Supporting Information for:

Proofreading Experimentally Assigned Stereochemistry Through Q2MM Predictions in Pd-Catalyzed Allylic Aminations

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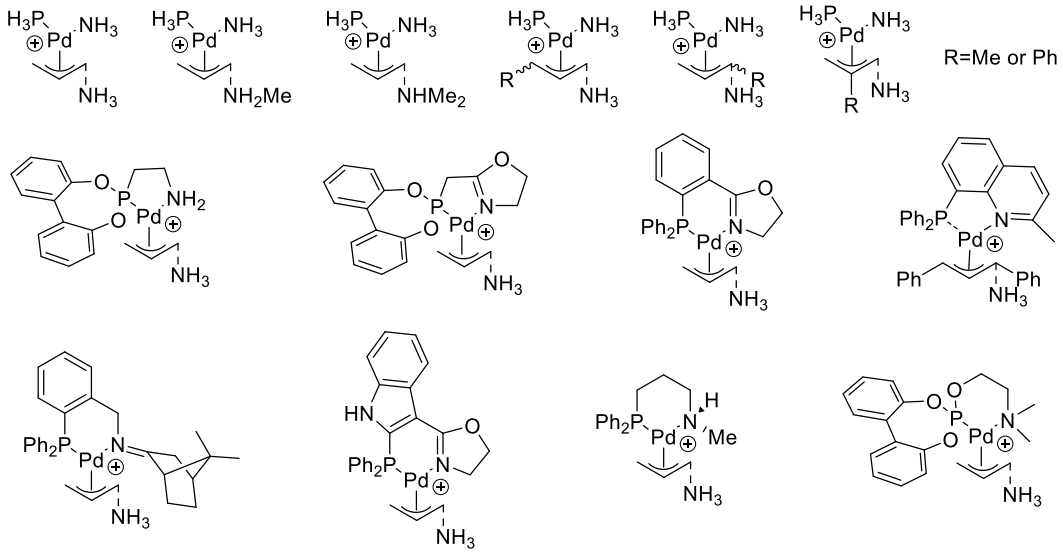
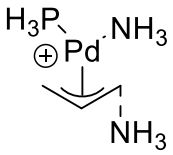


Figure S1. Training set structures used to fit the force field parameters

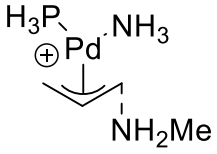
Table S1. Coordinates for the DFT optimized structures in the training set



TS 1.
Gibbs Free Energy: -699.798031
Imaginary Frequency: -333.18
Cartesian coordinates and point charges:

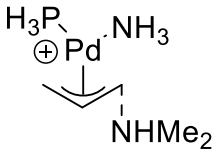
Pd	-0.43973	0.161508	0.102093	-0.17746
P	-2.5037	-0.94055	-0.30086	0.28649
H	-2.9894	-1.81422	0.692499	0.01425
H	-3.71257	-0.2516	-0.54564	0.0121
H	-2.5784	-1.83259	-1.38997	0.00364
N	-1.12861	2.324886	-0.01298	-0.64035
H	-1.55715	2.543185	-0.91141	0.28803
H	-1.83373	2.502176	0.701135	0.3054
H	-0.3901	3.010267	0.133721	0.28832
C	1.608243	-0.34529	0.693343	-0.03142
C	2.280925	0.411347	-0.2982	0.07537
C	0.832858	-1.4884	0.353728	-0.34887
H	2.566501	1.439726	-0.08438	0.0946

H	0.519335	-2.17281	1.142224	0.16335
H	2.070699	0.202237	-1.34705	0.09405
H	1.770133	-0.08597	1.740897	0.10638
N	4.152029	-0.22187	-0.40967	-0.5298
H	4.121833	-1.22629	-0.58902	0.27494
H	4.729114	0.217807	-1.12916	0.29212
H	4.605498	-0.08233	0.494163	0.27382
H	0.965259	-1.95778	-0.62608	0.15502



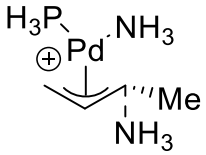
TS 2.
Gibbs Free Energy: -739.045407
Imaginary Frequency: -257.33
Cartesian coordinates and point charges:

Pd	0.795218	0.151145	-0.13183	-0.12461
P	2.873176	-0.77132	0.547701	0.23545
H	3.503667	-1.67004	-0.33565	0.02497
H	4.004071	0.017403	0.853521	0.02616
H	2.895393	-1.58427	1.698597	0.01675
N	1.305522	2.357937	-0.09612	-0.60022
H	1.431967	2.70453	0.853903	0.27696
H	2.176663	2.537285	-0.59371	0.28987
H	0.598434	2.946984	-0.53215	0.28433
C	-1.11037	-0.60051	-0.93203	-0.05376
C	-1.88922	0.242562	-0.11774	-0.16231
C	-0.30235	-1.62808	-0.37249	-0.27988
H	-2.23212	1.205658	-0.49124	0.15718
H	0.155982	-2.36284	-1.03449	0.14624
H	-1.83136	0.150562	0.966821	0.14265
H	-1.14806	-0.46399	-2.01365	0.12344
N	-3.86854	-0.44588	-0.07671	-0.19749
H	-3.8147	-1.43173	0.179738	0.21015
H	-4.22822	-0.40407	-1.03031	0.20713
H	-0.52397	-1.99808	0.633012	0.14486
C	-4.70035	0.318956	0.854749	-0.09178
H	-5.74178	-0.02494	0.884211	0.0761
H	-4.27813	0.237783	1.862495	0.07687
H	-4.69066	1.375	0.562255	0.07093



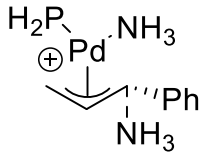
TS 3.
Gibbs Free Energy: -778.29767
Imaginary Frequency: -195.25
Cartesian coordinates and point charges:

Pd	1.070945	0.140616	-0.1082	-0.14318
P	3.211061	-0.72942	0.431691	0.25725
H	3.703296	-1.77835	-0.36961	0.02152
H	4.376135	0.068131	0.439088	0.02104
H	3.389561	-1.34104	1.688441	0.01915
N	1.591306	2.324256	-0.38814	-0.55815
H	1.953655	2.744459	0.466788	0.27289
H	2.311822	2.434345	-1.1004	0.27771
H	0.802401	2.896341	-0.68416	0.27175
C	-0.8955	-0.70025	-0.6302	0.05625
C	-1.53917	0.302162	0.110063	-0.21596
C	-0.04214	-1.64903	-0.00461	-0.33416
H	-1.91684	1.195846	-0.38445	0.15783
H	0.351189	-2.47849	-0.59212	0.16487
H	-1.40181	0.368672	1.188598	0.14717
H	-1.0291	-0.71893	-1.71298	0.10016
N	-3.61535	-0.25971	0.425236	-0.03392
H	-3.59021	-1.00748	1.118029	0.20131
H	-0.16698	-1.86322	1.060731	0.14966
C	-4.33893	0.895711	0.940758	-0.18694
H	-5.4063	0.686249	1.108315	0.09638
H	-3.89265	1.227804	1.885537	0.08143
H	-4.26524	1.715536	0.213412	0.08295
C	-4.13399	-0.76066	-0.84005	-0.098
H	-5.19371	-1.04942	-0.77555	0.07168
H	-4.03758	0.024656	-1.6025	0.07284
H	-3.55031	-1.6315	-1.16077	0.04646



TS 4.
Gibbs Free Energy: -739.059094
Imaginary Frequency: -327.40
Cartesian coordinates and point charges:

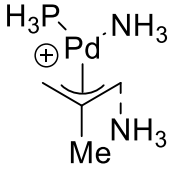
Pd	0.628012	0.143881	-0.182874	-0.17942
N	1.300373	2.320854	-0.152549	-0.59957
H	1.956442	2.48129	-0.9159	0.29072
H	0.549007	2.997713	-0.271055	0.26959
H	1.785444	2.568888	0.708383	0.28221
P	2.657647	-0.933085	0.371025	0.2524
H	3.843572	-0.231616	0.686264	0.01621
H	2.673087	-1.814759	1.471445	0.00948
H	3.215544	-1.811894	-0.579629	0.01847
C	-1.407701	-0.353186	-0.823073	-0.23463
C	-2.217438	0.399305	0.077685	0.51092
C	-0.653305	-1.499893	-0.452351	-0.21942
H	-2.49967	1.394407	-0.272825	0.00738
H	-0.306054	-2.170976	-1.238469	0.13962
H	-0.820048	-1.991177	0.509536	0.09832
H	-1.493028	-0.097569	-1.881554	0.11982
N	-4.067638	-0.308069	-0.218476	-0.68304
H	-4.054203	-1.286994	0.072753	0.29731
H	-4.832243	0.161155	0.270787	0.32614
H	-4.26928	-0.287941	-1.218743	0.3039
C	-2.170779	0.243333	1.56763	-0.43518
H	-3.035788	0.715054	2.04668	0.13049
H	-2.12865	-0.808567	1.874915	0.15221
H	-1.271193	0.733904	1.962074	0.1261



TS 5.
Gibbs Free Energy: -930.602498
Imaginary Frequency: -339.31
Cartesian coordinates and point charges:

Pd	1.380832	0.200234	0.197762	-0.24273
N	1.54318	-0.75283	2.267371	-0.56928
H	2.491174	-1.06337	2.473458	0.28843
H	1.268437	-0.13641	3.029804	0.26727
H	0.944299	-1.57595	2.314607	0.24977
Pd	2.99361	-1.05983	-0.99297	0.30405

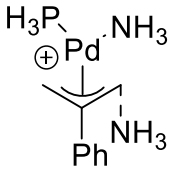
H	3.808554	-2.04938	-0.39563	-0.0008
H	2.575914	-1.82548	-2.10155	-0.00845
H	4.027738	-0.35336	-1.6412	0.00722
C	0.036209	1.902879	-0.08588	-0.08851
C	-1.17657	1.408527	0.5087	0.2216
C	0.627484	1.46981	-1.30139	-0.28913
H	1.389894	2.105865	-1.75189	0.14909
H	0.0868	0.846118	-2.01361	0.11343
N	-2.53882	2.695058	0.084409	-0.72574
H	-2.6005	2.751946	-0.93332	0.30782
H	-3.4585	2.436571	0.448754	0.30909
H	-2.28865	3.620059	0.438579	0.35932
H	-1.23388	1.603201	1.583651	0.0692
C	-3.20937	-2.23525	-0.45694	-0.08546
C	-2.8848	-1.9248	0.861323	-0.04938
C	-2.23102	-0.73189	1.151602	-0.19739
C	-1.87297	0.155143	0.129099	0.16641
C	-2.22326	-0.15738	-1.1905	-0.15716
C	-2.88545	-1.34502	-1.47988	-0.08876
H	-3.72854	-3.16355	-0.68732	0.12194
H	-3.15278	-2.60675	1.666206	0.11332
H	-1.98961	-0.48243	2.186964	0.11058
H	-1.99134	0.533812	-2.00108	0.12586
H	-3.15402	-1.57592	-2.50907	0.1231
H	0.470475	2.7741	0.410857	0.09531



TS 6.
Gibbs Free Energy: -739.057457
Imaginary Frequency: -358.98
Cartesian coordinates and point charges:

Pd	-0.5713	0.151886	-0.01702	-0.23428
N	-1.20329	2.34163	0.015895	-0.62788
H	-1.92544	2.487632	0.719714	0.29977
H	-0.45358	2.995884	0.231767	0.28355
H	-1.59908	2.632022	-0.87713	0.28392
P	-2.70466	-0.88835	-0.21492	0.33437
H	-3.93228	-0.19838	-0.09197	-0.0048
H	-3.0107	-1.58237	-1.40378	-0.0067

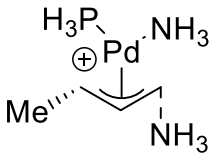
H	-2.99929	-1.93205	0.686142	0.00082
C	1.514618	-0.38754	0.392367	0.30403
C	2.085219	0.397488	-0.65438	0.00568
C	0.716889	-1.51425	0.046666	-0.49801
H	2.343718	1.436659	-0.44498	0.09423
H	0.468331	-2.24599	0.81749	0.18928
H	1.764847	0.206739	-1.67864	0.09605
H	0.757435	-1.92244	-0.96741	0.17111
N	3.908982	-0.15994	-0.91447	-0.53342
H	3.908203	-1.17184	-1.05234	0.27533
H	4.367816	0.276584	-1.71642	0.30311
H	4.461927	0.043975	-0.08065	0.28406
C	1.945354	-0.12524	1.81123	-0.29553
H	1.216564	-0.52016	2.52868	0.11113
H	2.907997	-0.61133	2.03984	0.0768
H	2.060717	0.949042	2.011183	0.08736



TS 7.
Gibbs Free Energy: -930.609145
Imaginary Frequency: -267.14
Cartesian coordinates and point charges:

Pd	-1.39357	0.07256	0.144667	-0.30152
N	-1.93811	-0.14181	2.335033	-0.47469
H	-1.57939	-1.02911	2.686941	0.25326
H	-1.5567	0.588102	2.934675	0.24554
H	-2.94467	-0.14819	2.491523	0.26185
P	-3.18039	-1.10233	-0.88804	0.36403
H	-4.25393	-1.67141	-0.16798	-0.00308
H	-3.94259	-0.43361	-1.86673	-0.00299
H	-2.84165	-2.23891	-1.6486	-0.00213
C	0.594038	0.799998	-0.47949	0.06308
C	0.39909	1.939718	0.330224	0.05356
C	-0.29248	0.599818	-1.57828	-0.3233
H	-0.10224	-0.22178	-2.26989	0.15046
H	-0.39258	2.648029	0.095918	0.1092
H	-0.81502	1.455269	-2.0146	0.15562

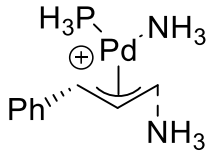
N	1.921661	3.263565	-0.22754	-0.59918
H	1.819391	3.466248	-1.22194	0.27453
H	2.008508	4.15381	0.264382	0.30064
H	2.799492	2.755535	-0.11052	0.22094
H	0.78367	1.96972	1.346277	0.08879
C	3.956238	-1.75823	0.267985	-0.09716
C	3.192428	-1.28839	1.3358	-0.05645
C	2.090568	-0.47431	1.100301	-0.21486
C	1.732131	-0.11462	-0.20599	0.21524
C	2.506785	-0.59125	-1.26915	-0.18932
C	3.609484	-1.40906	-1.03395	-0.05415
H	4.817824	-2.39682	0.452829	0.1149
H	3.45232	-1.56533	2.35613	0.1059
H	1.486309	-0.13438	1.944169	0.12215
H	2.254079	-0.30635	-2.29093	0.10688
H	4.202953	-1.768	-1.87294	0.11225



TS 8.
Gibbs Free Energy: -739.056054
Imaginary Frequency: -345.50
Cartesian coordinates and point charges:

Pd	-0.54154	0.305638	0.115982	-0.23144
N	-1.373	2.385541	-0.32489	-0.58724
H	-1.81584	2.432724	-1.24128	0.2718
H	-2.08695	2.628085	0.360688	0.29364
H	-0.67981	3.130619	-0.29555	0.27024
P	-2.51981	-0.98251	-0.13125	0.27405
H	-3.72075	-0.47193	-0.67389	0.01313
H	-2.46089	-2.15795	-0.9107	0.00219
H	-3.08046	-1.56026	1.02681	0.01103
C	1.522169	0.032331	0.793172	-0.264
C	2.190232	0.732818	-0.24306	0.26401
C	0.853826	-1.21463	0.598205	0.0788
H	2.390139	1.794304	-0.10551	0.05683
H	0.544637	-1.72069	1.517156	0.06518
H	2.032475	0.439747	-1.27991	0.04147
H	1.602571	0.433994	1.805044	0.12352
N	4.075207	0.221116	-0.24203	-0.56412

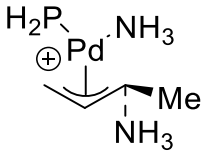
H	4.123287	-0.78751	-0.39338	0.28185
H	4.659582	0.680663	-0.94335	0.29593
H	4.466418	0.415618	0.680629	0.28519
C	1.133376	-2.14774	-0.5483	-0.22163
H	0.2828	-2.81466	-0.73391	0.08763
H	1.345668	-1.62829	-1.49181	0.07167
H	1.992208	-2.79953	-0.31922	0.0803



