

## Supporting Information

### Homogeneous catalyst modifier for alkyne semi-hydrogenation: systematic screening in an automated flow reactor and computational study on mechanisms

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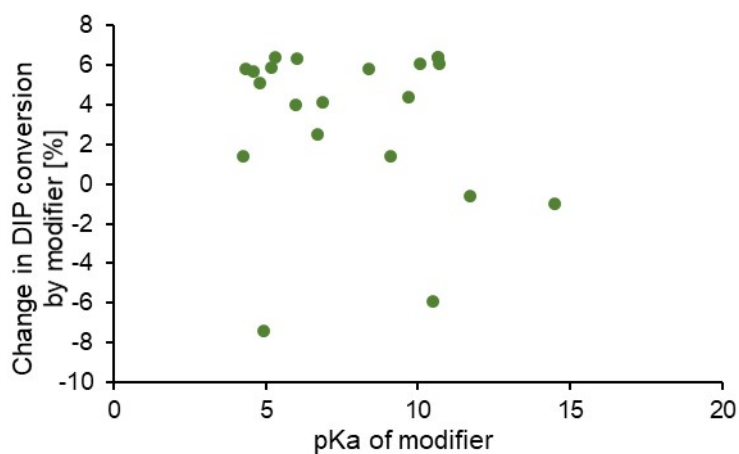


Figure S1. Change in DIP conversion at 3 mL/min and pKa value of modifiers

**Table S1.** List of conversion and selectivity with the liquid flow rate of 3 mL/min

Catalyst Modifier	MBY, Pd/C		MBY, Pd/ZnO		DLL, Pd/ZnO		DIP, Pd/ZnO	
	Conversion, -	Selectivity, -	Conversion, -	Selectivity, -	Conversion, -	Selectivity, -	Conversion, -	Selectivity, -
None	0.933	0.862	0.931	0.944	0.949	0.786	0.839	0.717
Quinoline	0.934	0.937	0.951	0.956	0.940	0.926	0.765	0.896
Pyridine	0.953	0.936	0.959	0.880	0.959	0.808	0.898	0.805
2,2'-bipyridine	0.959	0.949	0.962	0.947	0.951	0.909	0.897	0.882
1,10-phenanthroline	0.952	0.970	0.959	0.966	0.920	0.962	0.853	0.949
4,4'-bipyridine	0.946	0.956	0.964	0.940	0.943	0.913	0.890	0.886
2-phenylpyridine	0.949	0.944	0.958	0.945	0.950	0.901	0.903	0.830
2-methylpyridine	0.959	0.917	0.960	0.891	0.947	0.781	0.879	0.768
4-methylpyridine	0.963	0.912	0.959	0.899	0.964	0.798	0.902	0.792
2,4,6-trimethylpyridine	0.961	0.896	0.954	0.883	0.913	0.739	0.864	0.691
2-aminopyridine	0.924	0.857	0.930	0.848	0.959	0.822	0.880	0.862
2-hydroxypyridine	0.960	0.916	0.901	0.838	0.959	0.822	0.833	0.758
4-(dimethylamino)pyridine	0.927	0.858	0.971	0.906	0.963	0.840	0.883	0.817
imidazole	0.898	0.830	0.974	0.912	0.952	0.847	0.829	0.850
N-methylpiperidine	0.751	0.899	0.963	0.911	0.935	0.785	0.900	0.758
1-methylpiperazine	0.932	0.899	0.960	0.913	0.949	0.800	0.853	0.893
morpholine	0.940	0.872	0.962	0.894	0.928	0.799	0.897	0.818
N-methylcyclohexylamine	0.946	0.930	0.957	0.913	0.953	0.717	0.780	0.705
cyclohexylamine	0.953	0.936	0.964	0.888	0.948	0.786	0.903	0.750
hexylamine	0.891	0.731	0.958	0.891	0.941	0.788	0.903	0.781
propylamine	0.834	0.838	0.967	0.890	0.941	0.772	0.900	0.810
aniline	0.941	0.905	0.969	0.918	0.943	0.799	0.896	0.823

