

Electronic Supplementary Information

Palladium-Catalyzed Decarbonylative Suzuki–Miyaura Cross-Coupling of Amides by Carbon–Nitrogen Bond Activation

Tongliang Zhou,[†] Chong-Lei Ji,[‡] Xin Hong,^{*,‡} and Michal Szostak^{*,†}

[†]Department of Chemistry, Rutgers University, 73 Warren Street, Newark, New Jersey 07102, United States

[‡]Department of Chemistry, Zhejiang University, Hangzhou 310027, China

* Correspondence: hxchem@zju.edu.cn; michal.szostak@rutgers.edu

Table of Contents	S1
Computational Details	S2
Figure S1. DFT-Computed Transmetallation Barriers with and without Base	S3
Table S1. Energies in Figure 2	S4
Cartesian Coordinates of the Structures	S5
General Information	S38
Experimental Procedures	S39
Characterization Data	S44
Optimization and Mechanistic Studies	S72
References	S79
¹ H and ¹³ C NMR Spectra	S81

Computational Details

All density functional theory (DFT) calculations were performed with Gaussian 09 software package (1). Geometry optimizations and frequency calculations were conducted using B3LYP (2) functional with Grimme's D3(BJ) empirical dispersion correction (3), the LANL2DZ (4) basis set for Pd, and 6-31G(d) basis set for all the other elements. The vibrational frequencies were computed at the same level of theory to evaluate its zero-point vibrational energy (ZPVE) and thermal corrections at 298 K, and to check whether each optimized structure is an energy minimum or a transition state. The single point energies were calculated with the M06 functional (5) and a mixed basis set of SDD (6) for Pd and 6-311+G(d,p) for all other atoms. Solvation energy corrections were calculated using the SMD solvation model (7) with 1,4-dioxane as the solvent. All the calculated structures were visualized using CYLview (8). For thermal corrections are based on the ideal gas model, this approach ignores the solvent suppression on the rotational and translational freedoms of solutes, leading to overestimation of entropy contributions to the reaction free energies in solution (9).

To correct the entropy change in solution, An empirical approach proposed by Martin and co-workers was used (10), because there is currently no widely accepted quantum mechanics-based approach to correct entropy in solution. According to their approach, a correction of 4.3 kcal/mol applies to per component change for a reaction at 298.15 K and 1 atm (i.e., a reaction from m- to n-components has an additional correction of $(n-m) * 4.3$ kcal/mol). This approach has been validated through a number of computational and experimental studies (11). In order to adjust the Gibbs free energies from 1 atm to 1 mol/L, a correction of $RT\ln(c_s/c_g)$ (about 1.9 kcal/mol) is added to energies of all species except the carbon monoxide (CO), c_s is the standard molar concentration in solution (1 mol/L), c_g is the standard molar concentration in gas phase (0.0446 mol/L), and R is the gas constant.

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.;

- Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J., *Gaussian 09*, Revision D. 01 Gaussian, Inc., Wallingford CT (2010).
- (a) Head-Gordon, M.; Pople, J. A.; Frisch, M. *Chem. Phys. Lett.* **1988**, *153*, 503. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1988**, *37*, 785.
 - Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104.
 - (a) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 270. (b) Wadt, W. R.; Hay, P. J. *J. Chem. Phys.* **1985**, *82*, 284. (c) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299.
 - (a) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215. (b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157.
 - (a) von Szentpaly, L.; Fuentealba, P.; Preuss, H.; Stoll, H. *Chem. Phys. Lett.* **1982**, *93*, 555. (b) Dolg, M.; Wedig, U.; Stoll, H.; Preuss, H. *J. Chem. Phys.* **1987**, *86*, 866. (c) Schwerdtfeger, P.; Dolg, M.; Schwarz, W. H. E.; Bowmaker, G. A.; Boyd, P. D. W. *J. Chem. Phys.* **1989**, *91*, 1762.
 - Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378.
 - CYLVview, 1.0b; C. Y. Legault, Université de Sherbrooke, 2009 (<http://www.cylview.org>).
 - (a) Wertz, D. H. *J. Am. Chem. Soc.* **1980**, *102*, 5316. (b) Leung, B. O.; Reid, D. L.; Armstrong, D. A.; Rauk, A. *J. Phys. Chem. A* **2004**, *108*, 2720.
 - Martin, R. L.; Hay, P. J.; Pratt, L. R. *J. Phys. Chem. A* **1998**, *102*, 3565.
 - (a) Yu, Z.-X.; Houk, K. N. *J. Am. Chem. Soc.* **2003**, *125*, 13825. (b) Chen, Y.; Ye, S.; Jiao, L.; Liang, Y.; Sinha-Mahapatra, D. K.; Herndon, J. W.; Yu, Z.-X. *J. Am. Chem. Soc.* **2007**, *129*, 10773. (c) Liang, Y.; Liu, S.; Xia, Y.; Li, Y.; Yu, Z.-X. *Chem. - Eur. J.* **2008**, *14*, 4361. (d) Li, H.; Jiang, J.; Lu, G.; Huang, F.; Wang, Z.-X. *Organometallics* **2011**, *30*, 3131. (e) Li, H.; Wen, M.; Wang, Z.-X. *Inorg. Chem.* **2012**, *51*, 5716. (f) Wen, M.; Huang, F.; Lu, G.; Wang, Z.-X. *Inorg. Chem.* **2013**, *52*, 12098. (g) Qu, S.; Dang, Y.; Song, C.; Wen, M.; Huang, K.-W.; Wang, Z.-X. *J. Am. Chem. Soc.* **2014**, *136*, 4974. (h) Yu, J.-L.; Zhang, S.-Q.; Hong, X. *J. Am. Chem. Soc.* **2017**, *139*, 7224. (i) Liu, C.; Qin, Z.-X.; Ji, C.-L.; Hong, X.; Szostak, M. *Chem. Sci.* **2019**, *10*, 5736-5742.

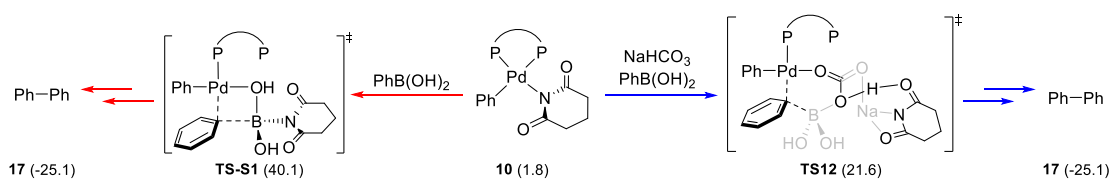


Figure S1. DFT-Computed Transmetalation Barriers with and without Base. Free energies in kcal/mol are shown in parenthesis.

Zero-point correction (*ZPE*), thermal correction to enthalpy (*TCH*), thermal correction to Gibbs free energy (*TCG*), energies (*E*), enthalpies (*H*), and Gibbs free energies (*G*) (in Hartree) of the structures calculated at the M06/6-311+G(d,p)-SDD-SMD(1,4-dioxane)//B3LYP-D3(BJ)/6-31G(d)-LANL2DZ level of theory

Table S1. Energies in Figure 2

Structures	<i>ZPE</i>	<i>TCH</i>	<i>TCG</i>	<i>E</i>	<i>H</i>	<i>G</i>	Imaginary Frequency
4	0.482706	0.515051	0.420618	-1871.496053	-1870.981002	-1871.075435	
5	0.482902	0.514905	0.420141	-1871.492841	-1870.977936	-1871.072700	
TS6	0.481177	0.513128	0.418427	-1871.474240	-1870.961112	-1871.055813	144.4i
7	0.482785	0.515272	0.419505	-1871.507580	-1870.992308	-1871.088075	
TS8	0.479845	0.512560	0.416681	-1871.461356	-1870.948796	-1871.044675	328.4i
9	0.480518	0.513848	0.416496	-1871.475670	-1870.961822	-1871.059174	
10	0.472577	0.503223	0.410969	-1758.190670	-1757.687447	-1757.779701	
11	0.629217	0.675675	0.545362	-2593.060814	-2592.385139	-2592.515452	
TS12	0.624653	0.670884	0.541557	-2593.030883	-2592.359999	-2592.489326	237.0i
13	0.174557	0.192328	0.125561	-1002.636148	-1002.443820	-1002.510587	
14	0.451167	0.479400	0.393397	-1590.420958	-1589.941558	-1590.027561	
TS15	0.448667	0.476895	0.390144	-1590.400694	-1589.923799	-1590.010550	398.8i
16	0.451711	0.480021	0.392845	-1590.454575	-1589.974554	-1590.061730	
17	0.182302	0.192100	0.147774	-463.048334	-462.856234	-462.900560	
CO	0.005036	0.008341	-0.014102	-113.285648	-113.277307	-113.299750	
NaHCO ₃	0.028633	0.034534	0.000151	-426.729179	-426.694645	-426.729028	
PhB(OH) ₂	0.125322	0.134140	0.091628	-408.123537	-407.989397	-408.031909	
TS-S1	0.596449	0.636466	0.520519	-2166.261148	-2165.624682	-2165.740629	269.8i

Cartesian coordinates of the structures

4

Pd	1.361437	-0.463500	-0.942581
P	2.354929	-1.084342	1.093209
P	1.233223	1.884867	-1.067187
C	1.320171	-2.153260	2.188257
C	4.013496	-1.904324	1.227723
C	2.603415	0.398832	2.190026
C	-0.335150	2.584669	-1.775488
C	2.485237	2.900935	-1.985488
C	1.213241	2.725513	0.597740
H	1.169796	-3.127400	1.715057
H	1.780227	-2.295991	3.173237
H	0.340165	-1.681314	2.304677
H	3.986666	-2.864468	0.702750
H	4.769564	-1.277769	0.743630
H	4.305066	-2.073800	2.271691
C	3.368559	1.535212	1.474329
H	1.598224	0.722098	2.481755
H	3.116728	0.092744	3.110442
H	-0.428748	2.279752	-2.822750
H	-0.381809	3.679103	-1.714957
H	-1.183206	2.162717	-1.229179
H	2.437996	2.651083	-3.050110
H	2.315442	3.977980	-1.863953
H	3.489761	2.656283	-1.628637
C	2.570069	2.839549	1.315379
H	0.508598	2.145956	1.203512

H	0.794216	3.735098	0.480656
H	3.688422	1.197341	0.479762
H	4.288222	1.766104	2.024859
H	3.196961	3.567673	0.784302
H	2.385541	3.266668	2.310839
C	-0.220541	-1.334722	-2.315974
C	-1.295495	-1.044582	-1.443909
C	0.576113	-2.479471	-2.028891
H	-0.100730	-0.779875	-3.240156
C	-1.627713	-1.912527	-0.402855
H	-1.872445	-0.140202	-1.596824
C	0.134262	-3.426391	-1.061837
H	1.383018	-2.748039	-2.704234
C	-0.954508	-3.159819	-0.269545
C	-2.611612	-1.559670	0.611635
H	0.690930	-4.351421	-0.938919
H	-1.285568	-3.846271	0.500931
N	-3.052649	-0.129783	0.610982
O	-3.050300	-2.281028	1.476755
C	-2.215250	0.780521	1.252978
C	-4.319792	0.136751	0.063371
C	-2.712004	2.211052	1.368454
O	-1.139793	0.425410	1.711736
C	-4.865574	1.532006	0.292481
O	-4.915208	-0.728534	-0.546195
C	-3.758551	2.586584	0.319429
H	-1.832591	2.859432	1.332540
H	-3.137599	2.312232	2.376868

H	-5.608675	1.719167	-0.485954
H	-5.396660	1.520918	1.255204
H	-4.175919	3.574325	0.539000
H	-3.289261	2.653562	-0.669751

5

Pd	0.731720	-0.007747	-0.493361
C	-1.382082	-0.001826	-0.972050
P	0.925408	0.673864	1.709389
N	-2.205921	-1.103522	-0.386994
C	-1.837710	1.364467	-0.585882
O	-0.797308	-0.245543	-2.079044
P	2.940049	-0.273089	-1.262316
O	-0.396109	-2.303677	0.371438
C	-0.206154	-0.178283	2.898635
C	0.636210	2.452968	2.107849
C	2.583218	0.353736	2.495337
C	-3.564650	-1.096938	-0.795433
C	-1.605121	-2.203827	0.231659
C	-1.449488	2.450277	-1.386754
C	-2.594590	1.616474	0.568451
C	3.396249	-1.979486	-1.811710
C	3.432539	0.733123	-2.734413
C	4.325436	0.141365	-0.091707
H	-1.240031	0.008329	2.595810
H	-0.025458	-1.255268	2.844982
H	-0.062903	0.171851	3.927802
H	-0.366720	2.734944	1.776555

H	1.358932	3.062519	1.556840
H	0.737372	2.654877	3.180930
C	3.216590	-0.969251	2.004038
H	3.224994	1.207832	2.249512
H	2.469810	0.360382	3.586054
C	-4.491756	-2.135364	-0.183931
O	-3.971050	-0.277591	-1.592112
C	-2.527142	-3.295743	0.749992
C	-1.784817	3.751066	-1.023916
H	-0.884267	2.246189	-2.289147
C	-2.937909	2.919720	0.923815
H	-2.917717	0.787497	1.190447
H	4.444871	-2.048914	-2.126224
H	3.214440	-2.686988	-0.997648
H	2.748656	-2.261138	-2.647465
H	3.348652	1.796027	-2.487159
H	2.738088	0.523518	-3.553519
H	4.457238	0.519451	-3.061949
C	4.469977	-0.781522	1.131543
H	4.146806	1.175299	0.228346
H	5.272284	0.144421	-0.648618
H	2.472865	-1.549233	1.443337
H	3.497417	-1.585853	2.865830
C	-3.925457	-2.782386	1.073626
H	-5.448142	-1.632252	-0.015338
H	-4.671615	-2.898504	-0.953879
H	-2.022577	-3.739931	1.611834
H	-2.582870	-4.076068	-0.022496

C	-2.527469	3.996989	0.135180
H	-1.473576	4.579953	-1.654362
H	-3.527920	3.093565	1.820103
H	4.808366	-1.769449	0.794238
H	5.280165	-0.381018	1.756559
H	-4.570603	-3.597491	1.417382
H	-3.873608	-2.047039	1.886802
H	-2.791999	5.013029	0.413687

TS6

Pd	0.594378	-0.280461	0.167832
P	1.474245	1.842394	-0.090070
C	-1.213933	0.374301	-0.784503
C	1.166422	2.702112	-1.688754
C	0.966855	3.108350	1.154564
C	3.323988	1.936392	0.076582
C	-1.904097	1.427114	0.042563
O	-1.031756	0.467366	-1.996793
H	1.384284	2.024342	-2.517048
H	1.771243	3.612064	-1.774881
H	0.107926	2.957109	-1.749195
H	1.229326	2.753018	2.155563
H	1.466124	4.066647	0.969251
H	-0.114432	3.249113	1.114666
C	4.143144	1.394128	-1.105366
H	3.576078	1.402388	1.000798
H	3.592700	2.988557	0.237558
C	-2.308589	2.608800	-0.584982

C	-2.074820	1.288722	1.424495
C	3.971635	-0.096369	-1.434624
H	3.913179	1.983143	-2.001577
H	5.203799	1.578789	-0.884842
C	-2.855491	3.651377	0.164339
H	-2.207063	2.677673	-1.662749
C	-2.630209	2.324060	2.171478
H	-1.751273	0.370931	1.907551
C	4.247986	-1.030339	-0.236024
H	4.658371	-0.338672	-2.254132
H	2.959781	-0.272958	-1.823396
C	-3.014148	3.515047	1.544757
H	-3.167651	4.567027	-0.331216
H	-2.757814	2.208766	3.244689
P	2.671701	-1.630586	0.554944
H	4.837793	-1.902886	-0.542666
H	4.839304	-0.509853	0.527635
H	-3.439482	4.326325	2.129143
C	2.339850	-3.149845	-0.447231
C	3.287264	-2.368981	2.138425
H	2.159995	-2.855612	-1.486182
H	3.173614	-3.861286	-0.411490
H	1.426812	-3.618846	-0.072429
H	3.617661	-1.573005	2.813573
H	4.117203	-3.066878	1.975245
H	2.463709	-2.903056	2.622704
N	-2.214891	-1.111402	-0.416363
C	-1.671603	-2.176514	0.183557

C	-3.505527	-1.094078	-0.962887
C	-2.455602	-3.465698	0.351201
O	-0.494003	-2.151504	0.619937
C	-4.293504	-2.400867	-0.935872
O	-3.969893	-0.082280	-1.451346
C	-3.964909	-3.240134	0.297009
H	-2.128018	-3.931229	1.284859
H	-2.143125	-4.134134	-0.464242
H	-5.351912	-2.138201	-1.000836
H	-4.038882	-2.960728	-1.847786
H	-4.496412	-4.197415	0.274457
H	-4.292253	-2.711373	1.201410

7

Pd	-0.337802	-0.072548	-0.321334
P	-2.145744	1.310101	0.520923
C	-2.129318	2.967621	-0.282697
C	-2.027295	1.721114	2.313265
C	-3.922874	0.801443	0.322371
H	-1.196395	3.466200	-0.009241
H	-2.130313	2.844399	-1.368421
H	-2.977991	3.584494	0.032527
H	-2.209903	0.823207	2.910905
H	-2.747280	2.496134	2.600655
H	-1.003861	2.045715	2.515721
C	-4.370437	-0.361870	1.226628
H	-4.052022	0.545228	-0.736120
H	-4.566395	1.669836	0.513209

C	-3.452726	-1.595580	1.237159
H	-4.467092	0.005031	2.255516
H	-5.378262	-0.668238	0.916093
C	-3.183650	-2.185582	-0.164891
H	-2.502806	-1.329706	1.719257
H	-3.909619	-2.358767	1.876681
P	-1.407315	-2.067649	-0.677470
H	-3.762612	-1.657155	-0.930173
H	-3.487202	-3.237532	-0.221971
C	-0.649838	-3.527226	0.152332
C	-1.449768	-2.534833	-2.452835
H	-1.185476	-4.449885	-0.097760
H	-0.668031	-3.378546	1.236080
H	0.395557	-3.615983	-0.153196
H	-1.839238	-3.548602	-2.595790
H	-0.437174	-2.451690	-2.854607
H	-2.081778	-1.821216	-2.990147
C	1.323187	-1.055458	-1.022196
C	2.332232	-1.527617	-0.015401
O	1.495630	-1.251424	-2.210593
C	2.176868	-1.279113	1.353219
C	3.430138	-2.278631	-0.466297
C	3.114319	-1.772141	2.261152
H	1.350259	-0.664795	1.694889
C	4.358600	-2.776626	0.442115
H	3.527971	-2.457836	-1.532376
C	4.200655	-2.523720	1.809392
H	2.998516	-1.562117	3.320662