TS 9.
Gibbs Free Energy: -930.605574
Imaginary Frequency: -321.61
Cartesian coordinates and point charges:

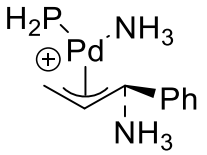
Pd	1.499123	0.090213	-0.08382	-0.16679
N	3.409384	0.636442	1.018866	-0.62432
H	4.22059	0.393497	0.451799	0.29427
H	3.490651	1.628469	1.232808	0.28447
H	3.505658	0.136045	1.901126	0.28663
P	1.69548	-2.26603	-0.26275	0.26537
H	2.658679	-3.04859	0.412039	0.02588
H	0.552303	-3.00697	0.104435	-0.02285
H	1.878912	-2.81524	-1.54812	0.01747
C	0.1369	1.621491	-0.85169	0.02507
C	-0.13971	2.365594	0.312578	0.03286
C	-0.35266	0.290383	-1.07953	-0.30484
H	-0.53919	1.876864	1.197426	0.07664
N	-1.91026	3.31421	0.019436	-0.51516
H	-2.58686	2.562033	-0.12139	0.19864
H	-2.24556	3.912945	0.775396	0.29247
H	-1.869	3.86724	-0.83657	0.27758
H	0.423213	3.276895	0.504196	0.09941
H	-0.26326	-0.04461	-2.11793	0.1374
C	-3.85936	-1.31635	0.813983	-0.11337
C	-3.80213	-1.13891	-0.56623	-0.04347
C	-2.64635	-0.63715	-1.15852	-0.21741
C	-1.52923	-0.29214	-0.38418	0.31856
C	-1.59612	-0.49473	1.002726	-0.17025
C	-2.7496	-0.99971	1.595695	-0.07585

H	-4.75928	-1.7165	1.277283	0.11762
H	-4.65751	-1.40066	-1.18676	0.10985
H	-2.60494	-0.50727	-2.2409	0.11323
H	-0.71719	-0.29438	1.619311	0.09546
H	-2.77675	-1.16042	2.67226	0.111
H	0.633365	2.135781	-1.67659	0.07445



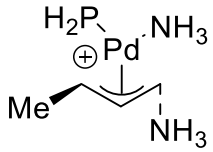
TS 10.
Gibbs Free Energy: -739.059048
Imaginary Frequency: -327.93
Cartesian coordinates and point charges:

Pd	-0.642894	0.103180	0.109908	-0.19354
N	-1.115447	2.333495	-0.006646	-0.57095
H	-0.535094	2.893555	0.616037	0.26982
H	-0.990196	2.705837	-0.947193	0.26041
H	-2.081501	2.525454	0.254439	0.28646
P	-2.795621	-0.795776	-0.313284	0.26288
H	-3.422005	-1.517270	0.723348	0.01918
H	-3.904854	0.004419	-0.670104	0.01260
H	-2.940216	-1.763690	-1.327973	0.00643
C	1.371873	-0.541110	0.683858	-0.15859
C	2.169341	0.078012	-0.320203	0.45967
C	0.501407	-1.626121	0.381288	-0.28430
H	0.139496	-2.262532	1.189273	0.15267
H	0.593254	-2.133428	-0.584881	0.12154
H	1.572341	-0.271375	1.724341	0.11363
N	3.851262	-0.994373	-0.369609	-0.62558
H	3.576443	-1.976323	-0.419275	0.28237
H	4.500458	-0.802565	-1.135091	0.31655
H	4.350278	-0.858038	0.511136	0.28750
H	1.923540	-0.181270	-1.353278	0.02459
C	2.767359	1.432603	-0.104201	-0.50568
H	3.591919	1.640686	-0.794398	0.15050
H	2.000696	2.197850	-0.280753	0.15654
H	3.122301	1.554900	0.927216	0.15530



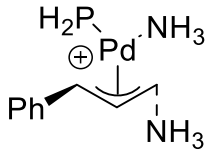
TS 11.
Gibbs Free Energy: -930.610452
Imaginary Frequency: -340.99
Cartesian coordinates and point charges:

Pd	1.438615	-0.121051	0.127361	-0.23041
N	0.451925	-2.180413	0.183590	-0.58363
H	0.968187	-2.914162	-0.298477	0.29773
H	0.339222	-2.483705	1.150101	0.27951
H	-0.482034	-2.154992	-0.226018	0.20049
P	3.698776	-0.654209	-0.359715	0.30658
H	4.359209	0.048881	-1.388703	-0.00570
H	4.658602	-0.439466	0.651003	0.00827
H	4.126841	-1.948934	-0.733377	-0.00367
C	0.119925	1.515394	0.657862	-0.03993
C	-0.903488	1.322325	-0.329801	0.16076
C	1.409013	1.984081	0.293531	-0.37729
H	2.078068	2.369981	1.062342	0.16991
H	-0.555486	1.416492	-1.362921	0.09671
H	1.569634	2.408905	-0.702094	0.14462
H	-0.149060	1.432291	1.713043	0.11030
N	-1.915334	2.960750	-0.384242	-0.68907
H	-1.279184	3.747995	-0.523742	0.35040
H	-2.636177	2.978764	-1.108672	0.31067
H	-2.373002	3.074388	0.522182	0.28544
C	-4.041652	-1.553049	0.072103	-0.08911
C	-3.557758	-1.203964	-1.186663	-0.05529
C	-2.543395	-0.256891	-1.300418	-0.15471
C	-1.996476	0.341348	-0.159281	0.18118
C	-2.49379	-0.01082	1.102074	-0.13975
C	-3.51006	-0.95305	1.214685	-0.08254
H	-4.83538	-2.29174	0.166048	0.11967
H	-3.97052	-1.66777	-2.08057	0.11453
H	-2.15672	0.011488	-2.28546	0.09342
H	-2.07954	0.440818	2.004205	0.09957
H	-3.8906	-1.22237	2.198233	0.12135



TS 12.
Gibbs Free Energy: -739.056954
Imaginary Frequency: -347.79
Cartesian coordinates and point charges:

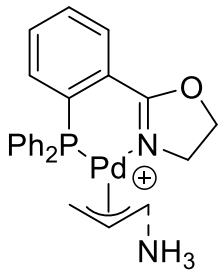
Pd	-0.476380	-0.328403	-0.071278	-0.25590
N	-1.226266	-2.455758	-0.448558	-0.54556
H	-1.608576	-2.876857	0.396900	0.25850
H	-1.976418	-2.445644	-1.137904	0.28187
H	-0.518059	-3.095939	-0.802137	0.26301
P	-2.501095	0.753341	0.546203	0.27643
H	-3.721931	0.098904	0.825568	0.01534
H	-2.488041	1.595727	1.678186	-0.00293
H	-3.010259	1.696049	-0.372659	0.00811
C	1.591697	0.237944	-0.524620	-0.18591
C	2.233630	-0.739256	0.279930	0.07536
C	0.854849	1.315037	0.047355	0.08894
H	2.479537	-1.706770	-0.155076	0.10871
H	1.998506	-0.768970	1.344206	0.08709
H	0.989710	1.489555	1.123101	0.06330
H	1.762856	0.216586	-1.604090	0.13255
N	4.087373	-0.220263	0.545753	-0.53659
H	4.087325	0.707326	0.972601	0.28088
H	4.642823	-0.846406	1.132357	0.29722
H	4.543775	-0.143085	-0.364307	0.28192
C	0.490601	2.527904	-0.757122	-0.29581
H	-0.373454	3.051910	-0.329856	0.10808
H	1.320180	3.251066	-0.779528	0.09315
H	0.249546	2.265352	-1.795254	0.10225



TS 13.
Gibbs Free Energy: -930.608964
Imaginary Frequency: -351.45
Cartesian coordinates and point charges:

Pd	-1.167300	-0.627673	0.061506	-0.19639

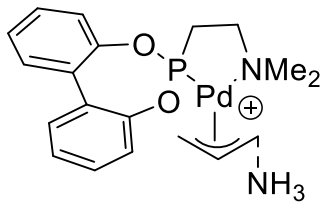
N	-2.953855	-1.723135	0.963254	-0.65986
H	-2.815537	-2.731785	0.972190	0.30029
H	-3.127276	-1.442742	1.926981	0.30663
H	-3.813334	-1.551121	0.444138	0.28274
P	0.173756	-2.393916	-0.821219	0.31347
H	-0.157216	-3.763379	-0.938129	0.00589
H	0.692314	-2.222924	-2.123254	-0.01886
H	1.407729	-2.552324	-0.152642	-0.01694
C	-0.858061	1.525496	0.393091	-0.07728
C	-2.073331	2.019892	-0.145157	0.17517
C	0.139946	0.961415	-0.457246	-0.30186
H	-2.328756	1.753925	-1.171523	0.05877
H	-0.008279	1.098467	-1.537102	0.14605
H	-0.639434	1.734092	1.442248	0.08886
N	-1.866820	3.907292	-0.514563	-0.48488
H	-1.050714	4.005264	-1.120612	0.25537
H	-2.663265	4.363918	-0.964371	0.28441
H	-1.664824	4.397686	0.357973	0.26319
H	-2.930907	2.147748	0.513470	0.06181
C	4.220396	0.148788	0.533582	-0.10283
C	3.815931	0.256194	-0.794808	-0.07869
C	2.487747	0.539687	-1.095851	-0.16558
C	1.539725	0.718959	-0.078788	0.25350
C	1.960333	0.605643	1.255371	-0.22324
C	3.287893	0.327659	1.556086	-0.02587
H	5.258542	-0.072765	0.773924	0.11352
H	4.537999	0.121857	-1.598311	0.11316
H	2.173989	0.621937	-2.138395	0.10288
H	1.241484	0.718012	2.067603	0.13055
H	3.598210	0.244350	2.596321	0.09600



TS 14.
Gibbs Free Energy: -1581.625685
Imaginary Frequency: -350.39
Cartesian coordinates and point charges:

N	-5.780870	2.222445	0.259987	-0.53399
H	-5.399968	3.138808	0.502922	0.28064
H	-6.244466	2.309995	-0.645837	0.28524
H	-6.478813	1.960016	0.959953	0.29673
Pd	-1.582508	0.512773	-0.400494	-0.17101
N	-1.354167	-1.701765	-0.373971	-0.32196
C	-2.336771	-2.573177	0.269987	0.01982
P	0.721115	0.424106	0.056040	-0.32827
C	-3.405312	1.613075	-0.882174	-0.03803
C	-2.317622	2.454114	-0.487406	-0.33520
C	-4.308456	1.063312	0.069928	0.06138
H	-1.835206	3.084300	-1.235343	0.14014
H	-4.884192	0.179724	-0.207487	0.09068
H	-2.304342	2.879701	0.521895	0.12823
H	-4.011788	1.084296	1.120393	0.11682
C	1.487911	-1.550232	4.166543	-0.06387
C	2.298741	-1.898122	3.088470	-0.11673
C	2.090074	-1.317631	1.839813	-0.09649
C	1.060969	-0.386876	1.660511	0.26789
C	0.244168	-0.050511	2.745803	-0.16111
C	0.462202	-0.621999	3.995788	-0.09656
H	1.654831	-2.003788	5.142203	0.10724
H	3.100176	-2.623485	3.219103	0.12212
H	2.735592	-1.592613	1.004068	0.05298
H	-0.564921	0.669268	2.604189	0.12111
H	-0.171525	-0.347596	4.837751	0.10823
C	3.438737	4.141424	-0.204898	-0.09864
C	2.383227	3.957821	-1.097637	-0.07046
C	1.567020	2.837757	-0.984166	-0.19506
C	1.813516	1.881153	0.007671	0.30153
C	2.874376	2.068775	0.898295	-0.18667
C	3.680118	3.200407	0.793076	-0.05507
H	4.071979	5.023364	-0.284591	0.11275
H	2.193172	4.693455	-1.877483	0.10632
H	0.736228	2.692172	-1.677727	0.13867
H	3.073287	1.332794	1.677400	0.07650
H	4.500855	3.344717	1.493698	0.11199
C	2.666251	-2.559393	-2.941787	-0.13525
C	1.494586	-2.905540	-2.276625	-0.00606
C	0.876454	-2.005252	-1.404668	-0.21819
C	1.467186	-0.745378	-1.156197	0.33584
C	2.648571	-0.422466	-1.823088	-0.18743
C	3.239609	-1.314357	-2.717804	-0.02188

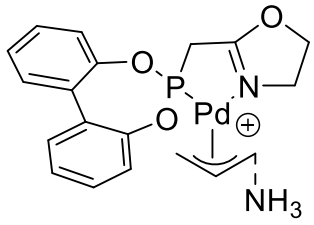
H	3.127446	-3.264952	-3.629743	0.12354
H	1.042670	-3.882086	-2.437324	0.10639
C	-0.371124	-2.436757	-0.757046	0.55367
H	3.126982	0.538960	-1.638748	0.08457
H	4.158175	-1.032781	-3.229703	0.11047
O	-0.492154	-3.757724	-0.554026	-0.42012
C	-1.784456	-3.986803	0.044179	0.29303
H	-3.323990	-2.420295	-0.185306	0.03763
H	-2.413792	-2.305471	1.334256	0.02467
H	-2.375784	-4.584803	-0.657855	0.03562
H	-1.626106	-4.559161	0.962592	0.01318
H	-3.645206	1.493296	-1.940496	0.09245



TS 15.
Gibbs Free Energy: -1466.472003
Imaginary Frequency: -355.67
Cartesian coordinates and point charges:

Pd	1.864663	-0.216322	-0.396740	-0.29811
N	2.130784	-2.157094	0.866745	0.07790
C	0.886623	-2.462480	1.614093	0.06103
P	-0.359845	-0.677683	0.001681	0.58694
C	3.445273	0.981178	-1.343211	0.01542
C	4.224582	1.298092	-0.201501	0.02614
C	2.131651	1.512669	-1.525075	-0.32428
H	1.661559	1.456403	-2.506691	0.15474
H	1.801236	2.362499	-0.918538	0.10671
H	3.918392	0.411901	-2.145610	0.09126
H	3.728020	1.777867	0.643649	0.12256
O	-1.080867	0.127428	1.243337	-0.44672
O	-1.511447	-0.673339	-1.148125	-0.46022
C	-5.578642	-1.076288	-0.394790	-0.10377
C	-4.879782	-2.093089	-1.041451	-0.08153
C	-3.511911	-1.960994	-1.260918	-0.21615
C	-2.861050	-0.814291	-0.828587	0.37400
C	-3.534116	0.224814	-0.173012	-0.03786
C	-4.910139	0.065526	0.031947	-0.11367
H	-6.647531	-1.175253	-0.216712	0.11922
H	-5.398205	-2.988254	-1.379404	0.11709

H	-2.942307	-2.726063	-1.786722	0.14793
H	-5.453995	0.851013	0.556485	0.11295
C	-2.743119	3.862118	0.529496	-0.10345
C	-1.523435	3.761689	1.196120	-0.09553
C	-0.953581	2.510107	1.411186	-0.18569
C	-1.615521	1.376914	0.959524	0.31310
C	-2.838008	1.445796	0.279472	0.02976
C	-3.389088	2.716283	0.077577	-0.13006
H	-3.192541	4.838409	0.358287	0.11888
H	-1.019581	4.657402	1.555050	0.11531
H	-0.012084	2.389946	1.946292	0.13146
H	-4.333882	2.799055	-0.459444	0.11452
C	-0.370309	-2.345942	0.762712	0.04676
C	2.449831	-3.236158	-0.077007	-0.25937
H	3.391194	-3.003976	-0.587862	0.11434
H	2.556837	-4.203770	0.446513	0.08997
H	1.669209	-3.329457	-0.839470	0.12375
C	3.231175	-2.011619	1.825302	-0.28202
H	4.170450	-1.850874	1.283524	0.11534
H	3.042179	-1.148735	2.475464	0.09080
H	3.339571	-2.915152	2.452319	0.10909
H	5.048468	0.641553	0.076489	0.09036
H	0.824799	-1.745463	2.445924	0.05460
H	0.967370	-3.471167	2.060387	0.01927
H	-1.271302	-2.483737	1.375904	-0.00265
H	-0.398867	-3.093620	-0.043247	0.02385
N	5.346481	2.814990	-0.611654	-0.50460
H	4.727163	3.564013	-0.924879	0.27538
H	5.926811	3.168432	0.152062	0.28700
H	5.955258	2.569148	-1.393521	0.26825