**Table S2.** List of conversion and selectivity with the liquid flow rate of 4 mL/min

Catalyst Modifier	MBY, Pd/C		MBY, Pd/ZnO		DLL, Pd/ZnO		DIP, Pd/ZnO	
	Conversion, -	Selectivity, -	Conversion, -	Selectivity, -	Conversion, -	Selectivity, -	Conversion, -	Selectivity, -
None	0.841	0.899	0.931	0.944	0.873	0.847	0.734	0.775
Quinoline	0.809	0.953	0.904	0.962	0.809	0.947	0.672	0.925
Pyridine	0.843	0.962	0.935	0.895	0.888	0.892	0.791	0.879
2,2'-bipyridine	0.852	0.971	0.874	0.969	0.833	0.959	0.785	0.925
1,10-phenanthroline	0.84	0.977	0.847	0.977	0.784	0.971	0.719	0.957
4,4'-bipyridine	0.825	0.971	0.867	0.971	0.816	0.959	0.766	0.921
2-phenylpyridine	0.832	0.967	0.85	0.971	0.831	0.958	0.688	0.916
2-methylpyridine	0.864	0.951	0.924	0.911	0.878	0.854	0.771	0.838
4-methylpyridine	0.873	0.954	0.939	0.908	0.888	0.896	0.79	0.873
2,4,6-trimethylpyridine	0.867	0.938	0.936	0.895	0.871	0.881	0.734	0.746
2-aminopyridine	0.843	0.908	0.911	0.901	0.835	0.955	0.775	0.909
2-hydroxypyridine	0.857	0.96	0.855	0.8	0.889	0.895	0.729	0.827
4-(dimethylamino)pyridine	0.846	0.906	0.938	0.923	0.886	0.933	0.777	0.865
imidazole	0.836	0.903	0.931	0.941	0.858	0.933	0.696	0.885
N-methylpiperidine	0.856	0.895	0.943	0.924	0.879	0.859	0.787	0.845
1-methylpiperazine	0.838	0.923	0.931	0.932	0.878	0.883	0.797	0.891
morpholine	0.84	0.921	0.945	0.907	0.876	0.891	0.796	0.889
N-methylcyclohexylamine	0.833	0.957	0.931	0.921	0.888	0.867	0.693	0.814
cyclohexylamine	0.84	0.963	0.94	0.901	0.889	0.883	0.8	0.84
hexylamine	0.808	0.917	0.933	0.88	0.861	0.858	0.77	0.847
propylamine	0.84	0.878	0.937	0.913	0.893	0.876	0.806	0.879
aniline	0.818	0.93	0.939	0.922	0.875	0.889	0.795	0.889

