Surprisingly Mild “Enolate-Counterion-free” Pd(0)-Catalyzed Intramolecular Allylic Alkylations

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Supporting Information

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General Remarks: Dichloromethane and triethylamine were distilled from CaH₂. All other reagents and solvents were used without further purification. ¹H NMR (400 MHz) and ¹³C NMR (100 MHz) were recorded on a Bruker ARX-400 spectrometer using the residual peak of chloroform-*d* as internal standard. IR spectra were recorded on a Bruker Tensor 27 (pike) instrument and only the strongest or structurally most important peaks are listed. Chromatographic purifications were conducted using 40-63 µm silica gel and analytical TLC was performed on Merck precoated silica 60-F₂₅₄ plates. Precursors of cyclization **1a**, **1c**, **1d**, **1e**, **1f**¹ and **3**² were prepared according to the literature. Cyclized products **2a**, **2c**, **2d**, **2e**, **2f**¹ and **4**² have already described.

(Z)-[para-Methoxybenzyl(malonyl)amino]-but-2-enyl acetate 1b :

To a solution of 2-butene-1,4-diol monoacetate¹ (6.15 g, 47.3 mmol.) in dry CH₃CN (200 ml) were added PPh₃ (18.6 g, 71 mmol.) and CCl₄ (13.7 ml, 142 mmol.), and the mixture was stirred at reflux for 2h. The CH₃CN was removed in vacuo and 200 ml of diethyl ether were added. The crude product was filtered and the liquid phase was evaporated. This operation was repeated four times to eliminate most of triphenylphosphine oxide. The resulting crude monoacetate monochloride (6.50 g, 43.8 mmol.) was dissolved as such in dry CH₃CN (150 ml) and *para*-methoxy benzylamine (17.1 ml, 131 mmol.) was added. The mixture was stirred at reflux for 30 min, then filtered and the liquid phase was evaporated. The residue was purified by silica gel flash chromatography (cyclohexane: EtOAc = 1:1) to afford the resulting unstable amine (6.50 g, 26.1 mmol.) that was then immediately dissolved in dry CH₂Cl₂ (230 ml). Et₃N (5.8 ml, 41.7 mmol.), methyl-3-chloro-3-oxopropionate (4.2 ml, 39.1 mmol.), and 4-DMAP (200 mg, catalytic quantity) were added at 0°C and the mixture was stirred overnight at room temperature. The reaction was quenched by addition of a saturated aqueous NH₄Cl solution (100 ml), the organic phase was separated, and the aqueous phase was extracted with CH₂Cl₂ (3 x 150 ml). The combined extracts were dried with anhydrous

¹ Giambastiani, G.; Pacini, B.; Porcelloni, M.; Poli, G. *J. Org. Chem.* **1998**, 63, 804-807.

² Lemaire, S.; Giambastiani, G.; Prestat, G.; Poli, G. *Eur. J. Org. Chem.* **2004**, 2840-2847.

MgSO₄ and the solvent was removed in vacuo. The residue was purified by silica gel flash chromatography (cyclohexane: EtOAc, 8:2) to afford **1b** (6.50 g, 39% yield).

¹H NMR (CDCl₃, 400 MHz): δ 7.21 (50%, d, J = 8.6 Hz, 2H), 7.12 (50%, d, J = 8.6 Hz, 2H), 6.89 (50%, d, J = 8.6 Hz, 2H), 6.86 (50%, d, J = 8.6 Hz, 2H), (5.73-5.42 (m, 2H), 4.58-4.42 (m, 4H), 4.08 (50%, d, J = 6.6 Hz, 2H), 3.92 (50%, d, J = 6.1 Hz, 2H), 3.81 (50%, s, 3H), 3.80 (50%, s, 3H), 3.77 (50%, s, 3H), 3.74 (50%, s, 3H), 3.53 (50%, s, 2H), 3.51 (50%, s, 2H), 2.06 (50%, s, 3H), 2.03 (50%, s, 3H).

¹³C NMR (CDCl₃, 100 MHz): δ 171.1 (s), 171.0 (s), 168.5 (s), 168.4 (s), 166.6 (s), 166.5 (s), 159.7 (s), 159.5 (s), 129.9 (d), 129.8 (d), 129.3 (d), 128.2 (d), 127.7 (d), 114.8 (d), 114.4 (d), 60.2 (t), 59.8 (t), 55.7 (q), 55.6 (q), 52.9 (q), 51.1 (t), 48.3 (t), 44.9 (t), 42.8 (t), 41.5 (t), 21.3 (q), 21.2 (q).