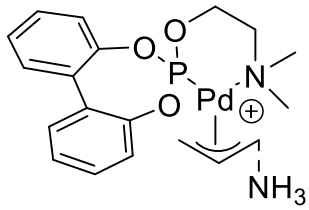


TS 16.
Gibbs Free Energy: -1539.310705
Imaginary Frequency: -353.53
Cartesian coordinates and point charges:

Pd	-1.866139	-0.435830	-0.101173	-0.27878
N	-2.285570	1.742077	-0.448881	-0.31287

C	-1.325196	2.526210	-0.792456	0.57593
P	0.288221	0.383583	-0.364020	0.60771
C	-3.271234	-2.101083	0.127623	0.05171
C	-4.021337	-1.581943	1.215327	0.04630
C	-1.907233	-2.488485	0.277777	-0.37570
H	-1.491942	-2.640888	1.278708	0.14940
H	-3.791633	-2.287925	-0.813448	0.08932
H	-3.484842	-1.297853	2.121455	0.12911
O	1.150461	0.554963	1.011579	-0.47511
O	1.419776	-0.108456	-1.441349	-0.42260
C	3.664167	-3.476031	-0.523727	-0.12204
C	2.621203	-3.566908	-1.443719	-0.07455
C	1.852862	-2.442971	-1.732267	-0.21053
C	2.144891	-1.245220	-1.096326	0.31692
C	3.179907	-1.121843	-0.162426	0.02005
C	3.937358	-2.267370	0.107885	-0.11041
H	4.265857	-4.352912	-0.292722	0.12403
H	2.408771	-4.511421	-1.941133	0.11362
H	1.040353	-2.470532	-2.457290	0.15727
H	4.741851	-2.204069	0.840360	0.10928
C	5.098992	1.836295	1.212577	-0.09861
C	4.075541	2.628444	1.727389	-0.10669
C	2.754804	2.202011	1.627370	-0.18294
C	2.473195	0.990857	1.009966	0.37105
C	3.480333	0.171817	0.481890	-0.04819
C	4.799626	0.624415	0.599852	-0.10266
H	6.133708	2.165518	1.282334	0.11910
H	4.302606	3.576376	2.211342	0.12223
H	1.934993	2.783286	2.047559	0.14289
H	5.599627	0.015221	0.179576	0.11025
C	0.079734	2.100537	-1.023727	-0.18564
H	-4.906184	-0.981476	1.007105	0.09076
H	0.789410	2.809674	-0.574034	0.06957
H	0.290478	2.085458	-2.103123	0.11523
O	-1.611690	3.813330	-0.973037	-0.41318
C	-3.029533	3.972904	-0.718701	0.23491
C	-3.503366	2.553368	-0.362827	0.03049
H	-1.429969	-3.086230	-0.498883	0.14049
H	-3.138116	4.698896	0.092601	0.04562
H	-3.480925	4.378951	-1.628842	0.03997
H	-4.252641	2.165702	-1.064262	0.05183
H	-3.923839	2.482985	0.648308	0.03935
N	-4.990323	-3.031962	2.055024	-0.56426

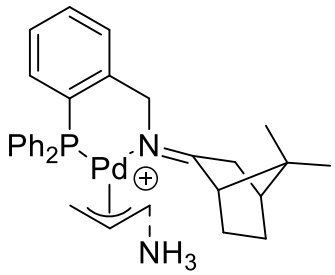
H	-4.300939	-3.740255	2.311248	0.28464
H	-5.529743	-2.785893	2.887561	0.30344
H	-5.623209	-3.447682	1.370441	0.28231



TS 17.
Gibbs Free Energy: -1541.679241
Imaginary Frequency: -352.77
Cartesian coordinates and point charges:

C	-1.69094	2.021803	1.010183	-0.23661
H	-1.42296	1.862706	2.059347	0.13818
C	-3.05176	1.883673	0.597165	-0.0077
C	-4.01086	1.232504	1.41401	0.01502
H	-3.65258	0.648838	2.263372	0.12499
H	-3.40028	2.380595	-0.31037	0.10023
Pd	-1.78988	0.156822	0.089912	-0.37161
N	-2.52232	-1.75499	-1.00553	0.18891
P	0.338871	-0.69767	0.023091	0.80798
H	-4.19009	3.054819	3.019876	0.27581
N	-4.9143	2.551179	2.505409	-0.53231
H	-5.59691	2.188843	3.174438	0.29733
C	-0.31586	-3.04855	-1.08658	0.18612
C	-1.44459	-2.34648	-1.82291	-0.05244
H	-0.67443	-3.95745	-0.58832	0.04077
H	0.418344	-3.35464	-1.84434	0.05997
C	-3.58601	-1.31314	-1.9165	-0.26219
H	-3.18584	-0.57607	-2.62309	0.11045
C	-3.06303	-2.72136	-0.04498	-0.17048
H	-3.40082	-3.64536	-0.54965	0.07265
H	-2.30917	-2.97586	0.708272	0.09625
H	-3.92094	-2.27217	0.469551	0.0571
H	-4.39257	-0.84384	-1.34126	0.09928
H	-1.04771	-1.54712	-2.46653	0.06586
O	0.378973	-2.30928	-0.08287	-0.4005
O	1.326596	-0.43179	1.267929	-0.47646
O	1.280458	-0.31828	-1.26745	-0.42667
C	1.883567	3.180407	-2.16613	-0.08329
C	1.296949	1.919791	-2.11173	-0.16066

C	1.834981	0.956716	-1.26907	0.28299
C	2.946802	1.209706	-0.4559	0.00876
H	1.475882	3.940702	-2.82983	0.11015
C	4.598548	-1.86808	2.038406	-0.06567
C	3.221719	-1.67358	2.000909	-0.22621
C	2.702319	-0.66909	1.199339	0.38592
C	3.5112	0.156925	0.410556	-0.0392
H	5.01677	-2.6541	2.664155	0.11402
C	2.995863	3.460708	-1.37409	-0.10877
C	3.518512	2.485296	-0.53158	-0.1104
C	5.434639	-1.05613	1.274651	-0.12833
C	4.893449	-0.0597	0.470821	-0.09295
H	-5.38378	3.220979	1.894542	0.27638
H	-1.03762	2.719552	0.4846	0.07458
H	-4.92278	0.847923	0.957293	0.10401
H	-1.87416	-3.11567	-2.49524	0.03075
H	-4.00407	-2.16287	-2.48675	0.08986
H	0.437899	1.658926	-2.72925	0.12692
H	2.539231	-2.28109	2.592202	0.15737
H	3.458062	4.445305	-1.41135	0.11863
H	4.377827	2.713521	0.098762	0.10433
H	6.512102	-1.20699	1.29622	0.12328
H	5.54688	0.554648	-0.14846	0.10757

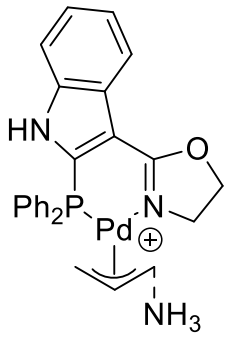


TS 18.
Gibbs Free Energy: -1780.032119
Imaginary Frequency: -347.81
Cartesian coordinates and point charges:

C	0.899509	3.294089	0.823943	-0.37371
H	1.647401	3.696783	0.131769	0.13947
C	-0.47635	3.64581	0.656718	-0.06575
C	-0.96262	4.245011	-0.5422	0.08414
H	-0.31801	4.205921	-1.42226	0.10371
H	-1.16126	3.581822	1.505415	0.10515
Pd	-0.00661	1.651592	-0.07974	-0.06727

N	-1.31536	0.242041	-1.17022	-0.49693
P	1.467687	-0.19225	-0.02096	-0.14162
H	-1.54372	6.359224	0.426677	0.26258
N	-0.9405	6.100795	-0.35585	-0.44131
H	0.016309	6.360748	-0.10916	0.25405
C	0.198732	-2.74061	3.632784	-0.13928
C	0.559494	-1.39948	3.772146	-0.017
C	0.936073	-0.66178	2.656379	-0.23271
C	0.979646	-1.25819	1.38799	0.42879
C	0.61005	-2.59962	1.255498	-0.21939
C	0.220809	-3.33538	2.37513	-0.01929
H	-0.10075	-3.31872	4.505398	0.11406
H	0.540845	-0.92746	4.753203	0.09737
H	1.205933	0.390795	2.76675	0.10236
H	0.619075	-3.07951	0.276293	0.07698
H	-0.06638	-4.37951	2.2586	0.09586
C	6.001026	0.56446	0.442159	-0.07407
C	5.236742	1.290968	-0.47036	-0.09707
C	3.870895	1.052268	-0.57589	-0.13331
C	3.259868	0.072894	0.215453	0.08989
C	4.031943	-0.65349	1.127106	0.00367
C	5.397771	-0.40332	1.241031	-0.12205
H	7.06901	0.75593	0.531979	0.10661
H	5.706448	2.048837	-1.09534	0.11232
H	3.266707	1.6287	-1.28044	0.10056
H	3.568049	-1.41789	1.751888	-0.01055
H	5.992452	-0.97155	1.954507	0.12427
C	1.189343	-3.2797	-3.46638	-0.06306
C	0.222339	-2.2862	-3.35699	-0.14861
C	0.295768	-1.29376	-2.37393	-0.00656
C	1.36534	-1.33415	-1.45744	0.14949
C	2.343267	-2.32771	-1.5891	-0.13804
C	2.266261	-3.29337	-2.58585	-0.07653
H	1.102746	-4.03679	-4.24383	0.1111
H	-0.61092	-2.2704	-4.06143	0.09771
H	3.182083	-2.34857	-0.892	0.07734
H	3.039608	-4.05482	-2.66854	0.11015
C	-0.72946	-0.18207	-2.44078	0.20387
H	-1.52257	-0.48283	-3.1432	0.02717
C	-2.32818	-0.38927	-0.70998	0.39062
C	-3.02935	-1.60142	-1.29053	-0.03074
C	-4.15768	-1.81496	-0.26739	-0.02441
C	-2.72745	-1.13956	1.561974	-0.02727

C	-3.49553	-2.36733	1.007349	-0.10484
H	-3.40096	-1.40467	-2.30753	0.04349
H	-2.3421	-2.45864	-1.36405	0.00225
H	-4.99496	-2.41593	-0.64578	0.00986
H	-1.64659	-1.30997	1.62858	-0.02206
H	-3.06493	-0.85361	2.566204	0.02052
H	-2.82558	-3.20826	0.779918	0.04294
H	-4.23877	-2.74204	1.721663	0.03472
C	-3.06071	-0.02517	0.545228	-0.08829
C	-4.51966	-0.35948	0.133083	0.45816
C	-5.03195	0.503348	-1.01926	-0.50704
H	-5.98608	0.112887	-1.40155	0.12592
H	-5.21635	1.529341	-0.66897	0.12143
H	-4.33951	0.574866	-1.86847	0.08936
C	-5.53195	-0.25605	1.266994	-0.36273
H	-6.51511	-0.61024	0.925039	0.07877
H	-5.26926	-0.83417	2.158763	0.10579
H	-5.6536	0.791555	1.577859	0.08056
H	-1.2259	6.635889	-1.17965	0.27817
H	-2.02391	4.147704	-0.77384	0.0547
H	1.286683	3.10847	1.827036	0.13325
H	-0.25049	0.708484	-2.87523	0.00795
H	-2.84987	0.997505	0.88933	-0.00567

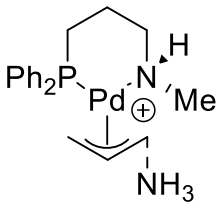


TS 19.
Gibbs Free Energy: -1713.095535
Imaginary Frequency: -351.35
Cartesian coordinates and point charges:

C	3.634355	0.70085	-0.44403	-0.38009
H	3.557686	1.024333	-1.4879	0.14665
C	4.146802	-0.60018	-0.14489	0.0057
C	4.259636	-1.60535	-1.14529	0.01845
H	4.586468	-0.80069	0.834148	0.09076
Pd	1.968999	-0.46158	0.018176	-0.1507

N	0.661237	-2.19084	0.496778	-0.4535
P	0.091821	0.926852	0.121182	-0.13966
H	6.173567	-2.20179	-2.65787	0.29306
N	5.992096	-1.54246	-1.89764	-0.50359
H	6.677113	-1.70182	-1.15742	0.26788
C	1.181162	-3.39676	1.142146	0.09216
C	-0.49917	4.621735	-2.58505	-0.1
C	0.163998	3.487962	-3.05406	-0.07048
C	0.36025	2.399916	-2.21033	-0.18041
C	-0.12133	2.429983	-0.89604	0.2185
C	-0.78512	3.570034	-0.42993	-0.15537
C	-0.96894	4.663357	-1.27442	-0.05575
H	-0.64614	5.476429	-3.24299	0.11418
H	0.532715	3.455594	-4.07795	0.11034
H	0.883643	1.51163	-2.5712	0.11251
H	-1.15633	3.606486	0.595328	0.06444
H	-1.48169	5.550122	-0.90542	0.11047
C	-0.8406	2.330288	4.41982	-0.10513
C	-1.82124	1.641746	3.710931	-0.04529
C	-1.57009	1.204353	2.411832	-0.17683
C	-0.32873	1.452149	1.81928	0.27603
C	0.659201	2.131555	2.542489	-0.19682
C	0.400754	2.576488	3.833928	-0.06088
H	-1.04098	2.672439	5.433686	0.11384
H	-2.78973	1.445003	4.167817	0.10236
H	-2.34685	0.666217	1.866767	0.08239
H	1.635354	2.315099	2.088053	0.12946
H	1.171431	3.10983	4.38795	0.10688
C	-0.61277	-2.3505	0.343809	0.6571
O	-1.11239	-3.542	0.715088	-0.35168
C	-0.00264	-4.36884	1.114642	0.18012
H	2.052365	-3.77505	0.59196	0.0131
H	-0.24775	-4.81383	2.08298	0.03784
H	0.104285	-5.16428	0.367438	0.04374
C	-1.57235	-1.40928	-0.18609	-0.39375
C	-1.35392	-0.05137	-0.37738	0.33191
N	-2.48632	0.502269	-0.90597	-0.54878
C	-3.45654	-0.46638	-1.07252	0.3096
C	-2.92091	-1.691	-0.61212	0.1317
C	-3.72178	-2.84381	-0.67037	-0.19119
C	-5.00281	-2.73433	-1.18198	-0.08519
C	-5.51053	-1.50371	-1.64146	-0.09095
C	-4.74525	-0.35152	-1.59599	-0.25445

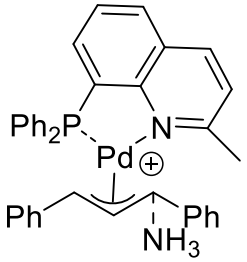
H	-3.34318	-3.79856	-0.31444	0.12239
H	-5.63603	-3.61847	-1.22862	0.1096
H	-6.5234	-1.45778	-2.03719	0.11618
H	-5.13165	0.603136	-1.94984	0.15169
H	1.513658	-3.15233	2.161115	0.05219
H	-2.57406	1.479575	-1.16347	0.3361
H	6.128568	-0.59252	-2.24735	0.27502
H	3.727125	-1.44834	-2.0848	0.11061
H	4.306128	-2.64927	-0.83503	0.11047
H	3.817662	1.51756	0.255887	0.14509



TS 20.
Gibbs Free Energy: -1317.236330
Imaginary Frequency: -348.64
Cartesian coordinates and point charges:

C	1.981679	0.951793	-1.64706	-0.20059
H	2.038905	1.918194	-1.13307	0.08516
C	3.081613	0.039796	-1.56676	-0.14184
C	4.122863	0.205962	-0.61102	0.11183
H	3.216897	-0.71828	-2.341	0.10887
Pd	1.39475	-0.48355	-0.26661	-0.2502
N	1.362588	-2.29709	1.1452	-0.11261
P	-0.80184	0.07084	0.366234	-0.06077
H	5.865346	0.705215	-2.19438	0.2685
N	5.513048	1.208663	-1.37849	-0.4635
H	5.098972	2.082335	-1.70902	0.26431
C	-4.26581	-1.89934	-1.96293	-0.0643
C	-4.50105	-1.40368	-0.68042	-0.10353
C	-3.47027	-0.79944	0.031854	-0.11545
C	-2.19288	-0.69001	-0.53146	0.24871
C	-1.96618	-1.19053	-1.81726	-0.17954
C	-3.00013	-1.78962	-2.53281	-0.09633
H	-5.07373	-2.37371	-2.5174	0.11207
H	-5.49108	-1.48774	-0.23517	0.11467
H	-3.66739	-0.40125	1.028898	0.10272
H	-0.96834	-1.10961	-2.25392	0.14195

