Supporting Information for
Pd(II)-Catalyzed Ortho Arylation of 6-Arylpurines with Aryl Iodides via Purine-Directed C–H Bond Activation: A New Strategy for Modification of 6-Arylpurine Derivatives

Hai-Ming Guo,* Li-Li Jiang, Hong-Ying Niu, Wei-Hao Rao, Lei Liang, Run-Ze Mao, De-Yang Li, and Gui-Rong Qu*

College of Chemistry and Environmental Science, Key Laboratory of Green Chemical Media and Reactions of Ministry of Education, Henan Normal University, Xinxiang 453007, Henan, China.
Fax: +86 373 3329276
E-mail: guohm518@hotmail.com; quguir@sina.com
School of Chemistry and Chemical Engineering, Henan Institute of Science and Technology, Xinxiang 453003, China

General information.....................................................................................................S1
General procedure.........................................................................................................S2
Characterization of compounds...................................................................................S3
References......................................................................................................................S10
Copies of 1H and 13C NMR spectra..............................................................................S11

General information: NMR spectra were recorded with a 400 MHz spectrometer for 1H NMR, 100 MHz for 13C NMR. Chemical shifts δ are given in ppm relative to the residual signals of tetramethylsilane in CDCl₃ or deuterated solvent CDCl₃ for 1H and 13C NMR. Multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), doublet of triplets (dt), triplet (t), quartet (q), multiplet (m). High resolution mass spectra were taken with a 3000 mass spectrometer, using Waters Q-TofMS/MS system. For column chromatography silica gel (200-300 mesh) was used as the stationary phase. All reactions were monitored by thin layer chromatography (TLC). All reagents and solvents were purchased from commercial sources and purified commonly before used. All starting materials (1a-1k) were synthesized by Suzuki cross-coupling reactions of 6-chloro-9-substituted purine with aryl boronic acid according to references 1 and 2.
**General procedure for the phenylation of 6-aryl-9-substituted purine**

A 25 mL Schlenk tube, containing a Teflon stirbar, was charged with 6-aryl-9-substituted purine (0.2 mmol), Pd(OAc)$_2$ (0.01 mmol, 2.3 mg), iodobenzene 2a (6 mmol), and AgOAc (0.4 mmol, 66.8 mg), then AcOH (0.5 mL) was added and the reaction mixture was heated at 120 °C for indicated hours under N$_2$ atmosphere via several vacuum-N$_2$ exchanges. The resulting mixture was cooled down to room temperature, filtered through a pad of celite, and the celite was rinsed with copious EtOAc. The filtrate was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc) affording the corresponding phenylated product.

**General procedure for the arylation of 9-butyl-6-phenylpurine**

A 25 mL Schlenk tube, containing a Teflon stirbar, was charged with 9-butyl-6-phenylpurine 1c (0.2 mmol, 50.5 mg), Pd(OAc)$_2$ (0.01 mmol, 2.3 mg), aryl iodides 2 (6 mmol), and AgOAc (0.4 mmol, 66.8 mg), then AcOH (0.5 mL) was added and the reaction mixture was heated at 120 °C for 60 hrs under N$_2$ atmosphere via several vacuum-N$_2$ exchanges. The resulting mixture was cooled down to room temperature, filtered through a pad of celite, and the celite was rinsed with copious EtOAc. The filtrate was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc) affording the corresponding monoarylated product.
Characterization of compounds

9-Benzyl-6-([1,1'-biphenyl]-2-yl)-9H-purine (3a):

White oil. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.89 (s, 1H), 7.86 (s, 1H), 7.80 (d, 1H), 7.55 (d, $J = 3.6$ Hz, 2H), 7.54-7.48 (m, 1H), 7.35 (d, $J = 6.4$ Hz, 3H), 7.21-7.19 (m, 2H), 7.14-7.10 (m, 5H), 5.4 (s, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 159.0, 152.4, 151.5, 144.2, 141.8, 141.2, 135.1, 134.3, 132.1, 130.8, 130.7, 129.8, 129.2, 129.1, 128.5, 127.7, 127.6, 127.3, 126.4, 47.1; HRMS: calcd for C$_{24}$H$_{19}$N$_4$ [M+H]$^+$ 363.1610, found 363.1603.

