Electronic Supplementary Material (ESI) for

Non-redox Metal Ions Promoted Oxidative Coupling of Indoles with Olefins by Palladium(II) Acetate Catalyst Through Dioxygen Activation: Experimental Results with DFT Calculations

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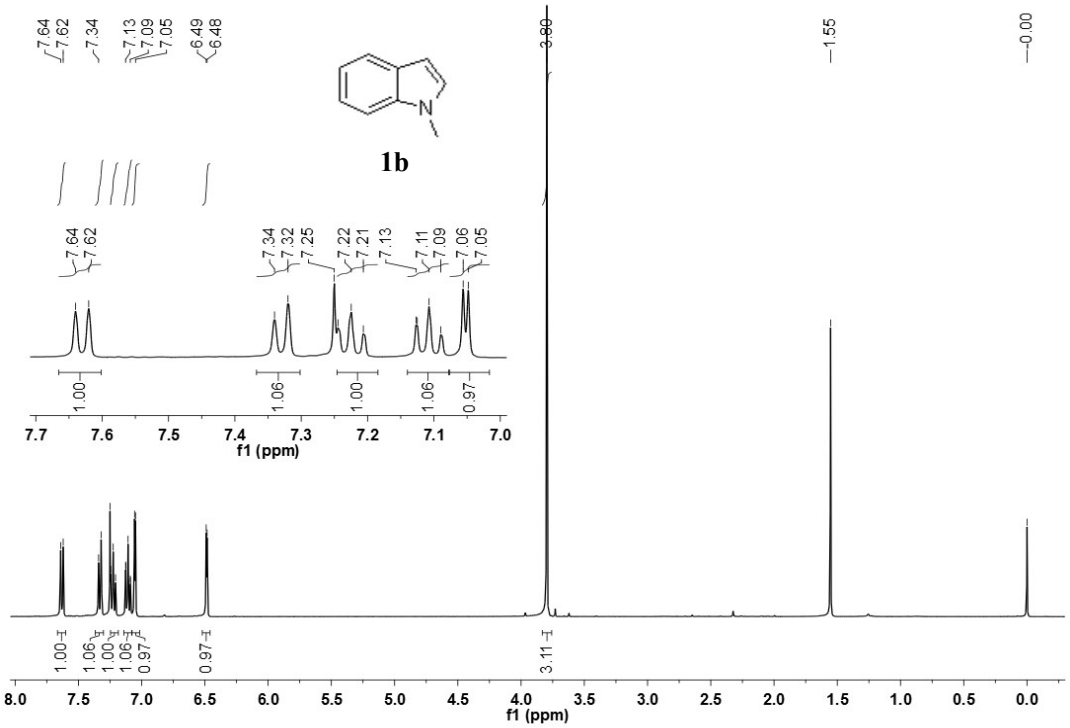
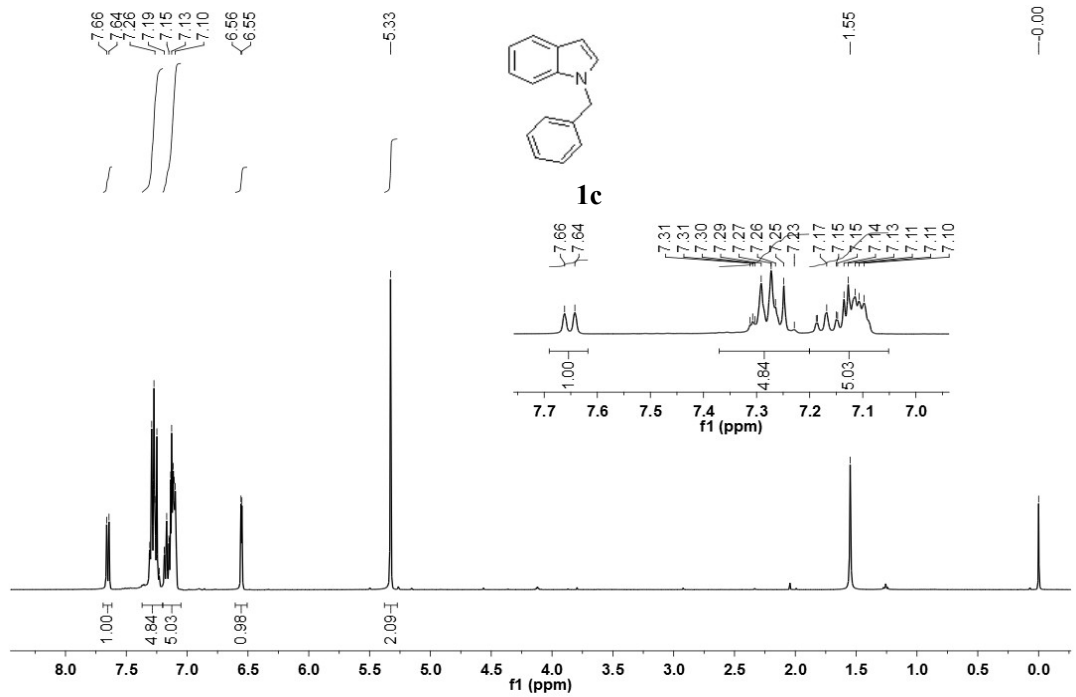
Procedure for synthesis of N-substituted indoles

1-methylindole (**1b**) was prepared according to the literature procedures.[1] Yield 82%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.9 Hz, 1H), 7.33 (d, *J* = 8.1 Hz, 1H), 7.23 (t, *J* = 8.1 Hz, 1H), 7.11 (t, *J* = 8.1 Hz, 1H), 7.05 (d, *J* = 3.1 Hz, 1H), 6.49 (d, *J* = 2.9 Hz, 1H), 3.80 (s, 3H).

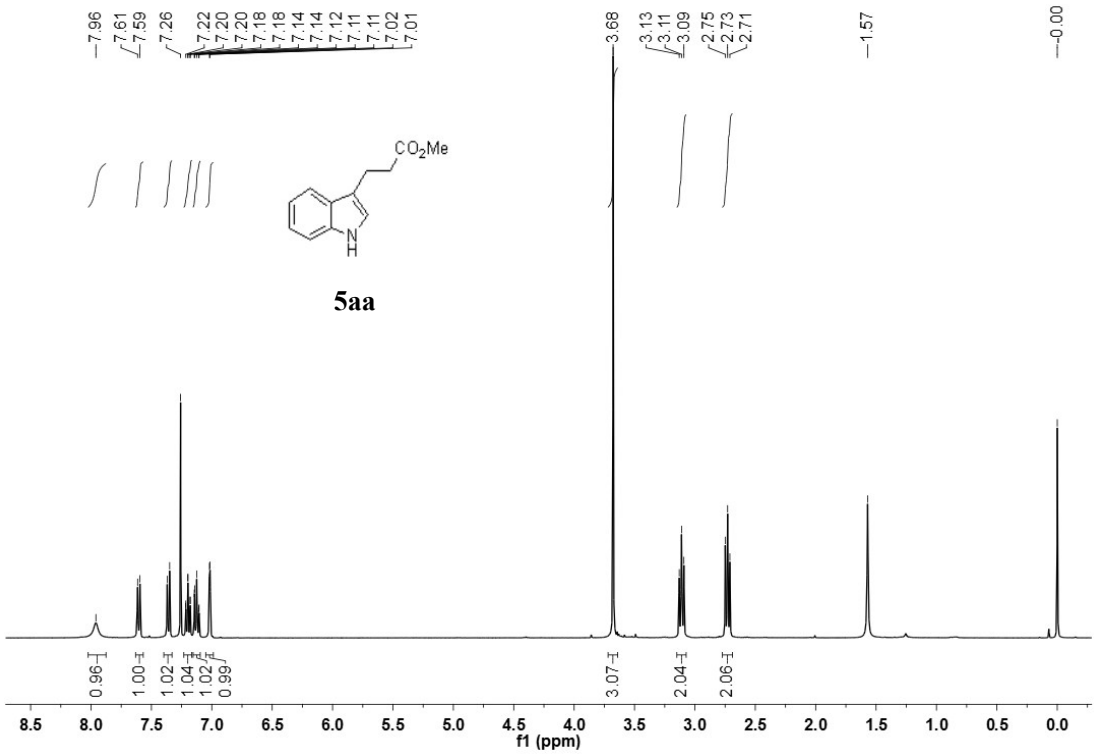


1-benzylindole (**1c**) was prepared according to the literature procedures.[1] Yield 75%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.7 Hz, 1H), 7.37-7.20 (m, 4H), 7.20-7.05 (m, 5H), 6.55 (d, *J* = 3.1 Hz, 1H), 5.33 (s, 2H).



Procedure for synthesis of intermediate methyl 3-(1*H*-indol-3-yl)propanoate (5aa)

3-(1H-indol-3-yl)propanoate (**5aa**) was synthesized according to the literature procedures.[2] Yield 89%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (s, 1H), 7.60 (d, J = 7.7 Hz, 1H), 7.36 (d, J = 8.1 Hz, 1H), 7.20 (td, J_1 = 8.0 Hz, J_2 = 1.0 Hz, 1H), 7.12 (td, J_1 = 8.0 Hz, J_2 = 1.0 Hz, 1H), 7.02 (d, J = 2.1 Hz, 1H), 3.68 (s, 3H), 3.11 (t, J = 7.7 Hz, 2H), 2.73 (t, J = 7.7 Hz, 2H).



^{1}H NMR studies on the interaction among $Pd(OAc)_2$, $Sc(OTf)_3$ and methyl acrylate (2a)

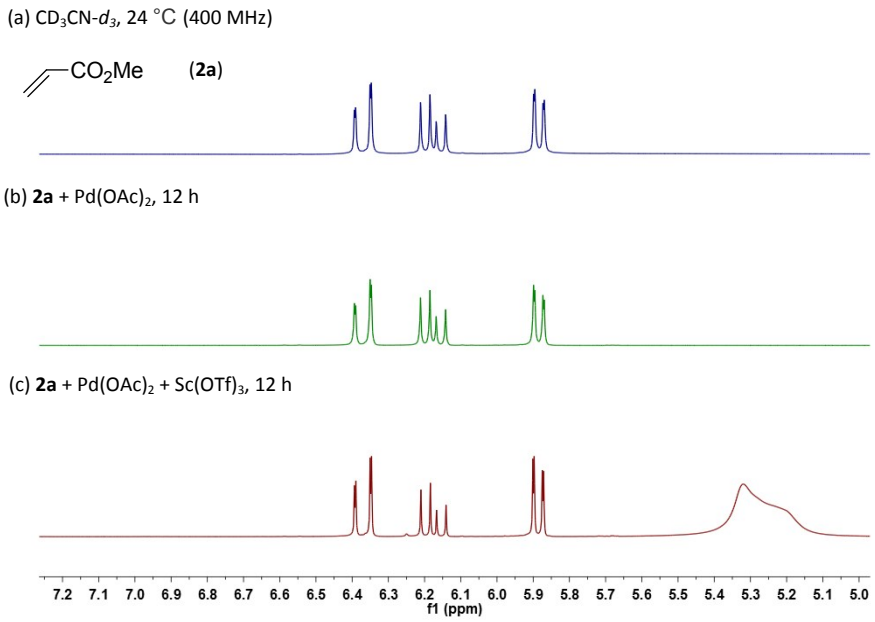


Figure S1. ^{1}H NMR studies on the interaction among $Pd(OAc)_2$, $Sc(OTf)_3$ and methyl acrylate (**2a**) in the absence of indole derivative at 25 °C. (a) ^{1}H NMR spectrum of indole in CD_3CN-d_3 ; (b) ^{1}H NMR spectrum of the reaction mixture after 12 h by the addition of $Pd(OAc)_2$; (c) ^{1}H NMR spectrum of the reaction mixture after 12 h by addition of $Pd(OAc)_2$ and $Sc(OTf)_3$.

^{1}H NMR kinetics of the interaction between $Pd(OAc)_2/Sc(OTf)_3$ and indole (1a)

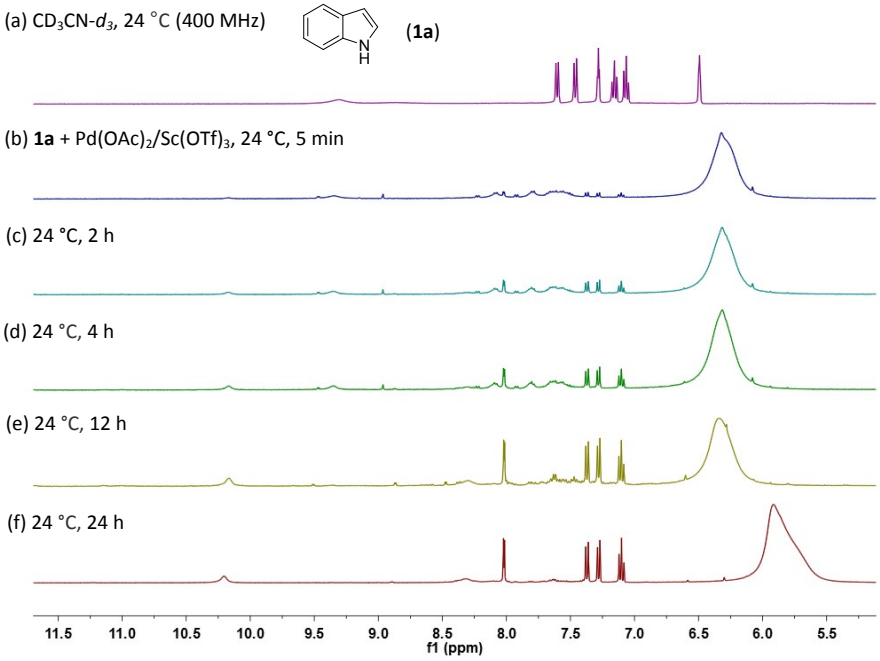


Figure S2. ^{1}H NMR kinetics of the interaction between $Pd(OAc)_2/Sc(OTf)_3$ and indole (**1a**) in the absence of acrylate substrate at 25 °C. (a) ^{1}H NMR spectrum of indole in CD_3CN-d_3. (b-f) ^{1}H NMR spectra of the reaction mixture after 5 min, 2, 4, 12 and 24 h by addition of $Pd(OAc)_2/Sc(OTf)_3$.

^{1}H NMR spectra of $Pd(OAc)_2$/$Sc(OTf)_3$ with related compounds

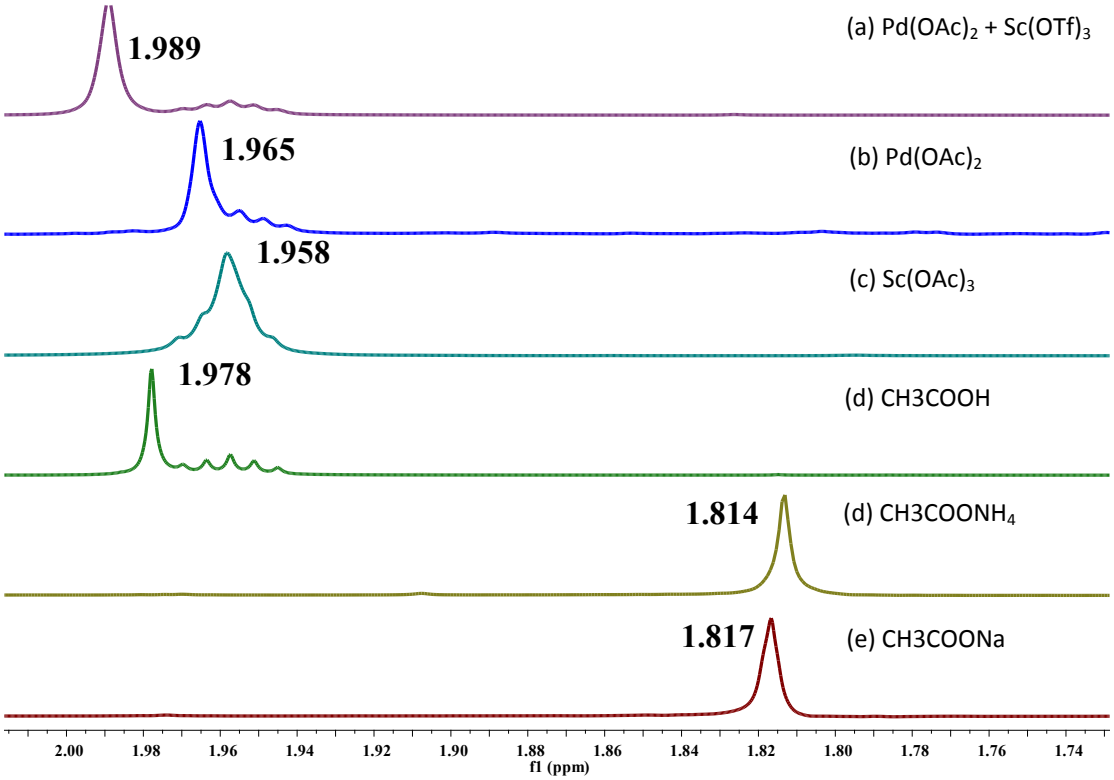


Figure S3. ^{1}H NMR spectra of $Pd(OAc)_2$/$Sc(OTf)_3$ with related compounds in CD_3CN.

^{13}C NMR spectra of $Pd(OAc)_2$, $Sc(OTf)_3$ and $Pd(OAc)_2$/$Sc(OTf)_3$

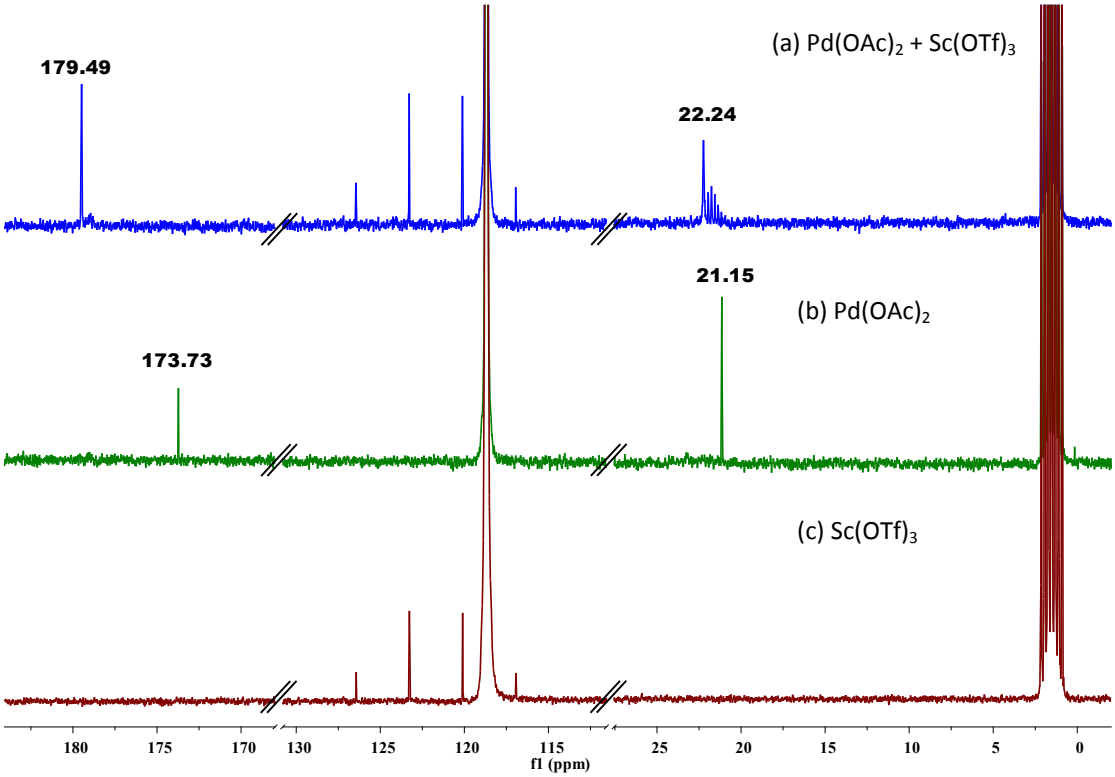
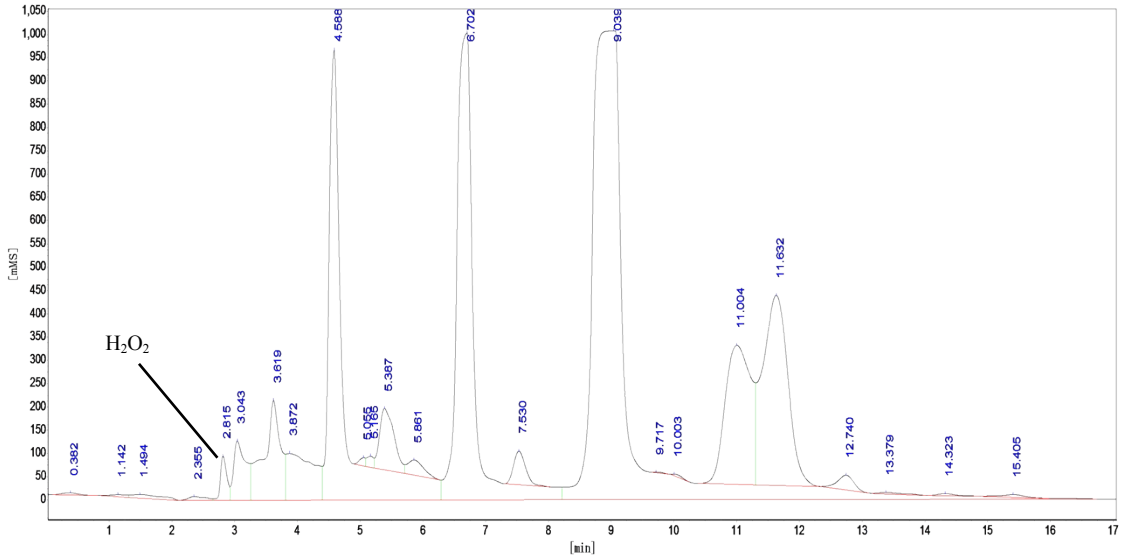


Figure S4. ^{13}C NMR spectra of $Pd(OAc)_2$, $Sc(OTf)_3$ and their mixture in CD_3CN

Detection of the formation of H_2O_2 through HPLC

(a)



(b)

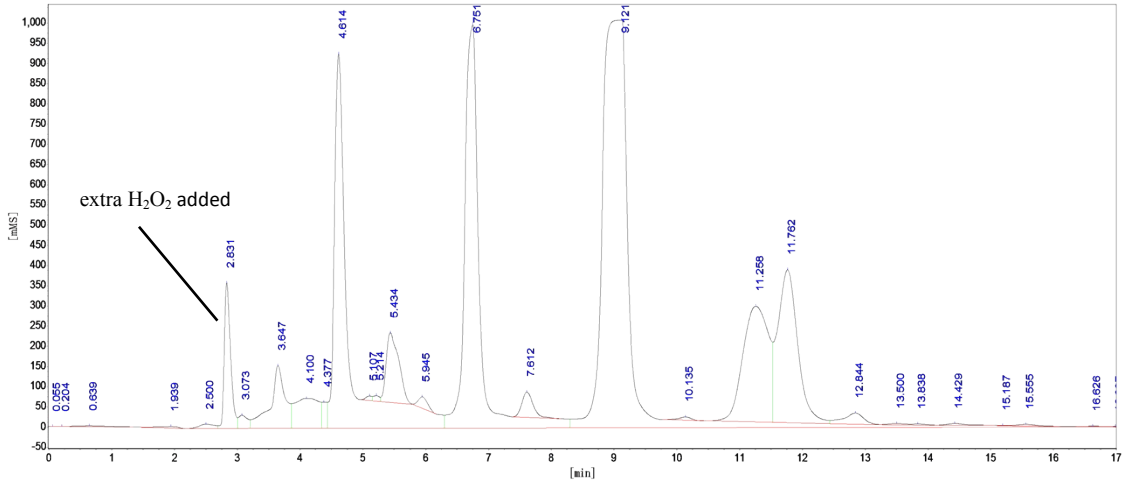
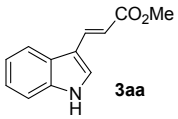


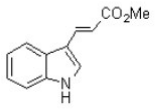
Figure S5. (a) HPLC graph of the reaction mixture between **1a** and **2a** in the presence of $Pd(OAc)_2/Sc(OTf)_3$ in CH_3CN; (b) the addition of extra H_2O_2 into (a). In Figure S5(a), after compared with authentic H_2O_2 sample, the peak at 2.851 min was attributed to H_2O_2. In Figure S5(b), after adding external H_2O_2 to the reaction mixture, this peak increases clearly.

Characterization data, ^{1}H NMR and ^{13}C NMR spectra of 3-vinylindoles and bis(indolyl) products

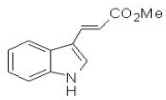


3aa

(*E*)-methyl 3-(1*H*-indol-3-yl)acrylate (3aa): Yield 6%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.96 (s, 1H), 7.92 (d, J = 16.0 Hz, 1H), 7.88 (dd, J_1 = 6.7 Hz, J_2 = 2.1 Hz, 1H), 7.43 – 7.35 (m, 2H), 7.28 – 7.19 (m, 2H), 6.46 (d, J = 16.0 Hz, 1H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.05, 138.81, 137.19, 129.26, 125.27, 123.29, 121.50, 120.37, 113.34, 112.61, 111.94, 51.50.



3aa



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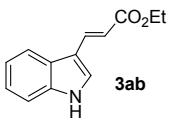
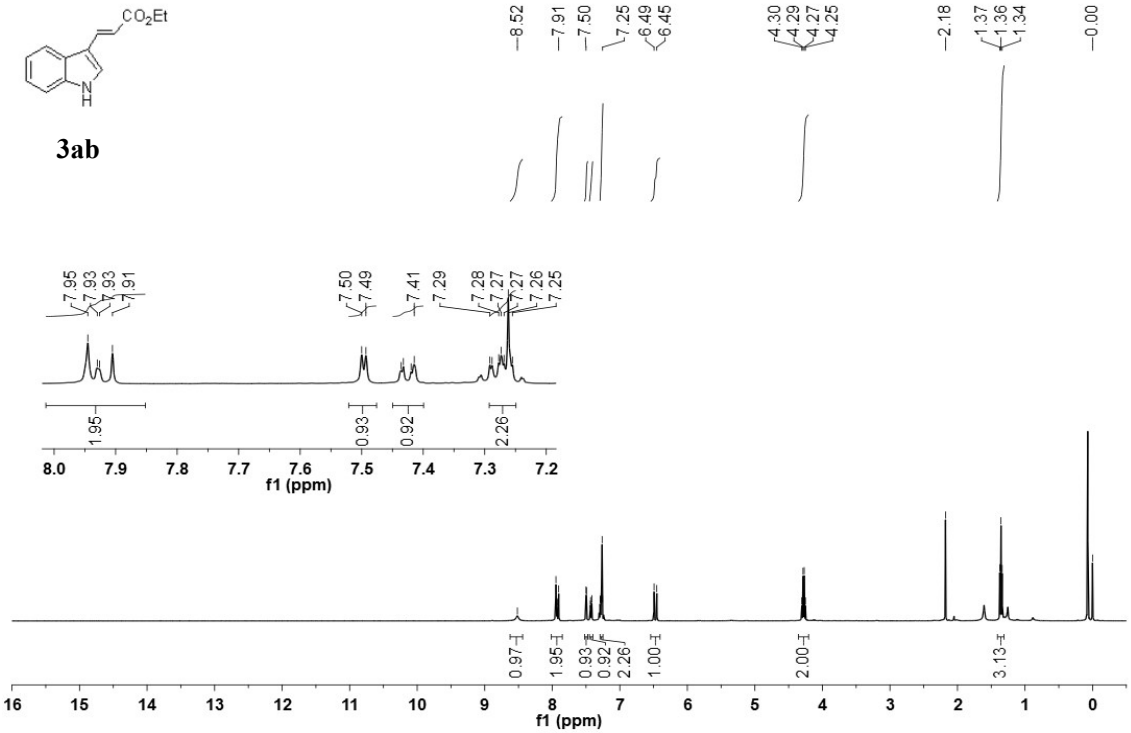
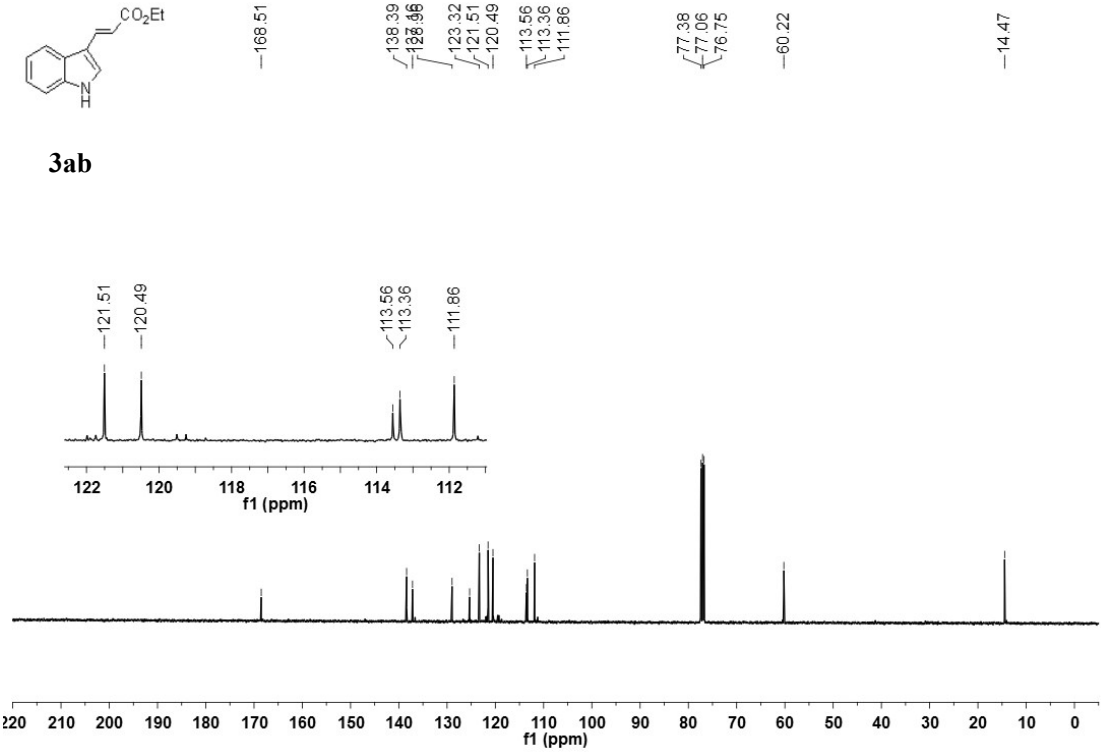
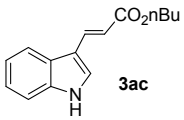


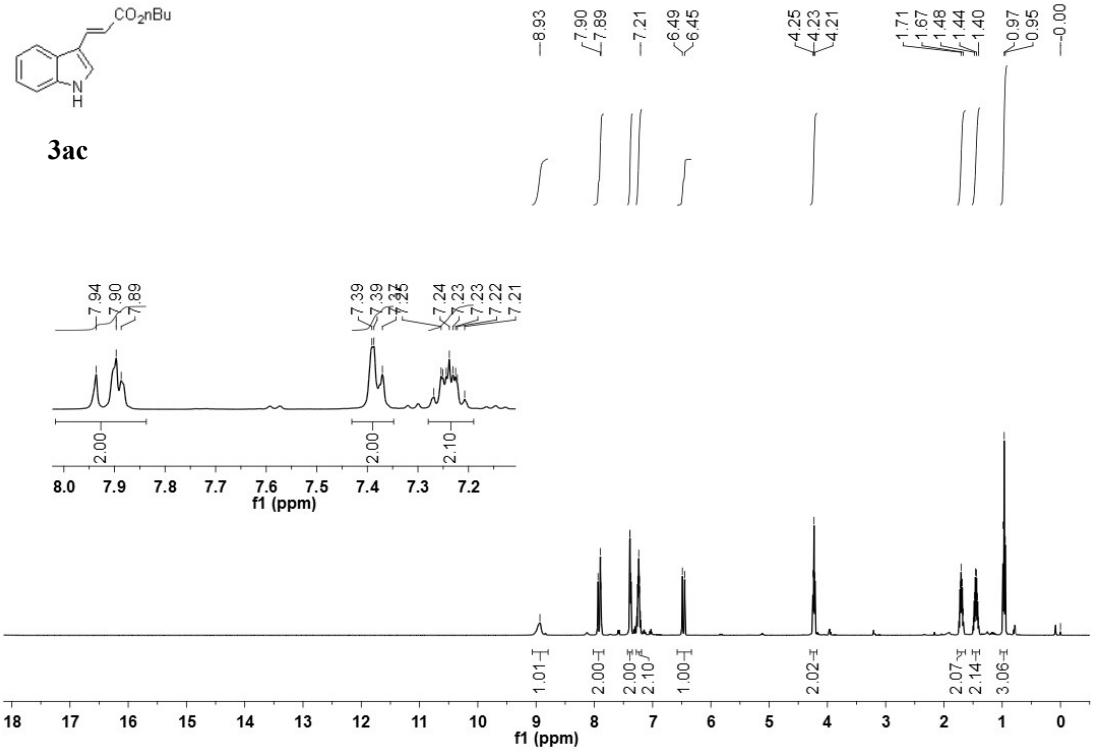
(*E*)-ethyl 3-(1*H*-indol-3-yl)acrylate (3ab): Yield 7%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (s, 1H), 8.01 – 7.85 (m, 2H), 7.50 (d, J = 2.7 Hz, 1H), 7.43 (dd, J = 6.8 Hz, J_2 = 1.7 Hz, 1H), 7.29 – 7.25 (m, 2H), 6.47 (d, J = 16.0 Hz, 1H), 4.28 (q, J = 7.1 Hz, 2H), 1.36 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.51, 138.39, 137.16, 128.96, 125.33, 123.32, 121.51, 120.49, 113.56, 113.36, 111.86, 60.22, 14.47.

