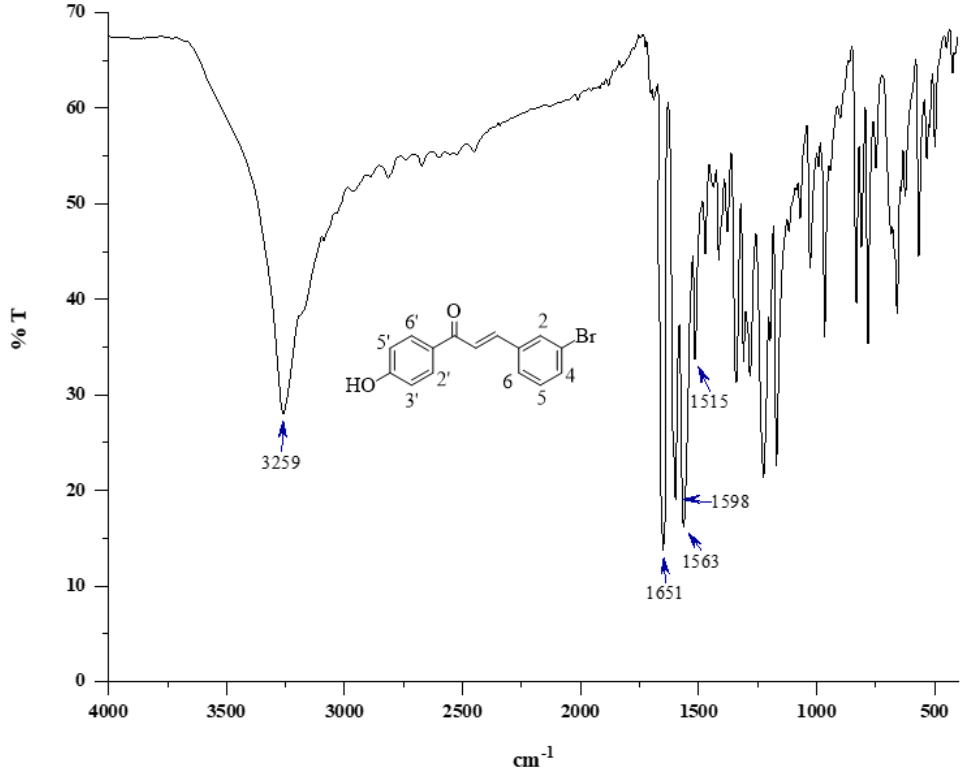
^{1}H NMR spectrum of (*E*)-3-(2-chlorophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one **(5d)**



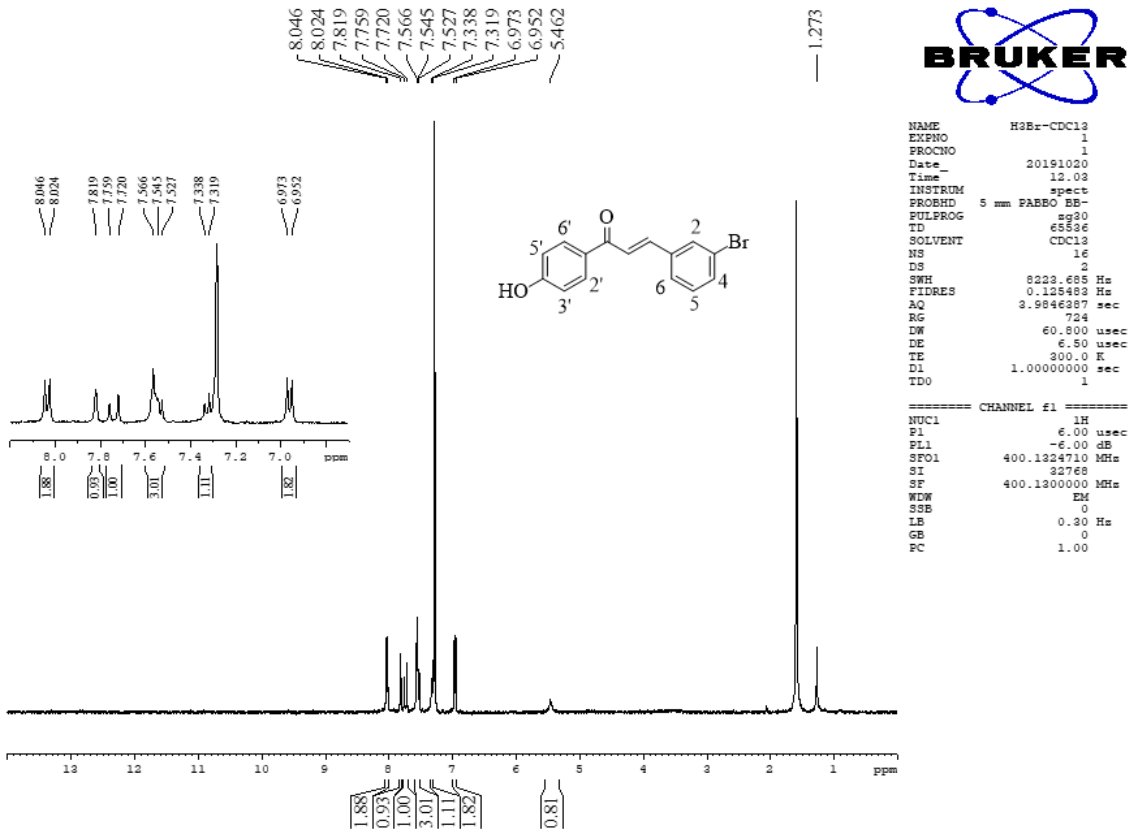
IR spectrum of (*E*)-3-(4-bromophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one **(5e)**



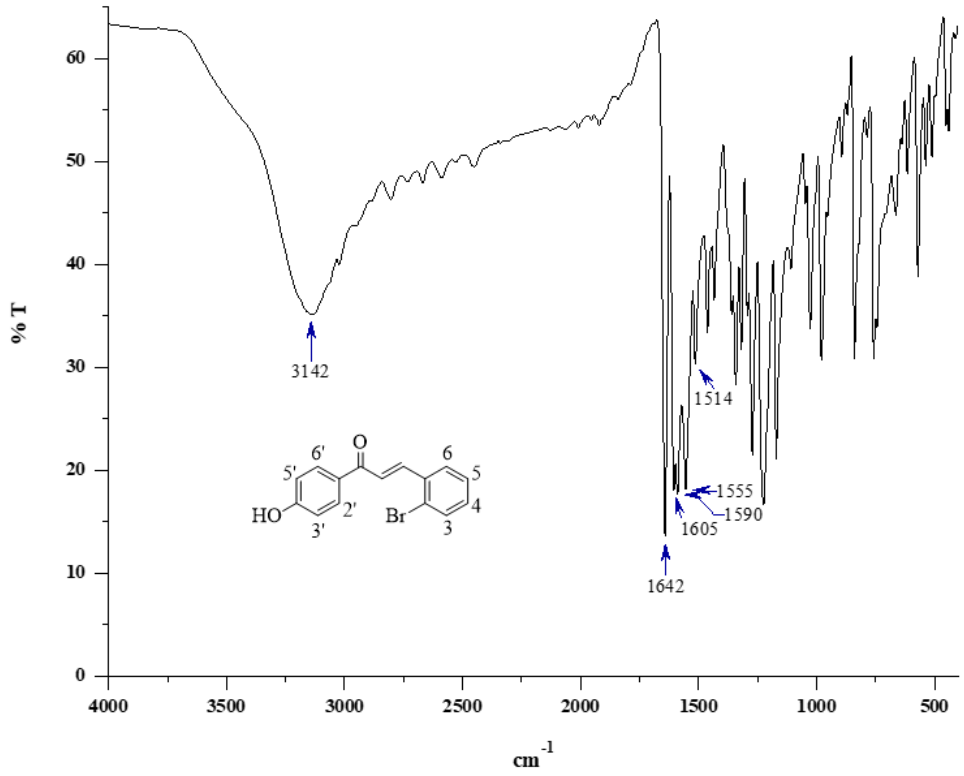
^{1}H NMR spectrum of (*E*)-3-(4-bromophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one **(5e)**



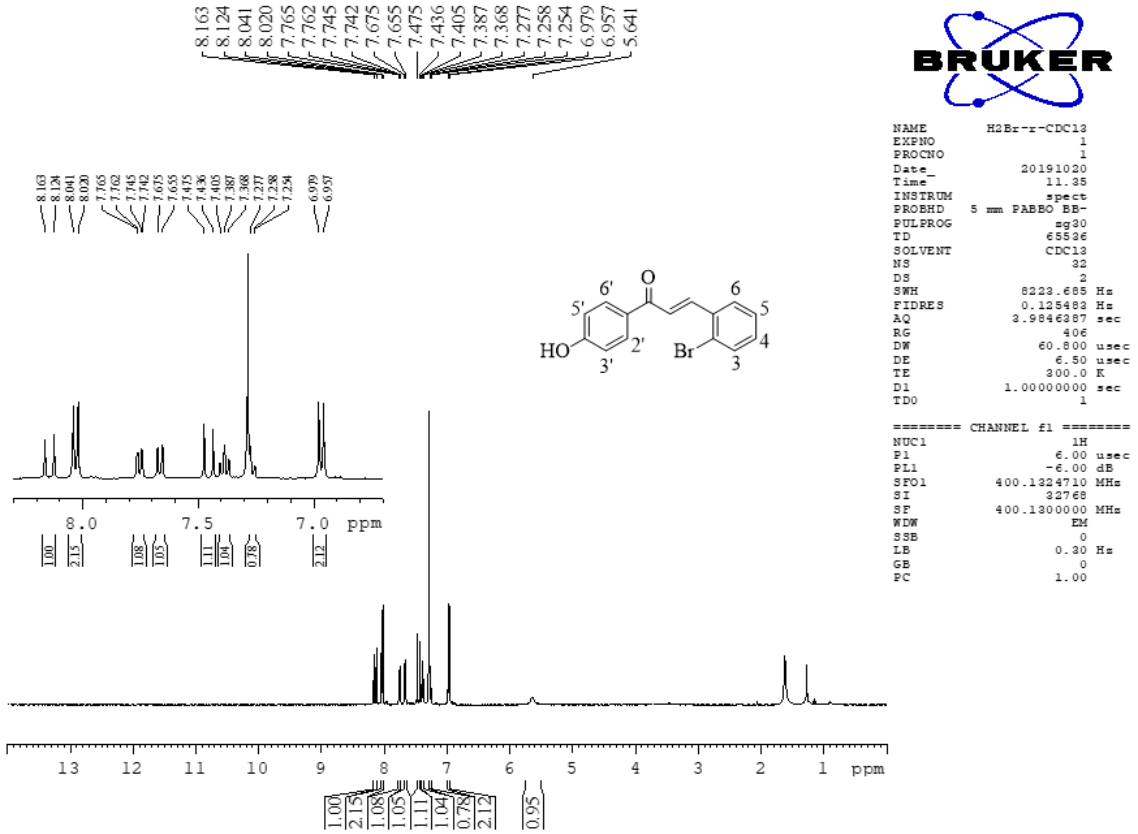
IR spectrum of (*E*)-3-(3-bromophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one **(5f)**



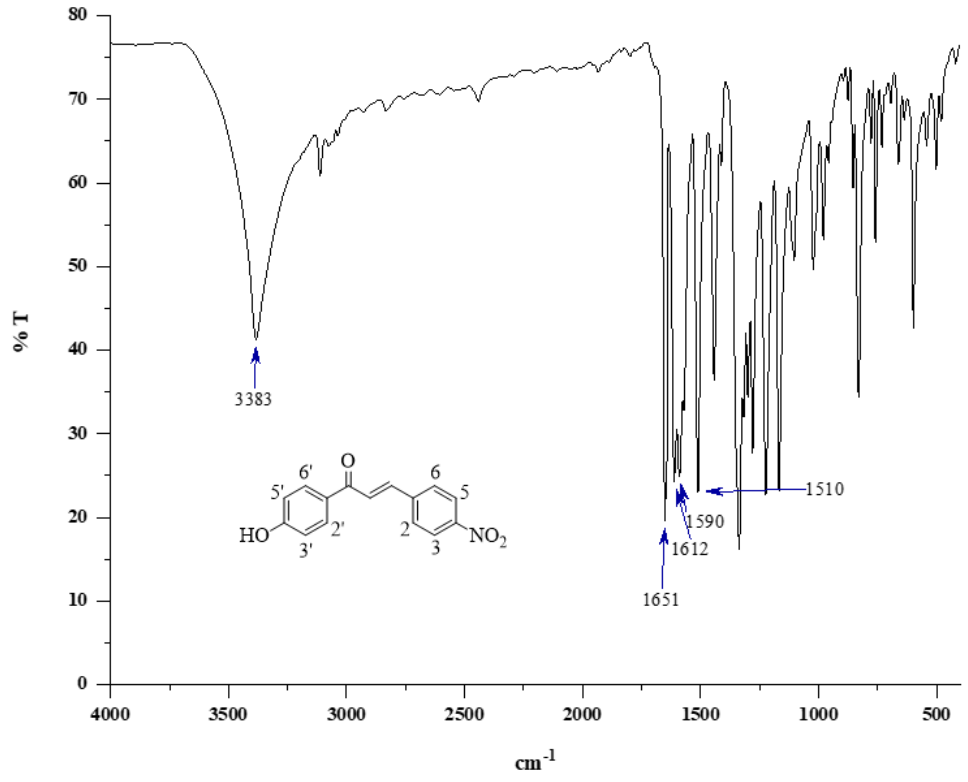
^{1}H NMR spectrum of (*E*)-3-(3-bromophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one **(5f)**



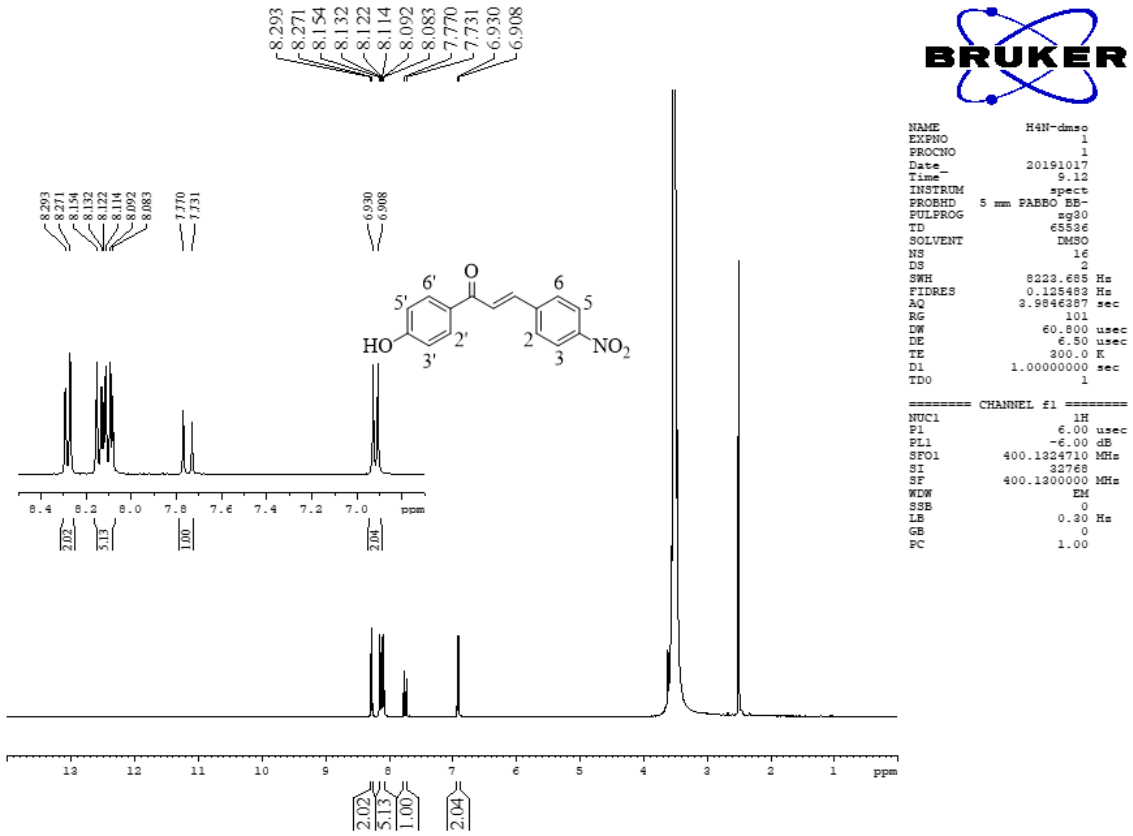
IR spectrum of (*E*)-3-(2-bromophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one **(5g)**



^{1}H NMR spectrum of (*E*)-3-(2-bromophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one **(5g)**



IR spectrum of (*E*)-1-(4-hydroxyphenyl)-3-(4-nitrophenyl)prop-2-en-1-one **(5h)**

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SOLVENT                 DMSO
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DE                   6.50 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                         1

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PL1                  -6.00 dB
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SF            400.1300000 MHz
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SSB                         0
LB                     0.30 Hz
GB                          0
PC                       1.00
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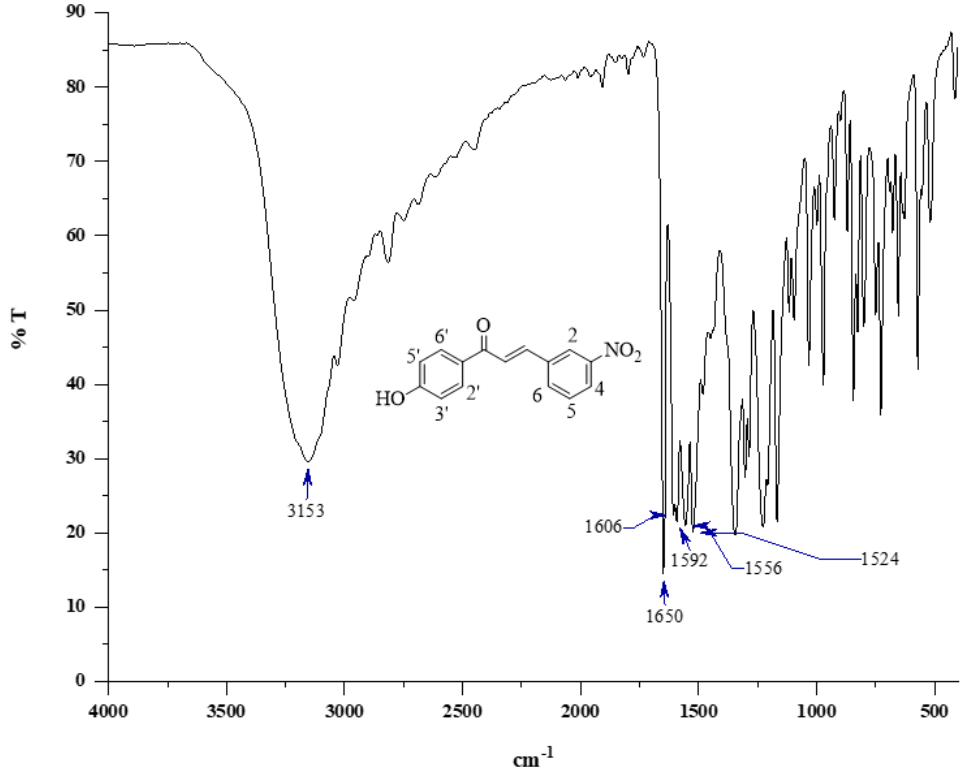
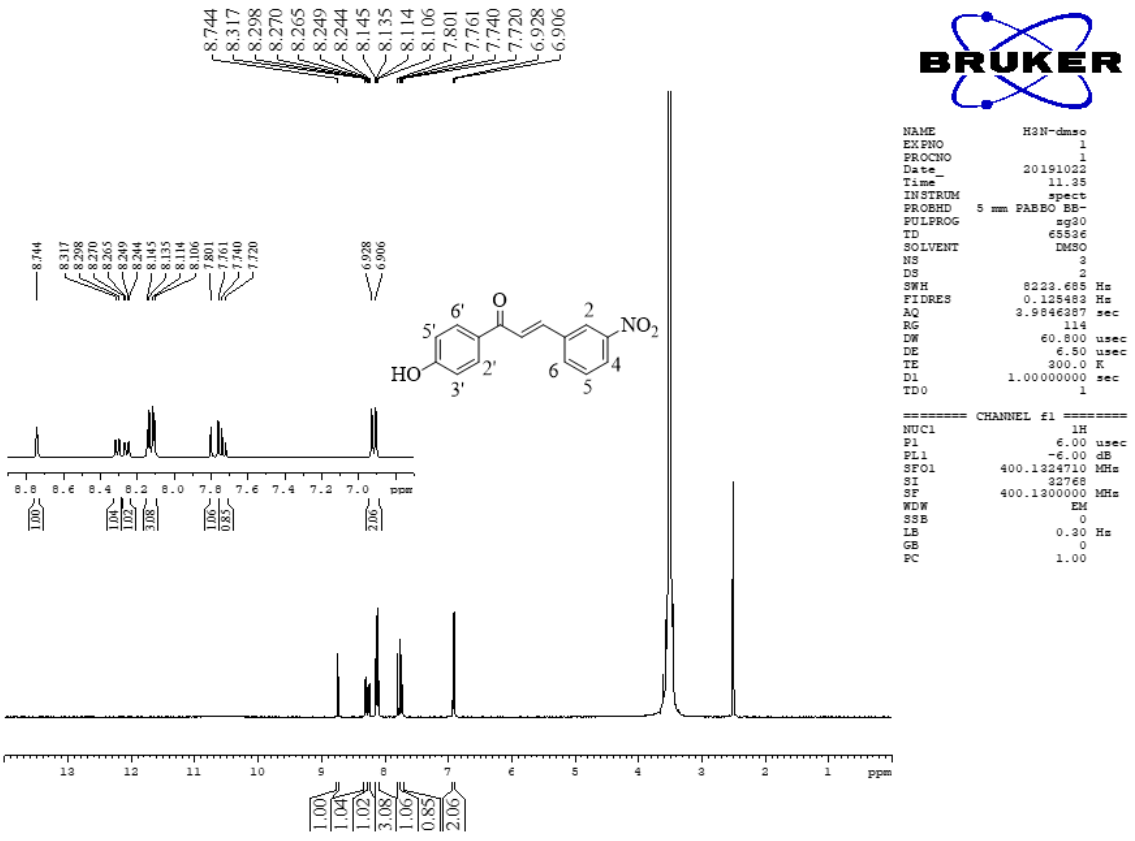
^{1}H NMR spectrum of (*E*)-1-(4-hydroxyphenyl)-3-(4-nitrophenyl)prop-2-en-1-one **(5h)**



IR spectrum of (*E*)-1-(4-hydroxyphenyl)-3-(3-nitrophenyl)prop-2-en-1-one **(5i)**



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PROCNO 1
Date_ 20191022
Time 11.35
INSTRUM spect
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SOLVENT DMSO
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RG 114
DW 60.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

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PL1 -6.00 dB
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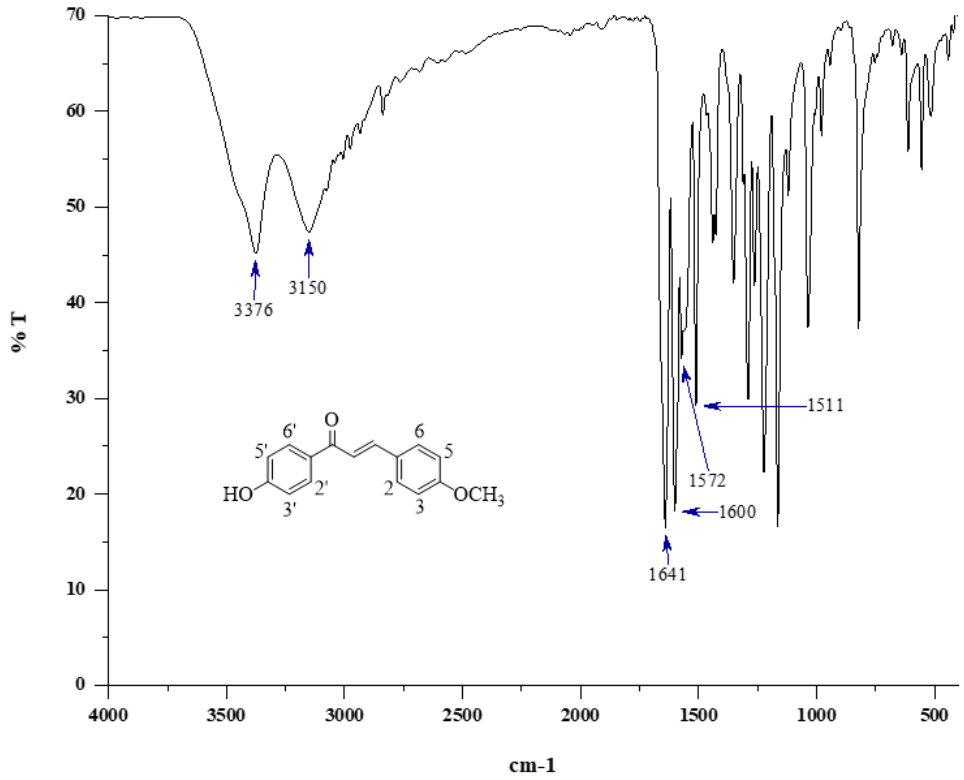
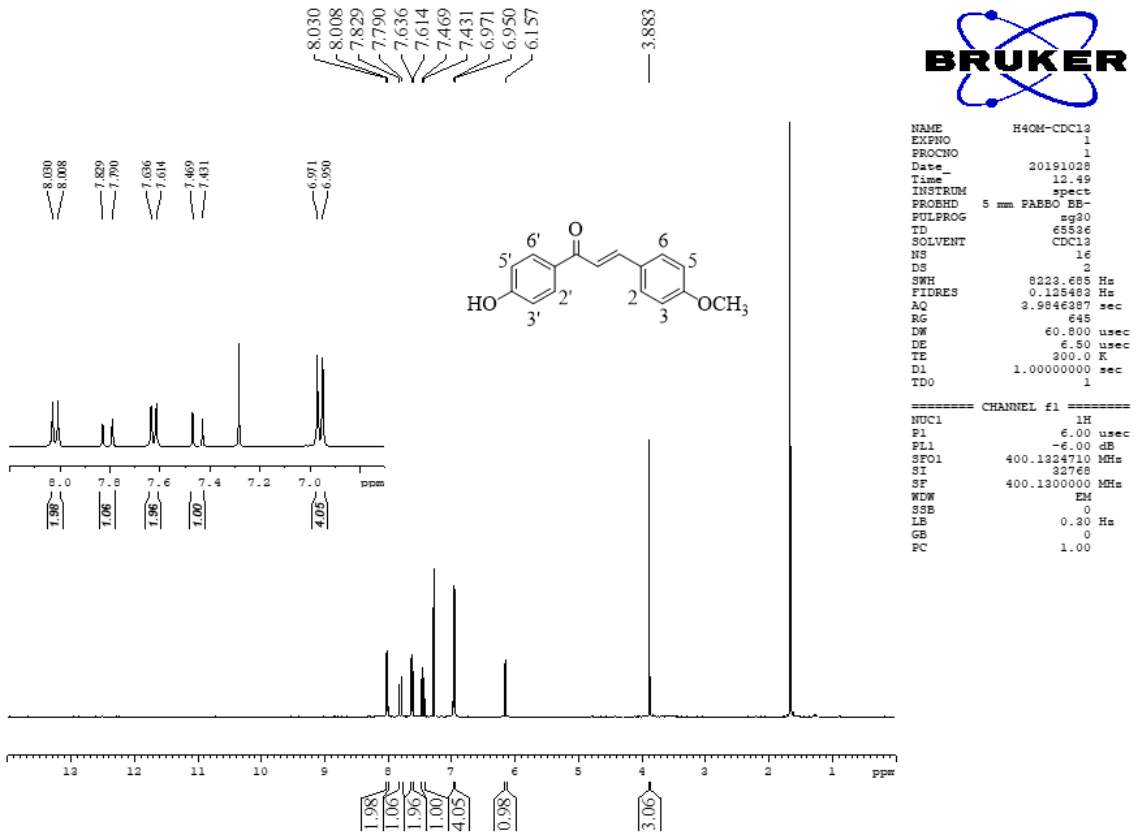
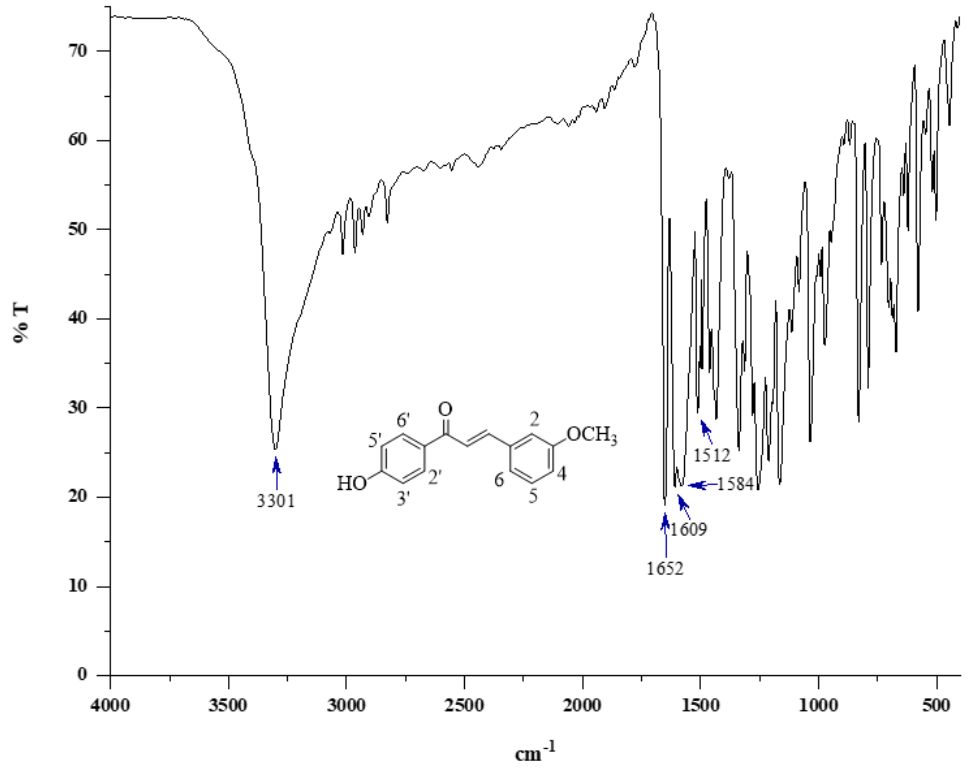
^{1}H NMR spectrum of (*E*)-1-(4-hydroxyphenyl)-3-(3-nitrophenyl)prop-2-en-1-one **(5i)**



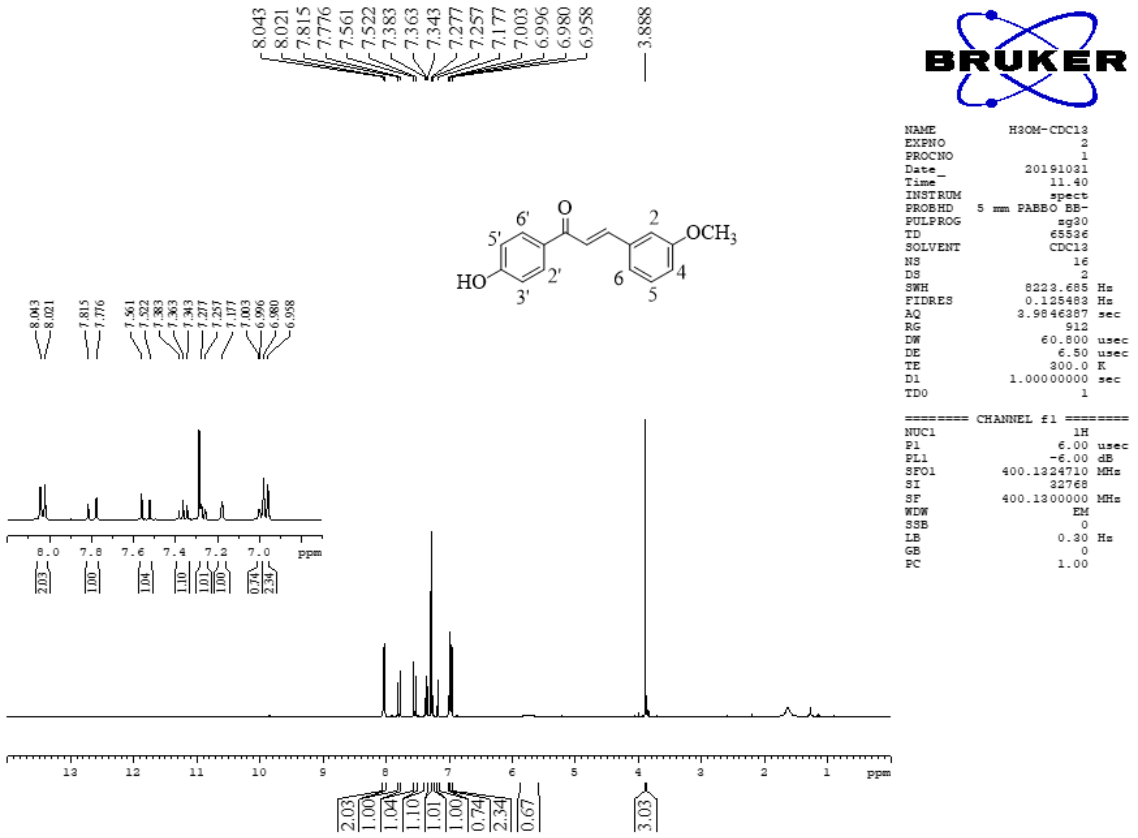
IR spectrum of (*E*)-1-(4-hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one **(5j)**



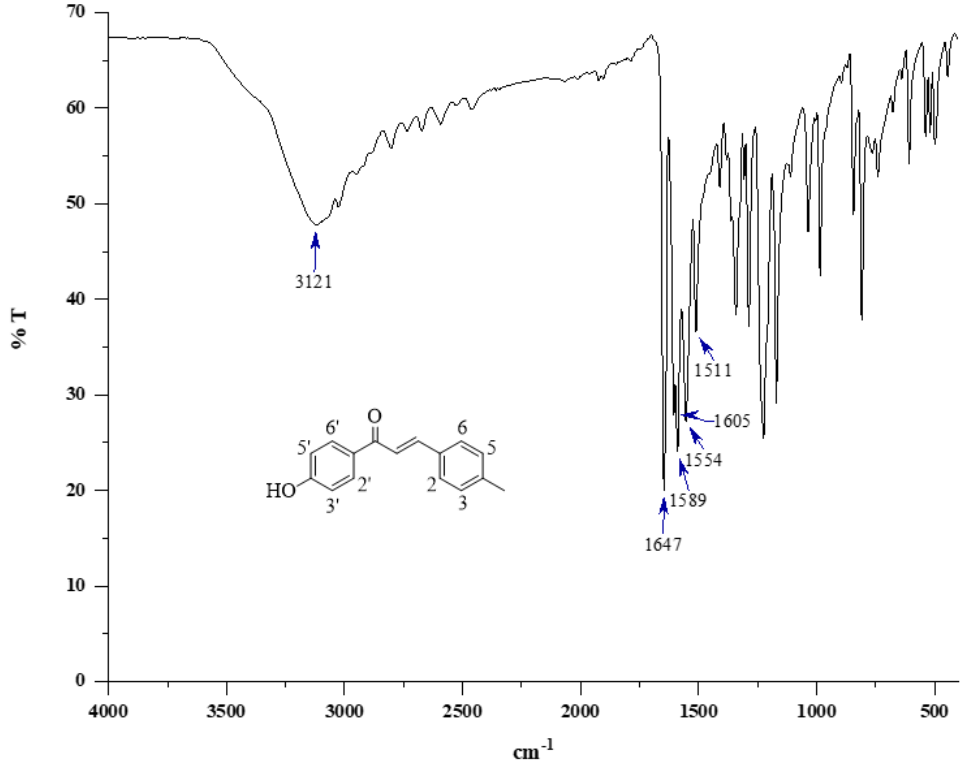
^{1}H NMR spectrum of (*E*)-1-(4-hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one **(5j)**



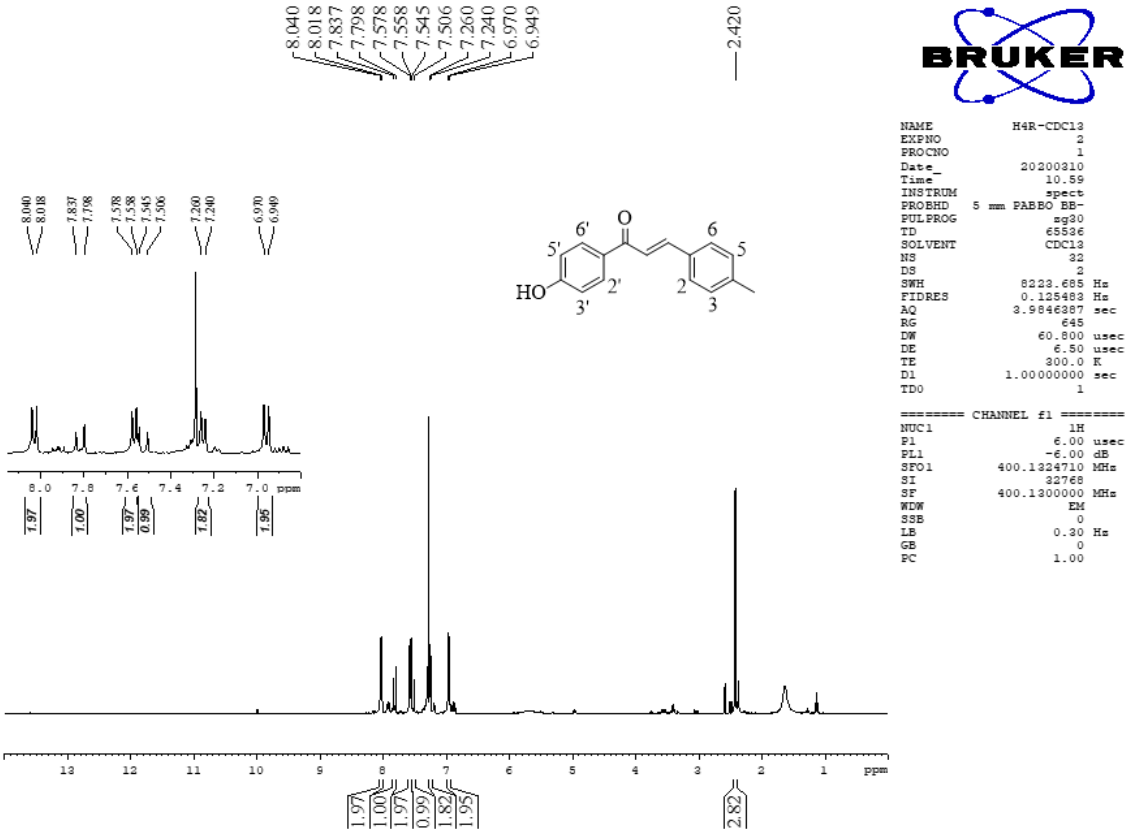
IR spectrum of (*E*)-1-(4-hydroxyphenyl)-3-(3-methoxyphenyl)prop-2-en-1-one **(5k)**



