

Supporting Information

Direct Organocatalytic Asymmetric Vinylogous Michael Reaction of α, β -Unsaturated Ketones with 2(5H)-furanone

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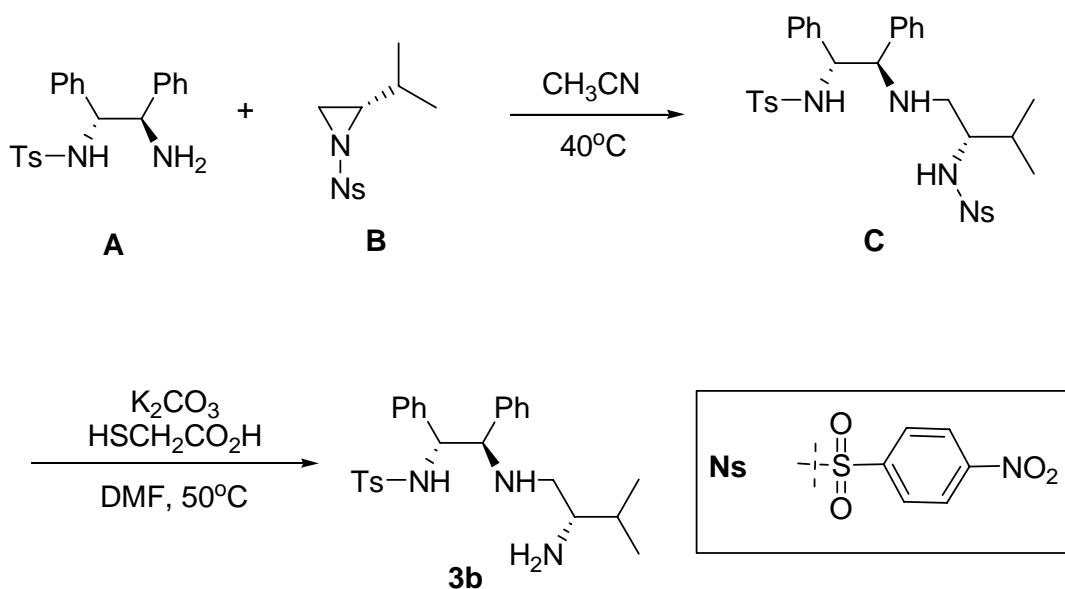
A: General Information and Starting Materials

General Information. Proton nuclear magnetic resonance (^1H NMR) spectra and carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded on a Bruker AV-400 spectrometer (400 MHz and 100 MHz). Chemical shifts for protons are reported in parts per million downfield from tetramethylsilane and are referenced to residual protium in the NMR solvent (CDCl_3 : δ 7.26) Chemical shifts for carbon are reported in parts per million downfield from tetramethylsilane and are referenced to the carbon resonances of the solvent (CDCl_3 : δ 77.16). Data are represented as follows: chemical shift, integration, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants in Hertz (Hz). Mass spectra (EI) were measured on a Waters Micromass GCT spectrometer. Optical rotations were measured on an Autopol III automatic polarimeter (Rudolph Research analytical). Melting points were measured on a XT3A apparatus. High performance liquid chromatography (HPLC) was performed on an Agilent 1200 Series chromatographs using a chiral columns (AS-H, AY-H, IA, IC) as noted.

Starting Materials. All solvents and inorganic reagents were from commercial sources and used without purification unless otherwise noted.

B: Experimental Procedure and Characterization of Catalysts

General procedure for the synthesis of new chiral catalysts¹.



To a solution of N-Ts DPEN **A** (2.93g, 8.0mmol) in CH₃CN (80.0 mL) was added **B** (2.16g, 8.0mmol). The reaction mixture was stirred at 40°C for 12h. TLC indicated the reaction was completed. The solvent was removed under reduced pressure and the residue was purified by silica gel chromatography to afford the pure product as a white solid **C** in 92% yield. ¹H NMR (400 MHz, CDCl₃): δ (ppm) 8.18 (d, *J* = 8.8 Hz, 2H), 7.90 (d, *J* = 8.4 Hz, 2H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.14-6.99 (m, 8H), 6.88-6.87 (m, 4H), 4.24 (d, *J* = 8.0 Hz, 1H), 3.58 (d, *J* = 8.0 Hz, 1H), 2.99-2.98 (m, 1H), 2.43-2.39 (m, 1H), 2.36 (s, 3H), 2.17-2.12 (m, 1H), 1.78-1.69 (m, 1H), 0.75 (d, *J* = 6.8 Hz, 3H), 0.70 (d, *J* = 6.8 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 149.6, 147.0, 143.1, 139.0, 138.2, 136.7, 129.3, 128.3, 128.2, 128.0, 127.6, 127.2, 127.1, 124.2, 68.1, 63.6, 59.7, 47.6, 29.8, 21.5, 18.8, 18.7.

To a stirred solution of **C** (3.18 g, 5.0 mmol) in DMF (30.0 mL) was added K₂CO₃ (2.07 g, 15.0 mmol), HSCH₂CO₂H (0.92 g, 10.0 mmol). The mixture was stirred at 50°C until TLC indicated that the reaction was completed. The mixture was then diluted with EtOAc (50 mL), and washed with 5M NaOH (3 × 100 mL). The aqueous layer was extracted with EtOAc (3 × 30 mL) and the combined organic layers were dried over MgSO₄ and concentrated. The residue was purified by silica gel chromatography to afford the pure product **3b** as a white solid in 80% yield.

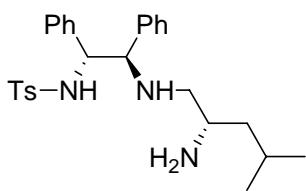
3a:N-((1*R*,2*R*)-2-((S)-2-amino-3-phenylpropylamino)-1,2-diphenylethyl)-4-methyl benzenesulfonamide

White solid. Mp 164-165°C; [α]²⁰_D - 20.3 (c 1.0, CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.40-7.38 (m, 2H), 7.32-7.29 (m, 2H), 7.25-7.21 (m, 1H), 7.16-7.11 (m, 5H), 7.07-7.01 (m, 5H), 6.96-6.93 (m, 4H), 4.32 (d, *J* = 8.0 Hz, 1H), 3.64 (d, *J* = 8.0 Hz, 1H), 3.03-2.98 (m, 1H), 2.72 (dd, *J* = 4.4, 13.2 Hz, 1H), 2.50 (dd, *J* = 4.0, 11.6 Hz, 1H), 2.44-2.39 (m, 1H), 2.34 (s, 3H), 2.26-2.21 (m, 1H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 142.5, 139.6, 138.9, 138.6, 137.6, 129.2, 129.1, 128.5, 128.3, 127.8, 127.6, 127.5, 127.4, 127.1, 127.0, 126.3, 68.6, 63.4, 53.5, 52.8, 42.3, 21.4; HRMS (EI): exact mass calculated for [(M+H)⁺] (C₃₀H₃₄N₃O₂S) requires m/z 500.2372, found m/z 500.2374.

3b:N-((1*R*,2*R*)-2-((S)-2-amino-3-methylbutylamino)-1,2-diphenylethyl)-4-methyl benzenesulfonamide

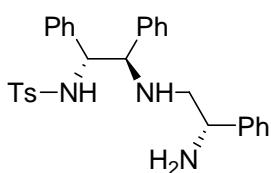
White solid. Mp 112-113°C; [α]²⁰_D - 34.1 (c 1.0, CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.40-7.39 (m, 2H), 7.15-7.13 (m, 3H), 7.07-7.02 (m, 5H), 6.96-6.95 (m, 4H), 4.34 (d, *J* = 8.0 Hz, 1H), 3.65 (d, *J* = 8.0 Hz, 1H), 2.50-2.44 (m, 2H), 2.34 (s, 3H), 2.18-2.13 (m, 1H), 1.55-1.51 (m, 1H), 0.83 (d, *J* = 6.8 Hz, 3H), 0.79 (d, *J* = 6.8 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 142.6, 139.6, 138.5, 137.2, 129.1, 128.3, 127.9, 127.6, 127.4, 127.2, 127.1, 68.6, 63.3, 57.0, 51.8, 31.7, 21.4, 19.5, 17.4; HRMS (EI): exact mass calculated for [(M+H)⁺] (C₂₆H₃₄N₃O₂S) requires m/z 452.2372, found m/z 452.2373.

3c:N-((1*R*,2*R*)-2-((*S*)-2-amino-4-methylpentylamino)-1,2-diphenylethyl)-4-methylbenzenesulfonamide



White solid. Mp 120-121°C; $[\alpha]^{20}_D$ - 39.3 (*c* 1.0, CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.41-7.39 (m, 2H), 7.16-7.15 (m, 3H), 7.06-7.03 (m, 5H), 6.96-6.94 (m, 4H), 4.33 (d, *J* = 8.0 Hz, 1H), 3.64 (d, *J* = 8.8 Hz, 1H), 2.80-2.74 (m, 1H), 2.45-2.41 (m, 1H), 2.35 (s, 3H), 2.15-2.10 (m, 1H), 1.66-1.60 (m, 1H), 1.13-1.09 (m, 1H), 0.88 (d, *J* = 6.8 Hz, 3H), 0.86 (d, *J* = 6.8 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 142.7, 139.6, 138.4, 137.3, 129.1, 128.3, 127.9, 127.6, 127.5, 127.4, 127.2, 127.1, 68.5, 63.3, 54.5, 49.1, 45.1, 24.6, 23.4, 22.0, 21.4; HRMS (EI): exact mass calculated for [(M+H)⁺] (C₂₇H₃₆N₃O₂S) requires m/z 466.2528, found m/z 466.2530.

3d:N-((1*R*,2*R*)-2-((*S*)-2-amino-2-phenylethylamino)-1,2-diphenylethyl)-4-methylbenzenesulfonamide



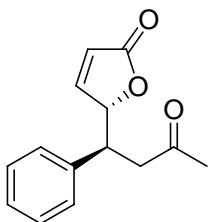
White crystals. Mp 79-80°C; $[\alpha]^{20}_D$ - 153.7 (*c* 1.0, CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.40-7.38 (m, 2H), 7.32-7.28 (m, 3H), 7.16-7.14 (m, 3H), 7.06-7.01 (m, 5H), 6.97-6.94 (m, 2H), 6.90-6.87 (m, 2H), 6.79-6.77 (m, 2H), 4.30 (d, *J* = 8.4 Hz, 1H), 3.42 (d, *J* = 8.4 Hz, 1H), 3.28-3.25 (m, 1H), 2.83 (dd, *J* = 4.4, 12.4 Hz, 1H), 2.71 (dd, *J* = 4.4, 12.4 Hz, 1H), 2.35 (s, 3H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 142.7, 141.2, 139.1, 138.2, 137.1, 129.1, 128.7, 128.3, 127.8, 127.7, 127.6, 127.5, 127.4, 127.3, 127.1, 64.3, 63.5, 61.7, 48.9, 21.4; HRMS (EI): exact mass calculated for [(M+H)⁺] (C₂₉H₃₂N₃O₂S) requires m/z 486.2215, found m/z 486.2216.

C: General Procedure for Asymmetric Michael Addition

To a solution of α , β -unsaturated ketones **5** (1.0 mmol, 2.0 equiv.) in CHCl₃ (1.0 mL) was added catalyst **3b** (0.05 mmol, 0.1 equiv.) and *N*-Boc-L-Phe (0.05 mmol, 0.1 equiv.) then followed by 2(5*H*)-furanone (35 μ L, 0.5 mmol, 1.0 equiv.). The reaction mixture was stirred at 50°C for 3 days and then the solvent was removed under vacuum. The residue was purified by silica gel chromatography to yield the desired addition product.

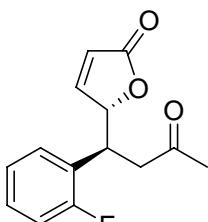
D: Characterization of Michael Addition Products

6a: 5-(3-oxo-1-phenylbutyl)furan-2(5H)-one



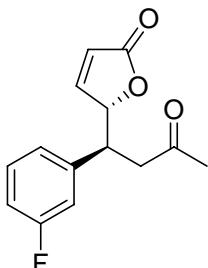
The product was obtained in 84% yield, white solid. Mp 77-78°C; $[\alpha]^{20}_D$ - 59.5 (*c* 1.0, CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.38-7.34 (m, 2H), 7.31-7.28 (m, 3H), 7.24-7.23 (m, 1H), 6.10 (dd, *J* = 1.2, 5.6 Hz, 1H), 5.18-5.16 (m, 1H), 3.49-3.44 (m, 1H), 3.05 (dd, *J* = 5.2, 17.6 Hz, 1H), 2.93 (dd, *J* = 8.0, 17.6 Hz, 1H), 2.08 (s, 3H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 205.9, 172.6, 155.5, 139.3, 129.0, 128.0, 127.7, 121.9, 85.7, 45.0, 44.2, 30.5; HRMS (EI): exact mass calculated for M⁺ (C₁₄H₁₄O₃) requires m/z 230.0943, found m/z 230.0944; The enantiomeric excess was determined by HPLC. [AY-H column, 220nm, n-Hexane: EtOH = 1:1, 0.60 mL/min]: 17.9 min (minor), 29.7 min (major), ee 98%.

6b: 5-(1-(2-fluorophenyl)-3-oxobutyl)furan-2(5H)-one



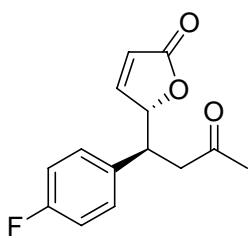
The product was obtained in 80% yield, white solid. Mp 89-91°C; $[\alpha]^{20}_D$ - 64.2 (*c* 1.0, CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.34-7.26 (m, 3H), 7.17-7.13 (m, 1H), 7.11-7.06 (m, 1H), 6.12 (dd, *J* = 1.2, 5.6 Hz, 1H), 5.27-5.25 (m, 1H), 3.78-3.72 (m, 1H), 3.10 (dd, *J* = 5.2, 17.6 Hz, 1H), 3.00 (dd, *J* = 7.6, 18.0 Hz, 1H), 2.11 (s, 3H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 205.6, 172.5, 161.8, 159.3, 155.4, 130.2, 130.2, 129.5, 129.4, 126.0, 125.9, 124.7, 124.7, 122.0, 116.0, 115.9, 84.4, 43.7, 38.5, 30.3; HRMS (EI): exact mass calculated for M⁺ (C₁₄H₁₃FO₃) requires m/z 248.0849, found m/z 248.0850; The enantiomeric excess was determined by HPLC. [AY-H column, 220nm, n-Hexane: EtOH = 7:3, 0.80 mL/min]: 24.2 min (minor), 42.9 min (major), ee 97%.

6c: 5-(1-(3-fluorophenyl)-3-oxobutyl)furan-2(5H)-one



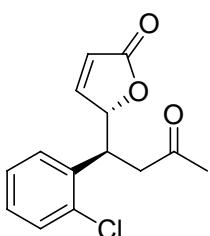
The product was obtained in 75% yield, white solid. Mp 80-82°C; $[\alpha]^{20}_D$ - 53.1 (*c* 1.0, CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.36-7.31 (m, 1H), 7.27 (d, *J* = 5.6 Hz, 1H), 7.11-7.09 (m, 1H), 7.04-6.09 (m, 2H), 6.14 (dd, *J* = 1.6, 5.6 Hz, 1H), 5.18-5.16 (m, 1H), 3.54-3.49 (m, 1H), 3.02 (dd, *J* = 5.2, 18.0 Hz, 1H), 2.89 (dd, *J* = 8.0, 18.0 Hz, 1H), 2.11 (s, 3H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 205.5, 172.4, 164.2, 161.7, 155.1, 142.1, 142.0, 130.6, 130.5, 123.9, 123.8, 122.2, 115.2, 115.2, 115.0, 114.8, 114.6, 85.2, 50.8, 44.5, 43.6, 30.5; HRMS (EI): exact mass calculated for M⁺ (C₁₄H₁₃FO₃) requires m/z 248.0849, found m/z 248.0852; The enantiomeric excess was determined by HPLC. [IA column, 220nm, n-Hexane: EtOH = 4:1, 1.0 L/min]: 12.3 min (major), 14.2 min (minor), ee 96%.

6d: 5-(1-(4-fluorophenyl)-3-oxobutyl)furan-2(5H)-one



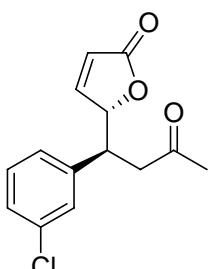
The product was obtained in 79% yield, colorless oil. $[\alpha]^{20}_D$ - 41.8 (*c* 1.0, CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.29-7.24 (m, 3H), 7.05-7.01 (m, 2H), 6.11 (dd, *J* = 1.6, 5.6 Hz, 1H), 5.15-5.13 (m, 1H), 3.52-3.47(m, 1H), 2.99 (dd, *J* = 5.2, 17.6 Hz, 1H), 2.87 (dd, *J* = 8.0, 18.0 Hz, 1H), 2.07 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 205.7, 172.5, 163.3, 160.9, 155.2, 135.2, 135.2, 129.8, 129.7, 122.1, 115.9, 115.7, 85.5, 44.7, 43.2, 30.5; HRMS (EI): exact mass calculated for M^+ ($\text{C}_{14}\text{H}_{13}\text{FO}_3$) requires m/z 248.0849, found m/z 248.0847; The enantiomeric excess was determined by HPLC. [AS-H column, 220nm, n-Hexane: *i*-PrOH = 1:1, 0.50 mL/min]: 37.3 min (major), 47.7 min (minor), ee 98%.

6e: 5-(1-(2-chlorophenyl)-3-oxobutyl)furan-2(5H)-one



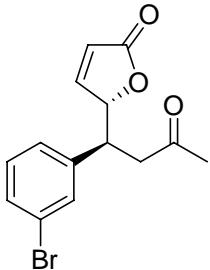
The product was obtained in 78% yield, brown oil. $[\alpha]^{20}_D$ - 3.5 (*c* 1.0, CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.42-7.36 (m, 2H), 7.33-7.31 (m, 1H), 7.28-7.21 (m, 2H), 6.11 (dd, *J* = 1.2, 6.0 Hz, 1H), 5.24-5.23 (m, 1H), 4.16-4.11(m, 1H), 2.98 (dd, *J* = 6.4, 17.6 Hz, 1H), 2.88 (dd, *J* = 6.8, 18.0 Hz, 1H), 2.08 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 205.5, 172.6, 155.7, 137.1, 133.8, 130.1, 129.1, 128.8, 127.4, 121.8, 84.6, 43.1, 39.5, 30.2; HRMS (EI): exact mass calculated for M^+ ($\text{C}_{14}\text{H}_{13}\text{ClO}_3$) requires m/z 264.0553, found m/z 264.0547; The enantiomeric excess was determined by HPLC. [AS-H column, 220nm, n-Hexane: *i*-PrOH = 1:1, 0.50 mL/min]: 32.2 min (minor), 57.6 min (major), ee 95%.

6f: 5-(1-(3-chlorophenyl)-3-oxobutyl)furan-2(5H)-one



The product was obtained in 81% yield, yellow oil. $[\alpha]^{20}_D$ - 28.4 (*c* 1.0, CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.30-7.28 (m, 3H), 7.27-7.26 (m, 1H), 7.22-7.19 (m, 1H), 6.14 (dd, *J* = 2.0, 5.6 Hz, 1H), 5.17-5.15 (m, 1H), 3.52-3.47(m, 1H), 3.00 (dd, *J* = 5.2, 18.0 Hz, 1H), 2.89 (dd, *J* = 8.0, 18.0 Hz, 1H), 2.10 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 205.4, 172.4, 155.2, 141.6, 134.7, 130.2, 128.2, 127.9, 126.5, 122.2, 85.2, 44.3, 43.5, 30.4; HRMS (EI): exact mass calculated for M^+ ($\text{C}_{14}\text{H}_{13}\text{ClO}_3$) requires m/z 264.0553, found m/z 264.0558; The enantiomeric excess was determined by HPLC. [AY-H column, 220nm, n-Hexane: *i*-PrOH = 1:1, 0.50 mL/min]: 36.9 min (minor), 62.8 min (major), ee 97%.

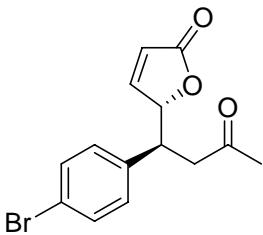
6g: 5-(1-(3-bromophenyl)-3-oxobutyl)furan-2(5H)-one



The product was obtained in 75% yield, yellow oil. $[\alpha]^{20}_D$ - 31.2 (*c* 1.0, CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.46-7.43 (m, 2H), 7.27-7.21 (m, 3H), 6.14 (dd, *J* = 2.0, 6.0 Hz, 1H), 5.17-5.15 (m, 1H), 3.51-3.46(m, 1H), 3.00 (dd, *J* = 5.2, 18.0 Hz, 1H), 2.88 (dd, *J* = 7.6, 18.0 Hz, 1H), 2.10 (s, 3H). ^{13}C NMR (100 MHz,

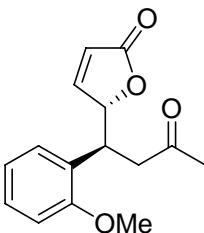
CDCl_3): δ (ppm) 205.4, 172.4, 155.1, 142.0, 131.0, 130.9, 130.5, 127.0, 122.9, 122.2, 85.2, 44.4, 43.5, 30.5; HRMS (EI): exact mass calculated for M^+ ($\text{C}_{14}\text{H}_{13}\text{BrO}_3$) requires m/z 308.0048, found m/z 308.0054; The enantiomeric excess was determined by HPLC. [AY-H column, 220nm, n-Hexane: EtOH = 1:1, 0.60 mL/min]: 14.0 min (minor), 17.3 min (major), ee 97%.

6h: 5-(1-(4-bromophenyl)-3-oxobutyl)furan-2(5H)-one



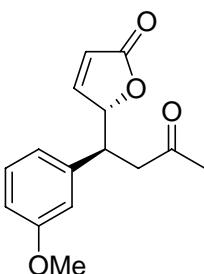
The product was obtained in 78% yield, white solid. Mp 91-92°C; $[\alpha]^{20}_D$ - 47.5 (c 1.0, CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.44 (d, J = 8.4 Hz, 2H), 7.24 (d, J = 5.6 Hz, 1H), 7.16 (d, J = 8.0 Hz, 2H), 6.08 (dd, J = 2.0, 5.6 Hz, 1H), 5.13-5.11 (m, 1H), 3.48-3.43 (m, 1H), 2.96 (dd, J = 5.2, 17.6 Hz, 1H), 2.85 (dd, J = 8.0, 18.0 Hz, 1H), 2.05 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 205.5, 172.4, 155.2, 138.5, 132.0, 129.9, 122.2, 121.6, 85.2, 44.391, 43.3, 30.5; HRMS (EI): exact mass calculated for M^+ ($\text{C}_{14}\text{H}_{13}\text{BrO}_3$) requires m/z 308.0048, found m/z 308.0055; The enantiomeric excess was determined by HPLC. [IC column, 220nm, n-Hexane: EtOH = 4:1, 1.0 mL/min]: 18.0 min (minor), 19.8 min (major), ee 95%.

6i: 5-(1-(2-methoxyphenyl)-3-oxobutyl)furan-2(5H)-one



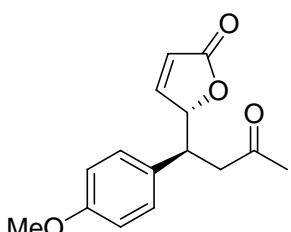
The product was obtained in 85% yield, colorless oil. $[\alpha]^{20}_D$ - 44.9 (c 1.0, CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.28-7.24 (m, 1H), 7.22-7.21 (m, 2H), 6.95-6.89 (m, 2H), 6.05 (dd, J = 1.6, 5.6 Hz, 1H), 5.33-5.31 (m, 1H), 3.86 (s, 3H), 3.80-3.75 (m, J = 5.2, 1H), 3.06-2.94 (m, 2H), 2.06 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 206.4, 172.9, 156.9, 156.4, 129.4, 128.8, 127.0, 121.2, 121.0, 111.0, 84.9, 55.4, 43.9, 39.2, 30.3; HRMS (EI): exact mass calculated for M^+ ($\text{C}_{14}\text{H}_{16}\text{O}_4$) requires m/z 260.1049, found m/z 260.1051; The enantiomeric excess was determined by HPLC. [AS-H column, 220nm, n-Hexane: EtOH = 4:1, 0.80 mL/min]: 26.5 min (minor), 38.7 min (major), ee 98%.

6j: 5-(1-(3-methoxyphenyl)-3-oxobutyl)furan-2(5H)-one



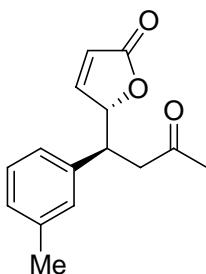
The product was obtained in 73% yield, colorless crystals. Mp 68-69°C; $[\alpha]^{20}_D$ - 47.9 (c 1.0, CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.27-7.22 (m, 2H), 6.84 (d, J = 7.6 Hz, 1H), 6.81-6.80 (m, 2H), 6.07 (dd, J = 1.2, 6.0 Hz, 1H), 5.14-5.12 (m, 1H), 3.79 (s, 3H), 3.42-3.37 (m, 1H), 3.02 (dd, J = 5.2, 17.6 Hz, 1H), 2.91 (dd, J = 8.0, 18.0 Hz, 1H), 2.06 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 205.9, 172.6, 159.8, 155.6, 140.8, 130.0, 121.8, 120.2, 114.1, 112.7, 85.6, 55.2, 45.0, 44.268, 30.5; HRMS (EI): exact mass calculated for M^+ ($\text{C}_{14}\text{H}_{16}\text{O}_4$) requires m/z 260.1049, found m/z 260.1046; The enantiomeric excess was determined by HPLC. [AS-H column, 220nm, n-Hexane: EtOH = 7:3, 0.80 mL/min]: 19.2 min (minor), 33.4 min (major), ee 97%.

6k: 5-(1-(4-methoxyphenyl)-3-oxobutyl)furan-2(5H)-one



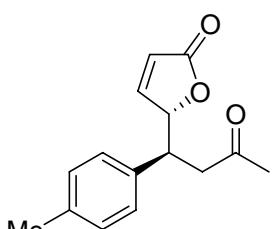
The product was obtained in 84% yield, colorless crystals. Mp 87-89°C; $[\alpha]^{20}_D$ - 53.4 (*c* 1.0, CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.22 (d, *J* = 5.6 Hz, 1H), 7.17 (d, *J* = 8.8 Hz 2H), 6.84 (d, *J* = 8.8 Hz 2H), 6.05 (dd, *J* = 1.6, 5.6 Hz, 1H), 5.11-5.09 (m, 1H), 3.76 (s, 3H), 3.40-3.35 (m, 1H), 2.98 (dd, *J* = 5.2, 17.2 Hz, 1H), 2.87 (dd, *J* = 8.4, 17.2 Hz, 1H), 2.03 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 206.1, 172.7, 158.9, 155.6, 131.1, 129.1, 121.8, 114.2, 85.9, 55.2, 45.2, 43.5, 30.5; HRMS (EI): exact mass calculated for M^+ ($\text{C}_{14}\text{H}_{16}\text{O}_4$) requires m/z 260.1049, found m/z 260.1052; The enantiomeric excess was determined by HPLC. [IC column, 220nm, n-Hexane: EtOH = 4:1, 1.0 mL/min]: 33.8 min (minor), 37.9 min (major), ee 96%.

6l: 5-(3-oxo-1-*m*-tolylbutyl)furan-2(5H)-one



The product was obtained in 83% yield, yellow oil. $[\alpha]^{20}_D$ - 26.2 (*c* 1.0, CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.23-7.20 (m, 2H), 7.09-7.05 (m, 3H), 6.07 (dd, *J* = 1.6, 5.6 Hz, 1H), 5.14-5.13 (m, 1H), 3.42-3.37 (m, 1H), 3.02 (dd, *J* = 5.2, 17.6 Hz, 1H), 2.91 (dd, *J* = 8.4, 17.6 Hz, 1H), 2.34 (s, 3H), 2.06 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 205.9, 172.6, 155.7, 139.2, 138.5, 128.8, 128.4, 125.0, 121.7, 85.8, 45.0, 44.2, 30.5, 21.4; HRMS (EI): exact mass calculated for M^+ ($\text{C}_{15}\text{H}_{16}\text{O}_3$) requires m/z 244.1099, found m/z 244.1100; The enantiomeric excess was determined by HPLC. [AY-H column, 220nm, n-Hexane: EtOH = 1:1, 0.60 mL/min]: 19.7 min (minor), 23.7 min (major), ee 97%.

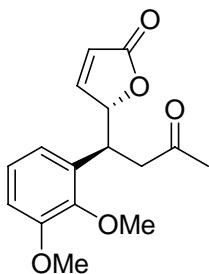
6m: 5-(3-oxo-1-*p*-tolylbutyl)furan-2(5H)-one



The product was obtained in 85% yield, yellow oil. $[\alpha]^{20}_D$ - 48.1 (*c* 1.0, CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.23 (d, *J* = 5.6 Hz, 1H), 7.16-7.15 (m, 4H), 6.09 (dd, *J* = 1.2, 5.6 Hz, 1H), 5.14-5.12 (m, 1H), 3.43-3.38 (m, 1H), 3.03 (dd, *J* = 5.2, 17.6 Hz, 1H), 2.91 (dd, *J* = 8.0, 17.6 Hz, 1H), 2.34 (s, 3H), 2.07 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 206.0, 172.7, 155.6, 137.4, 136.1, 129.6, 127.9, 121.8, 85.8, 45.2, 44.0, 30.5, 21.0; HRMS (EI): exact mass calculated for M^+ ($\text{C}_{15}\text{H}_{16}\text{O}_3$) requires m/z 244.1099, found m/z 244.1098; The enantiomeric excess was determined by HPLC. [IC column, 220nm, n-Hexane: EtOH = 4:1, 1.0 mL/min]: 24.2 min (minor), 27.6 min (major), ee 96%.

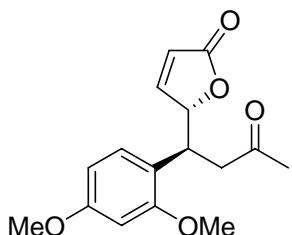
6n: 5-(1-(2,3-dimethoxyphenyl)-3-oxobutyl)furan-2(5H)-one

The product was obtained in 86% yield, yellow oil. $[\alpha]^{20}_D$ - 49.9 (*c* 1.0, CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.23 (d, *J* = 5.6 Hz, 1H) 7.07-7.03 (m, 1H),



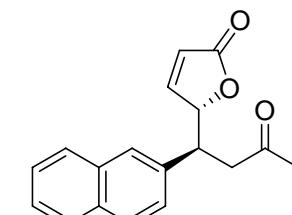
6.88-6.83 (m, 2H), 6.07 (dd, $J = 1.6, 5.6$ Hz, 1H), 5.14-5.12 (m, 1H), 3.92 (s, 3H), 3.88 (s, 3H), 3.86-3.82 (m, 1H), 3.07 (dd, $J = 5.2, 17.6$ Hz, 1H), 2.99 (dd, $J = 8.4, 17.6$ Hz, 1H), 2.10 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 206.1, 172.8, 156.1, 153.0, 146.8, 132.6, 124.3, 121.4, 119.8, 111.7, 85.4, 60.7, 55.7, 44.4, 38.0, 30.4; HRMS (EI): exact mass calculated for M^+ ($\text{C}_{16}\text{H}_{18}\text{O}_5$) requires m/z 290.1154, found m/z 290.1153; The enantiomeric excess was determined by HPLC. [AY-H column, 220nm, n-Hexane: EtOH = 1:1, 0.60 mL/min]: 38.2 min (major), 56.1 min (minor), ee 97%.

6o: 5-(1-(2,4-dimethoxyphenyl)-3-oxobutyl)furan-2(5H)-one



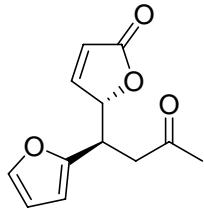
The product was obtained in 85% yield, yellow oil. $[\alpha]^{20}_D$ - 48.0 (c 1.0, CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.22 (d, $J = 6.0$ Hz, 1H), 7.12-7.10 (m, 1H), 6.47-6.45 (m, 2H), 6.04 (dd, $J = 1.2, 5.6$ Hz, 1H), 5.29-5.27 (m, 1H), 3.83 (s, 3H), 3.79 (s, 3H), 3.69-3.64 (m, 1H), 3.04-2.92 (m, 2H), 2.06 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 206.6, 172.9, 160.2, 157.9, 156.5, 130.0, 121.0, 119.1, 104.6, 98.8, 85.1, 55.4, 55.2, 44.2, 39.0, 30.2; HRMS (EI): exact mass calculated for M^+ ($\text{C}_{16}\text{H}_{18}\text{O}_5$) requires m/z 290.1154, found m/z 290.1157; The enantiomeric excess was determined by HPLC. [IA column, 220nm, n-Hexane: EtOH = 8:1, 1.0 mL/min]: 17.5 min (minor), 18.6 min (major), ee 98%.

6p: 5-(1-(naphthalen-2-yl)-3-oxobutyl)furan-2(5H)-one



The product was obtained in 86% yield, white solid. Mp 123-124°C; $[\alpha]^{20}_D$ - 59.8 (c 1.0, CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.87-7.83 (m, 3H), 7.77-7.76 (m, 1H), 7.54-7.48 (m, 2H), 7.44-7.41 (m, 1H), 7.25-7.24 (m, 1H), 6.11 (dd, $J = 1.6, 6.0$ Hz, 1H), 5.28-5.26 (m, 1H), 3.67-3.61 (m, 1H), 3.13 (dd, $J = 5.2, 17.6$ Hz, 1H), 3.04 (dd, $J = 8.0, 17.6$ Hz, 1H), 2.09 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 205.9, 172.6, 155.5, 136.9, 133.4, 132.8, 128.8, 127.8, 127.7, 127.0, 126.5, 126.2, 126.0, 122.0, 85.7, 45.1, 44.3, 30.5; HRMS (EI): exact mass calculated for M^+ ($\text{C}_{18}\text{H}_{16}\text{O}_3$) requires m/z 280.1099, found m/z 280.1096; The enantiomeric excess was determined by HPLC. [IA column, 220nm, n-Hexane: EtOH = 4:1, 1.0 mL/min]: 15.5 min (major), 20.1 min (minor), ee 98%.

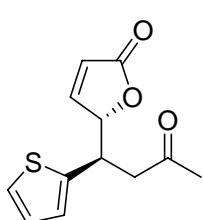
6q: 5-(1-(furan-2-yl)-3-oxobutyl)furan-2(5H)-one



The product was obtained in 79% yield, colorless oil. $[\alpha]^{20}_D$ - 105.8 (c 1.0, CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.36-7.34 (m, 2H), 6.32-6.31 (m, 1H), 6.19-6.18 (m, 1H), 6.10 (dd, $J = 1.6, 5.6$ Hz, 1H), 5.23-5.22 (m, 1H), 3.66-3.61 (m, 1H), 3.02-2.89 (m, 2H), 2.13 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 205.4, 172.4, 155.1, 152.0, 142.0, 121.9, 110.5, 107.5, 83.7, 42.5, 37.7,

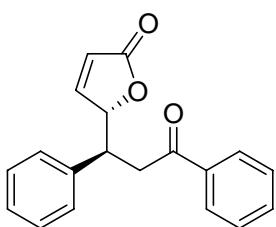
30.2; HRMS (EI): exact mass calculated for M^+ ($C_{12}H_{12}O_4$) requires m/z 220.0736, found m/z 220.0737; The enantiomeric excess was determined by HPLC. [AY-H column, 220nm, n-Hexane: EtOH = 1:1, 0.60 mL/min]: 23.4 min (minor), 27.4 min (major), ee 97%.

6r: 5-(3-oxo-1-(thiophen-2-yl)butyl)furan-2(5H)-one



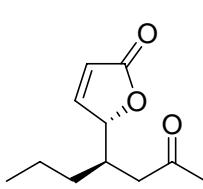
The product was obtained in 83% yield, brown solid. Mp 60-61°C; $[\alpha]^{20}_D$ - 73.6 (c 1.0, CH_2Cl_2); 1H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.32 (dd, J = 0.8, 6.0 Hz, 1H), 7.22-7.21 (m, 1H), 6.97-6.96 (m, 2H), 6.11 (dd, J = 1.6, 5.6 Hz, 1H), 5.20-5.18 (m, 1H), 3.84-3.79 (m, 1H), 3.05-2.90 (m, 2H), 2.11 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 205.4, 172.3, 155.0, 141.6, 127.1, 126.0, 124.7, 122.2, 85.2, 45.9, 39.4, 30.5; HRMS (EI): exact mass calculated for M^+ ($C_{12}H_{12}O_3S$) requires m/z 236.0507, found m/z 236.0506; The enantiomeric excess was determined by HPLC. [IA column, 220nm, n-Hexane: EtOH = 4:1, 1.0 mL/min]: 15.1 min (major), 45.3 min (minor), ee 98%.

6s: 5-(3-oxo-1,3-diphenylpropyl)furan-2(5H)-one



The product was obtained in 79% yield, white solid. Mp 83-85°C; $[\alpha]^{20}_D$ - 52.4 (c 1.0, CH_2Cl_2); 1H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.91-7.89 (m, 2H), 7.58-7.54 (m, 1H), 7.46-7.43 (m, 2H), 7.36-7.33 (m, 4H), 7.30-7.24 (m, 2H), 6.10-6.09 (m, 1H), 5.30-5.28 (m, 1H), 3.75-3.8270 (m, 1H), 3.59 (dd, J = 5.2, 17.6 Hz, 1H), 3.50 (dd, J = 7.6, 17.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 197.4, 172.7, 155.7, 139.6, 136.6, 133.4, 128.9, 128.7, 128.7, 128.4, 128.2, 128.1, 128.0, 127.7, 122.0, 85.8, 44.4, 40.1; HRMS (EI): exact mass calculated for M^+ ($C_{19}H_{16}O_3$) requires m/z 292.1099, found m/z 292.1101; The enantiomeric excess was determined by HPLC. [IC column, 220nm, n-Hexane: EtOH = 4:1, 1.0 mL/min]: 16.8 min (minor), 19.2 min (major), ee 97%.

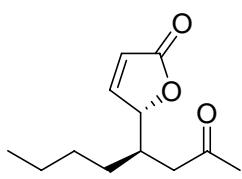
6t: 5-(2-oxoheptan-4-yl)furan-2(5H)-one



The product was obtained in 75% yield, yellow oil. $[\alpha]^{20}_D$ - 119.1 (c 1.0, CH_2Cl_2); 1H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.42 (dd, J = 1.6, 5.6 Hz, 1H), 6.10 (dd, J = 2.0, 5.6 Hz, 1H), 5.16-5.15 (m, 1H), 2.51-2.47 (m, 1H), 2.35-2.33 (m, 2H), 2.11 (s, 3H), 1.58-1.53 (m, 1H), 1.43-1.38 (m, 3H), 0.97-0.93 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 207.2, 173.0, 156.2, 121.5, 84.7, 41.9, 35.7, 34.0, 30.4, 20.2, 14.0; HRMS (EI): exact mass calculated for M^+ ($C_{11}H_{16}O_3$) requires m/z 196.1099, found m/z 196.1100; The enantiomeric excess was determined by HPLC. [AS-H column, 205nm, n-Hexane: EtOH = 8:1, 1.0 mL/min]: 15.0 min (minor), 32.2 min (major), ee 98%.

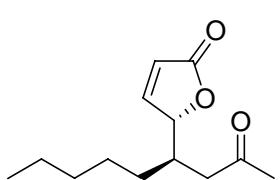
6u: 5-(2-oxooctan-4-yl)furan-2(5H)-one

The product was obtained in 74% yield, yellow oil. $[\alpha]^{20}_D$ - 128.0 (c 1.0, CH_2Cl_2); 1H



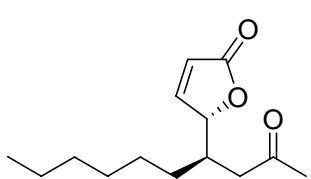
NMR (400 MHz, CDCl₃): δ (ppm) 7.42 (dd, *J* = 1.2, 5.6 Hz, 1H), 6.10 (dd, *J* = 1.6, 5.6 Hz, 1H), 5.16-5.15 (m, 1H), 2.51-2.43 (m, 1H), 2.35-2.34 (m, 2H), 2.11 (s, 3H), 1.60-1.56 (m, 1H) 1.44-1.31 (m, 5H), 0.94-0.91 (m, 3H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 207.2, 173.1, 156.2, 121.6, 84.8, 42.0, 35.9, 31.6, 30.5, 29.2, 22.6, 14.0; HRMS (EI): exact mass calculated for M⁺ (C₁₂H₁₈O₃) requires m/z 210.1056, found m/z 210.1259; The enantiomeric excess was determined by HPLC. [AS-H column, 205nm, n-Hexane: EtOH = 8:1, 1.0 mL/min]: 12.6min (minor), 18.8 min (major), ee 96%.

6v: 5-(2-oxononan-4-yl)furan-2(5H)-one



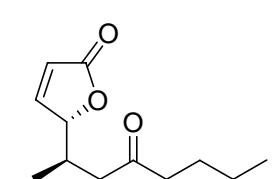
The product was obtained in 82% yield, yellow oil. [α]²⁰_D - 82.4 (*c* 1.0, CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.41 (dd, *J* = 1.6, 5.6 Hz, 1H), 6.09 (dd, *J* = 2.0, 5.6 Hz, 1H), 5.16-5.15 (m, 1H), 2.50-2.43 (m, 1H), 2.34-2.33 (m, 2H), 2.11 (s, 3H), 1.60-1.52 (m, 1H) 1.43-1.31 (m, 7H), 0.92-0.88 (m, 3H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 207.1, 173.0, 156.2, 121.5, 84.7, 41.9, 35.9, 31.7, 31.7, 30.4, 26.7, 22.4, 13.9; HRMS (EI): exact mass calculated for M⁺ (C₁₃H₂₀O₃) requires m/z 224.1412, found m/z 224.1415; The enantiomeric excess was determined by HPLC. [AS-H column, 205nm, n-Hexane: EtOH = 8:1, 1.0mL/min]: 11.6min (minor), 15.7 min (major), ee 97%.

6w: 5-(2-oxodecan-4-yl)furan-2(5H)-one



The product was obtained in 78% yield, yellow oil. [α]²⁰_D - 81.0 (*c* 1.0, CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.41 (dd, *J* = 1.6, 5.6 Hz, 1H), 6.09 (dd, *J* = 2.0, 5.6 Hz, 1H), 5.16-5.15 (m, 1H), 2.48-2.43 (m, 1H), 2.34-2.33 (m, 2H), 2.11 (s, 3H), 1.61-1.52 (m, 1H) 1.42-1.3129 (m, 9H), 0.91-0.88 (m, 3H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 207.2, 173.0, 156.2, 121.5, 84.7, 41.9, 35.9, 31.8, 31.6, 30.4, 29.2, 27.0, 22.5, 14.0; HRMS (EI): exact mass calculated for M⁺ (C₁₄H₂₂O₃) requires m/z 238.1569, found m/z 238.1572; The enantiomeric excess was determined by HPLC. [AS-H column, 205nm, n-Hexane: EtOH = 8:1, 1.0 mL/min]: 10.1min (minor), 13.8 min (major), ee 97%.

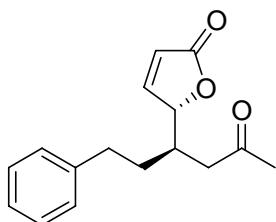
6x: 5-(4-oxooctan-2-yl)furan-2(5H)-one



The product was obtained in 65% yield, yellow oil. [α]²⁰_D - 85.6 (*c* 1.0, CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.45 (dd, *J* = 1.6, 5.6 Hz, 1H), 6.12 (dd, *J* = 2.0, 5.6 Hz, 1H), 4.99-4.98 (m, 1H), 2.53-2.47 (m, 2H) 2.39-2.30 (m, 3H) 1.58-1.50 (m, 2H), 1.33-1.26 (m, 2H), 1.11-1.10 (m, 3H), 0.93-0.89 (t, 3H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 209.3, 172.8, 155.4, 121.9, 86.5, 43.6, 43.1, 31.9, 25.8, 22.2, 16.8, 13.8; HRMS(EI): exact mass calculated for M⁺ (C₁₂H₁₈O₃) requires m/z 210.1256, found m/z 210.1257; The enantiomeric excess was determined by HPLC. [IC column,205nm, n-Hexane: EtOH = 4:1, 1.0 mL/min]:

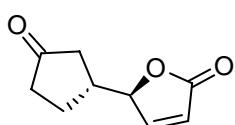
14.5 min (major), 15.7 min (minor), ee 99%.

