Supporting information

Hydroesterification of styrene derivatives catalyzed by an acidic resin supporting Palladium complexes

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Table S1. The physical properties of supports.

Entries	Samples	BET surface area /m^2g^{-1}	Mean pore diameter /nm	Pore volume /cm^3g^{-1}
1	LSI-600	42.4	19.1	0.17
2	LSCA-10	15.5	17.1	0.07
3	LSCA-30	15.7	17.0	0.11
4	CT-450	12.8	17.2	0.13
5	Amberlyst 15	44.5	40.0	0.36
6	Amberlist IR 120	0.8	-	<0.001
7	Silica gel	337.8	32.9	0.91
8	MCM-41	800	3.5	0.70
9	Quartz	1.2	-	<0.003

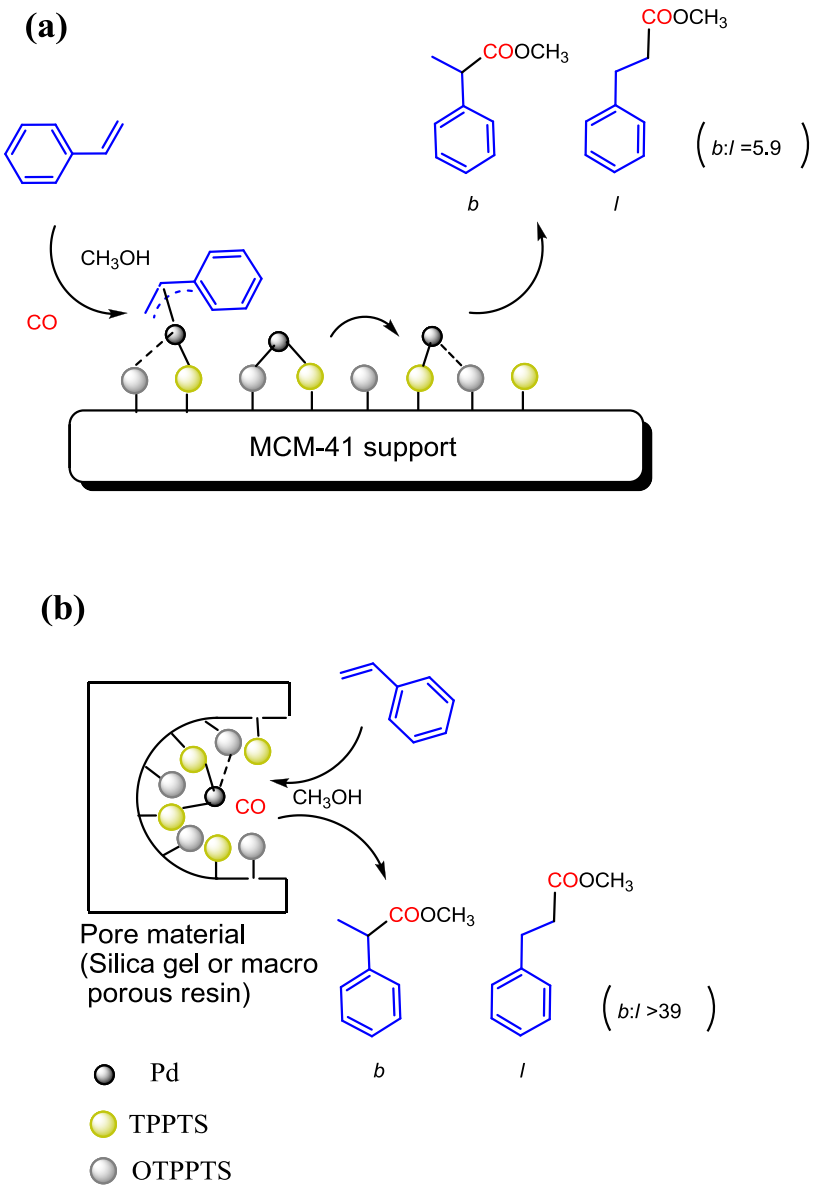


Figure S1. The steric confinement effect of the supports: (a) MCM-41 as the support (MCM-41 with an average pore size of 3.5 nm); (b) Silica gel and macro porous resins with an average pore size of 15-33 nm as support.

Nitrogen adsorption isotherms of resins and the Pd-P-OP/Resin catalyst.