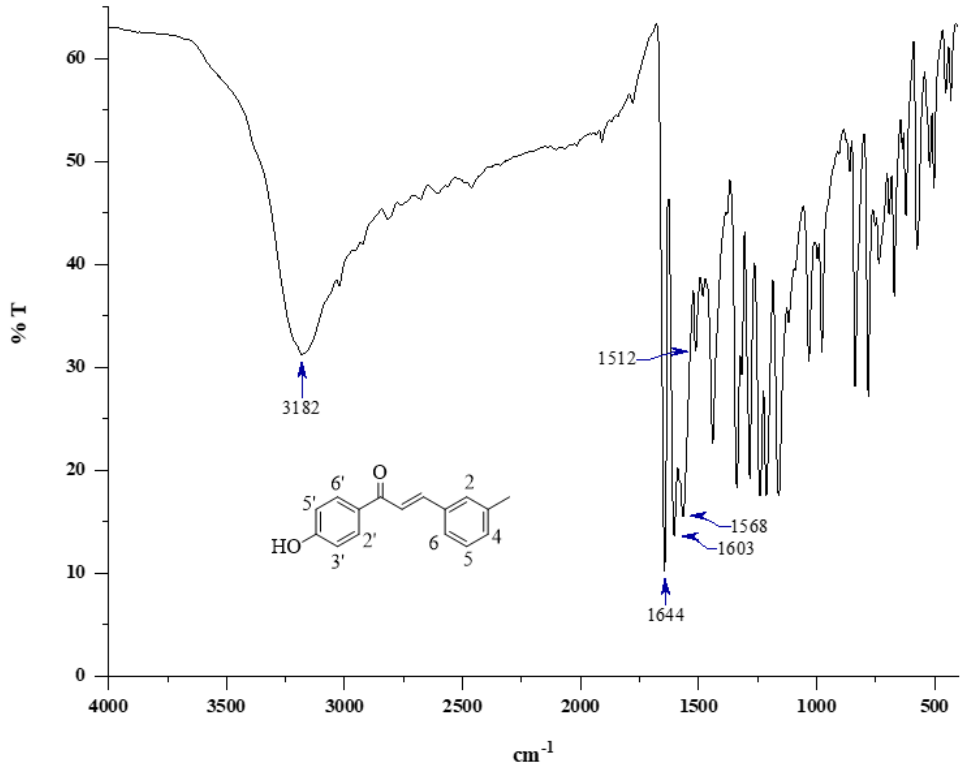
^{1}H NMR spectrum of (*E*)-1-(4-hydroxyphenyl)-3-(3-methoxyphenyl)prop-2-en-1-one **(5k)**



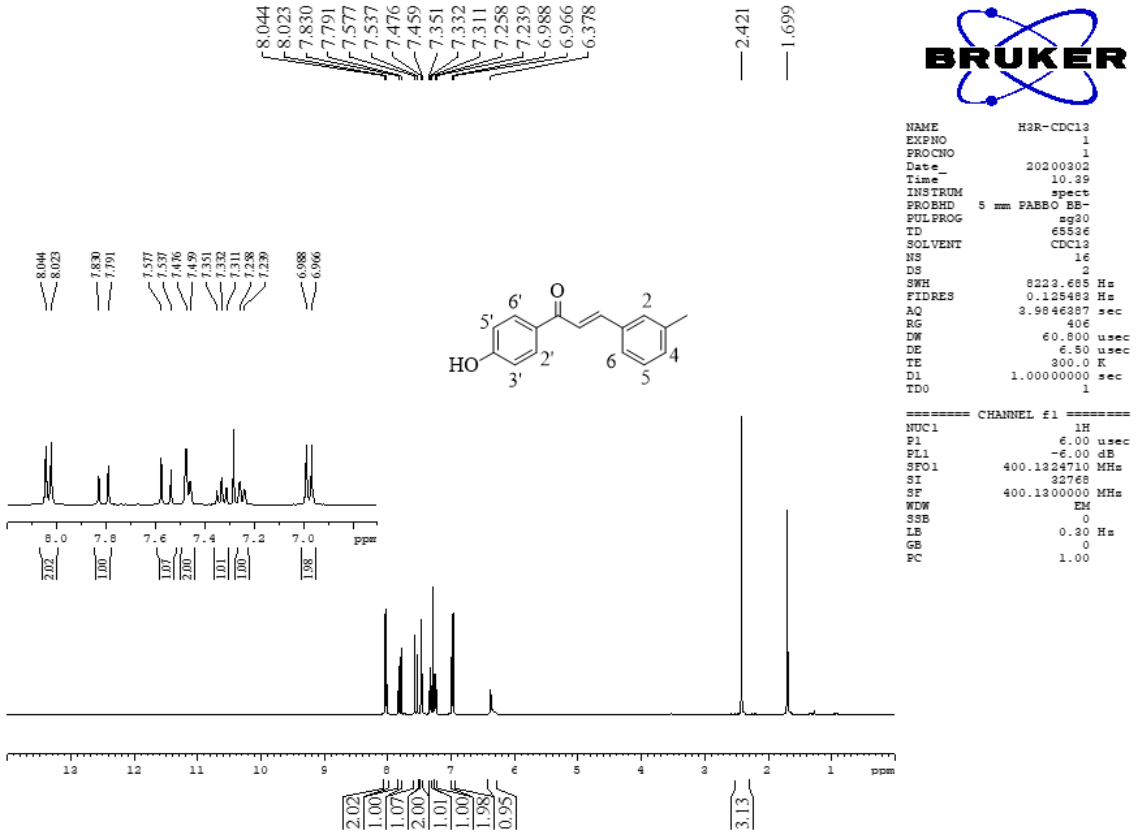
IR spectrum of (*E*)-1-(4-hydroxyphenyl)-3-(*p*-tolyl)prop-2-en-1-one **(5l)**



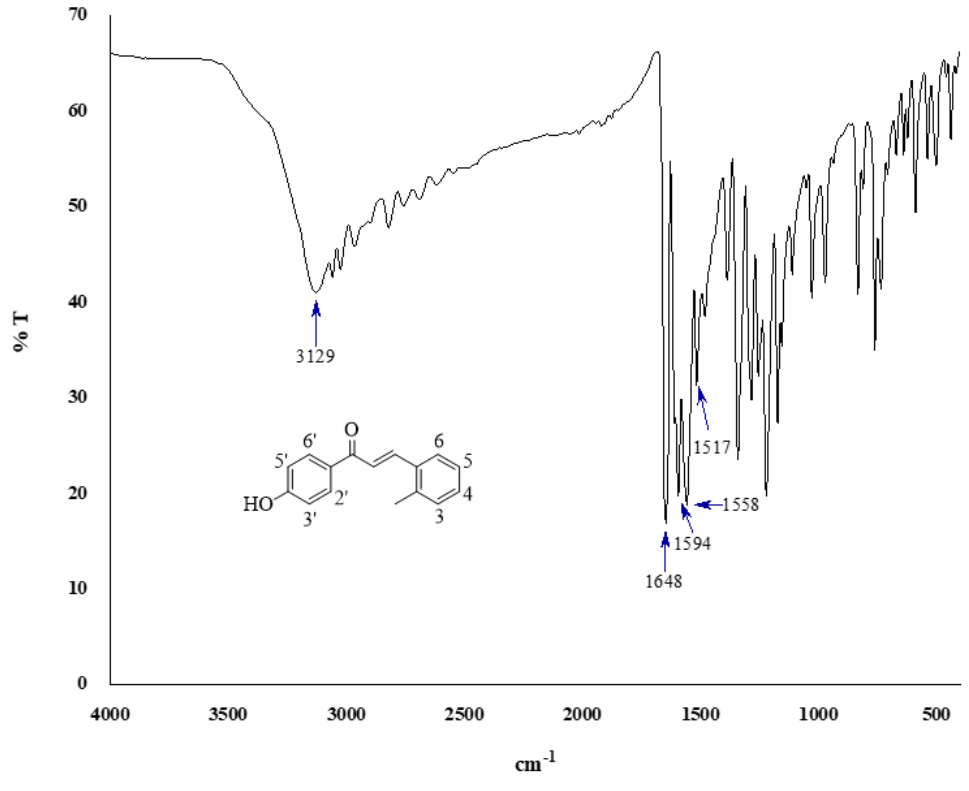
^{1}H NMR spectrum of (*E*)-1-(4-hydroxyphenyl)-3-(*p*-tolyl)prop-2-en-1-one **(5l)**



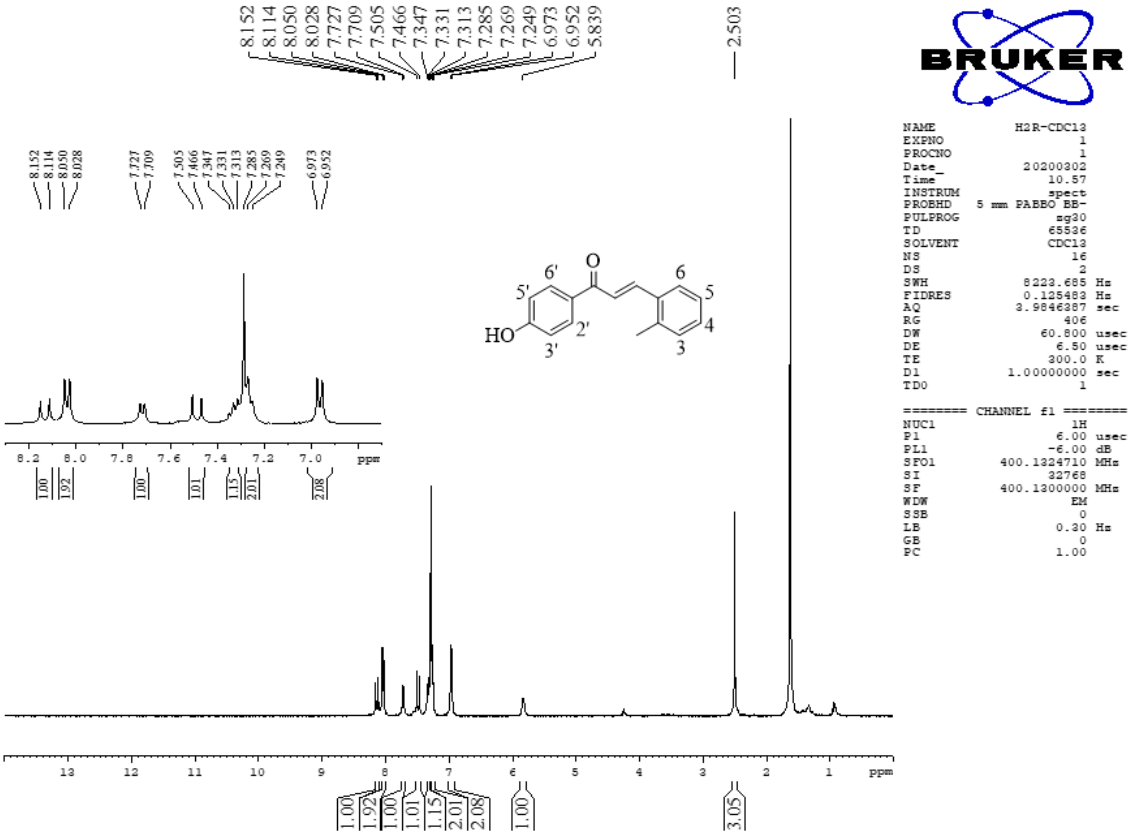
IR spectrum of (*E*)-1-(4-hydroxyphenyl)-3-(*m*-tolyl)prop-2-en-1-one **(5m)**



^{1}H NMR spectrum of (*E*)-1-(4-hydroxyphenyl)-3-(*m*-tolyl)prop-2-en-1-one **(5m)**



IR spectrum of (*E*)-1-(4-hydroxyphenyl)-3-(*o*-tolyl)prop-2-en-1-one **(5n)**



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PROCNO	1
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DS	2
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FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	406
DW	60.800 usec
DE	6.50 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
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P1	6.00 usec
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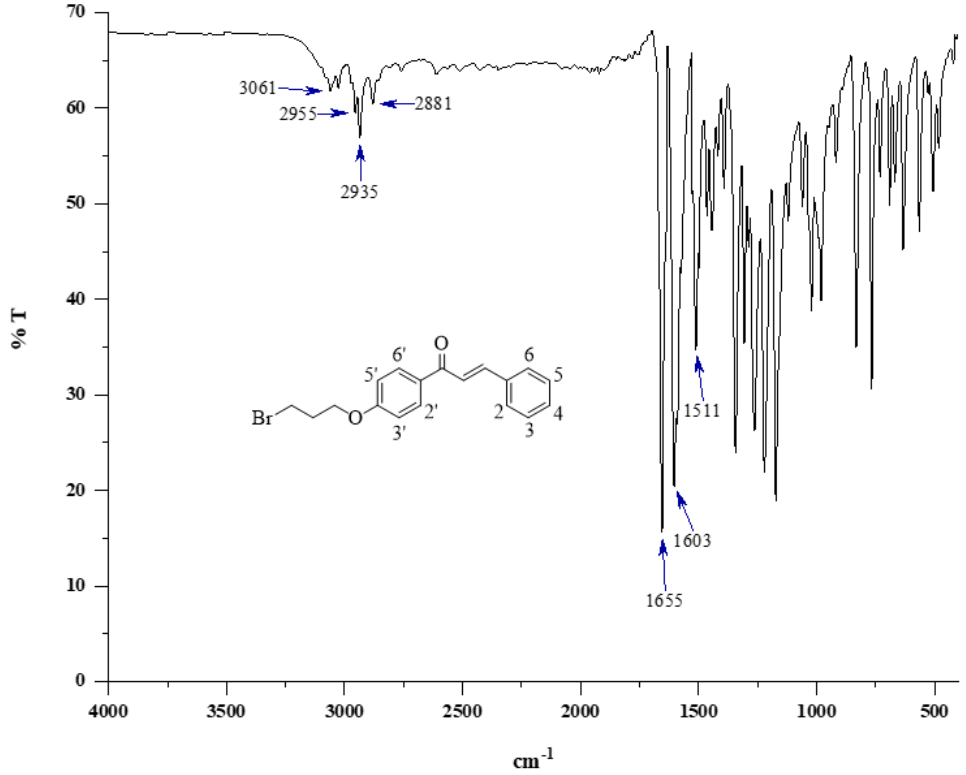
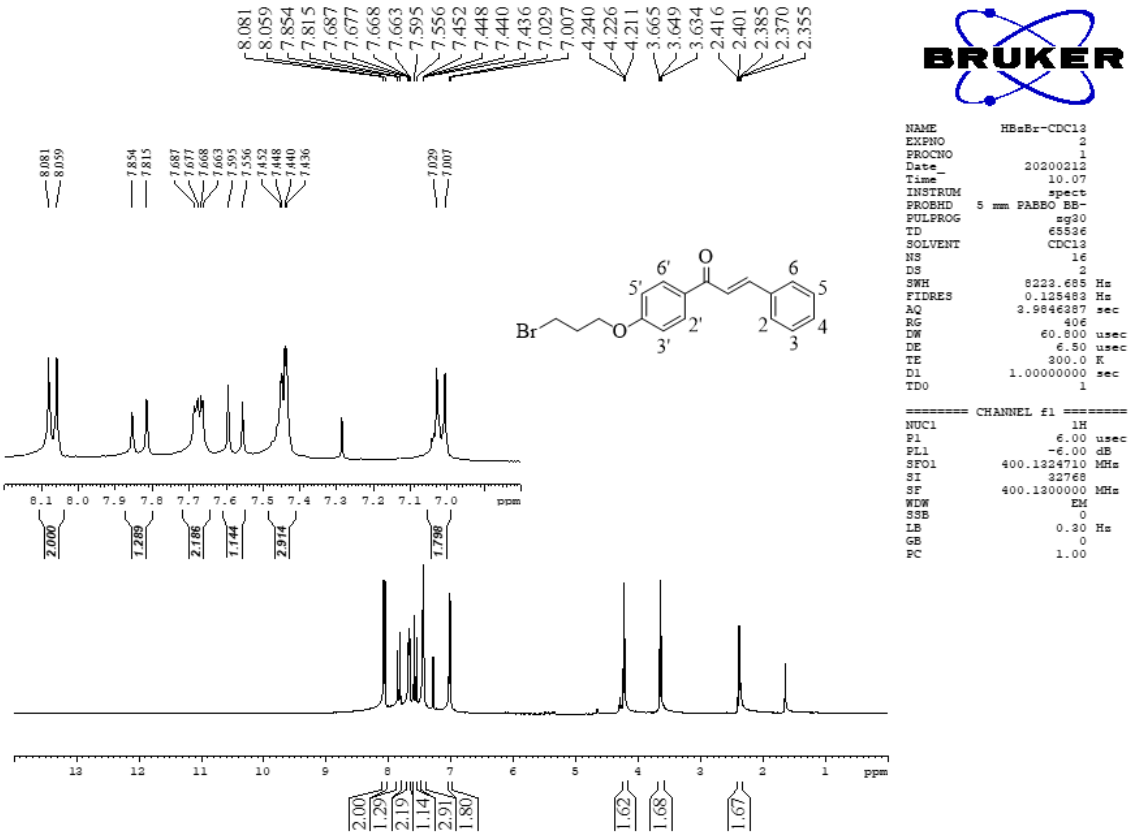
PC	1.00

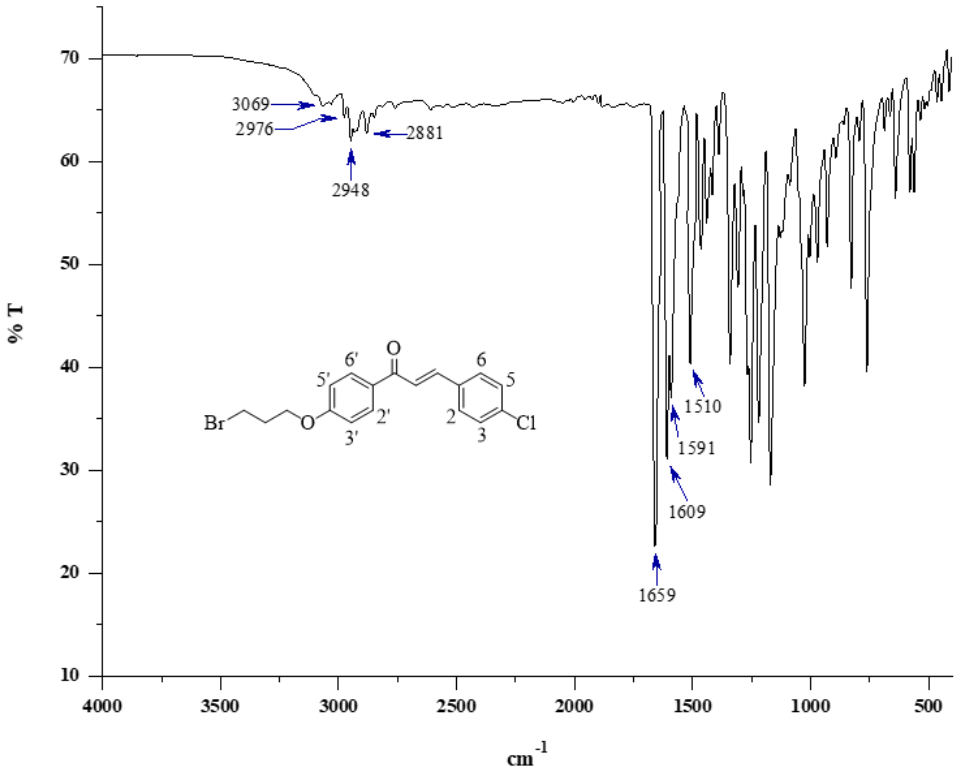
^{1}H NMR spectrum of *(E)*-1-(4-hydroxyphenyl)-3-(*o*-tolyl)prop-2-en-1-one **(5n)**



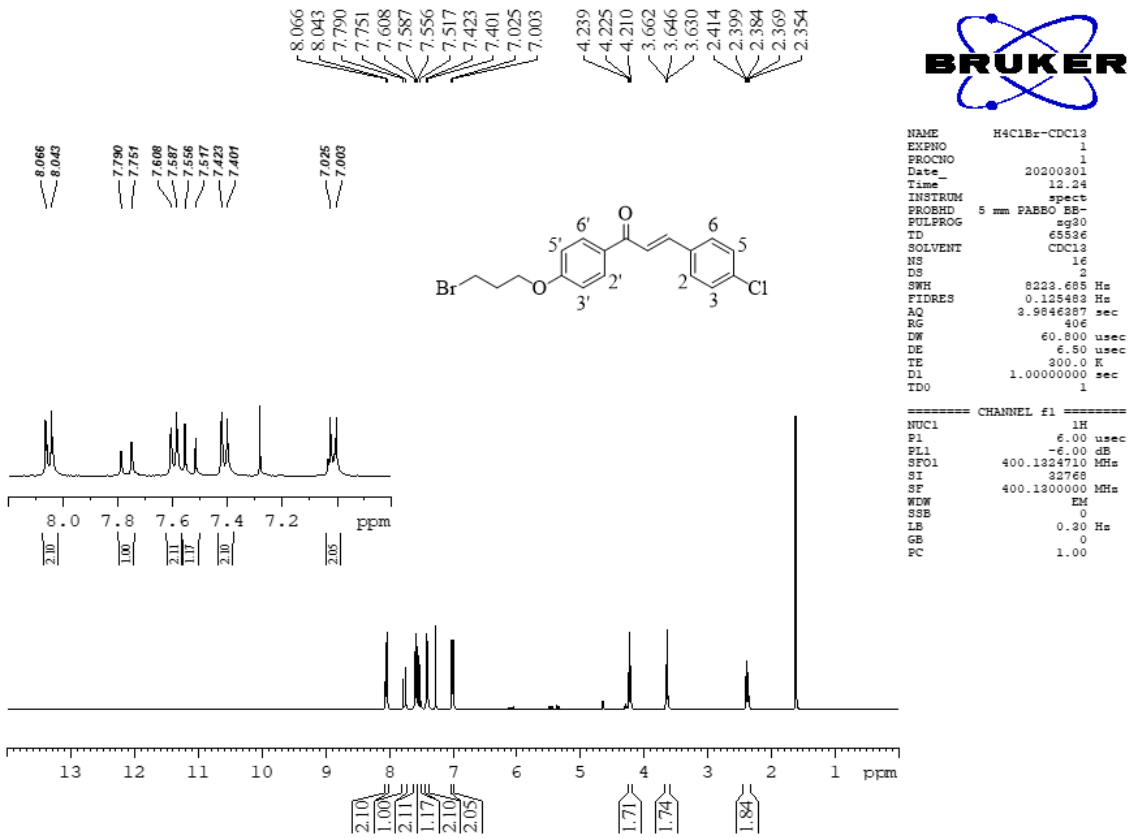
IR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-phenylprop-2-en-1-one **(7a)**



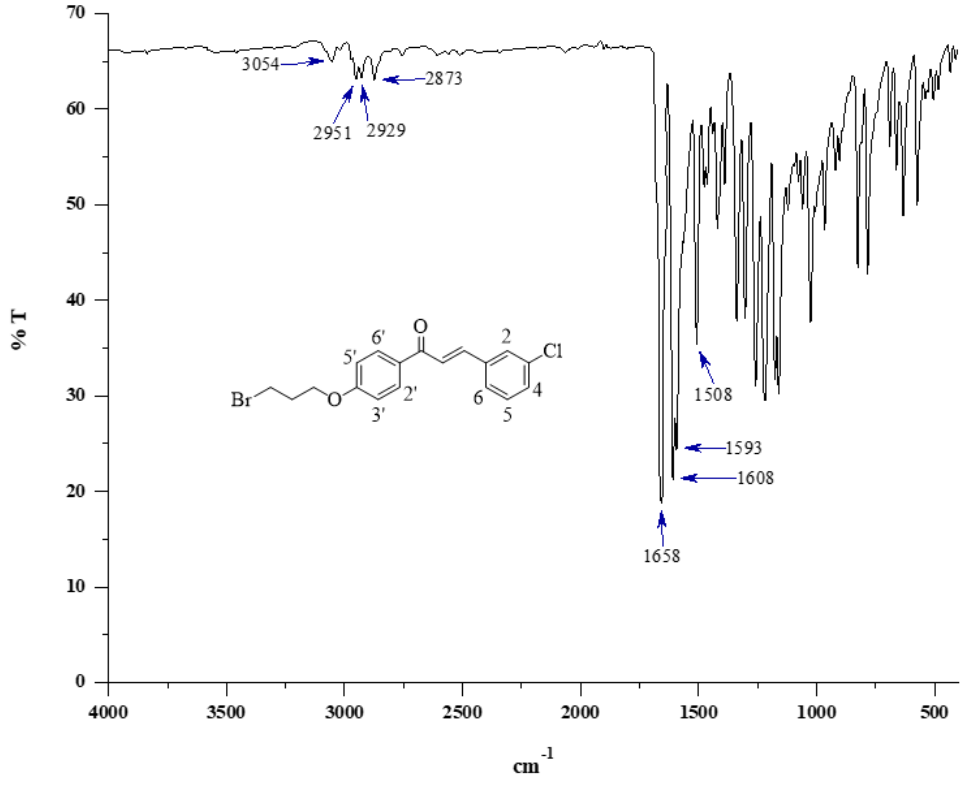
^{1}H NMR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-phenylprop-2-en-1-one **(7a)**



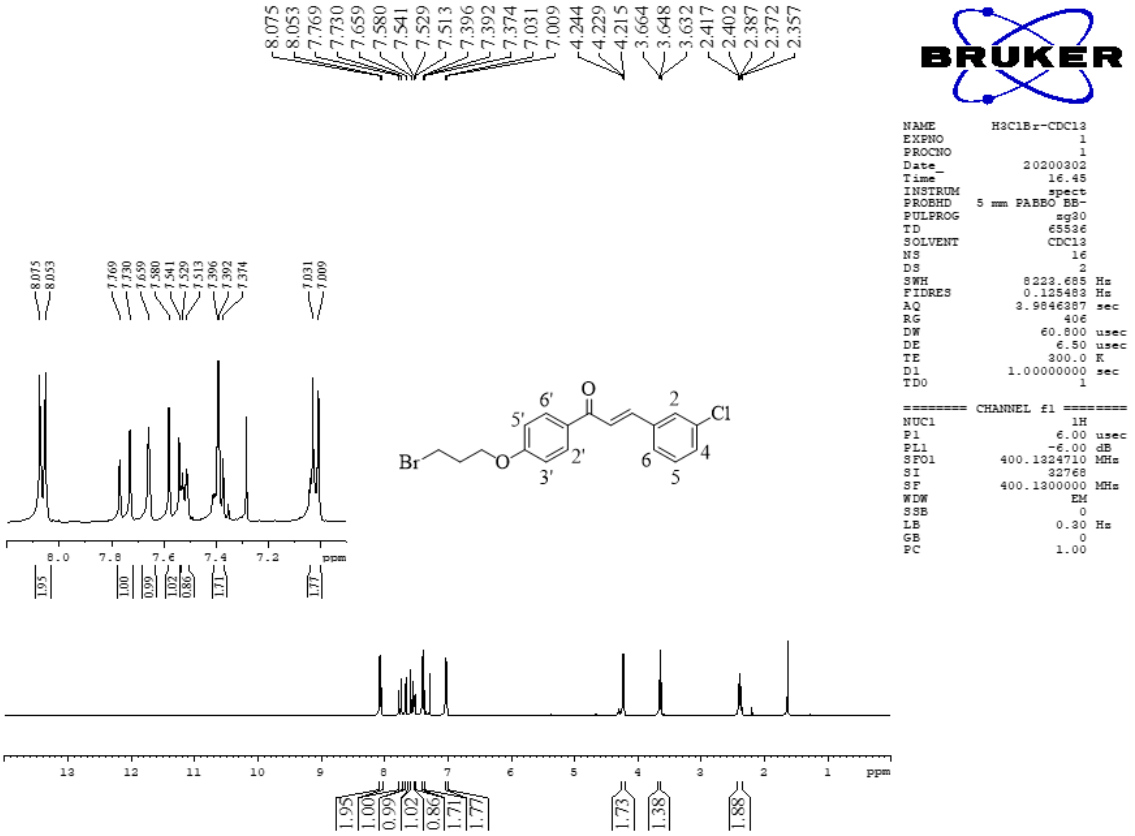
IR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(4-chlorophenyl)prop-2-en-1-one **(7b)**



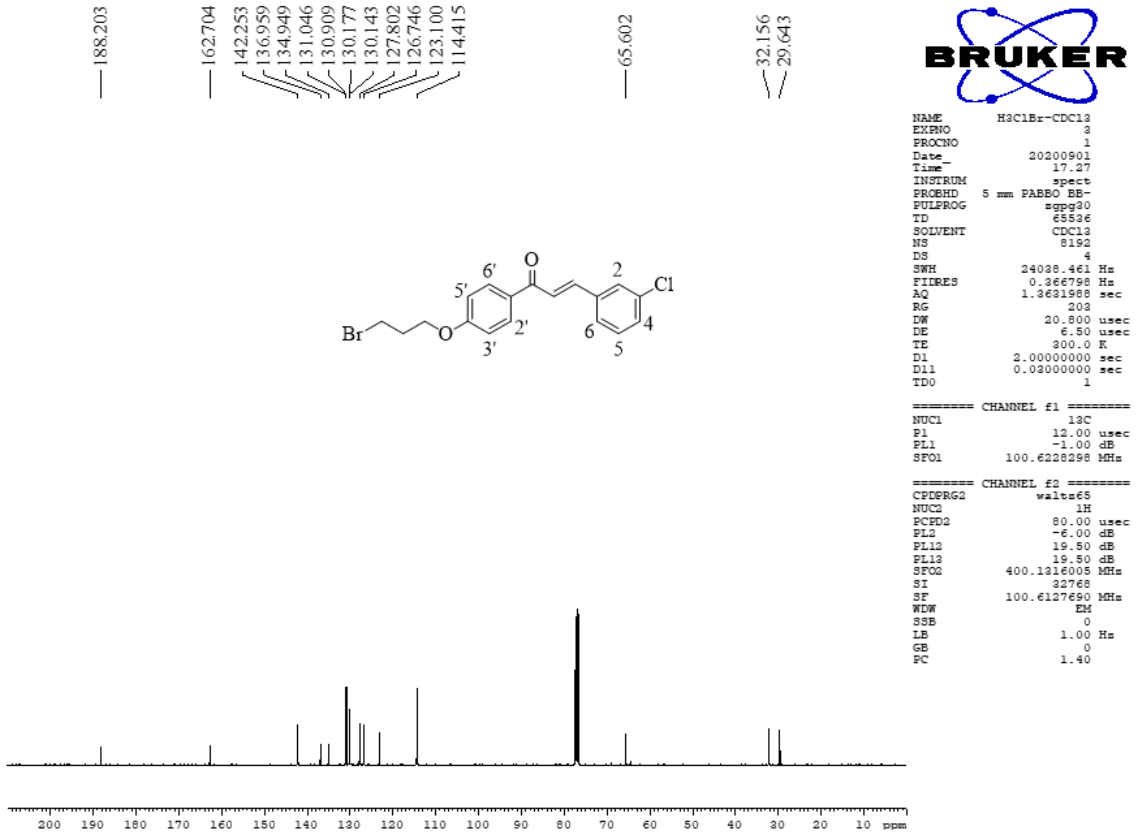
^{1}H NMR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(4-chlorophenyl)prop-2-en-1-one **(7b)**



IR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(3-chlorophenyl)prop-2-en-1-one **(7c)**



^{1}H NMR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(3-chlorophenyl)prop-2-en-1-one **(7c)**

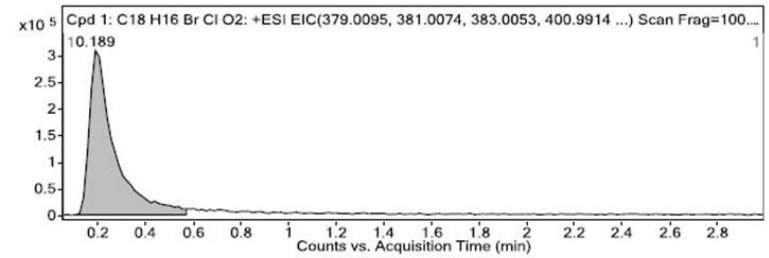


^{13}C NMR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(3-chlorophenyl)prop-2-en-1-one (**7c**)

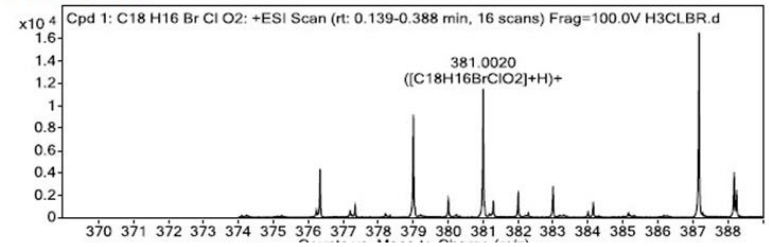
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C18 H16 Br Cl O2	0.189	377.9969	11569	C18 H16 Br Cl O2	378.0022	-14.17

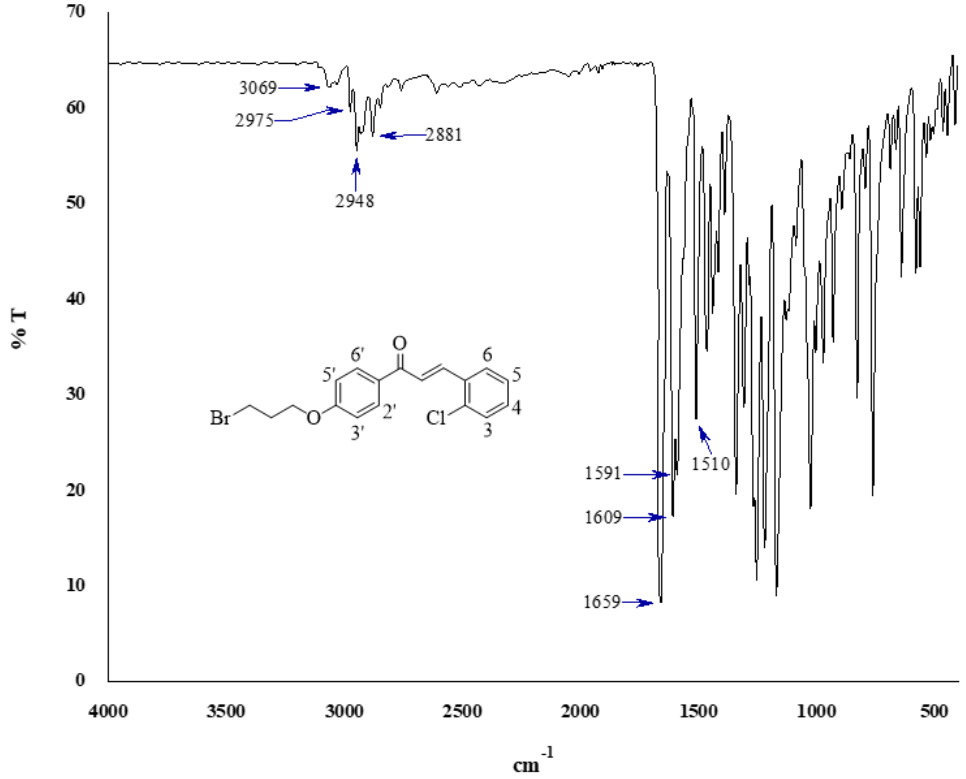
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C18 H16 Br Cl O2	381.002	0.189	Find By Formula	377.9969