H	-2.81659	-2.17575	-3.53405	0.11145
C	-1.66621	4.601997	0.680133	-0.1057
C	-0.57131	4.032021	1.32995	-0.08289
C	-0.33359	2.666804	1.221842	-0.14773
C	-1.19979	1.849712	0.483177	0.15709
C	-2.29069	2.428907	-0.17064	-0.14766
C	-2.51853	3.800819	-0.07289	-0.05077
H	-1.85001	5.672077	0.758946	0.11408
H	0.09996	4.655497	1.918726	0.10559
H	0.541606	2.23177	1.711139	0.11755
H	-2.96702	1.812526	-0.76305	0.05855
H	-3.37029	4.242847	-0.5873	0.11028
C	-0.87816	-2.01989	2.319044	0.14335
C	-0.98887	-0.50384	2.113725	-0.13952
C	0.003973	-2.83178	1.372773	0.04656
H	1.847343	-2.97992	0.563583	0.23424
H	-1.88	-2.46474	2.233019	-0.01559
H	-0.57014	-2.20235	3.359524	0.00073
H	-0.19273	0.023233	2.660863	0.07048
H	-0.47192	-2.91465	0.385424	-0.02291
C	2.130756	-2.13531	2.382931	-0.19838
H	1.726346	-1.30029	2.966501	0.10649
H	3.171656	-1.89774	2.135113	0.06497
H	2.110171	-3.04171	3.010971	0.08549
H	0.069556	-3.85435	1.785442	0.02606
H	-1.93378	-0.13582	2.539639	0.04747
H	1.370612	0.971736	-2.55084	0.10072
H	4.729834	-0.66025	-0.34483	0.06831
H	3.939095	0.886686	0.222652	0.09318
H	6.301922	1.429573	-0.76608	0.27841



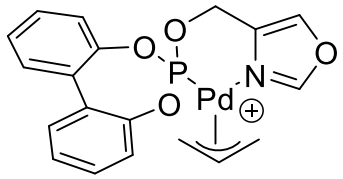
TS 21.
Gibbs Free Energy: -2006.153699
Imaginary Frequency: -265.98

Cartesian coordinates and point charges:

P	1.466722	0.743864	0.199137	0.02256
N	-1.17149	1.764606	-0.61844	-0.44063
C	-2.32579	2.071195	-1.19066	0.49435
Pd	-0.55543	-0.39794	-0.05281	-0.21908
C	-0.35797	-2.36699	0.599545	-0.26637
C	-1.71366	-2.25743	0.151568	-0.0374
C	-2.74975	-1.90766	1.090409	0.0977
N	-3.29779	-3.41892	1.904102	-0.62184
H	-2.02137	-2.64869	-0.82143	0.06505
H	-2.48135	-3.87965	2.313421	0.33305
H	-3.69401	-4.04349	1.198415	0.28824
H	-4.00289	-3.26392	2.629908	0.3085
H	-0.19412	-2.28929	1.684268	0.10586
H	-2.37316	-1.4124	1.9925	0.12979
C	0.738092	-3.05107	-0.10631	0.21209
C	0.618701	-3.54359	-1.41359	-0.25679
C	1.980924	-3.16421	0.536773	-0.09974
C	1.708326	-4.1236	-2.05571	-0.00927
H	-0.33111	-3.46446	-1.94344	0.12908
C	3.071811	-3.7332	-0.10927	-0.08586
H	2.095311	-2.77192	1.550408	0.03927
C	2.941024	-4.21701	-1.41027	-0.11566
H	1.594213	-4.50451	-3.06987	0.08815
H	4.029489	-3.79576	0.406322	0.09774
H	3.792606	-4.66722	-1.91746	0.10357
C	-4.02753	-1.32072	0.604741	0.1713
C	-4.50977	-0.1495	1.194653	-0.1904
C	-4.75107	-1.90971	-0.43805	-0.18036
C	-5.69295	0.43065	0.745069	-0.04545
H	-3.93926	0.323064	1.99614	0.08679
C	-5.93886	-1.33755	-0.87979	-0.07018
H	-4.37908	-2.81596	-0.92099	0.12366
C	-6.41133	-0.16524	-0.28926	-0.07987
H	-6.05626	1.347695	1.205982	0.10195
H	-6.49623	-1.80447	-1.68986	0.10952
H	-7.34174	0.280928	-0.63604	0.11014
C	4.250926	-0.51592	3.652053	-0.12718
C	4.742691	-0.50018	2.35066	-0.01701
C	3.93669	-0.06316	1.299833	-0.16988
C	2.627503	0.357917	1.548769	0.22739
C	2.134338	0.328555	2.860896	-0.12884
C	2.944462	-0.09447	3.907429	-0.06288

H	4.883432	-0.85453	4.470967	0.10869
H	5.761529	-0.82644	2.14709	0.09686
H	4.329049	-0.06082	0.28217	0.06217
H	1.105576	0.639108	3.059318	0.06024
H	2.557596	-0.10138	4.925438	0.10056
C	4.136585	0.792013	-3.55756	-0.09256
C	4.067411	1.940497	-2.7699	-0.0408
C	3.253884	1.963613	-1.64074	-0.21119
C	2.49868	0.83758	-1.29989	0.24619
C	2.561455	-0.30789	-2.10084	-0.21848
C	3.385561	-0.33243	-3.22206	-0.03506
H	4.776384	0.776724	-4.43855	0.10558
H	4.651842	2.820244	-3.03486	0.09932
H	3.210408	2.862695	-1.02461	0.09622
H	1.965243	-1.18516	-1.83937	0.14821
H	3.434479	-1.23091	-3.83604	0.07867
C	-0.42592	2.750454	-0.01798	0.33738
C	0.867573	2.443425	0.500478	-0.13572
C	1.586648	3.421732	1.158085	0.07762
C	1.078021	4.72861	1.308948	-0.14703
C	-0.14369	5.054237	0.771715	-0.15903
C	-0.91351	4.080014	0.093743	0.00676
H	2.569223	3.179724	1.56704	0.01408
H	1.664845	5.478055	1.836317	0.14172
H	-0.53966	6.066106	0.859875	0.13158
C	-2.86062	3.384685	-1.13835	-0.31655
C	-2.17281	4.369341	-0.48502	-0.01943
H	-3.821	3.582967	-1.6122	0.1445
H	-2.57391	5.380473	-0.41033	0.12519
C	-3.06548	1.007123	-1.931	-0.26099
H	-2.63011	0.020744	-1.7268	0.08756
H	-4.13096	0.995435	-1.66324	0.06414
H	-3.00473	1.193621	-3.01277	0.08251

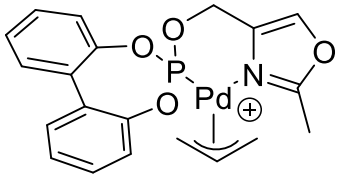
Table S2. Coordinates for the DFT optimized structures used to fit the oxazole moiety



TS 22.
Gibbs Free Energy: -1556.856130
Cartesian coordinates and point charges:

C	0.492092	2.305309	-1.47114	-0.13527
H	0.503473	1.897082	-2.48541	0.1536
C	1.630044	2.981227	-0.96478	0.10281
C	2.900079	2.531388	-1.331	-0.29647
H	3.061516	2.080794	-2.31345	0.18737
H	1.51769	3.636135	-0.0984	0.12451
Pd	1.692445	0.8335	-0.4749	-0.24239
P	-0.02335	-0.59673	0.093103	0.91585
C	1.54585	-2.06474	1.561332	0.06238
H	1.539865	-3.06781	1.997982	0.11796
H	1.326832	-1.35072	2.370307	0.07636
O	0.482574	-2.04505	0.599263	-0.36249
O	-1.07816	-0.93631	-1.05632	-0.46436
O	-0.93817	-0.15602	1.362951	-0.44058
C	-2.32292	3.233183	1.5169	-0.06921
C	-1.46672	2.152802	1.70773	-0.15913
C	-1.79065	0.927606	1.142228	0.31322
C	-2.952	0.726011	0.387112	0.00119
H	-2.08741	4.198029	1.961919	0.10963
C	-3.97876	-3.16173	-1.12101	-0.05328
C	-2.67957	-2.68697	-1.27087	-0.2121
C	-2.36739	-1.42696	-0.78903	0.3642
C	-3.30004	-0.60592	-0.14723	-0.06835
H	-4.23907	-4.14975	-1.49488	0.11704
C	-3.48238	3.070947	0.759042	-0.09409
C	-3.79241	1.832216	0.207567	-0.09965
C	-4.93897	-2.36937	-0.49563	-0.12441
C	-4.59969	-1.11034	-0.01407	-0.06901
H	-0.49606	2.532114	-1.07005	0.031
H	3.784032	2.904388	-0.81668	0.1609
H	-0.55945	2.236798	2.305408	0.11747
H	-1.90776	-3.271	-1.76819	0.15354
H	-4.15198	3.91387	0.600496	0.11808
H	-4.69624	1.712893	-0.38931	0.11001

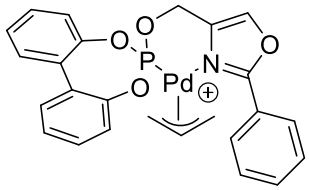
H	-5.95515	-2.73802	-0.37219	0.1261
H	-5.34567	-0.50602	0.501496	0.10449
C	2.875027	-1.78338	0.948805	0.05657
C	4.016652	-2.50728	1.001656	0.00448
C	4.408497	-0.70745	-0.09911	0.28624
N	3.153213	-0.61893	0.229805	-0.14322
O	4.989577	-1.81798	0.340741	-0.19004
H	4.298159	-3.45638	1.436404	0.17871
H	5.005606	-0.00634	-0.66923	0.13035



TS 23.
Gibbs Free Energy: -1596.128395
Cartesian coordinates and point charges:

C	0.312283	2.102724	-1.67415	-0.10558
H	0.207439	1.580525	-2.6291	0.14536
C	1.514451	2.78944	-1.36716	0.10228
C	2.728719	2.250911	-1.78896	-0.30185
H	2.783974	1.655855	-2.70348	0.1831
H	1.505358	3.553105	-0.5869	0.1177
Pd	1.544893	0.705462	-0.62268	-0.23079
P	-0.20333	-0.5705	0.165531	0.90266
C	1.332563	-2.6608	0.098081	0.07022
H	1.181196	-2.63876	-0.99324	0.07911
H	1.291749	-3.70631	0.417092	0.10355
O	0.236246	-2.0073	0.755443	-0.34984
O	-1.30711	-0.83631	-0.98081	-0.47517
O	-1.06267	-0.0835	1.437996	-0.46682
C	-2.35785	3.340246	1.562294	-0.046
C	-1.51894	2.243574	1.737091	-0.20393
C	-1.89951	1.015072	1.216683	0.39592
C	-3.0982	0.826253	0.520287	-0.05468
H	-2.07761	4.308644	1.972094	0.10874
C	-4.23207	-3.03471	-0.9726	-0.06167
C	-2.93496	-2.57063	-1.16799	-0.22836
C	-2.5887	-1.32028	-0.68312	0.36092
C	-3.48874	-0.50037	0.004818	-0.0294
H	-4.51802	-4.01484	-1.34863	0.11775

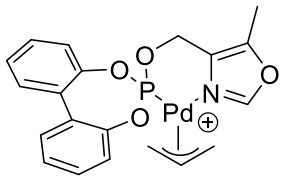
C	-3.55815	3.189234	0.869	-0.11787
C	-3.92186	1.94744	0.358813	-0.06782
C	-5.15815	-2.24146	-0.29857	-0.10979
C	-4.78734	-0.99145	0.183884	-0.09311
H	-0.62427	2.419508	-1.21323	0.01473
H	3.668869	2.660232	-1.42491	0.16203
H	-0.58203	2.316643	2.288153	0.12508
H	-2.19195	-3.15653	-1.70662	0.15863
H	-4.2159	4.044146	0.725749	0.12108
H	-4.8549	1.837192	-0.19323	0.10093
H	-6.17218	-2.6021	-0.13919	0.12351
H	-5.50625	-0.38456	0.73383	0.1128
C	2.642158	-2.06023	0.468368	0.07241
C	3.710172	-2.627	1.06898	-0.06484
C	4.176011	-0.55258	0.666527	0.54267
N	2.961773	-0.72409	0.21408	-0.23144
O	4.679953	-1.67628	1.188396	-0.21027
H	3.936138	-3.61246	1.452078	0.1981
C	5.017464	0.659288	0.666154	-0.4234
H	5.788697	0.581684	1.438263	0.14843
H	5.518949	0.784955	-0.30261	0.14899
H	4.405725	1.547068	0.856858	0.15591



TS 24.
Gibbs Free Energy: -1787.671865
Cartesian coordinates and point charges:

C	-0.241	1.984342	-1.54745	-0.12169
H	-0.37929	1.588201	-2.55733	0.14248
C	1.014465	2.513941	-1.15787	0.08769
C	2.175528	1.927751	-1.65276	-0.27319
H	2.181373	1.455245	-2.63818	0.19916
H	1.068546	3.168092	-0.28542	0.11954
Pd	0.844248	0.35651	-0.67421	-0.25645
P	-1.06416	-0.67584	0.110182	1.01368
C	0.168063	-2.96219	0.112434	0.11177
H	0.055034	-2.974	-0.98292	0.06402
H	-0.00499	-3.9786	0.477682	0.09486

O	-0.8697	-2.16261	0.701285	-0.38347
O	-2.22332	-0.74247	-1.01011	-0.51375
O	-1.80905	-0.05703	1.402065	-0.50966
C	-2.55581	3.519422	1.620608	-0.07345
C	-1.89711	2.301545	1.760354	-0.17629
C	-2.46922	1.158675	1.219401	0.40376
C	-3.69459	1.174542	0.54375	-0.04488
H	-2.12267	4.422911	2.045486	0.11404
C	-5.46744	-2.43283	-0.96112	-0.03212
C	-4.11591	-2.18423	-1.17839	-0.25936
C	-3.56037	-1.01282	-0.69015	0.3991
C	-4.30242	-0.06481	0.021434	-0.06039
H	-5.9162	-3.34894	-1.33956	0.10982
C	-3.77278	3.573369	0.941892	-0.11615
C	-4.33382	2.414359	0.416078	-0.07449
C	-6.23918	-1.5072	-0.26203	-0.13845
C	-5.66034	-0.34002	0.222649	-0.05828
H	-1.15069	2.3299	-1.05491	0.0249
H	3.145498	2.177268	-1.22728	0.1227
H	-0.95337	2.215145	2.297986	0.11733
H	-3.48884	-2.87713	-1.73677	0.16583
H	-4.28961	4.523676	0.824119	0.12329
H	-5.28065	2.462826	-0.12115	0.10152
H	-7.29529	-1.6996	-0.08492	0.1267
H	-6.26031	0.369364	0.792229	0.10187
C	1.530327	-2.50777	0.496211	-0.01289
C	2.43269	-3.12488	1.289177	0.02605
C	3.320696	-1.30169	0.534253	0.41299
N	2.108471	-1.3221	0.031951	-0.15984
O	3.561844	-2.36766	1.314769	-0.23412
H	2.43914	-4.04192	1.862322	0.17656
C	6.569889	1.332761	-0.13597	-0.06342
C	6.278093	0.910131	1.160151	-0.07145
C	5.209414	0.05163	1.38894	-0.11843
C	4.414941	-0.36574	0.315407	-0.01771
C	4.716277	0.047874	-0.98666	-0.03461
C	5.795025	0.895167	-1.20945	-0.05722
H	7.414655	1.996158	-0.31231	0.11003
H	6.890702	1.24491	1.994745	0.11542
H	4.982609	-0.29197	2.397284	0.12417
H	4.119079	-0.32264	-1.81971	0.05841
H	6.042209	1.203967	-2.22374	0.09402



TS 25.
Gibbs Free Energy: -1596.125961
Cartesian coordinates and point charges:

C	0.055207	-2.55369	-1.35642	-0.13614
H	0.028687	-2.21539	-2.39577	0.14922
C	-0.99976	-3.34637	-0.84056	0.11982
C	-2.30425	-3.09998	-1.27403	-0.32184
H	-2.48705	-2.74005	-2.28958	0.19081
H	-0.83403	-3.92347	0.071426	0.11808
Pd	-1.37502	-1.20262	-0.49873	-0.23234
P	0.103225	0.485454	0.024768	0.96447
C	-1.71323	1.791546	1.349146	0.08364
H	-1.8546	2.805314	1.735381	0.12445
H	-1.43085	1.153439	2.200869	0.07107
O	-0.6115	1.874583	0.42941	-0.39128
O	1.139852	0.90153	-1.11743	-0.4783
O	1.03068	0.248235	1.340184	-0.4456
C	2.859118	-2.9036	1.725662	-0.06868
C	1.857294	-1.94328	1.831091	-0.14032
C	2.029731	-0.71682	1.204914	0.28874
C	3.17707	-0.39814	0.468941	0.00371
H	2.742467	-3.86679	2.218738	0.10718
C	3.710061	3.498013	-1.25666	-0.08227
C	2.493577	2.839668	-1.40639	-0.18839
C	2.340175	1.58013	-0.85173	0.34879
C	3.355623	0.936487	-0.1371	-0.04769
H	3.844891	4.48794	-1.68754	0.12324
C	4.010693	-2.62325	0.990722	-0.09824
C	4.166589	-1.38524	0.376219	-0.09352
C	4.748648	2.885833	-0.55843	-0.10812
C	4.569013	1.623207	-0.00554	-0.09081
H	1.048441	-2.61707	-0.9107	0.02609
H	-3.14855	-3.55811	-0.76193	0.16736
H	0.948999	-2.12014	2.406534	0.11202
H	1.66603	3.279845	-1.95916	0.15138
H	4.794334	-3.37261	0.898861	0.11862
H	5.064909	-1.17461	-0.2035	0.106
H	5.700371	3.398349	-0.43462	0.12539

H	5.373591	1.159811	0.564938	0.10914
C	-2.96329	1.305956	0.703542	-0.04717
C	-4.19103	1.884869	0.659868	0.31951
C	-4.27976	-0.03408	-0.33388	0.26337
N	-3.04576	0.068896	0.056724	-0.16001
O	-5.02383	1.015529	0.000078	-0.24233
H	-4.74737	-0.84397	-0.88029	0.14006
C	-4.78068	3.147971	1.140904	-0.41497
H	-5.26164	3.69056	0.317963	0.16958
H	-5.54187	2.963737	1.909432	0.15318
H	-4.01045	3.795039	1.572346	0.13312

Table S3. Added TSFF parameters to the standard MM3* to described the Pd-catatlyzed allylic amination reaction

```
C  PdTS_Core OPT
 9  Pd(-C0-C0(-1)-C0(.1)[.NX])
-2
 1   1   2            2.1050    1.1549   -1.8195
 1   1   3            2.1805    1.7263   -2.5539
 1   1   4            2.7857    0.9661   -3.2640
 1   2   3            1.4082    5.5257   -1.2122
 1   2  C2             1.4739    3.8668   -1.4341
 1   2  C3             1.4958    4.5477    0.7841
 1   2  H1             1.0960    5.3315   -0.7789
 1   3   4            1.4262    5.0890   -2.4752
 1   3  C2             1.4463    4.3064   -0.7428
 1   3  C3             1.4995    3.9883    0.9457
 1   3  H1             1.0935    5.3544   -0.6048
 1   4  C2             1.4666    4.6409   -0.6953
 1   4  C3             1.4976    6.5450    1.2073
 1   4  H1             1.0933    5.4381   -0.5778
 2   2   1   3        38.9045    1.4600
 2   2   1   4        62.8828    5.3921
 2   3   1   4        31.1956    1.7451
 2   1   2   3        72.7904    0.8498
 2   1   2  C3        113.7095    1.3544
 2   1   2  C2        114.0944    2.0150
 2   1   2  H1        109.1846    0.5439
 2   3   2  C3        126.5077    0.8136
 2   3   2  C2        124.2861    0.9957
 2   3   2  H1        119.3245    0.6145
 2  H1   2  C3         118.4643    0.4969
 2  H1   2  C2         113.9745    0.1840
 2  H1   2  H1         116.4148    0.4719
 2   1   3   2        71.3746    0.1737
 2   1   3   4        97.7602    0.5804
 2   1   3  C2        117.8560    1.0981
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 2   1   3  C3          115.2384     2.5867
 2   1   3  H1          110.9192     0.4613
 2   2   3   4          122.3644     0.8526
 2   2   3  C2          124.5112     2.4193
 2   2   3  C3          123.6798     0.5464
 2   2   3  H1          116.5563     0.1281
 2   4   3  C2          118.9280     1.8938
 2   4   3  C3          120.9317     0.7171
 2   4   3  H1          117.1217     0.8904
 2   1   4   3           49.6771     0.1102
 2   1   4  C2          105.3175     0.1034
 2   1   4  C3          101.7406     0.1405
 2   1   4  H1           86.1229     0.1329
 2   3   4  C2          119.5362     0.3224
 2   3   4  C3          120.2062     0.4808
 2   3   4  H1          119.0980     0.5599
 2  H1   4  H1           113.9015     0.4620
 2  C2   4  H1           110.8934     0.3053
 2  C3   4  H1           116.0372     0.2697
 4  00   1   2  00        0.0000     0.0000     0.0000
 4   2   1   3  00        0.0000     0.0000     0.0000
 4   4   1   3  00        0.0000     0.0000     0.0000
 4  00   1   4  00        0.0000     0.0000     0.0000
 4  00   2   3  00        0.0000     0.0000     0.0000
 4  H1   2   3   4        0.0000     0.8902     0.0000
 4  C0   2   3   4        0.0000     1.7993     0.0000
 4  H1   2   3  H1         0.0000     0.0000     0.0000
 4  C0   2   3  H1         0.0000     0.0000     0.0000
 4  H1   2   3  C0         0.0000     0.0000     0.0000
 4  C0   2   3  C0         0.0000     0.0000     0.0000
 4  00   2  C2  00         0.0000     0.0000     0.0000
 4  00   2  C3  00         0.0000     0.0000     0.0000
 4  00   3   4  00        0.0000     0.0000     0.0000
 4   2   3   4  C2        0.0000    -0.1061     0.0000
 4   2   3   4  C3        0.0000     0.0000     1.4557
 4   2   3   4  H1        0.0000     4.0945     0.0000
 4   1   3   4  C2        0.0000     0.8770    -0.9674
 4   1   3   4  C3        0.0000     1.1033     0.0000
 4   1   3   4  H1        0.0000     0.0000    -0.8015
 4  00   3   4   1        0.0000     0.0000     0.0000
 4  00   3  C0  00         0.0000     0.0000     0.0000
 4   2   3  C2  C2         0.0000     0.0000     0.0000
 4   4   3  C2  C2         0.0000     0.0000     0.0000
 4  00   4  C3  00         0.0000     0.0000     0.0000
 4  00   4  C2  00         0.0000     0.0000     0.0000
 4   1   4  C2  00        0.0000     0.0000     0.0000
 5   4   3  00  00        0.0000     0.0000
-3
 C  PdTS_PP OPT
 9  Pd(-C0-C0(-1)-C0(.1)[.NX])(.P3)
-2
```

```
 1   1   6              2.3580     1.5684    -2.8961
 1   6  O3              1.6129     4.3412     1.9690
 1   6  C3              1.8392     3.6319    -0.4021
 1   6  C2              1.8390     3.2709    -1.3846
 1   6  H1              1.4138     3.5396     0.0321
 2   2   1   6         95.7465     0.1001
 2   3   1   6        149.9115     0.1005
 2   4   1   6        155.2452     0.1808
 2   1   6  H1        118.8123     0.1110
 2   1   6  C2        114.6107     0.2658
 2   1   6  C3        103.8950     4.7535
 2   1   6  O3        115.5134     1.1374
 2  H1   6  H1         98.7196     0.6170
 2  C2   6  C2        106.4260     2.7447
 2  C2   6  C3        103.5000     3.2797
 2   6  C2  N2        123.2000     0.5056
 2   6  O3  C3        125.0000     0.5000
 2   6  O3  C2        119.1945     0.2148
 4  00   1   6  00      0.0000     0.0000     0.0000
 4   6   1   2   3      0.0000     0.0000     0.0000
 4   6   1   3  00      0.0000     0.0000     0.0000
 4   4   3   1   6      0.0000     0.0000     0.9556
 4   2   3   1   6      0.0000     1.9210     0.0000
 4  H1   3   1   6      0.0000     0.0000     0.0000
 4   1   3   2   6      0.0000     0.0000     0.0000
 4   1   6  C2  C2      0.0000     0.0000     0.0000
 4   1   6  C2  N2      0.0000     1.0050     0.0000
 4   1   6  C3  00      0.0000     0.4001     0.0000
 4   1   6  C3  H1      0.0000     0.0000     0.0000
 4   1   6  C3  C0      0.0000     0.0000    -1.3260
 4   1   6  O3  C2      0.0000     0.0000     3.0462
 4   1   6  O3  C3      0.0000     0.0000     1.4410
 4   6   1   3  C0      0.0000     0.0000     0.0000
 4   6  O3  C0  C0      0.0000     0.0000     0.0000
-3
 C  PdTS_PN OPT
 9  Pd(-C0-C0(-1)-C0(.1)[.NX])(.P3)(.N0)
-2
 1   1   7              2.2482     1.5540    -3.0665
 2   2   1   7        165.3555     0.9410
 2   3   1   7        125.5870     0.1109
 2   4   1   7        103.8732     0.7572
 2   6   1   7         90.5092     0.1109
 4   7   1   2   3      0.0000     0.0000     0.0000
 4   7   1   3  00      0.0000     0.0000     0.0000
 4   7   1   3   2      0.0000     4.2795     0.0000
 4   7   1   3   4      0.0000     0.0000     1.9278
 4  00   1   6  00      0.0000     0.0000     0.0000
 4  00   1   7  00      0.0000     0.0000     0.0000
 4   6   2   3   7      0.0000     1.4028     0.0000
-3
```

```
 C  PdTS_N3 ligand OPT
 9  Pd.N3
-2
 1   2  H3              1.0203     6.9649    -1.4080
 1   2  C3              1.4570     3.2351    -0.3741
 2   1   2  H3         105.6811     0.1031
 2   1   2  C3         114.6750     2.0636
 2  H3   2  H3          112.9797     0.1956
 2  C3   2  C3          113.2437     1.1221
 4   1   2  C3  00        0.0000     0.0000     0.0000
-3
 C  PdTS_N2 ligand OPT
 9  Pd.N2
-2
 1   2  C3              1.4765     2.9993    -1.5609
 1   2  C2              1.3283     6.8499    -2.7262
 2   1   2  C3         112.1510     0.3768
 2   1   2  C2         123.3410     0.9884
 2  C3   2  C2          107.1845     0.1380
 4   1   2  C3  00        0.0000     0.0000    -2.5216
 4   1   2  C2  C2        0.0000     2.2465     0.0000
 4   1   2  C2  C3        0.0000     0.0000    -1.0000
 4   1   2  C2  O3        0.0000     0.6973     0.0000
 4   2  C2  C2  C2         0.0000     0.0000     0.0000
-3
 C  PdTS_amine OPT
 9  Pd-C0-C0(-1)-C0(.1).NX
-2
 1   4   5              1.9668     1.9093    -2.8841
 1   5  H3              1.0195     7.0392    -1.4042
 1   5  C3              1.4280     3.2872    -0.2903
 2   1   4   5         154.9079     0.1015
 2   3   4   5         106.5349     0.9533
 2   5   4  H1          93.3978     0.6182
 2   5   4  C2          99.5955     0.1251
 2   5   4  C3          97.7010     1.2985
 2   4   5  H3         110.6874     0.1069
 2   4   5  C0         111.0857     1.3239
 4   2   3   4   5        0.0000     0.0000     0.0000
 4   5   4  00  00        0.0000     0.0000     0.0000
 4  00   4   5  00        0.0000     0.0000     0.0000
 4   4   5  C0  00        0.0000     0.0000    -0.1909
-3
 C  Palladium oxazoline OPT
 9  Pd.N2=C2-O3-C3-C3-2
-2
 1   1   2              2.2505     1.3186    -2.9333
 1   2   3              1.2712    13.0304    -3.2480
 1   2   6              1.4724     7.9650    -0.8126
 1   3   4              1.3235     3.4594     0.6316
 1   4   5              1.4373     6.6772    -1.2473
```

```
 1   2  C0              1.4017     3.4671     0.1520
 1   4  C0              1.5151     2.5941     0.4716
 1   4   5              1.4440     5.1648    -1.9752
 2   1   2   3        130.6086     0.5693
 2   1   2   6        121.7180     0.0001
 2   3   2   6        107.8071     0.8095
 2   2   3   4        116.3343     0.6847
 2   2   3  C2         126.4541     0.5377
 2   2   3  C3         128.9152     0.3205
 2   4   3  C2         118.5661     1.6642
 2   4   4  C3         118.5277     0.4449
 2   3   4   5        112.6583     0.4766
 2   4   5   6        104.1000     0.6197
 4   1   2   3   4       0.0000     2.8509     0.0000
 4   1   2   3  C2       0.0000     2.8959     0.0000
 4   1   2   3  C3       0.0000     4.8651     0.0000
 4   1   2   6  00       0.0000     0.0000     0.0000
 5   2  00  00  00       0.0000     0.0000     0.0000
-3
 C  PdAllyl Oxazole OPT
 9  N2=C2-O2-C2=C2-1
-2
 1  Pd   1              2.1362     2.0971    -3.7679
 1   1   2              1.2849     5.2132    -1.9406
 1   1   5              1.3748     2.3660    -1.3658
 1   2   3              1.3209     3.4162     0.7539
 1   2  C0              1.4017     3.4671     0.1520
 1   3   4              1.3649     3.4196    -0.6118
 1   4  C0              1.5151     2.5941     0.4716
 1   4   5              1.3629     5.2176     0.3371
 2  Pd   1   2         124.4931     0.6121
 2  Pd   1   5         125.2020     2.3231
 2   2   1   5        103.2033     3.3837
 2   1   2   3        117.9564     2.4061
 2   1   2  C2         130.4264     0.2869
 2   1   2  C3         129.6924     0.1347
 2   1   5   4        104.1390     1.2007
 2   1   5  C3         121.5451     2.7335
 2   3   2  C2         117.3913     1.8003
 2   3   2  C3         120.5687     1.0388
 2   2   3   4        107.6874     2.1853
 2   3   4   5        102.3753     0.5901
 4   2   3   4   5       0.0000     0.6316     0.0000
 4   1   2   3   4       0.0000     0.4870     0.0000
 4   2   3   4  00       0.0000     0.0000     0.0000
 4  00   2   3   4       0.0000     0.0000     0.0000
 4  Pd   1   5   4       0.0000     1.1408     0.0000
 4  Pd   1   5  C3       0.0000     0.5337     0.0000
 4  Pd   1   2  00       0.0000     0.0000     0.0000
 4  Pd   1   2  C0       0.0000     0.4468     0.0000
-3
```

Details of Force Field Parameterization

The added substructures needed to describe the TS of this reaction was broken into eight different substructure. The first substructure described the atoms around the core, Pd-(C_{allyl}-C_{allyl}-C_{allyl}).N_{amine}, of the reaction which describes any of the parameters between the allyl and the metal center. There were four substructures developed to describe the P, N ligands. One substructure was used to describe the parameters between the metal and allyl with the phosphorus atom wjile a separate substructure was developed to describe the parameters metal and allyl with a general nitrogen atom. There were separate substructures to distinguish interactions between a N_{sp3} and a N_{sp2}. There was an two additional substructures developed to described an oxzaoline and oxazole moiety. The last substructure was used to describe the amine section.

With all of the substructures added to the MM3*, initial parameters needed to be estimated. The bond dipoles were all initially set to zero. The bond force constants were set to 1.0, with the exception of the force constant to describe the reaction coordinate which was set to 0.2. The angle force constants were set to 0.5, and the torsional terms were all set to zero. The equilibrium bond and angle values were set to the average of the interaction in the training set structures.