6-([1,1'-Biphenyl]-2-yl)-9-isopropyl-9H-purine (3b):

Light yellow crystal. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.82 (s, 1H), 8.00 (s, 1H), 7.79 (d, $J = 7.6$ Hz, 1H), 7.55 (d, $J = 3.6$ Hz, 2H), 7.52-7.48 (m, 1H), 7.17-7.11 (m, 5H), 4.90 (hept, $J = 6.8$ Hz, 1H), 1.62 (d, $J = 6.8$ Hz, 6H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 158.8, 151.7, 151.1, 142.0, 141.7, 141.2, 134.3, 132.6, 130.9, 130.7, 129.7, 129.1, 127.7, 127.2, 126.4, 47.2, 22.4; HRMS: calcd for C$_{20}$H$_{19}$N$_4$ [M+H]$^+$ 315.1610, found 315.1603.

6-([1,1'-Biphenyl]-2-yl)-9-butyl-9H-purine (3c):

Light yellow solid. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.84 (s, 1H), 7.88 (s, 1H), 7.79 (d, $J = 7.6$ Hz, 1H), 7.56-7.54 (m, 2H), 7.54-7.48 (m, 1H), 7.16-7.10 (m, 5H), 4.23 (t, $J = 7.2$ Hz, 2H),
1.91-1.84 (m, 2H), 1.37-1.27 (m, 2H), 0.95 (t, J = 7.6 Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 158.8, 152.0, 151.4, 144.3, 141.8, 141.2, 134.3, 132.2, 130.8, 130.6, 129.7, 129.1, 127.7, 127.2, 126.4, 43.6, 31.7, 19.8, 13.4; HRMS: calcd for C$_{21}$H$_{21}$N$_4$ [M+H$^+$] 329.1766, found 329.1763.

6-([1,1'-Biphenyl] -2-yl)-9-β-D-(2',3',5'-Tri-O-acetyl) ribofuranosyl -9H-purine (3d):

Light yellow solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.83 (s, 1H), 8.07 (s, 1H), 7.79 (d, J = 7.6 Hz, 1H), 7.59-7.49 (m, 3H), 7.15 (s, 5H), 6.20 (d, J = 4.8 Hz, 1H), 5.94-5.91 (m, 1H), 5.69 (t, J = 5.2 Hz, 1H), 4.49-4.45 (m, 2H), 4.36 (dd, J = 8.0, 5.2 Hz, 1H), 2.15 (s, 3H), 2.10 (s, 6H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 170.3, 169.5, 169.3, 159.5, 152.4, 151.0, 142.5, 141.9, 141.0, 133.9, 132.8, 131.1, 130.8, 129.9, 129.2, 127.9, 126.3, 86.5, 80.2, 73.1, 70.4, 62.9, 20.7, 20.5, 20.4; HRMS: calcd for C$_{28}$H$_{27}$N$_4$O$_7$ [M+H$^+$] 531.1880, found 531.1874.

9-Butyl-6-(5-methyl-[1,1'-biphenyl]-2-yl)-9H-purine (3e):

White solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.83 (s, 1H), 7.86 (s, 1H), 7.72 (d, J = 8.0 Hz, 1H), 7.36 (s, 1H), 7.32 (d, J = 7.6 Hz, 1H), 7.15-7.10 (m, 5H), 4.22 (t, J = 7.2 Hz, 2H), 2.47 (s, 3H), 1.91-1.84 (m, 2H), 1.37-1.28 (m, 2H), 0.95 (t, J = 7.6 Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 158.9, 152.0, 151.4, 144.1, 141.7, 141.4, 139.7, 132.3, 131.5, 131.5, 130.9, 129.1, 128.0, 127.7, 126.3, 43.6, 31.8, 21.4, 19.8, 13.4; HRMS: calcd for C$_{22}$H$_{23}$N$_4$ [M+H$^+$] 343.1923, found 343.1927.
9-Butyl-6-(5-methoxy-[1,1'-biphenyl]-2-yl)-9H-purine (3f):

Light blue oil. $^1\text{H NMR (400 MHz, CDCl}_3\delta$ 8.79 (s, 1H), 7.89 (s, 1H), 7.81 (d, $J = 8.8$ Hz, 1H), 7.17-7.11 (m, 5H), 7.07-7.03 (m, 2H), 4.21 (t, $J = 7.2$ Hz, 2H), 3.90 (s, 3H), 1.91-1.83 (m, 2H), 1.37-1.27 (m, 2H), 0.94 (t, $J = 7.6$ Hz, 3H); $^{13}\text{C NMR (100 MHz, CDCl}_3\delta$ 160.6, 158.5, 152.0, 151.4, 144.0, 143.6, 141.3, 132.7, 132.1, 129.1, 127.7, 127.0, 126.5, 116.2, 112.9, 55.4, 43.6, 31.8, 19.8, 13.4; HRMS: calcd for C$_{22}$H$_{23}$N$_4$O [M+H$^+$] 359.1872, found 359.1875.