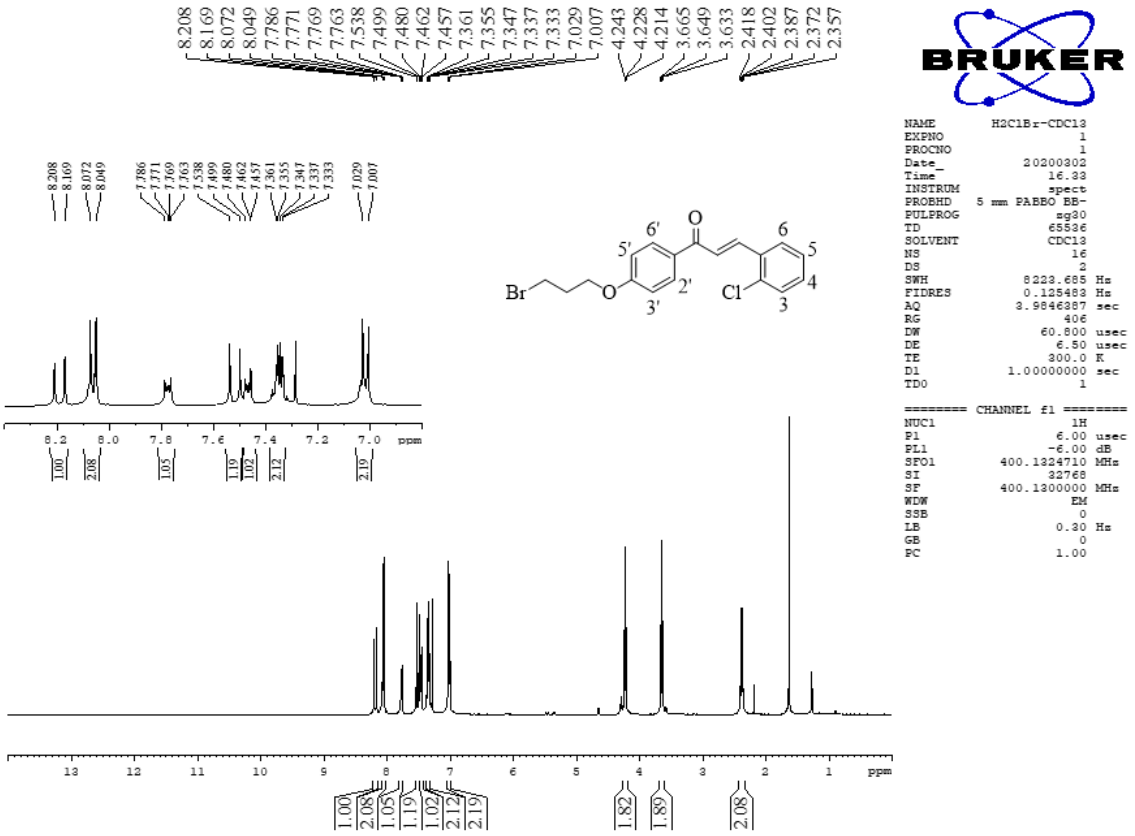
MS Zoomed Spectrum



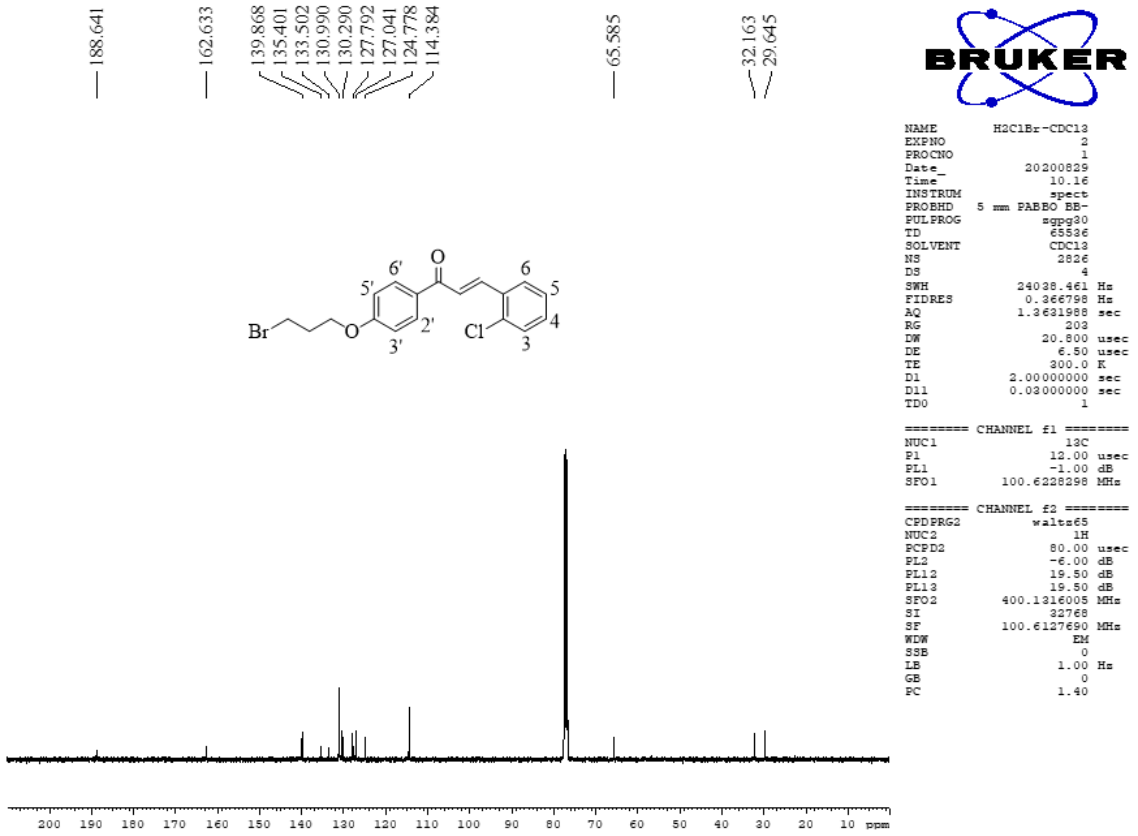
HRMS of compound **7c**



IR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(2-chlorophenyl)prop-2-en-1-one **(7d)**



^{1}H NMR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(2-chlorophenyl)prop-2-en-1-one **(7d)**

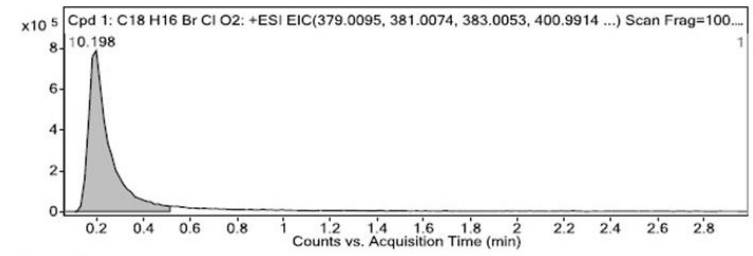


^{13}C NMR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(2-chlorophenyl)prop-2-en-1-one **(7d)**

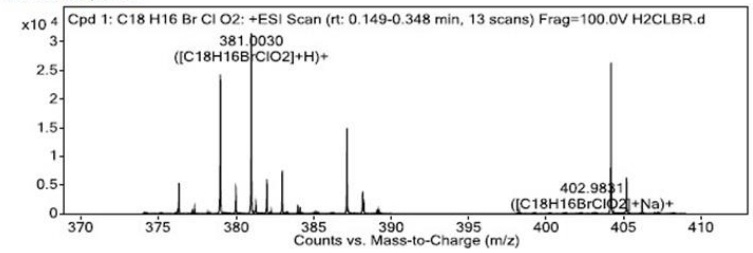
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C18 H16 Br Cl O2	0.198	377.9977	32030	C18 H16 Br Cl O2	378.0022	-11.9

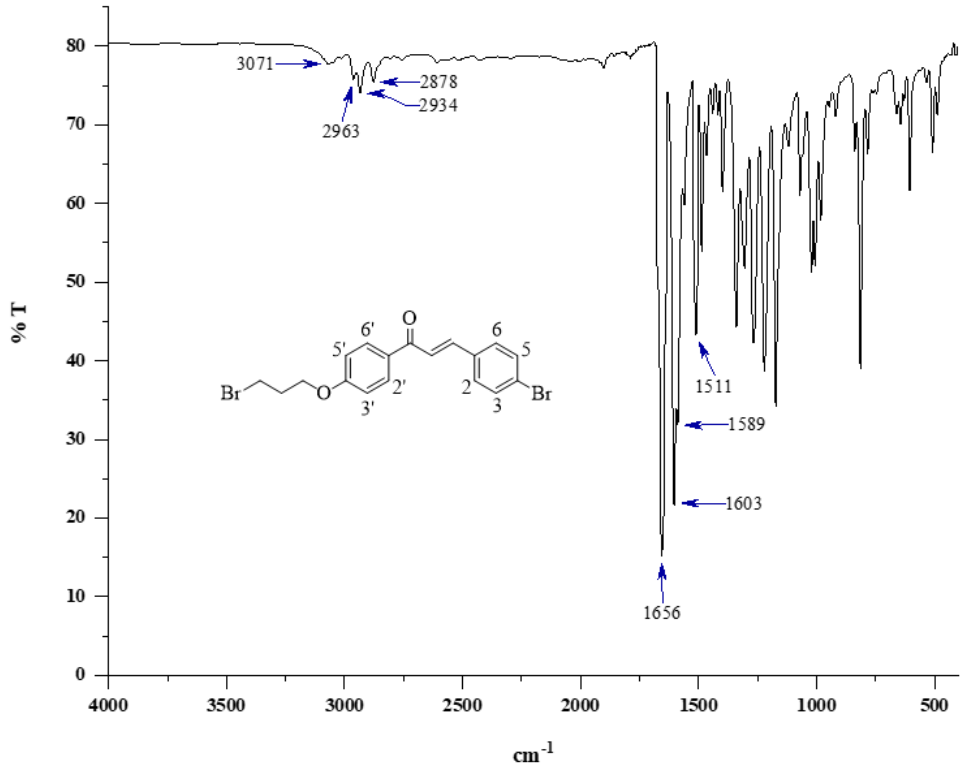
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C18 H16 Br Cl O2	381.003	0.198	Find By Formula	377.9977



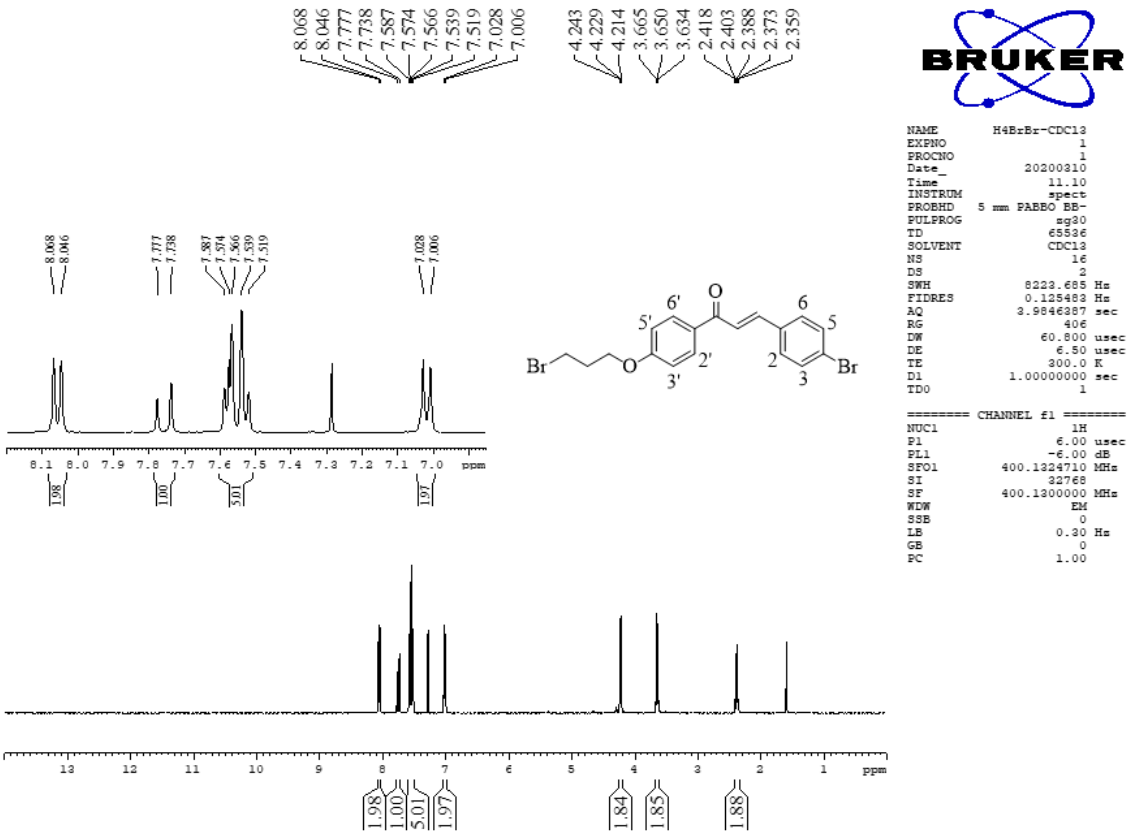
MS Zoomed Spectrum



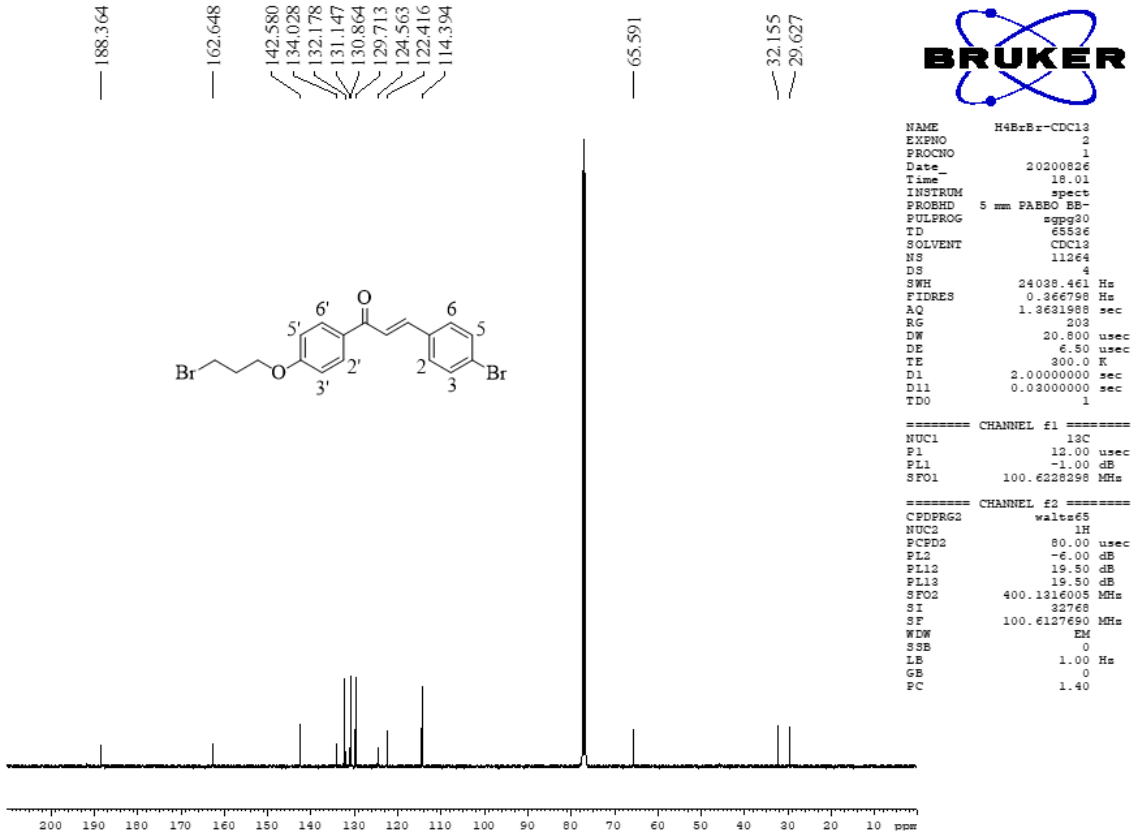
HRMS of compound **7d**



IR spectrum of (*E*)-3-(4-bromophenyl)-1-(4-(3-bromopropoxy)phenyl)prop-2-en-1-one **(7e)**



^{1}H NMR spectrum of (*E*)-3-(4-bromophenyl)-1-(4-(3-bromopropoxy)phenyl)prop-2-en-1-one **(7e)**



^{13}C NMR spectrum of (*E*)-3-(4-bromophenyl)-1-(4-(3-bromopropoxy)phenyl)prop-2-en-1-one (**7e**)

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C18 H16 Br2 O2	0.207	421.9465	83164	C18 H16 Br2 O2	421.9517	-12.4

Compound Label	*m/z*	RT	Algorithm	Mass
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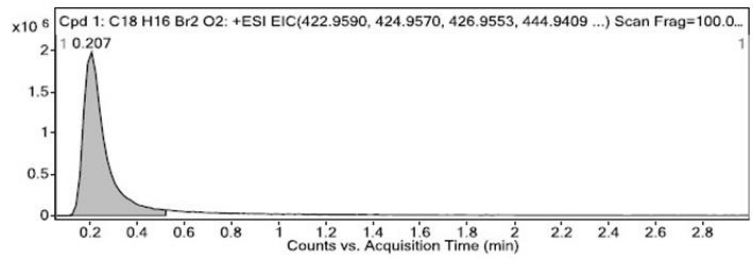
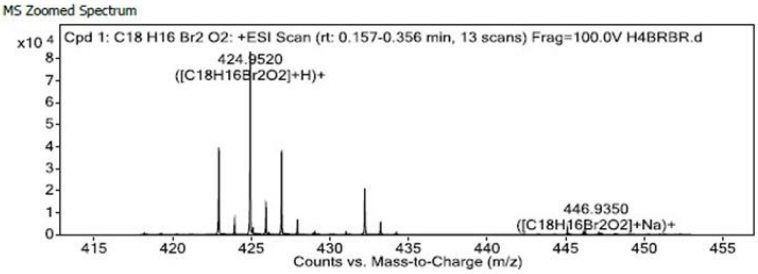
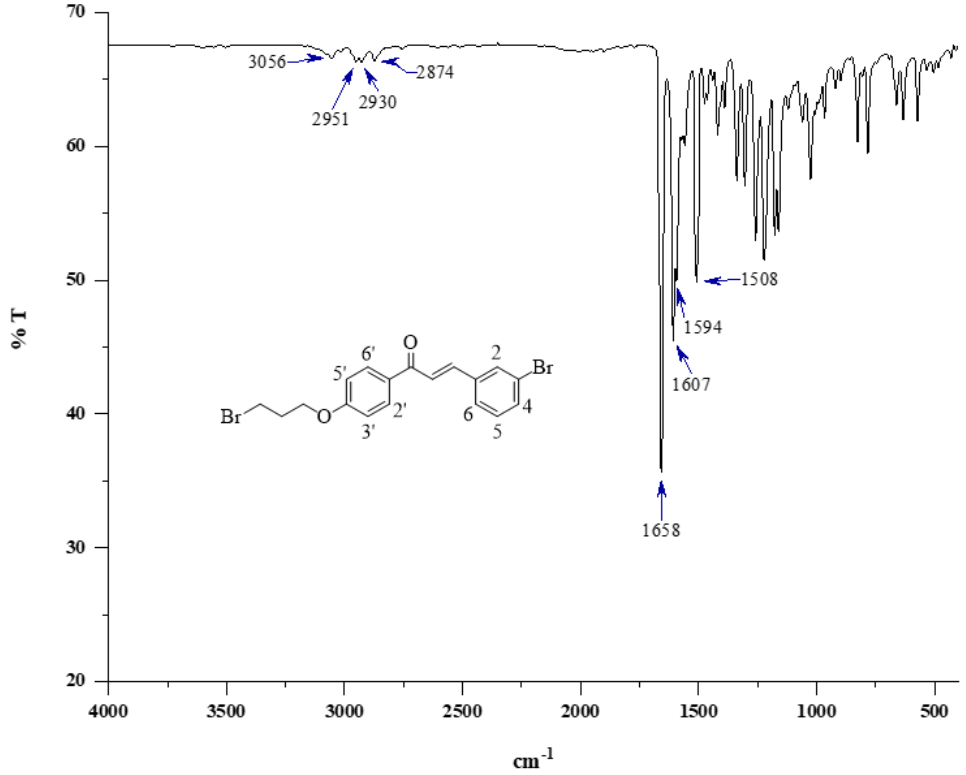


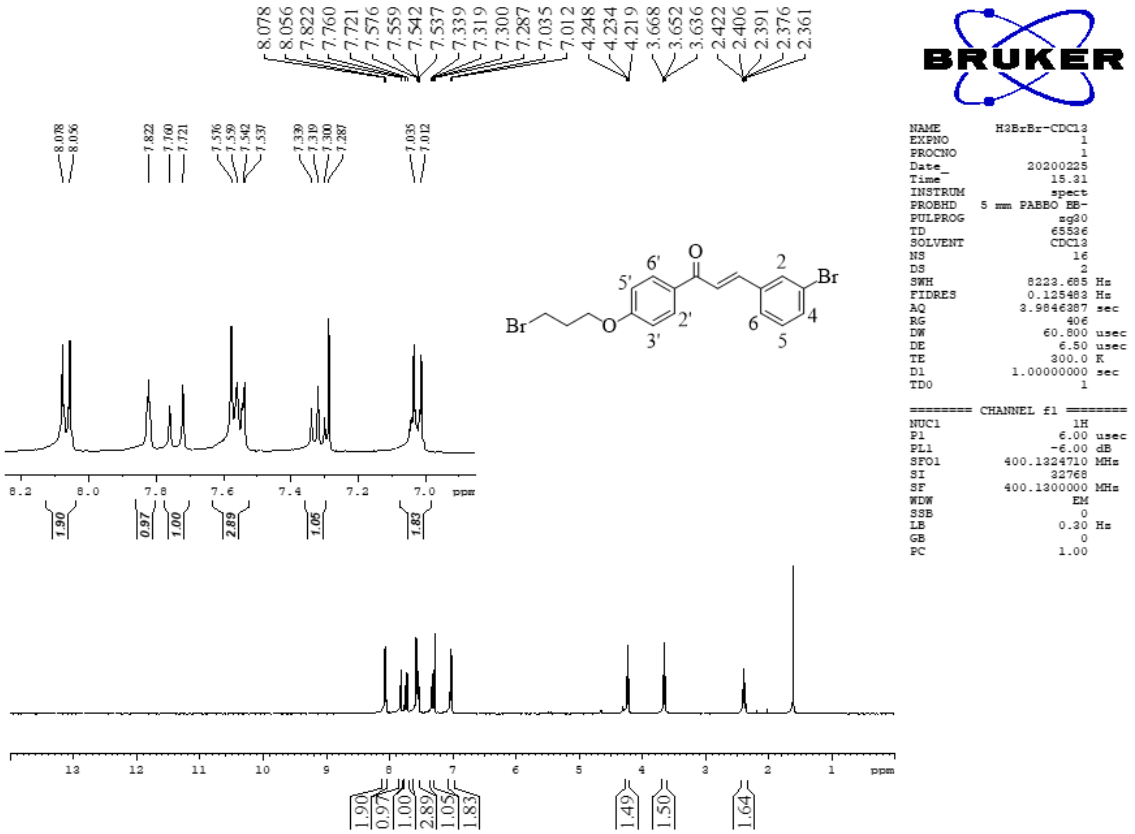
MS Zoomed Spectrum



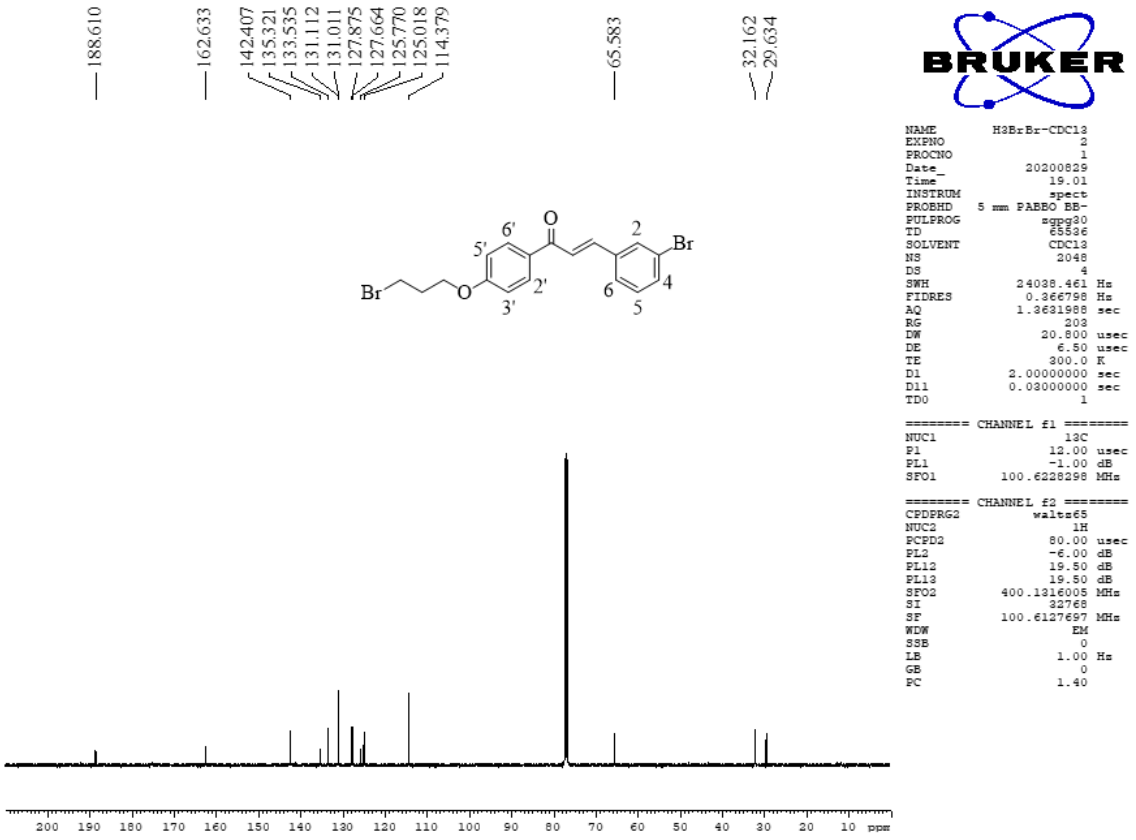
HRMS of compound **7e**



IR spectrum of (*E*)-3-(3-bromophenyl)-1-(4-(3-bromopropoxy)phenyl)prop-2-en-1-one **(7f)**



^{1}H NMR spectrum of (*E*)-3-(3-bromophenyl)-1-(4-(3-bromopropoxy)phenyl)prop-2-en-1-one **(7f)**

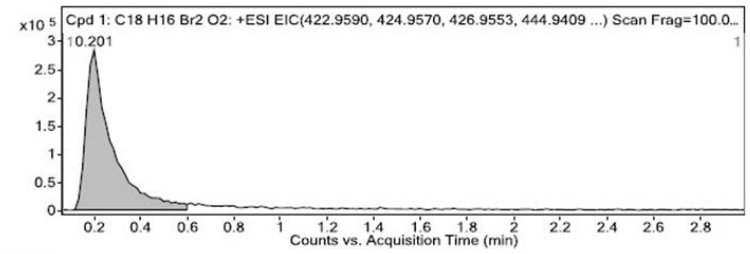


^{13}C NMR spectrum of (*E*)-3-(3-bromophenyl)-1-(4-(3-bromopropoxy)phenyl)prop-2-en-1-one **(7f)**

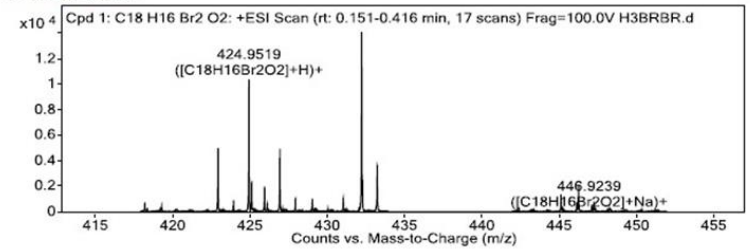
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C18 H16 Br2 O2	0.201	421.9464	10400	C18 H16 Br2 O2	421.9517	-12.51

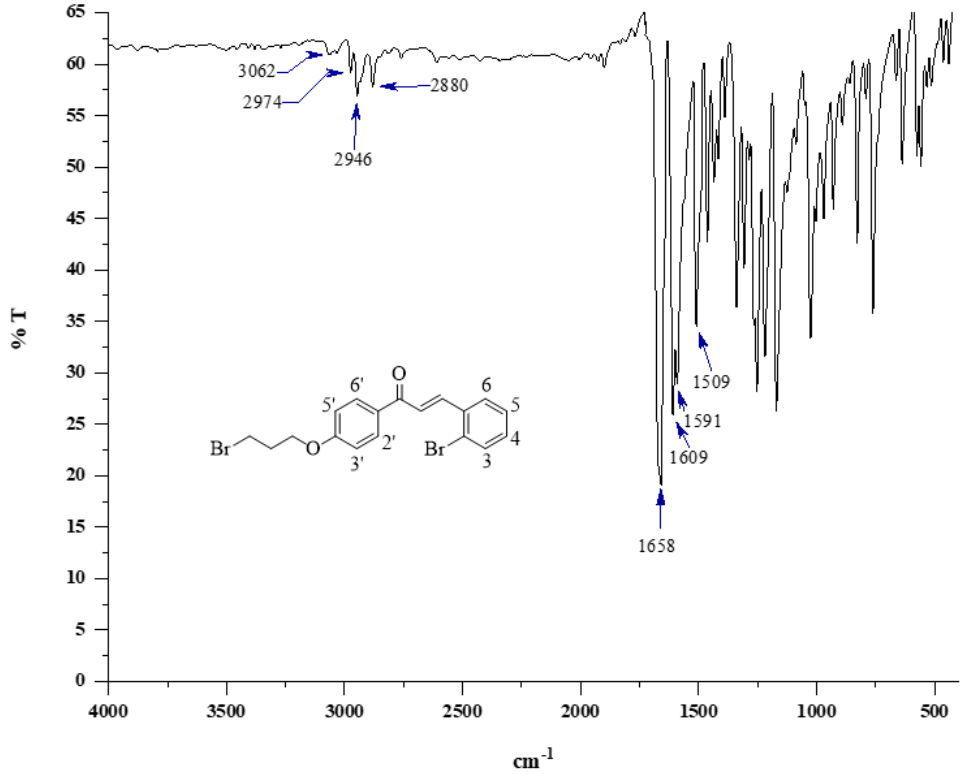
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C18 H16 Br2 O2	424.9519	0.201	Find By Formula	421.9464



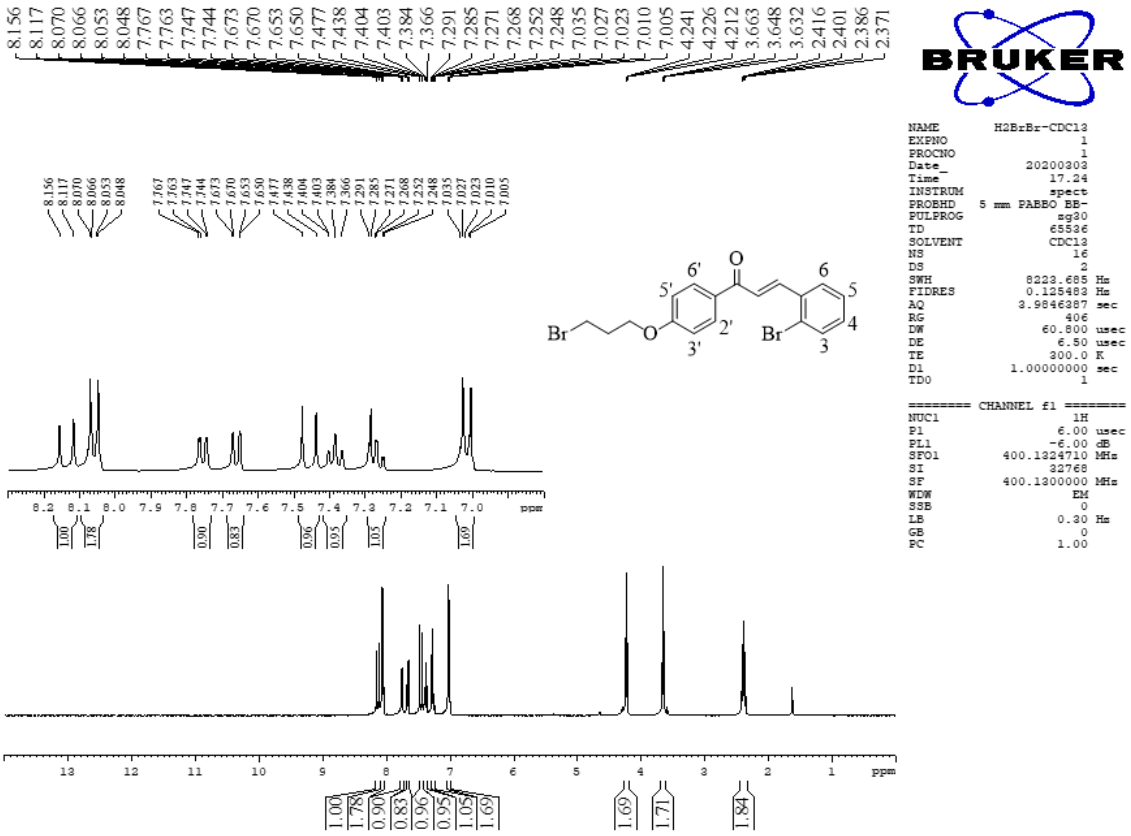
MS Zoomed Spectrum



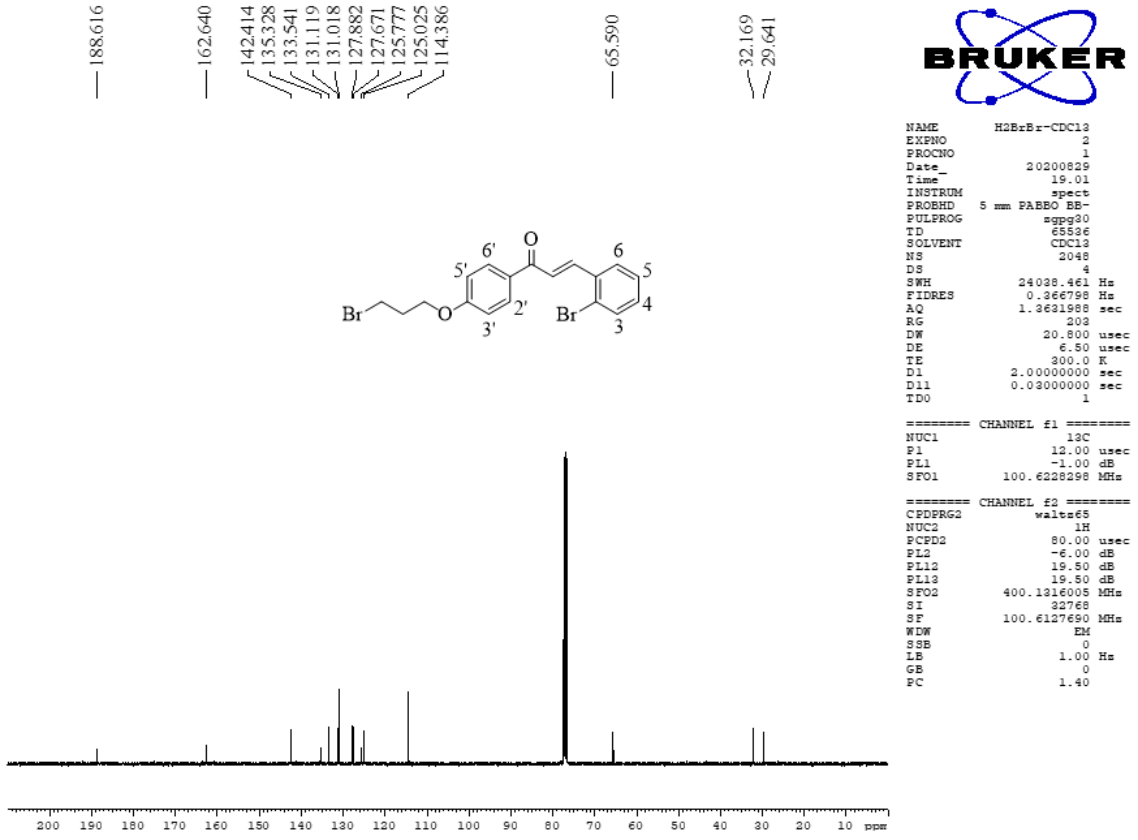
HRMS of compound **7f**



IR spectrum of (*E*)-3-(2-bromophenyl)-1-(4-(3-bromopropoxy)phenyl)prop-2-en-1-one **(7g)**



^{1}H NMR spectrum of (*E*)-3-(2-bromophenyl)-1-(4-(3-bromopropoxy)phenyl)prop-2-en-1-one **(7g)**

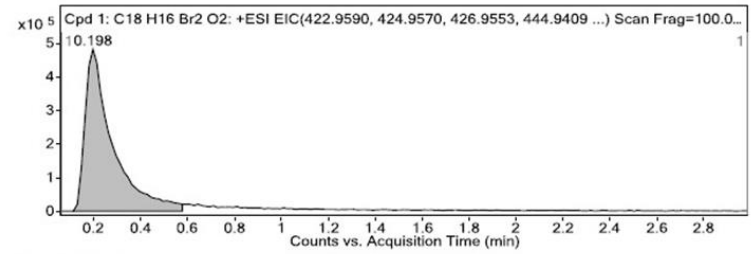


^{13}C NMR spectrum of (*E*)-3-(2-bromophenyl)-1-(4-(3-bromopropoxy)phenyl)prop-2-en-1-one (**7g**)

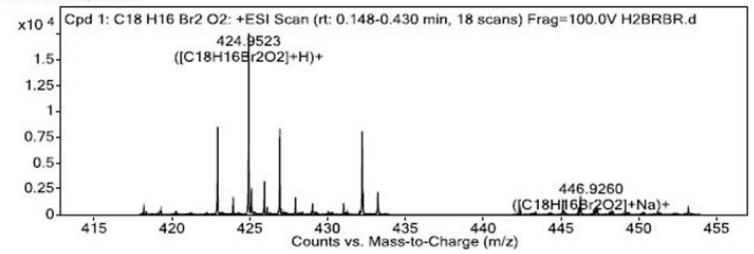
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C18 H16 Br2 O2	0.198	421.9467	17538	C18 H16 Br2 O2	421.9517	-11.74

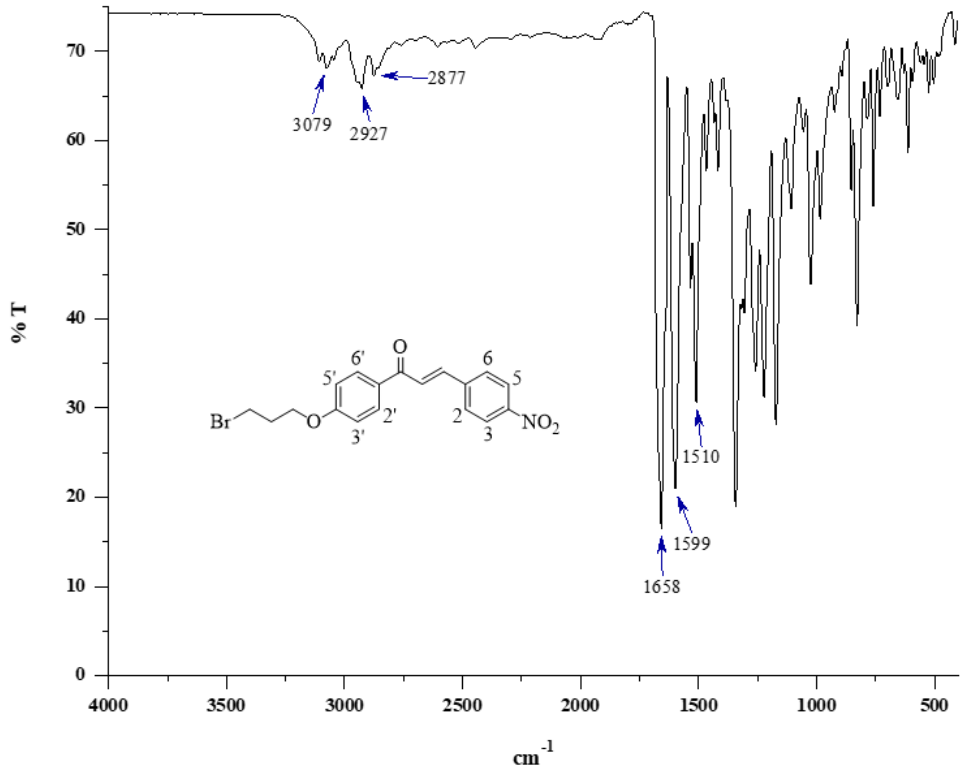
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C18 H16 Br2 O2	424.9523	0.198	Find By Formula	421.9467



