Supporting Information

Efficient Access to 2,3-diarylimidazo[1,2-a]pyridines via a One-pot, Ligand-free, Palladium-Catalyzed Three-Component Reaction under Microwave Irradiation

Yuanxiang Wang, Brendan Frett, and Hong-yu Li*

Department of Pharmacology and Toxicology, College of Pharmacy, The University of Arizona, Tucson, Arizona 85721, United States and The University of Arizona Cancer Center, Tucson, Arizona 85724, US

hongyuli@pharmacy.arizona.edu

Table of Contents

1. General Information……………………………………………….S2
2. General Procedure for the Synthesis of 4 and 6…………………...S2
3. Characterization of 4 and 6………………………………………..S2
4. Copies of NMR Spectra…………………………………………...S7
5. TGFβ-R1 Computational Modeling…………………………………..S32
General Information

Solvents were purchased from Aldrich or Acros and used without further purification. Other reagents were used as obtained from commercial providers except when otherwise noted. Analytical thin layer chromatography (TLC) was performed on pre-coated silica gel plates available from EMD. Visualization was accomplished with UV light. Column chromatography was performed using Biotage chromatographic systems. $^1$H NMR and $^{13}$C NMR spectra were recorded on Varian Inova instrument (400 MHz). Chemical shifts were quoted in parts per million (ppm) referenced to the residual undeuterated solvent peak or 0.0 ppm for tetramethylsilane. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants, $J$, were reported in Hertz unit (Hz). Low and high resolution mass spectra were obtained using ESI methods.

General procedure for the preparation of compounds 2 and 6

In a 25 mL microwave tube aminopyridine (1, 1 mmol), 2-bromophenylethanone (2, 1 mmol), phenyl bromide (3, 2 mmol), and K$_2$CO$_3$ (2 mmol) were taken in 6 mL DMF. The above mixture was purged with nitrogen for 1 minute and then Pd(OAc)$_2$ (10 mol %) was added. The tube was sealed with a pressure cap and irradiated in a Biotage microwave for indicated time at 160 °C. After cooling to room temperature, the mixture was diluted with ethyl acetate (20 mL) and washed with water, brine, and dried over anhydrous Na$_2$SO$_4$. The organic solvent was removed under vacuum to get the crude product, which is purified using Biotage chromatographic systems.

Characterization of 4 and 6

3-(4-nitrophenyl)-2-phenylimidazo[1,2-a]pyridine (4aaa)

Yellow solid; $^1$H NMR (400 MHz, CDCl$_3$) δ 8.38 – 8.27 (m, 2H), 8.08 (dt, $J$ = 7.0, 1.2 Hz, 1H), 7.71 (dt, $J$ = 9.1, 1.2 Hz, 1H), 7.67 – 7.61 (m, 2H), 7.37 – 7.26 (m, 4H), 6.84 (td, $J$ = 6.9, 1.2 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 147.3, 145.6, 144.4, 136.6, 133.4, 131.0, 128.5, 128.4, 128.1, 125.6, 124.6, 122.8, 118.7, 117.9, 113.1; [M+H]$^+$ = 316.

3-(2-phenylimidazo[1,2-a]pyridin-3-yl)benzonitrile (4aab)

Yellow solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.94 – 7.92 (m, 1H), 7.77 – 7.70 (m, 2H), 7.69 – 7.65 (m, 2H), 7.61 (dd, $J$ = 7.4, 0.8 Hz, 1H), 7.58 – 7.55 (m, 2H), 7.30 – 7.22 (m, 4H), 6.78 (td, $J$ = 6.8, 1.2 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 145.2, 143.5, 135.1, 133.8, 133.4, 132.1, 131.4, 130.5, 128.4, 128.1, 127.9, 125.3, 122.7, 118.4, 118.0, 117.7, 113.8, 112.9; [M+H]$^+$ = 296.
2-phenyl-3-(3-(trifluoromethyl)phenyl)imidazo[1,2-a]pyridine (4aac)

