

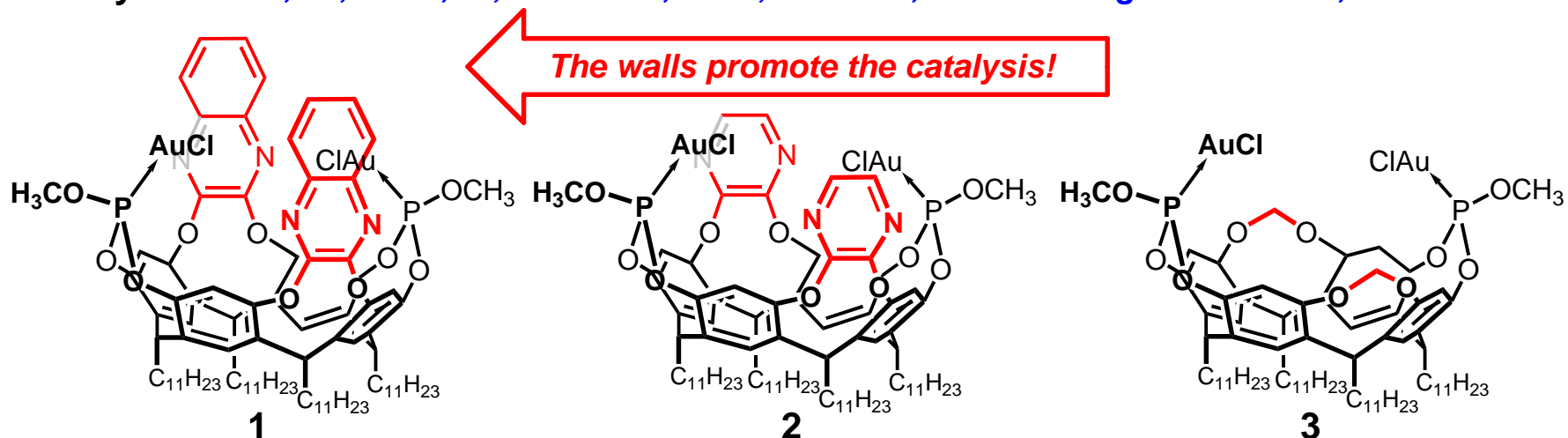


# Evaluation of Reactivity of Metallo-catalytic Cavities in the Dimerization of Terminal Alkynes

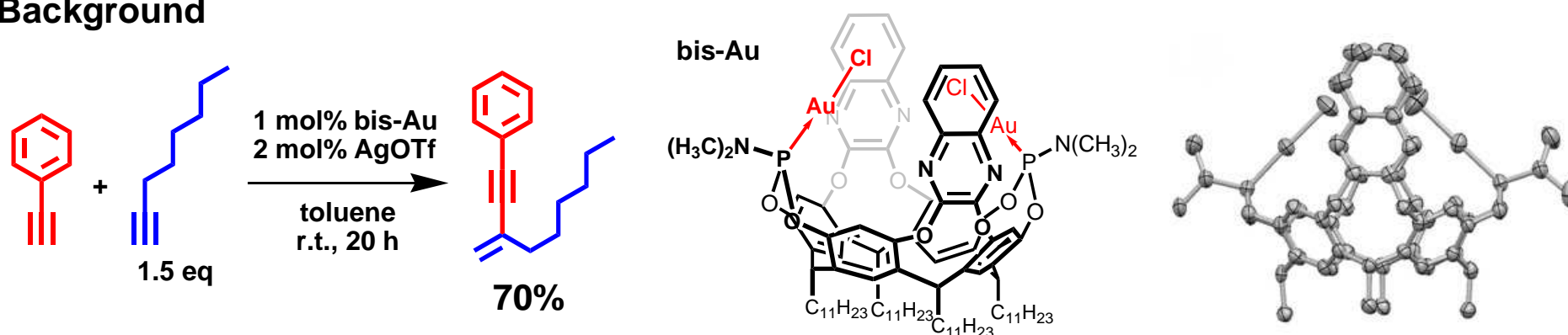
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## 1. Summary Kanaura, M.; Endo, N.; Schramm, M. P.; Iwasawa, T. *Eur. J. Org. Chem.* 2016, 4970-4975.



