

Supporting Information

Synthesis of tetrahydronaphthalene esters by intramolecular cyclization of ethyl *p*-azidophenyl-2-phenylalkanoates and evaluation of the inhibition of human tumor cells proliferation

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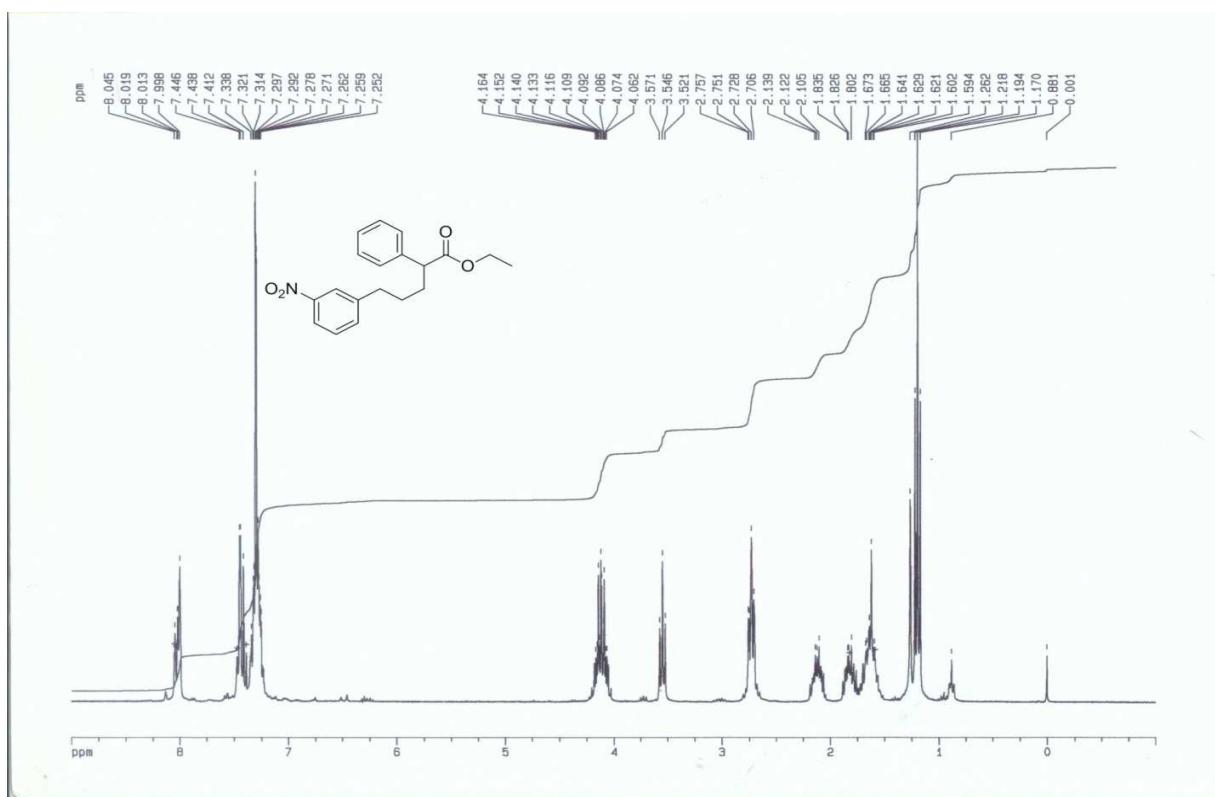


Figure S1. ¹H NMR spectrum of ethyl 5-(3-nitrophenyl)-2-phenylpentanoate (**16**).

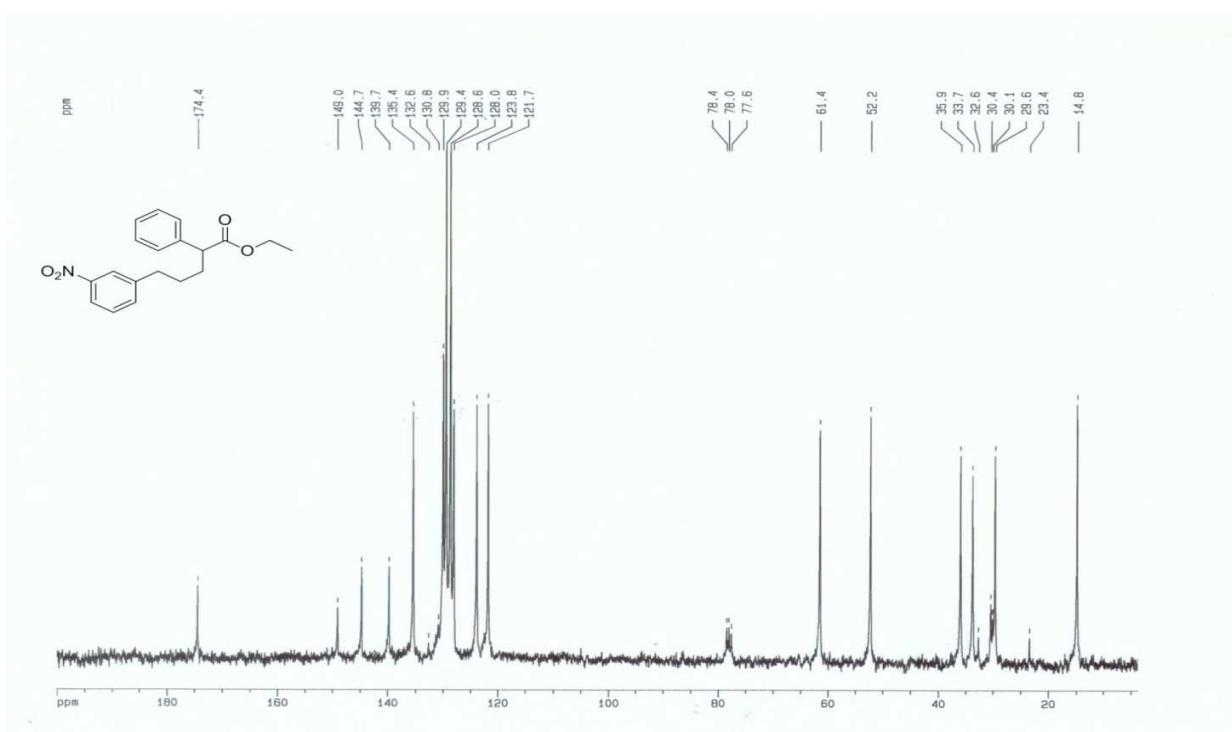


Figure S2.1¹³C NMR spectrum of ethyl 5-(3-nitrophenyl)-2-phenylpentanoate (**16**).

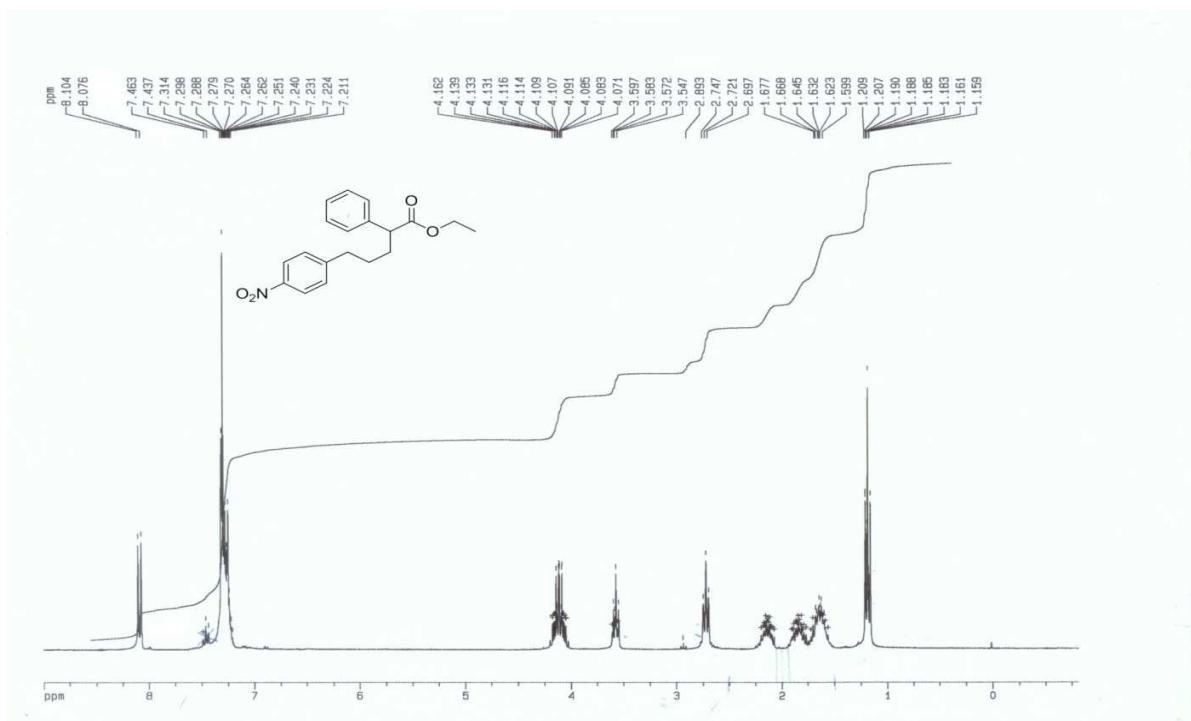


Figure S3. ¹H NMR spectrum of ethyl 5-(4-nitrophenyl)-2-phenylpentanoate(**17**).

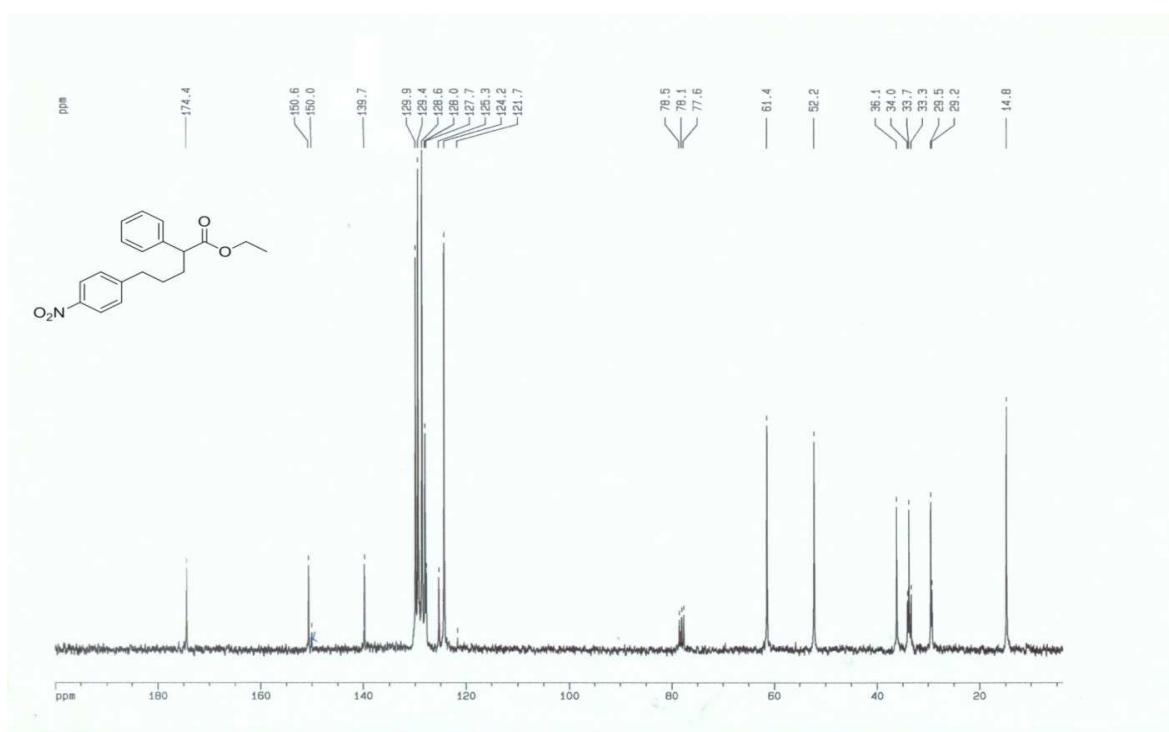


Figure S4. ^{13}C NMR spectrum of ethyl 5-(4-nitrophenyl)-2-phenylpentanoate (**17**).