Yellow solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.92 (dt, $J = 7.1$, 1.2 Hz, 1H), 7.75 (s, 1H), 7.75 – 7.69 (m, 2H), 7.66 – 7.54 (m, 4H), 7.32 – 7.19 (m, 4H), 6.76 (td, $J = 6.9$, 1.2 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 145.0, 143.1, 134.1 (q, $J = 1$ Hz), 133.5, 131.9 (q, $J = 33$ Hz), 130.7, 130.1, 128.3, 128.1, 127.8, 127.2 (q, $J = 3$ Hz), 125.5 (q, $J = 4$ Hz), 125.2, 123.7 (q, $J = 271$ Hz), 122.8, 119.3, 117.6, 112.8; [M+H]$^+$ = 339.

3-(4-fluorophenyl)-2-phenylimidazo[1,2-a]pyridine (4aad)

Yellow solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.89 (d, $J = 7.0$ Hz, 1H), 7.72 (d, $J = 9.0$ Hz, 1H), 7.70 – 7.55 (m, 2H), 7.48 – 7.35 (m, 2H), 7.33 – 7.18 (m, 6H), 6.76 (t, $J = 6.6$ Hz, 1H).

$^{13}$C NMR (100 MHz, CDCl$_3$) δ 162.9 (d, $J = 248$ Hz), 144.5, 142.1, 133.6, 132.7 (d, $J = 8$ Hz), 128.2 (d, $J = 32$ Hz), 128.0, 127.6, 125.6 (d, $J = 4$ Hz), 125.0, 123.1, 119.9, 117.4, 116.9, 116.7; [M+H]$^+$ = 289.

3-(3,4-dichlorophenyl)-2-phenylimidazo[1,2-a]pyridine (4aae)

White solid. $^1$H NMR (400 MHz, Chloroform-$d$) δ 7.93 (dt, $J = 7.0$, 1.2 Hz, 1H), 7.67 (dt, $J = 9.1$, 1.2 Hz, 1H), 7.66 – 7.59 (m, 2H), 7.61 – 7.52 (m, 2H), 7.33 – 7.18 (m, 5H), 6.82 – 6.75 (m, 1H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 144.0, 142.2, 132.6, 132.5, 132.0, 131.0, 130.5, 129.0, 128.8, 127.4, 127.0, 126.8, 124.1, 121.8, 117.3, 116.6, 111.7; [M+H]$^+$ = 339.

2-fluoro-4-(2-phenylimidazo[1,2-a]pyridin-3-yl)benzonitrile (4aaf)

White solid. $^1$H NMR (400 MHz, (CD$_3$)$_2$SO) δ 8.29 (dt, $J = 6.9$, 1.2 Hz, 1H), 8.16 – 8.00 (m, 1H), 7.79 (dd, $J = 10.3$, 1.5 Hz, 1H), 7.71 (dt, $J = 9.1$, 1.2 Hz, 1H), 7.63 – 7.52 (m, 2H), 7.49 (dd, $J = 8.0$, 1.5 Hz, 1H), 7.44 – 7.25 (m, 4H), 6.97 (td, $J = 6.8$, 1.2 Hz, 1H). $^{13}$C NMR (100 MHz, (CD$_3$)$_2$SO) δ 163.3 (d, $J = 246$ Hz), 154.2, 143.4, 137.5 (d, $J = 9$ Hz), 135.2, 133.9, 128.9, 128.5 (d, $J = 44$ Hz), 128.4, 128.3, 128.0 (d, $J = 4$ Hz), 126.6, 124.5, 118.6 (d, $J = 30$ Hz), 117.5, 114.3, 113.6; [M+H]$^+$ = 314; HRMS calculated for C$_{20}$H$_{13}$FN$_3$ [M+H]$^+$, 314.3352; found 314.3356.