9-Butyl-6-(4-methyl-[1,1'-biphenyl]-2-yl)-9H-purine (3g):

Light yellow solid. $^1\text{H NMR (400 MHz, CDCl}_3\delta$ 8.86 (s, 1H), 7.86 (s, 1H), 7.58 (s, 1H), 7.44 (d, $J = 8.0$ Hz, 1H), 7.36 (dd, $J = 6.8$, 1.2 Hz, 1H), 7.13-7.07 (m, 5H), 4.21 (t, $J = 7.2$ Hz, 2H), 2.45 (s, 3H), 1.89-1.82 (m, 2H), 1.35-1.25 (m, 2H), 0.94 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C NMR (100 MHz, CDCl}_3\delta$ 159.1, 152.0, 151.4, 144.2, 141.2, 139.0, 137.0, 134.2, 132.2, 131.3, 130.5, 129.1, 127.7, 126.1, 43.6, 31.8, 21.1, 19.8, 13.4; HRMS: calcd for C$_{22}$H$_{23}$N$_4$ [M+H$^+$] 343.1923, found 343.1917.

9-Butyl-6-(4-methoxy-[1,1'-biphenyl]-2-yl)-9H-purine (3h):

Light yellow liquid. $^1\text{H NMR (400 MHz, CDCl}_3\delta$ 8.88 (s, 1H), 7.87 (s, 1H), 7.46 (d, $J = 8.4$ Hz, 1H), 7.31 (d, $J = 2.4$ Hz, 1H), 7.11-7.06 (m, 6H), 4.21 (t, $J = 7.2$ Hz, 2H), 3.87 (s, 3H),
1.89-1.82 (m, 2H), 1.34-1.25 (m, 2H), 0.93 (t, \( J = 7.6 \) Hz, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \( \delta \) 158.7, 152.1, 151.5, 144.3, 140.9, 135.3, 134.5, 132.1, 131.8, 129.1, 127.7, 126.0, 115.9, 115.6, 55.4, 43.6, 31.8, 19.8, 13.4; HRMS: calcd for C\(_{22}\)H\(_{23}\)N\(_4\)O \([\text{M+H}^+]\) 359.1872, found 359.1868.

**9-Butyl-6-(4-nitro-[1,1'-biphenyl]-2-yl)-9\(^H\)-purine (3i):**

Yellow oil. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 8.89 (s, 1H), 8.69 (d, \( J = 2.0 \) Hz, 1H), 8.41 (dd, \( J = 6.0, 2.4 \) Hz, 1H), 7.93 (s, 1H), 7.72 (d, \( J = 8.4 \) Hz, 1H), 7.20-7.16 (m, 5H), 4.26 (t, \( J = 7.2 \) Hz, 2H), 1.93-1.86 (m, 2H), 1.38-1.29 (m, 2H), 0.96 (t, \( J = 7.6 \) Hz, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \( \delta \) 156.1, 152.2, 151.8, 148.3, 146.8, 145.0, 139.1, 135.7, 132.1, 131.7, 128.9, 128.1, 127.8, 126.3, 124.3, 43.8, 31.7, 19.8, 13.4; HRMS: calcd for C\(_{21}\)H\(_{20}\)N\(_5\)O\(_2\) \([\text{M+H}^+]\) 374.1617, found 374.1614.

**6-([4-Methyl-1,1'-biphenyl]-2-yl)-9-\(\beta\)-D-(2',3',5'-Tri-O-acetyl)ribofuranosyl-9\(^H\)-purine (3j):**

Light yellow solid. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 8.85 (s, 1H), 8.06 (s, 1H), 7.57 (s, 1H), 7.45 (d, \( J = 8.0 \) Hz, 1H), 7.37 (d, \( J = 8.0 \) Hz, 1H), 7.12 (s, 5H), 6.20 (d, \( J = 5.2 \) Hz, 1H), 5.91 (t, \( J = 5.2 \) Hz, 1H), 5.68 (t, \( J = 5.2 \) Hz, 1H), 4.48-4.44 (m, 2H), 4.36 (dd, \( J = 12.8, 5.2 \) Hz, 1H), 2.46 (s, 3H), 2.15 (s, 3H), 2.10 (s, 3H), 2.09 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \( \delta \) 170.3, 169.5, 169.3, 159.8, 152.4, 150.9, 142.5, 140.9, 139.1, 137.0, 133.7, 132.8, 131.5, 130.8, 130.7, 129.1, 127.8, 126.3, 86.4, 80.2, 73.1, 70.4, 62.9, 21.1, 20.7, 20.5, 20.4; HRMS: calcd for C\(_{29}\)H\(_{29}\)N\(_4\)O\(_7\) \([\text{M+H}^+]\) 545.2036, found 545.2034.
6-([4-Methoxyl-1,1'-biphenyl]-2-yl)-9-β-D-(2',3',5'-Tri-O-acetyl)ribofuranosyl-9H-purine (3k):