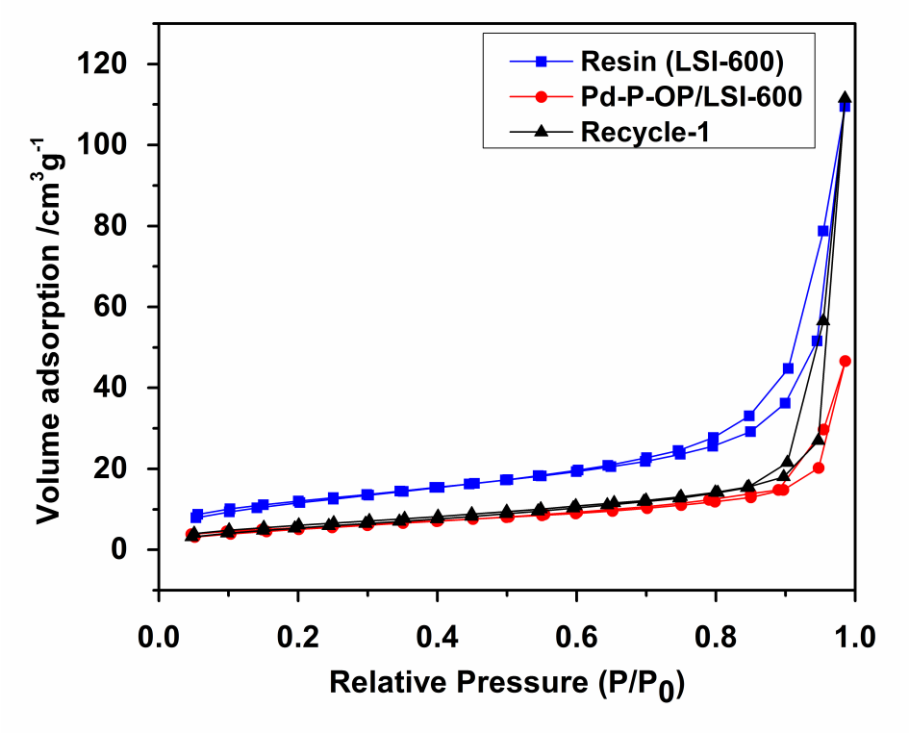


Figure S2. N_2 sorption isotherms of (■) LSI-600 resin, (●) fresh Pd-P-OP/LSI-600 catalyst and (▲) the third recycled Pd-P-OP/LSI-600 catalyst.

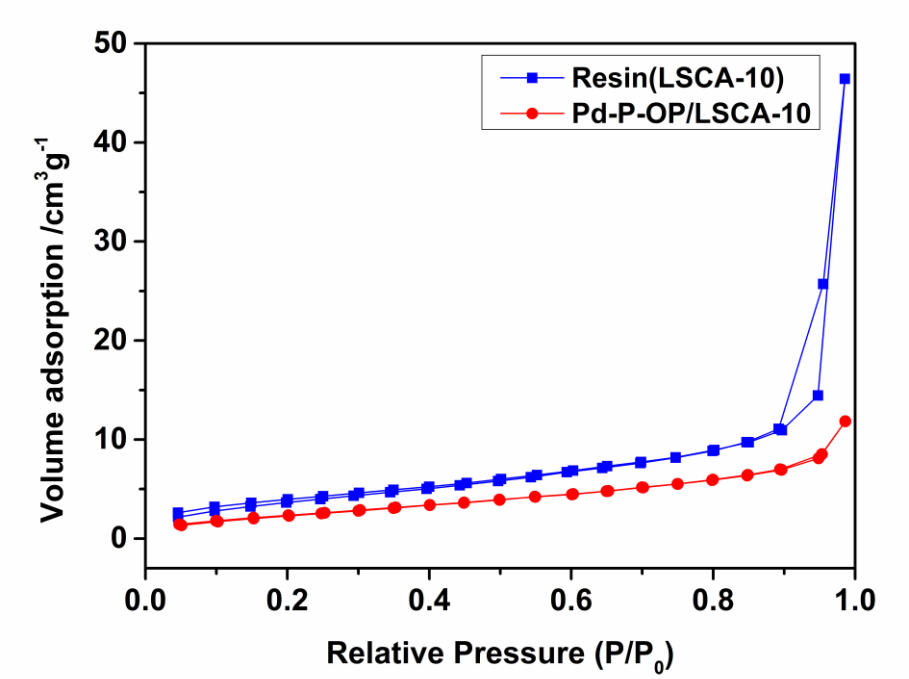


Figure S3. N_2 sorption isotherms of (■) LSCA-10 resin and (●) fresh Pd-P-OP/LSCA-10 catalyst.