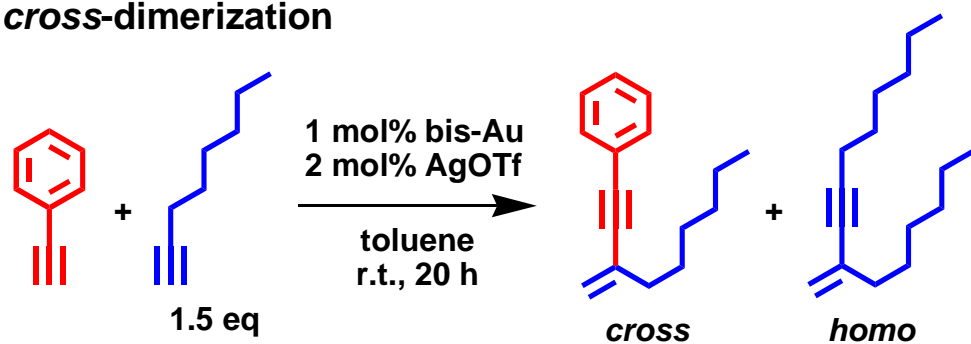
## 2. Background



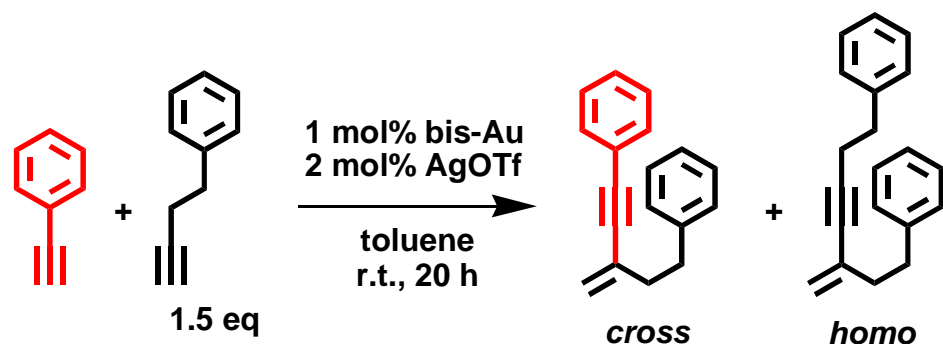
Endo, N.; Kanaura, M.; Schramm, M. P.; Iwasawa, T. *Eur. J. Org. Chem.* 2016, 2514-2521.

## 3. Comparison between 1, 2, and 3 in the dimerization reactions

### a) cross-dimerization

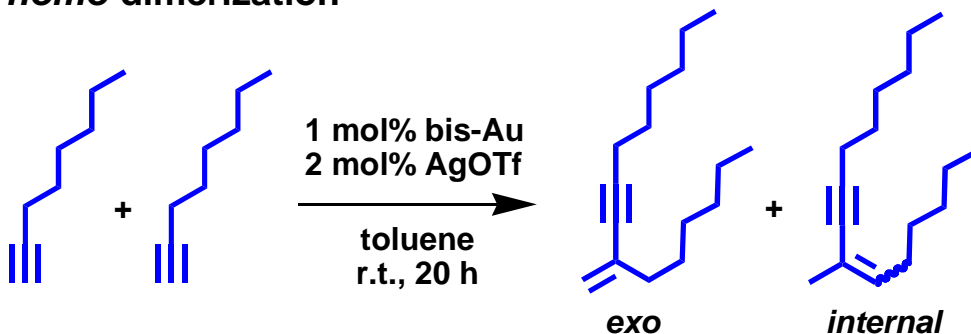


bis-Au	Yield (%) of cross	Molar ratios cross/homo
1	58	3.0/1
2	6	4.3/1
3	0	-

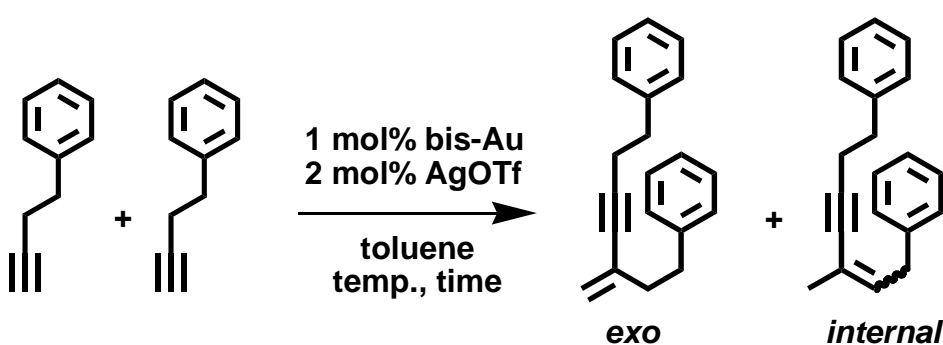


bis-Au	Yield (%) of cross	Molar ratios cross/homo
1	57	3.1/1
2	9	3.0/1
3	0	-

### b) homo-dimerization



bis-Au	Yield (%) of exo	Molar ratios exo/internal
1	63	~100/0
2	18	97/3
3	trace	>99/1



bis-Au	Temp./°C	Time/h	Yield (%) of exo	Molar ratios exo/internal
1	r.t.	20	65	94:6
	75	2	67	48:52
	110	2	40	2:98
2	r.t.	22	14	88:12
	75	22	28	16:84
	110	16	11	6:94
3	r.t.	18	trace	>99:1
	75	18	18	95:5
	110	16	12	51:49