6y: 5-(5-oxo-1-phenylhexan-3-yl)furan-2(5H)-one



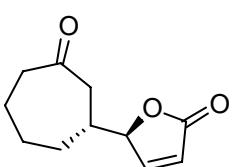
The product was obtained in 76% yield, yellow oil. $[\alpha]^{20}_D$ - 57.8 (*c* 1.0, CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.39 (dd, *J* = 1.2, 5.6 Hz, 1H), 7.33-7.30 (m, 2H), 7.24-7.19 (m, 3H), 6.10 (dd, *J* = 2.0, 6.0 Hz, 1H), 5.20-5.19 (m, 1H), 2.79-2.66 (m, 2H), 2.59-2.52 (m, 1H), 2.38-2.37 (m, 2H), 2.10 (s, 3H), 1.97-1.87 (m, 1H), 1.82-1.73 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 206.9, 173.0, 156.1, 141.1, 128.6, 128.3, 126.2, 121.7, 84.6, 41.8, 35.5, 33.5, 33.4, 30.4; HRMS (EI): exact mass calculated for M^+ ($\text{C}_{16}\text{H}_{18}\text{O}_3$) requires m/z 258.1256, found m/z 258.1255; The enantiomeric excess was determined by HPLC. [AY-H column, 220nm, n-Hexane: EtOH = 1:1, 0.60 mL/min]: 14.2min (minor), 15.4 min (major), ee 97%.

7a: 5-(3-oxocyclopentyl)furan-2(5H)-one



The product was obtained in 51% yield, yellow oil. $[\alpha]^{20}_D$ - 75.3 (*c* 1.0, CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.50-7.46 (m, 1H), 6.18-6.16 (m, 1H), 5.08-5.07 (m, 1H), 2.55-2.49 (m, 1H), 2.38-2.29 (m, 2H), 2.22-2.15 (m, 2H), 1.98-1.91 (m, 2H), 1.76-1.66 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 216.4, 172.5, 154.7, 122.6, 122.6, 122.4, 84.9, 84.6, 40.4, 39.4, 39.2, 37.8, 37.7, 25.4, 24.1; HRMS (EI): exact mass calculated for M^+ ($\text{C}_9\text{H}_{10}\text{O}_3$) requires m/z 166.0630, found m/z 166.0632; The enantiomeric excess was determined by HPLC. [IC column, 205nm, n-Hexane: EtOH = 1:1, 1.0 mL/min]: 19.2min (major), 21.2 min (minor), ee 97%.

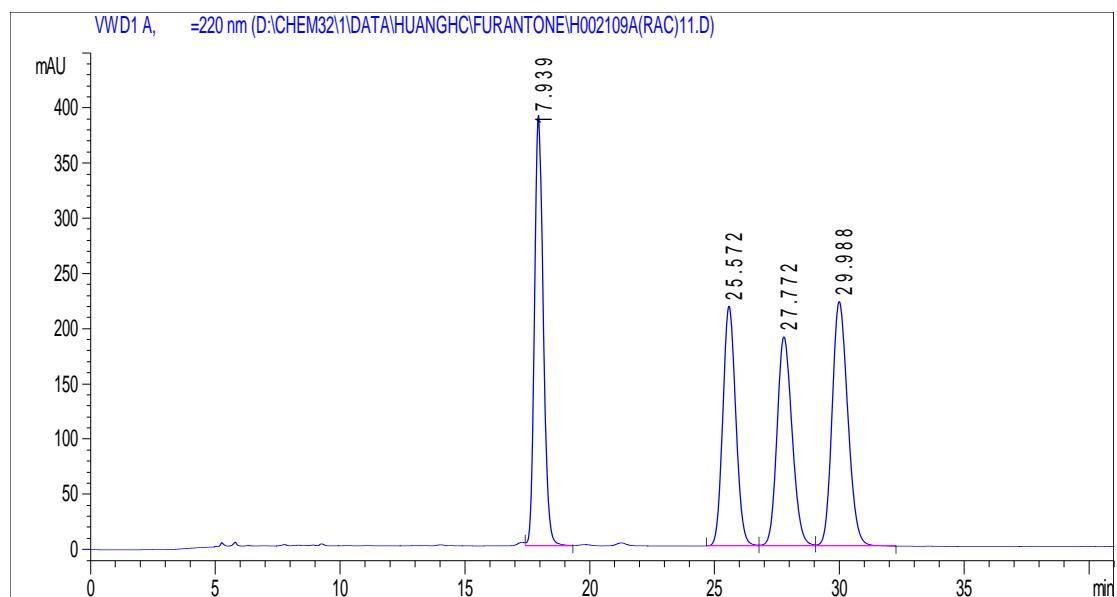
7b: 5-(3-oxocycloheptyl)furan-2(5H)-one



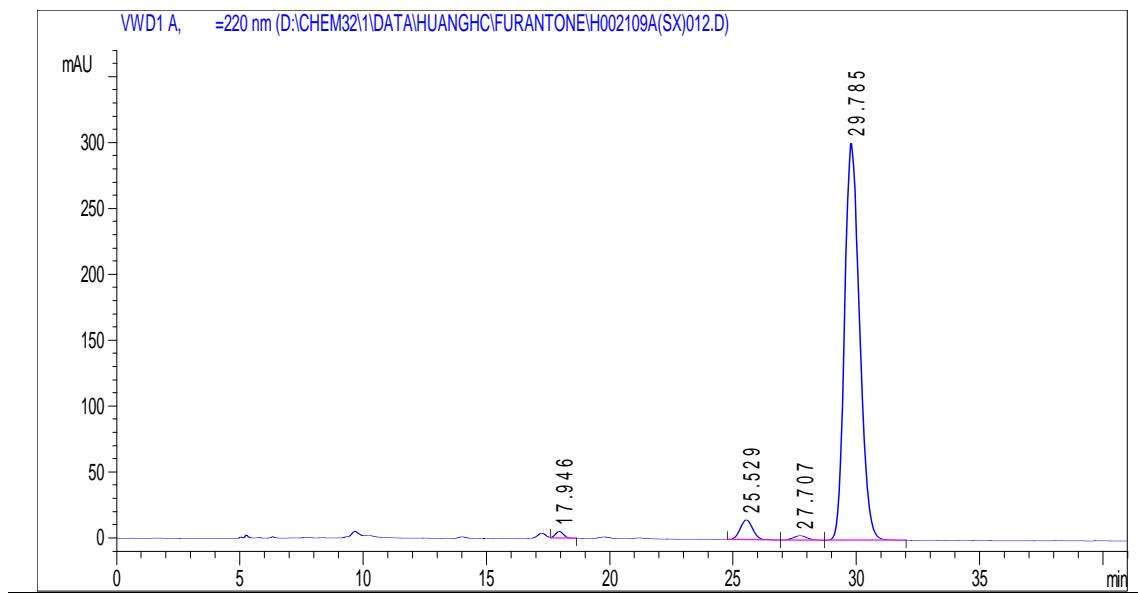
The product was obtained in 67% yield, yellow oil. $[\alpha]^{20}_D$ - 69.9 (*c* 1.0, CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.48-7.45 (m, 1H), 6.148-6.16 (m, 1H), 5.06-5.07 (m, 1H), 2.51-2.49 (m, 1H), 2.40-2.26 (m, 3H), 2.22-2.10 (m, 4H), 1.95-1.88 (m, 2H), 1.70-1.65 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 216.5, 216.4, 172.6, 154.7, 122.5, 122.4, 84.9, 84.7, 40.4, 39.3, 39.2, 37.8, 37.7, 25.4, 24.1; HRMS (EI): exact mass calculated for M^+ ($\text{C}_{11}\text{H}_{14}\text{O}_3$) requires m/z 194.0943, found m/z 194.0946; The enantiomeric excess was determined by HPLC. [IC column, 205nm, n-Hexane: EtOH = 1:1, 1.0 mL/min]: 22.7min (major), 25.6 min (minor), ee 97%.

E: HPLC Charts of Michael Addition Products

6a: 5-(3-oxo-1-phenylbutyl)furan-2(5H)-one

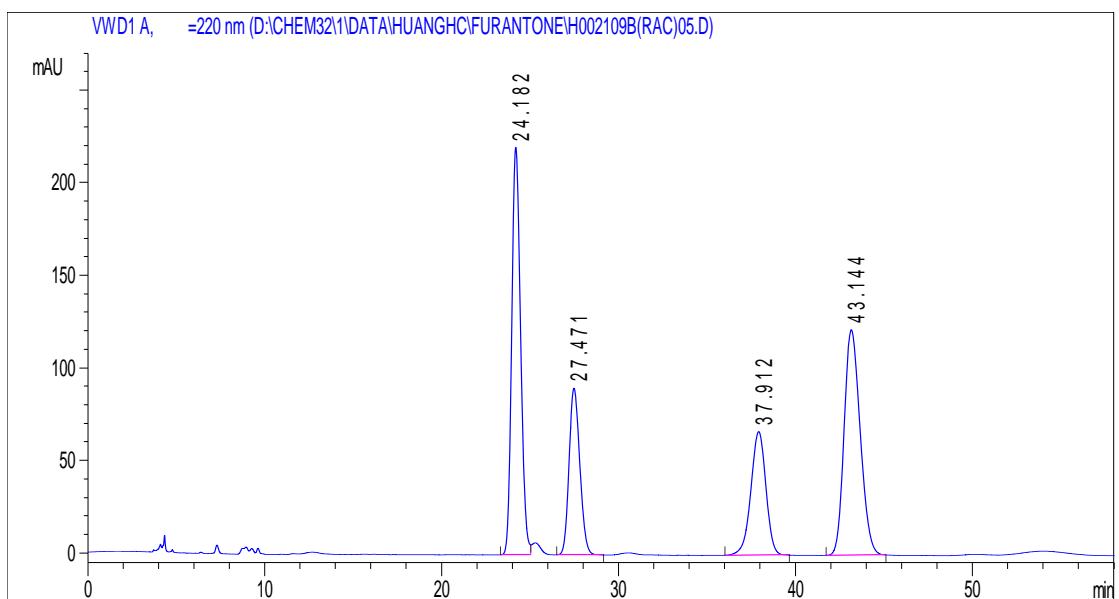


#	Time	Area	Height	Width	Symmetry	Area %
1	17.939	9578.3	390.1	0.3796	0.787	27.323
2	25.572	7837.6	217.3	0.5607	0.874	22.358
3	27.772	7977.3	189.6	0.6539	0.805	22.756
4	29.988	9662.2	221.6	0.6805	0.787	27.563

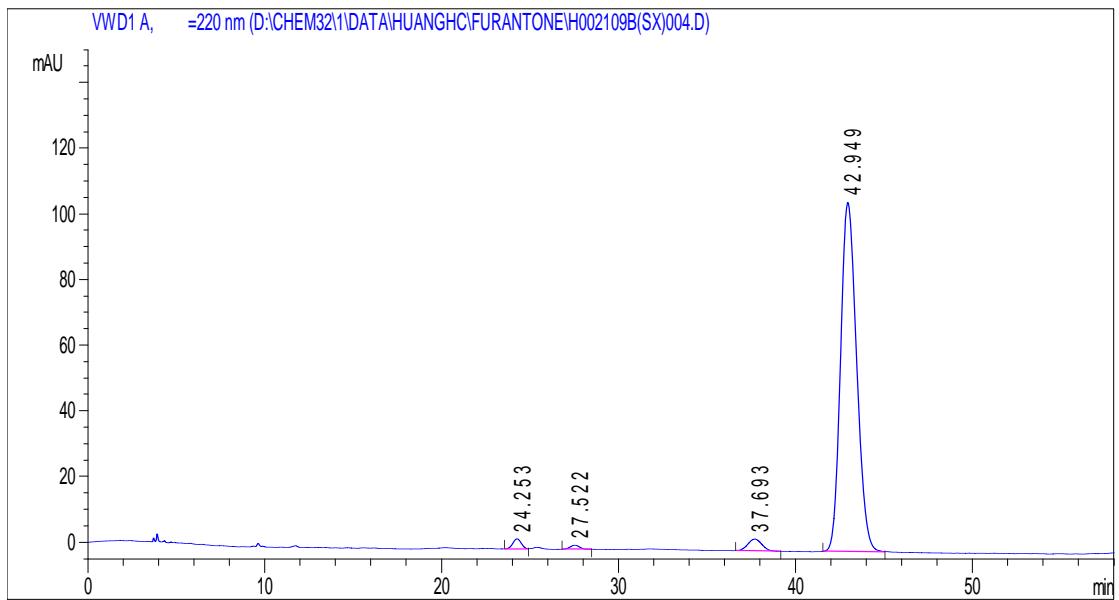


#	Time	Area	Height	Width	Symmetry	Area %
1	17.946	131.3	5.3	0.3802	0.917	0.966
2	25.529	535.3	15.1	0.5499	0.916	3.937
3	27.707	133.3	3.4	0.6251	0.894	0.980
4	29.785	12796	301.3	0.6586	0.759	94.117

6b: 5-(1-(2-fluorophenyl)-3-oxobutyl)furan-2(5H)-one

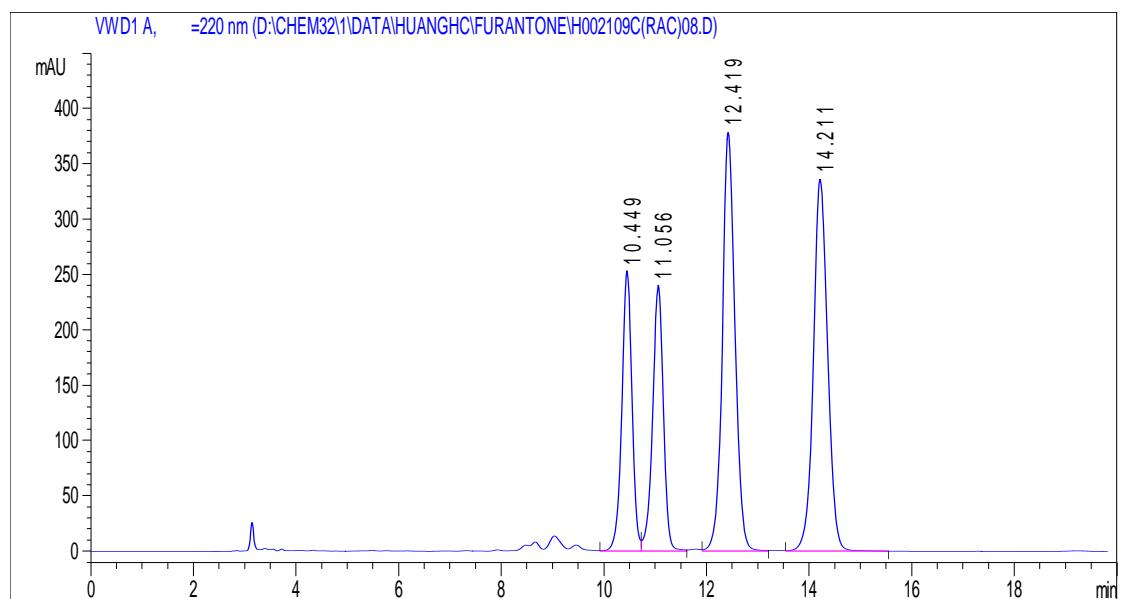


#	Time	Area	Height	Width	Symmetry	Area %
1	24.182	7669.4	220.2	0.5404	0.807	33.165
2	27.471	3803.1	90.1	0.6583	0.804	16.446
3	37.912	3957.5	66.8	0.915	1.067	17.114
4	43.144	7695	121.9	0.9871	0.768	33.276

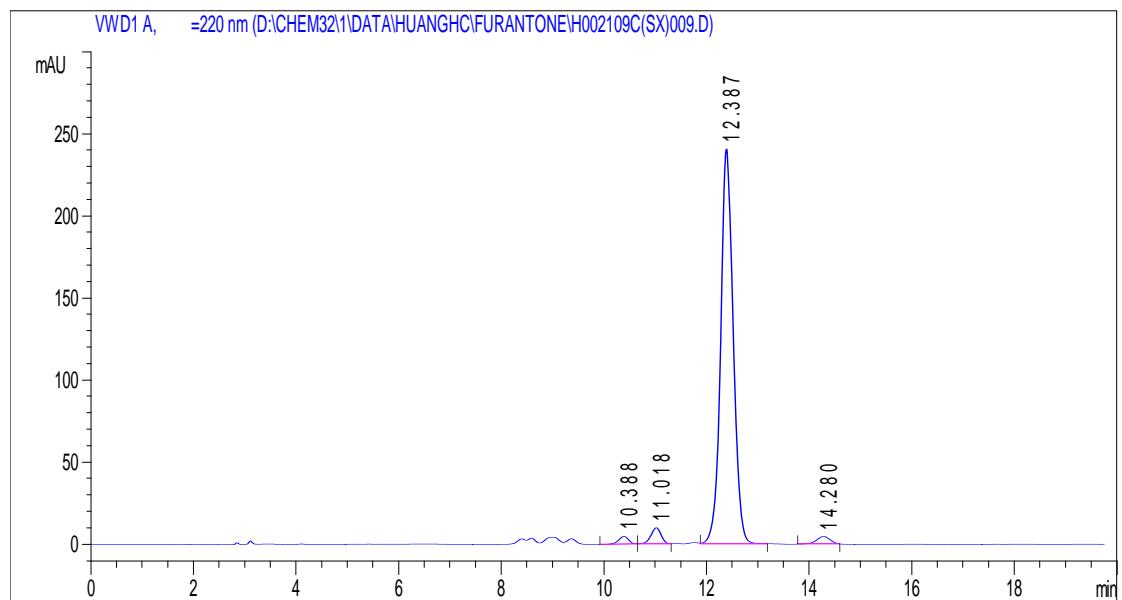


#	Time	Area	Height	Width	Symmetry	Area %
1	24.253	105.4	3.1	0.5317	0.96	1.491
2	27.522	48.5	1.3	0.5631	0.939	0.686
3	37.693	200.3	3.6	0.8183	0.958	2.833
4	42.949	6716.2	106.3	0.9843	0.788	94.990

6c: 5-(1-(3-fluorophenyl)-3-oxobutyl)furan-2(5H)-one

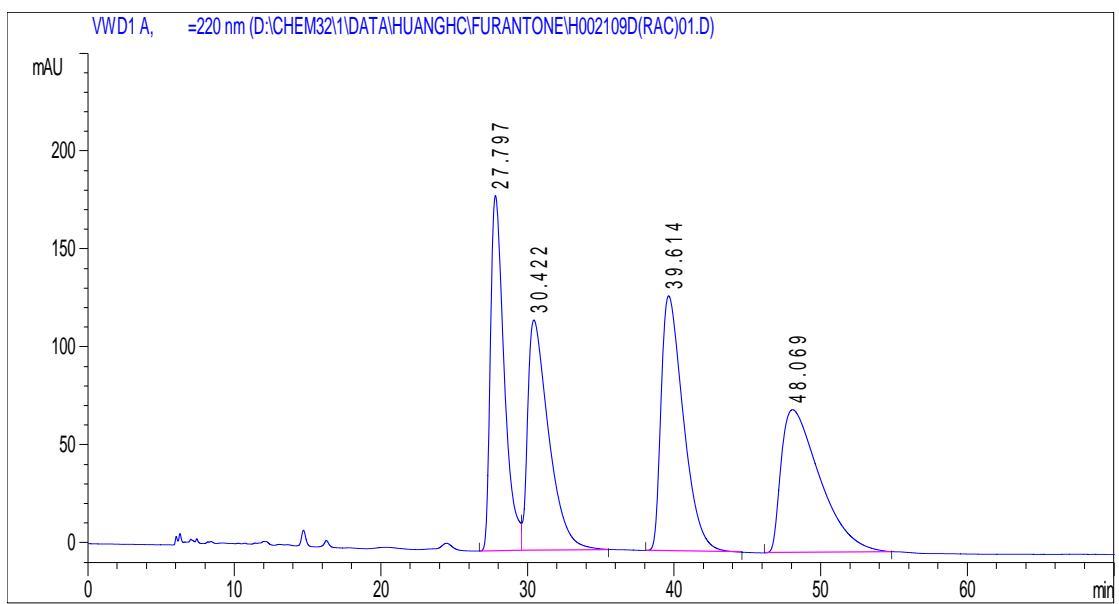


#	Time	Area	Height	Width	Symmetry	Area %
1	10.449	3502.8	253.4	0.2137	1.038	17.523
2	11.056	3505.4	240.4	0.2226	1.058	17.536
3	12.419	6481.1	378.4	0.261	0.833	32.422
4	14.211	6500.7	336.2	0.2955	0.87	32.520

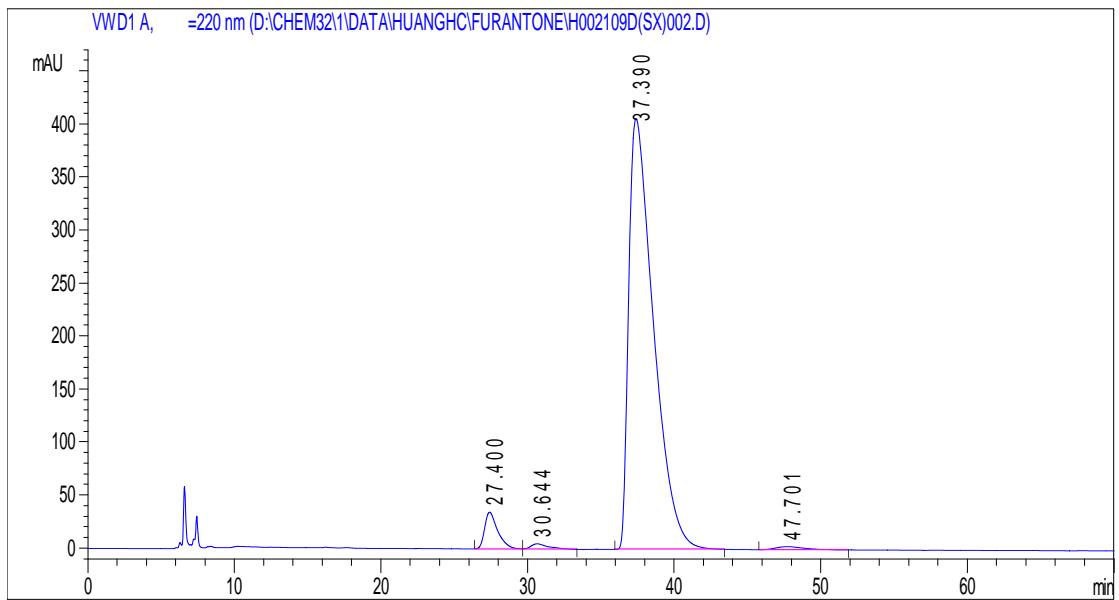


#	Time	Area	Height	Width	Symmetry	Area %
1	10.388	68.6	4.9	0.2141	1.082	1.559
2	11.018	144.8	10.1	0.2201	1.103	3.291
3	12.387	4102.2	240.6	0.2571	0.848	93.206
4	14.28	85.6	4.6	0.309	1.097	1.944

6d: 5-(1-(4-fluorophenyl)-3-oxobutyl)furan-2(5H)-one

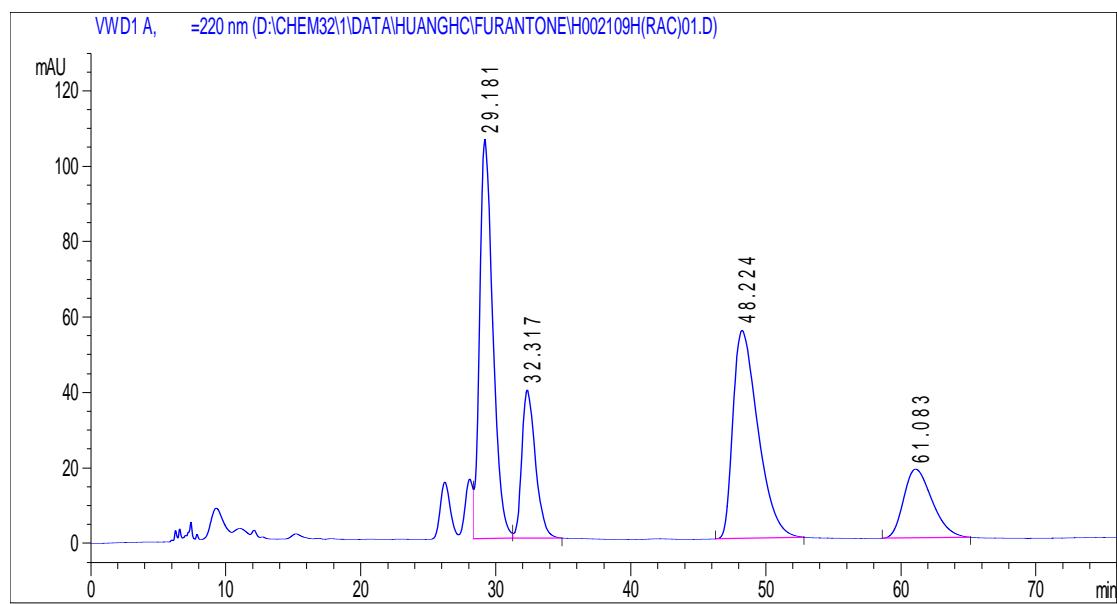


#	Time	Area	Height	Width	Symmetry	Area %
1	27.797	11874.1	181.5	0.9992	0.522	23.353
2	30.422	11781	117.7	1.4936	0.391	23.170
3	39.614	13761.8	130.3	1.6225	0.473	27.066
4	48.069	13428.6	73	2.7156	0.391	26.411

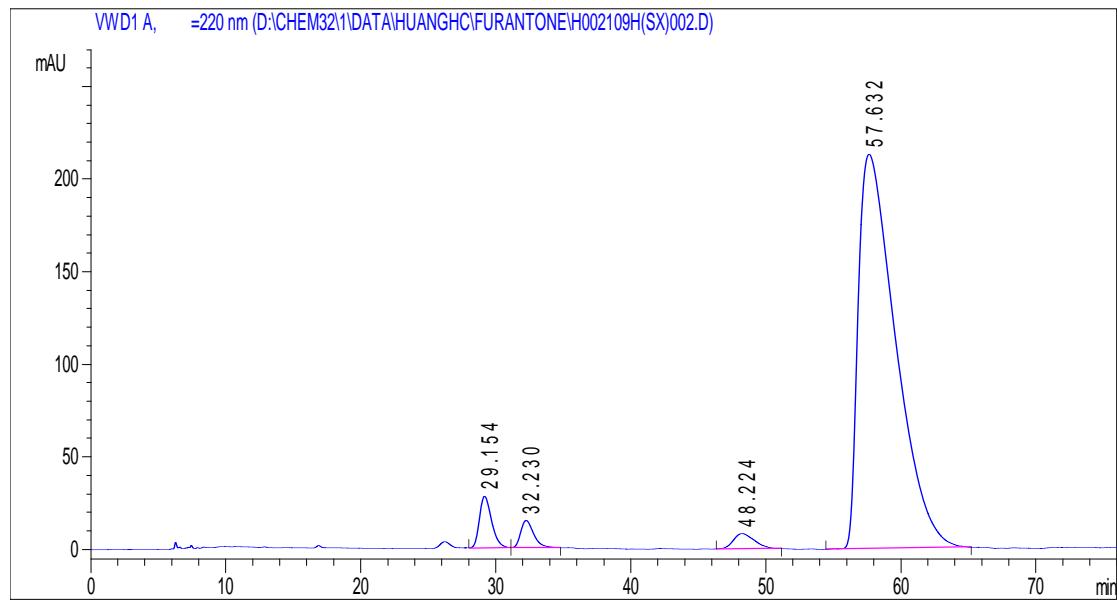


#	Time	Area	Height	Width	Symmetry	Area %
1	27.4	2162.5	34.8	0.9203	0.566	4.265
2	30.644	437	5.1	1.2081	0.484	0.862
3	37.39	47698.7	406.2	1.7601	0.388	94.067
4	47.701	408.7	3	1.6095	0.629	0.806

6e: 5-(1-(2-chlorophenyl)-3-oxobutyl)furan-2(5H)-one

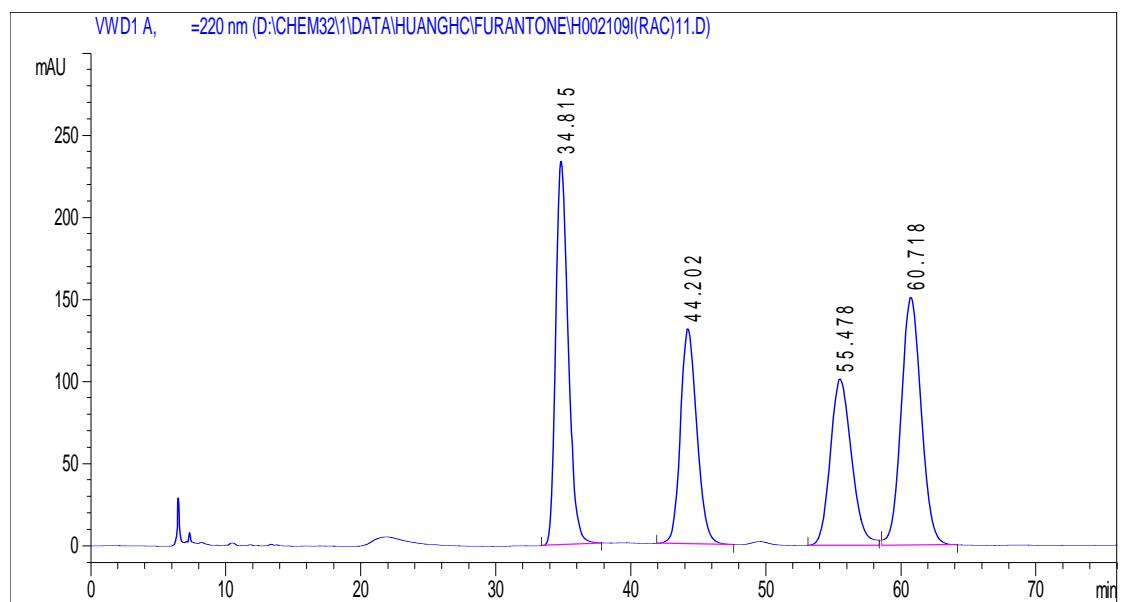


#	Time	Area	Height	Width	Symmetry	Area %
1	29.181	7264.1	106	1.0589	0.63	36.553
2	32.317	2787.8	39.4	1.0879	0.641	14.028
3	48.224	7113.1	55.2	1.9381	0.537	35.793
4	61.083	2708	18.3	2.1311	0.696	13.626

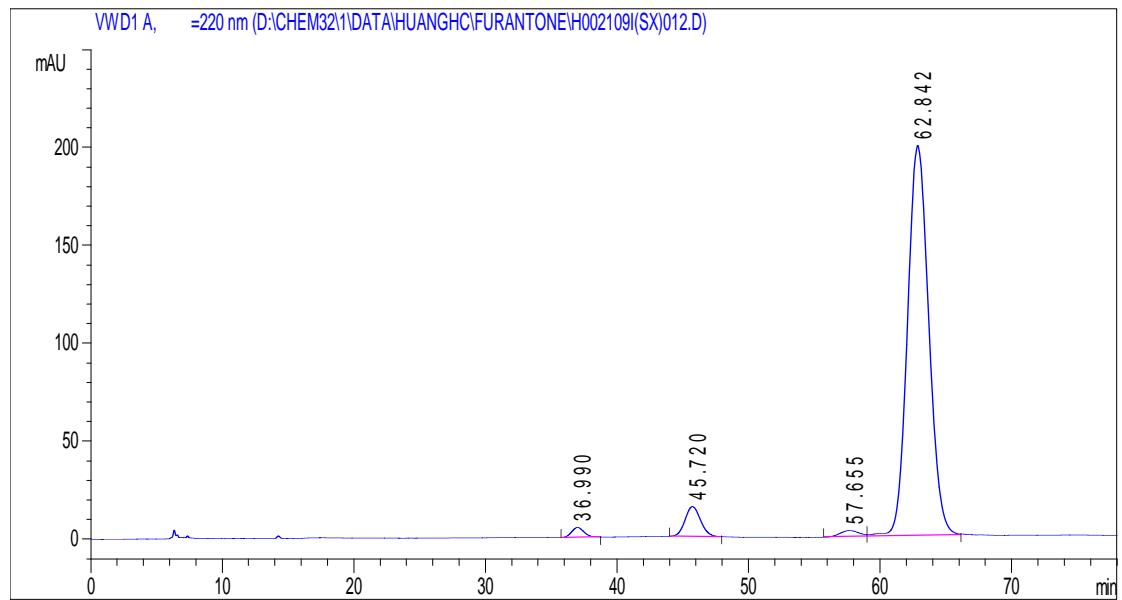


#	Time	Area	Height	Width	Symmetry	Area %
1	29.154	1777.8	28	0.9784	0.694	3.986
2	32.23	1012.4	14.9	1.015	0.677	2.270
3	48.224	914.7	8.3	1.5672	0.675	2.051
4	57.632	40893.7	213.2	2.8553	0.381	91.693

6f: 5-(1-(3-chlorophenyl)-3-oxobutyl)furan-2(5H)-one

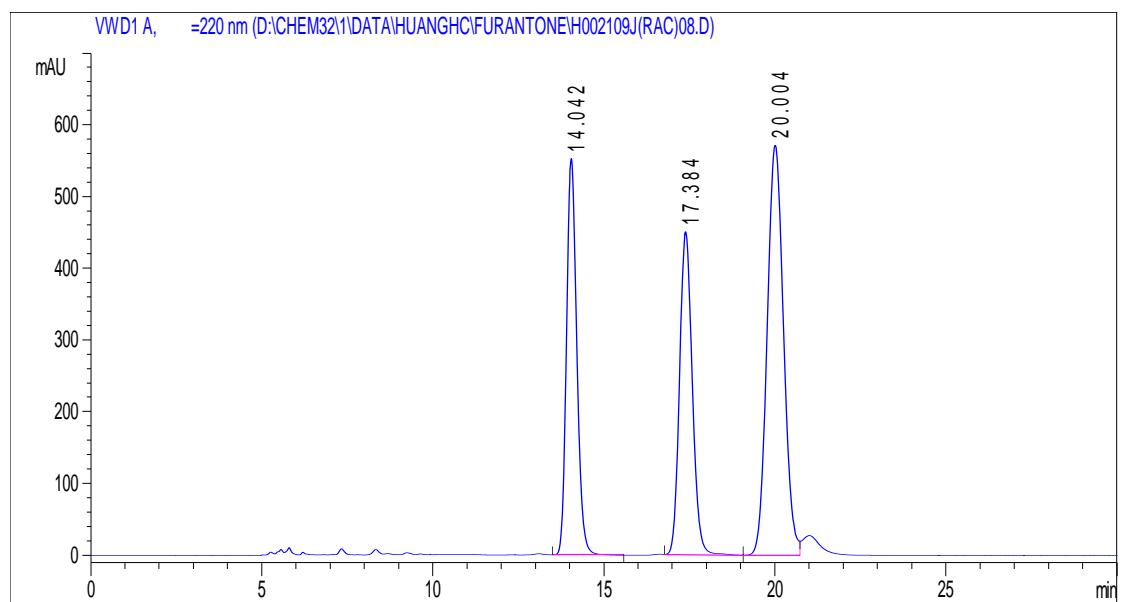


#	Time	Area	Height	Width	Symmetry	Area %
1	34.815	15033.7	233.6	0.9897	0.705	28.472
2	44.202	11099.4	131.1	1.3077	0.779	21.021
3	55.478	11089.7	101.4	1.5585	0.797	21.03
4	60.718	15578.6	150.9	1.5916	0.894	29.504

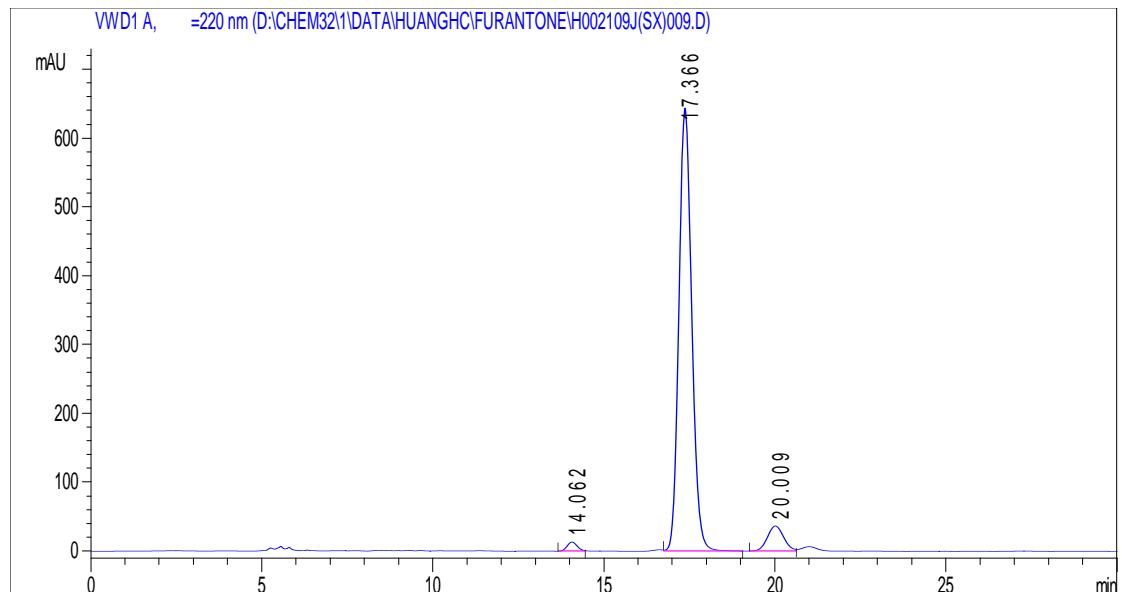


#	Time	Area	Height	Width	Symmetry	Area %
1	36.99	329	5	0.9838	0.875	1.355
2	45.72	1270.7	15.4	1.242	0.887	5.234
3	57.655	325.9	3.2	1.2231	0.958	1.342
4	62.842	22351.6	199.1	1.7405	0.894	92.068

6g: 5-(1-(3-bromophenyl)-3-oxobutyl)furan-2(5H)-one

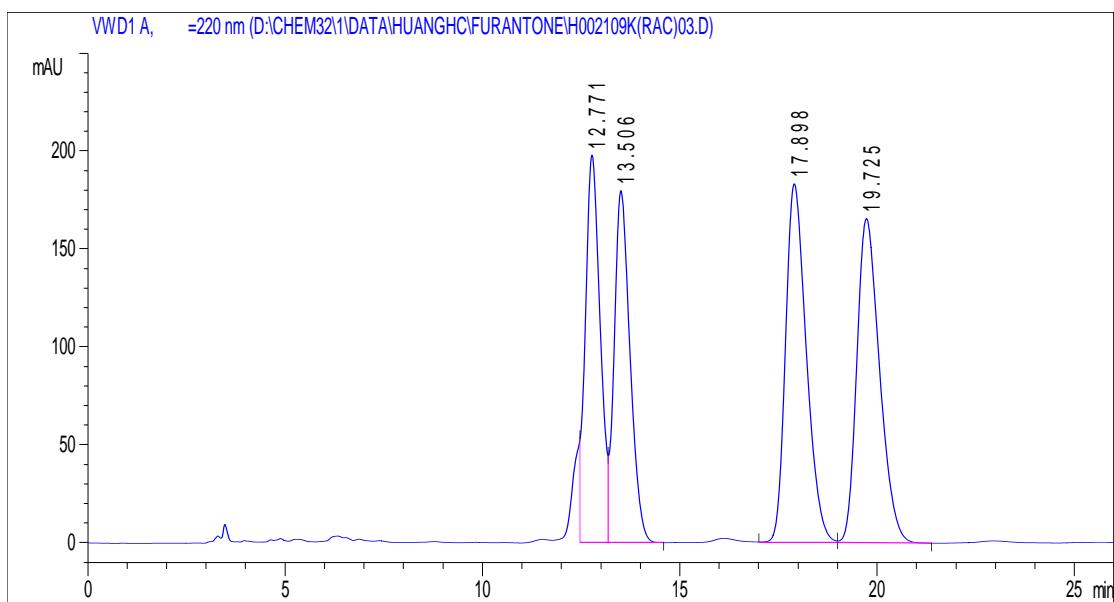


#	Time	Area	Height	Width	Symmetry	Area %
1	14.042	11548.2	553.1	0.3222	0.809	27.313
2	17.384	11722.4	451.3	0.402	0.848	27.725
3	20.004	19010.5	571.8	0.516	0.912	44.962

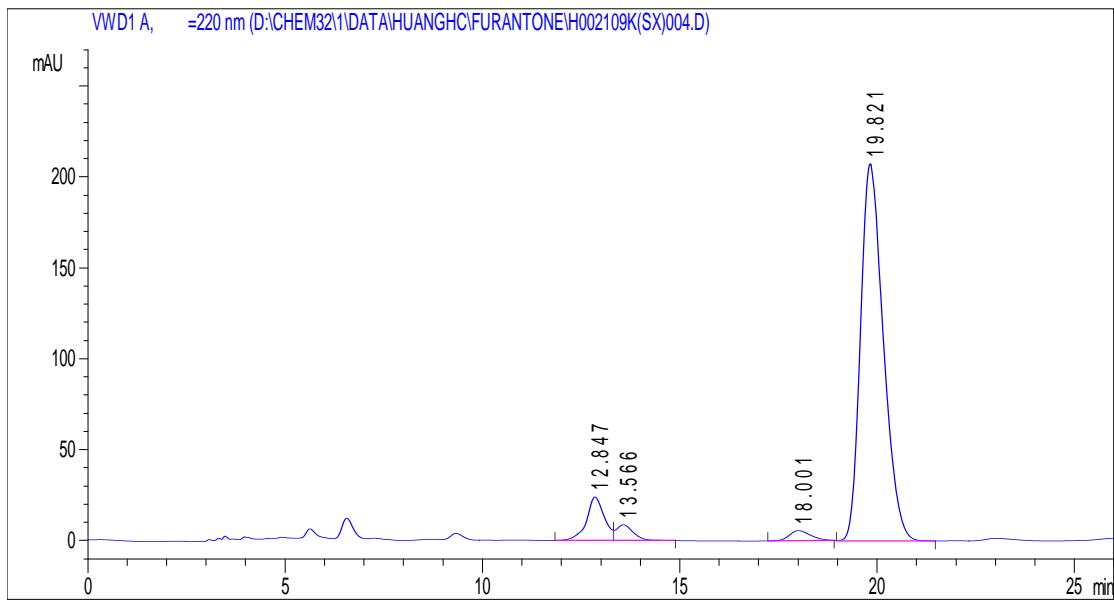


#	Time	Area	Height	Width	Symmetry	Area %
1	14.062	265.8	13.2	0.3363	0.927	1.453
2	17.366	16806.9	644.1	0.4063	0.843	91.873
3	20.009	1221	36.6	0.52	0.924	6.674

