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Supporting Information

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"Regio- and Stereoselective Construction of γ-Butenolides *via* Phosphine Catalyzed Substitution of Morita-Baylis-Hillman Acetates: An Organocatalytic Allylic Alkylation"

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Experimental Section

General. All reactions were run under an atmosphere of argon, unless otherwise indicated. Anhydrous solvents were transferred by an oven-dried syringe. Flasks were flame-dried and cooled under a stream of nitrogen. THF was distilled from sodium and degassed with Ar prior to use. Chemical reagents were purchased from Aldrich chemical company and used without further purification, unless otherwise noted. Substrates 1a-3a, 7a-9a were prepared according to the previously reported procedure.[1] 2-Trimethylsilyloxy furan as pronucleophile was also prepared according to the previously reported procedure.[2]

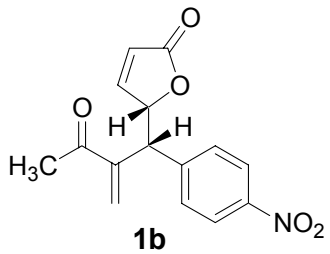
Analytical thin-layer chromatography (TLC) was carried out using 0.2-mm commercial silica gel plates (DC-Fertigplatten Krieselgel 60 F_{254}). Preparative column chromatography employing silica gel was performed according to the method of Still.[3] Melting points were determined on a Thomas-Hoover melting point apparatus in open capillaries and are uncorrected. Infrared spectra were recorded on a Perkin-Elmer 1420 spectrometer. High-resolution mass spectra (HRMS) were obtained on a Karatos MS9 and are reported as m/e (relative intensity). Accurate masses are reported for the molecular ion (M+1) or a suitable fragment ion.

Proton nuclear magnetic resonance (^{1}H NMR) spectra were recorded with a Varian Gemini (300 MHz) spectrometer, a Mercury (400 MHz) spectrometer. Chemical Shifts are reported in delta (δ) units, parts per million (ppm) downfield from trimethylsilane. Coupling constants are reported in Hertz (Hz). Carbon-13 nuclear magnetic resonance (^{13}C NMR) spectra were recorded with a Varian Gemini 300 (75 MHz) spectrometer, a Mercury 400 (100 MHz) spectrometer. Chemical shifts are reported in delta (δ) units, parts per million (ppm) relative to the center of the triplet at 77.00 ppm for deuteriochloroform. ^{13}C NMR spectra were routinely run with broadbrand decoupling.

Representative Procedure for the Phosphine Catalyzed Allylic Substitution

To a reaction vessel charged with substrate (0.5 mmol, 100 mol%), 2-trimethylsilyloxy furan (1.0 mmol, 200 mol%), and PPh_3 (0.1 mmol, 20 mol%), was added THF (1.6 mL, 0.3 M). The reaction was allowed to stir at ambient temperature until complete consumption of substrate was observed, at which point the reaction mixture was evaporated onto silica gel and the product was isolated by silica gel chromatography.

(1) Cho, C.-W.; Kong, J.-R.; Krische, M. J. *Org. Lett.* **2004**, *6*, 1337.
(2) Pelter, A.; Ward, R. S.; Sirit, A. *Tetrahedron: Asymmetry* **1994**, *5*, 1745.
(3) Still, W. C.; Kahn, M; Mitra, A. *J. Org. Chem.* **1978**, *43*, 2923.



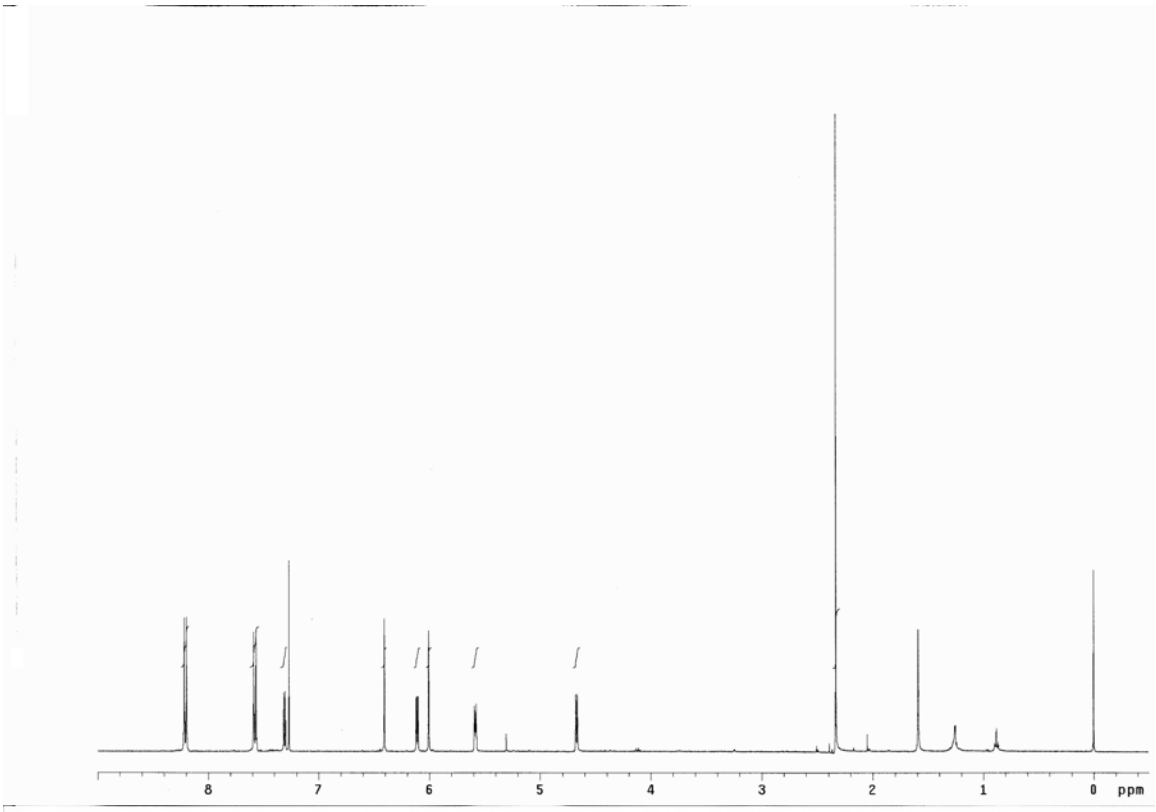
1b

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 9.2 Hz, 2H), 7.52 (d, *J* = 8.8 Hz, 2H), 7.26 (dd, *J* = 5.6, 1.2 Hz, 1H), 6.36 (s, 1H), 6.06 (dd, *J* = 5.6, 2.0 Hz, 1H), 5.97 (s, 1H), 5.55 (ddd, *J* = 5.6, 3.6, 1.6 Hz, 1H), 4.61 (d, *J* = 5.2 Hz, 1H), 2.29 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.1, 172.1, 155.0, 147.2, 146.7, 144.5, 130.9, 129.4, 124.0, 122.3, 82.2, 46.1, 25.5

HRMS calcd for $C_{15}H_{14}NO_5$ [M+1] 288.08665, found 288.08679

FTIR (neat) 3110, 2917, 1758, 1676, 1519, 1348, 1161, 1104 cm^{-1}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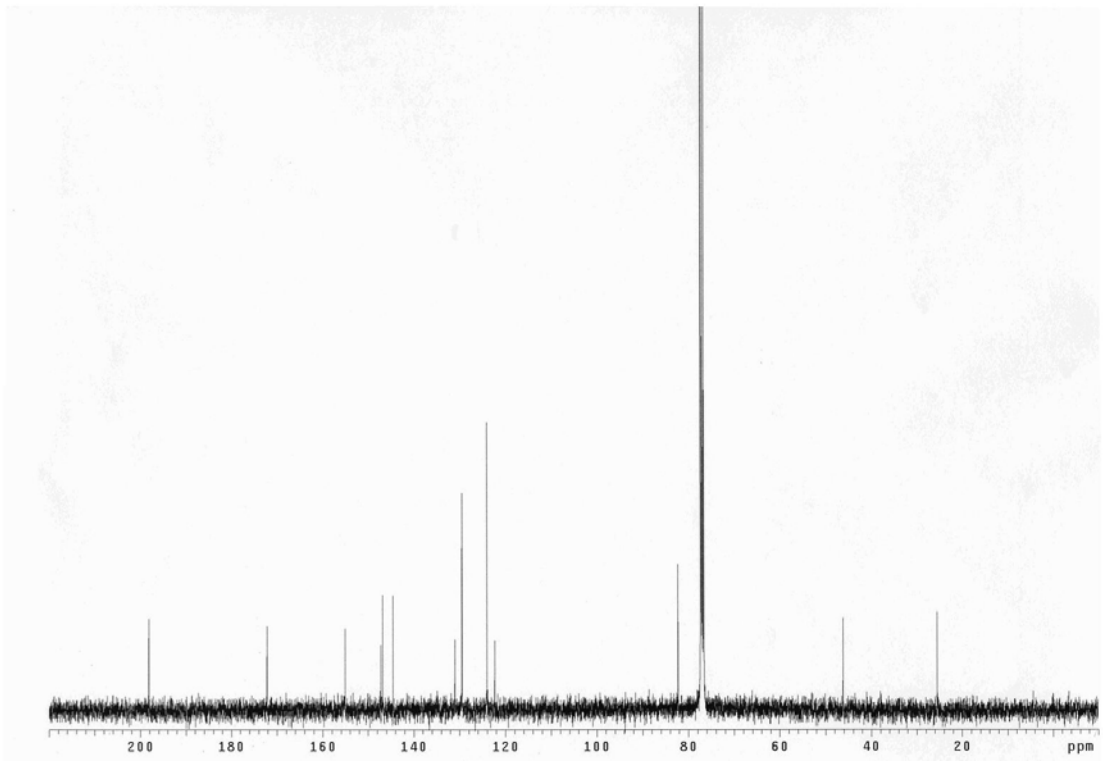
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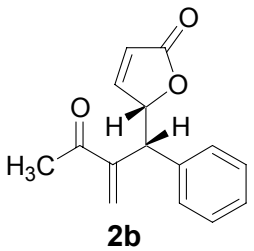

2b

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.26 (m, 6H), 6.35 (s, 1H), 6.07-6.05 (m, 2H), 5.55 (ddd, *J* = 6.8, 3.6, 1.6 Hz, 1H), 4.39 (d, *J* = 7.2 Hz, 1H), 2.30 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.4, 172.6, 155.9, 145.8, 138.8, 128.9, 128.7, 128.2, 127.4, 121.5, 83.3, 47.2, 25.7

HRMS calcd for $C_{15}H_{15}O_3$ [M+1] 243.10157, found 243.10132

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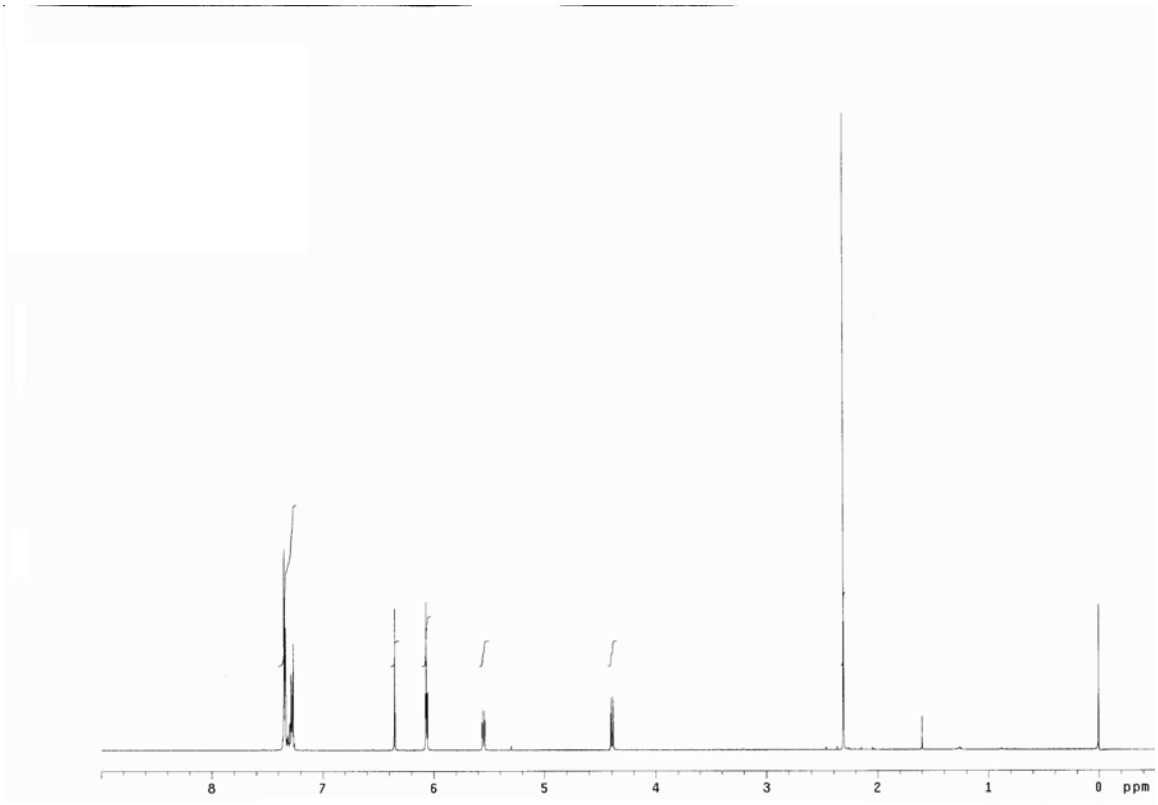
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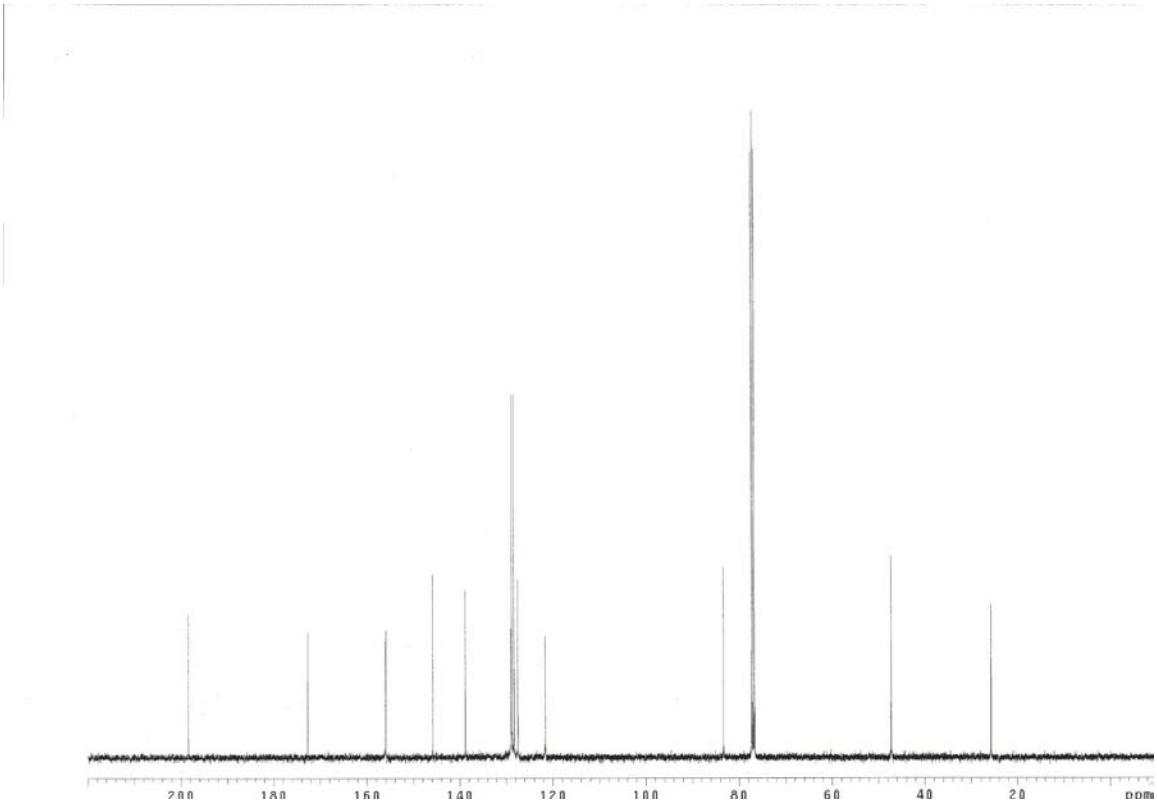
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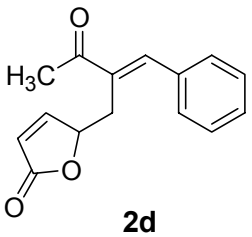


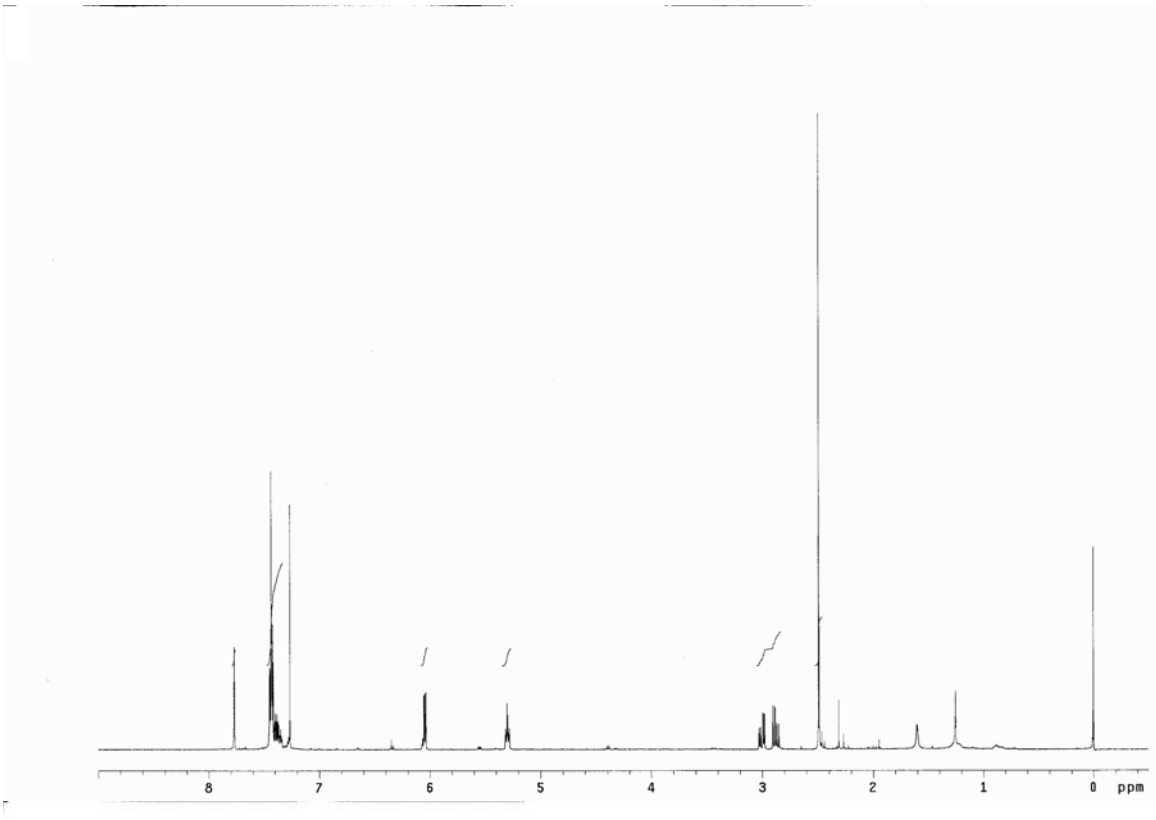
2d

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (s, 1H), 7.45-7.33 (m, 6H), 6.05 (dd, *J* = 5.6, 2.0 Hz, 1H), 5.32-5.27 (m, 1H), 3.02-2.85 (m, 2H), 2.49 (s, 3H)

^{13}C NMR (75 MHz, $CDCl_3$) δ 200.0, 172.7, 156.6, 144.7, 135.8, 134.6, 129.1, 129.0, 128.7, 120.9, 81.7, 29.9, 25.8

HRMS calcd for $C_{15}H_{15}O_3$ [M+1] 243.102120, found 243.102595

FTIR (neat) 2922, 1754, 1664, 1161, 1102, 818, 699 cm^{-1}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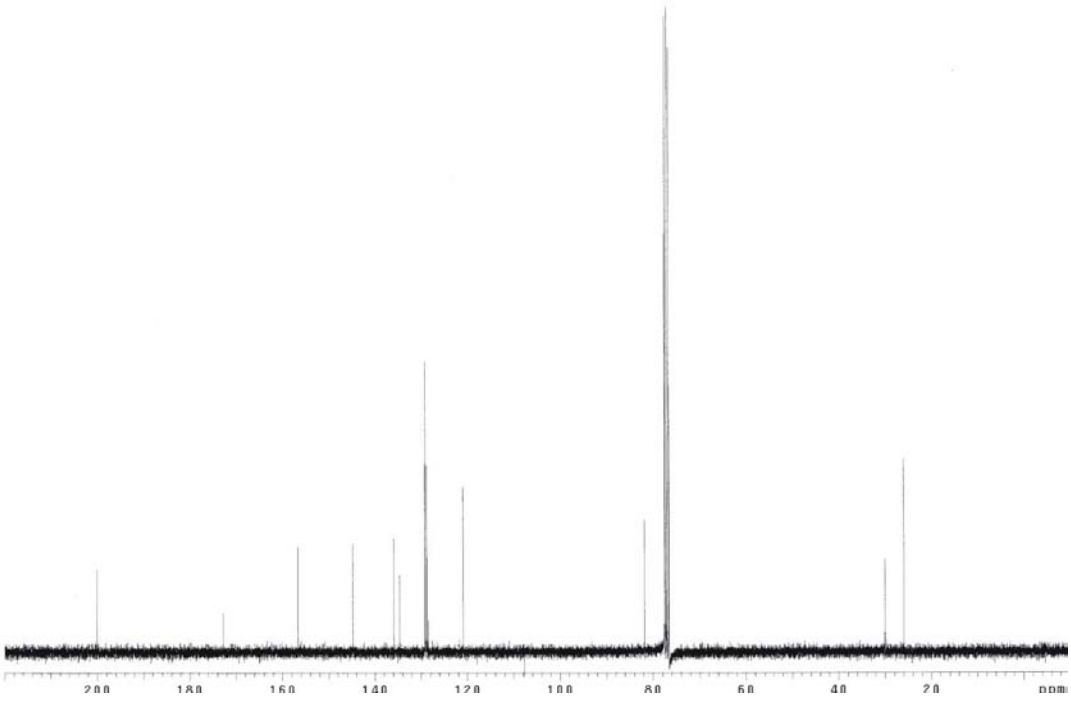
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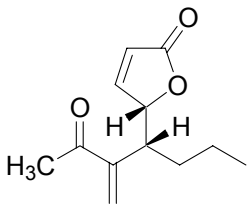


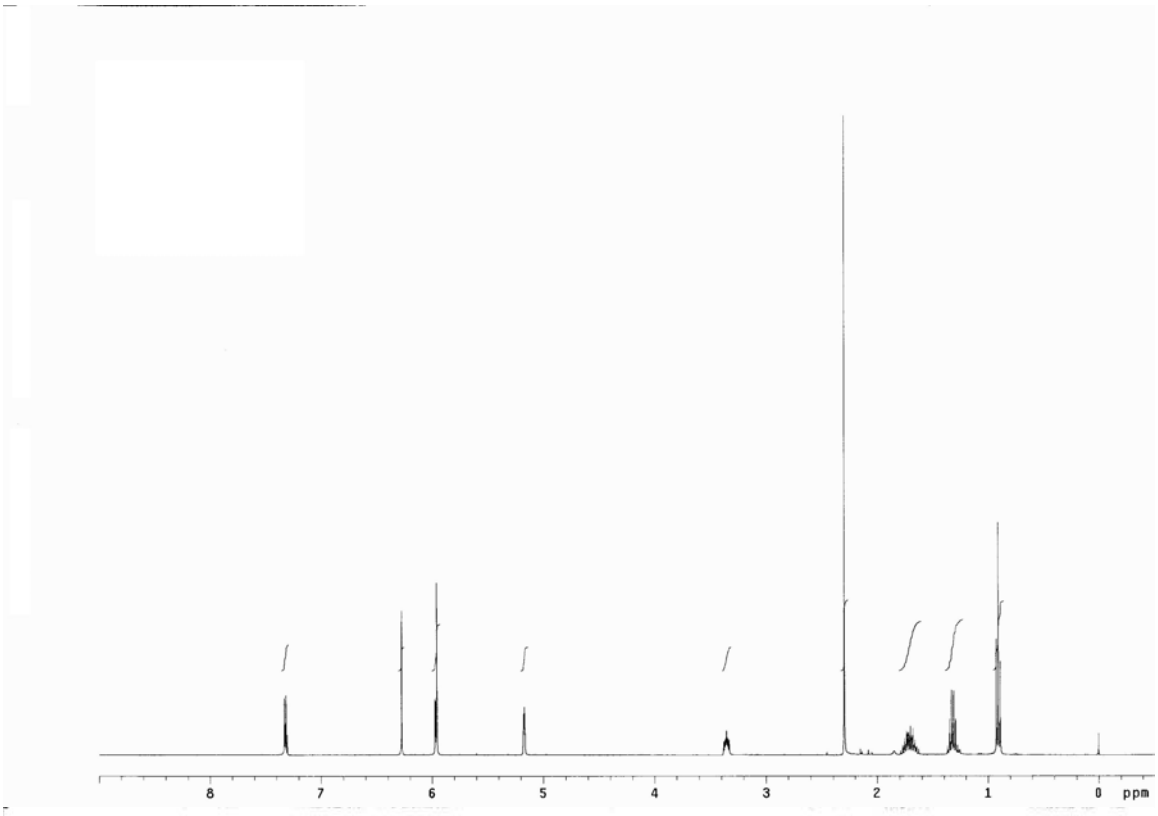
3b

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (dd, *J* = 6.0, 2.0 Hz, 1H), 6.27 (s, 1H), 5.97-5.95 (m, 2H), 5.18-5.16 (m, 1H), 3.37-3.31 (m, 1H), 2.29 (s, 3H), 1.79-1.62 (m, 2H), 1.36-1.25 (m, 2H), 0.90 (t, *J* = 7.2 Hz, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.3, 173.0, 155.7, 144.5, 129.1, 121.3, 84.0, 39.2, 33.2, 25.4, 20.2, 13.7

HRMS calcd for $C_{12}H_{17}O_3$ [M+1] 209.117770, found 209.116904

FTIR (neat) 3110, 2967, 1752, 1671, 1359, 1162, 1028, 822 cm^{-1}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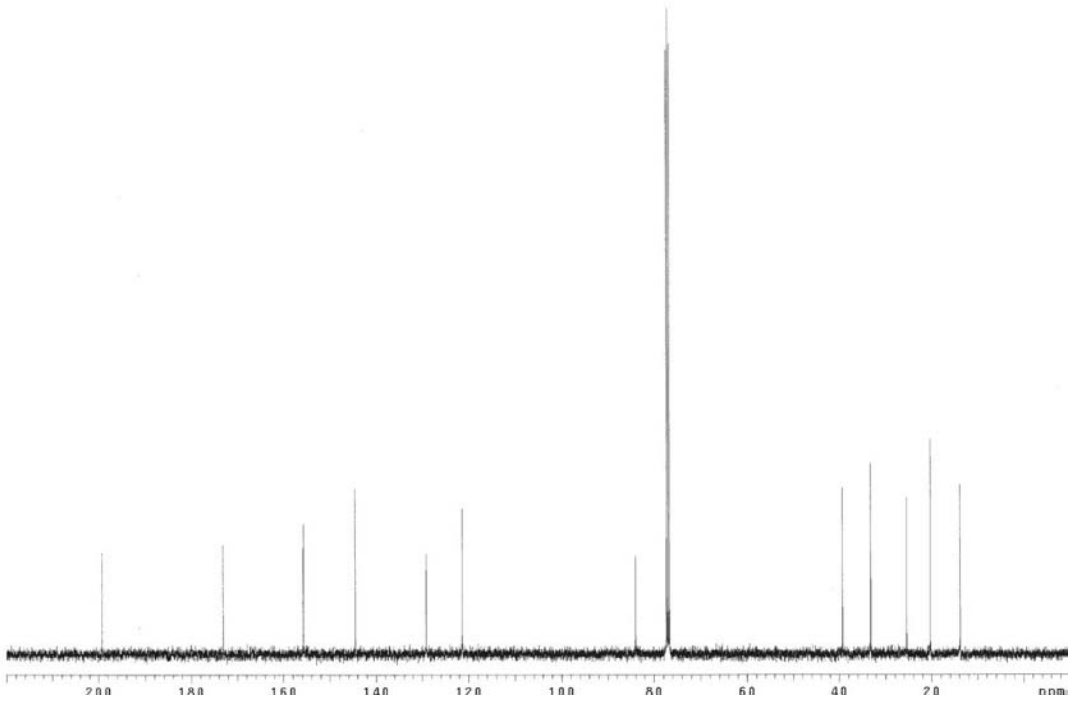
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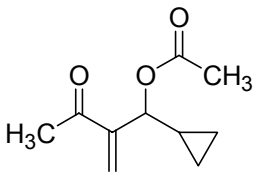


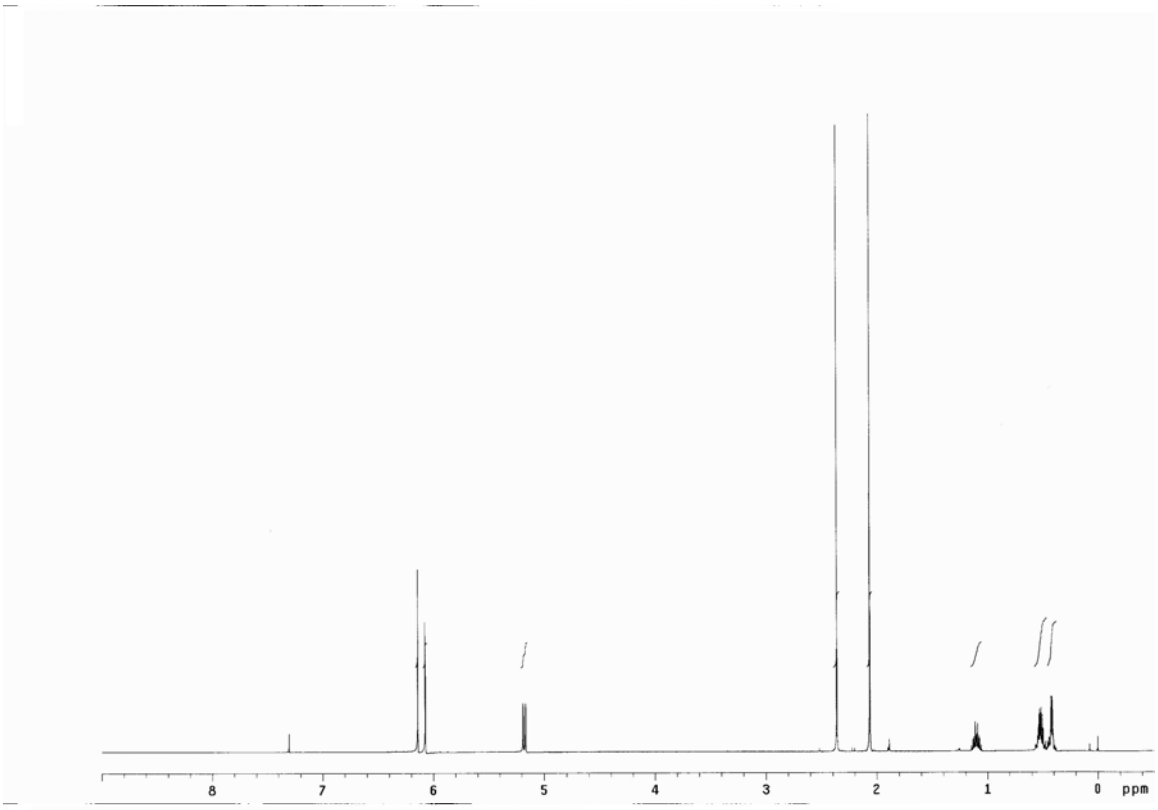
4a

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.14 (s, 1H), 6.07 (d, *J* = 0.8 Hz, 1H), 5.17 (dd, *J* = 8.4, 0.4 Hz, 1H), 2.36 (s, 3H), 2.06 (s, 3H), 1.14-1.05 (m, 1H), 0.56-0.47 (m, 2H), 0.45-0.39 (m, 2H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.6, 169.8, 148.0, 125.1, 74.0, 26.0, 21.0, 14.8, 3.7, 2.6

HRMS calcd for $C_{10}H_{15}O_3$ [M+1] 183.102120, found 183.102590

FTIR (neat) 3093, 3013, 1732, 1678, 1634, 1369, 1240, 1028 cm^{-1}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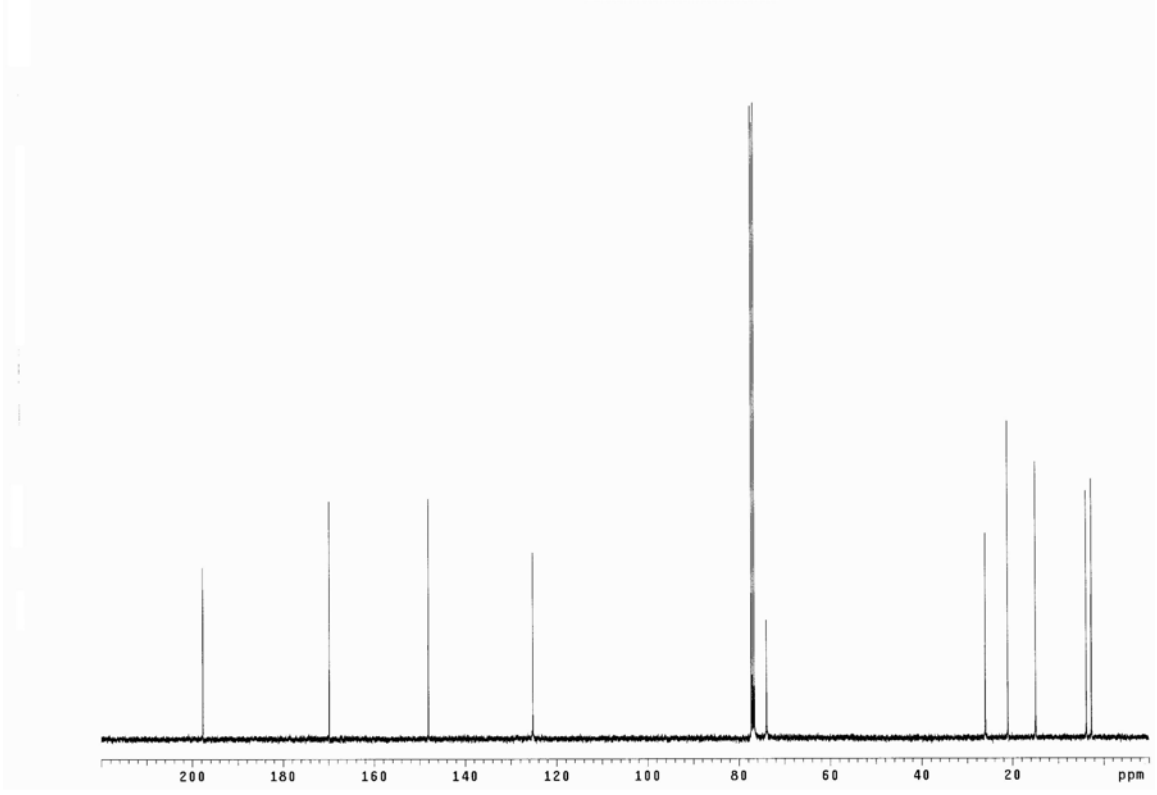
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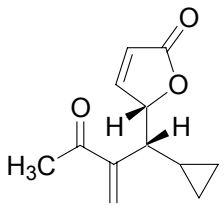