Colorless oil. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.86 (s, 1H), 8.05 (s, 1H), 7.47 (d, $J = 8.4$ Hz, 1H), 7.29 (d, $J = 2.4$ Hz, 1H), 7.13-7.10 (m, 6H), 6.19 (d, $J = 4.8$ Hz, 1H), 5.92 (t, $J = 5.2$ Hz, 1H), 5.68 (t, $J = 5.2$ Hz, 1H), 4.49-4.45 (m, 2H), 4.38-4.33 (m, 1H), 3.88 (s, 3H), 2.15 (s, 3H), 2.10 (s, 6H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 170.3, 169.5, 169.3, 159.4, 158.7, 152.4, 151.0, 142.6, 140.7, 134.8, 134.4, 132.8, 132.0, 129.1, 127.8, 126.1, 116.1, 115.8, 86.5, 80.1, 73.1, 70.4, 62.9, 55.4, 20.7, 20.5, 20.4; HRMS: calcd for C$_{29}$H$_{29}$N$_4$O$_8$ [M+H$^+$] 561.1985, found 561.1984.

9-Butyl-6-([4'-methyl-[1,1'-biphenyl]-2-yl]-9H-purine (3l):

Light yellow solid. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.85 (s, 1H), 7.90 (s, 1H), 7.76 (d, $J = 7.6$ Hz, 1H), 7.54-7.52 (m, 2H), 7.51-7.46 (m, 1H), 7.02 (d, $J = 8.0$ Hz, 2H), 6.92 (d, $J = 8.0$ Hz, 2H), 4.23 (t, $J = 7.2$ Hz, 2H), 2.23 (s, 3H), 1.92-1.84 (m, 2H), 1.36-1.23 (m, 2H), 0.95 (t, $J = 7.2$ Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 159.1, 152.0, 151.5, 144.3, 141.7, 138.2, 136.0, 134.3, 132.3, 130.8, 130.6, 129.7, 129.0, 128.5, 127.0, 43.6, 31.8, 21.0, 19.8, 13.5; HRMS: calcd for C$_{22}$H$_{23}$N$_4$ [M+H$^+$] 343.1923, found 343.1919.

9-Butyl-6-([4'-methoxy-[1,1'-biphenyl]-2-yl]-9H-purine (3m):
Colorless oil. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.88 (s, 1H), 7.90 (s, 1H), 7.75 (d, $J = 7.2$ Hz, 1H), 7.54-7.45 (m, 3H), 7.06 (d, $J = 8.8$ Hz, 2H), 6.66 (d, $J = 8.4$ Hz, 2H), 4.24 (t, $J = 7.2$ Hz, 2H), 3.72 (s, 3H), 1.93-1.85 (m, 2H), 1.41-1.29 (m, 2H), 0.96 (t, $J = 7.2$ Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 159.1, 158.2, 152.1, 151.5, 144.2, 141.3, 134.2, 133.7, 132.2, 130.8, 130.5, 130.2, 129.7, 126.9, 113.2, 55.1, 43.6, 31.8, 19.8, 13.5; HRMS: calcd for C$_{22}$H$_{23}$N$_4$O [M+H$^+$] 359.1872, found 359.1866.

9-Butyl-6-(3',5'-dimethyl-[1,1'-biphenyl]-2-yl)-9$^H$-purine (3n):

Light yellow solid. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.85 (s, 1H), 7.92 (s, 1H), 7.78-7.76 (m, 1H), 7.54-7.53 (m, 2H), 7.51-7.46 (m, 1H), 6.75 (s, 3H), 4.25 (t, $J = 7.2$ Hz, 2H), 2.11 (s, 6H), 1.95-1.85 (m, 2H), 1.37-1.27 (m, 2H), 0.95 (t, $J = 7.2$ Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 159.1, 152.0, 151.4, 144.2, 141.9, 140.9, 137.0, 134.3, 132.3, 130.7, 130.6, 129.6, 128.0, 127.0, 43.6, 31.8, 21.1, 19.8, 13.4; HRMS: calcd for C$_{23}$H$_{25}$N$_4$ [M+H$^+$] 357.2079, found 357.2082.

