Supporting Information

Metallation of *N*-vinylpyrroles and –indoles with Hg(OAc)$_2$: *N*-vinyl *vs.* pyrrole nucleophilic sites

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General information

IR spectra were obtained on a "Bruker IFS-25" spectrometer (400-4000 cm^{-1}, KBr pellets or thin films on KBr plates). ^{1}H (400.1 MHz), ^{13}C (100.6 MHz), ^{15}N (40.5 MHz) and ^{19}F (376.5 MHz) NMR spectra were recorded on a "Bruker Avance 400" instrument in $CDCl_3$. The assignment of signals in the ^{1}H NMR spectra was made using COSY and NOESY experiments. Resonance signals of carbon atoms were assigned based on ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC experiments. The values of the δ ^{15}N were measured through the 2D ^{1}H-^{15}N HMBC experiment. The ^{1}H and ^{13}C chemical shifts were referenced to HMDS, ^{15}N - CH_3NO_2, ^{19}F - $CFCl_3$, respectively. The chemical shifts were recorded in ppm.

Elemental analyses (C, H, N) were performed on an EA FLASH 1112 Series (CHN Analyzer) instrument for liquid compounds. Solid examples were analyzed on TM3000 Tabletop Microscope with Bruker Quantex 50 EDX. Fluorine content was determined on a SPECOL 11 (Carl Zeiss Jena, Germany) spectrophotometer.

Melting points were uncorrected.

N-Vinylpyrroles were prepared on Trofimov reaction[1] and formylated by method.[2] Cyanopyrrole **6** was prepared according to procedure.[3] Azopyrrole **3** was synthesized by method.[4]

Trifluoroacetylpyrrole **4** was prepared by reaction of 2-(4-bromophenyl)-1-vinylpyrrole with trifluoroacetic anhydride.[5]

Acetonitrile and dichloro methane were purified by distillation over P_2O_5.[6]

Addition of mercury (II) acetate to *N*-vinylpyrroles 2,4,6-8 (general procedure). A mixture of *N*-vinylpyrrole (1.0 mmol) and $Hg(OAc)_2$ (1.1 mmol) in dry acetonitrile (5 mL) was stirred up to full the pyrrole transformation (TLC) in conditions from Table. The solvent was removed in vacuo; the residue was stirred with dry dicloromethane (10 mL), filtered and washed by dry dicloromethane (5 mL). The solvent was removed off from combined solution to give mercuration product.

NMR spectra of organomercury compounds. The structures of the compounds synthesized were confirmed by 1D and 2D NMR spectra (COSY, NOESY, ^{1}H-^{13}C HSQC, ^{1}H-^{13}C HMBC).

In the ^{1}H NMR spectra of the compounds, signals of the CH_2 group (former C_β position) are shown as doublets of doublets with heminal constant of 12.5 Hz and vicinal constants of 6.9 Hz and 7.3 Hz. The corresponding spin-spin coupling constants are observed for methyne proton (former C_α position), the resonance signal of which appears as doublet of doublets. These data are supported by the correlations manifested themselves in the 2D COSY spectrum.

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(1) a) Mikhaleva, A. I.; Schmidt, E. Yu. In *Selected methods for synthesis and modification of heterocycles*; Kartsev, V. G., Ed.; IBS Press: Moscow, 2002, Vol. 1, pp 334-352. (b) *The Chemistry of Hydroxylamines, Oximes and Hydroxamic Acids*, Rappoport, Z.; Liebman, J. F., Eds.;. Wiley: Chichester, 2008, p 241. (c) Wang, Z. *Comprehensive Organic Name Reactions and Reagents*, Wiley: London; 2009, Part 3, pp 2793-2796.

(2) Mikhaleva, A. I.; Ivanov, A. V.; Skitaltseva, E. V.; Ushakov, I. A.; Vasiltsov, A. M.; Trofimov, B. A. *Synthesis*, **2009**, 587-590.

(3) Trofimov B.A., Vasil'tsov A.M., Mikhaleva A.I., Ivanov A.V., Skital'tseva E.V., Schmidt E.Yu., Senotrusova E.Yu., Ushakov I.A., Petrushenko K.B. *Tetrahedron Lett.*, **2009**, *50*, 97-100.

(4)Trofimov, B.A.; Schmidt, E.Yu.; Mikhaleva, A.I.; Vasil'tsov, A.M.; Zaitsev, A.B.; Smolyanina, N. S.; Senotrusova, E. Yu.; Afonin, A. V.; Ushakov, I. A.; Petrushenko, K. B.; Kazheva, O.N.; Dyachenko, O.A.; Smirnov, V.V., Schmidt, A.F.; Markova, M. V.; Morozova, L.V. *Eur. J. Org. Chem.*, **2006**, 4021-4033.

(5)Trofimov, B. A.; Mikhaleva, A. I.; Korostova, S. E.; Sobenina, L. N.; Vasil'ev, A. N.; Balashenko, L. V. *Zh. Org. Khim*. **1979**, *15*, 2042-2046; *Chem. Abstr*. **1980**, *92*, 76216.

(6) Gordon, A. G.; Ford, R. A. *The Chemist's Companion. A Handbook of Practical Data, Techniques, and Peferences.* Wiley: NY, 1972.

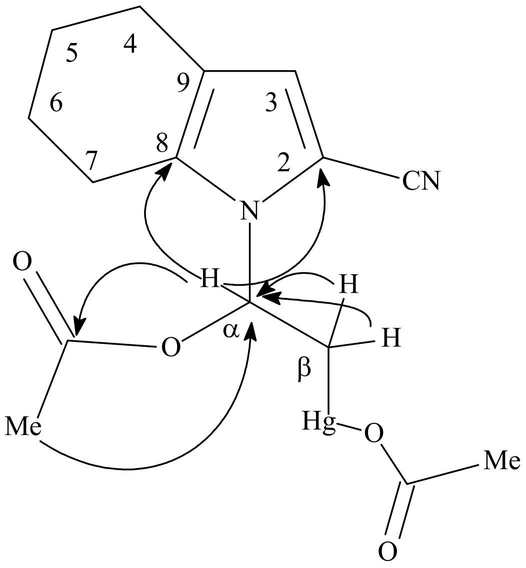
Besides, the ^{1}H NMR spectrum contains two singlets with intensity of three proton units and chemical shits of 2.0 and 2.1 ppm. These signals are assigned to two different Me groups of the acyl fragments.

In the ^{13}C NMR spectrum, the characteristic signals of the carbonyl groups of two acyl fragments are present at 169.3 and 176.9 ppm. A signal of methyne carbon atom is observed at 78.3 ppm, while that of the CH_2-moiety appears at 29.2 ppm. Carbon atom of the CN group has chemical shift at 115.1 ppm. Resonance signals of the pyrrole ring are slightly shifted (~ 2.0 ppm) as compared to the vinyl derivatives.

The assignment of acyl fragment signals has been performed using the 2D ^{1}H-^{13}C HMBC technique. So, Так, the observed correlations of methyne proton (6.72 ppm) and methyl group (2.1 ppm) signals relative to a signal with chemical shift at 169.3 ppm allows the signals of the acyl fragment in α position to be assigned. Additionally, methyne proton correlates with signals at 98.3 and 134.6 ppm which correspond to resonances of C-2 and C-8 atoms of the pyrrole moiety.