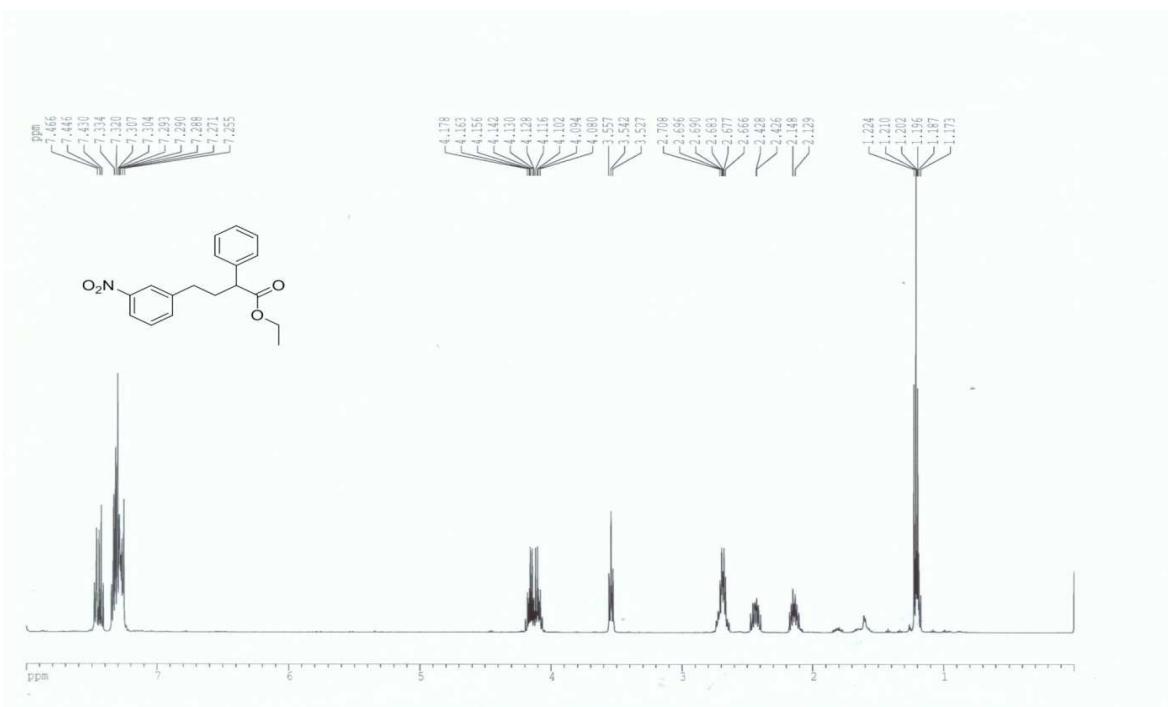


Figure S5. ^1H NMR spectrum of ethyl 4-(3-nitrophenyl)-2-phenylbutanoate (**18**).

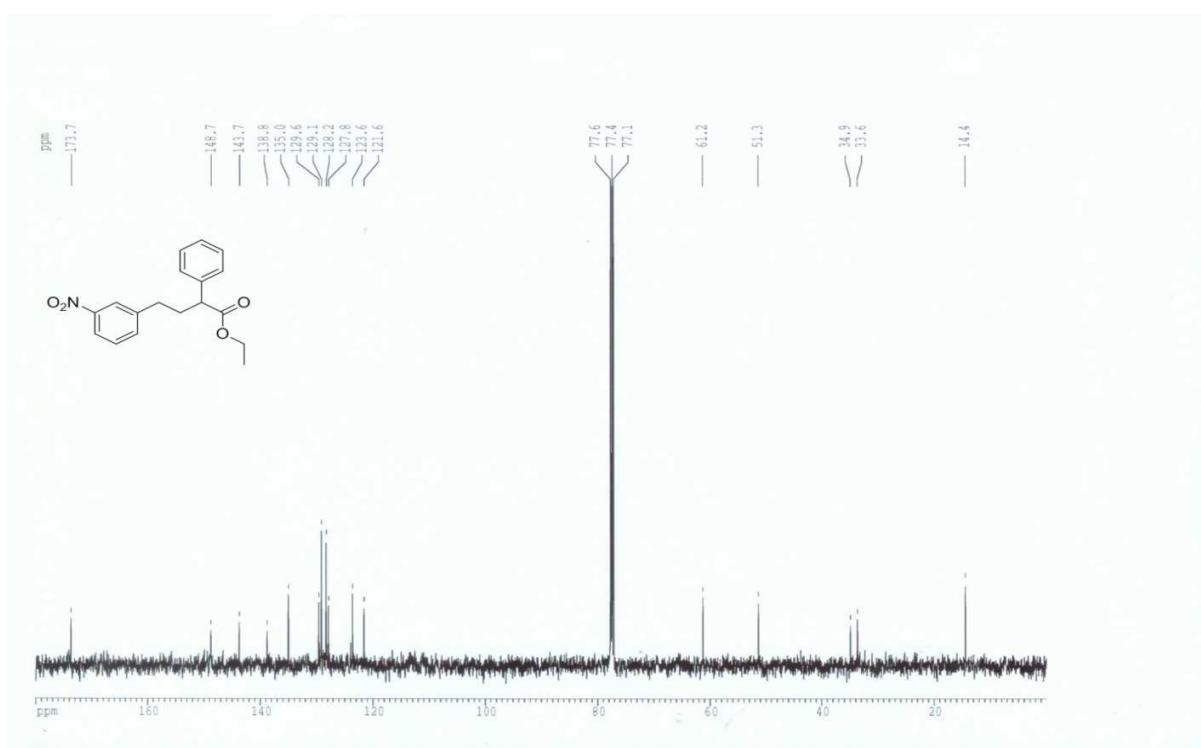


Figure S6. ¹³C NMR spectrum of ethyl 4-(3-nitrophenyl)-2-phenylbutanoate (**18**).

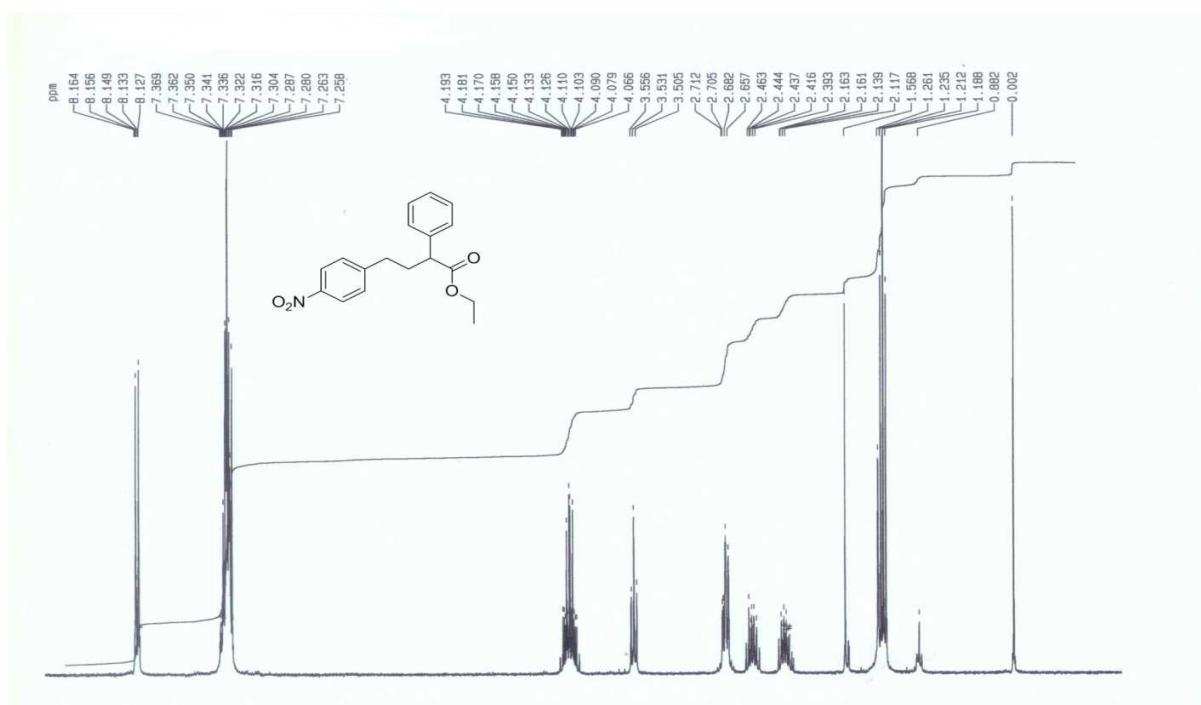


Figure S7. ¹H NMR spectrum of ethyl 4-(4-nitrophenyl)-2-phenylbutanoate (**19**).

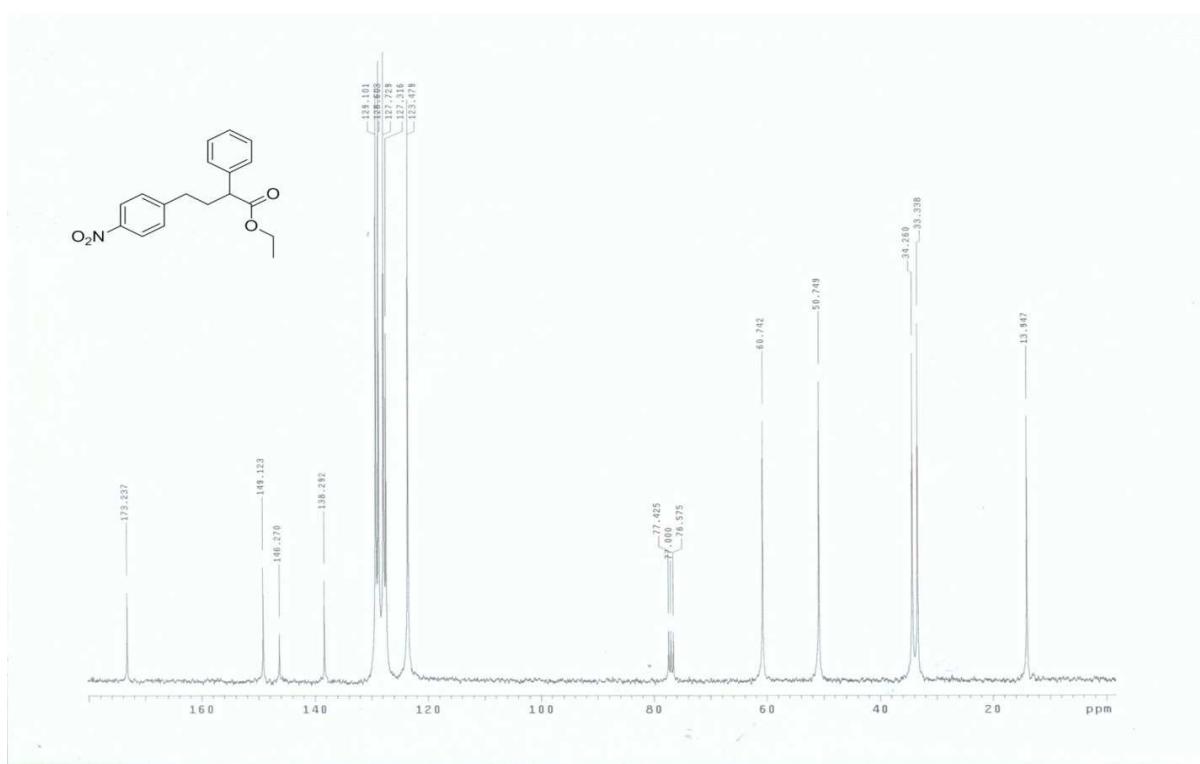


Figure S8. ^{13}C NMR spectrum of ethyl 4-(4-nitrophenyl)-2-phenylbutanoate (**19**).