H	5.205789	-3.359888	0.091041
H	4.927206	-2.910342	2.519372
N	0.914287	1.661597	-0.238551
C	1.066744	2.287516	-1.457895
C	1.481734	2.093981	0.926821
C	2.096072	3.405654	-1.579310
O	0.390102	1.947699	-2.425389
C	2.501004	3.227919	0.871603
O	1.195230	1.580341	2.014267
C	2.235205	4.196968	-0.279306
H	1.806883	4.031674	-2.427159
H	3.058429	2.937839	-1.833621
H	2.500007	3.720080	1.847641
H	3.490315	2.763940	0.745556
H	3.037500	4.939274	-0.357354
H	1.306982	4.752661	-0.086113

TS8

Pd	-0.318708	0.131304	0.545717
P	1.491737	1.285937	1.491903
P	-0.581358	1.335329	-1.523501
C	3.035335	0.314372	1.719665
C	1.144864	1.909999	3.193730
C	2.055360	2.802455	0.601106
C	-1.031927	-0.862033	2.000210
C	-0.638068	0.154739	-2.931851
C	-2.205451	2.203309	-1.671698
C	0.621456	2.605391	-2.126709

H	2.798613	-0.630612	2.216045
H	3.768044	0.870251	2.315311
H	3.448351	0.100065	0.732424
H	0.316886	2.624309	3.155557
H	2.022079	2.397548	3.634697
H	0.839028	1.071665	3.826623
C	0.872284	3.719144	0.210739
H	2.590529	2.440842	-0.281331
H	2.782996	3.330600	1.228867
O	-1.229436	-1.351236	3.037214
H	-1.325606	-0.657994	-2.681990
H	-0.964182	0.645245	-3.855871
H	0.364676	-0.255297	-3.061646
H	-2.291497	2.969455	-0.895428
H	-2.316816	2.675092	-2.654697
H	-3.012907	1.482254	-1.521641
C	0.696348	3.903226	-1.305236
H	1.580277	2.082148	-2.143910
H	0.362083	2.849212	-3.165261
H	1.001830	4.706195	0.668661
H	-0.062481	3.316808	0.624230
H	-0.207895	4.501084	-1.477317
H	1.533532	4.497910	-1.694578
C	-2.342138	-0.758006	0.589051
C	-2.554613	-1.896025	-0.197122
C	-3.391991	0.131165	0.850004
C	-3.814230	-2.113187	-0.760050
H	-1.739730	-2.597177	-0.335088

C	-4.650221	-0.096291	0.289661
H	-3.222888	0.998743	1.480891
C	-4.857713	-1.213852	-0.523592
H	-3.983159	-2.990131	-1.379469
H	-5.465226	0.595225	0.486640
H	-5.836544	-1.390828	-0.961003
N	1.207141	-1.520483	-0.489797
C	2.254970	-1.129671	-1.255328
C	1.061839	-2.803097	-0.042833
C	3.288771	-2.150393	-1.738125
O	2.407747	0.060845	-1.591748
C	2.057633	-3.885816	-0.466170
O	0.121916	-3.123455	0.696775
C	3.441449	-3.310825	-0.757906
H	4.225825	-1.615142	-1.914122
H	2.950637	-2.531194	-2.713632
H	2.070192	-4.647827	0.317329
H	1.657417	-4.364922	-1.372266
H	4.112995	-4.079800	-1.156971
H	3.892276	-2.946170	0.175288

9

Pd	0.161161	-0.370494	0.622129
P	-2.176540	-0.238070	1.178140
P	0.022368	-1.688665	-1.328000
C	-2.943885	1.424888	1.049737
C	-2.470316	-0.687108	2.946637
C	-3.389269	-1.338771	0.319285

C	0.732267	0.253104	2.409015
C	0.890760	-0.953583	-2.769180
C	0.789454	-3.358280	-1.181553
C	-1.630735	-2.057311	-2.075704
H	-2.316417	2.150504	1.573366
H	-3.952535	1.426773	1.477553
H	-2.985966	1.699031	-0.006128
H	-2.149294	-1.719139	3.118948
H	-3.528167	-0.590174	3.216246
H	-1.875602	-0.035932	3.593539
C	-2.833534	-2.765068	0.115001
H	-3.630378	-0.866804	-0.638307
H	-4.313420	-1.347837	0.909003
O	1.092910	0.522209	3.460014
H	1.911068	-0.685542	-2.491155
H	0.907206	-1.666152	-3.601203
H	0.339523	-0.056881	-3.060677
H	0.326347	-3.913635	-0.360999
H	0.669633	-3.923722	-2.112694
H	1.852820	-3.243619	-0.961226
C	-2.511350	-3.083814	-1.351329
H	-2.113393	-1.081388	-2.170563
H	-1.436805	-2.413676	-3.095614
H	-3.556672	-3.502384	0.481161
H	-1.927796	-2.903675	0.720961
H	-2.044840	-4.075613	-1.402909
H	-3.453837	-3.161477	-1.910034
C	2.203152	-0.560452	0.306078

C	2.874393	0.449212	-0.390259
C	2.932753	-1.639518	0.814141
C	4.252828	0.361552	-0.604451
H	2.315421	1.294242	-0.776450
C	4.313452	-1.726473	0.601059
H	2.428750	-2.420469	1.377050
C	4.975843	-0.727718	-0.112988
H	4.762935	1.150149	-1.152598
H	4.868245	-2.573017	0.998793
H	6.047759	-0.792897	-0.278940
N	-0.178780	1.860404	-0.438284
C	-0.871731	2.049913	-1.586768
C	0.365230	2.890977	0.276492
C	-0.911735	3.430549	-2.245874
O	-1.485323	1.114918	-2.136791
C	0.367157	4.307516	-0.302882
O	0.875981	2.702874	1.387663
C	-0.834058	4.554431	-1.213933
H	-1.813565	3.481831	-2.861708
H	-0.051461	3.495912	-2.929076
H	0.417845	5.010880	0.532189
H	1.298062	4.424076	-0.877913
H	-0.763462	5.533447	-1.701767
H	-1.753962	4.563829	-0.613130

10

Pd	-0.232754	0.046645	0.104227
P	-1.531203	-1.945746	0.248372

P	-1.866743	1.627789	0.257445
C	-1.669906	-2.653495	1.941656
C	-0.752805	-3.308522	-0.713663
C	-3.278847	-1.936949	-0.403471
N	1.489981	-1.153027	-0.066438
C	1.078892	1.616619	0.016617
C	-1.710667	2.716077	1.731749
C	-1.937996	2.815824	-1.143703
C	-3.618385	1.039378	0.410443
H	-0.661385	-2.683100	2.363957
H	-2.116231	-3.654144	1.941693
H	-2.275708	-1.987362	2.564654
H	-0.574858	-2.964124	-1.735742
H	-1.376233	-4.209254	-0.716598
H	0.217610	-3.535074	-0.266766
C	-3.516778	-0.812897	-1.434927
H	-3.961532	-1.829036	0.448055
H	-3.487205	-2.919495	-0.840992
C	2.100113	-1.563683	1.086649
C	1.994071	-1.319500	-1.330404
C	1.475349	2.162648	-1.211075
C	1.685305	2.086501	1.189115
H	-0.724237	3.185431	1.716745
H	-2.490722	3.485166	1.743213
H	-1.785793	2.108266	2.638584
H	-2.094114	2.272532	-2.079878
H	-2.743590	3.545597	-1.006487
H	-0.975914	3.329251	-1.208285

C	-4.235333	0.414740	-0.851939
H	-3.628295	0.323234	1.241197
H	-4.235133	1.891649	0.724217
H	-4.128019	-1.193976	-2.261021
H	-2.559158	-0.509797	-1.877582
C	3.494878	-2.176117	0.991934
O	1.531853	-1.464813	2.178114
C	3.380680	-1.937443	-1.480996
O	1.337348	-0.999303	-2.322593
C	2.444864	3.170129	-1.263588
H	1.047975	1.780334	-2.133556
C	2.655599	3.093547	1.137739
H	1.416288	1.650666	2.148045
H	-4.314289	1.182457	-1.631341
H	-5.266513	0.128508	-0.603845
C	4.247831	-1.693206	-0.246888
H	4.016469	-1.940877	1.923670
H	3.379648	-3.270019	0.959055
H	3.819752	-1.530094	-2.395629
H	3.251883	-3.018435	-1.641950
C	3.033853	3.642830	-0.089046
H	2.744243	3.580892	-2.225504
H	3.119308	3.444324	2.057256
H	4.453290	-0.619168	-0.153154
H	5.214170	-2.201575	-0.339972
H	3.786415	4.426121	-0.130055

Pd	0.665403	-1.154848	0.494704
P	1.903851	-2.062683	-1.142719
C	2.215212	-0.159741	1.271961
C	1.584148	-3.865743	-1.231091
C	1.355691	-1.419813	-2.770691
C	3.736742	-1.893577	-1.149199
C	3.258750	-0.757270	1.992385
C	2.201553	1.239709	1.141363
H	2.014785	-4.358393	-0.354527
H	2.014808	-4.298627	-2.140588
H	0.500232	-4.004128	-1.219160
H	1.526366	-0.341895	-2.818367
H	1.894661	-1.915151	-3.586029
H	0.284296	-1.605246	-2.868679
C	4.218055	-0.454802	-1.393426
H	4.079494	-2.240828	-0.168796
H	4.144327	-2.583523	-1.899746
C	4.275259	0.021808	2.552939
H	3.286681	-1.837154	2.114606
C	3.218332	2.018689	1.707166
H	1.400941	1.727313	0.588977
C	5.646465	-0.222263	-0.887575
H	3.558237	0.244054	-0.872004
H	4.150260	-0.218033	-2.462970
C	4.263498	1.411107	2.404265
H	5.082010	-0.456452	3.102616
H	3.193521	3.099606	1.592776
C	6.048652	1.254967	-0.952874

H	5.701666	-0.557322	0.154954
H	6.353886	-0.838599	-1.459151
H	5.063440	2.010637	2.828667
P	7.662441	1.607609	-0.079692
H	5.282180	1.850404	-0.441029
H	6.092273	1.602846	-1.995191
C	7.830895	3.411583	-0.520294
C	8.855974	0.893931	-1.323703
H	7.072325	3.991611	0.016170
H	7.714875	3.593071	-1.596099
H	8.814487	3.777582	-0.207245
H	9.878342	1.182866	-1.057576
H	8.648671	1.237720	-2.344963
H	8.805306	-0.199566	-1.303675
O	-0.521723	-0.116279	2.198163
B	-1.662934	0.560841	1.726948
H	0.198549	0.527377	2.338768
C	-3.030496	-0.201411	1.791239
O	-1.493925	1.857496	1.375817
C	-3.103286	-1.605079	1.843647
C	-4.236872	0.518879	1.836414
H	-2.145256	2.166361	0.703901
C	-4.334326	-2.262537	1.898617
H	-2.189882	-2.187901	1.809507
C	-5.471421	-0.126756	1.907787
H	-4.205542	1.604411	1.819315
C	-5.523480	-1.524663	1.930186
H	-4.366203	-3.348424	1.923475

H	-6.390878	0.451103	1.934296
H	-6.483147	-2.032657	1.982716
C	-1.852223	-1.425847	-0.990445
O	-2.921797	-1.785676	-1.512391
O	-1.505919	-0.108188	-0.931059
O	-0.978679	-2.201225	-0.467067
Na	-4.958282	-1.172664	-1.105686
H	-2.250607	0.519958	-1.135286
N	-5.005430	1.114343	-1.304208
C	-4.288933	2.193494	-0.961571
C	-6.367493	1.115248	-1.294792
C	-4.968845	3.523846	-0.667380
O	-3.039327	2.116419	-0.841081
C	-7.153843	2.406169	-1.107659
O	-6.973137	0.029682	-1.395530
C	-6.304113	3.642569	-1.405119
H	-4.271508	4.326135	-0.923364
H	-5.133624	3.581645	0.419778
H	-8.054503	2.350101	-1.725850
H	-7.494025	2.424097	-0.061354
H	-6.831139	4.557916	-1.115062
H	-6.116754	3.708118	-2.484491

TS12

Pd	0.341715	1.374972	0.544248
P	1.938024	1.361434	2.221017
C	1.068630	3.138316	-0.064181
C	2.615133	2.938986	2.871918

C	1.364478	0.450304	3.710679
C	3.426164	0.426776	1.645033
C	0.347178	4.313574	0.187442
C	2.293404	3.236064	-0.740002
H	1.798502	3.535413	3.288810
H	3.366925	2.758024	3.647408
H	3.059419	3.503214	2.048397
H	0.593983	1.040431	4.215941
H	2.188399	0.258013	4.406343
H	0.909606	-0.489270	3.389475
C	3.039496	-0.880960	0.941921
H	3.957613	1.085326	0.946096
H	4.097522	0.246889	2.495322
C	0.838857	5.553230	-0.228398
H	-0.612708	4.261546	0.693257
C	2.783403	4.477664	-1.160972
H	2.887435	2.346888	-0.942446
C	4.223679	-1.634952	0.330770
H	2.330611	-0.651851	0.139739
H	2.502847	-1.539340	1.636666
C	2.058553	5.641031	-0.904197
H	0.261777	6.453177	-0.029505
H	3.733318	4.530107	-1.687491
C	3.740365	-2.800773	-0.540927
H	4.820405	-0.946512	-0.282928
H	4.887782	-1.995660	1.128114
H	2.437911	6.606127	-1.228204
P	5.132167	-3.751740	-1.349314

H	3.103885	-2.404013	-1.343250
H	3.114335	-3.484704	0.050541
C	4.109976	-5.060711	-2.195819
C	5.706564	-4.749018	0.120305
H	4.767731	-5.832301	-2.609875
H	3.396553	-5.535796	-1.511067
H	3.553869	-4.612224	-3.025685
H	6.418514	-5.512957	-0.209856
H	4.872765	-5.243818	0.634454
H	6.225037	-4.100240	0.833880
C	-1.152065	1.365083	-1.082071
C	-1.077136	2.300793	-2.140034
C	-2.442901	1.075745	-0.581442
C	-2.217411	2.864673	-2.707529
H	-0.100903	2.558867	-2.540494
C	-3.593684	1.633632	-1.142820
H	-2.554818	0.374412	0.241563
C	-3.481651	2.524821	-2.212579
H	-2.128284	3.569131	-3.530991
H	-4.574375	1.368302	-0.757793
H	-4.374931	2.954884	-2.657917
B	-0.146715	-0.314033	-1.829636
O	1.135858	0.098784	-2.187595
O	-1.006032	-0.664356	-2.908029
O	-0.326544	-1.430874	-0.886362
H	1.543898	0.609891	-1.473277
H	-0.974682	0.014728	-3.595440
C	-0.519111	-1.549412	0.415982

O	-0.876272	-2.755583	0.749458
O	-0.404190	-0.618108	1.236166
N	-3.797107	-2.079908	0.312457
C	-3.827397	-2.251170	1.648839
C	-4.914880	-1.715577	-0.382300
C	-5.100221	-2.036104	2.455825
O	-2.799298	-2.578022	2.298636
C	-6.231071	-1.433122	0.325499
O	-4.847322	-1.582808	-1.620632
C	-6.357652	-2.246261	1.613490
H	-5.058443	-2.693585	3.327996
H	-5.070171	-1.004121	2.836012
H	-7.043699	-1.621033	-0.380653
H	-6.251643	-0.357831	0.559922
H	-7.254636	-1.959174	2.172592
H	-6.460792	-3.310598	1.365484
H	-1.635584	-2.704362	1.507774
Na	-2.582474	-1.871693	-1.769876

13

N	1.826066	0.186705	-0.023223
C	3.041509	0.794826	-0.019591
C	1.680441	-1.149129	-0.120431
C	4.326719	-0.015577	-0.093622
O	3.092510	2.044079	0.028660
C	2.897424	-2.060647	-0.210296
O	0.546313	-1.674955	-0.157401
C	4.125630	-1.431703	0.450941

H	5.109290	0.535676	0.434690
H	4.626526	-0.057852	-1.151223
H	2.630279	-3.025970	0.227586
H	3.095604	-2.240157	-1.277358
H	5.016889	-2.044850	0.279441
H	3.972429	-1.386385	1.537047
O	-1.755085	-0.613197	-0.082799
C	-2.067382	0.658686	-0.041866
H	-0.743351	-0.854282	-0.109525
O	-3.388775	0.857621	-0.002578
O	-1.301192	1.617086	-0.044076
B	-4.258521	-0.245168	0.062248
O	-4.809390	-0.644909	-1.118189
O	-4.537491	-0.725275	1.306781
H	-5.434773	-1.377961	-1.046284
H	-5.143976	-1.477064	1.326605
Na	0.780006	2.198673	0.036030

14

Pd	-0.006869	-0.024094	-0.093182
P	-1.237492	-2.045945	-0.100413
P	-1.755117	1.577715	-0.261217
C	-0.938565	-3.205171	-1.499815
C	-0.843779	-3.088226	1.368103
C	-3.091281	-1.959510	-0.007691
C	1.696123	-1.175716	-0.009024
C	1.304269	1.557790	0.044067
C	-1.967409	2.652217	1.221219

C	-1.449743	2.808771	-1.598147
C	-3.496106	1.062610	-0.666018
H	-1.468963	-4.153922	-1.362818
H	0.137059	-3.391084	-1.565634
H	-1.264588	-2.741340	-2.436181
H	0.237408	-3.242050	1.408810
H	-1.358977	-4.054526	1.326064
H	-1.144546	-2.560359	2.278622
C	-3.559891	-0.918244	1.036067
H	-3.458784	-1.704247	-1.008169
H	-3.484274	-2.957224	0.221131
C	2.312907	-1.494335	1.210205
C	2.257626	-1.709358	-1.179452
C	1.940872	2.094651	-1.085407
C	1.561943	2.164982	1.282998
H	-2.263335	2.046092	2.082636
H	-2.717070	3.433799	1.054214
H	-1.000325	3.111290	1.443932
H	-2.202281	3.605066	-1.593493
H	-0.452736	3.233753	-1.459838
H	-1.469771	2.300844	-2.567729
C	-4.261767	0.310749	0.435174
H	-3.420181	0.446665	-1.570832
H	-4.067038	1.957004	-0.947193
H	-2.704986	-0.579419	1.636524
H	-4.250435	-1.391167	1.743302
C	3.431317	-2.331996	1.263261
H	1.923875	-1.075236	2.135795

C	3.378242	-2.545813	-1.134994
H	1.820448	-1.468837	-2.146972
C	2.780729	3.208431	-0.987690
H	1.787133	1.635102	-2.059611
C	2.401990	3.278740	1.389577
H	1.106923	1.763220	2.186809
H	-4.494386	1.008931	1.248980
H	-5.228581	-0.001207	0.017547
C	3.967038	-2.865879	0.089277
H	3.889820	-2.561847	2.222955
H	3.792981	-2.944372	-2.058805
C	3.011113	3.809586	0.251589
H	3.261387	3.603331	-1.880531
H	2.583464	3.728747	2.363643
H	4.837594	-3.515598	0.127731
H	3.664509	4.674684	0.330138

TS15

Pd	-0.045209	-0.032469	-0.099086
P	-1.276063	-2.061342	-0.131702
P	-1.731238	1.645216	-0.227983
C	-0.992833	-3.244615	-1.521906
C	-0.916202	-3.126784	1.335139
C	-3.130627	-1.922120	-0.063260
C	1.925654	-0.768719	0.020177
C	1.680765	1.168113	0.067936
C	-1.382684	2.936586	-1.502898
C	-1.951041	2.682618	1.286814