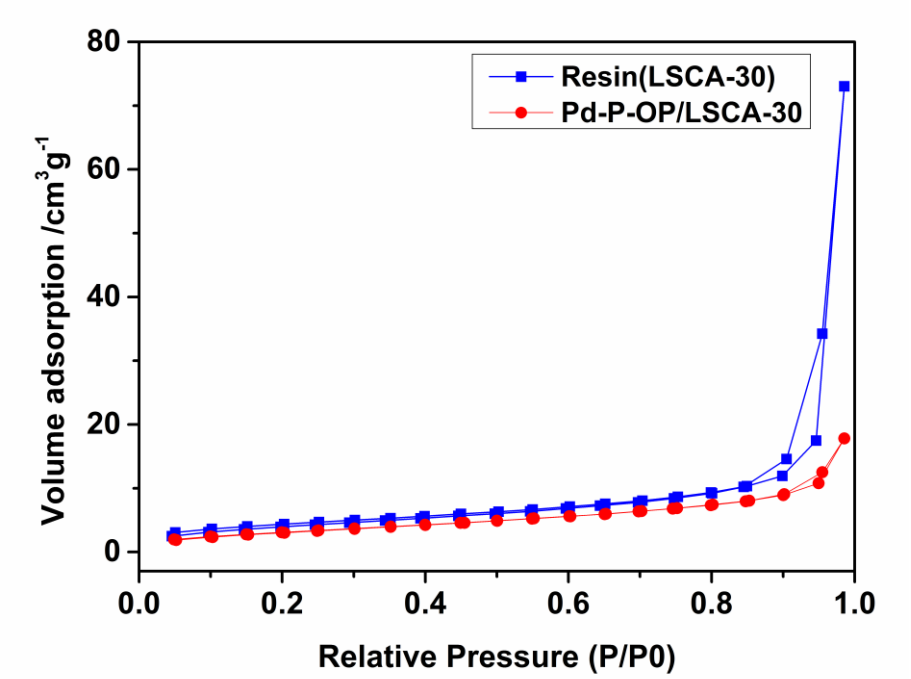


Figure S4. N_2 sorption isotherms of (■) LSCA-30 resin and (●) Pd-P-OP/LSCA-30 catalyst.

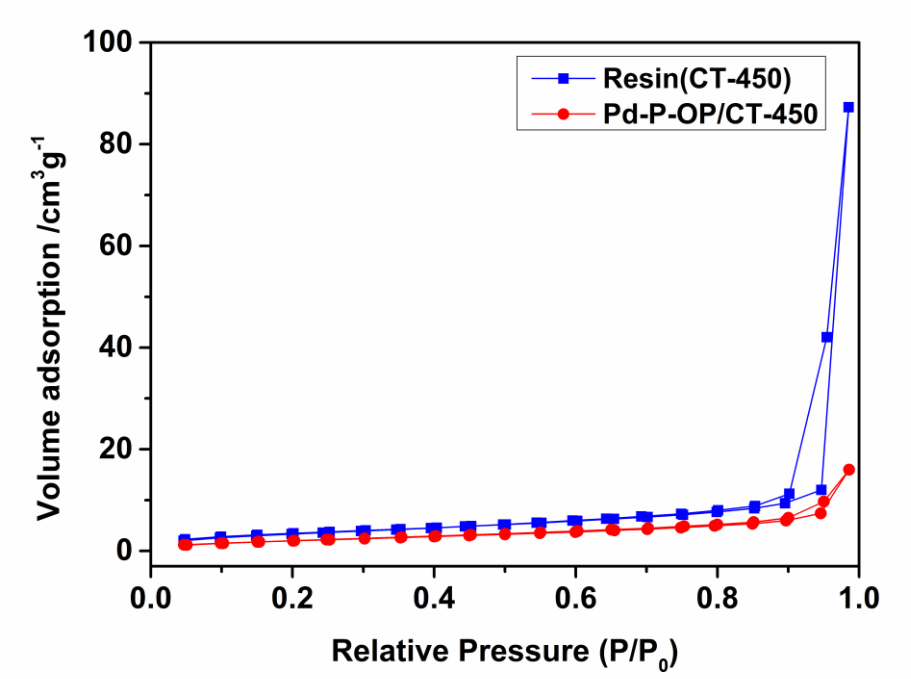


Figure S5. N_2 sorption isotherms of (■) CT-450 resin and (●) Pd-P-OP/CT-450 catalyst.

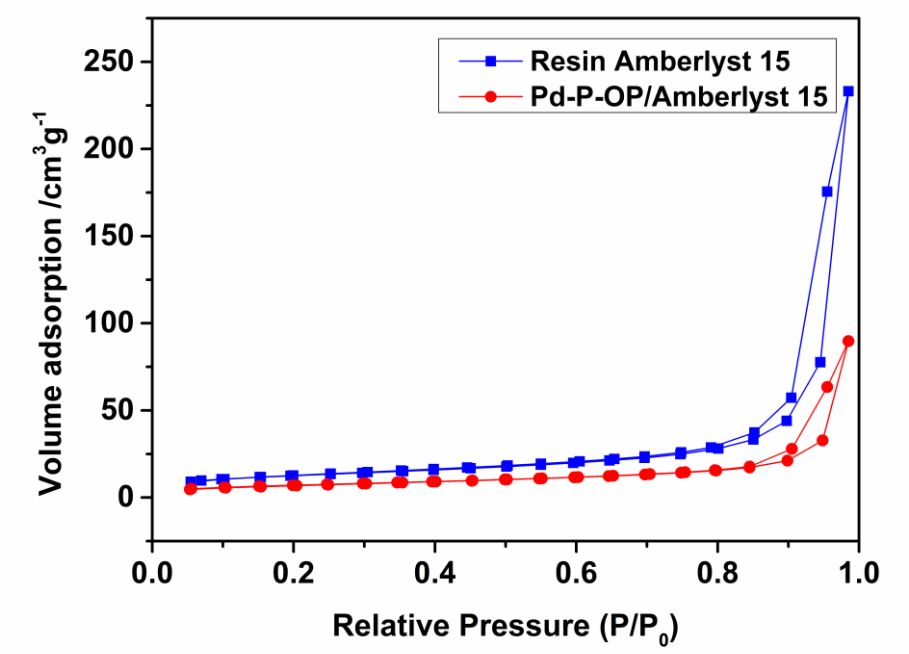


Figure S6. N_2 sorption isotherms of (■) Amberlyst 15 resin and (●) Pd-P-OP/Amberlyst 15 catalyst.