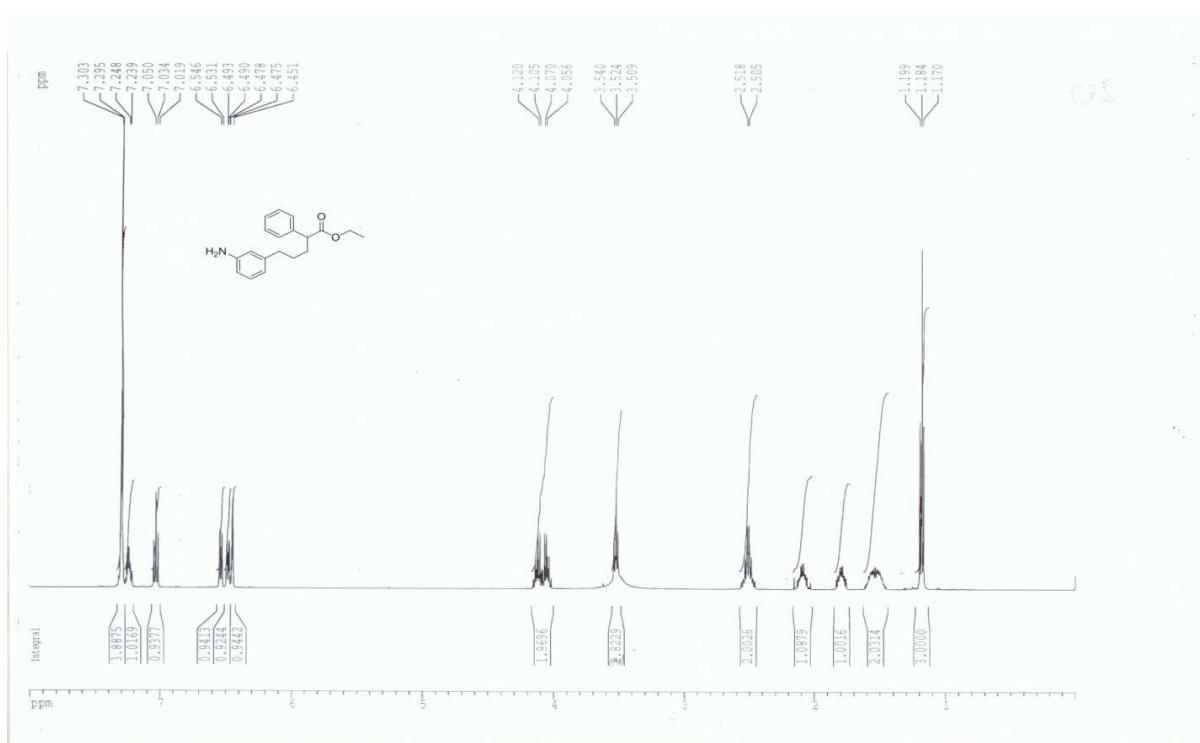


Figure S9. ^1H NMR spectrum of ethyl 5-(3-aminophenyl)-2-phenylpentanoate (**20**).

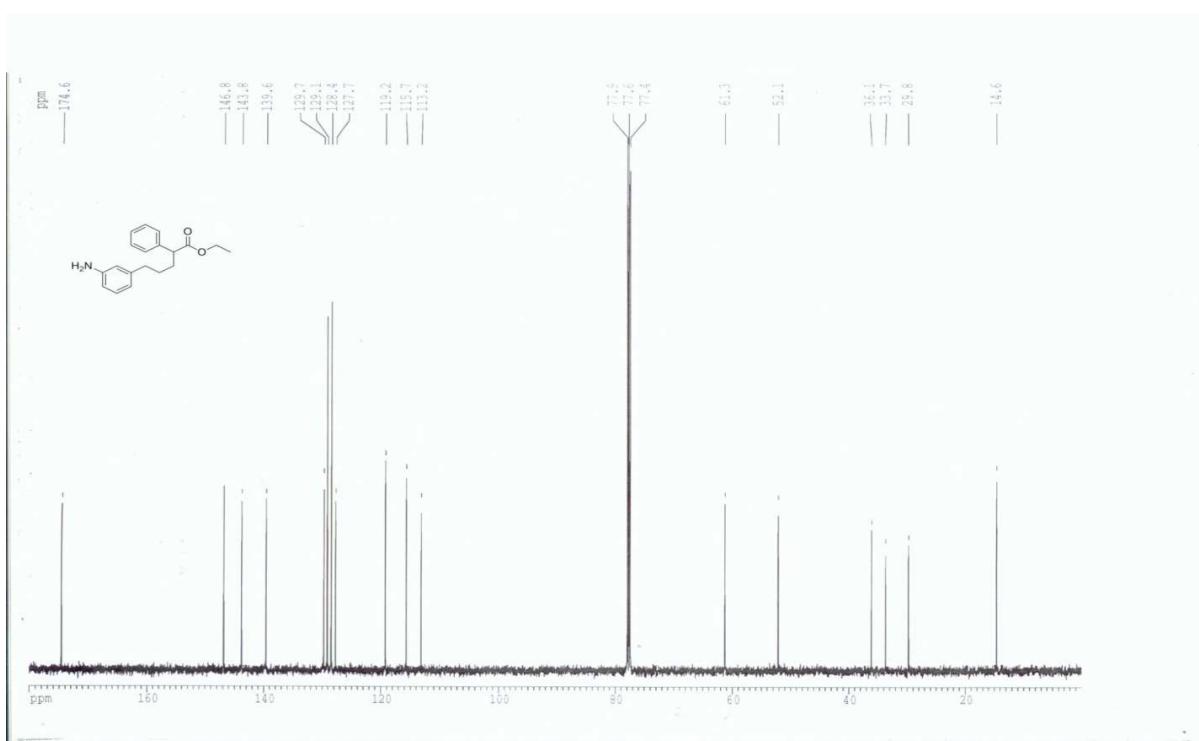


Figure S10. ¹³C NMR spectrum of ethyl 5-(3-aminophenyl)-2-phenylpentanoate (**20**).

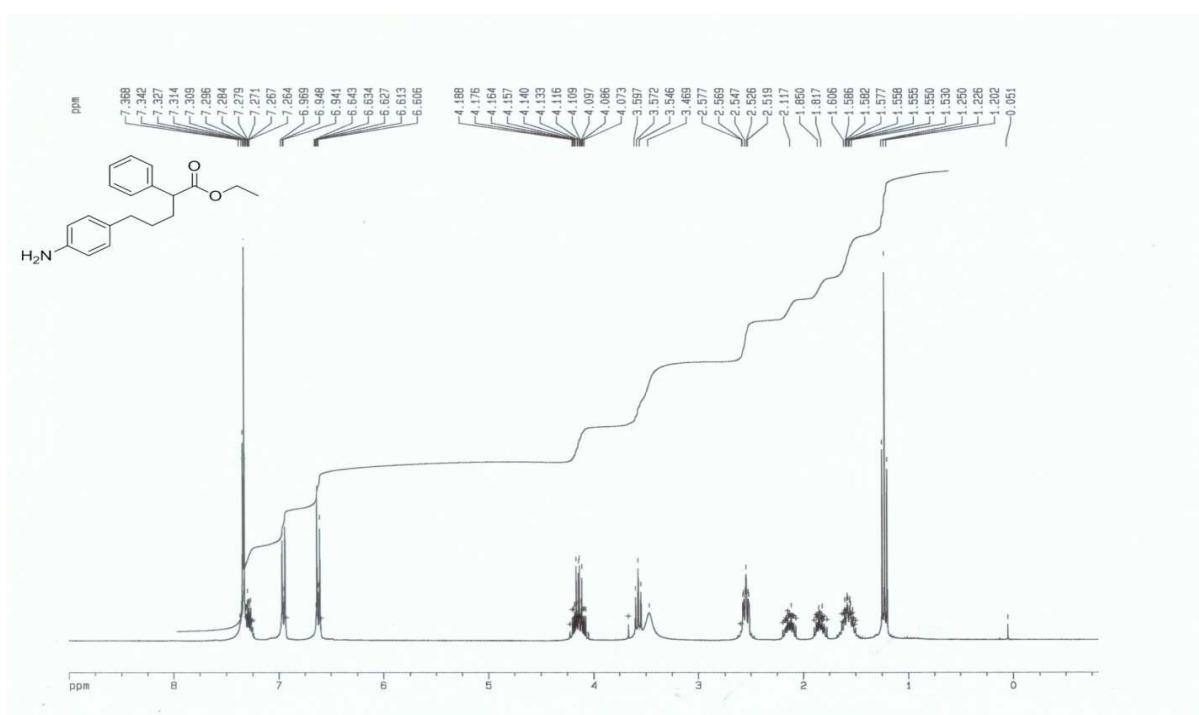


Figure S11. ¹H NMR spectrum of ethyl 5-(4-aminophenyl)-2-phenylpentanoate (**21**).

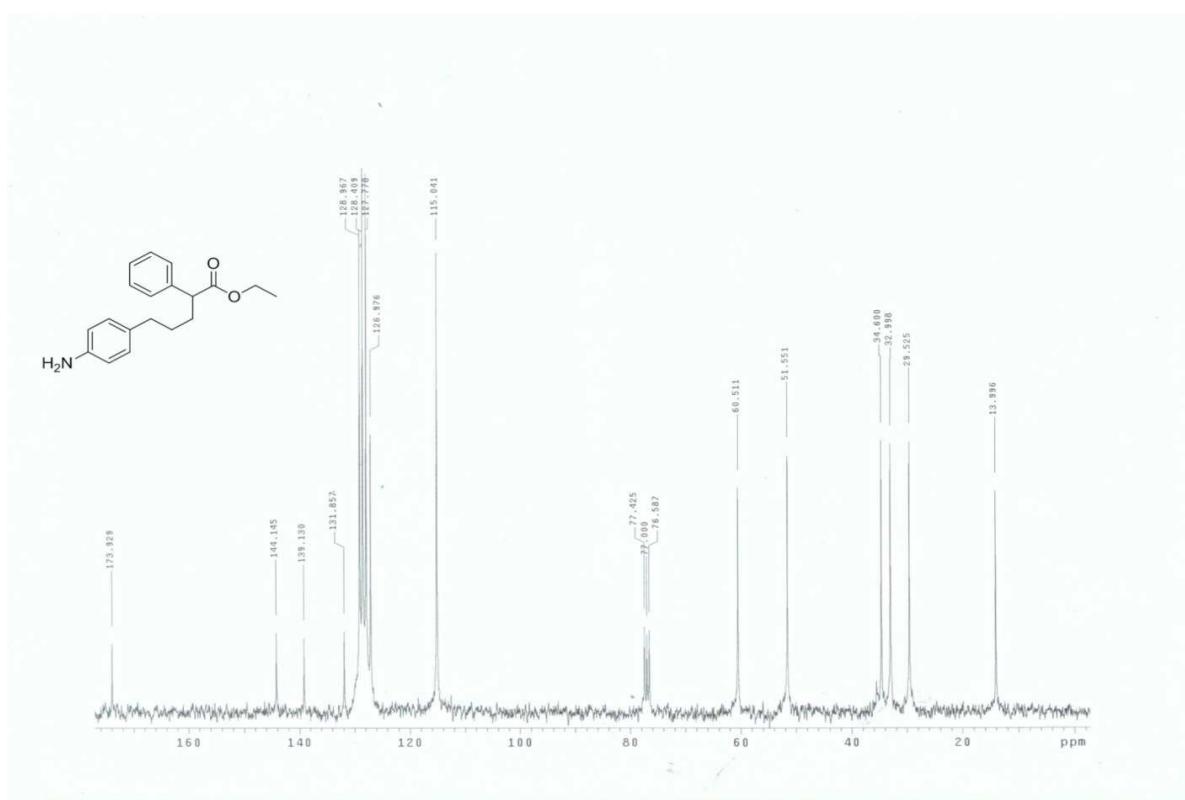


Figure S12. ^{13}C NMR spectrum of ethyl 5-(4-aminophenyl)-2-phenylpentanoate (**21**).