In the NMR spectra, the expected satellites due to the coupling to mercury generally were not observable because of scarce solubility ($CDCl_3$) of the products examined. Only in some cases, satellites of very low intensity have been detected.

Fig. 1. Main correlations in the 2D ^{1}H-^{13}C HMBC spectrum of **14**.



Synthetic Procedure for 9. A mixture of *N*-vinylpyrrole **1** (169 mg, 1.0 mmol) and $Hg(OAc)_2$ (1272 mg, 4.0 mmol) in dry acetonitrile (5 mL) was stirred at 40 °C for 0.5 h. Precipitate was filtered off, washed by dry acetonitrile (5 mL) and dried in vacuo to give 1175 mg (93%) of tetramercuric acetate **9**.

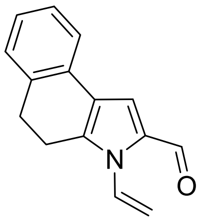
Synthetic Procedure for 11. A mixture of azopyrrole **3** (225 mg, 1.0 mmol) and $Hg(OAc)_2$ (318 mg, 1.0 mmol) in dry acetonitrile (5 mL) was stirred at room temperature for 2-2.5 h. Precipitate was filtered off, washed by dry acetonitrile (5 mL) and dried in vacuo to give 431 mg (89%) of *N*-vinylpyrrolomercurodiazolinium acetate **11**.

Synthetic Procedure for 13. A mixture of *N*-vinyl-4,5,6,7-tetrahydroindole **5** (147 mg, 1.0 mmol) and $Hg(OAc)_2$ (953 mg, 3.0 mmol) in dry acetonitrile (5 mL) was stirred at room temperature for 2-3 h. Precipitate was filtered off, washed by dry acetonitrile (5 mL) and dried in vacuo to give 885 mg (90%) of trimercuric acetate **13**.

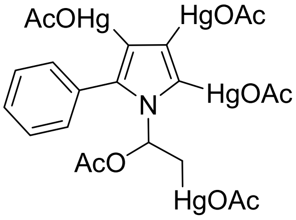
Synthetic Procedure for 17. A mixture of *N*-vinylpyrrole **4** (344 mg, 1.0 mmol) and $Hg(OAc)_2$ (954 mg, 3.0 mmol) in dry acetonitrile (5 mL) was stirred at 60 °C for 12 h. The solvent was removed in vacuo; the residue was stirred with dry dicloromethane (10 mL), filtered and washed by dry dicloromethane (5 mL). The solvent was removed off from combined solution to give 847 mg (92%) of dimercuric acetate **17**.

Synthetic Procedure for 19.

A mixture of dimercuric acetate **17** (92 mg, 0.1 mmol) and $NaBH_4$ (19 mg 0.5 mmol) in aqueous (10%) acetonitrile (3.3 mL) was stirred at room temperature for 30 min. The mixture was diluted by water (6 mL) and extracted by dichloromethane (3 mL × 3). Combined organic layers were washed by water and dried over Na_2SO_4. The solvent was removed off in vacuo to give 34 mg (96%) of 1-(5-(4-bromophenyl)-1-vinyl-1*H*-pyrrol-2-yl)-2,2,2-trifluoroethanol **19**.



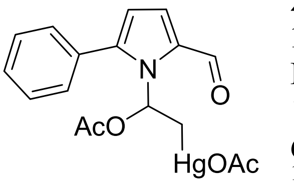
3-Vinyl-4,5-dihydro-3H-benzo[*e*]indole-2-carbaldehyde 8 was prepared by formylation of 3-vinyl-4,5-dihydro-3H-benzo[*e*]indole [7] according to procedure[2] in 90% yield. Light-brown crystals, mp 94-96 °C. Light-brown crystals, mp 94-96 °C. IR (KBr) ν/cm^{-1}: 3117, 3099, 3047, 3032, 3002, 2953, 2923, 2894, 2830, 1664, 1639, 1549, 1501, 1486, 1456, 1444, 1414, 1392, 1381, 1344, 1318, 1292, 1281, 1220, 1197, 1162, 1139, 1086, 1073, 1035, 964, 904, 887, 846, 831, 779, 757, 721, 706, 639, 580, 557, 526, 477, 445, 411. ^1H NMR, δ, ppm: 9.56 (s, CHO), 7.48 (dd, 1H, H-X, $^3J_{X\text{-}B}$ = 15.9 Hz, $^3J_{X\text{-}A}$ = 8.8 Hz), 7.40 (m, 1H, H-9), 7.04-7.14 (m, 3H, H-6, H-7, H-8), 5.18 (dd, 1H, H_A, $^2J_{B\text{-}A}$ = 1.0 Hz, $^3J_{X\text{-}A}$ = 8.8 Hz), 5.08 (dd, 1H, H_B, $^2J_{B\text{-}A}$ = 1.0 Hz, $^3J_{X\text{-}B}$ = 15.9 Hz), 2.89 (m, 4H, 5,4-CH_2). ^{13}C NMR, δ, ppm: 178.69 (C=O), 139.73 (C-3a), 133.34 (C-5a), 132.25 (C-2), 131.56 (C_α), 131.01 (C-9a), 128.14 (C-6), 127.14 (C-8), 126.33 (C-7), 122.37 (C-9), 122.37 (C-9b), 119.02 (C-1), 109.31 (C_β), 29.24 (C-5), 21.77 (C-4). Anal. Calcd for $C_{15}H_{13}NO$: C, 80.69; H, 6.27; N, 6.27. Found: C, 80.76; H, 6.10; N, 6.12.



Tetramercuric acetate 9. Dark-red crystals with metal luster, stable up to 350 °C, insoluble in organic solvents.

IR (KBr) ν/cm^{-1}: 3409, 2929, 2853, 1695, 1578, 1405, 1368, 1090, 1047, 1016, 921, 799, 764, 690, 648, 612 cm^{-1}.

Anal. Calcd. for $C_{22}H_{23}Hg_4NO_{10}$: C, 20.91; H, 1.83; Hg, 63.49; N, 1.11; O, 12.66. Found: C, 21.00; Hg, 63.51; N, 1.12, O, 12.70.



2-Acetoxy-2-(2-formyl-5-phenyl-1H-pyrrol-1-yl)ethylmercury acetate 10. Light-yellow viscous oil.

IR ν/cm^{-1}: 2932, 2848, 1750, 1714, 1660, 1599, 1503, 1453, 1424, 1370, 1311, 1226, 1140,1100, 1075, 1047, 1017, 958, 923, 830, 797, 763, 731, 697, 614, 508, 452.

^1H NMR, δ, ppm: 9.57 (s, 1H, CHO), 7.45-7.35 (m, 5H, Ph), 7.11 (d, H-3, $^3J_{4\text{-}3}$ = 3.9 Hz), 7.19 (dd, 1H, H_α, ^3J = 7.3 Hz, ^3J = 6.7 Hz), 6.28 (d, H-4, $^3J_{3\text{-}4}$ = 3.9 Hz), 2.54 (dd, 1H, H_β, ^2J = 12.5 Hz, ^3J = 6.7 Hz), 2.45 (dd, 1H, H_β, ^2J = 12.5 Hz, ^3J = 7.3 Hz), 2.01 (s, 3H, OAc), 1.97 (s, 3H, HgOAc).