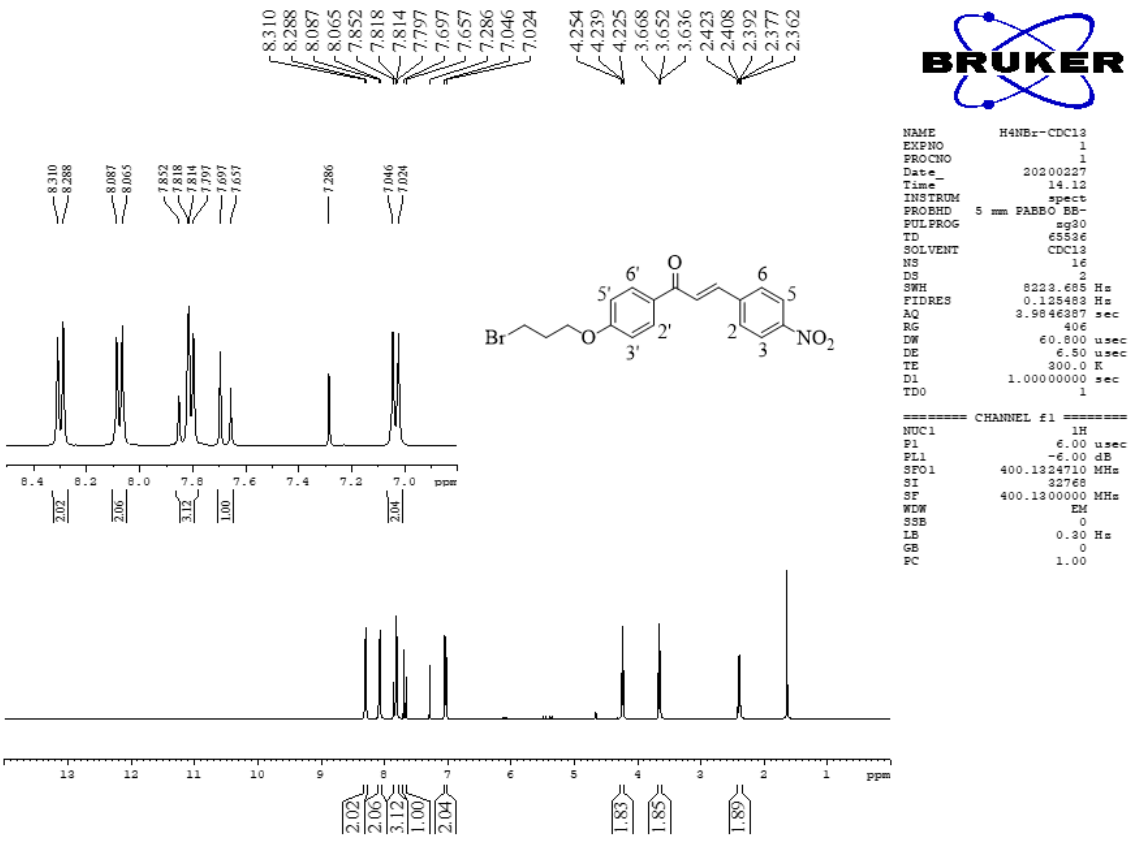
MS Zoomed Spectrum



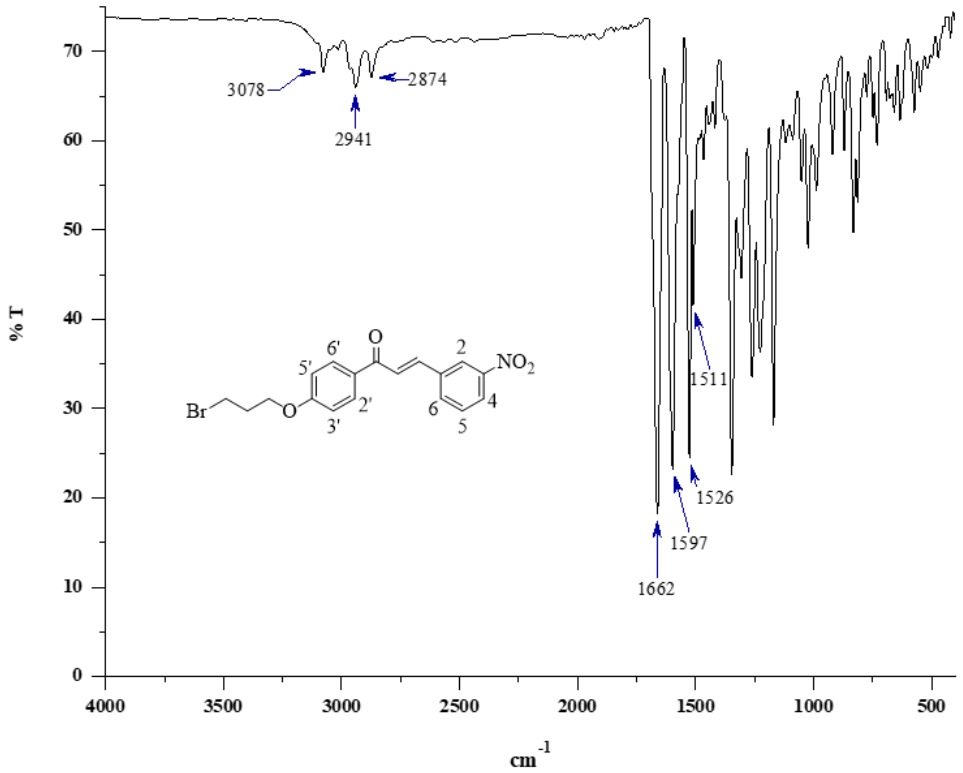
HRMS of compound **7g**



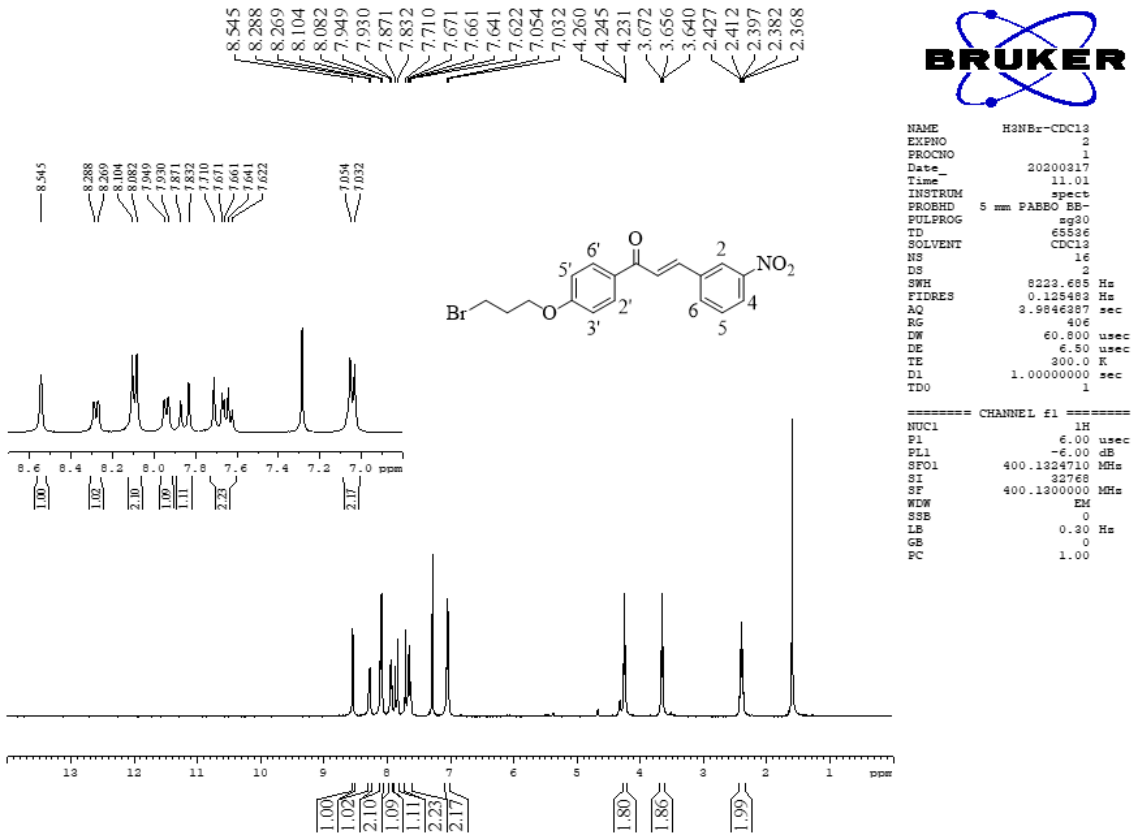
IR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(4-nitrophenyl)prop-2-en-1-one **(7h)**



^{1}H NMR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(4-nitrophenyl)prop-2-en-1-one **(7h)**



IR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(3-nitrophenyl)prop-2-en-1-one **(7i)**

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PROCNO                  1
Date_            20200317
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INSTRUM             spect
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PULPROG             zg30
TD                 65536
SOLVENT             CDC13
NS                     16
DS                      2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                    406
DW                60.800 usec
DE                 6.50 usec
TE                300.0 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
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PL1                -6.00 dB
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SI                  32768
SF            400.1300000 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
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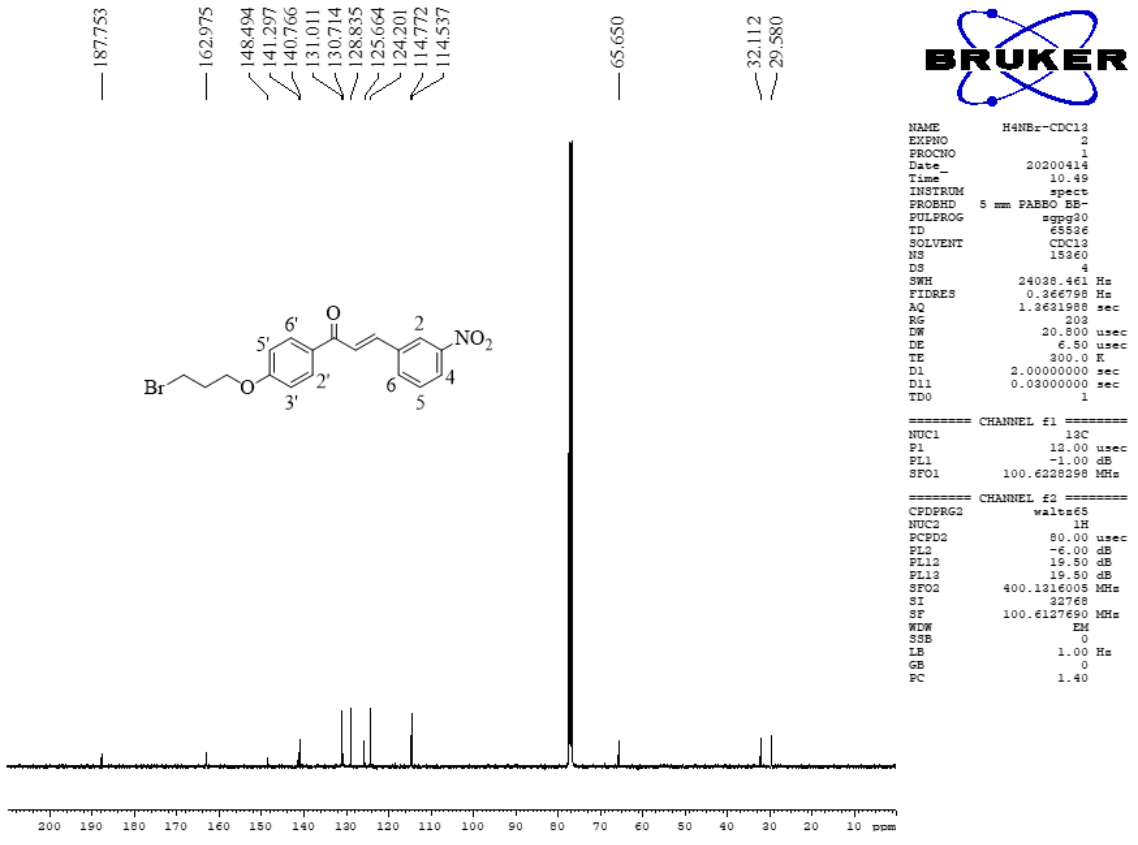
^{1}H NMR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(3-nitrophenyl)prop-2-en-1-one **(7i)**

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EXPNO                   2
PROCNO                  1
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TD                 65536
SOLVENT             CDC13
NS                  15360
DS                      4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                    203
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                12.00 usec
PL1               -1.00 dB
SFO1          100.6228298 MHz

