### **Supporting Information**

for

# Evaluation of a commercial packed bed flow hydrogenator for reaction screening, optimization, and synthesis

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#### Experimental queues and alternating Pd/quartz results

# Evaluation of a Commercial Packed Bed Flow Hydrogenator for Reaction Screening, Optimization, and Synthesis Supplemental Information

## Appendix A

		Experiment # in		Flow rate	Temperature	Pressure	
Entry	Queue date	queue	H2 mode	(mL/min)	(°C)	setting (bar)	Status
1	6/7/2010	1	full	1	60		Collected
		2	controlled	1	60	60	Collected with Error (instability detected)
		3	controlled	1	60	60	Collected
2	6/25/2010	1	controlled	0.5	60	60	Collected with Error (instability detected)
		2	controlled	1	60	60	Collected
3	9/22/2010	1	full	1	30		Collected
		2	full	1	30		Collected
		3	full	1	30		Collected
		4	controlled	1	30	100	Collected with Error (instability detected)
4	9/22/2010	1	full	1	30		Collected
		2	full	1	30		Collected
		3	full	1	30		Collected
		4	full	1	30		Collected
		5	controlled	1	30	10	Collected
		6	controlled	1	30	10	Collected
		/	controlled	1	30	10	Collected
		8	controlled	1	30	10	Collected
		9	controlled	1	30	10	Collected
		10	controlled	1	30	30	Collected
		11	controlled	1	30	30	Collected
		12	controlled	1	30	30	Collected
		13	controlled	1	30	30	Collected
		14	controlled	1	30	50 60	Collected
		16	controlled	1	30	60	Collected
		10	controlled	1	30	60	Collected
		18	controlled	1	30	60	Collected
		19	controlled	1	30	60	Collected
		20	controlled	1	30	80	Collected with Error (instability detected)
		21	controlled	1	30	80	Collected
		22	controlled	1	30	80	Collected
		23	controlled	1	30	80	Collected
		24	controlled	1	30	80	Collected
		25	controlled	1	30	100	Collected
		26	controlled	1	30	100	Collected
		27	controlled	1	30	100	Collected
		28	controlled	1	30	100	Collected
5	9/27/2010	1	controlled	1	30	10	Collected
		2	controlled	1	30	10	Collected
		3	controlled	1	30	10	Collected
		4	controlled	1	30	80	Collected with Error (instability detected)
		5	controlled	1	30	80	Collected
		6	controlled	1	30	80	Collected with Error (instability detected)
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6	9/27/2010		controlled	1	30	10	Collected with Error (instability detected)
		2	controlled	1	30	10	Collected
		3	controlled		30	80	Collected with Error (instability detected)
		4	controlled		30	80	Collected with Error (Instability detected)
~	A/15/2011	4	f II	1	20		Collected
/	4/15/2011		run	1	30	60	Collected with Error (instability data stad)
		2	controlled	1	30	60	Collected with Error (Instability detected)
		<u> </u>	controlled	1 1	30	60	Collected
	1		leoneoneu	_ <u> </u>	1 30	00	

Experimental queues for which an "instability detected" status was recorded by the auto sampler software during the run.

### Appendix B

Full data set for conversion of styrene to ethylbenzene over sequential reactions alternating 10% Pd/C with quartz on the AutoH<sup>3</sup> system.<sup>a</sup>



<sup>a</sup>All reactions were performed at a flow rate of 1.0 mL/min, temperature 30 °C, 0.5 M styrene in MeOH, 1 mL injection per reaction, run in order 1 through 6, then repeated in order 1 through 6. <sup>b</sup>Conversion based on GC-MS analysis using decane as an internal standard. <sup>c</sup>Data represented in blue correspond to reactions performed through a 30 mm 10% Pd/C CatCart<sup>™</sup>. <sup>d</sup>Data represented in red correspond to reactions performed through 30 mm quartz CatCart<sup>™</sup>.