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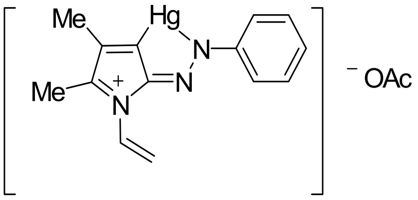
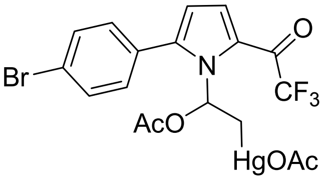
(7) Vasil'tsov, A. M.; Ivanov, A. V.; Mikhaleva, A. I.; Trofimov, B. A. *Tetrahedron Lett.,* **2010**, *51*, 1690–1692.

^{13}C NMR, δ, ppm: 179.09 (CHO), 176.83 (C=O, HgOAc), 169.23 (C=O, OAc), 144.61 (C-5), 133.25 (C_i), 131.980 (C_p), 129.77 (C_m), 128.66 (C_o), 127.90 (C-3), 124.24 (C-2), 112.71 (C-4), 80.50 (C_α), 29.22 (C_β), 22.50 (Me, HgOAc), 20.82 (Me, OAc).
Anal. Calcd. for $C_{17}H_{17}NO_5$, %: C, 39.58; H, 3.32; N, 2.71. Found: %: C, 40.03; H, 3.35; N, 2.92.

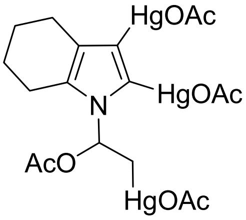


***N*-Vinylpyrrolomercurodiazolinium acetate 11.** Red-brown crystals with metal luster, decomposed at 278-280 °C, slightly soluble in organic solvents. IR (KBr) ν/cm^{-1}: 3425, 3061, 2971, 2921, 2852, 1699, 1637, 1597, 1494, 1439, 1396, 1375, 1287, 1223, 1148, 1072, 1017, 908, 764, 728, 690, 615, 562 cm^{-1}.

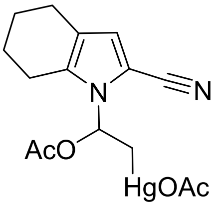
^{1}H NMR, δ, ppm: 7.75 (m, 2H, Ph-o), 7.43 (m, 2H, Ph-m), 7.32 (m, 1H, Ph-p), 7.27 (dd, 1H, H_X, $^3J_{X\text{-}B}$ = 16.0 Hz, $^3J_{X\text{-}A}$ = 9.1 Hz), 5.46 (d, 1H, H_B, $^3J_{X\text{-}B}$ = 16.0 Hz), 5.19 (d, 1H, H_A, $^3J_{X\text{-}A}$ = 9.1 Hz), 2.32 (s, 3H, Me), 2.12 (s, 3H, Me), 2.05 (s, 3H, OAc)
Anal. Calcd. for $C_{16}H_{17}HgN_3O_2$: C, 39.71; H, 3.54; Hg, 41.45; N, 8.68; O, 6.61. Found: C, 39.90; Hg, 42.00; N, 8.21, O, 6.72.



2-Acetoxy-2-(2-(4-bromophenyl)-5-(2,2,2-trifluoroacetyl)-1*H*-pyrrol-1-yl)ethylmercury acetate 12.
^{1}H NMR, δ, ppm: 7.62 (m, 2H, Ph-m), 7.34 (m, 2H, Ph-o), 7.34 (m, 1H, H-4), 7.19 (dd, 1H, H_α, ^3J = 8.6 Hz, ^3J = 6.8 Hz), 6.29 (d, 1H, H-3, ^3J = 4.3 Hz), 2.62 (dd, 1H, H_β, ^2J = 12.1 Hz, ^3J = 8.6 Hz), 2.37 (dd, 1H, H_β, ^2J = 12.1 Hz, ^3J = 6.8 Hz), 1.99 (s, 3H, HgOAc), 1.97 (s, 3H, OAc).
^{13}C NMR, δ, ppm: 177.10 (C=O, HgOAc), 169.77 (q, $\underline{C}OCF_3$, $^2J_{CF}$ = 35.7 Hz), 169.12 (C=O, OAc), 145.65 (C-2), 132.53 (Ph-i), 132.08 (Ph-m), 131.34 (Ph-o), 126.31 (C-4), 125.37 (C-5), 124.40 (Ph-p), 117.20 (q, CF_3, $^1J_{CF}$ = 290.0 Hz), 113.80 (C-3), 80.84 (C_α), 29.21 (C_β), 22.65 (Me, HgOAc), 20.87 (Me, OAc). ^{19}F NMR, δ, ppm: -70.3. ^{15}N NMR, δ, ppm: -198.4.

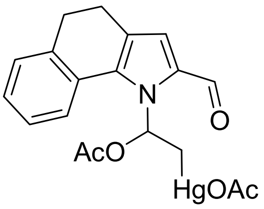


Trimercuric acetate 13. Dark-brown crystals with metal luster, stable up to 350 °C, insoluble in organic solvents. IR (KBr) ν/cm^{-1}: 3410, 2930, 2853, 1699, 1572, 1408, 1321, 1375, 1141, 1090, 1048, 1017, 923, 791, 754, 681, 649, 618 cm^{-1}. Anal. Calcd. for $C_{18}H_{23}Hg_3NO_8$: C, 21.99; H, 2.36; Hg, 61.21; N, 1.42; O, 13.02. Found: C, 22.12; Hg, 61.40; N, 1.37, O, 12.91.

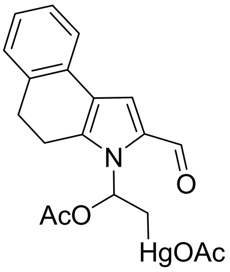


2-Acetoxy-2-(2-cyano-4,5,6,7-tetrahydroindol-1-yl)ethylmercury acetate 14. Light yellow viscous oil.
IR *ν*/cm^{-1}: 2936, 2856, 2208, 1751, 1734, 1601, 1479, 1444, 1370, 1299, 1223, 1132, 1065, 1016, 952, 832, 814, 732, 693, 647, 612, 507, 451.
^{1}H NMR, δ: 6.72 (dd, 1H, H_α, ^3J = 7.3 Hz, ^3J = 6.9 Hz), 6.63 (s, 1H, H-3), 2.75 (m, 2H, 7-CH_2), 2.58 (dd, 1H, H_β, ^3J = 7.3 Hz, ^2J = 12.5 Hz) 2.48 (dd, 1H, H_β, ^3J = 6.9 Hz, ^2J = 12.5 Hz), 2.42 (m, 2H, 4-CH_2), 2.06 (s, 3H, OAc), 2.00 (s, 3H, HgOAc), 1.81 (m, 2H, 6-CH_2), 1.69 (m, 2H, 5-CH_2). ^{13}C NMR, δ: 176.86 (C=O, HgOAc),

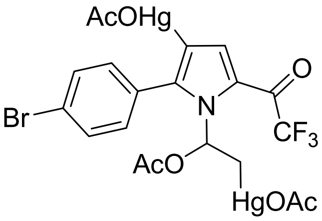
169.25 (C=O, OAc), 134.56 (C-8), 122.02 (C-3), 119.72 (C-9), 115.12 (C≡N), 98.31 (C-2), 78.33 (C_α), 29.22 (C_β), 22.74, 22.65, 22.62, 22.57 (C-4, C-5, C-6, C-7), 22.50 (Me, HgOAc), 20.82 (Me, OAc).
Anal. Calcd for $C_{15}H_{18}N_2O_4$: C, 36.70; H, 3.70; N, 5.71. Found: C, 36.36; H, 3.65; N, 5.84.