4b

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (dd, *J* = 6.0, 2.0 Hz, 1H), 6.27 (s, 1H), 6.10 (s, 1H), 5.99 (dd, *J* = 6.0, 2.0 Hz, 1H), 5.34-5.32 (m, 1H), 2.30 (s, 3H), 1.29-1.20 (m, 1H), 0.75-0.68 (m, 1H), 0.56-0.49 (m, 1H), 0.34-0.28 (m, 1H), 0.11-0.05 (m, 1H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 172.9, 155.6, 145.4, 129.3, 121.1, 84.6, 46.9, 25.5, 12.5, 6.0, 4.3

HRMS calcd for $C_{12}H_{15}O_3$ [M+1] 207.10157, found 207.10060

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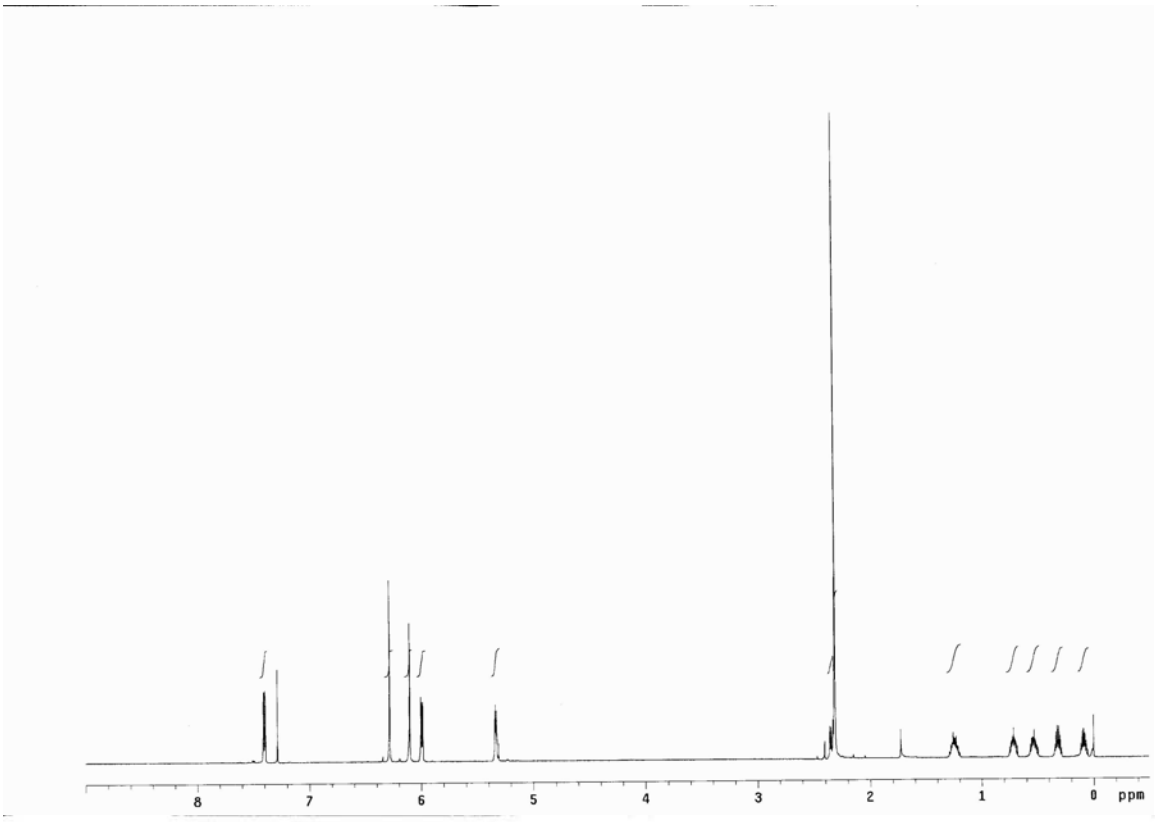
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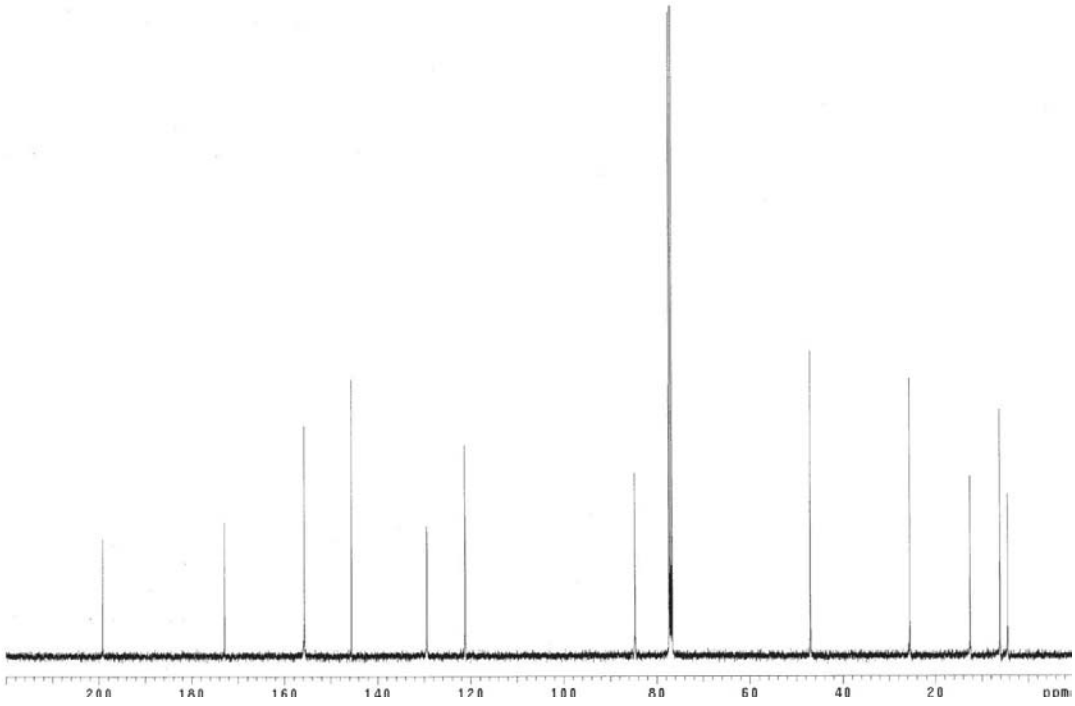
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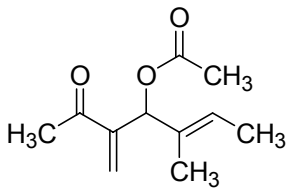


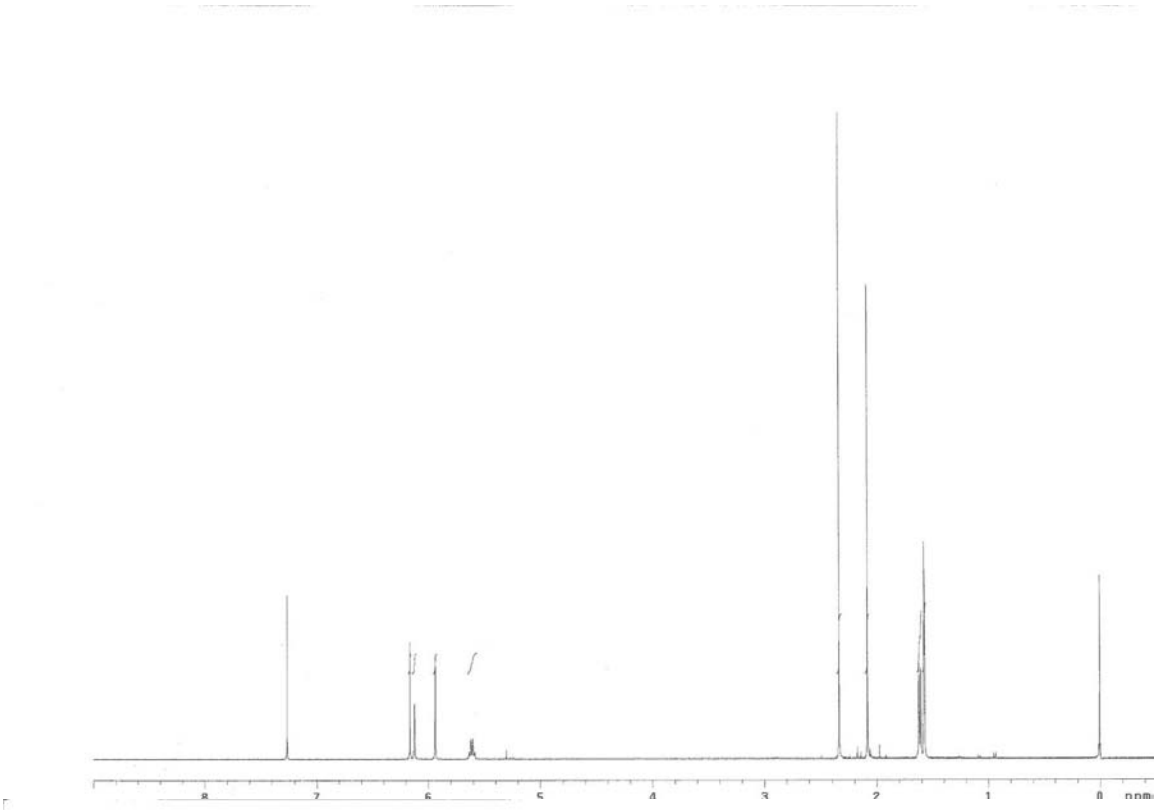
5a

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.16 (s, 1H), 6.12 (s, 1H), 5.93 (d, *J* = 1.2 Hz, 1H), 5.63-5.58 (m, 1H), 2.33 (s, 3H), 2.08 (s, 3H), 1.61 (d, *J* = 6.8 Hz, 3H), 1.57 (d, *J* = 0.8 Hz, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.3, 169.3, 146.2, 131.4, 125.0, 124.5, 74.9, 26.0, 20.9, 13.2, 12.1

HRMS calcd for $C_{11}H_{17}O_3$ [M+1] 197.117770, found 197.118635

FTIR (neat) 3095, 1734, 1644, 1372, 1233, 751, 637 cm^{-1}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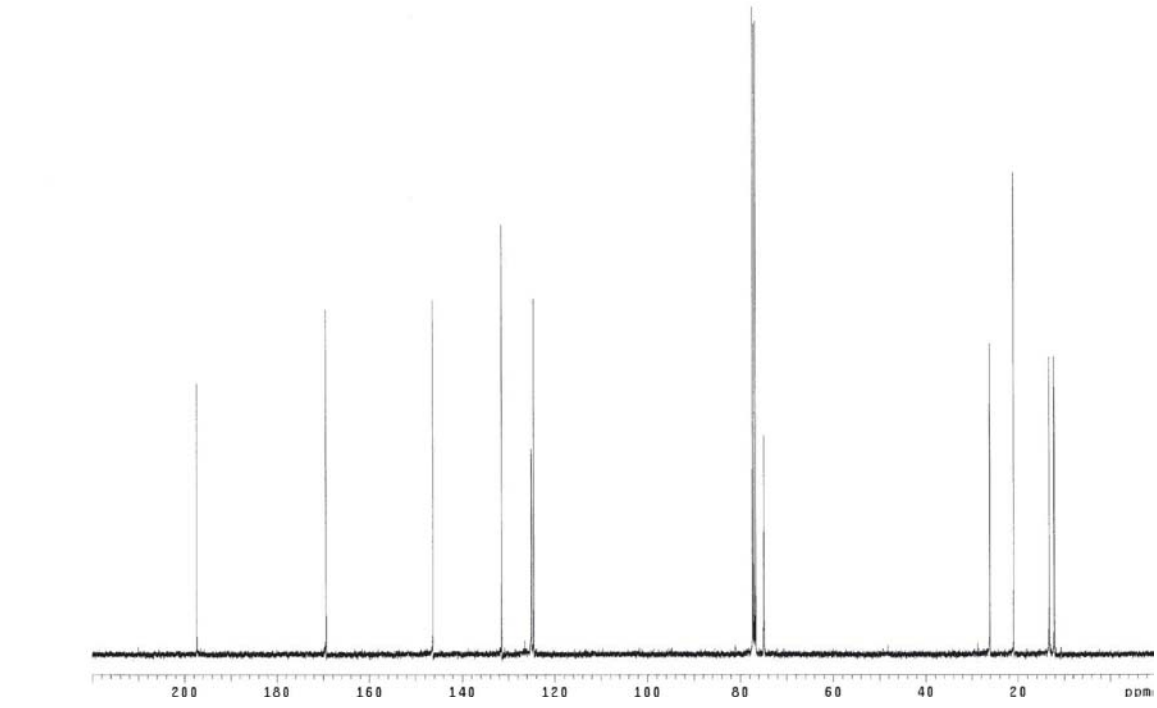
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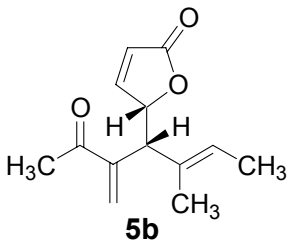

5b

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (dd, *J* = 6.0, 2.0 Hz, 1H), 6.29 (s, 1H), 6.01-5.99 (m, 2H), 5.71-5.66 (m, 1H), 5.37 (ddd, *J* = 5.6, 3.2, 1.6 Hz, 1H), 3.78 (d, *J* = 5.6 Hz, 1H), 2.31 (s, 3H), 1.65 (d, *J* = 6.4 Hz, 3H), 1.56 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9, 172.9, 156.4, 144.2, 133.1, 128.9, 122.5, 121.3, 82.8, 48.1, 25.6, 15.9, 13.5

HRMS calcd for $C_{13}H_{17}O_3$ [M+1] 221.117770, found 221.118383

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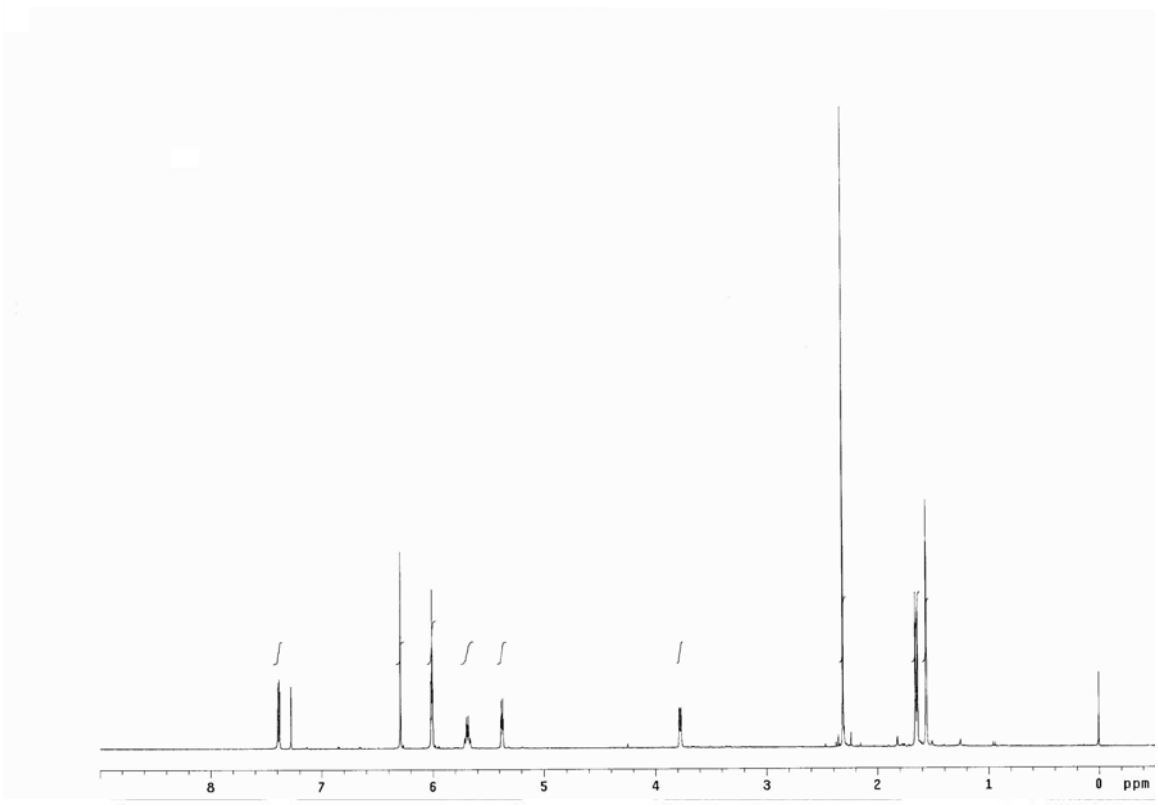
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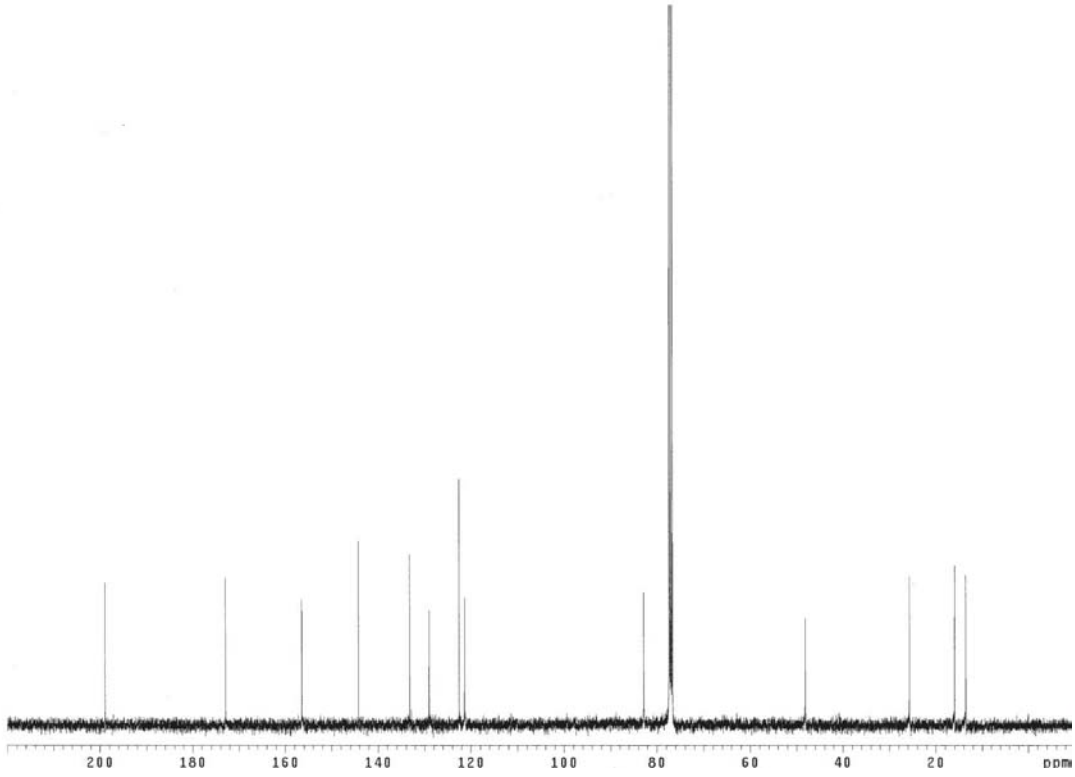
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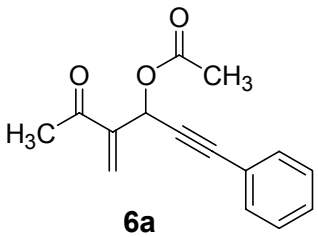


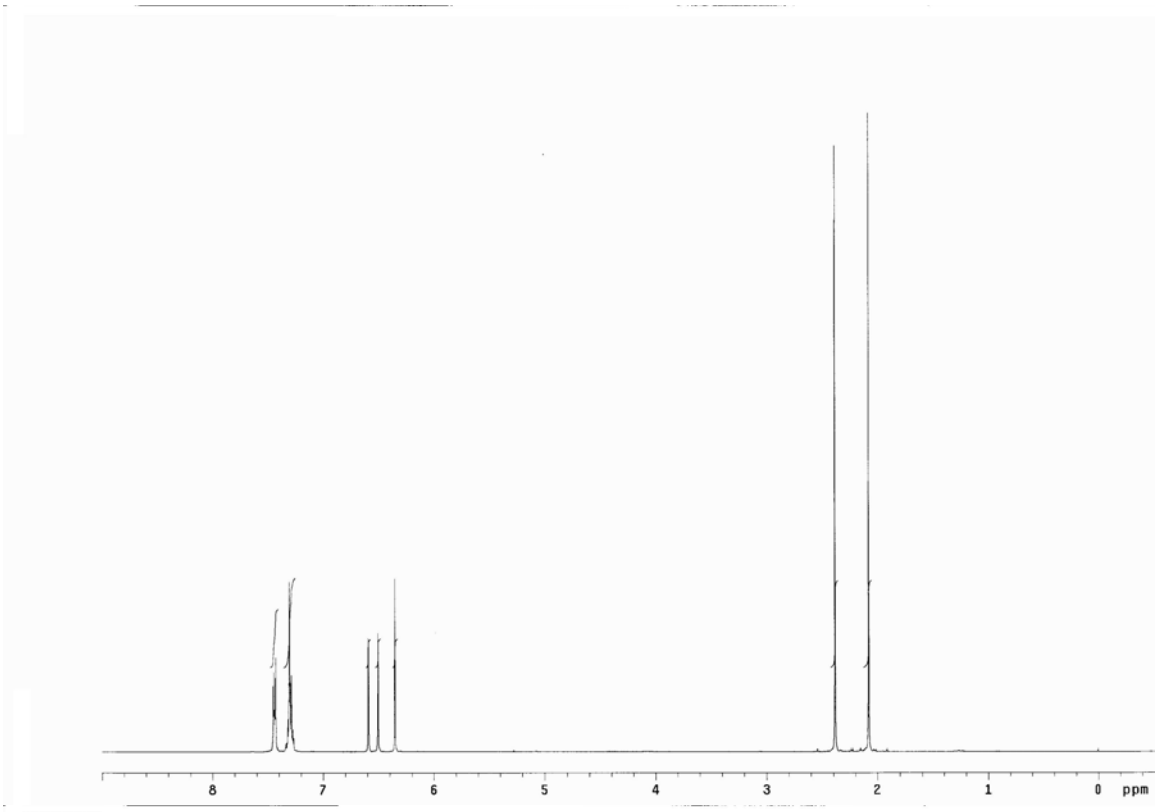
6a

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.43 (m, 2H), 7.33-7.26 (m, 3H), 6.59 (d, *J* = 0.8 Hz, 1H), 6.50 (d, *J* = 1.2 Hz, 1H), 6.35 (s, 1H), 2.38 (s, 3H), 2.07 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 196.0, 168.8, 144.0, 131.5, 128.5, 128.4, 127.9, 121.5, 86.6, 84.0, 60.9, 25.7, 20.4

HRMS calcd for $C_{15}H_{14}O_3$ [M+1] 242.094294, found 242.093681

FTIR (neat) 3112, 1746, 1680, 1369, 1223, 1036, 970, 758, 692 cm^{-1}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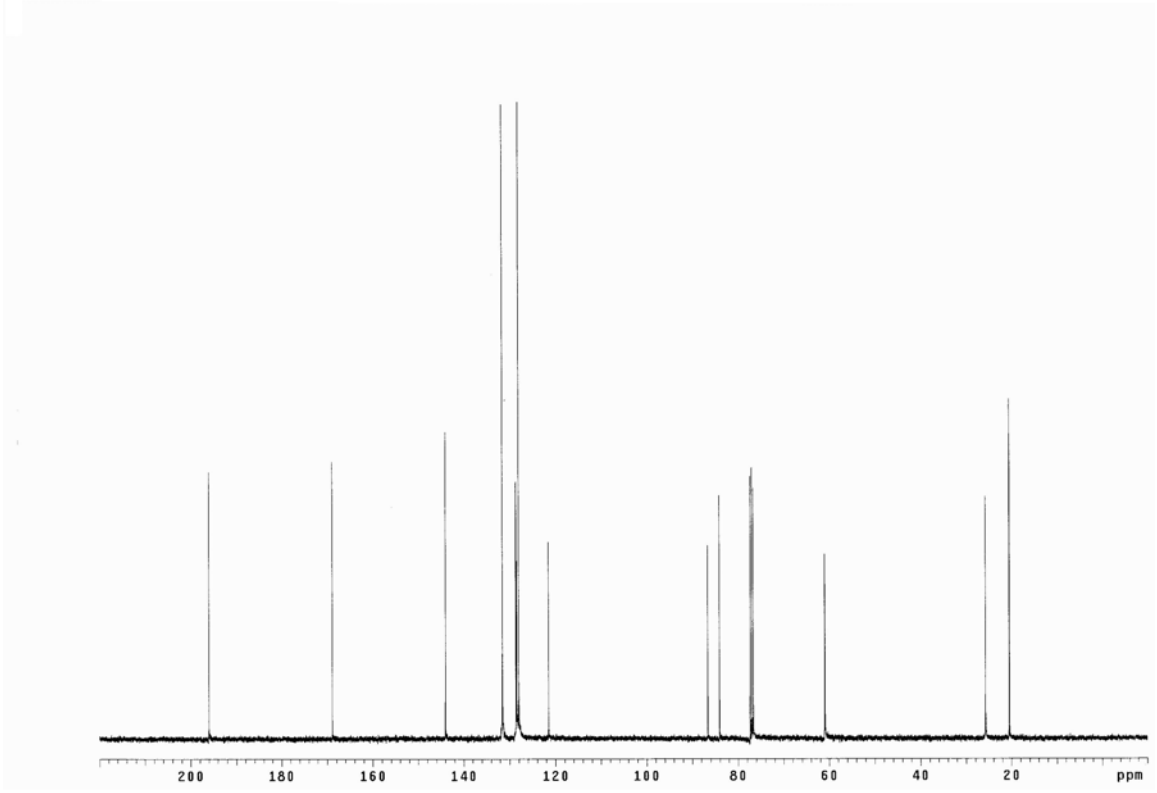
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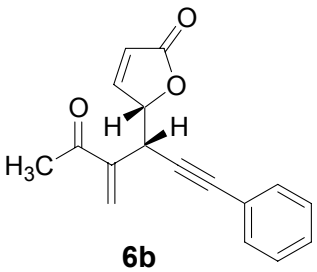


6b

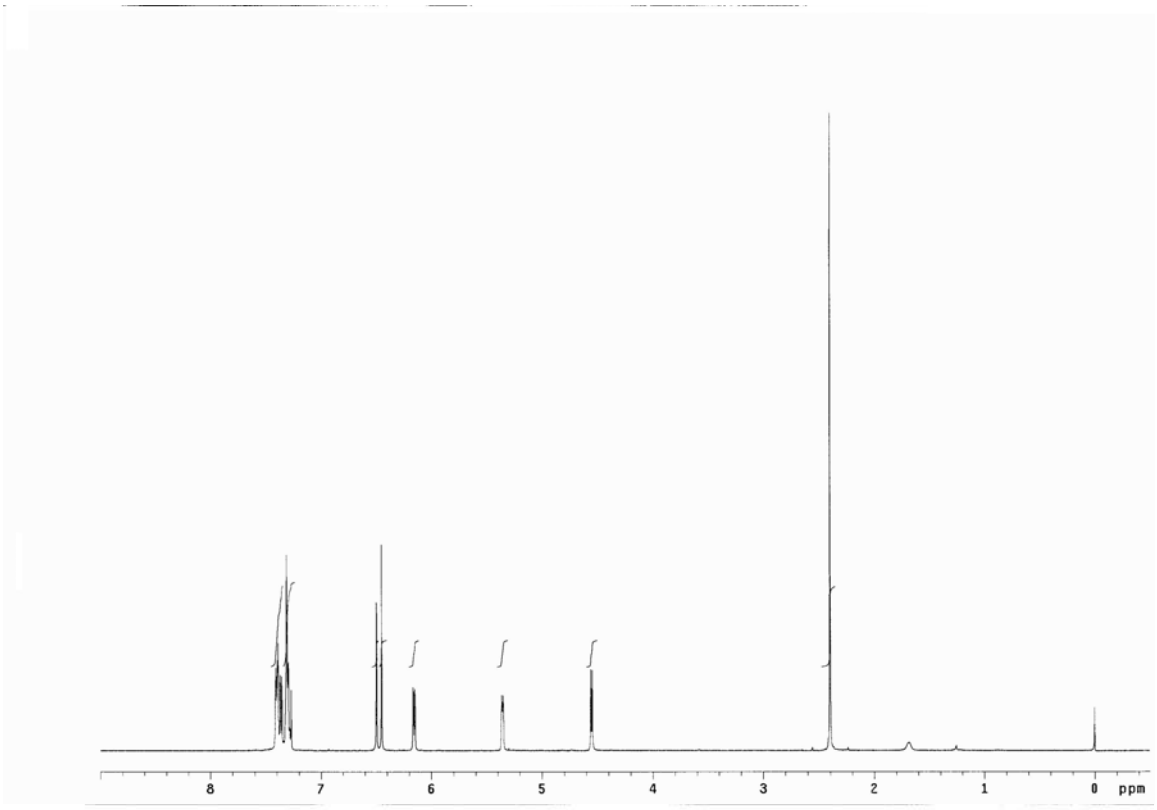
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.39 (m, 2H), 7.36 (dd, *J* = 6.0, 1.6 Hz, 1H), 7.31-7.28 (m, 3H), 6.49 (s, 1H), 6.44 (s, 1H), 6.15 (dd, *J* = 6.0, 2.0 Hz, 1H), 5.35 (m, 1H), 4.55 (d, *J* = 4.8 Hz,, 1H), 2.40 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.5, 172.3, 153.6, 142.7, 131.6, 131.3, 128.4, 128.2, 122.8, 122.3, 85.9, 84.6, 82.6, 36.1, 25.7

HRMS calcd for $C_{17}H_{15}O_3$ [M+1] 267.10157, found 267.10157

FTIR (neat) 3102, 3064, 1747, 1670, 1630, 1368, 1159, 1097, 1022, 908, 829, 758, 731, 692 cm^{-1}

M.P. 91~92 ^{o}C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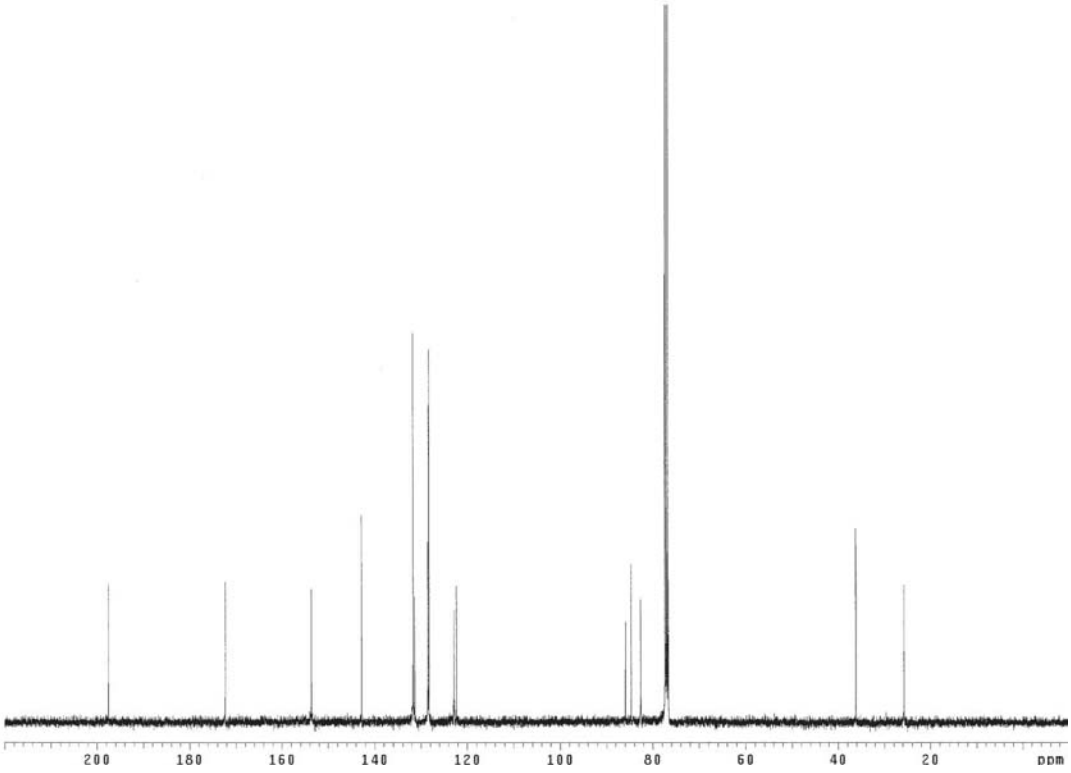
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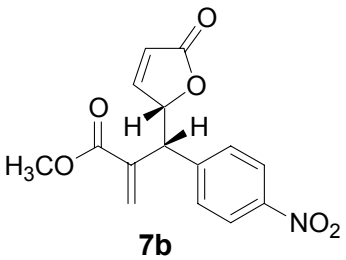