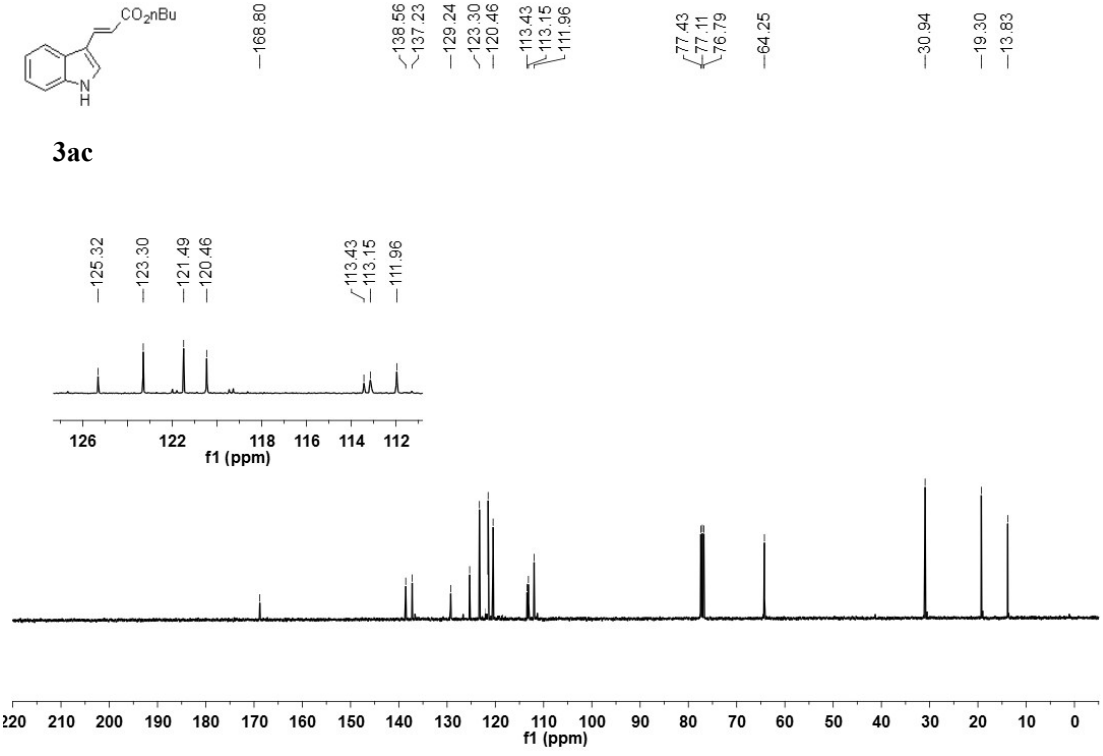


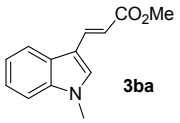




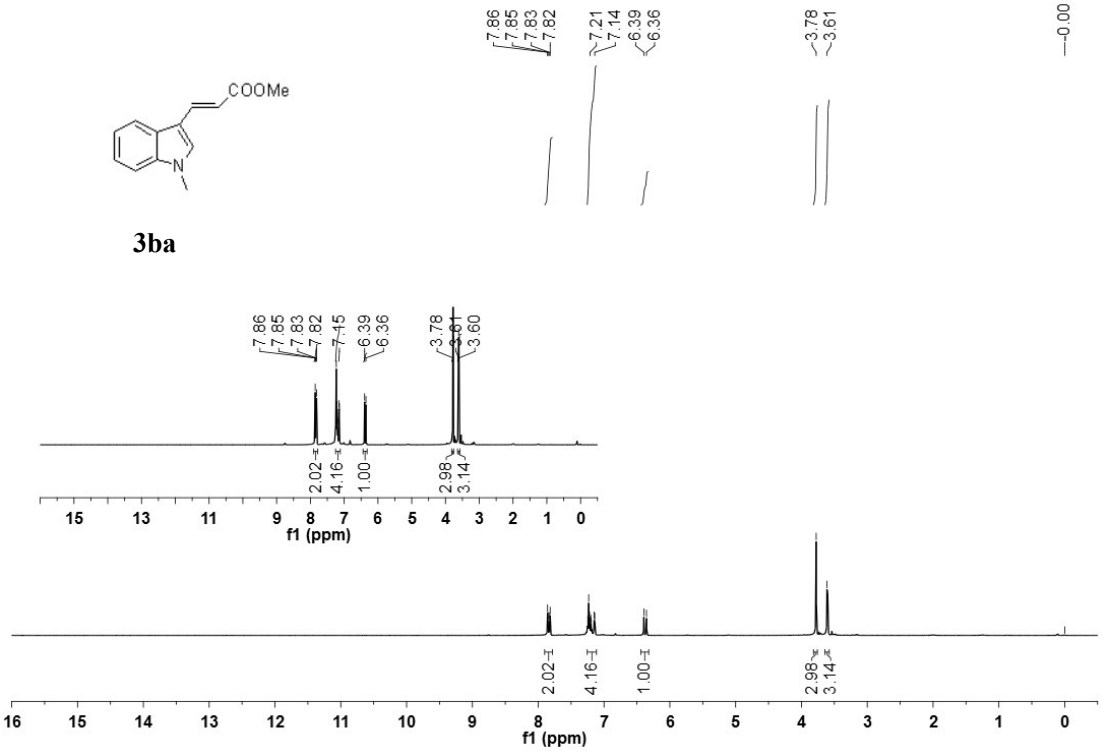
(*E*)-butyl 3-(1*H*-indol-3-yl)acrylate (3ac): Yield 5%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (s, 1H), 8.02 – 7.84 (m, 2H), 7.43 – 7.35 (m, 2H), 7.28 – 7.19 (m, 2H), 6.47 (d, *J* = 16.0 Hz, 1H), 4.23 (t, *J* = 6.7 Hz, 2H), 1.71 (q, *J* = 6.7 Hz, 2H), 1.52 – 1.39 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.80, 138.56, 137.23, 129.24, 125.32, 123.30, 121.49, 120.46, 113.43, 113.15, 111.96, 64.25, 30.94, 19.30, 13.83.

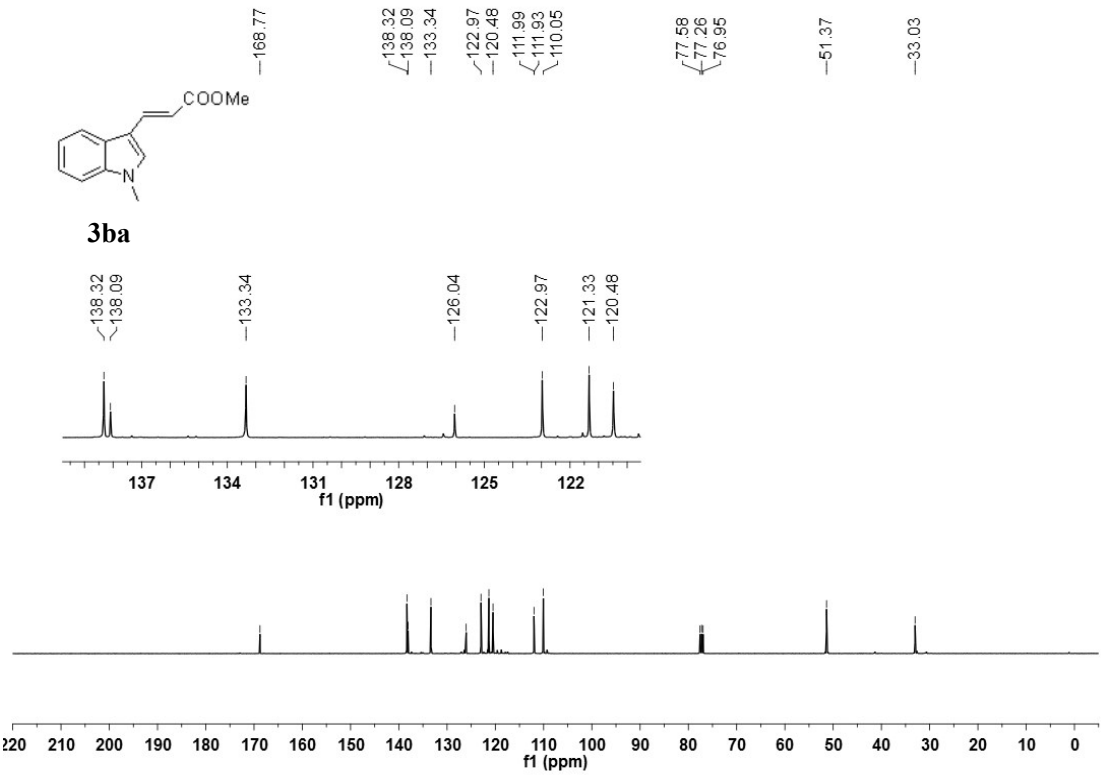


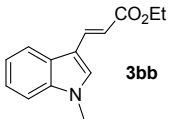




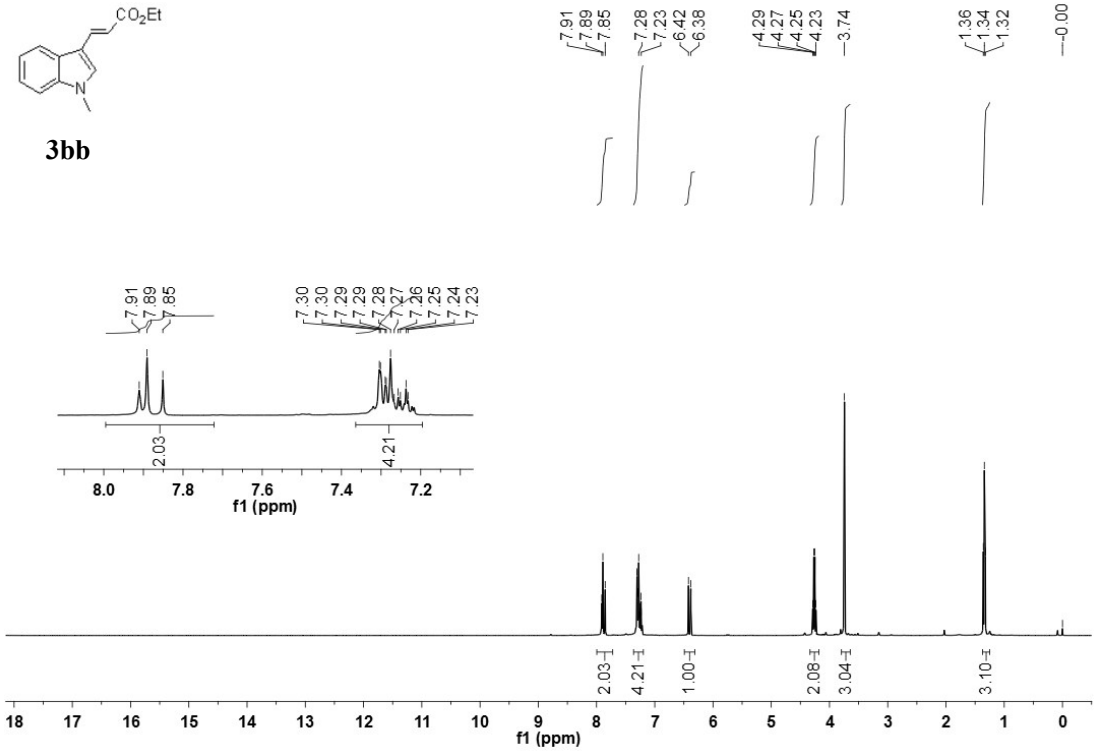
(*E*)-methyl 3-(1-methyl-1*H*-indol-3-yl)acrylate (3ba): Yield 21%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.78 (m, 2H), 7.26 – 7.12 (m, 4H), 6.37 (d, *J* = 15.9 Hz, 1H), 3.78 (s, 3H), 3.61 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.77, 138.32, 138.09, 133.34, 126.04, 122.97, 121.33, 120.48, 111.99, 111.93, 110.05, 51.37, 33.03.

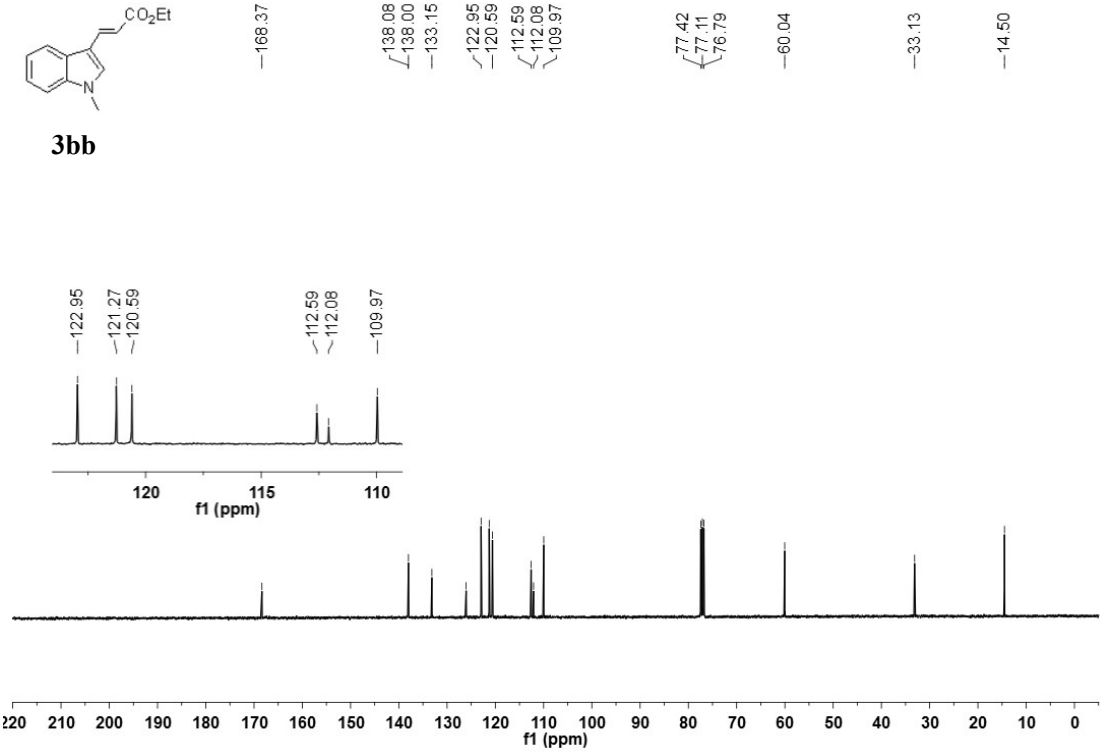


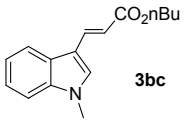




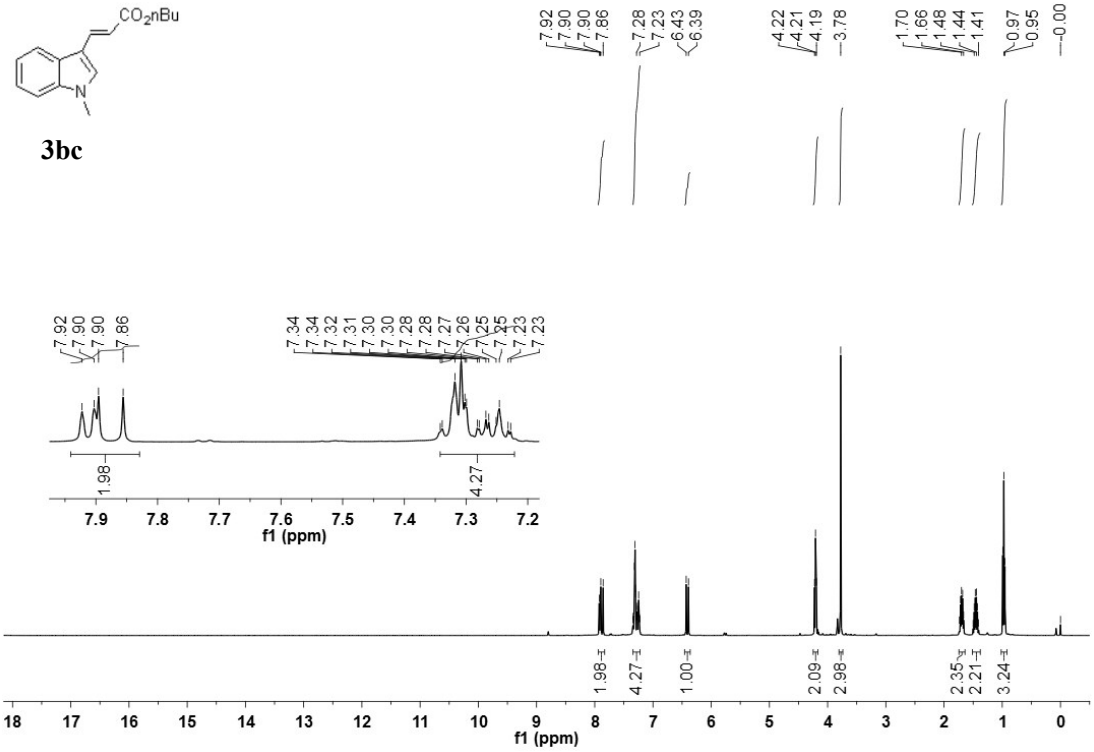
(*E*)-ethyl 3-(1-methyl-1*H*-indol-3-yl)acrylate (3bb): Yield 17%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.72 (t, *J* = 11.9 Hz, 2H), 7.36 – 7.20 (m, 4H), 6.40 (d, *J* = 15.9 Hz, 1H), 4.26 (q, *J* = 7.1 Hz, 2H), 3.74 (s, 3H), 1.34 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.37, 138.08, 138.00, 133.15, 126.05, 122.95, 121.27, 120.59, 112.59, 112.08, 109.97, 60.04, 33.13, 14.50.

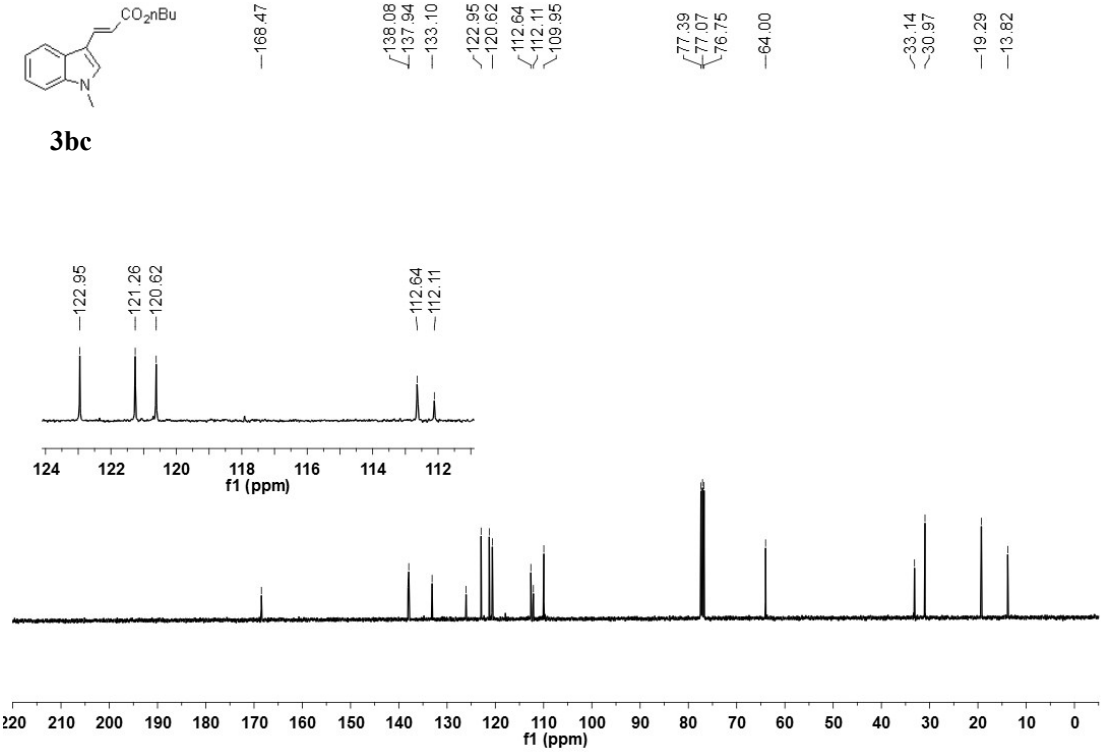


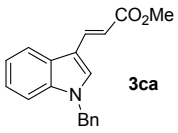




(*E*)-butyl 3-(1-methyl-1*H*-indol-3-yl)acrylate (3bc): Yield 21%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 – 7.83 (m, 2H), 7.34 – 7.22 (m, 4H), 6.41 (d, *J* = 15.9 Hz, 1H), 4.21 (t, *J* = 6.7 Hz, 2H), 3.78 (s, 3H), 1.70 (q, *J* = 6.8 Hz, 2H), 1.51 – 1.38 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.47, 138.08, 137.94, 133.10, 126.06, 122.95, 121.26, 120.62, 112.64, 112.11, 109.95, 64.00, 33.14, 30.97, 19.29, 13.82.

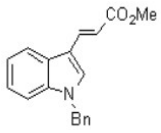






3ca

(*E*)-methyl 3-(1-benzyl-1*H*-indol-3-yl)acrylate (3ca): Yield 16%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.81 (m, 2H), 7.39 (s, 1H), 7.36 – 7.27 (m, 4H), 7.28 – 7.21 (m, 2H), 7.16 – 7.07 (m, 2H), 6.43 (d, *J* = 16.0 Hz, 1H), 5.30 (s, 2H), 3.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.65, 138.15, 137.67, 136.17, 132.44, 128.99, 128.09, 126.99, 126.33, 123.16, 121.50, 120.67, 112.63, 110.50, 51.39, 50.44.



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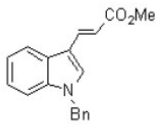

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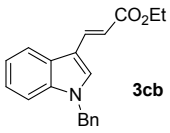
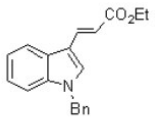


3cb

(*E*)-ethyl 3-(1-benzyl-1*H*-indol-3-yl)acrylate (3cb): Yield 21%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.83 (m, 2H), 7.37 (s, 1H), 7.33 – 7.27 (m, 4H), 7.26 – 7.22 (m, 2H), 7.18 – 7.04 (m, 2H), 6.43 (d, *J* = 16.0 Hz, 1H), 5.28 (s, 2H), 4.26 (d, *J* = 7.1 Hz, 2H), 1.34 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.23, 137.88, 137.67, 136.20, 132.38, 128.98, 128.08, 127.00, 126.34, 123.13, 121.46, 120.72, 113.13, 112.69, 110.48, 60.06, 50.42, 14.49.



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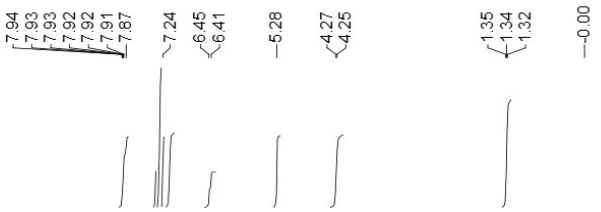
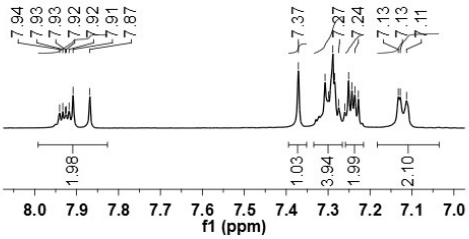
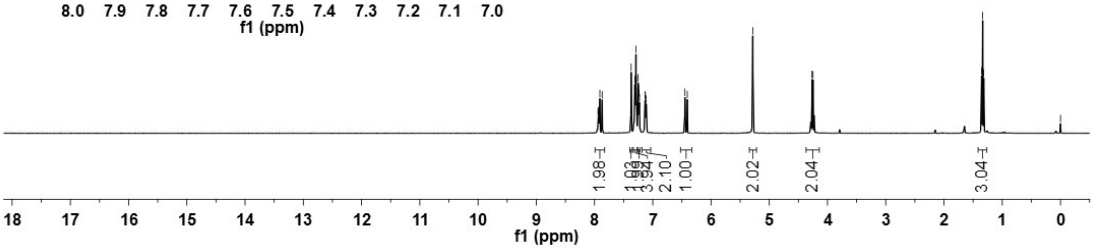
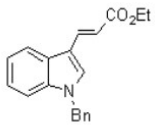
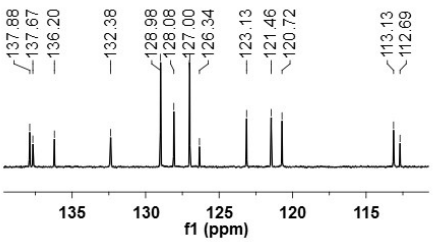


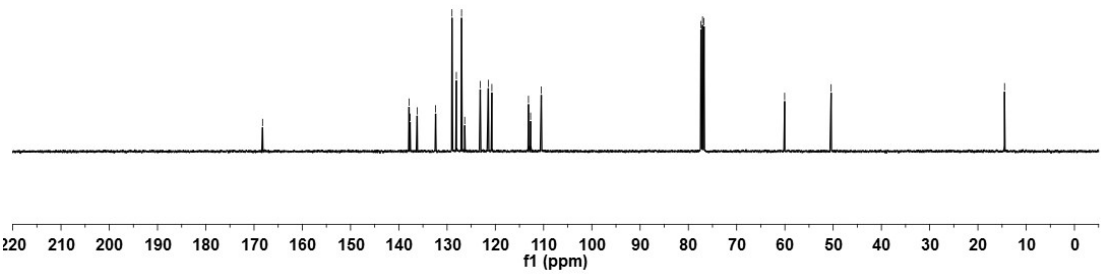


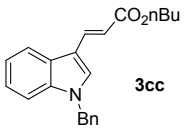




3cb

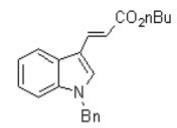




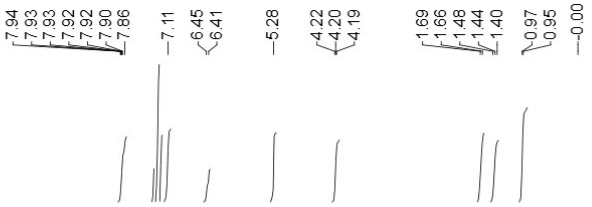


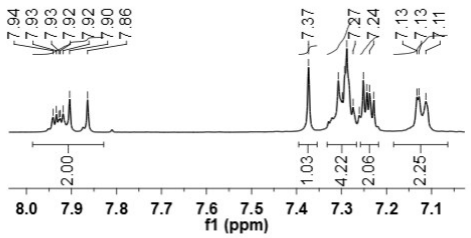
3cc

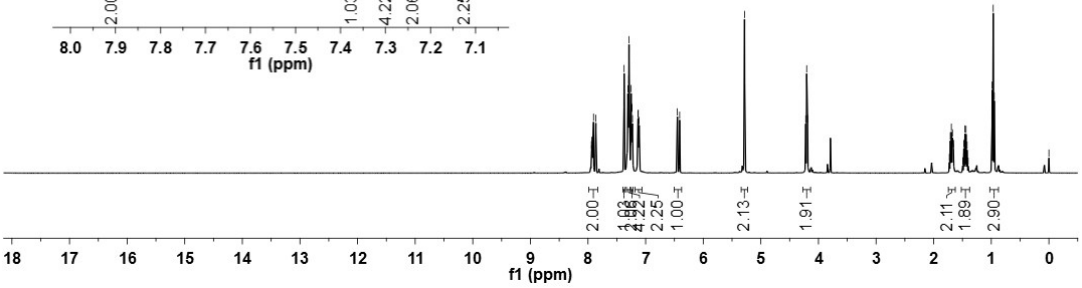
(*E*)-butyl 3-(1-benzyl-1*H*-indol-3-yl)acrylate (3cc): Yield 24%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.83 (m, 2H), 7.37 (s, 1H), 7.33 – 7.27 (m, 4H), 7.26 – 7.22 (m, 2H), 7.18 – 7.06 (m, 2H), 6.43 (d, *J* = 16.0 Hz, 1H), 5.28 (s, 2H), 4.20 (t, *J* = 6.7 Hz, 2H), 1.69 (q, *J* = 6.8 Hz, 2H), 1.52 – 1.38 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.34, 137.84, 137.67, 136.22, 132.36, 128.98, 128.08, 127.00, 126.34, 123.13, 121.45, 120.72, 113.15, 112.70, 110.48, 64.02, 50.42, 30.97, 19.29, 13.83. HRMS (ESI) m/z: calculated for $C_{22}H_{23}NO_2Na$ $[M+Na]^+$: 356.1626, found 356.1641.

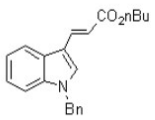


3cc

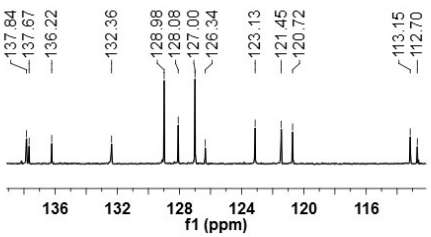


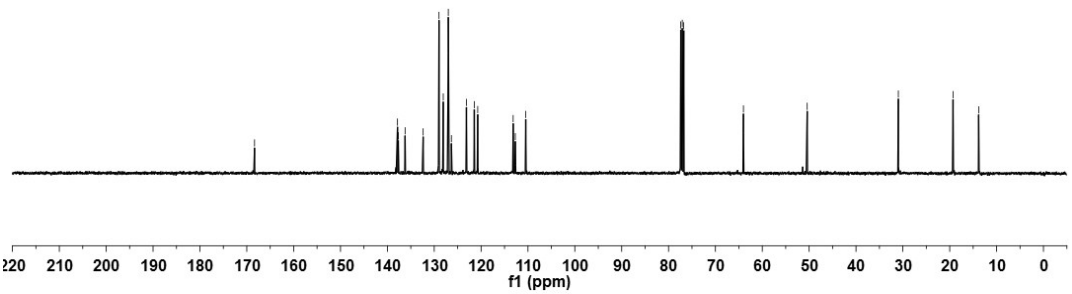


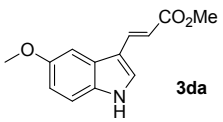




3cc

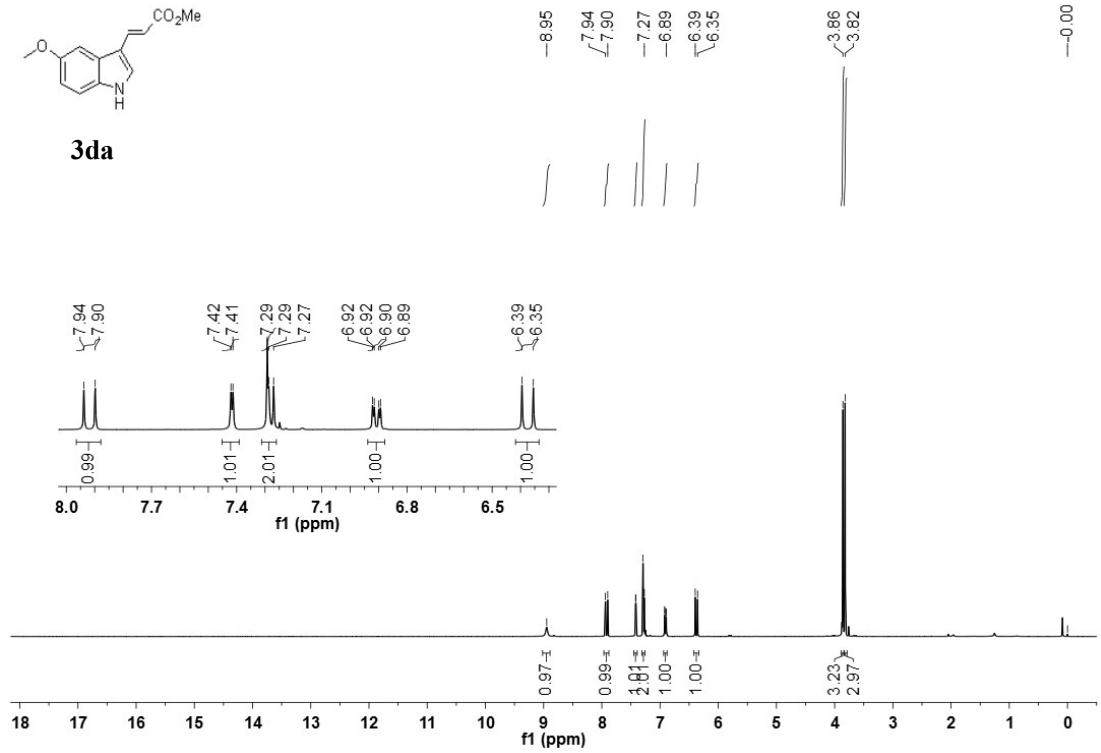


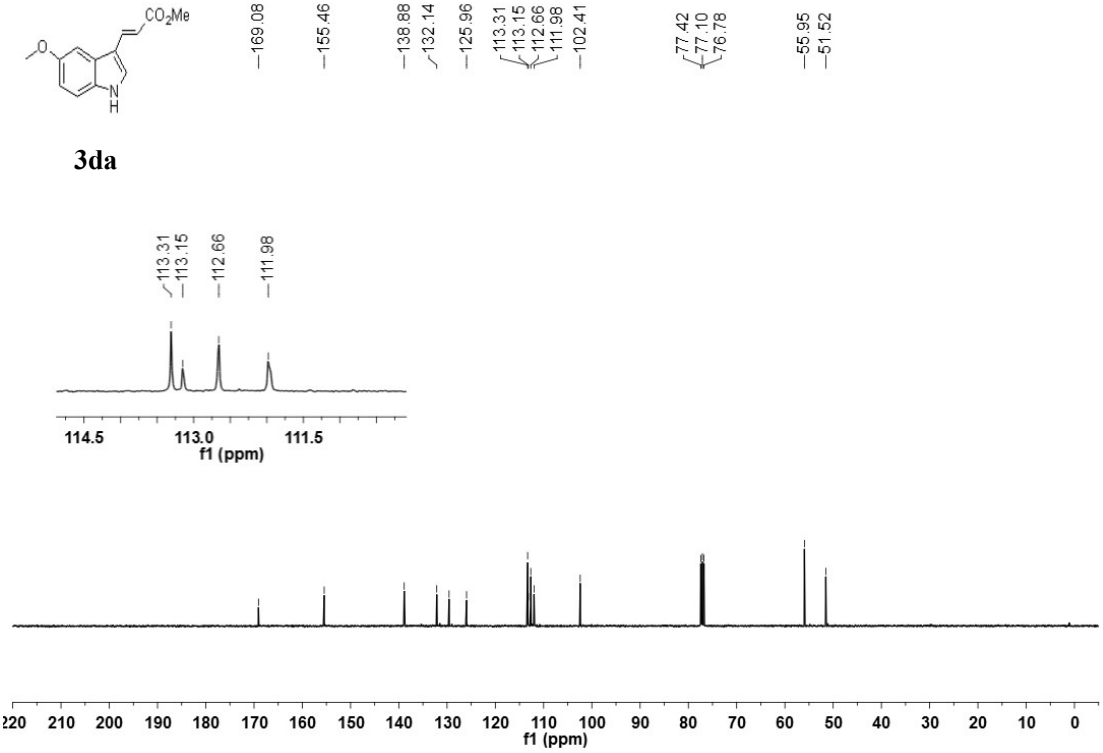


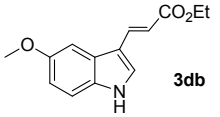


3da

(*E*)-methyl 3-(5-methoxy-1*H*-indol-3-yl)acrylate (3da): Yield 15%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (brs, 1H), 7.92 (d, J = 16.0 Hz, 1H), 7.42 (d, J = 2.8 Hz, 1H), 7.31 – 7.25 (m, 2H), 6.91 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 1H), 6.37 (d, J = 16.0 Hz, 1H), 3.86 (s, 3H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.08, 155.46, 138.88, 132.14, 129.59, 125.96, 113.31, 113.15, 112.66, 111.98, 102.41, 55.95, 51.52.

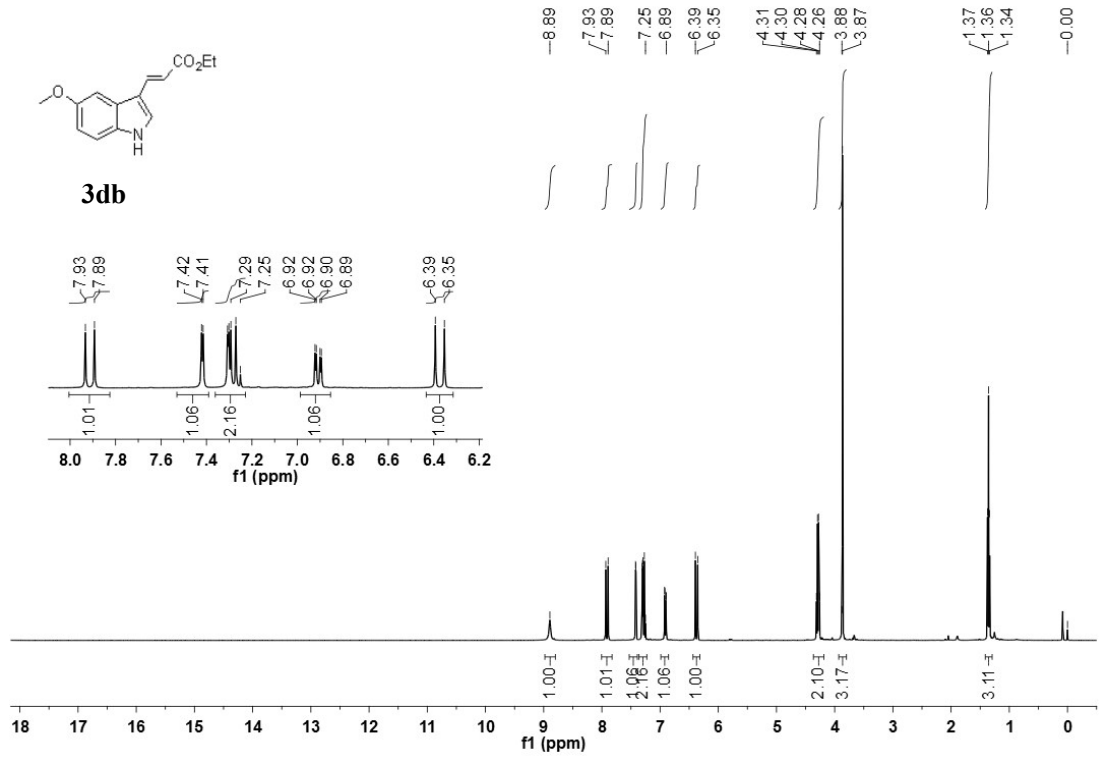


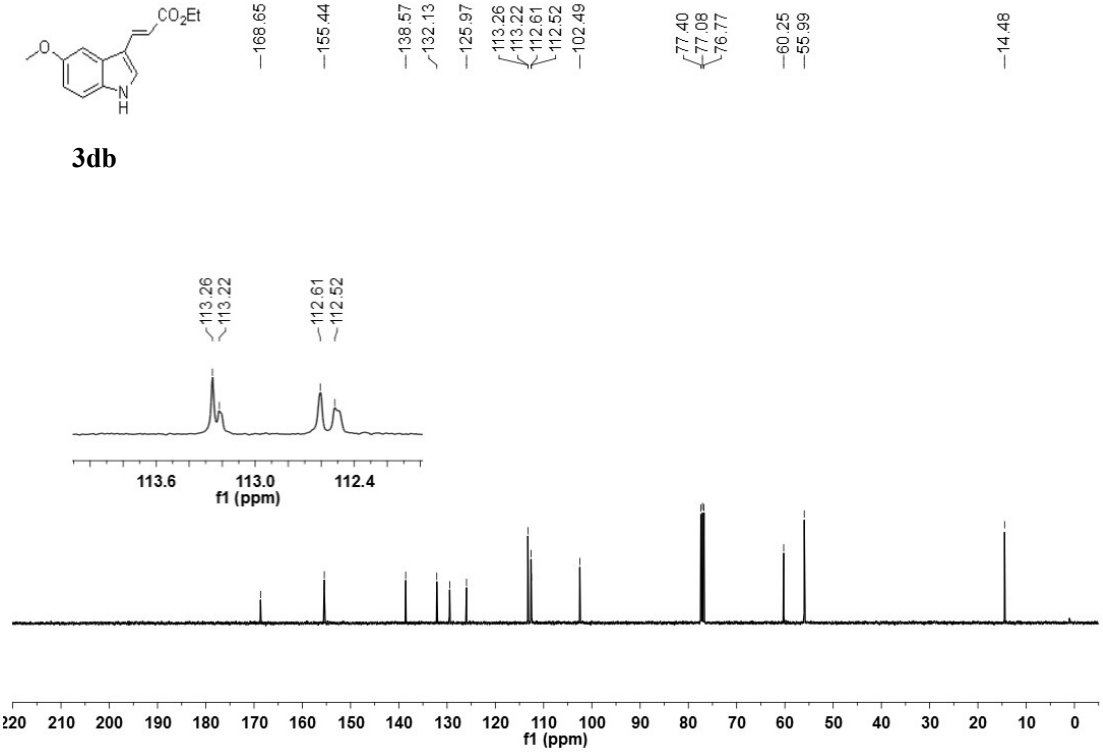


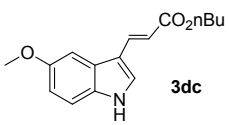


3db

(*E*)-ethyl 3-(5-methoxy-1*H*-indol-3-yl)acrylate (3db): Yield 10%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.89 (brs, 1H), 7.91 (d, J = 16.0 Hz, 1H), 7.42 (d, J = 2.8 Hz, 1H), 7.30 (d, J = 2.3 Hz, 1H), 7.28 (d, J = 8.8 Hz, 1H), 6.91 (dd, J_1 = 8.8, J_2 = 2.4 Hz, 1H), 6.37 (d, J = 16.0 Hz, 1H), 4.29 (q, J = 7.1 Hz, 2H), 3.87 (s, 3H), 1.36 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.65, 155.44, 138.57, 132.13, 129.46, 125.97, 113.26, 113.22, 112.61, 112.52, 102.49, 60.25, 55.99, 14.48.