IR (neat): ν = 2950, 1735, 1645, 1510, 1435, 1230, 1160, 1030 cm⁻¹.

MS (CI - NH₃) m/z : 350 (MH⁺), 290, 121.

HRMS m/z calculated for C₁₈H₂₄NO₆ (MH⁺) 350.1604, found 350.1608.

General procedure for palladium-catalyzed intramolecular allylic allylations under phase transfer conditions :

To a solution of tetrabutyl ammonium bromide or tetrabutyl ammonium hydrogensulfate (10 mol%) in dichloromethane (500 μ L) were added allylpalladium chloride dimer (5 mol%) and dppe (12.5 mol%). The solution was stirred at room temperature for 5 min. Then, a solution of acyclic substrate **1a-c** (0.157 mmol. in 1.5 mL of dichloromethane), 1.5 mL of water and 50% KOH aqueous solution (0.314 mmol.) were successively added. The resulting biphasic system was stirred vigorously at room temperature for 2 h. A saturated aqueous NH₄Cl solution was added and the aqueous phase was extracted three times with Et₂O. The collected organic phases were washed with brine, dried over MgSO₄ and the solvent was removed in vacuo. The crude product was purified by flash chromatography.

General procedure for palladium-catalyzed intramolecular allylic allylations in the presence of 15-crown-5 :

To a solution of Pd(OAc)₂ (5 mol%) in dry DMF (500 μ L) under nitrogen atmosphere was added dppe (12.5 mol%). In a separate flask, to a solution of acyclic substrate **1a** (50 mg,

0.157 mmol.) in dry DMF (2 mL) at 0°C under nitrogen atmosphere were successively added 15-crown-5 (0.188 mmol. or 0.016 mmol.) and NaH (60% in oil, 0.173 mmol. or 0.016 mmol.). The resulting mixture was stirred at 0°C for 15 min and, after warming to room temperature added to the reaction vessel containing the catalytic system. The reaction was monitored by TLC. A saturated aqueous NH₄Cl solution was added and the aqueous phase was extracted three times with Et₂O. The collected organic phases were washed three times with brine, dried over MgSO₄ and the solvent was removed in vacuo. The crude product was purified by flash chromatography.

(3,4-*trans*)-1-(*para*-methoxybenzyl)-3-(methoxycarbonyl)-4-vinylpyrrolidin-2-one 2b :

Purification by silica gel flash chromatography (cyclohexane: EtOAc, 8:2) to afford the product as a yellow oil.

¹H NMR (CDCl₃, 400 MHz): δ 7.17 (d, J = 8.6 Hz, 2H), 6.86 (d, J = 8.6 Hz, 2H), 5.78-5.65 (m, 1H), 5.13 (d, J = 18.7 Hz, 1H), 5.09 (d, J = 11.1 Hz, 1H), 4.45-4.36 (m, 2H), 3.81 (s, 3H), 3.80 (s, 3H), 3.49-3.31 (m, 3H), 3.05-2.95 (m, 1H).

¹³C NMR (CDCl₃, 100 MHz): δ 170.2 (s), 169.2 (s), 159.6 (s), 136.6 (d), 129.9 (d), 128.2 (s), 117.7 (t), 114.4 (d), 55.6 (q), 54.7 (d), 53.1 (q), 50.2 (t), 46.5 (t), 40.8 (d).

IR (neat): ν = 2950, 1735, 1685, 1512, 1435, 1245, 1165 cm⁻¹.

MS (CI - NH₃) m/z : 290 (MH⁺), 232, 121.

HRMS m/z calculated for C₁₆H₂₀NO₄ (MH⁺) 290.1392, found 290.1394.

dm 114 - purif

Current Data Parameters
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PROCNO 1

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RG 43500
DM 41.000 us
DE 98.57 us
TE 300.0 K
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D1 2.00000000 se
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DL5 23.00 dB
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SFO1 50.3277408 MHz
NUCLEUS 13C

F2 - Processing parameters
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GB 0
PC 1.40

10 NMR plot parameters
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F2P -10.000 pp
F2 -503.23 Hz
PPMCM 10.00000 pp
HZCM 503.22708 Hz

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PROCNO 1

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1D NMR plot parameters
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F1P 230.000 pp
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F2P -10.000 pp
F2 -503.23 Hz
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dm115f1

Current Data Parameters
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PROCNO 1