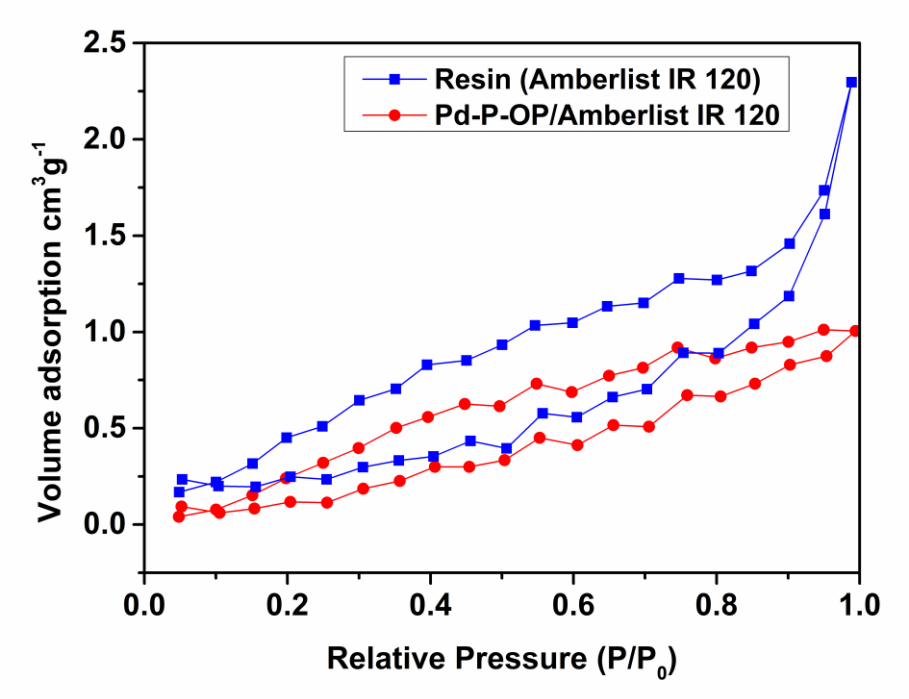
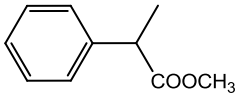


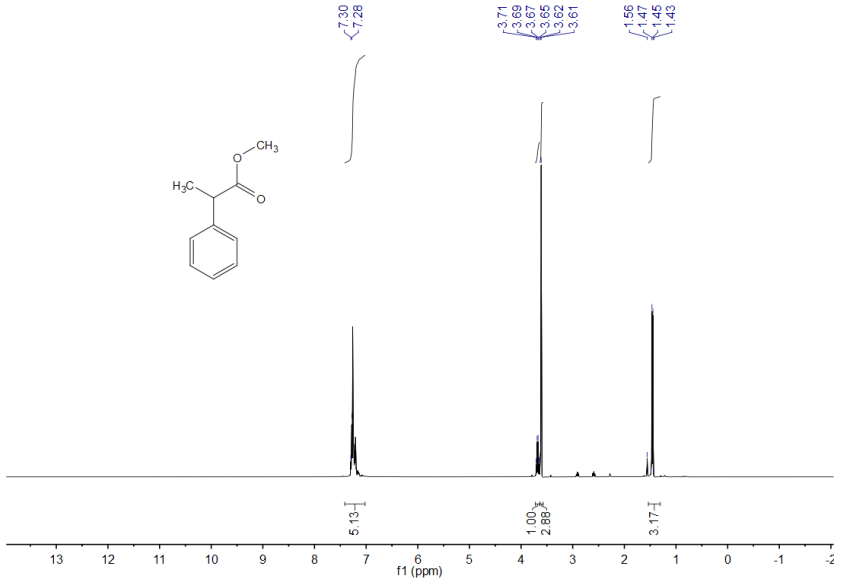
Figure S7. N_2 sorption isotherms of (■) Amberlist IR 120 resin and (●) Pd-P-OP/Amberlist IR 120 catalyst.