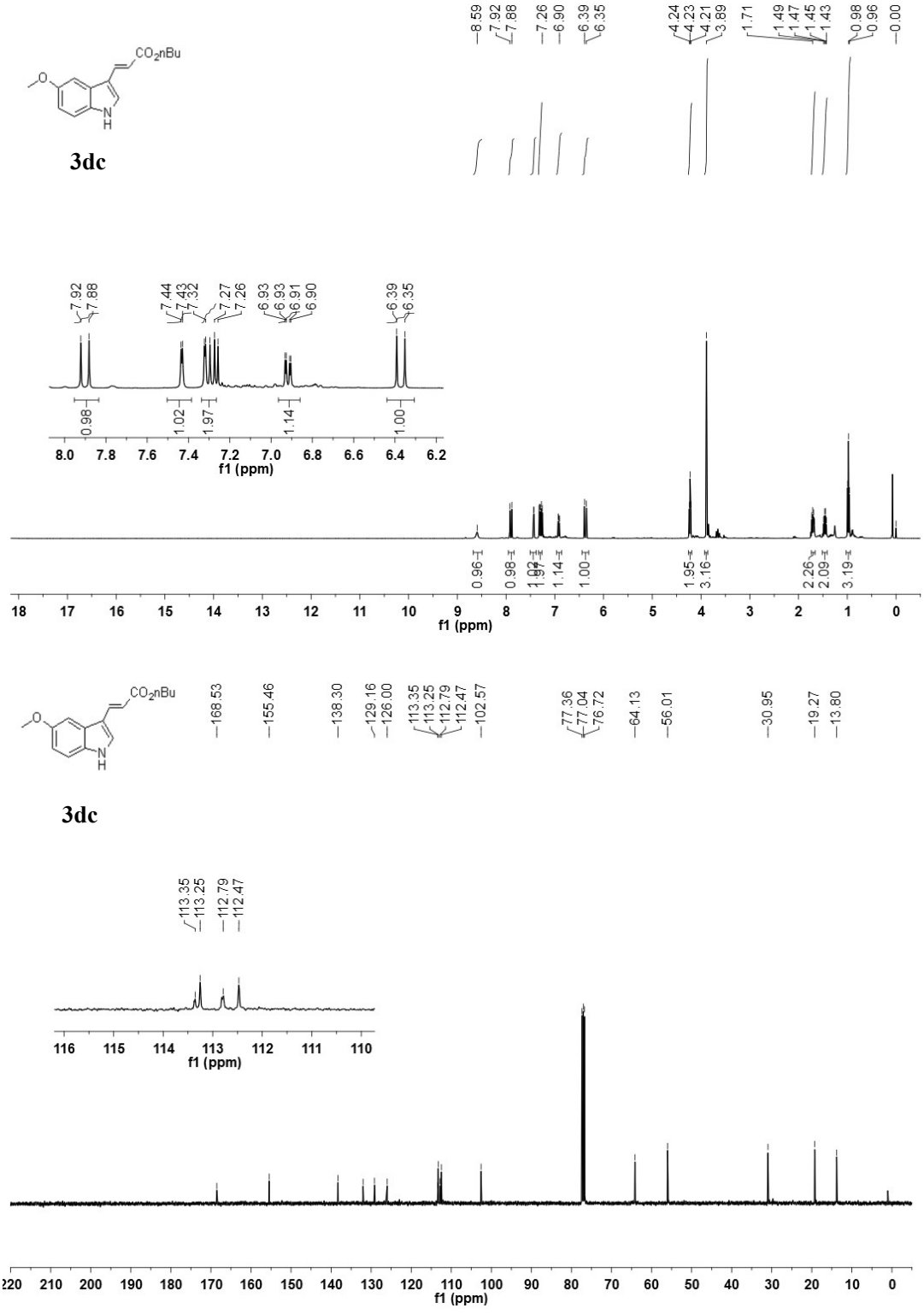


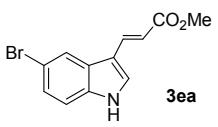




3dc

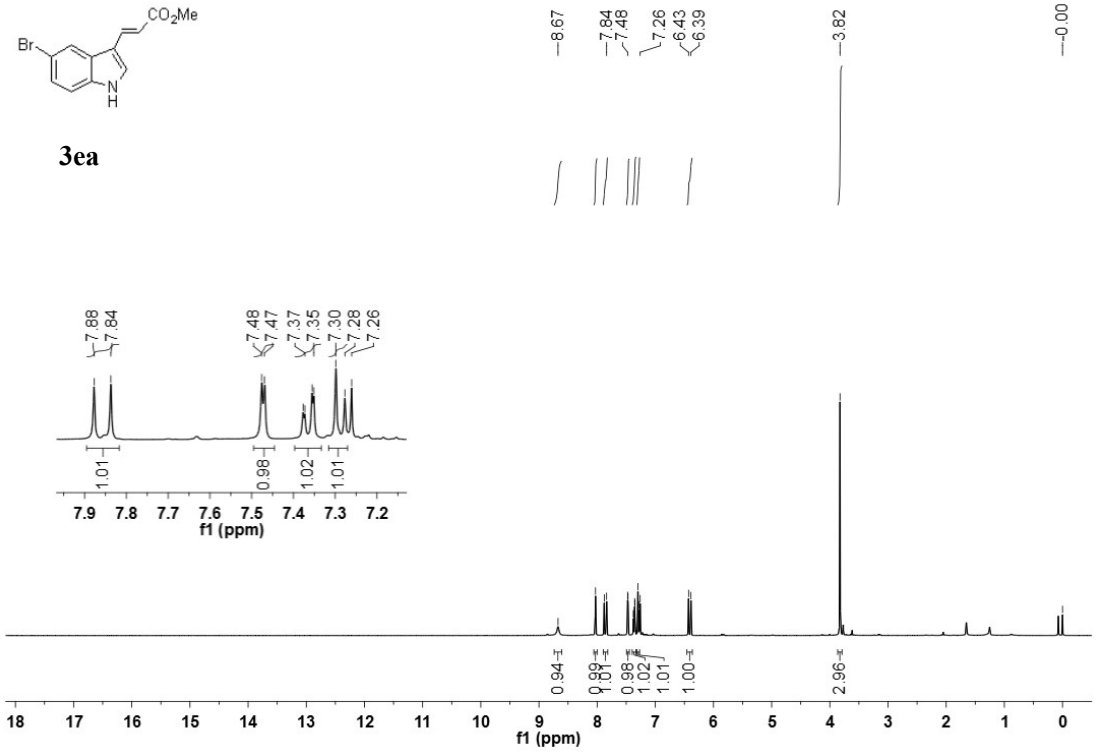
(*E*)-butyl 3-(5-methoxy-1*H*-indol-3-yl)acrylate (3dc): Yield 13%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (brs, 1H), 7.90 (d, J = 16.0 Hz, 1H), 7.43 (d, J = 2.8 Hz, 1H), 7.32 (d, J = 2.3 Hz, 1H), 7.28 (d, J = 8.8 Hz, 1H), 6.92 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 1H), 6.37 (d, J = 16.0 Hz, 1H), 4.23 (t, J = 6.7 Hz, 2H), 3.89 (s, 3H), 1.70 (q, J = 6.9 Hz, 2H), 1.52 – 1.39 (m, 2H), 0.98 (t, J = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.53, 155.46, 138.30, 132.02, 129.16, 126.00, 113.35, 113.25, 112.79, 112.47, 102.57, 64.13, 56.01, 30.95, 19.27, 13.80.

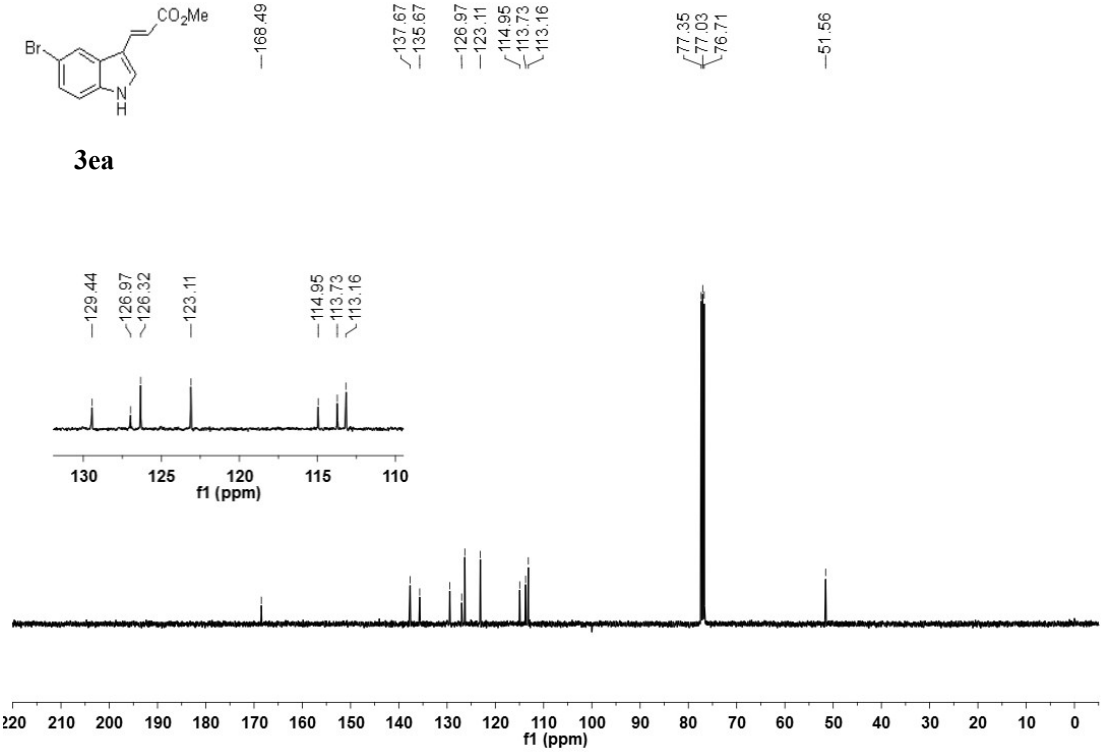


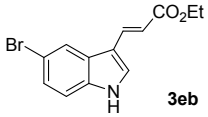


3ea

(*E*)-methyl 3-(5-bromo-1*H*-indol-3-yl)acrylate (3ea): Yield 10%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (brs, 1H), 8.03 (s, 1H), 7.86 (d, J = 16.0 Hz, 1H), 7.47 (d, J = 2.7 Hz, 1H), 7.36 (dd, J_1 = 8.6 Hz, J_2 = 1.7 Hz, 1H), 7.29 (d, J = 8.6 Hz, 1H), 6.41 (d, J = 16.0 Hz, 1H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.49, 137.67, 135.67, 129.44, 126.97, 126.32, 123.11, 114.95, 113.73, 113.16, 113.16, 51.56.

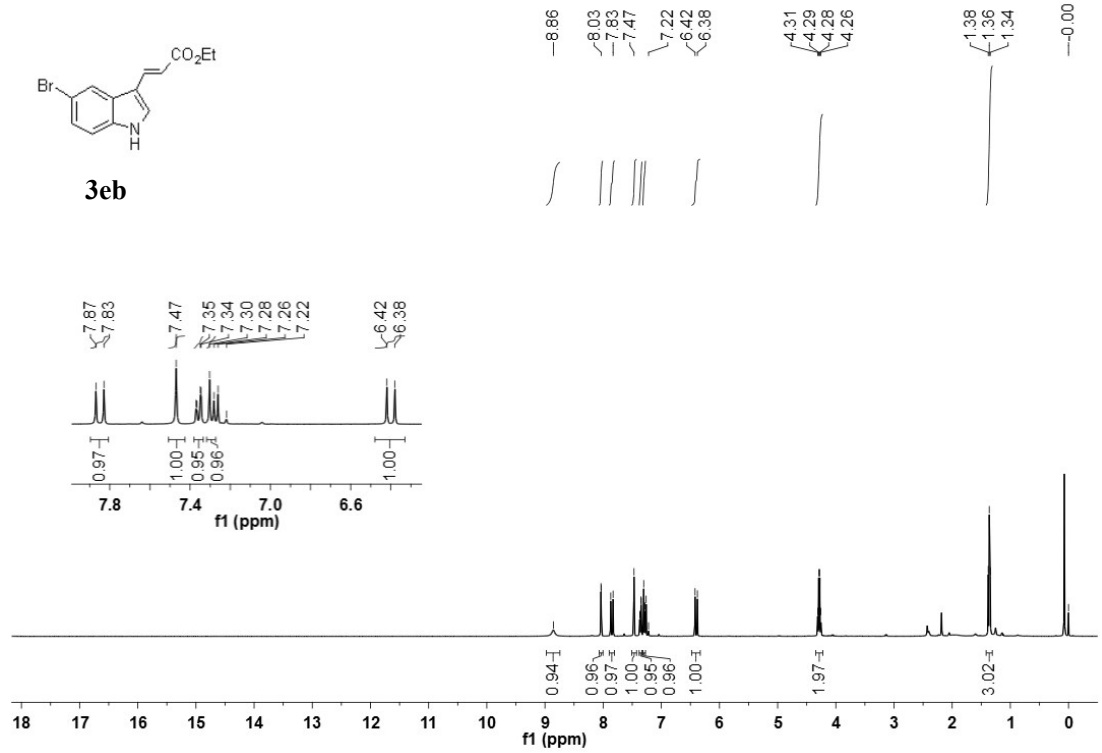


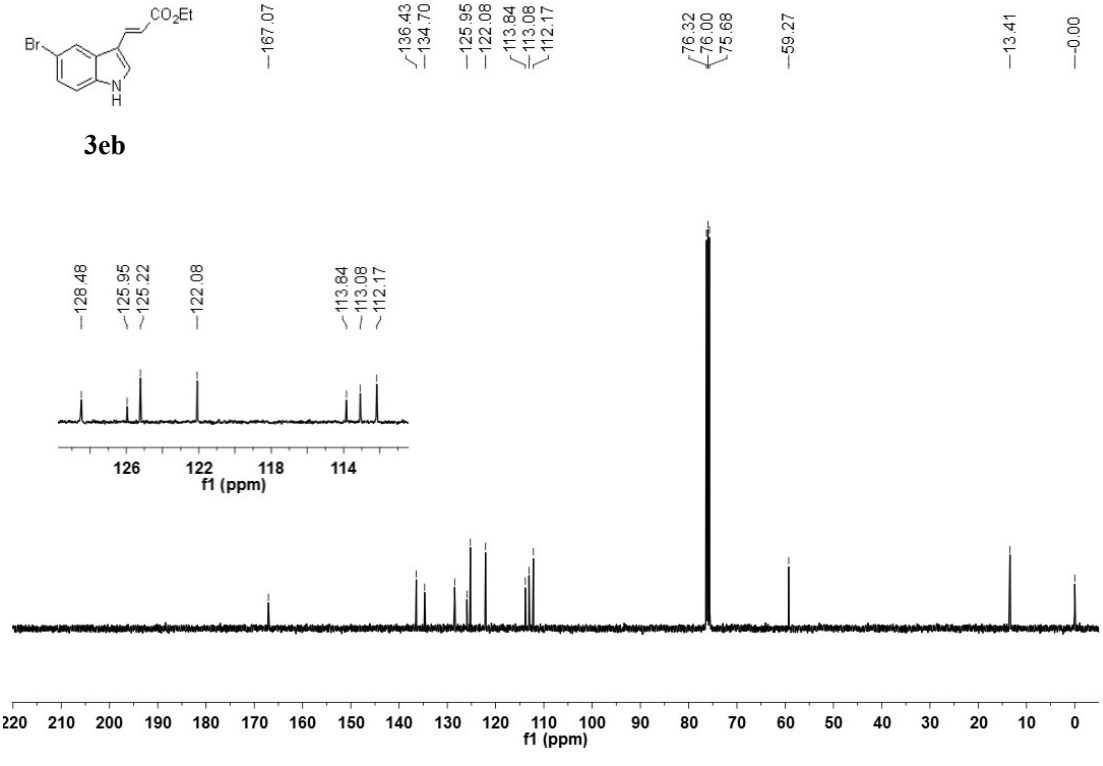


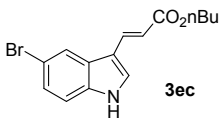


3eb

(*E*)-ethyl 3-(5-bromo-1*H*-indol-3-yl)acrylate (3eb): Yield 15%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86 (s, 1H), 8.04 (d, J = 1.4 Hz, 1H), 7.85 (d, J = 16.0 Hz, 1H), 7.47 (s, 1H), 7.36 (dd, J_1 = 8.6 Hz, J_2 = 1.6 Hz, 1H), 7.29 (d, J = 8.6 Hz, 1H), 6.40 (d, J = 16.0 Hz, 1H), 4.28 (q, J = 7.1 Hz, 2H), 1.36 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.07, 136.43, 134.70, 128.48, 125.95, 125.22, 122.08, 113.84, 113.08, 112.17, 112.15, 59.27, 13.41.

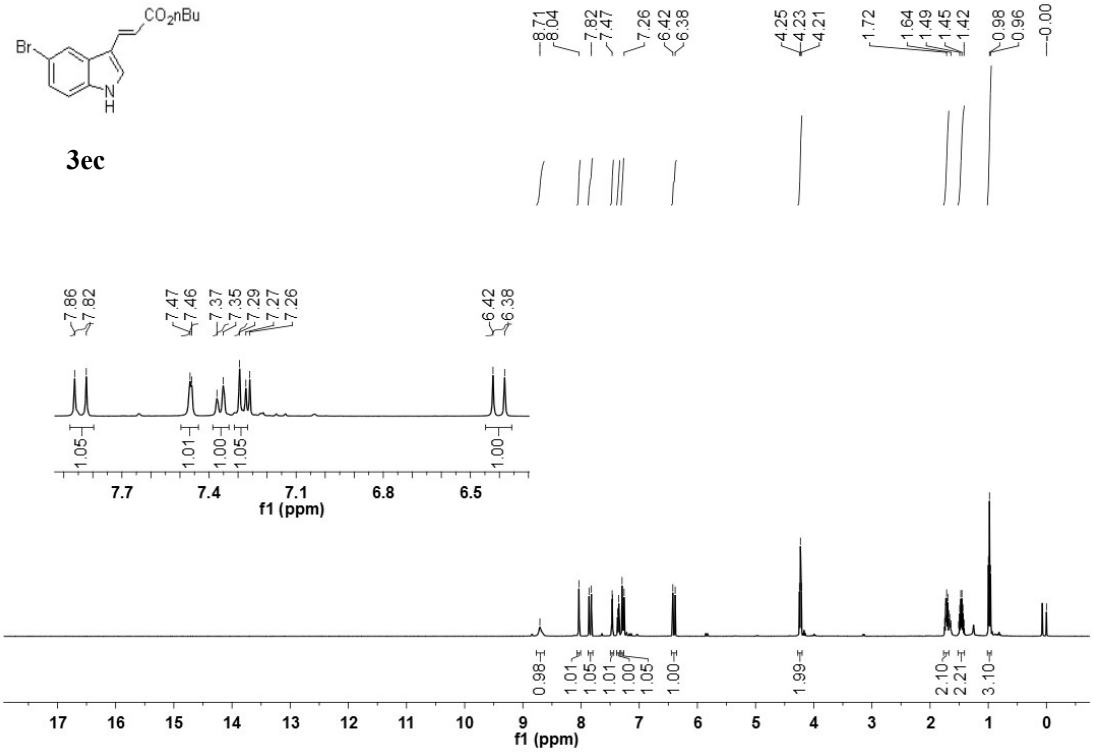


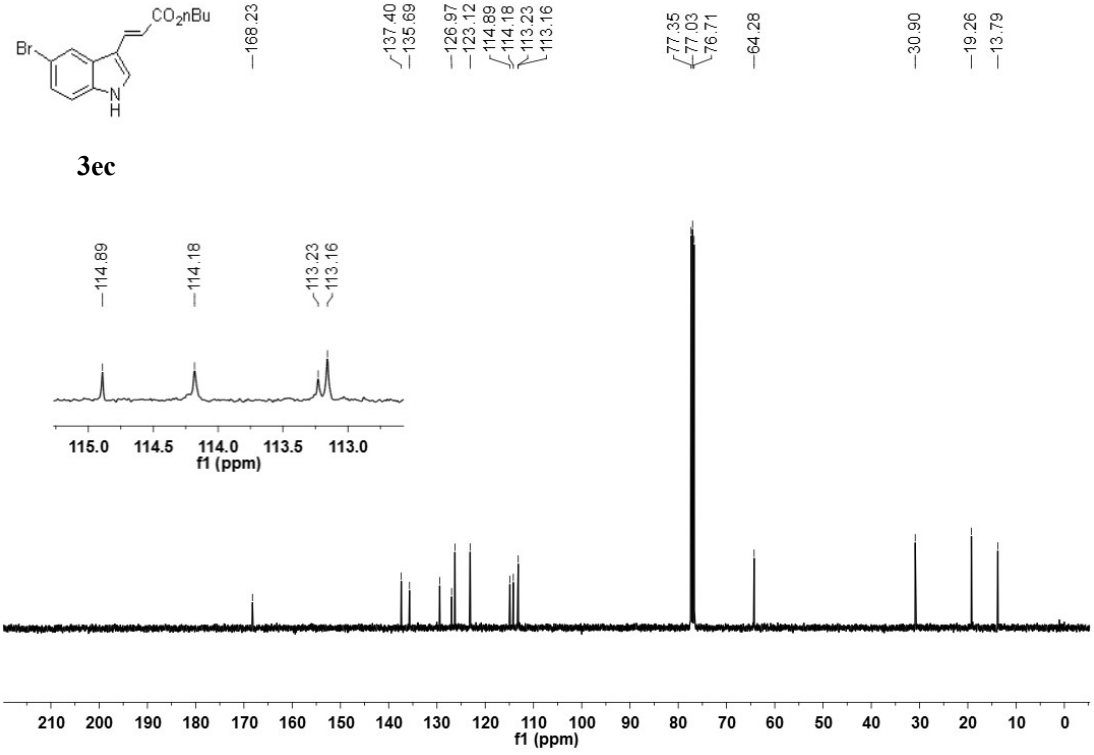


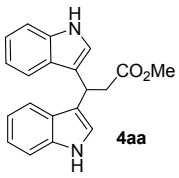


3ec

(*E*)-butyl 3-(5-bromo-1*H*-indol-3-yl)acrylate (3ec): Yield 10%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (s, 1H), 8.04 (s, 1H), 7.84 (d, *J* = 16.0 Hz, 1H), 7.46 (d, *J* = 2.4 Hz, 1H), 7.36 (d, *J* = 8.6 Hz, 1H), 7.28 (d, *J* = 8.6 Hz, 1H), 6.40 (d, *J* = 16.0 Hz, 1H), 4.23 (t, *J* = 6.7 Hz, 2H), 1.72 (q, *J* = 6.8 Hz, 2H), 1.52 – 1.39 (m, 2H), 0.98 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.23, 137.40, 135.69, 129.43, 126.97, 126.28, 123.12, 114.89, 114.18, 113.23, 113.16, 64.28, 30.90, 19.26, 13.79.

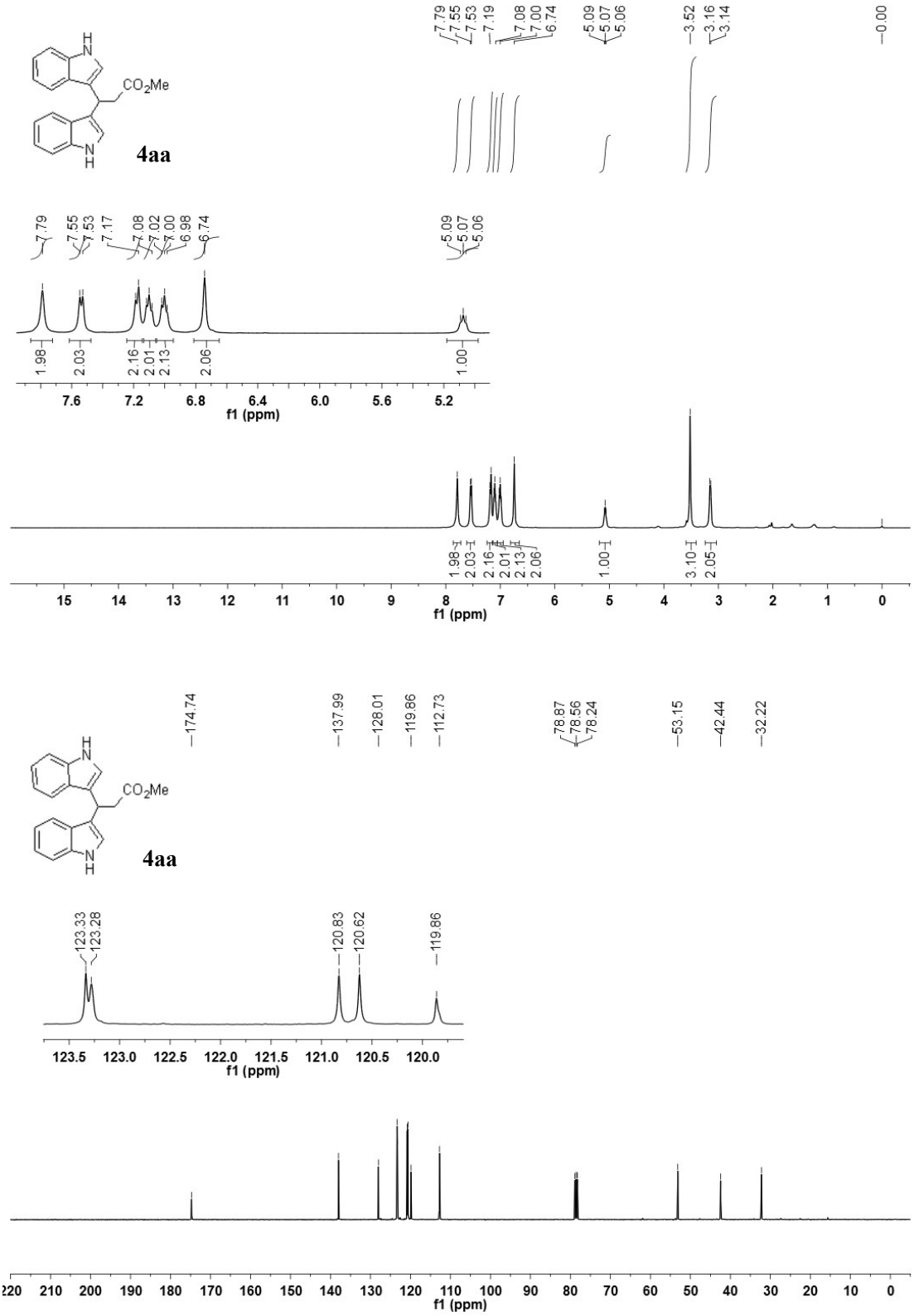


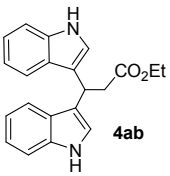




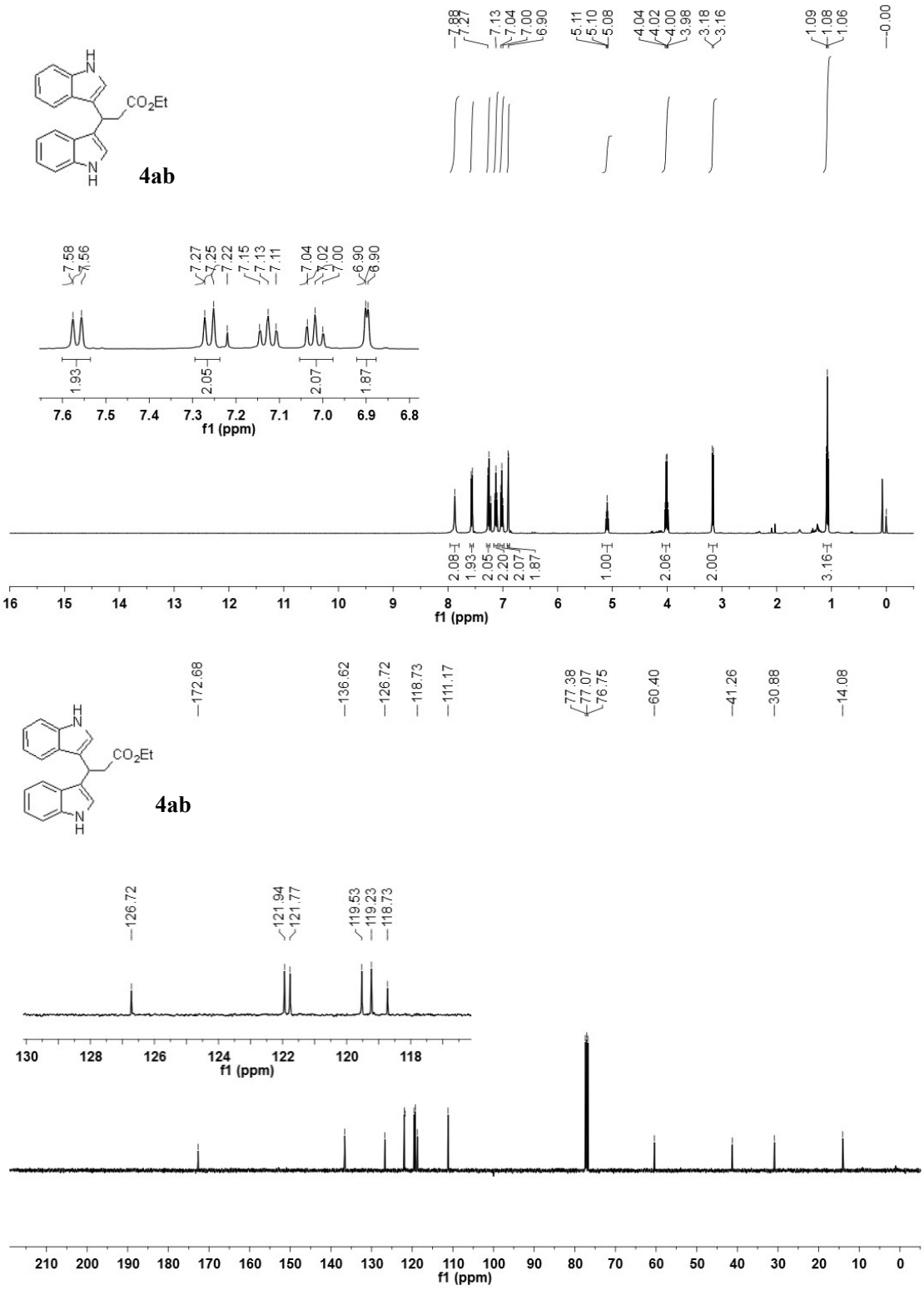
4aa

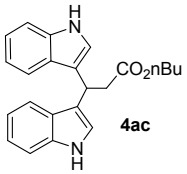
methyl 3,3-di(1*H*-indol-3-yl)propanoate (4aa): Yield 63%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (s, 2H), 7.54 (d, *J* = 7.5 Hz, 2H), 7.18 (d, *J* = 7.6 Hz, 2H), 7.10 (t, *J* = 7.0 Hz, 2H), 7.00 (t, *J* = 6.9 Hz, 2H), 6.74 (s, 2H), 5.07 (t, *J* = 6.9 Hz, 1H), 3.52 (s, 3H), 3.15 (d, *J* = 7.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.74, 137.99, 128.01, 123.33, 123.28, 120.83, 120.62, 119.86, 112.73, 53.15, 42.44, 32.22.



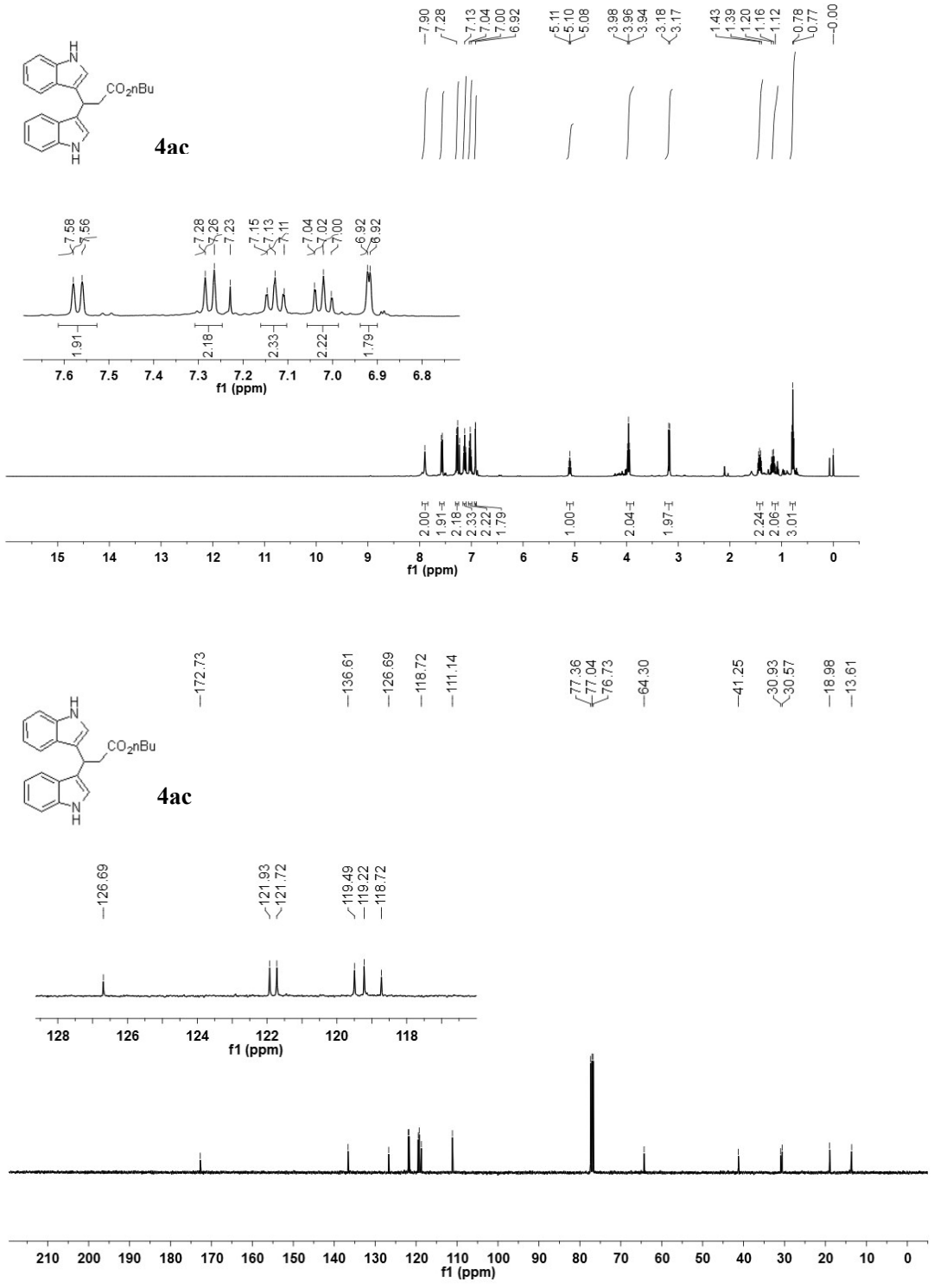


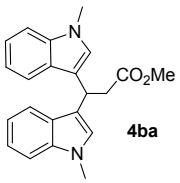
ethyl 3,3-di(1*H*-indol-3-yl)propanoate (4ab): Yield 70%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (s, 2H), 7.57 (d, *J* = 7.9 Hz, 2H), 7.26 (d, *J* = 8.1 Hz, 2H), 7.13 (t, *J* = 7.6 Hz, 2H), 7.02 (t, *J* = 7.1 Hz, 2H), 6.90 (d, *J* = 2.2 Hz, 2H), 5.10 (t, *J* = 7.7 Hz, 1H), 4.01 (q, *J* = 7.1 Hz, 2H), 3.17 (d, *J* = 7.7 Hz, 2H), 1.08 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.68, 136.62, 126.72, 121.94, 121.77, 119.53, 119.23, 118.73, 111.17, 60.40, 41.26, 30.88, 14.08.