6h: 5-(1-(4-bromophenyl)-3-oxobutyl)furan-2(5H)-one

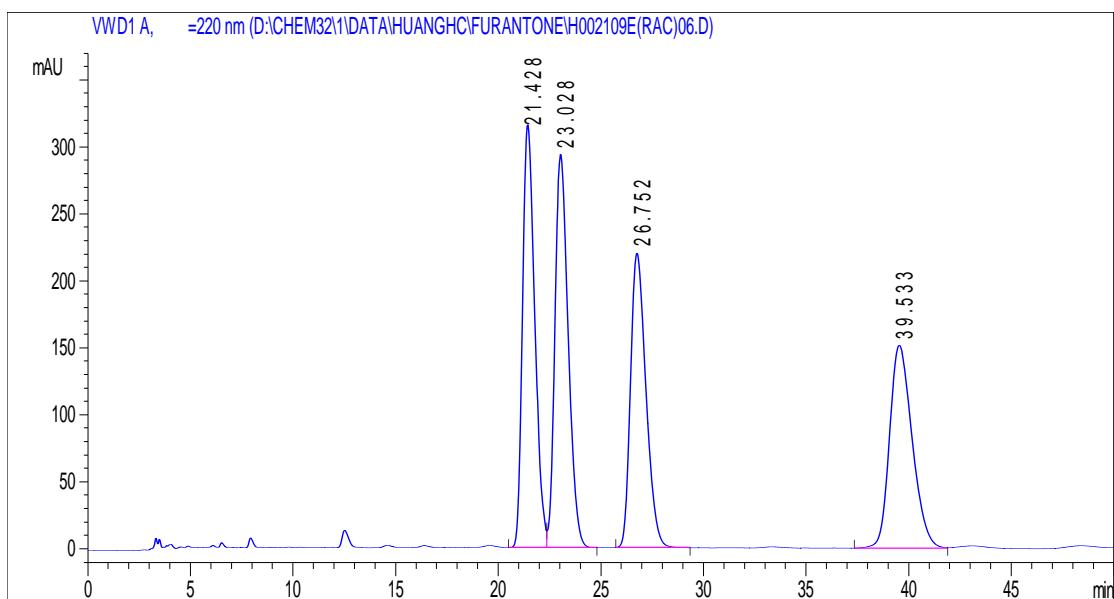


#	Time	Area	Height	Width	Symmetry	Area %
1	12.771	5173.9	198	0.4355	0.775	21.970
2	13.506	5027.4	179.8	0.4223	0.71	21.348
3	17.898	6708.9	183.4	0.5579	0.693	28.489
4	19.725	6639.3	165.8	0.6158	0.696	28.193

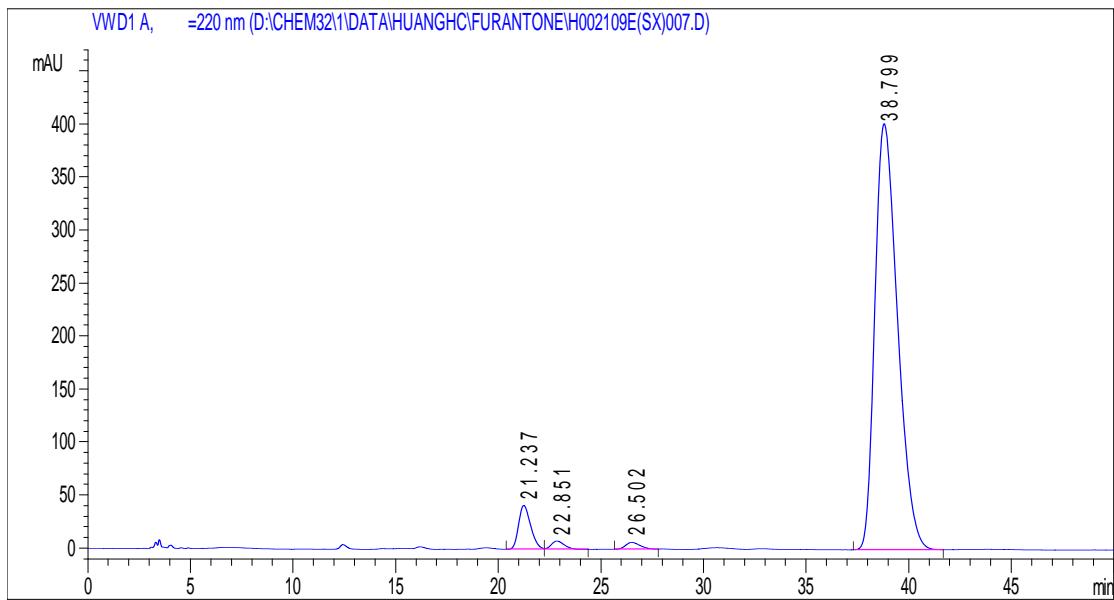


#	Time	Area	Height	Width	Symmetry	Area %
1	12.847	753.8	24	0.4619	0.915	7.888
2	13.566	265.8	8.7	0.4449	0.612	2.781
3	18.001	210.3	5.6	0.6294	0.741	2.201
4	19.821	8327.2	207.5	0.6168	0.701	87.131

6i: 5-(1-(2-methoxyphenyl)-3-oxobutyl)furan-2(5H)-one

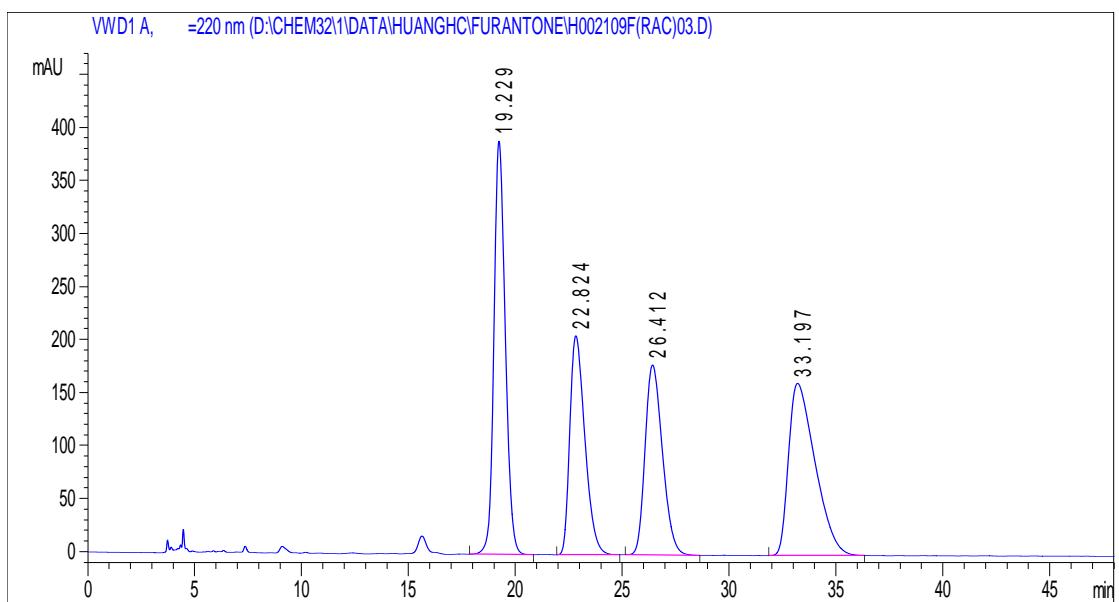


#	Time	Area	Height	Width	Symmetry	Area %
1	21.428	13098.7	315.7	0.6443	0.696	26.523
2	23.028	13199.3	293.6	0.6963	0.701	26.727
3	26.752	11477.4	219.7	0.8074	0.68	23.240
4	39.533	11610.7	151.5	1.1793	0.725	23.510

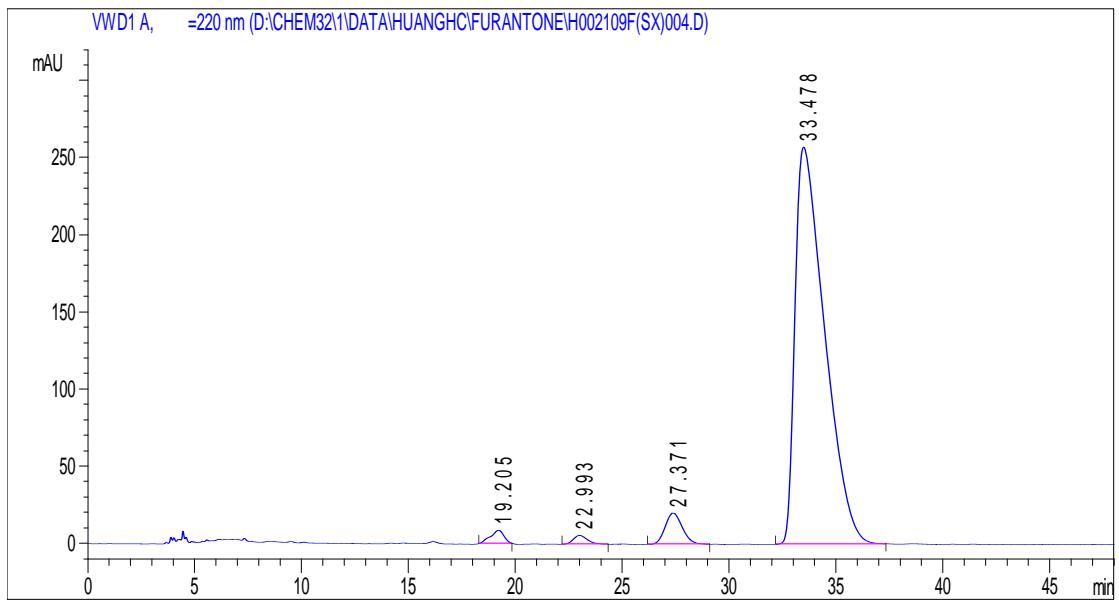


#	Time	Area	Height	Width	Symmetry	Area %
1	21.237	1699.7	41.4	0.6329	0.72	5.126
2	22.851	351.1	7.9	0.669	0.731	1.059
3	26.502	307.3	6.4	0.733	0.73	0.927
4	38.799	30800.7	401.8	1.1914	0.658	92.888

6j: 5-(1-(3-methoxyphenyl)-3-oxobutyl)furan-2(5H)-one

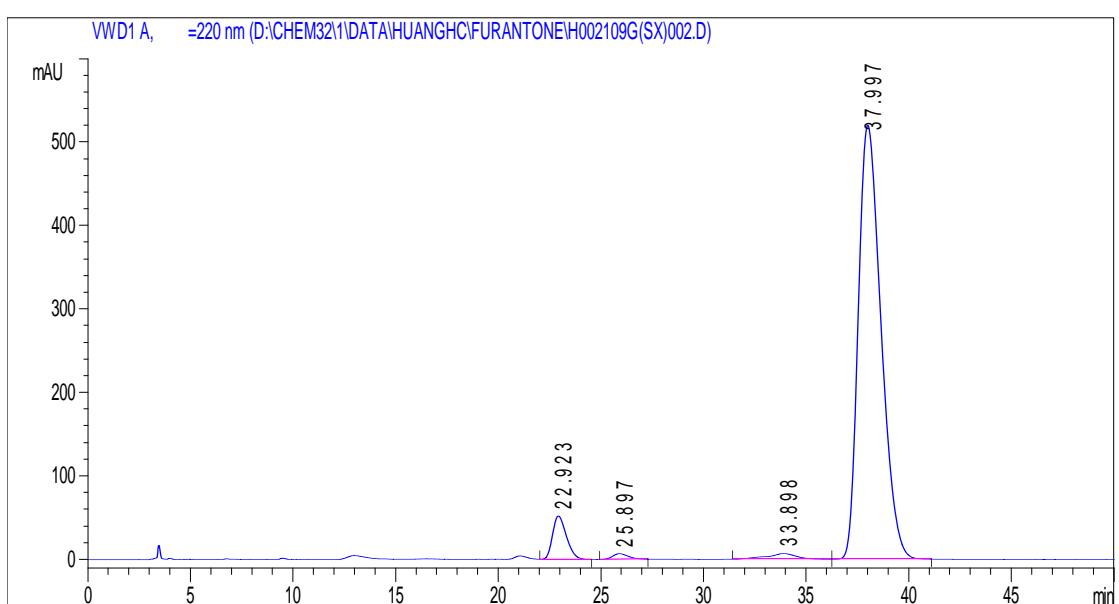
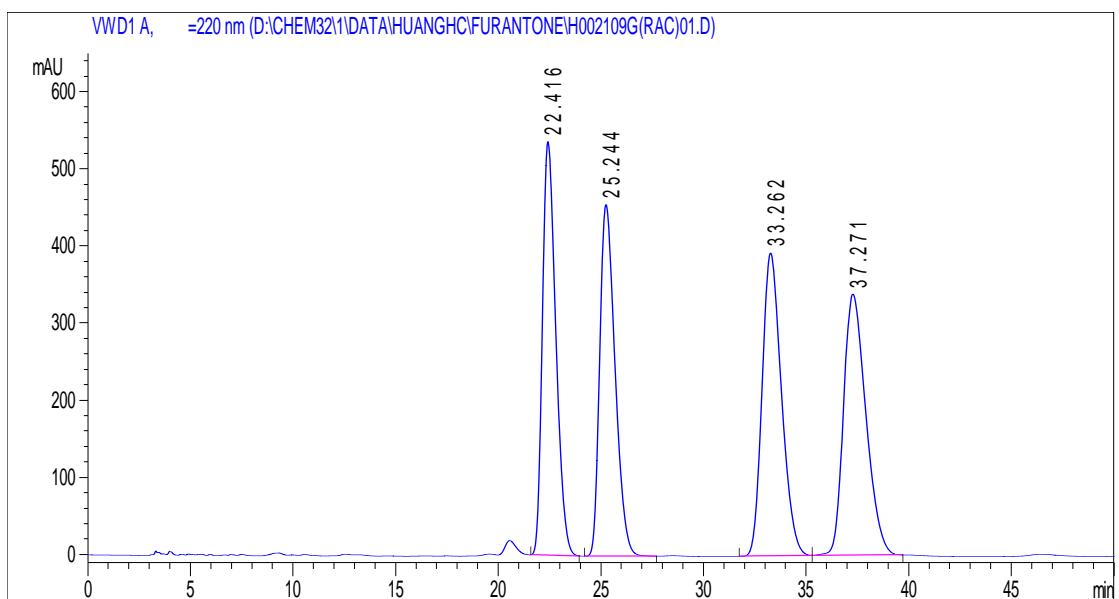


#	Time	Area	Height	Width	Symmetry	Area %
1	19.229	14344	389.7	0.5692	0.786	29.499
2	22.824	10132.5	206.7	0.7584	0.629	20.838
3	26.412	10157.2	179.4	0.8788	0.723	20.889
4	33.197	13991.5	162.4	1.3283	0.49	28.774

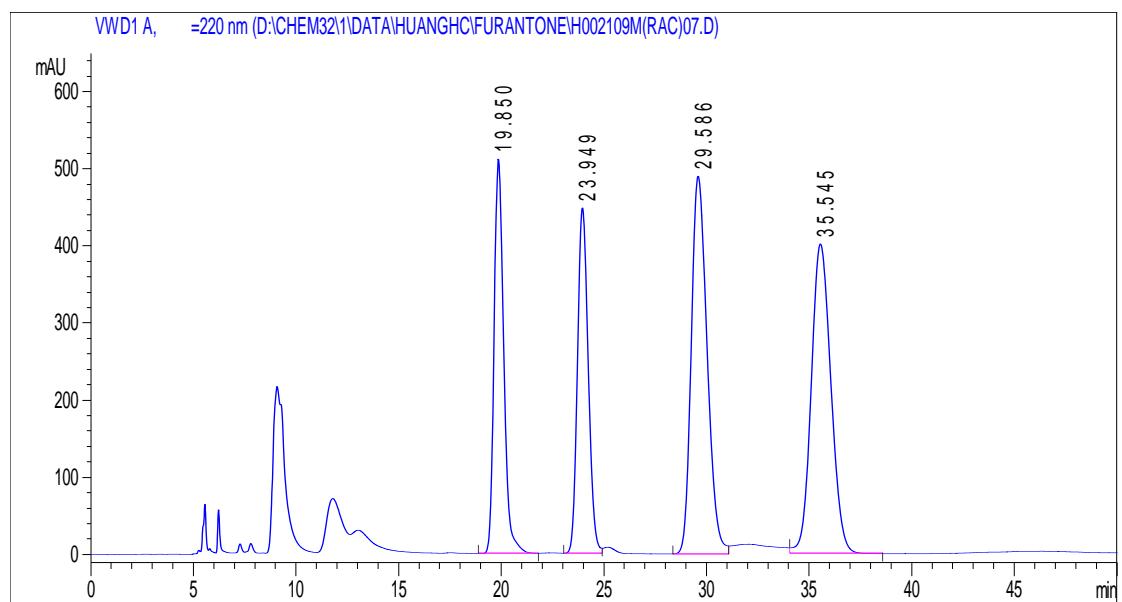


#	Time	Area	Height	Width	Symmetry	Area %
1	19.205	381.5	8.7	0.7319	1.427	1.438
2	22.993	263.5	5.8	0.697	0.747	0.993
3	27.371	1147.6	20.4	0.864	0.825	4.327
4	33.478	24731.2	257.4	1.45	0.385	93.242

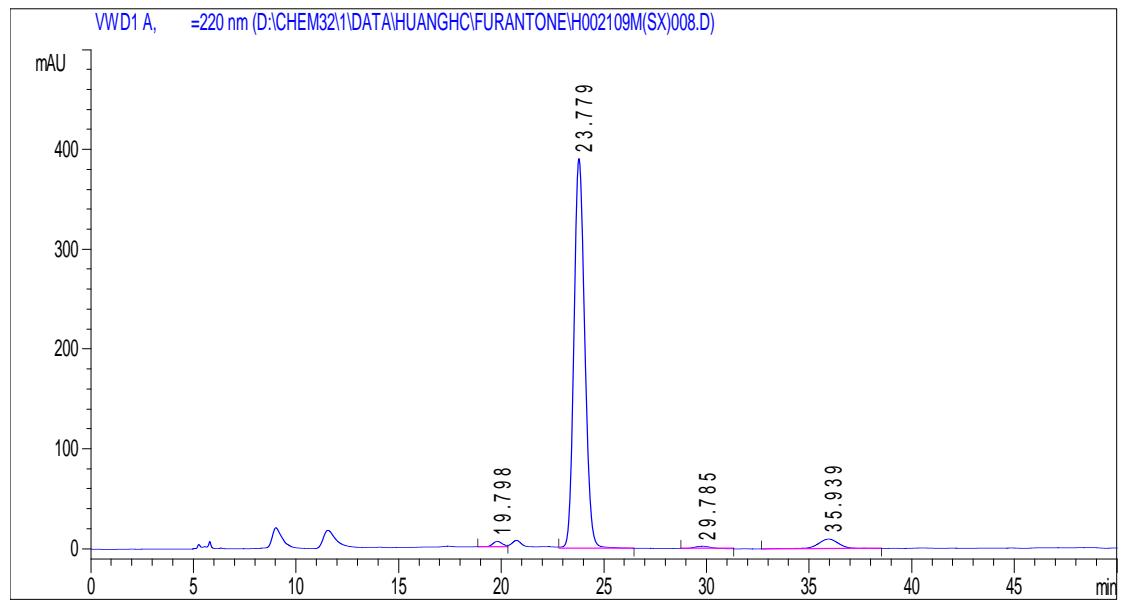
6k: 5-(1-(4-methoxyphenyl)-3-oxobutyl)furan-2(5H)-one



6l: 5-(3-oxo-1-*m*-tolylbutyl)furan-2(5H)-one

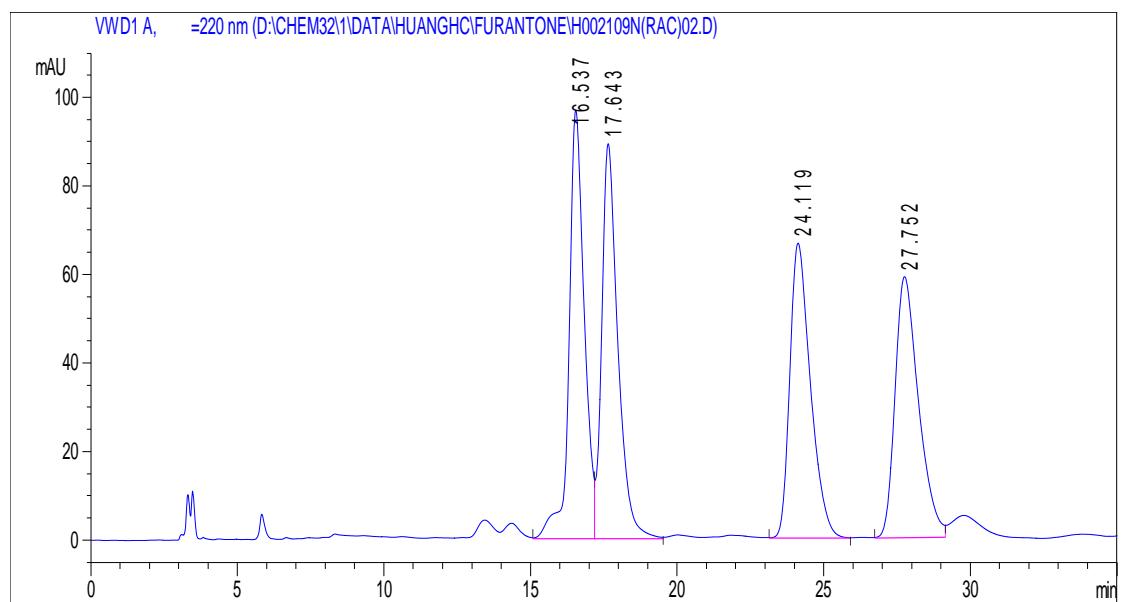


#	Time	Area	Height	Width	Symmetry	Area %
1	19.85	16788	511.5	0.5052	0.741	19.473
2	23.949	16384	448.5	0.5718	0.819	19.005
3	29.586	26245.7	489.6	0.8351	0.725	30.444
4	35.545	26792.3	401.7	1.0373	0.85	31.078

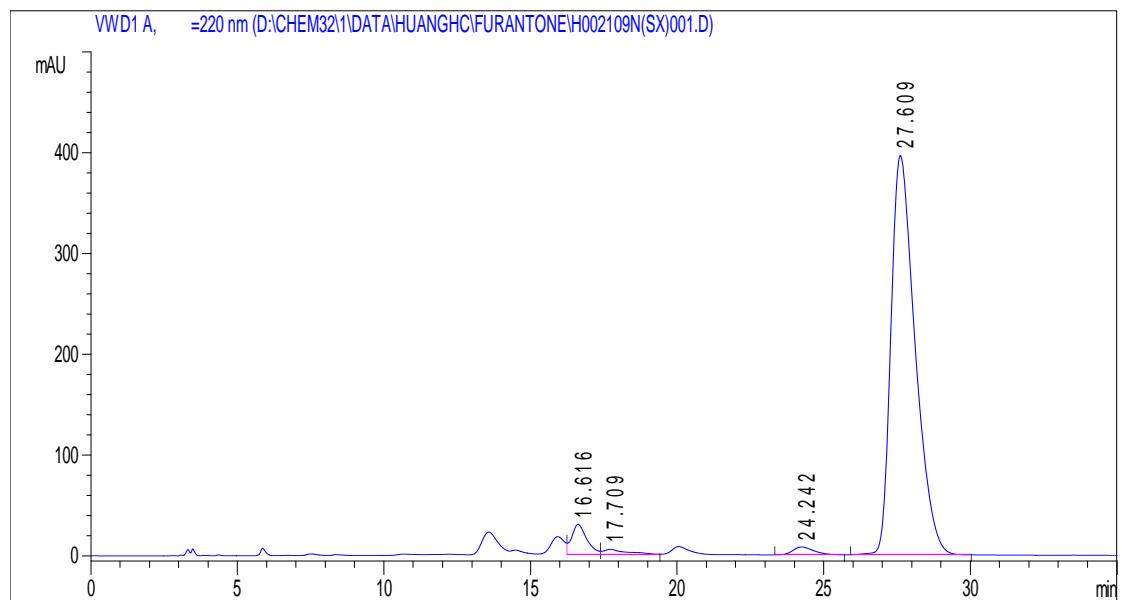


#	Time	Area	Height	Width	Symmetry	Area %
1	19.798	184.1	5.5	0.5617	0	1.196
2	23.779	14318.8	390.5	0.5705	0.826	93.064
3	29.785	139.3	2.5	0.7514	0.818	0.906
4	35.939	743.8	9.7	1.1239	1.021	4.834

6m: 5-(3-oxo-1-p-tolylbutyl)furan-2(5H)-one

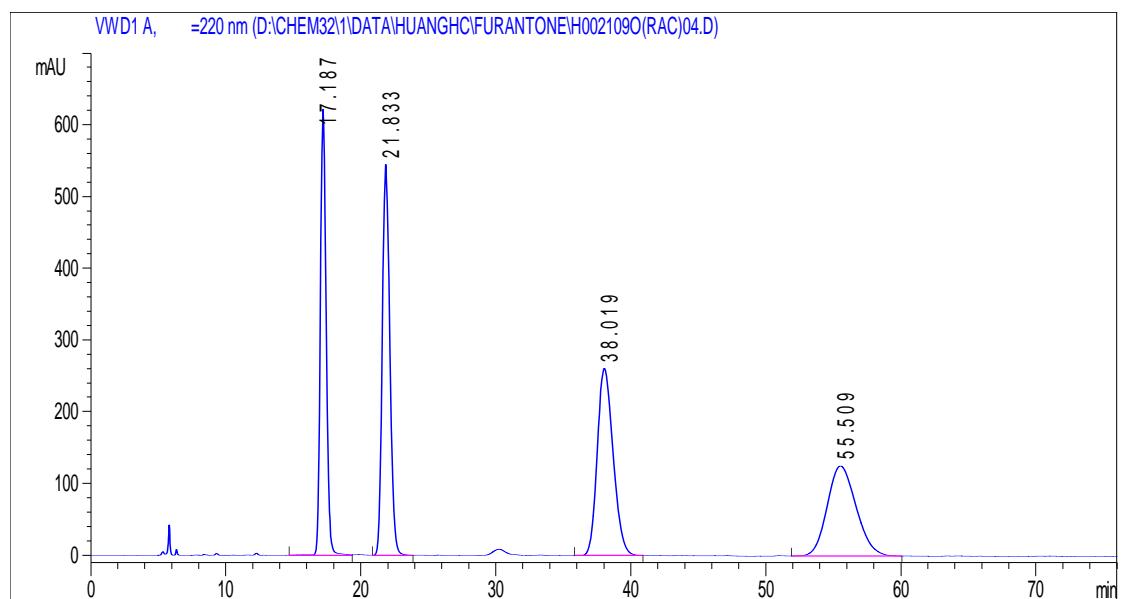


#	Time	Area	Height	Width	Symmetry	Area %
1	16.537	3510.6	96.9	0.5362	0.813	26.074
2	17.643	3397.9	89.3	0.5633	0.613	25.237
3	24.119	3265	66.7	0.7369	0.63	24.250
4	27.752	3290.7	59.1	0.8365	0.639	24.440

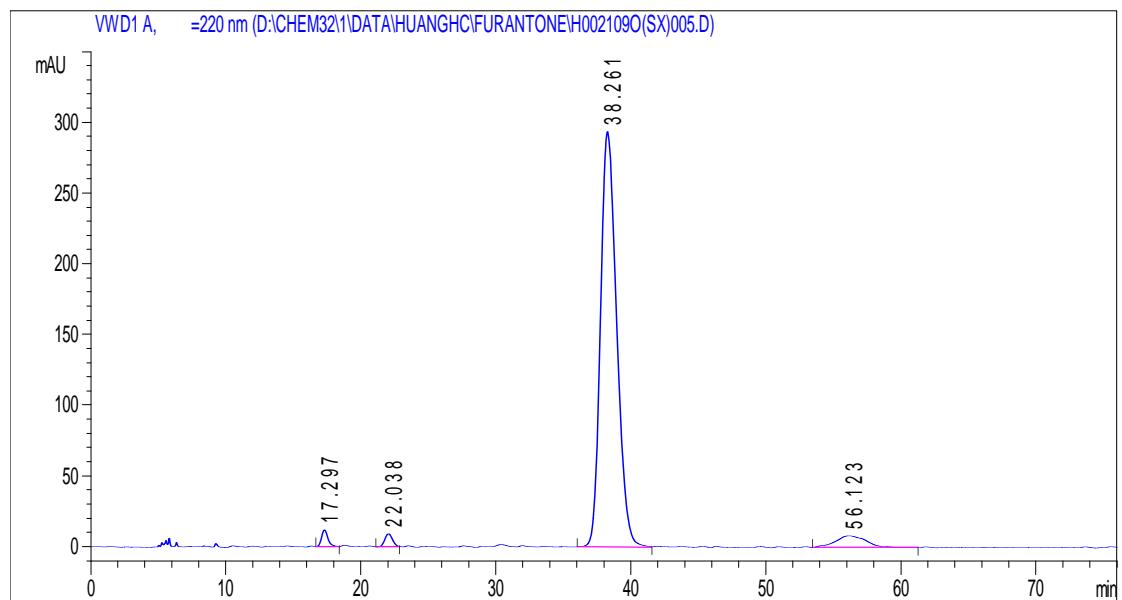


#	Time	Area	Height	Width	Symmetry	Area %
1	16.616	1110.9	30.5	0.5302	0.684	4.529
2	17.709	336	5.5	0.81	0.312	1.370
3	24.242	393.8	7.9	0.7484	0.683	1.605
4	27.609	22688.1	396.2	0.8662	0.6	92.496

6n: 5-(1-(2,3-dimethoxyphenyl)-3-oxobutyl)furan-2(5H)-one

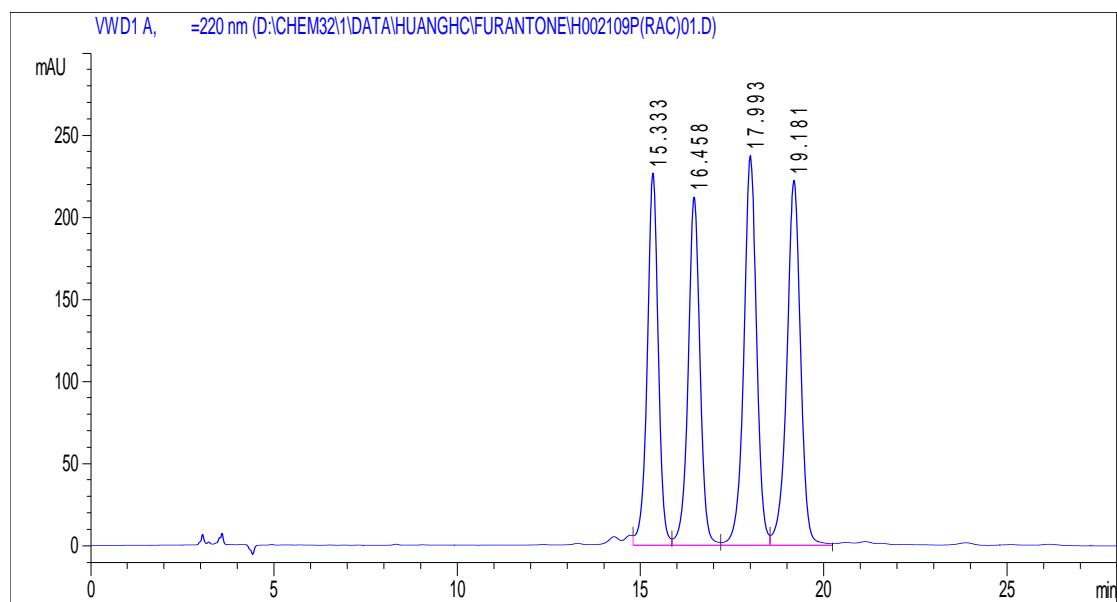


#	Time	Area	Height	Width	Symmetry	Area %
1	17.187	18712.3	622.3	0.4673	0.811	23.326
2	21.833	21308.3	545.2	0.6074	0.809	26.562
3	38.019	21353.7	261.5	1.2671	0.759	26.618
4	55.509	18847.7	126	2.2896	0.818	23.494

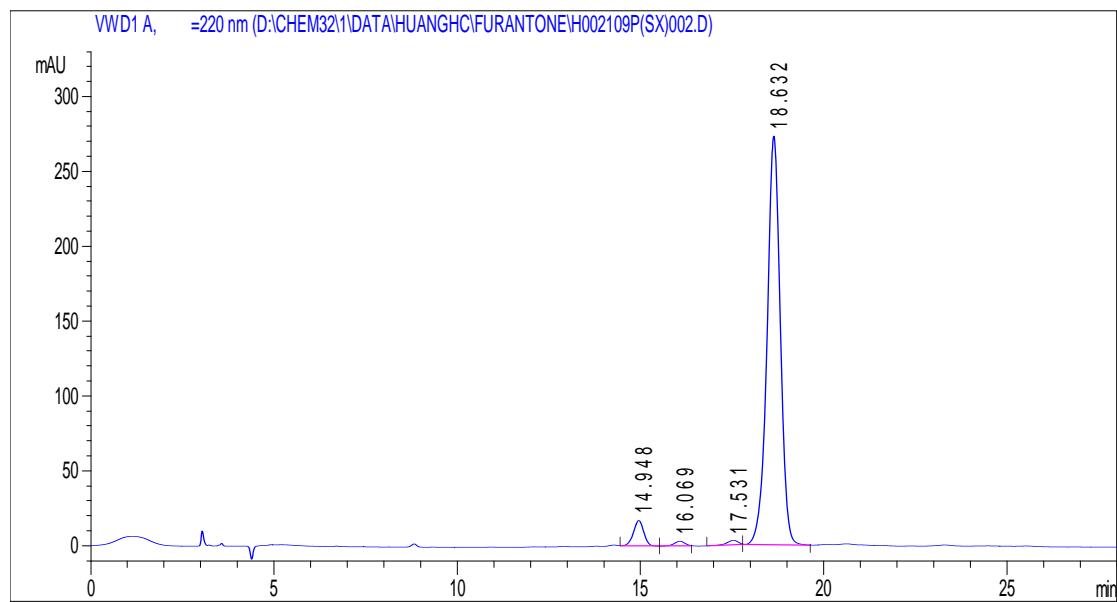


#	Time	Area	Height	Width	Symmetry	Area %
1	17.297	419.6	12.2	0.5216	0.756	1.581
2	22.038	364.7	9.2	0.6604	0.893	1.374
3	38.261	24404.8	293.8	1.2835	0.736	91.945
4	56.123	1353.7	8.3	2.2202	0.749	5.100

6o: 5-(1-(2,4-dimethoxyphenyl)-3-oxobutyl)furan-2(5H)-one

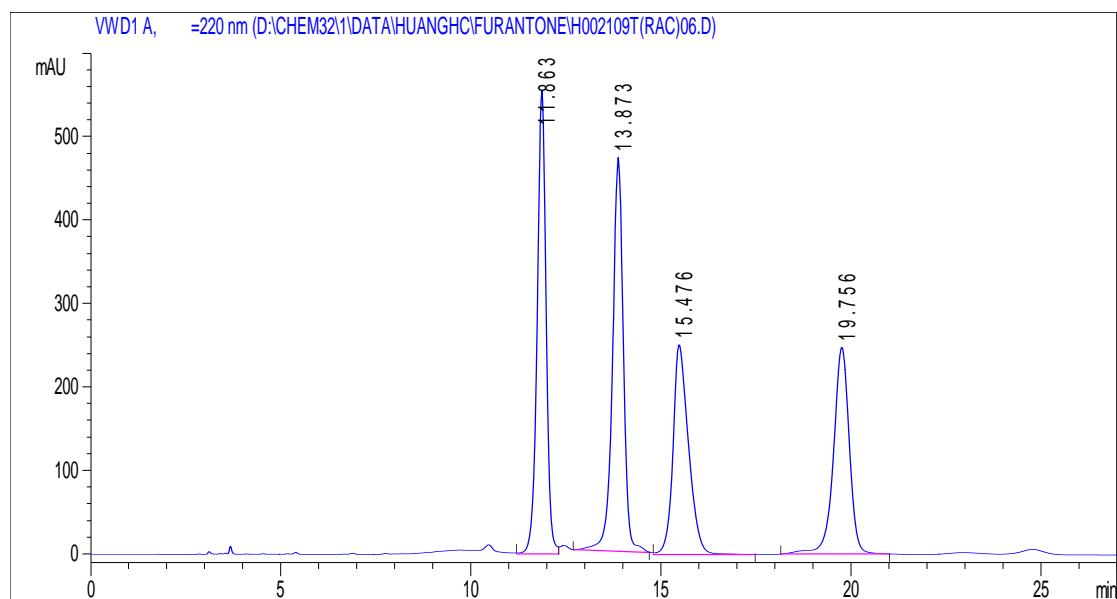


#	Time	Area	Height	Width	Symmetry	Area %
1	15.333	4719.3	226.7	0.3157	1.021	22.462
2	16.458	4758.8	212.1	0.3404	0.984	22.650
3	17.993	5743	237.4	0.3666	1.027	27.335
4	19.181	5788.7	222.3	0.3941	1.036	27.552

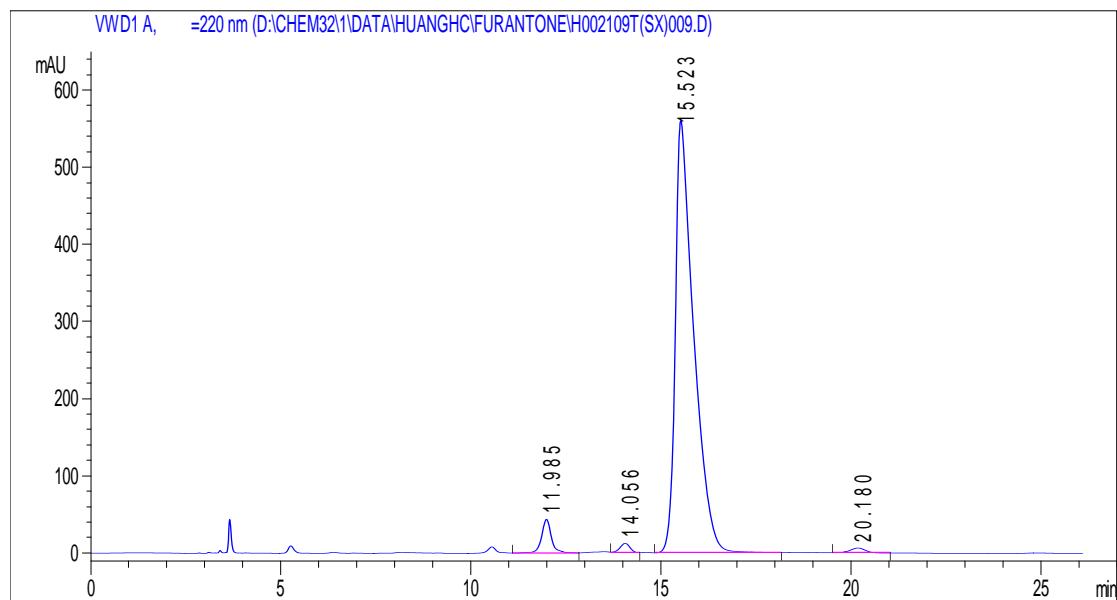


#	Time	Area	Height	Width	Symmetry	Area %
1	14.948	342.5	17.2	0.3324	1.027	4.668
2	16.069	76.7	3.4	0.373	1.067	1.045
3	17.531	72.1	3.2	0.3773	1.438	0.982
4	18.632	6847	273	0.418	0	93.305

6p: 5-(1-(naphthalen-2-yl)-3-oxobutyl)furan-2(5H)-one

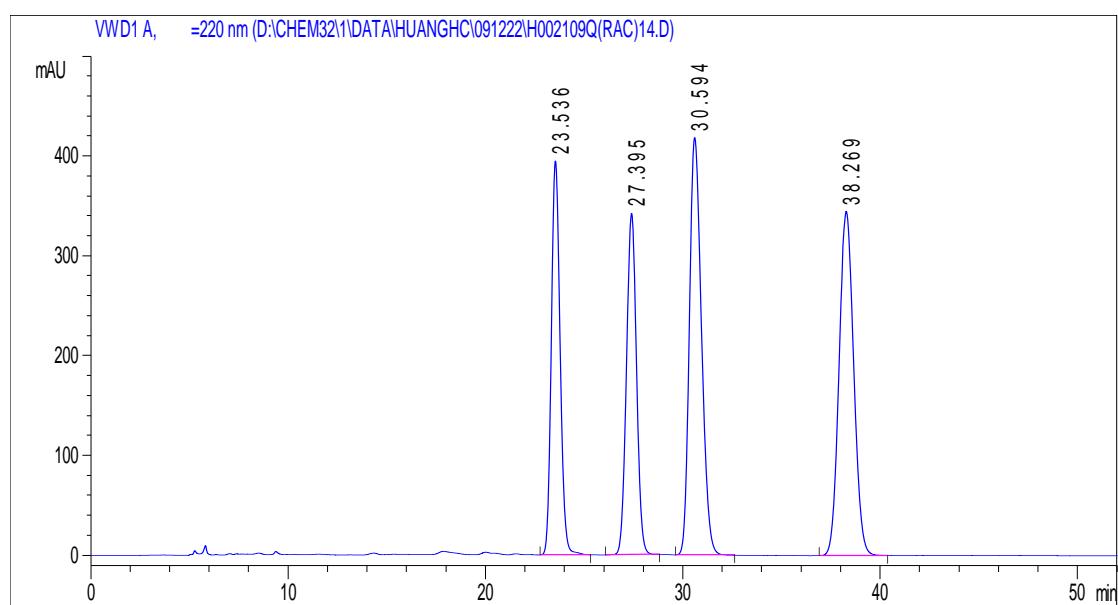


#	Time	Area	Height	Width	Symmetry	Area %
1	11.863	9083.3	555.3	0.2462	1.053	27.717
2	13.873	9387.4	472.4	0.3312	1.067	28.645
3	15.476	7135.8	251.4	0.4214	0.632	21.774
4	19.756	7165.3	247.7	0.4822	1.109	21.864

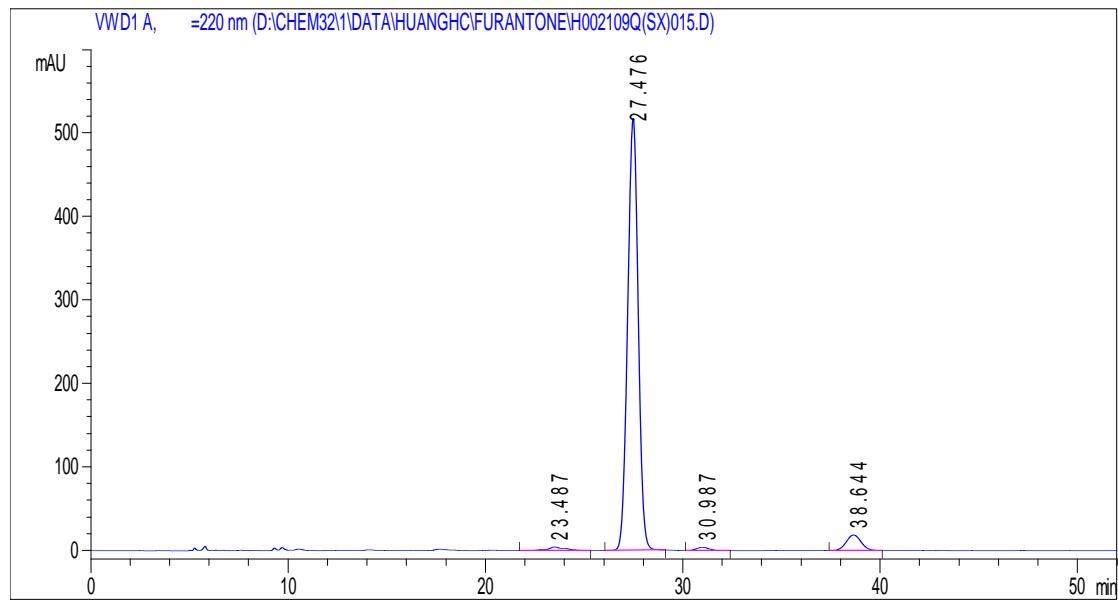


#	Time	Area	Height	Width	Symmetry	Area %
1	11.985	809.3	44	0.2729	0.967	4.047
2	14.056	236.9	12.4	0.2919	1.097	1.184
3	15.523	18783.3	560.3	0.4756	0.411	93.930
4	20.18	167.6	6.2	0.4155	1.077	0.838