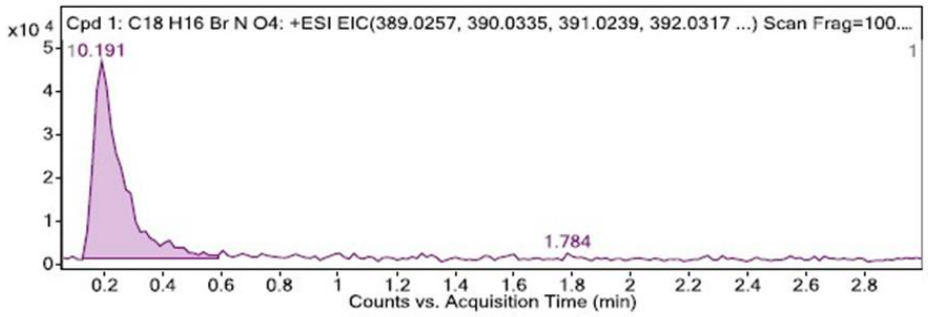
======== CHANNEL f2 ========
CPDPRG2          waltz65
NUC2                   1H
PCPD2             80.00 usec
PL2               -6.00 dB
PL12              19.50 dB
PL13              19.50 dB
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127690 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                   1.40
```

^{13}C NMR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(3-nitrophenyl)prop-2-en-1-one **(7i)**

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C18 H16 Br N O4	0.191	389.0273	1624	C18 H16 Br N O4	389.0263	2.59

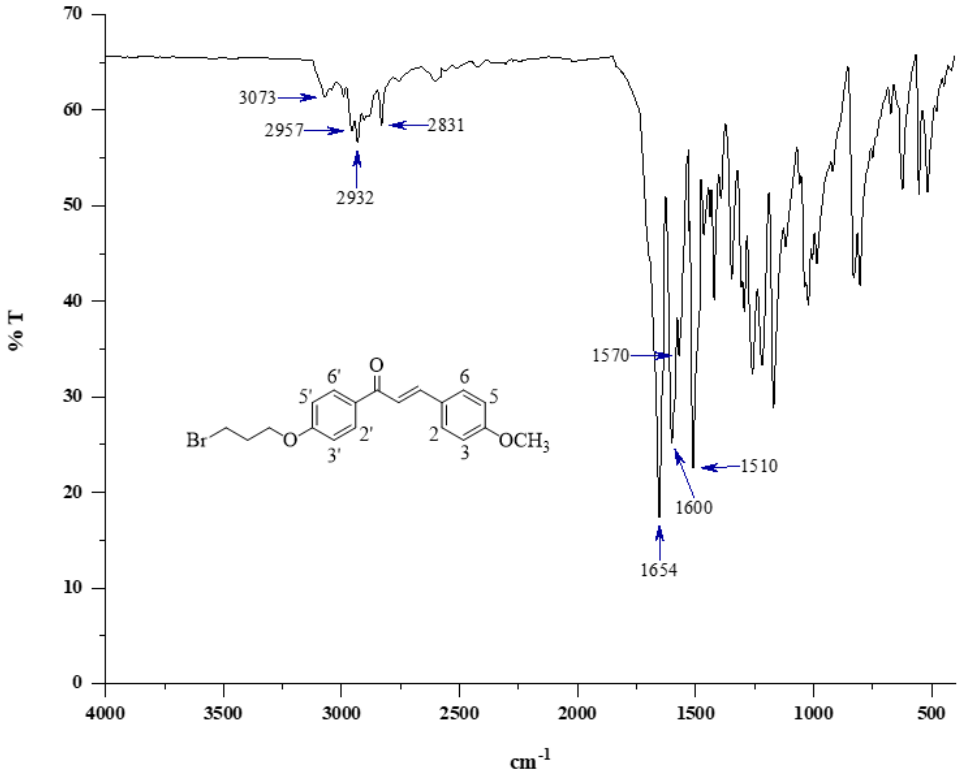
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C18 H16 Br N O4	390.0294	0.191	Find By Formula	389.0273



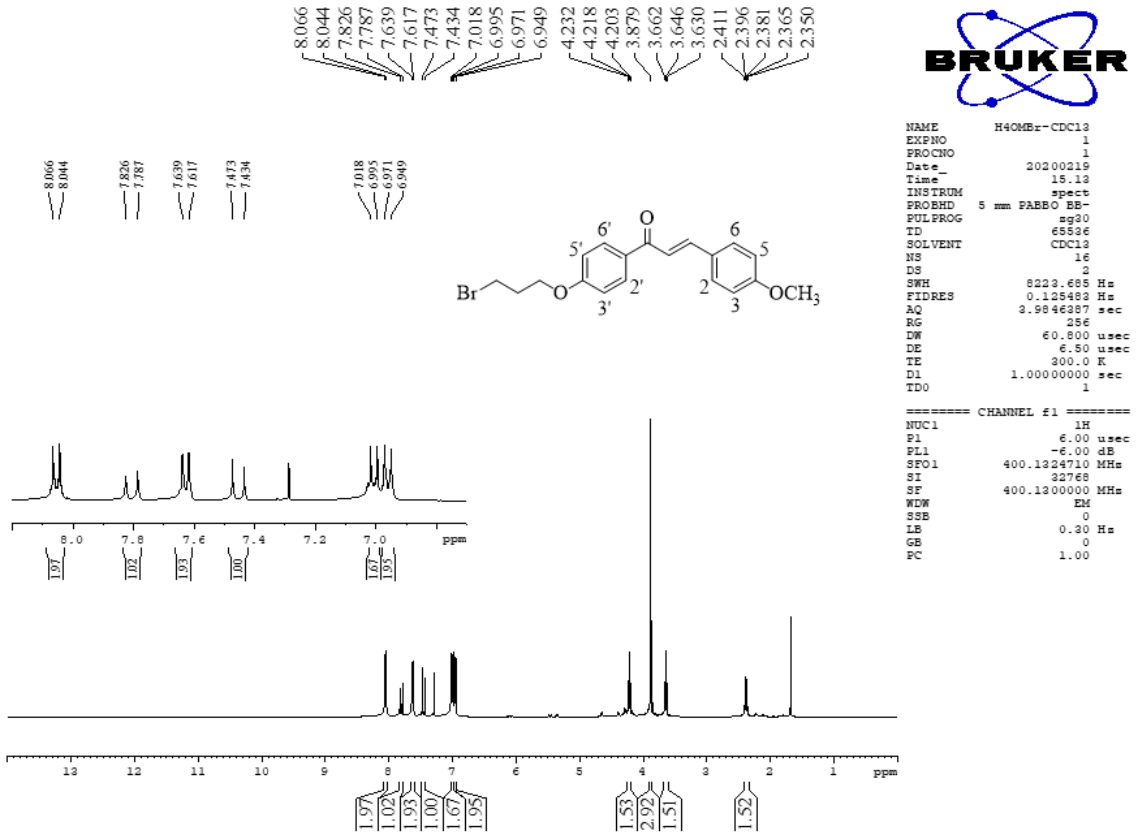
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
390.0294	390.029	-1.01	1	1623.55	C18H16BrNO4	M+
391.0339	391.0239	-25.7	1	307.43	C18H16BrNO4	M+
392.0269	392.0271	0.43	1	1518.64	C18H16BrNO4	M+

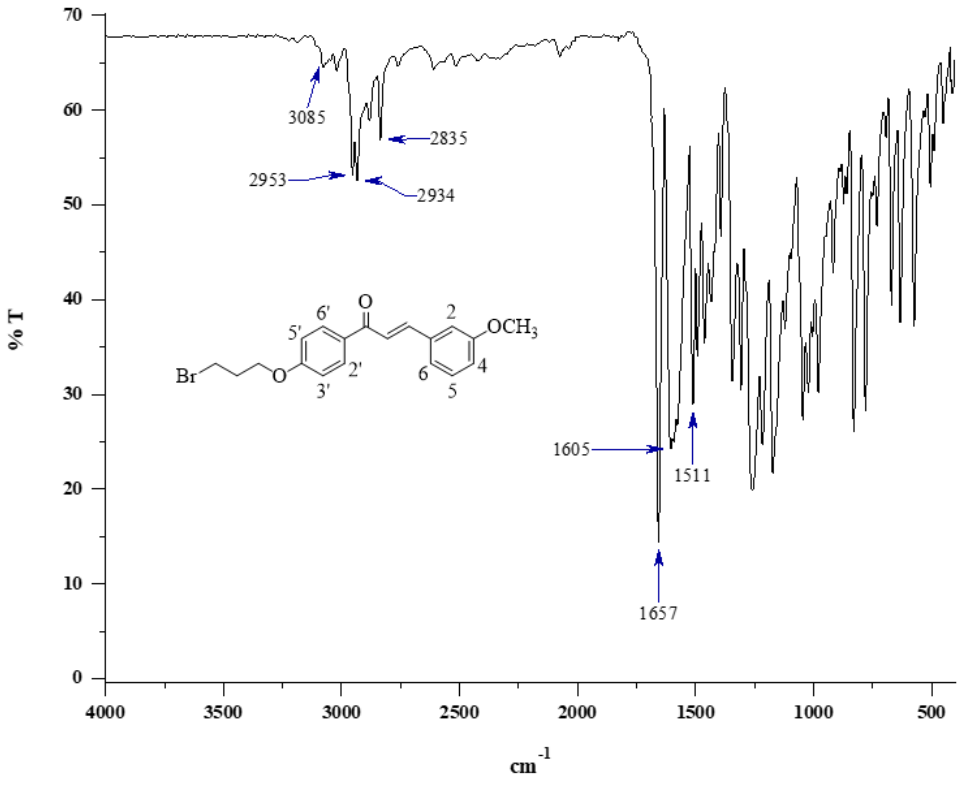
HRMS of compound **7i**



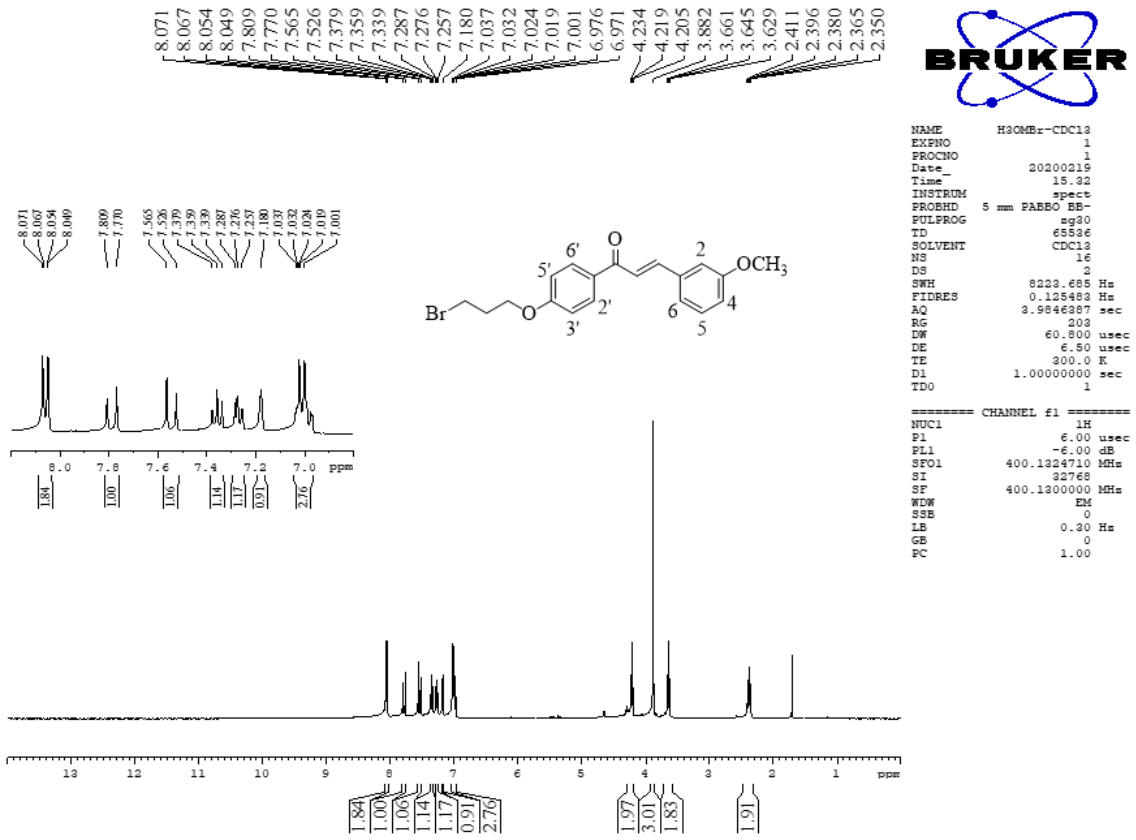
IR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(4-methoxyphenyl)prop-2-en-1-one **(7j)**



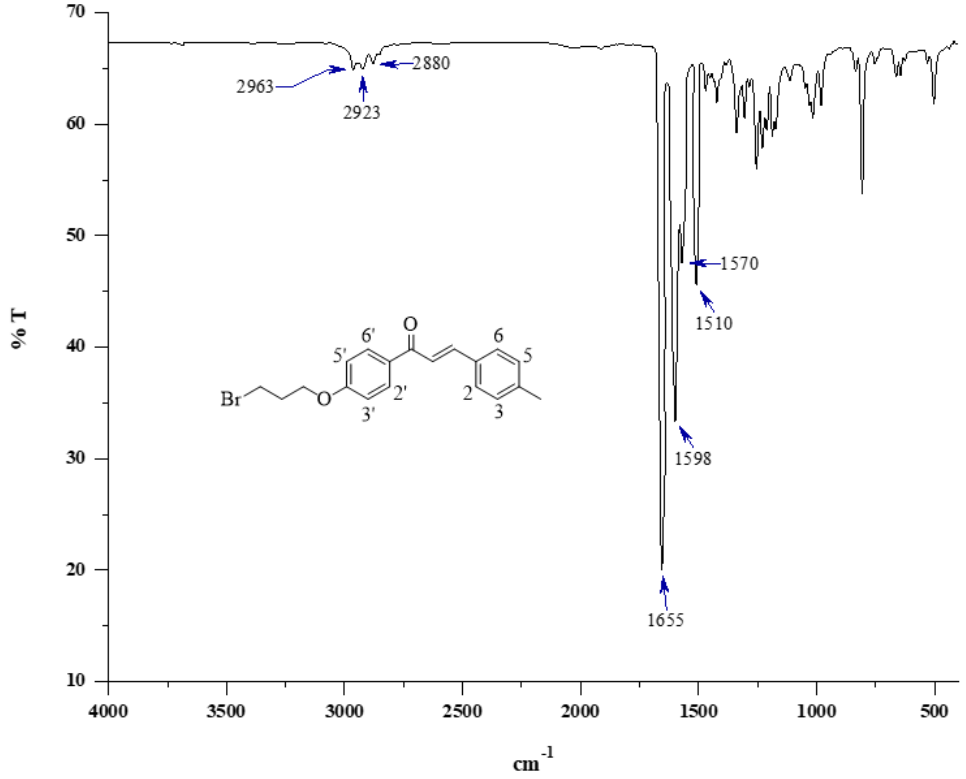
^{1}H NMR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(4-methoxyphenyl)prop-2-en-1-one **(7j)**



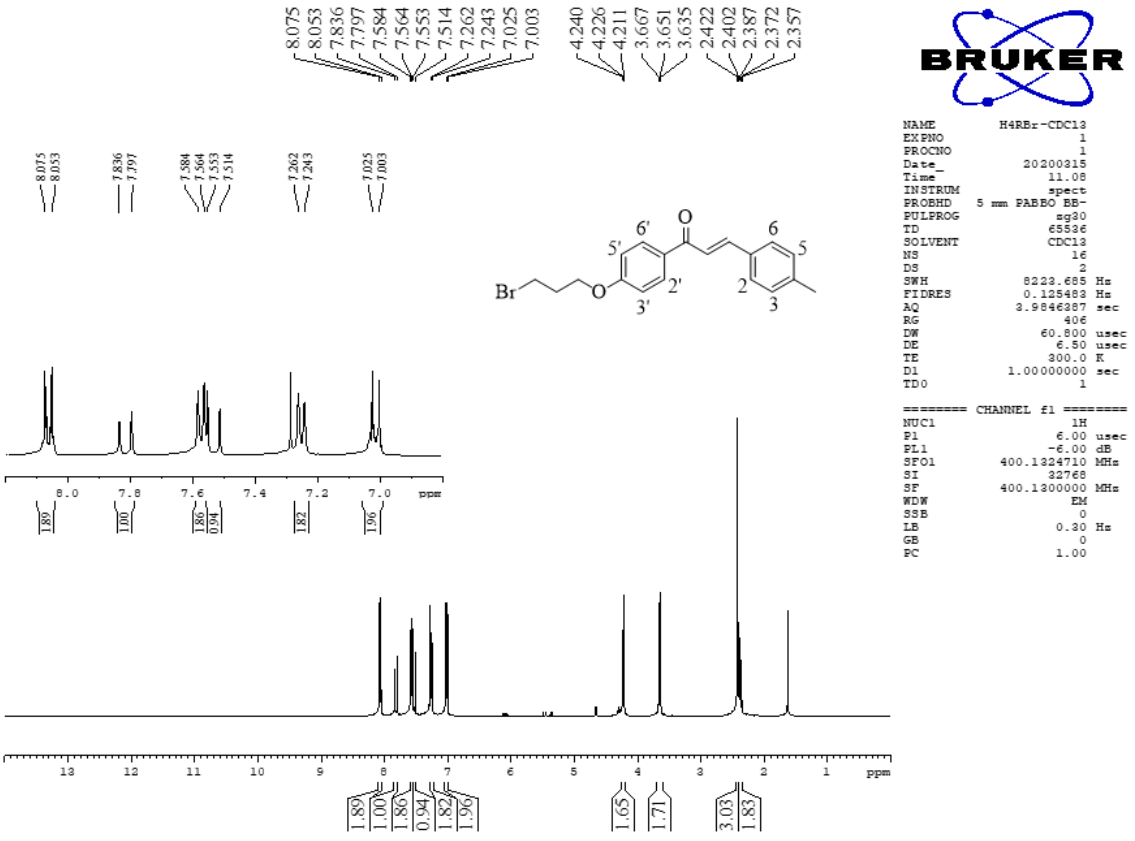
IR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(3-methoxyphenyl)prop-2-en-1-one **(7k)**



^{1}H NMR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(3-methoxyphenyl)prop-2-en-1-one **(7k)**



IR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(*p*-tolyl)prop-2-en-1-one **(7l)**



BRUKER

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PROCNO                  1
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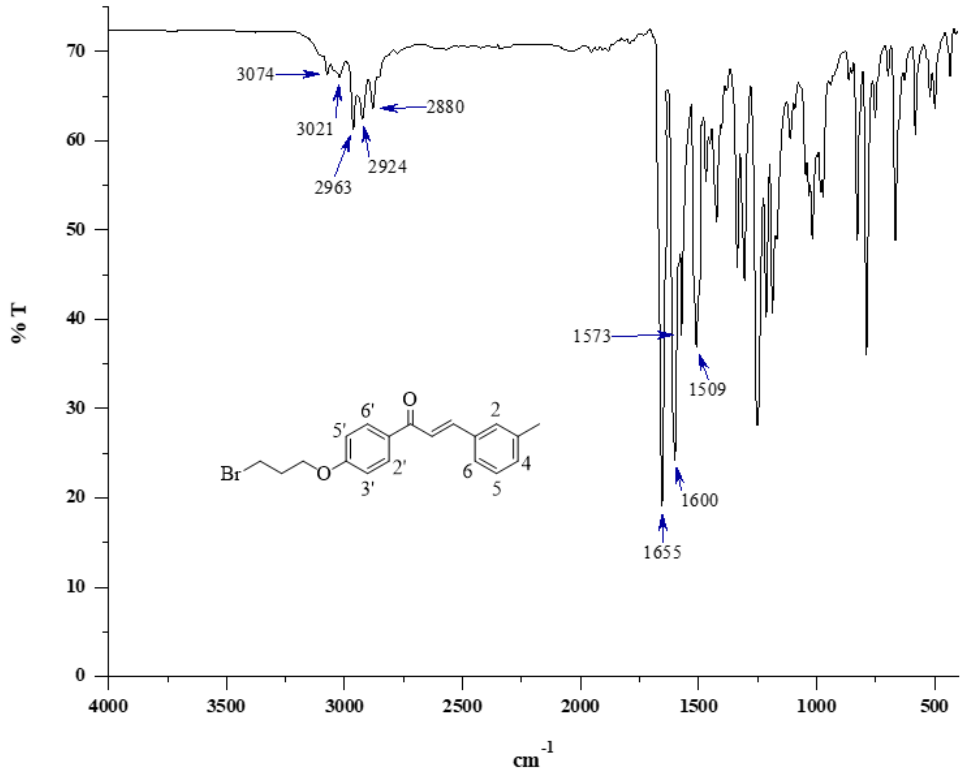
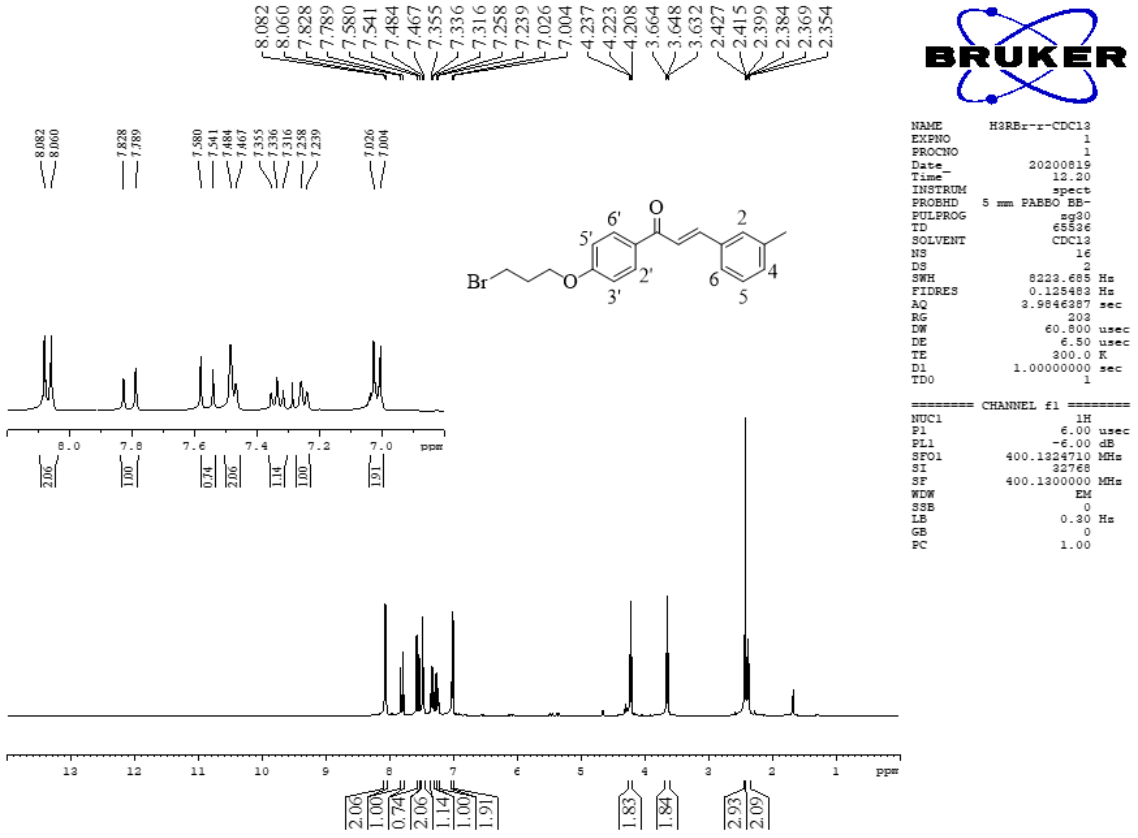
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                    16
DS                     2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                   406
DW              60.800 usec
DE               6.50 usec
TE                300.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 6.00 usec
PL1               -6.00 dB
SFO1        400.1324710 MHz
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

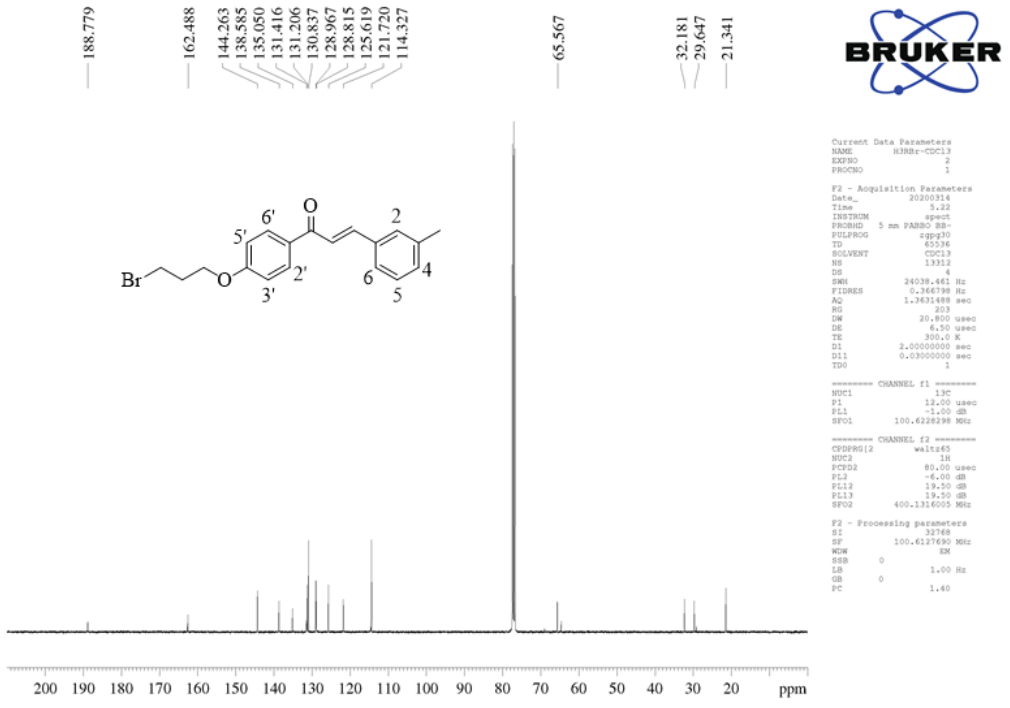
^{1}H NMR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(*p*-tolyl)prop-2-en-1-one **(7l)**



IR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(*m*-tolyl)prop-2-en-1-one **(7m)**



^{1}H NMR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(*m*-tolyl)prop-2-en-1-one **(7m)**

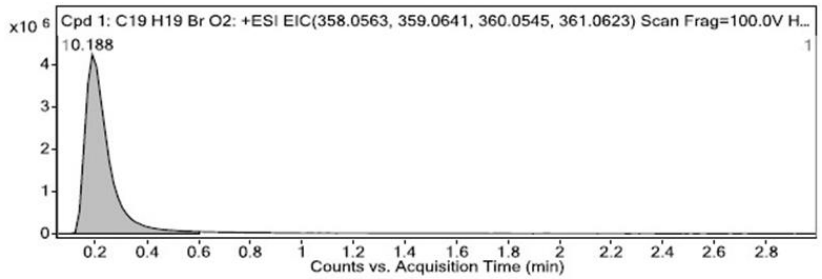


^{13}C NMR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(*m*-tolyl)prop-2-en-1-one **(7m)**

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C19 H19 Br O2	0.188	358.0535	99342	C19 H19 Br O2	358.0568	-9.4

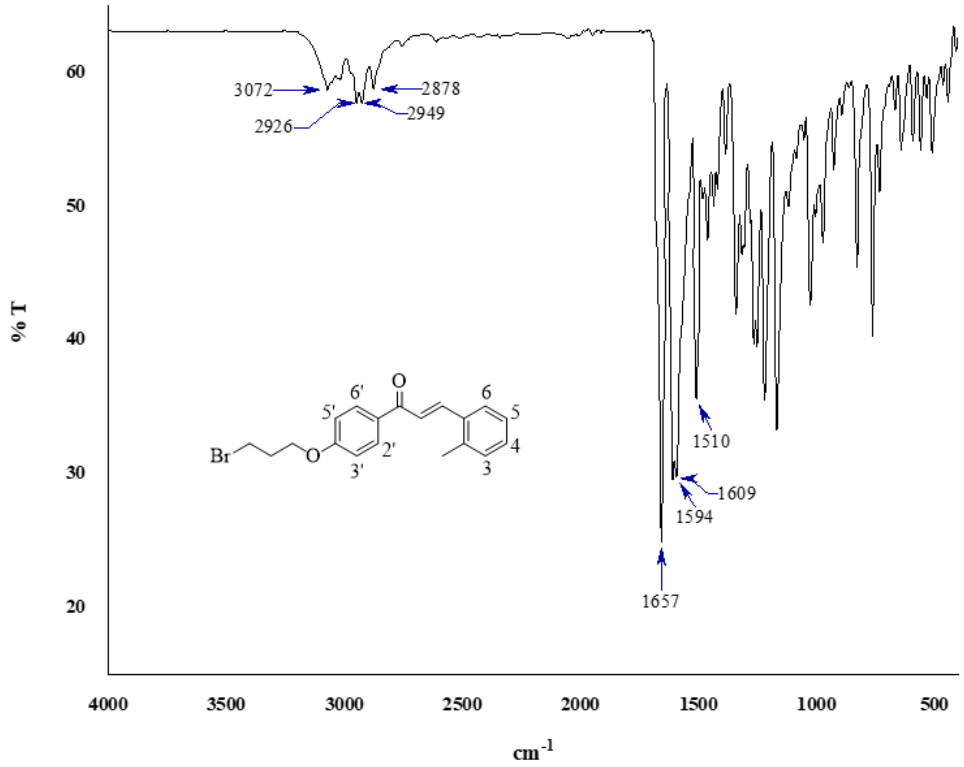
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C19 H19 Br O2	361.059	0.188	Find By Formula	358.0535



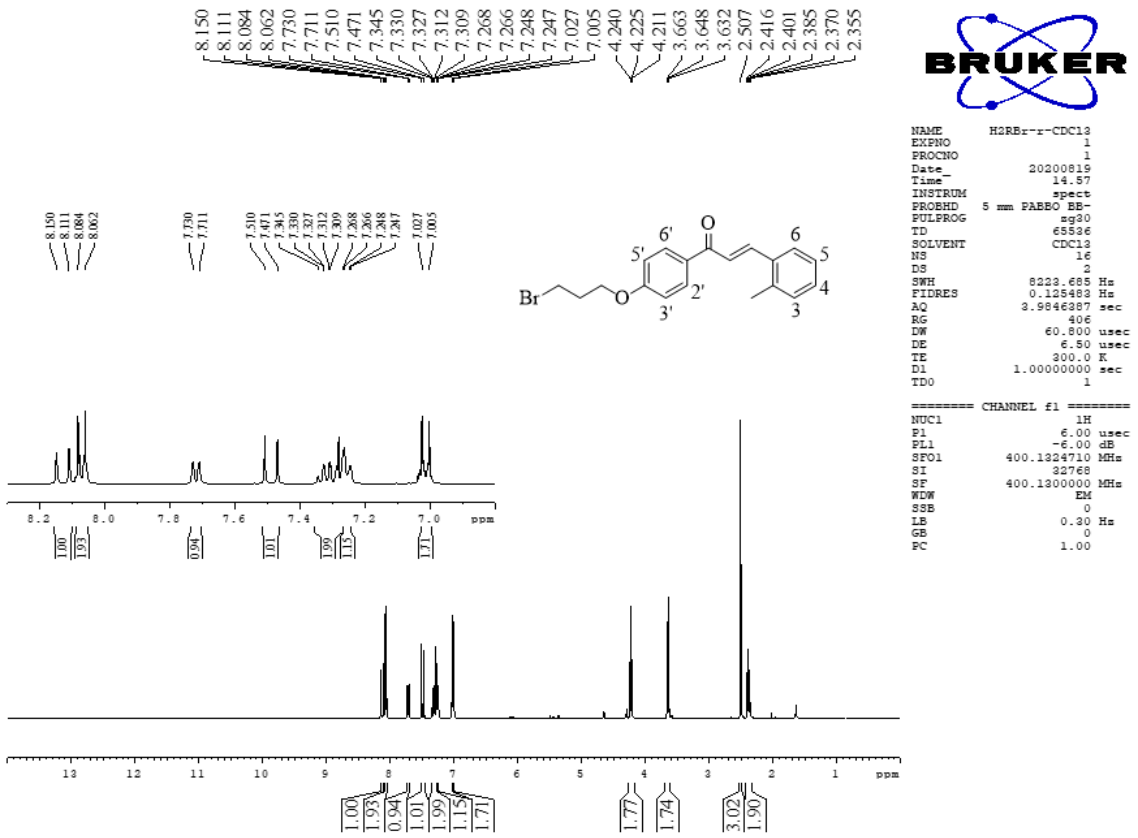
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
358.0488	358.0563	21.01	1	114.01	C19H19BrO2	M+
359.0609	359.0641	8.89	1	99164.11	C19H19BrO2	(M+H)+
360.0636	360.0675	10.8	1	18413.21	C19H19BrO2	(M+H)+
361.059	361.0623	9.22	1	99342.4	C19H19BrO2	(M+H)+
362.0617	362.0655	10.74	1	17730.4	C19H19BrO2	(M+H)+
363.0646	363.0685	10.63	1	2309.79	C19H19BrO2	(M+H)+
364.0665	364.0713	13.11	1	207.77	C19H19BrO2	(M+H)+

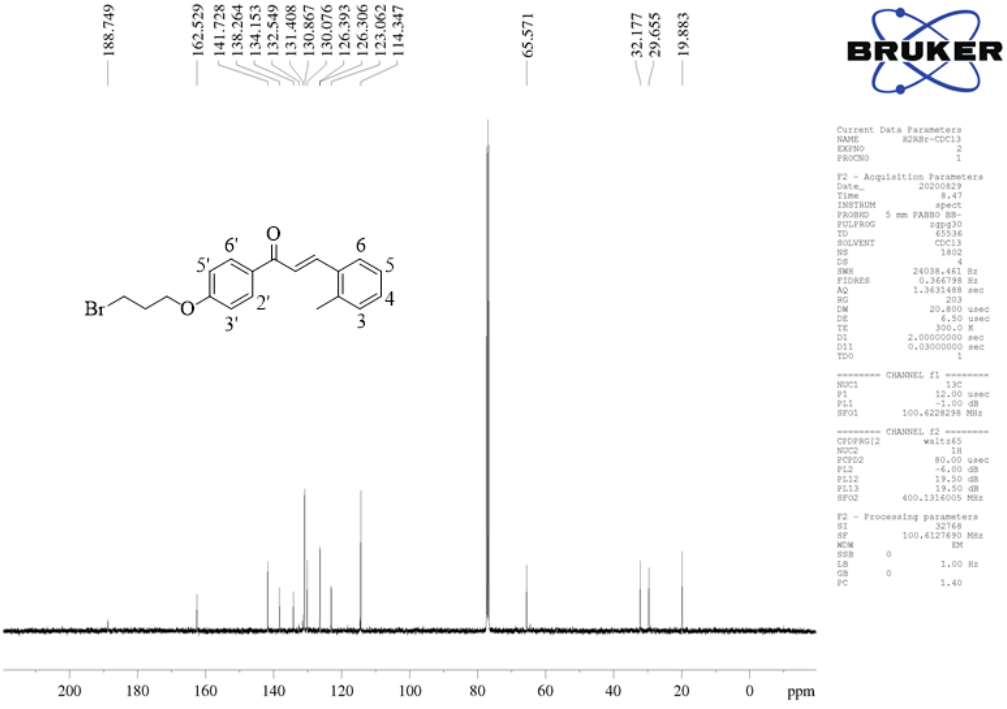
HRMS of compound **7m**



IR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(*o*-tolyl)prop-2-en-1-one (**7n**)



^{1}H NMR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(*o*-tolyl)prop-2-en-1-one **(7n)**

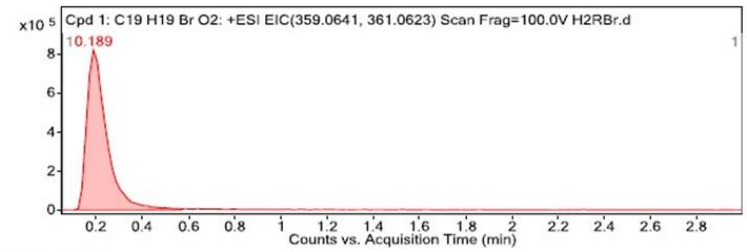


^{13}C NMR spectrum of (*E*)-1-(4-(3-bromopropoxy)phenyl)-3-(*o*-tolyl)prop-2-en-1-one **(7n)**

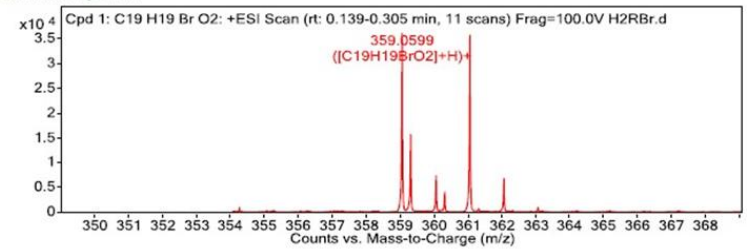
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C19 H19 Br O2	0.189	358.0526	36626	C19 H19 Br O2	358.0568	-11.86

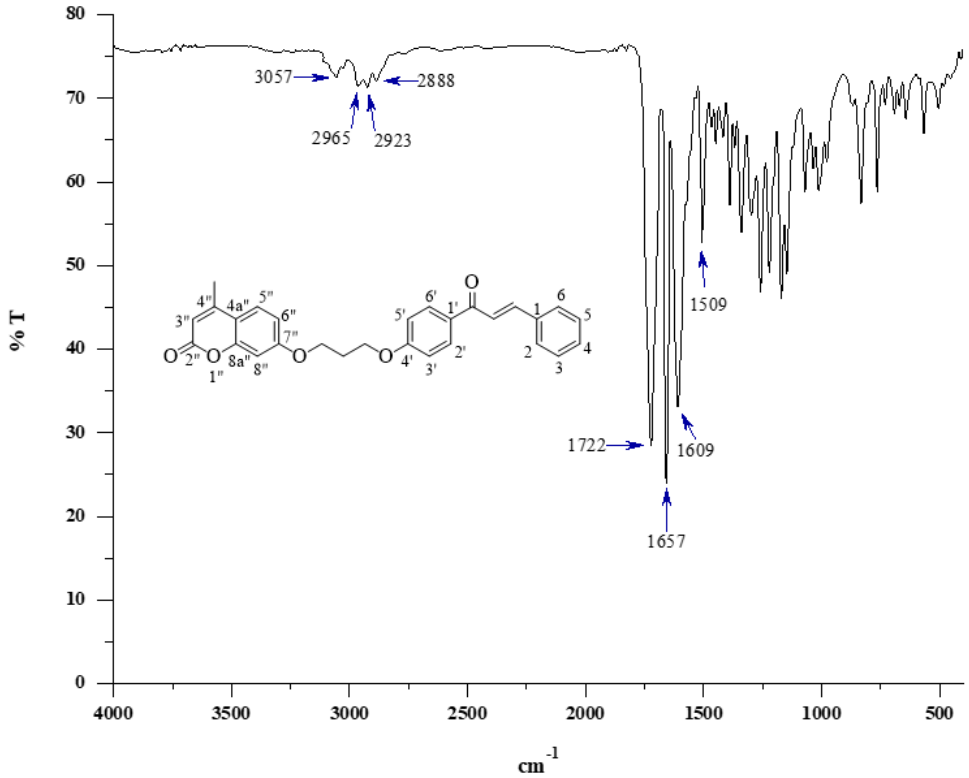
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C19 H19 Br O2	359.0599	0.189	Find By Formula	358.0526



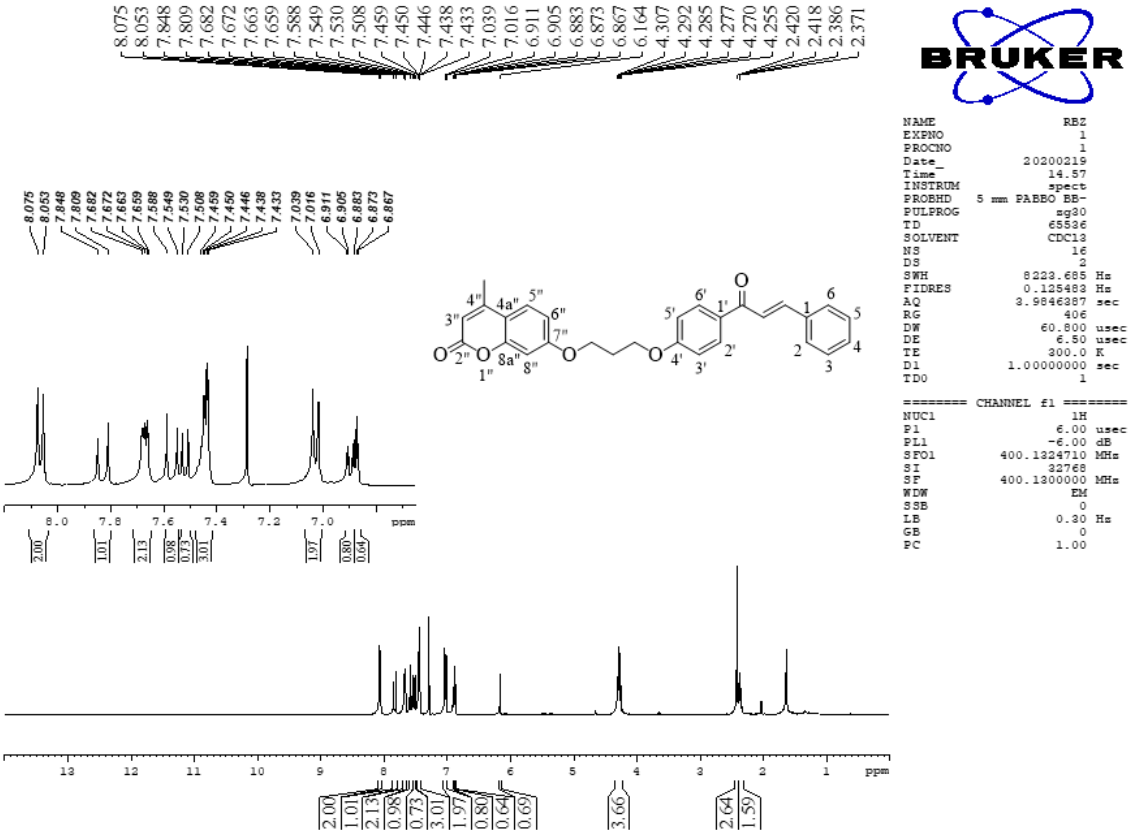
MS Zoomed Spectrum



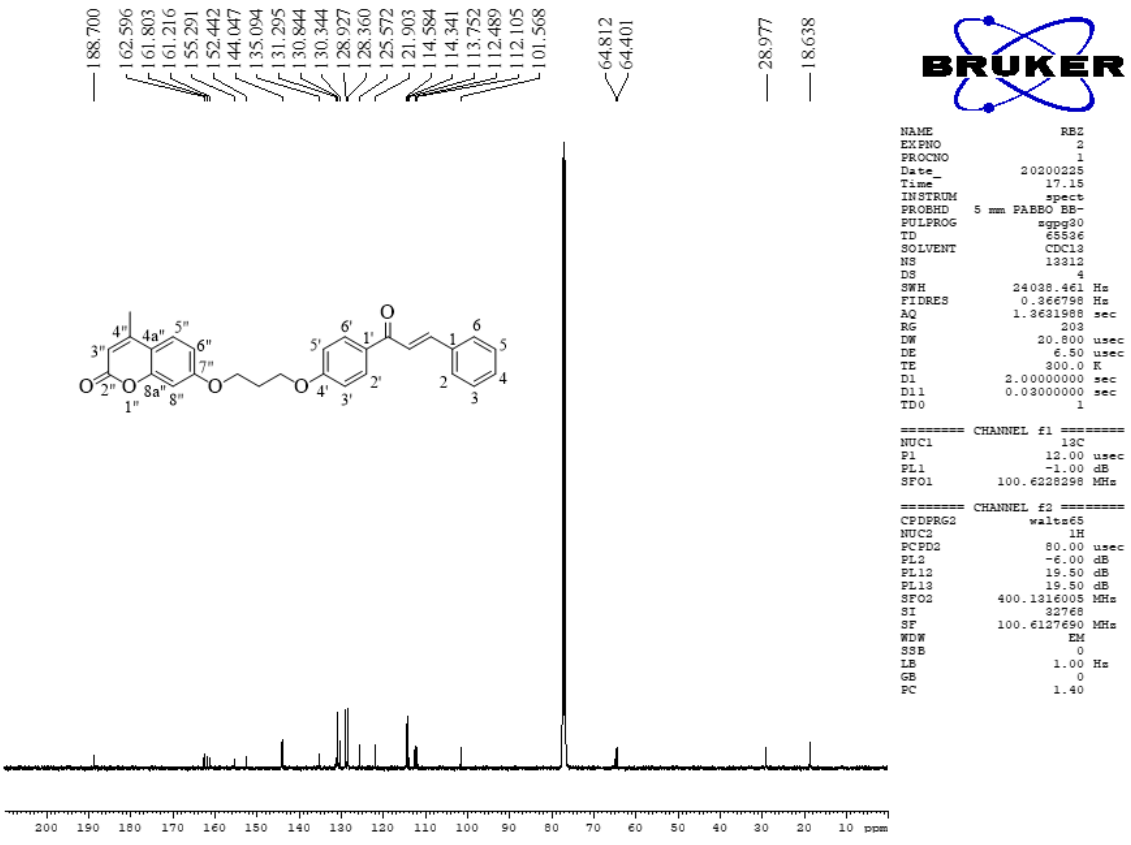
HRMS of compound **7n**



IR spectrum of 7-(3-(4-cinnamoylphenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8a)**



^{1}H NMR spectrum of 7-(3-(4-cinnamoylphenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8a)**

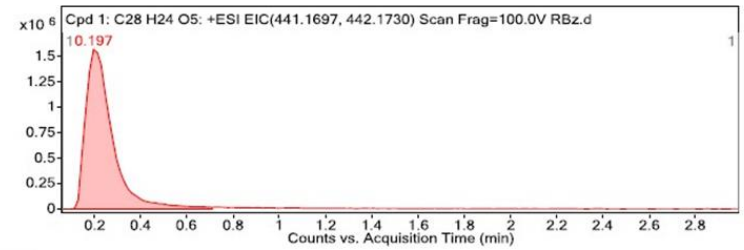


^{13}C NMR spectrum of 7-(3-(4-cinnamoylphenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8a)**

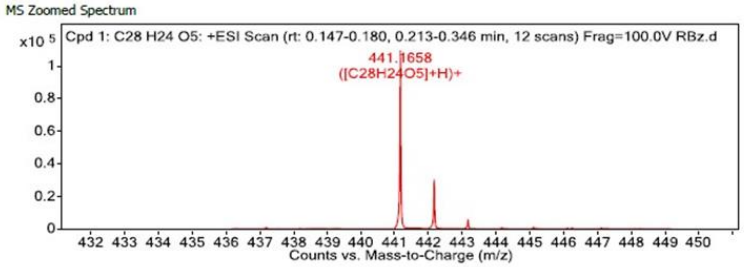
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C28 H24 O5	0.197	440.1583	109356	C28 H24 O5	440.1624	-9.19

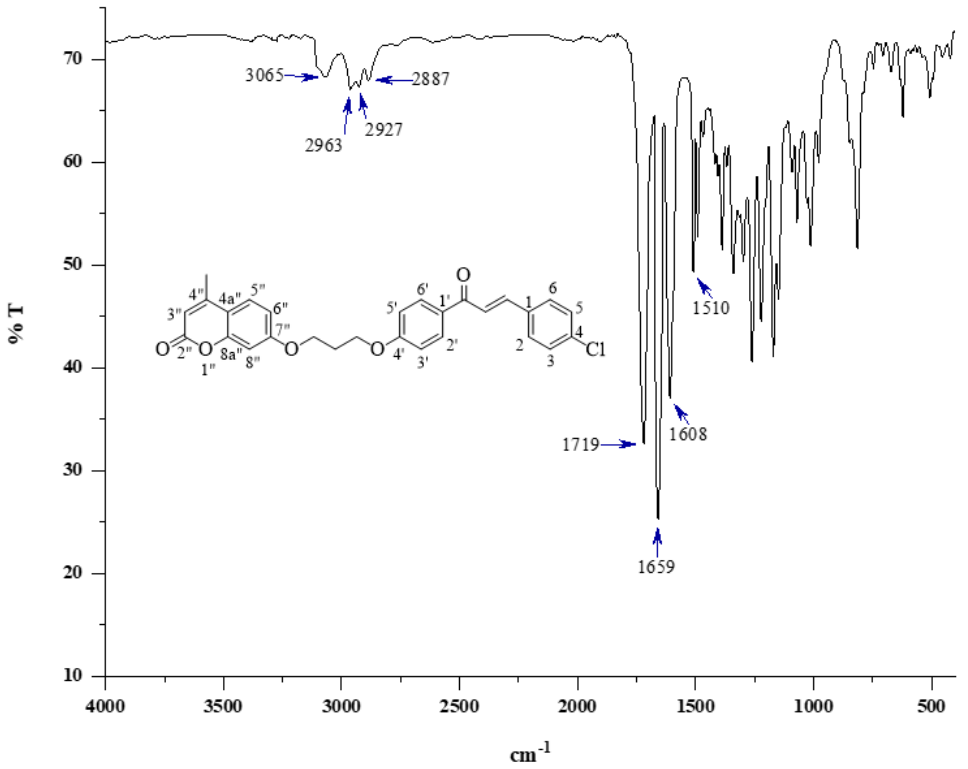
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C28 H24 O5	441.1658	0.197	Find By Formula	440.1583



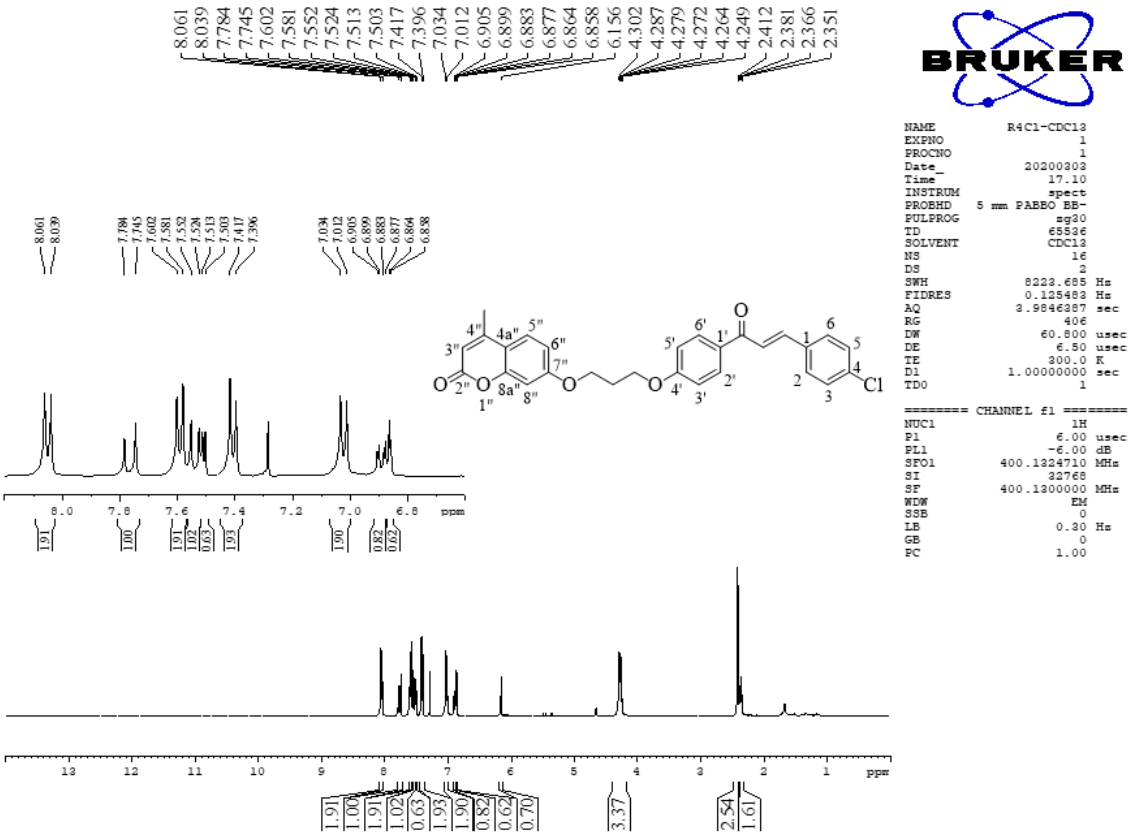
MS Zoomed Spectrum



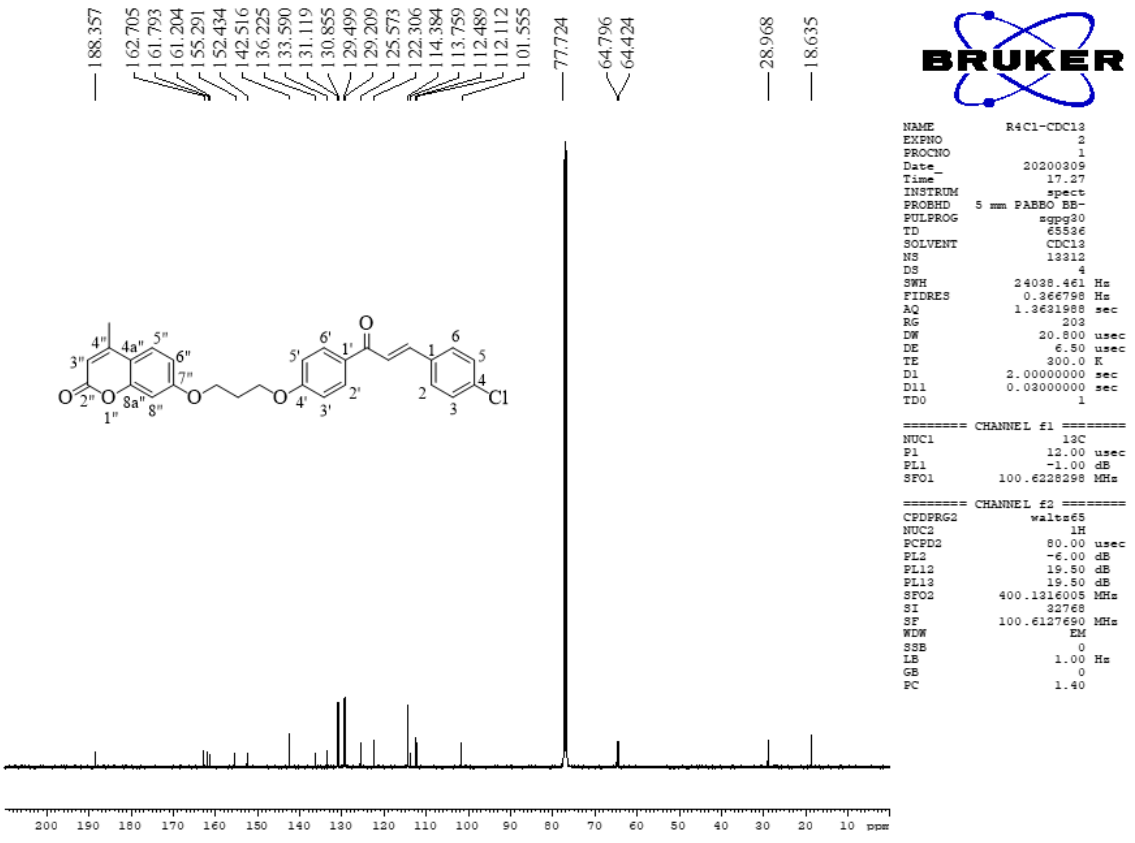
HRMS of compound **8a**



IR spectrum of (*E*)-7-(3-(4-(3-(4-chlorophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8b)**



^{1}H NMR spectrum of (*E*)-7-(3-(4-(3-(4-chlorophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8b)**

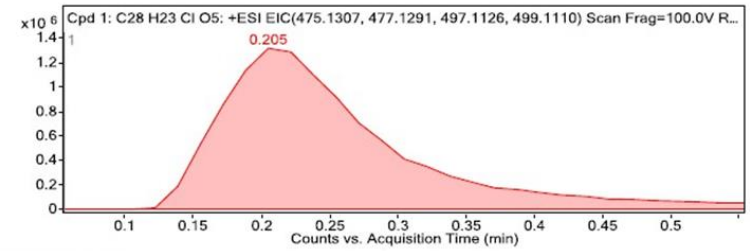


^{13}C NMR spectrum of (*E*)-7-(3-(4-(3-(4-chlorophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8b)**

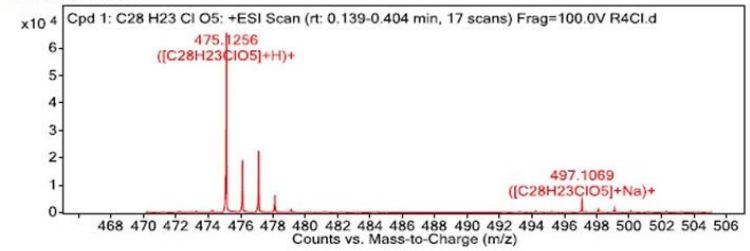
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C28 H23 Cl O5	0.205	474.118	66174	C28 H23 Cl O5	474.1234	-11.35

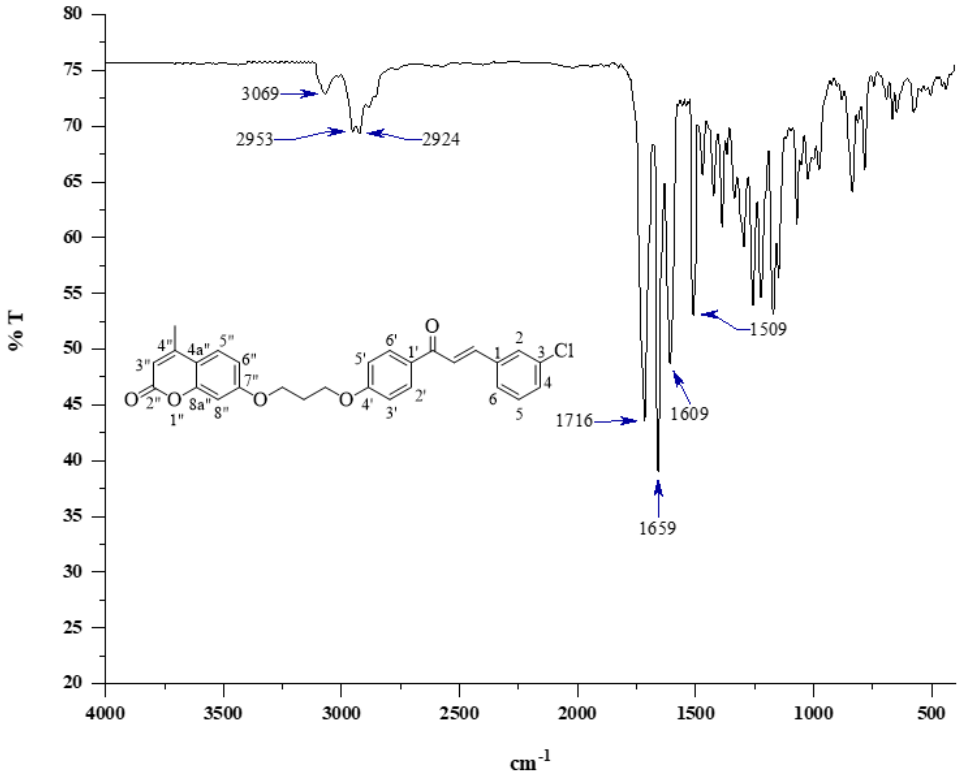
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C28 H23 Cl O5	475.1256	0.205	Find By Formula	474.118



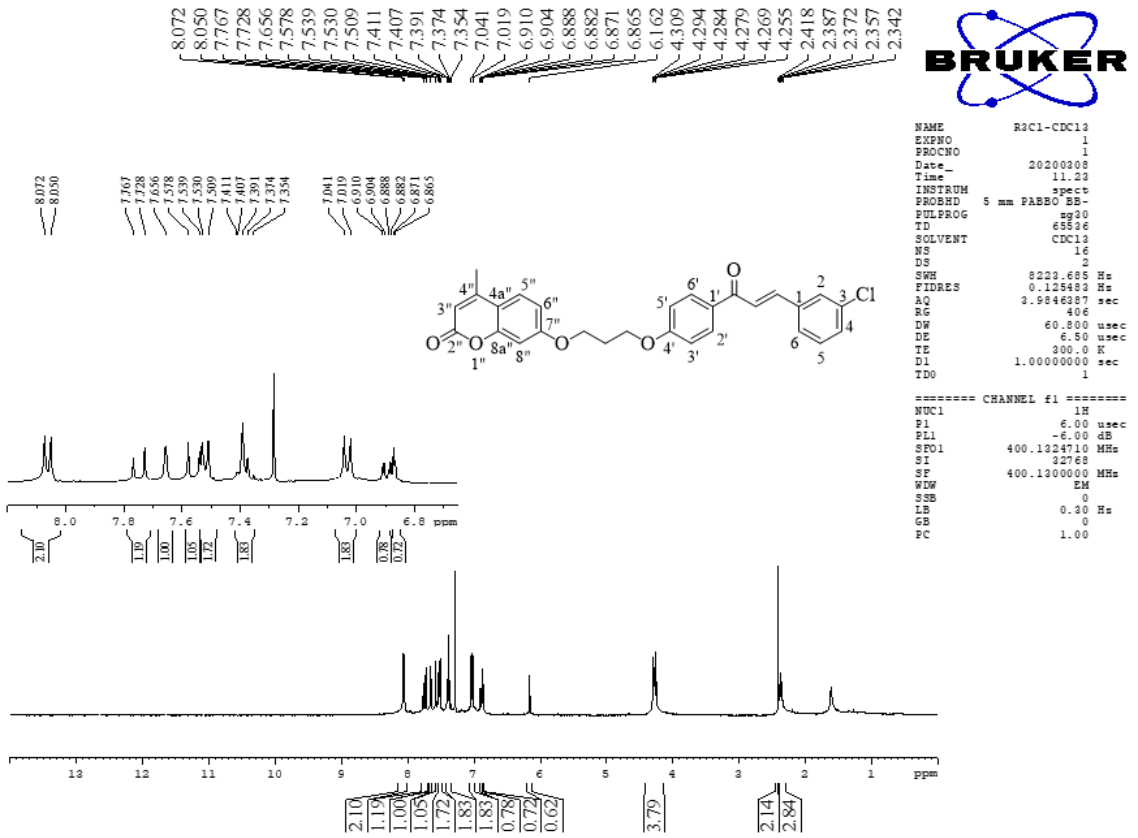
MS Zoomed Spectrum



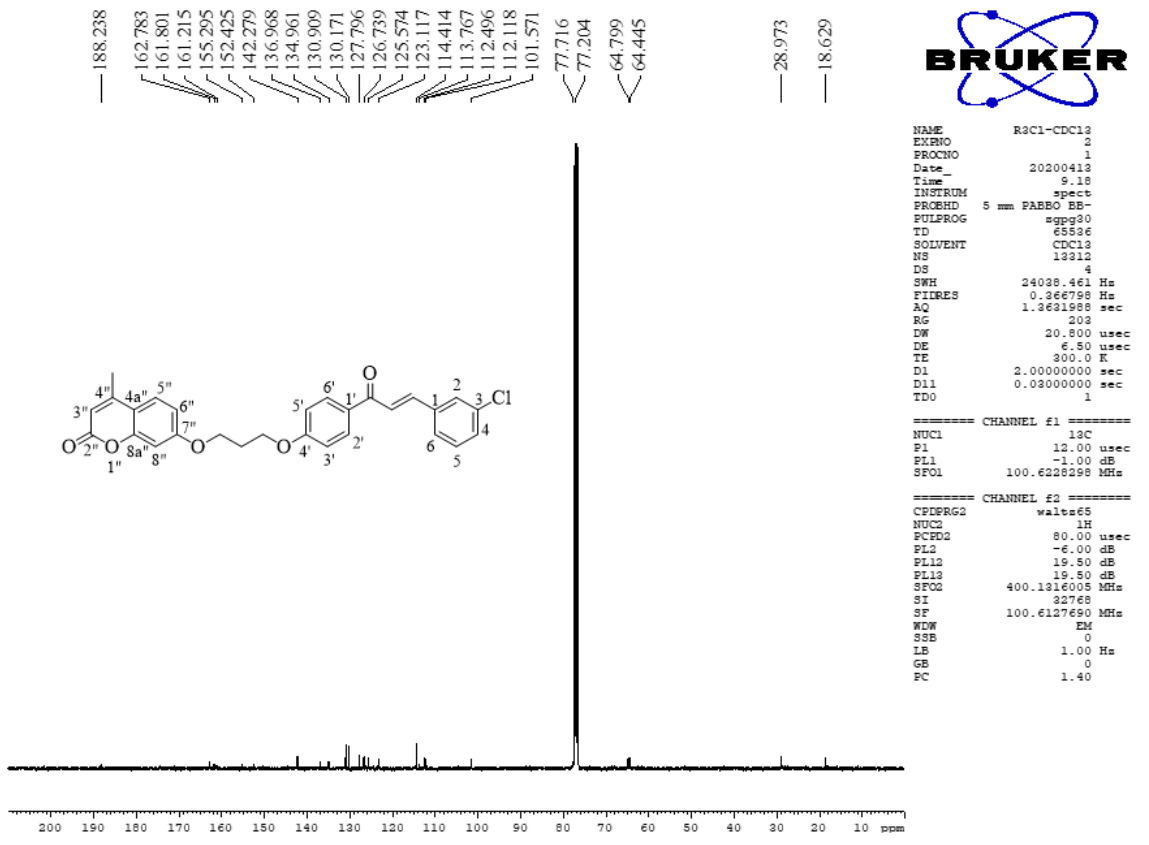
HRMS of compound **8b**



IR spectrum of (*E*)-7-(3-(4-(3-(3-chlorophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8c)**



^{1}H NMR spectrum of (*E*)-7-(3-(4-(3-(3-chlorophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8c)**

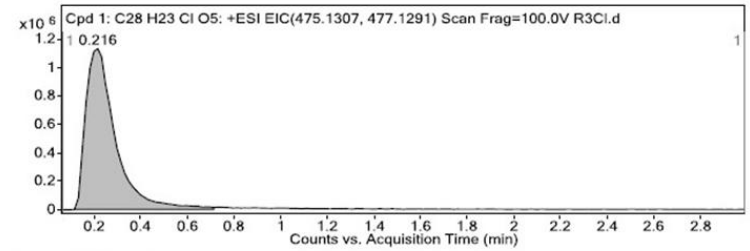


^{13}C NMR spectrum of (*E*)-7-(3-(4-(3-(3-chlorophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8c)**

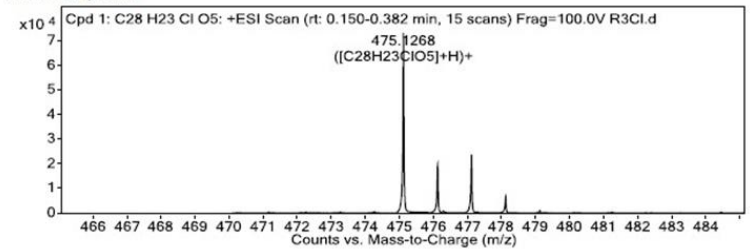
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C28 H23 Cl O5	0.216	474.1193	73562	C28 H23 Cl O5	474.1234	-8.7

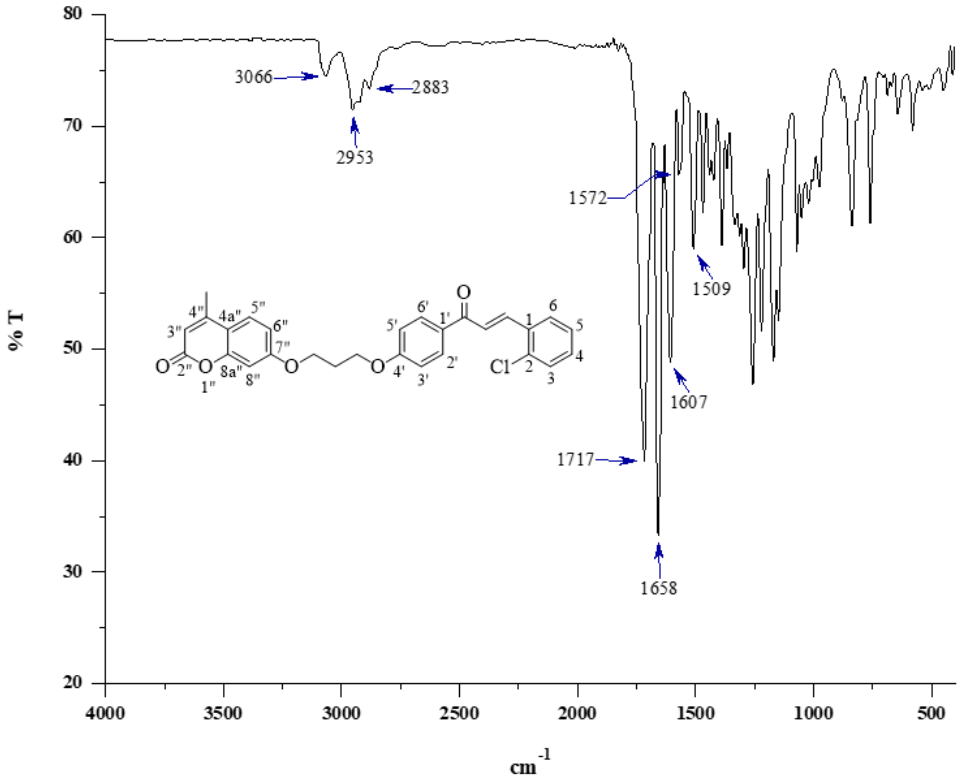
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C28 H23 Cl O5	475.1268	0.216	Find By Formula	474.1193



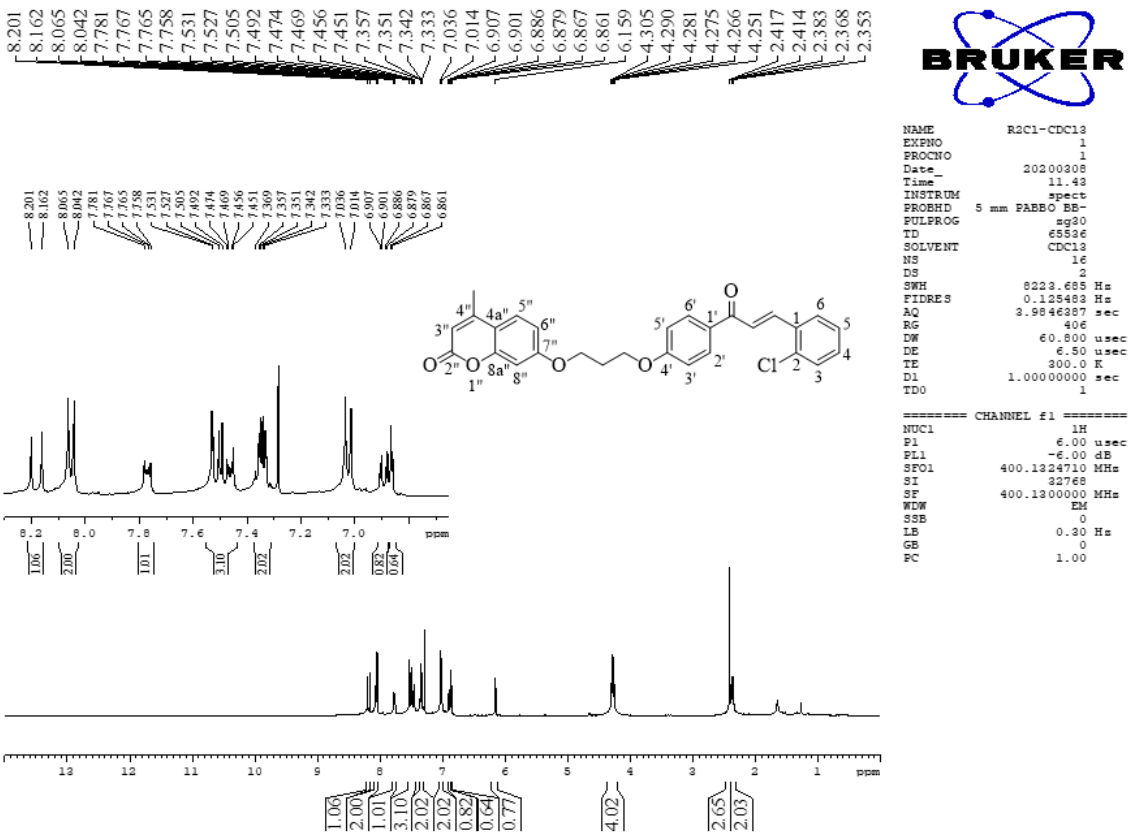
MS Zoomed Spectrum



HRMS of compound **8c**



IR spectrum of (*E*)-7-(3-(4-(3-(2-chlorophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8d)**



BRUKER

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PROCNO                   1
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PULPROG              zg30
TD                  65536
SOLVENT              CDC13
NS                      16
DS                       2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                     406
DW                60.800 usec
DE                 6.50 usec
TE                300.0 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
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P1                 6.00 usec
PL1                -6.00 dB
SFO1         400.1324710 MHz
SI                   32768
SF           400.1300000 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
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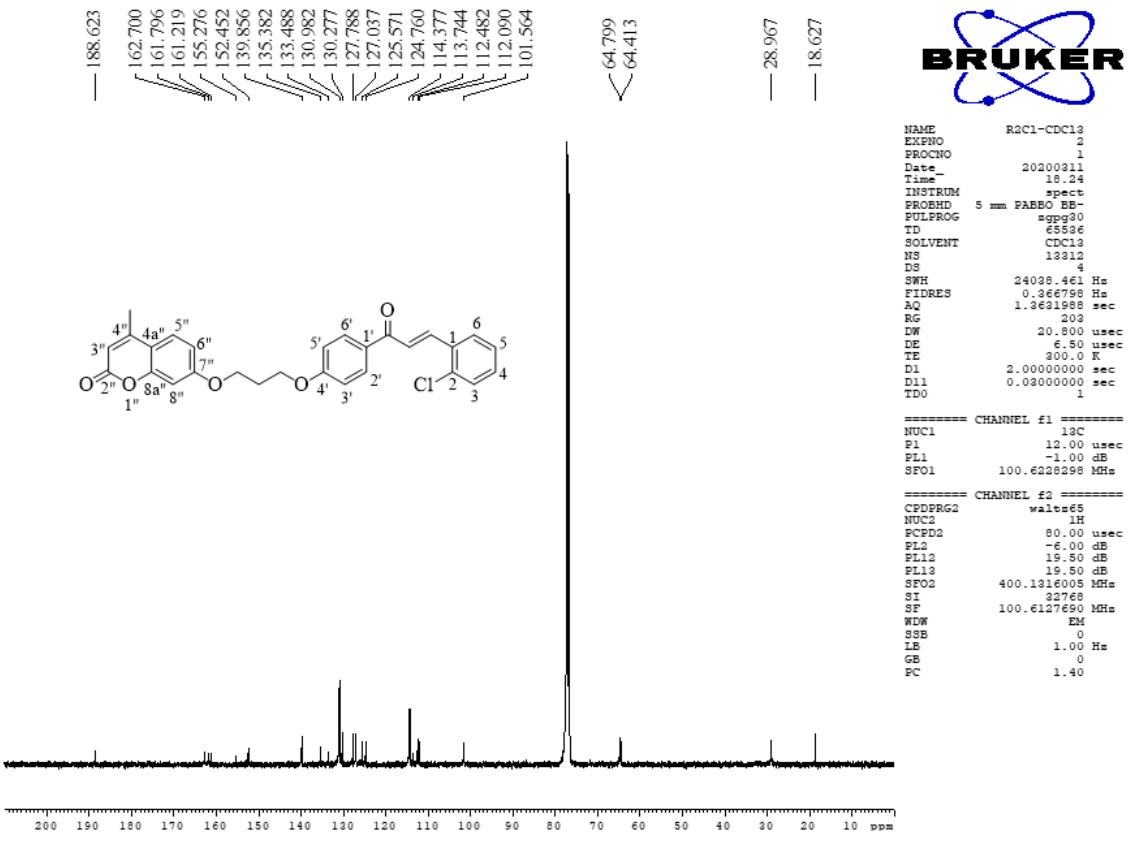
^{1}H NMR spectrum of (*E*)-7-(3-(4-(3-(2-chlorophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8d)**



BRUKER

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PROCNO                   1
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TD                  65536
SOLVENT              CDC13
NS                   13312
DS                       4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                     203
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                12.00 usec
PL1                -1.00 dB
SFO1         100.6228298 MHz

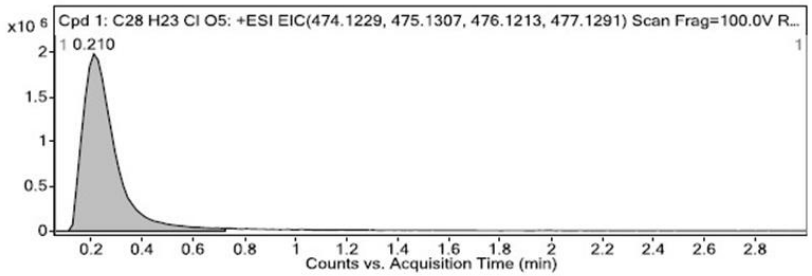
======== CHANNEL f2 ========
CPDPRG2            waltz65
NUC2                   1H
PCPD2              80.00 usec
PL2                -6.00 dB
PL12               19.50 dB
PL13               19.50 dB
SFO2         400.1316005 MHz
SI                   32768
SF           100.6127690 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                   1.40
```