2-phenyl-3-(pyridin-3-yl)imidazo[1,2-a]pyridine (4aag)

Yellow solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.74 (p, $J = 4.4$, 3.4 Hz, 2H), 7.99 – 7.93 (m, 1H), 7.78 (ddq, $J = 7.4$, 4.0, 1.9 Hz, 1H), 7.74 – 7.69 (m, 1H), 7.62 (dq, $J = 7.5$, 1.8 Hz, 2H), 7.46 (dq, $J = 7.4$, 3.0, 1.6 Hz, 1H), 7.36 – 7.23 (m, 4H), 6.79 (qd, $J = 5.9$, 5.3, 2.5 Hz, 1H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 151.3, 149.8, 145.3, 143.7, 138.2, 133.5, 128.4, 128.1, 127.8, 125.2, 122.8, 117.7, 117.4, 112.8; [M+H]$^+$ = 272.

2-phenyl-3-(pyridin-4-yl)imidazo[1,2-a]pyridine (4aah)

Yellow Solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.78 – 8.72 (m, 2H), 8.11 (dt, $J = 6.9$, 1.2 Hz, 2H), 7.71 (dt, $J = 9.0$, 1.2 Hz, 1H), 7.65 – 7.53 (m, 2H), 7.43 – 7.35 (m, 2H), 7.35 – 7.23 (m, 4H), 6.82 (td, $J = 6.9$, 1.2 Hz, 1H). $^{13}$C NMR (100 MHz,
CDCl$_3$ $\delta$ 144.7, 142.0, 133.7, 129.9, 129.5, 128.8, 128.3, 128.2, 127.5, 125.0, 123.3, 121.0, 117.3, 112.4; [M+H]$^+$ = 272.

2-phenyl-3-(pyrimidin-5-yl)imidazo[1,2-a]pyridine (4aai)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.31 (d, $J$ = 1.1 Hz, 1H), 8.86 (d, $J$ = 1.1 Hz, 2H), 8.00 (dt, $J$ = 6.9, 1.2 Hz, 1H), 7.74 (dd, $J$ = 9.1, 1.2 Hz, 1H), 7.59 – 7.57 (m, 2H), 7.32 (td, $J$ = 7.1, 6.6, 1.1 Hz, 4H), 6.88 – 6.85 (m, 1H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 158.2, 158.1, 145.9, 145.1, 133.0, 128.7, 128.2, 125.7, 125.0, 122.4, 118.1, 113.9, 113.3; [M+H]$^+$ = 273.

2,3-diphenylimidazo[1,2-a]pyridine (4aaj)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.96 – 7.94 (m, 1H), 7.77 (dd, $J$ = 9.1, 1.2 Hz, 1H), 7.69 – 7.65 (m, 2H), 7.52 – 7.43 (m, 5H), 7.30 – 7.19 (m, 4H), 6.75 – 6.71 (m, 1H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 144.7, 142.1, 130.7, 129.9, 129.5, 128.9, 128.3, 128.2, 128.1, 127.5, 124.9, 123.2, 117.4, 112.4; [M+H]$^+$ = 271.

2-phenyl-3-p-tolylimidazo[1,2-a]pyridine (4aak)

Yellow solid. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.93 (dd, $J$ = 6.9, 1.2 Hz, 1H), 7.73 – 7.64 (m, 3H), 7.33 – 7.21 (m, 7H), 7.19 – 7.14 (m, 1H), 6.72 – 6.67 (m, 1H), 2.45 (s, 3H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 144.7, 142.1, 138.8, 134.1, 130.5, 130.2, 128.2, 127.9, 127.3, 126.6, 124.5, 123.3, 121.1, 117.4, 112.1, 21.4; [M+H]$^+$ = 285.

2-phenyl-3-m-tolylimidazo[1,2-a]pyridine (4aal)

Yellow solid. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.92 (dt, $J$ = 6.9, 1.2 Hz, 1H), 7.75 – 7.58 (m, 3H), 7.40 (t, $J$ = 7.5 Hz, 1H), 7.32 – 7.19 (m, 6H), 7.17 (ddd, $J$ = 9.1, 6.7, 1.3 Hz, 1H), 6.70 (td, $J$ = 6.8, 1.2 Hz, 1H), 2.39 (s, 3H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 144.6, 142.1, 139.2, 134.2, 131.1, 129.7, 129.6, 129.4, 128.2, 128.0, 127.8, 127.4, 124.5, 123.3, 121.2, 117.4, 112.1, 21.4; [M+H]$^+$ = 285.