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RG 45500
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DE 58.57 us
TE 300.0 K
D12 0.000200 se
DL6 23.00 dB
D1 2.00000000 se
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DL5 23.00 dB
P1 5.50 us
SFO1 50.3277408 MHz
NUCLEUS 13C

F2 - Processing parameters
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SF 50.327090 MHz
WDW EM
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LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 24.00 cm
F1P 230.000 pp
F1 11574.22 Hz
F2P -10.000 pp
F2 -503.23 Hz
PPHMM 10.00000 pp
HZCM 503.22708 Hz

55.62
54.71
54.14
53.05
50.18
46.62
46.47
40.79
40.21

78.30
77.66
77.02

136.61
134.07
129.90
129.77
129.44
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114.43
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Current Data Parameters
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FIDRES 0.186983 Hz
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RG 45500
DM 41.000 us
DE 98.57 us
TE 300.0 K
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P3 7.70 us
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P31 100.00 us

F2 - Processing parameters
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SF 50.3227090 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 23.50 cm
F1P 230.000 pp
F1 11574.22 Hz
F2P -10.000 pp
F2 -503.23 Hz
PPMCM 10.21277 pp
HZCM 513.93408 Hz

Transition state structures optimized at B3LYP/LACVP* using the continuum solvent model PB-SCRF with parameters for CH₂Cl₂ (epsout=9.08,radprb=2.33237). Energies are reported in Hartree, and include solvation.

Table 2, entry 1: *Syn*, *Exo*, *E*

E_{sol}: -1329.69267405154

H	-0.41033	-0.22289	0.23648
P	-0.11935	-0.05530	1.60865
P	2.63952	0.17307	4.16829
H	3.36874	-0.31192	5.28010
H	-1.41975	-0.25823	2.12184
H	-0.09996	1.35754	1.64460
H	1.88128	1.15101	4.85086
H	3.63534	1.03071	3.64672
Pd	1.61925	-1.33556	2.59016
C	1.34307	-3.03782	1.28877
C	2.07291	-3.55889	2.38641
C	3.40288	-3.20064	2.63803
C	5.01230	-5.08942	1.80526
H	0.32591	-3.38280	1.12146
H	1.87600	-2.70581	0.39804
H	3.95007	-2.61314	1.90741
C	6.01054	-4.34792	2.54704
O	7.20237	-4.20750	2.19673
C	5.18386	-5.32693	0.42718
O	4.43303	-5.99182	-0.32344
H	6.08182	-4.83939	-0.01042

C	4.12237	-3.57488	3.91975
H	3.98376	-2.78547	4.66920
H	3.65605	-4.47898	4.34621
H	4.19130	-5.57981	2.31790
H	1.56203	-4.19313	3.11013
N	5.55166	-3.72882	3.70655
C	6.47743	-3.12129	4.64788
H	6.35913	-3.54447	5.65468
H	7.48886	-3.31819	4.29173
H	6.33432	-2.03292	4.71045

Table 2, entry 2: *Syn*, *Exo*, *Z*

E_{sol}: -1329.68767891354

H	0.23448	0.61889	0.28740
P	-0.04134	0.04059	1.54680
P	2.45577	0.12809	4.34880
H	3.32893	-0.39429	5.33252
H	-1.26088	-0.59334	1.22334
H	-0.56776	1.18325	2.18997
H	1.52143	0.72916	5.22238
H	3.19901	1.28575	4.02430
Pd	1.66893	-1.26293	2.55369
C	1.49002	-2.89692	1.14205
C	2.17100	-3.44739	2.25699
C	3.48012	-3.06680	2.56838
C	4.96700	-5.20974	1.89730
H	0.48622	-3.24207	0.90950
H	2.06586	-2.52113	0.29617

H	4.05114	-2.49063	1.84348
C	6.02037	-4.42178	2.50517
O	7.20360	-4.36283	2.12288
C	4.96643	-5.68258	0.56863
O	5.76973	-5.45412	-0.36214
H	4.08654	-6.33596	0.34899
C	4.19998	-3.43380	3.85036
H	4.12546	-2.60613	4.56572
H	3.69476	-4.28959	4.32674
H	4.16157	-5.57015	2.52803
H	1.63872	-4.10829	2.93988
N	5.61522	-3.67104	3.61609
C	6.59097	-2.97843	4.44176
H	6.49774	-3.26555	5.49810
H	7.58270	-3.25133	4.08062
H	6.48288	-1.88608	4.37064