C	-3.477919	1.172754	-0.670022
H	0.081582	-3.445302	-1.586616
H	-1.531726	-4.189640	-1.386691
H	-1.307310	-2.783305	-2.463670
H	-1.230113	-2.606905	2.246065
H	-1.424240	-4.096992	1.282342
H	0.166045	-3.279151	1.393546
C	-3.574819	-0.867473	0.980300
H	-3.466257	-1.640156	-1.068446
H	-3.573989	-2.902616	0.149922
C	2.451853	-1.303263	-1.174885
C	2.340516	-1.358134	1.232049
C	1.868894	1.794910	1.317941
C	2.118217	1.862961	-1.078109
H	-1.411566	2.479375	-2.497327
H	-2.100661	3.764283	-1.467706
H	-0.369823	3.317315	-1.339515
H	-0.977304	3.109311	1.548034
H	-2.674961	3.492997	1.139819
H	-2.278810	2.055948	2.121911
C	-4.258461	0.381808	0.395770
H	-3.394210	0.586164	-1.593858
H	-4.047204	2.076959	-0.924196
H	-4.272013	-1.327760	1.689939
H	-2.709894	-0.547131	1.576317
C	3.318731	-2.394469	-1.159457
H	2.171573	-0.862657	-2.128005
C	3.210615	-2.447333	1.246631

H	1.974556	-0.959548	2.174412
C	2.428950	3.067910	1.412282
H	1.565192	1.280664	2.226001
C	2.681355	3.134681	-0.982754
H	2.012772	1.402146	-2.056460
H	-4.502479	1.055703	1.227079
H	-5.220357	0.085406	-0.044711
C	3.703671	-2.978909	0.051182
H	3.698320	-2.790622	-2.098867
H	3.506901	-2.883707	2.198067
C	2.836543	3.751424	0.262503
H	2.549771	3.529294	2.390031
H	3.002237	3.647726	-1.886771
H	4.385826	-3.824161	0.063178
H	3.280204	4.740142	0.336811

16

Pd	-1.144326	-0.480645	-0.765202
P	-3.041158	-0.761033	0.562405
P	-0.520895	1.775267	-0.894404
C	-4.719885	-1.272303	-0.041610
C	-2.866077	-1.864119	2.045958
C	-3.456483	0.851108	1.406830
C	1.044306	2.194477	0.005733
C	-0.208501	2.606199	-2.524329
C	-1.713107	3.002303	-0.145235
H	-5.019441	-0.620248	-0.868290
H	-4.670357	-2.297400	-0.422574

H	-5.480474	-1.222461	0.747674
H	-3.734720	-1.807569	2.713731
H	-1.968046	-1.573942	2.600204
H	-2.733530	-2.899278	1.715875
C	-2.197312	1.543395	1.980353
H	-4.205213	0.678254	2.190751
H	-3.937948	1.483076	0.651458
H	1.256970	3.270510	-0.008448
H	1.878455	1.655058	-0.450237
H	0.973190	1.856386	1.043325
H	-1.118252	2.567483	-3.132088
H	0.101119	3.652576	-2.410802
H	0.574998	2.057455	-3.056420
C	-1.888650	2.927289	1.383129
H	-2.672686	2.833628	-0.649431
H	-1.395355	4.020770	-0.408216
H	-1.322077	0.897883	1.831263
H	-2.306678	1.660915	3.065012
H	-0.976330	3.308030	1.860098
H	-2.690405	3.624311	1.664423
C	0.615936	-1.684159	-1.826700
C	1.836964	-1.098668	-1.420575
C	-0.071466	-2.566171	-0.952063
H	0.297951	-1.587646	-2.861073
C	2.359165	-1.313426	-0.150739
H	2.343337	-0.423646	-2.104847
C	0.485631	-2.803052	0.332919
H	-0.875764	-3.193496	-1.319898

C	1.652525	-2.179677	0.727966
C	3.584276	-0.614790	0.293002
H	-0.011905	-3.495827	1.006251
H	2.068654	-2.389660	1.709032
C	4.644902	-0.363197	-0.594692
C	3.707863	-0.151802	1.614685
C	5.780361	0.329509	-0.179846
H	4.584078	-0.737565	-1.612440
C	4.845605	0.536510	2.032007
H	2.889309	-0.311760	2.310347
C	5.887891	0.782827	1.136609
H	6.589305	0.505656	-0.883926
H	4.913595	0.890655	3.057259
H	6.774358	1.320523	1.460844

17

C	-0.741072	-0.000008	-0.000102
C	-1.461524	1.139727	0.392245
C	-1.461592	-1.139580	-0.392574
C	-2.855150	1.140356	0.391848
H	-0.921916	2.021739	0.724333
C	0.741067	-0.000206	-0.000109
C	-2.855213	-1.140405	-0.391860
H	-0.921810	-2.021470	-0.724806
C	-3.558515	0.000037	0.000204
H	-3.392514	2.030401	0.707617
C	1.461465	1.139576	-0.392363
C	1.461628	-1.139727	0.392473

H	-3.392757	-2.030351	-0.707411
H	-4.644796	-0.000304	0.000677
C	2.855075	1.140473	-0.391811
H	0.921746	2.021399	-0.724863
C	2.855242	-1.140365	0.391892
H	0.922150	-2.021568	0.725322
C	3.558541	0.000077	-0.000036
H	3.392538	2.030719	-0.706753
H	3.392840	-2.030455	0.707052
H	4.644806	0.000158	-0.000010

CO

O	0.000000	0.000000	0.487597
C	0.000000	0.000000	-0.650130

NaHCO₃

C	-0.557990	0.042977	0.000008
O	-0.021948	-1.112520	-0.000015
O	-1.921419	0.097485	0.000009
Na	1.880065	-0.042255	0.000009
H	-2.209445	-0.830959	0.000012
O	0.052950	1.144773	-0.000014

PhB(OH)₂

C	0.179750	0.010246	-0.005823
C	-0.561414	1.202258	-0.062505
C	-0.534005	-1.199896	0.052517
C	-1.955571	1.195908	-0.057834

H	-0.050800	2.163043	-0.123966
B	1.744852	-0.002986	-0.004126
C	-1.927748	-1.217814	0.060401
H	0.020008	-2.132964	0.092397
C	-2.641449	-0.018425	0.005803
H	-2.505775	2.131628	-0.105492
O	2.522801	1.124989	0.107981
O	2.388553	-1.204730	-0.115400
H	-2.459360	-2.164354	0.108389
H	-3.728070	-0.029533	0.010852
H	2.002260	1.930601	0.226241
H	3.349262	-1.079225	-0.083798

TS-S1

Pd	0.440280	0.954635	0.336518
P	-0.941915	2.764505	-0.099608
C	-1.044071	0.033497	1.322514
C	-2.756102	2.452881	-0.125193
C	-0.563101	3.525505	-1.732744
C	-0.757680	4.170186	1.076656
C	-1.553184	0.561404	2.516765
C	-1.600631	-1.155092	0.829587
C	-3.139749	1.311039	-1.081996
H	-3.012998	2.171032	0.901366
H	-3.291011	3.381984	-0.359089
H	0.502210	3.771384	-1.769371
H	-1.155321	4.431199	-1.903840
H	-0.773962	2.801930	-2.525428

H	-1.021255	3.832509	2.083381
H	-1.401906	5.012689	0.801443
H	0.284726	4.502256	1.084725
C	-2.606367	-0.068155	3.190382
H	-1.130473	1.472633	2.934678
C	-2.657560	-1.779888	1.496345
H	-1.201313	-1.606531	-0.072790
C	-4.402817	0.570930	-0.625960
H	-2.320228	0.584987	-1.120614
H	-3.267791	1.699746	-2.100728
C	-3.170071	-1.236427	2.676492
H	-2.985615	0.359945	4.115526
H	-3.086082	-2.693020	1.090751
C	-4.674043	-0.685710	-1.457973
H	-4.271398	0.279387	0.422153
H	-5.266902	1.248298	-0.664045
H	-3.996735	-1.720752	3.188080
P	-6.051184	-1.739071	-0.757037
H	-3.771574	-1.311036	-1.456091
H	-4.887452	-0.425561	-2.505111
C	-6.166021	-2.996714	-2.129831
C	-7.517590	-0.680806	-1.217302
H	-5.272994	-3.630940	-2.121220
H	-6.255779	-2.530818	-3.119135
H	-7.035258	-3.642674	-1.966437
H	-8.441677	-1.242873	-1.044786
H	-7.490342	-0.363952	-2.267666
H	-7.548615	0.209978	-0.581665

C	1.731022	-0.790055	0.564130
C	1.883001	-1.386707	1.828263
C	1.531713	-1.650083	-0.540309
C	1.834057	-2.771246	1.993090
H	2.072304	-0.749040	2.685428
C	1.487844	-3.034391	-0.389818
H	1.426044	-1.224696	-1.536711
C	1.631343	-3.595152	0.885079
H	1.959102	-3.208435	2.980158
H	1.335730	-3.677891	-1.253584
H	1.592429	-4.674499	1.010136
B	3.052429	0.771165	0.288079
N	4.153320	-0.012189	-0.489839
O	2.317391	1.719357	-0.517185
O	3.433184	1.253904	1.535299
C	4.131680	-0.060291	-1.870380
C	5.021868	-0.849659	0.264640
H	2.434398	1.441840	-1.464632
H	2.856333	2.002001	1.748605
C	5.167239	-0.888263	-2.603246
O	3.277619	0.535659	-2.543553
C	6.148594	-1.574214	-0.460351
O	4.865888	-1.006288	1.455413
C	6.474983	-0.995053	-1.829512
H	5.281381	-0.440564	-3.593212
H	4.735526	-1.889473	-2.749601
H	7.002535	-1.573346	0.222302
H	5.830321	-2.621390	-0.562643

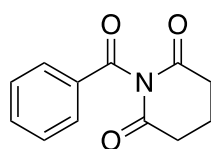
H	7.193843	-1.625921	-2.362382
H	6.929182	-0.001865	-1.725375

List of Known Compounds/General Methods

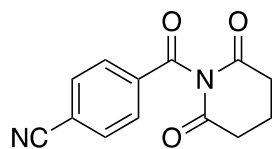
All starting materials reported in the manuscript have been previously described in literature and prepared by the method reported previously unless stated otherwise. Amides were prepared by standard methods.¹⁻⁵ All experiments involving palladium were performed using standard Schlenk techniques under nitrogen or argon unless stated otherwise. All solvents were purchased at the highest commercial grade and used as received or after purification by passing through activated alumina columns or distillation from sodium/benzophenone under nitrogen. All solvents were deoxygenated prior to use. All other chemicals were purchased at the highest commercial grade and used as received. Reaction glassware was oven-dried at 140 °C for at least 24 h or flame-dried prior to use, allowed to cool under vacuum and purged with argon (three cycles). All products were identified using ¹H NMR analysis and comparison with authentic samples. GC and/or GC/MS analysis was used for volatile products. All yields refer to yields determined by ¹H NMR and/or GC or GC/MS using an internal standard (optimization) and isolated yields (preparative runs) unless stated otherwise. ¹H NMR and ¹³C NMR spectra were recorded in CDCl₃ on Bruker spectrometers at 500 (¹H NMR), 125 (¹³C NMR) and 471 (¹⁹F NMR) MHz. All shifts are reported in parts per million (ppm) relative to residual CHCl₃ peak (7.26 and 77.16 ppm, ¹H NMR and ¹³C NMR, respectively). All coupling constants (*J*) are reported in hertz (Hz). Abbreviations are: s, singlet; d, doublet; t, triplet; q, quartet; brs, broad singlet. GC-MS chromatography was performed using Agilent HP6890 GC System and Agilent 5973A inert XL EI/CI MSD using helium as the carrier gas at a flow rate of 1 mL/min and an initial oven temperature of 50 °C. The injector temperature was 250 °C. The detector temperature was 250 °C. For runs with the initial oven temperature of 50 °C, temperature was increased with a 10 °C/min ramp after 50 °C hold for 3 min to a final temperature of 220 °C, then hold at 220 °C for 15 min (splitless mode of injection, total run time 22.0 min). High-resolution mass spectra were measured on a 7T Bruker Daltonics FT-MS instrument. All flash chromatography was performed using silica gel, 60 Å, 300 mesh. TLC analysis was carried out on glass plates coated with silica gel 60 F254, 0.2 mm thickness. The plates were visualized using a 254 nm ultraviolet lamp or aqueous potassium permanganate. ¹H NMR and ¹³C NMR data are given for all compounds in the Supplementary Experimental for characterization purposes. ¹H NMR, ¹³C NMR and HRMS data are given for all new compounds.

Experimental Procedures and Characterization Data

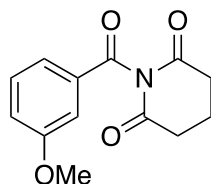
General Procedure for the Synthesis of Starting Materials. All amides used in this study have been previously reported and prepared by reported methods.¹⁻⁵ ¹H NMR and ¹³C NMR data are given for all starting materials in the section below for characterization purposes.



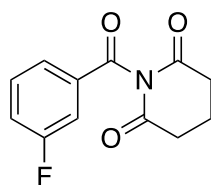
1-Benzoylpiperidine-2,6-dione (1a). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.89 (d, *J* = 7.8 Hz, 2 H), 7.67 (t, *J* = 7.5 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 2 H), 2.80 (t, *J* = 6.6 Hz, 4 H), 2.17 (q, *J* = 6.5 Hz, 2 H). ¹³C NMR (125 MHz, CDCl₃) δ 171.90, 170.74, 134.97, 131.78, 130.16, 129.14, 77.29, 77.24, 77.04, 76.78, 32.41, 17.51.



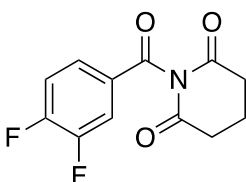
1-(4-Cyanobenzoyl)piperidine-2,6-dione (1b). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.97 (d, *J* = 8.5 Hz, 2 H), 7.82 (d, *J* = 8.5 Hz, 2 H), 2.82 (t, *J* = 6.5 Hz, 4 H), 2.20 (p, *J* = 6.6 Hz, 2 H). ¹³C NMR (125 MHz, CDCl₃) δ 171.89, 169.88, 135.23, 132.86, 130.30, 117.97, 117.48, 32.38, 17.43.



1-(3-Methoxybenzoyl)piperidine-2,6-dione (1c). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.48 (s, 1 H), 7.42-7.35 (m, 2 H), 7.20 (d, *J* = 7.5 Hz, 1 H), 3.87 (s, 3 H), 2.78 (t, *J* = 6.5 Hz, 4 H), 2.15 (m, 2 H). ¹³C NMR (125 MHz, CDCl₃) δ 171.90, 170.71, 160.11, 133.03, 130.11, 122.62, 121.55, 114.39, 55.56, 32.38, 17.50.

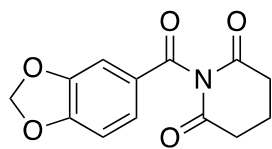


1-(3-Fluorobenzoyl)piperidine-2,6-dione (1d). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.64 (dt, *J* = 7.7, 1.3 Hz, 1 H), 7.54 (dt, *J* = 8.9, 2.0 Hz, 1 H), 7.47 (td, *J* = 8.0, 5.4 Hz, 1 H), 7.34 (td, *J* = 8.2, 2.5 Hz, 1 H), 2.77 (t, *J* = 6.6 Hz, 4 H), 2.14 (p, *J* = 6.6 Hz, 2 H). ¹³C NMR (125 MHz, CDCl₃) δ 172.08, 170.07, 163.89, 133.94, 131.02, 130.95, 125.93, 125.90, 122.25, 122.08, 116.92, 116.74, 32.37, 17.47. ¹⁹F NMR (471 MHz, CDCl₃) δ -111.07.

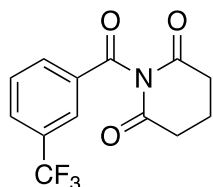


1-(3,4-Difluorobenzoyl)piperidine-2,6-dione (1e). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.81-7.60 (m, 2 H), 7.31 (dt, *J* = 16.1, 7.8 Hz, 1 H), 2.87-2.74 (m, 4 H), 2.25-2.11 (m, 2 H). ¹³C NMR (125 MHz, CDCl₃) δ

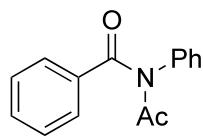
171.86, 168.94, 154.87 ($J^F = 243.8$ Hz), 150.73 ($J^F = 237.5$ Hz), 129.08, 127.37, 119.43 ($J^F = 18.8$ Hz), 118.25 ($J^F = 17.5$ Hz), 32.36, 17.43. ^{19}F NMR (471 MHz, CDCl_3) δ -125.85, -134.81.



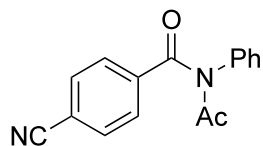
1-(Benzo[d][1,3]dioxole-5-carbonyl)piperidine-2,6-dione (1f). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.46 (d, $J = 8.2$ Hz, 1 H), 7.36 (s, 1 H), 6.89 (d, $J = 8.2$ Hz, 1 H), 6.11 (s, 2 H), 2.79 (t, $J = 6.4$ Hz, 4 H), 2.16 (m, 2 H). ^{13}C NMR (125 MHz, CDCl_3) δ 171.83, 169.33, 153.60, 148.62, 127.29, 126.25, 109.60, 108.55, 102.39, 32.43, 17.49.



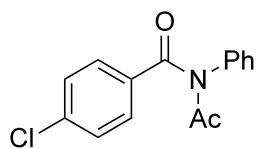
1-(3-(Trifluoromethyl)benzoyl)piperidine-2,6-dione (1g). White solid. ^1H NMR (500 MHz, CDCl_3) δ 8.13 (s, 1 H), 8.03 (d, $J = 7.9$ Hz, 1 H), 7.91 (d, $J = 7.8$ Hz, 1 H), 7.67 (t, $J = 7.8$ Hz, 1 H), 2.82 (t, $J = 6.5$ Hz, 4 H), 2.18 (m, 2 H). ^{13}C NMR (125 MHz, CDCl_3) δ 171.96, 169.98, 133.10, 132.66, 131.89 ($J^F = 32.5$ Hz), 131.30 ($J^F = 6.3$ Hz), 129.90, 126.77 ($J^F = 7.5$ Hz), 123.30 ($J^F = 270.0$ Hz), 32.36, 17.44. ^{19}F NMR (471 MHz, CDCl_3) δ -62.95.



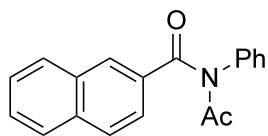
N-Acetyl-N-phenylbenzamide (1h). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.64-7.63 (d, $J = 7.1$ Hz, 2 H), 7.45-7.42 (t, $J = 7.4$ Hz, 1 H), 7.38-7.32 (m, 4 H), 7.31-7.29 (d, $J = 7.4$ Hz, 1 H), 7.19-7.18 (d, $J = 7.3$ Hz, 2 H), 2.46 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 173.55, 172.86, 139.14, 134.79, 132.06, 129.40, 129.24, 128.58, 128.28, 128.13, 25.69.