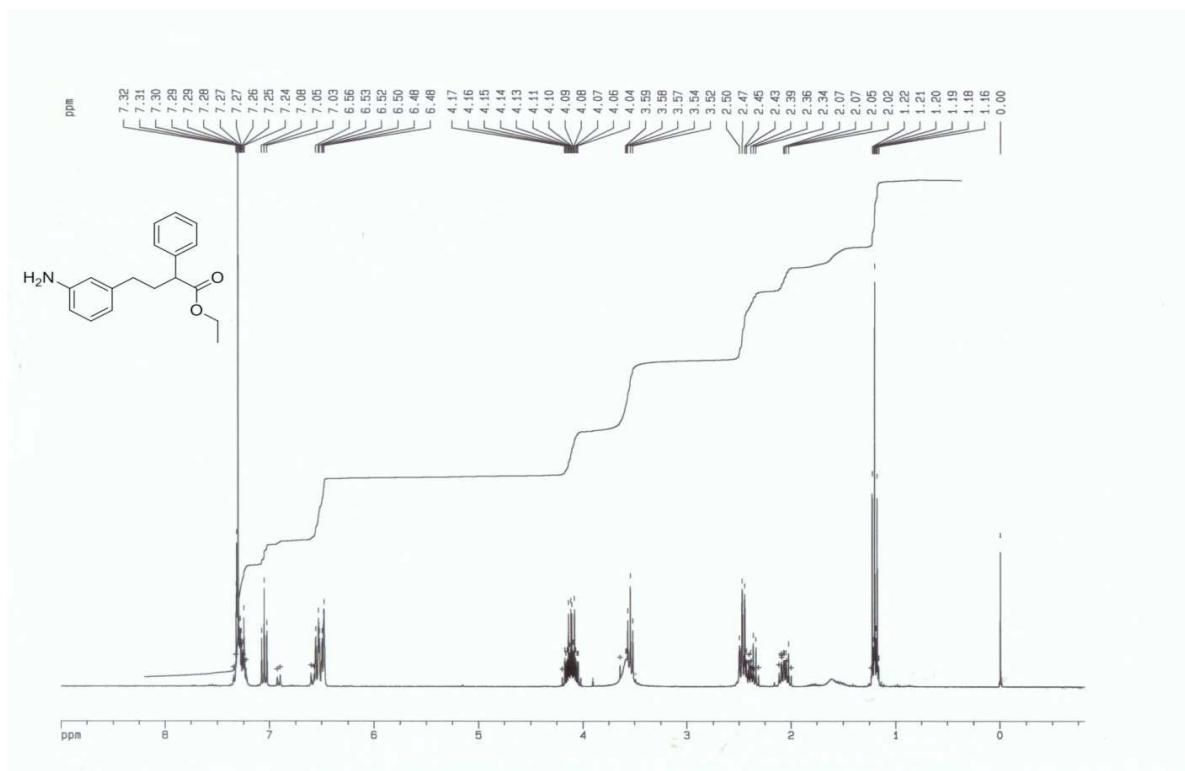


Figure S13. ^1H NMR spectrum of ethyl 4-(3-aminophenyl)-2-phenylbutanoate (**22**).

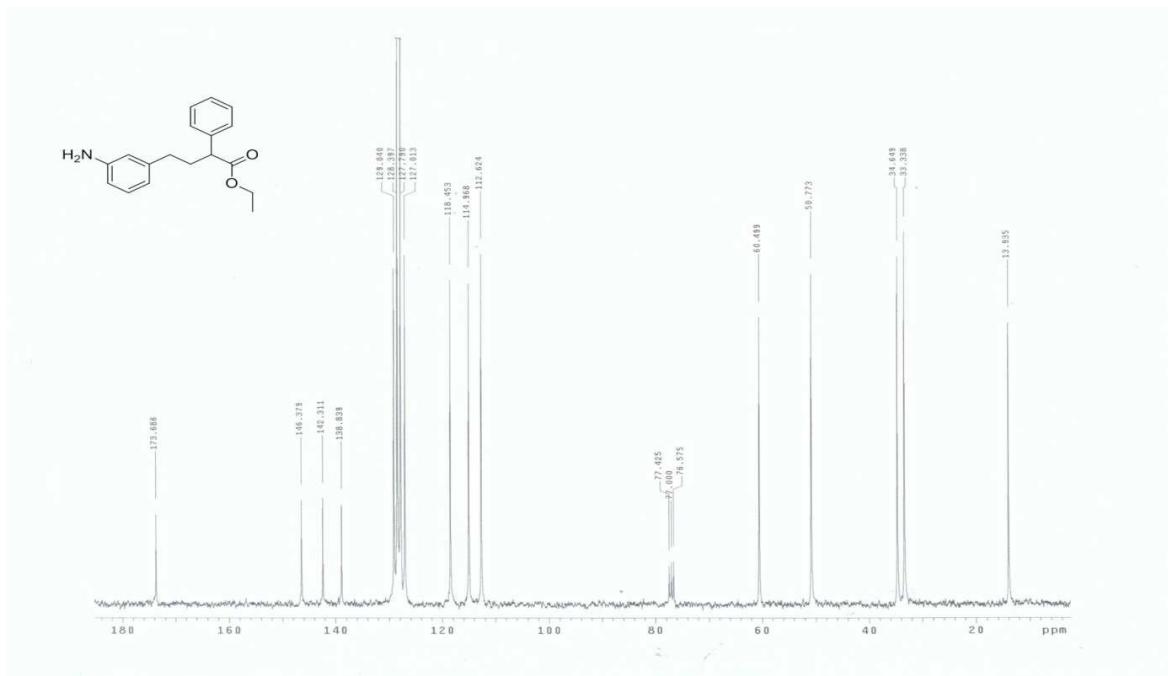


Figure S14. ^{13}C NMR spectrum of ethyl 4-(3-aminophenyl)-2-phenylbutanoate (**22**).

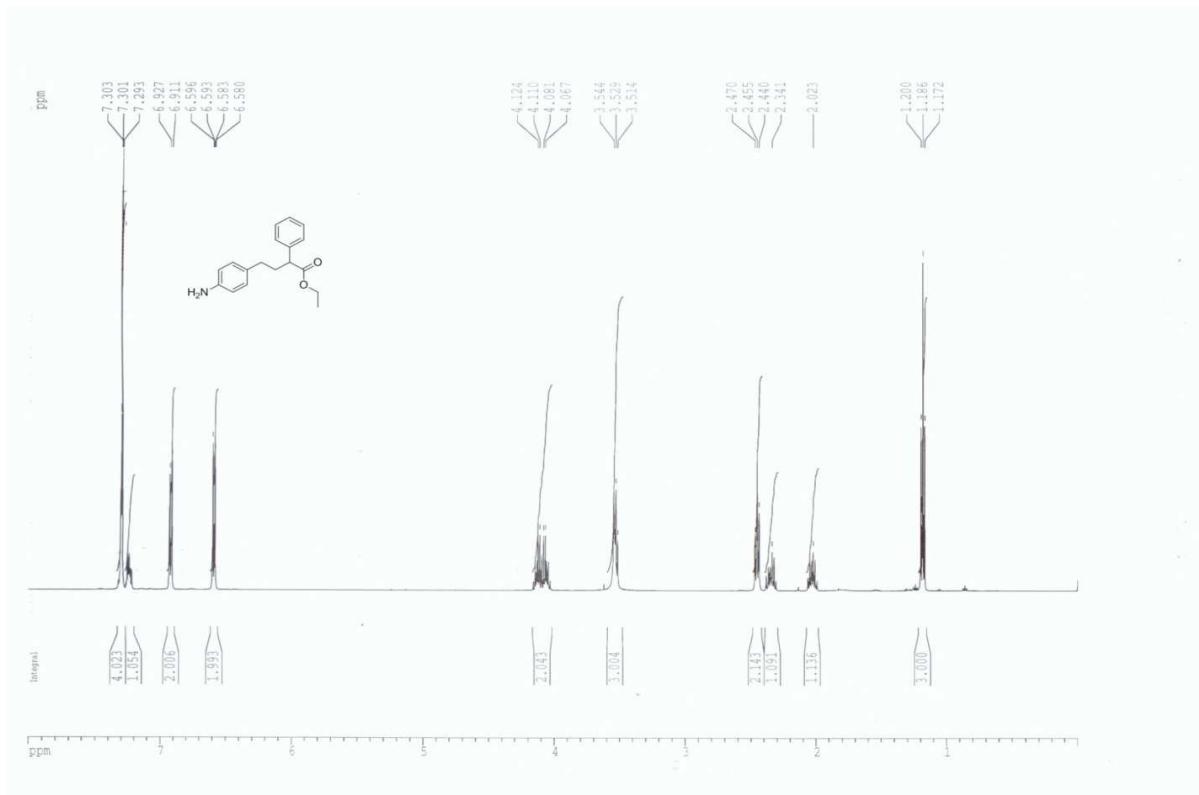


Figure S15. ^1H NMR spectrum of ethyl 4-(4-aminophenyl)-2-phenylbutanoate (**23**).

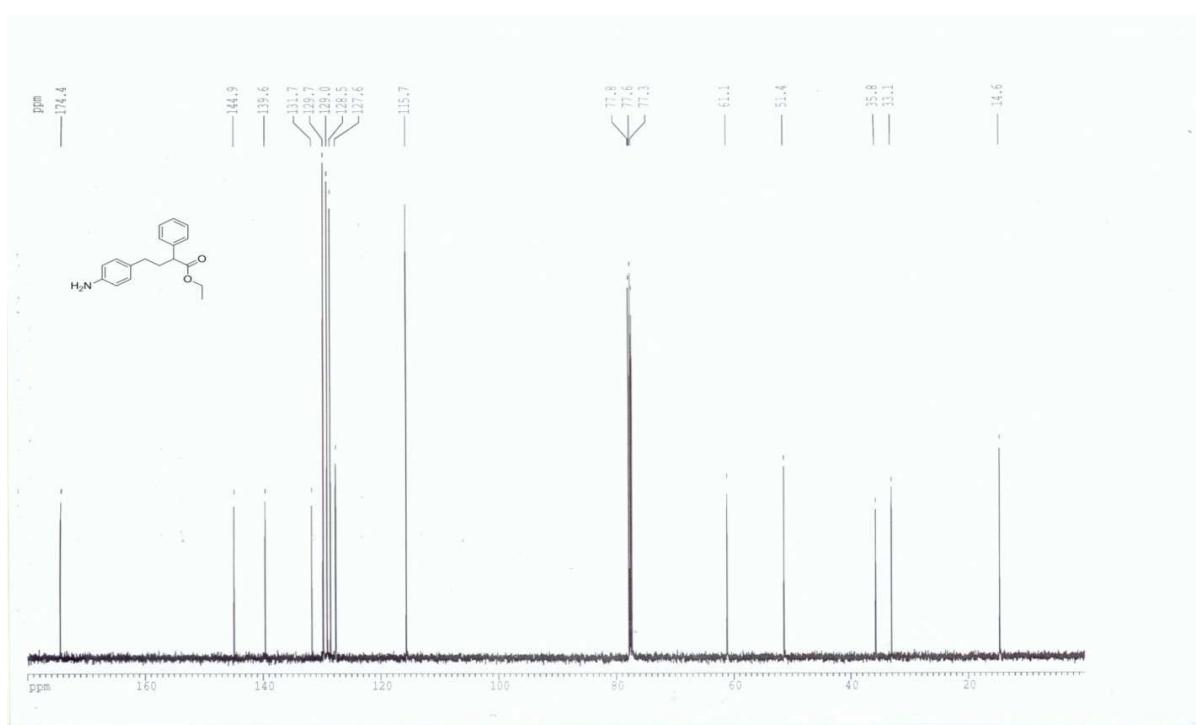


Figure S16. ¹³C NMR spectrum of ethyl 4-(4-aminophenyl)-2-phenylbutanoate (**23**).

