Supplementary Information

Selective formation of α, ω -ester amides from the aminocarbonylation of castor oil derived methyl 10-undecenoate and other unsaturated substrates

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1. Attempted aminocarbonylation of acrylate esters.



Scheme S1, Possible products from the aminocarbonylation of acrylate esters using aniline as the amine. R = H, R' = Me or Bu; R = Me, R' = Me.

Table S1	Products	from th	e aminocarbon	vlation c	of methy	l acryla	te with	anilinea
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Entry	T / °C	t / h	Conversion / %	Linear / %	Michael / %
1	85	3	27	1	22
2	115	3	45	0	45
3	70	16	52	4	41
4	85	16	75	7	54
5	115	16	87	0	82
6	85	64	93	9	69
7^{b}	100	6	100	55	30.5
8 ^c	100	6	60	47	4

^{*a*} Conditions: methyl acrylate (1.14 mL, 12.7 mmol), aniline (1.16 mL, 12.7 mmol), $[Pd_2(dba)_3]$ (114 mg, 0.0125 mmol), DTBPMB (251 mg, 0.0637 mmol), 1,4–dioxane (10 mL), MSA (10 μ L), 2–naphthol (1368 mg, 9.5 mmol), KI (10 mg, 0.064 mmol), $p_{CO} = 30$ bar,^{*b*} butyl acrylate(6 mmoles), aniline (11 mmol), $[PdCl_2]$ (32 mg, 0.2 mmoles), DTBPMB (98 mg, 0.25 mmoles), diethyl ether (10 ml), branched ester amide (14 %) and a trace of *N*-methylsuccinimide are also present. Conversions and selectivities were measured by GC FID using calculated¹ response factors and an internal standard and by GCMS ^{*c*} methyl methacrylate (6 mmol), conditions as for butyl acrylate, 1-phenyl – 3-methylsuccinimide (9 %) is also observed

2. Representative GC data

2.1 Aminocarbonylation of alkenes in the presence of 2-naphthol and NaI Response_



Fig. S1 Typical GC-FID trace from aminocarbonylation of 1-octene in the presence of 2naphthol and NaI. Conditions as in Table 2, entry 3. Note that almost no 1- octene remains.





Fig. S2 GCMS of products from the aminocarbonylation of ethyl-3-hexenoate with aniline at at 140°C for 65 h



2.3 Aminocarbonylation of methyl 10-undecenoate with aniline

Fig. S3 GCMS of crude product from the aminocarbonylation of methyl 10-undecenoate with aniline under the conditions of Table 5, entry 5



Fig. S4 ¹³C NMR spectrum of isolated methyl 12-oxo-12-(phenylamino)dodecanoate (21) from the aminocarbonylation of methyl-10-undecenoate with aniline under the conditions of Table 5, entry 5

2.4 Synthesis of N-phenylpyrrolidine from THF.



Fig. S5 GCMS of the products from reaction of THF with aniline; conditions as Table 6, Entry **1**)



Fig. S6 GCMS of the products from reaction of THF with aniline; conditions as Table 6, Entry **2**)

2.5 Synthesis of N-phenylpyrrolidone from γ-butyrolactone



Fig. S7 GCMS of the products from reaction of γ -butyrolactone with aniline; conditions as Table 6, Entry **6**)

1. J. C. Sternberg, D. T. Gallaway and L. Jones, in *Gas Chromatography*, eds. N. Brenner, N. S. Gallaway, J. E. Callen and D. Weiss, Academic Press, New York, 1962, pp. 231.