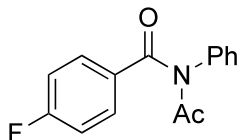
N-Acetyl-N-phenyl-4-cyanobenzamide (1i). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.72-7.61 (m, 4 H), 7.43 (t, $J = 7.4$ Hz, 2 H), 7.38 (t, $J = 7.4$ Hz, 1 H), 7.18 (d, $J = 7.3$ Hz, 2 H), 2.40 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 173.25, 171.11, 139.35, 138.33, 132.07, 129.81, 129.24, 128.98, 128.70, 117.85, 114.96, 25.71.



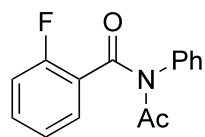
N-Acetyl-N-phenyl-4-chlorobenzamide (1j). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.54 (d, $J = 8.6$ Hz, 2 H), 7.37 (t, $J = 7.5$ Hz, 2 H), 7.33-7.27 (m, 3 H), 7.15 (d, $J = 7.0$ Hz, 1 H), 2.41 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 173.44, 171.75, 138.90, 138.34, 133.21, 130.59, 129.57, 128.63, 128.54, 128.38, 25.64.



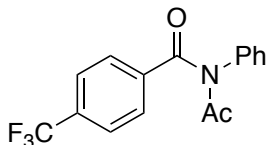
N-Acetyl-N-phenyl-2-naphthamide (1k). White solid. ^1H NMR (500 MHz, CDCl_3) δ 8.23 (s, 1 H), 7.86 (d, $J = 7.3$ Hz, 1 H), 7.82 (d, $J = 7.4$ Hz, 1 H), 7.77 (d, $J = 7.4$ Hz, 1 H), 7.67 (d, $J = 7.3$ Hz, 1 H), 7.57 (d, $J = 7.2$ Hz, 1 H), 7.54-7.50 (m, 1 H), 7.36 (t, $J = 7.4$ Hz, 2 H), 7.29-7.24 (m, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 173.58, 172.91, 139.19, 134.84, 132.33, 132.02, 130.89, 129.45, 129.18, 128.57, 128.33, 128.13, 128.08, 127.76, 126.84, 125.05, 25.72.



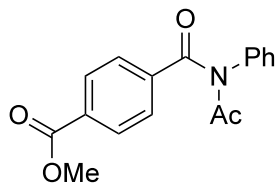
N-Acetyl-N-phenyl-4-fluorobenzamide (1l). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.67- 7.60 (m, 2 H), 7.36 (t, $J = 7.5$ Hz, 2 H), 7.29 (t, $J = 7.4$ Hz, 1 H), 7.19-7.12 (m, 2 H), 6.99 (t, $J = 8.6$ Hz, 2 H), 2.41 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 172.67 (d, $J^F = 226.9$ Hz), 164.91 (d, $J^F = 254.3$ Hz), 139.18, 132.96 (d, $J^F = 9.6$ Hz), 131.99 (d, $J^F = 9.1$ Hz), 130.99 (d, $J^F = 3.3$ Hz), 129.63, 128.62, 128.38, 115.65 (d, $J^F = 22.2$ Hz), 25.71. ^{19}F NMR (471 MHz, CDCl_3) δ -105.10.



N-Acetyl-N-phenyl-2-fluorobenzamide (1m). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.55-7.52 (m, 1 H), 7.41-7.33 (m, 4 H), 7.26-7.24 (d, $J = 7.6$ Hz, 2 H), 7.17-7.14 (t, $J = 7.6$ Hz, 1 H), 7.01-6.97 (t, $J = 9.8$ Hz, 1 H), 2.33 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 172.91, 168.43, 158.44 (d, $J^F = 248.6$ Hz), 138.51, 132.71 (d, $J^F = 8.5$ Hz), 129.88 (d, $J^F = 2.4$ Hz), 129.51, 128.89, 128.82, 125.00 (d, $J^F = 14.2$ Hz), 124.43 (d, $J^F = 3.4$ Hz), 115.64 (d, $J^F = 21.6$ Hz), 25.74. ^{19}F NMR (471 MHz, CDCl_3) δ - 114.28.

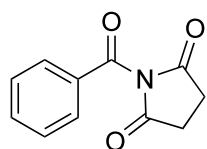


N-Acetyl-N-phenyl-4-(trifluoromethyl)benzamide (1n). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.68 (d, $J = 8.0$ Hz, 2 H), 7.58 (d, $J = 8.1$ Hz, 2 H), 7.40 (t, $J = 7.7$ Hz, 2 H), 7.36-7.30 (m, 1 H), 7.17 (d, $J = 6.5$ Hz, 2 H), 2.40 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 173.43, 171.66, 138.71, 138.65, 133.27 (q, $J^F = 32.8$ Hz), 129.82, 129.17, 128.82, 128.80, 125.43 (q, $J^F = 3.8$ Hz), 123.60 (q, $J^F = 272.6$ Hz). ^{19}F NMR (471 MHz, CDCl_3) δ -63.04.

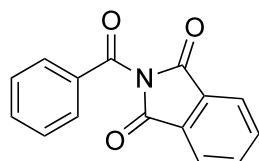


N-Acetyl-N-phenyl-4-(methoxycarbonyl)benzamide (1o). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.97 (d, $J = 6.5$ Hz, 2H), 7.62 (d, $J = 6.5$ Hz, 2H), 7.36 (t, $J = 6.8$ Hz, 2H), 7.29 (t, 1H), 7.15 (d, $J = 8.0$ Hz, 2H), 2.44 (s, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 173.39, 171.98, 166.07,

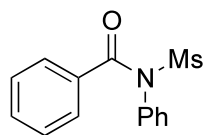
139.07, 138.68, 132.64, 129.58, 129.45, 128.70, 128.52, 52.42, 25.80.



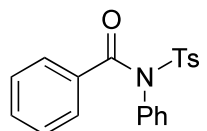
1-Benzoylpyrrolidine-2,5-dione (1p). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.88 (s, 1 H), 7.69 (t, $J = 7.5$ Hz, 1 H), 7.53 (t, $J = 7.8$ Hz, 1 H), 2.96 (s, 2 H). ^{13}C NMR (125 MHz, CDCl_3) δ 174.54, 167.62, 135.15, 131.40, 130.53, 128.97, 29.08.



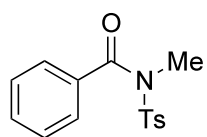
2-Benzoylisoindoline-1,3-dione (1q). White solid. ^1H NMR (500 MHz, CDCl_3) δ 8.02-7.98 (m, 2 H), 7.91-7.86 (m, 4 H), 7.70-7.65 (m, 1 H), 7.70 (t, $J = 8.0$ Hz, 2 H). ^{13}C NMR (125 MHz, CDCl_3) δ 167.07, 165.62, 135.32, 134.52, 132.60, 131.46, 130.46, 128.90, 128.67, 124.52.



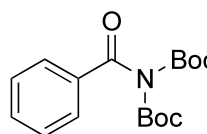
N-(Methylsulfonyl)-N-phenylbenzamide (1r). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.57-7.56 (d, $J = 7.2$ Hz, 2 H), 7.38-7.28 (m, 6 H), 7.26-7.23 (t, $J = 7.9$ Hz, 2 H), 3.46 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 171.10, 136.96, 133.14, 132.24, 129.82, 129.68, 129.47, 129.26, 128.21, 40.39.



N-Phenyl-N-tosylbenzamide (1s). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.86 (d, $J = 8.3$ Hz, 2 H), 7.46 (d, $J = 8.3$ Hz, 2 H), 7.34 (d, $J = 8.1$ Hz, 2 H), 7.29 (m, 4 H), 7.21-7.16 (m, 4 H), 2.47 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 169.90, 144.81, 137.43, 135.25, 133.67, 131.74, 130.40, 129.49, 129.25, 129.10, 129.03, 128.60, 127.98, 21.73.



N-Methyl-N-tosylbenzamide (1t). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.85 (d, $J = 8.0$ Hz, 2 H), 7.57 (d, $J = 8.2$ Hz, 2 H), 7.53 (t, $J = 8.0$ Hz, 1 H), 7.43 (t, $J = 7.6$ Hz, 2 H), 7.35 (d, $J = 8.1$ Hz, 2 H), 3.30 (s, 3H), 2.47 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 171.48, 144.91, 135.21, 134.52, 131.96, 129.62, 128.49, 128.42, 128.29, 35.60, 21.68.



N, N-Boc₂-Benzamide (1u). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.85 (d, $J = 7.7$ Hz, 2 H), 7.61 (t, $J = 7.4$ Hz, 1 H), 7.49 (t, $J = 7.3$ Hz, 2 H), 1.39 (s, 18 H). ^{13}C NMR (125 MHz, CDCl_3) δ 149.77, 133.41, 129.09, 128.67, 84.27, 27.59.

General Procedure for Biaryl Suzuki-Miyaura Cross-Coupling. N-Glutarimide Amides. An oven-dried vial equipped with a stir bar was charged with an amide substrate (neat, 1.0 equiv), boronic acid (typically, 1.2 equiv), NaHCO₃ (typically, 3 equiv) and Pd(dppb)Cl₂ or Pd(dppf)Cl₂ (typically, 5 mol%), placed under a positive pressure of argon, and subjected to three evacuation/backfilling cycles under high vacuum. Dioxane (typically, 0.125 M) was added with vigorous stirring at room temperature, the reaction mixture was placed in a preheated oil bath at 160 °C, and stirred for the indicated time at 160 °C. After the indicated time, the reaction mixture was cooled down to room temperature, diluted with CH₂Cl₂ (10 mL), filtered, and concentrated. The sample was analyzed by ¹H NMR (CDCl₃, 500 MHz) and GC-MS conversion and yield using internal standard and comparison with authentic samples. Purification by chromatography on silica gel (EtOAc/hexanes) afforded the title product.

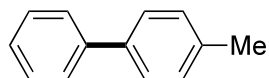
General Procedure for Biaryl Suzuki-Miyaura Cross-Coupling. N-Ac Amides. An oven-dried vial equipped with a stir bar was charged with an amide substrate (neat, 1.0 equiv), boronic acid (typically, 1.5 equiv), NaHCO₃ (typically, 3 equiv) and Pd(dppb)Cl₂ (typically, 5 mol%), placed under a positive pressure of argon, and subjected to three evacuation/backfilling cycles under high vacuum. Dioxane (typically, 0.125 M) was added with vigorous stirring at room temperature, the reaction mixture was placed in a preheated oil bath at 160 °C, and stirred for the indicated time at 160 °C. After the indicated time, the reaction mixture was cooled down to room temperature, diluted with CH₂Cl₂ (10 mL), filtered, and concentrated. The sample was analyzed by ¹H NMR (CDCl₃, 500 MHz) and GC-MS conversion and yield using internal standard and comparison with authentic samples. Purification by chromatography on silica gel (EtOAc/hexanes) afforded the title product.

Representative Procedure for Biaryl Suzuki-Miyaura Cross-Coupling. 1 Mmol scale. An oven-dried vial equipped with a stir bar was charged with 1-(4-cyanobenzoyl)piperidine-2,6-dione (neat, 242.2 mg, 1 mmol), (4-methylphenyl)boronic acid (163.2 mg, 1.2 mmol, 1.2 equiv), NaHCO₃ (252.0 mg, 3 mmol, 3 equiv), and Pd(dppb)Cl₂ (30.2 mg, 0.05 mmol 5 mol%), placed under a positive pressure of argon, and subjected to three evacuation/backfilling cycles under high vacuum. Dioxane (0.125 M) was added with vigorous stirring at room temperature, the flask was sealed with septum, the reaction was placed in a preheated oil bath at 170 °C, and stirred at 170 °C for 12 h. After the indicated time, the reaction mixture was cooled down to

room temperature, diluted with CH₂Cl₂ (50 mL), filtered, and concentrated. A sample was analyzed by ¹H NMR (CDCl₃, 500 MHz) and GC-MS to obtain conversion, yield and selectivity using internal standard and comparison with authentic samples. Purification by chromatography afforded the title product. Yield 87% (168.5 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.74-7.62 (m, 4 H), 7.50 (d, *J* = 8.2 Hz, 2 H), 7.29 (d, *J* = 7.9 Hz, 2 H), 2.42 (s, 3 H). ¹³C NMR (125 MHz, CDCl₃) δ 145.71, 138.87, 136.37, 132.67, 129.95, 127.57, 127.17, 119.16, 110.65, 21.31.

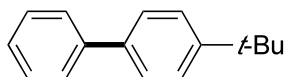
Biaryl Suzuki-Miyaura Coupling of N-Glutarimide Amides

4-Methylbiphenyl (Table 2, 3a)



According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), (4-(*tert*-butyl)phenyl)boronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 84% yield (28.3 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.59 (dd, *J* = 8.3, 1.3 Hz, 2 H), 7.51 (d, *J* = 8.1 Hz, 2 H), 7.44 (t, *J* = 7.7 Hz, 2 H), 7.33 (t, *J* = 7.4 Hz, 1 H), 7.26 (d, *J* = 8.1 Hz, 2 H), 2.41 (s, 3 H). ¹³C NMR (125 MHz, CDCl₃) δ 141.30, 138.50, 137.16, 129.61, 128.85, 127.13, 127.11, 127.11, 21.25. NMR spectroscopic data agreed with literature values.³

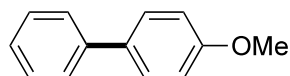
4-(*tert*-Butyl)biphenyl (Table 2, 3b)



According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), (4-(*tert*-butyl)phenyl)boronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 91% yield (38.3 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.61 (d, *J* = 7.1 Hz, 2 H), 7.56 (d, *J* = 8.5 Hz, 2 H), 7.49 (d, *J* = 8.4 Hz, 2 H), 7.44 (t, *J* = 7.8 Hz, 2 H), 7.34 (t, *J* = 7.4 Hz, 1 H), 1.38 (s, 9

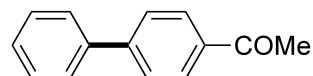
H). ^{13}C NMR (125 MHz, CDCl_3) δ 150.39, 141.21, 138.46, 128.83, 127.16, 127.11, 126.93, 125.85, 34.68, 31.53. NMR spectroscopic data agreed with literature values.¹

4-Methoxybiphenyl (Table 2, 3c)



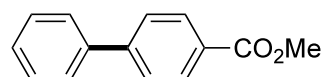
According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), (4-methoxyphenyl)boronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 86% yield (31.8 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.59-7.52 (m, 4 H), 7.43 (t, J = 7.8 Hz, 2 H), 7.31 (t, J = 7.4 Hz, 1 H), 6.99 (d, J = 8.8 Hz, 2 H), 3.86 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 159.28, 140.97, 133.92, 128.86, 128.29, 126.88, 126.79, 114.34, 55.49. NMR spectroscopic data agreed with literature values.⁶

4-Acetylbiphenyl (Table 2, 3d)



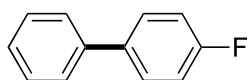
According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), (4-acetylphenyl)boronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 77% yield (30.5 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 8.04 (d, J = 8.4 Hz, 2 H), 7.69 (d, J = 8.4 Hz, 2 H), 7.63 (d, J = 7.0 Hz, 2 H), 7.48 (t, J = 7.5 Hz, 2 H), 7.41 (t, J = 7.3 Hz, 1 H), 2.64 (s, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 197.84, 145.87, 139.96, 135.95, 129.06, 129.02, 128.34, 127.37, 127.32, 26.78. NMR spectroscopic data agreed with literature values.³

Methyl 4-phenylbenzoate (Table 2, 3e)



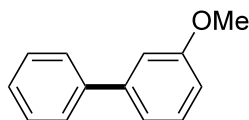
According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 69% yield (29.4 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 8.12 (d, *J* = 8.4 Hz, 2 H), 7.67 (d, *J* = 8.3 Hz, 2 H), 7.63 (d, *J* = 7.1 Hz, 2 H), 7.47 (t, *J* = 7.7 Hz, 2 H), 7.40 (t, *J* = 7.4 Hz, 1 H), 3.95 (s, 3 H). ¹³C NMR (125 MHz, CDCl₃) δ 167.09, 145.72, 140.08, 130.20, 129.02, 128.99, 128.24, 127.37, 127.14, 52.22. NMR spectroscopic data agreed with literature values.³

4-Fluorobiphenyl (Table 2, 3f)



According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), (4-fluorophenyl)boronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 71% yield (24.5 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.59- 7.52 (m, 4 H), 7.44 (t, *J* = 7.7 Hz, 2 H), 7.35 (t, *J* = 7.4 Hz, 1 H), 7.13 (t, *J* = 8.7 Hz, 2 H). ¹³C NMR (125 MHz, CDCl₃) δ 162.60 (d, *J*^F = 246.2 Hz), 140.40, 137.48 (d, *J*^F = 3.2 Hz), 128.96, 128.83 (d, *J*^F = 8.2 Hz), 127.40, 127.16, 115.75 (d, *J*^F = 21.4 Hz). ¹⁹F NMR (471 MHz, CDCl₃) δ -115.89. NMR spectroscopic data agreed with literature values.¹

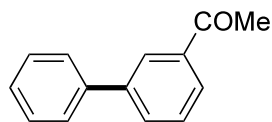
3-Methoxybiphenyl (Table 2, 3g)



According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), (3-methoxyphenyl)boronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 78% yield (28.8 mg). Colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 7.59 (d, *J* = 7.1 Hz, 2 H), 7.44 (t, *J* = 7.6 Hz, 2 H), 7.39- 7.33 (m, 2 H), 7.19 (d, *J* = 7.5 Hz, 1 H), 7.13 (t, *J* = 2.1 Hz, 1 H), 6.90 (dd, *J* = 8.2, 2.5 Hz, 1 H), 3.87 (s, 3 H). ¹³C NMR (125 MHz, CDCl₃) δ 160.07, 142.92, 141.25, 129.88,

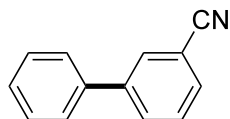
128.87, 127.55, 127.34, 119.83, 113.04, 112.82, 55.46. NMR spectroscopic data agreed with literature values.¹

3-Acetylbiphenyl (Table 2, 3h)



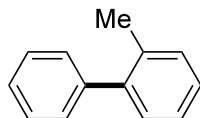
According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), (3-acetylphenyl)boronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 65% yield (25.6 mg). Colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 8.19 (t, *J* = 1.8 Hz, 1 H), 7.94 (ddd, *J* = 7.8, 1.8, 1.2 Hz, 1 H), 7.80 (ddd, *J* = 7.7, 1.9, 1.1 Hz, 1 H), 7.63 (dd, *J* = 8.3, 1.3 Hz, 2 H), 7.54 (t, *J* = 7.7 Hz, 1 H), 7.48 (t, *J* = 7.6 Hz, 2 H), 7.39 (t, *J* = 7.3 Hz, 1 H), 2.66 (s, 3 H). ¹³C NMR (125 MHz, CDCl₃) δ 198.23, 141.87, 140.32, 137.77, 131.88, 129.18, 129.06, 127.95, 127.33, 127.32, 127.10, 26.91. NMR spectroscopic data agreed with literature values.⁷