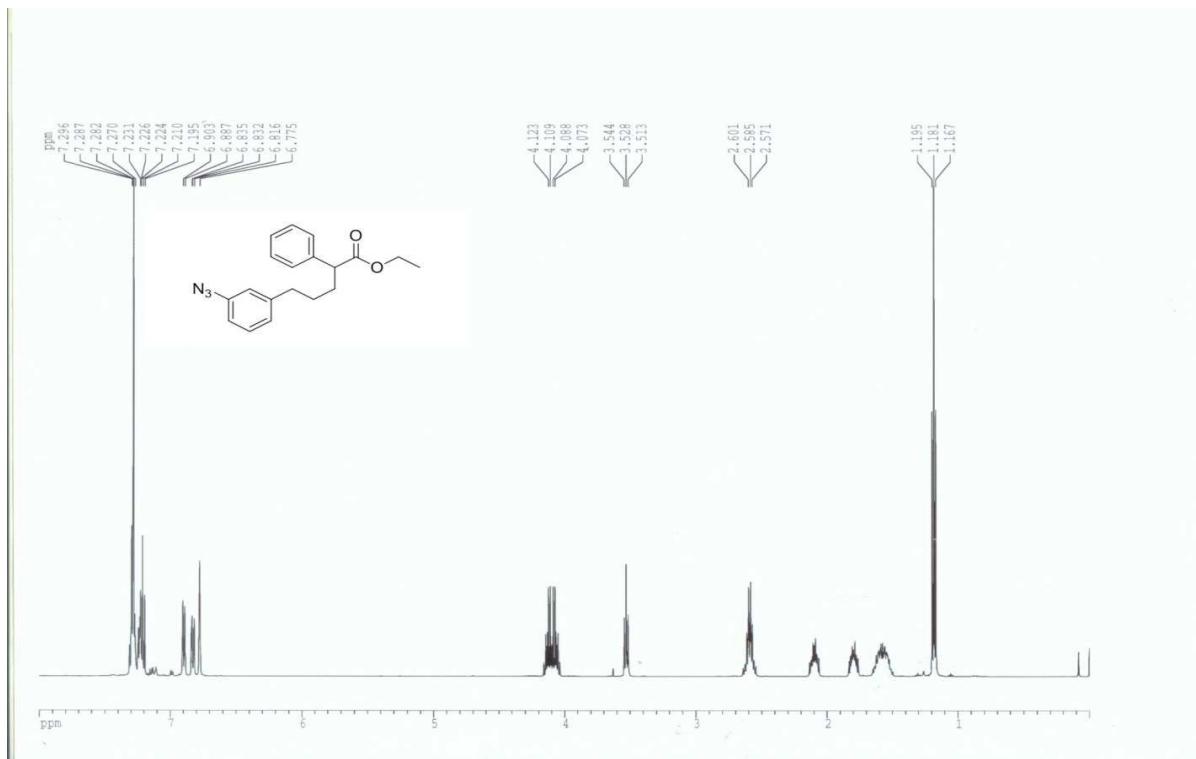


Figure S17. ¹H NMR spectrum of ethyl 5-(3-azidophenyl)-2-phenylpentanoate (**24**).

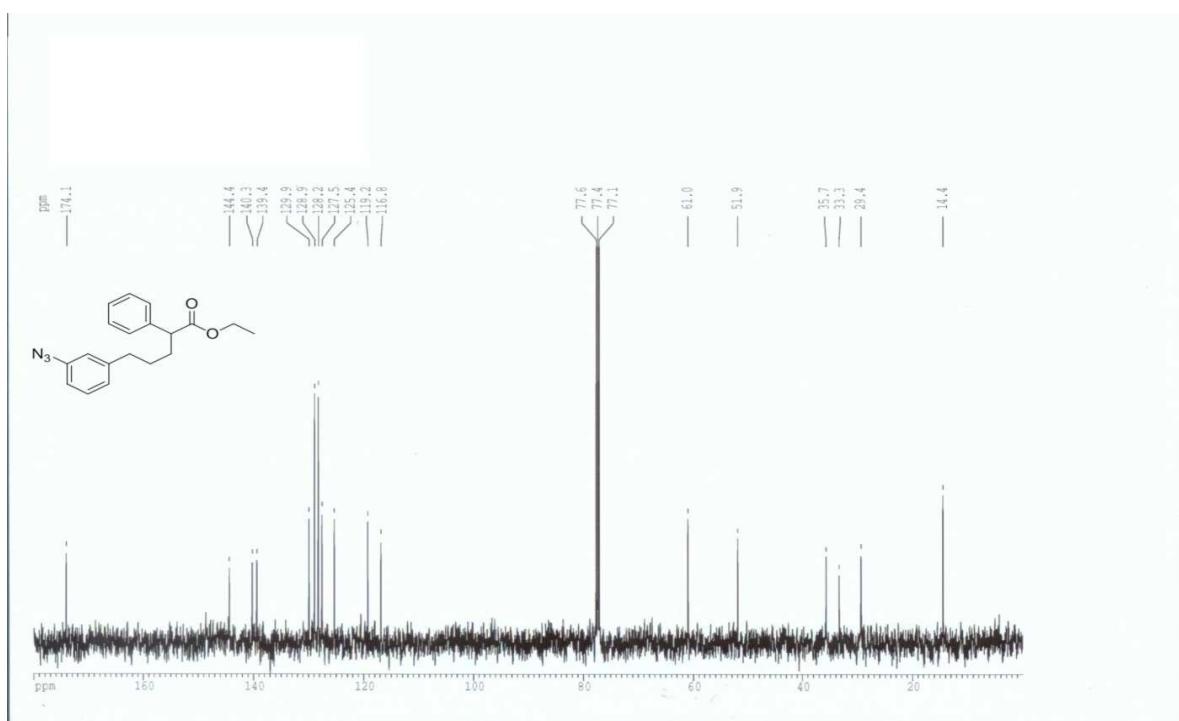


Figure S18. ^{13}C NMR spectrum of ethyl 5-(3-azidophenyl)-2-phenylpentanoate (**24**).

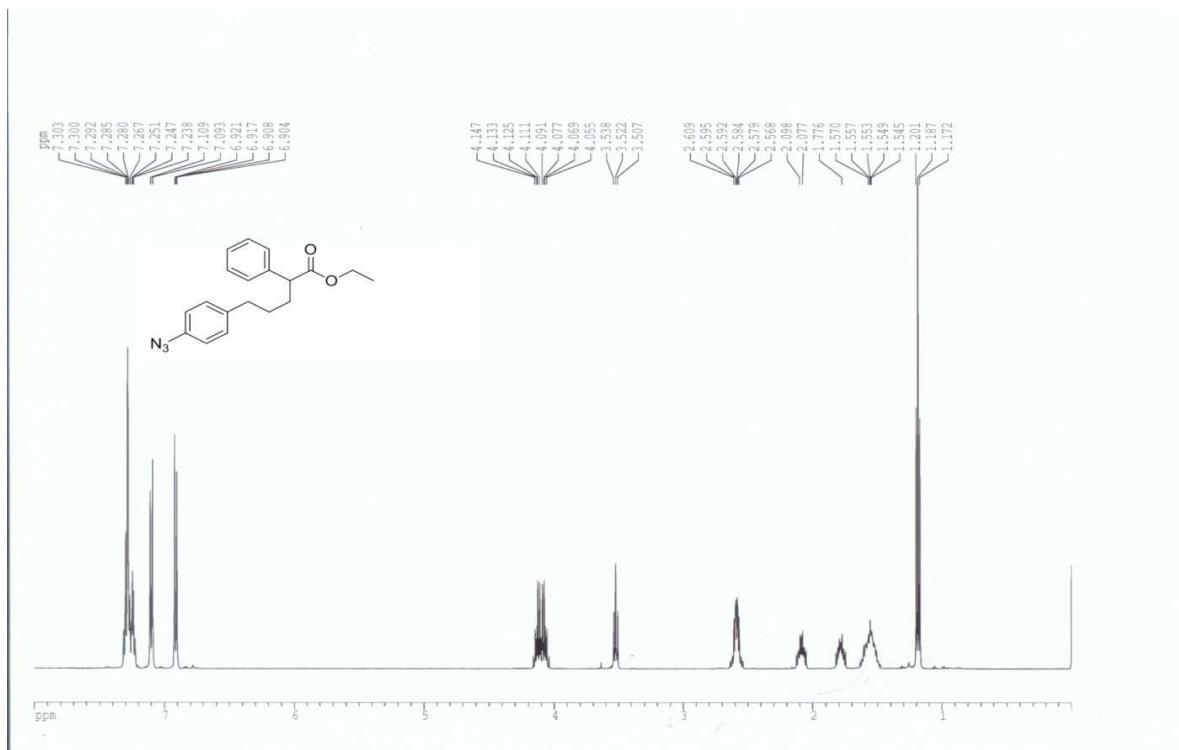


Figure S19. ^1H NMR spectrum of ethyl 5-(4-azidophenyl)-2-phenylpentanoate (**25**).

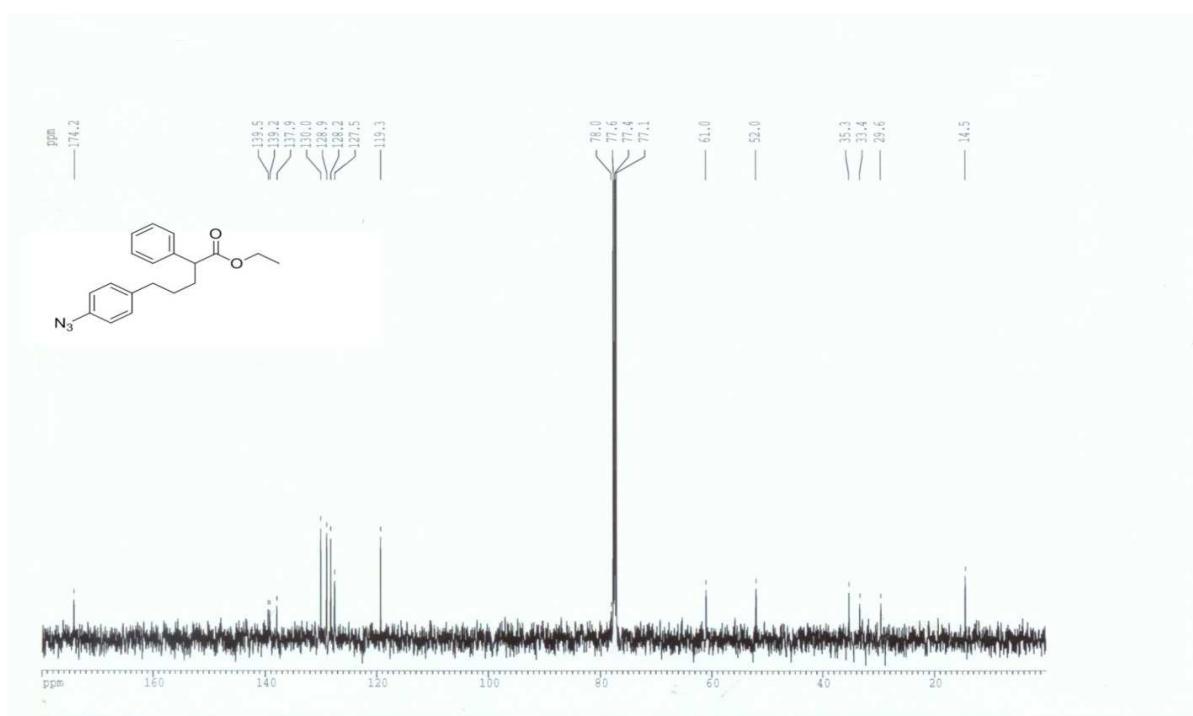


Figure S20. ^{13}C NMR spectrum of ethyl 5-(4-azidophenyl)-2-phenylpentanoate (**25**).