6q: 5-(1-(furan-2-yl)-3-oxobutyl)furan-2(5H)-one

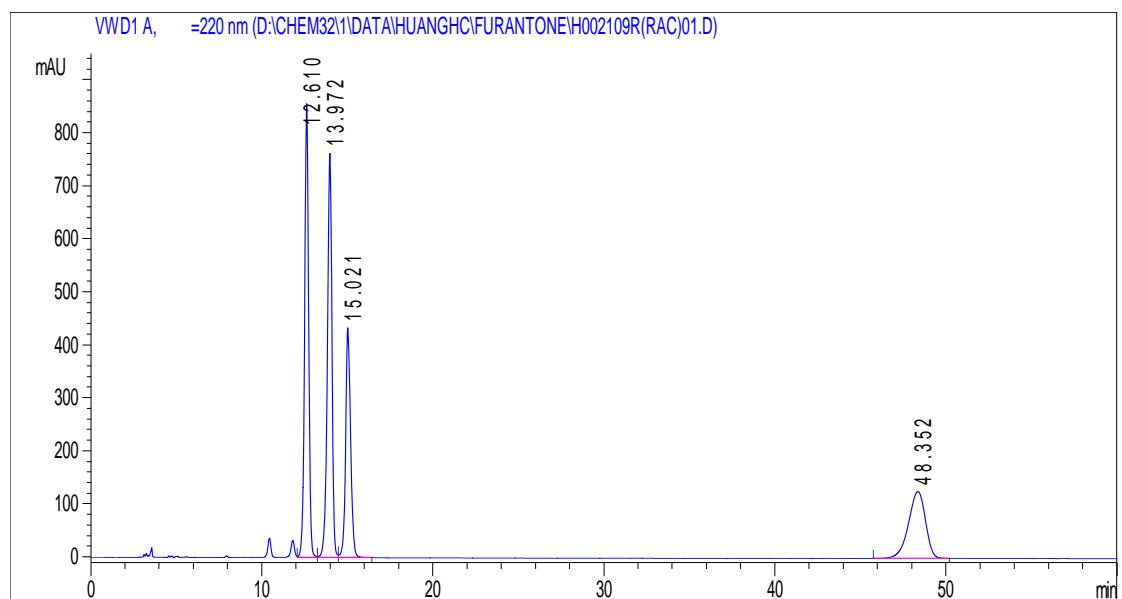


#	Time	Area	Height	Width	Symmetry	Area %
1	23.536	12151	394.7	0.4786	0.828	20.330
2	27.395	12104.6	342.1	0.5526	0.988	20.253
3	30.594	17736.7	418.2	0.6608	0.741	29.676
4	38.269	17775.2	345	0.8049	0.905	29.741

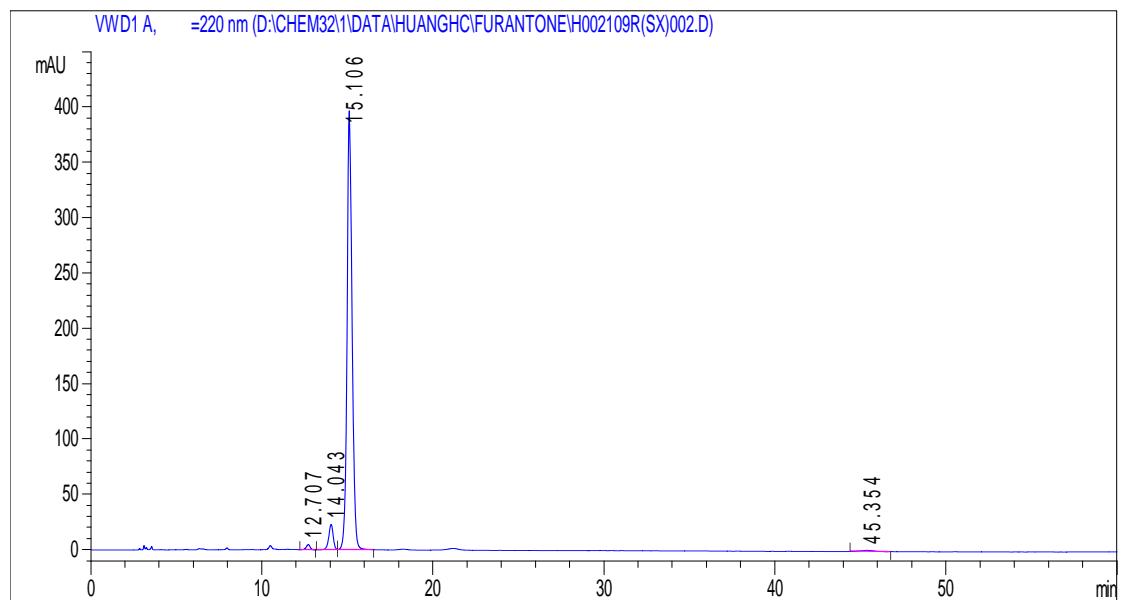


#	Time	Area	Height	Width	Symmetry	Area %
1	23.487	270.1	4.3	0.8347	0.749	1.310
2	27.476	19196.3	517.5	0.5783	1.039	93.099
3	30.987	174.8	3.9	0.6743	0.858	0.848
4	38.644	978	18.7	0.8148	0.938	4.743

6r: 5-(3-oxo-1-(thiophen-2-yl)butyl)furan-2(5H)-one

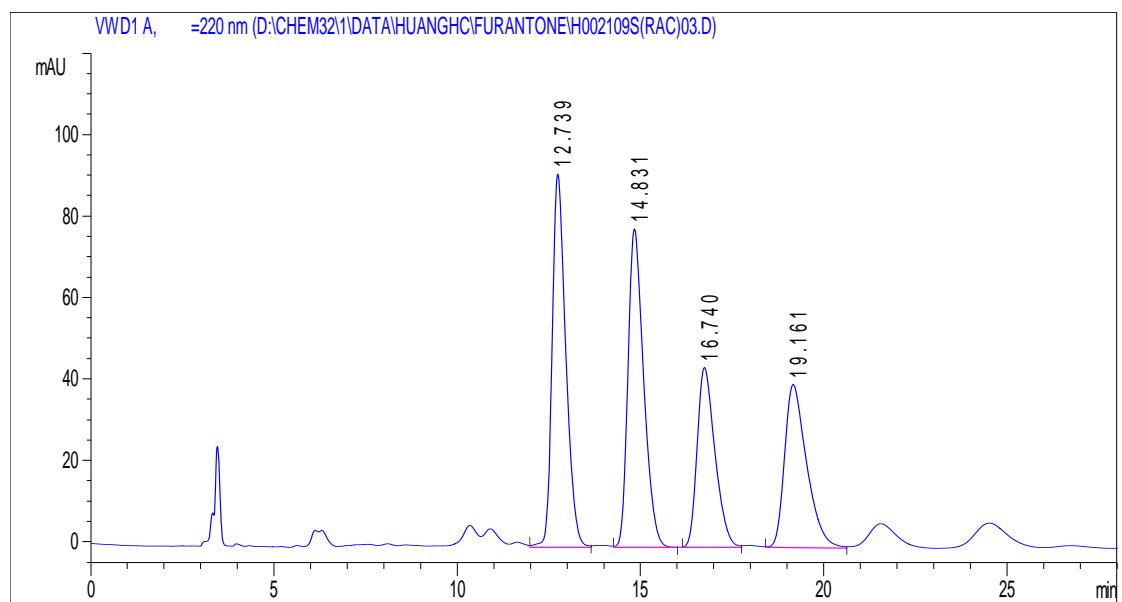


#	Time	Area	Height	Width	Symmetry	Area %
1	12.61	14104.5	856.1	0.2505	0.96	30.864
2	13.972	14143.5	762.3	0.2834	1.185	30.949
3	15.021	8771.4	433.5	0.303	0.775	19.194
4	48.352	8680.2	126	1.0746	1.23	18.994

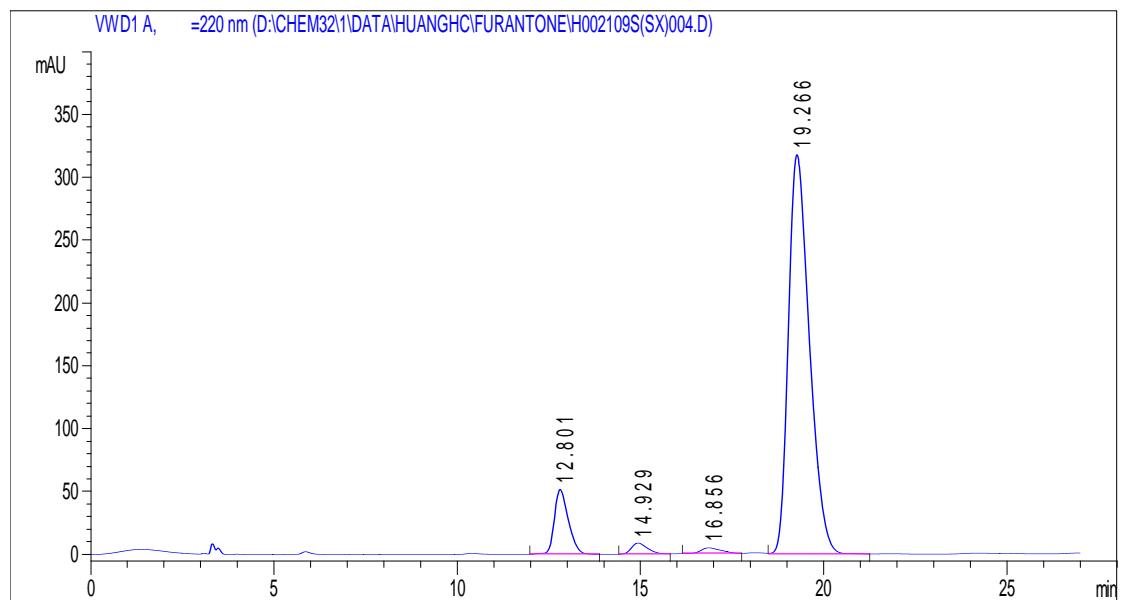


#	Time	Area	Height	Width	Symmetry	Area %
1	12.707	79.1	4.8	0.2531	1.169	0.917
2	14.043	419.9	23.1	0.2765	1.129	4.870
3	15.106	8063.9	396.7	0.307	0.786	93.522
4	45.354	59.6	1.1	0.7834	0.984	0.691

6s: 5-(3-oxo-1,3-diphenylpropyl)furan-2(5H)-one

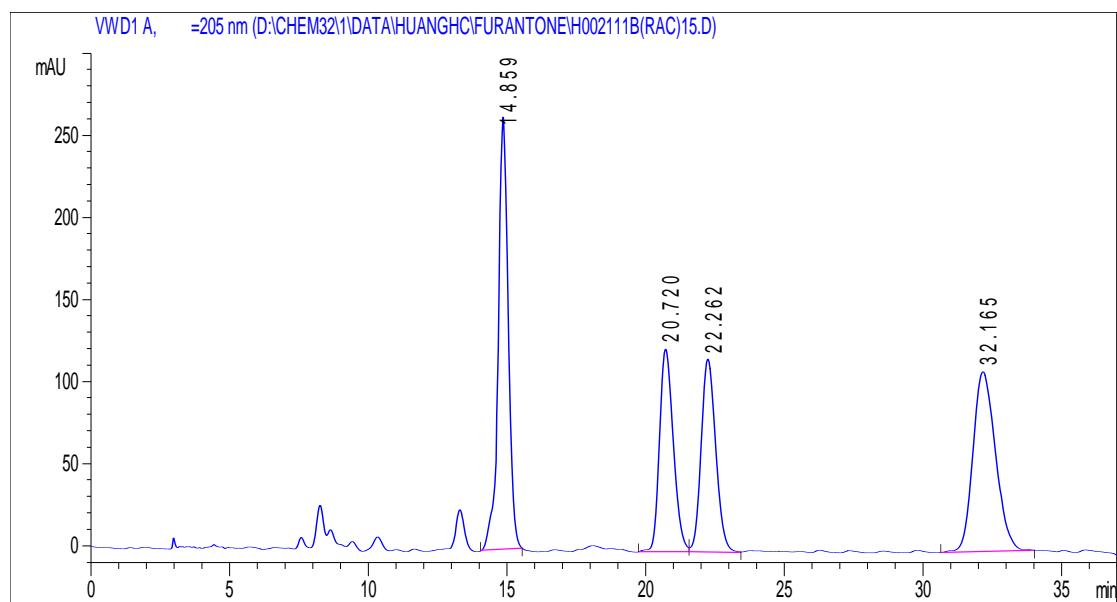


#	Time	Area	Height	Width	Symmetry	Area %
1	12.739	2378.4	91.7	0.3928	0.678	30.062
2	14.831	2335.8	78.3	0.4527	0.666	29.524
3	16.74	1505.4	44.3	0.5158	0.66	19.028
4	19.161	1692	40.2	0.6282	0.604	21.386

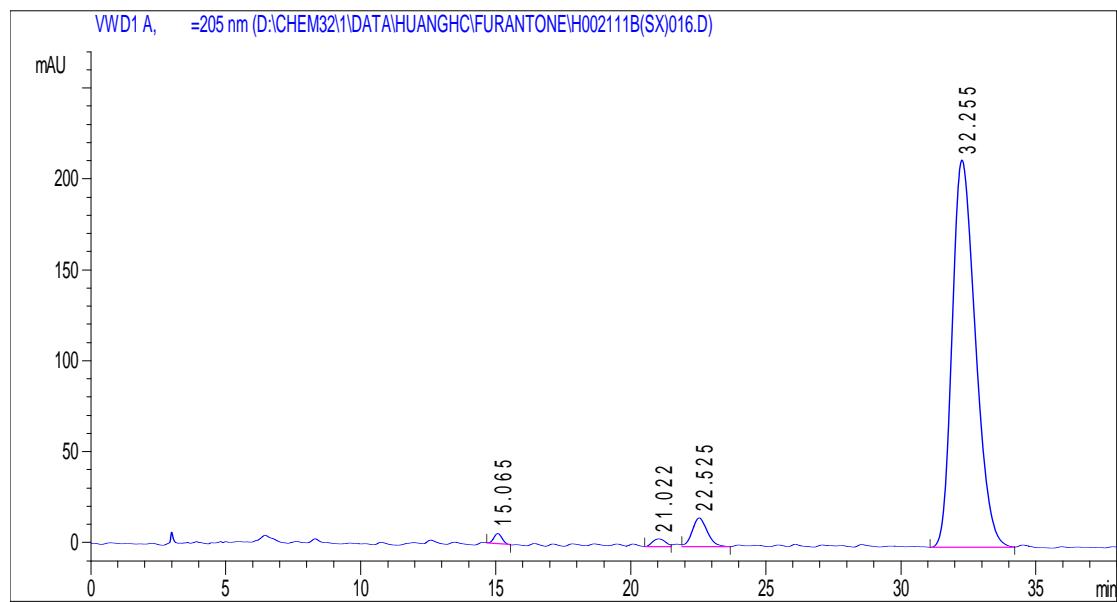


#	Time	Area	Height	Width	Symmetry	Area %
1	12.801	1373.7	51.7	0.4032	0.676	9.472
2	14.929	279	8.9	0.4723	0.64	1.924
3	16.856	166.1	4.5	0.6127	0.608	1.145
4	19.266	12684	317.9	0.6112	0.655	87.459

6t: 5-(2-oxoheptan-4-yl)furan-2(5H)-one

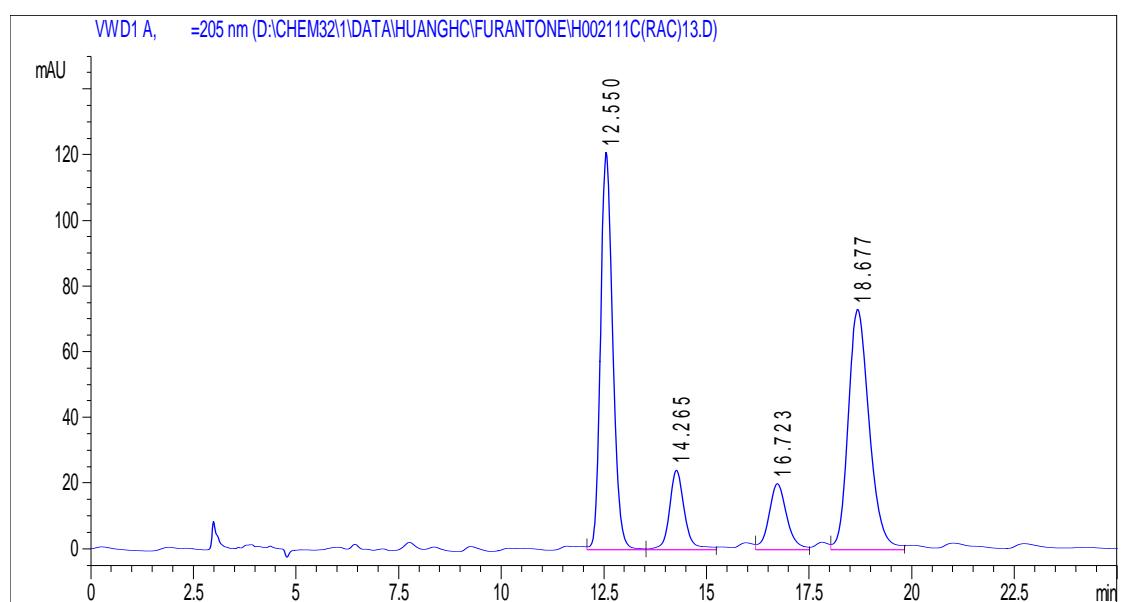


#	Time	Area	Height	Width	Symmetry	Area %
1	14.859	6595	263.3	0.4174	0.927	30.803
2	20.72	4294	123.6	0.579	0.765	20.056
3	22.262	4305.6	47.1	1.4594	0	20.110
4	32.165	6215.6	109.6	0.9451	0.789	29.031

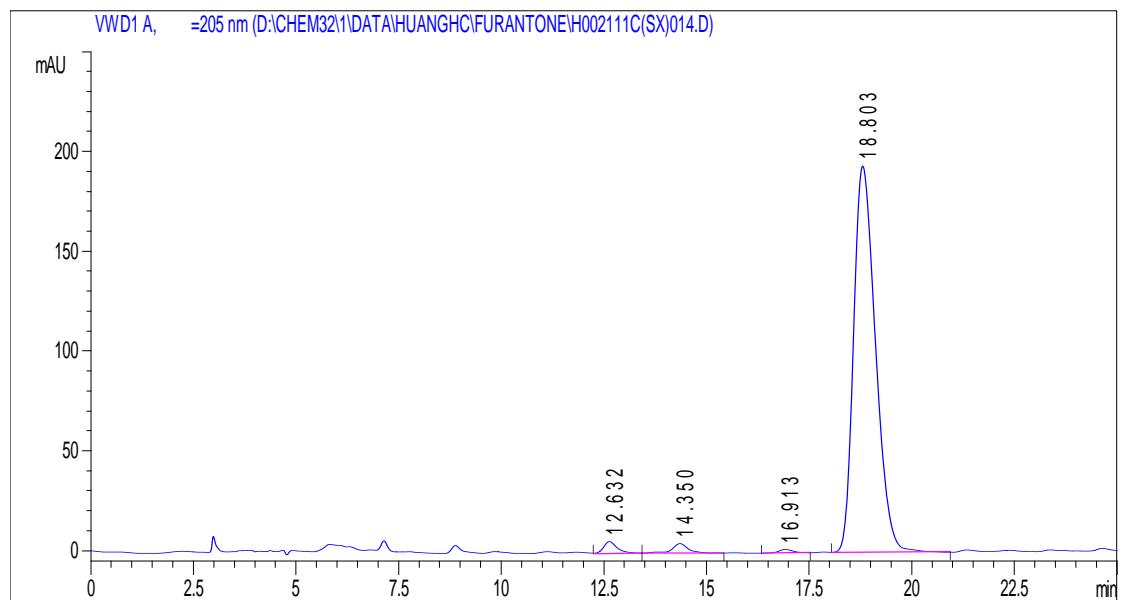


#	Time	Area	Height	Width	Symmetry	Area %
1	15.065	116.4	5.6	0.348	0.916	0.851
2	21.022	148.9	4.4	0.5653	0.888	1.088
3	22.525	632.5	16	0.6011	0.817	4.624
4	32.255	12781.1	213.3	0.9319	0.691	93.436

6u: 5-(2-oxooctan-4-yl)furan-2(5H)-one

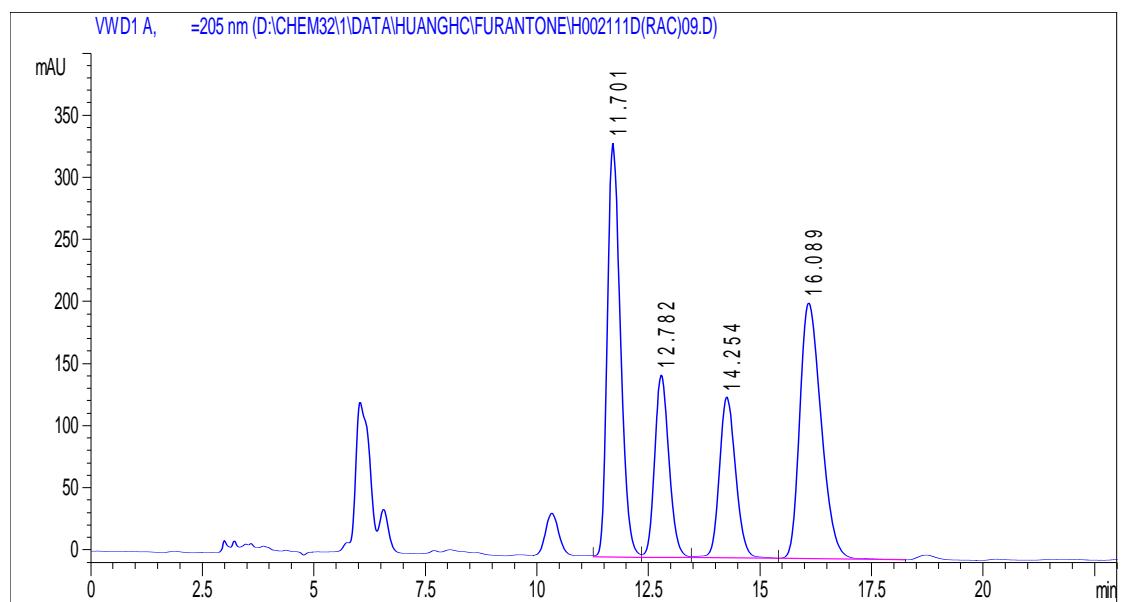


#	Time	Area	Height	Width	Symmetry	Area %
1	12.55	2505.8	121.1	0.32	0.781	39.436
2	14.265	624.5	24.3	0.3871	0.815	9.828
3	16.723	612.1	20.2	0.4589	0.848	9.634
4	18.677	2611.6	73.2	0.55	0.756	41.102

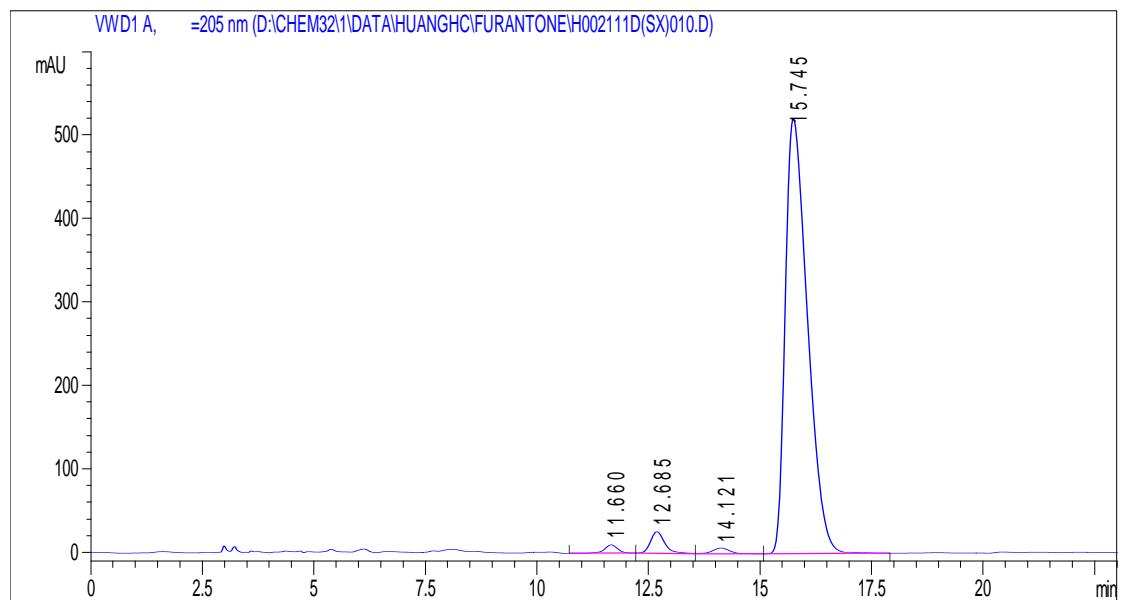


#	Time	Area	Height	Width	Symmetry	Area %
1	12.632	149	6.1	0.3576	0.659	1.974
2	14.35	157.6	5	0.4592	0.995	2.089
3	16.913	48.5	1.8	0.401	0.754	0.643
4	18.803	7191.9	193.7	0.5758	0.673	95.295

6v: 5-(2-oxanonan-4-yl)furan-2(5H)-one

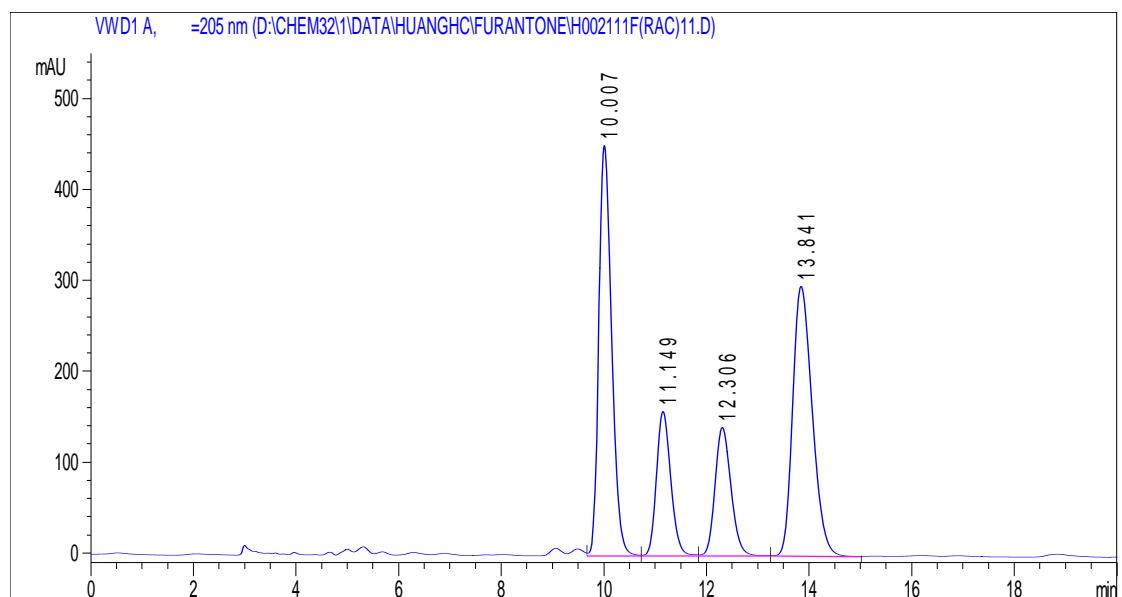


#	Time	Area	Height	Width	Symmetry	Area %
1	11.701	6858.3	333.6	0.3214	0.711	33.659
2	12.782	3295.6	147.3	0.3454	0.803	16.174
3	14.254	3339.9	130.1	0.3985	0.814	16.391
4	16.089	6882.2	206.2	0.5176	0.675	33.776

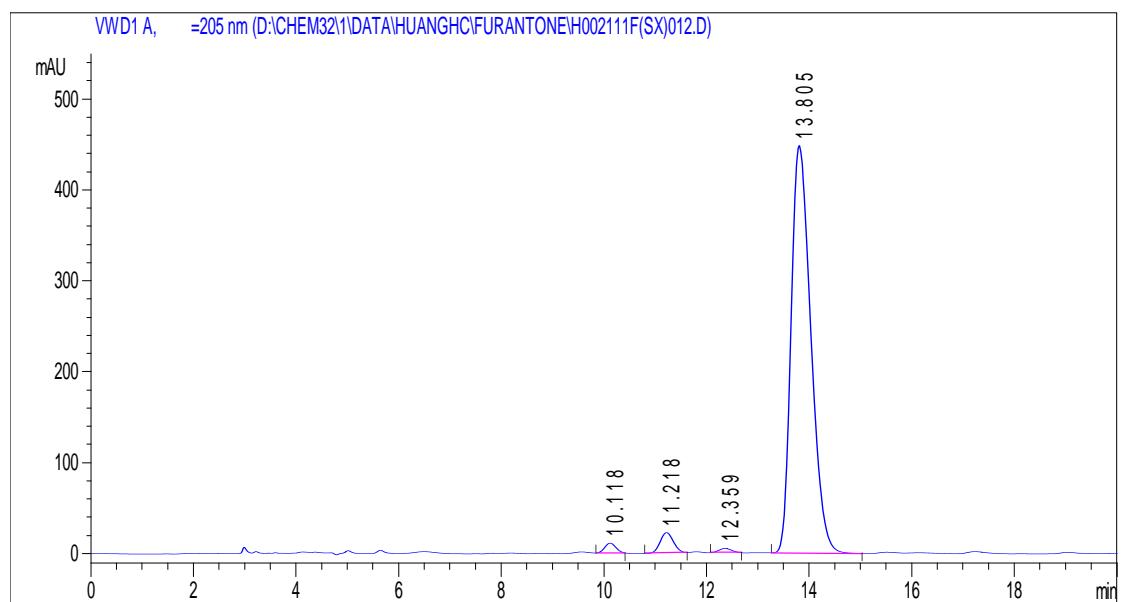


#	Time	Area	Height	Width	Symmetry	Area %
1	11.66	254.4	10.6	0.3492	1.053	1.331
2	12.685	615	26.5	0.3524	0.768	3.217
3	14.121	193	7	0.4237	0.96	1.09
4	15.745	18055.9	521.7	0.5377	0.539	94.443

6w: 5-(2-oxodecan-4-yl)furan-2(5H)-one

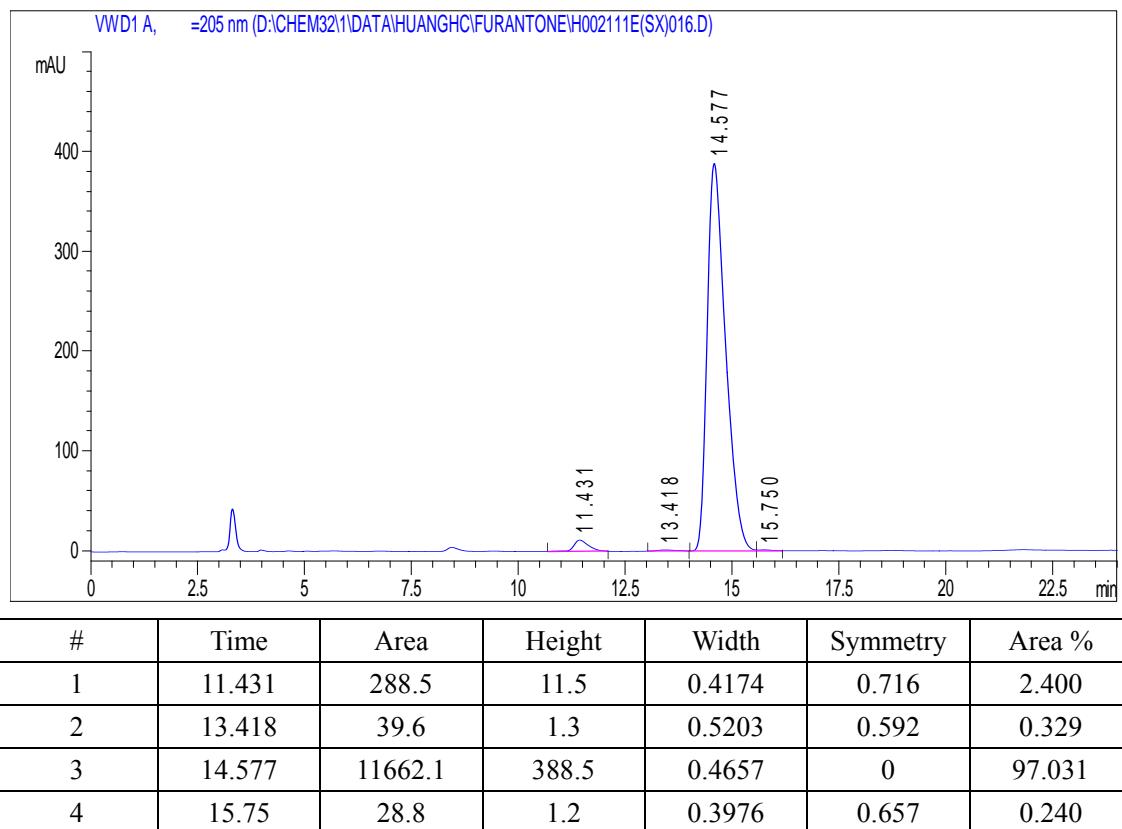
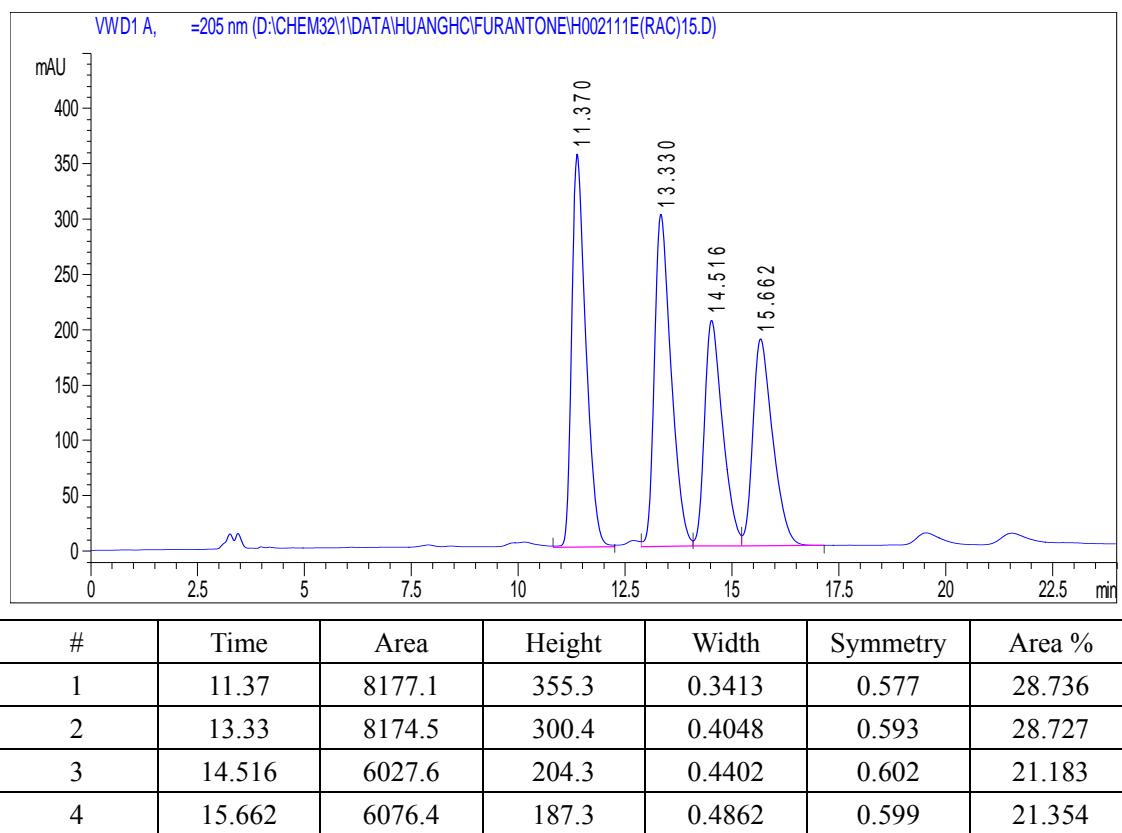


#	Time	Area	Height	Width	Symmetry	Area %
1	10.007	7838	451.5	0.2695	0.721	35.736
2	11.149	3109.4	159.3	0.3034	0.794	14.177
3	12.306	3103.7	142	0.3365	0.793	14.151
4	13.841	7882	297.4	0.4141	0.716	35.937

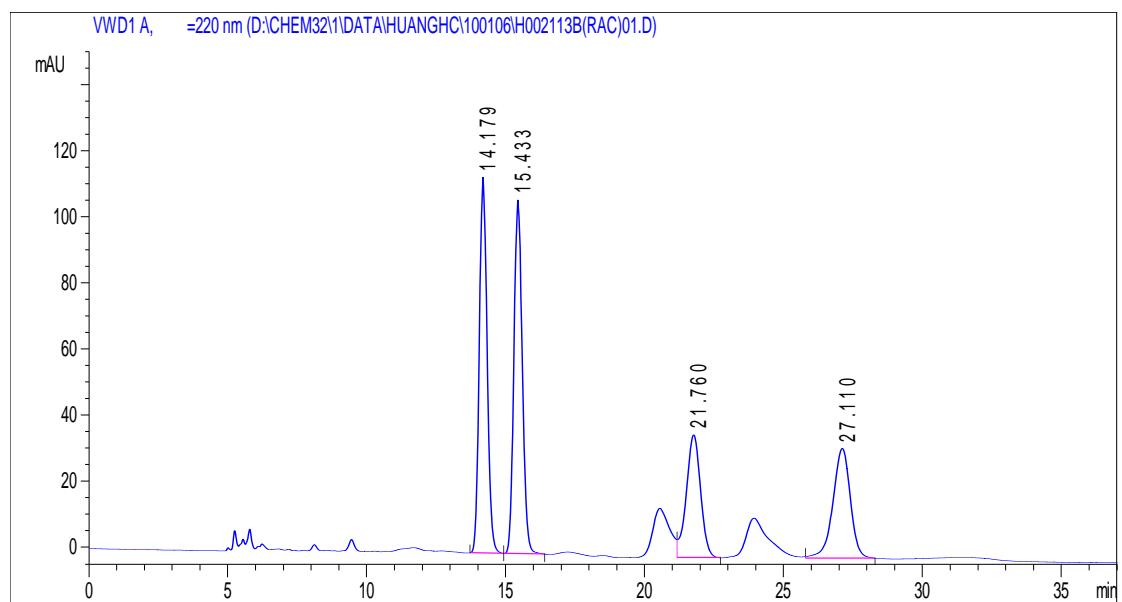


#	Time	Area	Height	Width	Symmetry	Area %
1	10.118	164.1	10.9	0.2502	0.875	1.300
2	11.218	406.8	22.6	0.2995	0.925	3.222
3	12.359	86.6	4.8	0.3006	0.922	0.686
4	13.805	11967.4	448.6	0.4149	0	94.792

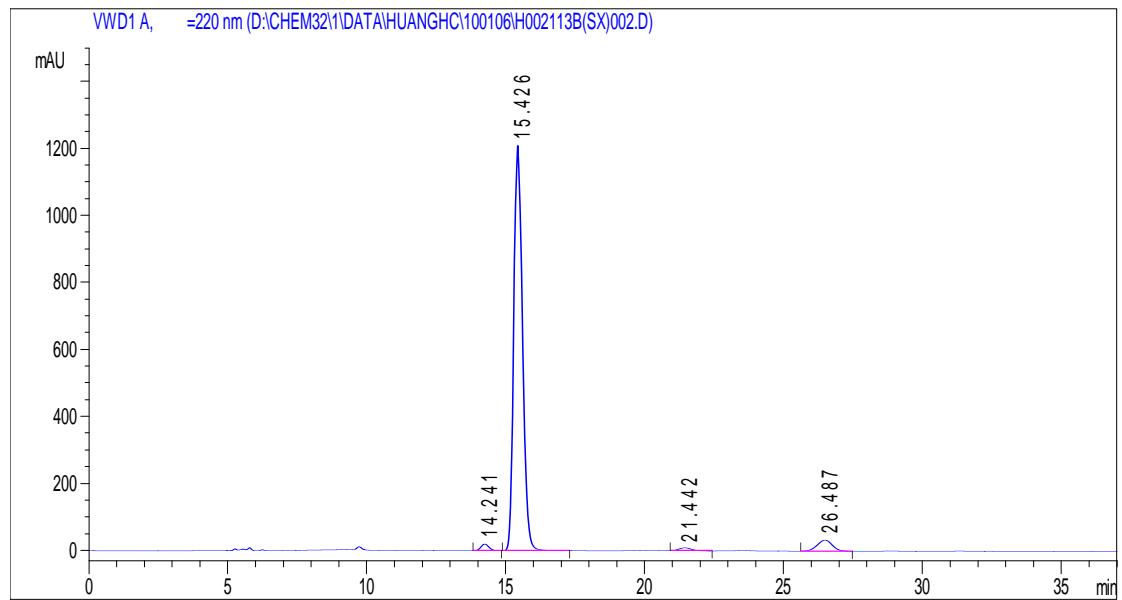
6x: 5-(4-oxooctan-2-yl)furan-2(5H)-one



6y: 5-(5-oxo-1-phenylhexan-3-yl)furan-2(5H)-one

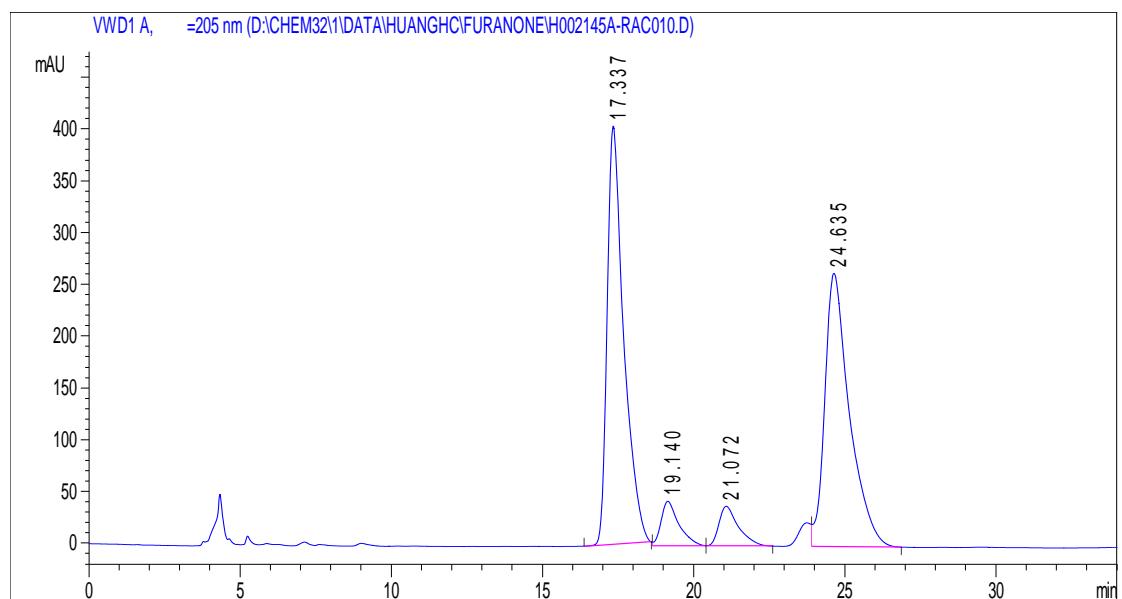


#	Time	Area	Height	Width	Symmetry	Area %
1	14.179	2234.1	113.7	0.305	0.876	30.748
2	15.433	2253.9	107	0.3288	0.867	31.020
3	21.76	1325	37.2	0.5469	1.032	18.235
4	27.11	1453	33.3	0.6712	1.149	19.997

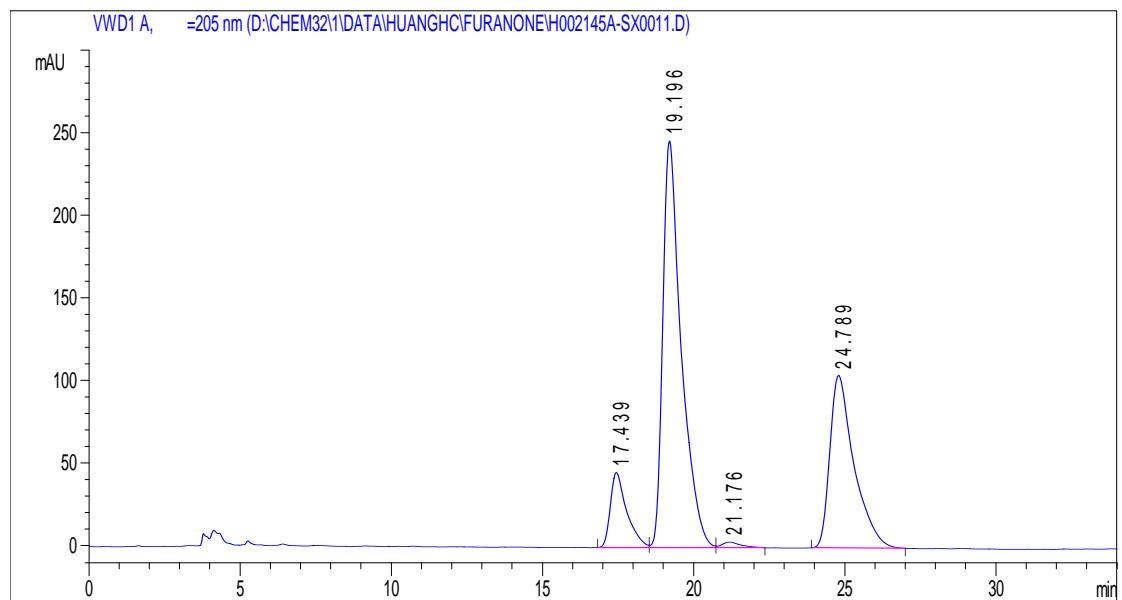


#	Time	Area	Height	Width	Symmetry	Area %
1	14.241	388.7	19.7	0.3054	0.878	1.364
2	15.426	26570	1209.1	0.3437	0.773	93.238
3	21.442	304.4	9.3	0.4984	0.937	1.068
4	26.487	1233.9	33	0.582	1.062	4.330