^{13}C NMR spectrum of (*E*)-7-(3-(4-(3-(2-chlorophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8d)**

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C28 H23 Cl O5	0.21	474.119	106185	C28 H23 Cl O5	474.1234	-9.39

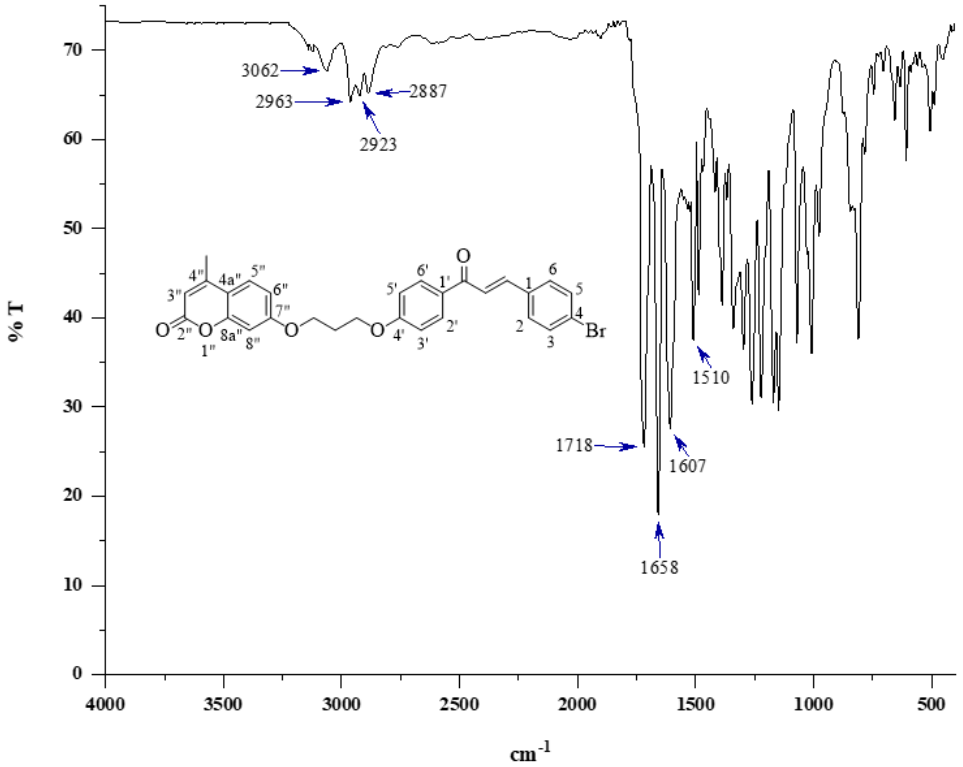
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C28 H23 Cl O5	475.1266	0.21	Find By Formula	474.119



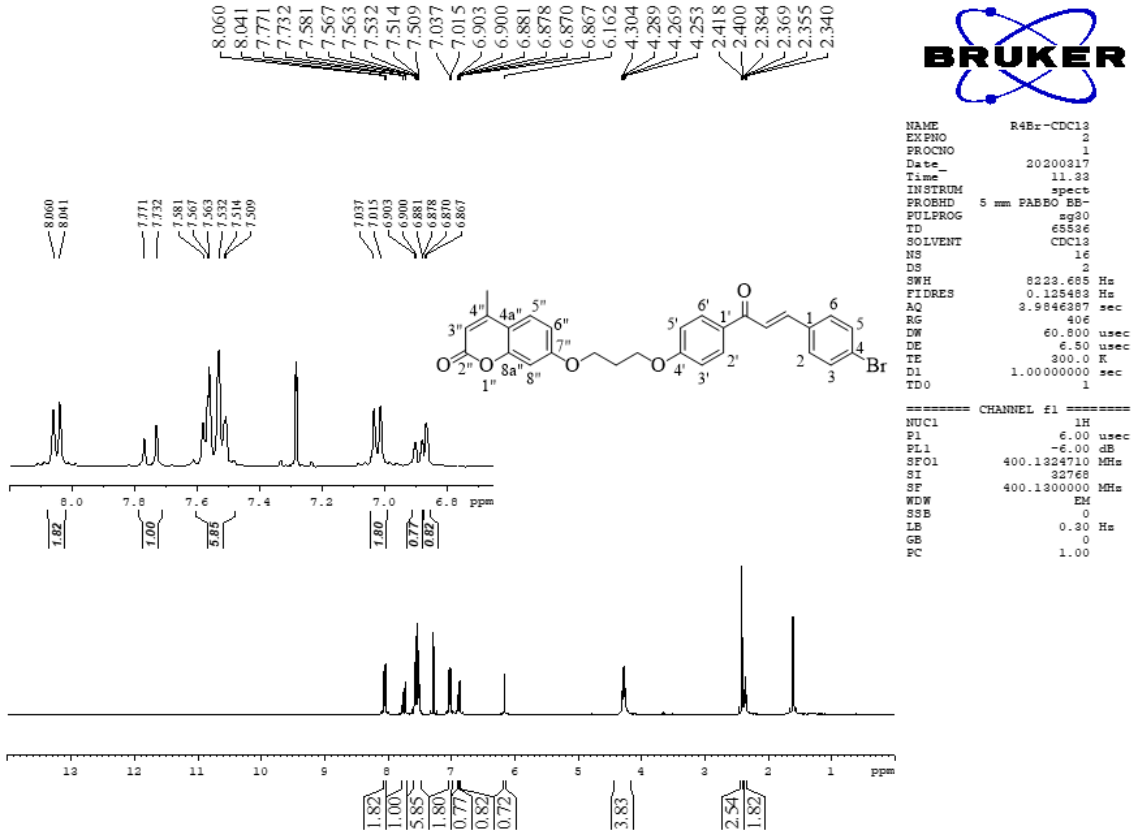
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
475.1266	475.1307	8.58	1	106185.4	C28H23ClO5	(M+H)+
476.1294	476.1341	9.79	1	29292.55	C28H23ClO5	(M+H)+
477.1239	477.1291	10.87	1	34881.14	C28H23ClO5	(M+H)+
478.1266	478.1317	10.79	1	9405.45	C28H23ClO5	(M+H)+
479.129	479.1344	11.26	1	1698.52	C28H23ClO5	(M+H)+
480.1348	480.1371	4.82	1	323.5	C28H23ClO5	(M+H)+
481.1335	481.1397	12.88	1	189.99	C28H23ClO5	(M+H)+

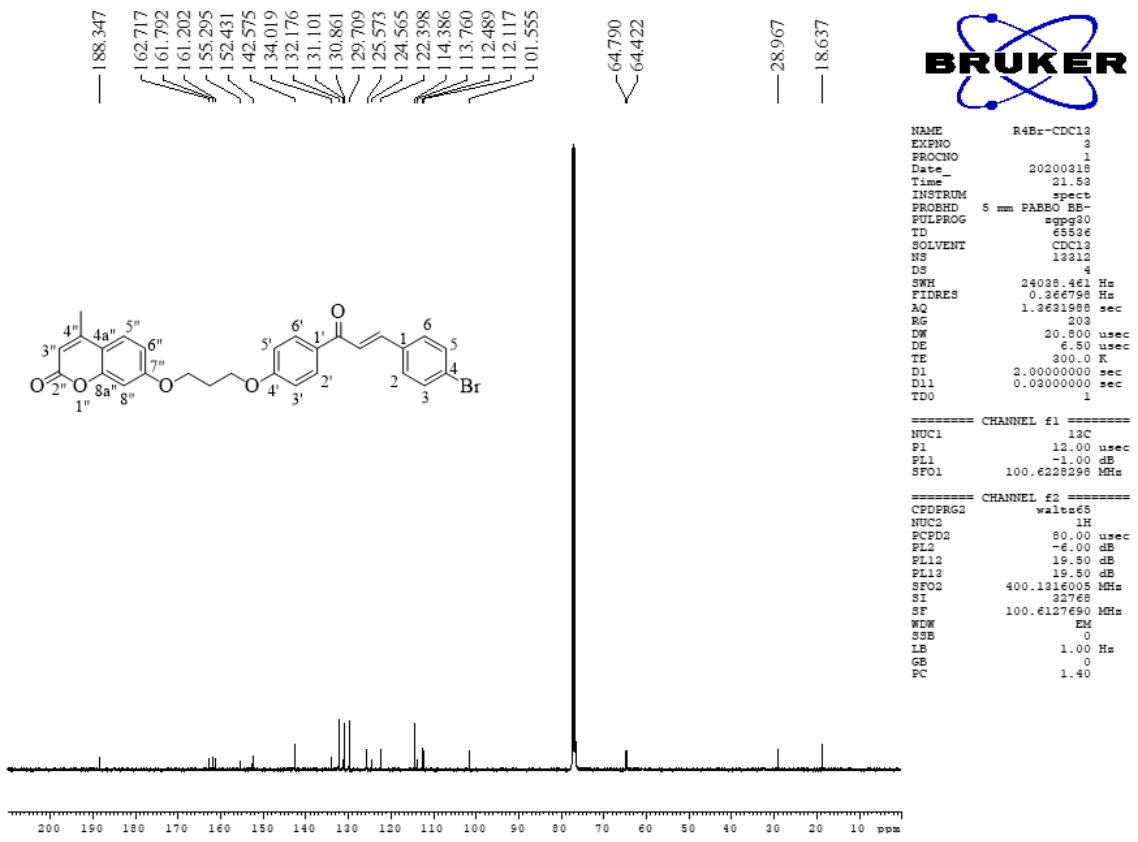
HRMS of compound **8d**



IR spectrum of (*E*)-7-(3-(4-(3-(4-bromophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8e)**



^{1}H NMR spectrum of (*E*)-7-(3-(4-(3-(4-bromophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8e)**

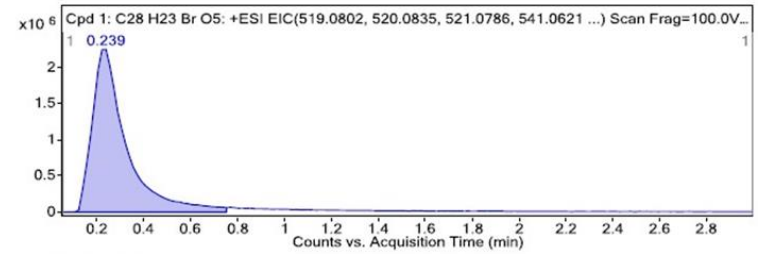


^{13}C NMR spectrum of (*E*)-7-(3-(4-(3-(4-bromophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8e)**

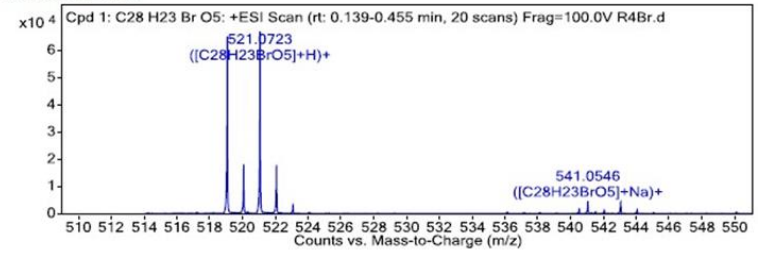
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C28 H23 Br O5	0.239	518.0664	67578	C28 H23 Br O5	518.0729	-12.48

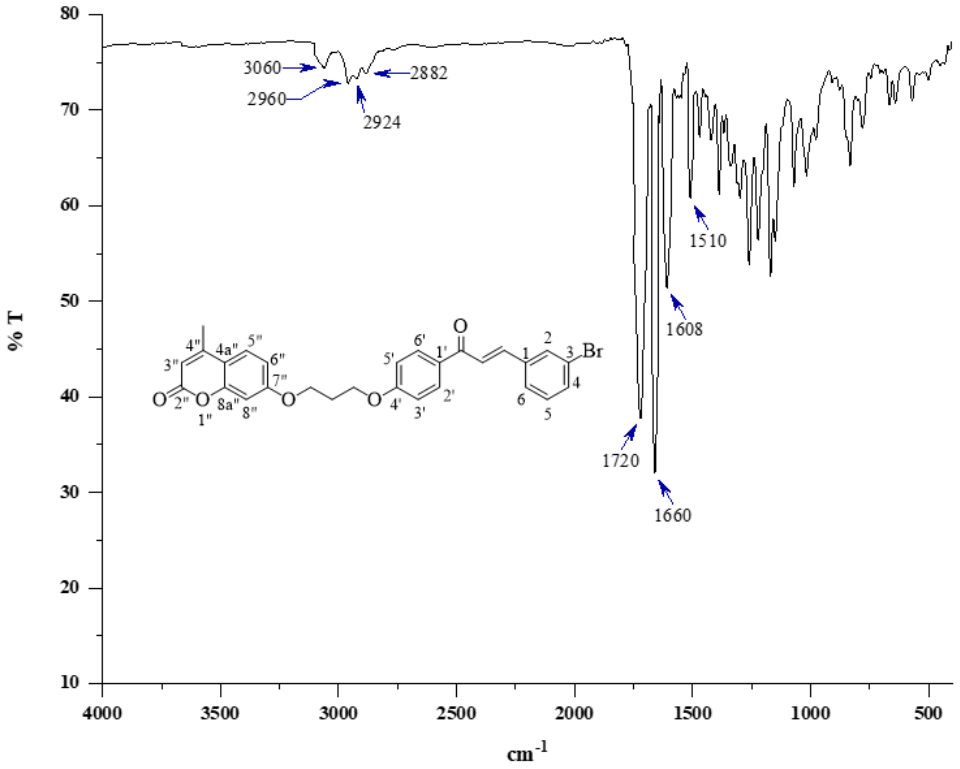
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C28 H23 Br O5	521.0723	0.239	Find By Formula	518.0664



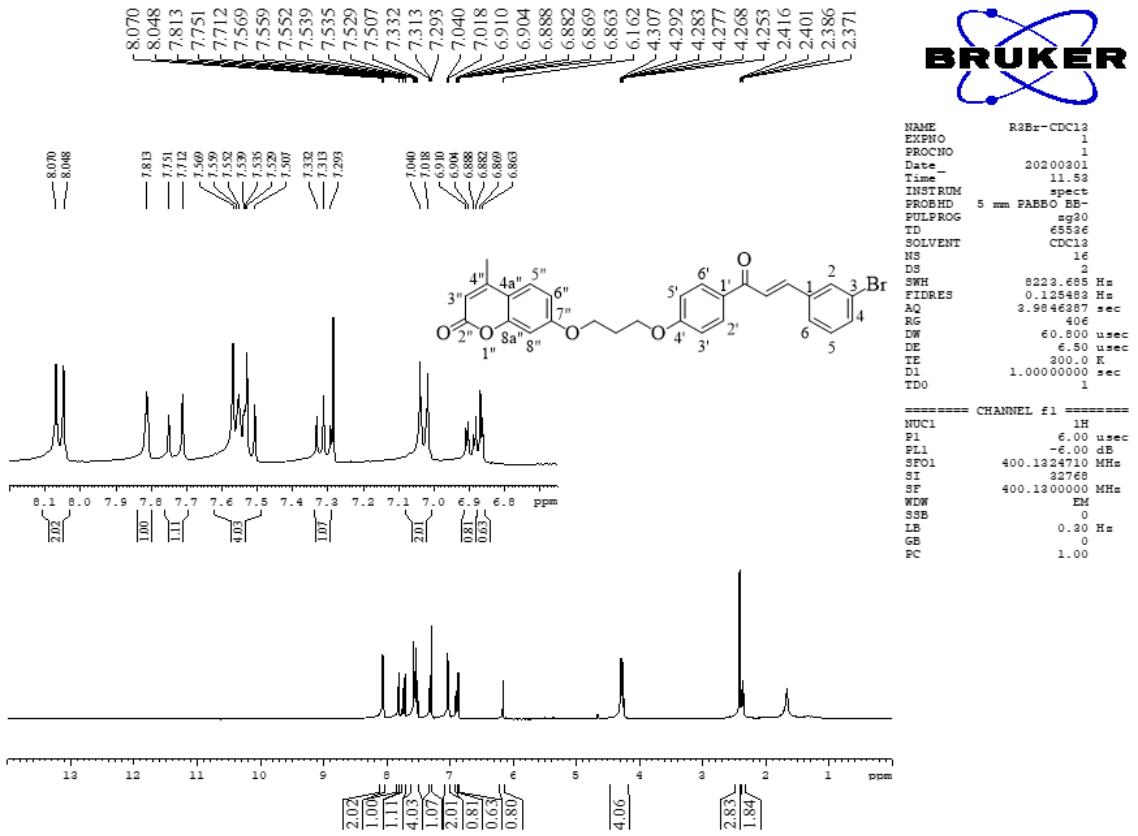
MS Zoomed Spectrum



HRMS of compound **8e**



IR spectrum of (*E*)-7-(3-(4-(3-(3-bromophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8f)**

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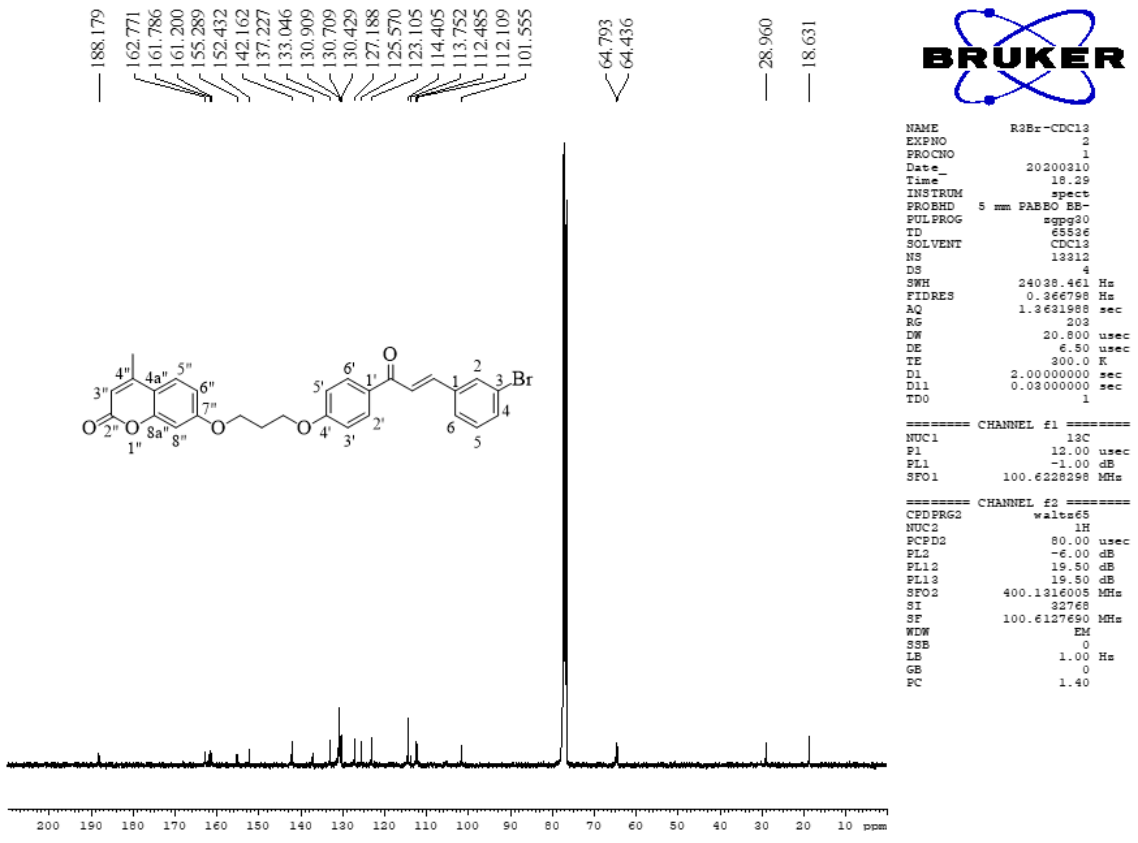
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      16
DS                       2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                     406
DW                60.800 usec
DE                 6.50 usec
TE                300.0 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   1H
P1                 6.00 usec
PL1                -6.00 dB
SFO1         400.1324710 MHz
SI                   32768
SF           400.1300000 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
```

^{1}H NMR spectrum of (*E*)-7-(3-(4-(3-(3-bromophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8f)**

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PROCNO                   1
Date_             20200310
Time                 18.29
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   13312
DS                       4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                     203
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                12.00 usec
PL1                -1.00 dB
SFO1         100.6228298 MHz

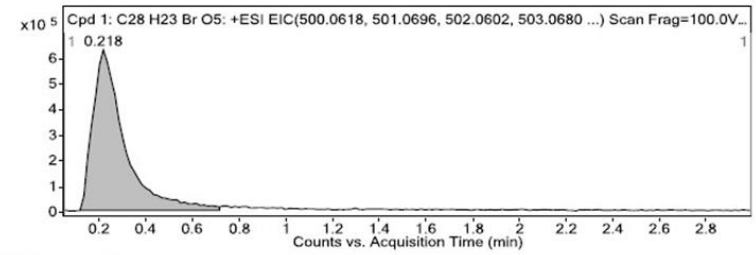
======== CHANNEL f2 ========
CPDPRG2            waltz65
NUC2                   1H
PCPD2              80.00 usec
PL2                -6.00 dB
PL12               19.50 dB
PL13               19.50 dB
SFO2         400.1316005 MHz
SI                   32768
SF           100.6127690 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                   1.40
```

^{13}C NMR spectrum of (*E*)-7-(3-(4-(3-(3-bromophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8f)**

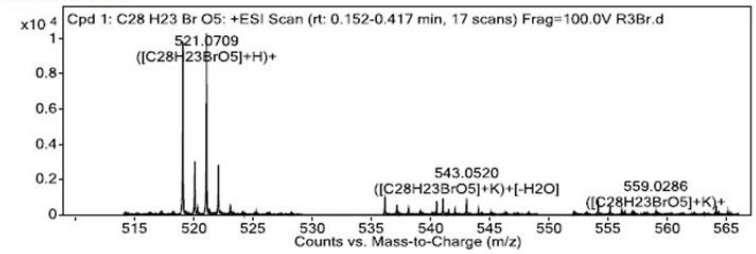
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C28 H23 Br O5	0.218	518.068	10308	C28 H23 Br O5	518.0729	-9.45

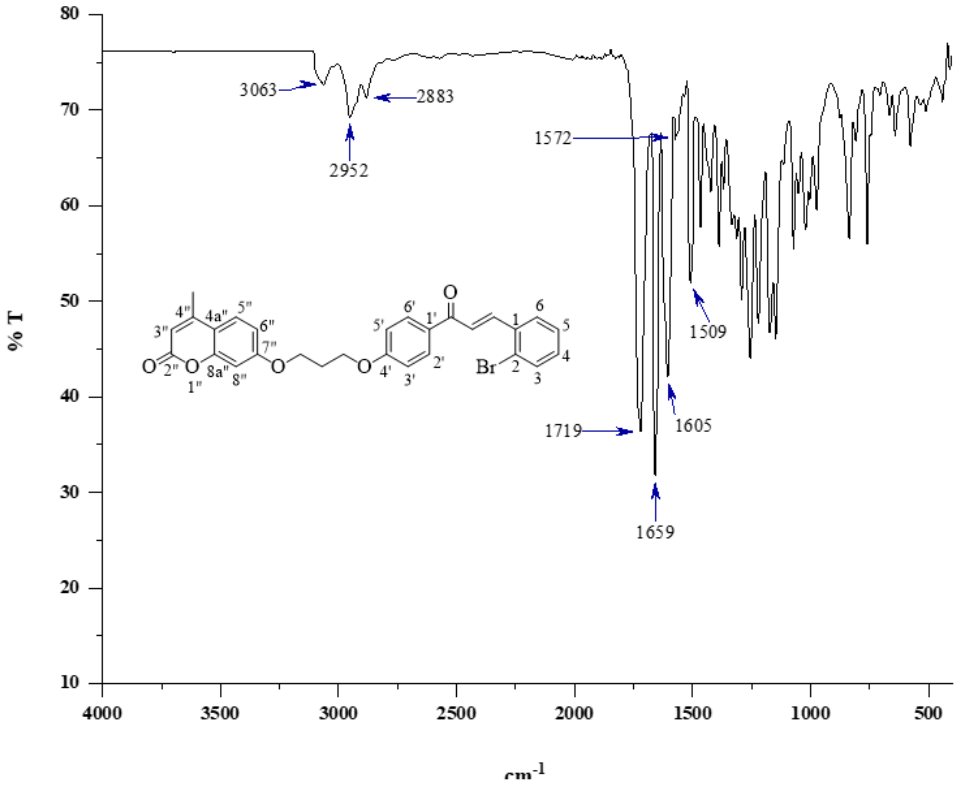
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C28 H23 Br O5	521.0709	0.218	Find By Formula	518.068