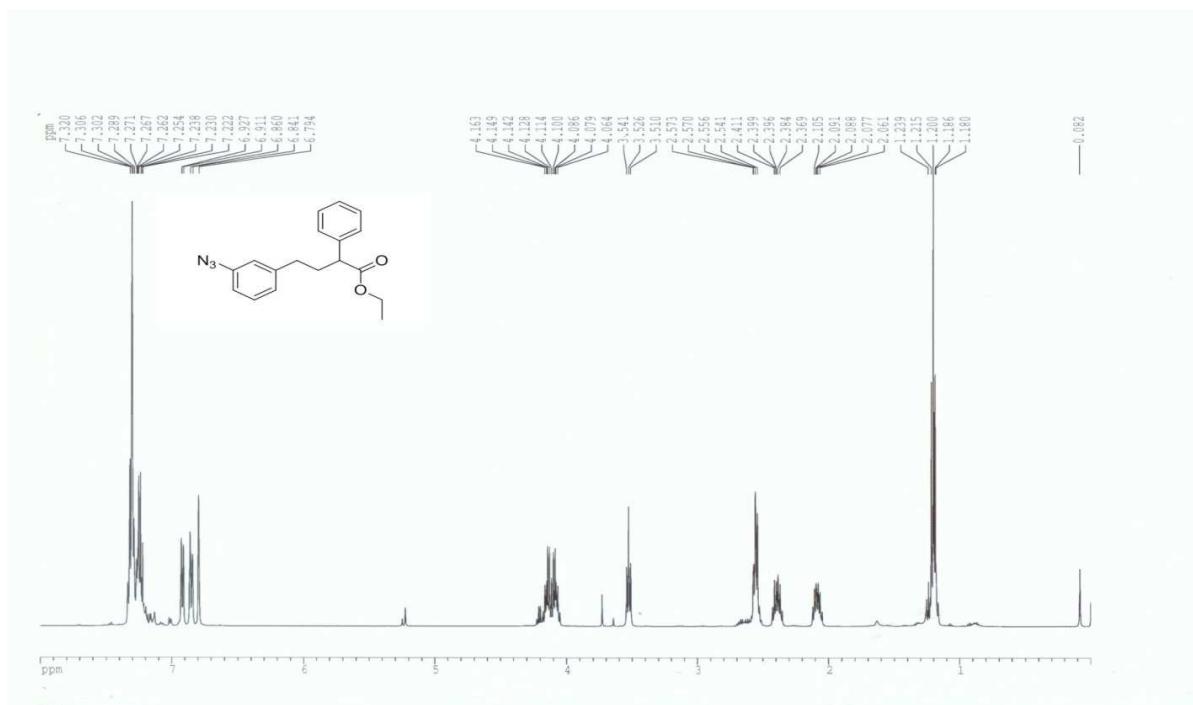


Figure S21. ^1H NMR spectrum of ethyl 4-(3-azidophenyl)-2-phenylbutanoate (**26**).

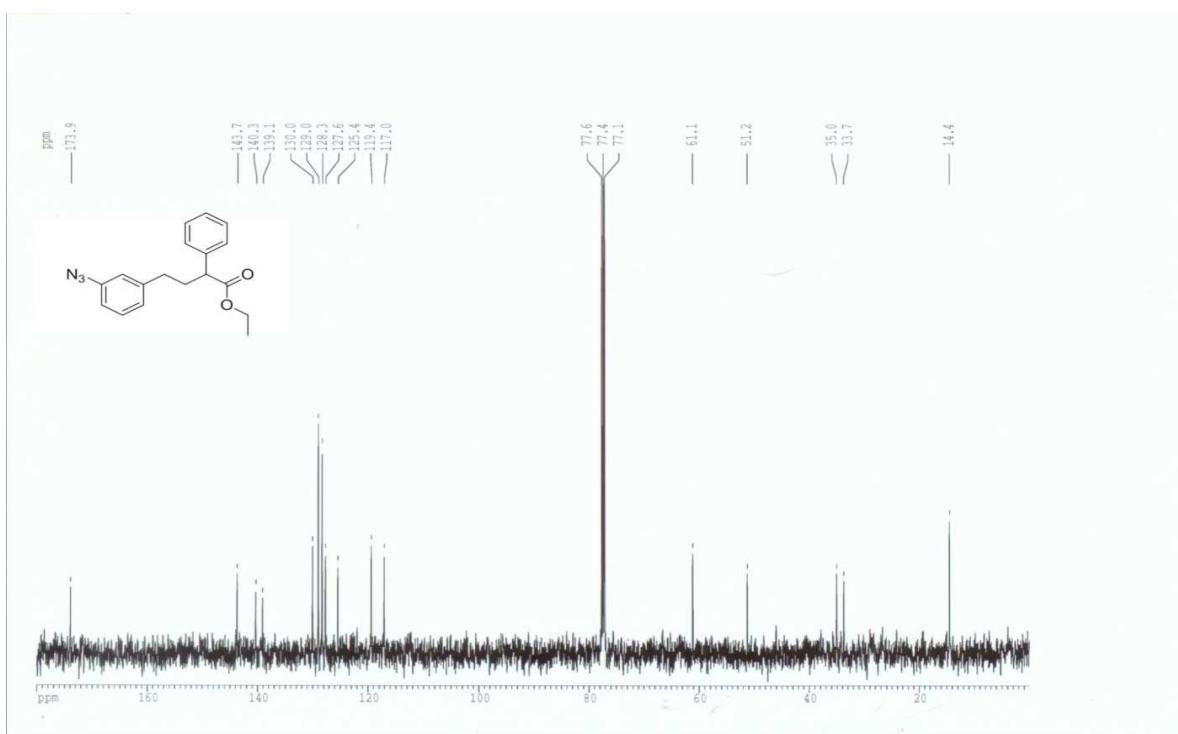


Figure S22. ^{13}C NMR spectrum of ethyl 4-(3-azidophenyl)-2-phenylbutanoate (**26**).

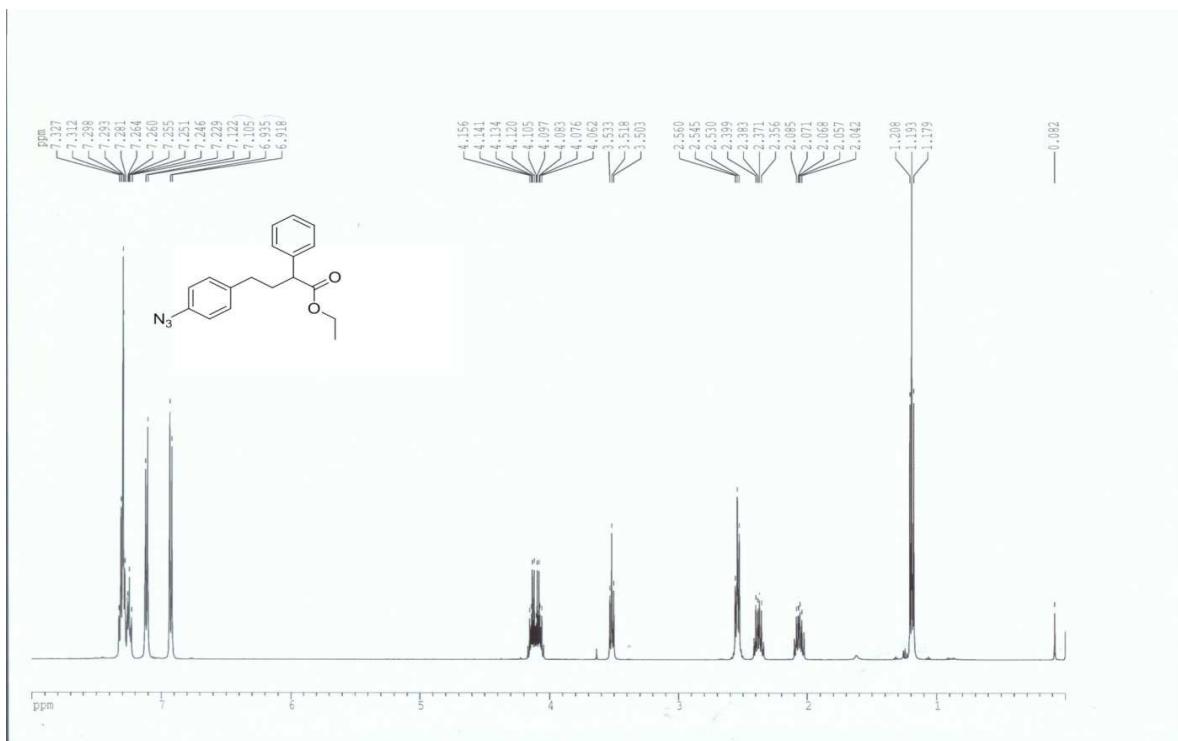


Figure S23. ^1H NMR spectrum of ethyl 4-(4-azidophenyl)-2-phenylbutanoate (**27**).

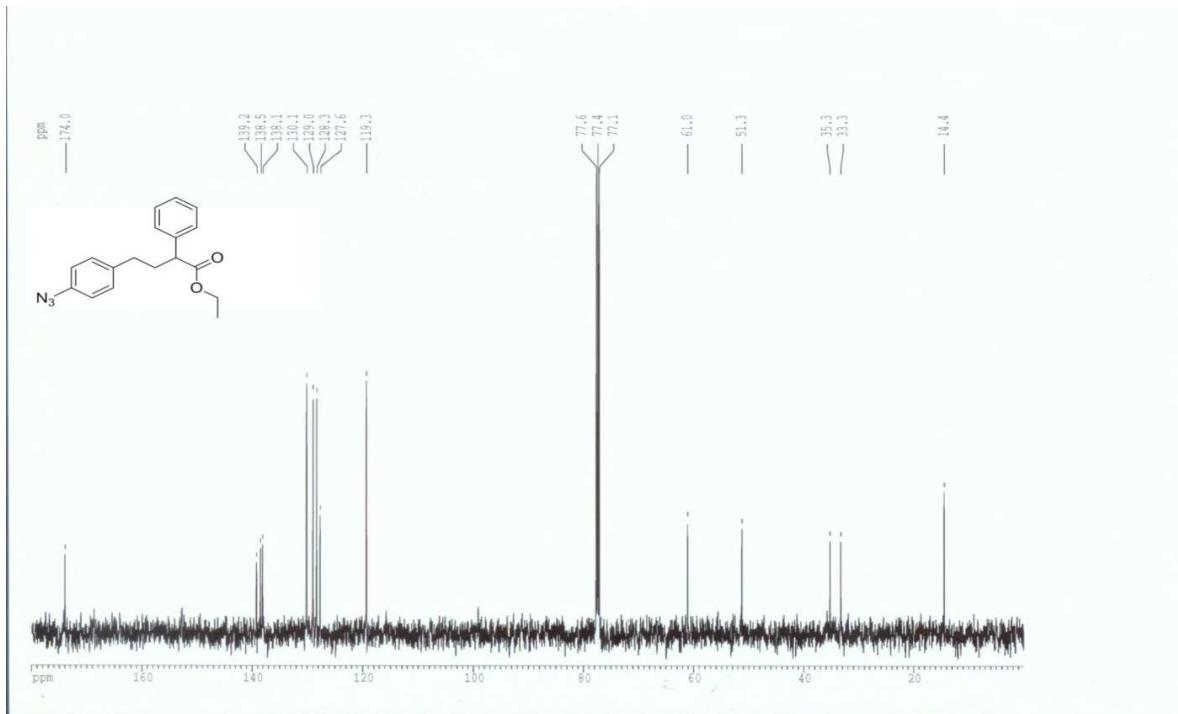


Figure S24. ^{13}C NMR spectrum of ethyl 4-(4-azidophenyl)-2-phenylbutanoate (**27**).

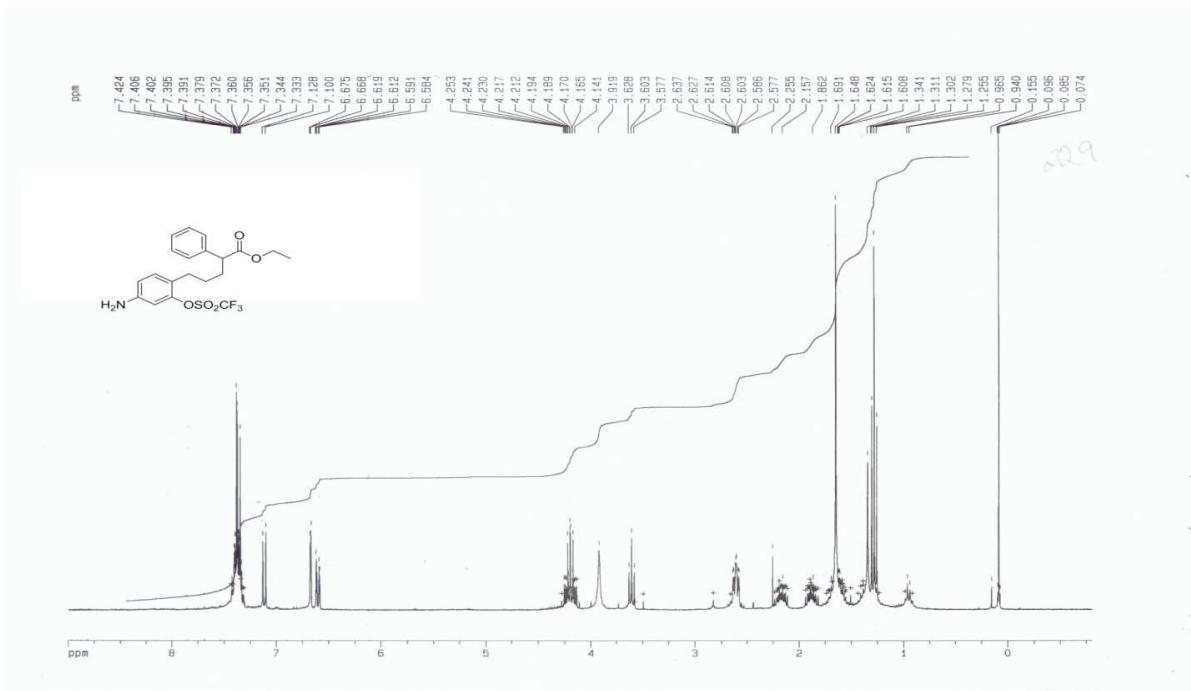


Figure S25. ^1H NMR spectrum of ethyl 5-[5-amino-2-(trifluoromethylsulfonyloxy)phenyl]-2-phenylpentanoate (**28**).