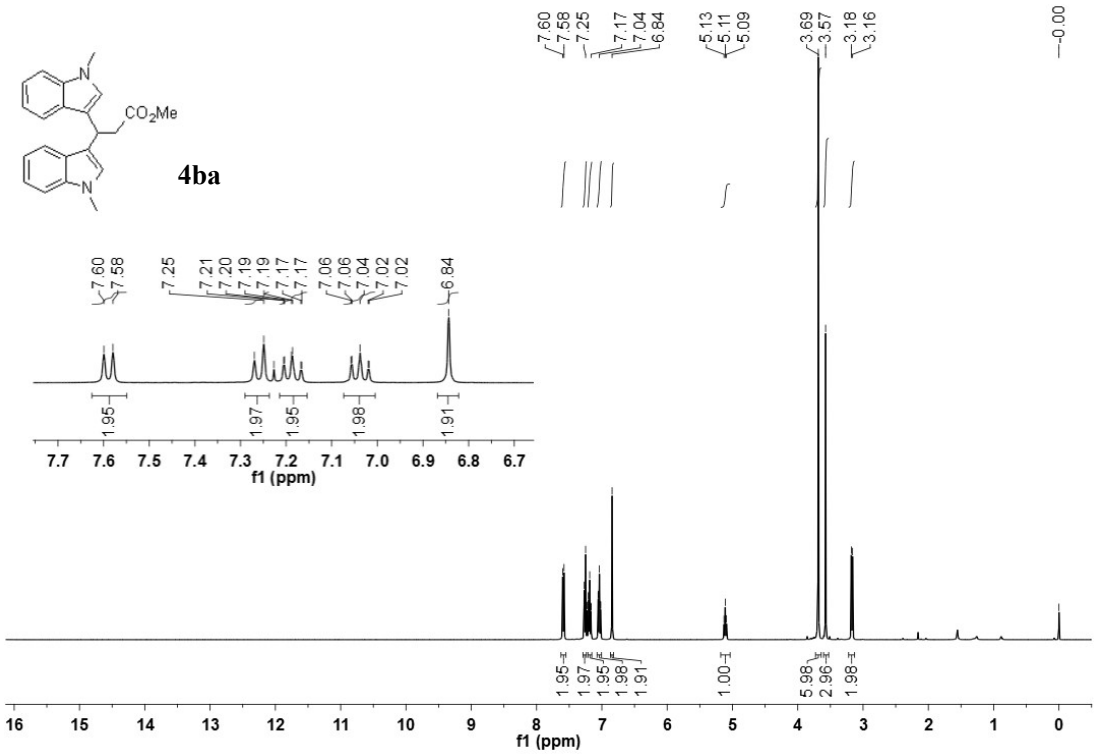


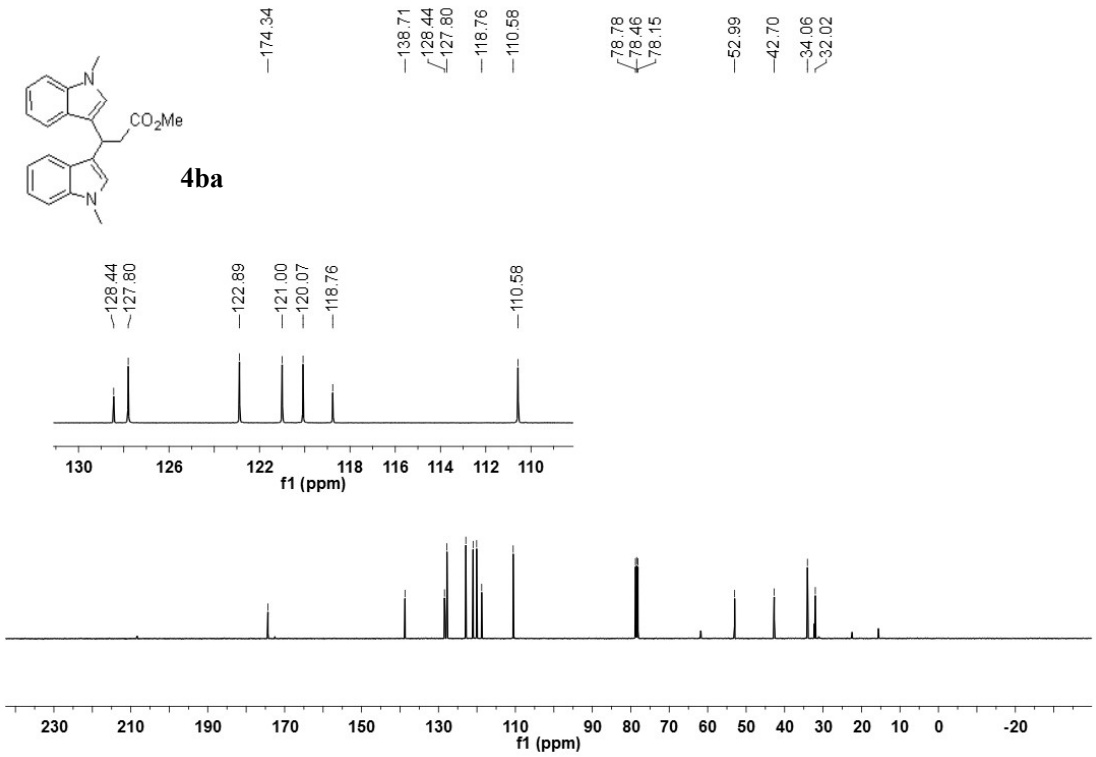
butyl 3,3-di(1*H*-indol-3-yl)propanoate (4ac): Yield 74%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (s, 2H), 7.57 (d, *J* = 7.9 Hz, 2H), 7.27 (d, *J* = 8.1 Hz, 2H), 7.13 (t, *J* = 7.6 Hz, 2H), 7.02 (t, *J* = 7.5 Hz, 2H), 6.92 (d, *J* = 2.2 Hz, 2H), 5.10 (t, *J* = 7.7 Hz, 1H), 3.96 (t, *J* = 6.6 Hz, 2H), 3.17 (d, *J* = 7.7 Hz, 2H), 1.43 (q, *J* = 6.7 Hz, 2H), 1.12 – 1.22 (m, 2H), 0.78 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.73, 136.61, 126.69, 121.93, 121.72, 119.49, 119.22, 118.72, 111.14, 64.30, 41.25, 30.93, 30.57, 18.98, 13.61. HRMS (ESI) m/z: calculated for $C_{23}H_{24}N_2O_2Na$ $[M+Na]^+$: 383.1735, found 383.1769.

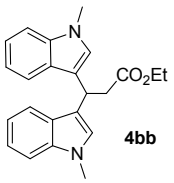




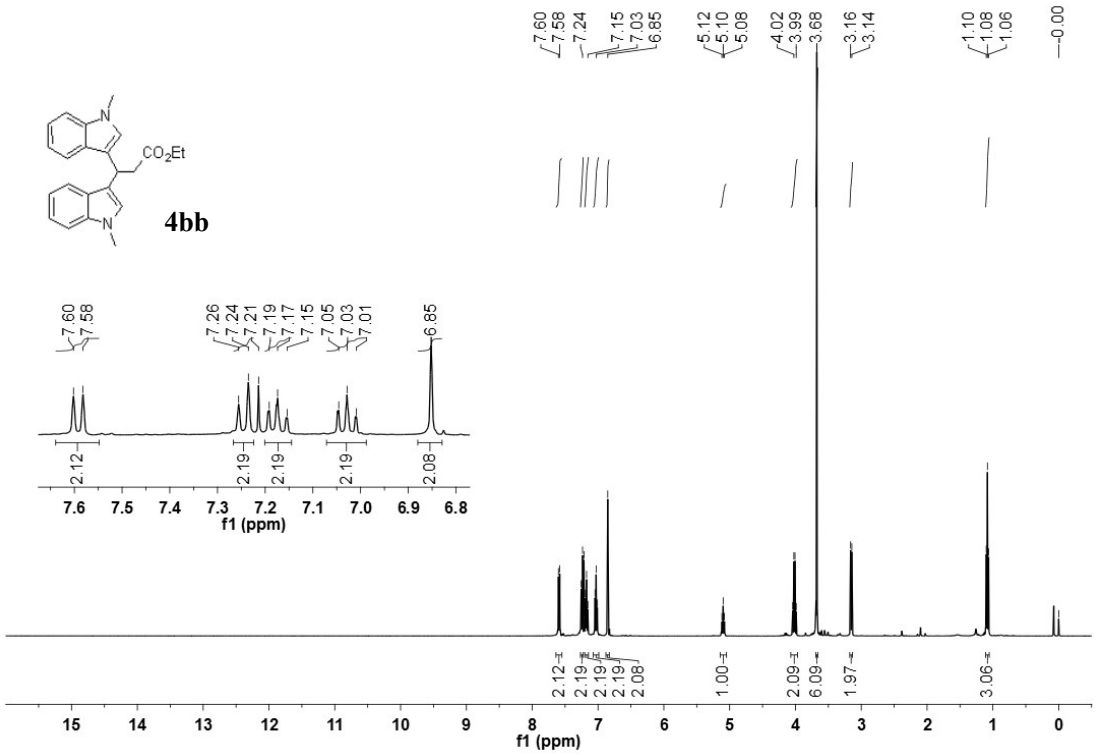
methyl 3,3-bis(1-methyl-1*H*-indol-3-yl)propanoate (4ba): Yield 77%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, J = 7.9 Hz, 2H), 7.26 (d, J = 8.2 Hz, 2H), 7.19 (td, J_1 = 7.0 Hz, J_2 = 0.9 Hz, 2H), 7.04 (td, J_1 = 7.0 Hz, J_2 = 0.9 Hz, 2H), 6.84 (s, 2H), 5.11 (t, J = 7.7 Hz, 1H), 3.69 (s, 6H), 3.57 (s, 3H), 3.17 (d, J = 7.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.34, 138.71, 128.44, 127.80, 122.89, 121.00, 120.07, 118.76, 110.58, 52.99, 42.70, 34.06, 32.02.

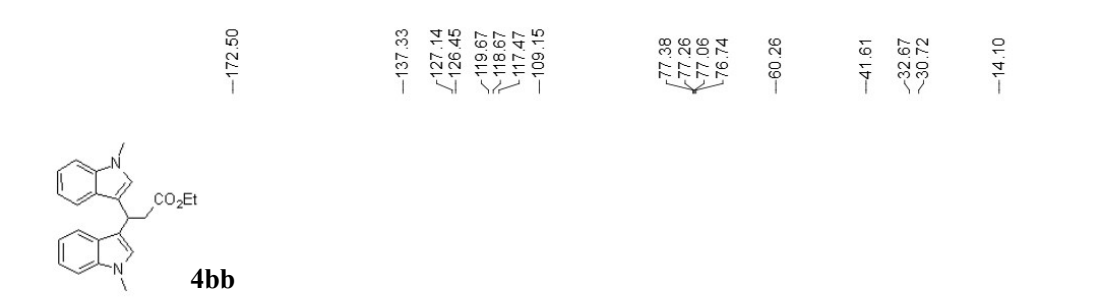


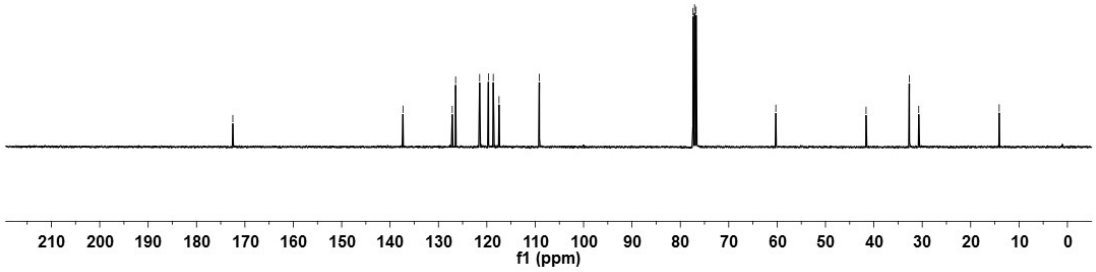


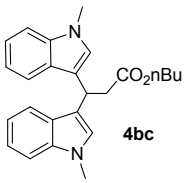


ethyl 3,3-bis(1-methyl-1*H*-indol-3-yl)propanoate (4bb): Yield 71%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.9 Hz, 2H), 7.25 (d, *J* = 8.2 Hz, 2H), 7.17 (t, *J* = 7.6 Hz, 2H), 7.03 (t, *J* = 7.4 Hz, 2H), 6.85 (s, 2H), 5.10 (t, *J* = 7.7 Hz, 1H), 4.02 (q, *J* = 7.1 Hz, 2H), 3.68 (s, 6H), 3.15 (d, *J* = 7.7 Hz, 2H), 1.08 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.50, 137.33 , 127.14, 126.45, 121.48, 119.67, 118.67, 117.47, 109.15, 60.26, 41.61, 32.67, 30.72, 14.10.

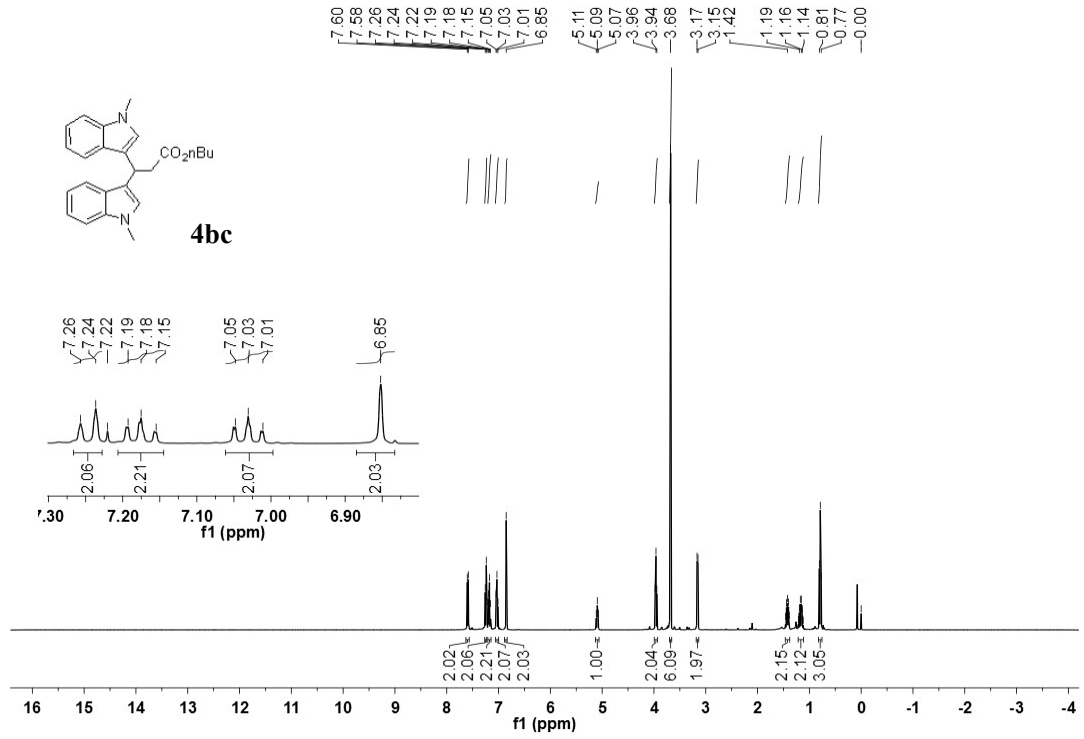


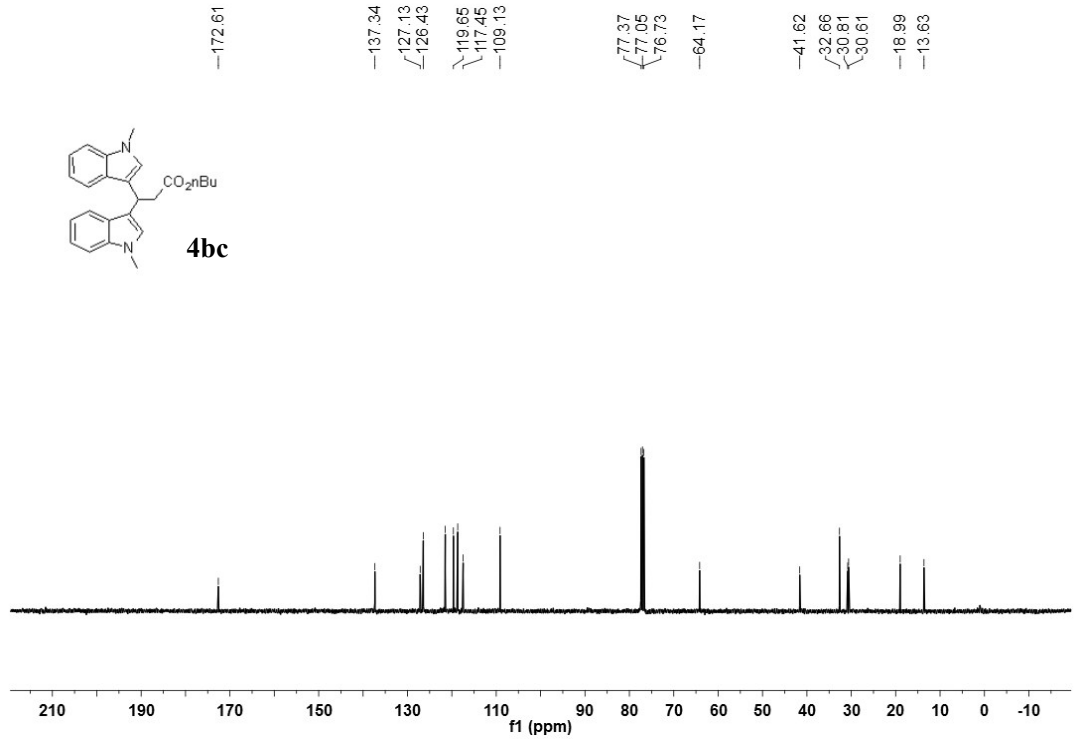


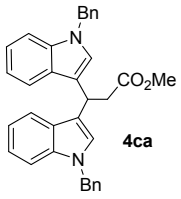




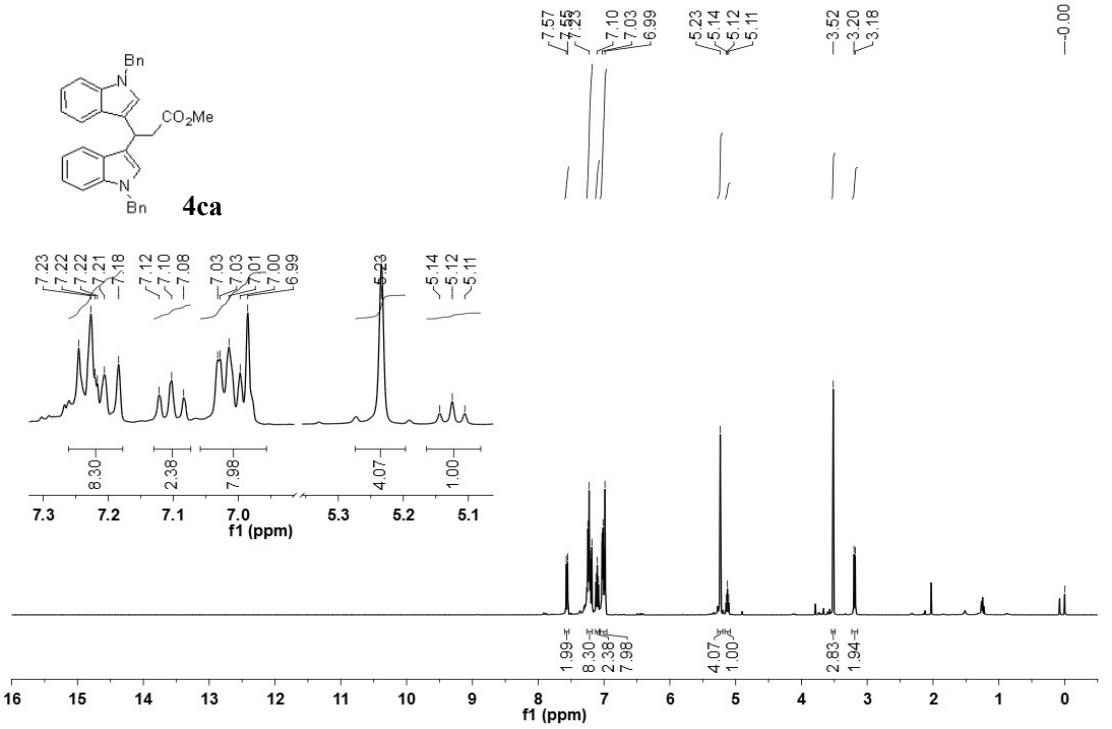
butyl 3,3-bis(1-methyl-1*H*-indol-3-yl)propanoate (4bc): Yield 73%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.9 Hz, 2H), 7.25 (d, *J* = 8.2 Hz, 2H), 7.17 (t, *J* = 7.6 Hz, 2H), 7.03 (t, *J* = 7.4 Hz, 2H), 6.85, 5.09 (t, *J* = 7.7 Hz, 1H), 3.96 (t, *J* = 6.6 Hz, 2H), 3.68 (s, 6H), 3.16 (d, *J* = 7.7 Hz, 2H), 1.42 (q, *J* = 6.7 Hz, 2H), 1.22 – 1.11 (m, 2H), 0.79 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.61, 137.34, 127.13, 126.43, 121.48, 119.65, 118.68, 117.45, 109.13, 64.17, 41.62, 32.66, 30.81, 30.61, 18.99, 13.63. HRMS (ESI) m/z: calculated for $C_{25}H_{28}N_2O_2Na$ $[M+Na]^+$: 411.2048, found 411.2046.

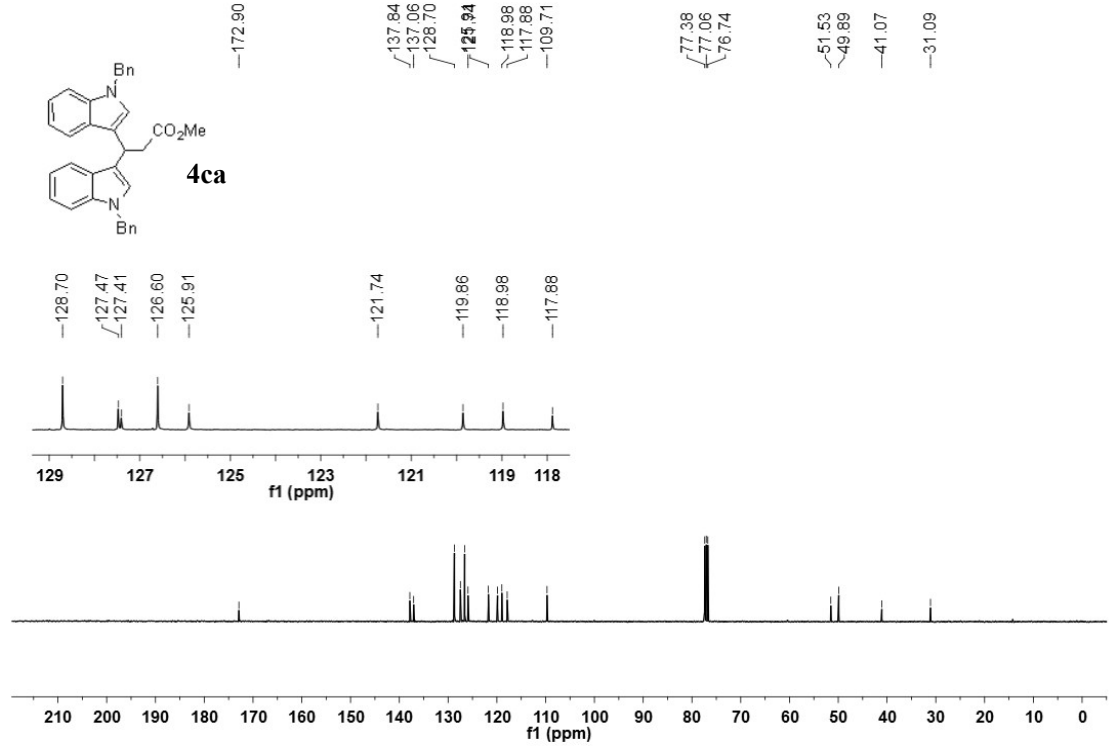


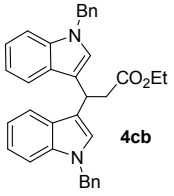




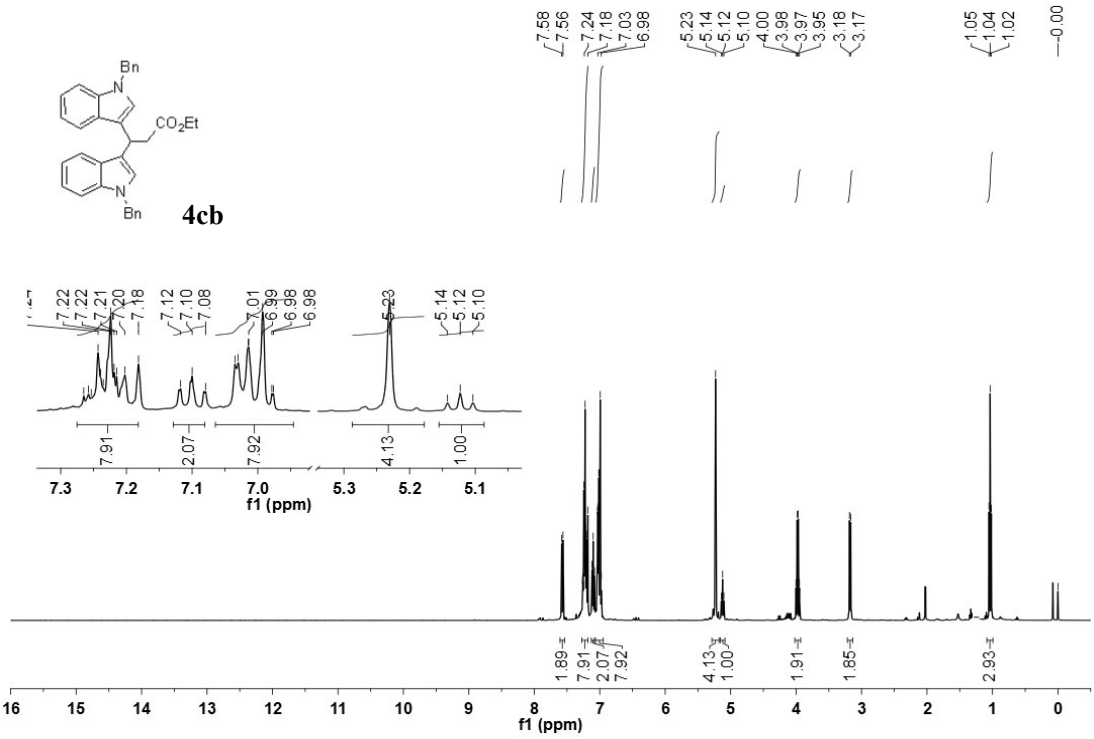
methyl 3,3-bis(1-benzyl-1*H*-indol-3-yl)propanoate (4ca): Yield 68%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.9 Hz, 2H), 7.31 – 7.17 (m, 8H), 7.10 (t, *J* = 7.6 Hz, 2H), 7.05 – 6.96 (m, 8H), 5.23 (s, 4H), 5.12 (t, *J* = 7.7 Hz, 1H), 3.52 (s, 3H), 3.19 (d, *J* = 7.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.90, 137.84, 137.06, 128.70, 127.47, 127.41, 126.60, 125.91, 121.74, 119.86, 118.98, 117.88, 109.71, 51.53, 49.89, 41.07, 31.09. HRMS (ESI) m/z: calculated for $C_{34}H_{30}N_2O_2$ $[M+Na]^+$: 498.2305, found 498.2347.

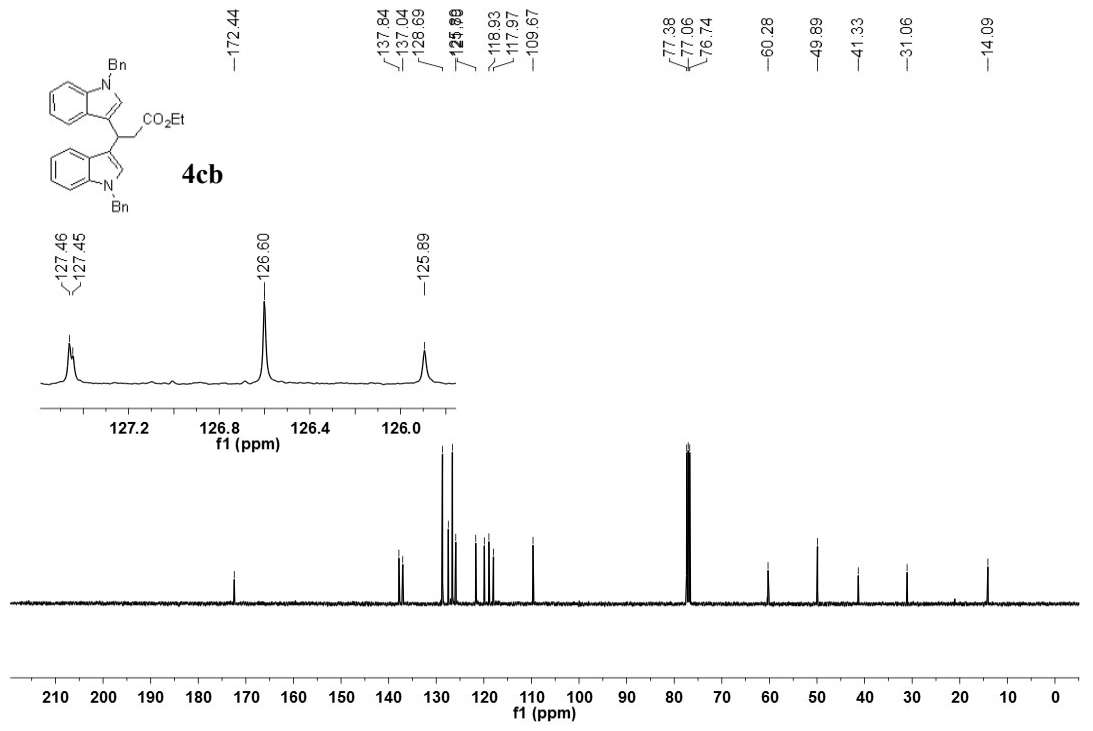


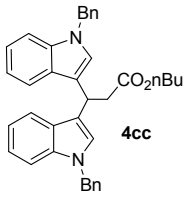




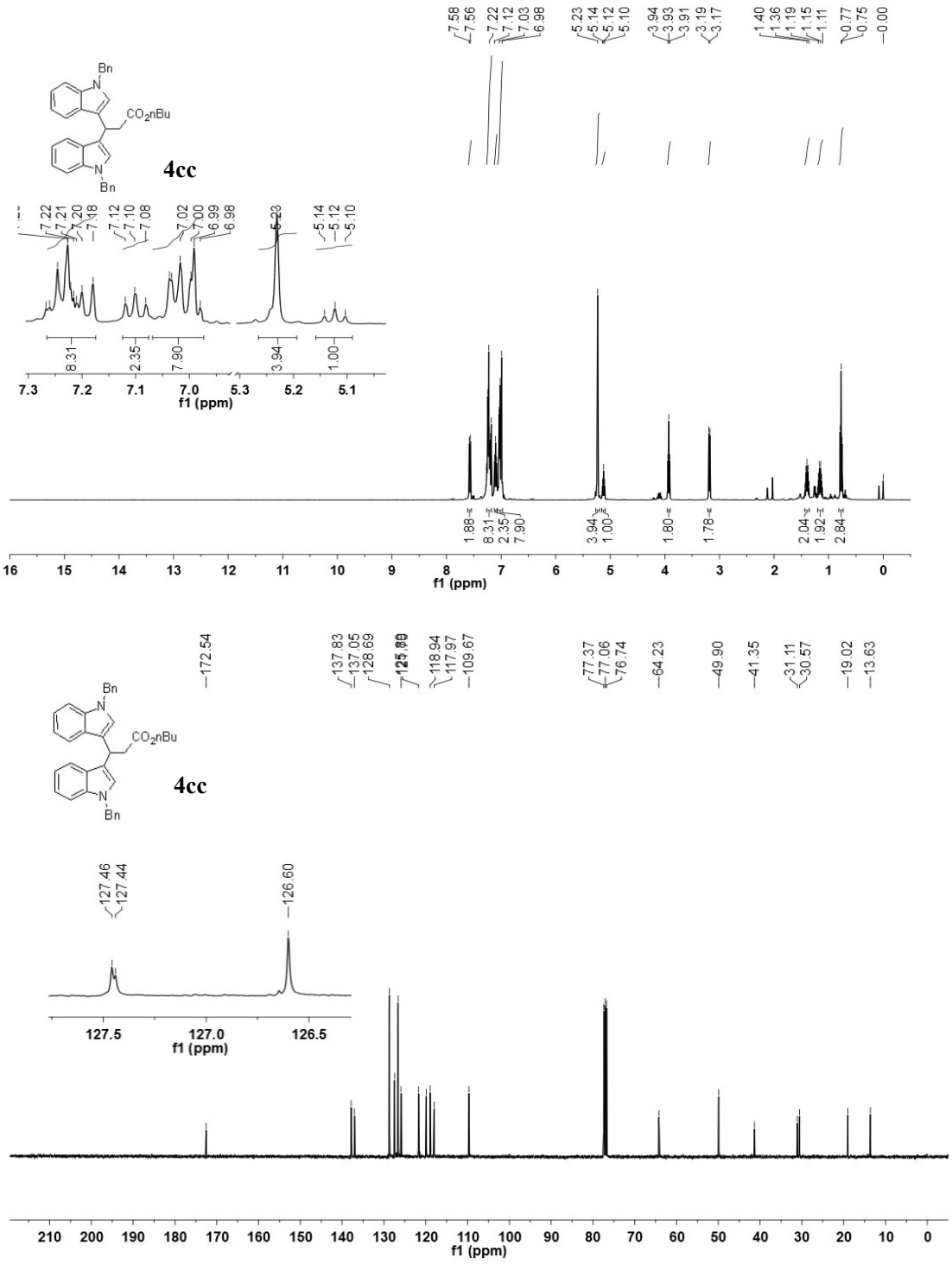
ethyl 3,3-bis(1-benzyl-1*H*-indol-3-yl)propanoate (4cb): Yield 69%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.9 Hz, 2H), 7.27 – 7.17 (m, 8H), 7.10 (t, *J* = 7.6 Hz, 2H), 7.06 – 6.95 (m, 8H), 5.23 (s, 4H), 5.12 (t, *J* = 7.7 Hz, 1H), 3.98 (q, *J* = 7.1 Hz, 2H), 3.18 (d, *J* = 7.7 Hz, 2H), 1.04 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.44, 137.84, 137.04, 128.69, 127.46, 127.45, 126.60, 125.89, 121.70, 119.89, 118.93, 117.97, 109.67, 60.28, 49.89, 41.33, 31.06, 14.09. HRMS (ESI) m/z: calculated for $C_{35}H_{32}N_2O_2Na$ $[M+Na]^+$: 535.2361, found 535.2404.