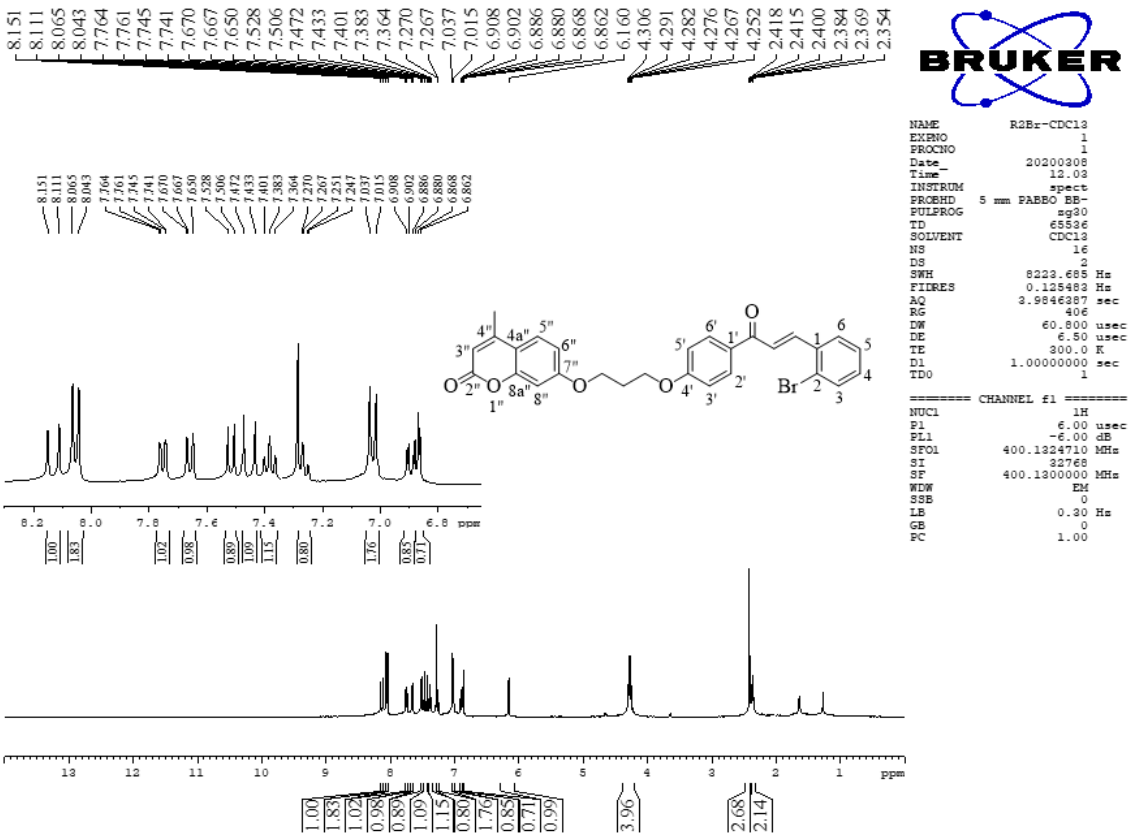
MS Zoomed Spectrum



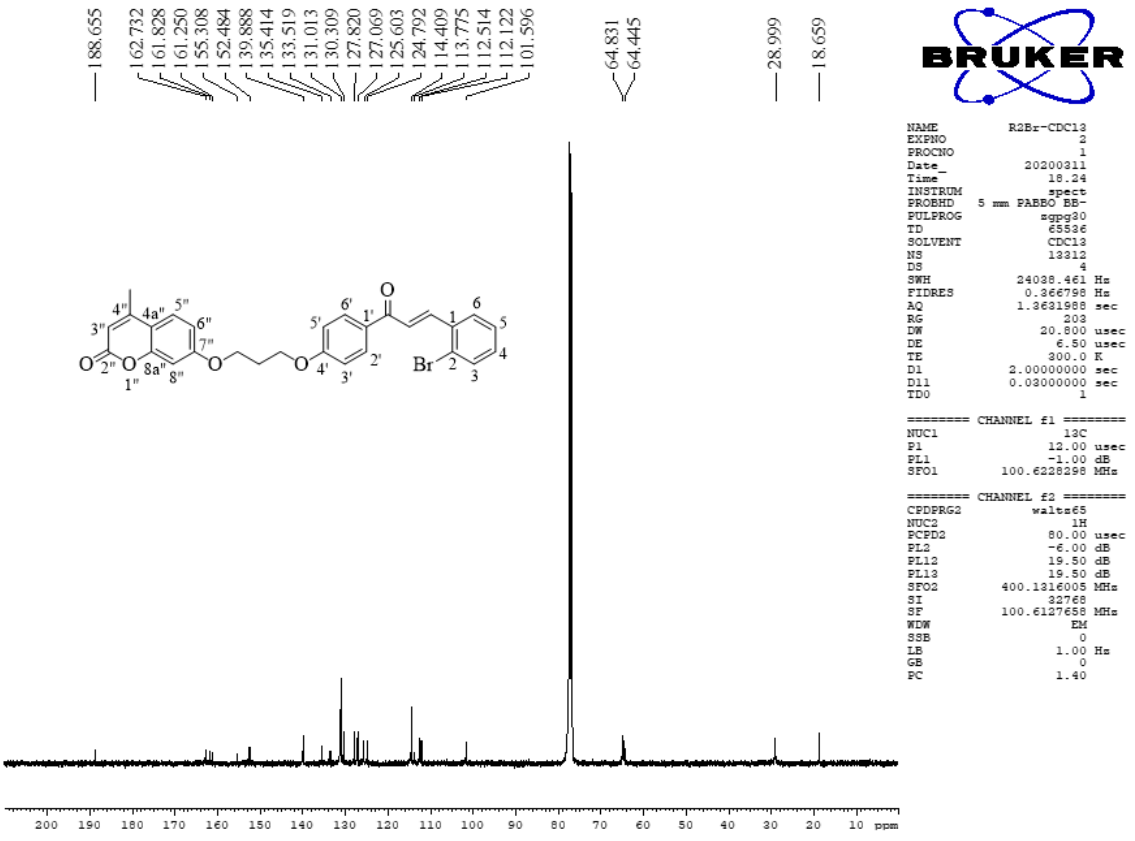
HRMS of compound **8f**



IR spectrum of (*E*)-7-(3-(4-(3-(2-bromophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8g)**



^{1}H NMR spectrum of (*E*)-7-(3-(4-(3-(2-bromophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8g)**

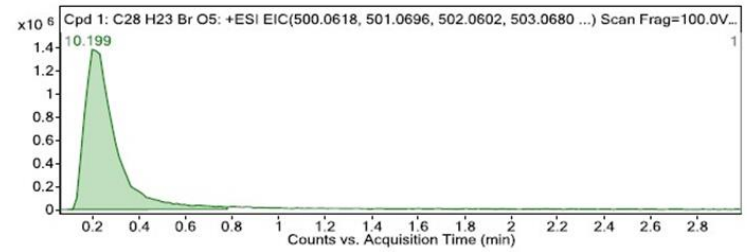


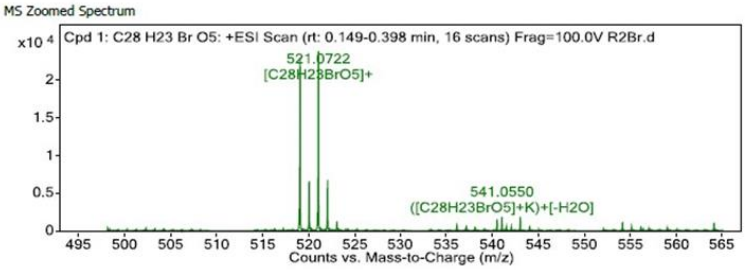
^{13}C NMR spectrum of (*E*)-7-(3-(4-(3-(4-bromophenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8g)**

Compound Table

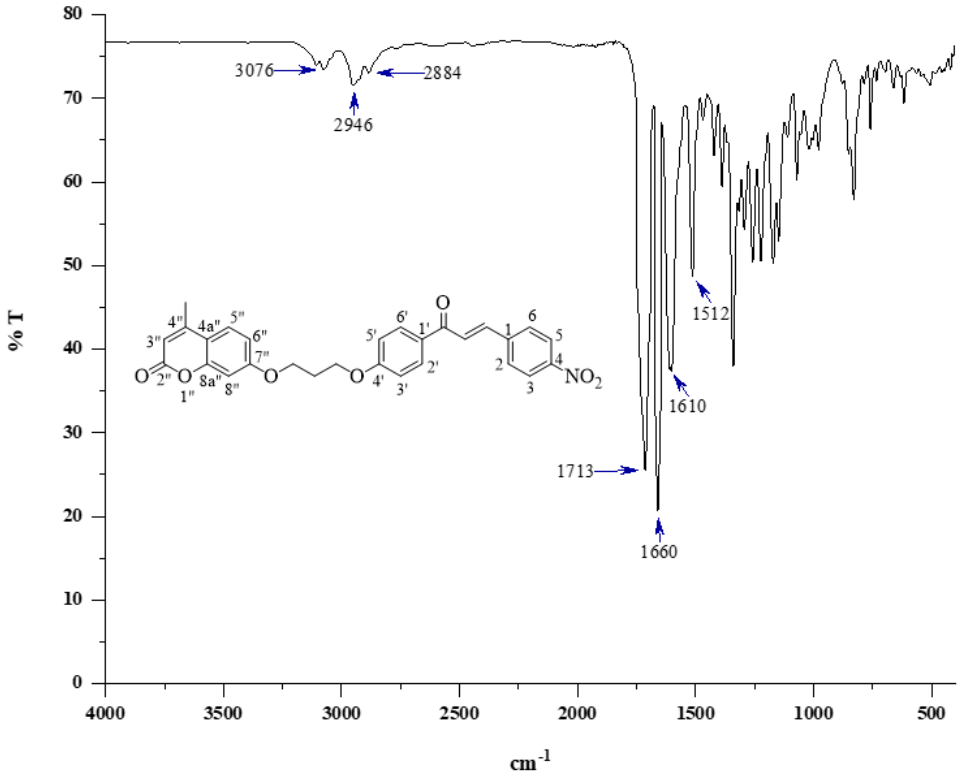
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C28 H23 Br O5	0.199	518.074	24025	C28 H23 Br O5	518.0729	2.24

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C28 H23 Br O5	521.0722	0.199	Find By Formula	518.074

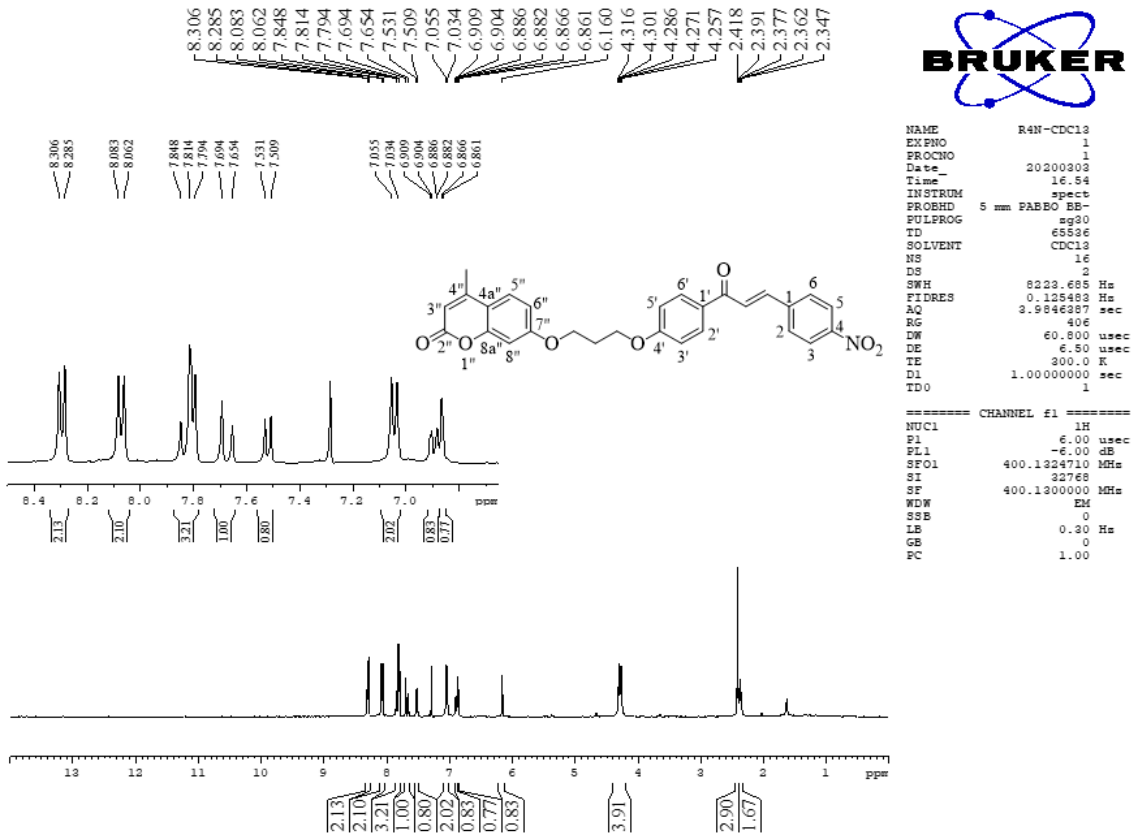




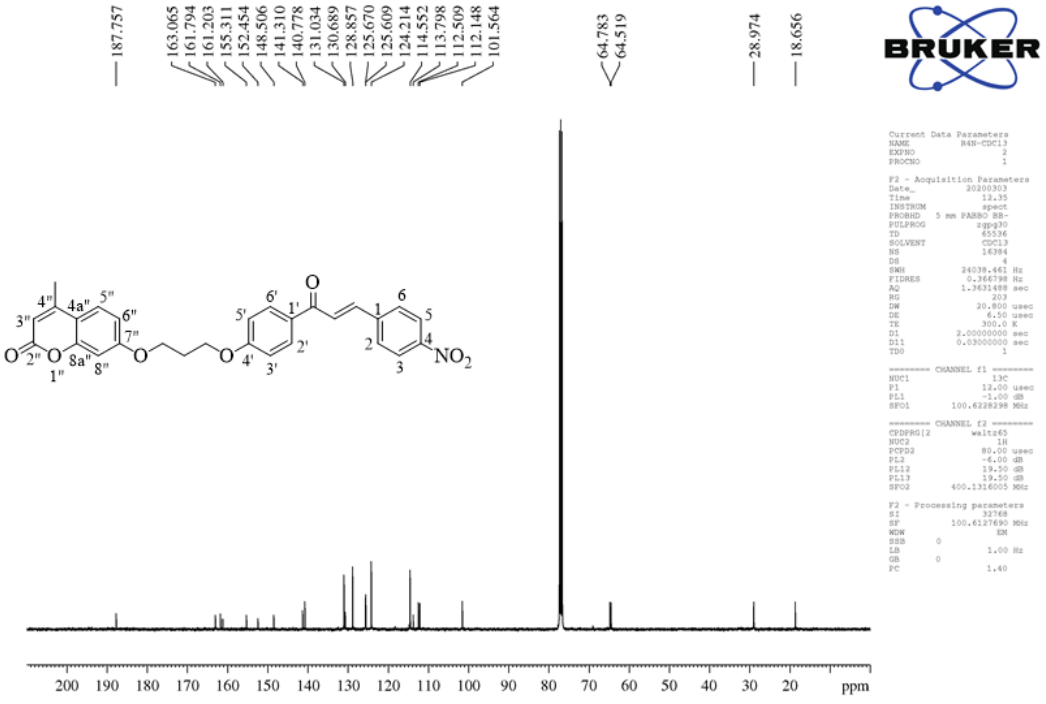
HRMS of compound **8g**



IR spectrum of (*E*)-4-methyl-7-(3-(4-(3-(4-nitrophenyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one **(8h)**



^{1}H NMR spectrum of (*E*)-4-methyl-7-(3-(4-(3-(4-nitrophenyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one **(8h)**

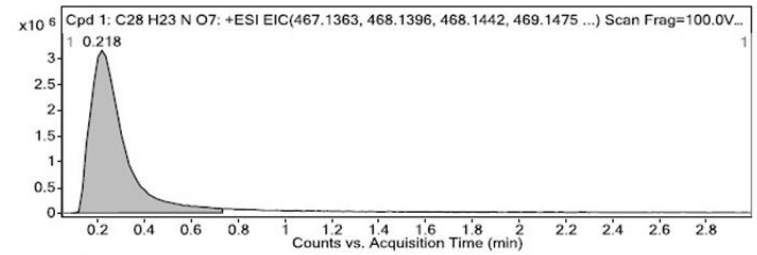


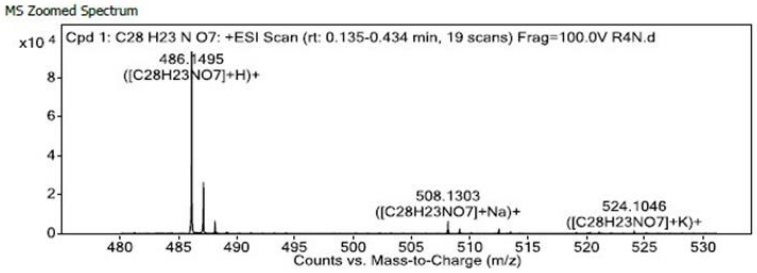
^{13}C NMR spectrum of (*E*)-4-methyl-7-(3-(4-(3-(4-nitrophenyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one **(8h)**

Compound Table

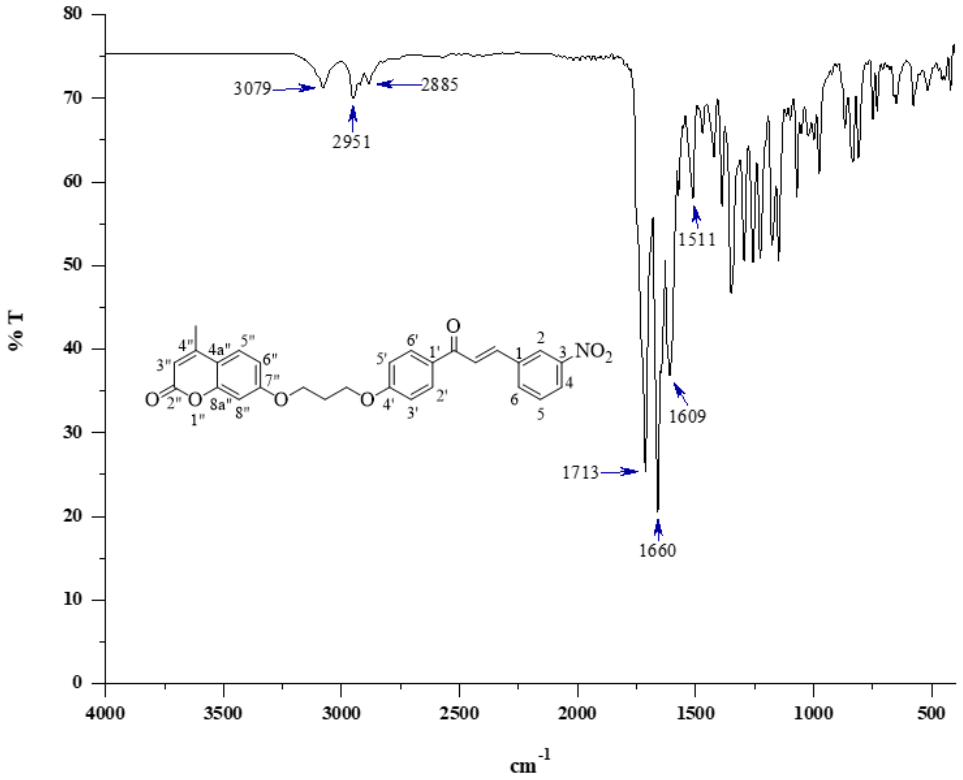
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C28 H23 N O7	0.218	485.1419	94265	C28 H23 N O7	485.1475	-11.4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C28 H23 N O7	486.1495	0.218	Find By Formula	485.1419

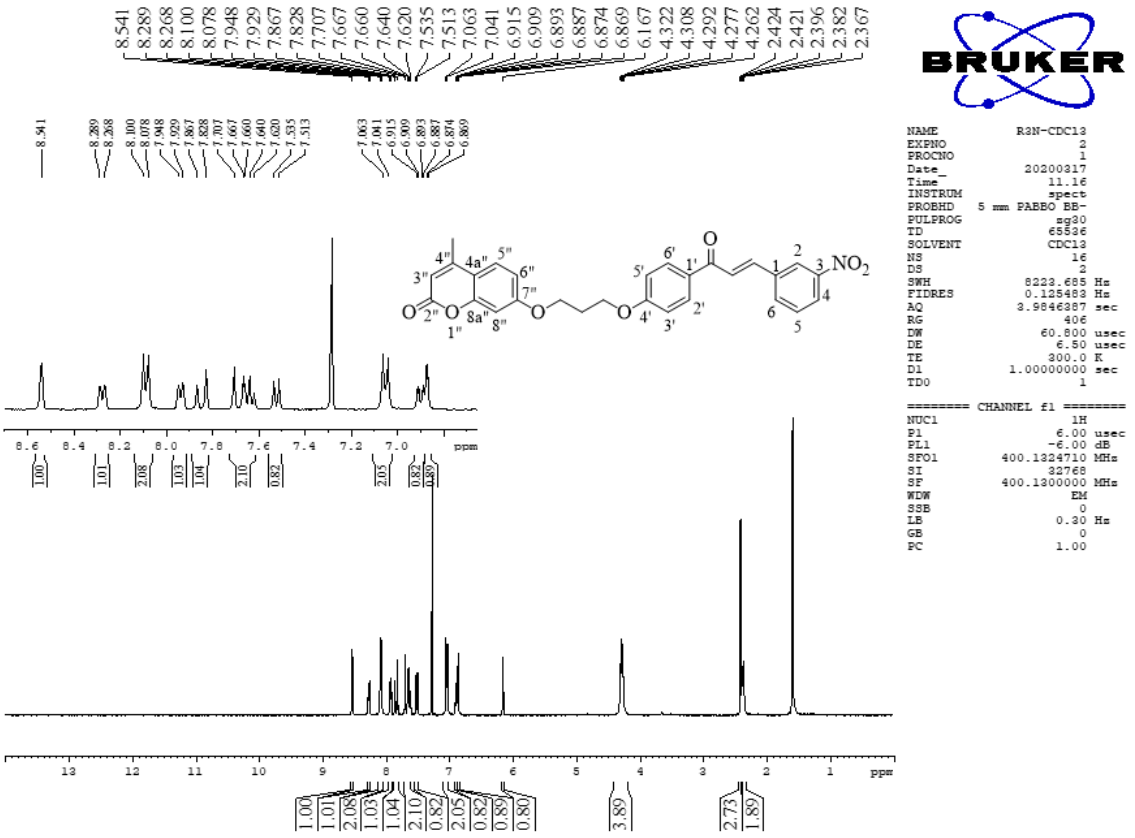




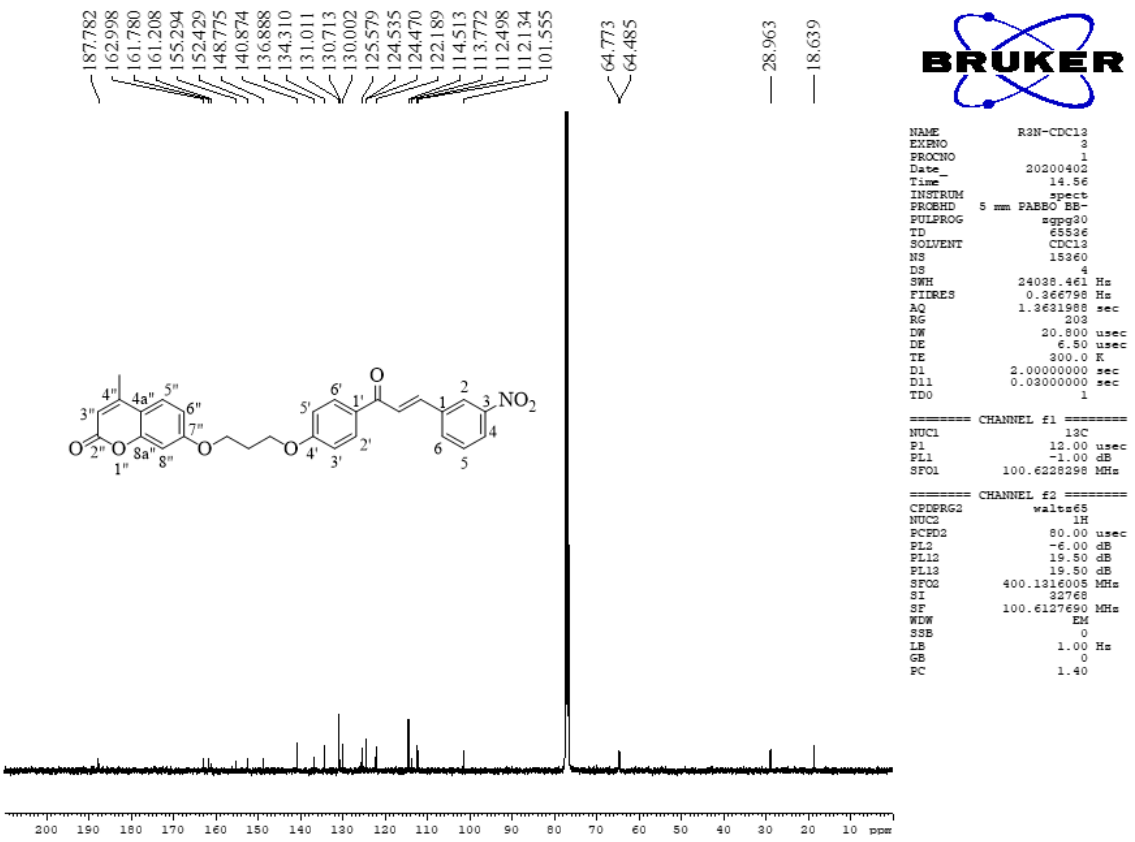
HRMS of compound **8h**



IR spectrum of (*E*)-4-methyl-7-(3-(4-(3-(3-nitrophenyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one **(8i)**



^{1}H NMR spectrum of (*E*)-4-methyl-7-(3-(4-(3-(3-nitrophenyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one **(8i)**

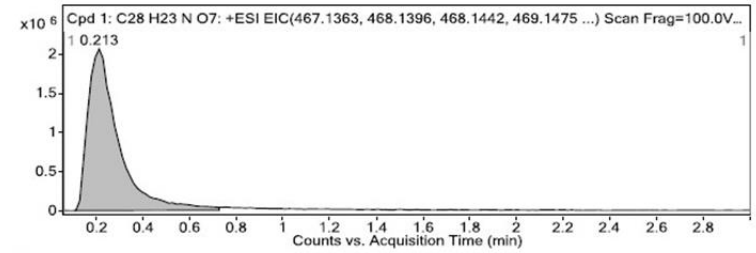


^{13}C NMR spectrum of (*E*)-4-methyl-7-(3-(4-(3-(3-nitrophenyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one **(8i)**

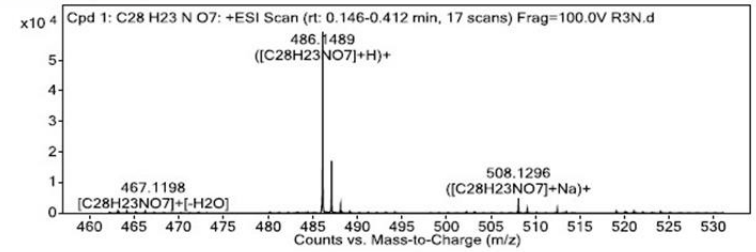
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C28 H23 N O7	0.213	485.1414	60022	C28 H23 N O7	485.1475	-12.5

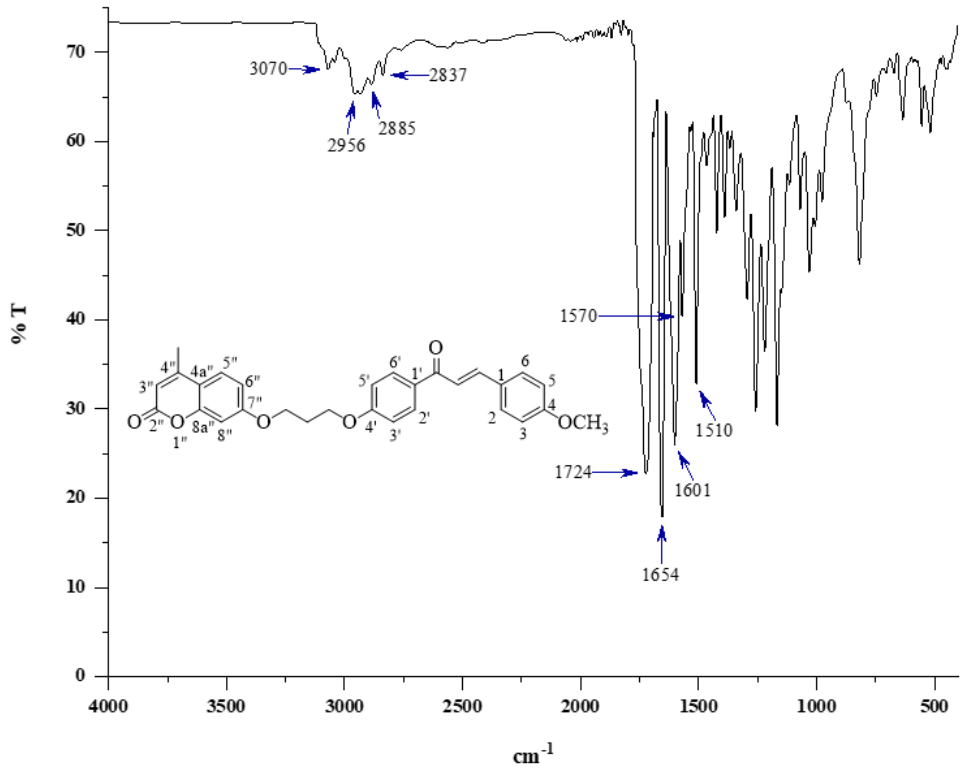
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C28 H23 N O7	486.1489	0.213	Find By Formula	485.1414



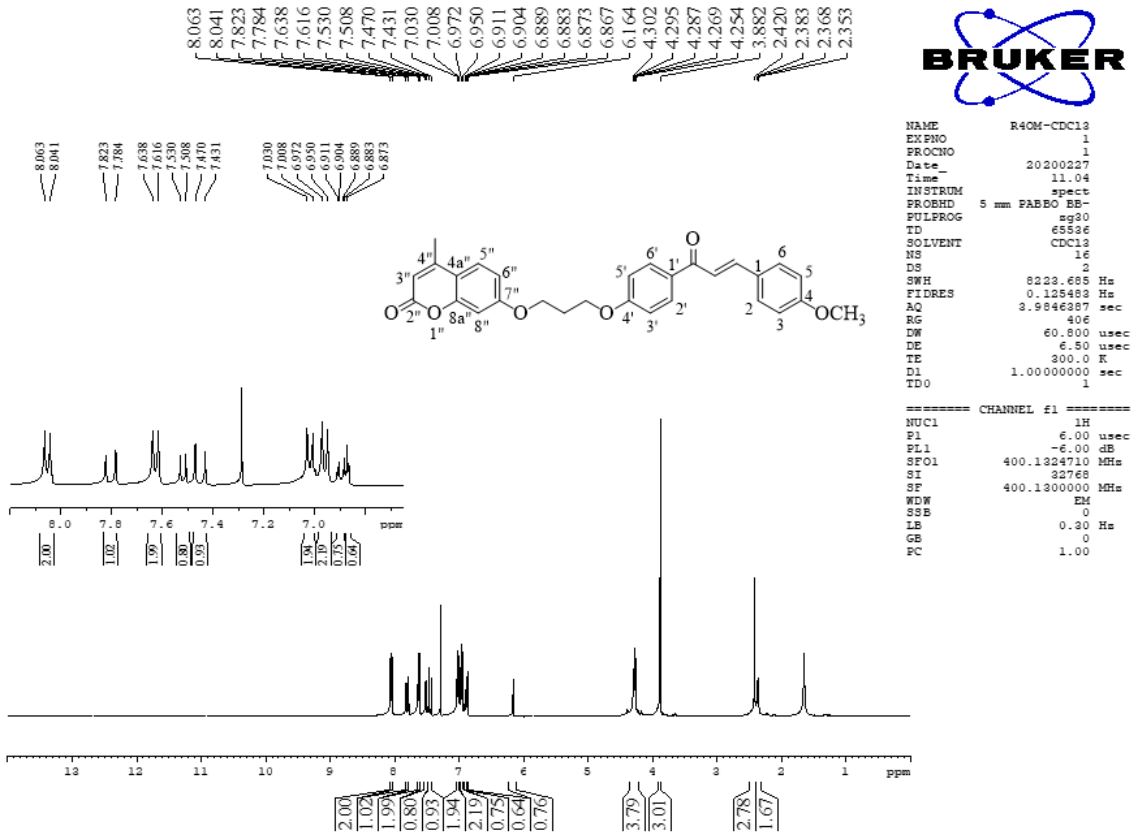
MS Zoomed Spectrum



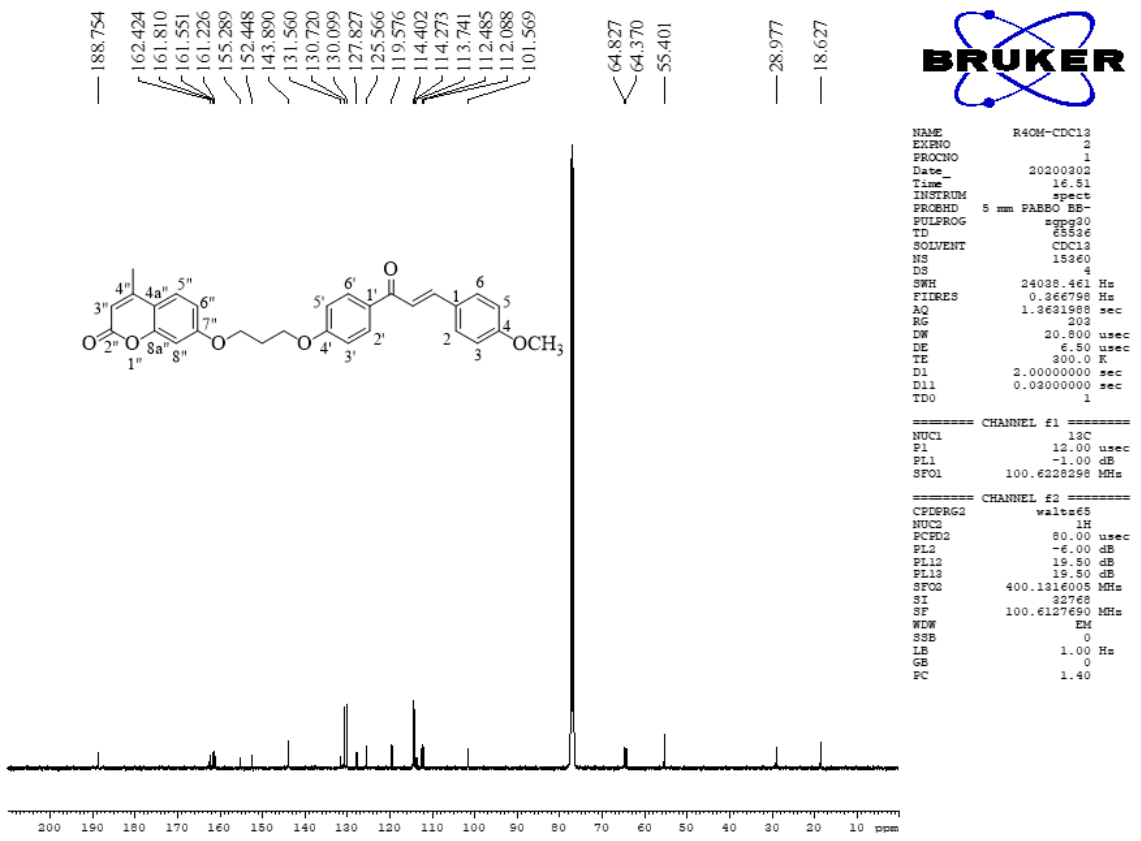
HRMS of compound **8i**



IR spectrum of (*E*)-7-(3-(4-(3-(4-methoxyphenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8j)**



^{1}H NMR spectrum of (*E*)-7-(3-(4-(3-(4-methoxyphenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8j)**

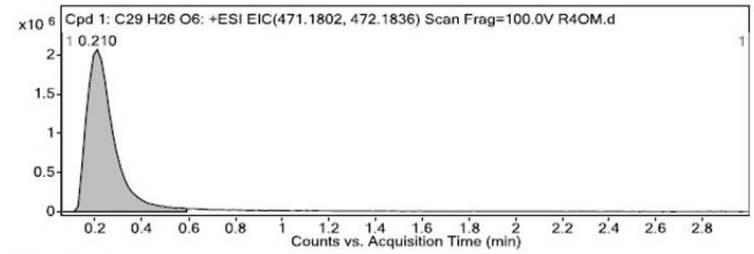


^{13}C NMR spectrum of (*E*)-7-(3-(4-(3-(4-methoxyphenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8j)**

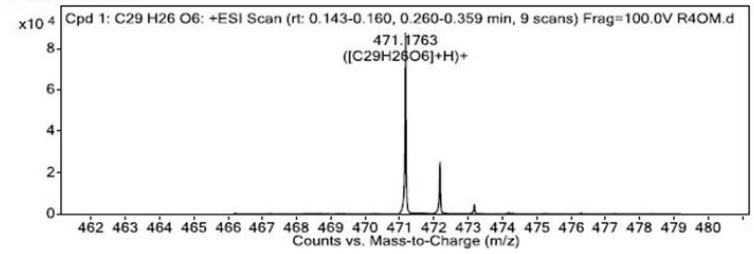
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C29 H26 O6	0.21	470.1688	87803	C29 H26 O6	470.1729	-8.8