3-Cyanobiphenyl (Table 2, 3i)



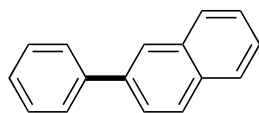
According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), (3-cyanophenyl)boronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 68% yield (24.5 mg). Colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 7.87 (t, *J* = 1.5 Hz, 1 H), 7.82 (dt, *J* = 8.0, 1.6 Hz, 1 H), 7.63 (dt, *J* = 7.7, 1.4 Hz, 1 H), 7.58-7.54 (m, 3 H), 7.48 (t, *J* = 7.5 Hz, 2 H), 7.42 (t, *J* = 7.3 Hz, 1 H). ¹³C NMR (125 MHz, CDCl₃) δ 142.59, 139.02, 131.63, 130.85, 130.83, 129.73, 129.27, 128.53, 127.22, 118.99, 113.10. NMR spectroscopic data agreed with literature values.⁸

2-Methylbiphenyl (Table 2, 3j)



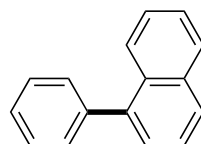
According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), (2-methylphenyl)boronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 59% yield (19.9 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.41 (t, J = 7.2 Hz, 2 H), 7.37-7.30 (m, 3 H), 7.28-7.22 (m, 4 H), 2.28 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 142.10, 142.07, 135.48, 130.43, 129.93, 129.33, 128.19, 127.37, 126.89, 125.89, 20.61. NMR spectroscopic data agreed with literature values.⁶

2-Phenylnaphthalene (Table 2, 3k)



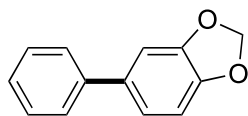
According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), naphthalen-2-ylboronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 81% yield (33.1 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 8.06 (s, 1H), 7.93 (t, J = 8.7 Hz, 2 H), 7.88 (d, J = 7.4 Hz, 1 H), 7.77 (dd, J = 8.6, 2.0 Hz, 1 H), 7.74 (d, J = 7.1 Hz, 2 H), 7.55-7.47 (m, 4 H), 7.40 (t, J = 7.3 Hz, 1 H). ^{13}C NMR (125 MHz, CDCl_3) δ 141.27, 138.70, 133.81, 132.75, 128.99, 128.55, 128.34, 127.78, 127.57, 127.49, 126.42, 126.07, 125.94, 125.74. NMR spectroscopic data agreed with literature values.¹

1-Phenylnaphthalene (Table 2, 3l)



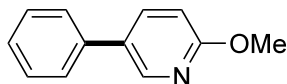
According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), naphthalen-1-ylboronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 66% yield (27.0 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.93 (dd, J = 8.3, 1.2 Hz, 2 H), 7.88 (dd, J = 8.2, 1.2 Hz, 1 H), 7.57- 7.49 (m, 6H), 7.47- 7.43 (m, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 140.91, 140.41, 133.94, 131.77, 130.21, 128.40, 128.39, 127.76, 127.37, 127.06, 126.17, 126.15, 125.89, 125.51. NMR spectroscopic data agreed with literature values.¹

3, 4-Methylenedioxybiphenyl (Table 2, 3m)



According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), 3,4-(methylenedioxy)phenylboronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 69% yield (27.4 mg). Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 7.52 (d, J = 7.9 Hz, 2 H), 7.41 (t, J = 7.5 Hz, 2 H), 7.32 (t, J = 7.5 Hz, 1 H), 7.11-7.03 (m, 2 H), 6.89 (d, J = 7.9 Hz, 1 H), 6.00 (s, 2 H). ^{13}C NMR (125 MHz, CDCl_3) δ 148.25, 147.20, 141.08, 135.78, 128.87, 127.07, 127.03, 120.77, 108.71, 107.83, 101.28. NMR spectroscopic data agreed with literature values.⁹

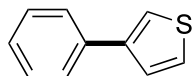
2-Methoxy-5-phenylpyridine (Table 2, 3n)



According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), (6-methoxy-3-pyridinyl)boronic acid (3 equiv), NaHCO_3 (4.5 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 64% yield (23.8 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 8.39 (d, J = 2.2 Hz, 1 H), 7.79 (dd, J = 8.6, 2.6 Hz, 1 H), 7.53 (d, J = 7.2 Hz, 2 H), 7.45 (t, J = 7.7 Hz, 2 H), 7.37 (t, J = 7.7 Hz, 1 H), 6.82 (d, J = 8.6 Hz, 1 H), 3.99 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 163.74, 145.12, 138.06, 137.61,

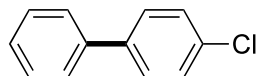
130.24, 129.11, 127.45, 126.83, 110.95, 53.69. NMR spectroscopic data agreed with literature values.¹⁰

3-Phenylthiophene (Table 2, 3o)



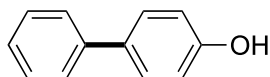
According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), 3-thiopheneboronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppf)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 67% yield (21.5 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.61 (dd, *J* = 8.2, 1.4 Hz, 2 H), 7.46 (dd, *J* = 2.7, 1.6 Hz, 1 H), 7.42- 7.38 (m, 4 H), 7.30 (t, *J* = 7.4 Hz, 1 H). ¹³C NMR (125 MHz, CDCl₃) δ 142.51, 136.00, 128.94, 127.27, 126.59, 126.48, 126.33, 120.40. NMR spectroscopic data agreed with literature values.¹¹

4-Chlorobiphenyl (Table 2, 3p)



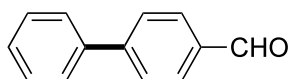
According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), 4-chlorophenylboronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppf)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 87% yield (32.8 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.55 (d, *J* = 7.4 Hz, 2 H), 7.52 (d, *J* = 8.5 Hz, 2 H), 7.44 (t, *J* = 7.7 Hz, 2 H), 7.41 (d, *J* = 8.5 Hz, 2 H), 7.36 (t, *J* = 7.4 Hz, 1 H). ¹³C NMR (125 MHz, CDCl₃) δ 140.00, 139.68, 133.38, 128.90, 128.87, 128.39, 127.58, 126.98. NMR spectroscopic data agreed with literature values.⁶

4-Phenylphenol (Table 2, 3q)



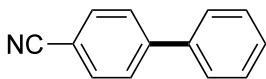
According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), 4-hydroxyphenylboronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 81% yield (27.6 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.54 (dd, J = 8.2, 1.2 Hz, 2 H), 7.48 (d, J = 8.6 Hz, 2 H), 7.42 (t, J = 7.7 Hz, 2 H), 7.31 (t, J = 7.4 Hz, 1 H), 6.91 (d, J = 8.6 Hz, 2 H), 4.81 (s, 1 H). ^{13}C NMR (125 MHz, CDCl_3) δ 155.19, 140.89, 134.19, 128.86, 128.54, 126.86, 126.85, 115.78. NMR spectroscopic data agreed with literature values.⁹

4-carbaldehydebiphenyl (Table 2, 3r)



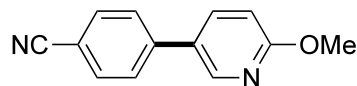
According to the general procedure, the reaction of 1-benzoylpiperidine-2,6-dione (0.20 mmol), 4-formylphenylboronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 74% yield (26.9 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 10.06 (s, 1 H), 7.96 (d, J = 8.3 Hz, 2 H), 7.76 (d, J = 8.3 Hz, 2 H), 7.64 (d, J = 7.0 Hz, 2 H), 7.49 (t, J = 7.5 Hz, 2 H), 7.42 (t, J = 7.4 Hz, 1 H). ^{13}C NMR (125 MHz, CDCl_3) δ 191.93, 147.21, 139.73, 135.20, 130.28, 129.02, 128.48, 127.70, 127.38. NMR spectroscopic data agreed with literature values.¹²

4-Cyanobiphenyl (Table 2, 3s)



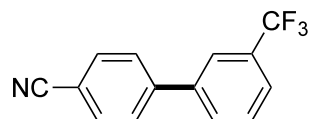
According to the general procedure, the reaction of 1-(4-cyanobenzoyl)piperidine-2,6-dione (0.20 mmol), phenylboronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 93% yield (33.3 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.76-7.66 (m, 4 H), 7.59 (d, J = 7.0 Hz, 2 H), 7.49 (t, J = 7.4 Hz, 2 H), 7.43 (t, J = 7.3 Hz, 1 H). ^{13}C NMR (125 MHz, CDCl_3) δ 145.89, 139.39, 132.81, 129.33, 128.88, 127.95, 127.45, 119.16, 111.14. NMR spectroscopic data agreed with literature values.¹²

4-(6-methoxypyridin-3-yl)benzonitrile (Table 2, 3t)



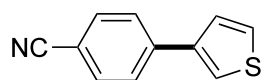
According to the general procedure, the reaction of 1-(4-cyanobenzoyl)piperidine-2,6-dione (0.20 mmol), (6-methoxy-3-pyridinyl)boronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 84% yield (35.3 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 8.41 (dd, $J = 2.6$, 0.8 Hz, 1 H), 7.79 (dd, $J = 8.7$, 2.6 Hz, 1 H), 7.73 (d, $J = 8.5$ Hz, 2 H), 7.62 (d, $J = 8.4$ Hz, 2 H), 6.85 (dd, $J = 8.7$, 0.7 Hz, 1 H), 3.99 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 164.58, 145.55, 142.59, 137.40, 132.94, 128.22, 127.24, 118.93, 111.46, 111.10, 53.88. NMR spectroscopic data agreed with literature values.¹³

4-(3-(Trifluoromethyl)phenyl)benzonitrile (Table 2, 3u)



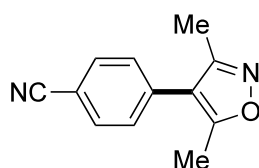
According to the general procedure, the reaction of 1-(4-cyanobenzoyl)piperidine-2,6-dione (0.20 mmol), 3-(trifluoromethyl)phenylboronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 88% yield (43.5 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.83 (s, 1 H), 7.80-7.74 (m, 3 H), 7.72-7.66 (m, 3 H), 7.62 (t, $J = 7.8$ Hz, 1 H). ^{13}C NMR (125 MHz, CDCl_3) δ 144.26, 140.15, 132.95, 131.77 (q, $J^F = 32.7$ Hz), 130.66, 129.82, 128.02, 125.45 (q, $J^F = 3.7$ Hz), 124.20 (q, $J^F = 3.8$ Hz), 124.05 (q, $J^F = 273.4$ Hz), 118.72, 112.02. ^{19}F NMR (471 MHz, CDCl_3) δ -62.70. NMR spectroscopic data agreed with literature values.¹⁴

4-(thiophen-3-yl)benzonitrile (Table 2, 3v)



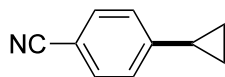
According to the general procedure, the reaction of 1-(4-cyanobenzoyl)piperidine-2,6-dione (0.20 mmol), 3-thiopheneboronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 75% yield (27.8 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.68 (s, 4 H), 7.58 (dd, $J = 2.9, 1.4$ Hz, 1 H), 7.45 (dd, $J = 5.0, 2.9$ Hz, 1 H), 7.40 (dd, $J = 5.1, 1.4$ Hz, 1 H). ^{13}C NMR (125 MHz, CDCl_3) δ 140.48, 140.14, 132.83, 127.29, 126.97, 126.06, 122.74, 119.07, 110.63. NMR spectroscopic data agreed with literature values.¹⁵

4-(3,5-dimethylisoxazol-4-yl)benzonitrile (Table 2, 3w)



According to the general procedure, the reaction of 1-(4-cyanobenzoyl)piperidine-2,6-dione (0.20 mmol), 3,5-dimethylisoxazole-4-boronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 66% yield (26.2 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.74 (d, $J = 8.4$ Hz, 2 H), 7.38 (d, $J = 8.4$ Hz, 2 H), 2.44 (s, 3 H), 2.29 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 166.26, 158.25, 135.66, 132.78, 129.72, 118.64, 115.57, 111.55, 11.88, 10.99. NMR spectroscopic data agreed with literature values.¹⁶

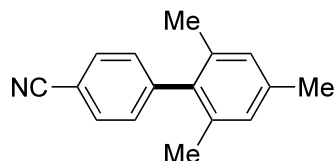
4-cyclopropylbenzonitrile (Table 2, 3x)



According to the general procedure, the reaction of 1-(4-cyanobenzoyl)piperidine-2,6-dione (0.20 mmol), cyclopropylboronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 77% yield (22.0 mg). Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 7.52 (d, $J = 8.2$ Hz, 2 H), 7.12 (d, $J = 8.2$ Hz, 2 H), 1.98-1.90 (m, 1 H), 1.13-1.03 (m, 2 H), 0.80-0.74 (m, 2 H). ^{13}C NMR (125

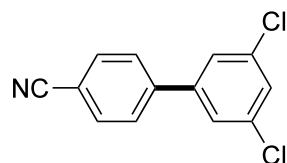
MHz, CDCl₃) δ 150.35, 132.23, 126.26, 119.38, 109.00, 16.00, 10.72. NMR spectroscopic data agreed with literature values.¹⁷

4-(2,4,6-(Trimethyl)phenyl)benzonitrile (Table 2, 3y)



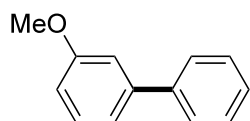
According to the general procedure, the reaction of 1-(4-cyanobenzoyl)piperidine-2,6-dione (0.20 mmol), (2,4,6-trimethylphenyl)boronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 67% yield (29.6 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.72 (d, *J* = 8.3 Hz, 2 H), 7.27 (d, *J* = 8.4 Hz, 2 H), 6.95 (s, 2 H), 2.33 (s, 3 H), 1.97 (s, 6 H). ¹³C NMR (125 MHz, CDCl₃) δ 146.66, 137.81, 137.37, 135.54, 132.54, 130.58, 128.58, 119.25, 110.88, 21.27, 20.85. NMR spectroscopic data agreed with literature values.¹⁸

4-((3,5-dichloro)phenyl)benzonitrile (Table 2, 3z)



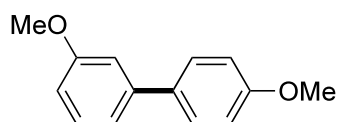
According to the general procedure, the reaction of 1-(4-cyanobenzoyl)piperidine-2,6-dione (0.20 mmol), (3,5-dichlorophenyl)boronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 73% yield (36.3 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.75 (d, *J* = 8.4 Hz, 2 H), 7.64 (d, *J* = 8.5 Hz, 2 H), 7.46 (d, *J* = 1.9 Hz, 2 H), 7.42 (t, *J* = 1.9 Hz, 1 H). ¹³C NMR (125 MHz, CDCl₃) δ 143.03, 142.23, 135.91, 132.98, 128.67, 127.92, 125.92, 118.57, 112.42. HRMS calcd for C₁₃H₇Cl₂NNa (M + Na⁺) 269.9853, found 269.9867.

3-Methoxybiphenyl (Table 2, 3g')



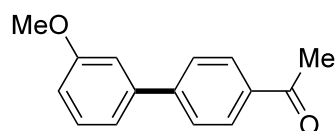
According to the general procedure, the reaction of 1-(3-methoxybenzoyl)piperidine-2,6-dione (0.20 mmol), phenylboronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 68% yield (25.1 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.59 (d, J = 7.1 Hz, 2 H), 7.44 (t, J = 7.6 Hz, 2 H), 7.39-7.33 (m, 2 H), 7.19 (d, J = 7.5 Hz, 1 H), 7.13 (t, J = 2.1 Hz, 1 H), 6.90 (dd, J = 8.2, 2.5 Hz, 1 H). ^{13}C NMR (125 MHz, CDCl_3) δ 160.07, 142.92, 141.25, 129.88, 128.87, 127.55, 127.34, 119.83, 113.04, 112.82, 55.46. NMR spectroscopic data agreed with literature values.¹

3, 4'-Dimethoxybiphenyl (Table 2, 3aa)



According to the general procedure, the reaction of 1-(3-methoxybenzoyl)piperidine-2,6-dione (0.20 mmol), (4-methoxyphenyl)boronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 78% yield (33.4 mg). Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 7.53 (d, J = 8.8 Hz, 2 H), 7.34 (t, J = 7.9 Hz, 1 H), 7.15 (ddd, J = 7.7, 1.7, 0.9 Hz, 1 H), 7.11-7.08 (m, 1 H), 6.98 (d, J = 8.8 Hz, 2 H), 6.86 (ddd, J = 8.2, 2.6, 1.0 Hz, 1 H), 3.87 (s, 3 H), 3.86 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 160.06, 159.38, 142.50, 133.76, 129.84, 128.33, 119.43, 114.30, 112.67, 112.16, 55.49, 55.43. NMR spectroscopic data agreed with literature values.¹²

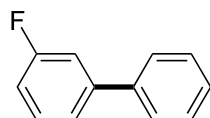
3-Methoxy-4'-acetylbiphenyl (Table 2, 3ab)



According to the general procedure, the reaction of 1-(3-methoxybenzoyl)piperidine-2,6-dione (0.20 mmol), (4-acetylphenyl)boronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0

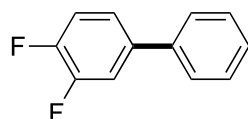
mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 72% yield (32.6 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 8.03 (d, *J* = 8.5 Hz, 2 H), 7.68 (d, *J* = 8.4 Hz, 2 H), 7.39 (t, *J* = 7.9 Hz, 1 H), 7.21 (ddd, *J* = 7.6, 1.7, 0.9 Hz, 1 H), 7.17-7.14 (m, 1 H), 6.95 (ddd, *J* = 8.2, 2.6, 0.9 Hz, 1 H). ¹³C NMR (125 MHz, CDCl₃) δ 197.88, 160.18, 145.79, 141.52, 136.12, 130.13, 129.02, 127.43, 119.90, 113.68, 113.22, 55.51, 26.83. NMR spectroscopic data agreed with literature values.¹⁹

3-Fluorobiphenyl (Table 2, 3ac)



According to the general procedure, the reaction of 1-(3-fluorobenzoyl)piperidine-2,6-dione (0.20 mmol), phenylboronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 62% yield (21.4 mg). Colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 7.60 (dd, *J* = 8.2, 1.4 Hz, 2 H), 7.47 (t, *J* = 7.6 Hz, 2 H), 7.43-7.36 (m, 3 H), 7.34-7.29 (m, 1 H), 7.09-7.03 (m, 1 H). ¹³C NMR (125 MHz, CDCl₃) δ 163.33 (d, *J*^F = 245.5 Hz), 143.64 (d, *J*^F = 7.7 Hz), 140.08 (d, *J*^F = 2.2 Hz), 130.34 (d, *J*^F = 8.5 Hz), 129.02, 127.97, 127.24, 122.89 (d, *J*^F = 2.8 Hz), 114.25 (d, *J*^F = 1.4 Hz), 114.07 (d, *J*^F = 2.3 Hz). ¹⁹F NMR (471 MHz, CDCl₃) δ -113.12. NMR spectroscopic data agreed with literature values.²⁰