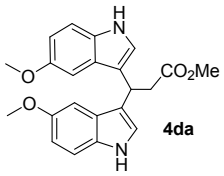




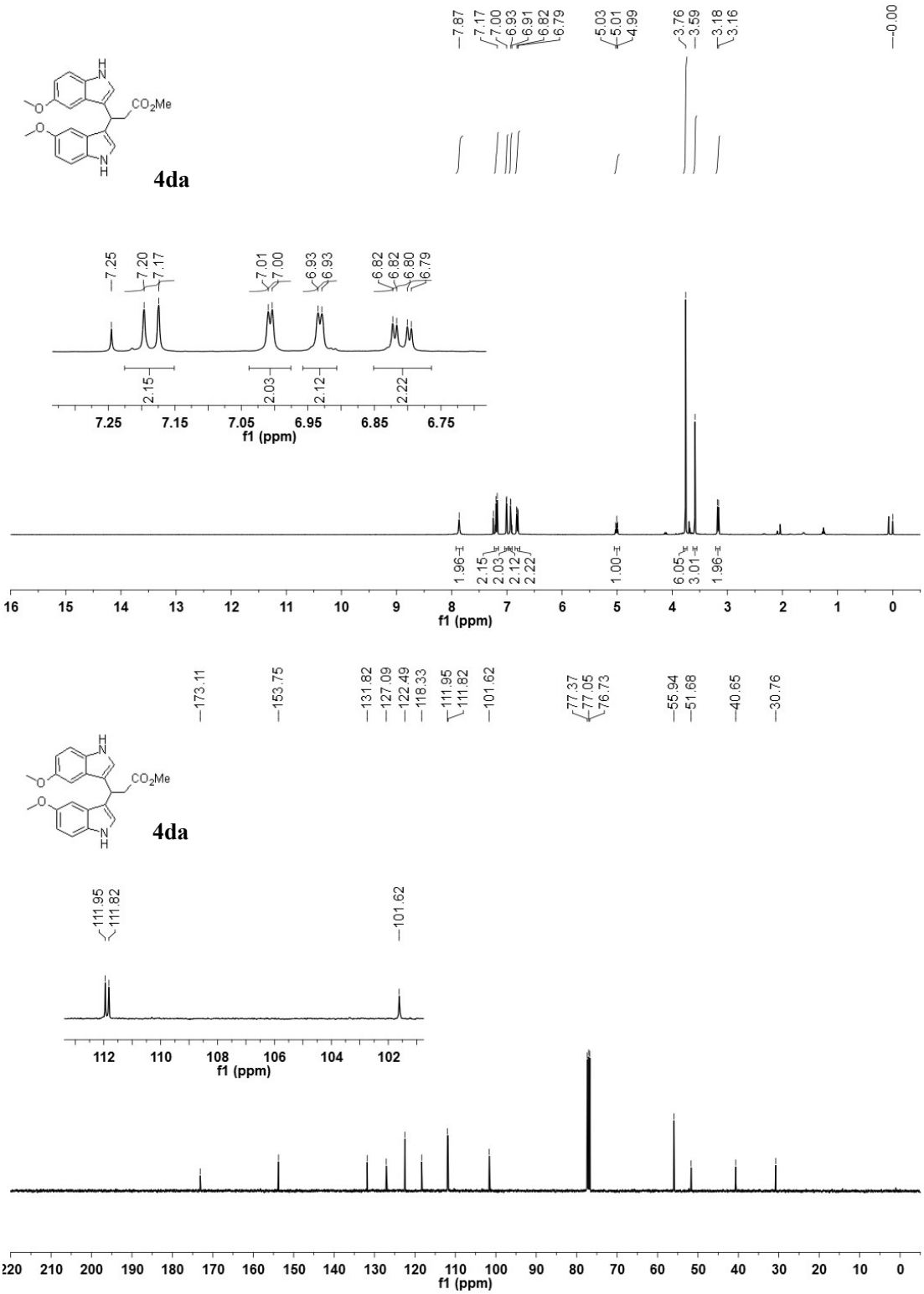


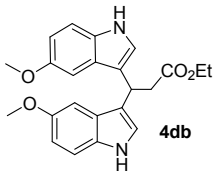
butyl 3,3-bis(1-benzyl-1*H*-indol-3-yl)propanoate (4cc): Yield 58%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.9 Hz, 2H), 7.30 – 7.16 (m, 8H), 7.10 (t, *J* = 7.6 Hz, 2H), 7.07 – 6.93 (m, 8H), 5.23 (s, 4H), 5.12 (t, *J* = 7.8 Hz, 1H), 3.93 (t, *J* = 6.7 Hz, 2H), 3.18 (d, *J* = 7.8 Hz, 2H), 1.40 (q, 6.8 Hz, 2H), 1.21 – 1.10 (m, 2H), 0.77 (t, *J* = 7.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.54, 137.83, 137.05, 128.69, 127.46, 127.44, 126.60, 125.89, 121.70, 119.87, 118.94, 117.97, 109.67, 64.23, 49.90, 41.35, 31.11, 30.57, 19.02, 13.63. HRMS (ESI) m/z: calculated for $C_{37}H_{36}N_2O_2Na$ $[M+Na]^+$: 563.2674, found 563.2712.



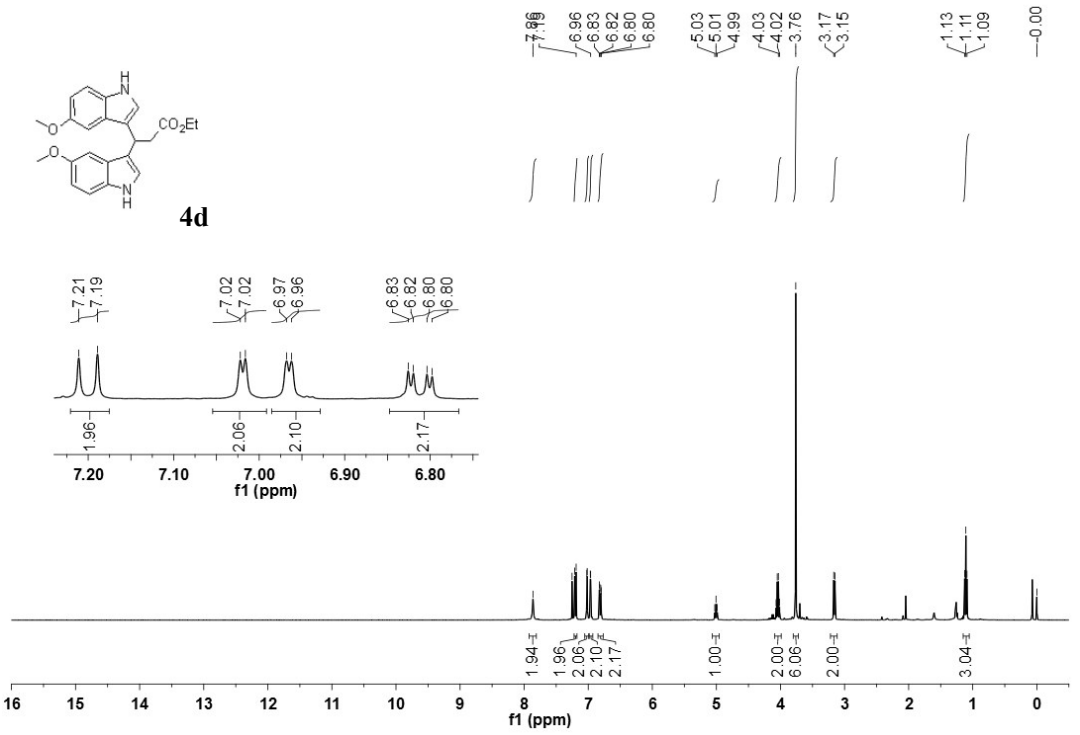


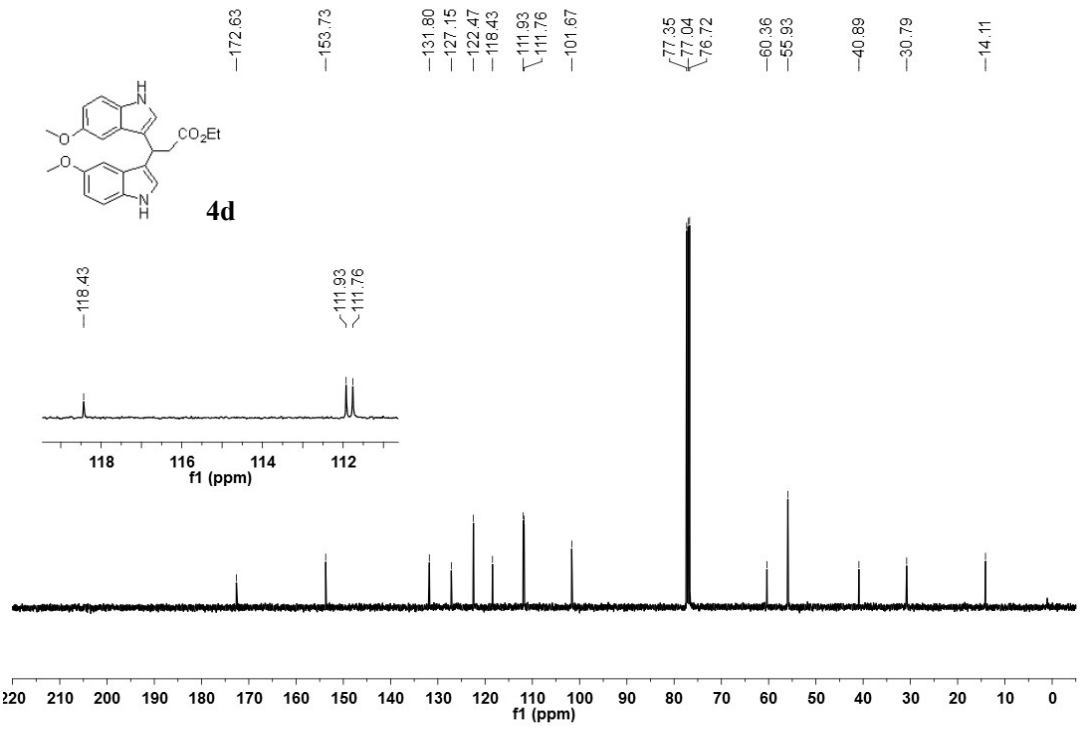
methyl 3,3-bis(5-methoxy-1*H*-indol-3-yl)propanoate (4da): Yield 55%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 2H), 7.19 (d, J = 8.8 Hz, 2H), 7.01 (d, J = 2.4 Hz, 2H), 6.93 (d, J = 2.3 Hz, 2H), 6.81 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 2H), 5.01 (t, J = 7.7 Hz, 1H), 3.76 (s, 6H), 3.59 (s, 3H), 3.17 (d, J = 7.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.11, 153.75, 131.82, 127.09, 122.49, 118.33, 111.95, 111.82, 101.62, 55.94, 51.68, 40.65, 30.76.

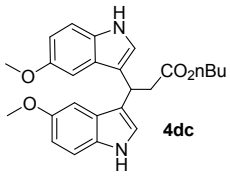




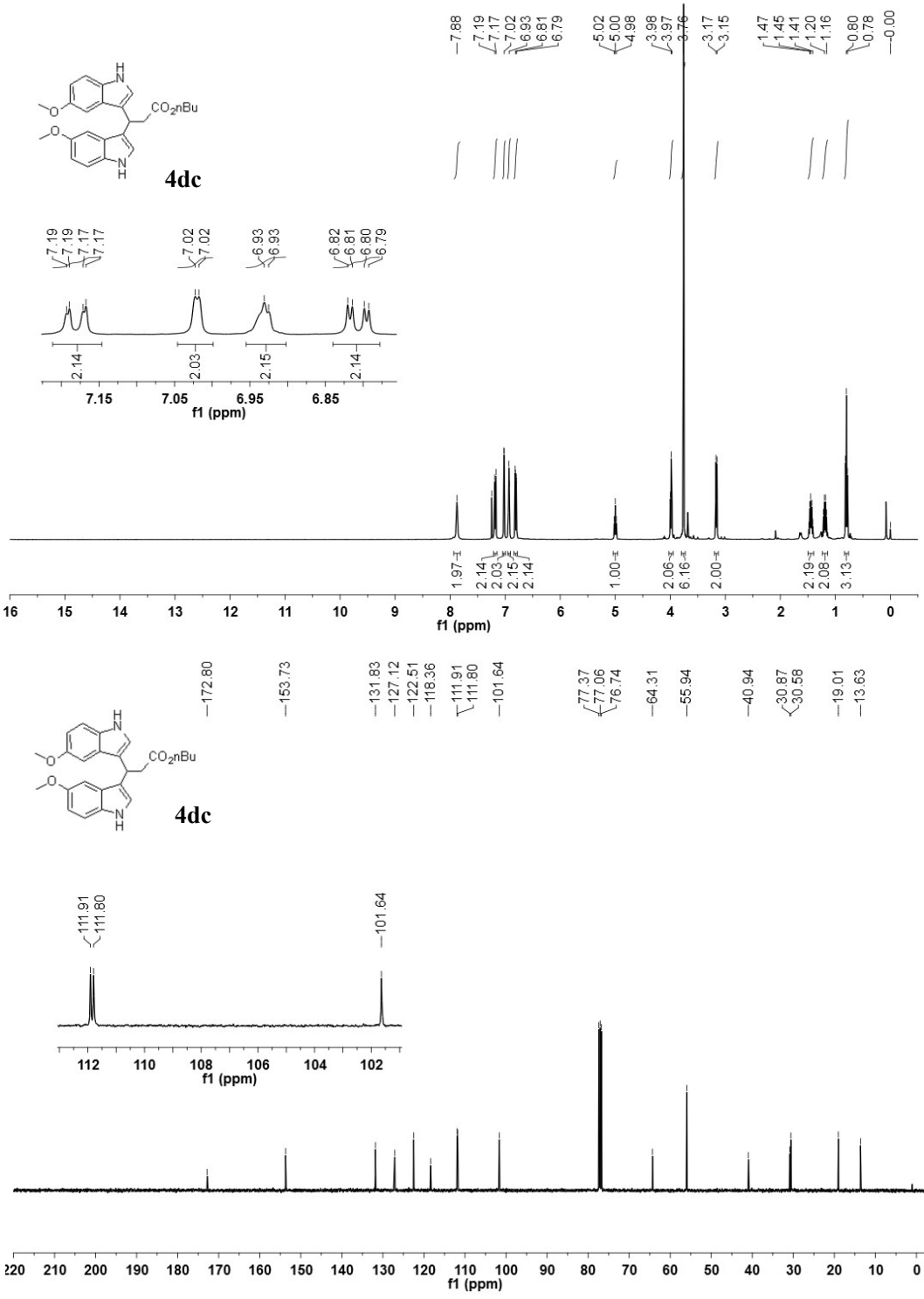
ethyl 3,3-bis(5-methoxy-1*H*-indol-3-yl)propanoate (4db): Yield 59%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (s, 2H), 7.20 (d, J = 8.8 Hz, 2H), 7.02 (d, J = 2.4 Hz, 2H), 6.97 (d, J = 2.3 Hz, 2H), 6.81 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 2H), 5.01 (t, J = 7.7 Hz, 1H), 4.04 (q, J = 7.1 Hz, 2H), 3.76 (s, 6H), 3.16 (d, J = 7.7 Hz, 2H), 1.11 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.63, 153.73, 131.80, 127.15, 122.47, 118.43, 111.93, 111.76, 101.67, 60.36, 55.93, 40.89, 30.79, 14.11. HRMS (ESI) m/z: calculated for $C_{23}H_{24}N_2O_4Na$ $[M+Na]^+$: 415.1634, found 415.1639.

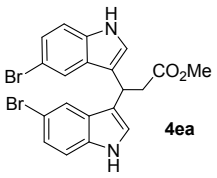




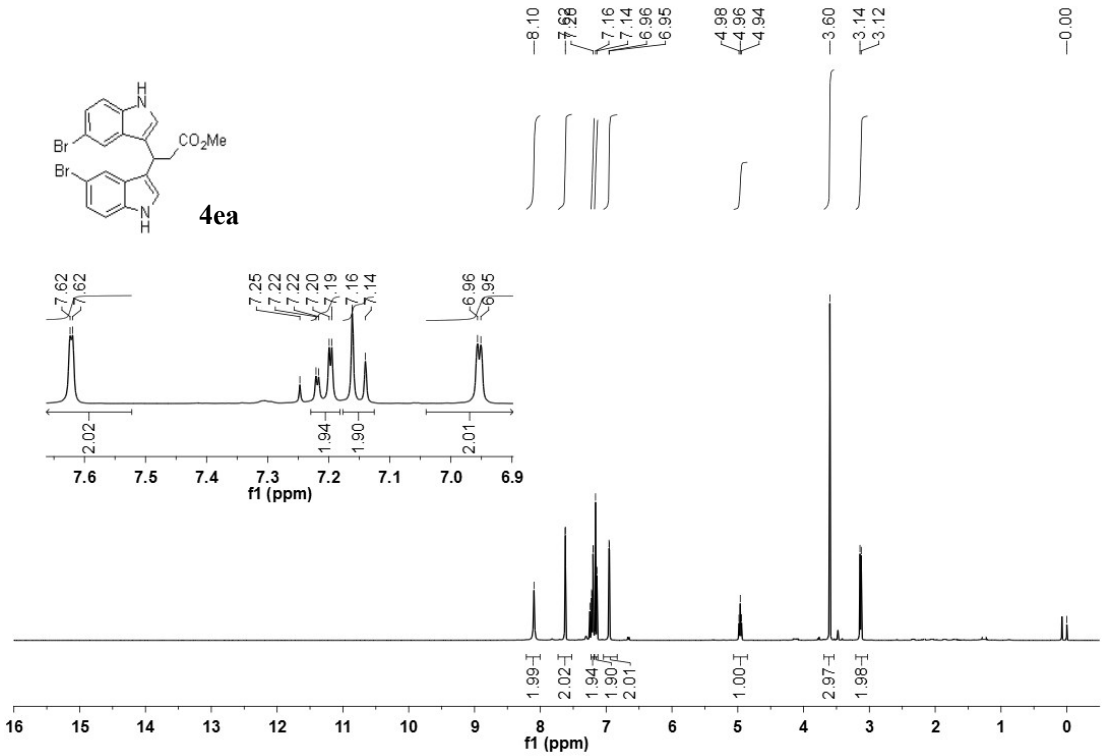


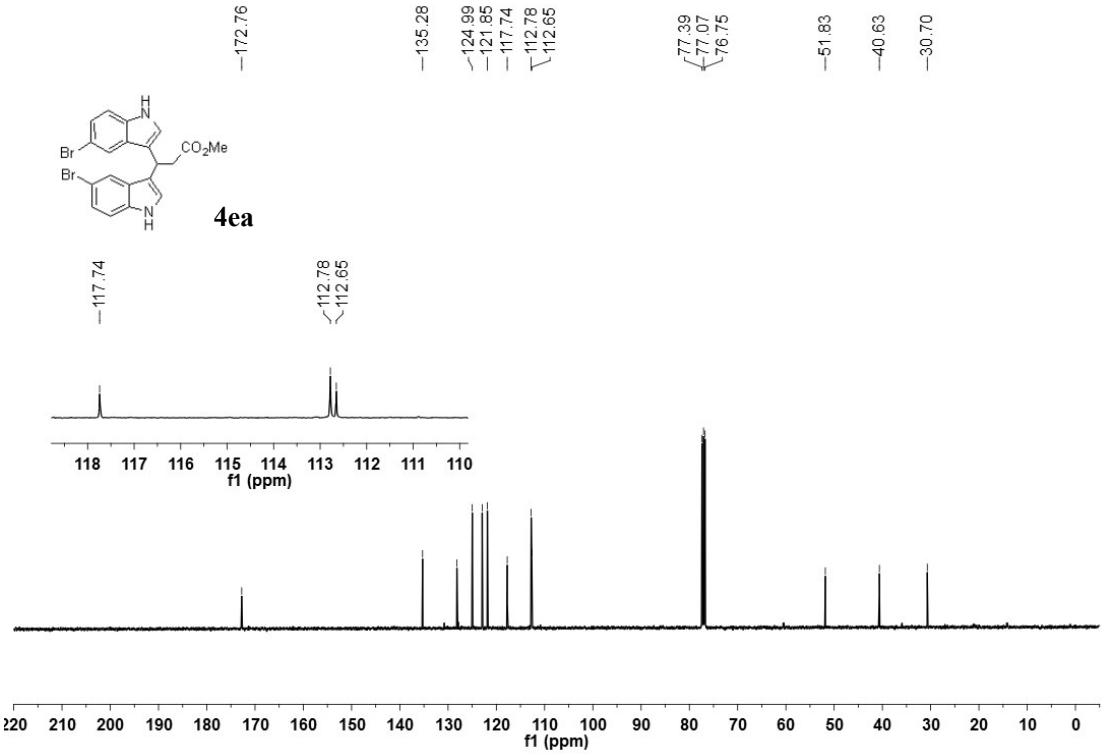
butyl 3,3-bis(5-methoxy-1*H*-indol-3-yl)propanoate (4dc): Yield 54%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (s, 2H), 7.18 (dd, J_1 = 8.8 Hz, J_2 = 1.5 Hz, 2H), 7.02 (d, J = 2.0 Hz, 2H), 6.93 (d, J = 2.3 Hz, 2H), 6.81 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 2H), 5.00 (t, J = 7.7 Hz, 1H), 3.98 (t, J = 6.6 Hz, 2H), 3.76 (s, 6H), 3.16 (d, J = 7.7 Hz, 2H), 1.45 (q, J = 6.7 Hz, 2H), 1.26 – 1.10 (m, 2H), 0.80 (t, J = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.80, 153.73, 131.83, 127.12, 122.51, 118.36, 111.91, 111.80, 101.64, 64.31, 55.94, 40.94, 30.87, 30.58, 19.01, 13.63. HRMS (ESI) m/z: calculated for $C_{25}H_{28}N_2O_4Na$ $[M+Na]^+$: 443.1947, found 443.1957.

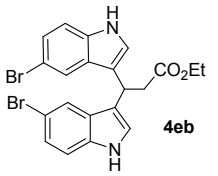




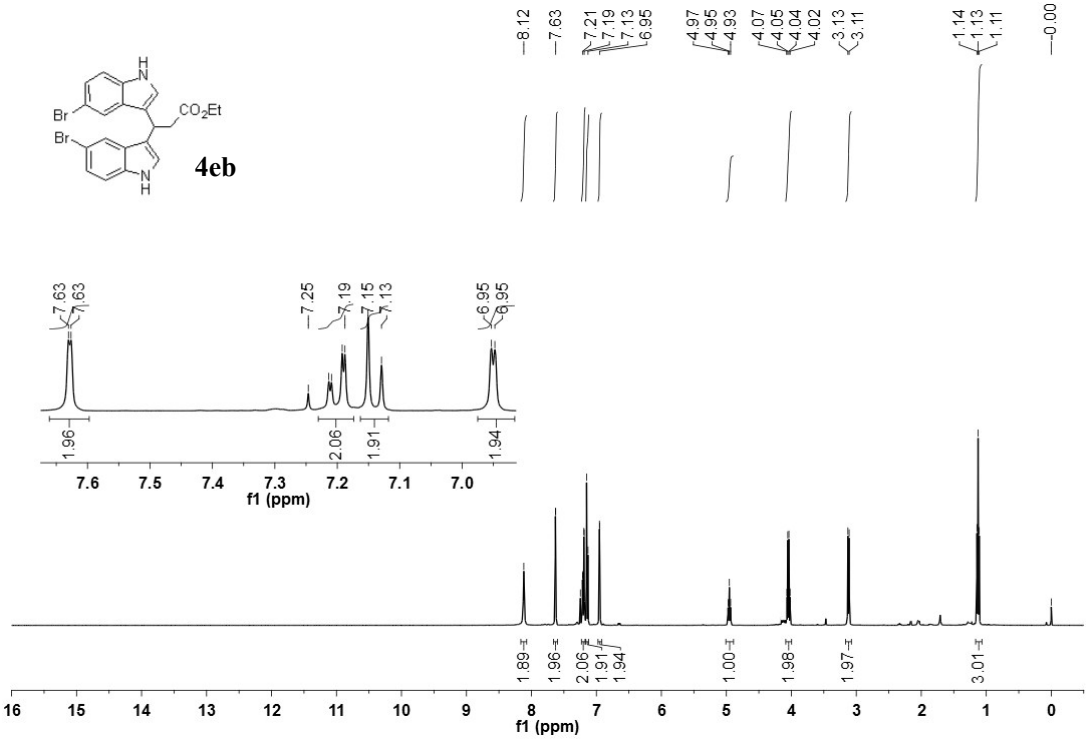
methyl 3,3-bis(5-bromo-1*H*-indol-3-yl)propanoate (4ea): Yield 61%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (s, 2H), 7.62 (d, J = 1.6 Hz, 2H), 7.21 (dd, J_1 = 8.6 Hz, J_2 = 1.8 Hz, 2H), 7.15 (d, J = 8.6 Hz, 2H), 6.95 (d, J = 2.2 Hz, 2H), 4.96 (t, J = 7.7 Hz, 1H), 3.60 (s, 3H), 3.13 (d, J = 7.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.76, 135.28, 128.17, 124.99, 122.93, 121.85, 117.74, 112.78, 112.65, 51.83, 40.63, 30.70.

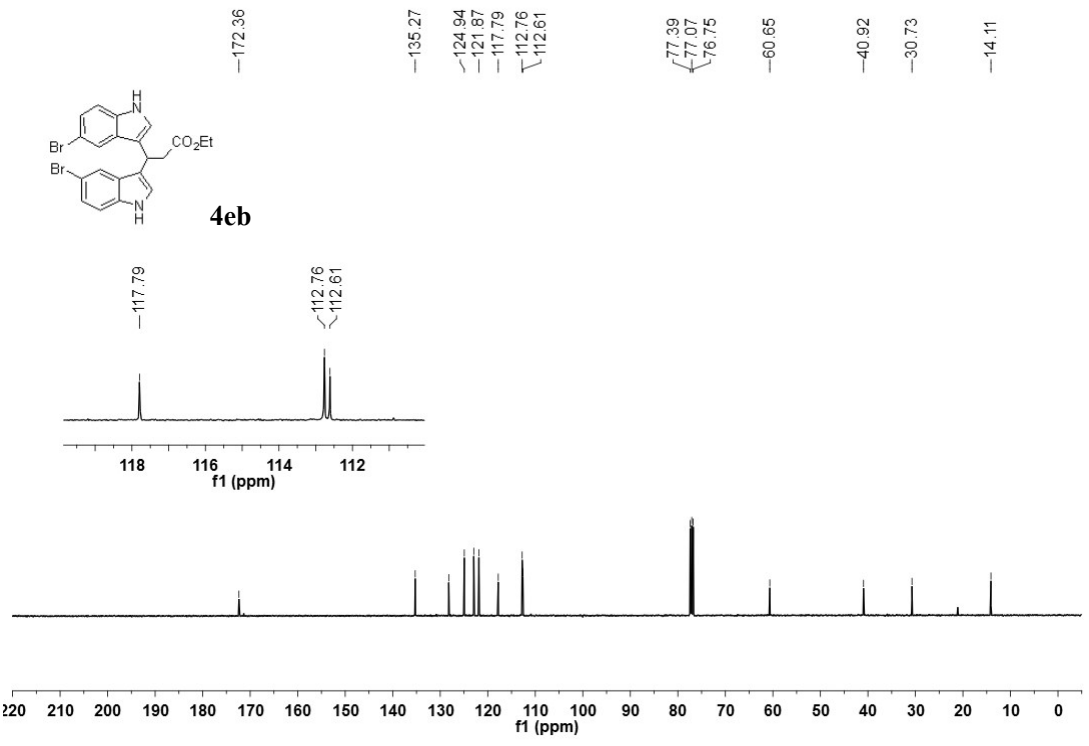


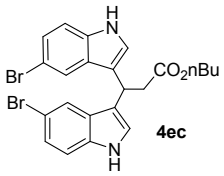




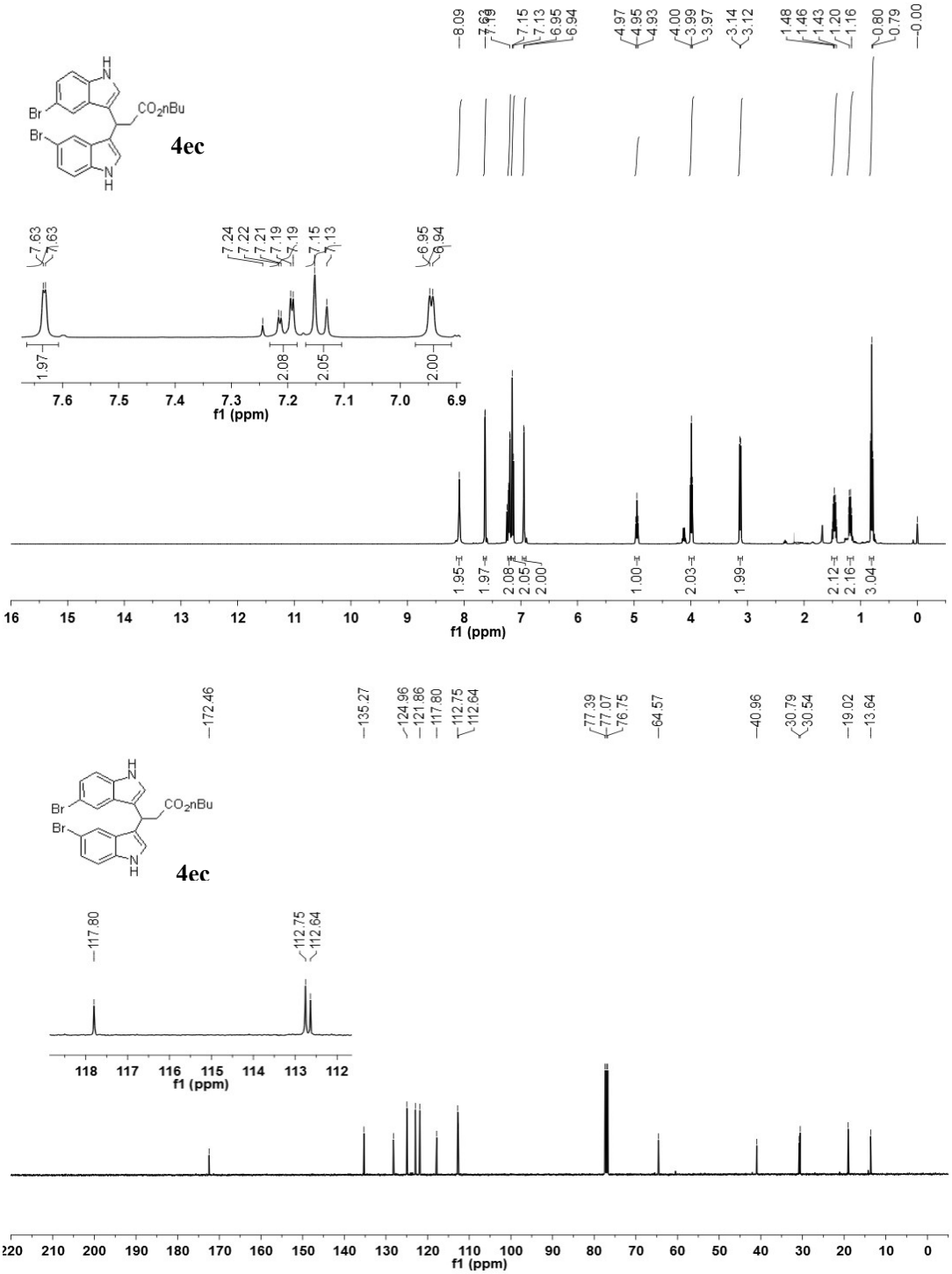
ethyl 3,3-bis(5-bromo-1*H*-indol-3-yl)propanoate (4eb): Yield 75%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 2H), 7.63 (d, J = 1.6 Hz, 2H), 7.20 (dd, J_1 = 8.6 Hz, J_2 = 1.8 Hz, 2H), 7.14 (d, J = 8.6 Hz, 2H), 6.95 (d, J = 2.2 Hz, 2H), 4.95 (t, J = 7.7 Hz, 1H), 4.05 (q, J = 7.1 Hz, 2H), 3.12 (d, J = 7.7 Hz, 2H), 1.13 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.36, 135.27, 128.21, 124.94, 122.94, 121.87, 117.79, 112.76, 112.61, 60.65, 40.92, 30.73, 14.11. HRMS (ESI) m/z: calculated for $C_{21}H_{18}N_2Br_2O_2Na$ $[M+Na]^+$: 510.9633, found 510.9611.







butyl 3,3-bis(5-bromo-1*H*-indol-3-yl)propanoate (4ec): Yield 75%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (s, 2H), 7.63 (d, J = 1.6 Hz, 2H), 7.20 (dd, J_1 = 8.6 Hz, J_2 = 1.8 Hz, 2H), 7.14 (d, J = 8.6 Hz, 2H), 6.95 (d, J = 2.2 Hz, 2H), 4.95 (t, J = 7.7 Hz, 1H), 3.99 (t, J = 6.6 Hz, 2H), 3.13 (d, J = 7.8 Hz, 2H), 1.47 (q, J = 6.7 Hz, 2H), 1.24 – 1.14 (m, *2*H), 0.80 (t, J = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.46, 135.27, 128.20, 124.96, 122.93, 121.86, 117.80, 112.75, 112.64, 64.57, 40.96, 30.79, 30.54, 19.02, 13.64. HRMS (ESI) m/z: calculated for $C_{23}H_{22}N_2Br_2O_2Na$ $[M+Na]^+$: 538.9946, found 538.9921.



References

[1] L. Zhang, C. Peng, D. Zhao, Y. Wang, H. Fu, Q. Shen, J. Li, *Chem. Commun.* **2012**, *48*, 5928.

[2] C. Shao, G. Shi, Y. Zhang, S. Pan, X. Guan, *Org. Lett.* **2015**, *17*, 2652.

Optimized structures for all stationary points

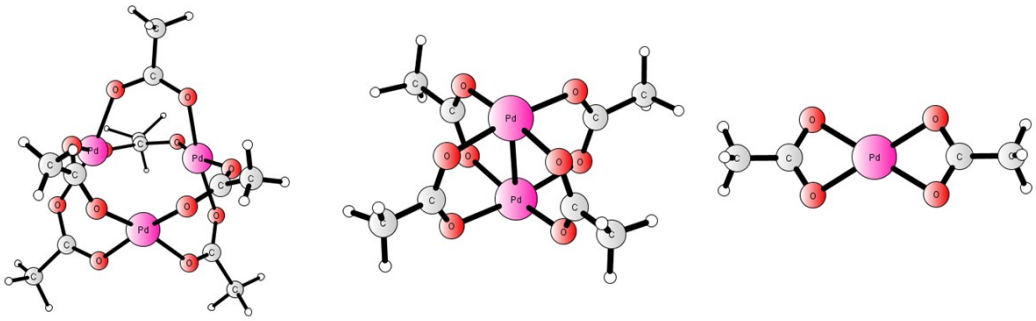


Figure S6. Optimized structures of the trimer, dimer, and monomer of palladium acetate.