7a:5-(3-oxocyclopentyl)furan-2(5H)-one

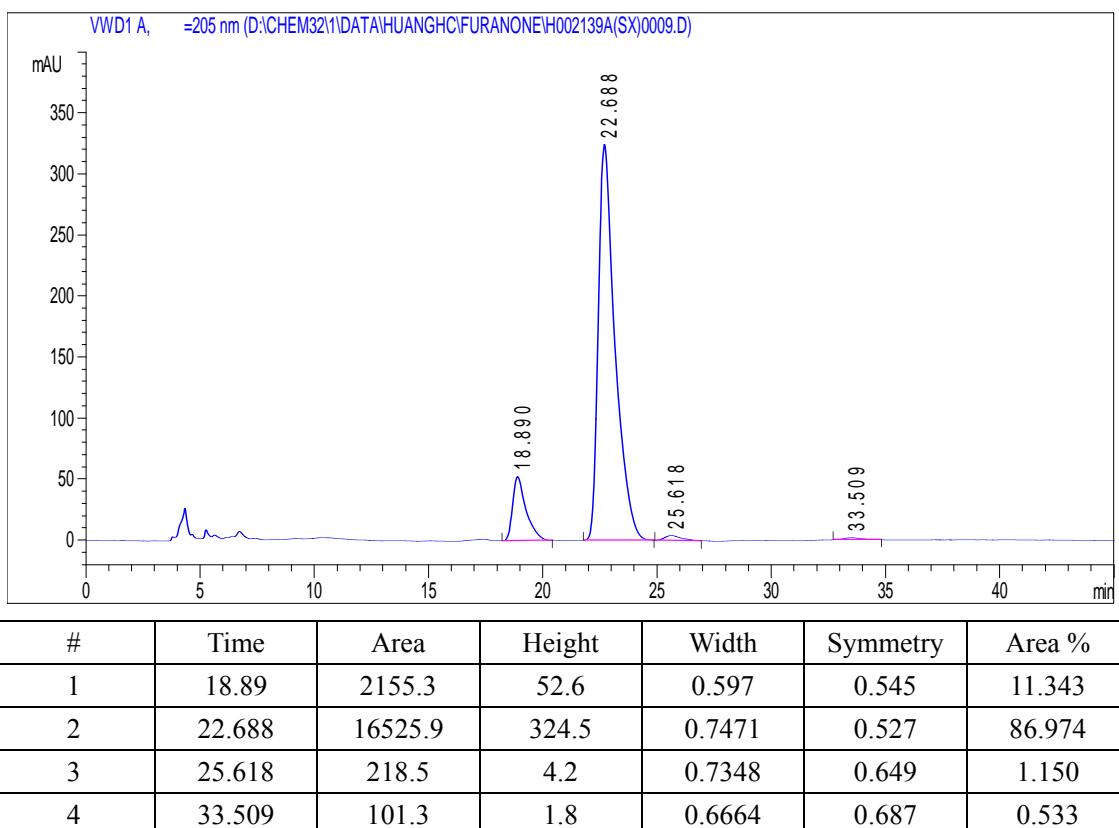
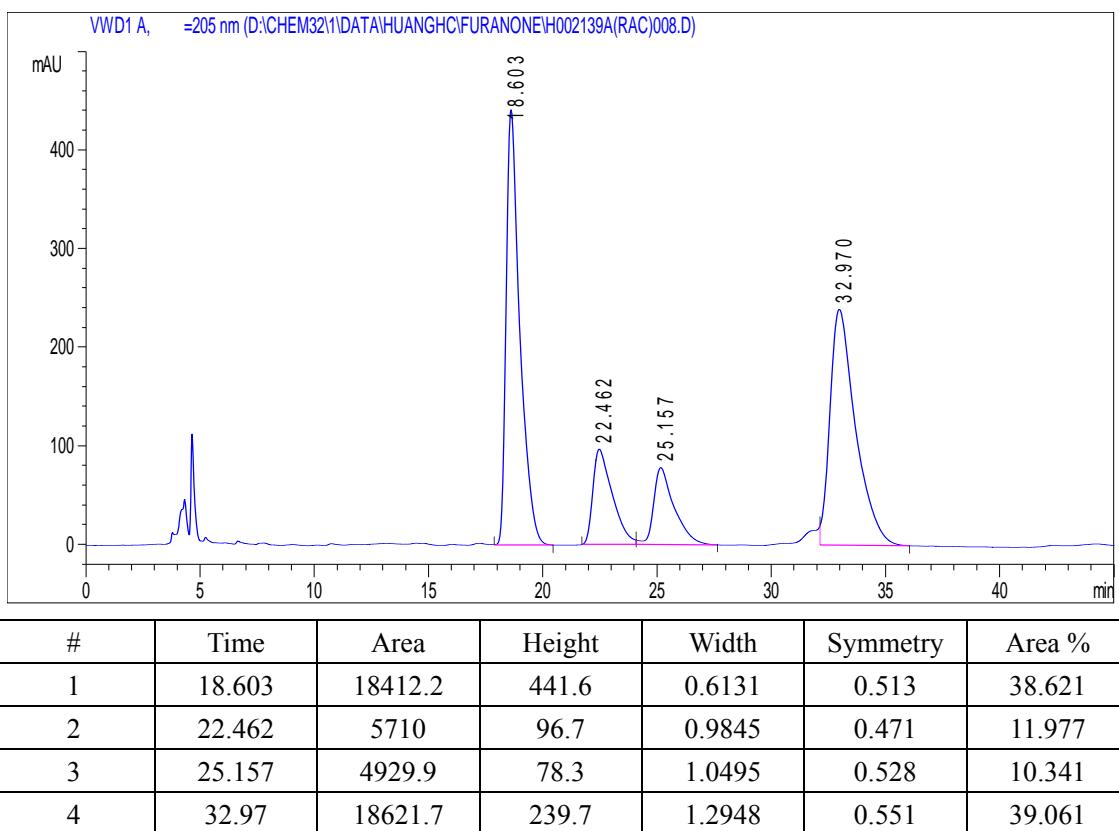


#	Time	Area	Height	Width	Symmetry	Area %
1	17.337	15372.1	403.8	0.6345	0.56	45.372
2	19.14	1802.7	43.4	0.6064	0.566	5.321
3	21.072	1743.1	38.6	0.6604	0.558	5.145
4	24.635	14962.5	264	0.8273	0.554	44.163



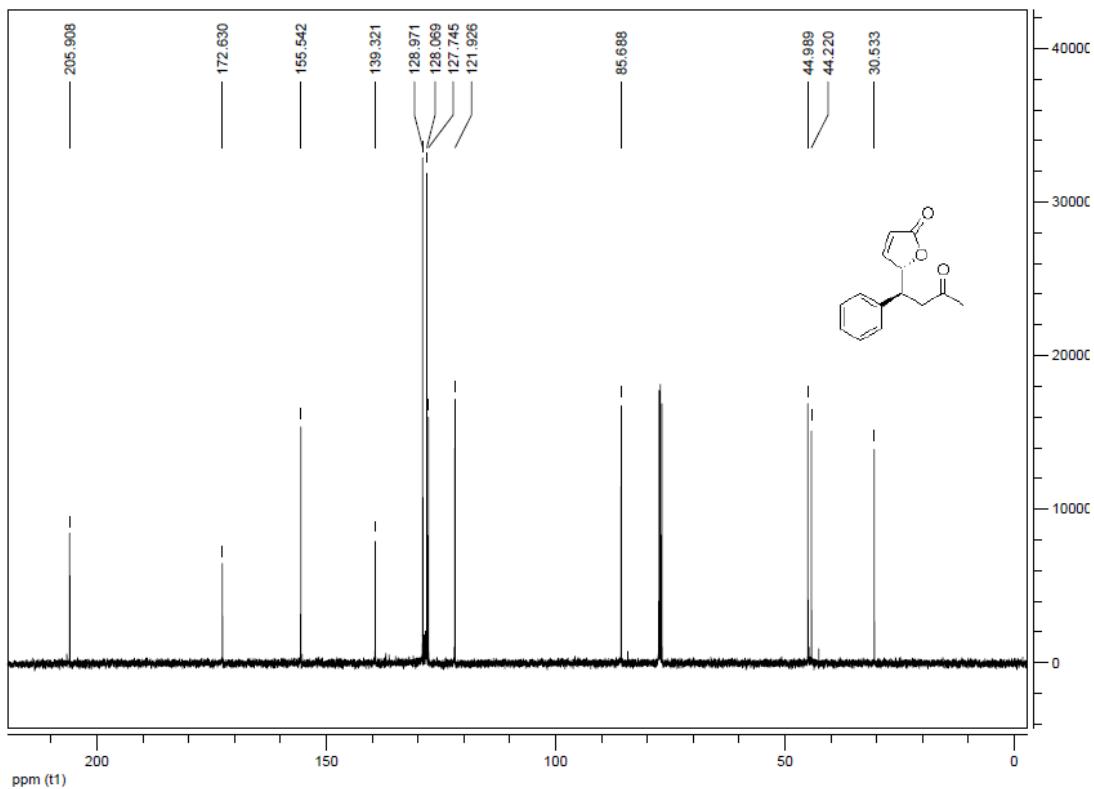
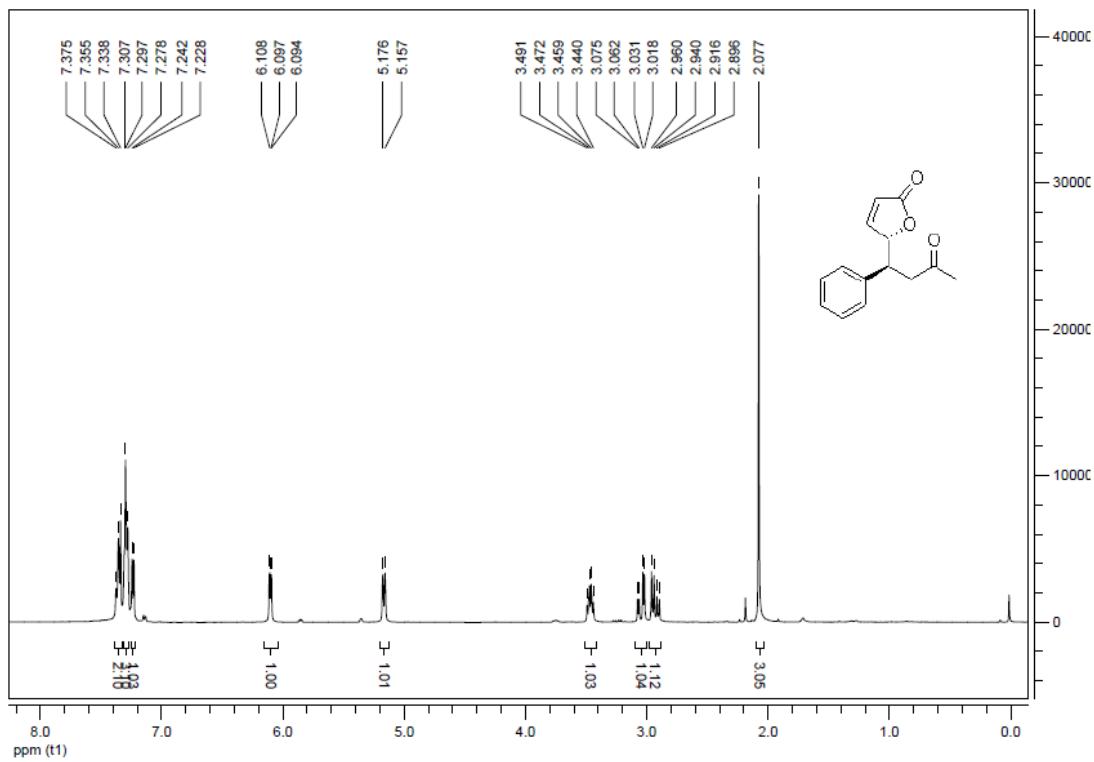
#	Time	Area	Height	Width	Symmetry	Area %
1	17.439	1717.1	45.4	0.55	0.538	9.460
2	19.196	10477.3	246.1	0.622	0.523	57.720
3	21.176	155.1	3.5	0.6428	0.573	0.854
4	24.789	5802.3	104.3	0.8133	0.53	31.966

7b:5-(3-oxocycloheptyl)furan-2(5H)-one

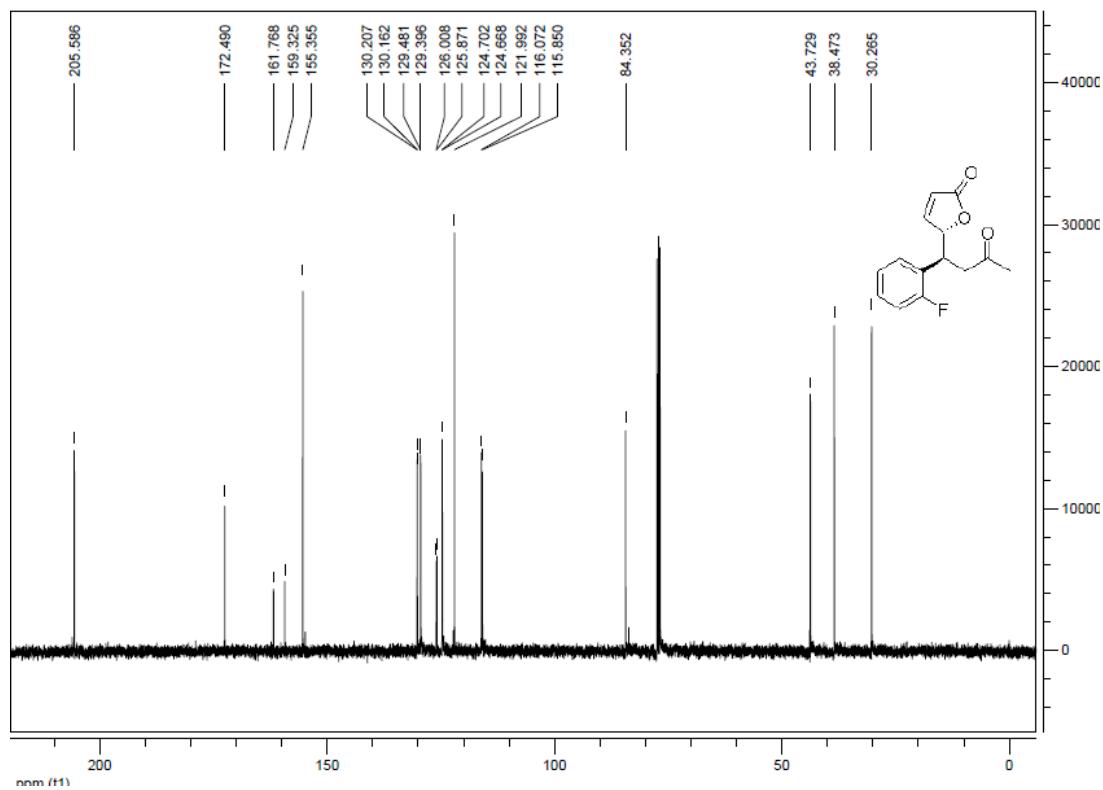
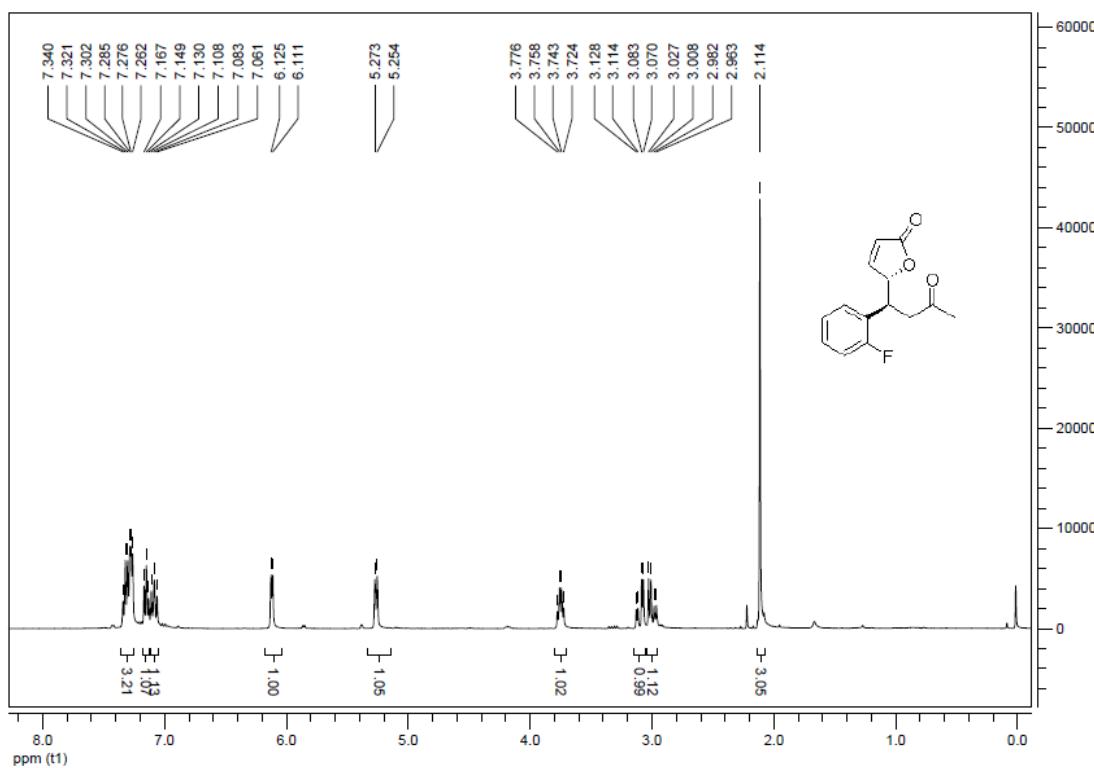


F: NMR Spectra of Michael Addition Products

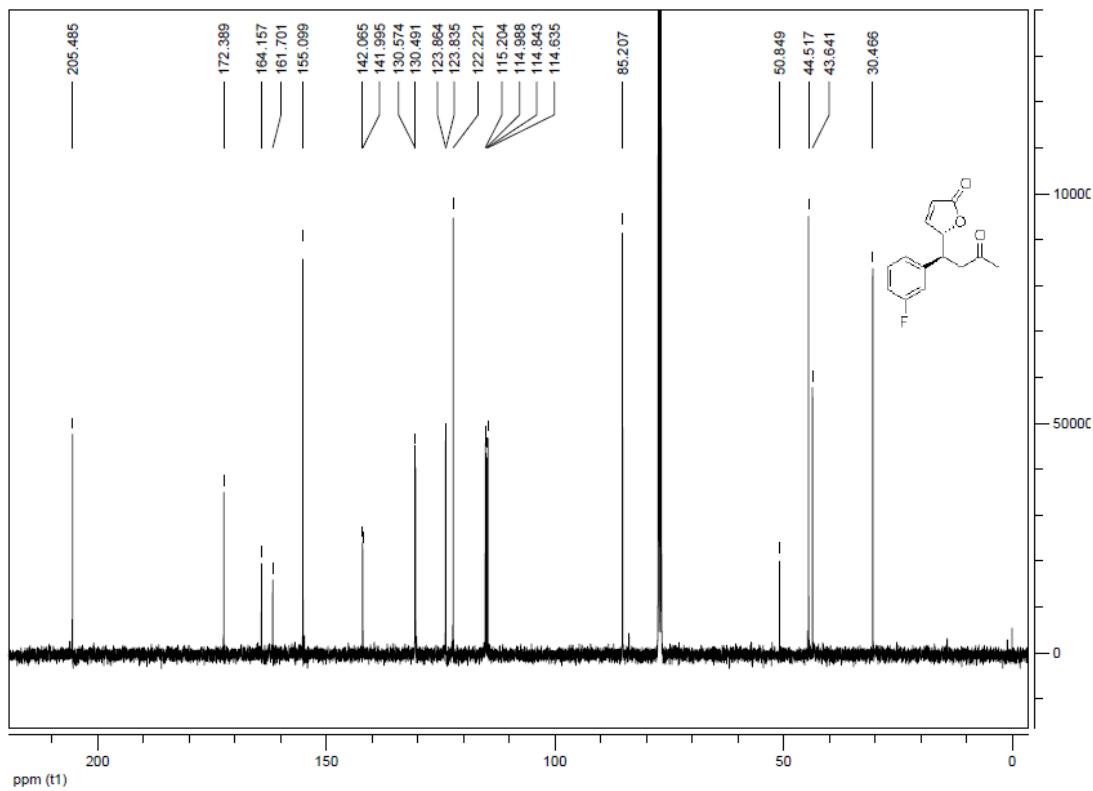
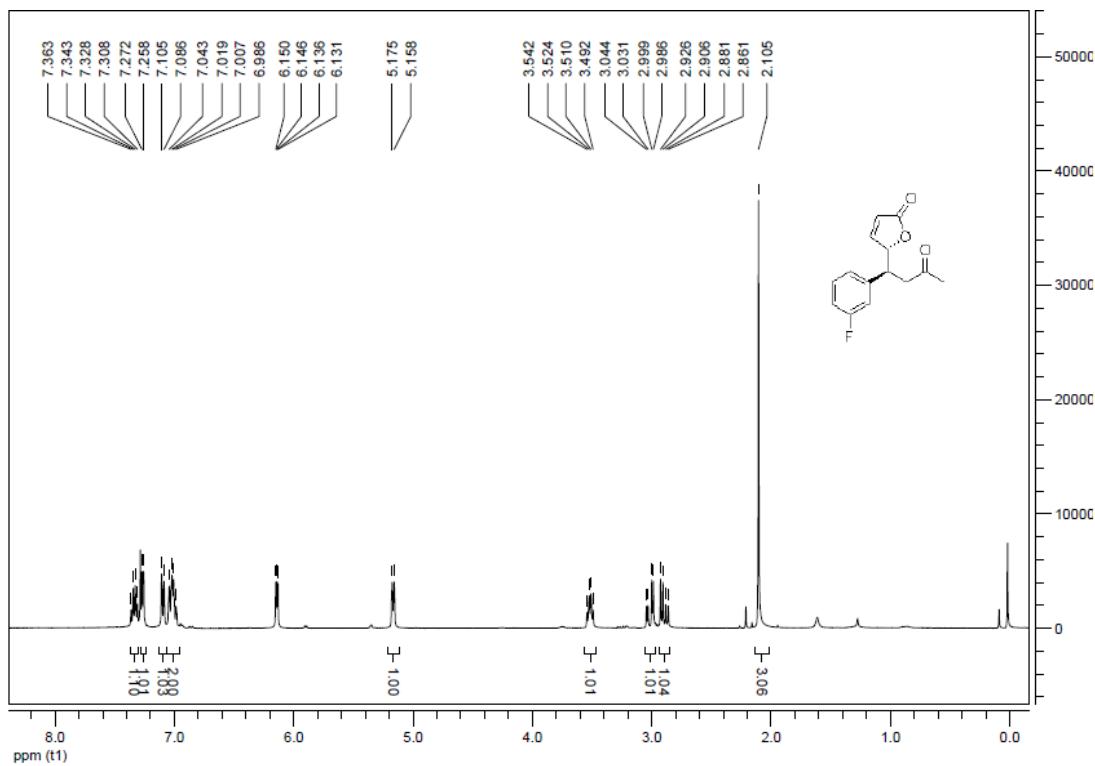
6a: 5-(3-oxo-1-phenylbutyl)furan-2(5H)-one



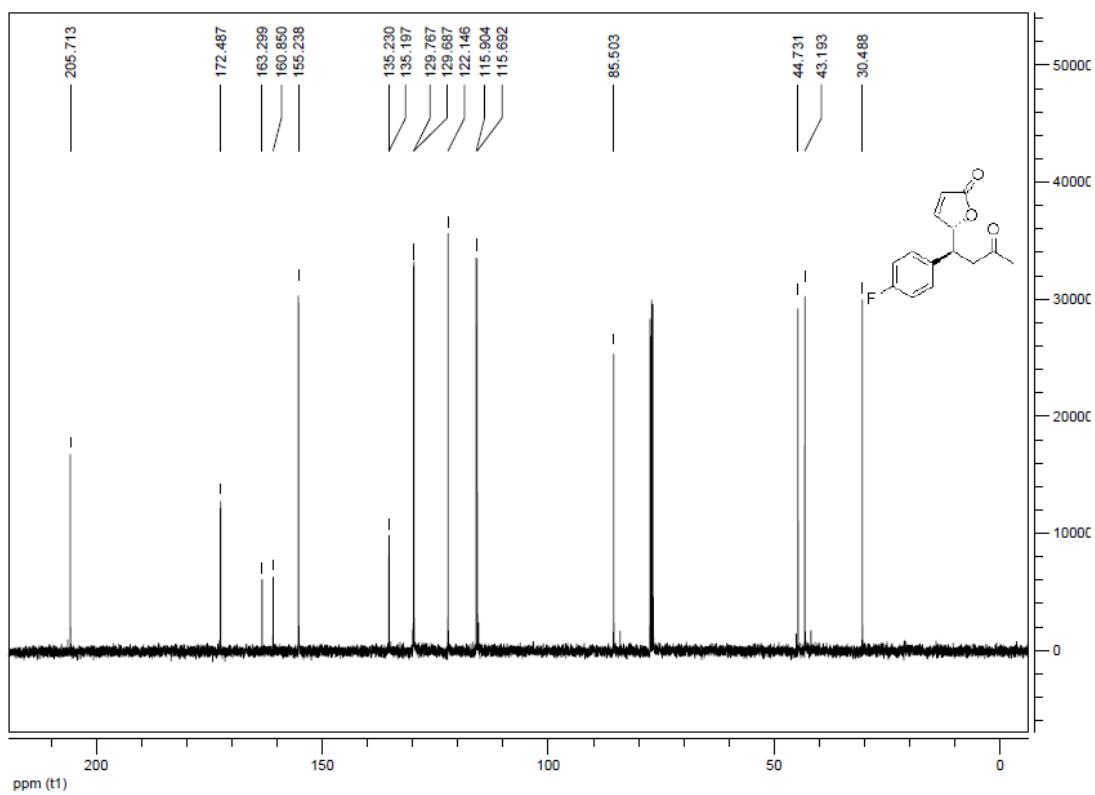
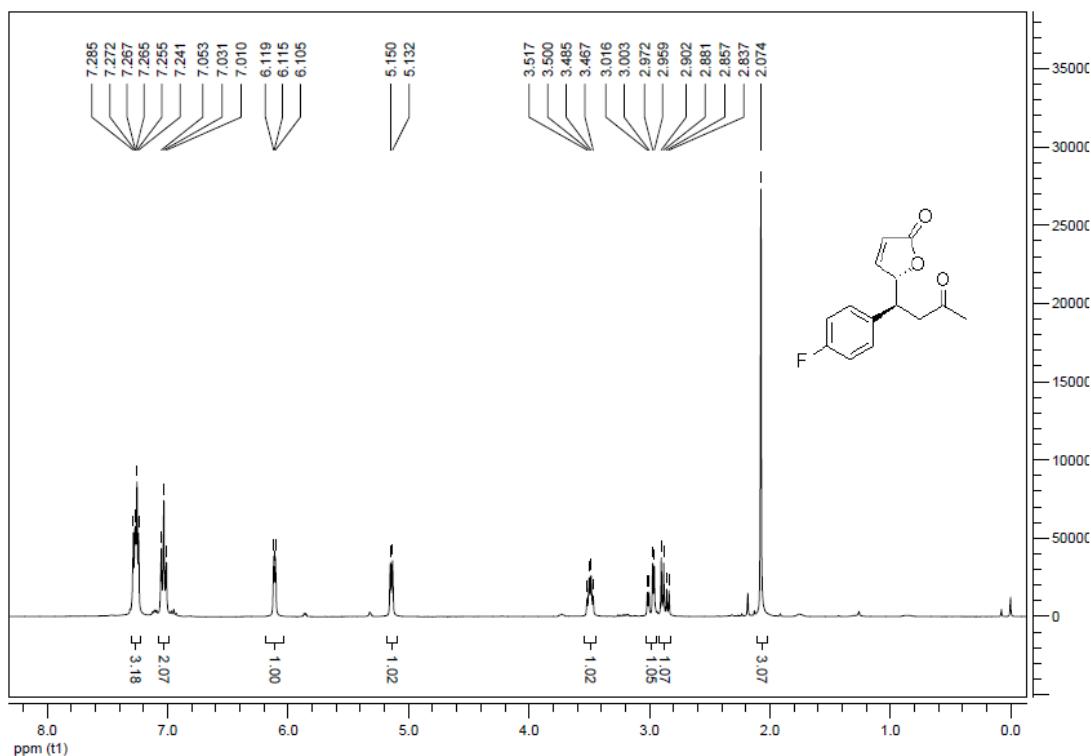
6b: 5-(3-oxo-1-phenylbutyl)furan-2(5H)-one



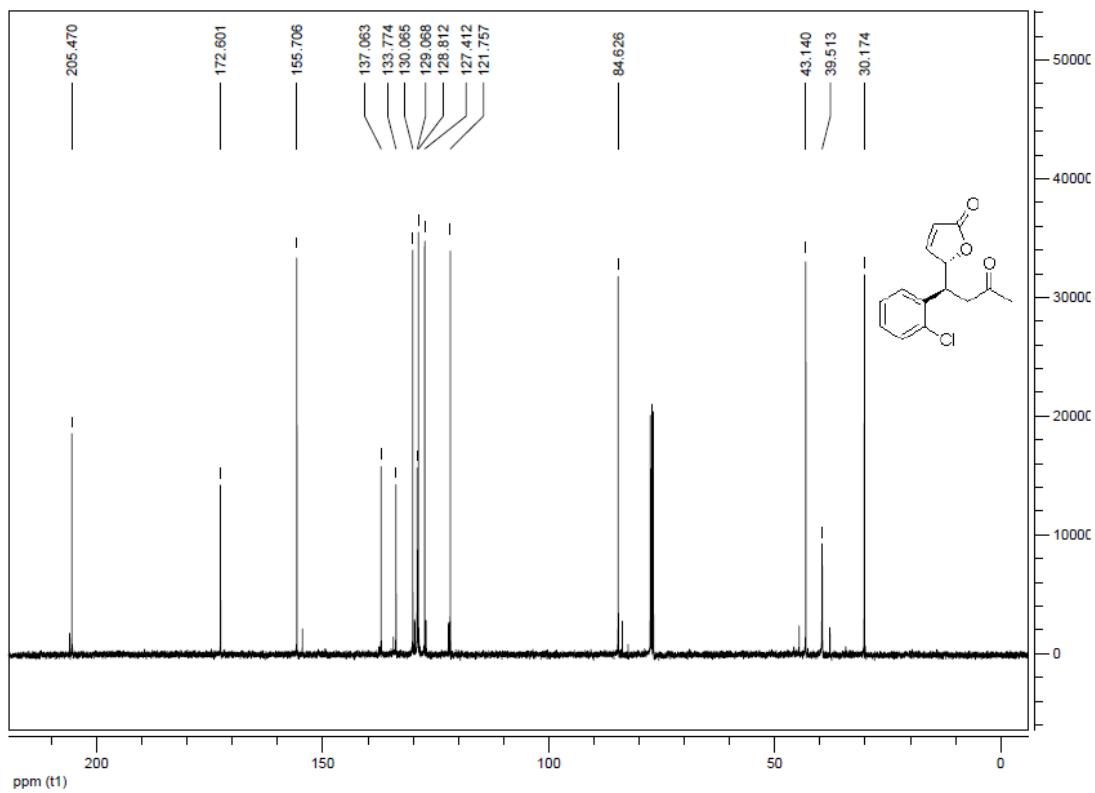
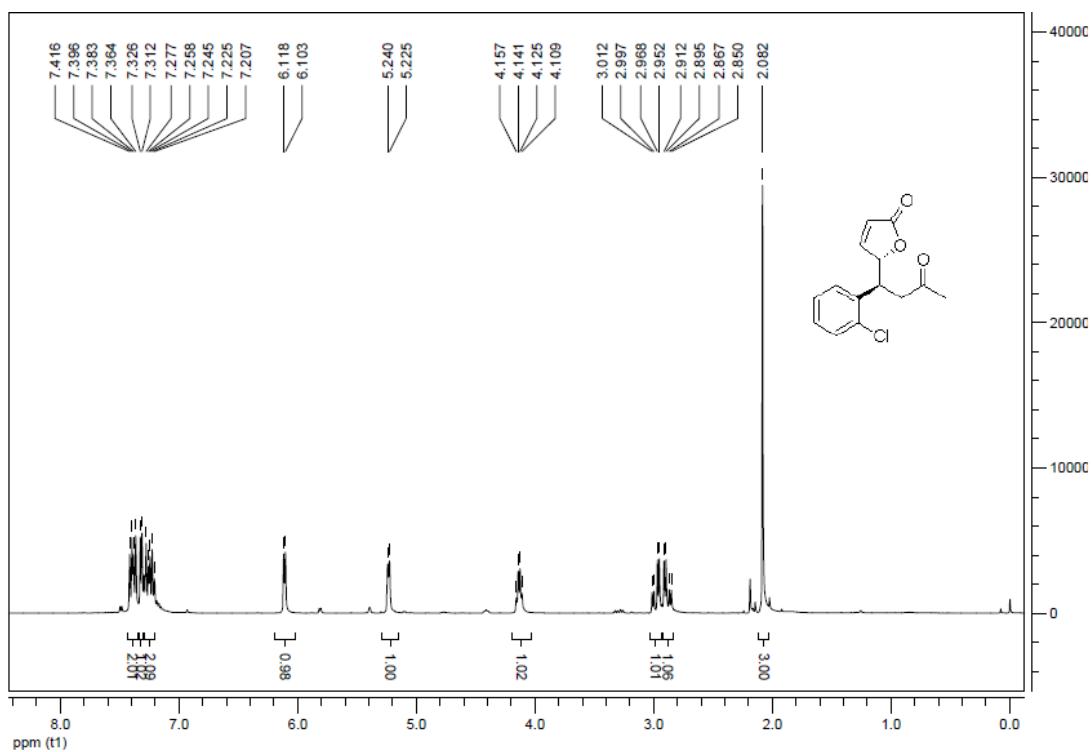
6c: 5-(3-oxo-1-phenylbutyl)furan-2(5H)-one



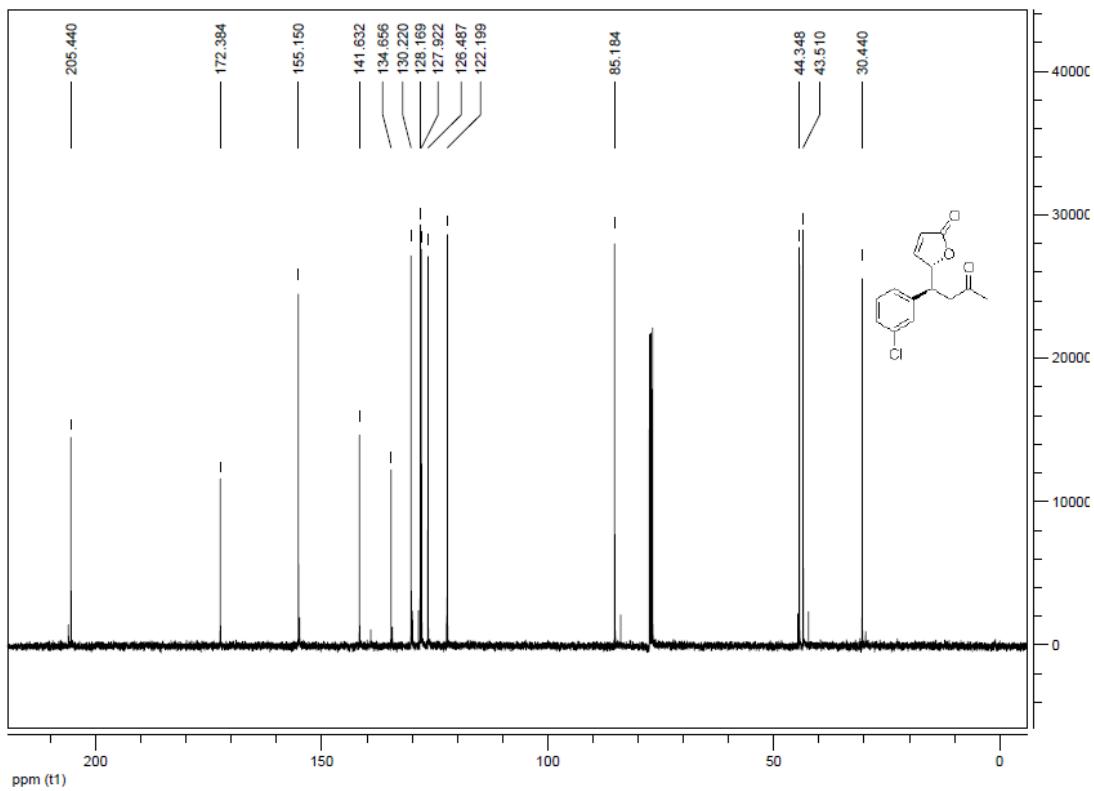
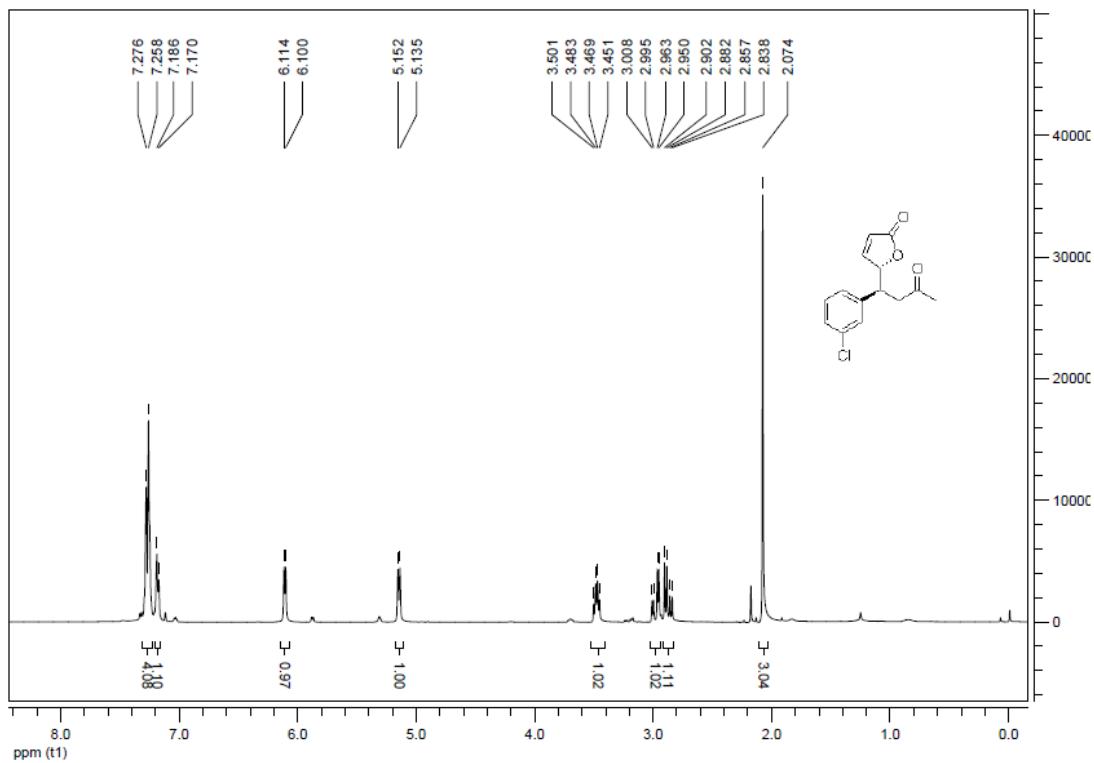
6d: 5-(1-(4-fluorophenyl)-3-oxobutyl)furan-2(5H)-one



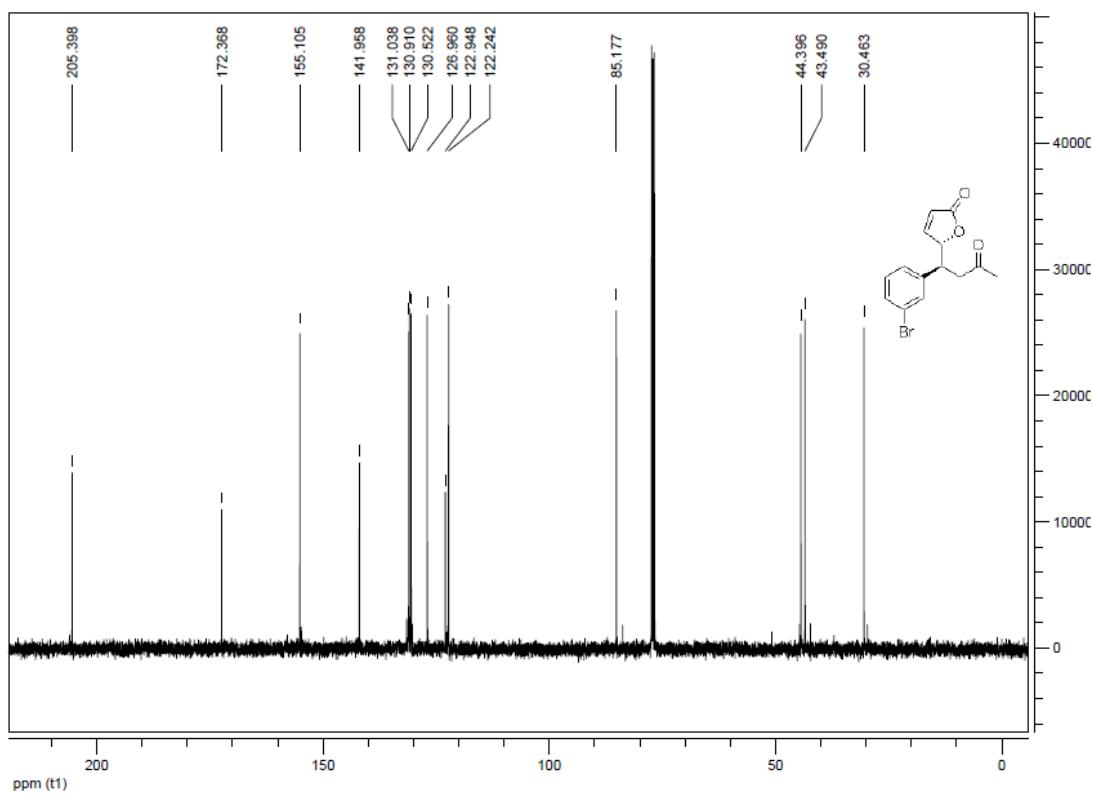
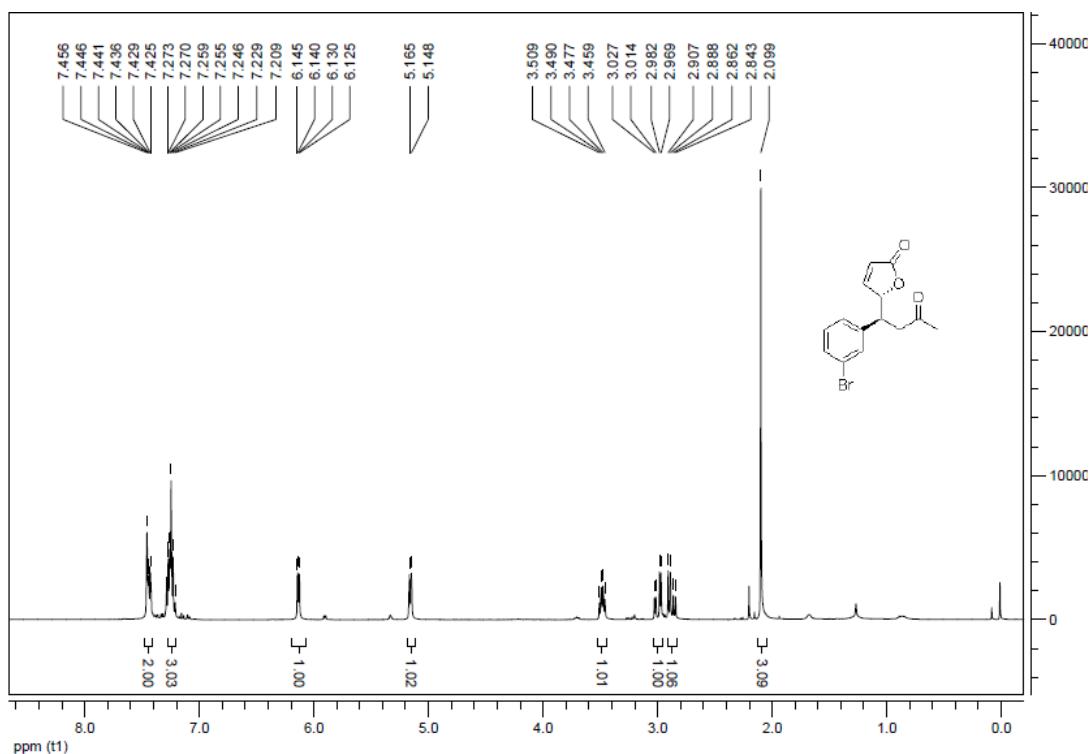
6e: 5-(1-(2-chlorophenyl)-3-oxobutyl)furan-2(5H)-one