2-((4-(2-phenylimidazo[1,2-a]pyridin-3-yl)phenyl)acetonitrile (4aam)

White solid. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.95 (dt, $J$ = 6.9, 1.2 Hz, 1H), 7.70 (dt, $J$ = 9.0, 1.2 Hz, 1H), 7.67 – 7.59 (m, 2H), 7.49 (d, $J$ = 1.4 Hz, 4H), 7.32 – 7.20 (m, 4H), 6.76 (td, $J$ = 6.8, 1.2 Hz, 1H), 3.86 (s, 2H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 144.9, 142.7, 133.8, 131.4, 130.6, 129.8, 129.2, 128.3, 128.0, 127.6, 124.9, 123.0, 120.0, 117.6, 117.4, 112.5, 23.5; [M+H]$^+$ = 310.

3-(biphenyl-3-yl)-2-phenylimidazo[1,2-a]pyridine (4aan)

White solid. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.02 (dt, $J$ = 6.9, 1.2 Hz, 1H), 7.80 – 7.64 (m, 5H), 7.62 – 7.52 (m, 3H), 7.46 – 7.39 (m, 3H), 7.37 – 7.24 (m, 4H), 7.20 (ddd, $J$ = 9.1, 6.7, 1.3 Hz, 1H), 6.74 (td, $J$ = 6.8, 1.2
$^{13}$C NMR (100 MHz, CDCl$_3$) δ 144.8, 142.5, 142.4, 140.2, 134.0, 130.4, 129.9, 129.5, 129.2, 128.8, 128.3, 128.1, 127.7, 127.6, 127.5, 127.1, 124.6, 123.2, 120.9, 117.6, 112.3; [M+H]$^+$ = 347; HRMS calculated for C$_{25}$H$_{19}$N$_2$ [M+H]$^+$, 347.4312; found 347.4310.

4-(2-phenylimidazo[1,2-a]pyridin-3-yl)isoquinoline (4aa)

White solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 9.45 – 9.41 (m, 1H), 8.62 (s, 1H), 8.13 (dt, $J = 8.3, 1.0$ Hz, 1H), 7.77 (dt, $J = 9.1, 1.2$ Hz, 1H), 7.67 – 7.56 (m, 4H), 7.49 (dt, $J = 6.9, 1.2$ Hz, 1H), 7.42 – 7.38 (m, 1H), 7.26 – 7.16 (m, 4H), 6.68 – 6.64 (m, 1H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 154.0, 146.1, 145.5, 144.5, 134.9, 133.6, 131.6, 128.6, 128.4, 128.3, 128.0, 127.7, 125.1, 124.0, 123.6, 121.4, 117.6, 115.4, 112.5; [M+H]$^+$ = 322; HRMS calculated for C$_{22}$H$_{16}$N$_3$ [M+H]$^+$, 322.3820; found 322.3825.

6-methyl-3-(4-nitrophenyl)-2-phenylimidazo[1,2-a]pyridine (4baa)

White solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.36 – 8.31 (m, 2H), 7.86 (dd, $J = 1.8, 1.0$ Hz, 1H), 7.65 – 7.60 (m, 3H), 7.57 – 7.53 (m, 2H), 7.32 – 7.27 (m, 3H), 7.13 (dd, $J = 9.2, 1.7$ Hz, 1H), 2.31 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 147.2, 144.6, 144.0, 136.8, 133.5, 131.0, 128.8, 128.4, 128.3, 128.0, 124.6, 122.9, 120.4, 118.5, 117.2, 18.3; [M+H]$^+$ = 330.