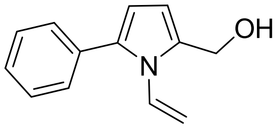
2-Acetoxy-2-(2-formyl-4,5-dihydrobenzo[*g*]indol-1-yl)ethylmercury acetate 15. Light yellow viscous oil.
IR (thin layer) ν/cm^{-1}: 2937, 2898, 2840, 1747, 1651, 1547, 1496, 1469, 1405, 1372, 1342, 1321, 1304, 1289, 1223, 1139, 1119, 1049, 1017, 958, 924, 845, 765, 739, 712, 648, 622, 599, 520, 471. ^{1}H NMR, δ, ppm: 9.48 (s, 1H, CHO), 7.79 (dd, 1H, H_α, ^3J = 5.6 Hz, ^3J = 9.1 Hz), 7.70 (m, 1H, H-9), 7.30-7.15 (m, 3H, H-6, H-7, H-8), 6.90 (s, 1H, H-3), 2.84 (m, 2H, H-4), 2.65-2.55 (m, 4H, H-5, H_β), 2.01 (s, 3H, OAc), 1.99 (s, 3H, HgOAc).
^{13}C NMR, δ: 178.55 (CHO), 177.18 (C=O, HgOAc), 169.33 (C=O, OAc), 139.60 (C-3a), 139.34 (C-5a), 132.48 (C-2), 129.17 (C-9a), 128.49 (C-6), 127.90 (C-8), 127.16 (C-7), 125.97 (C-9b), 125.93 (C-9), 125.35 (C-3), 80.20 (C_α), 30.80 (C-4), 28.67 (C_β), 23.03 (C-5), 22.07 (Me, HgOAc), 21.19 (Me, OAc).
Anal. Calcd for $C_{19}H_{19}HgNO_5$: C, 42.48; H, 3.42; N, 3.84. Found: C, 42.11; H, 3.53; N, 2.58.



2-Acetoxy-2-(2-formyl-4,5-dihydrobenzo[*e*]indol-3-yl)ethylmercury acetate 16. Light yellow viscous oil.
IR (thin layer) ν/cm^{-1}: 2937, 2894, 2836, 1750, 1725, 1651, 1547, 1496, 1469, 1405, 1372, 1342, 1321, 1304, 1289, 1223, 1139, 1119, 1049, 1017, 958, 924, 845, 765, 739, 712, 648, 622, 599, 520, 471.
^{1}H NMR, δ, ppm: 9.47 (s, 1H, CHO), 7.65 (dd, 1H, H_α, ^3J = 5.6 Hz, ^3J = 9.1 Hz), 7.42 (m, 1H, H-9), 7.31 (s, 1H, H-1), 7.25-7.15 (m, 3H, H-6, H-7, H-8), 3.18 (m, 1H, H-4), 3.08 (m, 1H, H-4), 3.07 (m, 2H, H-5), 2.52 (dd, 1H, H_β, ^3J = 5.6 Hz, ^2J = 12.2 Hz), 2.48 (dd, 1H, H_β, ^3J = 9.1 Hz, ^2J = 12.2 Hz), 2.06 (s, 3H, OAc), 1.99 (s, 3H, HgOAc). ^{13}C NMR, δ, ppm: 179.45 (CHO), 176.88 (C=O, HgOAc), 168.77 (C=O, OAc), 140.46 (C-3a), 132.90 (C-5a), 131.27 (C-2), 130.63 (C-9a), 128.14 (C-6), 127.21 (C-8), 126.48 (C-7), 122.76 (C-9b), 122.39 (C-9), 120.16 (C-1), 80.35 (C_α), 28.84 (C-4), 28.70 (C_β), 22.98 (C-5), 22.32 (Me, HgOAc), 20.90 (Me, OAc). Anal. Calcd for $C_{19}H_{19}HgNO_5$: C, 42.11; H, 3.53; N, 2.58. Found: C, 42.16; H, 3.55; N, 2.64.

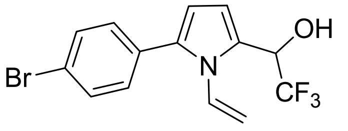


Dimercuric acetate 17. Yellow viscous oil. IR (thin layer) ν/cm^{-1}: 2922, 2855, 1738, 1657, 1561, 1518, 1445, 1406, 1269, 1151, 1074, 1113, 972, 908, 834, 733, 659.
^{1}H NMR, δ, ppm: 7.61 (m, 2H, Ph-m), 7.34 (m, 2H, Ph-o), 7.35 (m, 1H, H-3), 7.09 (dd, 1H, H_α, ^3J = 8.6 Hz, ^3J = 6.9 Hz), 2.57 (dd, 1H, H_β, ^2J = 12.0 Hz, ^3J = 8.6 Hz), 2.32 (dd, 1H, H_β, ^2J = 12.0 Hz, ^3J = 6.9 Hz,), 1.97 (s, 6H, HgOAc), 1.95 (s, 3H, OAc).
^{13}C NMR, δ, ppm: 177.20 (C=O, HgOAc), 169.68 (q, $\underline{C}OCF_3$, $^2J_{CF}$ = 35.6 Hz), 169.13 (C=O, OAc), 149.58 (C-5), 132.47 (Ph-m), 132.34 (C-3), 132.03 (Ph-i), 131.39 (Ph-o), 126.08 (C-4), 125.78 (C-2), 124.92 (Ph-p), 117.01 (q, CF_3, $^1J_{CF}$ = 290.7 Hz), 81.23 (C_α), 28.98 (C_β), 22.61 (Me, HgOAc), 20.86 (Me, OAc). ^{19}F NMR, δ, ppm: -70.4. ^{15}N NMR, δ, ppm: -199.5.
Anal. Calcd. for $C_{20}H_{17}BrF_3Hg_2NO$: C, 26.07; H, 1.86; Hg, 43.54; Br, 8.67; F, 6.19; N, 1.52. Found: C, 25.86; H, 1.70; Hg, 40.61; F, 23.63; N, 1.81.



(5-Phenyl-1-vinyl-pyrrol-2-yl)methanol 18. Light-brown viscous oil. IR (thin layer) ν/cm^{-1}: 3417, 3104, 3060, 3031, 2923, 2853, 1642, 1601, 1514, 1448, 1413, 1359, 1322, 1300, 1201, 1098, 1073, 1028, 972, 909, 759, 798, 661 cm^{-1}.