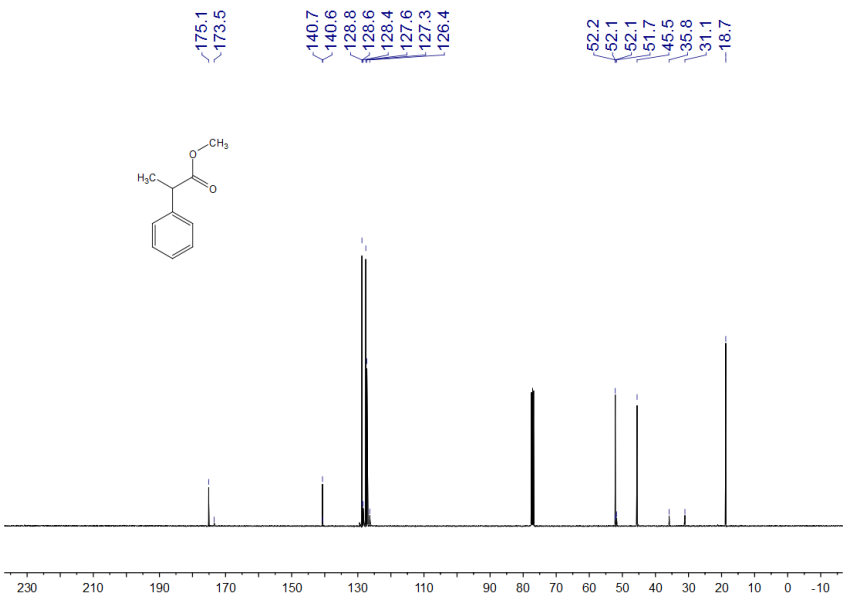


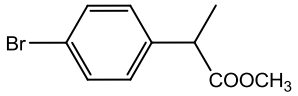
Methyl 2-phenylpropanoate[1]:

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21-7.28 (m, ArH, 5H), 3.68 (q, *J* = 7.2 Hz, CH, 1H), 3.61(s, CH_3, 3H), 1.46 (d, *J* = 7.2 Hz, CH_3, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.1, 140.7, 128.8, 127.6, 127.2, 52.1, 45.5, 18.7. GC MS: MS (EI): m/z calcd. for [$C_{10}H_{12}O_2$]:164.1, found 164.1.

^{1}H NMR (upper) and ^{13}C NMR (bottom)