8-methyl-3-(4-nitrophenyl)-2-phenylimidazo[1,2-a]pyridine (4caa)

$^1$H NMR (400 MHz, CDCl$_3$) δ 8.34 – 8.22 (m, 2H), 7.68 – 7.59 (m, 3H), 7.47 – 7.37 (m, 2H), 7.23 (dd, $J = 5.1, 2.0$ Hz, 3H), 7.17 (dd, $J = 9.0, 6.8$ Hz, 1H), 6.57 – 6.51 (m, 1H), 2.10 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 147.9, 146.6, 144.2, 139.8, 135.9, 133.7, 133.6, 128.3, 128.2, 127.7, 125.3, 122.9, 119.4, 116.0, 114.1, 22.2; [M+H]$^+$ = 330.

3-(4-nitrophenyl)-2-phenylimidazo[1,2-a]pyridine-6-carbonitrile (4daa)

Yellow solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.53 – 8.35 (m, 2H), 7.80 (dd, $J = 9.3, 1.0$ Hz, 1H), 7.73 – 7.61 (m, 3H), 7.60 – 7.55 (m, 2H), 7.38 (dd, $J = 9.3, 1.6$ Hz, 1H), 7.34 (dd, $J = 5.1, 2.0$ Hz, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 148.1, 146.3, 144.6, 134.9, 132.1, 129.0, 128.9, 128.7, 128.4, 125.2, 125.1, 119.7, 118.9, 116.2; [M+H]$^+$ = 341; HRMS calculated for C$_{20}$H$_{13}$N$_4$O$_2$ [M+H]$^+$, 341.3423; found 341.3424.

2-(4-fluorophenyl)-6-methyl-3-(4-nitrophenylimidazo[1,2-a]pyridine (4bba)

$^1$H NMR (400 MHz, CDCl$_3$) δ 8.42 – 8.28 (m, 2H), 7.85 (q, $J = 1.3$ Hz, 1H), 7.66 – 7.59 (m, 3H), 7.53 (dd, $J = 8.8, 5.4$ Hz, 2H), 7.14 (dd, $J = 9.2, 1.7$ Hz, 1H), 6.99 (t, $J = 8.7$ Hz, 2H), 2.32 (d, $J = 1.2$ Hz, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 162.5 (d, $J = 247$ Hz), 147.3, 144.7, 143.2, 136.6, 131.0, 130.1 (d, $J = 8$ Hz), 129.7 (d, $J = 8$ Hz), 128.9, 124.7, 123.0, 120.4, 118.3, 117.1, 115.5 (d, $J = 21$ Hz), 18.3; [M+H]$^+$ = 348.
6-methyl-3-(4-nitrophenyl)-2-(pyridin-4-yl)imidazo[1,2-a]pyridine (4bca)

Yellow solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.57 – 8.50 (m, 2H), 8.50 – 8.31 (m, 2H), 7.77 (q, $J = 1.3$ Hz, 1H), 7.72 – 7.56 (m, 3H), 7.54 – 7.41 (m, 2H), 7.19 (dd, $J = 9.2$, 1.7 Hz, 1H), 2.33 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 150.0, 147.9, 144.8, 141.3, 140.7, 136.0, 131.3, 129.4, 124.9, 123.6, 122.2, 120.5, 120.0, 117.5, 18.3; [M+H]$^+$ = 331.

6-methyl-3-(4-nitrophenyl)-2-(pyridin-2-yl)imidazo[1,2-a]pyridine (4bda)

Yellow solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.41 (ddd, $J = 4.8$, 1.8, 0.9 Hz, 1H), 7.75 – 7.66 (m, 2H), 7.62 – 7.56 (m, 2H), 7.50 – 7.44 (m, 2H), 7.21 (t, $J = 8.7$ Hz, 2H), 7.12 – 7.04 (m, 2H), 2.26 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 162.7 (d, $J = 250$ Hz), 153.3, 149.4, 143.9, 141.6, 135.9, 132.7 (d, $J = 11$ Hz), 128.2, 125.9 (d, $J = 6$ Hz), 122.3, 121.9, 121.6, 120.8, 117.3, 116.1 (d, $J = 21$ Hz), 18.3; [M+H]$^+$ = 304.