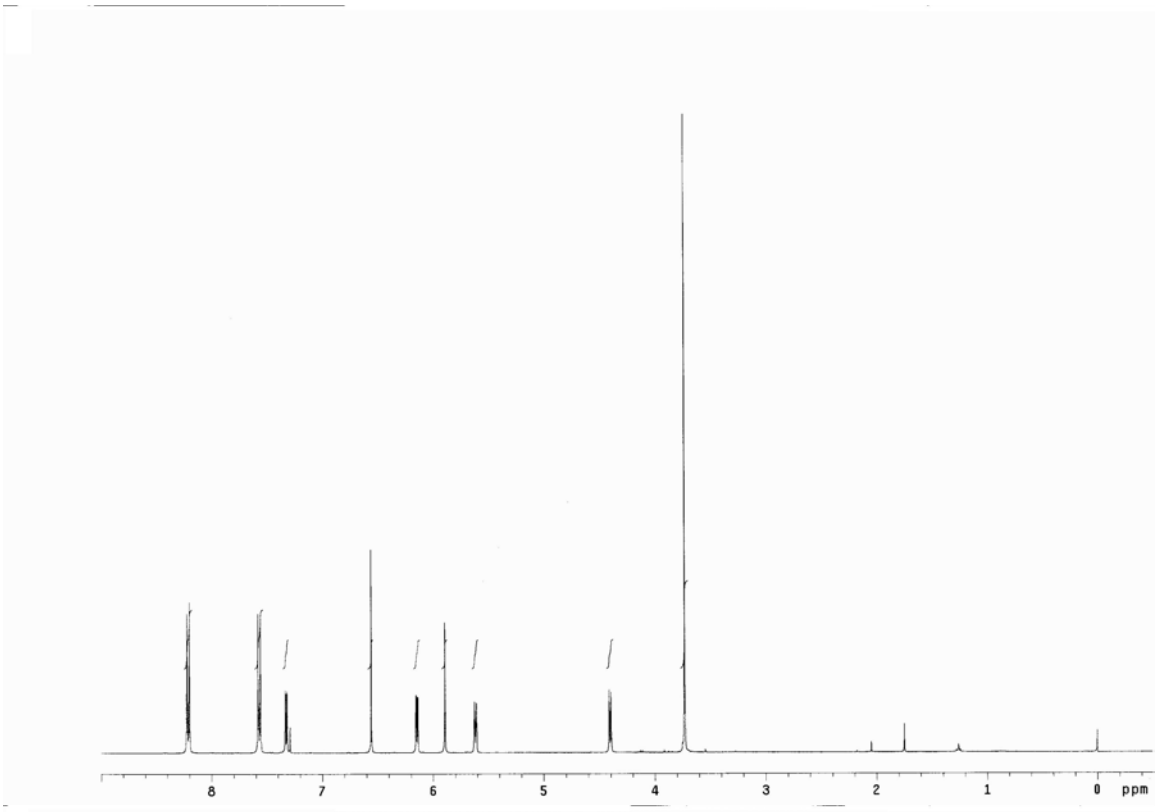
7b

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22-8.20 (m, 2H), 7.58-7.56 (m, 2H), 7.33 (dd, *J* = 5.6, 1.2 Hz, 1H), 6.55 (s, 1H), 6.15 (dd, *J* = 5.2, 1.6 Hz, 1H), 5.89 (s, 1H), 5.62 (ddd, *J* = 6.8, 3.6, 1.6 Hz, 1H), 4.40 (d, *J* = 6.8 Hz, 1H), 3.73 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.9, 166.2, 154.4, 147.2, 145.6, 136.5, 129.4, 129.4, 123.9, 122.6, 82.2, 52.3, 48.9

HRMS calcd for $C_{15}H_{14}NO_6$ [M+1] 304.082112, found 304.082322

FTIR (neat) 3126, 2952, 1757, 1715, 1521, 1348, 1152, 816, 709 cm^{-1}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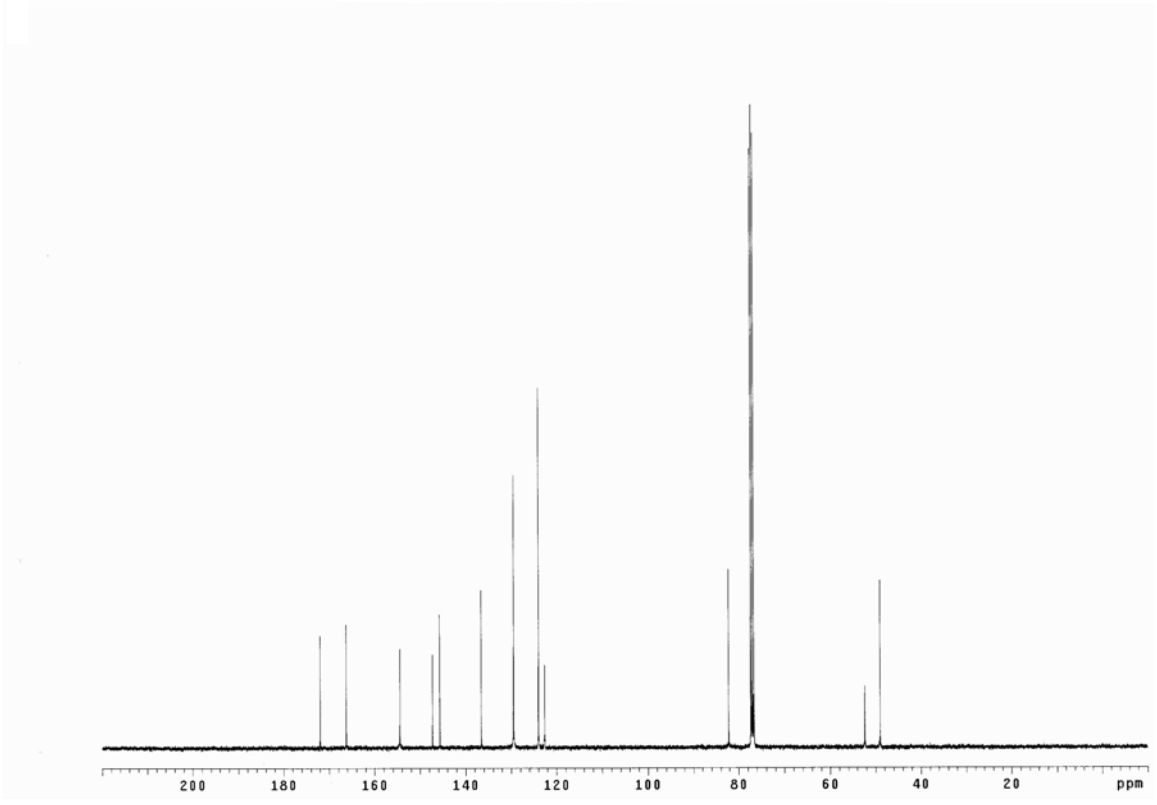
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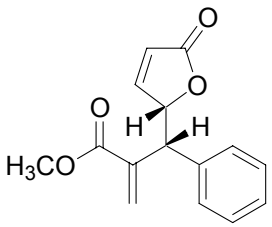


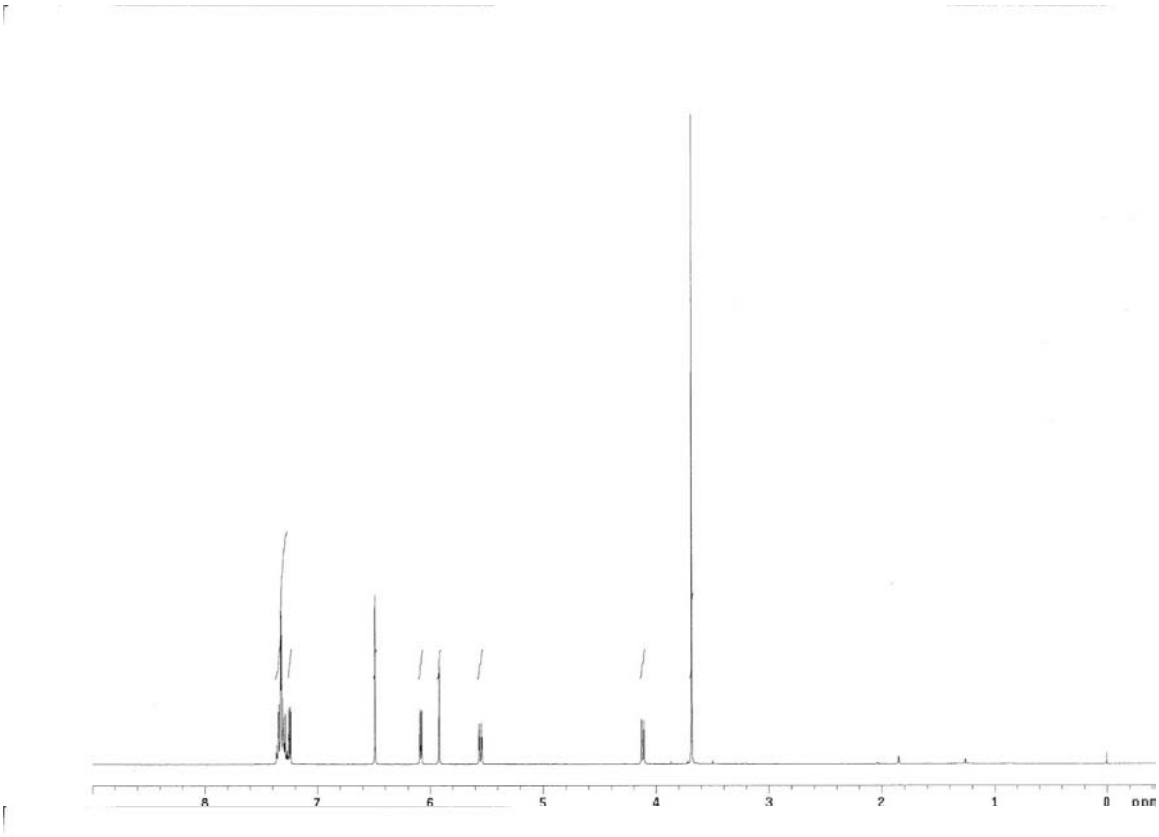
8b

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.26 (m, 5H), 7.25 (dd, *J* = 6.0, 2.0 Hz, 1H), 6.48 (s, 1H), 6.08 (dd, *J* = 6.0, 2.0 Hz, 1H), 5.92 (d, *J* = 0.8 Hz, 1H), 5.55 (ddd, *J* = 8.0, 3.2, 1.6 Hz, 1H), 4.12 (d, *J* = 8.4 Hz, 1H), 3.68 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.4, 166.5, 155.4, 138.0, 137.7, 128.8, 128.2, 127.6, 127.4, 121.8, 83.1, 52.0, 49.9

HRMS calcd for $C_{15}H_{15}O_4$ [M+1] 259.097034, found 259.097693

FTIR (neat) 3112, 2951, 1768, 1718, 1630, 1439, 1251, 1150, 899, 815, 704 cm^{-1}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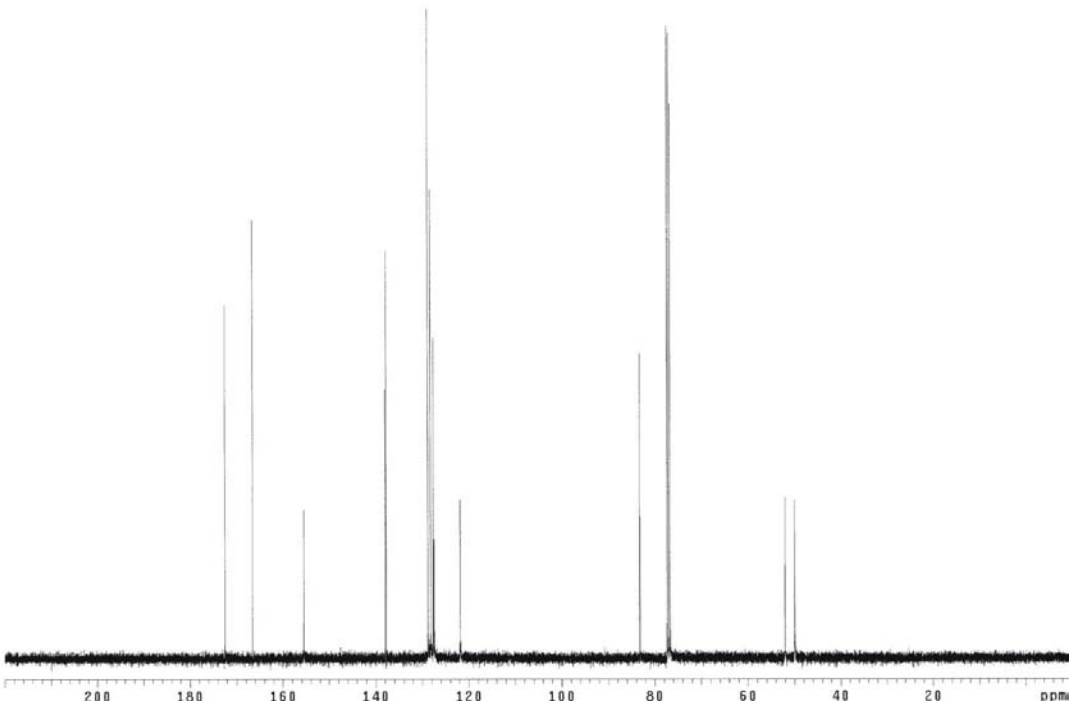
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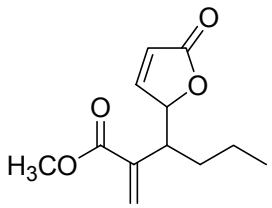


9b

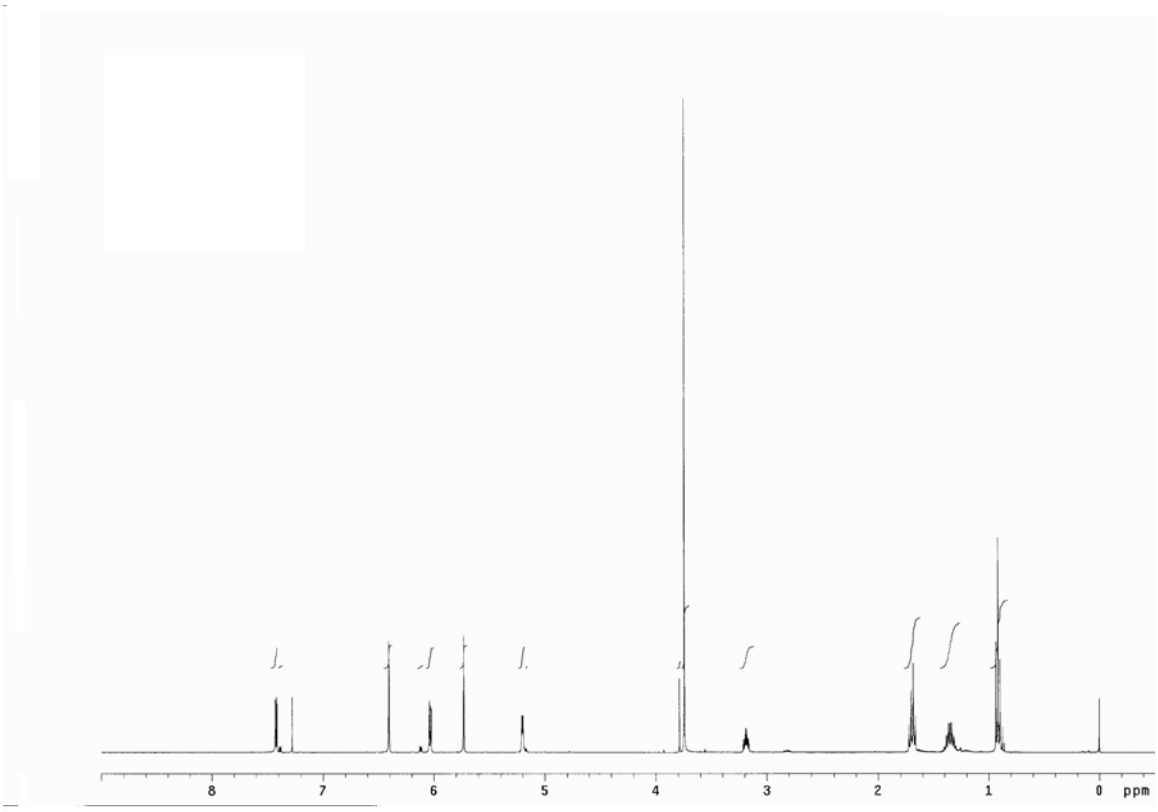
mixture of two diastereomers

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 and 7.39 (major: dd, *J* = 6.0, 2.0 Hz, minor: dd, *J* = 6.0, 1.6 Hz, 1H), 6.40 (s, 1H), 6.12 and 6.03 (major: dd, *J* = 6.0, 2.0 Hz, minor: dd, *J* = 5.6, 2.0 Hz, 1H), 5.73 (s, 1H), 5.21-5.19 and 5.18-5.16 (major: m, minor: m, 1H), 3.78 and 3.74 (major: s, minor: s, 3H), 3.21-3.16 and 2.86-2.79 (major: m, minor: m, 1H), 1.72-1.66 (m, 2H), 1.40-1.29 (m, 2H), 0.91 and 0.87 (major: t, *J* = 7.2 Hz, minor: t, *J* = 7.6 Hz, 3H)

^{13}C NMR (75 MHz, $CDCl_3$)
Major: δ 172.9, 167.3, 155.1, 136.2, 128.7, 121.9, 84.0, 52.1, 41.9, 32.7, 20.2, 13.8
Minor: δ 172.9, 167.3, 155.3, 138.5, 128.2, 121.8, 85.3, 52.1, 45.0, 31.6, 20.0, 13.8

HRMS calcd for $C_{12}H_{17}O_4$ [M+1] 225.11214, found 225.11217

FTIR (neat) 3095, 2959, 1705, 1628, 1279, 1159, 912, 819 cm^{-1}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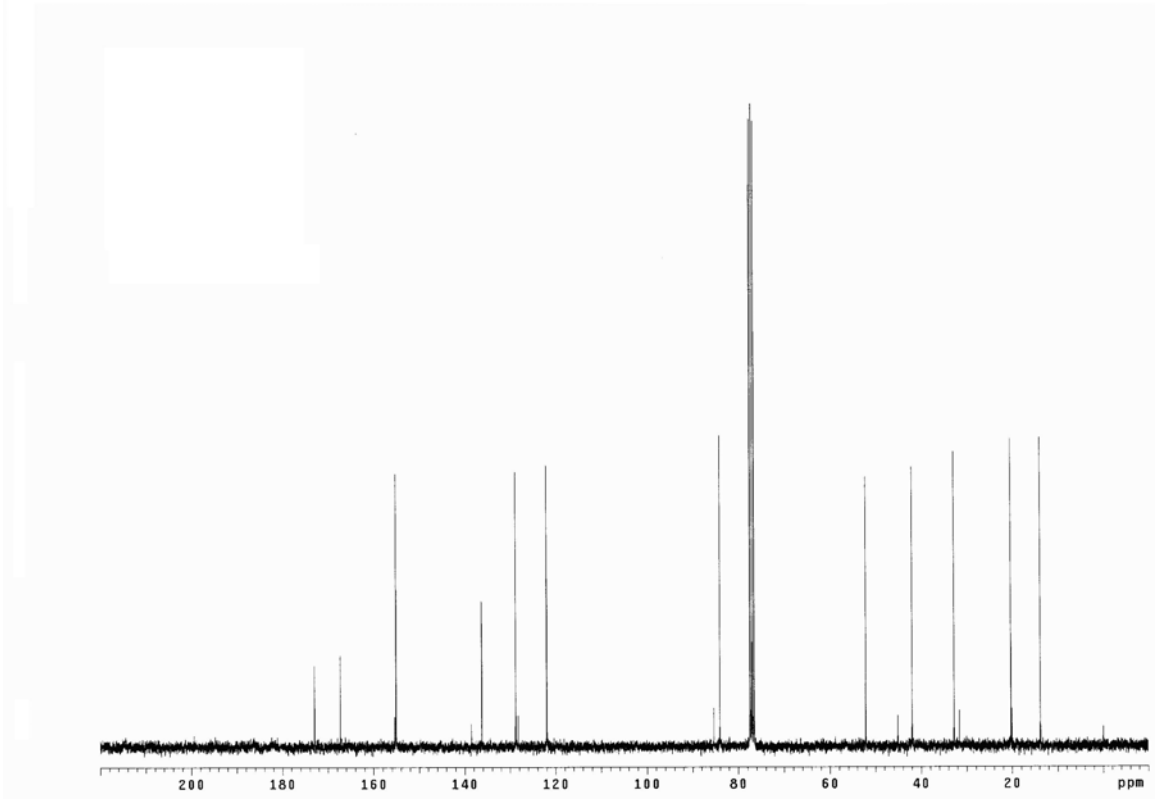
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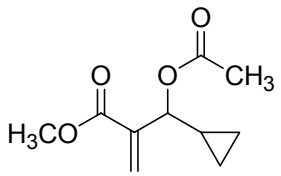


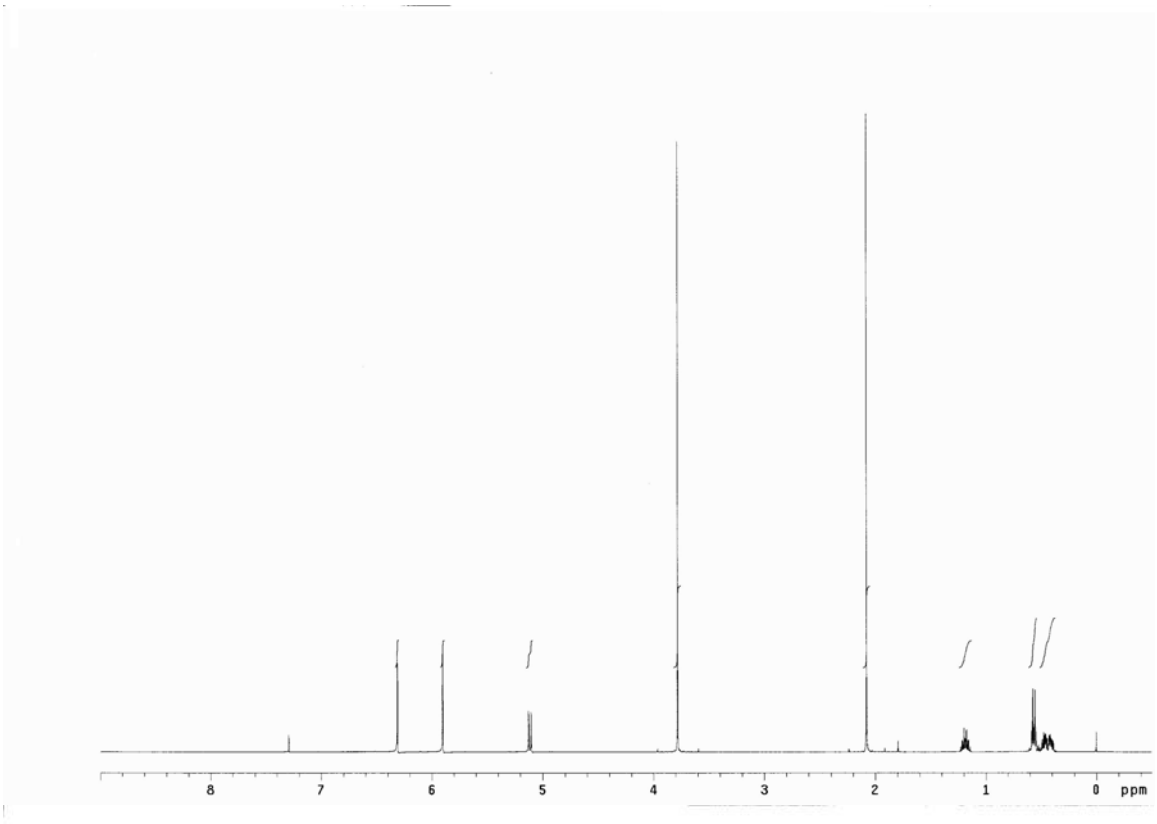
10a

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.31 (d, *J* = 0.8 Hz, 1H), 5.90 (t, *J* = 1.0 Hz, 1H), 5.11 (dd, *J* = 8.8, 1.2 Hz, 1H), 3.78 (s, 3H), 2.07 (s, 3H), 1.23-1.14 (m, 1H), 0.58-0.54 (m, 2H), 0.49-0.38 (m, 2H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.8, 165.8, 139.8, 125.8, 75.0, 51.8, 21.0, 14.5, 3.7, 2.8

HRMS calcd for $C_{10}H_{15}O_4$ [M+1] 199.097034, found 199.098354

FTIR (neat) 3012, 2955, 1736, 1268, 1246, 1030, 973, 816 cm^{-1}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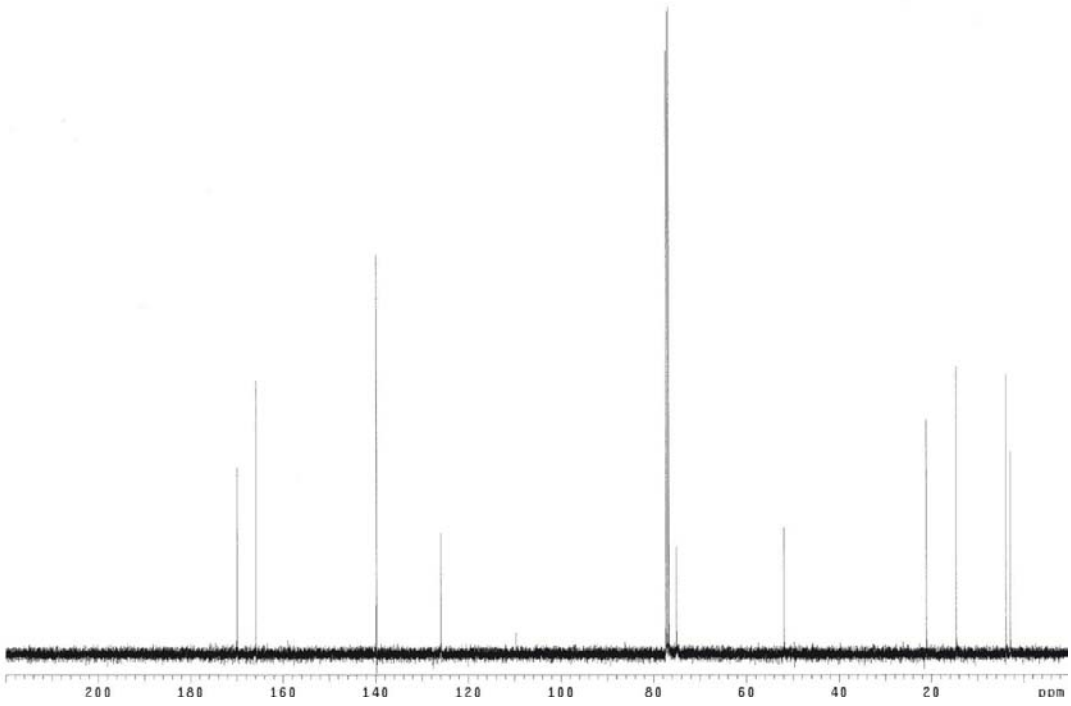
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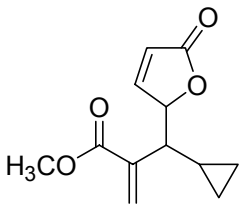


10b

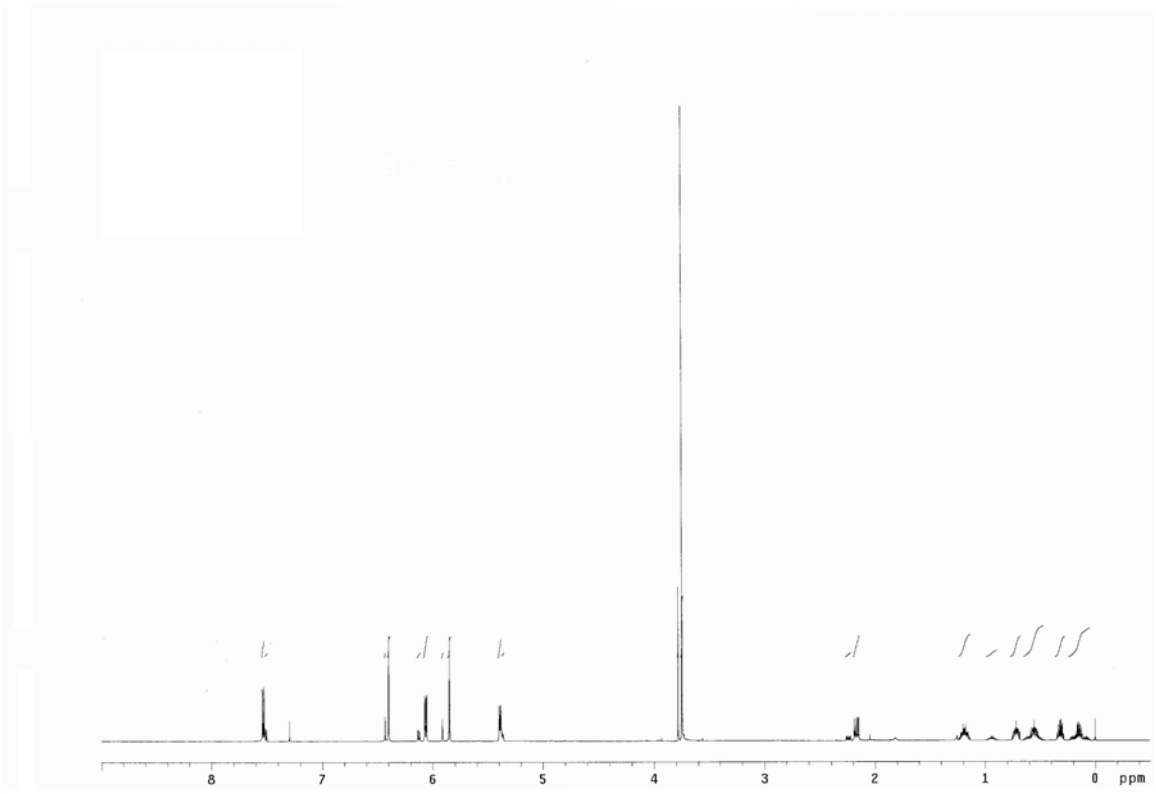
mixture of two diastereomers

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 and 7.51 (major: dd, *J* = 5.6, 1.6 Hz, minor: dd, *J* = 5.6, 1.2 Hz, 1H), 6.43 and 6.39 (minor: d, *J* = 0.4 Hz, major: d, *J* = 0.8 Hz, 1H), 6.13 and 6.06 (minor: dd, *J* = 5.6, 2.0 Hz, major: dd, *J* = 5.2, 1.6 Hz, 1H), 5.91 and 5.85 (minor: s, major: s, 1H), 5.40-5.36 (m, 1H), 3.78 and 3.75 (minor: s, major: s, 3H), 2.26-2.22 and 2.19-2.15 (major: m, minor: m, 1H), 1.25-1.44 and 0.98-0.89 (major: m, minor: m, 1H), 0.75-0.68 (m, 1H), 0.65-0.48 (m, 1H), 0.34-0.28 (m, 1H), 0.23-0.04 (m, 1H)

^{13}C NMR (75 MHz, $CDCl_3$)
Major: δ 173.1, 167.3, 155.5, 137.7, 129.0, 121.9, 84.9, 52.3, 49.8, 12.3, 6.5, 4.4
Minor: δ 173.4, 167.3, 155.9, 139.1, 128.6, 121.7, 85.0, 52.3, 49.4, 9.7, 7.4, 3.4

HRMS calcd for $C_{12}H_{15}O_4$ [M+1] 223.09649, found 223.09555

FTIR (neat) 3007, 1709, 1631, 1260, 1161, 953, 898, 818, 698 cm^{-1}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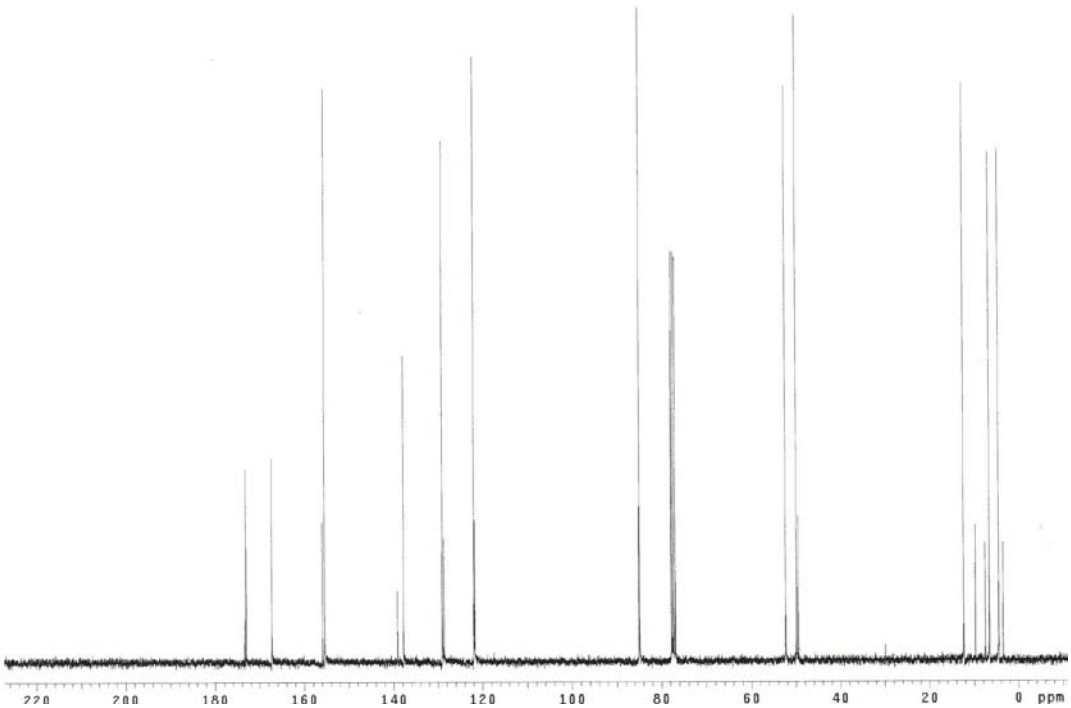
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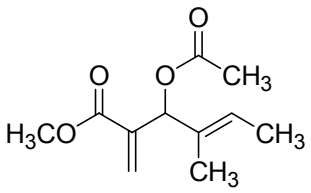