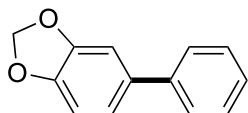
3,4-difluorobiphenyl (Table 2, 3ad)



According to the general procedure, the reaction of 1-(3,4-difluorobenzoyl)piperidine-2,6-dione (0.20 mmol), phenylboronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 77% yield (29.3 mg). Colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 7.59 (d, *J* = 7.0 Hz, 2 H), 7.52 (t, *J* = 7.7 Hz, 2 H), 7.48-7.42 (m, 2 H), 7.39-7.34 (m, 1 H), 7.33-7.27 (m, 1 H). ¹³C NMR (125 MHz,

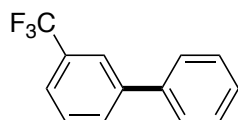
CDCl₃) δ 150.70 (dd, J^F = 248.2, 12.6 Hz), 150.10 (dd, J^F = 248.2, 12.8 Hz), 139.29 (d, J^F = 1.7 Hz), 138.48 (dd, J^F = 5.9, 3.7 Hz), 129.08, 127.95, 127.08, 123.12 (dd, J^F = 6.2, 3.4 Hz), 117.63 (d, J^F = 17.2 Hz), 116.13 (d, J^F = 17.7 Hz). ¹⁹F NMR (471 MHz, CDCl₃) δ -137.62, -140.36. NMR spectroscopic data agreed with literature values.⁹

3, 4-Methylenedioxybiphenyl (Table 2, 3m')



According to the general procedure, the reaction of 1-(benzo[*d*][1,3]dioxole-5-carbonyl)piperidine-2,6-dione (0.20 mmol), phenylboronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 60% yield (23.9 mg). Colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 7.52 (d, J = 7.9 Hz, 2 H), 7.41 (t, J = 7.5 Hz, 2 H), 7.32 (t, J = 7.5 Hz, 1 H), 7.11-7.03 (m, 2 H), 6.89 (d, J = 7.9 Hz, 1 H), 6.00 (s, 2 H). ¹³C NMR (125 MHz, CDCl₃) δ 148.25, 147.20, 141.08, 135.78, 128.87, 127.07, 127.03, 120.77, 108.71, 107.83, 101.28. NMR spectroscopic data agreed with literature values.⁹

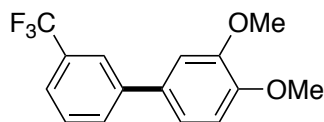
3-Trifluoromethylbiphenyl (Table 2, 3ae)



According to the general procedure, the reaction of 1-(3-trifluoromethylbenzoyl)piperidine-2,6-dione (0.20 mmol), phenylboronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 79% yield (35.1 mg). Colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 7.86 (s, 1 H), 7.78 (d, J = 7.6 Hz, 1 H), 7.66-7.60 (m, 3 H), 7.57 (t, J = 7.7 Hz, 1 H), 7.50 (t, J = 7.4 Hz, 2 H), 7.42 (t, J = 7.4 Hz, 1 H). ¹³C NMR (125 MHz, CDCl₃) δ 142.16, 139.91, 131.31 (q, J^F = 32.1 Hz), 130.56, 129.36, 129.14, 128.17, 127.33, 124.36 (q, J^F = 273.4 Hz), 124.88 (q, J = 3.8 Hz), 124.07 (q, J^F

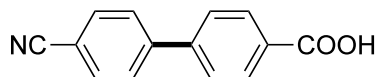
= 3.8 Hz). ^{19}F NMR (471 MHz, CDCl_3) δ -62.57. NMR spectroscopic data agreed with literature values.²¹

3, 4-dimethoxy-3'-(Trifluoromethyl)biphenyl (3af)



According to the general procedure, the reaction of 1-(3-trifluoromethylbenzoyl)piperidine-2,6-dione (0.20 mmol), (3,4-dimethoxyphenyl)boronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 89% yield (50.5 mg). Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 7.79 (s, 1 H), 7.73 (d, J = 7.5 Hz, 1 H), 7.60-7.51 (m, 2 H), 7.15 (dd, J = 8.3, 2.1 Hz, 1 H), 7.09 (d, J = 2.2 Hz, 1 H), 6.97 (d, J = 8.3 Hz, 1 H), 3.97 (s, 3 H), 3.94 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 149.49, 149.34, 141.97, 132.83, 131.11 (q, J^{F} = 34.02 Hz), 130.25, 129.31, 124.35 (q, J^{F} = 272.2 Hz), 123.7 (q, J^{F} = 3.8 Hz), 123.63 (q, J^{F} = 3.8 Hz), 119.77, 111.70, 110.47, 56.18, 56.15. ^{19}F NMR (471 MHz, CDCl_3) δ -62.56. NMR spectroscopic data agreed with literature values.²²

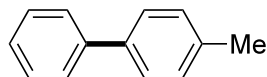
4'-cyanobiphenyl-4-carboxylic acid (Table 2, 3ag)



According to the general procedure, the reaction of 1-(4-cyanobenzoyl)piperidine-2,6-dione (0.20 mmol), (4-carboxyphenyl)boronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 49% yield (21.8 mg). White solid. ^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 13.10 (s, 1 H), 8.05 (d, J = 8.4 Hz, 2 H), 8.00-7.92 (m, 4 H), 7.88 (d, J = 8.4 Hz, 2 H). ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) δ 166.93, 143.48, 142.25, 132.94, 130.03, 130.00, 127.90, 127.30, 118.69, 110.82. NMR spectroscopic data agreed with literature values.²³

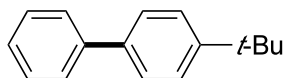
Biaryl Suzuki-Miyaura Coupling of N-Ac Amides

4-Methylbiphenyl (Table 3, 3a)



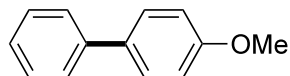
According to the general procedure, the reaction of *N*-Acetyl-*N*-phenylbenzamide (0.20 mmol), (4-methylphenyl)boronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 70% yield (23.6 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.59 (dd, *J* = 8.3, 1.3 Hz, 2 H), 7.51 (d, *J* = 8.1 Hz, 2 H), 7.44 (t, *J* = 7.7 Hz, 2 H), 7.33 (t, *J* = 7.4 Hz, 1 H), 7.26 (d, *J* = 8.1 Hz, 2 H), 2.41 (s, 3 H). ¹³C NMR (125 MHz, CDCl₃) δ 141.30, 138.50, 137.16, 129.61, 128.85, 127.13, 127.11, 127.11, 21.25. NMR spectroscopic data agreed with literature values.³

4-(*tert*-Butyl)biphenyl (Table 2, 3b)



According to the general procedure, the reaction of *N*-acetyl-*N*-phenylbenzamide (0.20 mmol), (4-(*tert*-butyl)phenyl)boronic acid (1.5 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 73% yield (30.7 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.61 (d, *J* = 7.1 Hz, 2 H), 7.56 (d, *J* = 8.5 Hz, 2 H), 7.49 (d, *J* = 8.4 Hz, 2 H), 7.44 (t, *J* = 7.8 Hz, 2 H), 7.34 (t, *J* = 7.4 Hz, 1 H), 1.38 (s, 9 H). ¹³C NMR (125 MHz, CDCl₃) δ 150.39, 141.21, 138.46, 128.83, 127.16, 127.11, 126.93, 125.85, 34.68, 31.53. NMR spectroscopic data agreed with literature values.¹

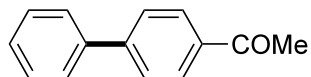
4-Methoxybiphenyl (Table 3, 3c)



According to the general procedure, the reaction of *N*-acetyl-*N*-phenylbenzamide (0.2 mmol), (4-methoxyphenyl)boronic acid (1.5 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 81% yield (29.8

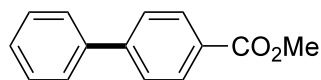
mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.59-7.52 (m, 4 H), 7.43 (t, $J = 7.8$ Hz, 2 H), 7.31 (t, $J = 7.4$ Hz, 1 H), 6.99 (d, $J = 8.8$ Hz, 2 H), 3.86 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 159.28, 140.97, 133.92, 128.86, 128.29, 126.88, 126.79, 114.34, 55.49. NMR spectroscopic data agreed with literature values.⁶

4-Acetylbiphenyl (Table 3, 3d)



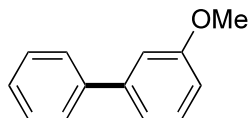
According to the general procedure, the reaction of *N*-acetyl-*N*-phenylbenzamide (0.20 mmol), (4-acetylphenyl)boronic acid (1.5 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 58% yield (22.8 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 8.04 (d, $J = 8.4$ Hz, 2 H), 7.69 (d, $J = 8.4$ Hz, 2 H), 7.63 (d, $J = 7.0$ Hz, 2 H), 7.48 (t, $J = 7.5$ Hz, 2 H), 7.41 (t, $J = 7.3$ Hz, 1 H), 2.64 (s, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 197.84, 145.87, 139.96, 135.95, 129.06, 129.02, 128.34, 127.37, 127.32, 26.78. NMR spectroscopic data agreed with literature values.³

Methyl 4-phenylbenzoate (Table 3, 3e)



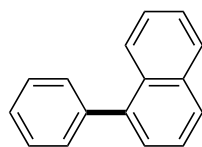
According to the general procedure, the reaction of *N*-acetyl-*N*-phenylbenzamide (0.20 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (1.5 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 52% yield (22.1 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 8.12 (d, $J = 8.4$ Hz, 2 H), 7.67 (d, $J = 8.3$ Hz, 2 H), 7.63 (d, $J = 7.1$ Hz, 2 H), 7.47 (t, $J = 7.7$ Hz, 2 H), 7.40 (t, $J = 7.4$ Hz, 1 H), 3.95 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 167.09, 145.72, 140.08, 130.20, 129.02, 128.99, 128.24, 127.37, 127.14, 52.22. NMR spectroscopic data agreed with literature values.³

3-Methoxybiphenyl (Table 3, 3g)



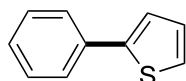
According to the general procedure, the reaction of *N*-acetyl-*N*-phenylbenzamide (0.20 mmol), (3-methoxyphenyl)boronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 67% yield (24.7 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.59 (d, *J* = 7.1 Hz, 2 H), 7.44 (t, *J* = 7.6 Hz, 2 H), 7.39-7.33 (m, 2 H), 7.19 (d, *J* = 7.5 Hz, 1 H), 7.13 (t, *J* = 2.1 Hz, 1 H), 6.90 (dd, *J* = 8.2, 2.5 Hz, 1 H), 3.87 (s, 3 H). ¹³C NMR (125 MHz, CDCl₃) δ 160.07, 142.92, 141.25, 129.88, 128.87, 127.55, 127.34, 119.83, 113.04, 112.82, 55.46. NMR spectroscopic data agreed with literature values.¹

1-Phenylnaphthalene (Table 3, 3l)



According to the general procedure, the reaction of *N*-acetyl-*N*-phenylbenzamide (0.20 mmol), naphthalen-1-ylboronic acid (1.5 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 54% yield (22.1 mg). Colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 7.93 (dd, *J* = 8.3, 1.2 Hz, 2 H), 7.88 (dd, *J* = 8.2, 1.2 Hz, 1 H), 7.57-7.49 (m, 6 H), 7.47-7.43 (m, 3 H). ¹³C NMR (125 MHz, CDCl₃) δ 140.91, 140.41, 133.94, 131.77, 130.21, 128.40, 128.39, 127.76, 127.37, 127.06, 126.17, 126.15, 125.89, 125.51. NMR spectroscopic data agreed with literature values.¹

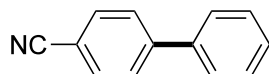
2-Phenylthiophene (Table 3, 3ah)



According to the general procedure, the reaction of *N*-acetyl-*N*-phenylbenzamide (0.20 mmol), 3-thiopheneboronic acid (1.5 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at

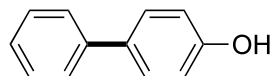
160 °C, afforded after work-up and chromatography the title compound in 73% yield (23.4 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.63 (d, *J* = 7.1 Hz, 2 H), 7.39 (t, *J* = 7.7 Hz, 2 H), 7.32 (dd, *J* = 3.6, 1.1 Hz, 1 H), 7.31-7.27 (m, 2 H), 7.09 (dd, *J* = 5.1, 3.6 Hz, 1 H). ¹³C NMR (125 MHz, CDCl₃) δ 144.57, 134.54, 129.01, 128.13, 127.59, 126.10, 124.93, 123.21. NMR spectroscopic data agreed with literature values.¹¹

4-Cyanobiphenyl (Table 3, 3s)



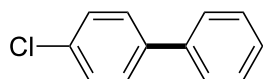
According to the general procedure, the reaction of *N*-acetyl-*N*-phenyl-4-cyanobenzamide (0.20 mmol), phenylboronic acid (1.5 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 91% yield (32.7 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.76-7.66 (m, 4 H), 7.59 (d, *J* = 7.0 Hz, 2 H), 7.49 (t, *J* = 7.4 Hz, 2 H), 7.43 (t, *J* = 7.3 Hz, 1 H). ¹³C NMR (125 MHz, CDCl₃) δ 145.89, 139.39, 132.81, 129.33, 128.88, 127.95, 127.45, 119.16, 111.14. NMR spectroscopic data agreed with literature values.⁹

4-Phenylphenol (Table 3, 3q)



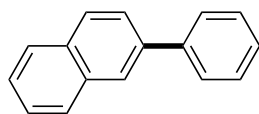
According to the general procedure, the reaction of *N*-acetyl-*N*-phenylbenzamide (0.20 mmol), 4-hydroxyphenylboronic acid (1.5 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 54% yield (18.4 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.54 (dd, *J* = 8.2, 1.2 Hz, 2 H), 7.48 (d, *J* = 8.6 Hz, 2 H), 7.42 (t, *J* = 7.7 Hz, 2 H), 7.31 (t, *J* = 7.4 Hz, 1 H), 6.91 (d, *J* = 8.6 Hz, 2 H), 4.81 (s, 1 H). ¹³C NMR (125 MHz, CDCl₃) δ 155.19, 140.89, 134.19, 128.86, 128.54, 126.86, 126.85, 115.78. NMR spectroscopic data agreed with literature values.⁹

4-chlorobiphenyl (Table 3, 3p')



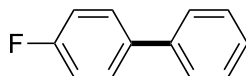
According to the general procedure, the reaction of *N*-acetyl-*N*-phenyl-4-chlorobenzamide (0.20 mmol), phenylboronic acid (1.5 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 77% yield (29.1 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.55 (d, *J* = 7.4 Hz, 2 H), 7.52 (d, *J* = 8.5 Hz, 2 H), 7.44 (t, *J* = 7.7 Hz, 2 H), 7.41 (d, *J* = 8.5 Hz, 2 H), 7.36 (t, *J* = 7.4 Hz, 1 H). ¹³C NMR (125 MHz, CDCl₃) δ 140.00, 139.68, 133.38, 128.90, 128.87, 128.39, 127.58, 126.98. NMR spectroscopic data agreed with literature values.⁶

2-Phenylnaphthalene (Table 3, 3k')



According to the general procedure, the reaction of *N*-acetyl-*N*-phenyl-2-naphthamide (0.20 mmol), phenylboronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 58% yield (23.7 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 8.06 (s, 1 H), 7.93 (t, *J* = 8.7 Hz, 2 H), 7.88 (d, *J* = 7.4 Hz, 1 H), 7.77 (dd, *J* = 8.6, 2.0 Hz, 1 H), 7.74 (d, *J* = 7.1 Hz, 2 H), 7.55-7.47 (m, 4 H), 7.40 (t, *J* = 7.3 Hz, 1 H). ¹³C NMR (125 MHz, CDCl₃) δ 141.27, 138.70, 133.81, 132.75, 128.99, 128.55, 128.34, 127.78, 127.57, 127.49, 126.42, 126.07, 125.94, 125.74. NMR spectroscopic data agreed with literature values.¹

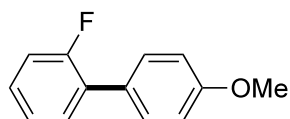
4-fluorobiphenyl (Table 3, 3f')



According to the general procedure, the reaction of *N*-acetyl-*N*-phenyl-4-fluorobenzamide (0.20 mmol), phenylboronic acid (1.5 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 65% yield (22.4

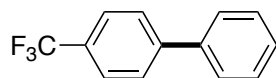
mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.59-7.52 (m, 4 H), 7.44 (t, $J = 7.7$ Hz, 2 H), 7.35 (t, $J = 7.4$ Hz, 1 H), 7.13 (t, $J = 8.7$ Hz, 2 H). ^{13}C NMR (125 MHz, CDCl_3) δ 162.60 (d, $J^F = 246.2$ Hz), 140.40, 137.48 (d, $J^F = 3.2$ Hz), 128.96, 128.83 (d, $J^F = 8.2$ Hz), 127.40, 127.16, 115.75 (d, $J^F = 21.4$ Hz). ^{19}F NMR (471 MHz, CDCl_3) δ -115.89. NMR spectroscopic data agreed with literature values.¹

2-Fluoro-4'-methoxybiphenyl (Table 3, 3ai)



According to the general procedure, the reaction of *N*-acetyl-*N*-phenyl-2-fluorobenzamide (0.20 mmol), (4-methoxyphenyl)boronic acid (1.5 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 65% yield (26.3 mg). Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 7.51 (dd, $J = 8.8, 1.7$ Hz, 2 H), 7.42 (td, $J = 7.8, 1.8$ Hz, 1 H), 7.31-7.26 (m, 1 H), 7.19 (td, $J = 7.5, 1.3$ Hz, 1 H), 7.14 (ddd, $J = 10.8, 8.1, 1.3$ Hz, 1 H), 6.99 (d, $J = 8.8$ Hz, 2 H), 3.86 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 159.88 (d, $J^F = 246.9$ Hz), 159.35, 130.64 (d, $J^F = 3.6$ Hz), 130.28 (d, $J^F = 3.0$ Hz), 128.83 (d, $J^F = 13.5$ Hz), 128.53 (d, $J^F = 8.2$ Hz), 128.32, 124.43 (d, $J^F = 3.7$ Hz), 116.18 (d, $J^F = 22.9$ Hz), 114.05, 55.45. ^{19}F NMR (471 MHz, CDCl_3) δ -118.24. NMR spectroscopic data agreed with literature values.²¹

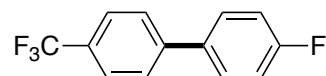
4-(Trifluoromethyl)biphenyl (Table 3, 3aj)



According to the general procedure, the reaction of *N*-acetyl-*N*-phenyl-4-(trifluoromethyl)benzamide (0.20 mmol), phenylboronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 81% yield (35.9 mg). Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 7.71 (s, 4 H), 7.63-7.59 (m, 2 H), 7.49 (t, $J = 7.5$ Hz, 2 H), 7.42 (t, $J = 7.3$ Hz, 1 H). ^{13}C NMR (125 MHz, CDCl_3) δ 144.88, 139.92, 129.50 (q, $J^F = 32.8$ Hz), 129.13, 128.33, 127.56, 127.42, 125.85 (q, J^F