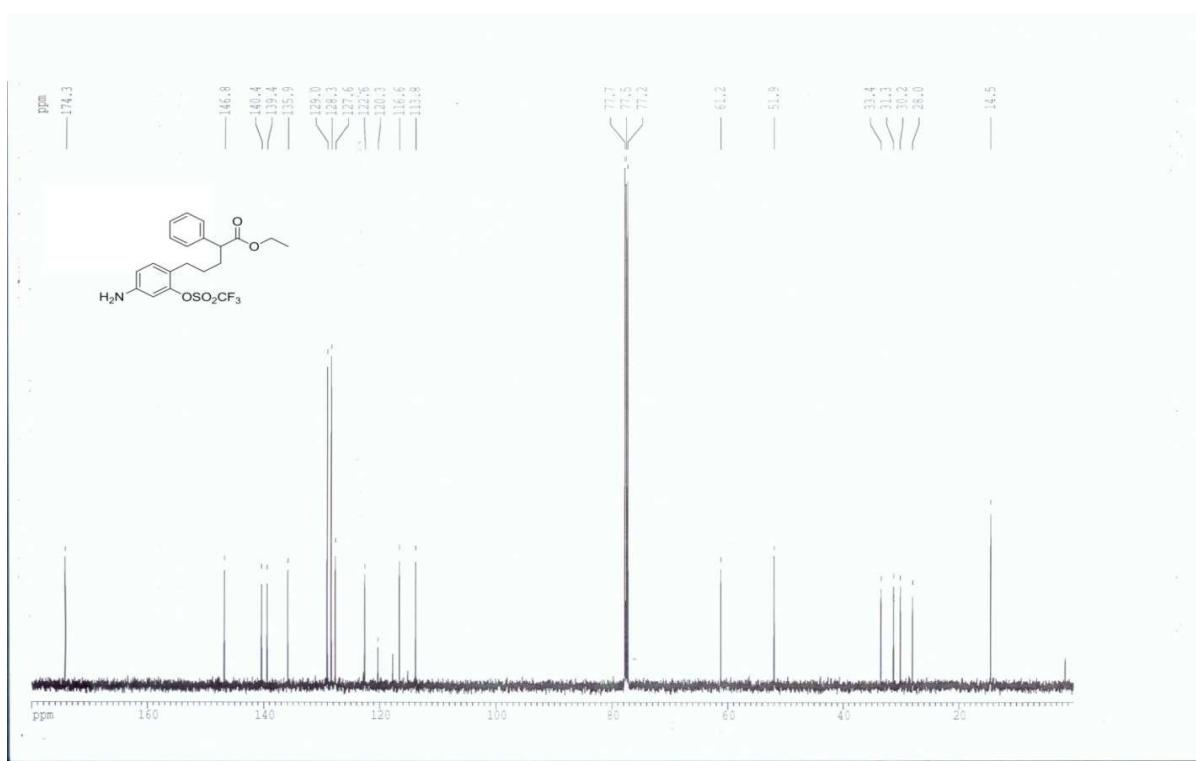


Figure S26. ^{13}C NMR spectrum of ethyl 5-[5-amino-2-(trifluoromethylsulfonyloxy)phenyl]-2-phenylpentanoate (**28**).

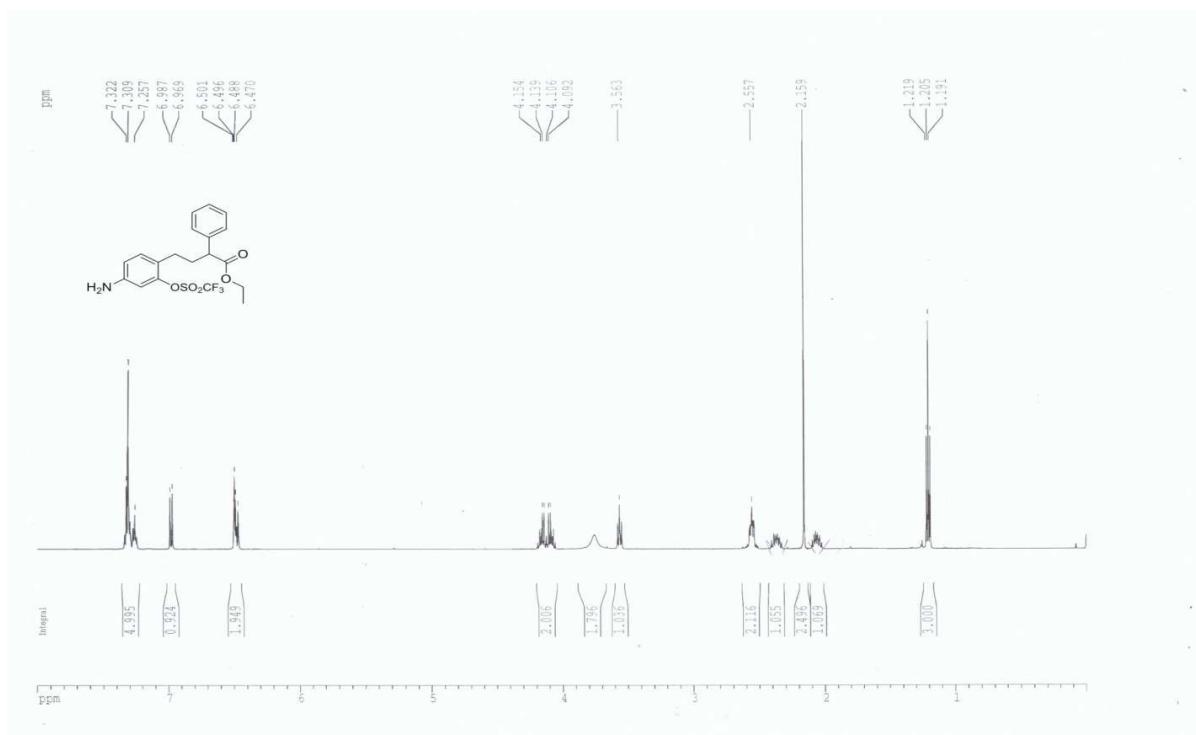


Figure S27. ^1H NMR spectrum of ethyl 4-[5-amino-2-(trifluoromethylsulfonyloxy)phenyl]-2-phenylbutanoate (**29**).

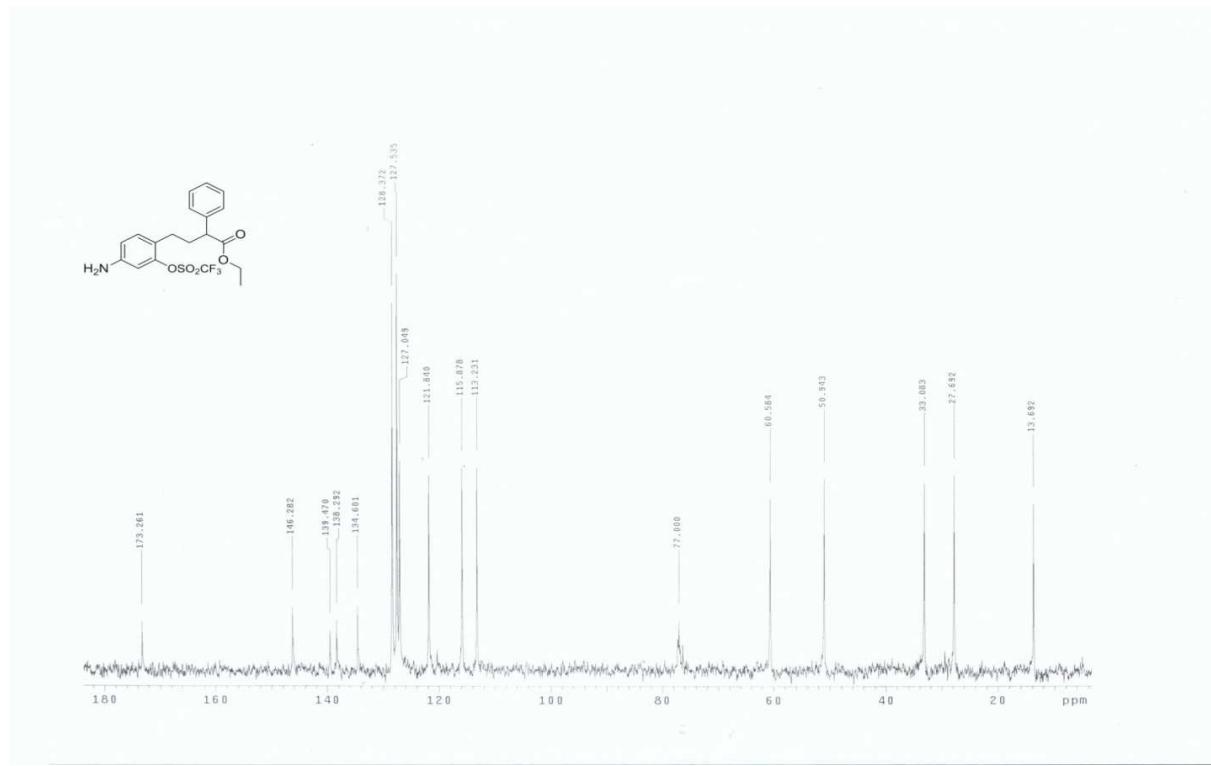


Figure S28. ^{13}C NMR spectrum of ethyl 4-[5-amino-2-(trifluoromethylsulfonyloxy)phenyl]-2-phenylbutanoate (**29**).

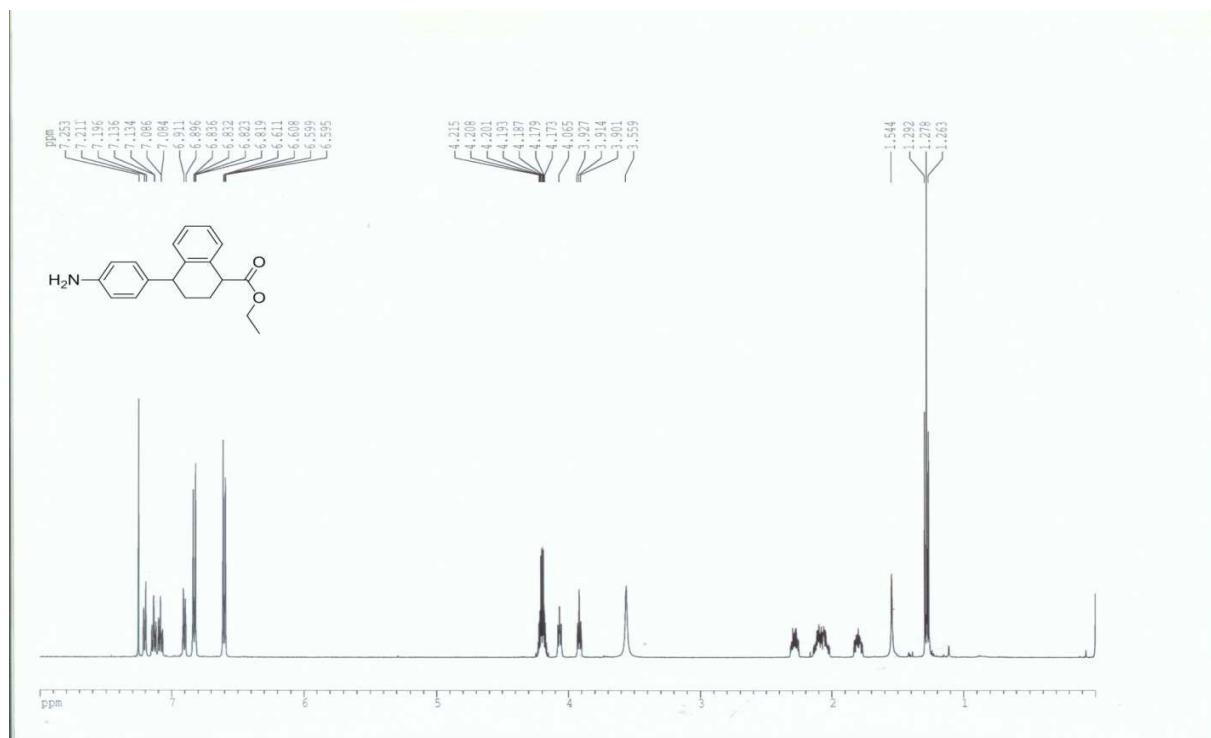


Figure S29. ^1H NMR spectrum of ethyl 4-(4-aminophenyl)-1,2,3,4-tetrahydronaphthalene-1-carboxylate (**30**).