The force field parameters were then optimized starting with the bond dipoles, followed by the bond and angle force constants, the equilibrium bond and angle values, and finally the torsional terms. The equilibrium bond and angle values were optimized by tethering to the average reference value from the DFT optimized training set. This ensures that the values don't deviate to unrealistic parameters during the parameterization process. Once all of the parameters have been optimized, various different data types calculated by DFT and MM were compared to see how well the added force field substructures could reproduce the structural informational and the Hessian matrix. The bond dipoles, bonds, angles, torsions, and diagonal eigenvalues were calculated from the MM optimized structures and compared to the DFT optimized structures

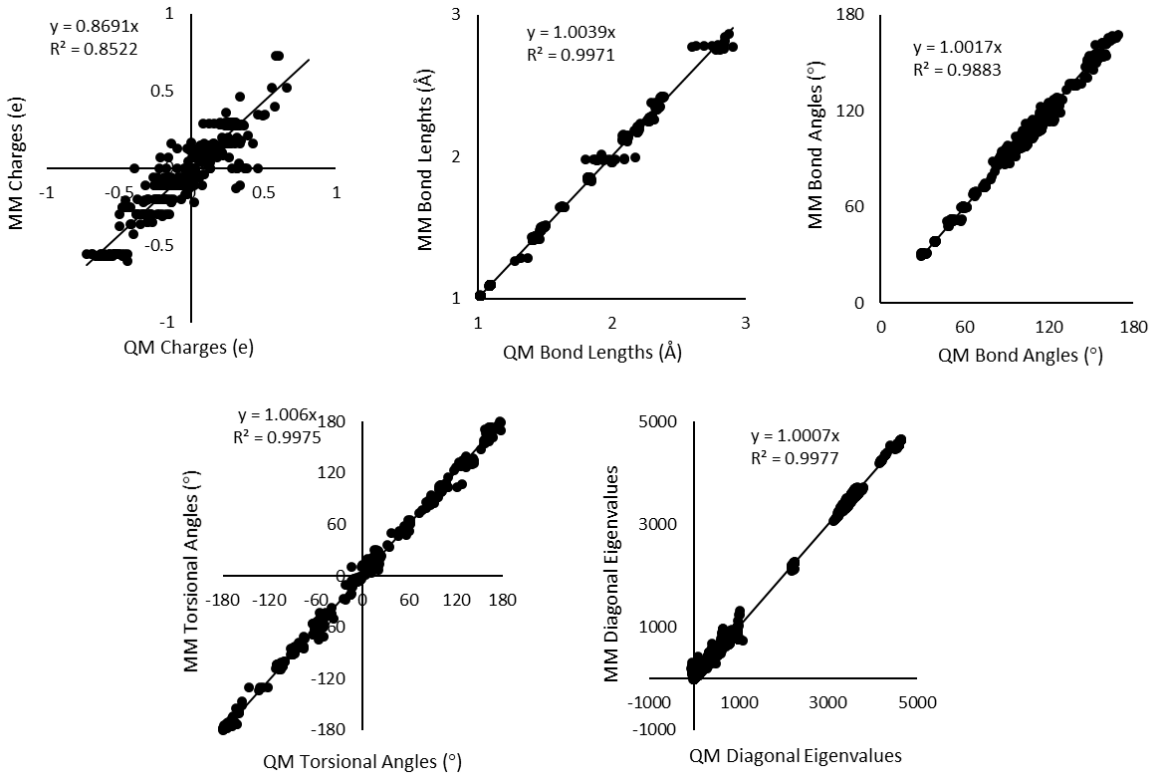


Figure S2. Data comparison between the QM optimized data and the MM optimized data

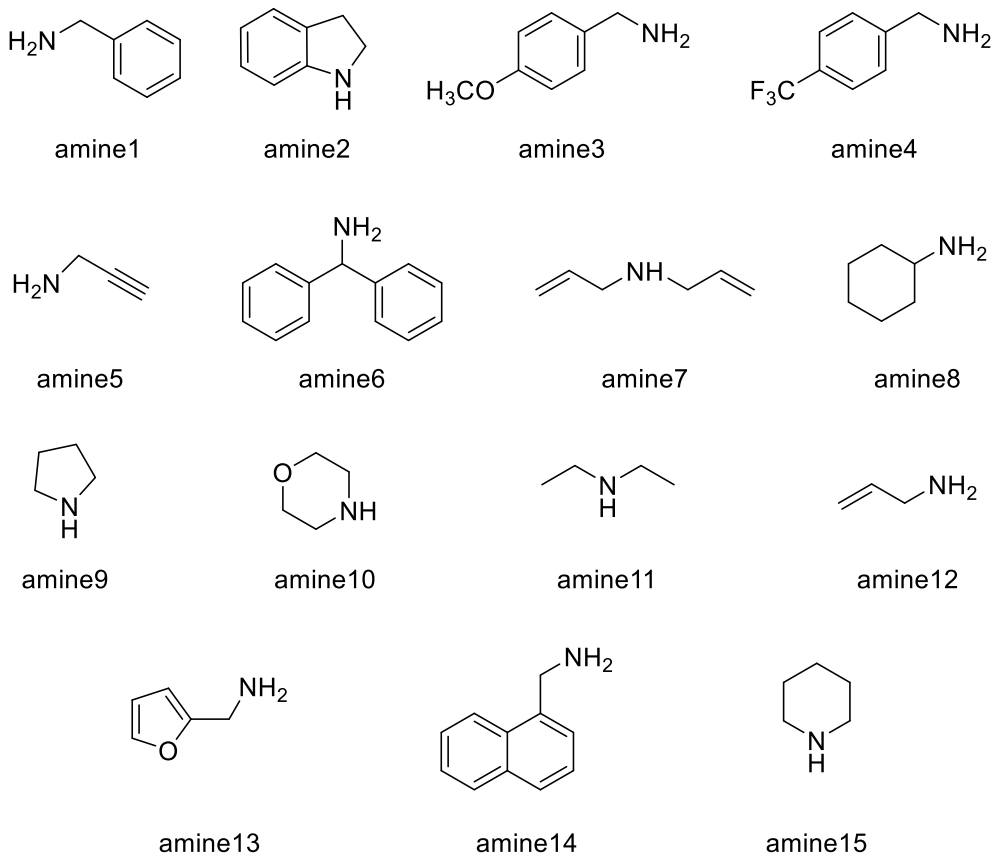
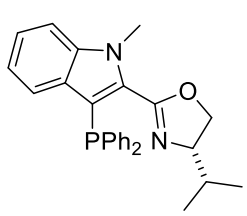


Figure S3. Structures of the Nucleophiles in the Validation Set



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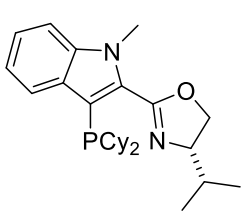

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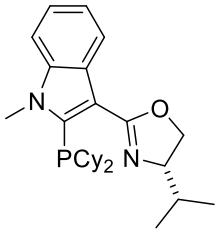

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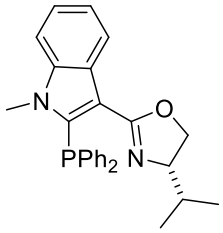

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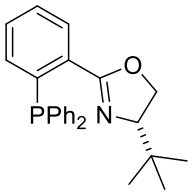

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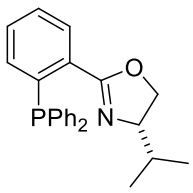

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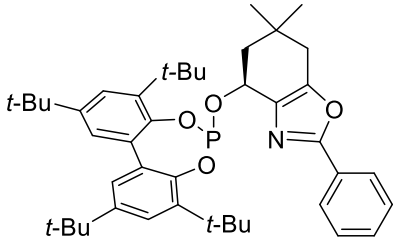

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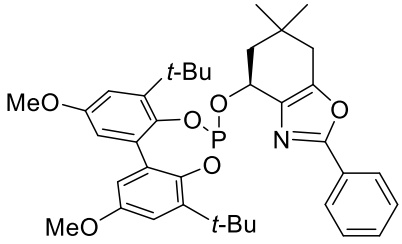

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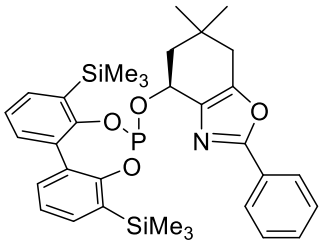

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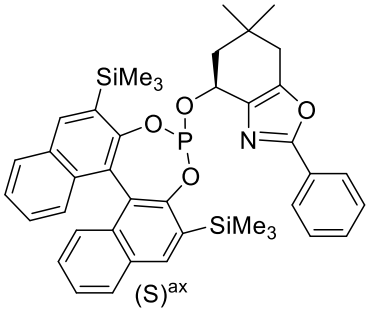

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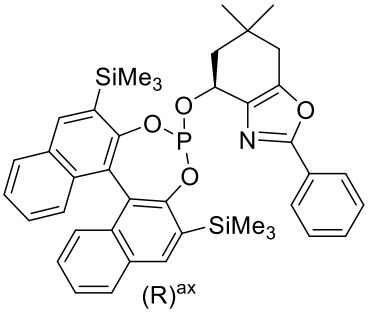

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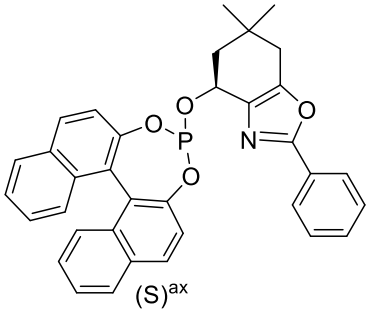

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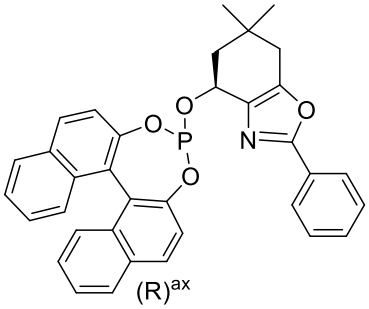

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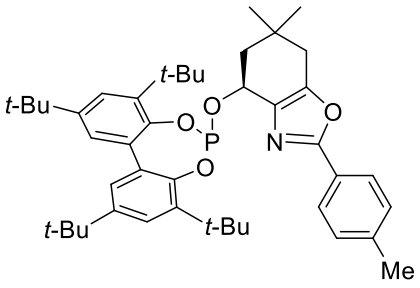

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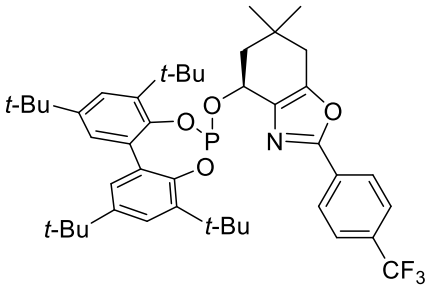

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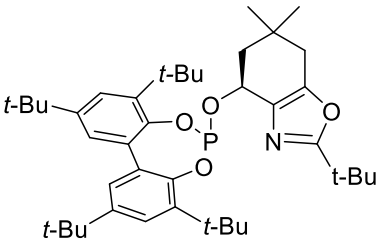

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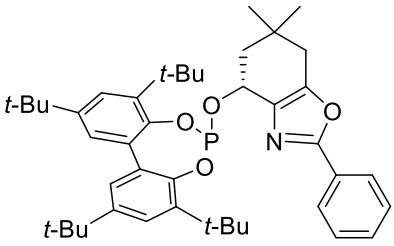

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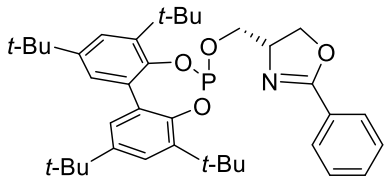

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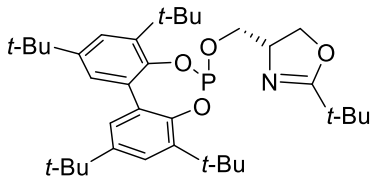

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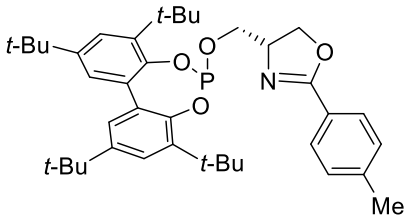

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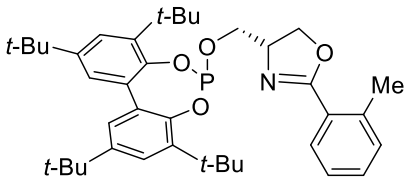

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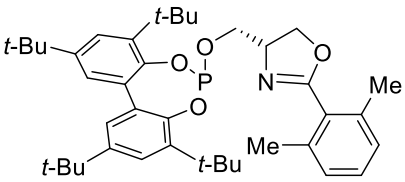

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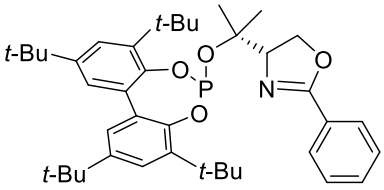

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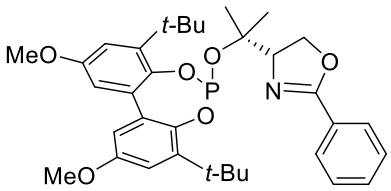

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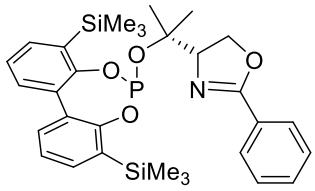

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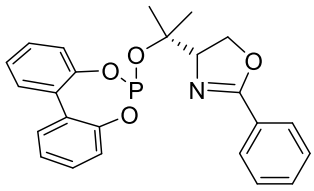

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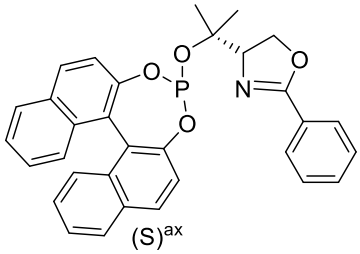

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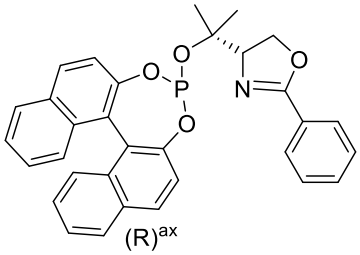

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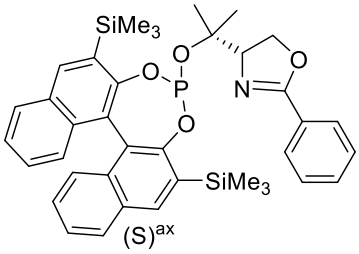

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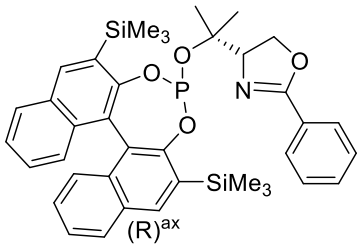

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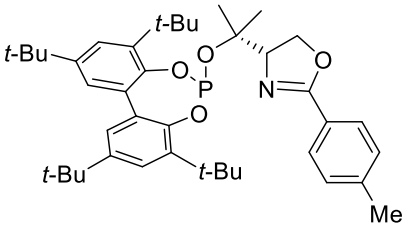

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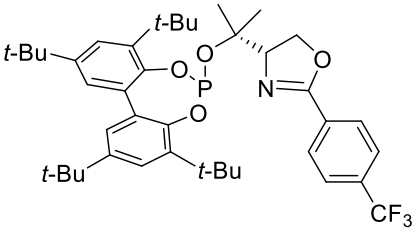

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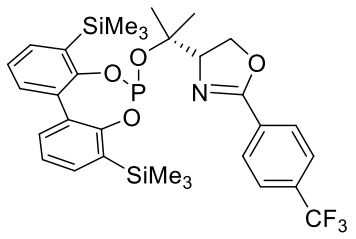

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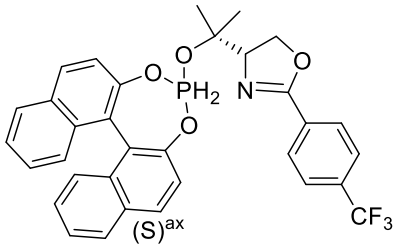

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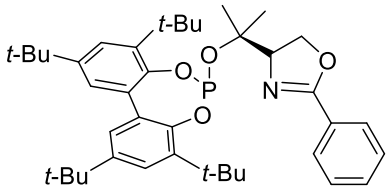

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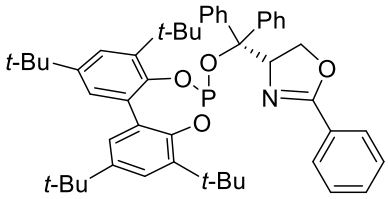