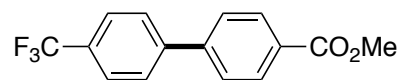
= 3.7 Hz), 124.47 (q, J^F = 272.2 Hz). ^{19}F NMR (471 MHz, CDCl_3) δ -62.38. NMR spectroscopic data agreed with literature values.¹

4-Fluoro-4'-(trifluoromethyl)biphenyl (Table 3, 3ak)



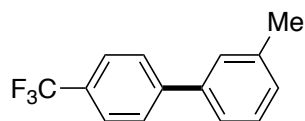
According to the general procedure, the reaction of *N*-acetyl-*N*-phenyl-4-(trifluoromethyl)benzamide (0.20 mmol), (4-fluorophenyl)boronic acid (1.5 equiv), NaHCO_3 (3 equiv) and $\text{Pd}(\text{dppb})\text{Cl}_2$ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 80% yield (38.4 mg). Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 7.72-7.63 (m, 4 H), 7.56 (dd, J = 8.4, 5.3 Hz, 2 H), 7.17 (t, J = 8.5 Hz, 2 H). ^{13}C NMR (125 MHz, CDCl_3) δ 163.11 (d, J^F = 247.9 Hz), 143.86, 136.03 (d, J^F = 3.3 Hz), 129.66 (q, J^F = 32.4 Hz), 129.07 (d, J^F = 8.2 Hz), 127.42, 125.93 (q, J^F = 3.8 Hz), 124.39 (q, J^F = 271.9 Hz), 116.09 (d, J^F = 21.6 Hz). ^{19}F NMR (471 MHz, CDCl_3) δ -62.44, -114.16. NMR spectroscopic data agreed with literature values.¹

Methyl 4'-(trifluoromethyl)biphenyl-4-carboxylate (Table 3, 3al)



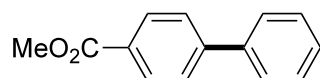
According to the general procedure, the reaction of *N*-acetyl-*N*-phenyl-4-(trifluoromethyl)benzamide (0.20 mmol), (4-methoxycarbonylphenyl)boronic acid (1.5 equiv), NaHCO_3 (3 equiv) and $\text{Pd}(\text{dppb})\text{Cl}_2$ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 73% yield (40.9 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 8.14 (d, J = 8.5 Hz, 2 H), 7.72 (s, 4 H), 7.67 (d, J = 8.4 Hz, 2 H), 3.96 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 166.90, 144.21, 143.68, 130.42, 130.32 (q, J^F = 32.8 Hz), 129.97, 127.77, 127.41, 126.02 (q, J^F = 3.7 Hz), 124.28 (q, J^F = 272.0 Hz), 52.39. ^{19}F NMR (471 MHz, CDCl_3) δ -62.54. NMR spectroscopic data agreed with literature values.¹

3-Methyl-4'-Trifluoromethylbiphenyl (Table 3, 3am)



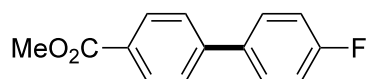
According to the general procedure, the reaction of *N*-acetyl-*N*-phenyl-4-(trifluoromethyl)benzamide (0.20 mmol), (3-methylphenyl)boronic acid (1.5 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 82% yield (38.7 mg). Colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 7.69 (s, 4 H), 7.41-7.36 (m, 3 H), 7.23 (d, *J* = 7.3 Hz, 1 H), 2.44 (s, 3 H). ¹³C NMR (125 MHz, CDCl₃) δ 145.02, 139.91, 138.79, 129.39 (q, *J*^F = 32.4 Hz), 129.06, 129.03, 128.19, 127.56, 125.78 (q, *J*^F = 3.8 Hz), 124.53, 124.48 (q, *J*^F = 272.2 Hz), 21.67. ¹⁹F NMR (471 MHz, CDCl₃) δ -62.37. NMR spectroscopic data agreed with literature values.¹

Methyl 4-phenylbenzoate (Table 3, 3d')



According to the general procedure, the reaction of *N*-acetyl-*N*-phenyl-4-(methoxycarbonyl)benzamide (0.20 mmol), phenylboronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 83% yield (35.2 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 8.12 (d, *J* = 8.4 Hz, 2 H), 7.67 (d, *J* = 8.3 Hz, 2 H), 7.63 (d, *J* = 7.1 Hz, 2 H), 7.47 (t, *J* = 7.7 Hz, 2 H), 7.40 (t, *J* = 7.4 Hz, 1 H), 3.95 (s, 3 H). ¹³C NMR (125 MHz, CDCl₃) δ 167.09, 145.72, 140.08, 130.20, 129.02, 128.99, 128.24, 127.37, 127.14, 52.22. NMR spectroscopic data agreed with literature values.³

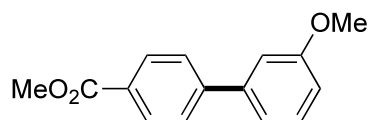
Methyl 4'-fluorobiphenyl-4-carboxylate (Table 3, 3an)



According to the general procedure, the reaction of *N*-acetyl-*N*-phenyl-4-(methoxycarbonyl)benzamide (0.20 mmol), (4-fluorophenyl)boronic acid (1.5 equiv), NaHCO₃

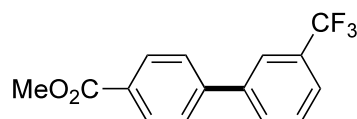
(3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 82% yield (37.8 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 8.10 (d, *J* = 8.5 Hz, 2 H), 7.64-7.55 (m, 4 H), 7.15 (t, *J* = 8.6 Hz, 2 H), 3.94 (s, 3 H). ¹³C NMR (125 MHz, CDCl₃) δ 167.05, 163.08 (d, *J*^F = 247.9 Hz), 144.73, 136.26 (d, *J*^F = 3.2 Hz), 130.30, 129.06 (d, *J*^F = 8.3 Hz), 127.02, 116.01 (d, *J*^F = 21.7 Hz), 52.30. ¹⁹F NMR (471 MHz, CDCl₃) δ -114.22. NMR spectroscopic data agreed with literature values.²⁴

Methyl 3'-methoxybiphenyl-4-carboxylate (Table 3, 3ao)



According to the general procedure, the reaction of *N*-acetyl-*N*-phenyl-4-(methoxycarbonyl)benzamide (0.20 mmol), (3-methoxyphenyl)boronic acid (1.5 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 78% yield (37.8 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 8.10 (d, *J* = 7.9 Hz, 2 H), 7.65 (d, *J* = 8.0 Hz, 2 H), 7.38 (t, *J* = 7.9 Hz, 1 H), 7.21 (d, *J* = 7.6 Hz, 1 H), 7.15 (d, *J* = 2.1 Hz, 1 H), 6.94 (dd, *J* = 8.2, 2.5 Hz, 1 H), 3.94 (s, 3 H), 3.88 (s, 3 H). ¹³C NMR (125 MHz, CDCl₃) δ 167.12, 160.16, 145.64, 141.65, 130.21, 130.08, 129.17, 127.24, 119.90, 113.64, 113.17, 55.50, 52.28. NMR spectroscopic data agreed with literature values.²⁵

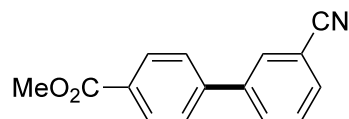
Methyl 3'-(trifluoromethyl)biphenyl-4-carboxylate (Table 3, 3ap)



According to the general procedure, the reaction of *N*-acetyl-*N*-phenyl-4-(methoxycarbonyl)benzamide (0.20 mmol), 3-(trifluoromethyl)phenylboronic acid (1.5 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 71% yield (39.8 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 8.14 (d, *J* = 7.9 Hz, 2 H), 7.86 (s, 1 H), 7.80 (d, *J* = 7.8 Hz, 1 H), 7.66 (t, *J* = 7.5 Hz, 3

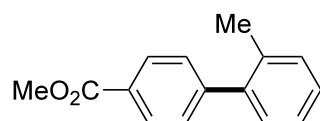
H), 7.59 (t, $J = 7.8$ Hz, 1 H), 3.96 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 166.91, 144.20, 140.99, 131.55 (q, $J^F = 32.5$ Hz), 130.71, 130.44, 129.84, 129.58, 127.31, 124.92 (q, $J^F = 3.7$ Hz), 124.22 (q, $J^F = 3.9$ Hz), 124.19 (q, $J^F = 272.16$ Hz), 52.38. ^{19}F NMR (471 MHz, CDCl_3) δ -62.65. NMR spectroscopic data agreed with literature values.²⁶

Methyl 3'-cyanobiphenyl-4-carboxylate (Table 3, 3aq)



According to the general procedure, the reaction of *N*-acetyl-*N*-phenyl-4-(methoxycarbonyl)benzamide (0.20 mmol), 3-cyanophenylboronic acid (1.5 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 63% yield (29.9 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 8.15 (d, $J = 8.7$ Hz, 2 H), 7.90 (t, $J = 1.5$ Hz, 1 H), 7.85 (ddd, $J = 7.9, 1.9, 1.2$ Hz, 1 H), 7.68 (dt, $J = 7.7, 1.4$ Hz, 1 H), 7.64 (d, $J = 8.6$ Hz, 2 H), 7.58 (t, $J = 7.8$ Hz, 1 H), 3.96 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 166.78, 143.27, 141.45, 131.73, 131.63, 130.99, 130.55, 130.18, 129.94, 127.23, 118.71, 113.38, 52.44. NMR spectroscopic data agreed with literature values.²⁷

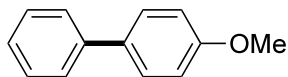
Methyl 2'-methylbiphenyl-4-carboxylate (Table 3, 3ar)



According to the general procedure, the reaction of *N*-acetyl-*N*-phenyl-4-(methoxycarbonyl)benzamide (0.02 mmol), (2-methylphenyl)boronic acid (1.5 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 74% yield (33.5 mg). Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 8.09 (d, $J = 8.3$ Hz, 2 H), 7.40 (d, $J = 8.2$ Hz, 2 H), 7.31-7.20 (m, 4 H), 3.95 (s, 3 H), 2.27 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 167.19, 146.89, 140.99, 135.30, 130.62, 129.66, 129.55, 129.40, 128.73, 127.96, 126.04, 52.27, 20.52. NMR spectroscopic data agreed with literature values.²⁸

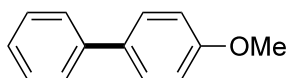
Biaryl Suzuki-Miyaura Coupling of Various Amides

4-Methoxybiphenyl (Table 4, from 1p, N-succinimide)



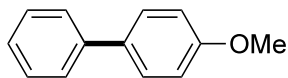
According to the general procedure, the reaction of 1-benzoylpyrrolidine-2,5-dione (0.20 mmol), (4-methoxyphenyl)boronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 77% yield (28.4 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.59-7.52 (m, 4 H), 7.43 (t, $J = 7.8$ Hz, 2 H), 7.31 (t, $J = 7.4$ Hz, 1 H), 6.99 (d, $J = 8.8$ Hz, 2 H), 3.86 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 159.28, 140.97, 133.92, 128.86, 128.29, 126.88, 126.79, 114.34, 55.49. NMR spectroscopic data agreed with literature values.⁶

4-Methoxybiphenyl (Table 4, from 1q, N-phthalimide)



According to the general procedure, the reaction of 2-benzoylisoindoline-1,3-dione (0.20 mmol), (4-methoxyphenyl)boronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2 (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 62% yield (22.9 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.59-7.52 (m, 4 H), 7.43 (t, $J = 7.8$ Hz, 2 H), 7.31 (t, $J = 7.4$ Hz, 1 H), 6.99 (d, $J = 8.8$ Hz, 2 H), 3.86 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 159.28, 140.97, 133.92, 128.86, 128.29, 126.88, 126.79, 114.34, 55.49. NMR spectroscopic data agreed with literature values.⁶

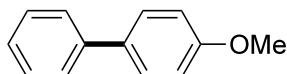
4-Methoxybiphenyl (Table 4, from 1r, N-Ms/Ph)



According to the general procedure, the reaction of *N*-(methylsulfonyl)-*N*-phenylbenzamide (0.20 mmol), (4-methoxyphenyl)boronic acid (1.2 equiv), NaHCO_3 (3 equiv) and Pd(dppb)Cl_2

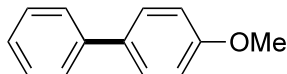
(5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 81% yield (29.5 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.59-7.52 (m, 4 H), 7.43 (t, J = 7.8 Hz, 2 H), 7.31 (t, J = 7.4 Hz, 1 H), 6.99 (d, J = 8.8 Hz, 2 H), 3.86 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 159.28, 140.97, 133.92, 128.86, 128.29, 126.88, 126.79, 114.34, 55.49. NMR spectroscopic data agreed with literature values.⁶

4-Methoxybiphenyl (Table 4, from 1s, N-Ts/Ph)



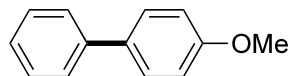
According to the general procedure, the reaction of *N*-phenyl-*N*-tosylbenzamide (0.20 mmol), (4-methoxyphenyl)boronic acid (1.2 equiv), NaHCO_3 (3 equiv) and $\text{Pd}(\text{dppb})\text{Cl}_2$ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 64% yield (23.6 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.59-7.52 (m, 4 H), 7.43 (t, J = 7.8 Hz, 2 H), 7.31 (t, J = 7.4 Hz, 1 H), 6.99 (d, J = 8.8 Hz, 2 H), 3.86 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 159.28, 140.97, 133.92, 128.86, 128.29, 126.88, 126.79, 114.34, 55.49. NMR spectroscopic data agreed with literature values.⁶

4-Methoxybiphenyl (Table 4, from 1t, N-Ts/Me)



According to the general procedure, the reaction of *N*-methyl-*N*-tosylbenzamide (0.20 mmol), (4-methoxyphenyl)boronic acid (1.2 equiv), NaHCO_3 (3 equiv) and $\text{Pd}(\text{dppb})\text{Cl}_2$ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 50% yield (18.4 mg). White solid. ^1H NMR (500 MHz, CDCl_3) δ 7.59-7.52 (m, 4 H), 7.43 (t, J = 7.8 Hz, 2 H), 7.31 (t, J = 7.4 Hz, 1 H), 6.99 (d, J = 8.8 Hz, 2 H), 3.86 (s, 3 H). ^{13}C NMR (125 MHz, CDCl_3) δ 159.28, 140.97, 133.92, 128.86, 128.29, 126.88, 126.79, 114.34, 55.49. NMR spectroscopic data agreed with literature values.⁶

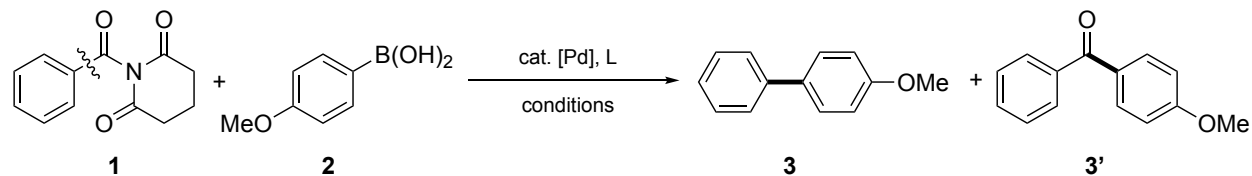
4-Methoxybiphenyl (Table 4, from 1u, N,N-Boc₂)



According to the general procedure, the reaction of N,N-Boc₂-benzamide (0.20 mmol), (4-methoxyphenyl)boronic acid (1.2 equiv), NaHCO₃ (3 equiv) and Pd(dppb)Cl₂ (5.0 mol%) for 12 h at 160 °C, afforded after work-up and chromatography the title compound in 28% yield (10.3 mg). White solid. ¹H NMR (500 MHz, CDCl₃) δ 7.59-7.52 (m, 4 H), 7.43 (t, *J* = 7.8 Hz, 2 H), 7.31 (t, *J* = 7.4 Hz, 1 H), 6.99 (d, *J* = 8.8 Hz, 2 H), 3.86 (s, 3 H). ¹³C NMR (125 MHz, CDCl₃) δ 159.28, 140.97, 133.92, 128.86, 128.29, 126.88, 126.79, 114.34, 55.49. NMR spectroscopic data agreed with literature values.⁶

Detailed Optimization Experiments

Table S2. Effect of Reaction Conditions on the Palladium-Catalyzed Suzuki-Miyaura Cross-Coupling of Amides.^a



Entry	[Pd]/(mol%)	2 (equiv)	Base/equiv	Yield of 3^b (%)	Yield of 3'^b (%)	Selectivity
1 ^c	Pd(PCy ₃) ₂ Cl ₂ /3	2	NaHCO ₃ /3	<2	10	<5:>95
2	Pd(PCy ₃) ₂ Cl ₂ /3	2	NaHCO ₃ /3	62	26	71:29
3 ^d	Pd(PCy ₃) ₂ Cl ₂ /3	2	NaHCO ₃ /3	16	13	55:45
4 ^e	Pd(PCy ₃) ₂ Cl ₂ /3	2	NaHCO ₃ /3	31	30	51:49
5	Pd(OAc) ₂ /PCy ₃ /3-6	2	NaHCO ₃ /3	<2	87	<5:>95
6	Pd(OAc) ₂ /PCyPh ₂ /3-6	2	NaHCO ₃ /3	<2	41	<5:>95
7	Pd(OAc) ₂ /dcype/3-6	2	NaHCO ₃ /3	<2	<2	-
8	Pd(OAc) ₂ /dcypp/3-6	2	NaHCO ₃ /3	<2	<2	-
9 ^f	Pd(PCy ₃) ₂ Cl ₂ /3	2	NaHCO ₃ /3	30	33	48:52
10	Pd(PCy ₃) ₂ Cl ₂ /3	2	NaHCO ₃ /5	47	35	57:43
11	Pd(PCy ₃) ₂ Cl ₂ /3	3	NaHCO ₃ /3	62	35	64:36
12	Pd(PCy ₃) ₂ Cl ₂ /3	1.5	NaHCO ₃ /3	66	28	70:30
13	Pd(PCy ₃) ₂ Cl ₂ /5	2	NaHCO ₃ /3	70	27	72:28
14 ^g	Pd(PCy ₃) ₂ Cl ₂ /5	2	NaHCO ₃ /3	12	33	27:73
15	Pd(PCy ₃) ₂ Cl ₂ /5	2	NaHCO ₃ /2	46	21	69:31
16	Pd(PCy ₃) ₂ Cl ₂ /5	1.2	NaHCO ₃ /3	83	16	84:16
17	Pd(PCy ₃) ₂ Cl ₂ /5	1.2	NaHCO ₃ /2	72	14	84:16
18	Pd(PCy ₃) ₂ Cl ₂ /5	3	NaHCO ₃ /4.5	56	42	57:43
19 ^h	Pd(PCy ₃) ₂ Cl ₂ /5	2	NaHCO ₃ /3	<2	<2	-
20	Pd(PCy ₃) ₂ Cl ₂ /5	2	NaHCO ₃ /-	<2	<2	-

Table S2. Continued.