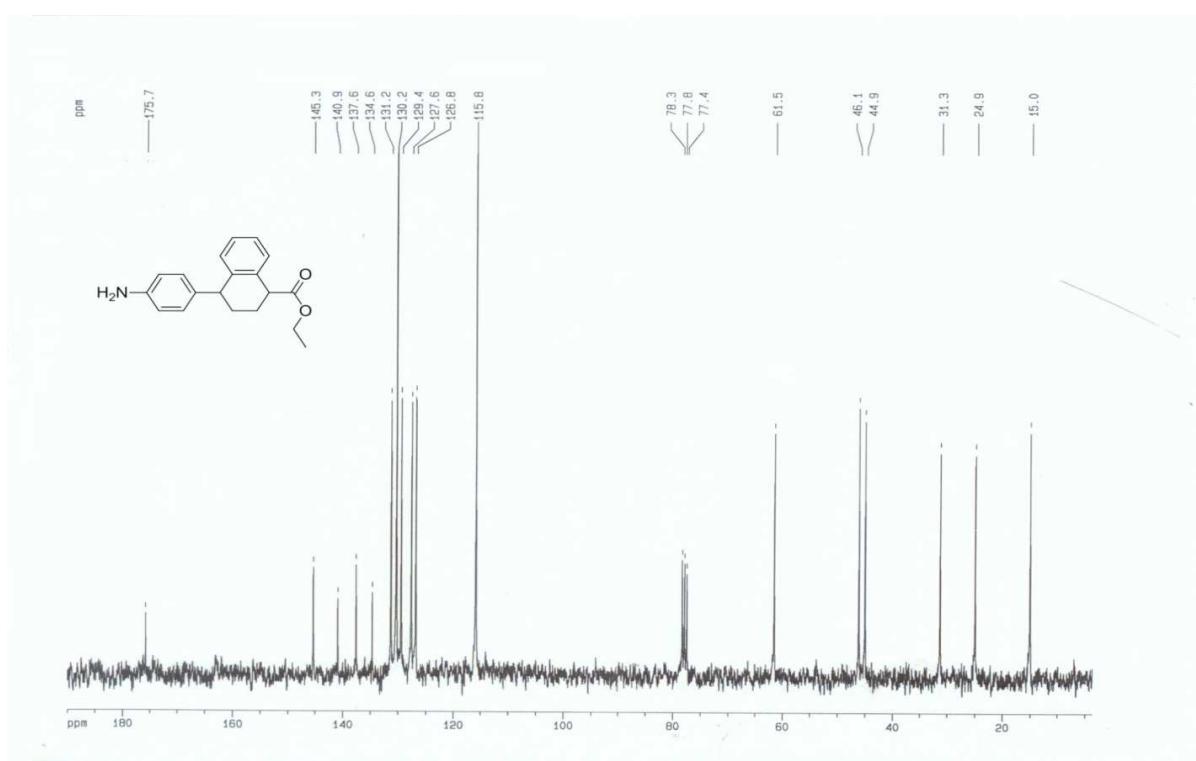


Figure S30. ^{13}C NMR spectrum of ethyl 4-(4-aminophenyl)-1,2,3,4-tetrahydronaphthalene-1-carboxylate (**30**).

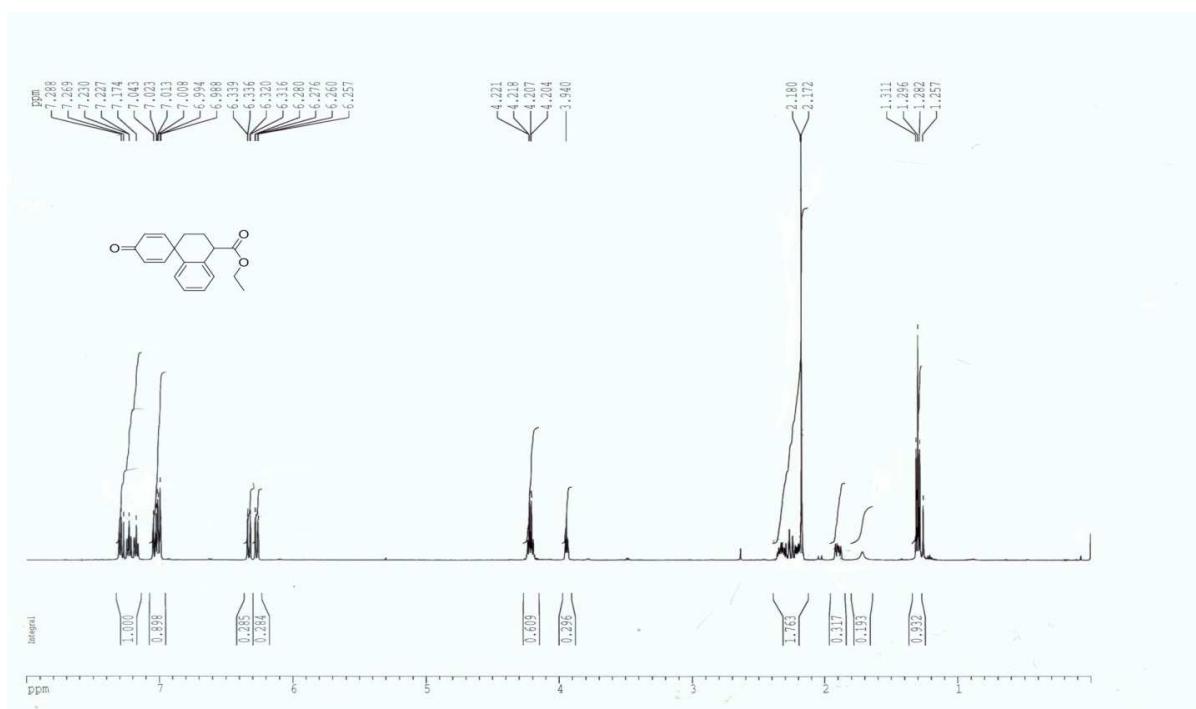


Figure S31. ^1H NMR spectrum of ethyl 4-oxo-3',4'-dihydro-2'H-spiro(cyclohexa[2,5]diene-1,1'-naphthalene)-4'-carboxylate (**31**).

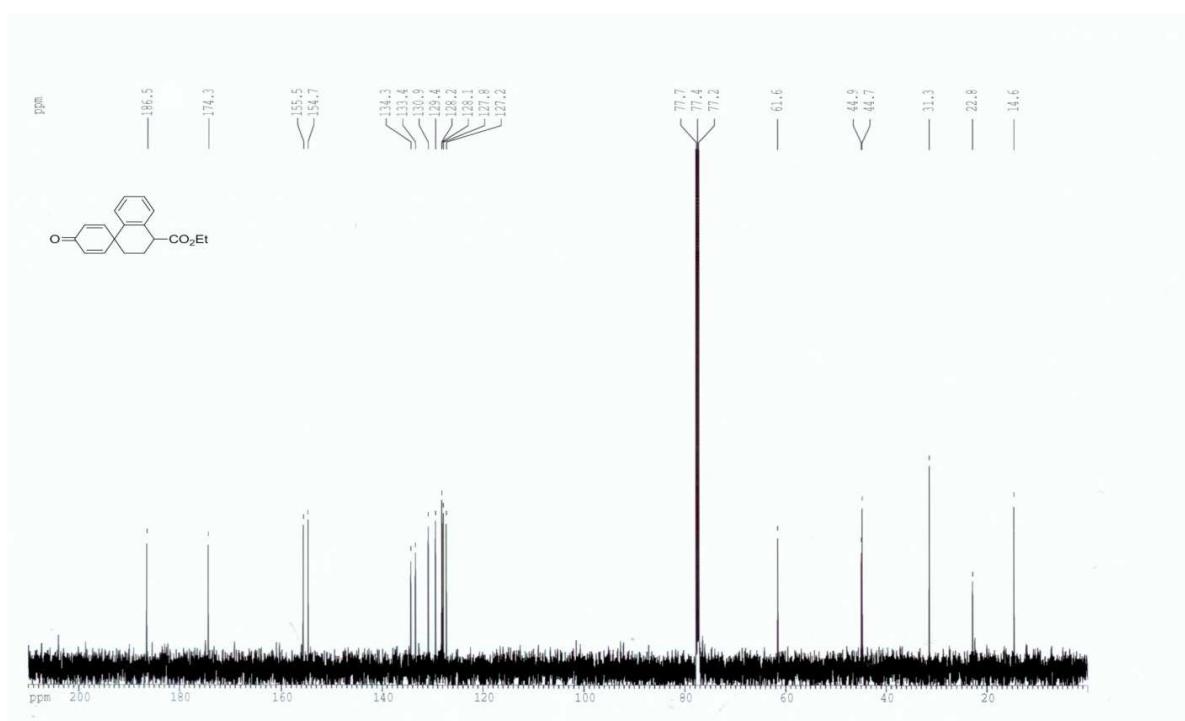


Figure S32. ^{13}C NMR spectrum of ethyl 4-oxo-3',4'-dihydro-2'H-spiro(cyclohexa[2,5]diene-1,1'-naphthalene)-4'-carboxylate (**31**).

Table S1. Crystal data and Structure Refinement for Compounds **30** and **31**.

	Compound 30	Compound 31
Empirical formula	C19 H21 N O2	C18 H18 O3
Formula weight	295.37	282.32
T/K	293(2)	293(2)
Wavelength/ \AA	1.54439	1.54439
Crystal size/mm	0.14 x 0.09 x 0.08	0.13 x 0.09 x 0.06
Color of crystal	colourless	colourless
Crystal system	Monoclinic	Monoclinic
Space group	P2 ₁	P2 ₁ /n
a/ \AA	11.077(2)	12.472(3)
b/ \AA	5.958(3)	9.898(2)
c/ \AA	12.778(2)	12.538(4)
β/deg	103.792(10)	104.47(2)

$V/\text{\AA}^3$	818.9(5)	1498.7(7)
Z	2	4
$\rho_{\text{calcd}}/\text{g}\cdot\text{cm}^{-3}$	1.198	1.251
μ/mm^{-1}	0.611	0.678
$F(000)$	316	600
θ limits/deg	3.56 - 66.77.	4.48 to 67.27
Limiting indices	-1 ≤ h ≤ 13 -1 ≤ k ≤ 7 -15 ≤ l ≤ 15	-14 ≤ h ≤ 14 -11 ≤ k ≤ 0 -14 ≤ l ≤ 14
Reflections collected/unique	2218 / 1909 [R(int) = 0.0382]	5301 / 2659 [R(int) = 0.1232]
Completeness to θ	100% ($\theta = 66.77$)	99.9% ($\theta = 67.27$)
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	1909 / 3 / 265	2659 / 1 / 234
GOF on F^2	1.082	1.015
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0602$	$R_1 = 0.0717$
R indices (all data)	$R_1 = 0.0648$	$R_1 = 0.1409$
Absolute structure parameter	0.6(11)	-
Extinction coefficient	0.025(3)	-
Largest diff. peak and hole/e. \AA^{-3}	0.321 and -0.226	0.400 and -0.329