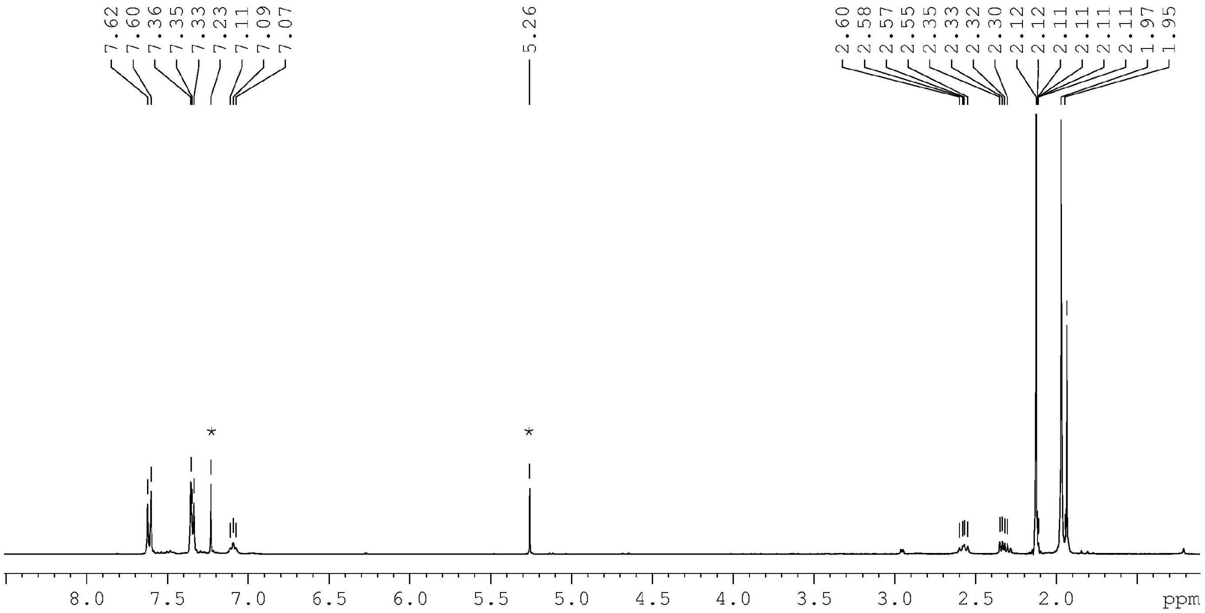
^{1}H NMR, δ, ppm: 7.35 (m, 5H, Ph), 6.83 (dd, 1H, H_X, $^3J_{X\text{-}B}$ = 15.9 Hz, $^3J_{X\text{-}A}$ = 8.9 Hz), 6.26 (d, 1H, H-4, $^3J_{3\text{-}4}$ = 3.9 Hz), 6.20 (d, 1H, H-3, $^3J_{4\text{-}3}$ = 3.9 Hz,), 5.34 (d, 1H, H_B, $^3J_{X\text{-}B}$ = 15.9 Hz), 4.99 (d, 1H, H_A, $^3J_{X\text{-}A}$ = 8.9 Hz), 4.65 (s, 2H, CH_2), 1.63 (br s, 1H, OH). ^{13}C NMR, δ, ppm: 135.31 (C-5), 132.88 (Ph-i), 132.71 (C-2), 131.10 (C_α), 128.56 (Ph-m), 127.43 (Ph-o), 126.68 (Ph-p), 110.64 (C_β), 108.83 (C-4), 107.44 (C-3), 56.68 (CH_2).
Anal. Calcd. for $C_{13}H_{13}NO$: C, 78.36; H, 6.58; N, 7.03. Found: C, 78.55; H, 6.62; N, 6.96.



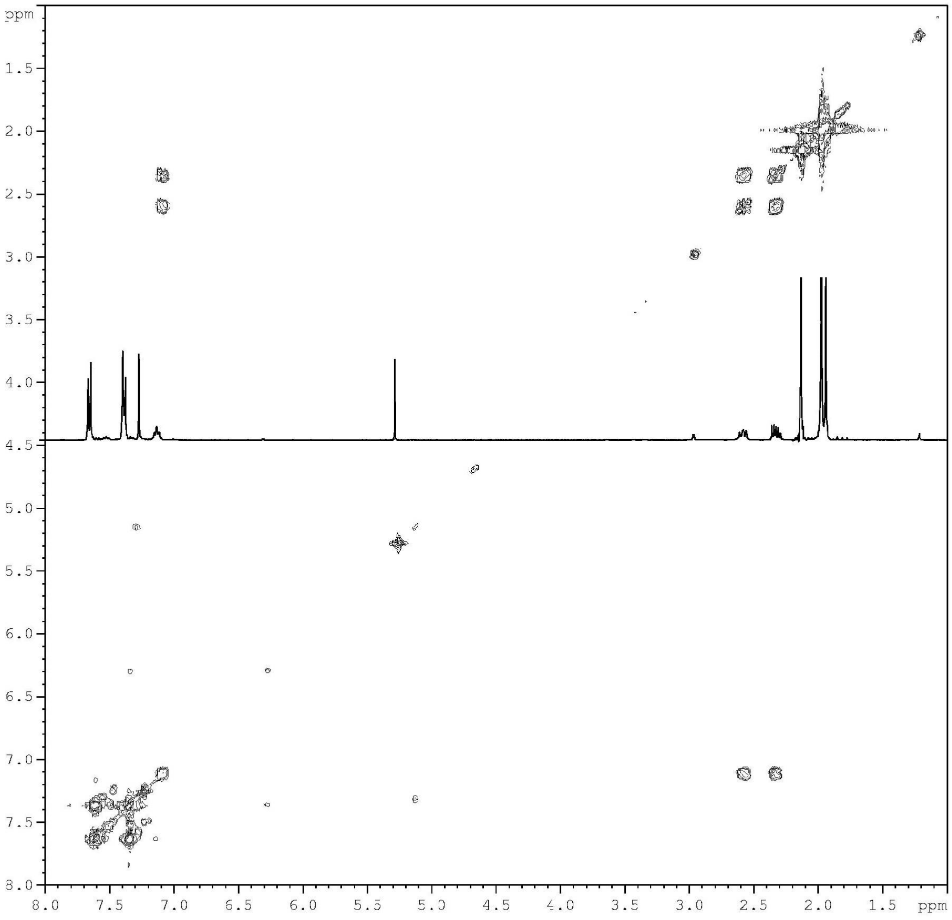
1-(5-(4-Bromophenyl)-1-vinyl-1*H*-pyrrol-2-yl)-2,2,2-trifluoroethanol 19. Colorless crystals; mp 59-60 °C. IR (KBr) ν/cm^{-1}: 3584, 3400, 2932, 2853, 1641, 1557, 1518, 1469, 1437, 1382, 1281, 1177, 1136, 1098, 1044, 1011, 969, 909, 860, 829, 777, 735, 651 cm^{-1}.