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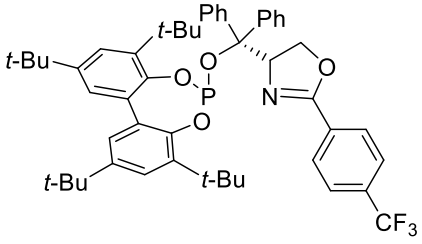

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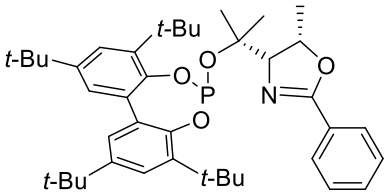

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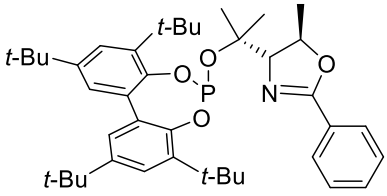

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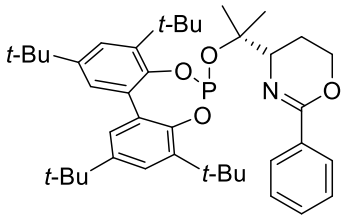

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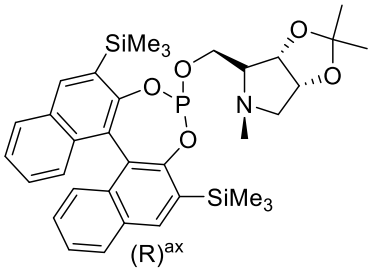

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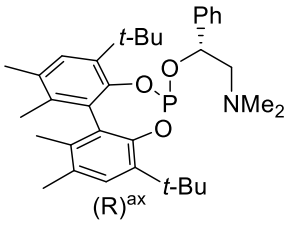

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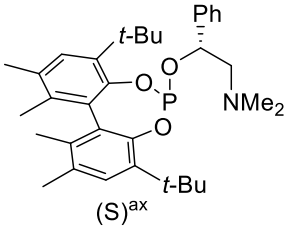

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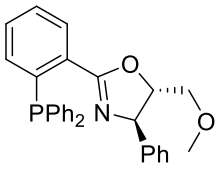

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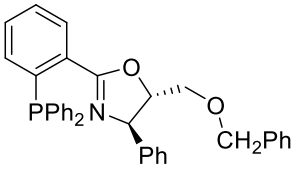

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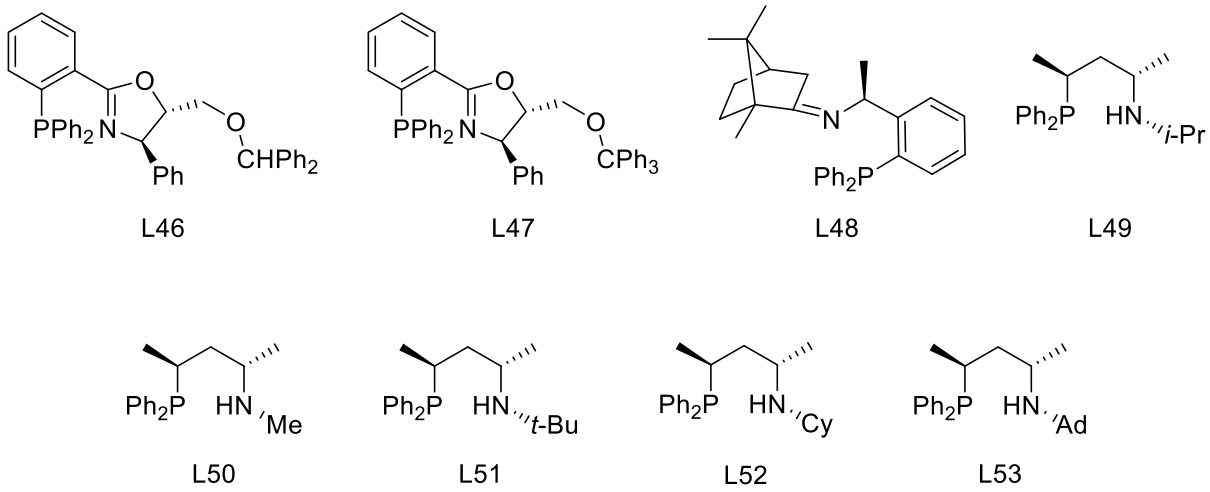


Figure S4. Structures of the Ligands in the Validation Set

Table S3. Results for the Validation Set

	Nucleophile	Ligand	Abs. Conf (exp)	% ee (exp)	temp	ln(er) (exp.)	ln(er) (calc.)
Structure01	amine1	L1	R	-52	rt	-2.88	-8.76
Structure02	amine1	L2	R	-62	rt	-3.62	-18.96
Structure03	amine1	L3	R	-23	rt	-1.17	-18.96
Structure04	amine1	L4	R	-94	rt	-8.67	-5.96
Structure05	amine2	L5	S	95	rt	9.14	-18.96
Structure06	amine2	L6	S	86	rt	6.45	-8.59
Structure07	amine1	L7	R	-84	296	-6.01	5.10
Structure08	amine1	L8	R	-80	296	-5.41	2.75
Structure09	amine1	L9	R	-69	296	-4.17	2.67
Structure10	amine1	L10	R	-71	296	-4.37	6.29
Structure11	amine1	L11	R	-41	296	-2.14	3.61
Structure12	amine1	L12	R	-7	296	-0.35	4.88
Structure13	amine1	L13	S	5	296	0.25	5.98
Structure14	amine1	L14	R	-32	296	-1.63	1.35
Structure15	amine1	L15	R	-82	296	-5.69	6.62
Structure16	amine1	L16	R	-25	296	-1.26	6.93
Structure17	amine1	L17	S	84	296	6.01	-4.83
Structure18	amine1	L18	R	-55	rt	-3.08	-4.65
Structure19	amine1	L19	R	-9	rt	-0.45	-10.05
Structure20	amine1	L20	R	-50	rt	-2.74	-3.40
Structure21	amine1	L21	R	-32	rt	-1.65	-0.91
Structure22	amine1	L22	R	-5	rt	-0.25	-2.33
Structure23	amine1	L23	R	-87	rt	-6.65	-3.28

Structure24	amine1	L24	R	-86	rt	-6.45	-5.34
Structure25	amine1	L25	R	-92	rt	-7.93	-6.32
Structure26	amine1	L26	R	-92	rt	-7.93	-5.28
Structure27	amine1	L27	R	-93	rt	-8.27	-5.38
Structure28	amine1	L28	R	-91	rt	-7.62	-3.44
Structure29	amine1	L29	R	-57	rt	-3.23	-7.93
Structure30	amine1	L30	R	-90	rt	-7.34	-6.02
Structure31	amine1	L31	R	-83	rt	-5.93	-2.29
Structure32	amine1	L32	R	-93	rt	-8.27	-2.17
Structure33	amine1	L33	R	-96	rt	-9.71	-7.27
Structure34	amine1	L34	R	-84	rt	-6.09	-3.13
Structure35	amine1	L35	S	88	rt	6.86	3.34
Structure36	amine1	L36	R	-89	rt	-7.09	-8.71
Structure37	amine1	L37	R	-88	rt	-6.86	-8.27
Structure38	amine1	L38	R	-62	rt	-3.62	-0.31
Structure39	amine1	L39	R	-84	rt	-6.09	-2.77
Structure40	amine1	L40	S	8	rt	0.40	-8.09
Structure41	amine1	L41	S	91	273	6.93	5.62
Structure42	amine3	L41	S	90	273	6.68	5.48
Structure43	amine4	L41	S	91	273	6.93	4.42
Structure44	amine1	L42	S	97	296	10.30	2.37
Structure45	amine1	L43	R	-99	296	-13.03	-8.31
Structure46	amine1	L44	S	95	rt	9.14	10.12
Structure47	amine5	L44	S	94	rt	8.67	9.46
Structure48	amine6	L44	S	97	rt	10.44	13.20
Structure49	amine7	L44	s	96	rt	9.71	10.05
Structure50	amine8	L44	S	99	rt	13.20	9.71
Structure51	amine1	L45	S	84	rt	6.09	7.99
Structure52	amine1	L46	S	83	rt	5.93	4.63
Structure53	amine1	L47	S	88	rt	6.86	3.68
Structure54	amine1	L6	R	-96	313	-10.12	-8.51
Structure55	amine1	L48	S	99	rt	13.20	8.63
Structure56	amine9	L48	S	97	rt	10.44	11.34
Structure57	amine10	L48	S	86	rt	6.45	8.94
Structure58	amine11	L48	S	86	rt	6.45	9.71
Structure59	amine12	L48	S	98	rt	11.46	9.91
Structure60	amine13	L48	S	98	rt	11.46	10.61
Structure61	amine2	L48	S	87	rt	6.65	8.09
Structure62	amine4	L48	S	99	rt	13.20	9.71
Structure63	amine5	L48	S	97	rt	10.44	10.80
Structure64	amine14	L48	S	99	rt	13.20	12.54
Structure65	amine15	L48	S	98	rt	11.46	8.20
Structure66	amine7	L48	S	98	rt	11.46	11.87

Structure67	amine6	L48	S	94	rt	8.67	11.34
Structure68	amine1	L49	S	78	rt	5.21	9.64
Structure69	amine9	L49	S	61	rt	3.54	7.12
Structure70	amine12	L49	S	90	rt	7.34	10.05
Structure71	amine11	L49	S	82	rt	5.77	6.89
Structure72	amine16	L49	S	86	rt	6.45	5.45
Structure73	amine10	L49	S	80	rt	5.48	10.27
Structure74	amine16	L50	S	20	rt	1.01	0.24
Structure75	amine16	L51	S	54	rt	3.01	5.31
Structure76	amine16	L52	S	88	rt	6.86	7.29
Structure77	amine16	L53	S	62	rt	3.62	13.20

Pd-catalyzed amination of (*rac*)-1,3-diphenylallyl acetate with indoline using phosphine-oxazoline ligand L5.

A degassed solution of $[PdCl(\eta^3\text{-}C_3H_5)]_2$ (3.65 mg, 0.01 mmol) and **L5** (8.52 mg, 0.022 mmol) in dichloromethane (1 mL) was stirred for 30 min. Subsequently, a solution of the corresponding (*rac*)-1,3-diphenylallyl acetate (50.4 mg, 0.2 mmol) in dichloromethane (1 mL), indoline (27 µL, 0.24 mmol) and sodium carbonate (42.2 mg, 0.4 mmol) were added. The reaction mixture was stirred at room temperature for 18 hours. The reaction mixture was diluted with Et_2O (5 mL) and extracted with brine (3 x 10 mL) and the extract dried over $MgSO_4$. Solvent was removed and the product was purified by column chromatography (hexane/EtOAc 9:1).

Characterization of 1-(1,3-diphenylallyl)indoline.[1,2] ^{1}H NMR ($CDCl_3$, 401 MHz): δ 2.95–2.99 (m, 2H), 3.39–3.45 (m, 2H), 5.12 (d, *J* = 7.7 Hz, 1H), 6.36 (d, *J* = 7.9 Hz, 1H), 6.49 (dd, *J* = 15.9, 7.7 Hz, 1H), 6.61–6.68 (m, 2H), 6.95 (m, 1H), 7.08 (dd, *J* = 7.1, 1.4 Hz, 1H), 7.21–7.48 (m, 10H). ^{13}C NMR ($CDCl_3$, 100 MHz,): δ 28.4, 50.6, 64.1, 108.4, 117.5, 124.4, 126.5, 127.0, 127.3, 127.7, 127.8, 128.5, 130.5, 132.7, 136.7, 140.8, 151.3.

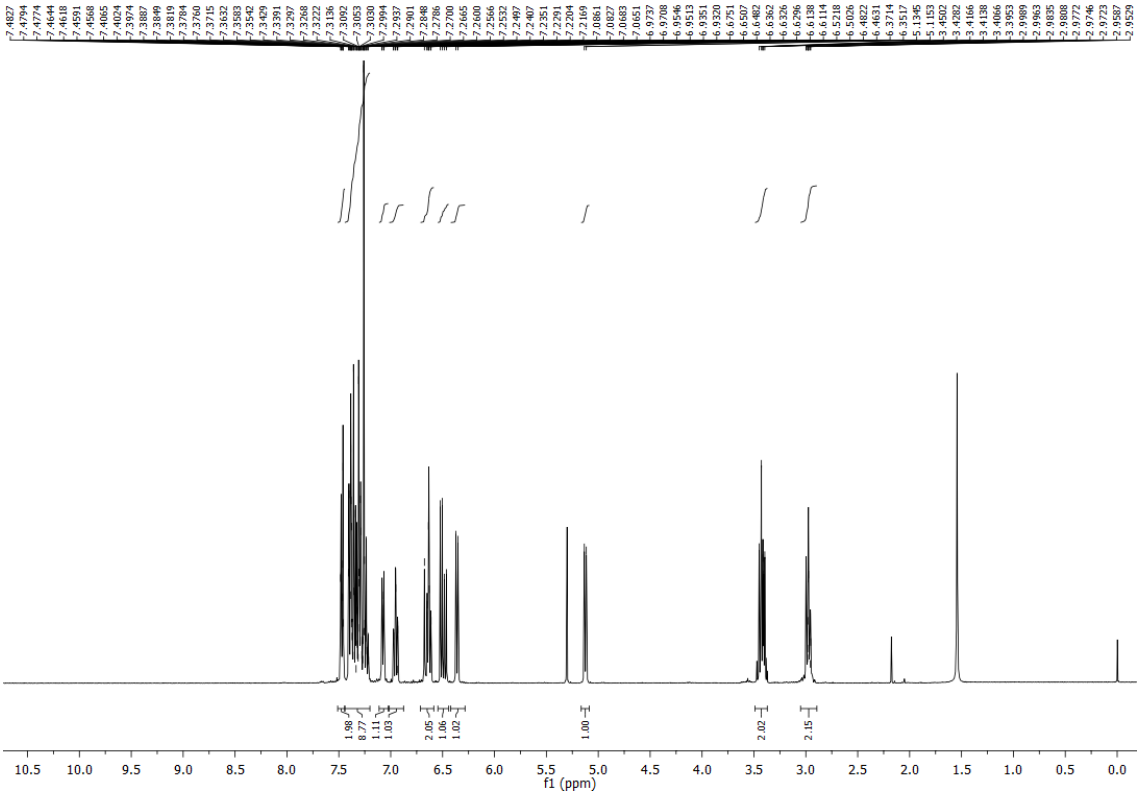


Figure S6. ^{1}H NMR of 1-(1,3-diphenylallyl)indoline in $CDCl_3$.

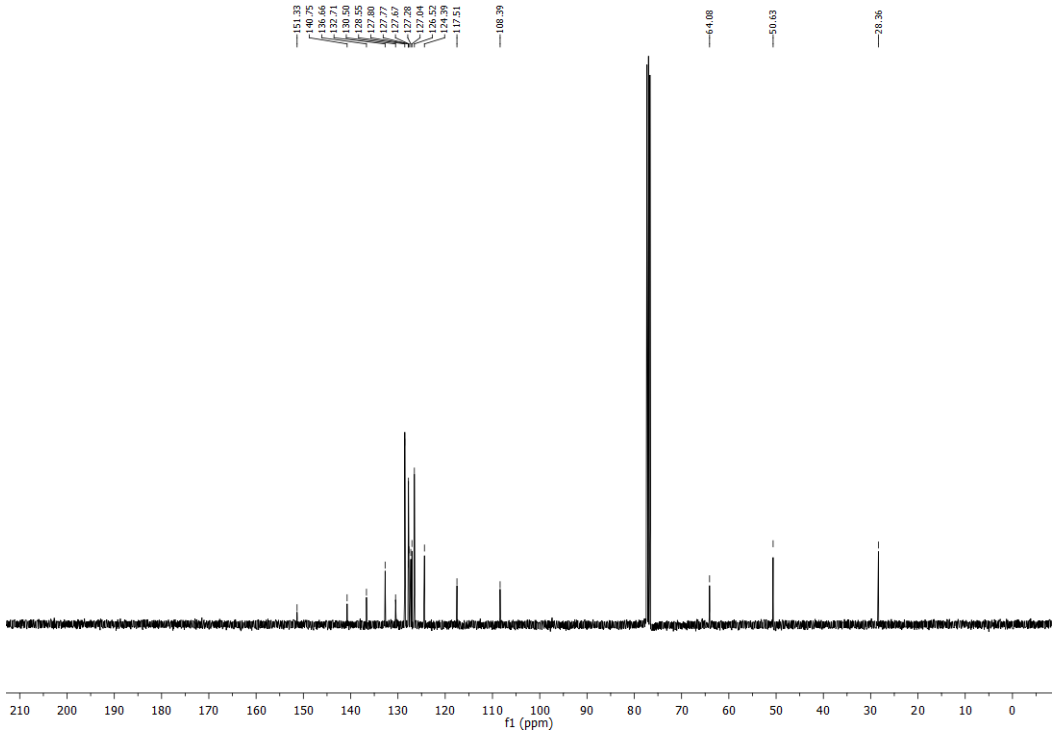


Figure S7. $^{13}C\{^{1}H\}$ NMR of 1-(1,3-diphenylallyl)indoline in $CDCl_3$

Enantiomeric excess determination of 1-(1,3-diphenylallyl)indoline.[1,2] Enantiomeric excess was determined by HPLC using Chiralcel OD-H column (98% hexane/2-propanol, flow 0.5 mL/min). t_R 16.0 min (*S*, minor); t_R 17.2 min (*R*, major). The preferential formation of the (*R*) enantiomer was further confirmed by comparing the optical rotation of the sample $[\alpha]_D^{24}$: –6.8 (c 1.97 in $CDCl_3$) with those found in the literature $[\alpha]_D^{25}$: –10.8 (c 3.32 in $CDCl_3$), 86%(*R*) ee[1] and $[\alpha]_D^{23}$: +7.08 (c 2.36 in $CDCl_3$), 87%(*S*) ee[2].