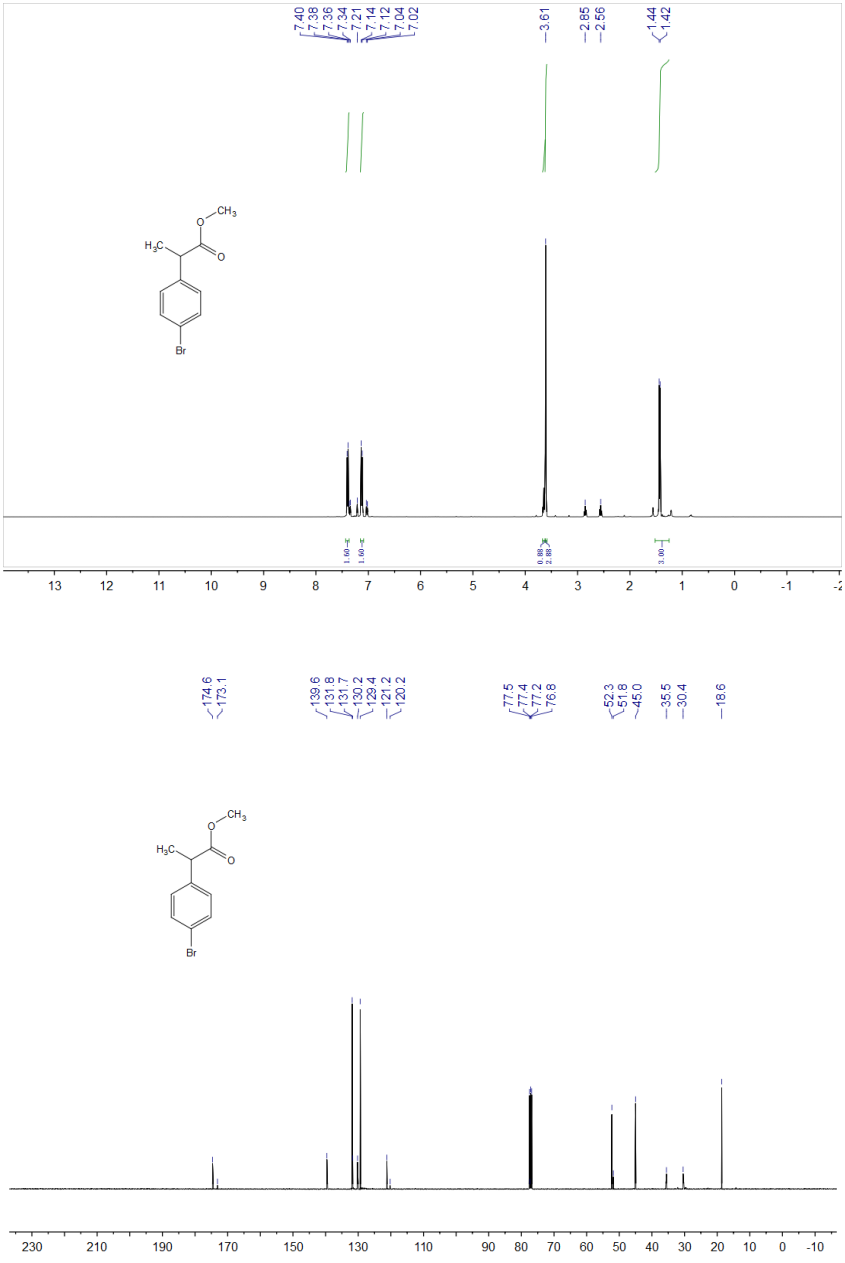


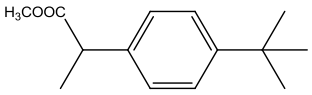


Methyl 2-(4-bromophenyl)propanoate:

^{1}H NMR (400 MHz, $CDCl_3$) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, J=8.2, 2H), 7.18 (d, J=8.2, 2H), 3.69 (dd, J=7.16, 1H), 3.69(s, OCH_3, 3H), 1.48 (d, J=7.2, CH_3, 3H).^{13}C NMR (101 MHz, $cdcl_3$) δ 174.6, 139.6,131.9, 129.4, 121.2, 52.3, 45.0, 18.6. GC MS: MS (EI): m/z calcd. for [$C_{10}H_{11}O_2Br$]: 242.9 found 242.0.

^{1}H NMR (upper) and ^{13}C NMR (bottom)

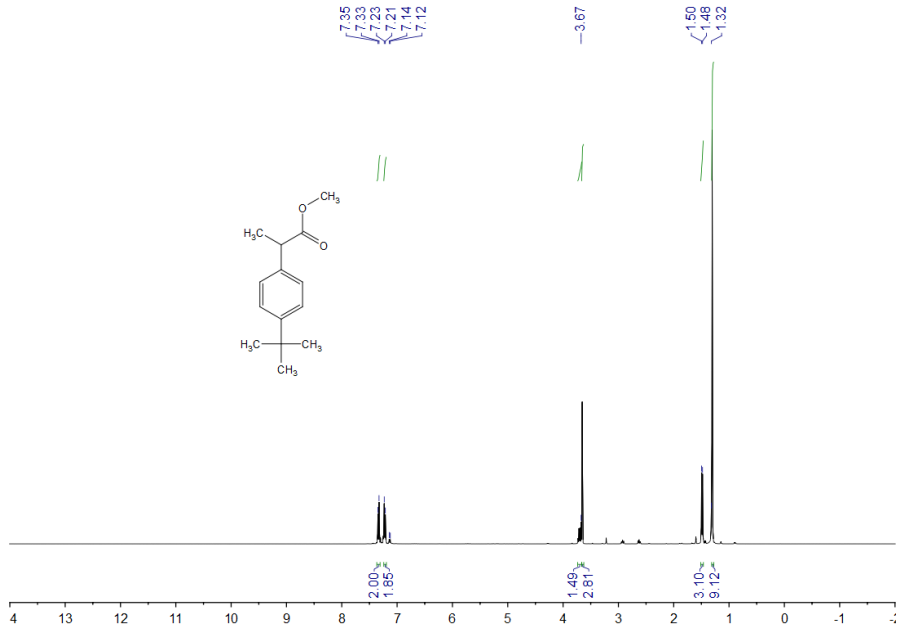


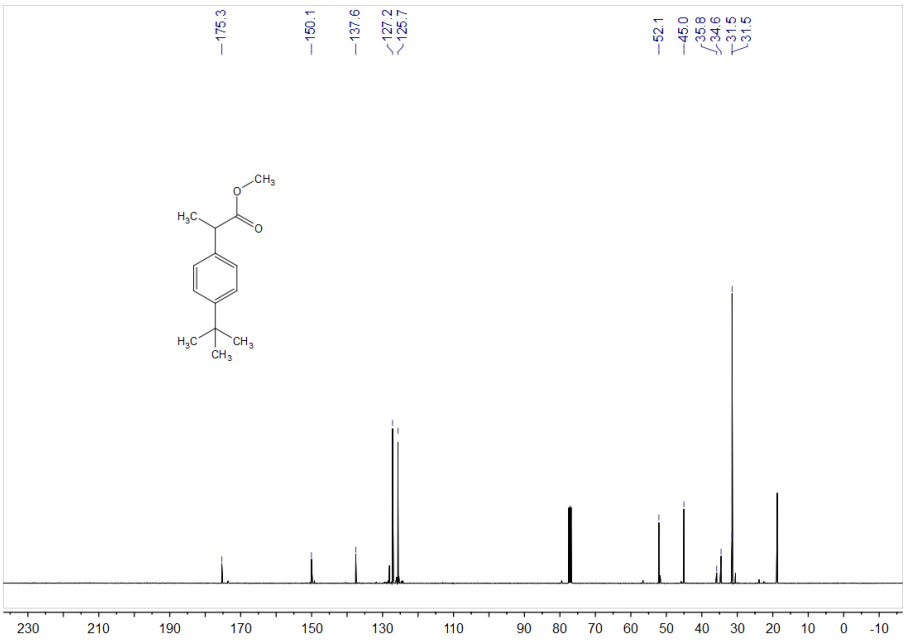


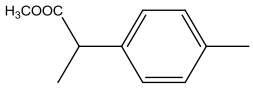
Methyl 2-(4-*tert*-butylphenyl)propanoate:

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.3 Hz, 2H), 7.18 (d, *J* = 8.3 Hz, 2H), 3.68 (dd, *J* = 14.3, 7.2 Hz, 1H), 3.61 (s, 3H), 1.45 (d, *J* = 7.2 Hz, 3H), 1.27 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.3, 150.1, 137.6, 127.2, 125.7, 52.1, 45.0, 34.6, 31.5, 18.7. GC MS: MS (EI): m/z calcd. for [$C_{14}H_{20}O_2$]: 220.1, found 220.2.

^{1}H NMR (upper) and ^{13}C NMR (bottom)



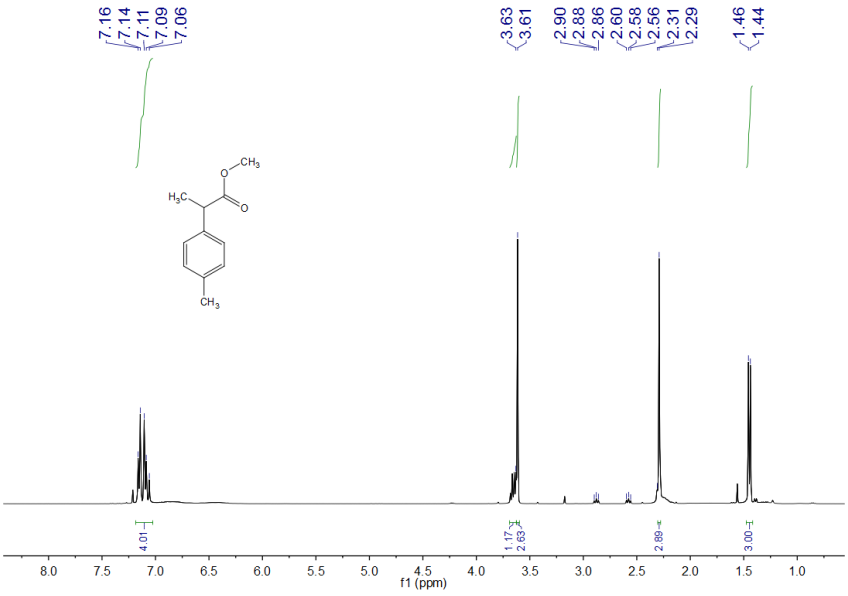


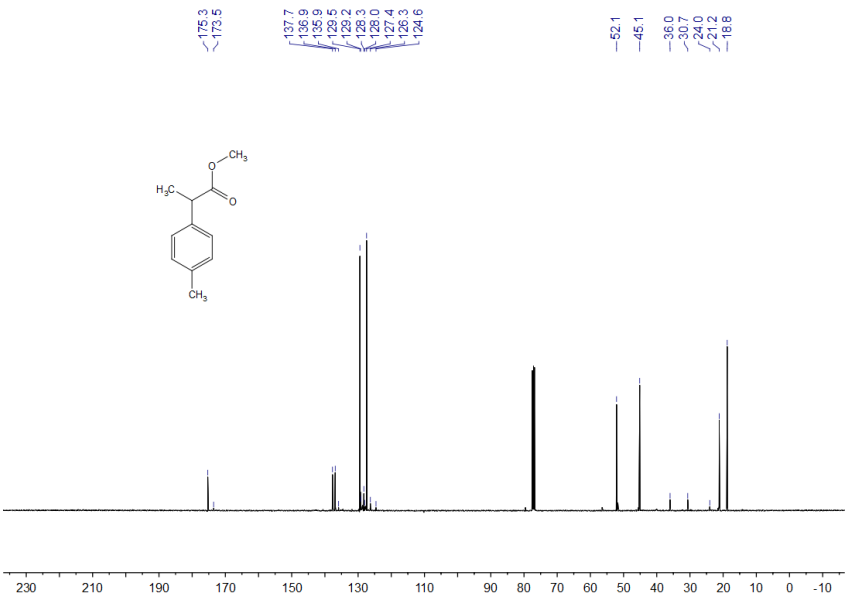


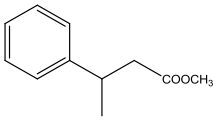
Methyl 2-*p*-tolylpropanoate:

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 (d, *J* = 7.9 Hz, 2H), 7.10 (d, *J* = 7.9 Hz, 2H), 3.66 (dd, *J* = 13.2, 6.0 Hz, 1H), 3.61 (s, 3H), 2.29 (s, 3H), 1.45 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.3, 137.7, 136. 9, 129. 5, 127. 4, 52.1, 45.1, 21.2, 18.8. GC MS: MS (EI): m/z calcd. for [$C_{11}H_{14}O_2$]: 178.1, found 178.1.