Entry	[Pd]/(mol%)	2 (equiv)	Base/equiv	Yield of 3^b (%)	Yield of 3^b (%)	Selectivity
21 ^h	Pd(PCy ₃) ₂ Cl ₂ /5	2	NaHCO ₃ /-	<2	<2	-
22	Pd(PCy ₃) ₂ Cl ₂ /5	2	KHCO ₃ /3	56	40	58:42
23	Pd(PCy ₃) ₂ Cl ₂ /5	2	Na ₂ CO ₃ /3	21	16	57:43
24	Pd(PPh ₃) ₂ Cl ₂ /5	2	NaHCO ₃ /3	67	30	67:33
25	Pd(dcyph)Cl ₂ /5	2	NaHCO ₃ /3	82	13	86:14
26	Pd(dppf)Cl ₂ /5	2	NaHCO ₃ /3	82	13	86:14
27	Pd(dppb)Cl ₂ /5	2	NaHCO ₃ /3	86	12	88:12
28	Pd(PCy ₃) ₂ Cl ₂ /5	1.05	NaHCO ₃ /3	83	15	85:15
29	Pd(PCy ₃) ₂ Cl ₂ /5	1.05	NaHCO ₃ /1.5	46	11	81:19
30 ⁱ	Pd(PPh ₃) ₂ Cl ₂ /3	2	NaHCO ₃ /3	57	38	60:40
31 ⁱ	Pd(PCy ₃) ₂ Cl ₂ /3	2	NaHCO ₃ /3	61	36	63:37
32	Pd(PCy ₃) ₂ Cl ₂ /3	2	Na ₂ CO ₃ /3	15	12	56:44
33	Pd(PCy ₃) ₂ Cl ₂ /3	2	K ₂ CO ₃ /3	6	92	6:94
34	Pd(PCy ₃) ₂ Cl ₂ /3	2	K ₃ PO ₄ /3	<2	93	<5:>95
35	Pd(PCy ₃) ₂ Cl ₂ /3	2	KHCO ₃ /3	50	45	53:47
36	Pd(PCy ₃) ₂ Cl ₂ /3	2	K ₂ HPO ₄ /3	13	33	28:72
37	Pd(PCy ₃) ₂ Cl ₂ /3	2	KH ₂ PO ₄ /3	<2	<2	-
38	Pd(PCy ₃) ₂ Cl ₂ /3	2	KF/3	<2	98	<5:>95
39	Pd(PCy ₃) ₂ Cl ₂ /3	2	KOAc/3	<2	99	<5:>95
40	Pd(PCy ₃) ₂ Cl ₂ /3	2	Li ₂ CO ₃ /3	20	12	63:37
41	Pd(PCy ₃) ₂ Cl ₂ /3	2	LiBr/3	<2	<2	-
42	Pd(PCy ₃) ₂ Cl ₂ /3	2	CaCO ₃ /3	<2	<2	-
43	Pd(PCy ₃) ₂ Cl ₂ /3	2	KOH/3	10	88	10:90
44	Pd(PCy ₃) ₂ Cl ₂ /3	2	LiOH/3	30	48	39:61
45	Pd(PCy ₃) ₂ Cl ₂ /3	2	KOt-Bu/3	<2	14	<5:>95
46	Pd(PCy ₃) ₂ Cl ₂ /10	1.2	NaHCO ₃ /3	76	20	79:21
47	Pd(dppf)Cl ₂ /10	1.2	NaHCO ₃ /3	91	9	>10:1

Table S2. Continued.

Entry	[Pd]/(mol%)	2 (equiv)	Base/equiv	Yield of 3^b (%)	Yield of 3^b (%)	Selectivity
48	Pd(dppb)Cl ₂ /10	1.2	NaHCO ₃ /3	88	10	90:10
49	Pd(dppf)Cl ₂ /5	1.2	NaHCO ₃ /3	90	8	>10:1
50	Pd(dppb)Cl ₂ /5	1.2	NaHCO ₃ /3	88	10	90:10
51	Pd(OAc) ₂ /PCy ₃ /10-20	1.2	NaHCO ₃ /3	<2	71	<5:>95
52	PdCl ₂ /PCy ₃ /10-20	1.2	NaHCO ₃ /3	63	17	79:21
53	Pd(OAc) ₂ /dppf/10-20	1.2	NaHCO ₃ /3	25	<2	>95:5
54	PdCl ₂ /dppf/10-20	1.2	NaHCO ₃ /3	10	<2	>95:5

^aConditions: amide (0.20 mmol), boronic acid (1.05-3 equiv), [Pd] (x mol%), base (1.5-4.5 equiv), solvent (0.125 M), 160 °C, 12 h. All reactions carried out using standard Schlenk techniques. ^bDetermined by ¹H NMR and/or GC-MS. **3'**: (4-methoxyphenyl)(phenyl)methanone. Note a complete switch of the decarbonylation selectivity using strong bases. ^cToluene. ^dDME. ^eNMP. ^f0.25 M. ^g0.83 M. ^hH₃BO₃ (2.0 equiv). ⁱ150 °C.

Selectivity Studies – Boronic Acids

General Procedure. An oven-dried vial equipped with a stir bar was charged with an amide substrate (0.10 mmol, 1.0 equiv), sodium bicarbonate (3 equiv), two boronic acid substrates (each 2.0 equiv) and Pd(dppb)Cl₂ (0.05 equiv), placed under a positive pressure of argon, and subjected to three evacuation/backfilling cycles under high vacuum. Dioxane (0.125 M) was added with vigorous stirring at room temperature, the reaction mixture was placed in a preheated oil bath at 160 °C, and stirred for the indicated time at 160 °C. After the indicated time, the reaction mixture was cooled down to room temperature, diluted with CH₂Cl₂ (10 mL), filtered, and concentrated. The sample was analyzed by ¹H NMR (CDCl₃, 500 MHz) and GC-MS to obtain conversion and yield using internal standard and comparison with authentic samples.

Table S3. Selectivity Study in the Palladium-Catalyzed Suzuki-Miyaura Cross-Coupling of Amides.^a

Reaction scheme: Amide **1** (Ph-C(=O)-N(R')R'') reacts with boronic acids **2-I** (R₁-C₆H₄-B(OH)₂) and **2-II** (R₂-C₆H₄-B(OH)₂) in the presence of Pd(dppb)Cl₂ (5 mol%), NaHCO₃ (3 equiv), dioxane, 160 °C, 12 h to yield biaryl products **3-I** (Ph-C₆H₄-R₁) and **3-II** (Ph-C₆H₄-R₂).

Entry	NR'R''	2-I (R ₁)	2-II (R ₂)	Boronic acid (equiv)	3-I:3-II (R ₁ :R ₂) ^b
1	glutarimide	-Ac	-MeO	2.0	93:7
2	N-Ph/Ac	-Ac	-MeO	2.0	92:8

^aConditions: amide (0.10 mmol), boronic acid (2.0 equiv), Pd(dppb)Cl₂ (5 mol%), base (3 equiv), dioxane (0.125 M), 160 °C, 12 h. All reactions carried out using standard Schlenk techniques. ^bDetermined by ¹H NMR and/or GC-MS.

Selectivity Studies – Amides

General Procedure. An oven-dried vial equipped with a stir bar was charged with two amide substrates (1.0 equiv each), sodium bicarbonate (3 equiv), boronic acid (0.10 mmol) and Pd(dppb)Cl₂ (0.05 equiv), placed under a positive pressure of argon, and subjected to three evacuation/backfilling cycles under high vacuum. Dioxane (0.125 M) was added with vigorous stirring at room temperature, the reaction mixture was placed in a preheated oil bath at 160 °C, and stirred for the indicated time at 160 °C. After the indicated time, the reaction mixture was cooled down to room temperature, diluted with CH₂Cl₂ (10 mL), filtered, and concentrated. The sample was analyzed by ¹H NMR (CDCl₃, 500 MHz) and GC-MS to obtain conversion and yield using internal standard and comparison with authentic samples.

Table S4. Selectivity Study in the Palladium-Catalyzed Suzuki-Miyaura Cross-Coupling of Amides.^a

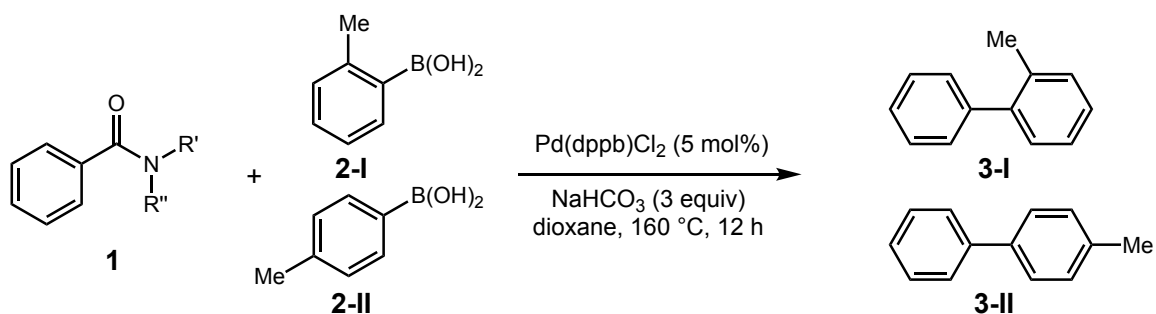
Entry	NR'R''	1-I (R ₁)	1-II (R ₂)	Amide (equiv)	3-I:3-II (R ₁ :R ₂) ^b
1	glutarimide	-CN	-H	2.0	>95:<5
2	N-Ph/Ac	-CF ₃	-H	2.0	82:18

^aConditions: amide (0.20 mmol), boronic acid (1.0 equiv), Pd(dppb)Cl₂ (5 mol%), base (3 equiv), dioxane (0.125 M), 160 °C, 12 h. All reactions carried out using standard Schlenk techniques. ^bDetermined by ¹H NMR and/or GC-MS.

Selectivity Studies – Sterics

General Procedure. An oven-dried vial equipped with a stir bar was charged with an amide substrate (0.10 mmol, 1.0 equiv), sodium bicarbonate (3 equiv), two boronic acid substrates (each 2.0 equiv) and Pd(dppb)Cl₂ (0.05 equiv), placed under a positive pressure of argon, and subjected to three evacuation/backfilling cycles under high vacuum. Dioxane (0.125 M) was added with vigorous stirring at room temperature, the reaction mixture was placed in a preheated oil bath at 160 °C, and stirred for the indicated time at 160 °C. After the indicated time, the reaction mixture was cooled down to room temperature, diluted with CH₂Cl₂ (10 mL), filtered, and concentrated. The sample was analyzed by ¹H NMR (CDCl₃, 500 MHz) and GC-MS to obtain conversion and yield using internal standard and comparison with authentic samples.

Table S5. Selectivity Study in the Palladium-Catalyzed Suzuki-Miyaura Cross-Coupling of Amides.^a



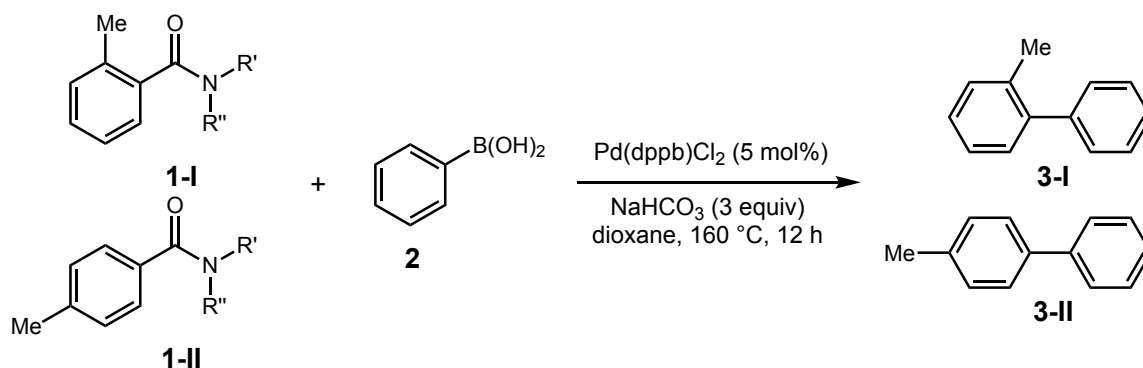
Entry	NR'R''	2-I (Ar)	2-II (Ar)	Boronic acid (equiv)	3-I:3-II (R ₁ :R ₂) ^b
1	glutarimide	-2-Me	-4-Me	2.0	46:54
2	N-Ph/Ac	-2-Me	-4-Me	2.0	53:47

^aConditions: amide (0.10 mmol), boronic acid (2.0 equiv), Pd(dppb)Cl₂ (5 mol%), base (3 equiv), dioxane (0.125 M), 160 °C, 12 h. All reactions carried out using standard Schlenk techniques. ^bDetermined by ¹H NMR and/or GC-MS.

Selectivity Studies – Sterics

General Procedure. An oven-dried vial equipped with a stir bar was charged with two amide substrates (1.0 equiv each), sodium bicarbonate (3 equiv), boronic acid (0.10 mmol) and Pd(dppb)Cl₂ (0.05 equiv), placed under a positive pressure of argon, and subjected to three evacuation/backfilling cycles under high vacuum. Dioxane (0.125 M) was added with vigorous stirring at room temperature, the reaction mixture was placed in a preheated oil bath at 160 °C, and stirred for the indicated time at 160 °C. After the indicated time, the reaction mixture was cooled down to room temperature, diluted with CH₂Cl₂ (10 mL), filtered, and concentrated. The sample was analyzed by ¹H NMR (CDCl₃, 500 MHz) and GC-MS to obtain conversion and yield using internal standard and comparison with authentic samples.

Table S6. Selectivity Study in the Palladium-Catalyzed Suzuki-Miyaura Cross-Coupling of Amides.^a



Entry	NR'R''	1-I (Ar)	1-II (Ar)	Amide (equiv)	3-I:3-II (R ₁ :R ₂) ^b
1	N-Ph/Ac	-2-Me	-4-Me	2.0	45:55

^aConditions: amide (0.20 mmol), boronic acid (1.0 equiv), Pd(dppb)Cl₂ (5 mol%), base (3 equiv), dioxane (0.125 M), 160 °C, 12 h. All reactions carried out using standard Schlenk techniques. ^bDetermined by ¹H NMR and/or GC-MS.

References

1. Shi, S.; Meng, G.; Szostak, M. *Angew. Chem. Int. Ed.* **2016**, *55*, 6959.
2. Shi, S.; Szostak, M. *Org. Lett.* **2017**, *19*, 3095.
3. Liu, C.; Li, G.; Shi, S.; Meng, G.; Lalancette, R.; Szostak, R.; Szostak, M. *ACS Catal.* **2018**, *8*, 9131.
4. Cui, M.; Wu, H.; Jian, J.; Wang, H.; Liu, C.; Daniel, S.; Zeng, Z. *Chem. Commun.* **2016**, *52*, 12076.
5. Meng, G.; Shi, S.; Lalancette, R.; Szostak, R.; Szostak, M. *J. Am. Chem. Soc.* **2018**, *140*, 727.
6. Monguchi, Y.; Hattori, T.; Miyamoto, Y.; Yanase, T.; Sawama, Y.; Sajiki, H. *Adv. Synth. Catal.* **2012**, *354*, 2561.
7. Huang, C. Y.; Doyle, A. G. *J. Am. Chem. Soc.* **2012**, *134*, 9541.
8. Shu, Z.; Ye, Y.; Deng, Y.; Zhang, Y.; Wang, J. *Angew. Chem., Int. Ed.* **2013**, *52*, 10573.
9. Scheuermann, G. M.; Rumi, L.; Steurer, P.; Bannwarth, W.; Mülhaupt, R. *J. Am. Chem. Soc.* **2009**, *131*, 8262.
10. Kuriyama, M.; Matsuo, S.; Shinozawa, M.; Onomura, O. *Org. Lett.* **2013**, *15*, 2716.
11. Tang, D.-T. D.; Collins, K. D.; Ernst, J. B.; Glorius, F. *Angew. Chem. Int. Ed.* **2014**, *53*, 1809.
12. Li, P.; Wang, L.; Zhang, L.; Wang, G. W. *Adv. Synth. Catal.* **2012**, *354*, 1307.
13. Isley, N. A.; Gallou, F.; Lipshutz, B. H. *J. Am. Chem. Soc.* **2013**, *135*, 17707.
14. Lipshutz, B. H.; Nihan, D. M.; Vinogradova, E.; Taft, B. R.; Boskovic, Z. V. *Org. Lett.* **2008**, *10*, 4279.
15. Mattiello, S.; Rooney, M.; Sanzone, A.; Brazzo, P.; Sassi, M.; Beverina, L. *Org. Lett.* **2017**, *19*, 654.
16. Oberli, M. A.; Buchwald, S. L. *Org. Lett.* **2012**, *14*, 4606.
17. Shu, C.; Sidhu, K.; Zhang, L.; Wang, X. J.; Krishnamurthy, D.; Senanayake, C. H. *J. Org. Chem.* **2010**, *75*, 6677.
18. Crespi, S.; Protti, S.; Fagnoni, M. *J. Org. Chem.* **2016**, *81*, 9612.
19. Zinser, C. M.; Warren, K. G.; Meadows, R. E.; Nahra, F.; Al-Majid, A. M.; Barakat, A.; Islam, M. S.; Nolan, S. P.; Cazin, C. S. *Green Chem.* **2018**, *20*, 3246.

20. Biafora, A.; Krause, T.; Hackenberger, D.; Belitz, F.; Gooßen, L. J. *Angew. Chem. Int. Ed.* **2016**, *55*, 14752.
21. Roesner, S.; Buchwald, S. L. *Angew. Chem. Int. Ed.* **2016**, *55*, 10463.
22. Ciana, C. L.; Phipps, R. J.; Brandt, J. R.; Meyer, F. M.; Gaunt, M. J. *Angew. Chem., Int. Ed.* **2011**, *50*, 458.
23. Ardeleanu, R.; Dascalu, A.; Shova, S.; Nicolescu, A.; Roşca, I.; Bratanovici, B.; Lozan, V.; Roman G. *J. Mol. Struct.* **2018**, *1173*, 63.
24. Kloss, F.; Neuwirth, T.; Haensch, V. G.; Hertweck, C. *Angew. Chem. Int. Ed.* **2018**, *57*, 14476.
25. Leowanawat, P.; Zhang, N.; Safi, M.; Hoffman, D. J.; Fryberger, M. C.; George, A.; Percec, V. *J. Org. Chem.* **2012**, *77*, 2885.
26. Amatore, M.; Gosmini, C. *Angew. Chem. Int. Ed.* **2008**, *47*, 2089.
27. Zhu, L.; Duquette, J.; Zhang, M. *J. Org. Chem.* **2003**, *68*, 3729.
28. Guan, B. T.; Wang, Y.; Li, B. J.; Yu, D. G.; Shi, Z. J. *J. Am. Chem. Soc.* **2008**, *130*, 14468.