^{1}H NMR, δ, ppm: 7.47 (m, 2H, Ph-m), 7.25 (m, 2H, Ph-o), 6.73 (dd, 1H, H_X, $^3J_{X\text{-}B}$ = 15.9 Hz, $^3J_{X\text{-}A}$ = 8.6 Hz), 6.51 (m, 1H, H-3), 6.27 (d, 1H, H-4, $^3J_{3\text{-}4}$ = 3.9 Hz), 5.29 (d, 1H, H_B, $^3J_{X\text{-}B}$ = 15.9 Hz), 5.24 (d, 1H, H_A, $^3J_{X\text{-}A}$ = 8.6 Hz), 5.11 (q, 1H, $CHCF_3$, $^3J_{HF}$ = 6.7 Hz), 2.96 (br s, 1H, OH).
^{13}C NMR, δ, ppm: 134.78 (C-5), 131.55 (Ph-m), 130.37 (Ph-o), 131.58 (Ph-i), 131.12 (C_α), 127.17 (C-2), 124.41 (q, CF_3, $^1J_{CF}$ = 282.0 Hz), 121.60 (Ph-p), 112.99 (C_β), 110.48 (C-3), 109.98 (C-4), 65.72 (q, $\underline{C}HCF_3$, $^2J_{CF}$ = 33.2 Hz). ^{19}F NMR, δ, ppm: -76.16 (dd, J_{HF} = 1.2 Hz, J_{HF} = 6.7 Hz). ^{15}N NMR, δ, ppm: -213.0.
Anal. Calcd. for $C_{12}H_{11}BrF_3NO$: C, 48.58; H, 3.20; Br, 23.08. Found: C, 48.31.75; H, 3.31; Br, 23.01.

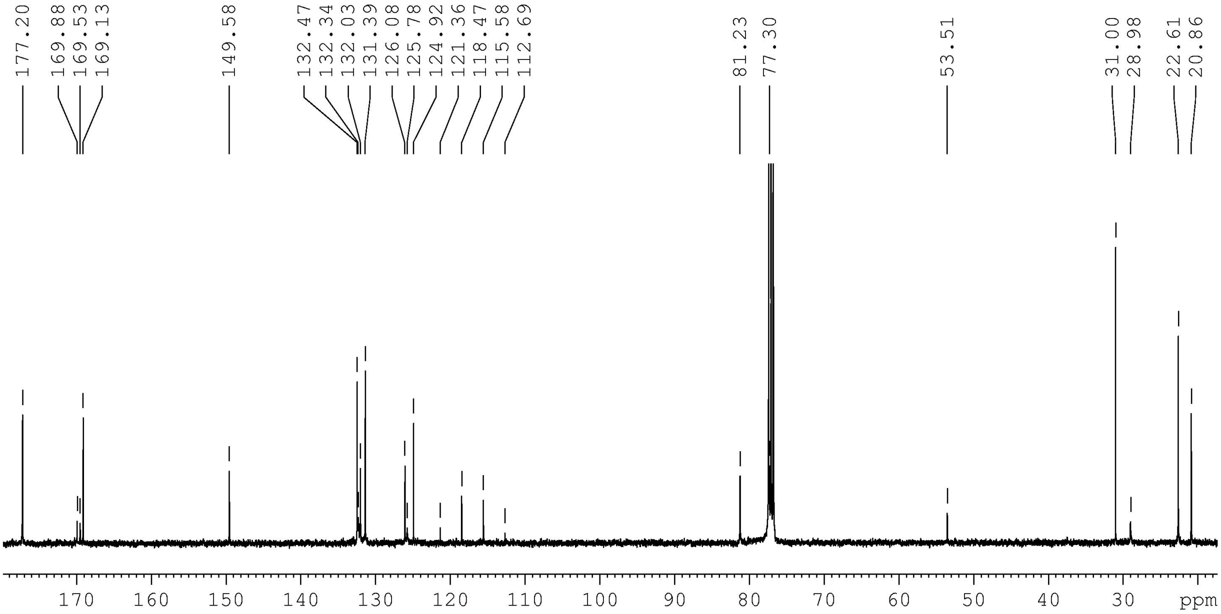
Representative NMR Spectra



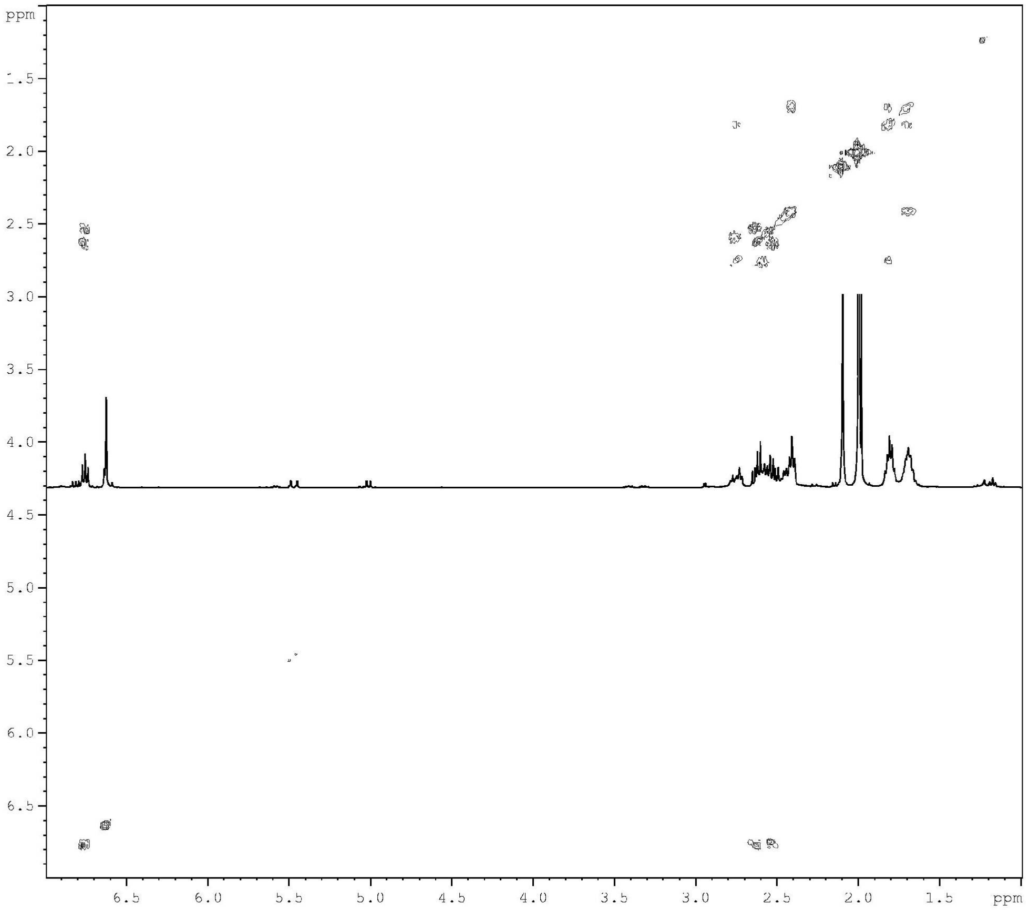
^{1}H NMR spectrum of **17** (400.1 MHz, $CDCl_3$)