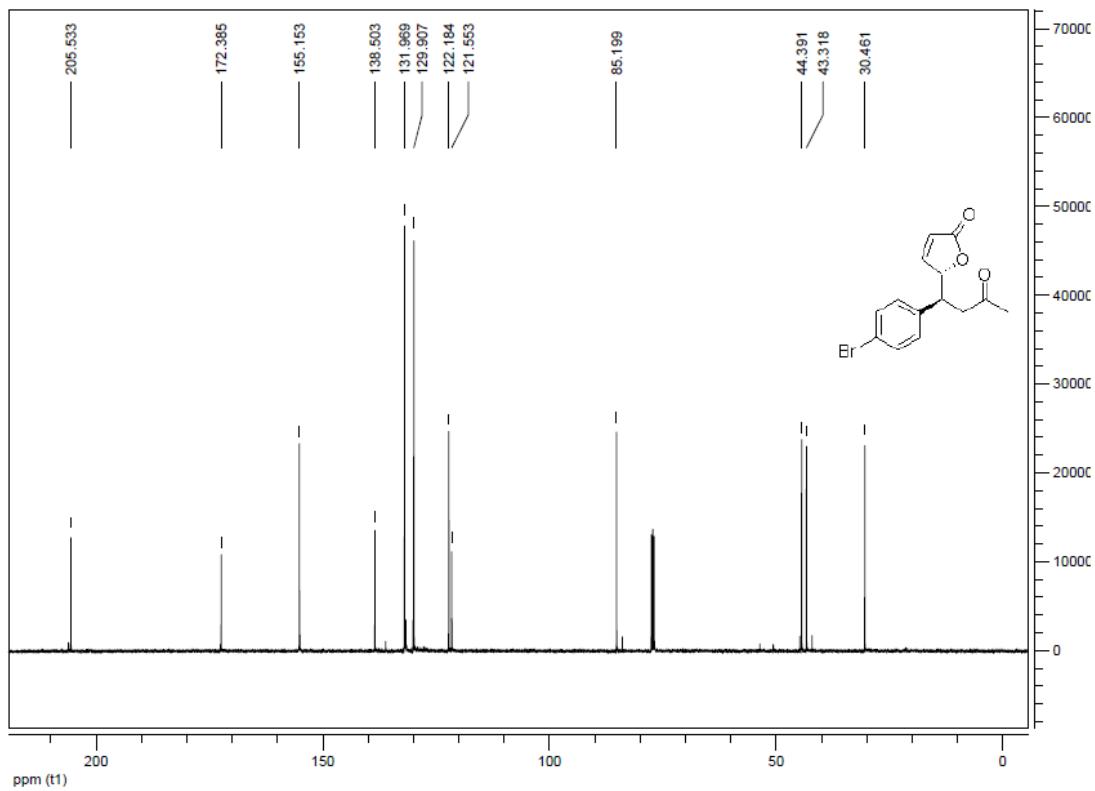
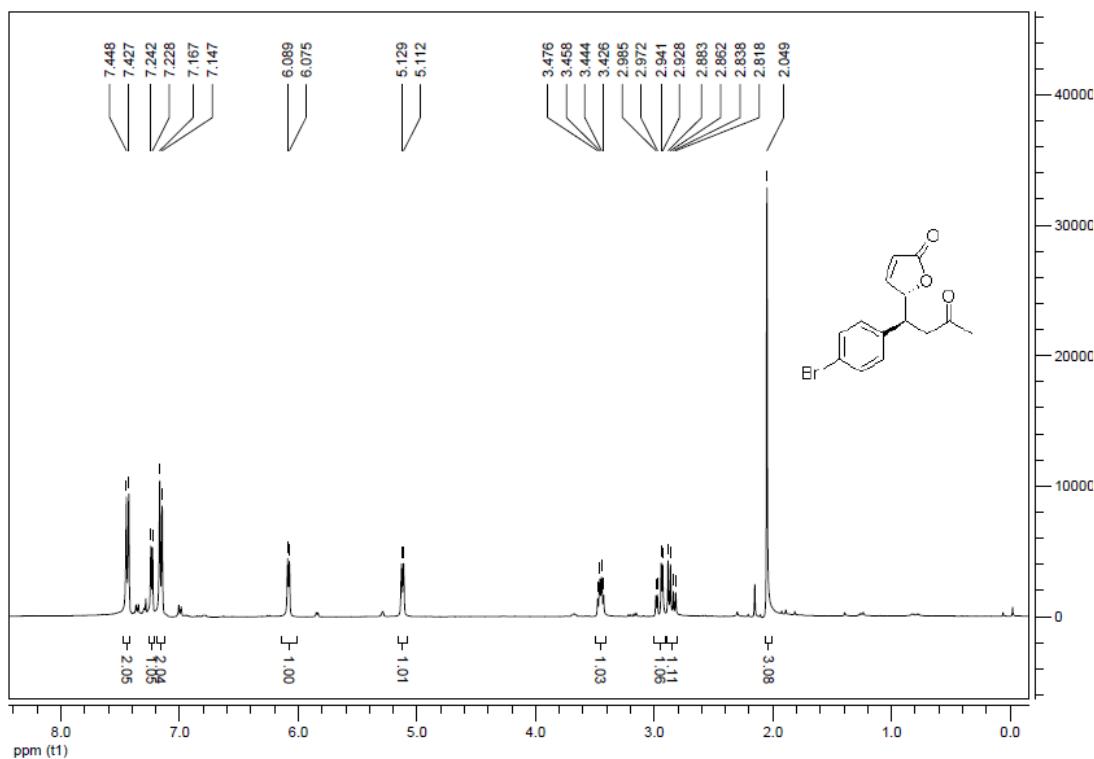
6f: 5-(1-(3-chlorophenyl)-3-oxobutyl)furan-2(5H)-one



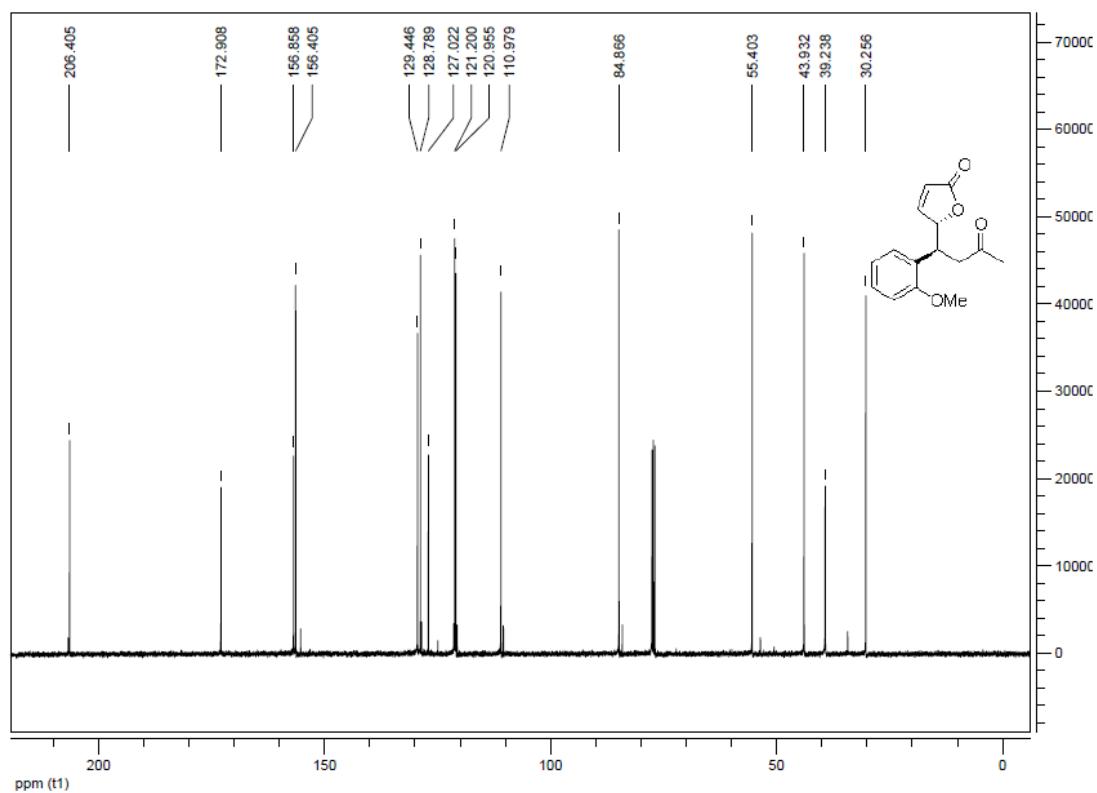
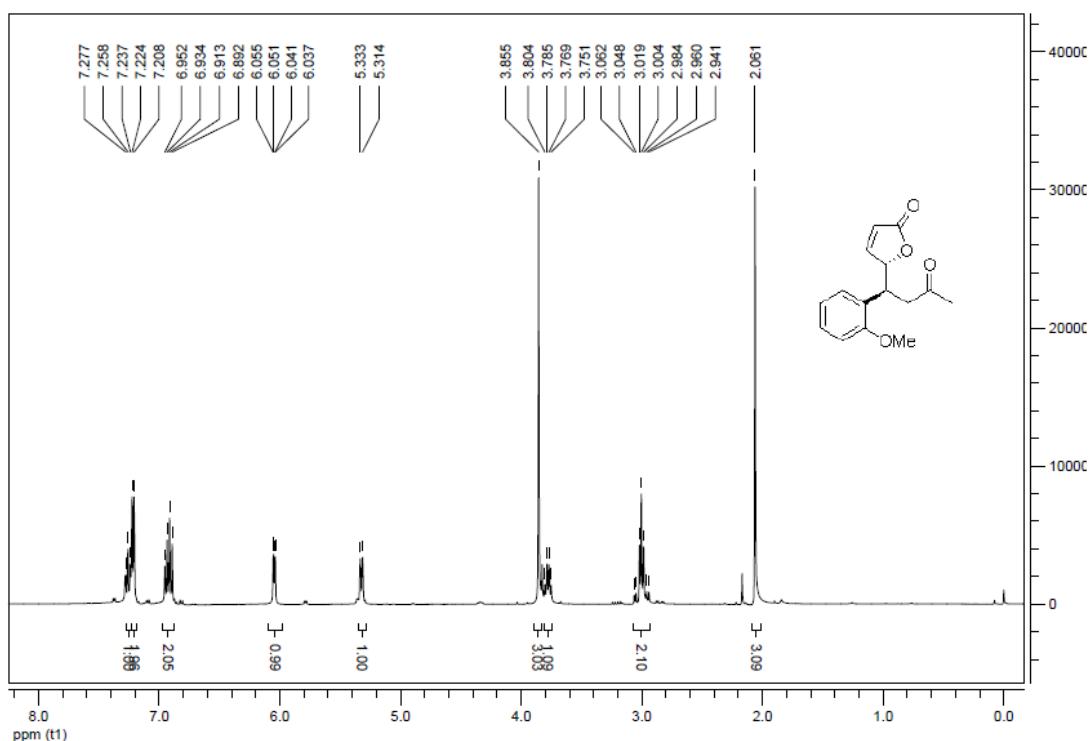
6g: 5-(1-(3-bromophenyl)-3-oxobutyl)furan-2(5H)-one



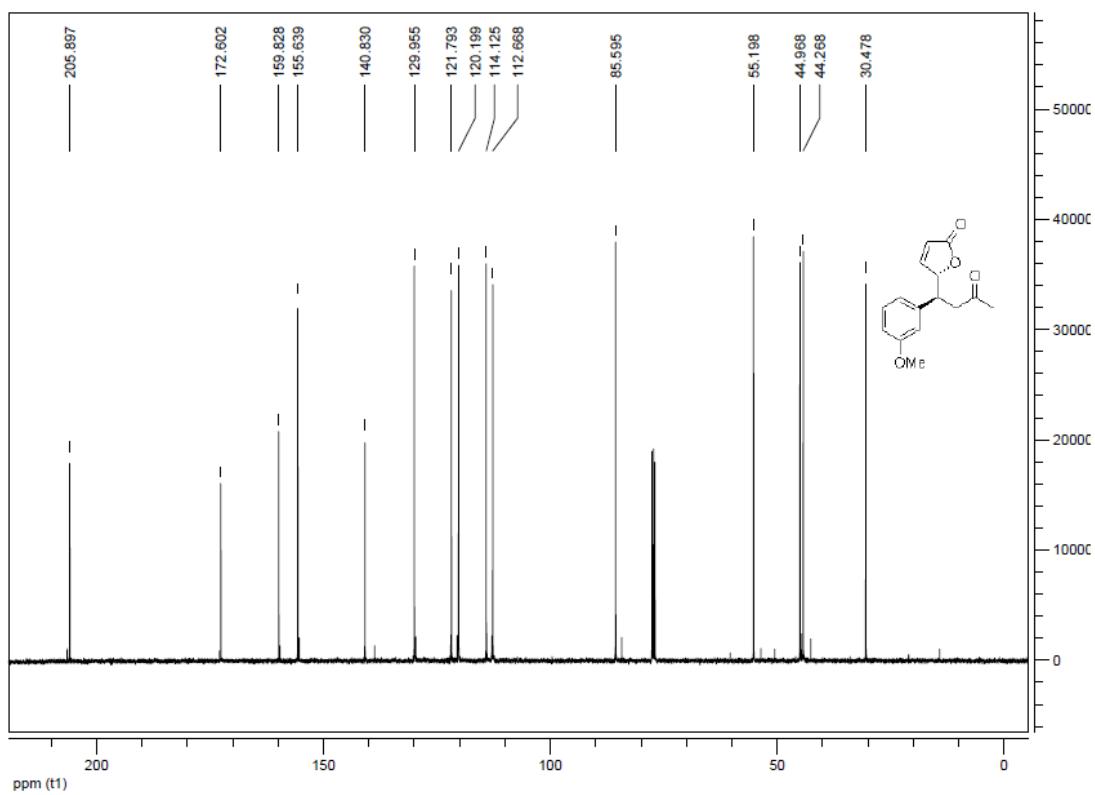
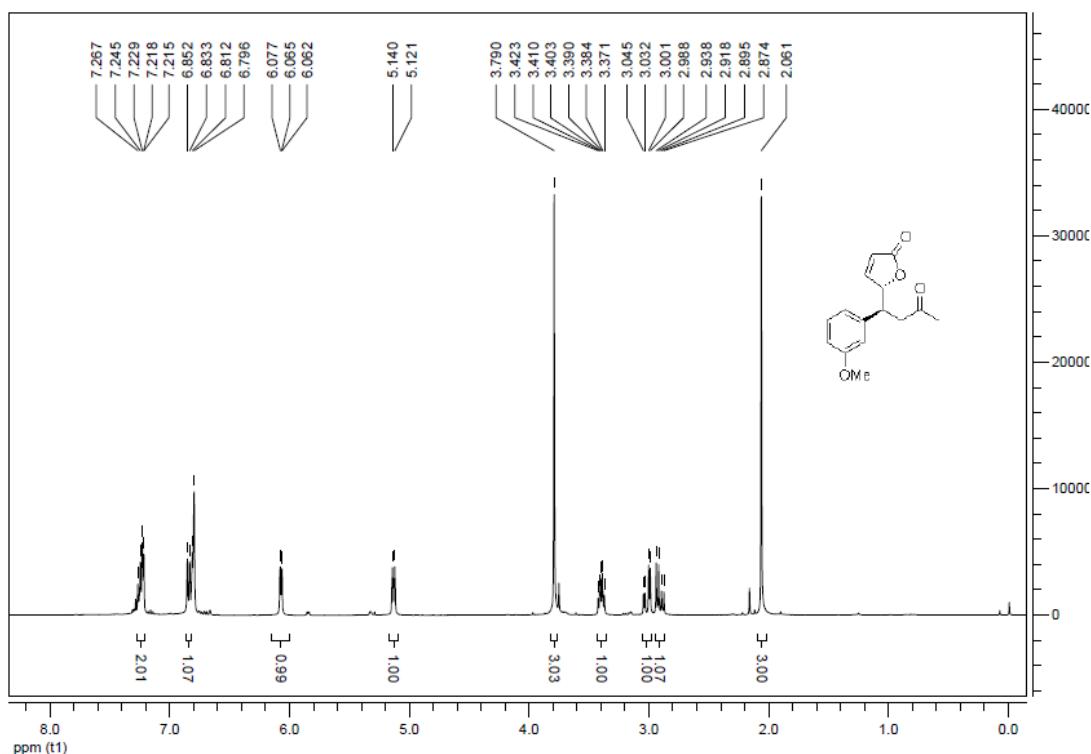
6h: 5-(1-(4-bromophenyl)-3-oxobutyl)furan-2(5H)-one



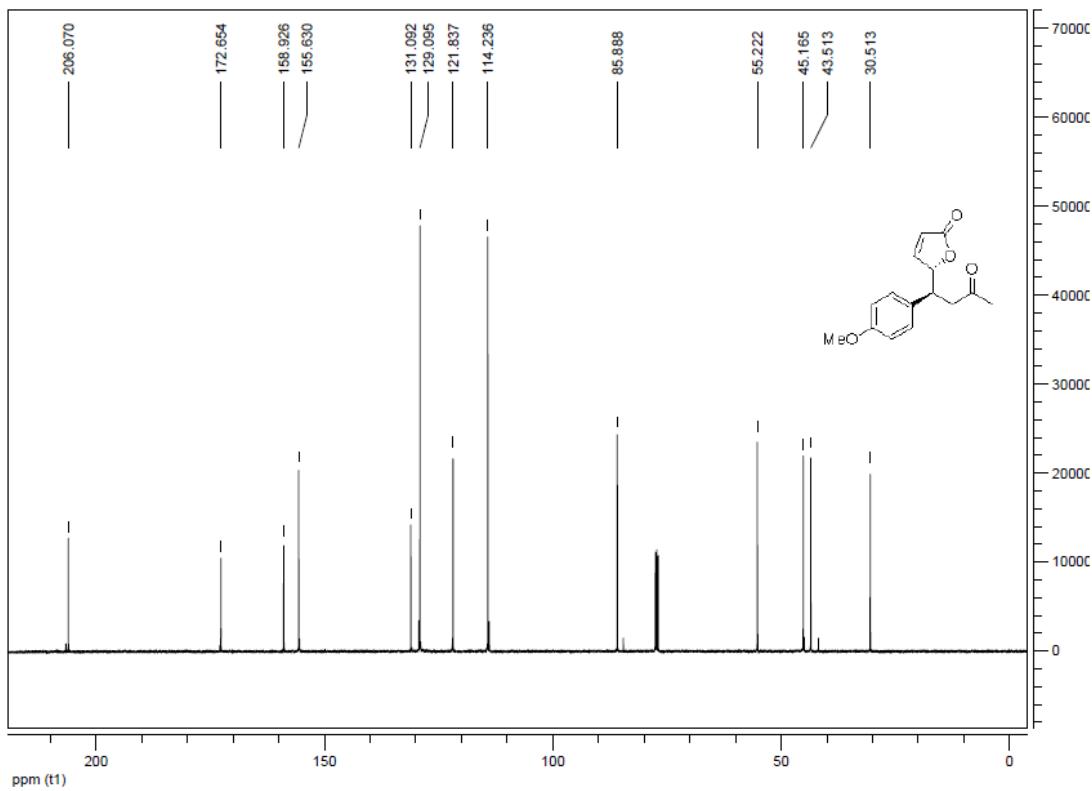
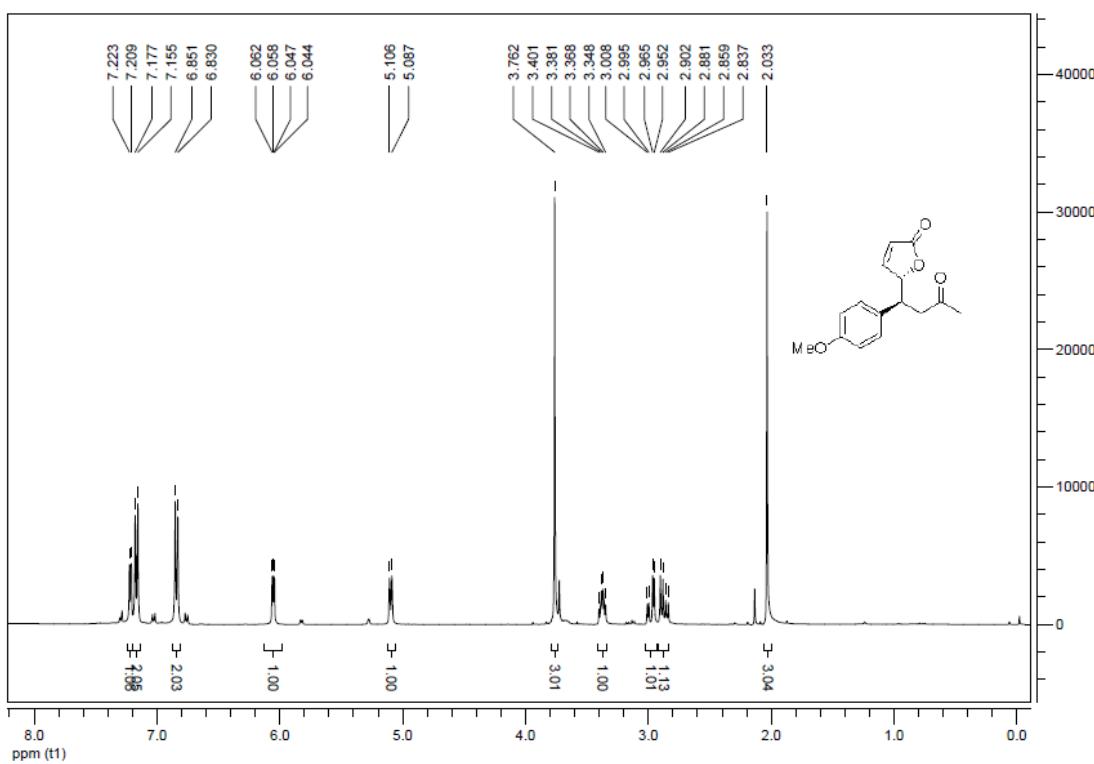
6i: 5-(1-(2-methoxyphenyl)-3-oxobutyl)furan-2(5H)-one



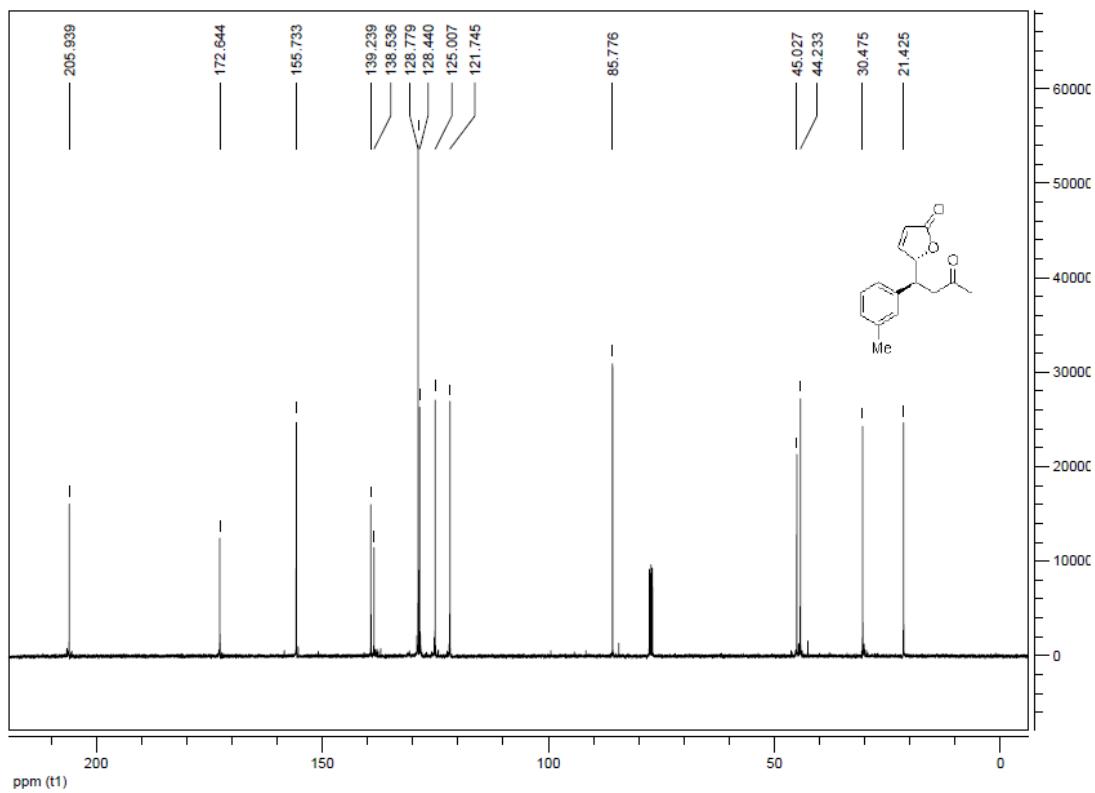
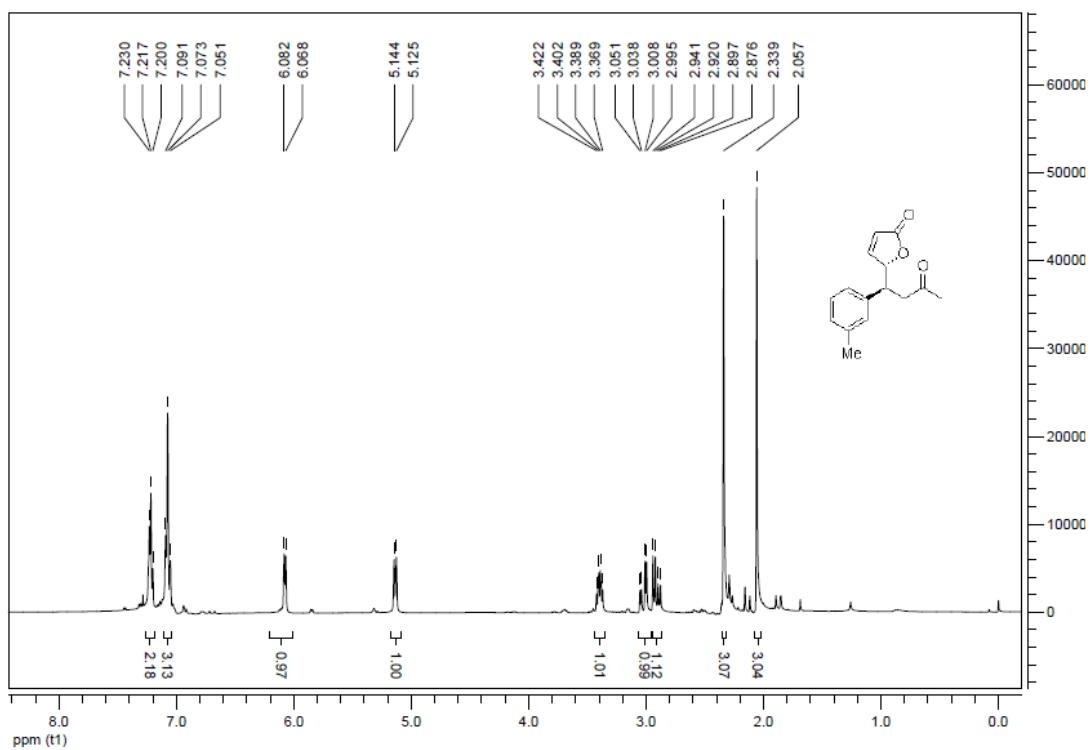
6j: 5-(1-(2-methoxyphenyl)-3-oxobutyl)furan-2(5H)-one



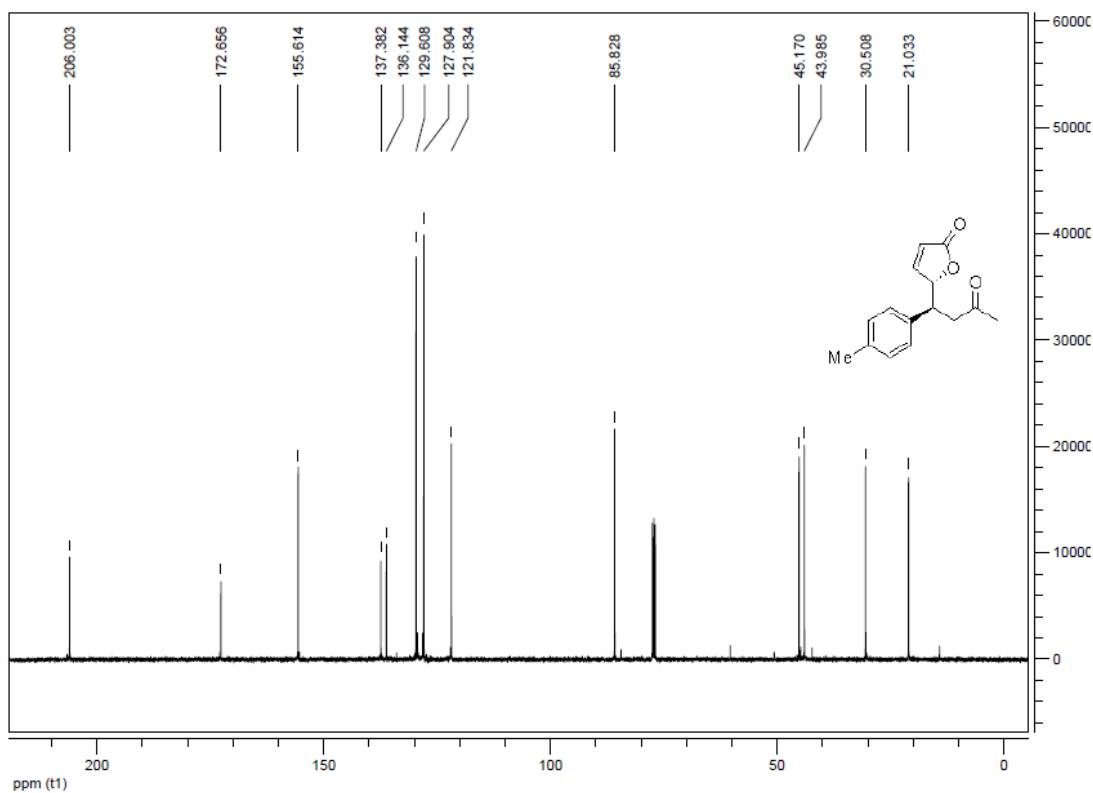
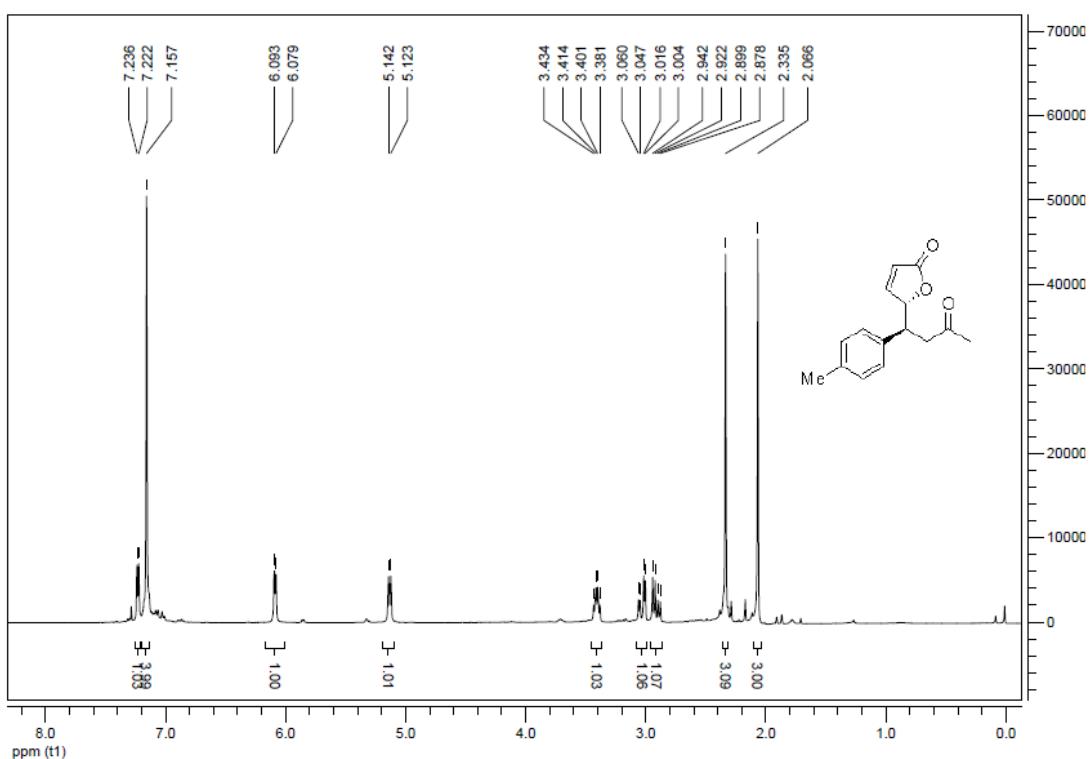
6k: 5-(1-(4-methoxyphenyl)-3-oxobutyl)furan-2(5H)-one



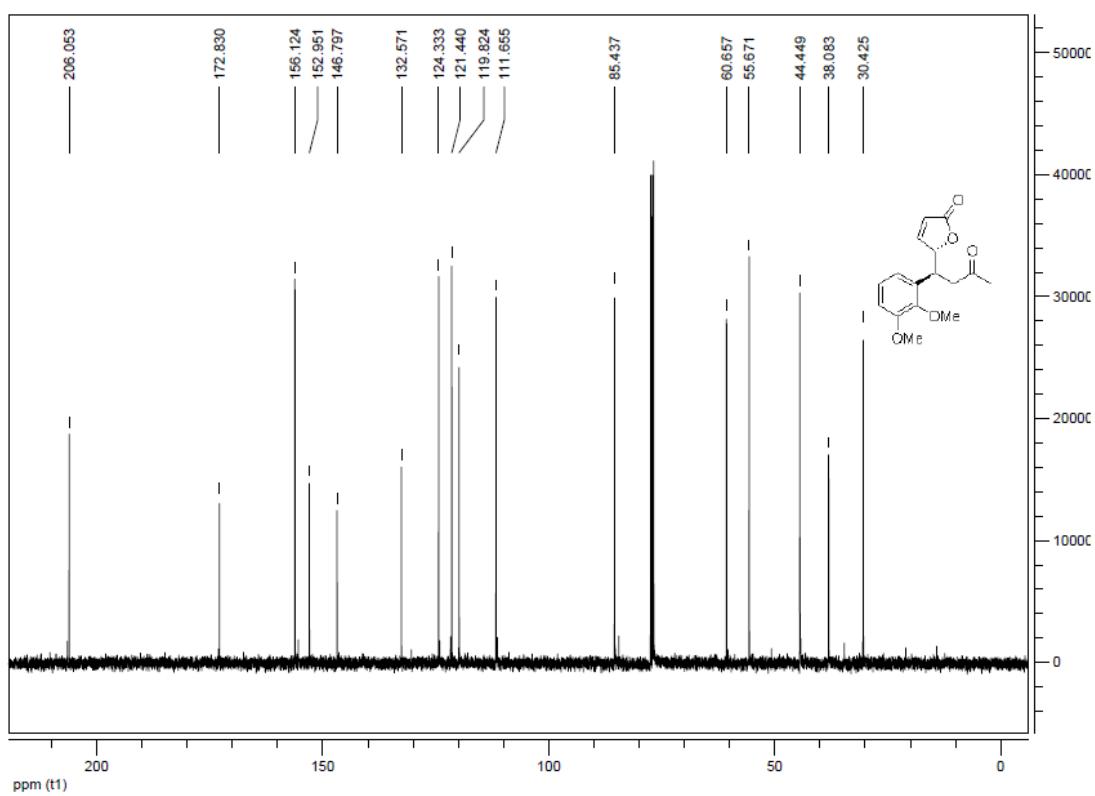
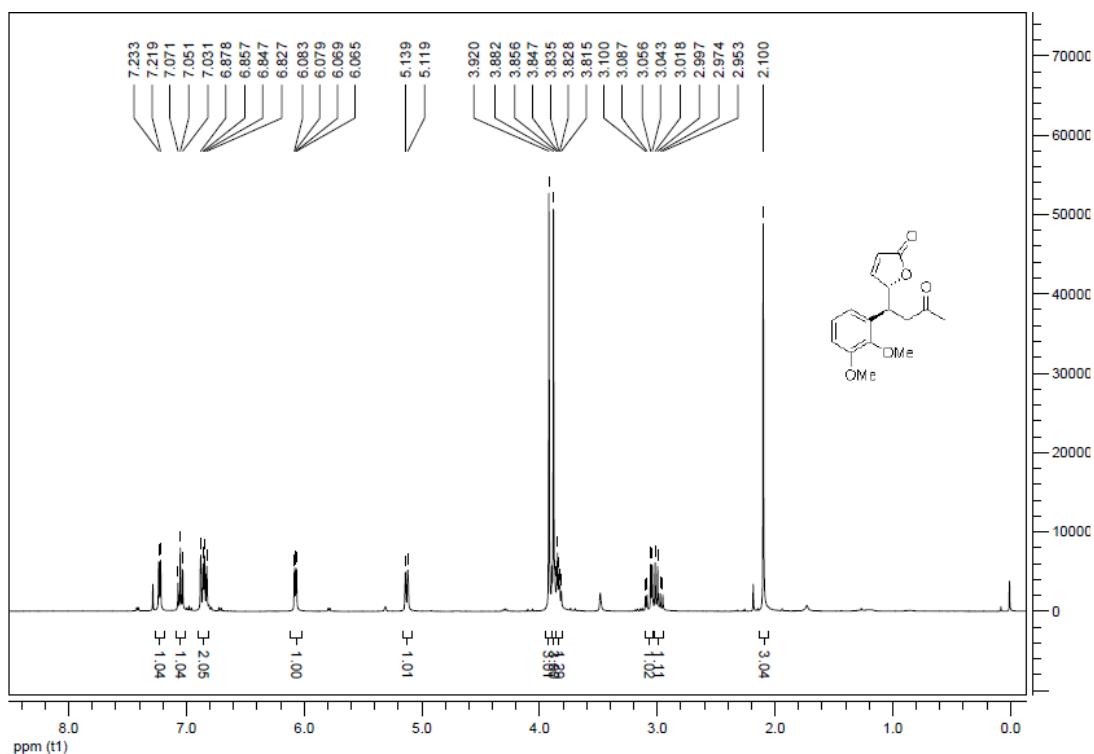
6l: 5-(3-oxo-1-*m*-tolylbutyl)furan-2(5H)-one



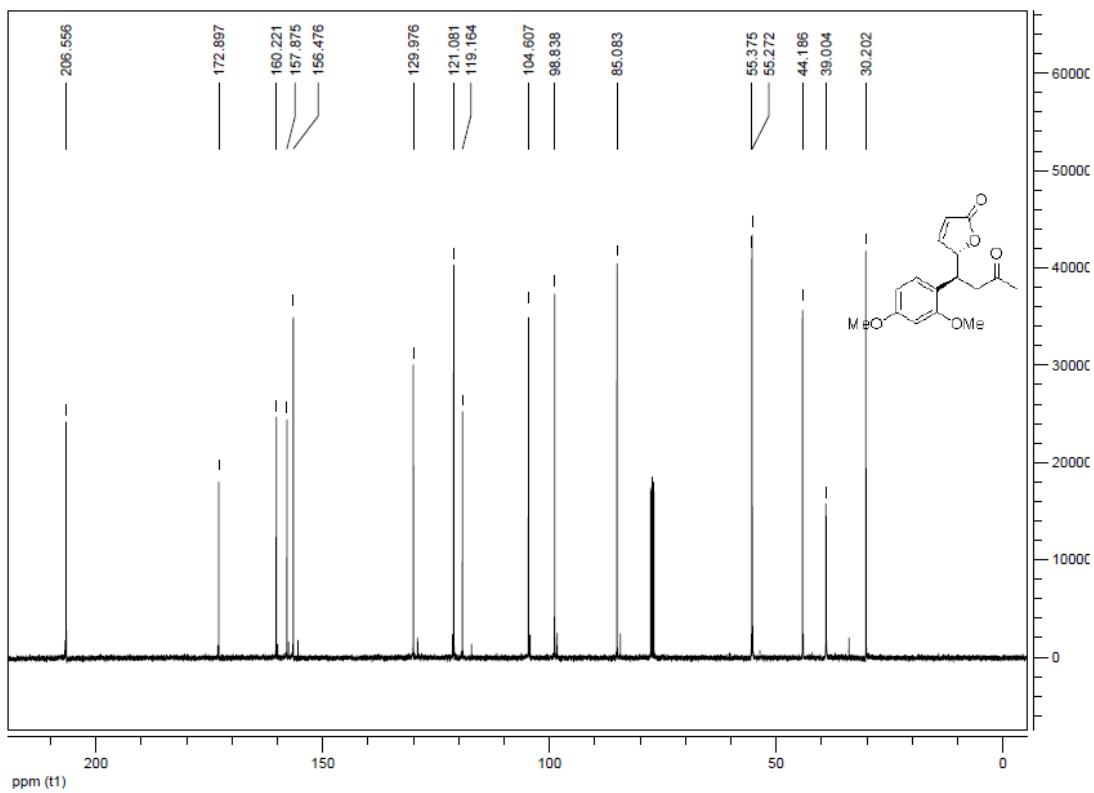
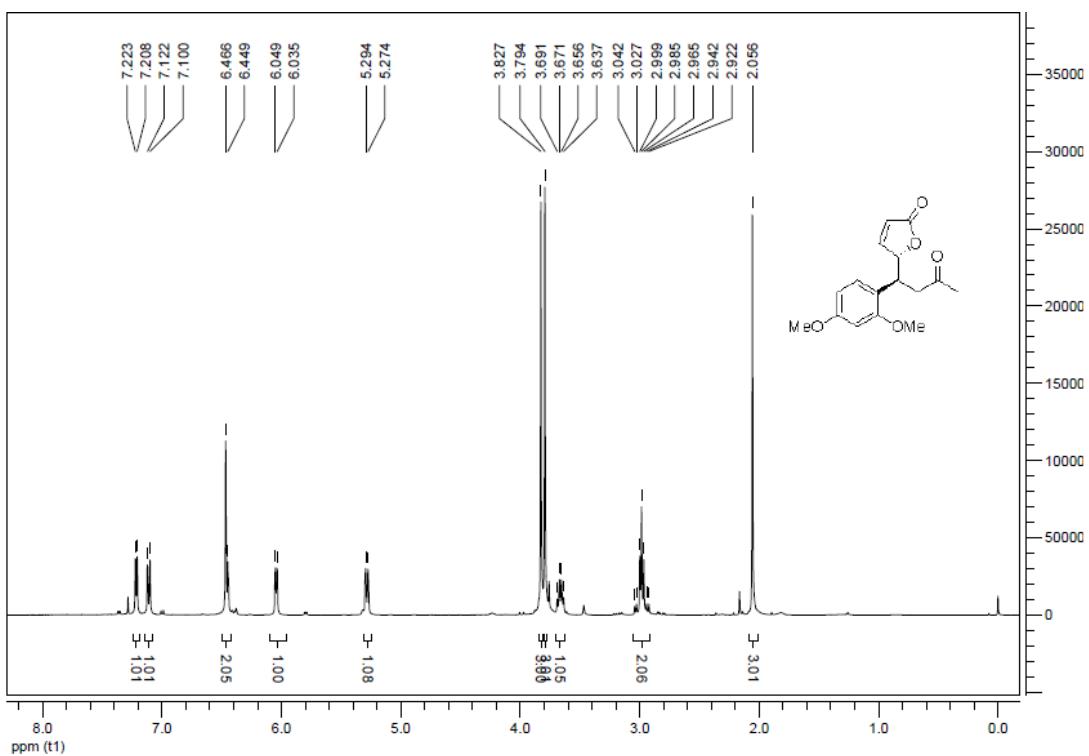
6m: 5-(3-oxo-1-*p*-tolylbutyl)furan-2(5*H*)-one