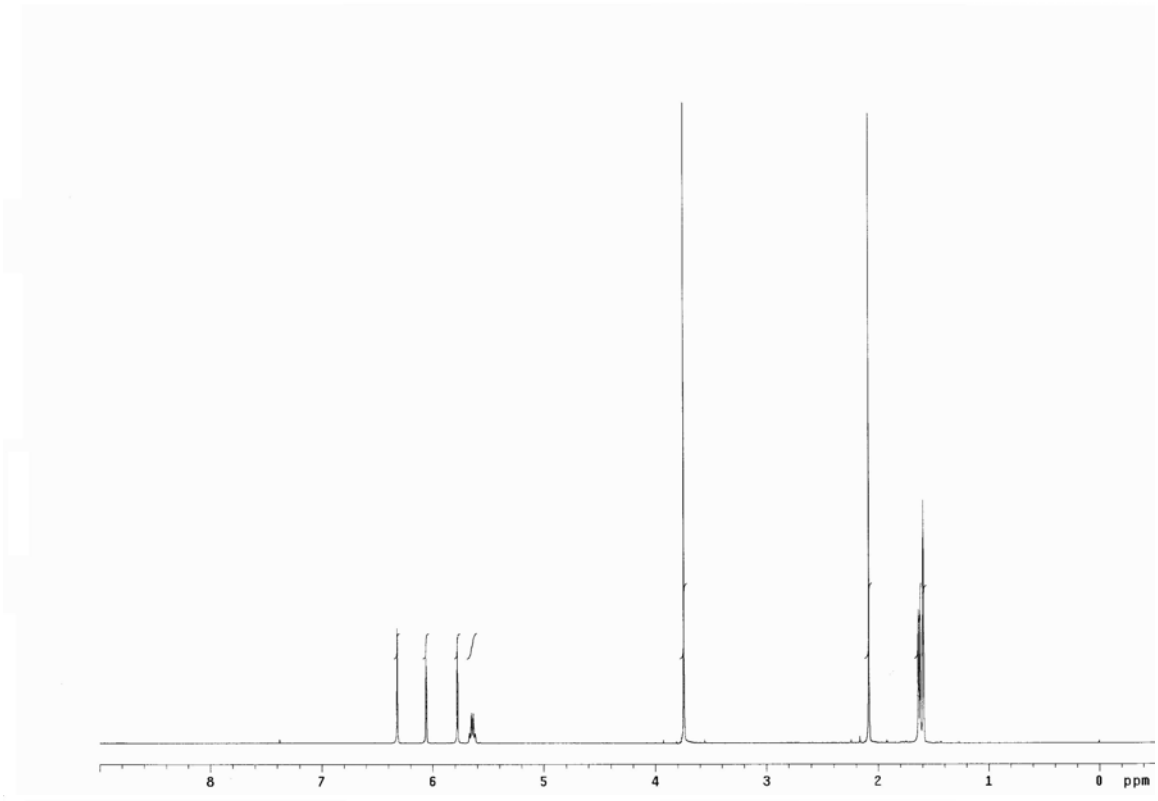
11a

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.33 (d, *J* = 0.4 Hz, 1H), 6.06 (s, 1H), 5.77 (t, *J* = 1.2 Hz, 1H), 5.67-5.62 (m, 1H), 3.75 (s, 3H), 2.09 (s, 3H), 1.63 (d, *J* = 6.8 Hz, 3H), 1.59 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.0, 165.3, 138.2, 131.0, 124.9, 124.6, 75.4, 51.5, 20.6, 13.0, 11.7

HRMS calcd for $C_{11}H_{16}O_4$ [M+1] 212.104859, found 212.105449

FTIR (neat) 2996, 2924, 1717, 1632, 1439, 1372, 1232, 1147, 1022, 979, 818 cm^{-1}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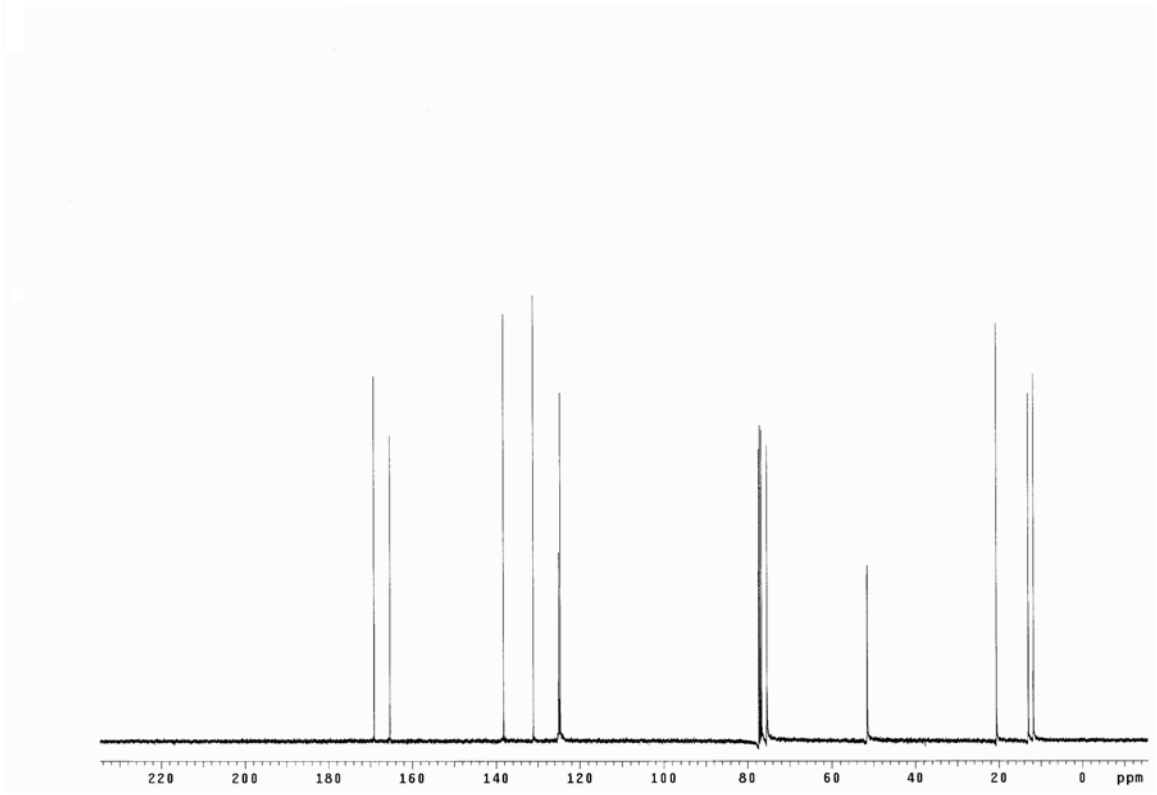
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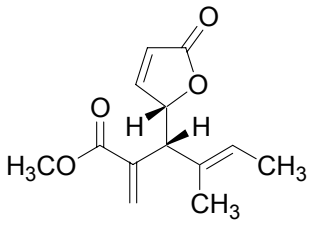


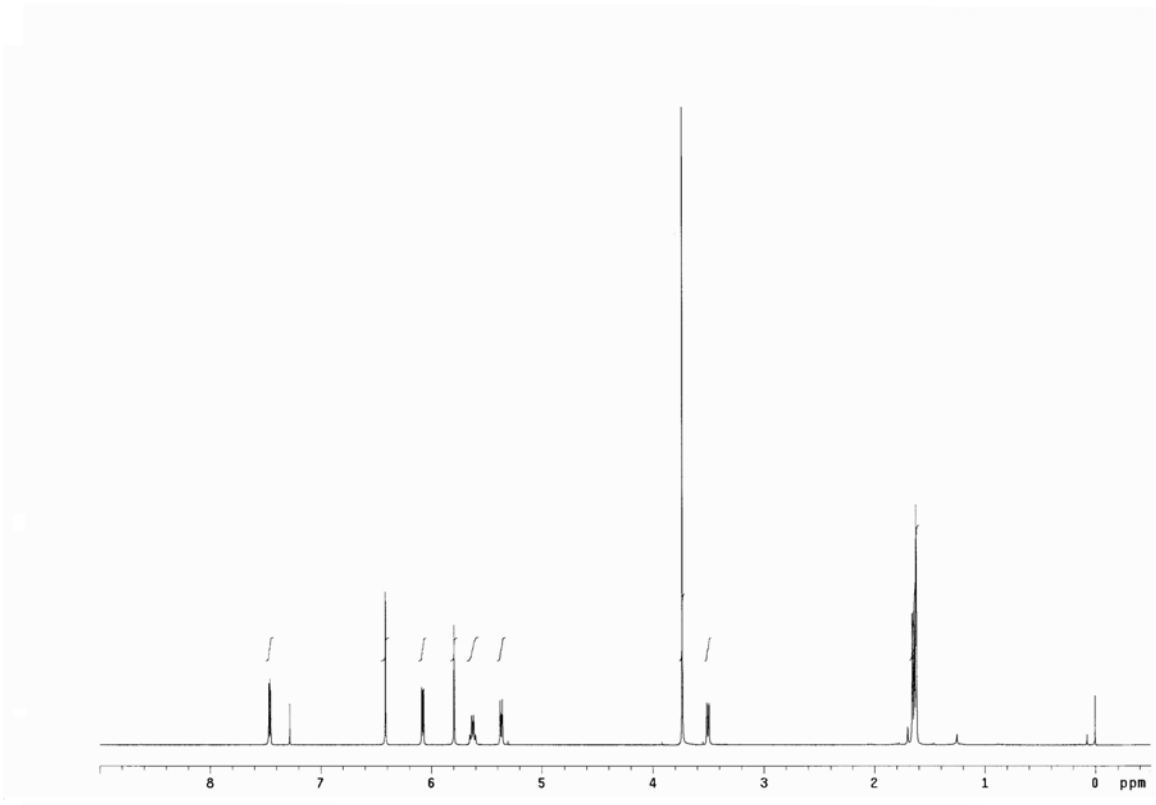
11b

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (dd, *J* = 6.0, 1.6 Hz, 1H), 6.41 (s, 1H), 6.08 (dd, *J* = 6.0, 2.0 Hz, 1H), 5.79 (s, 1H), 5.63 (q, *J* = 13.2, 6.4 Hz, 1H), 5.37 (ddd, *J* = 7.2, 3.2, 1.6 Hz, 1H), 3.73 (s, 3H), 3.51 (d, *J* = 7.2 Hz, 3H), 1.64 (d, *J* = 7.2 Hz, 3H), 1.62 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.7, 167.0, 155.8, 132.3, 127.4, 123.3, 121.6, 82.7, 52.0, 51.0, 15.6, 13.5

HRMS calcd for $C_{13}H_{17}O_4$ [M+1] 237.112684, found 237.112807

FTIR (neat) 3112, 2953, 2922, 1757, 1714, 1630, 1439, 1263, 1234, 1151, 817, 732 cm^{-1}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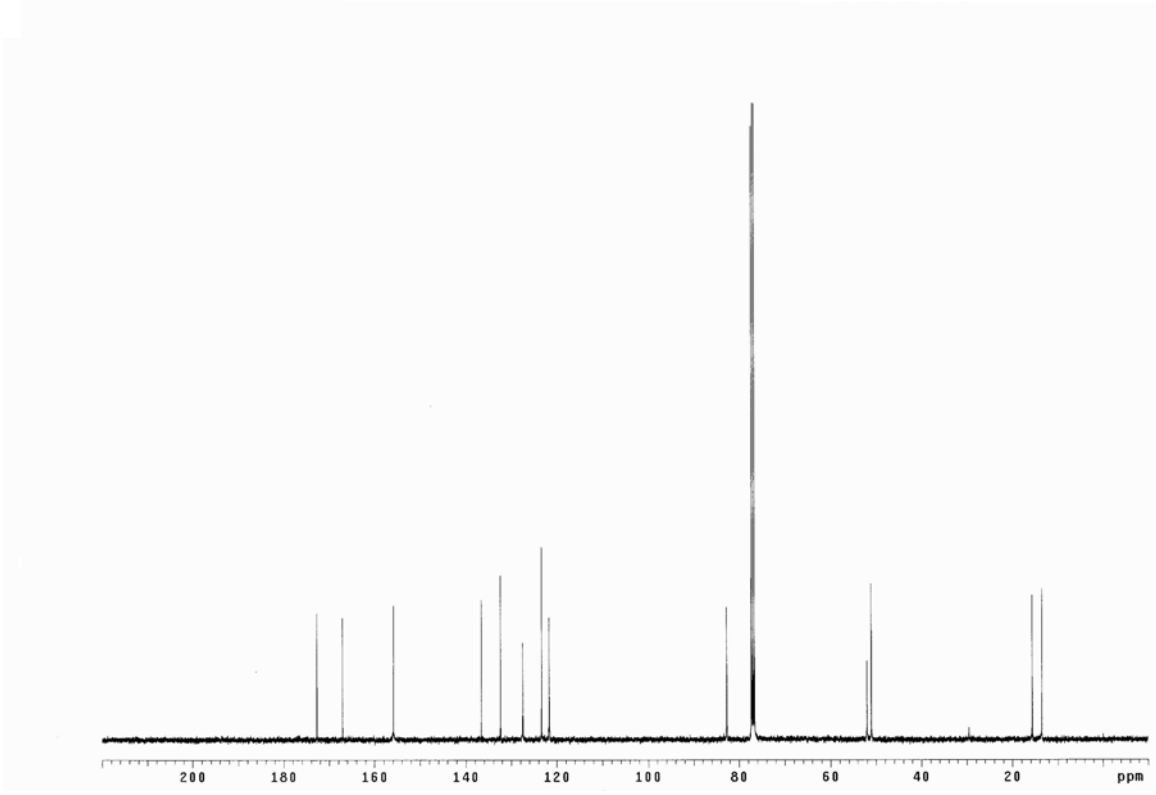
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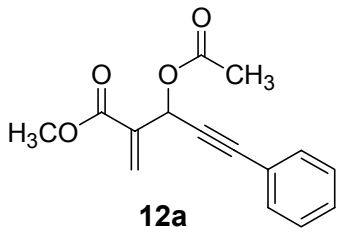


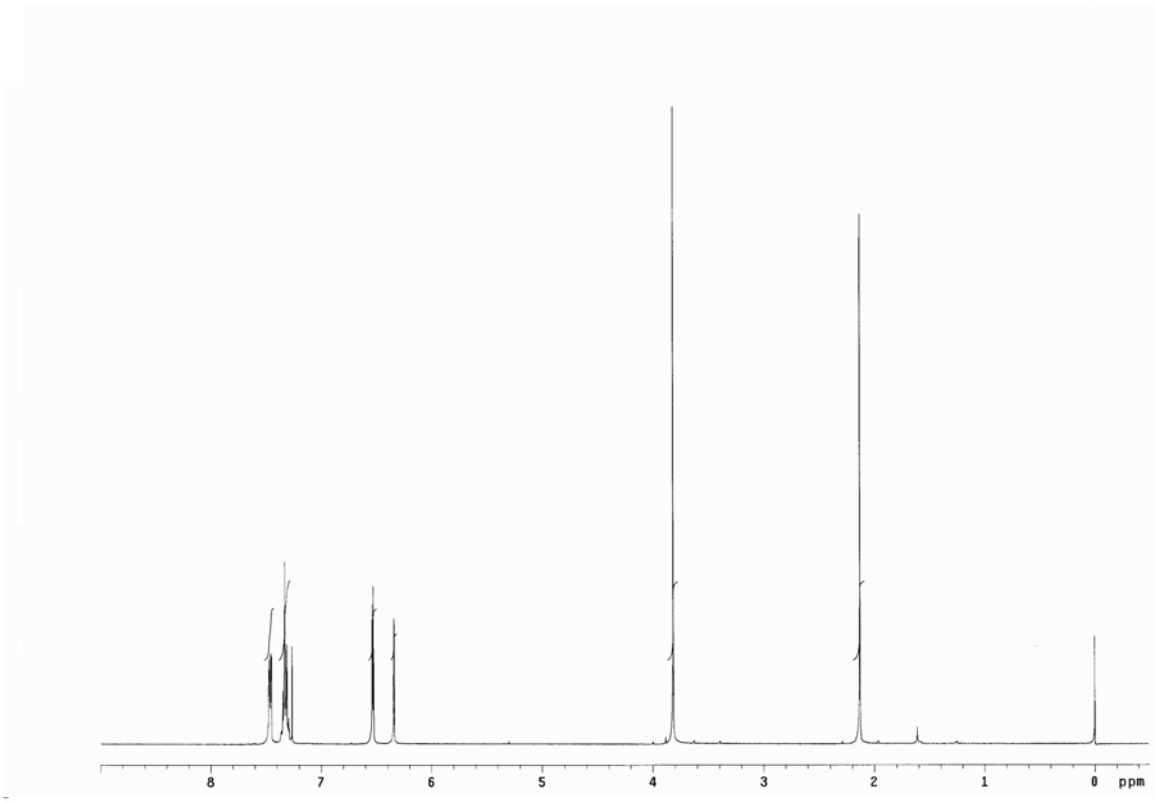
12a

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47-7.45 (m, 2H), 7.36-7.28 (m, 3H), 6.53 (s, 1H), 6.52 (s, 1H), 6.34 (d, *J* = 0.8 Hz, 1H), 3.81 (s, 3H), 2.13 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.2, 164.8, 136.5, 131.8, 129.1, 128.8, 128.2, 121.7, 87.1, 83.6, 62.0, 52.2, 20.8

HRMS calcd for $C_{15}H_{14}O_4$ [M+1] 258.089209, found 258.089292

FTIR (neat) 2953, 2233, 1747, 1440, 1369, 1253, 1222, 1147, 1042, 998, 758, 692 cm^{-1}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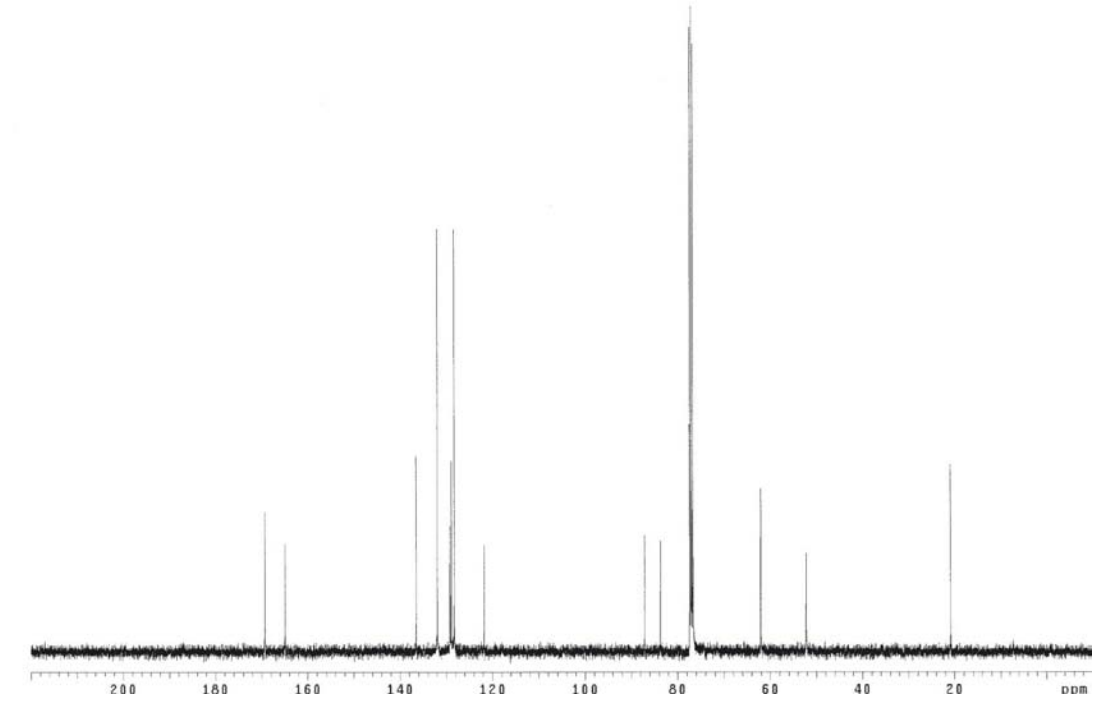
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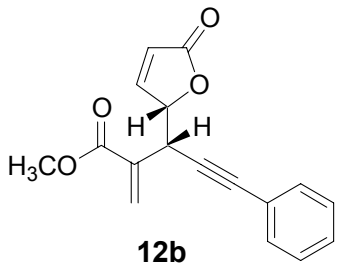


12b

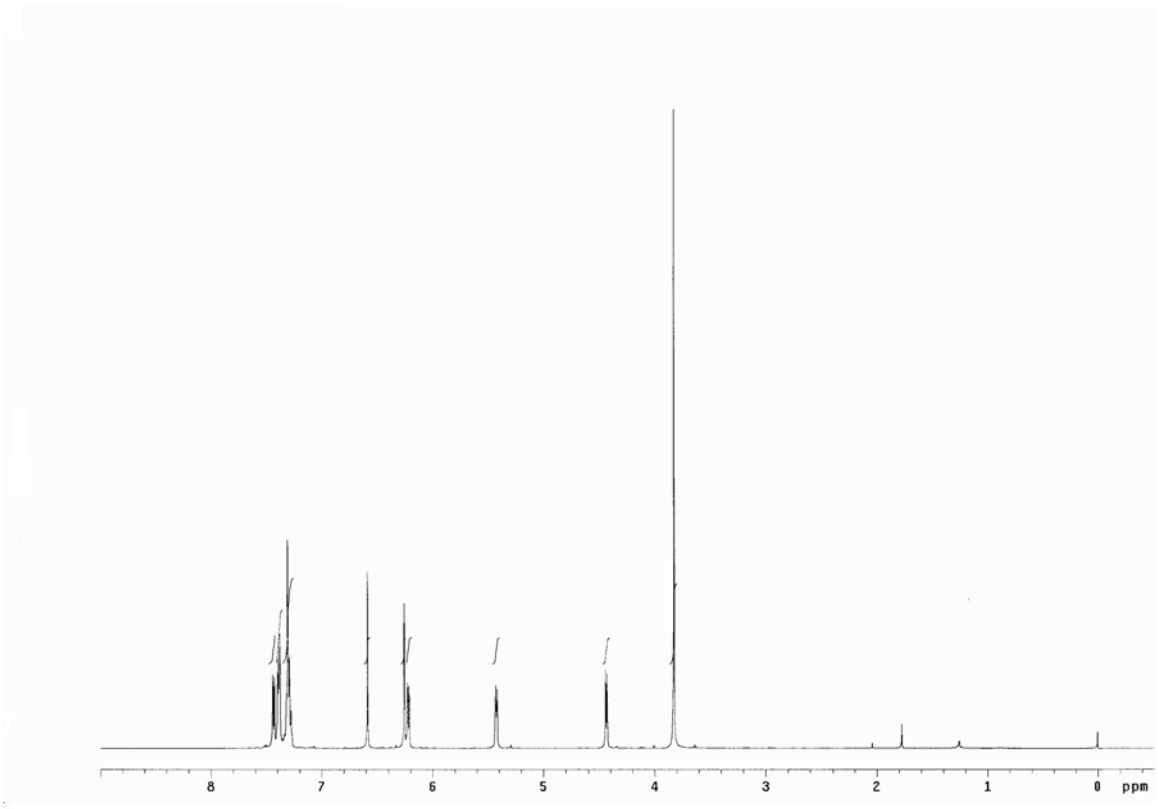
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (dd, *J* = 6.0, 1.6 Hz, 1H), 7.40-7.37 (m, 2H), 7.32-7.27 (m, 3H), 6.58 (s, 1H), 6.25 (s, 1H), 6.22 (dd, *J* = 6.0, 2.0 Hz, 1H), 5.42 (ddd, *J* = 5.6, 2.8, 1.2 Hz, 1H), 4.44 (d, *J* = 4.8 Hz,, 1H), 3.82 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.1, 165.7, 153.2, 134.7, 131.6, 130.7, 128.4, 128.2, 123.1, 122.1, 86.7, 83.4, 82.3, 52.4, 38.2

HRMS calcd for $C_{17}H_{15}O_4$ [M+1] 283.097034, found 283.097888

FTIR (neat) 3096, 2950, 2101, 1759, 1636, 1145, 822, 758. 692 cm^{-1}

M.P. 103~105 ^{o}C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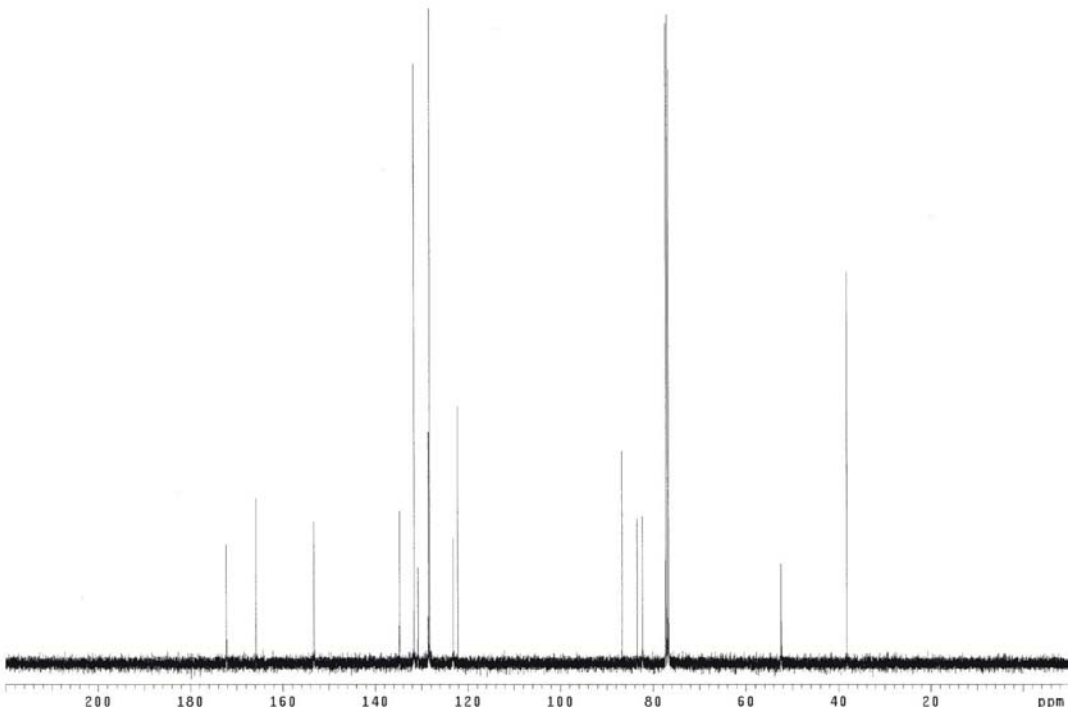
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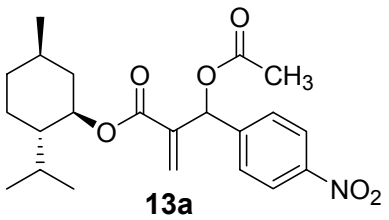


13a

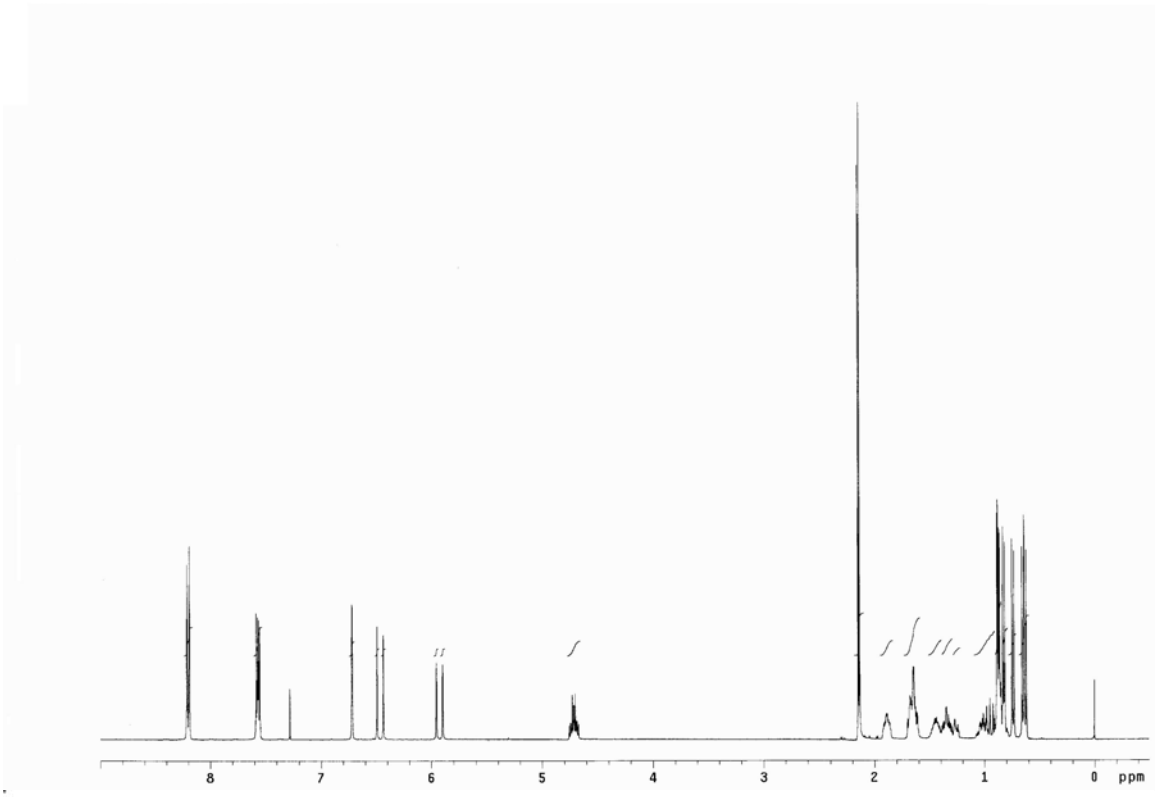
mixture of two diastereomers (dr = 50 : 50)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21-8.19 (m, 2H), 7.58-7.55 (m, 2H), 6.71 (s, 1H), 6.49 (s, 0.5H) and 6.43 (s, 0.5H), 5.95 (t, *J* = 1.2 Hz, 0.5H) and 5.89 (t, *J* = 1.6 Hz,, 0.5H), 4.75-4.67 (m, 1H), 2.14 (s, 1.5H) and 2.13 (s, 1.5H), 1.91-1.85 (m, 1H), 1.70-1.23 (m, 5H), 1.06-0.78 (m, 3H), 0.88 (d, *J* = 2.8 Hz, 1.5H) and 0.86 (d, *J* = 3.2 Hz, 1.5H), 0.81 (d, *J* = 7.6 Hz, 1.5H) and 0.74 (d, *J* = 6.8 Hz, 1.5H), 0.65 (d, *J* = 6.8 Hz, 1.5H) and 0.63 (d, *J* = 7.2 Hz, 1.5H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 164.0 and 163.9, 147.6, 145.2 and 145.1, 139.0 and 138.7, 128.6 and 128.3, 126.6 and 126.3, 123.5, 75.3 and 75.2, 72.2 and 72.1, 46.9, 40.6 and 40.5, 34.0 and 33.9, 31.2, 26.2 and 25.8, 23.2 and 22.9, 21.8 and 20.8, 20.6, 16.1 and 15.8

HRMS calcd for $C_{22}H_{30}NO_6$ [M+1] 404.207313, found 404.207630

FTIR (neat) 2959, 2870, 1744, 1710, 1530, 1350, 1230, 1035, 913, 735 cm^{-1}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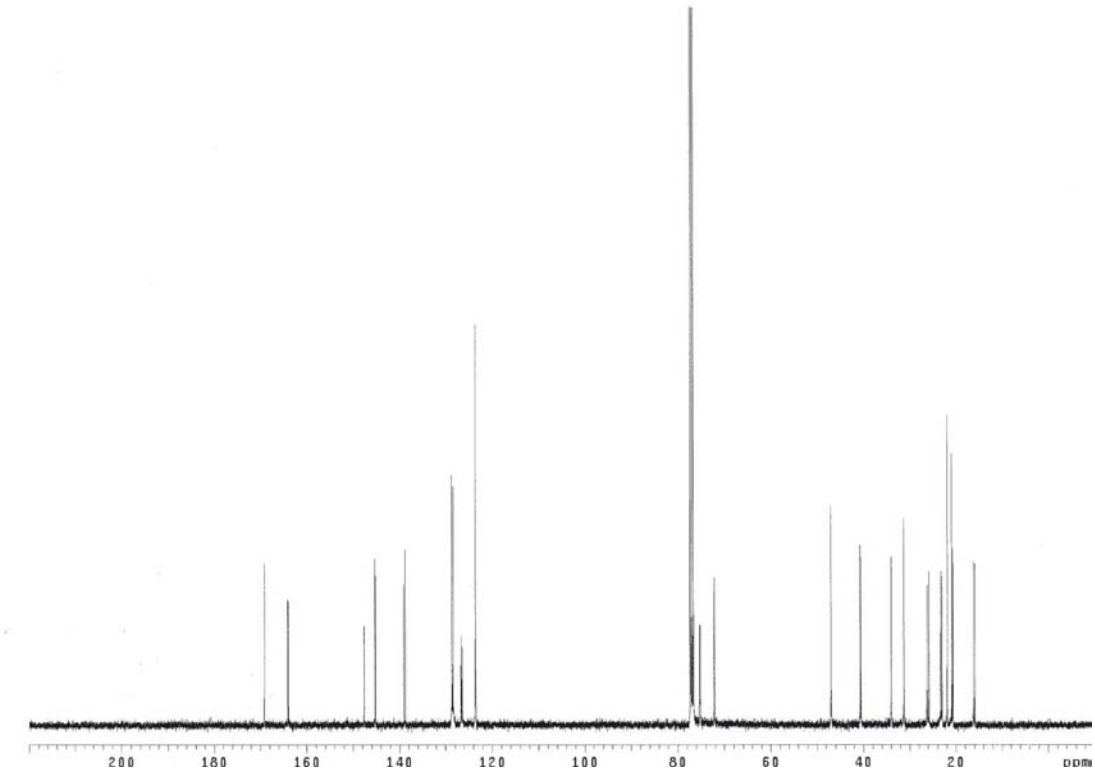
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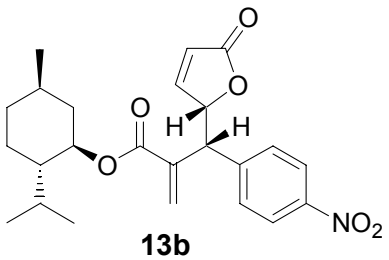