Table 2, entry 3: *Syn*, *Endo*, *E*

E_{sol}: -1329.66141674652

H	0.14273	-0.65103	0.06844
P	0.02033	0.01192	1.31252
P	3.91171	-0.15170	1.60022
H	3.88357	-0.85719	0.37452
H	-1.00057	-0.80843	1.84901
H	-0.81352	1.06644	0.87008

H	4.79817	-1.00658	2.29554
H	4.84990	0.83980	1.23180
Pd	1.95044	0.52870	2.70329
C	0.67848	1.21023	5.58371
C	1.53901	1.68610	4.62026
C	2.88483	1.17533	4.49944
C	2.24358	2.92035	7.13725
H	-0.27005	1.69789	5.79539
H	0.89368	0.29297	6.12618
H	3.06494	0.23075	5.02065
C	3.44930	2.13753	7.28730
O	3.74842	1.54441	8.34662
C	1.32627	3.04193	8.21044
O	0.32256	3.78706	8.24059
H	1.54290	2.38875	9.07876
N	4.36264	2.06584	6.20937
C	5.56577	1.26776	6.45104
H	5.87537	1.39679	7.48705
H	5.40256	0.19208	6.28164
H	6.36198	1.61084	5.78293
C	3.98270	2.18752	4.78417
H	4.89208	2.02074	4.20083
H	3.63827	3.20371	4.55917
H	2.11645	3.58330	6.28923
H	1.33784	2.68134	4.22279

Table 2, entry 4: *Syn*, *Endo*, *Z*

E_{sol}: -1329.65454030963

H	0.07260	0.02148	-0.08418
P	0.00539	-0.01514	1.32879
P	3.91034	-0.08051	1.52482
H	3.89879	-0.49862	0.17324
H	-0.62438	-1.27753	1.44304
H	-1.15993	0.77648	1.46769
H	4.77881	-1.07534	2.03066
H	4.86379	0.95538	1.39352
Pd	1.95290	0.43742	2.71614
C	0.69916	1.15416	5.64020
C	1.56465	1.56409	4.64971
C	2.89721	1.01800	4.53460
C	2.30514	2.88333	7.10484
H	-0.24762	1.65767	5.81881
H	0.89939	0.26127	6.22751
H	3.04785	0.06439	5.04913
C	3.46602	2.04749	7.33188
O	3.73336	1.50729	8.41994
C	1.34117	3.24035	8.08786
O	1.19909	2.82904	9.25331
H	0.61170	3.99248	7.70236
N	4.37614	1.86951	6.25692
C	5.52761	1.00706	6.52718

H	5.79837	1.09768	7.57770
H	5.31817	-0.05484	6.32397
H	6.36778	1.32153	5.89921
C	4.02822	1.98999	4.82398
H	4.94046	1.77523	4.26081
H	3.73243	3.01638	4.57814
H	2.25377	3.45957	6.18949
H	1.38727	2.55206	4.22238

Table 2, entry 5: *Anti, Exo, E*

E_{sol}: -1329.69068526416

H	0.70442	0.57453	-0.25006
P	0.24138	0.03402	0.97060
P	3.93661	-0.21206	1.86035
H	4.14744	0.00429	0.47989
H	-0.50815	-1.04288	0.44571
H	-0.82309	0.93221	1.20297
H	4.91863	-1.21135	2.04986
H	4.68299	0.88569	2.34632
Pd	1.71788	-0.48108	2.75760
C	0.16151	-0.85287	4.26593
C	1.40215	-0.77004	4.94095
C	2.40022	-1.75360	4.82549
C	2.42932	-3.20248	7.02475
H	-0.56072	-0.05169	4.39684
H	-0.25551	-1.81724	3.98203

H	3.40139	-1.49683	5.15359
C	3.38469	-4.00104	6.28606
O	4.38049	-4.56686	6.78626
C	2.77585	-2.66282	8.28018
O	2.03100	-2.01767	9.05333
H	3.83468	-2.83065	8.57248
N	3.15931	-4.07730	4.91395
C	3.90507	-5.00271	4.07732
H	3.23734	-5.70826	3.56392
H	4.49603	-4.47080	3.31858
H	4.58553	-5.55732	4.72357
C	2.21003	-3.16844	4.29513
H	1.16643	-3.48850	4.44140
H	2.38501	-3.19815	3.21183
H	1.39683	-3.13103	6.70081
H	1.66319	0.15080	5.45783