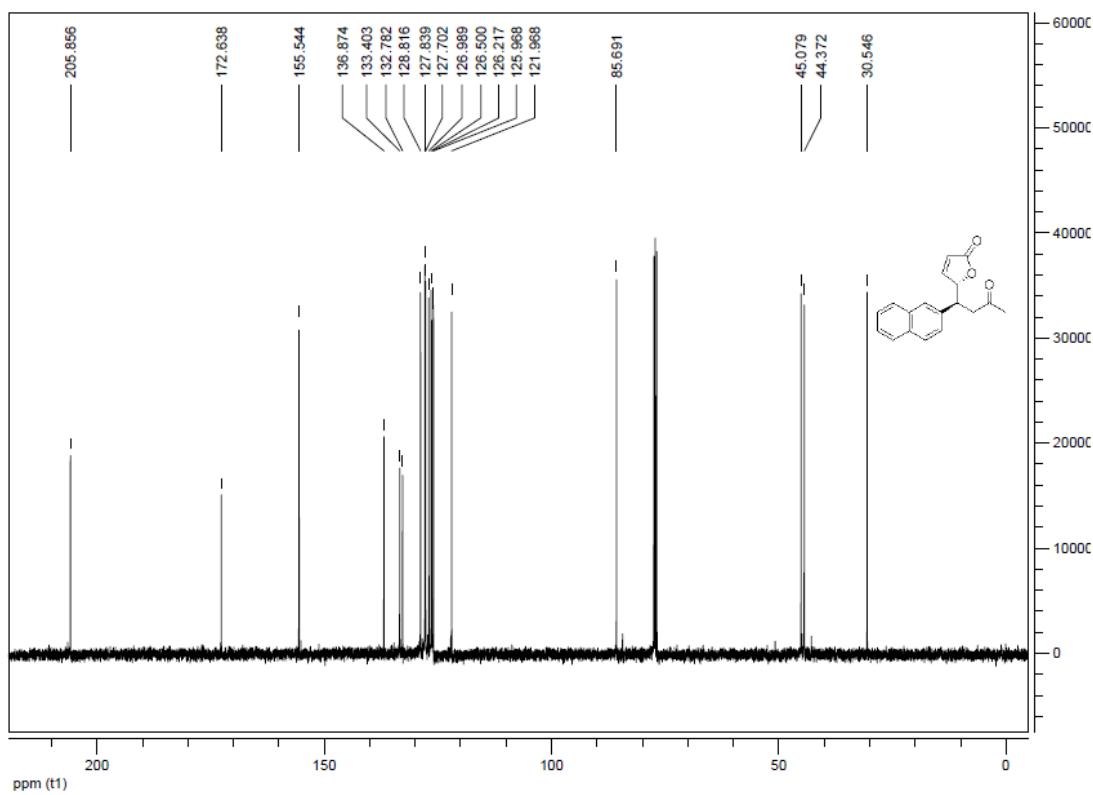
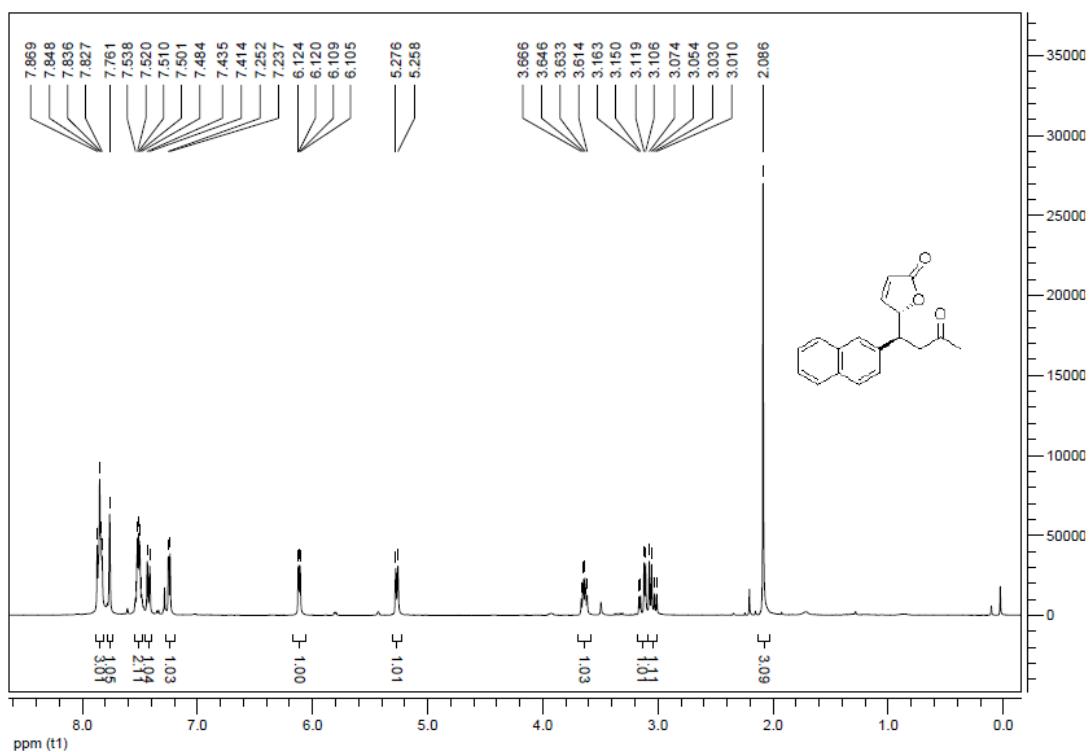
6n: 5-(1-(2,3-dimethoxyphenyl)-3-oxobutyl)furan-2(5H)-one



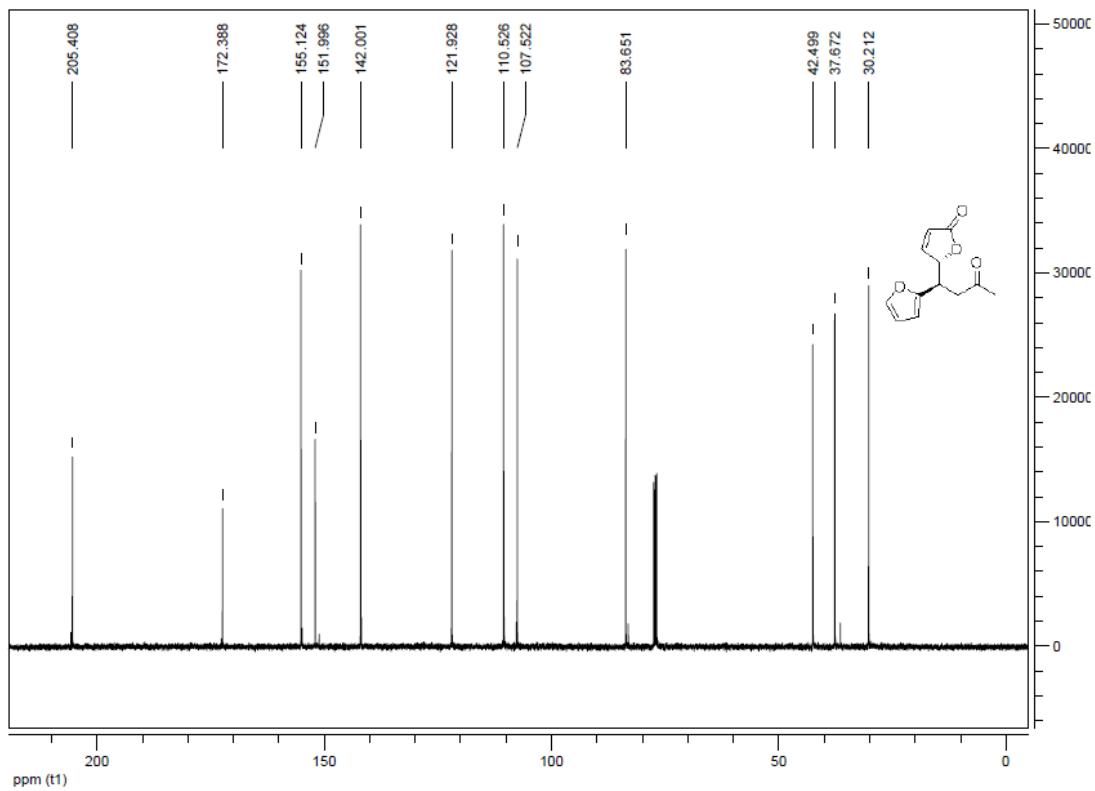
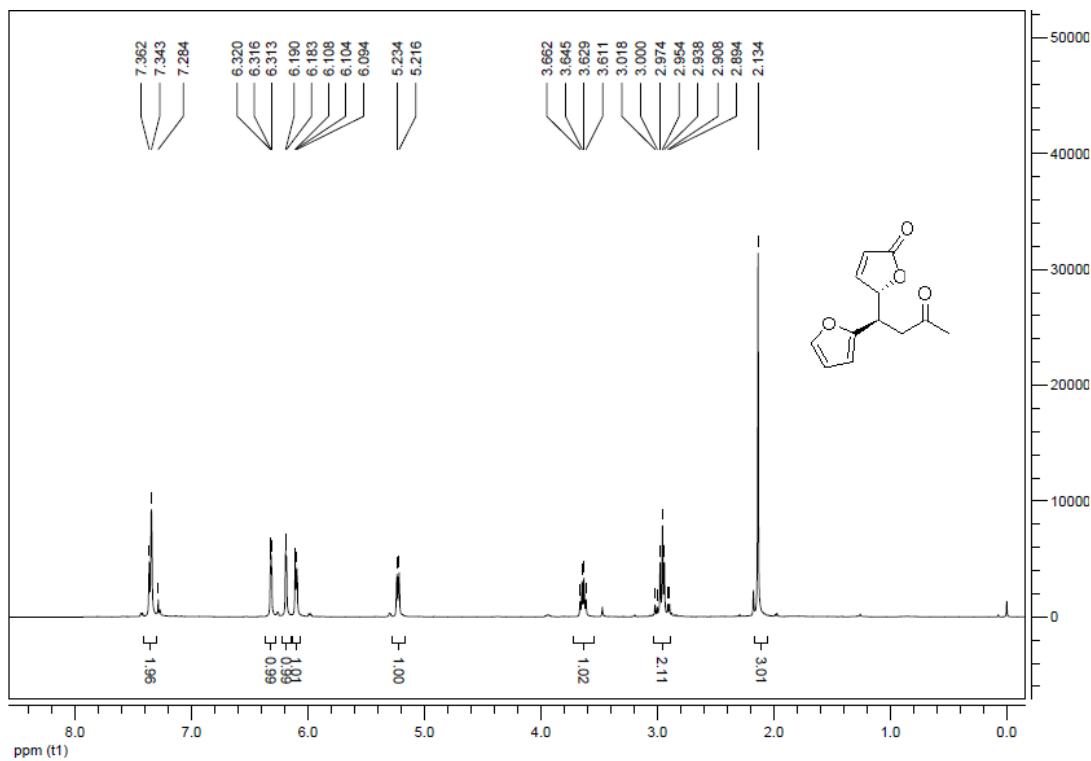
6o: 5-(1-(2,4-dimethoxyphenyl)-3-oxobutyl)furan-2(5H)-one



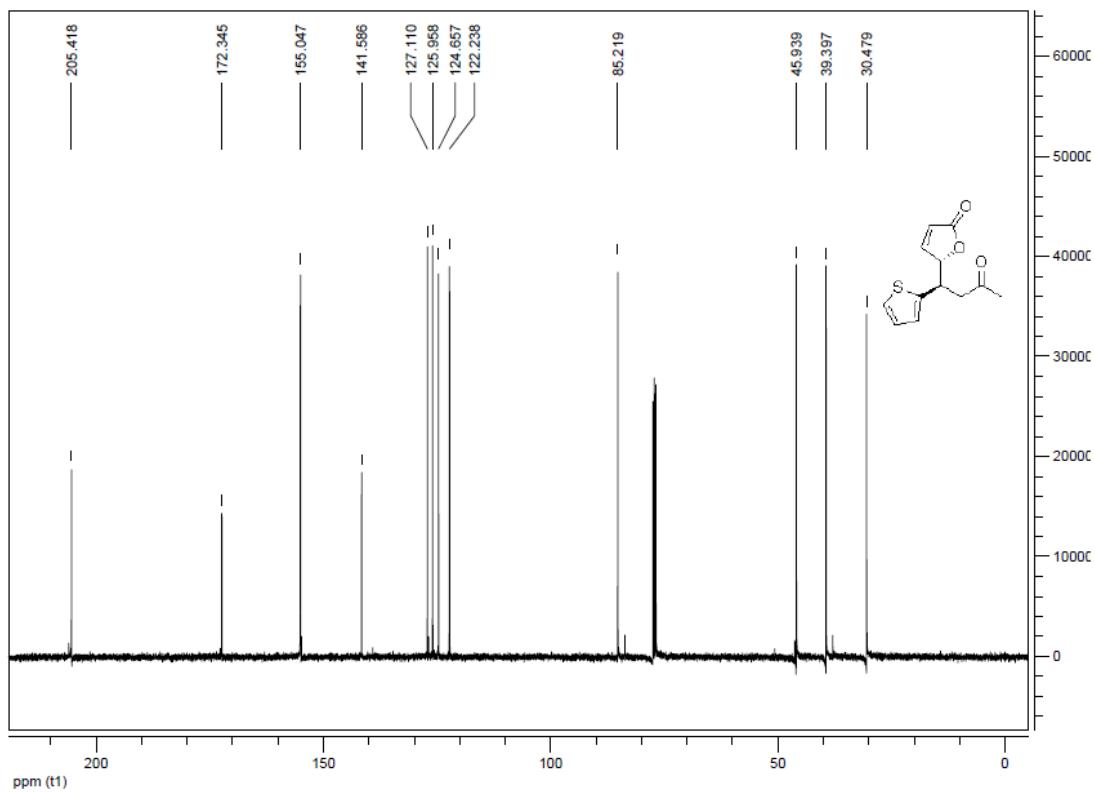
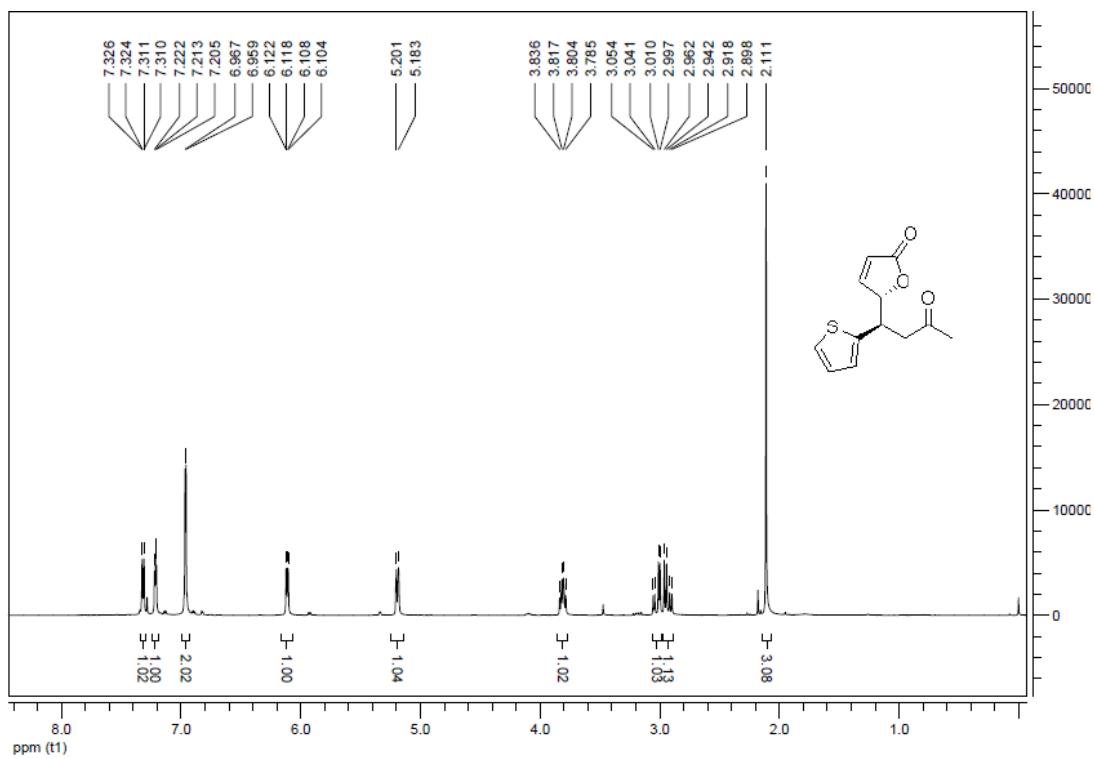
6p: 5-(1-(naphthalen-2-yl)-3-oxobutyl)furan-2(5H)-one



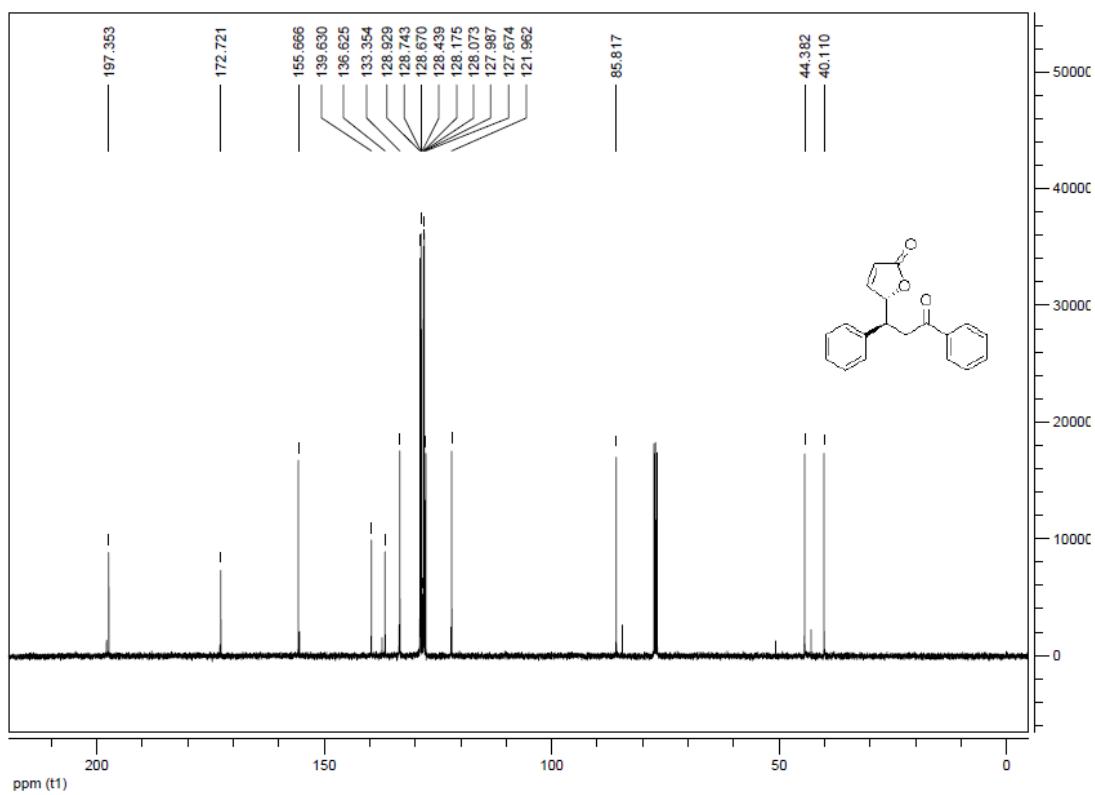
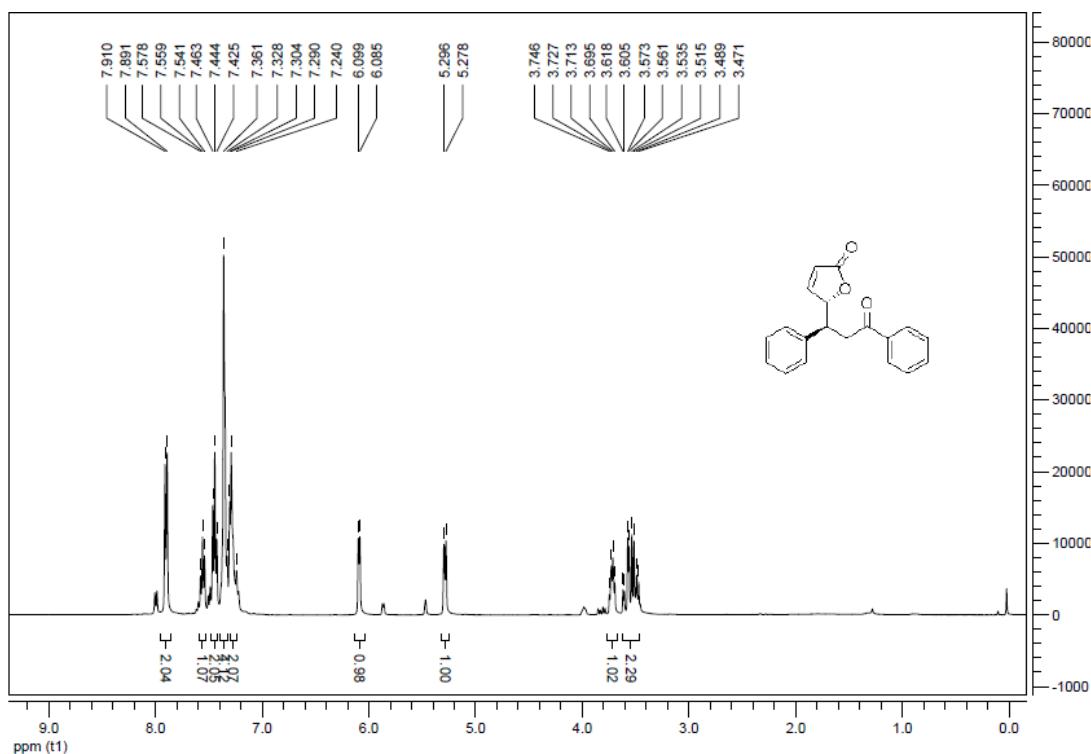
6q: 5-(1-(furan-2-yl)-3-oxobutyl)furan-2(5H)-one



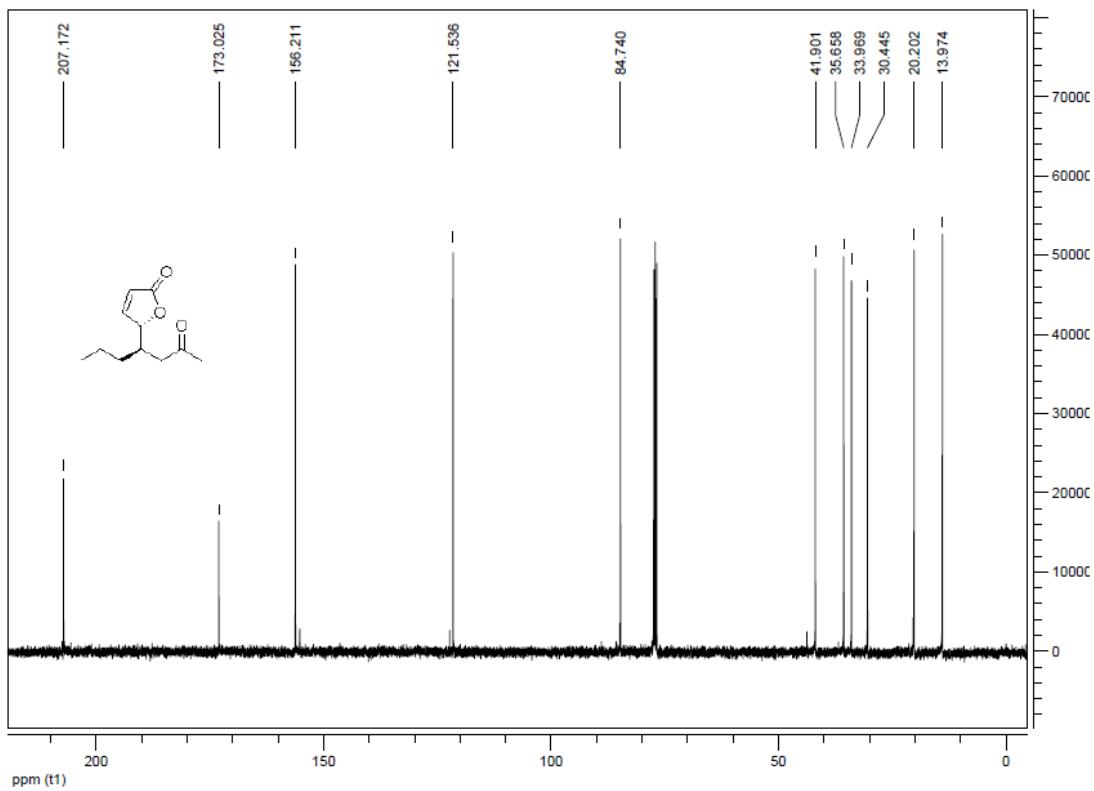
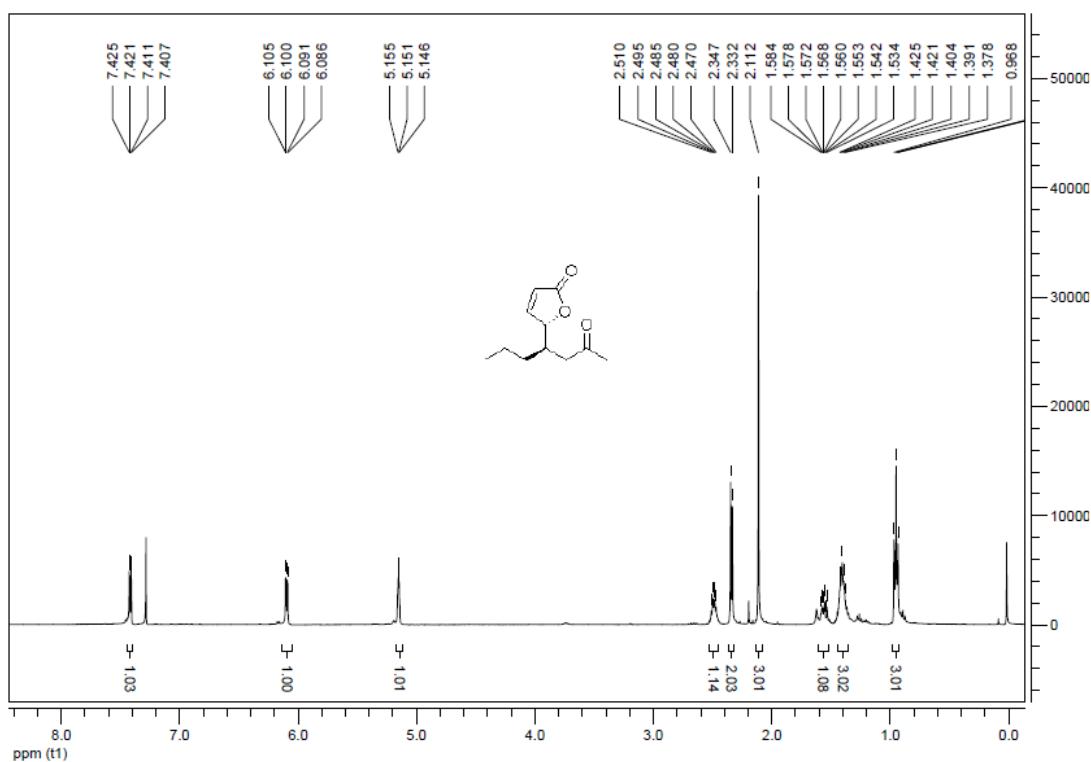
6r: 5-(3-oxo-1-(thiophen-2-yl)butyl)furan-2(5H)-one



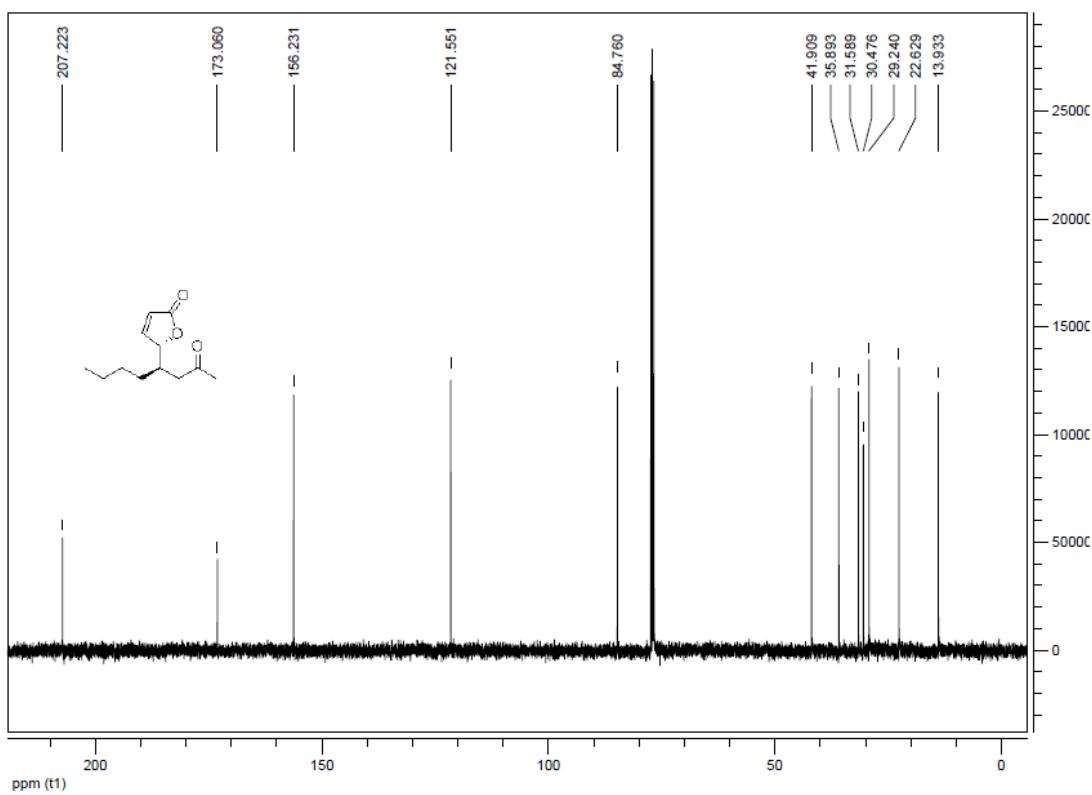
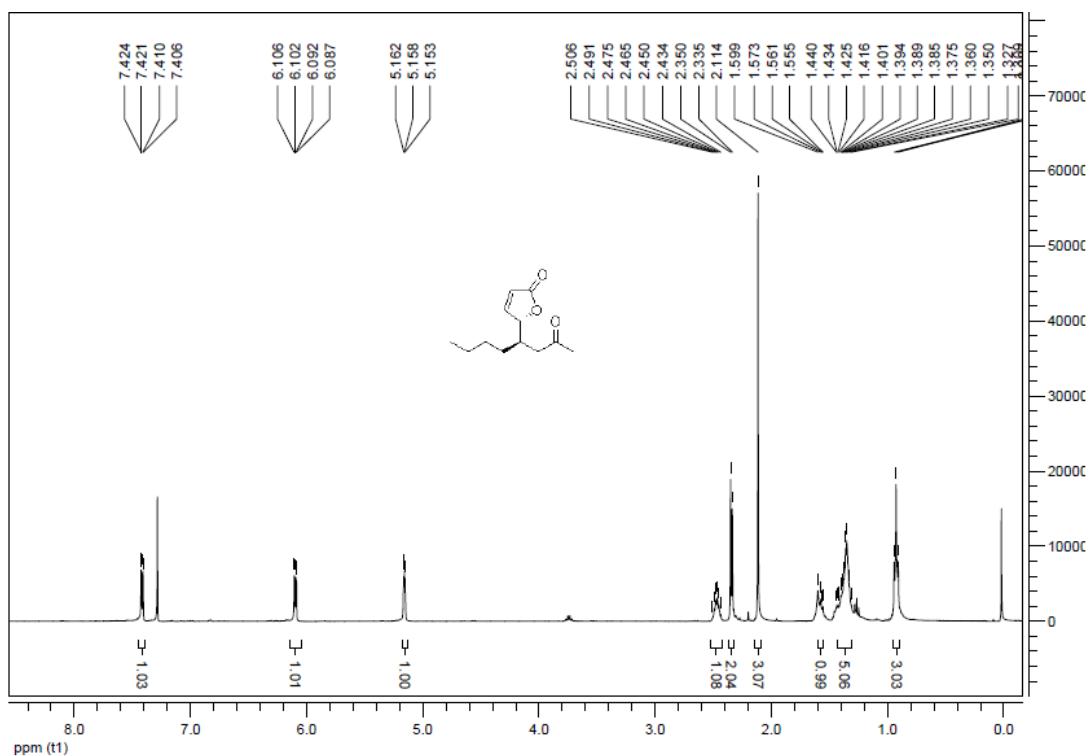
6s: 5-(3-oxo-1,3-diphenylpropyl)furan-2(5H)-one



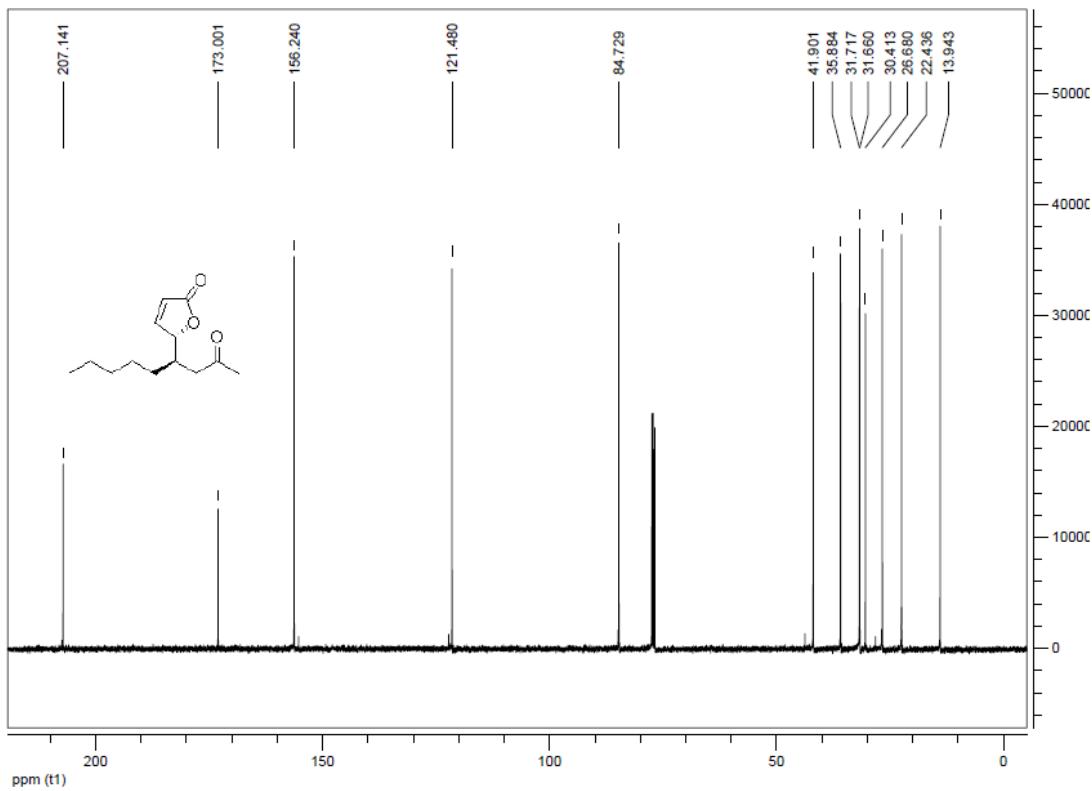
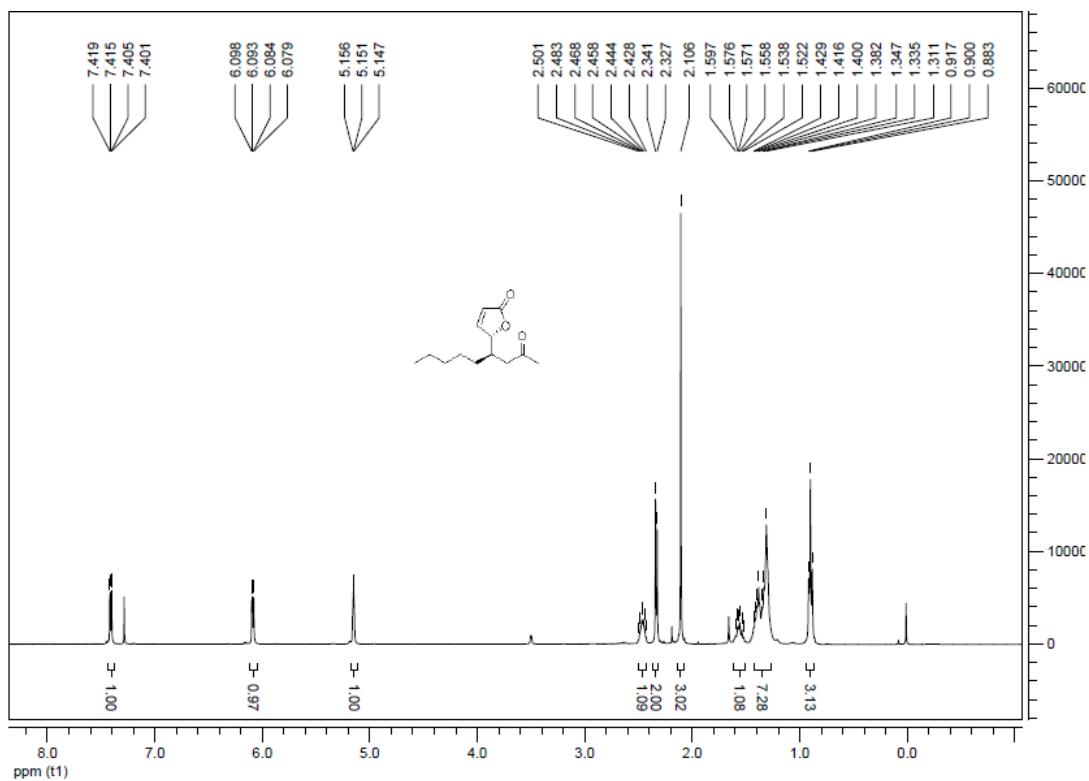
6t: 5-(2-oxoheptan-4-yl)furan-2(5H)-one



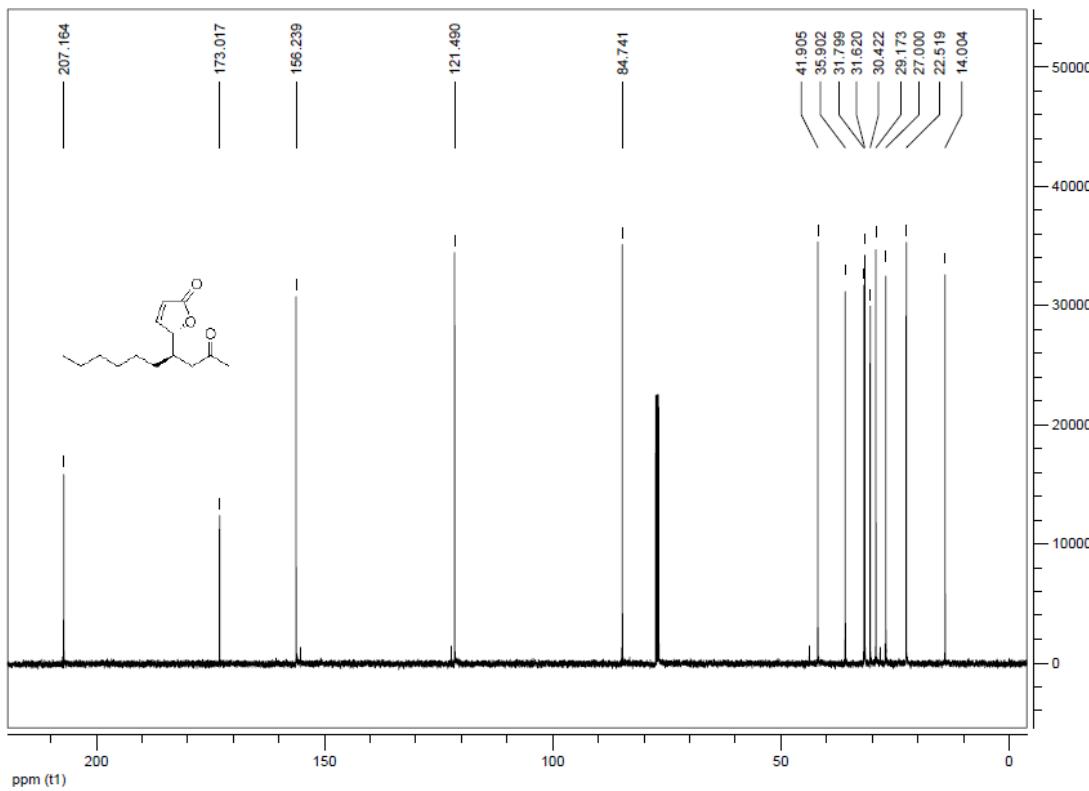
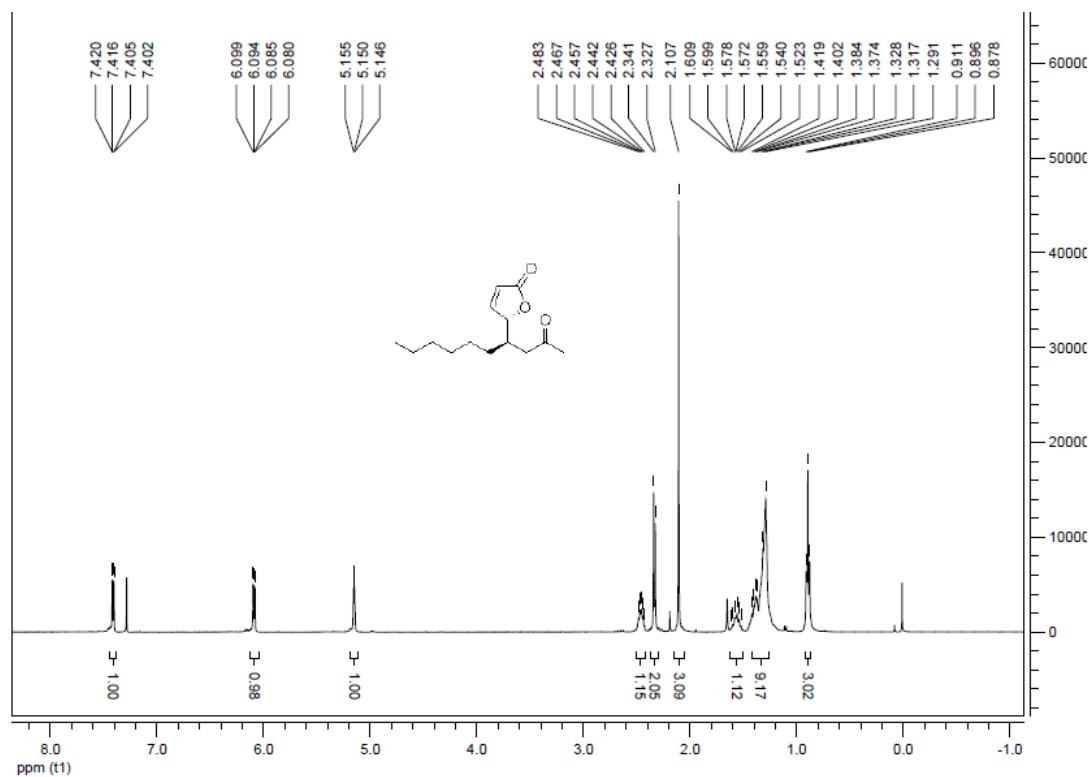
6u: 5-(2-oxooctan-4-yl)furan-2(5H)-one