**Table S3.** List of conversion and selectivity with the liquid flow rate of 5 mL/min

Catalyst Modifier	MBY, Pd/C		MBY, Pd/ZnO		DLL, Pd/ZnO		DIP, Pd/ZnO	
	Conversion, -	Selectivity, -	Conversion, -	Selectivity, -	Conversion, -	Selectivity, -	Conversion, -	Selectivity, -
None	0.703	0.896	0.819	0.969	0.779	0.896	0.651	0.768
Quinoline	0.704	0.95	0.778	0.975	0.714	0.926	0.611	0.909
Pyridine	0.744	0.966	0.844	0.97	0.807	0.909	0.7	0.883
2,2'-bipyridine	0.742	0.972	0.737	0.974	0.727	0.954	0.694	0.929
1,10-phenanthroline	0.715	0.978	0.728	0.978	0.674	0.966	0.646	0.957
4,4'-bipyridine	0.705	0.971	0.748	0.971	0.718	0.954	0.672	0.926
2-phenylpyridine	0.71	0.969	0.73	0.972	0.717	0.952	0.696	0.914
2-methylpyridine	0.753	0.959	0.833	0.956	0.79	0.897	0.683	0.851
4-methylpyridine	0.754	0.962	0.768	0.959	0.808	0.911	0.699	0.878
2,4,6-trimethylpyridine	0.741	0.951	0.845	0.946	0.756	0.905	0.643	0.773
2-aminopyridine	0.75	0.93	0.817	0.967	0.687	0.889	0.695	0.903
2-hydroxypyridine	0.755	0.962	0.729	0.937	0.792	0.911	0.652	0.837
4-(dimethylamino)pyridine	0.757	0.915	0.832	0.968	0.782	0.954	0.682	0.866
imidazole	0.724	0.892	0.83	0.967	0.762	0.929	0.62	0.887
N-methylpiperidine	0.941	0.864	0.851	0.963	0.783	0.888	0.69	0.857
1-methylpiperazine	0.729	0.92	0.829	0.931	0.792	0.905	0.705	0.901
morpholine	0.736	0.921	0.852	0.955	0.784	0.907	0.713	0.891
N-methylcyclohexylamine	0.717	0.962	0.812	0.963	0.809	0.892	0.66	0.809
cyclohexylamine	0.724	0.967	0.837	0.96	0.796	0.901	0.719	0.844
hexylamine	0.719	0.914	0.851	0.952	0.776	0.881	0.7	0.846
propylamine	0.735	0.918	0.834	0.961	0.799	0.911	0.721	0.872
aniline	0.732	0.934	0.84	0.965	0.781	0.92	0.694	0.901

**Table S4.** List of conversion and selectivity with the liquid flow rate of 6 mL/min

Catalyst Modifier	MBY, Pd/C		MBY, Pd/ZnO		DLL, Pd/ZnO		DIP, Pd/ZnO	
	Conversion, -	Selectivity, -	Conversion, -	Selectivity, -	Conversion, -	Selectivity, -	Conversion, -	Selectivity, -
None	0.640	0.906	0.728	0.968	0.687	0.904	0.601	0.789
Quinoline	0.622	0.958	0.689	0.974	0.627	0.944	0.559	0.918
Pyridine	0.643	0.966	0.776	0.960	0.717	0.932	0.606	0.884
2,2'-bipyridine	0.640	0.968	0.659	0.974	0.624	0.943	0.610	0.923
1,10-phenanthroline	0.639	0.976	0.651	0.978	0.584	0.966	0.575	0.954
4,4'-bipyridine	0.609	0.968	0.672	0.966	0.622	0.938	0.599	0.917
2-phenylpyridine	0.628	0.967	0.635	0.971	0.625	0.934	0.653	0.760
2-methylpyridine	0.651	0.951	0.730	0.945	0.709	0.916	0.603	0.851
4-methylpyridine	0.653	0.962	0.739	0.966	0.692	0.922	0.613	0.874
2,4,6-trimethylpyridine	0.643	0.947	0.765	0.954	0.698	0.898	0.606	0.777
2-aminopyridine	0.669	0.938	0.754	0.964	0.667	0.857	0.603	0.905
2-hydroxypyridine	0.723	0.912	0.761	0.956	0.608	0.940	0.607	0.862
4-(dimethylamino)pyridine	0.746	0.919	0.735	0.970	0.647	0.938	0.623	0.893
imidazole	0.720	0.693	0.748	0.967	0.553	0.908	0.586	0.881
N-methylpiperidine	0.729	0.922	0.777	0.965	0.705	0.908	0.606	0.849
1-methylpiperazine	0.646	0.941	0.756	0.969	0.691	0.920	0.665	0.884
morpholine	0.670	0.935	0.774	0.958	0.695	0.931	0.654	0.885
N-methylcyclohexylamine	0.617	0.959	0.740	0.960	0.714	0.869	0.606	0.855
cyclohexylamine	0.608	0.964	0.750	0.947	0.702	0.925	0.643	0.879
hexylamine	0.800	0.930	0.781	0.963	0.680	0.895	0.642	0.858
propylamine	0.850	0.870	0.749	0.968	0.725	0.928	0.630	0.887
aniline	0.651	0.939	0.747	0.963	0.705	0.922	0.609	0.893