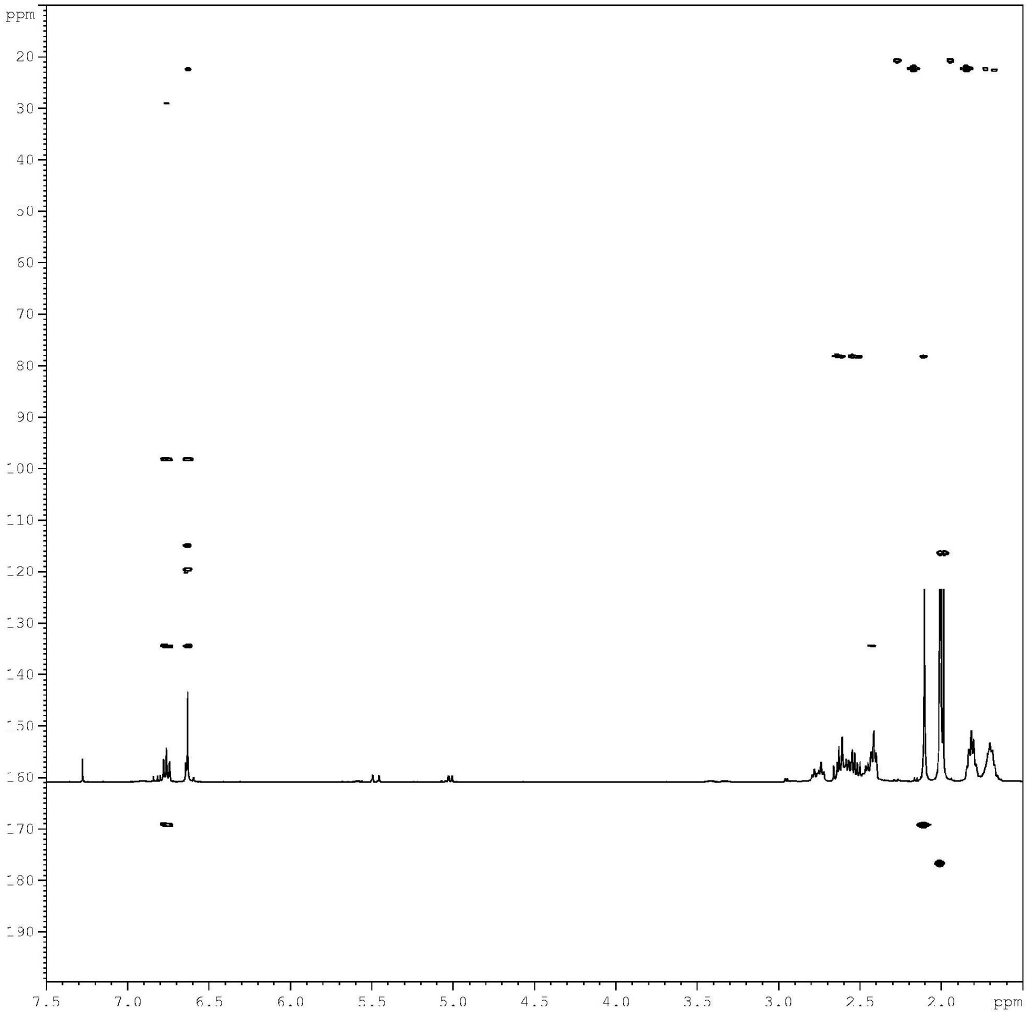
2D COSY spectrum of **17** (400.13 MHz, $CDCl_3$)



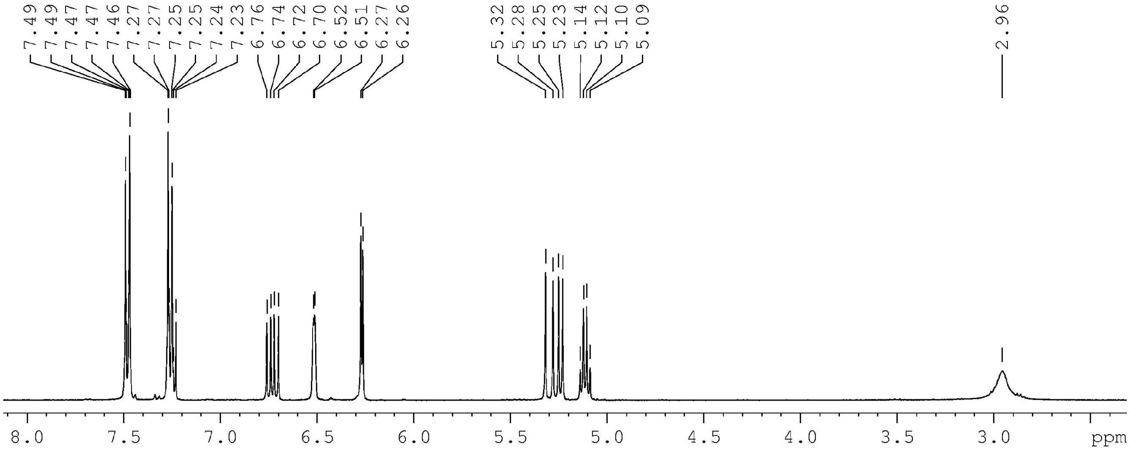
^{13}C NMR spectrum of **17** (100.6 MHz, CDCl$_3$)



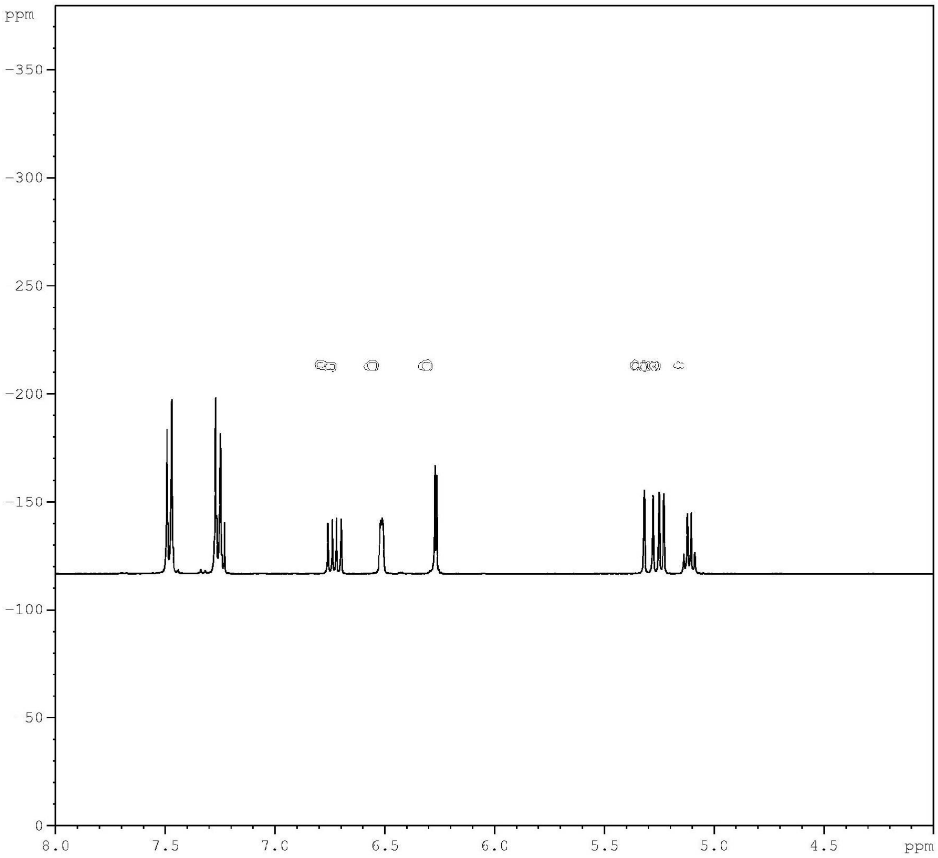
2D COSY spectrum of **14** (400.1 MHz, CDCl$_3$)