Table 2, entry 6: *Anti*, *Exo*, *Z*

E_{sol}: -1329.68394475154

H	0.44582	0.44452	-0.16325
P	0.12820	0.13006	1.17693
P	3.89015	-0.28544	1.63141
H	3.93352	-0.01298	0.24569
H	-0.89309	-0.81560	0.93502
H	-0.68728	1.24578	1.46805
H	4.78685	-1.37827	1.64451

H	4.79000	0.71649	2.05928
Pd	1.77922	-0.46283	2.77291
C	0.32521	-0.84654	4.36443
C	1.60175	-0.77797	4.97125
C	2.60017	-1.74585	4.78050
C	2.31118	-3.28614	6.98653
H	-0.38978	-0.05268	4.56258
H	-0.10696	-1.80677	4.08812
H	3.60522	-1.49176	5.10607
C	3.37395	-4.04449	6.35763
O	4.29743	-4.63684	6.94604
C	2.35437	-2.73573	8.28443
O	3.30512	-2.66942	9.09353
H	1.38036	-2.27674	8.58465
N	3.31561	-4.07571	4.95813
C	4.13768	-5.00022	4.19411
H	3.52444	-5.70935	3.61969
H	4.79573	-4.46781	3.49302
H	4.75650	-5.55241	4.90151
C	2.43890	-3.16163	4.24494
H	1.38396	-3.47258	4.28225
H	2.72722	-3.19701	3.18701
H	1.35216	-3.22862	6.48464
H	1.88730	0.13090	5.49729

Table 2, entry 7: *Anti*, *Endo*, *E*

E_{sol}: -1329.67270330206

H	-0.09862	-0.14970	0.20840
P	-0.07086	0.47066	1.47897
P	3.66752	-0.41830	1.48011
H	3.37792	-1.16957	0.31760
H	-1.04875	-0.33813	2.10376
H	-0.90599	1.56938	1.16889
H	4.39394	-1.41068	2.17807
H	4.76843	0.30836	0.97201
Pd	1.99660	0.79889	2.65720
C	0.91492	1.80128	4.83493
C	2.13014	2.26651	4.32369
C	3.29876	1.46749	4.34030
C	1.75563	2.20106	7.24322
H	0.02684	2.42500	4.79368
H	0.78232	0.79592	5.20891
H	4.22239	1.94767	4.02309
C	2.36695	0.91329	7.43494
O	1.90974	0.02722	8.17794
C	0.54246	2.53149	7.90760
O	0.01666	3.66099	7.96017
H	0.04046	1.67600	8.40391
N	3.62274	0.66934	6.74301
C	4.41003	-0.37060	7.42936
H	4.49837	-0.11597	8.48870
H	3.96468	-1.37366	7.35997
H	5.41275	-0.39532	6.98992
C	3.46772	0.30066	5.29812
H	2.65091	-0.43020	5.19180
H	4.38375	-0.22542	5.01828
H	2.33984	3.00553	6.81335
H	2.17576	3.28270	3.93704

Table 2, entry 8: *Anti*, *Endo*, *Z*

E_{sol}: -1329.66750523156

H	0.01108	-0.18316	0.13602
P	-0.02863	0.03111	1.53527
P	3.78815	0.02425	1.39365
H	3.66877	-0.90258	0.33200
H	-0.54285	-1.23730	1.90328
H	-1.24675	0.75250	1.58319
H	4.91684	-0.54831	2.02370
H	4.45893	1.04727	0.68549
Pd	1.94105	0.72596	2.71680
C	0.74929	1.46248	4.96170
C	1.87552	2.11455	4.45246
C	3.14827	1.49694	4.42550
C	1.66461	1.89245	7.35855
H	-0.22180	1.94874	4.94387
H	0.76803	0.44199	5.31749
H	3.98921	2.12384	4.13626
C	2.39502	0.65790	7.50866
O	2.07056	-0.27330	8.25678
C	0.44355	2.20670	8.02072
O	-0.30839	1.46523	8.67801
H	0.14815	3.27466	7.88634
N	3.64010	0.55250	6.76203
C	4.51839	-0.48093	7.33897
H	4.61200	-0.31807	8.41457
H	4.14556	-1.50442	7.18623
H	5.50883	-0.39329	6.88077

C	3.49013	0.29678	5.29290
H	2.77043	-0.52299	5.13781
H	4.45710	-0.08296	4.95368
H	2.18513	2.72574	6.90410
H	1.76631	3.14041	4.10607