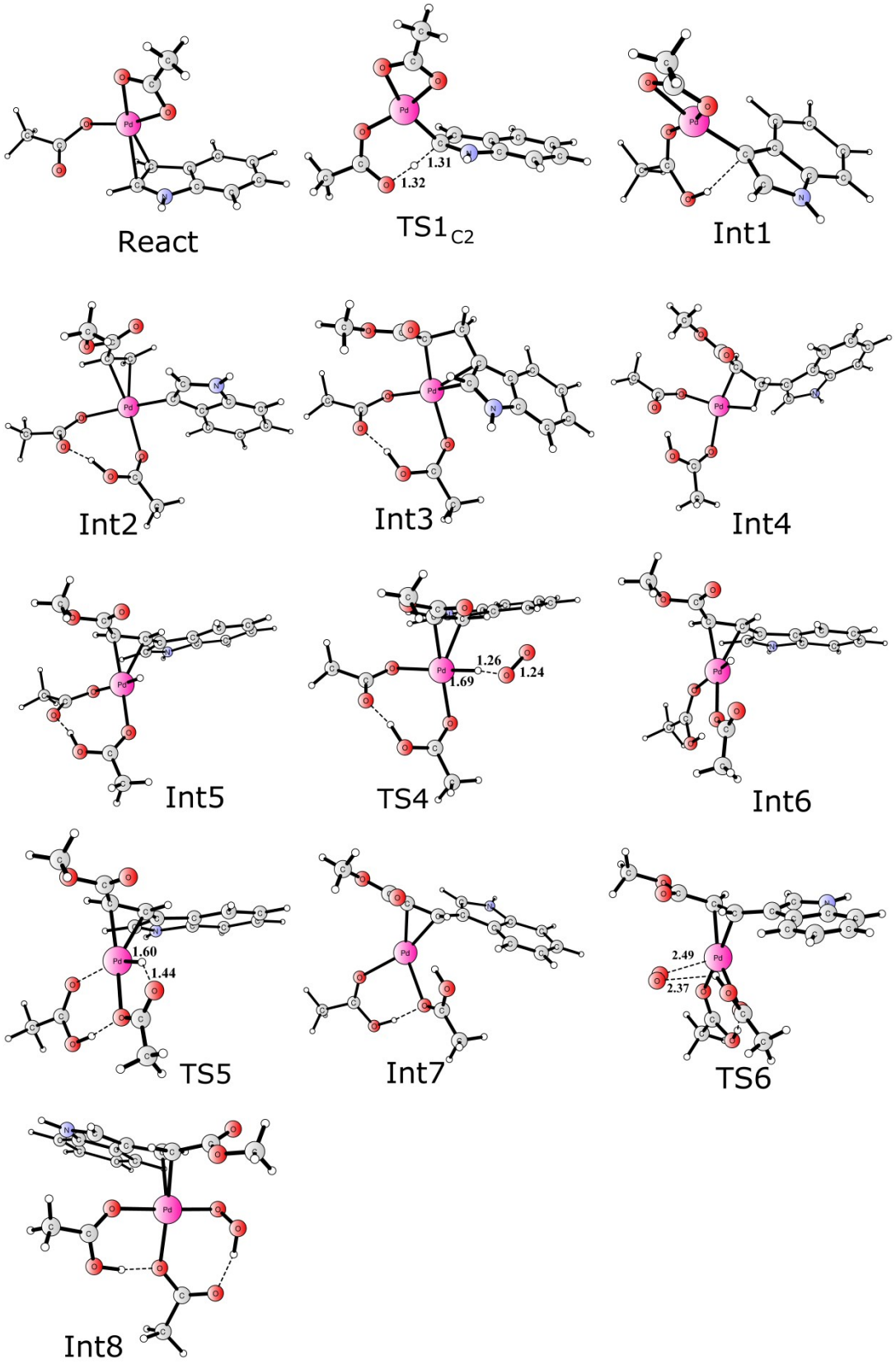


Figure S7. Optimized structures of the reactant, transition states, and intermediates for the $Pd(OAc)_2$-catalyzed oxidative coupling of indole with methyl acrylate.

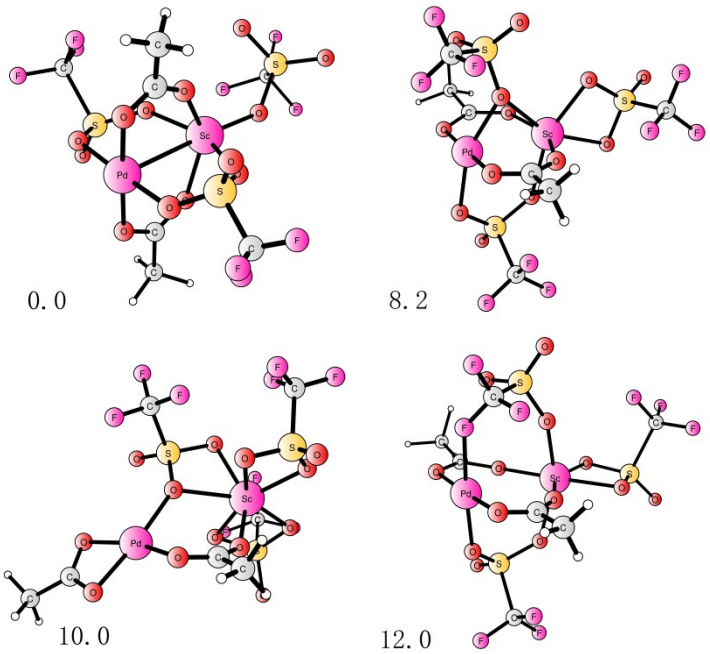


Figure S8. Optimized structures of possible isomers of $Pd(OAc)_2/Sc(OTf)_3$. Relative energies are given in kcal/mol.

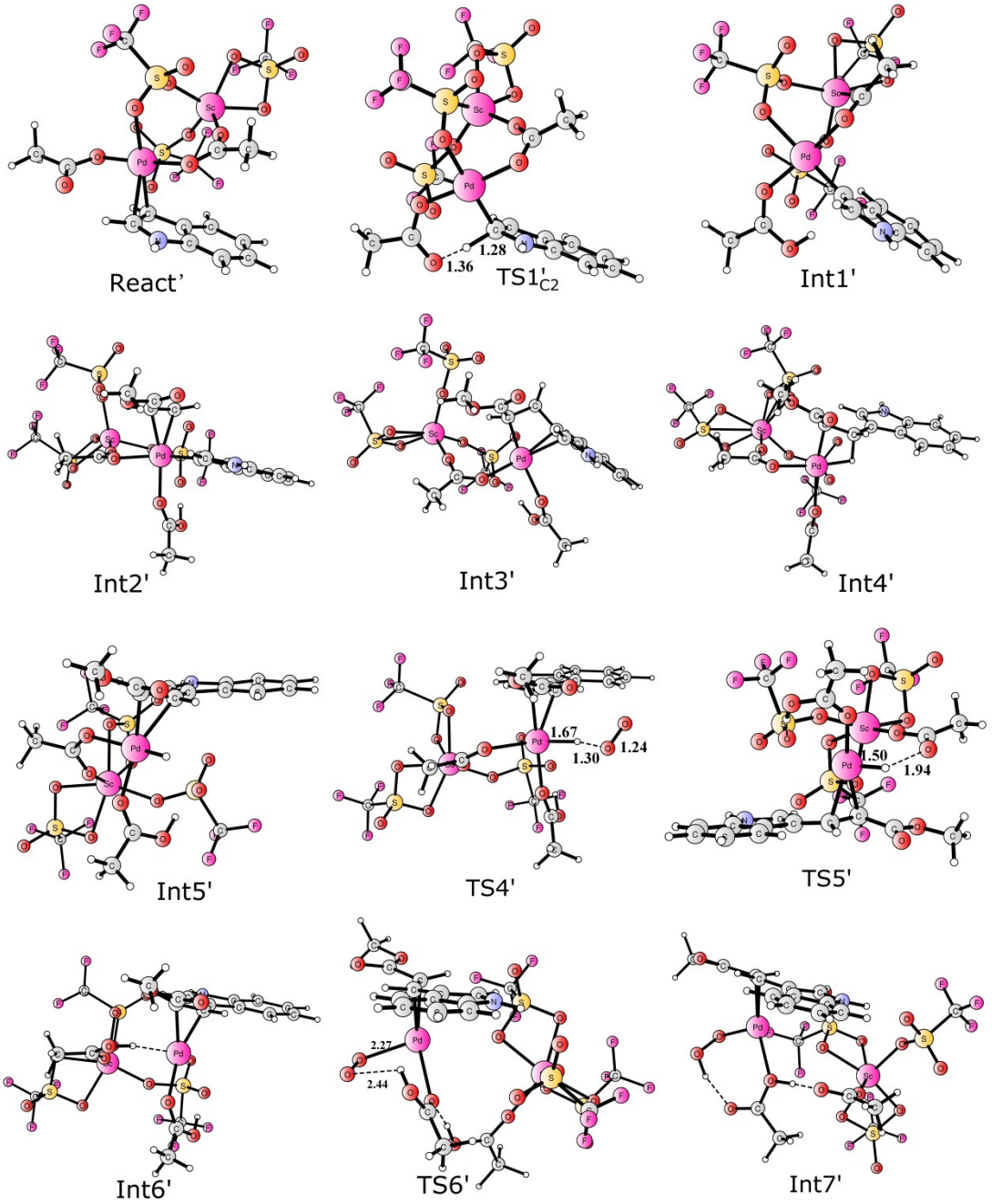


Figure S9. Optimized structures of the reactant, transition states, and intermediates for the $Pd(OAc)_2/Sc(OTf)_3$-catalyzed oxidative coupling of indole with methyl acrylate.

Cartesian coordinates for all stationary points

The electronic energies obtained from (SMD-B3LYP/def2-TZVPPD) are given below.

$Pd_3(OAc)_6$ E=-1755.674784

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.961810	1.410288	-0.041845
2	8	0	2.163266	1.563641	-1.314773
3	8	0	-2.152412	1.159231	1.569955
4	6	0	1.240732	2.148463	-1.932169
5	8	0	-0.011172	2.027156	-1.701789
6	6	0	-2.724954	0.063842	1.846929
7	8	0	-2.477107	-1.034777	1.265378
8	6	0	1.616070	3.101077	-3.036799
9	1	0	1.623327	4.122148	-2.620811
10	1	0	2.616126	2.865206	-3.420426
11	1	0	0.865697	3.071235	-3.837848
12	6	0	-3.744692	0.054772	2.948588
13	1	0	-4.553258	-0.647586	2.704203
14	1	0	-3.253513	-0.303760	3.868074
15	1	0	-4.136463	1.064735	3.120705
16	46	0	-0.920041	-1.434949	0.035634
17	8	0	0.234383	2.461117	1.193011
18	8	0	-2.115202	-1.221151	-1.577413
19	6	0	1.340681	2.254031	1.791597
20	8	0	2.126485	1.299282	1.568104
21	6	0	-2.716343	-0.142246	-1.858341
22	8	0	-2.501289	0.963689	-1.277508
23	6	0	1.703485	3.242753	2.868218
24	1	0	2.755247	3.126427	3.155414
25	1	0	1.504198	4.265362	2.518164
26	1	0	1.058474	3.061389	3.742846
27	6	0	-3.730713	-0.163263	-2.964721
28	1	0	-4.550108	0.531469	-2.735597
29	1	0	-3.238827	0.186786	-3.887158
30	1	0	-4.107139	-1.181222	-3.123899
31	46	0	2.029094	0.030826	0.000330
32	8	0	2.205576	-1.498255	1.315180
33	8	0	2.165266	-1.233442	-1.567618
34	6	0	1.412475	-2.215964	-1.787525
35	8	0	0.306676	-2.450504	-1.199537
36	6	0	1.298188	-2.106171	1.932980
37	8	0	0.044049	-2.019464	1.699826
38	6	0	1.697180	-3.044572	3.041507
39	1	0	2.694840	-2.788258	3.418073
40	1	0	0.950828	-3.022311	3.846662
41	1	0	1.719216	-4.068470	2.633130
42	6	0	1.851518	-3.230114	-2.810786
43	1	0	2.360009	-4.052737	-2.281371
44	1	0	0.984429	-3.647187	-3.338840
45	1	0	2.563825	-2.774625	-3.510201

$Pd_2(OAc)_4$ E=-1170.421434

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.000933	-0.000088	1.309901
2	8	0	-1.445749	1.447918	-1.136712
3	8	0	1.444900	-1.448285	1.136358

4	6	0	-1.847666	1.844981	-0.000255
5	8	0	-1.446798	1.447902	1.136786
6	6	0	1.847546	-1.845000	-0.000167
7	8	0	1.447645	-1.447339	-1.137151
8	6	0	-2.948493	2.881923	0.000966
9	1	0	-2.862500	3.527832	0.884533
10	1	0	-2.921275	3.471946	-0.923989
11	1	0	-3.917753	2.359485	0.052092
12	6	0	2.947512	-2.882832	0.003381
13	1	0	2.940689	-3.454192	-0.933441
14	1	0	3.915581	-2.362721	0.088974
15	1	0	2.841151	-3.546295	0.871753
16	46	0	0.001014	0.000235	-1.309909
17	8	0	1.445613	1.447879	1.136828
18	8	0	-1.444712	-1.448140	-1.136490
19	6	0	1.847437	1.845292	0.000470
20	8	0	1.446571	1.448475	-1.136671
21	6	0	-1.847275	-1.845193	-0.000067
22	8	0	-1.447390	-1.447768	1.137017
23	6	0	2.948158	2.882350	-0.000560
24	1	0	2.861798	3.528706	-0.883766
25	1	0	2.921189	3.471897	0.924704
26	1	0	3.917452	2.360037	-0.052315
27	6	0	-2.947643	-2.882598	-0.003743
28	1	0	-2.939660	-3.455427	0.932182
29	1	0	-3.915658	-2.361984	-0.086920
30	1	0	-2.842835	-3.544715	-0.873315

$Pd(OAc)_2$ E=-585.1844957

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.000001	0.000058	-0.010130
2	8	0	-1.762221	-1.082066	-0.010266
3	8	0	1.762197	-1.082108	-0.010248
4	6	0	-2.433764	0.000113	-0.005025
5	8	0	-1.762215	1.082238	-0.010243
6	6	0	2.433761	0.000050	-0.005000
7	8	0	1.762237	1.082196	-0.010223
8	6	0	-3.928374	-0.000094	0.037579
9	1	0	-4.321579	0.911020	-0.432957
10	1	0	-4.321494	-0.898878	-0.456397
11	1	0	-4.253008	-0.014664	1.090969
12	6	0	3.928373	-0.000124	0.037561
13	1	0	4.321566	0.908944	-0.436967
14	1	0	4.253062	-0.009803	1.090988
15	1	0	4.321459	-0.901025	-0.452534

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indole E=-363.983575

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.251522	-0.673191	-0.000051
2	6	0	0.250435	0.753760	-0.000064
3	6	0	-0.985200	1.431183	-0.000011
4	6	0	-2.163246	0.691711	0.000009
5	6	0	-2.138373	-0.720921	0.000037
6	6	0	-0.934929	-1.420694	0.000018
7	6	0	2.391719	0.027926	0.000033
8	6	0	1.627875	1.170006	0.000038
9	7	0	1.568547	-1.080746	-0.000038

10	1	0	2.004656	2.190724	0.000082
11	1	0	3.474321	-0.086851	0.000049
12	1	0	1.883056	-2.041265	0.000123
13	1	0	-0.917937	-2.513736	-0.000071
14	1	0	-3.080891	-1.274374	0.000067
15	1	0	-3.126586	1.208009	0.000044
16	1	0	-1.015269	2.524035	-0.000074

React E=-949.1890647

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.319820	-0.914349	0.821778
2	6	0	1.822930	-1.228496	-0.468563
3	6	0	2.696730	-1.222357	-1.565723
4	6	0	4.035049	-0.895481	-1.353908
5	6	0	4.505687	-0.569707	-0.066360
6	6	0	3.656896	-0.571196	1.040494
7	6	0	0.119487	-1.384285	1.069342
8	6	0	0.399808	-1.501402	-0.318019
9	7	0	1.267474	-1.038041	1.722850
10	46	0	-0.775707	0.359473	-0.177495
11	8	0	0.610398	1.826953	0.294238
12	8	0	-2.368722	-0.681438	-0.785709
13	6	0	-3.137194	-1.308492	0.068730
14	8	0	-2.877226	-1.511531	1.248347
15	6	0	-0.231276	2.763959	0.060379
16	8	0	-1.400429	2.436585	-0.289593
17	6	0	0.185788	4.201146	0.169320
18	6	0	-4.443224	-1.773703	-0.559821
19	1	0	-0.219393	-2.051548	-1.025282
20	1	0	-0.804513	-1.650607	1.589888
21	1	0	1.308588	-0.779696	2.700962
22	1	0	4.026268	-0.318651	2.036890
23	1	0	5.558839	-0.311415	0.069239
24	1	0	4.730842	-0.886943	-2.196045
25	1	0	2.331463	-1.465777	-2.566259
26	1	0	-4.255261	-2.275835	-1.520242
27	1	0	-4.969363	-2.445824	0.130043
28	1	0	-5.074608	-0.895620	-0.769427
29	1	0	0.990566	4.312492	0.908616
30	1	0	0.568768	4.533759	-0.809406
31	1	0	-0.677175	4.827841	0.431682

TS1 E=-949.1615658

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.929232	-0.154951	0.738607
2	6	0	1.873663	-0.311864	-0.194906
3	6	0	2.152460	-0.135314	-1.559290
4	6	0	3.452431	0.183625	-1.948892
5	6	0	4.484825	0.328412	-1.000032
6	6	0	4.238644	0.159373	0.361841
7	6	0	1.068360	-0.662124	1.893616
8	6	0	0.658346	-0.662384	0.548867
9	7	0	2.388338	-0.376357	2.003317
10	46	0	-1.143836	0.247008	0.085263
11	8	0	-0.511554	2.201479	0.263213
12	8	0	-2.195365	-1.470297	-0.208737
13	6	0	-1.717391	-2.641304	-0.248361

14	8	0	-0.506931	-2.931606	-0.039351
15	6	0	-1.663482	2.661172	-0.058626
16	8	0	-2.590928	1.841750	-0.304284
17	6	0	-1.868382	4.146571	-0.158389
18	6	0	-2.668674	-3.765440	-0.594375
19	1	0	0.110779	-1.826456	0.245432
20	1	0	0.477397	-0.880502	2.783089
21	1	0	2.913525	-0.361287	2.869634
22	1	0	5.037251	0.269263	1.099785
23	1	0	5.494267	0.577566	-1.336276
24	1	0	3.679031	0.326073	-3.008434
25	1	0	1.356155	-0.240526	-2.300023
26	1	0	-2.480535	-4.073277	-1.635634
27	1	0	-2.468098	-4.634186	0.048194
28	1	0	-3.711373	-3.439229	-0.499079
29	1	0	-1.405897	4.649950	0.703048
30	1	0	-1.367473	4.517653	-1.067043
31	1	0	-2.938915	4.381835	-0.215092

Int1 E=-949.1740697

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.698640	1.437021	0.484009
2	6	0	1.785173	0.609488	-0.236360
3	6	0	2.232882	-0.024610	-1.412573
4	6	0	3.546832	0.164308	-1.830067
5	6	0	4.435122	0.980554	-1.095487
6	6	0	4.024185	1.626132	0.067470
7	6	0	0.724905	1.467137	1.567946
8	6	0	0.522774	0.633452	0.481933
9	7	0	2.022185	1.943509	1.572626
10	46	0	-1.216163	-0.140448	-0.075828
11	8	0	-2.367590	1.546056	0.088422
12	8	0	-0.404933	-2.048756	-0.317964
13	6	0	0.357462	-2.640451	0.454884
14	8	0	0.954287	-2.066441	1.467223
15	6	0	-3.434835	0.957400	-0.320406
16	8	0	-3.387553	-0.266559	-0.601603
17	6	0	-4.694570	1.765822	-0.474540
18	6	0	0.677606	-4.094303	0.276163
19	1	0	0.789132	-1.080798	1.422112
20	1	0	0.019550	1.783586	2.334751
21	1	0	2.417309	2.556681	2.273064
22	1	0	4.711348	2.261104	0.633054
23	1	0	5.461367	1.111631	-1.448020
24	1	0	3.899250	-0.319861	-2.744432
25	1	0	1.547508	-0.648598	-1.991731
26	1	0	1.719558	-4.185896	-0.070707
27	1	0	0.606187	-4.614568	1.242331
28	1	0	0.001998	-4.544027	-0.460065
29	1	0	-4.800095	2.471683	0.361645
30	1	0	-4.628606	2.356437	-1.402737
31	1	0	-5.567038	1.102576	-0.536003

Methyl acrylate E=-306.6151856

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.317802	-0.645999	-0.000098
2	1	0	1.237036	-1.736046	-0.000233

3	6	0	2.496663	-0.015689	0.000135
4	1	0	2.533502	1.077659	0.000243
5	1	0	3.441042	-0.565615	0.000163
6	6	0	0.041881	0.120129	-0.000089
7	8	0	-0.059021	1.324863	-0.000086
8	8	0	-1.018410	-0.713572	-0.000025
9	6	0	-2.303656	-0.096084	0.000098
10	1	0	-2.435655	0.535765	-0.891743
11	1	0	-3.037124	-0.911956	0.000164
12	1	0	-2.435492	0.535719	0.892007

Int2 E=-1255.812253

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.494675	-0.952610	0.427753
2	6	0	-2.543224	-0.167267	-0.293506
3	6	0	-3.020044	0.819352	-1.180519
4	6	0	-4.391954	0.997952	-1.329049
5	6	0	-5.313553	0.209090	-0.605405
6	6	0	-4.877710	-0.772950	0.279712
7	6	0	-1.431339	-1.641391	1.015056
8	6	0	-1.230038	-0.630934	0.101839
9	7	0	-2.787813	-1.833410	1.214175
10	46	0	0.476733	0.195530	-0.514306
11	8	0	3.011115	1.852867	0.752020
12	8	0	-0.329282	1.977544	0.273324
13	6	0	-0.085009	2.555539	1.352867
14	8	0	1.008475	2.441432	2.015406
15	6	0	3.121375	1.696425	-0.490724
16	8	0	2.247867	1.178356	-1.250642
17	6	0	4.411749	2.168744	-1.136704
18	6	0	-1.115055	3.491307	1.930145
19	1	0	1.841693	2.054406	1.436468
20	1	0	-0.715435	-2.274730	1.531024
21	1	0	-3.193054	-2.519999	1.835511
22	1	0	-5.590433	-1.384621	0.839592
23	1	0	-6.385764	0.371434	-0.742664
24	1	0	-4.766287	1.761577	-2.015767
25	1	0	-2.316422	1.441406	-1.738321
26	1	0	-1.055028	3.490670	3.026871
27	1	0	-0.890504	4.513707	1.583267
28	1	0	-2.119330	3.215020	1.586592
29	1	0	4.482400	3.262910	-1.030166
30	1	0	5.268014	1.740322	-0.594083
31	1	0	4.457018	1.897489	-2.198656
32	6	0	1.616299	-1.585473	-1.094074
33	1	0	2.580844	-1.114379	-1.289298
34	6	0	0.569717	-1.412969	-1.986453
35	1	0	-0.312533	-2.052881	-1.925740
36	1	0	0.720840	-0.839556	-2.904960
37	6	0	1.638227	-2.675528	-0.070890
38	8	0	0.802947	-3.537522	0.067898
39	8	0	2.752470	-2.585308	0.676215
40	6	0	2.926960	-3.577661	1.687189
41	1	0	2.898799	-4.587931	1.251881
42	1	0	3.905559	-3.381675	2.141471
43	1	0	2.135501	-3.502374	2.448632

TS2 E=-1255.802248

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-3.571394	-0.781476	0.788913
2	6	0	-2.674830	-0.537171	-0.293176
3	6	0	-3.205500	-0.140563	-1.534902
4	6	0	-4.584232	-0.007115	-1.672473
5	6	0	-5.453017	-0.255782	-0.587650
6	6	0	-4.959311	-0.642840	0.655907
7	6	0	-1.477177	-1.149343	1.532864
8	6	0	-1.336038	-0.768545	0.208012
9	7	0	-2.808233	-1.147002	1.881669
10	46	0	0.367532	0.059311	-0.532182
11	8	0	2.867254	1.560302	0.680855
12	8	0	-0.511623	1.970505	-0.135580
13	6	0	-0.228044	2.767465	0.774019
14	8	0	0.843714	2.737626	1.493869
15	6	0	3.031009	1.322871	-0.540921
16	8	0	2.124652	0.906191	-1.329666
17	6	0	4.408835	1.507847	-1.148615
18	6	0	-1.175086	3.894762	1.100828
19	1	0	1.627169	2.114513	1.140786
20	1	0	-0.707788	-1.453983	2.240703
21	1	0	-3.171669	-1.383663	2.795588
22	1	0	-5.632127	-0.831644	1.496577
23	1	0	-6.531154	-0.140648	-0.724791
24	1	0	-5.004493	0.300857	-2.633127
25	1	0	-2.539058	0.069145	-2.375457
26	1	0	-1.309999	3.961293	2.190393
27	1	0	-0.725587	4.845134	0.770827
28	1	0	-2.138122	3.747714	0.598445
29	1	0	5.056039	2.089166	-0.479733
30	1	0	4.851451	0.511815	-1.311367
31	1	0	4.329669	1.994523	-2.131423
32	6	0	1.224656	-1.824810	-0.911022
33	1	0	1.732630	-1.610154	-1.854705
34	6	0	-0.125543	-2.232145	-0.882780
35	1	0	-0.438710	-2.921989	-0.103337
36	1	0	-0.704680	-2.254495	-1.807172
37	6	0	2.085536	-2.169007	0.258361
38	8	0	1.674640	-2.605115	1.313064
39	8	0	3.381313	-1.919093	0.009293
40	6	0	4.283545	-2.082724	1.105861
41	1	0	4.154099	-3.067064	1.578203
42	1	0	5.293071	-1.985473	0.687929
43	1	0	4.110377	-1.296228	1.856311

Int3 E=-1255.851962

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.079695	-0.349830	0.764865
2	6	0	-2.564027	-1.196490	-0.252829
3	6	0	-3.369209	-1.514009	-1.358427
4	6	0	-4.652184	-0.976710	-1.432430
5	6	0	-5.140844	-0.125554	-0.419984
6	6	0	-4.364322	0.201750	0.690009
7	6	0	-0.983962	-0.924685	1.382611
8	6	0	-1.212027	-1.564760	0.144456
9	7	0	-2.112118	-0.228191	1.746016
10	46	0	0.314353	0.001639	-0.359000
11	8	0	2.731881	1.979848	0.293130
12	8	0	-0.754841	1.890696	-0.101163
13	6	0	-0.451932	2.947097	0.473344
14	8	0	0.710210	3.234483	0.957263

15	6	0	2.836553	1.441979	-0.834184
16	8	0	1.914667	0.795186	-1.428200
17	6	0	4.157814	1.525817	-1.574593
18	6	0	-1.485808	4.035596	0.637443
19	1	0	1.506092	2.578495	0.693557
20	1	0	-0.181075	-1.124976	2.091803
21	1	0	-2.173987	0.381787	2.550396
22	1	0	-4.748844	0.856895	1.475311
23	1	0	-6.150740	0.283345	-0.505188
24	1	0	-5.290629	-1.214054	-2.286531
25	1	0	-2.995145	-2.167915	-2.149810
26	1	0	-1.399605	4.497964	1.631163
27	1	0	-1.285824	4.823528	-0.107037
28	1	0	-2.494200	3.637312	0.471848
29	1	0	4.828737	2.249893	-1.095593
30	1	0	4.622133	0.526748	-1.566229
31	1	0	3.985786	1.795223	-2.626956
32	6	0	1.050305	-1.885777	-0.606700
33	1	0	1.511584	-1.900727	-1.600601
34	6	0	-0.283983	-2.615240	-0.448616
35	1	0	-0.218127	-3.505809	0.198190
36	1	0	-0.667494	-2.928137	-1.429311
37	6	0	2.030378	-2.109792	0.489392
38	8	0	1.748944	-2.488917	1.612123
39	8	0	3.295446	-1.822902	0.118938
40	6	0	4.288739	-1.917174	1.138591
41	1	0	4.295674	-2.919874	1.591575
42	1	0	5.249585	-1.712950	0.649721
43	1	0	4.105420	-1.175240	1.931147

Int4 E=-1255.829618

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.531000	0.945698	0.713999
2	6	0	3.728547	0.167509	-0.170218
3	6	0	4.360409	-0.716527	-1.066879
4	6	0	5.748925	-0.799060	-1.065085
5	6	0	6.525985	-0.017520	-0.181291
6	6	0	5.930467	0.862222	0.717991
7	6	0	2.373755	1.452494	1.108076
8	6	0	2.352490	0.509760	0.103595
9	7	0	3.675542	1.713131	1.475551
10	46	0	-0.999021	0.432337	0.146970
11	8	0	-3.960273	-0.609983	-0.133407
12	8	0	-2.037598	2.304806	-0.211759
13	6	0	-3.086003	2.533648	-0.835393
14	8	0	-3.955774	1.645737	-1.189480
15	6	0	-3.485571	-0.840500	0.998577
16	8	0	-2.376934	-0.385281	1.440963
17	6	0	-4.237339	-1.744164	1.958182
18	6	0	-3.436991	3.943859	-1.238239
19	1	0	-3.821535	0.687401	-0.779355
20	1	0	1.540676	1.966046	1.586558
21	1	0	3.957529	2.378648	2.182246
22	1	0	6.533322	1.464597	1.402278
23	1	0	7.615006	-0.106040	-0.203319
24	1	0	6.250561	-1.480229	-1.756757
25	1	0	3.770853	-1.329982	-1.753172
26	1	0	-3.674882	3.971944	-2.312193
27	1	0	-4.344784	4.256896	-0.698664
28	1	0	-2.612473	4.628821	-1.009290
29	1	0	-5.246653	-1.953343	1.582526
30	1	0	-3.678156	-2.687149	2.066091

31	1	0	-4.284394	-1.280628	2.954505
32	6	0	0.335642	-1.085098	0.172571
33	1	0	0.623552	-1.336499	1.198957
34	6	0	1.152243	-0.083599	-0.564332
35	1	0	0.429636	0.846405	-0.831889
36	1	0	1.350936	-0.417097	-1.594518
37	6	0	-0.214675	-2.220793	-0.625895
38	8	0	-0.163575	-2.308030	-1.834216
39	8	0	-0.797528	-3.144803	0.159018
40	6	0	-1.425809	-4.235281	-0.515833
41	1	0	-0.714354	-4.750487	-1.178255
42	1	0	-1.780434	-4.916110	0.267938
43	1	0	-2.273213	-3.878052	-1.121091

TS3 E=-1255.823376

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.519819	-0.144558	0.902414
2	6	0	3.601435	-0.164274	-0.183329
3	6	0	4.042173	0.243545	-1.456261
4	6	0	5.363752	0.650270	-1.611857
5	6	0	6.259890	0.657710	-0.520648
6	6	0	5.852119	0.260539	0.749833
7	6	0	2.539166	-0.868417	1.692021
8	6	0	2.337484	-0.637285	0.341516
9	7	0	3.836204	-0.578941	2.022863
10	46	0	-0.712111	0.407638	0.204303
11	8	0	-3.834442	0.052351	-0.164473
12	8	0	-1.270730	2.470274	0.168168
13	6	0	-2.247859	2.981036	-0.406442
14	8	0	-3.254123	2.341968	-0.898520
15	6	0	-3.462870	-0.354428	0.964638
16	8	0	-2.317156	-0.142838	1.471103
17	6	0	-4.420054	-1.185634	1.798376
18	6	0	-2.317029	4.479495	-0.567917
19	1	0	-3.363187	1.317997	-0.622731
20	1	0	1.835780	-1.210575	2.448826
21	1	0	4.230629	-0.668355	2.950026
22	1	0	6.545493	0.267379	1.594432
23	1	0	7.291804	0.981746	-0.675937
24	1	0	5.717617	0.970003	-2.594901
25	1	0	3.360752	0.242760	-2.310752
26	1	0	-2.503759	4.725621	-1.624106
27	1	0	-3.171847	4.865435	0.009428
28	1	0	-1.389107	4.950017	-0.222952
29	1	0	-5.443348	-1.113118	1.408707
30	1	0	-4.088371	-2.235964	1.762377
31	1	0	-4.382106	-0.867356	2.850201
32	6	0	-0.035666	-1.550271	0.020457
33	1	0	-0.056351	-2.009828	1.012149
34	6	0	1.111258	-0.833241	-0.434609
35	1	0	0.526271	0.712154	-0.708406
36	1	0	1.245434	-0.845709	-1.521294
37	6	0	-0.921218	-2.172961	-1.008941
38	8	0	-0.799680	-2.033304	-2.205784
39	8	0	-1.892625	-2.906464	-0.436482
40	6	0	-2.895463	-3.423649	-1.314967
41	1	0	-2.439948	-3.931136	-2.177165
42	1	0	-3.488053	-4.130235	-0.720525
43	1	0	-3.535600	-2.602753	-1.673139

Int5 E=-1255.829542

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.034113	0.788295	0.808538
2	6	0	3.369942	-0.038466	-0.137046
3	6	0	4.056442	-0.423637	-1.302336
4	6	0	5.362141	0.021013	-1.492590
5	6	0	6.002525	0.840305	-0.538651
6	6	0	5.348311	1.234339	0.626177
7	6	0	1.966245	0.375756	1.606682
8	6	0	2.043606	-0.304205	0.394018
9	7	0	3.145259	1.015633	1.847523
10	46	0	-0.848169	0.115635	-0.518983
11	8	0	-3.326250	0.849115	1.485646
12	8	0	-1.710387	1.804858	-1.451950
13	6	0	-2.879311	2.235504	-1.473070
14	8	0	-3.821765	1.881770	-0.675064
15	6	0	-2.230520	0.858453	2.098977
16	8	0	-1.083755	0.815798	1.557139
17	6	0	-2.263903	0.900825	3.618422
18	6	0	-3.266350	3.269369	-2.501264
19	1	0	-3.522294	1.336403	0.207121
20	1	0	1.104187	0.489008	2.261723
21	1	0	3.327092	1.603122	2.651143
22	1	0	5.842981	1.867667	1.366694
23	1	0	7.028597	1.171147	-0.716500
24	1	0	5.903560	-0.268842	-2.396349
25	1	0	3.575920	-1.059264	-2.050067
26	1	0	-4.171483	2.935807	-3.030741
27	1	0	-3.521011	4.210082	-1.988114
28	1	0	-2.448035	3.439190	-3.210431
29	1	0	-3.285232	1.066943	3.982831
30	1	0	-1.885247	-0.054328	4.016971
31	1	0	-1.596103	1.695025	3.985431
32	6	0	-0.113283	-1.690157	0.339610
33	1	0	-0.319040	-1.574579	1.405555
34	6	0	1.031979	-1.118880	-0.240761
35	1	0	-0.734290	-0.454047	-1.921984
36	1	0	1.301640	-1.525107	-1.220266
37	6	0	-0.753045	-2.869410	-0.318401
38	8	0	-0.414983	-3.366625	-1.367250
39	8	0	-1.768461	-3.335616	0.433498
40	6	0	-2.476733	-4.457966	-0.090258
41	1	0	-1.801435	-5.314940	-0.235475
42	1	0	-3.251033	-4.702249	0.647281
43	1	0	-2.937939	-4.210934	-1.058679

TS4 E=-1406.204405

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.010742	-0.939847	-0.995224
2	6	0	3.343282	0.001293	-0.166223
3	6	0	4.014870	0.516309	0.956959
4	6	0	5.314050	0.088099	1.216919
5	6	0	5.960147	-0.843344	0.376299
6	6	0	5.318215	-1.370669	-0.741816
7	6	0	1.956156	-0.612586	-1.863940
8	6	0	2.026512	0.211411	-0.743008
9	7	0	3.131899	-1.286805	-2.009782
10	46	0	-0.797173	-0.144111	0.296571
11	8	0	-3.403245	-1.186766	-1.349941

12	8	0	-1.554040	-1.660036	1.574239
13	6	0	-2.692461	-2.138047	1.741975
14	8	0	-3.690310	-1.982965	0.948069
15	6	0	-2.378847	-1.258622	-2.072585
16	8	0	-1.183387	-1.118780	-1.672403
17	6	0	-2.573786	-1.492897	-3.562906
18	6	0	-2.969680	-2.983080	2.960042
19	1	0	-3.475803	-1.542845	-0.010228
20	1	0	1.104732	-0.797455	-2.516377
21	1	0	3.318503	-1.968765	-2.733764
22	1	0	5.816650	-2.093385	-1.392492
23	1	0	6.980654	-1.158146	0.607448
24	1	0	5.845034	0.477736	2.088755
25	1	0	3.524231	1.231855	1.620993
26	1	0	-3.869606	-2.606812	3.469146
27	1	0	-3.186885	-4.014367	2.639922
28	1	0	-2.111628	-2.976297	3.641982
29	1	0	-3.573339	-1.899267	-3.763388
30	1	0	-2.472320	-0.529333	-4.089250
31	1	0	-1.797063	-2.166869	-3.951883
32	6	0	-0.153821	1.530484	-0.887509
33	1	0	-0.365280	1.229770	-1.914958
34	6	0	1.007256	1.098921	-0.228984
35	1	0	-0.550056	0.659648	1.762474
36	1	0	1.270535	1.648782	0.682620
37	6	0	-0.872758	2.742670	-0.404415
38	8	0	-0.630714	3.353004	0.612667
39	8	0	-1.848888	3.090342	-1.265133
40	6	0	-2.631369	4.227870	-0.904853
41	1	0	-1.998245	5.121958	-0.799537
42	1	0	-3.358387	4.367475	-1.714279
43	1	0	-3.152720	4.056799	0.049356
44	8	0	-0.347976	1.085123	2.935669
45	8	0	0.749389	1.661133	3.049994