13b

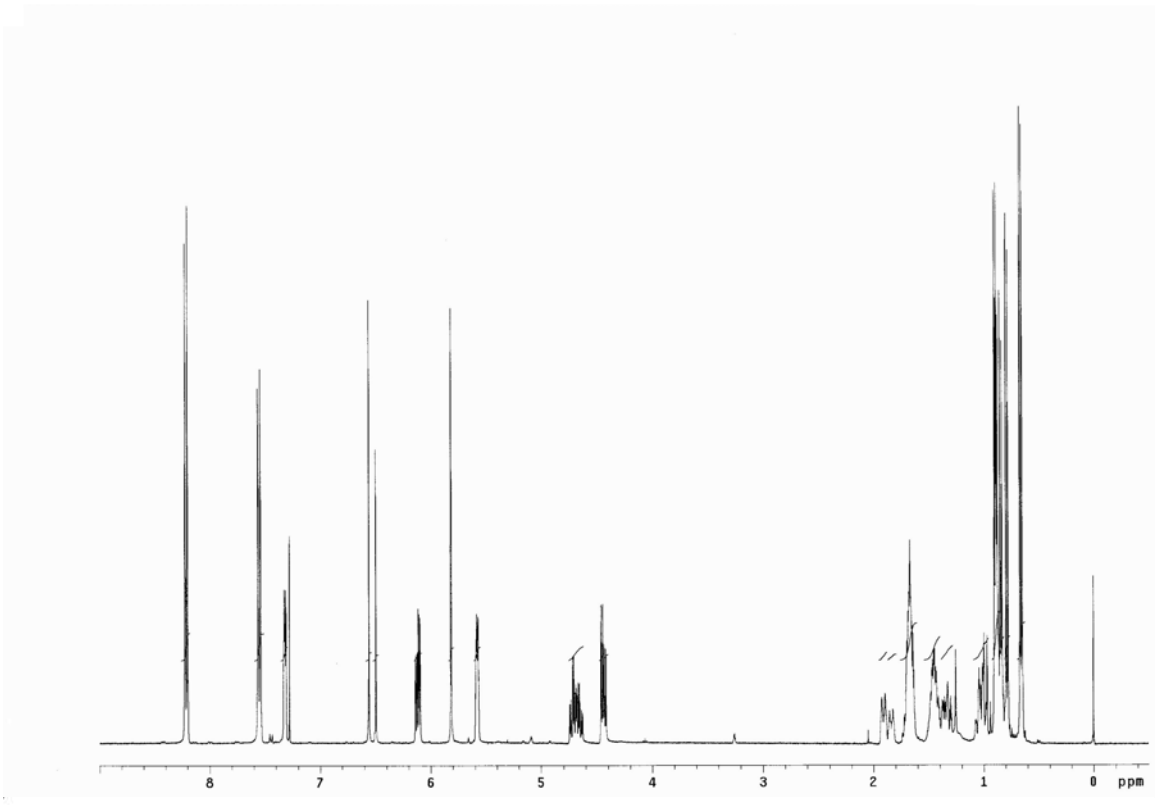
mixture of two diastereomers (dr = 59 : 41)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22-8.19 (m, 2H), 7.56-7.53 (m, 2H), 7.33-7.30 (m, 1H), 6.55 and 6.49 (major: s, minor: s, 1H), 6.13 and 6.10 (minor: dd, *J* = 6.0, 2.0 Hz, major: dd, *J* = 5.6, 2.0 Hz, 1H), 5.81 (s, 1H), 5.59-5.56 (m, 1H), 4.45 and 4.43 (major: d, *J* = 6.0 Hz, minor: d, *J* = 6.4 Hz, 1H), 1.91 and 1.84 (major: m, minor: m, 1H), 1.72-1.29 (m, 5H), 1.07-0.94 (m, 2H), 0.89 and 0.88 (major: d, *J* = 6.4 Hz, minor: d, *J* = 6.4 Hz, 3H), 0.84 and 0.79 (minor: d, *J* = 7.2 Hz, major: d, *J* = 6.8 Hz, 3H), 0.66 (d, *J* = 6.8 Hz, 3H)

^{13}C NMR (75 MHz, $CDCl_3$)
Major: δ 172.0, 165.3, 154.4, 147.2, 145.9, 136.9, 129.5, 129.1, 123.9, 122.5, 82.2, 75.5, 48.7, 47.0, 40.7, 34.0, 31.3, 26.0, 23.1, 21.8, 20.6, 16.0
Minor: δ 172.0, 165.5, 154.4, 147.2, 145.8, 137.3, 129.5, 128.5, 123.9, 122.5, 82.2, 75.5, 49.0, 46.9, 40.4, 34.0, 31.2, 26.4, 23.4, 21.8, 20.5, 16.3

HRMS calcd for $C_{24}H_{30}NO_6$ [M+1] 428.207313, found 428.208949

FTIR (neat) 3111, 2959, 2870, 1758, 1707, 1527, 1347, 1159, 1102, 909, 815, 732 cm^{-1}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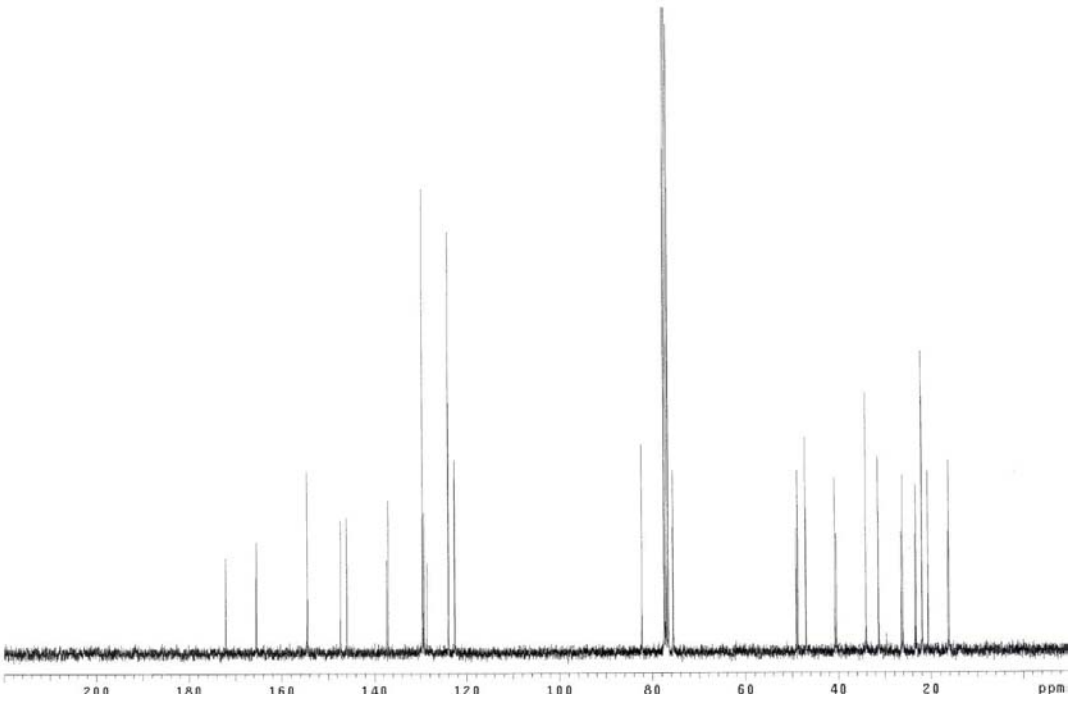
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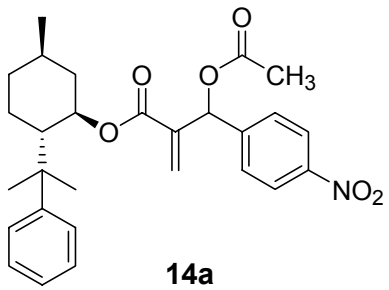


14a

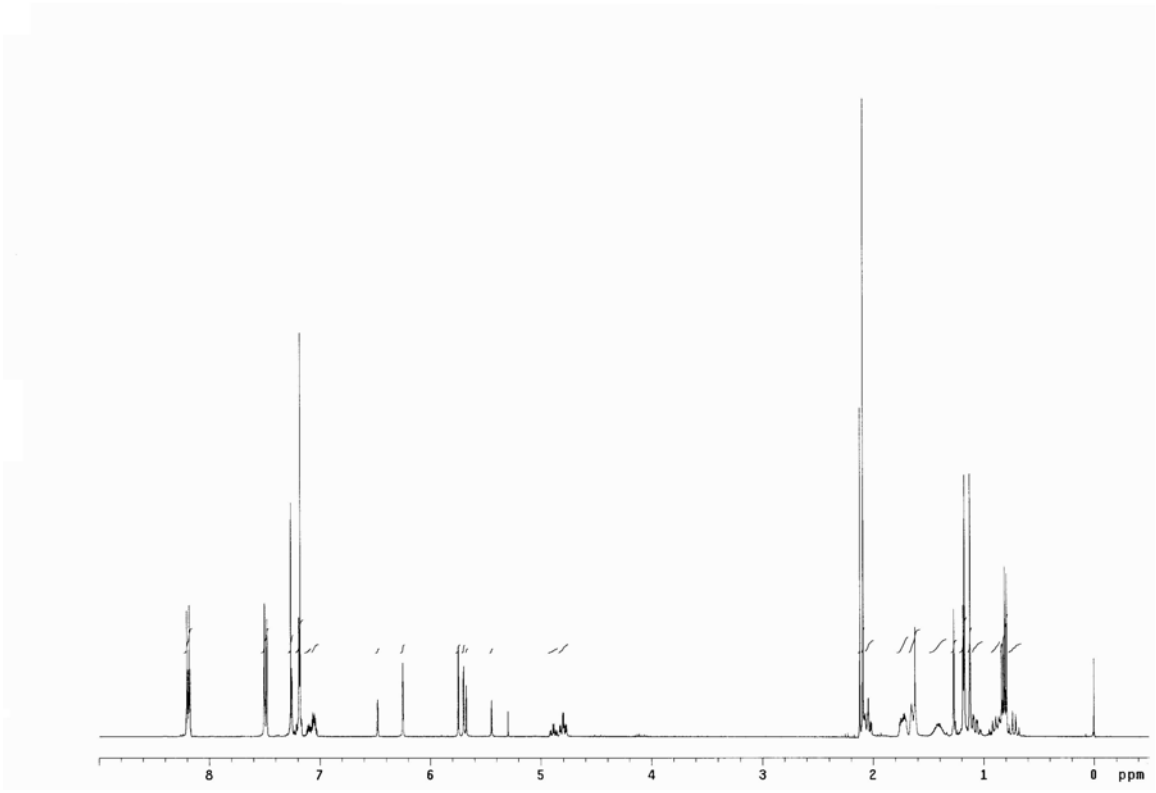
mixture of two diastereomers (dr = 67 : 33)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21-8.16 (m, 2H), 7.50-7.47 (m, 2H), 7.26-7.02 (m, 5H), 6.47 and 6.25 (minor: s, major: s, 1H), 5.74 and 5.67 (major: s, minor: s, 1H), 5.70 and 5.44 (major: d, *J* = 0.8 Hz, minor: d, *J* = 1.6 Hz, 1H), 4.89 and 4.80 (minor: dt, *J* = 10.4, 4.4 Hz, major: dt, *J* = 10.8, 4.4 Hz, 1H), 2.12 and 2.09 (minor: s, major: s, 3H), 2.08-2.01 (m, 1H), 1.76-1.68 (m, 7H), 1.23 and 1.15 (minor: d, *J* = 33.6 Hz, major: d, *J* = 20.0 Hz, 6H), 0.83 and 0.80 (minor: d, *J* = 6.4 Hz, major: d, *J* = 6.4 Hz, 3H)

^{13}C NMR (100 MHz, $CDCl_3$)
Major: δ 169.1, 163.7, 151.9, 147.8, 145.8, 138.4, 128.9, 128.3, 125.4, 125.2, 123.6, 75.6, 72.3, 50.5, 41.5, 39.6, 34.6, 31.4, 28.8, 26.6, 24.3, 21.1
Minor: δ 169.2, 164.0, 151.8, 147.8, 145.6, 138.7, 128.5, 128.3, 126.1, 125.6, 123.8, 75.5, 72.2, 50.4, 41.8, 39.7, 34.6, 31.4, 28.5, 26.7, 24.8, 21.9

HRMS calcd for $C_{28}H_{34}NO_6$ [M+1] 480.23807, found 480.23997

FTIR (neat) 2956, 2924, 1747, 1707, 1524, 1348, 1227, 1154, 1031, 701 cm^{-1}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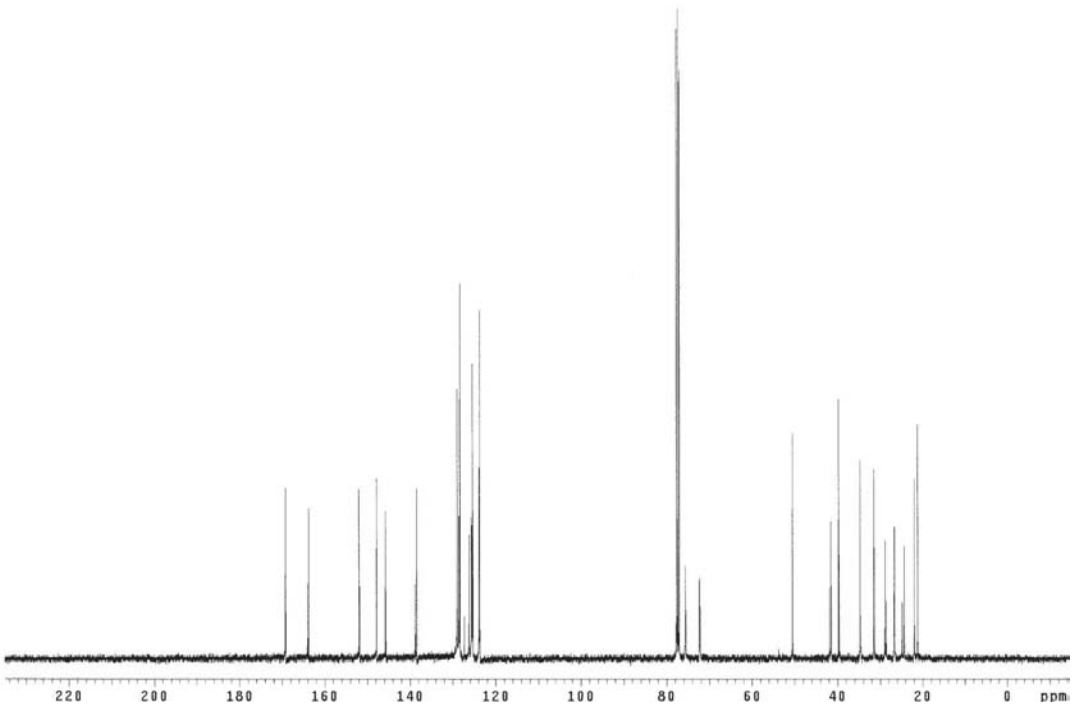
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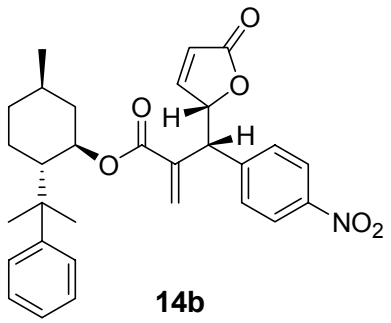


14b

single diastereomer (dr = >98 : 2)

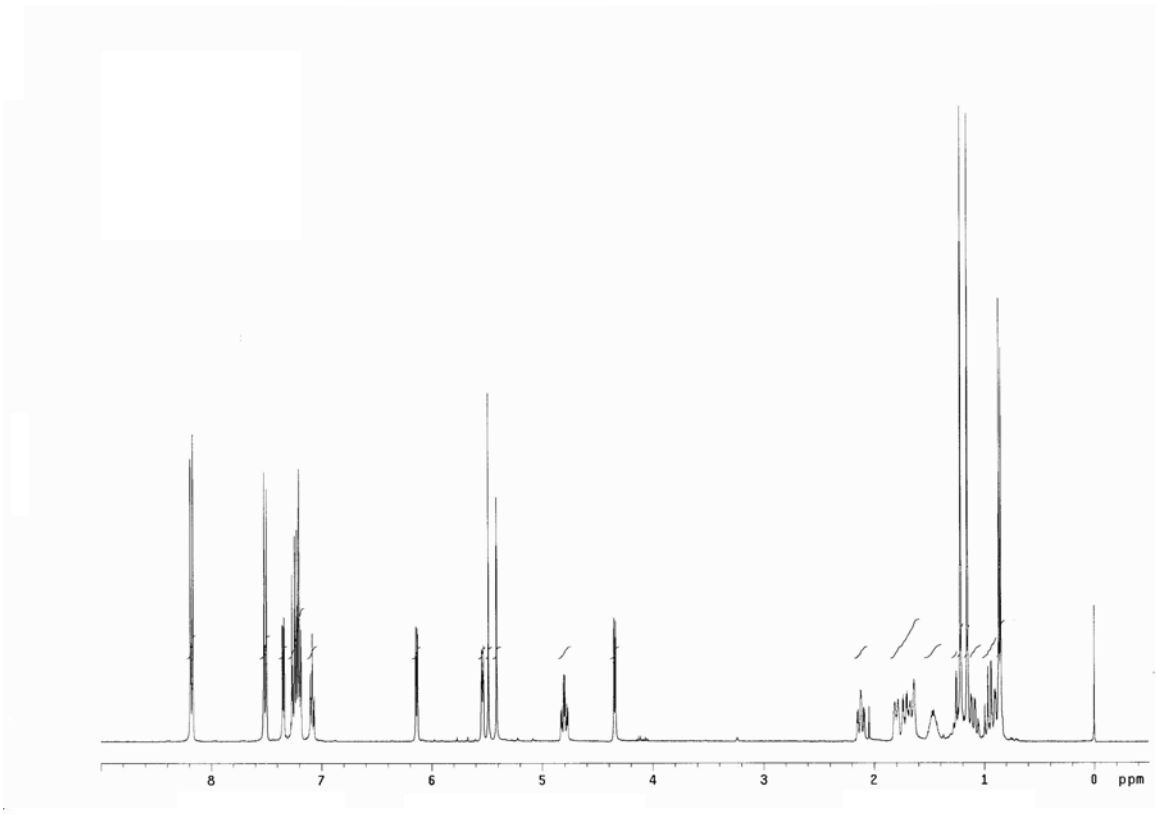
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19-8.16 (m, 2H), 7.52-7.50 (m, 2H), 7.34 (dd, *J* = 6.0, 1.6 Hz, 1H), 7.26-7.18 (m, 4H), 7.10-7.06 (m, 1H), 6.14 (dd, *J* = 6.0, 2.0 Hz, 1H), 5.54 (ddd, *J* = 5.6, 3.6, 1.6 Hz, 1H), 5.48 (s, 1H), 5.41 (s, 1H), 4.80 (dt, *J* = 10.4, 4.4 Hz, 1H), 4.35 (d, *J* = 6.0 Hz, 1H), 2.12 (dt, *J* = 10.4, 3.6 Hz, 1H), 1.81-1.64 (m, 3H), 1.52-1.41 (m, 1H), 1.28-0.89 (m, 3H), 1.18 (d, *J* = 24.4 Hz, 6H), 0.86 (d, *J* = 6.4 Hz, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.0, 165.1, 154.7, 151.5, 147.1, 146.4, 135.7, 130.7, 129.4, 128.1, 125.1, 123.8, 122.4, 82.2, 76.2, 50.1, 48.3, 41.4, 39.4, 34.4, 31.3, 28.2, 26.5, 24.7, 21.6

FTIR (neat) 2956, 2923, 1759, 1699, 1522, 1348, 1156, 910, 732, 702 cm^{-1}

M.P. 179~181 °C

X-Ray Crystallographic Data for 14b: S49-S87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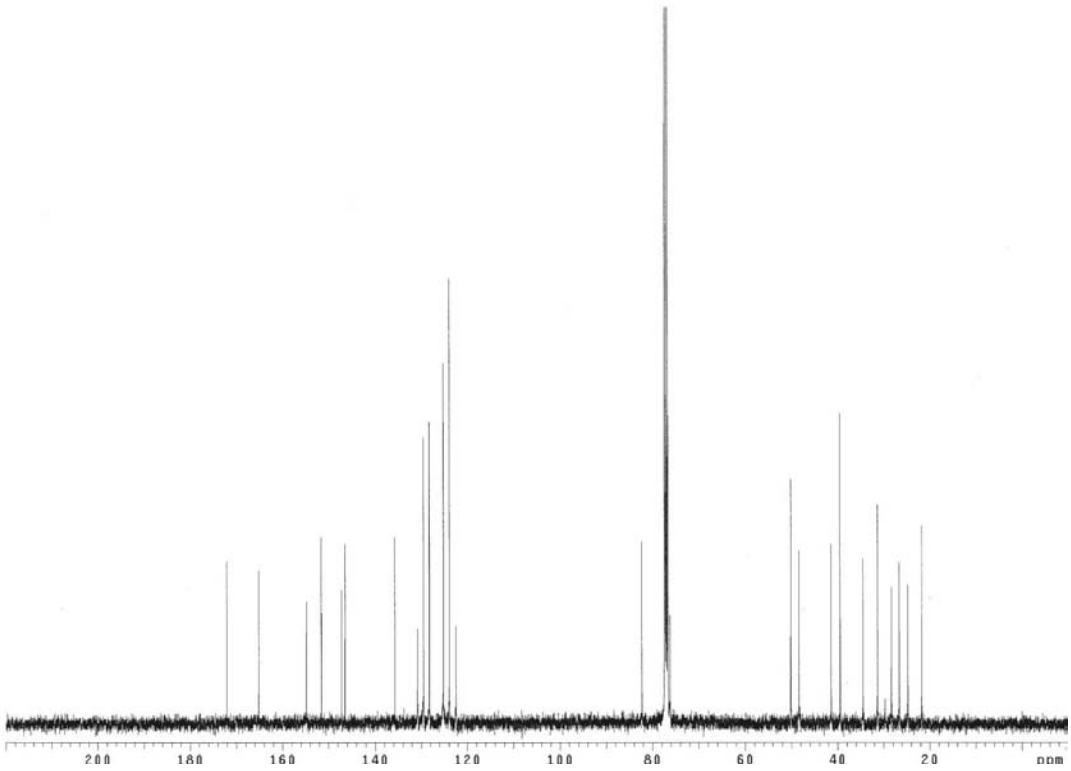
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Crystallographic Material for **14b**.

X-ray Experimental.

Table 1. Crystallographic Data for **14b**.

Table 2. Fractional coordinates and equivalent isotropic thermal parameters ($Å^2$) for the non-hydrogen atoms of **14b**.

Table 3. Bond Lengths (Å) and Angles (^{o}) for the non-hydrogen atoms of **14b**.

Table 4. Anisotropic thermal parameters for the non-hydrogen atoms of **14b**.

Table 5. Fractional coordinates and isotropic thermal parameters ($Å^2$) for the hydrogen atoms of **14b**.

Table 6. Torsion Angles (^{o}) for the non-hydrogen atoms of **14b**.

Table 7. Observed and calculated structure factor amplitudes for **14b**. Values for Fo, Fc and σ(Fo) have been multiplied by 10.

Figure 1. View of **14b** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level.

Figure 2. Unit cell packing diagram for **14b**. The view is approximately down the **a** axis.

X-ray Experimental for **14b**: Crystals grew very thin, colorless needles by slow evaporation from acetone-hexanes. The data crystal was cut from a long needle and had approximate dimensions; 0.56 x 0.08 x 0.06 mm. The data were collected on a Nonius Kappa CCD diffractometer using a graphite monochromator with MoKα radiation (λ = 0.71073Å). A total of 544 frames of data were collected using ω-scans with a scan range of 0.7° and a counting time of 101 seconds per frame. The data were collected at 153 K using an Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in Table 1. Data reduction were performed using DENZO-SMN.[1] The structure was solved by direct methods using SIR97[2] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-97.[3] The hydrogen atoms on carbon were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms). The function, $\Sigma w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.0373*P)^2 + (0.8544*P)]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. $R_w(F^2)$ refined to 0.127, with R(F) equal to 0.0620 and a goodness of fit, S, = 1.04. Definitions used for calculating R(F), $R_w(F^2)$ and the goodness of fit, S, are given below.[4] The data were corrected for secondary extinction effects. The correction takes the form: $F_{corr} = kF_c/[1 + (1.99(13)x10^{-5})* F_c^2 \lambda^3/(\sin 2\theta)]^{0.25}$ where k is the overall scale factor. The absolute configuration was assigned by internal comparison to the known configuration of the cyclohexyl moiety. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).[5] All figures were generated using SHELXTL/PC.[6] Tables of positional and thermal parameters, bond lengths and angles, torsion angles, figures and lists of observed and calculated structure factors are located in tables 1 through 7.

References

1) DENZO-SMN. (1997). Z. Otwinowski and W. Minor, Methods in Enzymology, **276**: Macromolecular Crystallography, part A, 307 – 326, C. W. Carter, Jr. and R. M. Sweets, Editors, Academic Press.

2) SIR97. (1999). A program for crystal structure solution. Altomare A., Burla M.C., Camalli M., Cascarano G.L., Giacovazzo C. , Guagliardi A., Moliterni A.G.G., Polidori G.,Spagna R. J. Appl. Cryst. 32, 115-119.

3) Sheldrick, G. M. (1994). SHELXL97. Program for the Refinement of Crystal Structures. University of Gottingen, Germany.

4) $R_W(F^2) = \{\Sigma w(|F_O|^2 - |F_C|^2)^2/\Sigma w(|F_O|)^4\}^{1/2}$ where w is the weight given each reflection.
$R(F) = \Sigma(|F_O| - |F_C|)/\Sigma|F_O|\}$ for reflections with $F_O > 4(\sigma(F_O))$.
$S = [\Sigma w(|F_O|^2 - |F_C|^2)^2/(n - p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters.

5) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, A. J. C. Wilson, editor, Boston: Kluwer Academic Press.

6) Sheldrick, G. M. (1994). SHELXTL/PC (Version 5.03). Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.

Table 1. Crystal data and structure refinement for **14b**.

Empirical formula	C30 H33 N O6	
Formula weight	503.57	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P212121	
Unit cell dimensions	a = 6.02730(10) Å	α= 90°.
	b = 18.1164(5) Å	β= 90°.
	c = 23.7715(7) Å	γ = 90°.
Volume	2595.68(11) $Å^3$	
Z	4	
Density (calculated)	1.289 Mg/m^3	
Absorption coefficient	0.089 mm^{-1}	
F(000)	1072	
Crystal size	0.56 x 0.08 x 0.06 mm	
Theta range for data collection	3.42 to 25.00°.	
Index ranges	-7<=h<=7, -21<=k<=21, -27<=l<=28	
Reflections collected	4561	
Independent reflections	4561	
Completeness to theta = 25.00°	99.7 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4561 / 0 / 335	
Goodness-of-fit on F^2	1.039	
Final R indices [I>2sigma(I)]	R1 = 0.0620, wR2 = 0.1036	
R indices (all data)	R1 = 0.1533, wR2 = 0.1273	
Extinction coefficient	$1.99(13)x10^{-5}$	
Largest diff. peak and hole	0.272 and -0.257 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **14b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C1	2697(7)	5362(2)	156(2)	32(1)
C2	1157(7)	4746(2)	-46(2)	34(1)
C3	435(8)	4940(2)	-647(2)	43(1)
C4	-661(7)	5693(2)	-677(2)	42(1)
C5	835(7)	6307(2)	-462(2)	40(1)
C6	1642(7)	6119(2)	131(2)	36(1)
O7	3296(4)	5205(1)	743(1)	31(1)
C8	5270(7)	5455(2)	920(2)	35(1)
O9	6521(5)	5811(2)	627(1)	44(1)
C10	5796(7)	5248(2)	1504(2)	31(1)
C11	4541(7)	4765(2)	1775(2)	46(1)
C12	7903(6)	5606(2)	1735(2)	31(1)
C13	8603(6)	5313(2)	2315(2)	34(1)
O14	10817(4)	5602(2)	2431(1)	38(1)
C15	10807(8)	5973(2)	2935(2)	39(1)
C16	8555(7)	5935(2)	3162(2)	35(1)
C17	7287(7)	5559(2)	2812(2)	37(1)
O18	12459(5)	6261(2)	3110(1)	56(1)
C19	7741(7)	6437(2)	1749(2)	33(1)
C20	5882(7)	6786(2)	1964(2)	38(1)
C21	5810(9)	7549(3)	2004(2)	49(1)
C22	7609(10)	7954(2)	1831(2)	47(1)
C23	9451(9)	7634(2)	1615(2)	50(1)
C24	9528(7)	6873(2)	1578(2)	39(1)
N25	7521(11)	8765(3)	1882(2)	73(2)
O26	9284(9)	9111(2)	1790(2)	105(2)
O27	5751(9)	9049(2)	2002(2)	93(2)
C28	2131(7)	3952(2)	29(2)	34(1)

C29	4555(7)	3940(2)	-181(2)	44(1)
C30	863(7)	3397(2)	-348(2)	46(1)
C31	1913(7)	3661(2)	629(2)	32(1)
C32	-87(7)	3719(2)	918(2)	41(1)
C33	-431(8)	3387(2)	1438(2)	46(1)
C34	1240(8)	2966(2)	1681(2)	47(1)
C35	3236(8)	2907(2)	1404(2)	46(1)
C36	3579(8)	3254(2)	891(2)	42(1)
C37	-298(8)	7061(2)	-480(2)	53(1)

Table 3. Bond lengths [Å] and angles [°] for **14b**.

C1-O7	1.469(4)	O14-C15	1.374(5)
C1-C6	1.512(5)	C15-O18	1.198(5)
C1-C2	1.529(5)	C15-C16	1.463(6)
C1-H1	0.96	C16-C17	1.318(5)
C2-C3	1.535(5)	C16-H16	0.96
C2-C28	1.563(5)	C17-H17	0.96
C2-H2	0.96	C19-C20	1.385(5)
C3-C4	1.518(6)	C19-C24	1.396(5)
C3-H3A	0.96	C20-C21	1.386(6)
C3-H3B	0.96	C20-H20	0.96
C4-C5	1.521(6)	C21-C22	1.372(6)
C4-H4A	0.96	C21-H21	0.96
C4-H4B	0.96	C22-C23	1.352(6)
C5-C37	1.527(6)	C22-N25	1.476(6)
C5-C6	1.529(5)	C23-C24	1.384(6)
C5-H5	0.96	C23-H23	0.96
C6-H6A	0.96	C24-H24	0.96
C6-H6B	0.96	N25-O27	1.218(6)
O7-C8	1.341(5)	N25-O26	1.252(6)
C8-O9	1.212(5)	C28-C31	1.526(5)
C8-C10	1.474(6)	C28-C29	1.544(6)
C10-C11	1.324(5)	C28-C30	1.548(5)
C10-C12	1.528(5)	C29-H29A	0.96
C11-H11A	0.96	C29-H29B	0.96
C11-H11B	0.96	C29-H29C	0.96
C12-C19	1.508(5)	C30-H30A	0.96
C12-C13	1.537(5)	C30-H30B	0.96
C12-H12	0.96	C30-H30C	0.96
C13-O14	1.460(4)	C31-C32	1.392(5)
C13-C17	1.492(5)	C31-C36	1.394(6)
C13-H13	0.96	C32-C33	1.390(6)

C32-H32	0.96	C35-H35	0.96
C33-C34	1.389(6)	C36-H36	0.96
C33-H33	0.96	C37-H37A	0.96
C34-C35	1.375(6)	C37-H37B	0.96
C34-H34	0.96	C37-H37C	0.96
C35-C36	1.386(6)		

O7-C1-C6	108.4(3)	C37-C5-C6	111.6(3)
O7-C1-C2	107.8(3)	C4-C5-H5	107.3
C6-C1-C2	113.2(3)	C37-C5-H5	107.8
O7-C1-H1	109.4	C6-C5-H5	108.2
C6-C1-H1	109.5	C1-C6-C5	111.9(3)
C2-C1-H1	108.4	C1-C6-H6A	109.4
C1-C2-C3	107.3(3)	C5-C6-H6A	109.1
C1-C2-C28	114.1(3)	C1-C6-H6B	109.0
C3-C2-C28	115.0(3)	C5-C6-H6B	109.0
C1-C2-H2	106.3	H6A-C6-H6B	108.3
C3-C2-H2	106.6	C8-O7-C1	116.8(3)
C28-C2-H2	107.0	O9-C8-O7	123.5(4)
C4-C3-C2	111.8(3)	O9-C8-C10	122.9(4)
C4-C3-H3A	110.0	O7-C8-C10	113.6(4)
C2-C3-H3A	109.7	C11-C10-C8	120.2(4)
C4-C3-H3B	108.5	C11-C10-C12	125.6(4)
C2-C3-H3B	108.4	C8-C10-C12	114.1(4)
H3A-C3-H3B	108.3	C10-C11-H11A	120.4
C3-C4-C5	112.6(4)	C10-C11-H11B	119.6
C3-C4-H4A	107.7	H11A-C11-H11B	120.0
C5-C4-H4A	107.4	C19-C12-C10	112.2(3)
C3-C4-H4B	110.5	C19-C12-C13	110.0(3)
C5-C4-H4B	110.6	C10-C12-C13	113.8(3)
H4A-C4-H4B	107.9	C19-C12-H12	105.9
C4-C5-C37	112.3(4)	C10-C12-H12	106.6
C4-C5-C6	109.5(3)	C13-C12-H12	107.9

O14-C13-C17	103.3(3)	C19-C24-H24	118.2
O14-C13-C12	107.3(3)	O27-N25-O26	125.0(5)
C17-C13-C12	117.6(3)	O27-N25-C22	118.1(6)
O14-C13-H13	109.1	O26-N25-C22	117.0(6)
C17-C13-H13	110.3	C31-C28-C29	112.2(3)
C12-C13-H13	108.9	C31-C28-C30	105.9(3)
C15-O14-C13	109.6(3)	C29-C28-C30	105.7(3)
O18-C15-O14	120.8(4)	C31-C28-C2	113.0(3)
O18-C15-C16	131.6(4)	C29-C28-C2	109.4(3)
O14-C15-C16	107.6(4)	C30-C28-C2	110.3(3)
C17-C16-C15	109.3(4)	C28-C29-H29A	110.4
C17-C16-H16	125.9	C28-C29-H29B	109.2
C15-C16-H16	124.8	H29A-C29-H29B	109.5
C16-C17-C13	110.2(4)	C28-C29-H29C	108.8
C16-C17-H17	125.4	H29A-C29-H29C	109.5
C13-C17-H17	124.3	H29B-C29-H29C	109.5
C20-C19-C24	118.2(4)	C28-C30-H30A	110.1
C20-C19-C12	121.1(4)	C28-C30-H30B	108.2
C24-C19-C12	120.5(4)	H30A-C30-H30B	109.5
C19-C20-C21	120.4(4)	C28-C30-H30C	110.1
C19-C20-H20	119.0	H30A-C30-H30C	109.5
C21-C20-H20	120.6	H30B-C30-H30C	109.5
C22-C21-C20	119.2(4)	C32-C31-C36	116.3(4)
C22-C21-H21	119.9	C32-C31-C28	120.7(4)
C20-C21-H21	120.9	C36-C31-C28	122.7(4)
C23-C22-C21	122.3(4)	C33-C32-C31	122.4(4)
C23-C22-N25	119.1(5)	C33-C32-H32	120.2
C21-C22-N25	118.6(5)	C31-C32-H32	117.4
C22-C23-C24	118.6(5)	C32-C33-C34	120.0(4)
C22-C23-H23	119.8	C32-C33-H33	120.2
C24-C23-H23	121.6	C34-C33-H33	119.9
C23-C24-C19	121.3(4)	C35-C34-C33	118.5(4)
C23-C24-H24	120.4	C35-C34-H34	120.3

C33-C34-H34	121.2	C5-C37-H37A	111.6
C34-C35-C36	121.1(4)	C5-C37-H37B	108.1
C34-C35-H35	119.1	H37A-C37-H37B	109.5
C36-C35-H35	119.8	C5-C37-H37C	108.6
C35-C36-C31	121.7(4)	H37A-C37-H37C	109.5
C35-C36-H36	119.2	H37B-C37-H37C	109.5
C31-C36-H36	119.1		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **14b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C1	32(3)	37(2)	27(3)	0(2)	-1(2)	1(2)
C2	30(2)	42(3)	29(2)	-4(2)	2(2)	-7(2)
C3	42(3)	55(3)	32(3)	-3(2)	-1(2)	-7(2)
C4	37(3)	52(3)	35(3)	4(2)	-2(2)	0(2)
C5	41(3)	44(3)	34(3)	6(2)	3(2)	3(2)
C6	33(3)	37(3)	39(3)	0(2)	3(2)	-4(2)
O7	28(2)	39(2)	28(2)	1(1)	0(1)	-5(1)
C8	33(3)	34(3)	39(3)	-2(2)	0(2)	1(2)
O9	40(2)	63(2)	29(2)	3(2)	-2(2)	-14(2)
C10	32(2)	31(2)	30(3)	-5(2)	3(2)	-3(2)
C11	53(3)	48(3)	37(3)	-4(2)	-5(3)	-7(2)
C12	25(2)	34(2)	34(3)	-1(2)	5(2)	1(2)
C13	35(3)	34(2)	33(3)	1(2)	-5(2)	2(2)
O14	25(2)	51(2)	37(2)	-4(2)	-5(1)	7(2)
C15	41(3)	49(3)	26(3)	0(2)	-1(2)	8(3)
C16	36(3)	42(3)	28(3)	-2(2)	2(2)	2(2)
C17	37(3)	37(3)	39(3)	4(2)	2(2)	3(2)
O18	35(2)	79(2)	52(2)	-12(2)	-8(2)	-7(2)
C19	33(3)	39(3)	27(3)	-3(2)	-6(2)	0(2)
C20	34(3)	40(3)	40(3)	-3(2)	-1(2)	6(2)
C21	57(3)	53(3)	37(3)	-5(2)	-9(3)	23(3)
C22	75(4)	31(3)	36(3)	-5(2)	-15(3)	-2(3)
C23	69(4)	41(3)	39(3)	1(2)	-7(3)	-15(3)
C24	36(3)	44(3)	36(3)	-4(2)	-11(2)	-4(2)
N25	124(5)	54(4)	41(3)	-5(2)	-25(3)	2(4)
O26	151(4)	53(3)	111(4)	-12(2)	-27(4)	-27(3)
O27	163(4)	62(3)	54(3)	-13(2)	-25(3)	49(3)
C28	30(2)	34(2)	40(3)	-6(2)	4(2)	-2(2)

C29	43(3)	46(3)	42(3)	-1(2)	5(2)	3(2)
C30	48(3)	49(3)	43(3)	-7(2)	0(2)	-8(3)
C31	32(3)	30(2)	35(3)	-4(2)	-1(2)	-3(2)
C32	35(3)	45(3)	42(3)	5(2)	-5(2)	-2(2)
C33	51(3)	49(3)	37(3)	2(3)	3(3)	-11(3)
C34	49(3)	41(3)	51(3)	9(2)	-6(3)	-9(2)
C35	47(3)	36(3)	55(3)	1(2)	-11(3)	-1(2)
C36	44(3)	31(2)	51(3)	-3(2)	2(2)	4(2)
C37	52(3)	54(3)	54(3)	8(3)	-2(3)	12(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **14b**.

	x	y	z	U(eq)
H1	4011	5356	-72	38
H2	-149	4774	184	40
H3A	-561	4568	-786	51
H3B	1729	4945	-883	51
H4A	-1948	5681	-439	50
H4B	-1146	5796	-1053	50
H5	2103	6327	-706	48
H6A	2700	6483	249	43
H6B	404	6132	385	43
H11A	4908	4617	2151	55
H11B	3251	4565	1593	55
H12	9068	5494	1473	37
H13	8667	4784	2301	41
H16	8084	6157	3508	42
H17	5740	5456	2866	45
H20	4643	6493	2084	45
H21	4522	7796	2149	58
H23	10672	7937	1496	59
H24	10815	6631	1428	47
H29A	5166	3453	-146	66
H29B	4594	4090	-568	66
H29C	5412	4279	41	66
H30A	1490	2913	-308	70
H30B	-660	3388	-229	70
H30C	944	3547	-734	70
H32	-1258	3994	742	49
H33	-1816	3451	1631	55

H34	1015	2717	2033	57
H35	4411	2627	1573	55
H36	4999	3211	711	50
H37A	-805	7179	-852	80
H37B	-1540	7049	-227	80
H37C	741	7428	-357	80

Table 6. Torsion angles [°] for **14b**.