6-(3'-Bromo-[1,1'-biphenyl]-2-yl)-9-butyl-9$^H$-purine (3o):

Light yellow solid. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.86 (s, 1H), 7.91 (s, 1H), 7.84-7.82 (m, 1H), 7.58-7.50 (m, 3H), 7.36 (t, $J = 1.6$ Hz, 1H), 7.24 (d, $J = 7.6$ Hz, 1H), 7.01 (d, $J = 8.0$ Hz, 1H), 6.95 (t, $J = 8.0$ Hz, 1H), 4.25 (t, $J = 7.2$ Hz, 2H), 1.93-1.86 (m, 2H), 1.38-1.25 (m, 2H), 0.96 (t, $J = 7.2$ Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 158.1, 152.1, 151.6, 144.5, 143.3, 140.3, 134.4, 132.1, 132.0, 131.0, 130.5, 129.8, 129.4, 129.1, 127.9, 127.8, 121.7, 43.7, 31.8, 19.8, 13.5; HRMS: calcd for C$_{21}$H$_{20}$BrN$_4$ [M+H$^+$] 407.0871, found 407.0869.
6-(4'-Bromo-[1,1'-biphenyl]-2-yl)-9-butyl-9H-purine (3p):

![Chemical structure of 3p]

Light yellow solid. \( ^1 \)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 8.87 (s, 1H), 8.00 (s, 1H), 7.81-7.79 (m, 1H), 7.57-7.48 (m, 3H), 7.25-7.22 (m, 2H), 7.02-7.00 (m, 2H), 4.24 (t, \( J = 7.2 \) Hz, 2H), 1.92-1.85 (m, 2H), 1.37-1.27 (m, 2H), 0.95 (t, \( J = 7.6 \) Hz, 3H); \( ^{13} \)C NMR (100 MHz, CDCl\(_3\)) \( \delta \) 158.3, 152.1, 151.5, 144.4, 140.6, 140.2, 134.3, 132.1, 131.0, 130.8, 130.4, 129.8, 127.7, 120.7, 43.7, 31.7, 19.8, 13.5; HRMS: calcd for C\(_{21}H\(_{20}\)BrN\(_4\) [M+H\(^+\)] 407.0871, found 407.0870.

Ethyl 2'-(9-butyl-9H-purin-6-yl)-[1,1'-biphenyl]-4-carboxylate (3q):

![Chemical structure of 3q]

Light yellow crystal. \( ^1 \)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 8.85 (s, 1H), 7.91 (s, 1H), 7.86-7.75 (m, 3H), 7.61-7.52 (m, 3H), 7.22 (d, \( J = 8.4 \) Hz, 2H), 4.32 (q, \( J = 7.2 \) Hz, 2H), 4.24 (t, \( J = 7.2 \) Hz, 2H), 1.92-1.85 (m, 2H), 1.37-1.29 (m, 5H), 0.95 (t, \( J = 7.6 \) Hz, 3H); \( ^{13} \)C NMR (100 MHz, CDCl\(_3\)) \( \delta \) 166.5, 158.2, 152.1, 151.5, 146.0, 144.5, 140.9, 137.7, 134.3, 132.0, 131.4, 131.1, 130.5, 129.9, 129.1, 129.0, 128.4, 127.9, 60.8, 43.7, 31.7, 19.8, 14.3, 13.4; HRMS: calcd for C\(_{24}H\(_{25}\)N\(_4\)O\(_2\) [M+H\(^+\)] 401.1978, found 401.1974.

9-Butyl-6-(3'-nitro-[1,1'-biphenyl]-2-yl)-9H-purine (3r):

![Chemical structure of 3r]

Light yellow liquid. \( ^1 \)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 8.82 (s, 1H), 8.09-8.08 (m, 1H), 8.00 (ddd, \( J = 8.0, 2.0, 0.8 \) Hz, 1H), 7.93 (s, 1H), 7.92-7.91 (m, 1H), 7.64-7.59 (m, 2H), 7.58-7.55 (m, 1H), 7.43 (dt, \( J = 7.6, 1.2 \) Hz, 1H), 7.27 (t, \( J = 8.0 \) Hz, 1H), 4.25 (t, \( J = 7.2 \) Hz, 2H), 1.92-1.85
(m, 2H), 1.37-1.28 (m, 2H), 0.95 (t, $J = 7.6$ Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 157.4, 152.1, 151.8, 147.8, 144.7, 143.1, 139.4, 135.2, 134.4, 132.1, 131.4, 130.6, 130.1, 128.5, 128.4, 124.1, 121.4, 43.7, 31.7, 19.8, 13.4; HRMS: calcd for C$_{21}$H$_{19}$N$_5$NaO$_2$ [M+Na$^+$] $\text{396.1436}$, found 396.1424.

References:

Copies of $^1$H and $^{13}$C NMR spectra