Int6 E=-1255.833447

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.948886	-0.337628	0.559121
2	6	0	-3.066260	0.372660	-0.298345
3	6	0	-3.466803	0.635163	-1.620913
4	6	0	-4.717463	0.194742	-2.044314
5	6	0	-5.580426	-0.505059	-1.173469
6	6	0	-5.209115	-0.781682	0.139795
7	6	0	-2.085834	0.133728	1.736460
8	6	0	-1.873753	0.673423	0.473982
9	7	0	-3.314464	-0.463353	1.783655
10	46	0	1.017411	0.018881	-0.241537
11	8	0	1.917946	-2.996575	1.151703
12	8	0	2.374729	-0.907398	-3.045068
13	6	0	2.432805	-1.780644	-2.207784
14	8	0	1.946130	-1.670000	-0.977565
15	6	0	1.343180	-2.215300	2.019103
16	8	0	0.897021	-1.090981	1.761343
17	6	0	1.256669	-2.796271	3.407815
18	6	0	3.077314	-3.134546	-2.468235
19	1	0	1.972892	-2.546528	0.219288
20	1	0	-1.420909	0.117243	2.596565
21	1	0	-3.702811	-0.924237	2.596100
22	1	0	-5.875831	-1.324561	0.814347
23	1	0	-6.556104	-0.836985	-1.536640
24	1	0	-5.039183	0.391310	-3.069810
25	1	0	-2.807708	1.170974	-2.308145

26	1	0	3.892922	-3.309753	-1.748859
27	1	0	2.337309	-3.937627	-2.323846
28	1	0	3.470434	-3.172548	-3.491483
29	1	0	0.704094	-3.747992	3.374986
30	1	0	2.270318	-3.026161	3.770806
31	1	0	0.764842	-2.094320	4.091221
32	6	0	0.395362	1.832079	0.723985
33	1	0	0.491743	1.616501	1.791353
34	6	0	-0.721689	1.409882	-0.009871
35	1	0	1.227895	0.704899	-1.563099
36	1	0	-0.846637	1.888428	-0.985724
37	6	0	1.213089	2.976199	0.224231
38	8	0	1.025859	3.585674	-0.802377
39	8	0	2.203552	3.266988	1.091830
40	6	0	3.069761	4.336927	0.716830
41	1	0	2.504080	5.271672	0.583614
42	1	0	3.795917	4.443388	1.532282
43	1	0	3.587479	4.107534	-0.227107

TS5 E=-1255.818909

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.942914	-0.617841	-0.577508
2	6	0	3.147531	0.318950	0.139116
3	6	0	3.677411	0.913307	1.299411
4	6	0	4.960890	0.564879	1.709514
5	6	0	5.733593	-0.366046	0.981427
6	6	0	5.236867	-0.968940	-0.171259
7	6	0	1.973306	-0.423094	-1.654521
8	6	0	1.887283	0.438283	-0.569321
9	7	0	3.194511	-1.045796	-1.657898
10	46	0	-0.990059	0.029181	0.165458
11	8	0	-2.343453	-3.235668	-0.444225
12	8	0	-1.912863	0.304740	2.821519
13	6	0	-2.223905	-0.880963	2.562391
14	8	0	-1.967975	-1.422422	1.430637
15	6	0	-1.812139	-2.756042	-1.552448
16	8	0	-1.244810	-1.674954	-1.637865
17	6	0	-1.979045	-3.687693	-2.727374
18	6	0	-2.916125	-1.722885	3.606754
19	1	0	-2.231623	-2.605435	0.323776
20	1	0	1.220251	-0.663073	-2.402688
21	1	0	3.494197	-1.727787	-2.341751
22	1	0	5.834924	-1.689127	-0.735384
23	1	0	6.738843	-0.617789	1.328352
24	1	0	5.381276	1.018639	2.610328
25	1	0	3.091103	1.635817	1.872336
26	1	0	-3.859633	-2.113750	3.196038
27	1	0	-2.282625	-2.590019	3.850060
28	1	0	-3.113477	-1.140106	4.513947
29	1	0	-1.538598	-4.668404	-2.490373
30	1	0	-3.051422	-3.853565	-2.914598
31	1	0	-1.505116	-3.262574	-3.619677
32	6	0	-0.303377	1.666518	-1.015592
33	1	0	-0.360191	1.335199	-2.056730
34	6	0	0.771641	1.296779	-0.190726
35	1	0	-1.291552	0.713894	1.583122
36	1	0	0.924753	1.914256	0.699290
37	6	0	-1.104293	2.876416	-0.688050
38	8	0	-0.964547	3.586405	0.282067
39	8	0	-2.030992	3.110329	-1.644910
40	6	0	-2.871763	4.241305	-1.436179
41	1	0	-2.278632	5.165642	-1.359585

42	1	0	-3.541926	4.290621	-2.303819
43	1	0	-3.457040	4.130776	-0.509993

Int7 E=-1255.838301

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.798925	0.553467	-1.314199
2	6	0	2.921471	0.588848	-0.191833
3	6	0	3.372513	0.070973	1.037899
4	6	0	4.658794	-0.456049	1.120895
5	6	0	5.512131	-0.478364	-0.004226
6	6	0	5.094525	0.024457	-1.233904
7	6	0	1.860293	1.493358	-1.969400
8	6	0	1.679609	1.194685	-0.631345
9	7	0	3.121682	1.109199	-2.376870
10	46	0	-0.993663	-0.057485	-0.068103
11	8	0	-2.436294	-3.247275	-1.016319
12	8	0	0.317949	-1.315305	2.355338
13	6	0	0.137674	-2.372444	1.600419
14	8	0	-0.433554	-2.294263	0.510484
15	6	0	-3.201174	-2.186748	-1.227806
16	8	0	-2.918182	-1.056736	-0.859368
17	6	0	-4.466050	-2.512320	-1.976376
18	6	0	0.708730	-3.645500	2.149346
19	1	0	-1.636697	-2.987339	-0.495772
20	1	0	1.173475	1.962447	-2.670950
21	1	0	3.496931	1.240329	-3.305986
22	1	0	5.755614	0.006857	-2.104377
23	1	0	6.517812	-0.895702	0.091556
24	1	0	5.019396	-0.855204	2.072528
25	1	0	2.722236	0.077179	1.915788
26	1	0	0.290193	-4.510931	1.622112
27	1	0	1.800557	-3.624704	1.997234
28	1	0	0.525426	-3.716489	3.230423
29	1	0	-4.212053	-2.950315	-2.954266
30	1	0	-5.041418	-3.269931	-1.422315
31	1	0	-5.065423	-1.605213	-2.113641
32	6	0	-0.719413	2.016139	-0.235941
33	1	0	-0.856955	2.327905	-1.275814
34	6	0	0.494026	1.421429	0.209829
35	1	0	-0.063001	-0.532172	1.847222
36	1	0	0.714935	1.553047	1.276417
37	6	0	-1.590651	2.712476	0.739401
38	8	0	-1.448164	2.744946	1.944368
39	8	0	-2.613557	3.346247	0.113316
40	6	0	-3.540094	4.018204	0.956915
41	1	0	-3.039611	4.788086	1.564917
42	1	0	-4.281235	4.482925	0.293471
43	1	0	-4.036916	3.312575	1.641675

O_2 E=-150.39076

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.599983
2	8	0	0.000000	0.000000	-0.599983

TS6 E=-1406.23622

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.889761	0.583780	-1.312558
2	6	0	2.993441	0.753587	-0.217654
3	6	0	3.457220	0.482693	1.084284
4	6	0	4.771133	0.057217	1.261917
5	6	0	5.641289	-0.104125	0.161189
6	6	0	5.213415	0.157022	-1.137896
7	6	0	1.912287	1.282990	-2.130884
8	6	0	1.725497	1.202304	-0.761390
9	7	0	3.198583	0.912311	-2.458255
10	46	0	-0.926592	-0.063905	-0.179874
11	8	0	-1.961519	-3.417875	-1.149394
12	8	0	0.778410	-1.356771	2.283804
13	6	0	0.610120	-2.340673	1.427307
14	8	0	-0.125313	-2.233157	0.447342
15	6	0	-2.818133	-2.453430	-1.455132
16	8	0	-2.668928	-1.284143	-1.137700
17	6	0	-4.005496	-2.948189	-2.237268
18	6	0	1.412128	-3.567765	1.741705
19	1	0	-1.222374	-3.052865	-0.604530
20	1	0	1.210794	1.583028	-2.906513
21	1	0	3.580543	0.906990	-3.394052
22	1	0	5.887572	0.034616	-1.989628
23	1	0	6.668476	-0.436412	0.331736
24	1	0	5.140010	-0.150196	2.269639
25	1	0	2.797531	0.601278	1.946420
26	1	0	1.100283	-4.402839	1.103972
27	1	0	2.475519	-3.342126	1.559114
28	1	0	1.308952	-3.827954	2.804921
29	1	0	-3.662762	-3.473239	-3.142028
30	1	0	-4.565496	-3.677908	-1.631685
31	1	0	-4.654685	-2.107397	-2.506696
32	6	0	-0.691302	2.011661	-0.540108
33	1	0	-0.797300	2.198794	-1.612772
34	6	0	0.511232	1.500009	0.011162
35	1	0	0.215917	-0.596624	2.003267
36	1	0	0.677066	1.729399	1.070352
37	6	0	-1.612758	2.788683	0.321924
38	8	0	-1.491292	2.980798	1.513212
39	8	0	-2.647994	3.288398	-0.395342
40	6	0	-3.620059	4.019842	0.342492
41	1	0	-3.163561	4.879420	0.857633
42	1	0	-4.364341	4.366129	-0.386388
43	1	0	-4.101442	3.382091	1.100492
44	8	0	-2.499107	-0.085989	1.749637
45	8	0	-1.963783	-0.218059	2.845216

$Int8_{triplet}$ E=-1406.247785

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.116591	-0.684771	0.473327
2	6	0	-3.247553	0.206261	-0.212065
3	6	0	-3.573478	0.605643	-1.520969
4	6	0	-4.744865	0.122836	-2.097448
5	6	0	-5.599098	-0.754667	-1.394830
6	6	0	-5.297242	-1.172388	-0.101132
7	6	0	-2.387485	-0.226150	1.844396
8	6	0	-2.141986	0.496360	0.683824
9	7	0	-3.557529	-0.923602	1.717257
10	46	0	0.803130	0.041586	-0.192643

11	8	0	2.076998	-2.986526	1.196802
12	8	0	3.011759	-0.727568	-2.782154
13	6	0	2.973268	-1.583256	-1.880883
14	8	0	2.116507	-1.586994	-0.923727
15	6	0	1.367491	-2.305875	2.058166
16	8	0	0.811690	-1.236033	1.806616
17	6	0	1.279151	-2.951769	3.418209
18	6	0	3.978747	-2.717555	-1.890475
19	1	0	2.121057	-2.491201	0.300079
20	1	0	-1.788880	-0.295553	2.749622
21	1	0	-3.958638	-1.516521	2.431837
22	1	0	-5.955959	-1.855140	0.441389
23	1	0	-6.511601	-1.115348	-1.875863
24	1	0	-5.009055	0.424286	-3.113930
25	1	0	-2.913735	1.273938	-2.079469
26	1	0	4.470044	-2.796150	-0.908554
27	1	0	3.451212	-3.668642	-2.067579
28	1	0	4.726513	-2.563067	-2.677731
29	1	0	0.833169	-3.953831	3.321359
30	1	0	2.292682	-3.088886	3.825655
31	1	0	0.681548	-2.334964	4.099407
32	6	0	0.049147	1.682982	1.202991
33	1	0	0.182580	1.219090	2.182129
34	6	0	-1.033827	1.383508	0.392582
35	1	0	1.977223	0.227989	-2.966861
36	1	0	-1.137904	2.004615	-0.502972
37	6	0	0.891348	2.873103	0.922216
38	8	0	0.756128	3.643666	-0.000538
39	8	0	1.855395	3.006071	1.862213
40	6	0	2.735479	4.115088	1.699744
41	1	0	2.177574	5.064158	1.696394
42	1	0	3.428861	4.084407	2.549709
43	1	0	3.291933	4.040018	0.752553
44	8	0	0.514646	1.124974	-2.089484
45	8	0	1.207511	0.932027	-3.182520

$Int8_{singlet}$ E=-1406.273981

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.107823	0.411846	0.137460
2	6	0	-2.962329	0.728952	-0.640058
3	6	0	-3.026661	0.588756	-2.037926
4	6	0	-4.216776	0.152589	-2.614044
5	6	0	-5.345358	-0.150608	-1.822466
6	6	0	-5.307651	-0.026738	-0.435718
7	6	0	-2.480176	1.059212	1.554855
8	6	0	-1.922444	1.144904	0.284899
9	7	0	-3.771942	0.623815	1.465575
10	46	0	0.952657	-0.093190	0.055309
11	8	0	0.241396	-3.129662	1.431967
12	8	0	3.123283	-2.016520	-1.993772
13	6	0	2.313640	-2.652775	-1.328006
14	8	0	1.485428	-2.128483	-0.462712
15	6	0	-0.119637	-2.125558	2.164330
16	8	0	0.062382	-0.933569	1.865323
17	6	0	-0.811494	-2.495720	3.449961
18	6	0	2.204770	-4.161411	-1.466974
19	1	0	0.759186	-2.805931	0.577156
20	1	0	-2.034103	1.291813	2.519152
21	1	0	-4.402123	0.515492	2.249647
22	1	0	-6.180435	-0.263381	0.177875
23	1	0	-6.264638	-0.490159	-2.305767
24	1	0	-4.280678	0.040796	-3.698999

25	1	0	-2.158457	0.813992	-2.661888
26	1	0	2.329055	-4.644255	-0.484735
27	1	0	1.201752	-4.427252	-1.836949
28	1	0	2.965976	-4.532633	-2.163966
29	1	0	-1.744673	-3.031965	3.216094
30	1	0	-0.176617	-3.187901	4.023353
31	1	0	-1.029938	-1.601013	4.044129
32	6	0	0.471317	1.876299	0.787464
33	1	0	0.385437	1.728297	1.868265
34	6	0	-0.595479	1.590821	-0.073016
35	1	0	3.287929	-0.417040	-1.667441
36	1	0	-0.459434	1.923172	-1.107812
37	6	0	1.540838	2.828502	0.341403
38	8	0	1.433496	3.614412	-0.566447
39	8	0	2.634809	2.705851	1.113081
40	6	0	3.777881	3.457980	0.701653
41	1	0	3.532033	4.526107	0.606715
42	1	0	4.538918	3.305677	1.477069
43	1	0	4.140816	3.082658	-0.266721
44	8	0	1.807549	0.713043	-1.493990
45	8	0	3.173616	0.516334	-1.317366

$Sc(OTf)_3$ E=-3646.290346

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	21	0	-0.445419	-0.196403	0.215892
2	8	0	1.093710	-1.245518	0.633508
3	16	0	2.080390	-2.412620	0.178564
4	8	0	1.557365	-3.026706	-1.031253
5	8	0	2.501560	-3.182828	1.330561
6	6	0	3.530531	-1.338754	-0.336939
7	8	0	-1.902608	-1.095473	-1.029637
8	16	0	-2.911955	-1.385441	0.087622
9	8	0	-2.143270	-0.891292	1.313885
10	8	0	-3.544272	-2.678536	0.134135
11	6	0	-4.226473	-0.069638	-0.170861
12	8	0	-0.393490	1.724519	1.137772
13	16	0	0.026612	2.487981	-0.122109
14	8	0	-0.683982	3.694749	-0.463740
15	8	0	0.081148	1.354843	-1.149342
16	6	0	1.828139	2.927439	0.183172
17	9	0	3.128826	-0.465677	-1.259860
18	9	0	4.007541	-0.680069	0.710387
19	9	0	4.475468	-2.114472	-0.844956
20	9	0	-5.080021	-0.105323	0.834694
21	9	0	-4.849610	-0.298089	-1.311128
22	9	0	-3.622190	1.114720	-0.212609
23	9	0	2.476884	1.836587	0.566202
24	9	0	1.883912	3.843805	1.132178
25	9	0	2.347030	3.395340	-0.936940

$Pd(OAc)_2$-$Sc(OTf)_3$ E= -4231.556786

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.578715	-1.666155	0.053279
2	8	0	-0.324057	0.323577	1.901760
3	8	0	-1.436934	-1.790733	-1.958518
4	6	0	-0.987430	-0.514800	2.582010
5	8	0	-1.651173	-1.464989	2.062591

6	6	0	-0.722056	-0.916807	-2.541274
7	8	0	-0.092627	-0.012031	-1.916541
8	6	0	-0.961368	-0.420446	4.079602
9	1	0	-1.772734	-1.006352	4.527182
10	1	0	0.006508	-0.828226	4.415735
11	1	0	-1.011200	0.632556	4.388978
12	6	0	-0.660191	-0.945230	-4.039665
13	1	0	-1.319701	-0.143956	-4.411948
14	1	0	0.363173	-0.723555	-4.372750
15	1	0	-1.007111	-1.908779	-4.431232
16	21	0	0.257379	0.741946	-0.035901
17	8	0	1.580703	-0.885328	0.214394
18	16	0	1.411912	-2.308338	0.700296
19	8	0	0.076714	-2.871381	0.221248
20	8	0	1.740533	-2.542721	2.093323
21	6	0	2.620514	-3.260868	-0.371819
22	8	0	-1.668955	1.608471	-0.242061
23	16	0	-3.004145	1.034036	-0.663007
24	8	0	-3.170634	-0.380418	-0.114401
25	8	0	-3.364542	1.223863	-2.054765
26	6	0	-4.217684	1.984213	0.404851
27	8	0	1.394335	2.326443	-0.021809
28	16	0	2.695132	2.787772	-0.784912
29	8	0	2.607496	4.185505	-1.162897
30	8	0	3.085970	1.755168	-1.739045
31	6	0	3.906145	2.685740	0.642462
32	9	0	2.335675	-3.045740	-1.647334
33	9	0	3.844404	-2.840506	-0.104359
34	9	0	2.512305	-4.549399	-0.095865
35	9	0	-5.439790	1.540920	0.166392
36	9	0	-4.132814	3.268055	0.100211
37	9	0	-3.912022	1.803176	1.681984
38	9	0	3.872331	1.465618	1.176204
39	9	0	3.594705	3.577727	1.574140
40	9	0	5.128363	2.930241	0.187056

React’ E=-4595.554486

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.175420	-2.952569	-1.683945
2	6	0	2.201097	-2.828597	-0.664103
3	6	0	0.981154	-3.509255	-0.780190
4	6	0	0.759320	-4.281683	-1.921253
5	6	0	1.733197	-4.378501	-2.934309
6	6	0	2.958609	-3.715106	-2.833688
7	6	0	4.074676	-1.624972	-0.088476
8	6	0	2.758231	-1.944212	0.355923
9	7	0	4.293216	-2.215339	-1.289890
10	46	0	2.527949	0.188983	-0.081976
11	8	0	2.149992	-0.063599	-2.111001
12	8	0	2.808558	0.528624	1.846276
13	6	0	4.011368	0.758836	2.320423
14	8	0	5.055743	0.588096	1.706718
15	6	0	1.012924	-0.073741	-2.625076
16	8	0	-0.069173	-0.051217	-1.930326
17	6	0	0.870808	-0.083157	-4.119760
18	6	0	3.971244	1.274488	3.748705
19	1	0	2.416528	-1.916404	1.390773
20	1	0	4.853427	-1.078004	0.450954
21	1	0	5.115578	-2.057134	-1.860223
22	1	0	3.714516	-3.800078	-3.617627
23	1	0	1.530054	-4.991448	-3.815954
24	1	0	-0.183382	-4.822285	-2.032479

25	1	0	0.232736	-3.424719	0.009085
26	1	0	3.337014	0.627422	4.372294
27	1	0	4.989932	1.322986	4.153451
28	1	0	3.518652	2.278426	3.757389
29	1	0	0.535295	0.921360	-4.426970
30	1	0	1.827133	-0.310995	-4.604403
31	1	0	0.095045	-0.801781	-4.419619
32	21	0	-1.386752	0.377138	-0.536568
33	8	0	-3.071533	1.662256	-0.952164
34	16	0	-3.975686	0.582407	-1.542670
35	8	0	-4.674287	0.868576	-2.774116
36	8	0	-3.084519	-0.647720	-1.477260
37	6	0	-5.258562	0.294833	-0.205950
38	8	0	-1.264379	-0.795790	1.007975
39	16	0	-0.951813	-1.427247	2.406642
40	8	0	0.262156	-2.235841	2.333728
41	8	0	-1.157907	-0.465861	3.474142
42	6	0	-2.366928	-2.653340	2.489709
43	8	0	-0.342609	2.026825	0.079913
44	16	0	0.747301	2.881237	-0.577315
45	8	0	2.101516	2.324029	-0.284943
46	8	0	0.452911	3.233862	-1.959168
47	6	0	0.677078	4.440755	0.458045
48	9	0	-5.956022	-0.790452	-0.500907
49	9	0	-4.638565	0.128907	0.956762
50	9	0	-6.061654	1.343865	-0.140016
51	9	0	-0.523770	4.985219	0.332622
52	9	0	0.907591	4.146660	1.726752
53	9	0	1.599186	5.282559	0.015416
54	9	0	-3.530595	-2.017959	2.409052
55	9	0	-2.299314	-3.305522	3.642364
56	9	0	-2.275226	-3.523950	1.485772

TS1’ E= -4595.532206

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.650578	-2.601416	-2.097680
2	6	0	2.874802	-2.127192	-1.012005
3	6	0	1.719542	-2.835791	-0.647451
4	6	0	1.366950	-3.967227	-1.383259
5	6	0	2.150225	-4.412205	-2.466851
6	6	0	3.313506	-3.737906	-2.838133
7	6	0	4.691328	-0.783976	-1.276950
8	6	0	3.553372	-0.946628	-0.454638
9	7	0	4.748672	-1.745041	-2.219072
10	46	0	2.524727	0.798948	-0.078641
11	8	0	2.148874	0.916323	-2.118685
12	8	0	2.818044	0.795511	1.903810
13	6	0	3.400789	-0.106439	2.592534
14	8	0	4.042143	-1.072846	2.115667
15	6	0	1.030218	0.745171	-2.639825
16	8	0	-0.007765	0.374930	-1.972398
17	6	0	0.843537	1.010219	-4.106429
18	6	0	3.254966	0.014151	4.090406
19	1	0	3.861892	-1.047586	0.785394
20	1	0	5.471809	-0.025939	-1.210828
21	1	0	5.500789	-1.859908	-2.889525
22	1	0	3.933847	-4.090088	-3.665930
23	1	0	1.847589	-5.304650	-3.019802
24	1	0	0.468221	-4.523880	-1.107388
25	1	0	1.121391	-2.514162	0.205216
26	1	0	2.306852	-0.481754	4.354124
27	1	0	4.080793	-0.499269	4.598700

28	1	0	3.192111	1.067405	4.392717
29	1	0	0.317402	1.974973	-4.199130
30	1	0	1.810212	1.076932	-4.619313
31	1	0	0.208493	0.234074	-4.556252
32	21	0	-1.417838	0.316178	-0.609439
33	8	0	-3.356457	1.155866	-1.030714
34	16	0	-3.939475	-0.073594	-1.725972
35	8	0	-4.657860	0.117104	-2.964866
36	8	0	-2.768895	-1.040897	-1.699771
37	6	0	-5.141470	-0.764774	-0.464258
38	8	0	-1.077767	-0.898792	0.882394
39	16	0	-0.785392	-1.311704	2.362479
40	8	0	0.633087	-1.610845	2.537232
41	8	0	-1.491795	-0.454686	3.299357
42	6	0	-1.658899	-2.970007	2.367961
43	8	0	-0.851545	2.097004	0.208294
44	16	0	0.188778	3.153723	-0.185438
45	8	0	1.551501	2.747133	0.256168
46	8	0	0.028526	3.632154	-1.552778
47	6	0	-0.248692	4.555752	0.975476
48	9	0	-5.577361	-1.943622	-0.879704
49	9	0	-4.514302	-0.901246	0.698105
50	9	0	-6.158959	0.070127	-0.329074
51	9	0	-1.489017	4.950080	0.726073
52	9	0	-0.149362	4.150709	2.229997
53	9	0	0.590562	5.558709	0.758333
54	9	0	-2.950272	-2.809138	2.100745
55	9	0	-1.522577	-3.520279	3.567395
56	9	0	-1.121243	-3.774349	1.452694

Int1’ E= -4595.543497

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.320312	-2.245883	-1.828645
2	6	0	3.217891	-1.680370	-1.118580
3	6	0	2.138782	-2.516954	-0.766839
4	6	0	2.173884	-3.856893	-1.135326
5	6	0	3.270455	-4.392761	-1.846844
6	6	0	4.358060	-3.598861	-2.196485
7	6	0	4.774832	-0.069130	-1.473418
8	6	0	3.536430	-0.281629	-0.893342
9	7	0	5.242998	-1.241269	-2.029220
10	46	0	2.365308	1.174291	-0.241259
11	8	0	1.850070	1.501308	-2.211587
12	8	0	2.794234	0.956981	1.757474
13	6	0	3.390537	0.097846	2.422551
14	8	0	4.129296	-0.841131	1.899520
15	6	0	0.747729	1.210613	-2.712348
16	8	0	-0.183451	0.599175	-2.061966
17	6	0	0.448875	1.609026	-4.129122
18	6	0	3.275676	0.073422	3.913234
19	1	0	4.085572	-0.780105	0.906319
20	1	0	5.354936	0.848715	-1.552910
21	1	0	6.142362	-1.355818	-2.477936
22	1	0	5.212100	-4.015257	-2.736977
23	1	0	3.268444	-5.450849	-2.120353
24	1	0	1.341820	-4.509141	-0.860370
25	1	0	1.301463	-2.125137	-0.189849
26	1	0	2.407198	-0.565040	4.144916
27	1	0	4.172910	-0.362588	4.370714
28	1	0	3.078941	1.083279	4.293276
29	1	0	-0.234480	2.473634	-4.091208
30	1	0	1.366318	1.896973	-4.655556

31	1	0	-0.067651	0.791719	-4.652026
32	21	0	-1.507168	0.206638	-0.673123
33	8	0	-3.556940	0.793708	-0.964893
34	16	0	-3.991142	-0.447385	-1.744609
35	8	0	-4.778856	-0.261885	-2.941242
36	8	0	-2.696830	-1.236821	-1.833709
37	6	0	-5.031696	-1.404088	-0.512974
38	8	0	-0.925817	-1.084518	0.693324
39	16	0	-0.645840	-1.439082	2.188699
40	8	0	0.791935	-1.467994	2.448836
41	8	0	-1.548154	-0.728258	3.080138
42	6	0	-1.196004	-3.229946	2.166428
43	8	0	-1.151533	1.940870	0.327992
44	16	0	-0.285038	3.180564	0.060461
45	8	0	1.130065	2.921916	0.434759
46	8	0	-0.554327	3.794098	-1.233584
47	6	0	-0.896304	4.347380	1.389866
48	9	0	-5.297828	-2.601625	-1.009757
49	9	0	-4.352053	-1.528527	0.621018
50	9	0	-6.158672	-0.747633	-0.290559
51	9	0	-2.189582	4.569830	1.208125
52	9	0	-0.695777	3.816312	2.585219
53	9	0	-0.228917	5.488675	1.288339
54	9	0	-2.482490	-3.305965	1.844294
55	9	0	-1.013674	-3.744372	3.376452
56	9	0	-0.481736	-3.921589	1.283284

Int2’ E= -4902.169196

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.262941	-0.427651	-0.403826
2	6	0	4.845332	-0.616405	-0.361863
3	6	0	4.312476	-1.819509	-0.868724
4	6	0	5.173953	-2.785358	-1.378041
5	6	0	6.570992	-2.581825	-1.399558
6	6	0	7.130640	-1.402900	-0.916094
7	6	0	5.347088	1.426110	0.487933
8	6	0	4.292439	0.584103	0.221466
9	7	0	6.532585	0.815000	0.122325
10	46	0	2.421009	0.928829	0.773753
11	8	0	0.536409	1.437817	1.773176
12	8	0	2.850943	-0.214694	2.530718
13	6	0	2.997146	-1.362251	2.955851
14	8	0	2.585288	-2.446228	2.359099
15	6	0	-0.646302	1.082142	1.741374
16	8	0	-1.069772	0.116026	0.987611
17	6	0	-1.677590	1.789148	2.583508
18	6	0	3.714475	-1.620864	4.250798
19	1	0	2.077346	-2.298201	1.518943
20	1	0	5.354588	2.433822	0.895169
21	1	0	7.448116	1.239812	0.180176
22	1	0	8.211469	-1.239700	-0.938708
23	1	0	7.222539	-3.358855	-1.807165
24	1	0	4.760073	-3.715844	-1.774380
25	1	0	3.236677	-1.990077	-0.875594
26	1	0	3.223319	-2.428746	4.810143
27	1	0	4.738673	-1.952876	4.013108
28	1	0	3.767030	-0.701423	4.845237
29	1	0	-2.342249	1.060176	3.069387
30	1	0	-1.196160	2.439052	3.323857
31	1	0	-2.289428	2.404925	1.904752
32	21	0	-2.451195	-0.817669	-0.028667
33	8	0	-4.315477	-1.968305	-0.317418

34	16	0	-4.792539	-1.831810	1.115310
35	8	0	-5.282793	-3.001879	1.806193
36	8	0	-3.655664	-1.037774	1.760404
37	6	0	-6.199747	-0.596617	1.027210
38	8	0	-2.850638	0.651000	-1.280100
39	16	0	-2.402849	2.083899	-1.713529
40	8	0	-1.417856	2.627563	-0.774640
41	8	0	-2.177411	2.158837	-3.144697
42	6	0	-3.991399	3.008351	-1.355347
43	8	0	-1.255922	-2.281475	-0.739750
44	16	0	0.257622	-2.398925	-0.998248
45	8	0	0.737258	-1.407073	-1.954214
46	8	0	0.994680	-2.588443	0.261486
47	6	0	0.335912	-4.061418	-1.852885
48	9	0	-6.623647	-0.335006	2.254735
49	9	0	-5.763714	0.522507	0.458541
50	9	0	-7.186203	-1.107862	0.309757
51	9	0	-0.169945	-5.000416	-1.066801
52	9	0	-0.343373	-4.013950	-2.988429
53	9	0	1.611000	-4.335548	-2.107602
54	9	0	-4.986926	2.520163	-2.081322
55	9	0	-3.818563	4.291788	-1.644848
56	9	0	-4.296619	2.891783	-0.059986
57	6	0	1.928999	2.583217	-0.588600
58	1	0	0.919545	2.841139	-0.259597
59	6	0	2.141279	1.446534	-1.351356
60	1	0	3.081398	1.325268	-1.893025
61	1	0	1.313278	0.792022	-1.632886
62	6	0	2.927057	3.699784	-0.523215
63	8	0	3.984709	3.742481	-1.104133
64	8	0	2.466954	4.684249	0.268411
65	6	0	3.290463	5.844214	0.385937
66	1	0	3.482400	6.287064	-0.602971
67	1	0	2.738270	6.547837	1.020336
68	1	0	4.257254	5.593108	0.848811

TS2’ E= -4902.158415

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.298098	0.156949	-0.433870
2	6	0	4.925103	-0.235504	-0.470168
3	6	0	4.606312	-1.539060	-0.900192
4	6	0	5.635288	-2.404137	-1.260330
5	6	0	6.986453	-1.998849	-1.204326
6	6	0	7.334621	-0.715227	-0.792847
7	6	0	5.067201	1.923313	0.227698
8	6	0	4.160708	0.908251	-0.021239
9	7	0	6.345361	1.468622	-0.006437
10	46	0	2.336751	0.906393	0.833974
11	8	0	0.599704	1.062794	2.102803
12	8	0	3.187844	-0.327328	2.413784
13	6	0	3.340080	-1.519808	2.674598
14	8	0	2.762449	-2.511692	2.045806
15	6	0	-0.606618	0.823064	1.968665
16	8	0	-1.109234	0.325954	0.883498
17	6	0	-1.567206	1.123353	3.091305
18	6	0	4.264096	-1.966123	3.773378
19	1	0	2.133791	-2.237075	1.327775
20	1	0	4.878389	2.953258	0.525652
21	1	0	7.187879	2.017633	0.102886
22	1	0	8.379971	-0.397775	-0.755092
23	1	0	7.771636	-2.701580	-1.494033
24	1	0	5.393367	-3.414670	-1.598455

25	1	0	3.566502	-1.859278	-0.969311
26	1	0	3.812186	-2.787951	4.346051
27	1	0	5.187620	-2.351291	3.310804
28	1	0	4.513312	-1.120926	4.425120
29	1	0	-2.189125	0.239123	3.295352
30	1	0	-1.026362	1.438298	3.991371
31	1	0	-2.243985	1.928324	2.763443
32	21	0	-2.396835	-0.653518	-0.218535
33	8	0	-3.945858	-2.199925	-0.503087
34	16	0	-4.367969	-2.261507	0.951510
35	8	0	-4.534745	-3.551251	1.580824
36	8	0	-3.411352	-1.262620	1.604690
37	6	0	-6.026484	-1.388995	1.000837
38	8	0	-3.291189	0.801586	-1.207045
39	16	0	-2.803788	2.048408	-2.017348
40	8	0	-1.351509	1.996388	-2.179351
41	8	0	-3.673785	2.326046	-3.143908
42	6	0	-3.146598	3.388687	-0.748103
43	8	0	-1.051127	-1.738446	-1.269202
44	16	0	0.441643	-2.086862	-1.179692
45	8	0	1.273528	-1.275979	-2.060214
46	8	0	0.846957	-2.252092	0.230155
47	6	0	0.446280	-3.816081	-1.893965
48	9	0	-6.421045	-1.280428	2.261458
49	9	0	-5.901323	-0.180802	0.466991
50	9	0	-6.908346	-2.095441	0.312914
51	9	0	-0.358075	-4.599950	-1.190219
52	9	0	0.050033	-3.784899	-3.156290
53	9	0	1.689648	-4.284040	-1.827781
54	9	0	-4.453682	3.539998	-0.579226
55	9	0	-2.621382	4.534225	-1.169357
56	9	0	-2.594550	3.069849	0.427390
57	6	0	1.487852	2.167216	-0.642599
58	1	0	0.484775	1.745957	-0.739459
59	6	0	2.537323	1.652018	-1.417903
60	1	0	3.333933	2.320298	-1.734786
61	1	0	2.381536	0.735448	-1.989091
62	6	0	1.562607	3.589916	-0.187941
63	8	0	2.559012	4.279314	-0.208742
64	8	0	0.368604	4.016600	0.249885
65	6	0	0.292819	5.371498	0.693610
66	1	0	0.632222	6.059129	-0.095143
67	1	0	-0.762345	5.553063	0.928852
68	1	0	0.918474	5.524544	1.586306

Int3’ E= -4902.216631

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.592881	-1.038079	-0.708940
2	6	0	-4.394882	-0.711166	-1.397207
3	6	0	-4.407931	0.318647	-2.350871
4	6	0	-5.605321	0.992299	-2.589928
5	6	0	-6.782549	0.659564	-1.890814
6	6	0	-6.794244	-0.358026	-0.936140
7	6	0	-3.999482	-2.437610	0.061316
8	6	0	-3.355235	-1.609662	-0.893223
9	7	0	-5.316710	-2.094859	0.148824
10	46	0	-2.419961	-0.866536	0.943087
11	8	0	-1.183139	-0.350516	2.620531
12	8	0	-4.077293	0.264383	1.925971
13	6	0	-4.483678	1.424206	1.875167
14	8	0	-3.864679	2.416579	1.286986
15	6	0	-0.022714	0.053861	2.757612

16	8	0	0.763376	0.321652	1.768031
17	6	0	0.543949	0.280636	4.137158
18	6	0	-5.802180	1.822557	2.481756
19	1	0	-2.985860	2.179864	0.882125
20	1	0	-3.606607	-3.349076	0.512260
21	1	0	-5.967601	-2.484351	0.818980
22	1	0	-7.709043	-0.622018	-0.400027
23	1	0	-7.705555	1.205071	-2.102640
24	1	0	-5.631908	1.796558	-3.328731
25	1	0	-3.491886	0.602421	-2.870633
26	1	0	-5.728400	2.812698	2.952075
27	1	0	-6.546078	1.892390	1.671119
28	1	0	-6.129627	1.067543	3.206179
29	1	0	0.720782	1.359434	4.276875
30	1	0	-0.145640	-0.082212	4.908411
31	1	0	1.519953	-0.220496	4.221824
32	21	0	2.029937	0.691896	0.349810
33	8	0	3.375437	2.380428	0.435438
34	16	0	4.443126	1.722554	1.307678
35	8	0	4.992113	2.487523	2.404618
36	8	0	3.835571	0.363736	1.598289
37	6	0	5.834112	1.359896	0.104264
38	8	0	2.326454	-0.839375	-0.808151
39	16	0	2.539342	-1.893040	-1.943644
40	8	0	1.360657	-2.739710	-2.081551
41	8	0	3.170430	-1.283922	-3.102114
42	6	0	3.851783	-2.943769	-1.116521
43	8	0	0.768428	1.803003	-0.800851
44	16	0	-0.700367	2.182593	-0.990147
45	8	0	-1.326433	1.489598	-2.110075
46	8	0	-1.408527	2.206962	0.309042
47	6	0	-0.540166	3.979389	-1.486933
48	9	0	6.738175	0.599899	0.702573
49	9	0	5.337605	0.724269	-0.949505
50	9	0	6.387856	2.499653	-0.279133
51	9	0	0.102998	4.654668	-0.543603
52	9	0	0.118592	4.075006	-2.631802
53	9	0	-1.762229	4.482563	-1.633895
54	9	0	4.910658	-2.198239	-0.813743
55	9	0	4.219109	-3.908198	-1.951718
56	9	0	3.374789	-3.492243	-0.000147
57	6	0	-1.082700	-1.860768	-0.227162
58	1	0	-0.217300	-1.201608	-0.320662
59	6	0	-1.976717	-1.942050	-1.458797
60	1	0	-1.957943	-2.928608	-1.946993
61	1	0	-1.679792	-1.179724	-2.188848
62	6	0	-0.729750	-3.154955	0.420723
63	8	0	-1.379083	-4.179116	0.336728
64	8	0	0.397056	-3.062732	1.152855
65	6	0	0.831822	-4.258499	1.799227
66	1	0	1.016316	-5.052450	1.060803
67	1	0	1.763981	-4.003413	2.317457
68	1	0	0.076724	-4.614059	2.517070