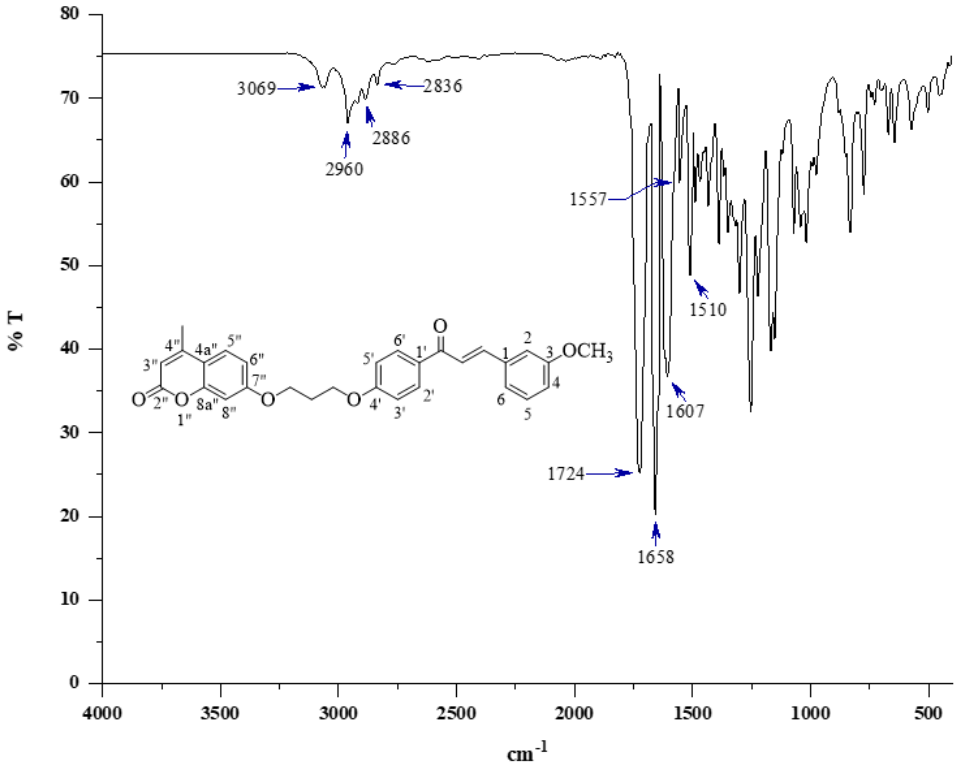
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C29 H26 O6	471.1763	0.21	Find By Formula	470.1688



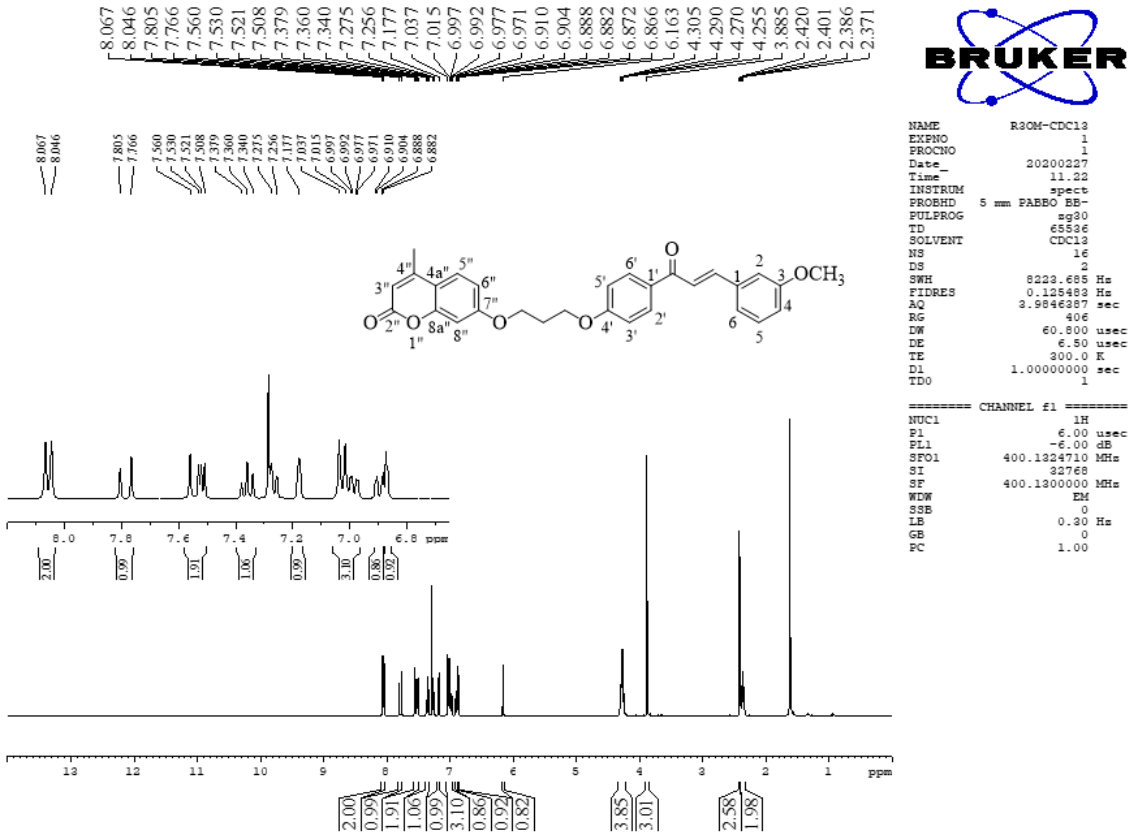
MS Zoomed Spectrum



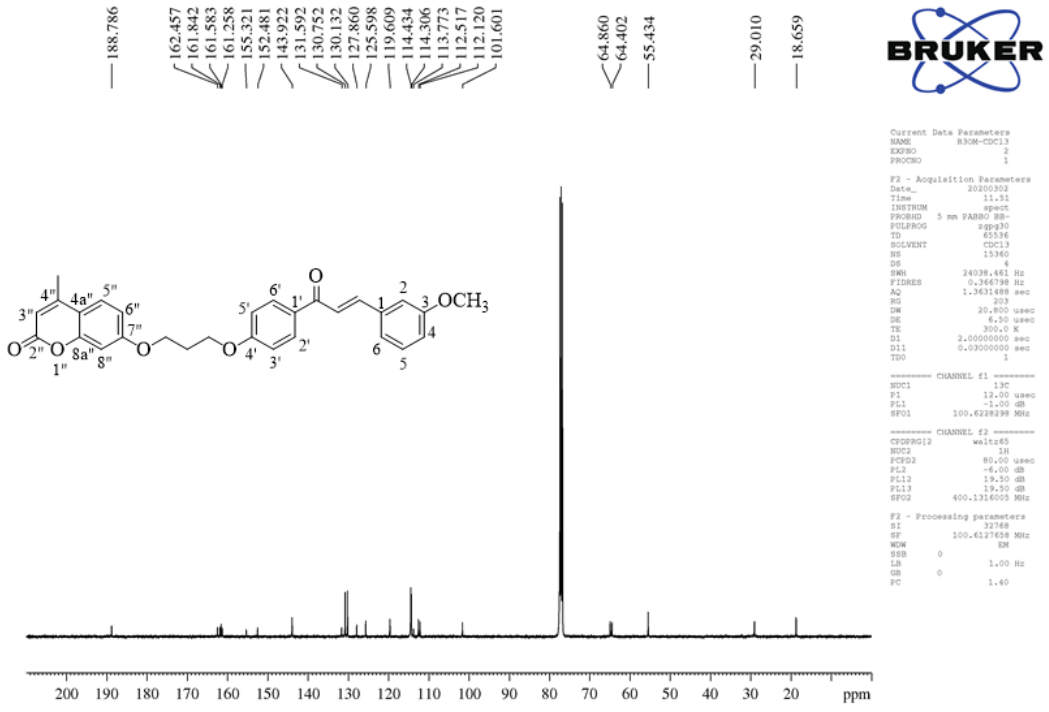
HRMS of compound **8j**



IR spectrum of (*E*)-7-(3-(4-(3-(3-methoxyphenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8k)**



^{1}H NMR spectrum of (*E*)-7-(3-(4-(3-(3-methoxyphenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8k)**

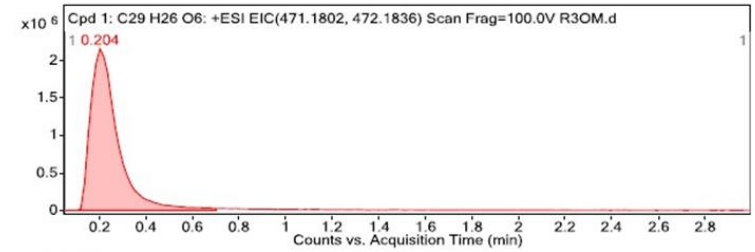


^{13}C NMR spectrum of (*E*)-7-(3-(4-(3-(3-methoxyphenyl)acryloyl)phenoxy)propoxy)-4-methyl-2*H*-chromen-2-one **(8k)**

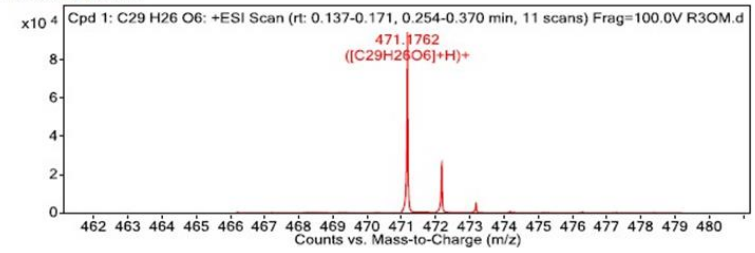
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C29 H26 O6	0.204	470.1688	94882	C29 H26 O6	470.1729	-8.87

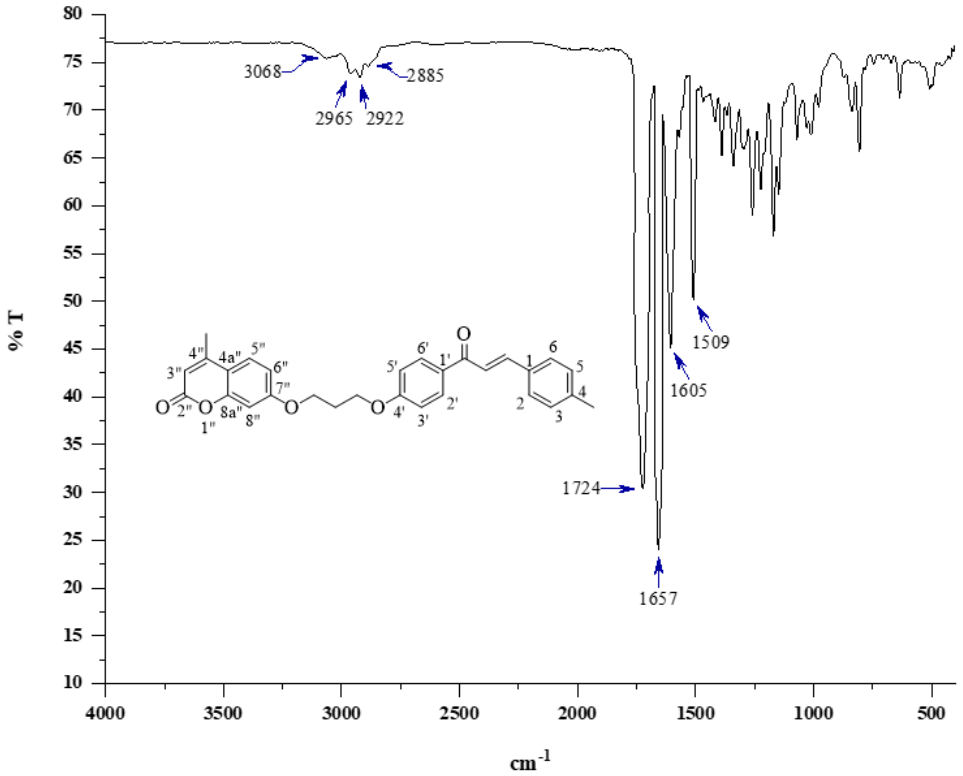
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C29 H26 O6	471.1762	0.204	Find By Formula	470.1688



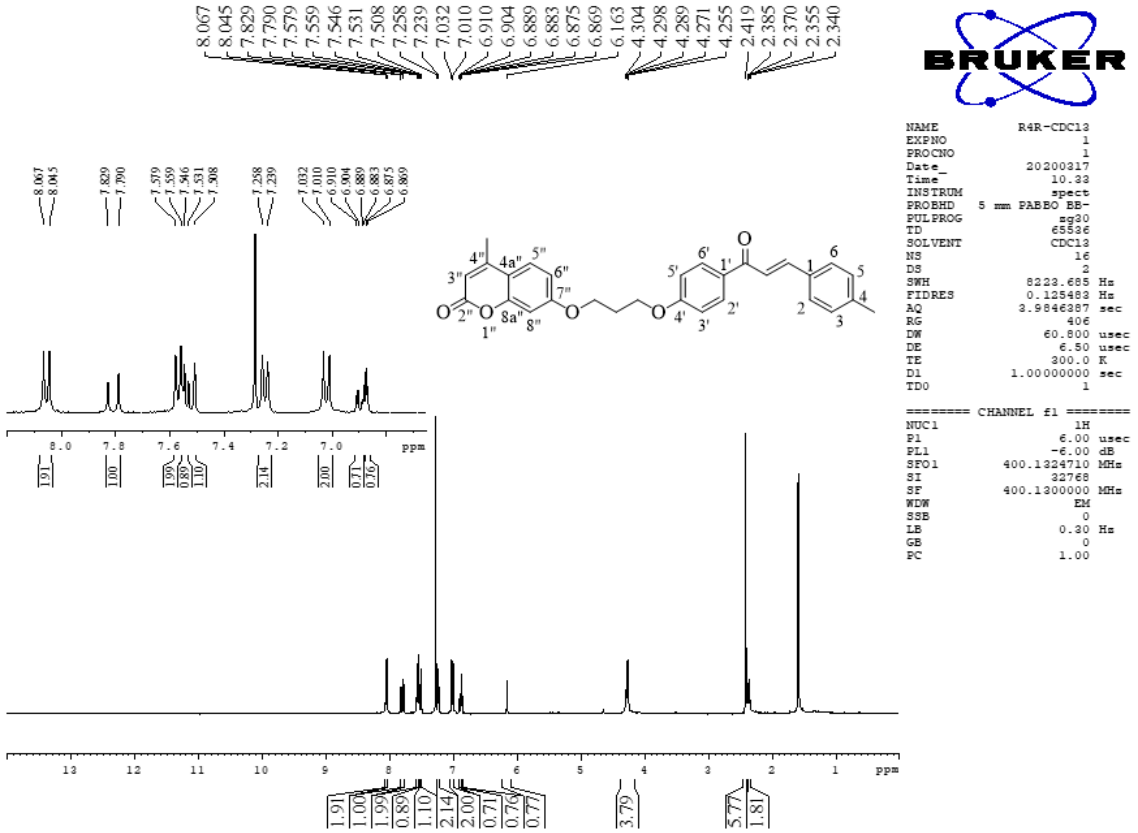
MS Zoomed Spectrum



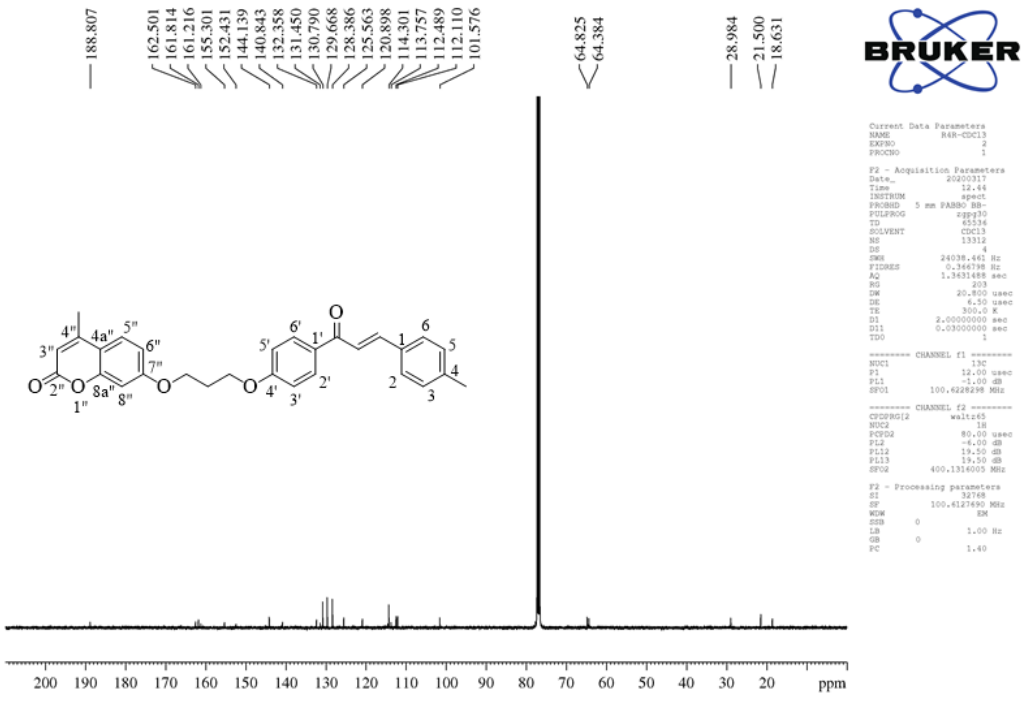
HRMS of compound **8k**



IR spectrum of (*E*)-4-methyl-7-(3-(4-(3-(*p*-tolyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one **(8l)**



^{1}H NMR spectrum of (*E*)-4-methyl-7-(3-(4-(3-(*p*-tolyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one **(8l)**

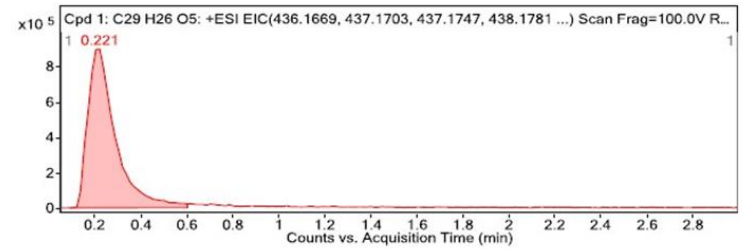


^{13}C NMR spectrum of (*E*)-4-methyl-7-(3-(4-(3-(*p*-tolyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one **(8l)**

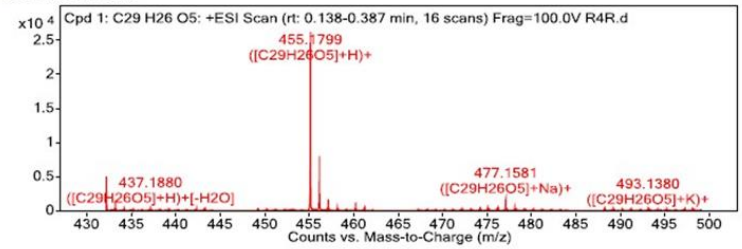
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C29 H26 O5	0.221	454.1729	26214	C29 H26 O5	454.178	-11.39

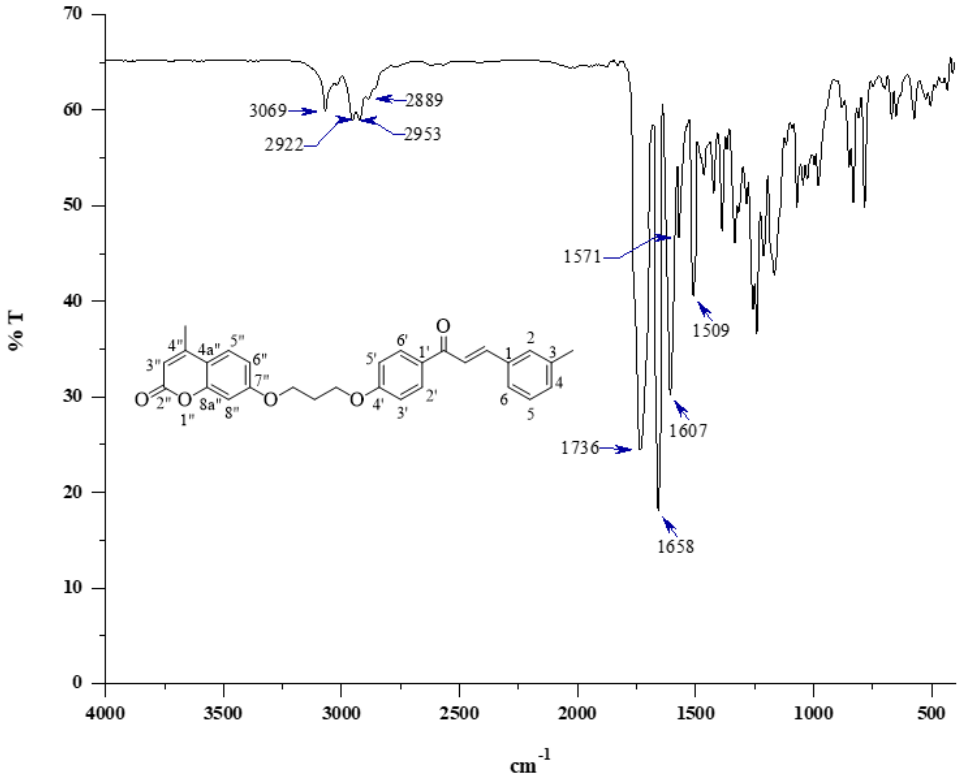
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C29 H26 O5	455.1799	0.221	Find By Formula	454.1729



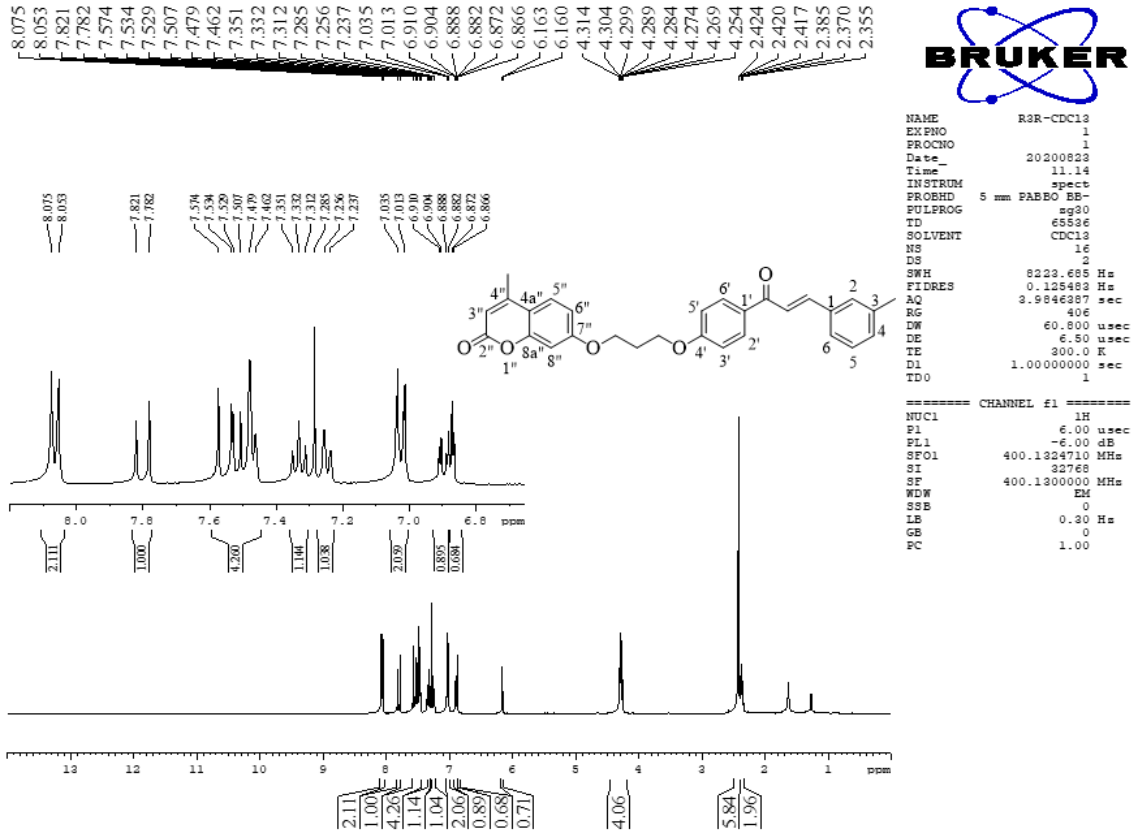
MS Zoomed Spectrum



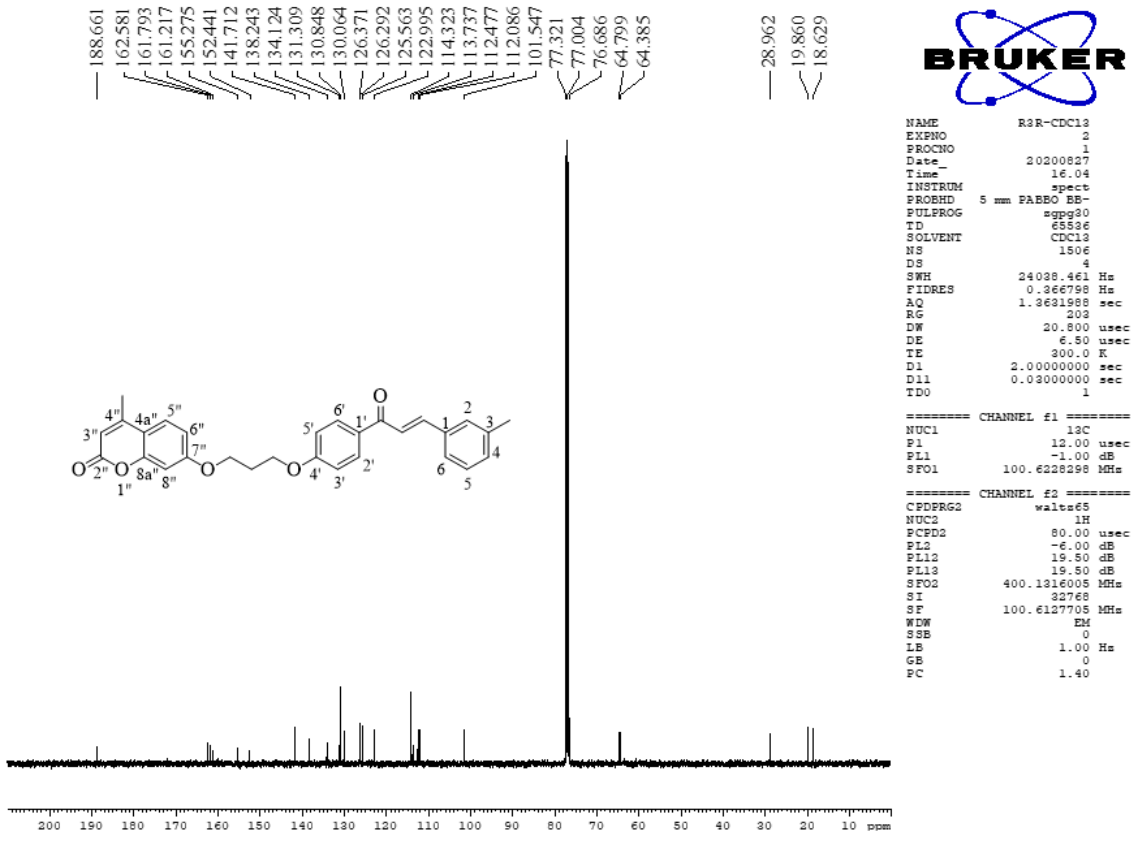
HRMS of compound **8l**



IR spectrum of (*E*)-4-methyl-7-(3-(4-(3-(*m*-tolyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one **(8m)**



^{1}H NMR spectrum of (*E*)-4-methyl-7-(3-(4-(3-(*m*-tolyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one **(8m)**

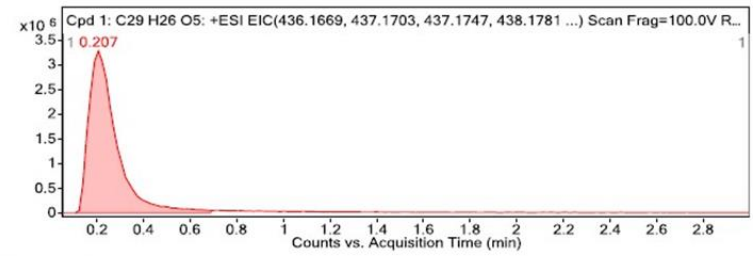


^{13}C NMR spectrum of (*E*)-4-methyl-7-(3-(4-(3-(*m*-tolyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one **(8m)**

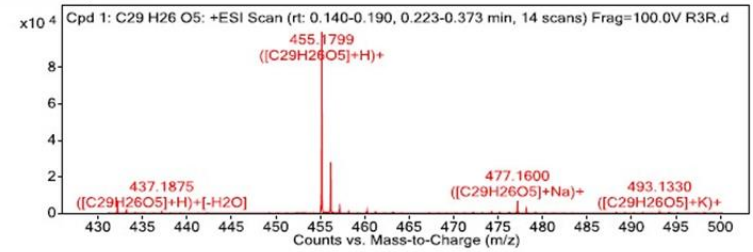
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C29 H26 O5	0.207	454.1725	100141	C29 H26 O5	454.178	-12.11

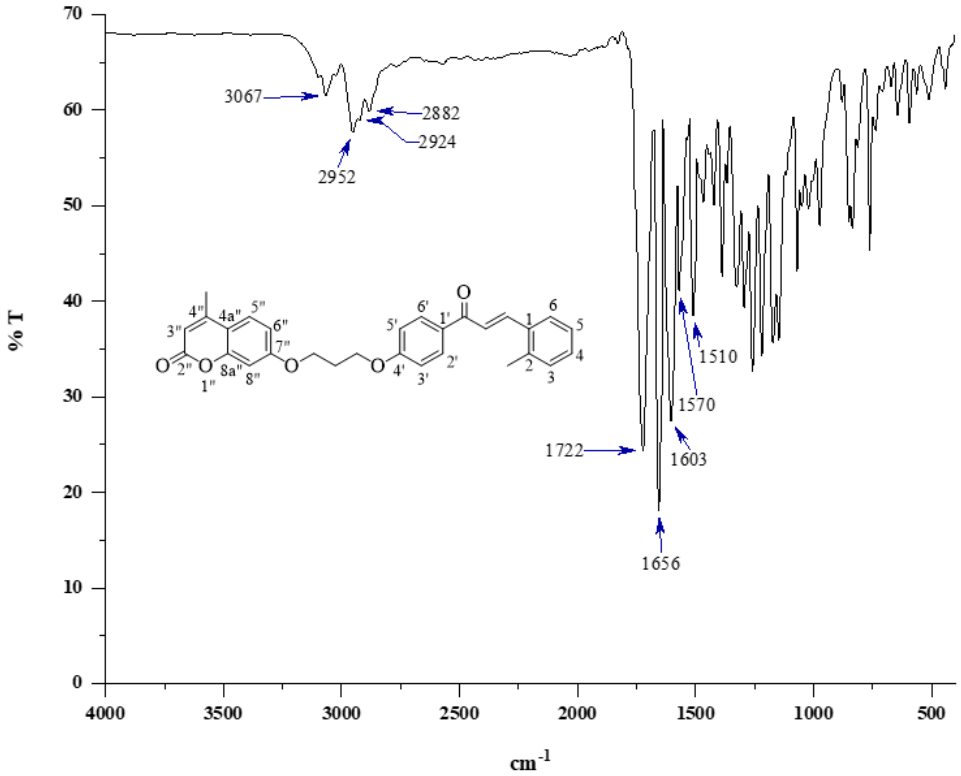
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C29 H26 O5	455.1799	0.207	Find By Formula	454.1725



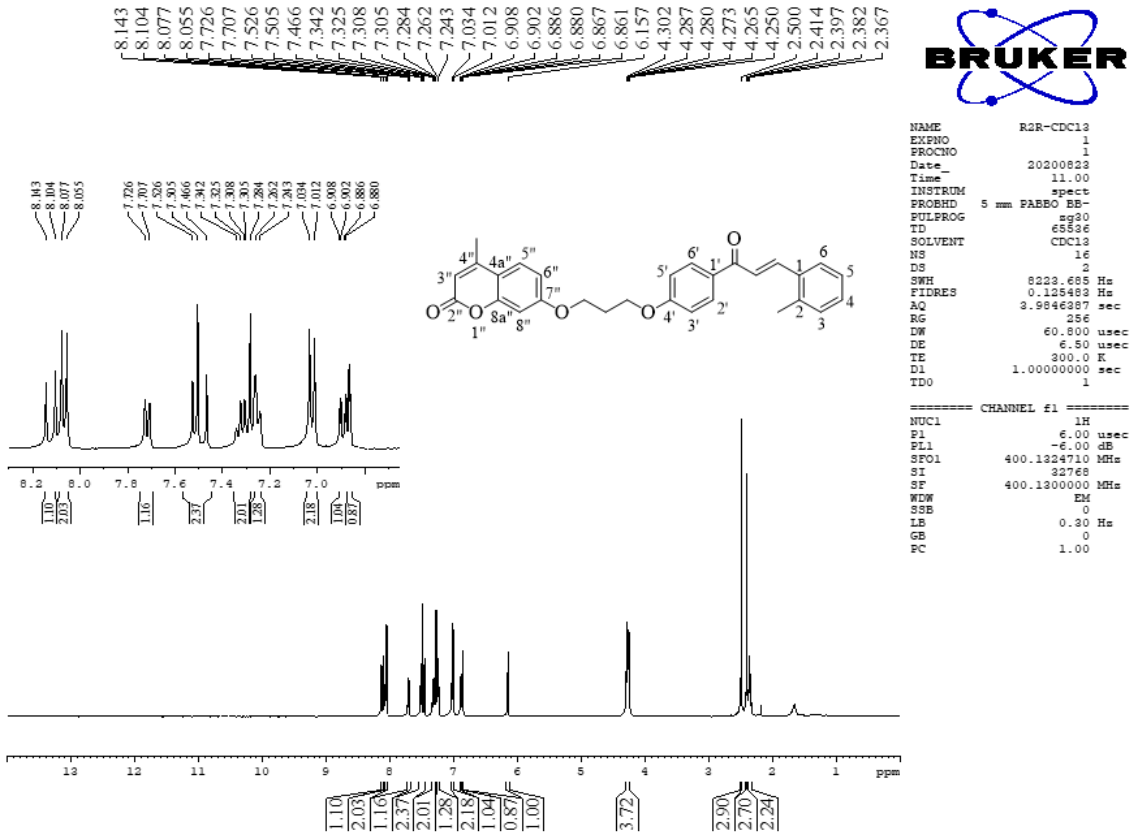
MS Zoomed Spectrum



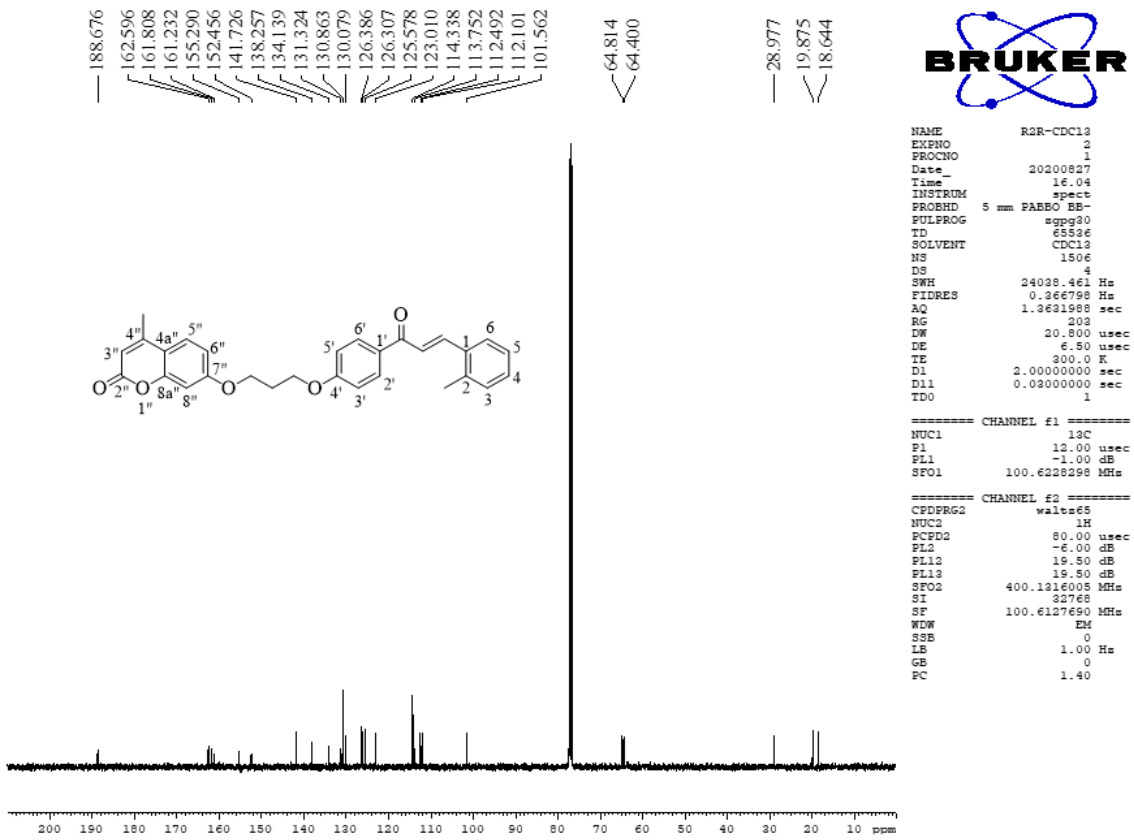
HRMS of compound **8m**



IR spectrum of (*E*)-4-methyl-7-(3-(4-(3-(*o*-tolyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one **(8n)**



^{1}H NMR spectrum of (*E*)-4-methyl-7-(3-(4-(3-(*o*-tolyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one **(8n)**

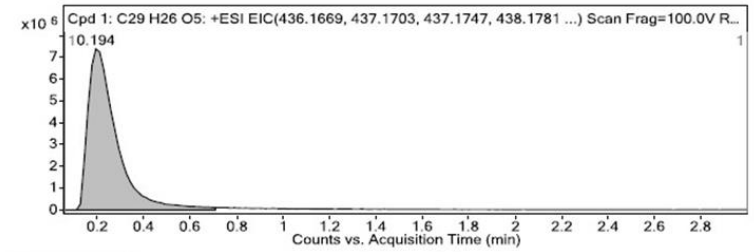


^{13}C NMR spectrum of (*E*)-4-methyl-7-(3-(4-(3-(*o*-tolyl)acryloyl)phenoxy)propoxy)-2*H*-chromen-2-one **(8n)**

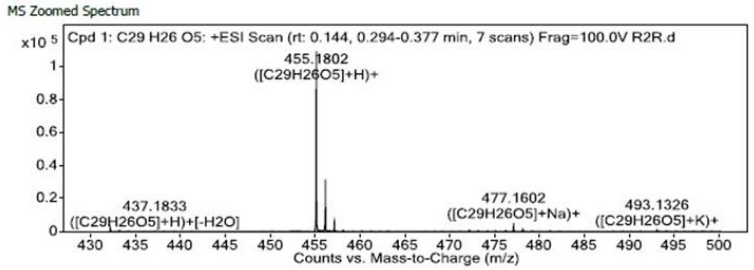
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C29 H26 O5	0.194	454.1727	109754	C29 H26 O5	454.178	-11.83

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C29 H26 O5	455.1802	0.194	Find By Formula	454.1727



MS Zoomed Spectrum



HRMS of compound **8n**

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