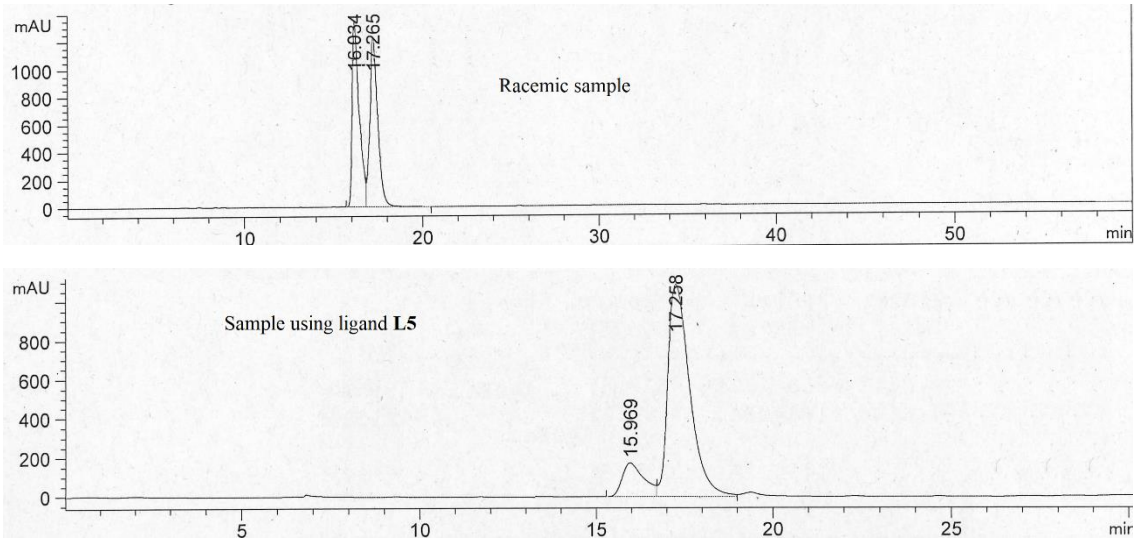


Figure S8: Traces for chiral HPLC separation of 1-(1,3-diphenylallyl)indoline formed in a reaction catalyzed by **L5**

Experimental details for Pd-catalyzed amination of (*rac*)-1,3-diphenylallyl acetate with benzylamine using phosphite-oxazole ligands L7–L16.

Typical procedure. A degassed solution of $[PdCl(\eta^3\text{-}C_3H_5)]_2$ (0.9 mg, 0.0025 mmol) and the corresponding ligand (0.0055 mmol) in dichloromethane (0.5 mL) was stirred for 30 min. Subsequently, a solution of the corresponding (*rac*)-1,3-diphenylallyl acetate (0.5 mmol, 126.1 mg) in dichloromethane (1.5 mL) and benzylamine (131 μL, 1.5 mmol) were added. The reaction mixture was stirred at room temperature. After the desired reaction time, the reaction mixture was diluted with Et_2O (5 mL) and saturated NH_4Cl (aq) (25 mL) was added. The mixture was extracted with Et_2O (3 x 10 mL) and the extract dried over $MgSO_4$. Solvent was removed the product was purified by column chromatography (hexane/EtOAc 3:1). Enantiomeric excesses were measured by HPLC and the results are shown in Table S5

Enantiomeric excess determination of *N*-benzyl-1,3-diphenylprop-2-en-1-amine.[3] Enantiomeric excess was determined by HPLC using Chiralcel OD-H column (99% hexane/2-propanol, flow 0.5 mL/min). t_R 27.2 min (*R*); t_R 31.8 min (*S*), see Fig. S8. The preferential formation of the (*S*) enantiomer was further confirmed by comparing the optical rotation of the sample with 84% ee ($[\alpha]_D^{23}$: +15.4 (c 0.87 in $CDCl_3$)) with that found in the literature $[\alpha]_D^{23}$: +16.4 (c 0.85 in $CDCl_3$), 95%(*S*) ee.

Characterization of *N*-benzyl-1,3-diphenylprop-2-en-1-amine.[4] ^{1}H NMR ($CDCl_3$, 400 MHz), δ: 3.70 (m, 2H), 4.31 (dd, 1H, *J*= 7.6, 3.6 Hz), 6.24 (m, 1H), 6.49 (dd, 1H, *J*= 16, 3.6 Hz), 7.10-7.36 (m, 15H). ^{13}C NMR ($CDCl_3$), δ: 51.4, 64.6, 126.5, 127.0, 127.3, 127.4, 127.5, 128.2, 128.5, 128.6, 128.7, 130.5, 132.6, 137.0, 140.3, 142.8. HRMS (ESI+): m/z calcd. for $C_{22}H_{22}N$ $[M+H]^+$: 300.1747, found: 300.1746.

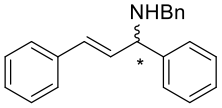
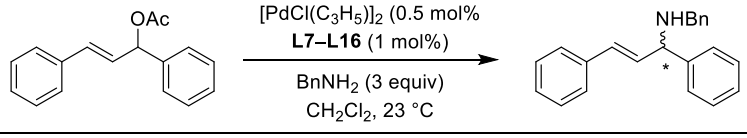
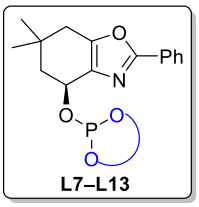
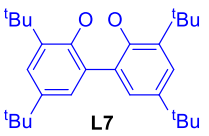
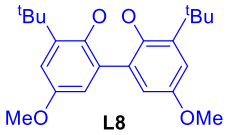
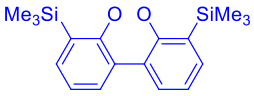
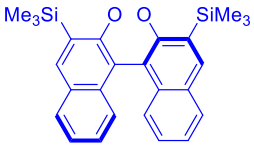
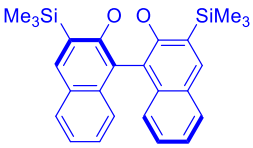


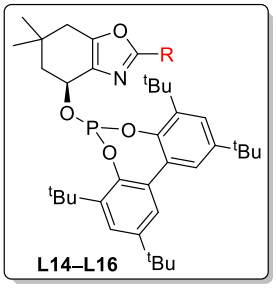
Table S5. Enantiomeric excesses attained in the allylic amination using ligands **L7–L16**.





	% ee
 **L7**	84 (*S*)
 **L8**	80 (*S*)
 **L9**	69 (*S*)
 **L10** $(S)^{ax}$	71 (*S*)

	% ee
 **L11** $(R)^{ax}$	41 (*S*)
 **L12** $(S)^{ax}$	7 (*S*)
 **L13** $(R)^{ax}$	5 (*R*)



Ligand	R	% ee
L14	4-Me-C_6H_4	32 (*S*)
L15	4-CF_3-C_6H_4	82 (*S*)
L16	^{t}Bu	25 (*S*)

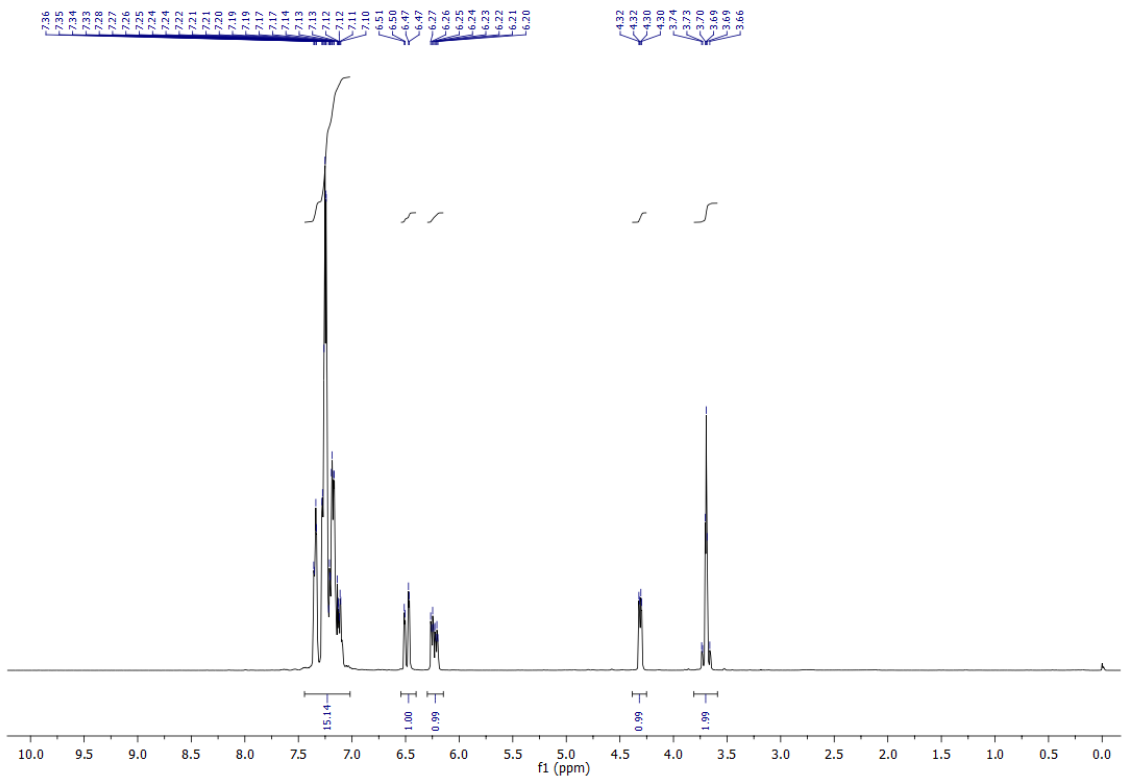


Figure S9. ^{1}H NMR of *N*-benzyl-1,3-diphenylprop-2-en-1-amine in $CDCl_3$.

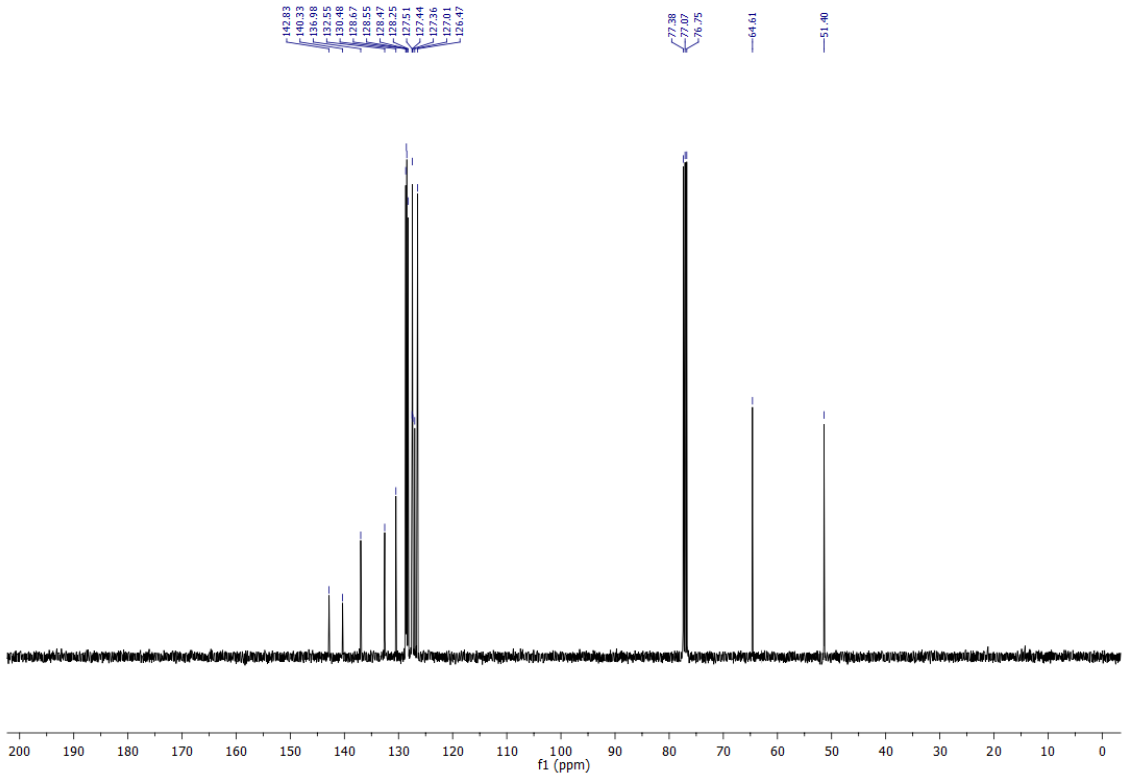


Figure S10. ^{13}C{^{1}H} NMR of *N*-benzyl-1,3-diphenylprop-2-en-1-amine in $CDCl_3$

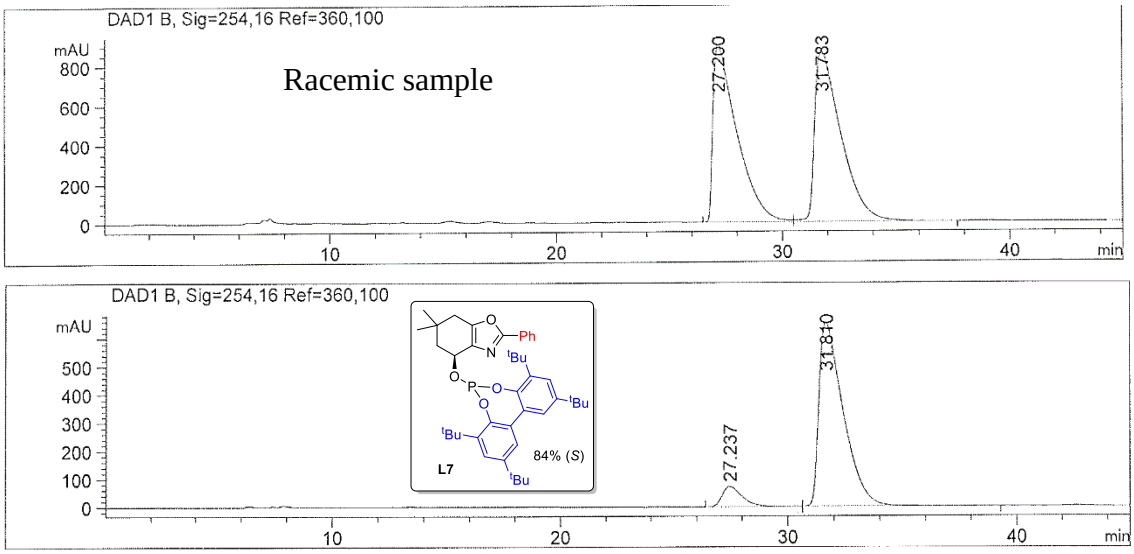


Figure S11: Traces for chiral HPLC separation of *N*-benzyl-1,3-diphenylprop-2-en-1-amine formed in a reaction catalyzed by L7

References

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