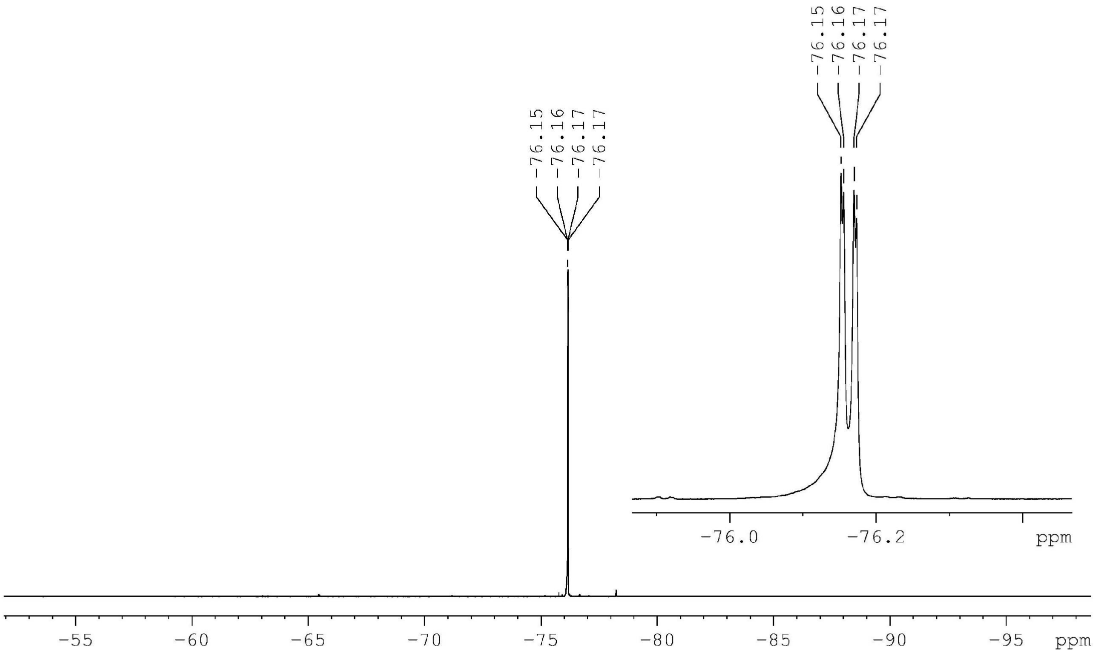
2D ^{1}H-^{13}C HMBC spectrum of **14** ($CDCl_3$)



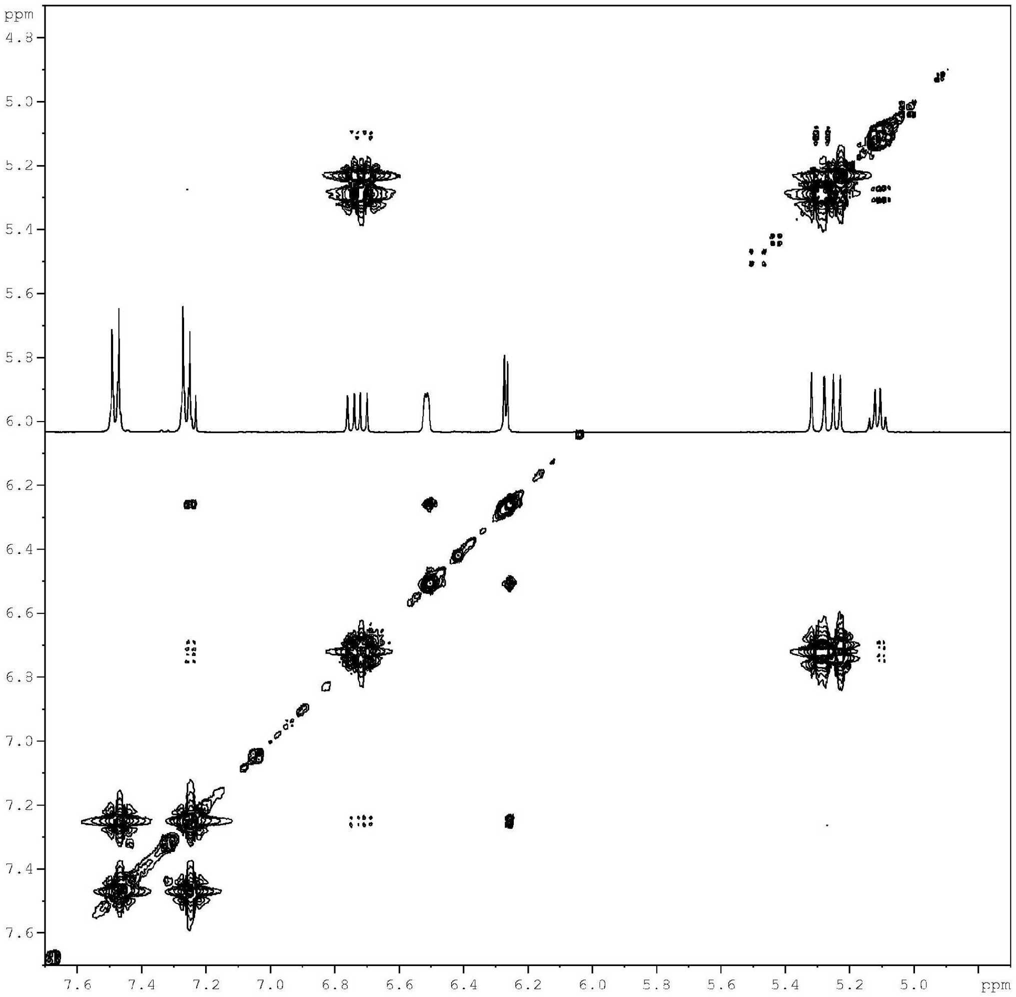
^{1}H NMR spectrum of **19** (400.1 MHz, $CDCl_3$)



2D ^{1}H-^{15}N HMBC spectrum of **19** ($CDCl_3$)



^{19}F NMR spectrum of **19** (376.5 MHz, CDCl$_3$)



2D NOESY spectrum of **19** (400.1 MHz, CDCl$_3$)