O7-C1-C2-C3	176.8(3)	C13-O14-C15-O18	-179.4(4)
C6-C1-C2-C3	56.8(4)	C13-O14-C15-C16	0.0(4)
O7-C1-C2-C28	-54.7(4)	O18-C15-C16-C17	179.5(5)
C6-C1-C2-C28	-174.6(3)	O14-C15-C16-C17	0.2(4)
C1-C2-C3-C4	-56.6(4)	C15-C16-C17-C13	-0.3(5)
C28-C2-C3-C4	175.4(3)	O14-C13-C17-C16	0.2(4)
C2-C3-C4-C5	57.9(5)	C12-C13-C17-C16	-117.6(4)
C3-C4-C5-C37	-178.7(4)	C10-C12-C19-C20	47.0(5)
C3-C4-C5-C6	-54.1(5)	C13-C12-C19-C20	-80.8(5)
O7-C1-C6-C5	-176.5(3)	C10-C12-C19-C24	-137.2(4)
C2-C1-C6-C5	-56.9(5)	C13-C12-C19-C24	95.0(4)
C4-C5-C6-C1	53.1(5)	C24-C19-C20-C21	0.3(6)
C37-C5-C6-C1	178.1(3)	C12-C19-C20-C21	176.2(4)
C6-C1-O7-C8	-85.7(4)	C19-C20-C21-C22	-0.4(7)
C2-C1-O7-C8	151.3(3)	C20-C21-C22-C23	0.7(7)
C1-O7-C8-O9	1.9(6)	C20-C21-C22-N25	-179.3(4)
C1-O7-C8-C10	-177.4(3)	C21-C22-C23-C24	-1.0(7)
O9-C8-C10-C11	-169.4(4)	N25-C22-C23-C24	179.0(4)
O7-C8-C10-C11	9.9(6)	C22-C23-C24-C19	1.0(7)
O9-C8-C10-C12	7.8(6)	C20-C19-C24-C23	-0.7(6)
O7-C8-C10-C12	-172.9(3)	C12-C19-C24-C23	-176.6(4)
C11-C10-C12-C19	-121.4(5)	C23-C22-N25-O27	170.0(5)
C8-C10-C12-C19	61.6(4)	C21-C22-N25-O27	-10.0(7)
C11-C10-C12-C13	4.3(6)	C23-C22-N25-O26	-9.1(7)
C8-C10-C12-C13	-172.6(3)	C21-C22-N25-O26	170.9(4)
C19-C12-C13-O14	-63.3(4)	C1-C2-C28-C31	79.8(4)
C10-C12-C13-O14	169.9(3)	C3-C2-C28-C31	-155.6(3)
C19-C12-C13-C17	52.4(5)	C1-C2-C28-C29	-46.0(4)
C10-C12-C13-C17	-74.5(4)	C3-C2-C28-C29	78.6(4)
C17-C13-O14-C15	-0.1(4)	C1-C2-C28-C30	-161.9(3)
C12-C13-O14-C15	124.7(3)	C3-C2-C28-C30	-37.3(5)

C29-C28-C31-C32	171.4(4)
C30-C28-C31-C32	-73.7(4)
C2-C28-C31-C32	47.1(5)
C29-C28-C31-C36	-16.1(5)
C30-C28-C31-C36	98.8(4)
C2-C28-C31-C36	-140.4(4)
C36-C31-C32-C33	-0.6(6)
C28-C31-C32-C33	172.4(4)
C31-C32-C33-C34	-1.4(7)
C32-C33-C34-C35	1.9(7)
C33-C34-C35-C36	-0.5(7)
C34-C35-C36-C31	-1.5(7)
C32-C31-C36-C35	2.0(6)
C28-C31-C36-C35	-170.8(4)

__ Table 7. Observed and calculated structure factors for **14b**

Page 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	458	470	6	5	13	0	0	29	1	-2	4	1	475	495	5	6	10	1	0	19	1	1	19	1	76	79	58
4	0	0	59	12	59	0	14	0	187	185	12	-1	4	1	592	623	7	-6	11	1	95	47	47	2	19	1	59	41	59
6	0	0	95	167	51	1	14	0	199	199	8	0	4	1	1278	1229	16	-5	11	1	67	38	67	3	19	1	84	72	84
1	1	0	964	948	11	2	14	0	164	161	7	1	4	1	598	623	6	-4	11	1	0	25	1	-2	20	1	0	6	1
2	1	0	214	205	3	3	14	0	18	32	17	2	4	1	480	495	5	-3	11	1	248	241	5	-1	20	1	115	61	30
3	1	0	118	121	8	4	14	0	0	59	1	3	4	1	54	50	17	-2	11	1	0	18	1	0	20	1	0	9	1
4	1	0	167	152	8	5	14	0	25	61	25	4	4	1	347	342	5	-1	11	1	148	144	4	1	20	1	54	61	53
5	1	0	76	88	25	1	15	0	47	44	47	5	4	1	131	127	10	0	11	1	18	40	17	2	20	1	0	6	1
6	1	0	72	69	53	2	15	0	196	190	6	6	4	1	54	28	53	1	11	1	150	143	3	-1	21	1	36	37	35
7	1	0	0	21	1	3	15	0	0	2	1	7	4	1	82	53	82	2	11	1	67	18	16	0	21	1	111	45	70
1	2	0	374	378	3	4	15	0	40	24	40	-6	5	1	47	65	47	3	11	1	250	241	5	1	21	1	0	37	1
2	2	0	152	133	4	5	15	0	54	77	53	-5	5	1	153	152	8	4	11	1	0	25	1	1	0	2	584	597	6
3	2	0	31	1	31	0	16	0	76	80	40	-4	5	1	86	87	12	5	11	1	57	38	56	2	0	2	151	148	4
4	2	0	57	61	20	1	16	0	0	52	1	-3	5	1	322	308	4	6	11	1	78	47	78	3	0	2	289	254	6
5	2	0	138	112	10	2	16	0	74	34	11	-2	5	1	227	223	3	-5	12	1	126	110	25	4	0	2	25	17	25
6	2	0	18	3	17	3	16	0	135	150	12	-1	5	1	398	418	4	-4	12	1	170	163	10	5	0	2	435	415	6
7	2	0	0	34	1	4	16	0	88	112	37	0	5	1	1152	1137	14	-3	12	1	223	219	7	6	0	2	215	231	9
1	3	0	764	780	8	1	17	0	0	40	1	1	5	1	403	418	4	-2	12	1	113	125	10	7	0	2	78	47	78
2	3	0	236	243	3	2	17	0	67	67	67	2	5	1	220	224	4	-1	12	1	72	72	9	-7	1	2	0	26	1
3	3	0	206	200	4	3	17	0	57	86	56	3	5	1	317	309	4	0	12	1	80	13	18	-6	1	2	155	153	14
4	3	0	428	424	5	4	17	0	0	17	1	4	5	1	88	87	11	1	12	1	69	72	7	-5	1	2	113	123	13
5	3	0	120	94	12	0	18	0	118	119	31	5	5	1	152	152	7	2	12	1	119	125	8	-4	1	2	146	123	6
6	3	0	31	15	31	1	18	0	18	27	17	6	5	1	74	65	48	3	12	1	213	219	7	-3	1	2	258	248	5
7	3	0	0	57	1	2	18	0	62	7	62	-6	6	1	0	26	1	4	12	1	162	163	11	-2	1	2	119	117	5
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1	4	0	304	308	3	1	19	0	0	0	1	-4	6	1	336	317	5	-5	13	1	47	23	47	1	1	2	955	958	10
2	4	0	404	401	4	2	19	0	0	72	1	-3	6	1	522	500	5	-4	13	1	0	27	1	2	1	2	114	117	5
3	4	0	97	103	8	3	19	0	0	68	1	-2	6	1	222	229	3	-3	13	1	372	352	6	3	1	2	259	248	6
4	4	0	183	179	6	0	20	0	82	13	82	-1	6	1	319	341	4	-2	13	1	106	104	9	4	1	2	120	123	11
5	4	0	246	240	6	1	20	0	72	38	71	0	6	1	244	238	4	-1	13	1	84	89	24	5	1	2	115	123	13
6	4	0	0	28	1	2	20	0	0	3	1	1	6	1	318	341	4	0	13	1	95	109	14	6	1	2	151	153	14
7	4	0	74	71	73	1	21	0	44	78	43	2	6	1	236	228	3	1	13	1	93	89	15	7	1	2	0	26	1
1	5	0	114	100	4	1	0	1	65	74	5	3	6	1	520	500	5	2	13	1	100	104	8	-7	2	2	65	39	64
2	5	0	163	157	3	2	0	1	266	262	4	4	6	1	324	317	5	3	13	1	367	352	6	-6	2	2	40	67	40
3	5	0	206	191	4	3	0	1	91	103	7	5	6	1	106	106	9	4	13	1	62	27	36	-5	2	2	91	108	13
4	5	0	91	95	11	4	0	1	44	28	43	6	6	1	51	26	50	5	13	1	0	23	1	-4	2	2	139	140	7
5	5	0	290	292	6	5	0	1	0	11	1	-6	7	1	0	33	1	-5	14	1	116	11	34	-3	2	2	338	320	4
6	5	0	76	75	28	6	0	1	137	154	14	-5	7	1	69	72	18	-4	14	1	67	93	67	-2	2	2	401	401	4
0	6	0	283	299	7	7	0	1	67	7	67	-4	7	1	358	338	5	-3	14	1	51	59	32	-1	2	2	209	213	2
1	6	0	108	101	3	-7	1	1	0	68	1	-3	7	1	57	71	9	-2	14	1	100	103	11	1	2	2	209	213	3
2	6	0	0	12	1	-6	1	1	67	47	36	-2	7	1	421	418	4	-1	14	1	59	69	28	2	2	2	400	401	4
3	6	0	187	176	4	-5	1	1	62	45	36	-1	7	1	356	362	4	0	14	1	80	97	20	3	2	2	336	320	4
4	6	0	54	44	17	-4	1	1	279	269	5	0	7	1	88	98	7	1	14	1	59	69	28	4	2	2	147	140	7
5	6	0	127	106	10	-3	1	1	160	158	6	1	7	1	350	362	4	2	14	1	108	103	11	5	2	2	91	108	17

```
   6  6  0   44    5  43    -2  1  1  132  119   6     2  7  1  420  418   6     3 14  1   62   59  22     6  2  2   67
67  36
   1  7  0  424  431   5    -1  1  1 1261 1197  12     3  7  1   69   71   9     4 14  1   74   93  38     7  2  2    0
39   1
   2  7  0  272  272   4     1  1  1 1266 1197  13     4  7  1  350  338   6     5 14  1    0   11   1    -7  3  2   54
56  53
   3  7  0   80   92   6     2  1  1  119  118   5     5  7  1   65   72  28    -5 15  1   69   56  69    -6  3  2   98
88  24
   4  7  0   57   33  16     3  1  1  153  158   6     6  7  1    0   33   1    -4 15  1   25   39  25    -5  3  2   65
54  20
   5  7  0    0   19   1     4  1  1  277  269   6    -6  8  1   93   90  36    -3 15  1   18   69  17    -4  3  2  116
111   8
   6  7  0   47   52  47     5  1  1   78   45  27    -5  8  1  113  101  10    -2 15  1  134  135   8    -3  3  2  289
283   4
   0  8  0   57   49  25     6  1  1   54   47  53    -4  8  1   18    5  17    -1 15  1  235  233   8    -2  3  2  178
187   3
   1  8  0  672  649   8     7  1  1    0   68   1    -3  8  1  183  178   5     0 15  1   25   10  25    -1  3  2  724
744   6
   2  8  0  109  105   6    -7  2  1   31   22  31    -2  8  1  287  272   3     1 15  1  236  232   8     0  3  2   31
20  13
   3  8  0   74   55  11    -6  2  1  103  140  20    -1  8  1  194  196   4     2 15  1  142  135   8     1  3  2  722
744   7
   4  8  0  146  147   5    -5  2  1  137  130  11     0  8  1  822  789  12     3 15  1   47   68  47     2  3  2  195
187   3
   5  8  0    0   13   1    -4  2  1  118  114   8     1  8  1  200  196   4     4 15  1   54   40  53     3  3  2  290
284   4
   6  8  0   80   44  49    -3  2  1  250  237   4     2  8  1  286  272   5     5 15  1    0   56   1     4  3  2  137
111   8
   1  9  0  826  807  10    -2  2  1  374  373   4     3  8  1  185  178   6    -4 16  1   40   26  40     5  3  2   54
54  28
   2  9  0  162  153   6    -1  2  1  582  602   5     4  8  1    0    5   1    -3 16  1    0   51   1     6  3  2   59
87  59
   3  9  0   36   30  35     1  2  1  576  602   5     5  8  1   86  101  21    -2 16  1   40    8  40     7  3  2    0
56   1
   4  9  0  336  328   7     2  2  1  373  373   4     6  8  1    0   90   1    -1 16  1   44   54  43    -7  4  2    0
21   1
   5  9  0  193  193   6     3  2  1  248  237   4    -6  9  1   69   18  69     0 16  1  112  109  17    -6  4  2   74
51  30
   6  9  0   67   75  67     4  2  1   76  114  19    -5  9  1  138  129   7     1 16  1   67   54  31    -5  4  2   76
82  16
   0 10  0  178  196   9     5  2  1  126  130  17    -4  9  1    0   58   1     2 16  1    0    8   1    -4  4  2  216
202   6
   1 10  0  186  172   4     6  2  1  124  140  15    -3  9  1  100  103   8     3 16  1   54   51  53    -3  4  2  269
265   4
   2 10  0   72   62  12     7  2  1    0   22   1    -2  9  1  222  233   4     4 16  1    0   27   1    -2  4  2  226
229   3
   3 10  0   78   47  13    -7  3  1   74   59  73    -1  9  1  185  184   4    -4 17  1    0   62   1    -1  4  2  949
948  10
   4 10  0  152  149   9    -6  3  1   36   74  35     0  9  1   65   95  17    -3 17  1   82   65  82     0  4  2  245
261   3
   5 10  0   40   52  40    -5  3  1  178  175   7     1  9  1  184  184   4    -2 17  1    0   65   1     1  4  2  946
948  10
   6 10  0  111  109  32    -4  3  1  234  232   5     2  9  1  235  233   5    -1 17  1   25   50  25     2  4  2  224
229   3
   1 11  0  108   95   4    -3  3  1  271  249   4     3  9  1  122  103   8     0 17  1   78  126  38     3  4  2  275
265   3
   2 11  0  189  181   6    -2  3  1  311  312   4     4  9  1   25   58  25     1 17  1   31   50  31     4  4  2  214
202   4
   3 11  0   40    6  40    -1  3  1  643  666   6     5  9  1  127  129  11     2 17  1   47   65  47     5  4  2   78
82  16
   4 11  0  116  113  14     0  3  1  224  238   2     6  9  1   57   18  56     3 17  1   82   65  46     6  4  2   59
51  41
   5 11  0   82   40  38     1  3  1  642  666   6    -6 10  1    0   19   1     4 17  1   25   62  25     7  4  2   80
21  80
   6 11  0  115   68  40     2  3  1  310  312   3    -5 10  1   57   84  56    -3 18  1   84   41  84    -6  5  2   78
62  42
   0 12  0  269  260   9     3  3  1  267  248   4    -4 10  1  135  143   8    -2 18  1   76   50  45    -5  5  2   80
72  18
   1 12  0    0   46   1     4  3  1  242  232   5    -3 10  1   31   46  31    -1 18  1    0   15   1    -4  5  2  216
217   5
   2 12  0  354  334   5     5  3  1  180  175   9    -2 10  1  113  106   7     0 18  1    0   40   1    -3  5  2  340
324   4
   3 12  0  169  156   7     6  3  1   40   74  40    -1 10  1  220  216   4     1 18  1   62   15  62    -2  5  2  297
301   3
   4 12  0  228  230   8     7  3  1    0   59   1     0 10  1  236  224   6     2 18  1   90   50  32    -1  5  2  245
254   3
   5 12  0  109   55  23    -7  4  1   98   53  54     1 10  1  222  216   3     3 18  1  112   41  47     0  5  2 1204
1175  15
   1 13  0  264  263   7    -6  4  1   40   28  40     2 10  1  113  106   8    -3 19  1   59   72  59     1  5  2  251
254   3
   2 13  0   62   44  18    -5  4  1  123  126   9     3 10  1   59   46  19    -2 19  1   65   41  64     2  5  2  296
301   3
   3 13  0  293  277   6    -4  4  1  342  342   5     4 10  1  126  143  14    -1 19  1   65   79  64     3  5  2  338
324   5
   4 13  0   98   90  22    -3  4  1   57   50  16     5 10  1   31   84  31     0 19  1   54   57  53     4  5  2  222
217   4
```

Table 7. Observed and calculated structure factors for **14b**
Page 2

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
5	5	2	74	72	14	2	12	2	196	186	5	-4	1	3	132	145	7	-1	7	3	283	279	4	0	14	3	352	342	8
6	5	2	40	62	40	3	12	2	167	156	7	-3	1	3	102	109	8	0	7	3	62	71	8	1	14	3	196	188	5
-6	6	2	90	104	25	4	12	2	36	79	35	-2	1	3	253	266	3	1	7	3	282	279	4	2	14	3	72	52	15
-5	6	2	138	152	9	5	12	2	0	21	1	-1	1	3	599	639	6	2	7	3	243	240	4	3	14	3	194	178	7
-4	6	2	169	161	6	-5	13	2	31	65	31	1	1	3	596	638	6	3	7	3	132	139	6	4	14	3	0	22	1
-3	6	2	59	70	12	-4	13	2	80	76	36	2	1	3	259	266	4	4	7	3	256	255	5	5	14	3	0	44	1
-2	6	2	233	233	4	-3	13	2	204	200	6	3	1	3	95	109	10	5	7	3	93	90	19	-5	15	3	151	34	28
-1	6	2	323	341	4	-2	13	2	255	248	6	4	1	3	145	144	9	6	7	3	100	30	63	-4	15	3	51	66	50
0	6	2	562	587	6	-1	13	2	185	188	4	5	1	3	166	190	9	-6	8	3	0	32	1	-3	15	3	98	101	14
1	6	2	334	342	3	0	13	2	209	192	7	6	1	3	109	127	21	-5	8	3	132	152	10	-2	15	3	67	90	19
2	6	2	239	233	3	1	13	2	191	188	6	7	1	3	40	7	40	-4	8	3	95	72	10	-1	15	3	115	112	13
3	6	2	74	70	11	2	13	2	258	248	5	-7	2	3	109	54	41	-3	8	3	40	33	40	0	15	3	18	47	17
4	6	2	163	161	8	3	13	2	213	200	6	-6	2	3	103	112	20	-2	8	3	164	161	5	1	15	3	119	112	12
5	6	2	148	152	5	4	13	2	82	76	22	-5	2	3	51	62	32	-1	8	3	609	596	7	2	15	3	82	90	10
6	6	2	131	104	21	5	13	2	111	65	34	-4	2	3	36	33	35	0	8	3	0	16	1	3	15	3	97	101	14
-6	7	2	80	14	49	-5	14	2	95	80	38	-3	2	3	219	215	4	1	8	3	607	596	6	4	15	3	57	66	56
-5	7	2	54	5	35	-4	14	2	113	103	31	-2	2	3	166	167	4	2	8	3	167	161	3	5	15	3	25	34	25
-4	7	2	112	113	8	-3	14	2	212	211	7	-1	2	3	795	811	8	3	8	3	0	33	1	-4	16	3	84	98	44
-3	7	2	522	514	5	-2	14	2	312	305	6	0	2	3	804	829	14	4	8	3	36	72	35	-3	16	3	88	86	23
-2	7	2	448	446	5	-1	14	2	152	132	9	1	2	3	791	811	8	5	8	3	153	152	8	-2	16	3	57	86	31
-1	7	2	592	596	7	0	14	2	25	18	25	2	2	3	163	167	5	6	8	3	0	32	1	-1	16	3	0	54	1
0	7	2	349	368	4	1	14	2	133	132	10	3	2	3	219	215	4	-6	9	3	108	50	33	0	16	3	51	29	50
1	7	2	594	597	6	2	14	2	296	305	5	4	2	3	40	33	40	-5	9	3	204	206	8	1	16	3	0	54	1
2	7	2	448	446	4	3	14	2	210	211	7	5	2	3	51	62	50	-4	9	3	206	209	8	2	16	3	93	86	15
3	7	2	518	514	5	4	14	2	62	103	62	6	2	3	103	112	18	-3	9	3	161	166	8	3	16	3	76	86	19
4	7	2	115	113	8	5	14	2	103	80	40	7	2	3	0	54	1	-2	9	3	112	98	7	4	16	3	112	98	38
5	7	2	0	5	1	-5	15	2	0	27	1	-7	3	3	0	36	1	-1	9	3	301	300	4	-4	17	3	95	42	94
6	7	2	31	13	31	-4	15	2	67	54	67	-6	3	3	65	87	46	0	9	3	0	4	1	-3	17	3	62	47	62
-6	8	2	40	9	40	-3	15	2	93	106	15	-5	3	3	80	74	18	1	9	3	298	301	3	-2	17	3	122	115	12
-5	8	2	109	104	10	-2	15	2	74	56	17	-4	3	3	162	164	7	2	9	3	91	98	5	-1	17	3	80	72	26
-4	8	2	326	322	5	-1	15	2	201	204	9	-3	3	3	432	420	5	3	9	3	170	166	3	0	17	3	0	71	1
-3	8	2	54	73	17	0	15	2	0	12	1	-2	3	3	198	203	4	4	9	3	210	209	6	1	17	3	31	72	31
-2	8	2	59	70	12	1	15	2	212	204	9	-1	3	3	245	250	3	5	9	3	202	206	8	2	17	3	97	115	29
-1	8	2	397	395	4	2	15	2	54	56	17	0	3	3	80	87	6	6	9	3	0	50	1	3	17	3	78	47	47
0	8	2	390	409	5	3	15	2	88	106	16	1	3	3	241	249	2	-6	10	3	93	66	45	4	17	3	0	42	1
1	8	2	404	395	4	4	15	2	67	54	49	2	3	3	204	203	3	-5	10	3	0	59	1	-3	18	3	88	77	87
2	8	2	57	70	16	5	15	2	65	27	64	3	3	3	437	420	5	-4	10	3	0	53	1	-2	18	3	59	74	59
3	8	2	76	73	6	-4	16	2	86	76	35	4	3	3	167	164	6	-3	10	3	76	84	13	-1	18	3	44	22	43
4	8	2	327	323	5	-3	16	2	113	109	13	5	3	3	93	74	15	-2	10	3	101	108	8	0	18	3	0	90	1
5	8	2	91	104	19	-2	16	2	140	123	10	6	3	3	78	87	30	-1	10	3	222	225	4	1	18	3	91	23	24
6	8	2	0	9	1	-1	16	2	57	64	38	7	3	3	0	36	1	0	10	3	149	160	5	2	18	3	0	74	1
-6	9	2	86	51	50	0	16	2	0	57	1	-7	4	3	59	49	59	1	10	3	220	225	3	3	18	3	76	77	76
-5	9	2	120	117	9	1	16	2	82	63	22	-6	4	3	179	189	13	2	10	3	106	108	7	-3	19	3	67	53	67
-4	9	2	151	158	8	2	16	2	115	123	13	-5	4	3	220	234	6	3	10	3	91	84	13	-2	19	3	0	57	1