^{1}H NMR (upper) and ^{13}C NMR (bottom)



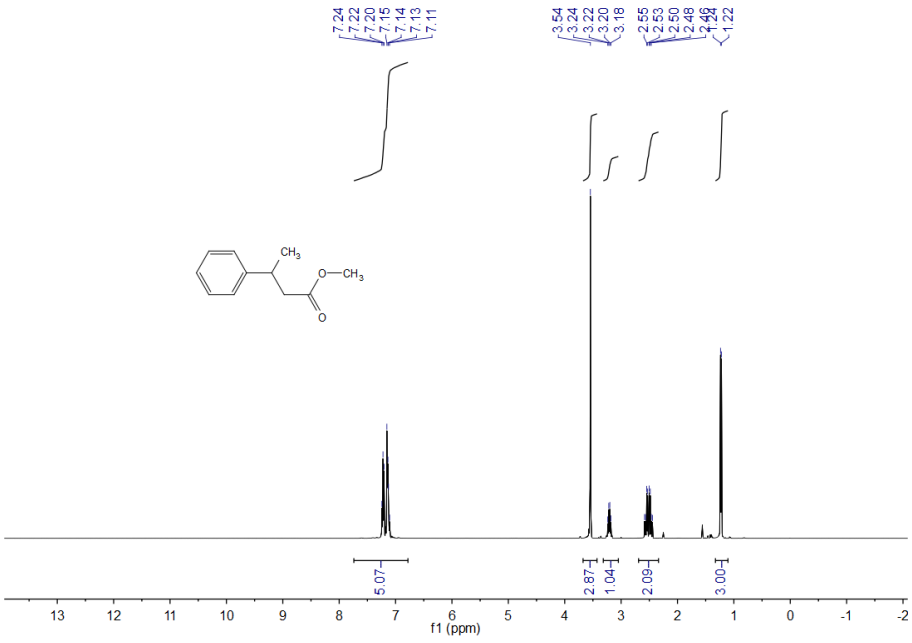


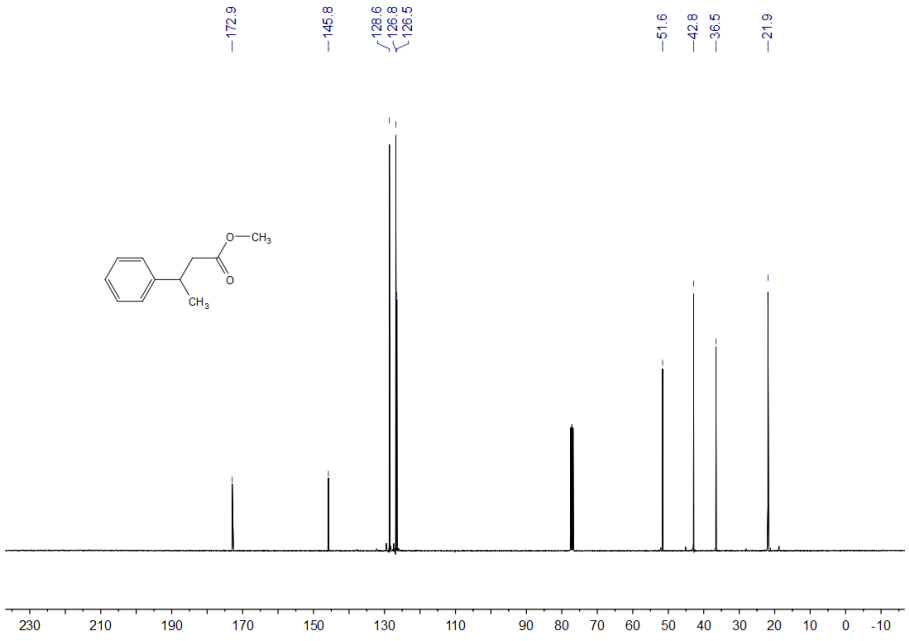


Methyl 3-p-tolylbutanoate[1]:

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25–7.10 (m, 5H), 3.54 (s, 3H), 3.21 (m, *J* = 14.5, 7.2 Hz, 1H), 2.56 (dd, *J* = 15.2, 6.8 Hz, 1H), 2.47 (dd, J=15.1, 8.2 Hz, 1H), 1.23 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.9, 145.8, 128.6, 126.8, 126.52, 51.6, 42.9, 36.6, 21.9. GC MS: MS (EI): m/z calcd. for $[C_{11}H_{14}O_2]$:178.1, found 178.1.

^{1}H NMR (upper) and ^{13}C NMR (bottom)





Reference

[1] T. M. Konrad, J. T. Durrani, C. J. Cobley, M. L. Clarke. *Chem. Commun.*, **2013**, *49*, 3306.