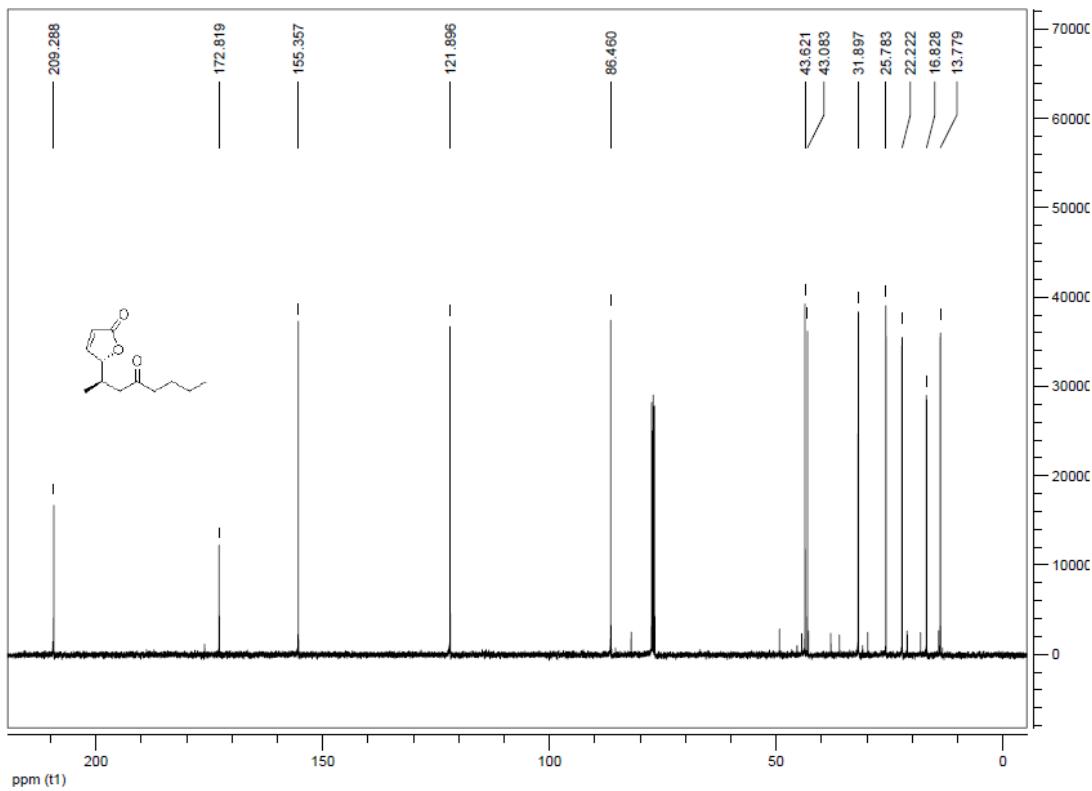
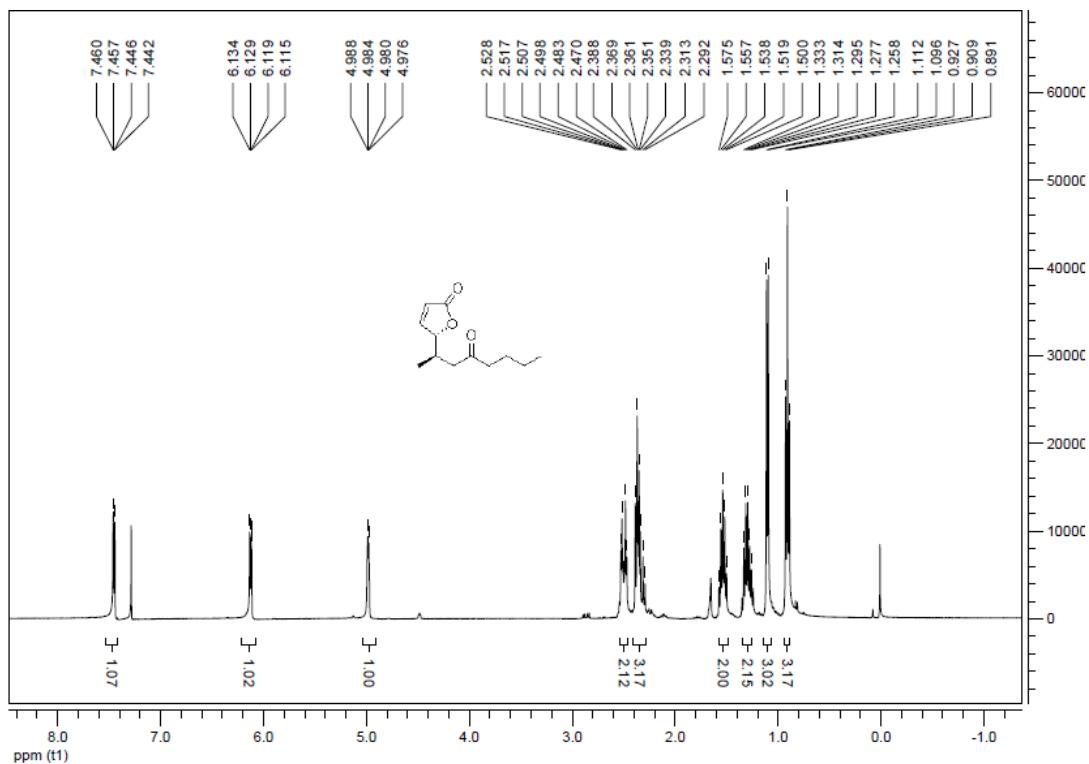
6v: 5-(2-oxanonan-4-yl)furan-2(5H)-one



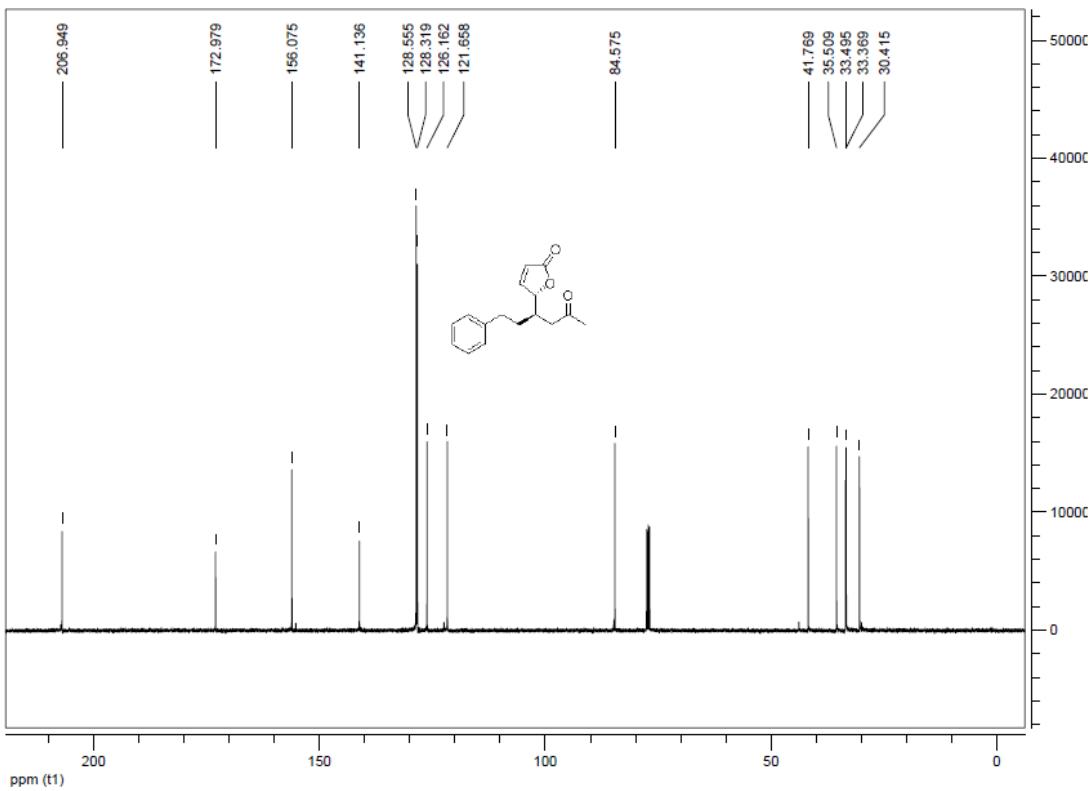
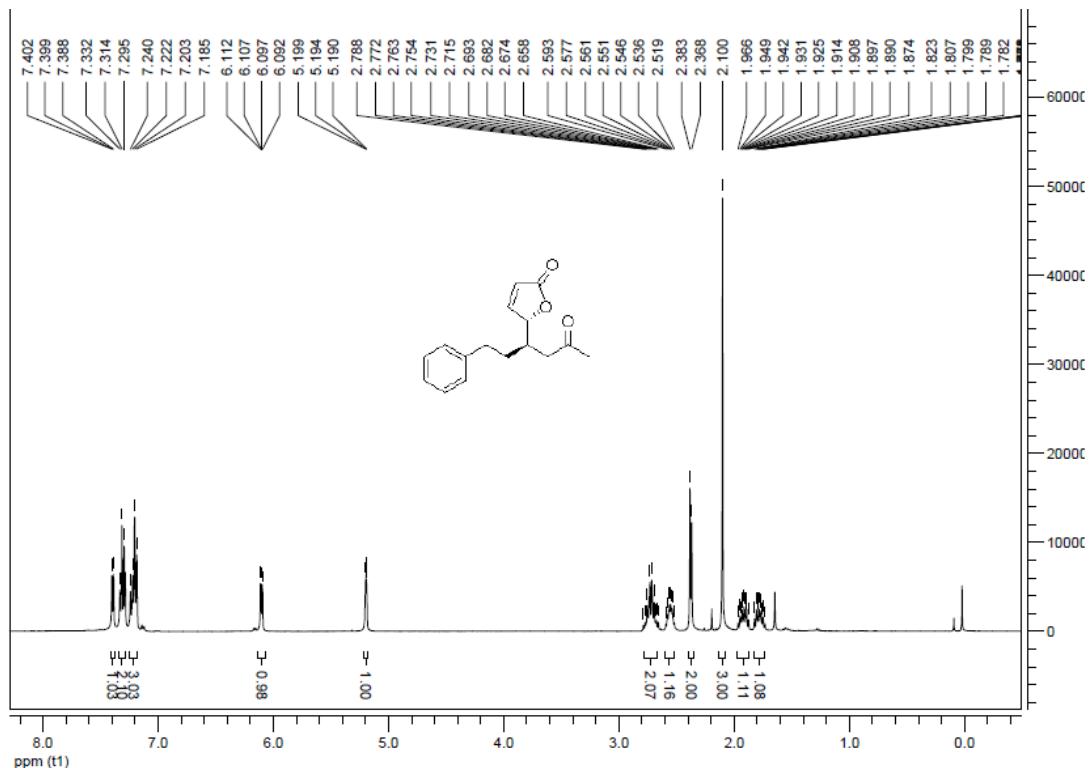
6w: 5-(2-oxodecan-4-yl)furan-2(5H)-one



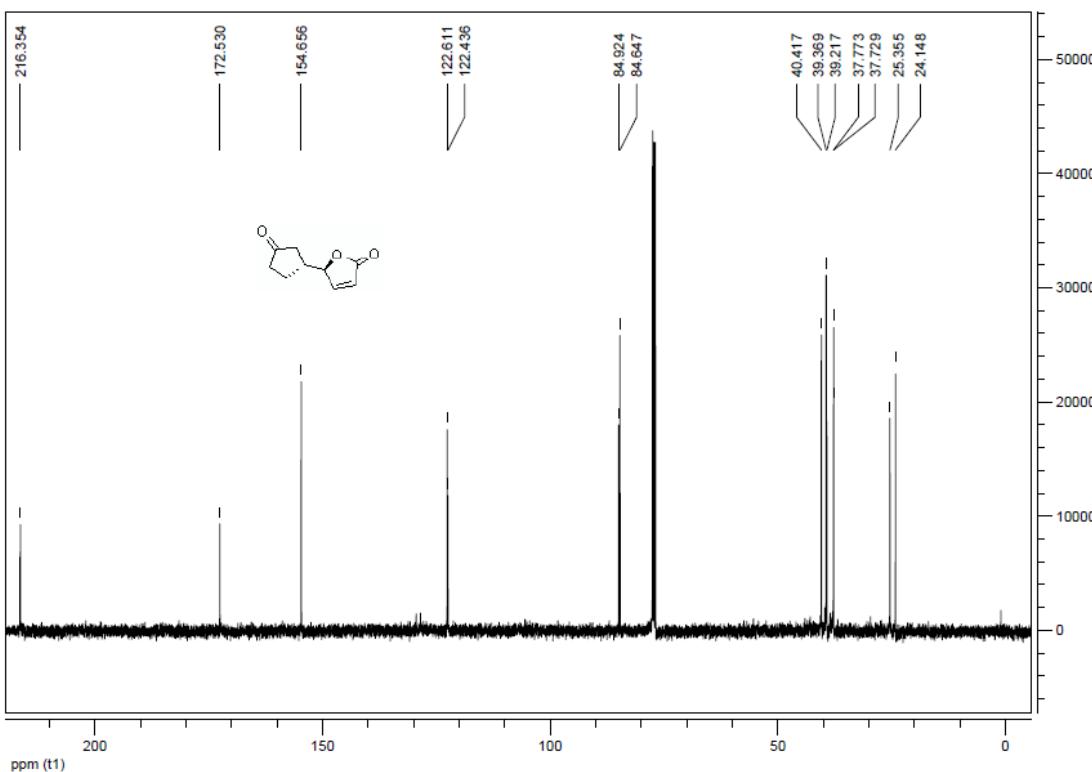
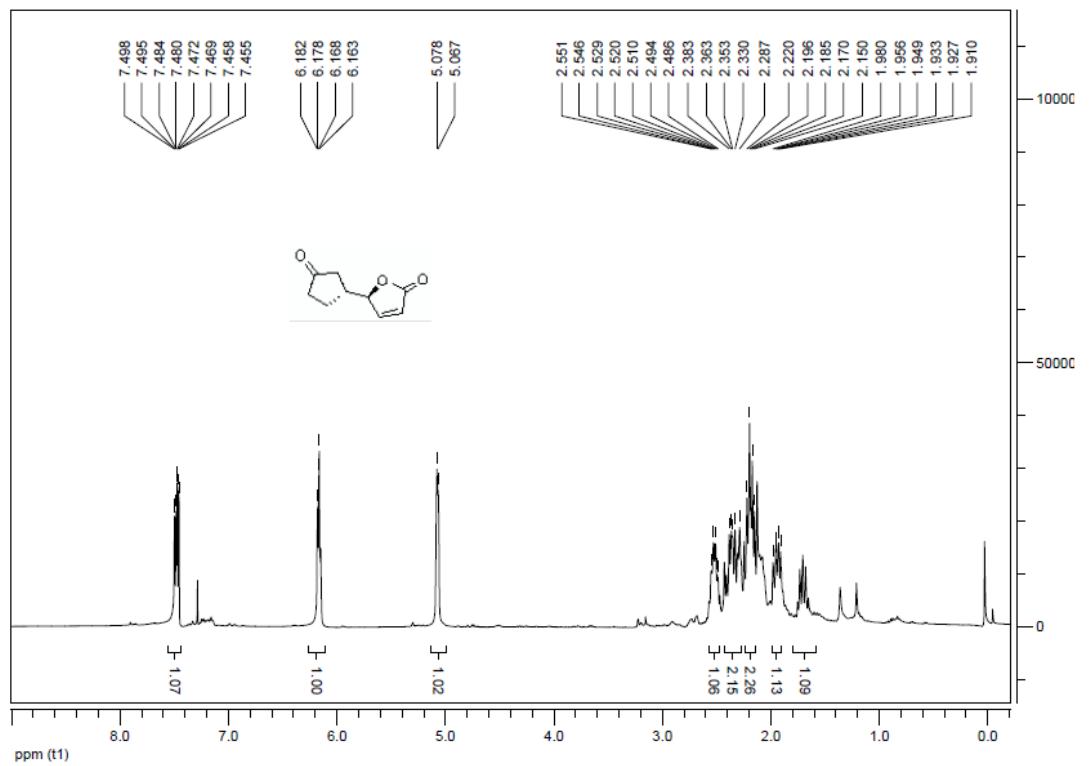
6x: 5-(4-oxooctan-2-yl)furan-2(5H)-one



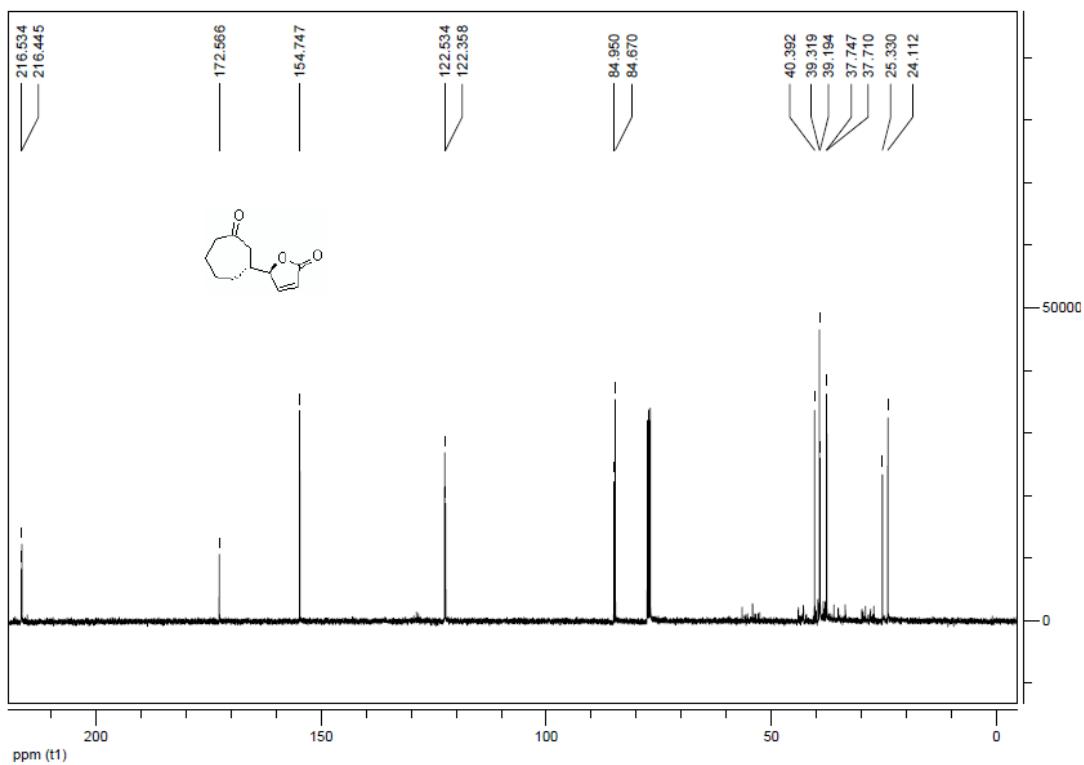
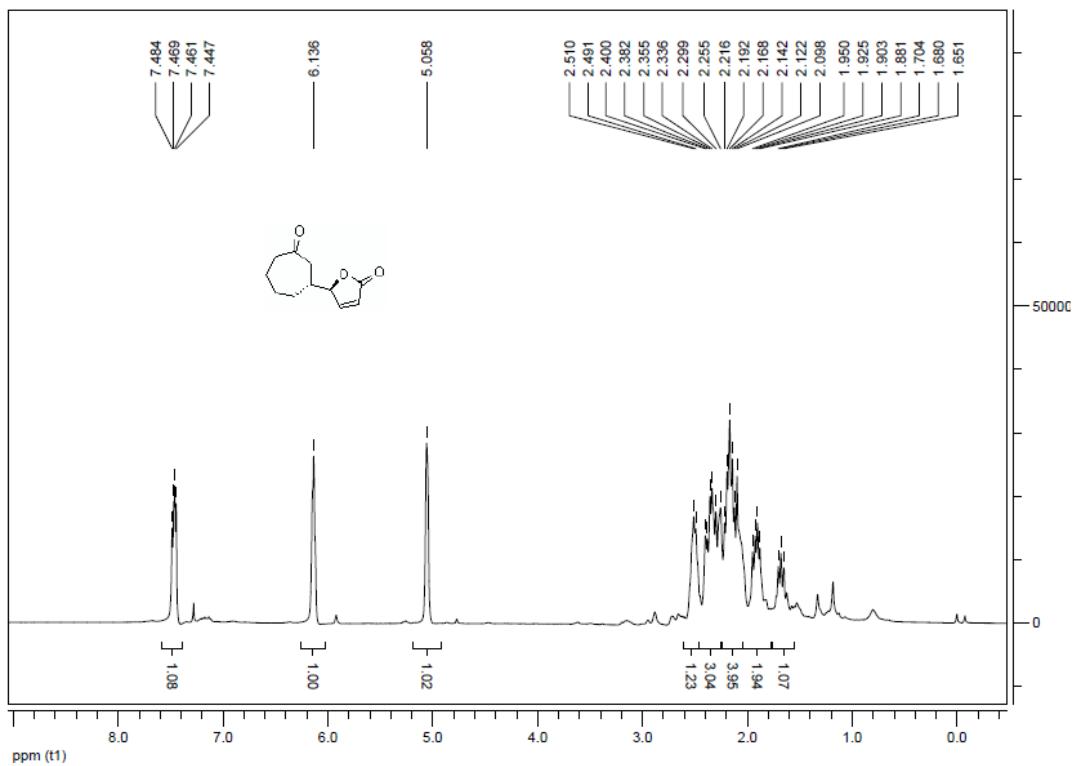
6y: 5-(5-oxo-1-phenylhexan-3-yl)furan-2(5H)-one



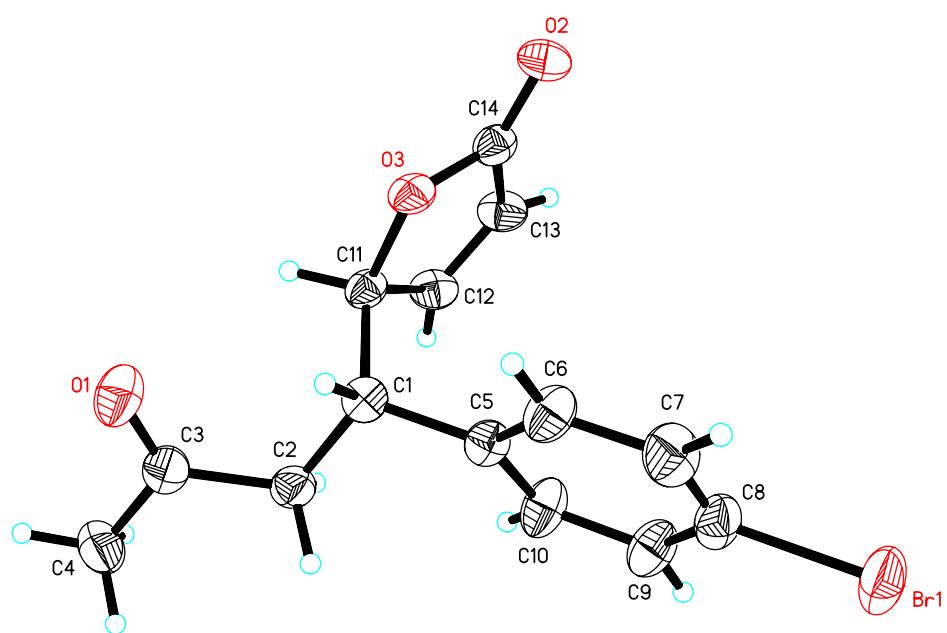
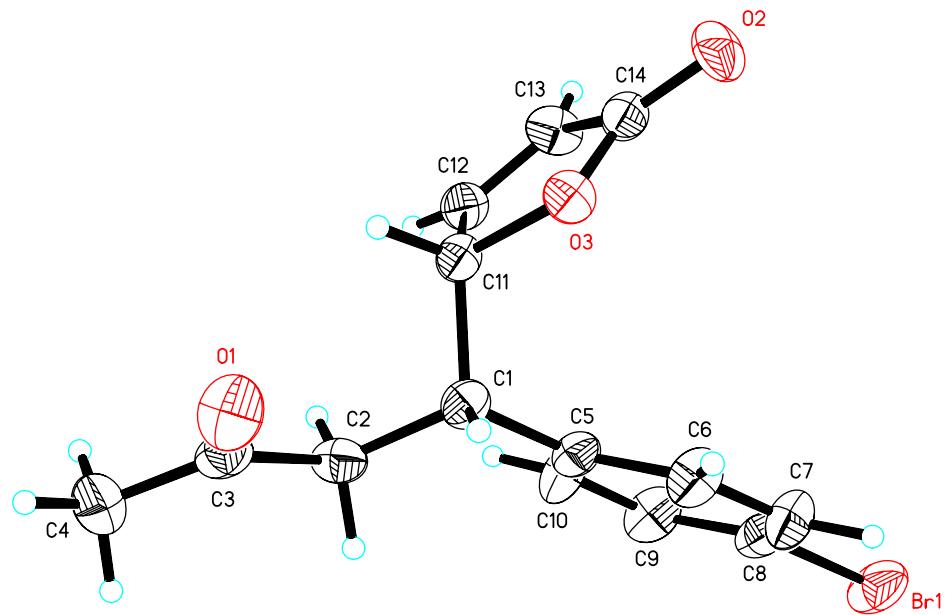
7a: 5-(3-oxocyclopentyl)furan-2(5H)-one

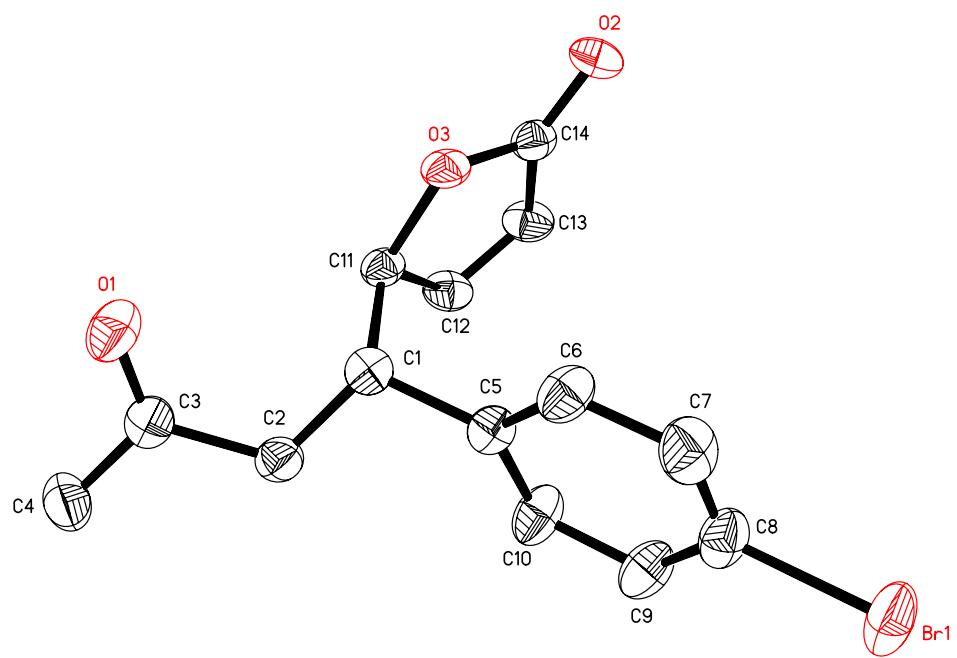
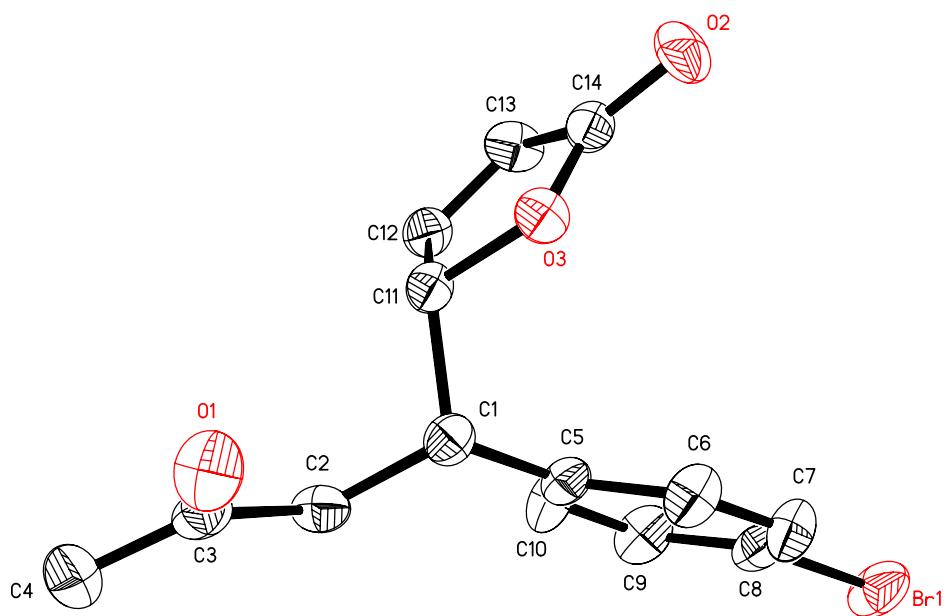


7b: 5-(3-oxocycloheptyl)furan-2(5H)-one



G: Absolute Configuration and X-Ray Analysis Data





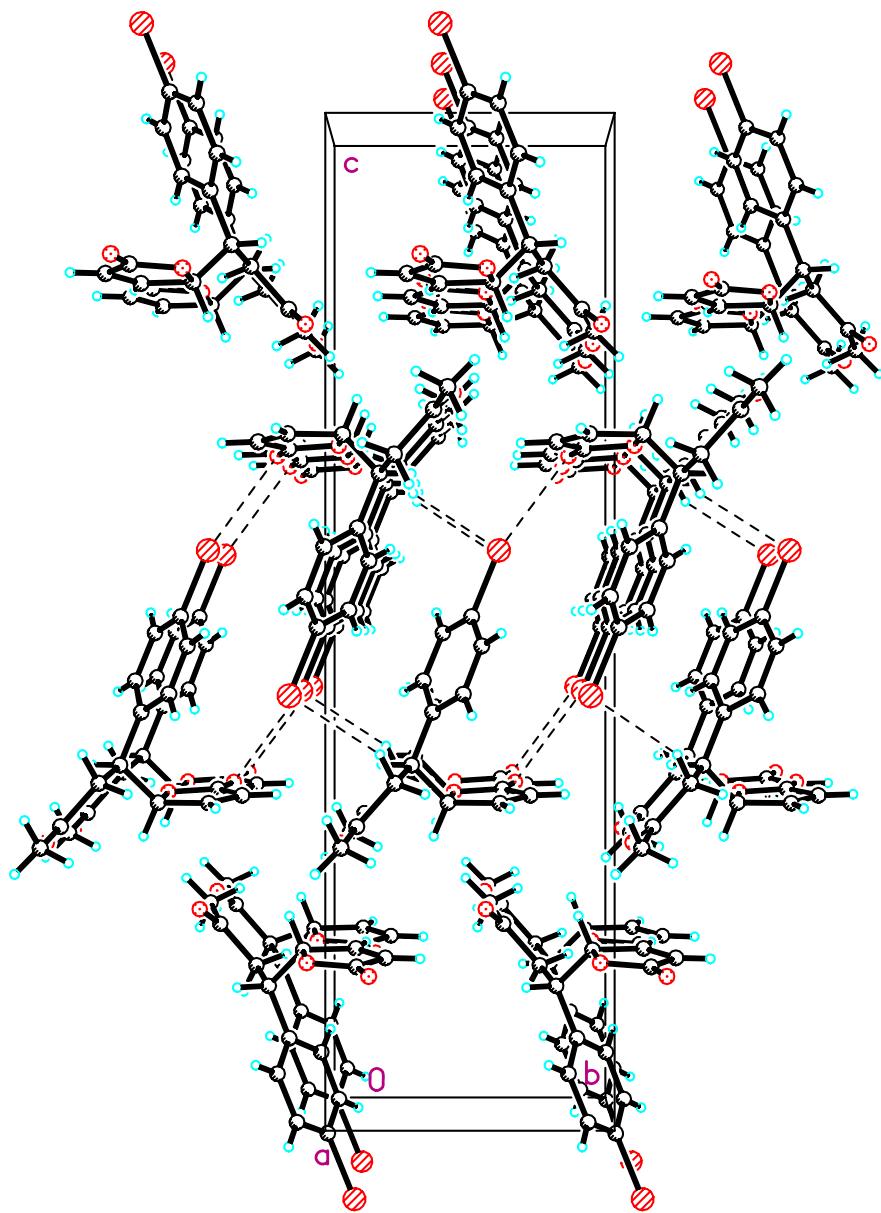


Table 1. Crystal data and structure refinement for cd20181.

Identification code	cd20181
Empirical formula	C14 H13 Br O3
Formula weight	309.15
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	$a = 6.5631(11)$ Å $\alpha = 90$ deg. $b = 7.7659(12)$ Å $\beta = 90$ deg. $c = 27.286(4)$ Å $\gamma = 90$ deg.
Volume	1390.7(4) Å ³
Z, Calculated density	4, 1.477 Mg/m ³

Absorption coefficient	2.953 mm ⁻¹
F(000)	624
Crystal size	0.425 x 0.340 x 0.308 mm
Theta range for data collection	2.73 to 27.50 deg.
Limiting indices	-8<=h<=8, -9<=k<=10, -19<=l<=35
Reflections collected / unique	8391 / 3168 [R(int) = 0.0517]
Completeness to theta = 27.50	99.5 %
Absorption correction	Empirical
Max. and min. transmission	1.0000 and 0.4111
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3168 / 0 / 165

Goodness-of-fit on F^2	0.847
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0414, wR2 = 0.0838
R indices (all data)	R1 = 0.0765, wR2 = 0.0910
Absolute structure parameter	0.036(12)
Extinction coefficient	0.0309(15)
Largest diff. peak and hole	0.615 and -0.574 e. \AA^{-3}

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic

displacement parameters ($\text{\AA}^2 \times 10^3$) for cd20181.

$U(\text{eq})$ is defined as one third of the trace of the orthogonalized

U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Br(1)	9345(1)	10993(1)	-699(1)	83(1)
O(1)	8262(5)	5554(4)	2143(1)	73(1)
O(2)	14229(4)	11606(3)	1619(1)	62(1)
O(3)	12042(3)	9439(3)	1696(1)	45(1)
C(1)	8985(5)	7999(5)	1398(1)	45(1)
C(2)	6833(6)	7466(5)	1552(1)	50(1)
C(3)	6748(7)	6181(5)	1966(1)	52(1)
C(4)	4654(6)	5714(6)	2141(2)	75(1)
C(5)	9068(6)	8721(4)	882(1)	45(1)
C(6)	10710(6)	8385(5)	582(1)	58(1)
C(7)	10802(7)	9061(6)	111(2)	70(1)

C(8)	9260(8)	10062(5)	-51(1)	61(1)
C(9)	7600(7)	10403(5)	234(2)	64(1)
C(10)	7536(6)	9778(5)	699(2)	61(1)
C(11)	9883(4)	9238(5)	1774(1)	41(1)
C(12)	9101(5)	11036(5)	1771(1)	49(1)
C(13)	10608(6)	12092(5)	1713(1)	52(1)
C(14)	12505(6)	11150(5)	1669(1)	45(1)

Table 3. Bond lengths [Å] and angles [deg] for cd20181.

Br(1)-C(8)	1.911(4)
O(1)-C(3)	1.207(5)
O(2)-C(14)	1.194(4)
O(3)-C(14)	1.365(4)
O(3)-C(11)	1.441(4)
C(1)-C(5)	1.516(5)
C(1)-C(11)	1.526(5)
C(1)-C(2)	1.531(5)
C(1)-H(1)	0.9800
C(2)-C(3)	1.509(5)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.498(5)
C(4)-H(4A)	0.9600
C(4)-H(4B)	0.9600
C(4)-H(4C)	0.9600
C(5)-C(6)	1.379(5)
C(5)-C(10)	1.391(5)

C(6)-C(7)	1.390(5)
C(6)-H(6)	0.9300
C(7)-C(8)	1.350(6)
C(7)-H(7)	0.9300
C(8)-C(9)	1.364(6)
C(9)-C(10)	1.359(5)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(11)-C(12)	1.487(5)
C(11)-H(11)	0.9800
C(12)-C(13)	1.295(5)
C(12)-H(12)	0.9300
C(13)-C(14)	1.448(5)
C(13)-H(13)	0.9300
C(14)-O(3)-C(11)	109.4(3)
C(5)-C(1)-C(11)	112.2(3)
C(5)-C(1)-C(2)	112.8(3)
C(11)-C(1)-C(2)	110.0(3)
C(5)-C(1)-H(1)	107.2
C(11)-C(1)-H(1)	107.2
C(2)-C(1)-H(1)	107.2

C(3)-C(2)-C(1)	114.7(3)
C(3)-C(2)-H(2A)	108.6
C(1)-C(2)-H(2A)	108.6
C(3)-C(2)-H(2B)	108.6
C(1)-C(2)-H(2B)	108.6
H(2A)-C(2)-H(2B)	107.6
O(1)-C(3)-C(4)	122.1(4)
O(1)-C(3)-C(2)	122.3(4)
C(4)-C(3)-C(2)	115.6(4)
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(6)-C(5)-C(10)	117.6(3)
C(6)-C(5)-C(1)	120.6(3)
C(10)-C(5)-C(1)	121.7(3)
C(5)-C(6)-C(7)	120.8(4)
C(5)-C(6)-H(6)	119.6
C(7)-C(6)-H(6)	119.6
C(8)-C(7)-C(6)	119.2(4)

C(8)-C(7)-H(7)	120.4
C(6)-C(7)-H(7)	120.4
C(7)-C(8)-C(9)	121.6(4)
C(7)-C(8)-Br(1)	119.9(3)
C(9)-C(8)-Br(1)	118.5(3)
C(10)-C(9)-C(8)	119.1(4)
C(10)-C(9)-H(9)	120.4
C(8)-C(9)-H(9)	120.4
C(9)-C(10)-C(5)	121.6(4)
C(9)-C(10)-H(10)	119.2
C(5)-C(10)-H(10)	119.2
O(3)-C(11)-C(12)	103.7(3)
O(3)-C(11)-C(1)	110.4(3)
C(12)-C(11)-C(1)	117.0(3)
O(3)-C(11)-H(11)	108.5
C(12)-C(11)-H(11)	108.5
C(1)-C(11)-H(11)	108.5
C(13)-C(12)-C(11)	109.4(3)
C(13)-C(12)-H(12)	125.3
C(11)-C(12)-H(12)	125.3
C(12)-C(13)-C(14)	110.3(3)
C(12)-C(13)-H(13)	124.9

C(14)-C(13)-H(13)	124.9
O(2)-C(14)-O(3)	120.4(3)
O(2)-C(14)-C(13)	132.4(4)
O(3)-C(14)-C(13)	107.2(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for cd20181.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Br(1)	141(1)	65(1)	42(1)	2(1)	7(1)	-12(1)
O(1)	78(2)	70(2)	70(2)	17(2)	-1(2)	18(2)
O(2)	29(1)	80(2)	76(2)	7(1)	-2(1)	0(2)
O(3)	31(1)	51(2)	52(2)	2(1)	-5(1)	11(1)
C(1)	45(2)	44(2)	46(2)	-4(2)	3(2)	6(2)
C(2)	58(2)	41(2)	51(2)	-3(2)	-10(2)	-2(2)
C(3)	72(3)	40(2)	45(2)	-10(2)	-2(2)	2(2)
C(4)	83(3)	71(3)	70(3)	9(3)	5(2)	-22(3)
C(5)	52(2)	42(2)	40(2)	-6(2)	2(2)	4(2)
C(6)	61(3)	63(3)	50(3)	2(2)	0(2)	18(2)
C(7)	74(3)	81(3)	56(3)	-11(3)	21(2)	2(3)
C(8)	92(3)	51(2)	41(2)	-5(2)	3(3)	-7(3)

C(9)	80(3)	59(3)	53(3)	5(2)	-6(2)	21(2)
C(10)	71(3)	70(3)	43(2)	4(2)	12(2)	25(2)
C(11)	33(2)	51(2)	38(2)	1(2)	-1(1)	7(2)
C(12)	34(2)	61(2)	50(2)	-11(2)	3(2)	7(2)
C(13)	43(2)	44(2)	69(3)	-5(2)	-8(2)	9(2)
C(14)	39(2)	56(3)	39(2)	0(2)	-1(2)	6(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for cd20181.

	x	y	z	U(eq)
H(1)	9828	6957	1402	54
H(2A)	6088	8490	1649	60
H(2B)	6143	6978	1270	60
H(4A)	4753	4849	2391	112
H(4B)	3872	5275	1871	112
H(4C)	3997	6718	2271	112
H(6)	11769	7697	696	70
H(7)	11911	8827	-90	84
H(9)	6525	11054	111	77
H(10)	6442	10064	900	73
H(11)	9670	8754	2102	49
H(12)	7741	11352	1805	58
H(13)	10490	13285	1700	62

Table 6. Torsion angles [deg] for cd20181.

C(5)-C(1)-C(2)-C(3)	158.6(3)
C(11)-C(1)-C(2)-C(3)	-75.3(4)
C(1)-C(2)-C(3)-O(1)	-4.0(5)
C(1)-C(2)-C(3)-C(4)	176.9(3)
C(11)-C(1)-C(5)-C(6)	91.8(4)
C(2)-C(1)-C(5)-C(6)	-143.3(3)
C(11)-C(1)-C(5)-C(10)	-86.4(4)
C(2)-C(1)-C(5)-C(10)	38.5(5)
C(10)-C(5)-C(6)-C(7)	-1.0(5)
C(1)-C(5)-C(6)-C(7)	-179.3(4)
C(5)-C(6)-C(7)-C(8)	0.2(6)
C(6)-C(7)-C(8)-C(9)	-1.1(6)
C(6)-C(7)-C(8)-Br(1)	-179.6(3)
C(7)-C(8)-C(9)-C(10)	2.8(6)
Br(1)-C(8)-C(9)-C(10)	-178.7(3)
C(8)-C(9)-C(10)-C(5)	-3.6(6)
C(6)-C(5)-C(10)-C(9)	2.7(6)
C(1)-C(5)-C(10)-C(9)	-179.0(4)

C(14)-O(3)-C(11)-C(12)	2.2(4)
C(14)-O(3)-C(11)-C(1)	128.3(3)
C(5)-C(1)-C(11)-O(3)	-66.6(4)
C(2)-C(1)-C(11)-O(3)	166.9(3)
C(5)-C(1)-C(11)-C(12)	51.6(4)
C(2)-C(1)-C(11)-C(12)	-74.9(4)
O(3)-C(11)-C(12)-C(13)	-1.5(4)
C(1)-C(11)-C(12)-C(13)	-123.3(3)
C(11)-C(12)-C(13)-C(14)	0.3(4)
C(11)-O(3)-C(14)-O(2)	177.9(3)
C(11)-O(3)-C(14)-C(13)	-2.1(4)
C(12)-C(13)-C(14)-O(2)	-178.8(4)
C(12)-C(13)-C(14)-O(3)	1.1(4)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for cd20181 [A and deg.].

D-H...A $d(D-H)$ $d(H \dots A)$ $d(D \dots A)$ $\angle(DHA)$

H: References

¹ Fukuyama, T.; Cheung, M.; Kan, T. *synlett.* **1999**, 8, 1301-1303.