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  -3  9  2  154  143   7     3 16  2   95  109  16    -4  4  3  106  101   9     4 10  3   25   53  25    -1 19  3   54
81  53
  -2  9  2  206  214   5     4 16  2   69   76  69    -3  4  3  218  216   4     5 10  3    0   59   1     0 19  3   59
15  59
  -1  9  2  175  166   3    -4 17  2    0   12   1    -2  4  3  250  248   3     6 10  3   59   66  59     1 19  3   57
81  56
   0  9  2  662  643   7    -3 17  2  140  111  35    -1  4  3  498  518   5    -6 11  3  108   32  35     2 19  3    0
57   1
   1  9  2  168  166   3    -2 17  2   62   59  62     0  4  3  407  419   4    -5 11  3   91  101  31     3 19  3  133
53  48
   2  9  2  213  214   5    -1 17  2    0   13   1     1  4  3  503  518   5    -4 11  3   44   40  43    -2 20  3    0
37   1
   3  9  2  151  143   7     0 17  2   47   61  47     2  4  3  245  248   4    -3 11  3  144  148   9    -1 20  3    0
2   1
   4  9  2  163  158   5     1 17  2    0   13   1     3  4  3  217  216   2    -2 11  3   59   60  15     0 20  3   40
6  40
   5  9  2  124  117  13     2 17  2   44   59  43     4  4  3  112  101   7    -1 11  3  131  141   6     1 20  3   67
2  67
   6  9  2    0   51   1     3 17  2  132  111  24     5  4  3  228  234   6     0 11  3  174  173   5     2 20  3   40
37  40
  -6 10  2  112   76  29     4 17  2    0   12   1     6  4  3  173  189  11     1 11  3  147  141   5    -1 21  3    0
78   1
  -5 10  2   84   73  30    -3 18  2   74   39  73     7  4  3  113   49  59     2 11  3   76   60  11     0 21  3   90
10  89
  -4 10  2  144  151   9    -2 18  2   59   55  59    -6  5  3   54   24  53     3 11  3  137  148   8     1 21  3   31
78  31
  -3 10  2   69   62  15    -1 18  2   47   46  47    -5  5  3   54   79  28     4 11  3   31   40  31     0  0  4  597
613  12
  -2 10  2  234  225   4     0 18  2   25   49  25    -4  5  3  213  211   5     5 11  3  131  101  24     1  0  4 1453
1363  18
  -1 10  2  154  151   5     1 18  2   65   46  46    -3  5  3  314  304   4     6 11  3   40   32  40     2  0  4  230
235   4
   0 10  2  157  133   5     2 18  2   57   55  56    -2  5  3  474  475   5    -5 12  3   47   41  47     3  0  4  282
265   4
   1 10  2  163  151   4     3 18  2   97   39  65    -1  5  3  433  447   5    -4 12  3  101  134  15     4  0  4  141
117  10
   2 10  2  242  225   5    -3 19  2  115   74  58     0  5  3   51   47   6    -3 12  3  245  238   7     5  0  4  222
214   8
   3 10  2   82   62  15    -2 19  2   18   47  17     1  5  3  430  447   4    -2 12  3   51   41  19     6  0  4  140
155  14
   4 10  2  123  151  13    -1 19  2   88   36  40     2  5  3  480  475   4    -1 12  3   31   27  31     7  0  4    0
20   1
   5 10  2   18   73  17     0 19  2  122   84  26     3  5  3  307  304   5     0 12  3  351  345   5    -7  1  4  109
47  68
   6 10  2   74   76  73     1 19  2    0   36   1     4  5  3  217  211   3     1 12  3   44   27  18    -6  1  4  147
171  13
  -6 11  2  101   65  44     2 19  2   72   47  71     5  5  3   78   79  13     2 12  3   47   42  29    -5  1  4  349
329   5
  -5 11  2    0   30   1     3 19  2   31   74  31     6  5  3    0   24   1     3 12  3  265  238   6    -4  1  4  126
133  10
  -4 11  2  178  170   9    -2 20  2    0   39   1    -6  6  3   18   58  17     4 12  3  142  134  14    -3  1  4  361
352   4
  -3 11  2  103   97   6    -1 20  2    0   33   1    -5  6  3   51   54  50     5 12  3    0   41   1    -2  1  4  735
734   7
  -2 11  2   91   92   9     0 20  2   72   77  71    -4  6  3  184  191   7    -5 13  3    0   36   1    -1  1  4  615
640   6
  -1 11  2  147  142   5     1 20  2    0   33   1    -3  6  3  193  183   5    -4 13  3   62   92  36     0  1  4  505
524   6
   0 11  2  177  147   8     2 20  2   98   39  54    -2  6  3   84   78   5    -3 13  3  158  176   6     1  1  4  610
641   7
   1 11  2  155  142   4    -1 21  2    0    5   1    -1  6  3  229  247   4    -2 13  3  225  218   6     2  1  4  733
734   8
   2 11  2   98   92  10     0 21  2  124   96  42     0  6  3  123  126   3    -1 13  3  160  154   5     3  1  4  363
352   4
   3 11  2   97   96  12     1 21  2    0    5   1     1  6  3  225  247   3     0 13  3  280  266   7     4  1  4  128
133  11
   4 11  2  158  170  13     1  0  3 1225 1194  14     2  6  3   62   79   8     1 13  3  152  154   7     5  1  4  336
329   6
   5 11  2  101   30  29     2  0  3  590  588   6     3  6  3  184  183   4     2 13  3  212  218   6     6  1  4  159
171  12
   6 11  2   47   65  47     3  0  3  462  435   5     4  6  3  194  191   6     3 13  3  164  176   9     7  1  4  141
47  41
  -5 12  2   97   21  34     4  0  3  166  161   5     5  6  3   65   54  39     4 13  3   65   93  28    -7  2  4  126
59  51
  -4 12  2   36   79  35     5  0  3  144  151  11     6  6  3  111   58  30     5 13  3    0   36   1    -6  2  4   76
40  28
  -3 12  2  167  156   5     6  0  3  160  175  13    -6  7  3   84   30  40    -5 14  3    0   43   1    -5  2  4  204
204   6
  -2 12  2  188  186   6     7  0  3    0   10   1    -5  7  3   80   89  18    -4 14  3    0   22   1    -4  2  4   31
71  31
  -1 12  2   65   78  13    -7  1  3   25    7  25    -4  7  3  262  256   5    -3 14  3  186  178   7    -3  2  4  333
321   4
   0 12  2   51   45  32    -6  1  3   90  127  25    -3  7  3  131  139   6    -2 14  3   44   52  43    -2  2  4  291
303   4
   1 12  2   76   78   6    -5  1  3  177  190   6    -2  7  3  238  240   3    -1 14  3  182  188   4    -1  2  4  613
646   7
```

Table 7. Observed and calculated structure factors for **14b**
Page 3

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
0	2	4	951	947	13	6	8	4	47	62	47	-1	16	4	97	88	20	-6	4	5	0	52	1	3	10	5	88	82	9
1	2	4	620	646	6	-6	9	4	36	73	35	0	16	4	59	55	59	-5	4	5	176	179	8	4	10	5	258	255	5
2	2	4	289	303	5	-5	9	4	105	97	13	1	16	4	69	88	25	-4	4	5	0	13	1	5	10	5	97	85	60
3	2	4	329	321	5	-4	9	4	139	151	7	2	16	4	40	46	40	-3	4	5	232	222	4	6	10	5	40	80	40
4	2	4	72	71	12	-3	9	4	177	182	7	3	16	4	59	69	28	-2	4	5	139	139	4	-6	11	5	0	65	1
5	2	4	209	204	8	-2	9	4	253	243	4	4	16	4	0	73	1	-1	4	5	201	200	3	-5	11	5	0	77	1
6	2	4	40	40	40	-1	9	4	120	117	5	-4	17	4	97	25	96	0	4	5	456	484	7	-4	11	5	97	107	20
7	2	4	101	59	101	0	9	4	604	579	7	-3	17	4	108	75	50	1	4	5	200	200	3	-3	11	5	78	40	18
-7	3	4	106	81	41	1	9	4	116	117	5	-2	17	4	54	56	35	2	4	5	146	139	4	-2	11	5	91	59	9
-6	3	4	54	15	53	2	9	4	248	244	3	-1	17	4	118	131	19	3	4	5	242	222	4	-1	11	5	244	235	5
-5	3	4	113	88	11	3	9	4	186	182	6	0	17	4	69	5	44	4	4	5	57	14	12	0	11	5	169	151	3
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-3	3	4	229	222	4	5	9	4	25	97	25	2	17	4	36	56	35	6	4	5	47	52	47	2	11	5	62	59	8
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3	3	4	225	222	4	-2	10	4	329	322	5	0	18	4	18	77	17	-1	5	5	538	556	7	-4	12	5	25	36	25
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-6	4	4	57	60	56	3	10	4	54	67	22	-2	19	4	57	60	56	4	5	5	115	114	8	1	12	5	259	251	5
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0	5	4	1703	1582	21	-3	12	4	308	299	6	6	0	5	215	216	10	-3	7	5	82	87	10	-2	14	5	158	167	6
1	5	4	779	803	9	-2	12	4	111	112	9	7	0	5	0	25	1	-2	7	5	606	602	6	-1	14	5	132	138	6

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   3  5  4  119  117   8     0 12  4   88   97   9    -6  1  5  124  117  16     0  7  5  136  143   4     1 14  5  129
138  11
   4  5  4  115  119   7     1 12  4  153  158   5    -5  1  5  120  133   9     1  7  5  271  281   4     2 14  5  161
167   7
   5  5  4  103   82   8     2 12  4  111  112   9    -4  1  5   47   11  29     2  7  5  613  602   6     3 14  5   76
37  19
   6  5  4   78   42  78     3 12  4  294  299   6    -3  1  5  535  525   6     3  7  5   95   87   8     4 14  5  115
115  16
  -6  6  4    0   25   1     4 12  4   65   88  28    -2  1  5  170  171   4     4  7  5  113  109   8     5 14  5   82
44  82
  -5  6  4  207  216   7     5 12  4  103   48  43    -1  1  5  534  563   7     5  7  5  112  128  18    -4 15  5  128
135  25
  -4  6  4   47   47  29    -5 13  4    0   61   1     0  1  5  768  784   9     6  7  5  105  104  64    -3 15  5   31
31  31
  -3  6  4  284  266   5    -4 13  4  183  188  10     1  1  5  531  563   6    -6  8  5   67   56  67    -2 15  5  150
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135   5
   0  6  4  504  512   6    -1 13  4  296  299   5     4  1  5    0   11   1    -3  8  5  187  178   6     1 15  5   95
104  14
   1  6  4  271  268   3     0 13  4   91   79  11     5  1  5  149  133  12    -2  8  5  101  103   4     2 15  5  154
151  10
   2  6  4  186  178   3     1 13  4  313  299   6     6  1  5   95  117  20    -1  8  5  336  340   5     3 15  5    0
31   1
   3  6  4  280  267   4     2 13  4  147  168   7     7  1  5   78   37  78     0  8  5   59   65  12     4 15  5  152
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125  22
   5  6  4  224  216  10     4 13  4  170  188   9    -6  2  5   76   71  40     2  8  5  109  103   6    -3 16  5   51
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58  31
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93  15
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   0  7  4  234  245   4     1 14  4   78   69  13     2  2  5  314  322   4    -3  9  5  148  153   8    -4 17  5  105
49 104
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27  31
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54  98
   4  8  4   36   53  35    -3 16  4   80   69  26     5  3  5  109  100  14     1 10  5  205  199   4    -2 19  5  119
103  45
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37   1
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Table 7. Observed and calculated structure factors for **14b**
Page 4

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
0	19	5	44	3	43	-2	6	6	198	187	4	-1	13	6	224	225	5	-3	2	7	158	149	6	6	8	7	160	122	33
1	19	5	91	37	37	-1	6	6	399	406	5	0	13	6	18	10	17	-2	2	7	540	534	6	-6	9	7	155	118	23
2	19	5	97	103	42	0	6	6	185	185	4	1	13	6	228	225	5	-1	2	7	174	184	4	-5	9	7	86	75	26
3	19	5	128	54	43	1	6	6	399	407	5	2	13	6	80	96	8	0	2	7	251	255	4	-4	9	7	111	99	10
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3	0	6	261	247	5	-2	7	6	109	100	6	1	14	6	93	104	7	-3	3	7	153	150	6	6	9	7	108	118	76
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5	0	6	44	4	43	0	7	6	183	189	4	3	14	6	140	153	10	-1	3	7	335	345	4	-5	10	7	140	144	19
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1	2	6	371	390	4	-3	9	6	51	52	25	-2	17	6	44	79	43	-4	5	7	199	193	7	-5	12	7	0	39	1
2	2	6	202	195	4	-2	9	6	380	371	5	-1	17	6	112	102	8	-3	5	7	266	263	5	-4	12	7	154	146	14
3	2	6	116	112	8	-1	9	6	528	520	7	0	17	6	0	38	1	-2	5	7	166	157	4	-3	12	7	112	111	13
4	2	6	67	52	16	0	9	6	323	329	5	1	17	6	91	102	13	-1	5	7	209	222	4	-2	12	7	173	177	6
5	2	6	259	262	5	1	9	6	523	520	6	2	17	6	101	79	29	0	5	7	356	371	4	-1	12	7	109	111	10
6	2	6	118	107	17	2	9	6	378	371	4	3	17	6	118	83	31	1	5	7	212	222	4	0	12	7	84	91	10

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  -5  3  6   36   37  35     4  9  6   74   85  14    -3 18  6  118   32  81     3  5  7  270  263   4     2 12  7  183
176   5
  -4  3  6  111  100   9     5  9  6  115   81  11    -2 18  6   54   99  53     4  5  7  192  193   7     3 12  7  103
111   9
  -3  3  6  164  161   6     6  9  6    0   44   1    -1 18  6   67   42  41     5  5  7   65   32  24     4 12  7  152
146   7
  -2  3  6  195  197   4    -6 10  6    0   13   1     0 18  6   88   62  28     6  5  7  129  172  26     5 12  7   25
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  -1  3  6  115  114   4    -5 10  6  113  102  21     1 18  6   98   42  24    -6  6  7  126  139  28    -5 13  7   69
 30  69
   0  3  6  876  886  13    -4 10  6   59   60  34     2 18  6  126   99  25    -5  6  7  103  111  17    -4 13  7   57
 55  56
   1  3  6  109  113   6    -3 10  6   47   50  47     3 18  6    0   32   1    -4  6  7  142  127  10    -3 13  7   78
 83  21
   2  3  6  198  197   4    -2 10  6  315  316   5    -3 19  6  103   49 103    -3  6  7   54   69  17    -2 13  7  168
163   6
   3  3  6  153  161   7    -1 10  6  265  265   6    -2 19  6   54   47  53    -2  6  7  292  281   4    -1 13  7  129
146   7
   4  3  6   97  100  12     0 10  6  402  391   5    -1 19  6    0   85   1    -1  6  7  435  440   6     0 13  7  133
126   6
   5  3  6   47   37  47     1 10  6  270  265   4     0 19  6  116  151  24     0  6  7  657  679   9     1 13  7  137
146   7
   6  3  6   98   25  28     2 10  6  315  316   4     1 19  6   72   85  71     1  6  7  435  440   5     2 13  7  152
163   5
  -6  4  6    0   70   1     3 10  6   44   50  25     2 19  6   69   47  69     2  6  7  277  281   4     3 13  7   82
 83  12
  -5  4  6  205  197   8     4 10  6   67   60  16     3 19  6   69   49  69     3  6  7   86   69   9     4 13  7    0
 55   1
  -4  4  6  165  165   6     5 10  6   91  102  55    -2 20  6   90   94  89     4  6  7  127  127   9     5 13  7    0
 30   1
  -3  4  6  183  176   5     6 10  6    0   13   1    -1 20  6   18   25  17     5  6  7   95  111  16    -5 14  7    0
 72   1
  -2  4  6  370  364   4    -5 11  6   62   51  62     0 20  6   88   97  87     6  6  7  115  140  55    -4 14  7  177
186  15
  -1  4  6  384  407   5    -4 11  6    0   56   1     1 20  6    0   25   1    -6  7  7   88  106  62    -3 14  7   91
 97  19
   0  4  6  379  408   5    -3 11  6   57   71  31     2 20  6  116   94  42    -5  7  7   88   91  20    -2 14  7  157
156   8
   1  4  6  394  407   5    -2 11  6  231  230   4     0 21  6    0   12   1    -4  7  7  151  164   8    -1 14  7   82
 85  10
   2  4  6  367  364   4    -1 11  6   95   86  10     1  0  7  243  251   4    -3  7  7   51   66  19     0 14  7   80
100  15
   3  4  6  187  176   4     0 11  6   76   57   8     2  0  7   25   24  25    -2  7  7   84   81  10     1 14  7   76
 85   8
   4  4  6  175  165   5     1 11  6   72   86   9     3  0  7  256  257   5    -1  7  7  169  171   4     2 14  7  160
156   6
   5  4  6  193  197   8     2 11  6  244  230   4     4  0  7  166  165   6     0  7  7   62   27  11     3 14  7  103
 97  15
   6  4  6   51   70  50     3 11  6   98   71  12     5  0  7  258  236   6     1  7  7  165  171   4     4 14  7  186
186  11
  -6  5  6   86  114  38     4 11  6   74   56  11     6  0  7  152  139  15     2  7  7   97   81   6     5 14  7    0
 72   1
  -5  5  6   80   73  20     5 11  6   18   51  17    -6  1  7   57   95  56     3  7  7   74   66  11    -4 15  7   78
 54  52
  -4  5  6   36   28  35    -5 12  6   93   77  31    -5  1  7   72   58  17     4  7  7  162  164   7    -3 15  7   76
 67  28
  -3  5  6   80   79  10    -4 12  6   67   62  31    -4  1  7  149  140   7     5  7  7   82   91  15    -2 15  7  124
119   9
  -2  5  6  195  178   4    -3 12  6  204  213   8    -3  1  7  356  344   5     6  7  7  122  106  47    -1 15  7  159
160   7
  -1  5  6  256  265   4    -2 12  6  318  319   5    -2  1  7  188  180   5    -6  8  7  137  122  30     0 15  7  173
179   8
   0  5  6  257  273   4    -1 12  6  129  129   7    -1  1  7  518  539   6    -5  8  7   57   70  56     1 15  7  140
160   8
   1  5  6  257  265   4     0 12  6   88   90   7     0  1  7  466  473   5    -4  8  7  112  127  12     2 15  7  129
119   7
   2  5  6  187  178   4     1 12  6  132  129   7     1  1  7  517  539   5    -3  8  7  127  131   7     3 15  7   31
 67  31
   3  5  6   88   79  11     2 12  6  324  319   5     2  1  7  176  180   4    -2  8  7   86   75   9     4 15  7   93
 54  28
   4  5  6   40   28  40     3 12  6  215  214   5     3  1  7  353  344   6    -1  8  7   88   99   9    -4 16  7   98
 69  38
   5  5  6    0   73   1     4 12  6   78   62  24     4  1  7  146  140   6     0  8  7  285  274   4    -3 16  7  111
 89  22
   6  5  6  112  114  24     5 12  6  150   78  27     5  1  7    0   58   1     1  8  7  118   99   5    -2 16  7   98
114  14
  -6  6  6  148  161  24    -5 13  6   91   37  47     6  1  7   67   95  41     2  8  7   95   75   7    -1 16  7   86
 75  14
  -5  6  6  139  146  10    -4 13  6  101  102  21    -6  2  7   25   18  25     3  8  7  128  131   7     0 16  7  131
122  11
  -4  6  6  203  216   7    -3 13  6   98  131  16    -5  2  7   67   98  23     4  8  7  118  127  11     1 16  7   74
 75  20
  -3  6  6  141  141   7    -2 13  6  100   96   8    -4  2  7   59   67  19     5  8  7   69   70  25     2 16  7   82
114  10
```

Table 7. Observed and calculated structure factors for **14b**
Page 5

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
3	16	7	84	89	24	-4	5	8	120	126	9	-5	12	8	44	49	43	2	1	9	198	193	4	-2	8	9	74	78	14
4	16	7	119	69	56	-3	5	8	69	59	15	-4	12	8	203	194	10	3	1	9	410	401	5	-1	8	9	247	231	5
-4	17	7	0	107	1	-2	5	8	198	198	4	-3	12	8	62	54	31	4	1	9	162	163	7	0	8	9	0	35	1
-3	17	7	185	83	29	-1	5	8	263	265	4	-2	12	8	163	158	6	5	1	9	31	52	31	1	8	9	244	231	5
-2	17	7	25	70	25	0	5	8	0	44	1	-1	12	8	133	128	10	6	1	9	62	54	62	2	8	9	82	77	10
-1	17	7	128	133	11	1	5	8	266	265	4	0	12	8	178	172	6	-6	2	9	54	65	53	3	8	9	133	149	7
0	17	7	59	36	19	2	5	8	198	198	4	1	12	8	115	128	8	-5	2	9	62	100	26	4	8	9	215	212	8
1	17	7	118	133	17	3	5	8	80	59	13	2	12	8	168	158	5	-4	2	9	36	75	35	5	8	9	222	215	11
2	17	7	36	70	35	4	5	8	124	126	9	3	12	8	67	54	13	-3	2	9	137	125	7	6	8	9	139	88	39
3	17	7	67	83	67	5	5	8	88	101	11	4	12	8	198	194	10	-2	2	9	267	251	5	-6	9	9	69	67	69
4	17	7	127	107	46	6	5	8	95	28	76	5	12	8	103	49	52	-1	2	9	395	414	5	-5	9	9	128	121	17
-3	18	7	76	24	76	-6	6	8	0	17	1	-5	13	8	0	83	1	0	2	9	431	441	5	-4	9	9	132	139	11
-2	18	7	0	30	1	-5	6	8	78	69	21	-4	13	8	0	33	1	1	2	9	393	415	4	-3	9	9	109	118	14
-1	18	7	90	56	38	-4	6	8	120	140	9	-3	13	8	101	87	17	2	2	9	256	251	4	-2	9	9	129	133	7
0	18	7	0	48	1	-3	6	8	207	204	6	-2	13	8	185	198	6	3	2	9	127	125	7	-1	9	9	236	237	6
1	18	7	78	56	60	-2	6	8	135	121	6	-1	13	8	90	95	11	4	2	9	93	74	12	0	9	9	248	241	5
2	18	7	0	30	1	-1	6	8	162	158	5	0	13	8	54	25	22	5	2	9	95	100	12	1	9	9	245	237	6
3	18	7	82	24	64	0	6	8	203	215	4	1	13	8	84	95	10	6	2	9	18	65	17	2	9	9	129	133	6
-2	19	7	0	39	1	1	6	8	153	158	5	2	13	8	195	198	5	-6	3	9	106	85	27	3	9	9	122	118	8
-1	19	7	0	48	1	2	6	8	123	121	6	3	13	8	84	87	14	-5	3	9	86	113	16	4	9	9	144	139	9
0	19	7	0	7	1	3	6	8	213	204	5	4	13	8	25	33	25	-4	3	9	116	132	10	5	9	9	115	121	23
1	19	7	44	48	43	4	6	8	123	140	9	5	13	8	86	83	86	-3	3	9	197	183	4	6	9	9	108	67	56
2	19	7	0	38	1	5	6	8	82	70	15	-5	14	8	51	56	50	-2	3	9	331	334	5	-5	10	9	59	71	59
-1	20	7	142	133	27	6	6	8	80	17	62	-4	14	8	187	184	15	-1	3	9	576	581	6	-4	10	9	67	104	31
0	20	7	0	22	1	-6	7	8	51	75	50	-3	14	8	67	36	36	0	3	9	405	430	5	-3	10	9	95	99	18
1	20	7	86	133	86	-5	7	8	76	53	19	-2	14	8	287	291	6	1	3	9	576	582	7	-2	10	9	67	62	13
0	0	8	2217	1951	36	-4	7	8	62	79	22	-1	14	8	112	109	10	2	3	9	338	334	4	-1	10	9	198	171	7
1	0	8	189	183	4	-3	7	8	129	123	7	0	14	8	262	248	4	3	3	9	191	182	5	0	10	9	51	21	19
2	0	8	123	120	6	-2	7	8	82	87	10	1	14	8	105	109	7	4	3	9	123	132	9	1	10	9	190	171	6
3	0	8	142	130	6	-1	7	8	523	516	7	2	14	8	295	291	6	5	3	9	131	113	8	2	10	9	69	62	12
4	0	8	80	81	13	0	7	8	185	186	5	3	14	8	76	36	16	6	3	9	103	85	77	3	10	9	100	99	10
5	0	8	139	135	9	1	7	8	514	516	6	4	14	8	179	184	14	-6	4	9	109	121	26	4	10	9	106	105	12
6	0	8	103	33	29	2	7	8	67	86	10	5	14	8	62	56	62	-5	4	9	69	61	25	5	10	9	113	71	56
-6	1	8	142	141	16	3	7	8	138	123	7	-4	15	8	93	46	42	-4	4	9	111	118	12	-5	11	9	69	78	69
-5	1	8	88	73	16	4	7	8	106	79	12	-3	15	8	179	172	11	-3	4	9	164	154	6	-4	11	9	93	104	21
-4	1	8	145	153	8	5	7	8	18	53	17	-2	15	8	65	87	24	-2	4	9	293	295	5	-3	11	9	201	194	9
-3	1	8	90	97	9	6	7	8	69	75	69	-1	15	8	122	111	8	-1	4	9	289	283	5	-2	11	9	150	147	7
-2	1	8	360	344	5	-6	8	8	135	62	33	0	15	8	65	74	24	0	4	9	214	222	4	-1	11	9	185	195	8
-1	1	8	418	429	5	-5	8	8	59	28	41	1	15	8	100	111	10	1	4	9	294	283	4	0	11	9	31	66	31
0	1	8	160	134	5	-4	8	8	80	106	15	2	15	8	80	87	13	2	4	9	293	295	4	1	11	9	192	195	7
1	1	8	412	429	4	-3	8	8	65	53	17	3	15	8	173	172	10	3	4	9	168	154	5	2	11	9	151	147	7
2	1	8	349	344	4	-2	8	8	62	43	14	4	15	8	0	46	1	4	4	9	106	118	9	3	11	9	193	194	5
3	1	8	101	97	10	-1	8	8	151	148	6	-4	16	8	0	54	1	5	4	9	62	61	18	4	11	9	80	104	18
4	1	8	140	153	8	0	8	8	233	240	5	-3	16	8	116	125	19	6	4	9	78	121	78	5	11	9	105	78	42

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   5  1  8   40   73  40     1  8  8  144  148   6    -2 16  8   88   93  18    -6  5  9   62   24  62    -5 12  9   95
46  38
   6  1  8  147  141  17     2  8  8   40   43  22    -1 16  8  100   94  11    -5  5  9  138  133  12    -4 12  9  106
108  20
  -6  2  8  134  159  19     3  8  8   51   53  25     0 16  8  115  143  13    -4  5  9   54   37  28    -3 12  9  120
148  14
  -5  2  8    0   49   1     4  8  8   95  107  12     1 16  8   88   94  16    -3  5  9   51   47  19    -2 12  9   44
42  43
  -4  2  8    0   53   1     5  8  8   36   28  35     2 16  8   84   93  14    -2  5  9  175  163   5    -1 12  9  313
308   7
  -3  2  8  158  146   6     6  8  8   67   62  67     3 16  8  123  124  21    -1  5  9  188  193   5     0 12  9   95
97  12
  -2  2  8   74   88  11    -6  9  8    0   41   1     4 16  8    0   55   1     0  5  9  226  230   4     1 12  9  309
308   5
  -1  2  8  106  106   6    -5  9  8  164  172  14    -3 17  8   44   70  43     1  5  9  192  193   4     2 12  9   47
42  22
   0  2  8  122  116   5    -4  9  8  255  246   7    -2 17  8   54   64  53     2  5  9  168  163   5     3 12  9  135
147   7
   1  2  8  106  106   6    -3  9  8   82   82  17    -1 17  8    0   41   1     3  5  9   47   47  16     4 12  9   95
108  14
   2  2  8   76   88   8    -2  9  8   88   90  11     0 17  8   84   66  36     4  5  9   25   37  25     5 12  9  133
46  39
   3  2  8  158  146   6    -1  9  8  296  300   7     1 17  8   69   41  33     5  5  9  129  133  14    -5 13  9    0
53   1
   4  2  8   88   53  13     0  9  8   47    1  22     2 17  8   54   64  53     6  5  9   40   25  40    -4 13  9   88
113  28
   5  2  8    0   49   1     1  9  8  298  300   6     3 17  8  101   70  41    -6  6  9  198  218  22    -3 13  9  132
140  12
   6  2  8  144  159  25     2  9  8   97   90   8    -3 18  8    0   32   1    -5  6  9  190  188  11    -2 13  9   44
36  43
  -6  3  8   82  104  38     3  9  8   69   82  18    -2 18  8    0   59   1    -4  6  9   93  103  15    -1 13  9   62
31  18
  -5  3  8   76  102  22     4  9  8  253  246   5    -1 18  8   57   53  56    -3  6  9  132  139   8     0 13  9   47
14  29
  -4  3  8   40   82  40     5  9  8  173  172  11     0 18  8  178  182  16    -2  6  9  122  130   6     1 13  9    0
31   1
  -3  3  8  147  140   7     6  9  8    0   41   1     1 18  8  116   53  28    -1  6  9  146  135   6     2 13  9    0
36   1
  -2  3  8  160  150   5    -6 10  8   74   39  73     2 18  8    0   59   1     0  6  9   72   66   9     3 13  9  132
140   7
  -1  3  8  235  241   4    -5 10  8   90  128  30     3 18  8    0   32   1     1  6  9  142  135   5     4 13  9  103
113  20
   0  3  8  167  166   3    -4 10  8   90   96  20    -2 19  8    0   81   1     2  6  9  133  130   6     5 13  9    0
53   1
   1  3  8  235  241   4    -3 10  8  100  104  13    -1 19  8  119  106  36     3  6  9  129  139   7    -4 14  9    0
25   1
   2  3  8  151  150   5    -2 10  8  314  304   6     0 19  8   90   93  45     4  6  9  111  104  12    -3 14  9    0
28   1
   3  3  8  141  140   7    -1 10  8  251  252   6     1 19  8  123  106  33     5  6  9  182  188  10    -2 14  9   44
44  43
   4  3  8   74   82  17     0 10  8  242  256   6     2 19  8  116   81  42     6  6  9  209  218  18    -1 14  9  250
238   7
   5  3  8   91  102  11     1 10  8  257  252   5    -1 20  8    0   35   1    -6  7  9   51   43  50     0 14  9   59
40  23
   6  3  8   54  104  53     2 10  8  303  304   4     0 20  8   97   17  65    -5  7  9  164  158  11     1 14  9  246
238   5
  -6  4  8  118  126  21     3 10  8  111  104   9     1 20  8    0   35   1    -4  7  9   67   86  23     2 14  9   47
44  29
  -5  4  8   82   52  20     4 10  8  100   96  12     1  0  9  757  756   8    -3  7  9   82  106  15     3 14  9    0
28   1
  -4  4  8   44   51  43     5 10  8  113  128  35     2  0  9   18    6  17    -2  7  9  180  180   5     4 14  9    0
25   1
  -3  4  8   84   75  12     6 10  8   36   39  35     3  0  9  120  114   8    -1  7  9   57   68  16    -4 15  9   54
77  53
  -2  4  8  433  414   5    -5 11  8   69  105  69     4  0  9   47   56  47     0  7  9  112  119   7    -3 15  9   78
99  30
  -1  4  8    0   28   1    -4 11  8  116  118  16     5  0  9   76   53  19     1  7  9   72   68  12    -2 15  9   57
54  25
   0  4  8  569  573   7    -3 11  8   74   55  23     6  0  9  157  163  16     2  7  9  180  180   5    -1 15  9  224
218   7
   1  4  8   47   29  16    -2 11  8  324  315   5    -6  1  9    0   55   1     3  7  9  109  106   9     0 15  9   47
31  22
   2  4  8  425  414   5    -1 11  8  131  144  10    -5  1  9   40   52  40     4  7  9  106   87  11     1 15  9  218
218   6
   3  4  8   65   75  13     0 11  8   67   50  13    -4  1  9  158  162   8     5  7  9  151  158   9     2 15  9   69
54  18
   4  4  8   47   51  29     1 11  8  145  144   6    -3  1  9  410  401   5     6  7  9   65   43  64     3 15  9  101
99  17
   5  4  8   82   52  12     2 11  8  321  315   5    -2  1  9  202  192   5    -6  8  9   18   88  17     4 15  9   36
77  35
   6  4  8  120  126  48     3 11  8   44   55  25    -1  1  9  522  535   6    -5  8  9  203  215   9    -4 16  9   54
61  53
  -6  5  8   36   28  35     4 11  8  124  118   9     0  1  9  506  544   6    -4  8  9  218  212   7    -3 16  9  108
77  23
  -5  5  8   97  101  18     5 11  8   65  105  64     1  1  9  527  534   6    -3  8  9  151  149   7    -2 16  9   80
83  20
```

Table 7. Observed and calculated structure factors for **14b**
Page 6

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-1	16	9	106	109	12	-6	5	10	0	52	1	-3	12	10	139	143	12	-5	2	11	167	185	10	4	8	11	88	114	13
0	16	9	115	59	14	-5	5	10	65	48	33	-2	12	10	57	68	25	-4	2	11	86	85	16	5	8	11	88	47	28
1	16	9	106	109	9	-4	5	10	156	160	9	-1	12	10	160	161	8	-3	2	11	93	78	11	6	8	11	0	69	1
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111  10
   4  1 10  150  151   8     0  8 10  337  328   6     3 16 10    0   44   1     1  5 11  189  185   6     4 12 11   18
 49  17
   5  1 10   90   39  17     1  8 10  229  211   5     4 16 10   97   58  96     2  5 11  176  170   5     5 12 11    0
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   6  1 10    0   71   1     2  8 10  148  156   6    -3 17 10  174  122  42     3  5 11   44   62  43    -4 13 11   25
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  -6  2 10   82   84  42     3  8 10   57   66  20    -2 17 10    0   64   1     4  5 11  185  167   6    -3 13 11  128
108  14
  -5  2 10   88   69  20     4  8 10   82   55  15    -1 17 10   74   49  26     5  5 11  129  139  14    -2 13 11  281
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160   8
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 77  13
  -1  2 10   78   46   8    -4  9 10  193  199   9     3 17 10  113  122  48    -4  6 11   84  107  17     2 13 11  288
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 63  39
   3  2 10  237  217   4     0  9 10  298  281   6     0 18 10   80   61  32     0  6 11  247  245   5    -3 14 11   67
106  41
   4  2 10  191  193   7     1  9 10  178  177   6     1 18 10  120   88  27     1  6 11  126  138   7    -2 14 11  173
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106  22
  -3  3 10  212  208   6    -4 10 10  164  178  11     1 19 10   84   31  58    -6  7 11   93   27  67     4 14 11   80
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 22   1
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 95  19
  -4  4 10  153  163   8    -3 11 10  247  257   8    -3  1 11   82   90  15     6  7 11  100   27  74    -1 16 11   98
121  24
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  -2  4 10  317  316   5    -1 11 10  123  113  10    -1  1 11  516  513   5    -5  8 11    0   47   1     1 16 11  118
121  14
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   0  4 10  493  495   6     1 11 10  101  113  11     1  1 11  525  513   6    -3  8 11  128  119   6     3 16 11    0
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   4  4 10  163  163   8     5 11 10  109   71  41     5  1 11   51   46  50     1  8 11  332  312   6     0 17 11  109
 91  37
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 16  34
   6  4 10  123   42  49    -4 12 10  176  174  13    -6  2 11   62   96  62     3  8 11  122  119   9     2 17 11   60
134  59
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Table 7. Observed and calculated structure factors for **14b**

Page 7

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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0	18	11	106	72	25	3	6	12	209	219	6	2	14	12	0	28	1	2	4	13	67	38	13	-3	12	13	59	63	59
1	18	11	72	78	71	4	6	12	78	60	21	3	14	12	100	115	17	3	4	13	201	205	5	-2	12	13	47	96	47
2	18	11	0	15	1	5	6	12	187	203	11	4	14	12	59	57	59	4	4	13	224	231	7	-1	12	13	78	93	18
-1	19	11	25	63	25	6	6	12	0	33	1	-4	15	12	122	87	33	5	4	13	59	59	34	0	12	13	180	177	9
0	19	11	47	26	47	-6	7	12	0	52	1	-3	15	12	76	88	76	6	4	13	0	45	1	1	12	13	84	93	14
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0	0	12	817	797	10	-4	7	12	188	191	9	-1	15	12	177	172	10	-5	5	13	90	81	22	3	12	13	72	63	17
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2	0	12	142	133	6	-2	7	12	97	110	10	1	15	12	167	172	8	-3	5	13	141	149	9	-4	13	13	105	71	26
3	0	12	219	213	6	-1	7	12	112	111	8	2	15	12	200	196	9	-2	5	13	106	119	11	-3	13	13	124	95	18
4	0	12	18	29	17	0	7	12	95	73	10	3	15	12	76	88	58	-1	5	13	129	113	9	-2	13	13	84	88	21
5	0	12	182	177	10	1	7	12	109	111	9	4	15	12	0	87	1	0	5	13	350	345	6	-1	13	13	80	77	20
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  -4  3 12  313  316   6    -3 10 12   90   72   9    -5  1 13   74   70  26     5  7 13   54   84  53    -1 17 13   67
25  67
  -3  3 12  180  175   7    -2 10 12  154  154   8    -4  1 13  156  172   9    -5  8 13   80   47  36     0 17 13    0
23   1
  -2  3 12   93   79  11    -1 10 12  341  345   7    -3  1 13   36   12  35    -4  8 13   74   51  26     1 17 13    0
25   1
  -1  3 12  232  248   5     0 10 12   31   27  31    -2  1 13  105   97   9    -3  8 13  166  174   7     2 17 13    0
31   1
   0  3 12  350  340   5     1 10 12  338  345   7    -1  1 13  144  149   6    -2  8 13  118  108  11    -2 18 13    0
36   1
   1  3 12  247  248   5     2 10 12  157  154   7     0  1 13  270  261   4    -1  8 13  233  214   7    -1 18 13  109
57  46
   2  3 12   82   79  10     3 10 12   54   72  28     1  1 13  153  149   6     0  8 13  135  128   7     0 18 13   67
82  67
   3  3 12  181  175   7     4 10 12   90  100  17     2  1 13  112   97   8     1  8 13  221  214   7     1 18 13  124
57  48
   4  3 12  320  316   6     5 10 12  112   39  64     3  1 13   18   13  17     2  8 13  109  108   9     2 18 13   47
36  47
   5  3 12    0   59   1    -5 11 12   74   45  73     4  1 13  152  172   8     3  8 13  179  174   7     0 19 13    0
13   1
   6  3 12   18   49  17    -4 11 12   36   64  35     5  1 13   59   70  59     4  8 13    0   51   1     0  0 14  239
227   7
  -6  4 12    0   80   1    -3 11 12   51   54  50     6  1 13    0   12   1     5  8 13   54   47  53     1  0 14  427
431   5
  -5  4 12  220  224   9    -2 11 12  159  156  10    -6  2 13   18   42  17    -5  9 13   78   47  60     2  0 14   67
70  16
  -4  4 12  163  164   9    -1 11 12   84   81  17    -5  2 13   98   72  20    -4  9 13  139  129  12     3  0 14   74
77  17
  -3  4 12   36   50  35     0 11 12  128  127   9    -4  2 13  246  270   7    -3  9 13   67   81  19     4  0 14   88
97  16
  -2  4 12  227  202   6     1 11 12   95   81  12    -3  2 13  106  109  11    -2  9 13  186  190   7     5  0 14   18
24  17
  -1  4 12  232  230   6     2 11 12  134  156   8    -2  2 13  171  179   7    -1  9 13  147  147   9     6  0 14    0
94   1
   0  4 12  293  284   5     3 11 12   82   54  15    -1  2 13  166  158   6     0  9 13  149  141   7    -6  1 14  129
38  31
   1  4 12  238  230   5     4 11 12   88   64  18     0  2 13  331  307   4     1  9 13  146  147   9    -5  1 14  176
169  13
   2  4 12  216  202   5     5 11 12   78   45  78     1  2 13  165  158   5     2  9 13  199  190   6    -4  1 14   82
65  17
   3  4 12   57   50  16    -5 12 12   88   25  87     2  2 13  184  179   6     3  9 13   90   81  13    -3  1 14  213
209   6
   4  4 12  167  164   7    -4 12 12    0   34   1     3  2 13  109  109  10     4  9 13  115  129  16    -2  1 14  197
213   6
   5  4 12  233  224   8    -3 12 12  167  165  10     4  2 13  256  270   6     5  9 13    0   47   1    -1  1 14  438
428   6
   6  4 12  145   80  28    -2 12 12  165  169  10     5  2 13   97   72  16    -5 10 13   80   51  80     0  1 14  853
794   9
  -6  5 12   62   41  62    -1 12 12  191  189   7     6  2 13   54   42  53    -4 10 13    0   76   1     1  1 14  446
428   5
  -5  5 12    0   26   1     0 12 12  120  117  11    -6  3 13   51    7  50    -3 10 13   91  118  15     2  1 14  213
213   6
  -4  5 12  113  125  15     1 12 12  192  188   7    -5  3 13   97  101  20    -2 10 13  196  204   8     3  1 14  203
209   7
  -3  5 12  207  201   7     2 12 12  168  169   8    -4  3 13  113  121  13    -1 10 13  168  172   8     4  1 14   57
65  31
  -2  5 12  182  172   6     3 12 12  166  165   7    -3  3 13   36   34  35     0 10 13   88   81  13     5  1 14  194
169  11
  -1  5 12  256  246   5     4 12 12    0   34   1    -2  3 13   57   37  20     1 10 13  180  172   8     6  1 14    0
38   1
   0  5 12  229  242   5     5 12 12    0   25   1    -1  3 13  166  169   6     2 10 13  187  204   8    -6  2 14    0
42   1
   1  5 12  262  246   6    -4 13 12  106  114  27     0  3 13  180  180   5     3 10 13  111  118  12    -5  2 14   90
120  22
   2  5 12  171  173   5    -3 13 12    0   62   1     1  3 13  172  169   6     4 10 13   74   76  26    -4  2 14   76
67  19
   3  5 12  198  201   5    -2 13 12   59   67  34     2  3 13   40   38  40     5 10 13    0   51   1    -3  2 14  229
218   7
   4  5 12  118  125   9    -1 13 12  126  128  13     3  3 13    0   34   1    -5 11 13    0   25   1    -2  2 14  129
126   9
   5  5 12   57   26  56     0 13 12   31   20  31     4  3 13  106  122  11    -4 11 13  115  106  21    -1  2 14   82
71  12
   6  5 12  137   41  32     1 13 12  124  129  10     5  3 13  120  101  15    -3 11 13   62   84  22     0  2 14  314
328   4
  -6  6 12    0   33   1     2 13 12   76   67  19     6  3 13    0    7   1    -2 11 13  106   99  14     1  2 14   67
71  16
  -5  6 12  185  203  11     3 13 12   98   63  14    -6  4 13   18   45  17    -1 11 13   98  115  14     2  2 14  137
126   7
  -4  6 12   59   60  28     4 13 12  135  114  19    -5  4 13   74   59  33     0 11 13    0   18   1     3  2 14  226
218   6
  -3  6 12  216  219   6    -4 14 12    0   57   1    -4  4 13  236  231   8     1 11 13  113  115  10     4  2 14   95
66  14
  -2  6 12   31   65  31    -3 14 12   62  115  44    -3  4 13  206  205   7     2 11 13   97   99  14     5  2 14  108
120  16
  -1  6 12   47   53  29    -2 14 12    0   28   1    -2  4 13   31   38  31     3 11 13  101   84  13     6  2 14   25
42  25
```