Int4’ E= -4902.196269

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.445694	-1.460300	-2.572793
2	6	0	4.746785	-0.307133	-1.791606
3	6	0	6.090260	-0.026892	-1.478201
4	6	0	7.083814	-0.885749	-1.939944
5	6	0	6.763758	-2.023379	-2.712230
6	6	0	5.444161	-2.324959	-3.039754

7	6	0	2.504121	-0.439628	-2.085415
8	6	0	3.484851	0.332309	-1.493594
9	7	0	3.076493	-1.497299	-2.735371
10	46	0	2.137129	1.611363	1.368301
11	8	0	0.400632	2.488019	2.206163
12	8	0	2.672598	0.916664	3.370179
13	6	0	2.498172	-0.047841	4.112720
14	8	0	2.001883	-1.201287	3.743202
15	6	0	-0.759214	2.081630	2.020536
16	8	0	-1.019950	1.014334	1.348378
17	6	0	-1.927492	2.843869	2.588980
18	6	0	2.858715	0.007789	5.571983
19	1	0	1.834370	-1.282075	2.763199
20	1	0	1.425559	-0.318851	-2.085942
21	1	0	2.545040	-2.246012	-3.161652
22	1	0	5.196953	-3.204854	-3.638684
23	1	0	7.566062	-2.678695	-3.060267
24	1	0	8.130239	-0.678124	-1.703011
25	1	0	6.354667	0.850828	-0.881987
26	1	0	1.988733	-0.286230	6.178431
27	1	0	3.656862	-0.723056	5.776286
28	1	0	3.192939	1.015326	5.843331
29	1	0	-2.572503	2.167485	3.169888
30	1	0	-1.585333	3.679720	3.210069
31	1	0	-2.541471	3.218059	1.754396
32	21	0	-1.919094	-0.293224	0.194200
33	8	0	-3.563417	-0.949967	1.425524
34	16	0	-4.502375	0.216131	1.129955
35	8	0	-5.080528	0.913823	2.260605
36	8	0	-3.728915	1.026138	0.109106
37	6	0	-5.922383	-0.552873	0.177030
38	8	0	-2.590890	-1.210184	-1.729028
39	16	0	-1.623822	-0.440386	-2.598923
40	8	0	-0.897898	0.449380	-1.585613
41	8	0	-0.804642	-1.156351	-3.554567
42	6	0	-2.684915	0.748645	-3.587962
43	8	0	-0.746821	-1.870984	0.653527
44	16	0	0.623494	-2.538650	0.468825
45	8	0	0.878631	-2.938988	-0.906823
46	8	0	1.678233	-1.787786	1.182475
47	6	0	0.364948	-4.106505	1.459507
48	9	0	-6.727775	0.416542	-0.234512
49	9	0	-5.457772	-1.221683	-0.865704
50	9	0	-6.582654	-1.373571	0.980156
51	9	0	0.160122	-3.798142	2.735780
52	9	0	-0.680804	-4.769233	0.988718
53	9	0	1.452546	-4.859716	1.357335
54	9	0	-3.464737	0.047878	-4.397991
55	9	0	-1.889368	1.534497	-4.299984
56	9	0	-3.427166	1.482616	-2.774606
57	6	0	2.009359	2.237641	-0.562208
58	1	0	1.130975	1.796466	-1.045363
59	6	0	3.303856	1.545037	-0.659196
60	1	0	3.550682	1.151638	0.511725
61	1	0	4.139549	2.258023	-0.725733
62	6	0	2.030845	3.732089	-0.564458
63	8	0	3.021486	4.419847	-0.456276
64	8	0	0.787752	4.232800	-0.687619
65	6	0	0.676071	5.655939	-0.654880
66	1	0	1.276620	6.113991	-1.455047
67	1	0	-0.387461	5.882520	-0.799222
68	1	0	1.023192	6.051921	0.311733

TS3’ E= -4902.19134

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.340277	-1.783751	-2.308074
2	6	0	4.690127	-0.531575	-1.730458
3	6	0	6.044660	-0.253308	-1.475929
4	6	0	7.001128	-1.212996	-1.799166
5	6	0	6.632121	-2.448271	-2.372367
6	6	0	5.297884	-2.750540	-2.635742
7	6	0	2.434678	-0.640305	-1.982329
8	6	0	3.449825	0.191782	-1.527535
9	7	0	2.963699	-1.799270	-2.450941
10	46	0	2.221459	1.727891	1.196882
11	8	0	0.422174	2.727956	1.873697
12	8	0	2.584195	1.210334	3.254922
13	6	0	2.492282	0.244432	4.011426
14	8	0	2.141346	-0.964407	3.657853
15	6	0	-0.738155	2.313755	1.758036
16	8	0	-1.015786	1.158621	1.243447
17	6	0	-1.903836	3.151517	2.217134
18	6	0	2.792310	0.373524	5.479679
19	1	0	1.962264	-1.089884	2.684950
20	1	0	1.360551	-0.483236	-1.992848
21	1	0	2.398043	-2.593474	-2.727765
22	1	0	5.010220	-3.706516	-3.079554
23	1	0	7.406191	-3.180539	-2.614409
24	1	0	8.057077	-1.007827	-1.606895
25	1	0	6.347916	0.699077	-1.033208
26	1	0	1.921456	0.038630	6.063545
27	1	0	3.630639	-0.291632	5.738981
28	1	0	3.042514	1.411098	5.727019
29	1	0	-2.546322	2.567672	2.893505
30	1	0	-1.555729	4.066396	2.710581
31	1	0	-2.523499	3.404635	1.342255
32	21	0	-1.926862	-0.242075	0.236300
33	8	0	-3.550976	-0.791475	1.548030
34	16	0	-4.498307	0.340193	1.161612
35	8	0	-5.061111	1.139204	2.231229
36	8	0	-3.745781	1.053308	0.056094
37	6	0	-5.930644	-0.517241	0.308246
38	8	0	-2.623261	-1.315267	-1.602599
39	16	0	-1.658018	-0.630502	-2.541547
40	8	0	-0.908817	0.329996	-1.613535
41	8	0	-0.857462	-1.430051	-3.445698
42	6	0	-2.717984	0.486934	-3.611494
43	8	0	-0.753929	-1.789540	0.812719
44	16	0	0.573642	-2.524832	0.596918
45	8	0	0.721758	-3.044795	-0.756716
46	8	0	1.703745	-1.765747	1.170728
47	6	0	0.327858	-3.998689	1.724427
48	9	0	-6.740109	0.407689	-0.189120
49	9	0	-5.479713	-1.288859	-0.667511
50	9	0	-6.582613	-1.251762	1.197306
51	9	0	0.198897	-3.582817	2.979512
52	9	0	-0.757817	-4.665839	1.362669
53	9	0	1.389013	-4.790319	1.629047
54	9	0	-3.525181	-0.267140	-4.343231
55	9	0	-1.924042	1.193679	-4.404035
56	9	0	-3.431841	1.302276	-2.851895
57	6	0	2.090858	2.248084	-0.822004
58	1	0	1.161492	1.827664	-1.219164
59	6	0	3.306452	1.500964	-0.922205
60	1	0	3.577223	1.147238	0.688544
61	1	0	4.213198	2.115102	-0.885856
62	6	0	2.189639	3.738812	-0.862137
63	8	0	3.213774	4.378756	-0.777301
64	8	0	0.973575	4.295303	-1.010157

65	6	0	0.932257	5.722163	-1.028941
66	1	0	1.562939	6.121763	-1.837228
67	1	0	-0.117269	5.995392	-1.193814
68	1	0	1.287808	6.134686	-0.072409

Int5’ E= -4902.196407

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.497091	3.484758	-0.936558
2	6	0	-3.551633	2.641987	-0.502035
3	6	0	-4.601509	3.195065	0.250642
4	6	0	-4.565241	4.553888	0.552497
5	6	0	-3.502588	5.373078	0.114535
6	6	0	-2.453183	4.850474	-0.636190
7	6	0	-2.038929	1.420229	-1.689061
8	6	0	-3.252268	1.308721	-1.000737
9	7	0	-1.606817	2.702002	-1.654469
10	46	0	-2.868041	-1.669800	0.189474
11	8	0	-1.351116	-2.363043	-1.282784
12	8	0	-1.834063	-2.737717	1.707283
13	6	0	-1.372022	-2.587887	2.840865
14	8	0	-1.246247	-1.447322	3.458451
15	6	0	-0.119128	-2.423260	-1.222963
16	8	0	0.571407	-1.818548	-0.303462
17	6	0	0.666457	-3.204164	-2.247073
18	6	0	-0.867231	-3.764620	3.628245
19	1	0	-1.442734	-0.638290	2.901970
20	1	0	-1.439170	0.647528	-2.166250
21	1	0	-0.675968	2.995072	-1.950267
22	1	0	-1.624485	5.477483	-0.971658
23	1	0	-3.502600	6.435040	0.371883
24	1	0	-5.372468	4.996327	1.141356
25	1	0	-5.431073	2.574841	0.599051
26	1	0	0.234331	-3.766588	3.583115
27	1	0	-1.153641	-3.665609	4.684606
28	1	0	-1.247625	-4.700478	3.203042
29	1	0	1.401606	-3.849441	-1.743792
30	1	0	-0.001976	-3.797390	-2.882245
31	1	0	1.236601	-2.493470	-2.866985
32	21	0	1.881939	-0.414892	0.039016
33	8	0	3.264926	-1.338896	1.411995
34	16	0	4.180158	-1.970045	0.365744
35	8	0	4.522593	-3.367083	0.517870
36	8	0	3.558010	-1.514510	-0.939514
37	6	0	5.768460	-0.985137	0.504723
38	8	0	2.817684	1.519723	-0.596374
39	16	0	2.042712	1.657491	-1.884604
40	8	0	1.186713	0.400871	-1.916835
41	8	0	1.365376	2.913565	-2.170936
42	6	0	3.303024	1.446240	-3.258208
43	8	0	0.906606	0.510847	1.541797
44	16	0	-0.155057	1.554030	1.925529
45	8	0	-0.175848	2.695647	1.024912
46	8	0	-1.432732	0.887237	2.256267
47	6	0	0.529977	2.149169	3.563264
48	9	0	6.599125	-1.372234	-0.452559
49	9	0	5.501683	0.306528	0.370154
50	9	0	6.315070	-1.208659	1.690141
51	9	0	0.583628	1.135614	4.419760
52	9	0	1.746782	2.646133	3.386704
53	9	0	-0.269340	3.091984	4.043858
54	9	0	4.183598	2.432205	-3.181671
55	9	0	2.667919	1.499832	-4.421254

56	9	0	3.918755	0.282659	-3.139044
57	6	0	-4.051625	-1.079988	-1.479253
58	1	0	-3.387530	-1.242797	-2.331769
59	6	0	-4.072420	0.152766	-0.804148
60	1	0	-3.984094	-1.358869	1.163813
61	1	0	-4.951760	0.304154	-0.169907
62	6	0	-5.286323	-1.924349	-1.464128
63	8	0	-6.283362	-1.710222	-0.814281
64	8	0	-5.155359	-2.969378	-2.303534
65	6	0	-6.268275	-3.859131	-2.378680
66	1	0	-7.176113	-3.325707	-2.698882
67	1	0	-5.997118	-4.626482	-3.114151
68	1	0	-6.464717	-4.322353	-1.399556

TS4’ E= -5052.571584

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.311152	3.148765	-1.755560
2	6	0	-3.379872	2.294735	-1.380074
3	6	0	-4.565917	2.862463	-0.885448
4	6	0	-4.650465	4.249763	-0.782755
5	6	0	-3.573208	5.078996	-1.157235
6	6	0	-2.385209	4.540018	-1.647792
7	6	0	-1.622893	1.045314	-2.123734
8	6	0	-2.929536	0.932715	-1.621502
9	7	0	-1.272693	2.344859	-2.205725
10	46	0	-2.741062	-1.534759	0.343711
11	8	0	-1.075816	-3.019125	-0.071000
12	8	0	-2.327112	-1.786162	2.440180
13	6	0	-2.086937	-1.217003	3.505755
14	8	0	-1.786417	0.046137	3.635915
15	6	0	0.143263	-2.908216	0.068315
16	8	0	0.718719	-1.774180	0.342646
17	6	0	1.057175	-4.100498	-0.084849
18	6	0	-2.109318	-1.964804	4.810513
19	1	0	-1.686566	0.554848	2.780840
20	1	0	-0.913914	0.266711	-2.396994
21	1	0	-0.326691	2.657833	-2.425985
22	1	0	-1.542711	5.175234	-1.928034
23	1	0	-3.669364	6.162731	-1.056271
24	1	0	-5.566012	4.705142	-0.397625
25	1	0	-5.401316	2.232316	-0.573329
26	1	0	-1.093682	-1.975953	5.236686
27	1	0	-2.755594	-1.436536	5.527349
28	1	0	-2.462569	-2.990524	4.656987
29	1	0	1.748155	-4.160774	0.769487
30	1	0	0.475190	-5.024992	-0.177724
31	1	0	1.680318	-3.959864	-0.982665
32	21	0	2.029244	-0.348172	0.218672
33	8	0	3.429211	-0.836968	1.784294
34	16	0	4.285445	-1.808407	0.977189
35	8	0	4.549539	-3.111533	1.550575
36	8	0	3.660709	-1.742660	-0.402043
37	6	0	5.933363	-0.932814	0.802321
38	8	0	3.102209	1.351248	-0.835183
39	16	0	2.349220	1.196103	-2.130345
40	8	0	1.451499	-0.010190	-1.877198
41	8	0	1.705627	2.358256	-2.726337
42	6	0	3.615377	0.619611	-3.388523
43	8	0	1.032617	0.999814	1.346894
44	16	0	0.056089	2.183572	1.363244
45	8	0	0.253164	3.098374	0.248228
46	8	0	-1.316062	1.717233	1.653641

47	6	0	0.625105	3.075901	2.908028
48	9	0	6.721626	-1.658940	0.022578
49	9	0	5.747577	0.262208	0.261901
50	9	0	6.483254	-0.803292	2.000200
51	9	0	0.450665	2.293993	3.967618
52	9	0	1.907773	3.391059	2.795425
53	9	0	-0.093260	4.181611	3.051749
54	9	0	4.476366	1.603066	-3.602372
55	9	0	2.984589	0.321465	-4.516103
56	9	0	4.254090	-0.446059	-2.937132
57	6	0	-3.290481	-1.583485	-1.712044
58	1	0	-2.367267	-1.784154	-2.261698
59	6	0	-3.673414	-0.267571	-1.390594
60	1	0	-4.158946	-0.849085	0.891823
61	1	0	-4.722010	-0.138767	-1.096788
62	6	0	-4.343518	-2.635026	-1.825505
63	8	0	-5.486508	-2.530098	-1.439450
64	8	0	-3.858058	-3.736737	-2.424596
65	6	0	-4.764580	-4.830538	-2.563410
66	1	0	-5.653630	-4.532199	-3.139175
67	1	0	-4.213633	-5.618616	-3.091144
68	1	0	-5.093534	-5.191350	-1.576829
69	8	0	-5.200717	-0.452325	1.553115
70	8	0	-6.035795	0.117450	0.828666

TS5’ E= -4902.185153

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.581757	-0.481611	-2.639532
2	6	0	-4.693925	-0.995924	-1.319795
3	6	0	-5.944161	-0.957847	-0.678672
4	6	0	-7.032932	-0.418743	-1.360223
5	6	0	-6.898555	0.085899	-2.670914
6	6	0	-5.671273	0.061381	-3.329697
7	6	0	-2.542585	-1.211962	-2.033018
8	6	0	-3.371073	-1.458589	-0.936583
9	7	0	-3.261473	-0.640985	-3.030679
10	46	0	-1.929902	-0.364055	1.499024
11	8	0	0.175912	-1.281111	3.703086
12	8	0	-2.134243	1.412033	2.767660
13	6	0	-2.831619	2.424139	2.727597
14	8	0	-3.456079	2.841522	1.647357
15	6	0	1.204267	-0.942329	3.140780
16	8	0	1.217630	-0.379768	1.944163
17	6	0	2.568780	-1.142166	3.762828
18	6	0	-3.027338	3.307569	3.924990
19	1	0	-3.154094	2.314341	0.863889
20	1	0	-1.478885	-1.396013	-2.165487
21	1	0	-2.855912	-0.306483	-3.896724
22	1	0	-5.564627	0.451639	-4.344572
23	1	0	-7.771913	0.502678	-3.178209
24	1	0	-8.010538	-0.385354	-0.873278
25	1	0	-6.064042	-1.344260	0.336557
26	1	0	-2.477960	4.249152	3.763431
27	1	0	-4.091244	3.564935	4.031815
28	1	0	-2.652676	2.811951	4.827604
29	1	0	3.134437	-0.198226	3.760196
30	1	0	2.467942	-1.524085	4.785897
31	1	0	3.144715	-1.854220	3.150541
32	21	0	1.819037	0.184907	0.208110
33	8	0	3.178191	1.812424	0.685819
34	16	0	4.399500	0.940766	0.948477

35	8	0	5.103336	1.123733	2.201823
36	8	0	3.905359	-0.452369	0.604400
37	6	0	5.610053	1.384472	-0.413032
38	8	0	2.375139	0.110141	-2.019752
39	16	0	1.671366	-1.196640	-2.262443
40	8	0	1.127968	-1.566399	-0.879504
41	8	0	0.739625	-1.316677	-3.369155
42	6	0	3.029530	-2.449337	-2.580459
43	8	0	0.284667	1.469391	-0.279120
44	16	0	-0.965502	1.900605	-1.027732
45	8	0	-0.948539	1.618846	-2.454053
46	8	0	-2.183585	1.484790	-0.270667
47	6	0	-0.883404	3.760748	-0.818859
48	9	0	6.641596	0.553696	-0.345987
49	9	0	5.028687	1.280420	-1.596217
50	9	0	6.025142	2.629257	-0.225087
51	9	0	-0.828842	4.064320	0.475833
52	9	0	0.190485	4.230066	-1.430777
53	9	0	-1.974687	4.298776	-1.349219
54	9	0	3.649110	-2.124563	-3.706534
55	9	0	2.483479	-3.651632	-2.701469
56	9	0	3.893724	-2.449759	-1.578301
57	6	0	-1.683524	-2.378384	0.711330
58	1	0	-0.846621	-2.317852	0.010516
59	6	0	-2.985496	-2.017069	0.332931
60	1	0	-1.488042	-1.092373	2.733312
61	1	0	-3.788727	-2.347605	1.000220
62	6	0	-1.517767	-3.379766	1.812910
63	8	0	-2.398486	-3.777585	2.539865
64	8	0	-0.246171	-3.809942	1.875727
65	6	0	0.062517	-4.706237	2.943969
66	1	0	-0.622933	-5.566210	2.946832
67	1	0	1.094401	-5.038584	2.774968
68	1	0	-0.015563	-4.181709	3.908339

Int6’ E= -4902.188871

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.297353	-3.458277	-0.801924
2	6	0	4.149583	-2.347205	-0.540446
3	6	0	5.361796	-2.564838	0.140533
4	6	0	5.687564	-3.856503	0.544046
5	6	0	4.825181	-4.943397	0.279534
6	6	0	3.621919	-4.759687	-0.396455
7	6	0	2.307579	-1.626788	-1.640094
8	6	0	3.496535	-1.173597	-1.086536
9	7	0	2.198249	-2.981730	-1.484645
10	46	0	2.675925	1.424624	0.143438
11	8	0	0.149689	4.049372	0.192231
12	8	0	1.496103	2.456349	1.732694
13	6	0	1.621489	2.513235	2.969742
14	8	0	1.831333	1.467520	3.707197
15	6	0	-0.795108	3.399108	-0.395396
16	8	0	-0.948094	2.171917	-0.216288
17	6	0	-1.705703	4.177091	-1.288833
18	6	0	1.571984	3.816203	3.712893
19	1	0	1.779743	0.602944	3.193244
20	1	0	1.511724	-1.061918	-2.119551
21	1	0	1.344649	-3.493801	-1.676273
22	1	0	2.953211	-5.599321	-0.601482
23	1	0	5.107528	-5.945984	0.611090
24	1	0	6.625611	-4.036259	1.075558

25	1	0	6.037724	-1.732535	0.352592
26	1	0	1.215918	3.669130	4.740399
27	1	0	2.596895	4.221777	3.758187
28	1	0	0.944233	4.541714	3.179229
29	1	0	-2.739223	4.056702	-0.927390
30	1	0	-1.426180	5.236165	-1.317678
31	1	0	-1.666061	3.741754	-2.299343
32	21	0	-1.774229	0.307782	-0.034560
33	8	0	-3.337916	0.896567	1.311492
34	16	0	-4.309790	1.444981	0.266699
35	8	0	-4.820860	2.786258	0.470337
36	8	0	-3.600373	1.147448	-1.036560
37	6	0	-5.770862	0.270104	0.324449
38	8	0	-2.440584	-1.722759	-0.533238
39	16	0	-1.664331	-1.818361	-1.833877
40	8	0	-1.011447	-0.439810	-1.922436
41	8	0	-0.825568	-2.975996	-2.068881
42	6	0	-2.960930	-1.850030	-3.192978
43	8	0	-0.574844	-0.326578	1.415723
44	16	0	0.319779	-1.452958	1.988945
45	8	0	0.418082	-2.597109	1.102078
46	8	0	1.545569	-0.873994	2.568657
47	6	0	-0.718309	-1.972097	3.461581
48	9	0	-6.621678	0.609868	-0.631618
49	9	0	-5.350040	-0.969792	0.133778
50	9	0	-6.355798	0.372327	1.506813
51	9	0	-0.783301	-0.970469	4.333111
52	9	0	-1.942854	-2.285259	3.056964
53	9	0	-0.156544	-3.024266	4.036294
54	9	0	-3.598230	-3.008432	-3.128007
55	9	0	-2.344973	-1.737644	-4.359599
56	9	0	-3.818665	-0.856163	-3.039356
57	6	0	3.545591	1.284828	-1.796161
58	1	0	2.754777	1.164436	-2.542573
59	6	0	3.995781	0.196062	-1.023229
60	1	0	0.717116	3.445703	0.785178
61	1	0	4.984695	0.316961	-0.566220
62	6	0	4.413254	2.470353	-1.982251
63	8	0	5.505006	2.660380	-1.490319
64	8	0	3.835605	3.364251	-2.830974
65	6	0	4.583679	4.545500	-3.086261
66	1	0	5.572936	4.307933	-3.507656
67	1	0	3.998556	5.133842	-3.805591
68	1	0	4.739011	5.125665	-2.162287

TS6’ E= -5052.587842

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.143598	2.162799	-2.004964
2	6	0	-4.692415	1.006884	-1.380608
3	6	0	-6.021150	1.048213	-0.917619
4	6	0	-6.754468	2.220605	-1.078537
5	6	0	-6.188804	3.357439	-1.696249
6	6	0	-4.879040	3.343830	-2.168863
7	6	0	-2.549553	0.582100	-1.991844
8	6	0	-3.650296	-0.003420	-1.373544
9	7	0	-2.847289	1.858875	-2.370581
10	46	0	-2.363852	-1.298578	0.990706
11	8	0	0.475492	0.179357	3.782166
12	8	0	-1.711391	0.413710	2.477941
13	6	0	-2.447890	1.408295	2.601159
14	8	0	-3.661039	1.424809	2.126923
15	6	0	1.585446	0.336107	3.151230

16	8	0	1.612404	0.642980	1.938077
17	6	0	2.841045	0.118239	3.932477
18	6	0	-2.001742	2.675450	3.256971
19	1	0	-3.871916	0.549088	1.724388
20	1	0	-1.561741	0.165168	-2.176007
21	1	0	-2.140250	2.521138	-2.680559
22	1	0	-4.440870	4.220996	-2.650968
23	1	0	-6.790791	4.262659	-1.808291
24	1	0	-7.787179	2.263875	-0.723702
25	1	0	-6.475301	0.175031	-0.441676
26	1	0	-1.439522	3.243614	2.496962
27	1	0	-2.861406	3.268919	3.590538
28	1	0	-1.330637	2.454115	4.097660
29	1	0	3.570565	0.907702	3.703485
30	1	0	2.635163	0.064434	5.007560
31	1	0	3.289955	-0.828478	3.589676
32	21	0	2.263238	0.388742	0.007487
33	8	0	4.234567	1.233977	0.062272
34	16	0	4.942246	0.067470	0.750364
35	8	0	5.752574	0.369817	1.912603
36	8	0	3.830088	-0.952415	0.903512
37	6	0	6.085443	-0.634523	-0.561368
38	8	0	2.418077	-0.689806	-1.880937
39	16	0	1.202333	-1.572897	-1.650437
40	8	0	0.771122	-1.165879	-0.243098
41	8	0	0.186165	-1.613947	-2.682829
42	6	0	1.873416	-3.316887	-1.470138
43	8	0	1.372533	1.982449	-0.732536
44	16	0	0.320542	3.120102	-0.795359
45	8	0	-0.246687	3.228559	-2.137206
46	8	0	-0.559059	3.095922	0.370659
47	6	0	1.443743	4.602732	-0.577839
48	9	0	6.662865	-1.722219	-0.073989
49	9	0	5.387873	-0.940544	-1.642478
50	9	0	7.003709	0.271107	-0.855803
51	9	0	2.072257	4.511263	0.591532
52	9	0	2.334796	4.652192	-1.555770
53	9	0	0.702388	5.703149	-0.592905
54	9	0	2.398934	-3.685166	-2.627707
55	9	0	0.876911	-4.120879	-1.145485
56	9	0	2.801660	-3.339930	-0.526624
57	6	0	-2.822499	-2.370775	-0.849929
58	1	0	-1.927086	-2.294525	-1.471726
59	6	0	-3.744593	-1.317839	-0.758284
60	1	0	-0.360214	0.296388	3.192819
61	1	0	-4.728407	-1.592619	-0.361115
62	6	0	-3.247821	-3.745950	-0.494580
63	8	0	-4.336984	-4.078456	-0.082678
64	8	0	-2.238762	-4.628332	-0.698902
65	6	0	-2.525844	-5.986667	-0.383374
66	1	0	-3.373073	-6.360861	-0.978731
67	1	0	-1.616889	-6.555149	-0.618809
68	1	0	-2.779074	-6.099489	0.682439
69	8	0	-3.496141	-2.183523	2.748851
70	8	0	-4.333195	-1.361530	3.169660

Int7'$_{triplet}$ E= -5052.607425

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.969456	3.914648	-0.338622
2	6	0	-3.165009	3.162807	-0.202721
3	6	0	-4.228669	3.698019	0.542289
4	6	0	-4.071189	4.954622	1.124368

5	6	0	-2.872860	5.684096	0.977931
6	6	0	-1.802771	5.175193	0.243875
7	6	0	-1.658534	2.005573	-1.472354
8	6	0	-2.959875	1.920767	-0.934356
9	7	0	-1.089112	3.173685	-1.116045
10	46	0	-2.893103	-0.544856	0.316510
11	8	0	-0.505464	1.630250	2.908286
12	8	0	-2.008860	-0.275746	2.423443
13	6	0	-2.454459	-0.835787	3.538906
14	8	0	-3.246564	-1.766220	3.501153
15	6	0	0.708660	1.702805	2.648930
16	8	0	1.311521	0.827166	1.916853
17	6	0	1.548632	2.823387	3.194619
18	6	0	-1.928066	-0.294323	4.841855
19	1	0	-3.655669	-2.654349	2.333722
20	1	0	-1.122191	1.282638	-2.084518
21	1	0	-0.125155	3.452456	-1.349222
22	1	0	-0.871795	5.733247	0.123971
23	1	0	-2.782590	6.666652	1.447237
24	1	0	-4.890435	5.385132	1.705134
25	1	0	-5.162876	3.144654	0.665805
26	1	0	-1.933254	0.804212	4.846631
27	1	0	-2.526960	-0.697709	5.666403
28	1	0	-0.881021	-0.616292	4.965656
29	1	0	2.070659	3.323619	2.363990
30	1	0	0.932225	3.531944	3.760150
31	1	0	2.330234	2.397874	3.844516
32	21	0	2.001543	-0.120751	0.349317
33	8	0	4.110718	-0.375355	0.720821
34	16	0	3.993907	-1.660797	1.534450
35	8	0	4.676796	-1.724441	2.807316
36	8	0	2.500072	-1.935664	1.499232
37	6	0	4.751798	-2.983736	0.442715
38	8	0	1.904021	-1.291437	-1.568401
39	16	0	0.407758	-1.472481	-1.549804
40	8	0	-0.007369	-0.830697	-0.226157
41	8	0	-0.355540	-1.085393	-2.724937
42	6	0	0.136869	-3.312772	-1.302353
43	8	0	2.201117	1.532320	-0.791094
44	16	0	2.668079	2.998962	-0.882245
45	8	0	1.624314	3.821168	-1.515723
46	8	0	3.289837	3.473220	0.348920
47	6	0	4.028746	2.853775	-2.159840
48	9	0	4.601378	-4.158617	1.038159
49	9	0	4.149399	-3.000347	-0.736353
50	9	0	6.040627	-2.723086	0.284419
51	9	0	4.953137	2.005054	-1.730972
52	9	0	3.523335	2.418064	-3.306219
53	9	0	4.573542	4.049981	-2.341401
54	9	0	0.540507	-3.950015	-2.390020
55	9	0	-1.154739	-3.533923	-1.103362
56	9	0	0.828731	-3.727369	-0.253464
57	6	0	-3.666968	-0.362120	-1.751711
58	1	0	-2.774781	-0.532328	-2.360591
59	6	0	-3.905935	0.848799	-1.094461
60	1	0	-1.320527	0.527594	2.576187
61	1	0	-4.926688	1.013737	-0.733527
62	6	0	-4.809315	-1.291283	-1.976603
63	8	0	-5.926131	-1.145109	-1.532665
64	8	0	-4.436298	-2.331692	-2.738666
65	6	0	-5.426152	-3.334822	-2.964750
66	1	0	-6.318719	-2.904544	-3.443280
67	1	0	-4.961372	-4.079878	-3.621959
68	1	0	-5.726096	-3.799420	-2.013261
69	8	0	-3.704646	-2.601007	0.451383
70	8	0	-3.906362	-3.276662	1.556779

Int7'$_{singlet}$ E= -5052.628832

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.094680	3.718148	0.288675
2	6	0	-3.315491	3.001073	0.285064
3	6	0	-4.394876	3.477095	1.043899
4	6	0	-4.223768	4.649938	1.778568
5	6	0	-2.998738	5.347266	1.770062
6	6	0	-1.912084	4.891668	1.024484
7	6	0	-1.778077	1.956266	-1.060849
8	6	0	-3.112479	1.845737	-0.584810
9	7	0	-1.200241	3.045863	-0.541688
10	46	0	-2.959024	-0.482773	0.346614
11	8	0	-0.323972	1.507097	2.727905
12	8	0	-1.706394	-0.557979	2.261305
13	6	0	-1.461721	-1.574848	3.112792
14	8	0	-2.208403	-2.526965	3.171641
15	6	0	0.872235	1.720478	2.494167
16	8	0	1.585983	0.939585	1.741950
17	6	0	1.591131	2.898854	3.093944
18	6	0	-0.212678	-1.456319	3.945571
19	1	0	-3.690392	-2.540652	2.371479
20	1	0	-1.244212	1.308617	-1.754000
21	1	0	-0.217818	3.326486	-0.701008
22	1	0	-0.959161	5.424142	1.009818
23	1	0	-2.899337	6.262367	2.358471
24	1	0	-5.053738	5.036626	2.374349
25	1	0	-5.348508	2.944445	1.064141
26	1	0	-0.151010	-0.467395	4.421866
27	1	0	-0.216675	-2.247624	4.703975
28	1	0	0.670718	-1.577518	3.296944
29	1	0	2.119419	3.453183	2.304315
30	1	0	0.890177	3.544858	3.635586
31	1	0	2.365436	2.525155	3.783646
32	21	0	2.193032	-0.072682	0.191489
33	8	0	4.218867	-0.644291	0.613065
34	16	0	3.907068	-1.887834	1.442890
35	8	0	4.558691	-2.030219	2.725361
36	8	0	2.389809	-1.944750	1.390637
37	6	0	4.475311	-3.319580	0.372551
38	8	0	1.954420	-1.169314	-1.756053
39	16	0	0.451038	-1.266899	-1.677482
40	8	0	0.130738	-0.642996	-0.321756
41	8	0	-0.342993	-0.789005	-2.799815
42	6	0	0.080068	-3.098545	-1.491887
43	8	0	2.518357	1.595813	-0.918750
44	16	0	2.738025	3.110885	-0.741267
45	8	0	1.447958	3.827001	-0.776801
46	8	0	3.677285	3.439903	0.322317
47	6	0	3.570738	3.519515	-2.366083
48	9	0	4.158660	-4.452623	0.982278
49	9	0	3.877533	-3.265302	-0.808692
50	9	0	5.787508	-3.245197	0.214911
51	9	0	4.715706	2.859463	-2.461539
52	9	0	2.776336	3.182222	-3.374654
53	9	0	3.805223	4.825073	-2.406100
54	9	0	0.436435	-3.712380	-2.609777
55	9	0	-1.217760	-3.252112	-1.285663
56	9	0	0.761063	-3.590472	-0.470188
57	6	0	-3.750305	-0.325443	-1.656912
58	1	0	-2.843896	-0.416193	-2.263738
59	6	0	-4.071464	0.837519	-0.935524
60	1	0	-1.080983	0.258926	2.389881

61	1	0	-5.111756	0.959746	-0.617329
62	6	0	-4.841274	-1.310196	-1.936243
63	8	0	-6.000614	-1.152395	-1.636229
64	8	0	-4.355842	-2.386179	-2.564536
65	6	0	-5.281412	-3.449753	-2.799922
66	1	0	-6.129122	-3.101123	-3.408486
67	1	0	-4.721424	-4.228239	-3.331685
68	1	0	-5.664675	-3.837400	-1.844523
69	8	0	-3.699810	-2.304493	0.530733
70	8	0	-4.411200	-2.363976	1.708510

H_2O_2 E= -151.6343747

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.720983	-0.052431
2	1	0	0.829842	0.896146	0.419445
3	8	0	0.000000	-0.720983	-0.052431
4	1	0	-0.829842	-0.896146	0.419445

(E)-methyl 3-(1H-indol-3-yl)acrylate E= -669.4123873

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.777486	0.776624	0.000073
2	6	0	1.750070	-0.206218	-0.000211
3	6	0	2.112183	-1.565986	-0.000373
4	6	0	3.462138	-1.904234	-0.000304
5	6	0	4.465367	-0.910532	-0.000063
6	6	0	4.138075	0.442642	0.000168
7	6	0	0.798386	1.851439	0.000172
8	6	0	0.480702	0.499441	-0.000016
9	7	0	2.158003	2.013127	0.000348
10	1	0	0.137423	2.716110	0.000261
11	1	0	2.635516	2.904802	-0.001640
12	1	0	4.913778	1.212501	0.000328
13	1	0	5.516686	-1.208692	-0.000070
14	1	0	3.754551	-2.957119	-0.000419
15	1	0	1.347119	-2.346123	-0.000475
16	6	0	-2.033593	0.507183	0.000054
17	1	0	-2.141212	1.594457	-0.000452
18	6	0	-0.830993	-0.111018	0.000299
19	1	0	-0.858296	-1.206308	0.000689
20	6	0	-3.277797	-0.282539	0.000190
21	8	0	-3.360254	-1.492329	0.000872
22	8	0	-4.365863	0.525410	-0.000513
23	6	0	-5.629303	-0.129635	-0.000400
24	1	0	-5.746025	-0.764627	0.891833
25	1	0	-6.388330	0.663201	-0.002327
26	1	0	-5.744609	-0.767751	-0.890560