3-(4-fluorophenyl)-6-methyl-2-(pyridin-2-yl)imidazo[1,2-a]pyridine (4bdd)

Yellow solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.52 (ddd, $J = 4.8$, 1.9, 0.9 Hz, 1H), 7.75 – 7.66 (m, 2H), 7.62 – 7.56 (m, 2H), 7.50 – 7.44 (m, 2H), 7.21 (t, $J = 8.7$ Hz, 2H), 7.12 – 7.04 (m, 2H), 2.26 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 162.7 (d, $J = 250$ Hz), 153.3, 149.4, 143.9, 141.6, 135.9, 132.7 (d, $J = 11$ Hz), 128.2, 125.9 (d, $J = 6$ Hz), 122.3, 121.9, 121.6, 120.8, 117.3, 116.1 (d, $J = 21$ Hz), 18.3; [M+H]$^+$ = 304.

3-(4-nitrophenyl)imidazo[1,2-a]pyridine (6)

$^1$H NMR (400 MHz, CDCl$_3$) δ 8.44 (dt, $J = 7.0$, 1.2 Hz, 1H), 8.43 – 8.35 (m, 2H), 7.87 (s, 1H), 7.80 – 7.70 (m, 3H), 7.34 – 7.28 (m, 1H), 6.95 (td, $J = 6.9$, 1.2 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 147.3, 146.7, 135.8, 134.6, 127.4, 125.4, 124.7, 123.7, 123.2, 118.7, 113.6; [M+H]$^+$ = 240.
Copies of NMR Spectra

$^1$H-NMR of 4aaa

$^{13}$C-NMR of 4aaa
1H-NMR of 4aac

13C-NMR of 4aac
$^1$H-NMR of 4aad

$^{13}$C-NMR of 4aad
$^1$H-NMR of 4aae

$^{13}$C-NMR of 4aae
\(^1\)H-NMR of 4aaf

\(^{13}\)C-NMR of 4aaf
$^1$H-NMR of 4aah

$^{13}$C-NMR of 4aah
$^1$H-NMR of 4aai

$^{13}$C-NMR of 4aai
$^1$H-NMR of 4aaj

$^{13}$C-NMR of 4aaj
$^1$H-NMR of 4aak

$^{13}$C-NMR of 4aak
$^1$H-NMR of 4aal

$^{13}$C-NMR of 4aal
$^1$H-NMR of 4aam

$^{13}$C-NMR of 4aam
$^1$H-NMR of 4aan

$^{13}$C-NMR of 4aan
$^1$H-NMR of 4aao

$^{13}$C-NMR of 4aao
$^1$H-NMR of 4baa

$^{13}$C-NMR of 4baa
$^1$H-NMR of 4caa

$^{13}$C-NMR of 4caa
$^1$H-NMR of 4daa

$^{13}$C-NMR of 4daa
$^1$H-NMR of 4bba

$^{13}$C-NMR of 4bba
$^1$H-NMR of 4bca

$^{13}$C-NMR of 4bca
$^1$H-NMR of 4bdd

$^{13}$C-NMR of 4bdd
$^1$H-NMR of 4bdh

$^{13}$C-NMR of 4bdh
$^1$H-NMR of 4bea

$^{13}$C-NMR of 4bea
TGFβ-R1 Computational Modeling.

Computational modeling studies were completed using AutoDock Vina, AutoDock Tools, and Discovery Studio 3.5. Using AutoDock Tools, the TGFβ-R1 crystal structure (PDB: 3FFA) was prepared as follows: 1) All waters and ligands were removed from the structure, 2) All hydrogens were added as ‘Polar Only’, and 3) A grid box for the ATP binding site was created (center x = 75.827, center y = 23.317, center z = 93.636 / size x = 18, size y = 22, size z = 22). Compounds to be computationally modeled were assigned appropriate rotatable bonds using AutoDock Tools. To computational model the compounds, AutoDock Vina was employed. After the modeling study, the results were visualized and analyzed with Discovery Studio 3.5.