Table 7. Observed and calculated structure factors for **14b**

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-6	3	14	0	46	1	-1	10	14	165	176	9	-5	2	15	62	13	62	4	9	15	153	137	13	-2	2	16	129	148	10
-5	3	14	59	63	59	0	10	14	86	92	14	-4	2	15	76	111	22	5	9	15	103	27	103	-1	2	16	135	130	8
-4	3	14	101	89	13	1	10	14	186	176	8	-3	2	15	0	26	1	-5	10	15	76	71	76	0	2	16	338	325	5
-3	3	14	330	318	6	2	10	14	95	98	16	-2	2	15	62	72	18	-4	10	15	147	152	18	1	2	16	135	130	8
-2	3	14	100	78	11	3	10	14	72	16	24	-1	2	15	264	263	6	-3	10	15	62	51	36	2	2	16	154	148	7
-1	3	14	88	104	11	4	10	14	98	74	20	0	2	15	160	142	7	-2	10	15	0	15	1	3	2	16	177	186	8
0	3	14	54	71	17	5	10	14	95	58	63	1	2	15	266	263	6	-1	10	15	98	107	14	4	2	16	129	136	13
1	3	14	101	104	10	-5	11	14	86	36	86	2	2	15	82	72	12	0	10	15	317	319	6	5	2	16	44	49	43
2	3	14	90	78	11	-4	11	14	93	87	33	3	2	15	40	26	40	1	10	15	111	107	12	-5	3	16	62	63	62
3	3	14	320	319	6	-3	11	14	74	65	20	4	2	15	100	111	17	2	10	15	18	15	17	-4	3	16	67	78	27
4	3	14	97	89	14	-2	11	14	88	83	18	5	2	15	0	13	1	3	10	15	62	51	26	-3	3	16	306	295	7
5	3	14	97	63	20	-1	11	14	127	125	11	6	2	15	0	53	1	4	10	15	156	152	12	-2	3	16	250	239	6
6	3	14	59	46	59	0	11	14	98	90	14	-5	3	15	82	119	28	5	10	15	109	71	65	-1	3	16	312	283	6
-6	4	14	0	45	1	1	11	14	113	125	11	-4	3	15	54	99	53	-4	11	15	91	95	31	0	3	16	180	181	6
-5	4	14	93	30	21	2	11	14	62	83	31	-3	3	15	223	223	7	-3	11	15	0	20	1	1	3	16	284	283	6
-4	4	14	224	224	8	3	11	14	36	65	35	-2	3	15	80	82	15	-2	11	15	44	43	43	2	3	16	255	239	6
-3	4	14	293	294	6	4	11	14	82	87	34	-1	3	15	313	300	6	-1	11	15	122	131	11	3	3	16	304	295	6
-2	4	14	59	90	23	5	11	14	0	36	1	0	3	15	74	77	14	0	11	15	31	62	31	4	3	16	0	78	1
-1	4	14	268	275	6	-4	12	14	131	118	21	1	3	15	316	300	5	1	11	15	133	131	11	5	3	16	0	63	1
0	4	14	290	281	6	-3	12	14	166	167	14	2	3	15	74	82	14	2	11	15	36	42	35	-5	4	16	72	40	40
1	4	14	279	275	6	-2	12	14	59	103	34	3	3	15	214	223	7	3	11	15	54	20	53	-4	4	16	54	67	53
2	4	14	90	90	11	-1	12	14	18	41	17	4	3	15	100	99	15	4	11	15	62	95	62	-3	4	16	103	100	13
3	4	14	306	294	5	0	12	14	95	112	14	5	3	15	132	119	18	-4	12	15	0	47	1	-2	4	16	335	331	6
4	4	14	227	224	7	1	12	14	0	41	1	-5	4	15	72	40	35	-3	12	15	40	77	40	-1	4	16	150	138	8
5	4	14	25	30	25	2	12	14	59	102	59	-4	4	15	268	274	7	-2	12	15	80	99	36	0	4	16	250	245	6
6	4	14	100	45	37	3	12	14	139	167	13	-3	4	15	162	165	8	-1	12	15	18	32	17	1	4	16	154	138	7
-6	5	14	97	55	96	4	12	14	113	118	23	-2	4	15	36	29	35	0	12	15	301	285	8	2	4	16	348	330	6
-5	5	14	44	52	43	-4	13	14	122	167	28	-1	4	15	196	200	6	1	12	15	47	32	47	3	4	16	93	100	12
-4	5	14	144	145	11	-3	13	14	86	74	26	0	4	15	203	197	6	2	12	15	108	99	16	4	4	16	80	67	23
-3	5	14	0	34	1	-2	13	14	54	35	53	1	4	15	199	200	6	3	12	15	86	77	18	5	4	16	25	40	25
-2	5	14	93	103	12	-1	13	14	91	115	19	2	4	15	51	29	25	4	12	15	101	47	34	-5	5	16	0	24	1
-1	5	14	98	94	12	0	13	14	220	226	8	3	4	15	152	165	8	-4	13	15	31	36	31	-4	5	16	98	101	18
0	5	14	65	22	17	1	13	14	93	115	17	4	4	15	274	274	7	-3	13	15	131	88	22	-3	5	16	206	206	7
1	5	14	74	94	17	2	13	14	40	35	40	5	4	15	91	40	34	-2	13	15	44	68	43	-2	5	16	57	28	31
2	5	14	100	103	10	3	13	14	72	74	24	-5	5	15	82	108	31	-1	13	15	84	86	21	-1	5	16	186	181	7
3	5	14	65	34	17	4	13	14	155	167	22	-4	5	15	54	87	53	0	13	15	122	141	17	0	5	16	244	240	6
4	5	14	152	145	9	-4	14	14	0	62	1	-3	5	15	189	194	8	1	13	15	100	86	15	1	5	16	182	181	9
5	5	14	69	52	69	-3	14	14	124	74	27	-2	5	15	267	266	6	2	13	15	51	68	50	2	5	16	0	28	1
6	5	14	112	55	112	-2	14	14	74	59	73	-1	5	15	76	56	16	3	13	15	98	88	26	3	5	16	202	205	7
-5	6	14	31	45	31	-1	14	14	90	93	22	0	5	15	59	40	23	4	13	15	112	36	33	4	5	16	95	101	18
-4	6	14	74	98	26	0	14	14	112	117	17	1	5	15	54	56	28	-3	14	15	0	19	1	5	5	16	36	24	35
-3	6	14	74	65	20	1	14	14	98	93	20	2	5	15	284	266	5	-2	14	15	123	124	21	-5	6	16	0	47	1
-2	6	14	176	171	7	2	14	14	18	59	17	3	5	15	193	193	6	-1	14	15	0	31	1	-4	6	16	112	128	18
-1	6	14	158	171	8	3	14	14	88	75	31	4	5	15	95	87	18	0	14	15	98	52	20	-3	6	16	57	36	31

```
   0  6 14   47   57  29     4 14 14   31   62  31     5  5 15  111  108  26     1 14 15    0   31   1    -2  6 16    0
31   1
   1  6 14  188  171   6    -3 15 14  101   42  31    -5  6 15   74   13  42     2 14 15   98  124  24    -1  6 16  124
125  12
   2  6 14  171  171   7    -2 15 14  118  110  29    -4  6 15  203  210   8     3 14 15    0   19   1     0  6 16  250
230   6
   3  6 14   36   64  35    -1 15 14   54   95  53    -3  6 15  138  137   9    -3 15 15   74    4  73     1  6 16  111
125  10
   4  6 14  123   98  18     0 15 14   65   15  33    -2  6 15   95   84  14    -2 15 15   72   55  71     2  6 16    0
31   1
   5  6 14    0   45   1     1 15 14   84   95  24    -1  6 15  157  139   9    -1 15 15  120   98  20     3  6 16   44
36  43
  -5  7 14   72   15  46     2 15 14  100  110  21     0  6 15  219  214   6     0 15 15   62    4  62     4  6 16  122
128  17
  -4  7 14   47   58  47     3 15 14    0   42   1     1  6 15  140  139   9     1 15 15   95   98  27     5  6 16   40
47  40
  -3  7 14   54   27  28    -3 16 14    0   64   1     2  6 15  103   84  11     2 15 15   67   55  67    -5  7 16   59
68  59
  -2  7 14  182  163   7    -2 16 14   88   75  87     3  6 15  145  137  10     3 15 15    0    4   1    -4  7 16  106
101  20
  -1  7 14  171  168   8    -1 16 14   95   80  32     4  6 15  197  211  10    -2 16 15  101   38  70    -3  7 16  135
132  11
   0  7 14   31   50  31     0 16 14   88   74  37     5  6 15    0   13   1    -1 16 15    0   32   1    -2  7 16   86
77  18
   1  7 14  163  168   8     1 16 14   78   80  60    -5  7 15    0   28   1     0 16 15   65   54  64    -1  7 16  131
136  10
   2  7 14  163  163   8     2 16 14    0   75   1    -4  7 15   65  103  46     1 16 15    0   32   1     0  7 16   76
99  16
   3  7 14   18   27  17     3 16 14    0   64   1    -3  7 15  266  240   7     2 16 15  166   38  55     1  7 16  132
136  10
   4  7 14   31   58  31    -2 17 14    0  102   1    -2  7 15  108  123  11    -2 17 15   78   21  78     2  7 16   40
77  40
   5  7 14    0   16   1    -1 17 14   78   80  78    -1  7 15  109   98  12    -1 17 15   80   53  80     3  7 16  109
132  12
  -5  8 14    0   82   1     0 17 14  113   58  27     0  7 15   54   32  28     0 17 15    0   43   1     4  7 16   91
101  19
  -4  8 14  119   94  15     1 17 14   69   80  69     1  7 15  101   98  11     1 17 15   88   53  62     5  7 16   51
68  50
  -3  8 14   62   43  22     2 17 14  148  102  46     2  7 15  118  123  10     2 17 15  128   21  63    -5  8 16  109
59  41
  -2  8 14   51   24  32    -1 18 14  106   68  41     3  7 15  242  240   8    -1 18 15   84   17  84    -4  8 16  158
181  15
  -1  8 14  271  266   7     0 18 14    0    5   1     4  7 15   98  103  18     0 18 15   65   37  64    -3  8 16   76
112  25
   0  8 14  105   87   9     1 18 14   67   68  67     5  7 15    0   28   1     1 18 15   47   17  47    -2  8 16  213
221  10
   1  8 14  271  266   6     1  0 15   72   65  15    -5  8 15    0   11   1     0  0 16  399  401   8    -1  8 16   54
54  53
   2  8 14    0   24   1     2  0 15  291  278   5    -4  8 15  115  105  18     1  0 16  259  259   6     0  8 16  144
144   9
   3  8 14   51   43  32     3  0 15  320  318   6    -3  8 15   25   19  25     2  0 16  388  380   6     1  8 16   80
54  20
   4  8 14   57   94  38     4  0 15   82  112  20    -2  8 15  106  119  16     3  0 16  398  388   6     2  8 16  229
221   7
   5  8 14   25   82  25     5  0 15   82   45  25    -1  8 15  212  218   7     4  0 16   76   69  22     3  8 16  116
112  11
  -5  9 14   67   36  67     6  0 15    0   68   1     0  8 15   88   88  13     5  0 16   84  123  30     4  8 16  193
181  12
  -4  9 14   90   91  22    -6  1 15  127   44  35     1  8 15  220  218   7    -5  1 16  167  159  15     5  8 16   76
59  76
  -3  9 14  190  186   8    -5  1 15   51   30  50     2  8 15  109  119  14    -4  1 16  144  110  11    -5  9 16  103
85  49
  -2  9 14  261  261   7    -4  1 15  154  158   9     3  8 15    0   19   1    -3  1 16   65   83  24    -4  9 16    0
6   1
  -1  9 14  199  194   8    -3  1 15  193  197   7     4  8 15   69  105  33    -2  1 16  115  117  11    -3  9 16   91
95  19
   0  9 14   84   90  14    -2  1 15  108  101  11     5  8 15   69   11  69    -1  1 16  375  361   6    -2  9 16  156
181  11
   1  9 14  201  194   7    -1  1 15  181  178   7    -5  9 15   78   27  78     0  1 16   47   53  22    -1  9 16  162
169  10
   2  9 14  264  261   6     0  1 15   78   18  13    -4  9 15  129  137  18     1  1 16  372  361   6     0  9 16   51
36  50
   3  9 14  170  186   7     1  1 15  178  178   7    -3  9 15  101   74  15     2  1 16  100  118  12     1  9 16  165
169  10
   4  9 14   88   91  23     2  1 15   98  102  10    -2  9 15  152  150  10     3  1 16   76   83  16     2  9 16  179
181  10
   5  9 14   18   36  17     3  1 15  204  198   7    -1  9 15  122  113  11     4  1 16   98  110  18     3  9 16   93
95  17
  -5 10 14   93   58  57     4  1 15  144  158  10     0  9 15  148  159   8     5  1 16  163  159  15     4  9 16   65
6  39
  -4 10 14   86   74  26     5  1 15   36   30  35     1  9 15  100  113  13    -5  2 16   65   49  64     5  9 16   97
85  65
  -3 10 14   84   16  19     6  1 15  101   45  44     2  9 15  137  150  11    -4  2 16  137  136  11    -4 10 16   65
46  64
  -2 10 14   59   98  28    -6  2 15   80   53  80     3  9 15   82   74  17    -3  2 16  192  186   8    -3 10 16   78
81  34
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Table 7. Observed and calculated structure factors for **14b**
Page 9

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-2	10	16	62	27	36	-1	3	17	252	255	7	3	11	17	67	85	41	-4	5	18	113	134	21	-2	15	18	0	38	1
-1	10	16	76	99	22	0	3	17	190	174	6	4	11	17	31	25	31	-3	5	18	97	105	18	-1	15	18	31	61	31
0	10	16	226	226	8	1	3	17	263	255	6	-4	12	17	151	24	25	-2	5	18	44	61	43	0	15	18	0	38	1
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0	12	16	0	23	1	-3	5	17	47	67	47	-1	14	17	0	15	1	5	6	18	18	61	17	2	1	19	200	206	8
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0	14	16	120	118	15	3	6	17	101	112	15	1	0	18	78	59	18	1	8	18	221	226	8	-3	3	19	93	85	23
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3	14	16	82	67	82	-5	7	17	0	4	1	4	0	18	31	9	31	4	8	18	131	95	17	0	3	19	198	196	8
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34   1
   1 15 16   54   67  53     0  7 17    0    7   1    -2  1 18  360  353   8     0  9 18   47   24  47     5  3 19    0
18   1
   2 15 16   44   91  43     1  7 17  176  189   9    -1  1 18  252  242   7     1  9 18  193  194  10    -5  4 19    0
94   1
   3 15 16   57   37  56     2  7 17  166  185  10     0  1 18  176  169   7     2  9 18   86  108  26    -4  4 19    0
41   1
  -2 16 16   67   12  67     3  7 17  135  124  12     1  1 18  250  242   7     3  9 18   69   37  33    -3  4 19  122
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243   8
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132  14
   1 17 16    0   26   1    -1  8 17   74   95  23    -3  2 18  165  175  11     1 10 18    0   12   1     4  4 19   69
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147  10
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72  25
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186  10
  -1  1 17  131  136  10    -1  9 17  198  203   9    -4  3 18   51   69  50     2 11 18   44   52  43     3  5 19    0
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   0  1 17  202  197   6     0  9 17  186  199   8    -3  3 18   57   81  38     3 11 18  105  111  22     4  5 19   59
74  59
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309   9
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64  25
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70  23
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309   9
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  -4  3 17  105   65  20     0 11 17  221  229   9     4  4 18   84   91  21     0 14 18   97   93  24     3  7 19   40
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56  26
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59   1
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Table 7. Observed and calculated structure factors for **14b**
Page 10

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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-2	8	19	145	155	19	1	3	20	102	132	15	0	15	20	132	66	36	2	10	21	0	43	1	3	7	22	76	84	76
-1	8	19	100	92	19	2	3	20	93	115	19	1	0	21	31	20	31	3	10	21	93	48	42	-3	8	22	118	39	52
0	8	19	0	19	1	3	3	20	93	75	19	2	0	21	201	213	12	-3	11	21	72	59	71	-2	8	22	69	17	69
1	8	19	105	92	18	4	3	20	0	57	1	3	0	21	113	92	20	-2	11	21	112	97	40	-1	8	22	0	48	1
2	8	19	168	155	18	-4	4	20	59	23	59	4	0	21	122	77	25	-1	11	21	57	75	56	0	8	22	0	5	1
3	8	19	59	51	59	-3	4	20	59	6	59	-4	1	21	80	49	62	0	11	21	44	47	43	1	8	22	0	49	1
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-3	9	19	36	77	35	0	4	20	76	99	25	-1	1	21	95	103	16	3	11	21	54	60	53	-3	9	22	159	136	54
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1	9	19	101	115	19	4	4	20	62	23	62	3	1	21	86	103	29	1	12	21	135	122	29	1	9	22	0	37	1
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-3	12	19	62	43	62	-3	7	20	116	123	26	-4	4	21	51	25	50	1	1	22	84	130	24	-1	13	22	0	73	1
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1	12	19	144	157	17	1	7	20	31	60	31	0	4	21	31	2	31	-4	2	22	0	30	1	2	0	23	157	133	16
2	12	19	115	95	26	2	7	20	0	68	1	1	4	21	44	60	43	-3	2	22	167	176	18	3	0	23	44	81	43
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0	13	19	84	71	30	-2	8	20	0	59	1	-3	5	21	0	32	1	2	2	22	138	124	16	-1	1	23	78	78	30

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   1 13 19  161  182  16    -1  8 20  201  203  11    -2  5 21  103  102  24     3  2 22  178  176  18     0  1 23   95
120  20
   2 13 19   59   56  59     0  8 20   54   45  53    -1  5 21  105  109  20     4  2 22    0   30   1     1  1 23   90
 78  27
   3 13 19    0   24   1     1  8 20  199  203  12     0  5 21   51   46  50    -4  3 22   25   63  25     2  1 23   86
 64  32
  -2 14 19    0   20   1     2  8 20    0   59   1     1  5 21   90  109  25    -3  3 22    0   39   1     3  1 23  169
119  20
  -1 14 19    0  124   1     3  8 20  119   89  22     2  5 21   74  102  33    -2  3 22  187  179  13     4  1 23  126
115  28
   0 14 19    0   41   1     4  8 20  103   10  31     3  5 21    0   32   1    -1  3 22  108  122  21    -4  2 23    0
 54   1
   1 14 19  138  124  22    -4  9 20   18   27  17     4  5 21  100   69  40     0  3 22    0   14   1    -3  2 23  118
113  26
   2 14 19    0   20   1    -3  9 20   69   54  69    -4  6 21   18   71  17     1  3 22  112  122  18    -2  2 23  123
 65  24
  -1 15 19    0   37   1    -2  9 20  122  106  23    -3  6 21  103  104  26     2  3 22  195  179  12    -1  2 23    0
 27   1
   0 15 19    0   21   1    -1  9 20  119  107  20    -2  6 21   74   88  42     3  3 22   62   39  62     0  2 23   44
 61  43
   1 15 19   93   37  49     0  9 20   90  133  25    -1  6 21  119  135  19     4  3 22   25   63  25     1  2 23   44
 27  43
   0  0 20   67   83  36     1  9 20   82  107  34     0  6 21   93  118  23    -4  4 22  112   63  55     2  2 23   93
 66  28
   1  0 20  170  169   9     2  9 20   95  106  30     1  6 21  132  134  16    -3  4 22   78   86  47     3  2 23   93
113  42
   2  0 20  285  297   8     3  9 20   40   54  40     2  6 21  109   88  24    -2  4 22   40   86  40     4  2 23   36
 54  35
   3  0 20  210  241  12     4  9 20    0   27   1     3  6 21  103  104  33    -1  4 22  123  135  18    -4  3 23    0
 41   1
   4  0 20  101   47  27    -3 10 20   31   90  31     4  6 21   47   71  47     0  4 22  100  109  23    -3  3 23  172
188  18
   5  0 20    0   66   1    -2 10 20  112  126  25    -4  7 21    0   42   1     1  4 22  144  135  14    -2  3 23    0
 32   1
  -5  1 20    0   22   1    -1 10 20    0   89   1    -3  7 21   59   72  59     2  4 22   82   85  28    -1  3 23   98
123  24
  -4  1 20   80   48  36     0 10 20   51   35  50    -2  7 21   88   35  43     3  4 22   86   86  35     0  3 23  141
116  15
  -3  1 20  141  128  14     1 10 20   72   89  40    -1  7 21  124   97  16     4  4 22  103   63  49     1  3 23  108
123  23
  -2  1 20  399  379   9     2 10 20   78  126  42     0  7 21   57   38  56    -4  5 22   88   55  87     2  3 23   82
 32  34
  -1  1 20  111  107  13     3 10 20  106   90  32     1  7 21  108   98  19    -3  5 22   36   63  35     3  3 23  210
188  17
   0  1 20   36    0  35    -3 11 20  156   15  40     2  7 21   31   35  31    -2  5 22  113   96  23     4  3 23  108
 41  38
   1  1 20   47  107  47    -2 11 20  113   69  25     3  7 21  109   72  30    -1  5 22   93   61  26    -3  4 23    0
 35   1
   2  1 20  410  379   8    -1 11 20  103   79  22     4  7 21   84   42  40     0  5 22    0   16   1    -2  4 23   72
  6  46
   3  1 20  148  128  13     0 11 20   31    5  31    -3  8 21  139  124  25     1  5 22   36   60  35    -1  4 23  118
114  22
   4  1 20   74   48  48     1 11 20   74   79  38    -2  8 21   95   75  32     2  5 22   98   97  26     0  4 23  199
190  15
   5  1 20   86   23  54     2 11 20   78   69  47    -1  8 21  129  129  17     3  5 22   97   63  27     1  4 23   44
114  43
  -5  2 20   91   69  51     3 11 20    0   14   1     0  8 21   18   28  17     4  5 22   59   55  59     2  4 23    0
  5   1
  -4  2 20    0   77   1    -3 12 20  111   51 110     1  8 21   95  129  23    -4  6 22  116   55  56     3  4 23    0
 35   1
  -3  2 20  105   78  22    -2 12 20   40   62  40     2  8 21    0   75   1    -3  6 22   31   79  31    -3  5 23   78
 48  78
  -2  2 20  133  136  14    -1 12 20  210  199  13     3  8 21   78  124  78    -2  6 22  115  137  25    -2  5 23   25
 52  25
  -1  2 20    0   31   1     0 12 20   65   12  64    -3  9 21    0   34   1    -1  6 22   98   72  26    -1  5 23   95
 31  35
   0  2 20  175  187   8     1 12 20  197  199  14    -2  9 21   51   23  50     0  6 22  122  118  20     0  5 23  229
226  16
   1  2 20   65   31  28     2 12 20   86   62  50    -1  9 21  112   84  20     1  6 22   98   72  33     1  5 23    0
 31   1
   2  2 20  122  137  17     3 12 20   18   51  17     0  9 21   25   39  25     2  6 22  167  137  17     2  5 23    0
 52   1
   3  2 20   62   78  44    -2 13 20   90   53  49     1  9 21   69   84  51     3  6 22    0   79   1     3  5 23    0
 49   1
   4  2 20   67   77  67    -1 13 20    0   42   1     2  9 21    0   23   1     4  6 22  109   55  35    -3  6 23   31
 55  31
   5  2 20   72   69  71     0 13 20    0   57   1     3  9 21    0   34   1    -3  7 22    0   84   1    -2  6 23   67
 52  67
  -4  3 20   59   57  59     1 13 20    0   42   1    -3 10 21    0   48   1    -2  7 22  142  122  24    -1  6 23   93
 35  33
  -3  3 20   65   75  46     2 13 20   86   53  42    -2 10 21   51   43  50    -1  7 22    0   38   1     0  6 23    0
 22   1
  -2  3 20  106  115  20    -1 14 20  105   57  37    -1 10 21   91  103  31     0  7 22   97   80  27     1  6 23    0
 35   1
  -1  3 20  128  132  14     0 14 20  148  106  23     0 10 21    0    5   1     1  7 22    0   39   1     2  6 23   47
 52  47
```

Table 7. Observed and calculated structure factors for **14b**

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
3	6	23	51	56	50	-2	2	24	88	60	40	2	8	24	0	46	1	0	5	25	25	26	25	1	4	26	93	45	49
-3	7	23	0	48	1	-1	2	24	112	69	29	-2	9	24	0	19	1	1	5	25	78	73	60	2	4	26	0	36	1
-2	7	23	82	72	51	0	2	24	116	116	23	-1	9	24	0	33	1	2	5	25	0	1	1	-2	5	26	153	60	56
-1	7	23	44	48	43	1	2	24	36	69	35	0	9	24	0	6	1	-2	6	25	127	19	126	-1	5	26	0	80	1
0	7	23	105	121	32	2	2	24	101	60	29	1	9	24	0	33	1	-1	6	25	95	60	47	0	5	26	62	10	62
1	7	23	47	48	47	3	2	24	132	123	24	2	9	24	0	19	1	0	6	25	44	25	43	1	5	26	25	80	25
2	7	23	76	72	58	-3	3	24	111	64	45	-1	10	24	65	57	64	1	6	25	76	60	76	2	5	26	69	60	69
3	7	23	80	48	44	-2	3	24	103	113	24	0	10	24	51	53	50	2	6	25	0	19	1	-1	6	26	44	25	43
-3	8	23	95	46	94	-1	3	24	69	77	69	1	10	24	101	57	39	-2	7	25	0	33	1	0	6	26	51	102	50
-2	8	23	57	67	56	0	3	24	98	84	24	0	11	24	31	86	31	-1	7	25	78	83	78	1	6	26	18	25	17
-1	8	23	100	87	35	1	3	24	74	77	42	1	0	25	84	77	36	0	7	25	74	3	73	-1	7	26	0	50	1
0	8	23	0	34	1	2	3	24	67	113	67	2	0	25	101	84	39	1	7	25	103	83	38	0	7	26	0	76	1
1	8	23	57	87	56	3	3	24	95	64	41	3	0	25	67	46	67	2	7	25	0	33	1	1	7	26	0	50	1
2	8	23	109	67	28	-3	4	24	69	30	69	-3	1	25	0	20	1	-2	8	25	0	34	1	0	8	26	82	61	82
3	8	23	40	46	40	-2	4	24	0	47	1	-2	1	25	146	140	25	-1	8	25	0	17	1	1	0	27	0	6	1
-2	9	23	0	42	1	-1	4	24	0	24	1	-1	1	25	111	96	30	0	8	25	31	33	31	2	0	27	0	0	1
-1	9	23	65	66	64	0	4	24	0	50	1	0	1	25	80	109	40	1	8	25	78	17	78	-2	1	27	57	71	56
0	9	23	59	58	59	1	4	24	36	24	35	1	1	25	40	96	40	2	8	25	0	34	1	-1	1	27	0	35	1
1	9	23	0	66	1	2	4	24	18	47	17	2	1	25	124	140	26	-1	9	25	0	12	1	0	1	27	109	58	44
2	9	23	54	42	53	3	4	24	18	30	17	3	1	25	0	20	1	0	9	25	69	54	69	1	1	27	44	35	43
-2	10	23	93	48	93	-3	5	24	80	17	80	-3	2	25	0	23	1	1	9	25	0	12	1	2	1	27	84	71	84
-1	10	23	0	30	1	-2	5	24	0	22	1	-2	2	25	69	59	69	0	10	25	101	60	76	-2	2	27	36	42	35
0	10	23	88	49	69	-1	5	24	74	68	73	-1	2	25	0	48	1	0	0	26	18	42	17	-1	2	27	134	69	94
1	10	23	25	30	25	0	5	24	90	108	42	0	2	25	59	1	59	1	0	26	0	10	1	0	2	27	108	31	42
2	10	23	86	48	42	1	5	24	57	68	56	1	2	25	51	48	50	2	0	26	0	8	1	1	2	27	103	69	43
-1	11	23	0	56	1	2	5	24	59	22	59	2	2	25	59	59	59	-2	1	26	0	49	1	2	2	27	0	41	1
0	11	23	47	32	47	3	5	24	51	17	50	3	2	25	0	22	1	-1	1	26	128	62	25	-1	3	27	127	74	73
1	11	23	0	56	1	-3	6	24	148	89	63	-3	3	25	119	71	78	0	1	26	95	61	35	0	3	27	0	74	1
-1	12	23	84	56	84	-2	6	24	100	61	32	-2	3	25	76	17	76	1	1	26	31	62	31	1	3	27	112	74	38
0	12	23	0	8	1	-1	6	24	0	45	1	-1	3	25	84	38	44	2	1	26	0	49	1	-1	4	27	0	73	1
1	12	23	86	56	54	0	6	24	0	27	1	0	3	25	84	46	44	-2	2	26	0	98	1	0	4	27	65	51	64
0	0	24	119	131	31	1	6	24	103	45	33	1	3	25	44	38	43	-1	2	26	0	34	1	1	4	27	67	73	67
1	0	24	0	64	1	2	6	24	74	61	73	2	3	25	59	17	59	0	2	26	91	38	37	-1	5	27	0	14	1
2	0	24	131	122	27	3	6	24	139	89	26	3	3	25	91	70	60	1	2	26	86	34	38	0	5	27	165	90	46
3	0	24	0	77	1	-2	7	24	44	48	43	-3	4	25	101	120	101	2	2	26	78	98	52	1	5	27	0	14	1
-3	1	24	240	232	16	-1	7	24	115	66	34	-2	4	25	0	66	1	-2	3	26	150	97	48	0	6	27	0	90	1
-2	1	24	65	35	64	0	7	24	0	49	1	-1	4	25	0	33	1	-1	3	26	84	43	58	0	0	28	74	36	73
-1	1	24	78	61	38	1	7	24	84	66	48	0	4	25	109	119	30	0	3	26	44	13	43	0	1	28	91	77	91
0	1	24	0	29	1	2	7	24	0	48	1	1	4	25	59	34	59	1	3	26	108	43	27	0	2	28	93	105	93
1	1	24	31	61	31	-2	8	24	98	46	98	2	4	25	62	66	62	2	3	26	93	97	36						
2	1	24	76	35	58	-1	8	24	93	28	49	3	4	25	111	120	26	-2	4	26	0	36	1						
3	1	24	238	232	16	0	8	24	95	33	41	-2	5	25	0	1	1	-1	4	26	0	45	1						
-3	2	24	134	123	28	1	8	24	74	28	73	-1	5	25	59	73	59	0	4	26	84	82	53						

Figure 1. View of **14b** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level.

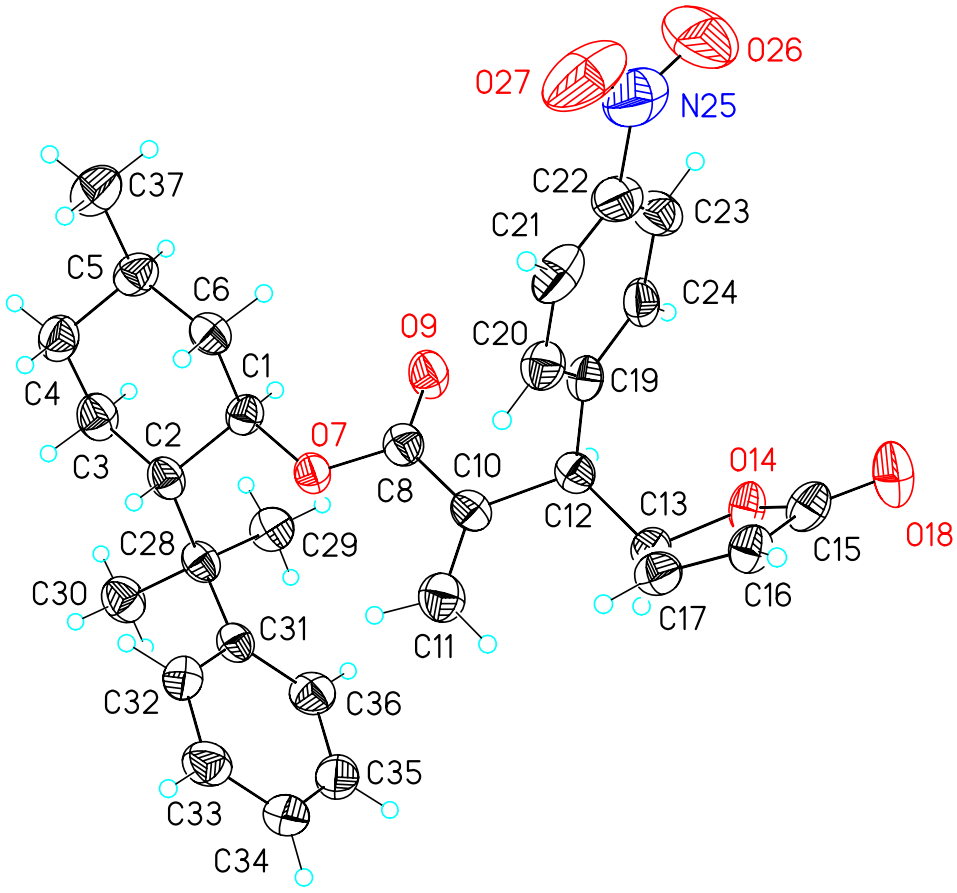

Figure 2. Unit cell packing diagram for **14b**. The view is approximately down the **a** axis.