

Brønsted Acid-Catalyzed, Enantioselective Synthesis of 1,4-Dihydroquinoline-3-Carboxylates via In Situ Generated *ortho*-Quinone Methide Imines

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Supporting Information

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Important note:

Minor impurities in some NMR-spectra and HPLC-chromatograms relate to decomposed products. This decomposition takes place during work-up and chromatography and cannot be fully suppressed.

¹H and ¹³C APT NMR Spectral Characterization of the Novel Compounds

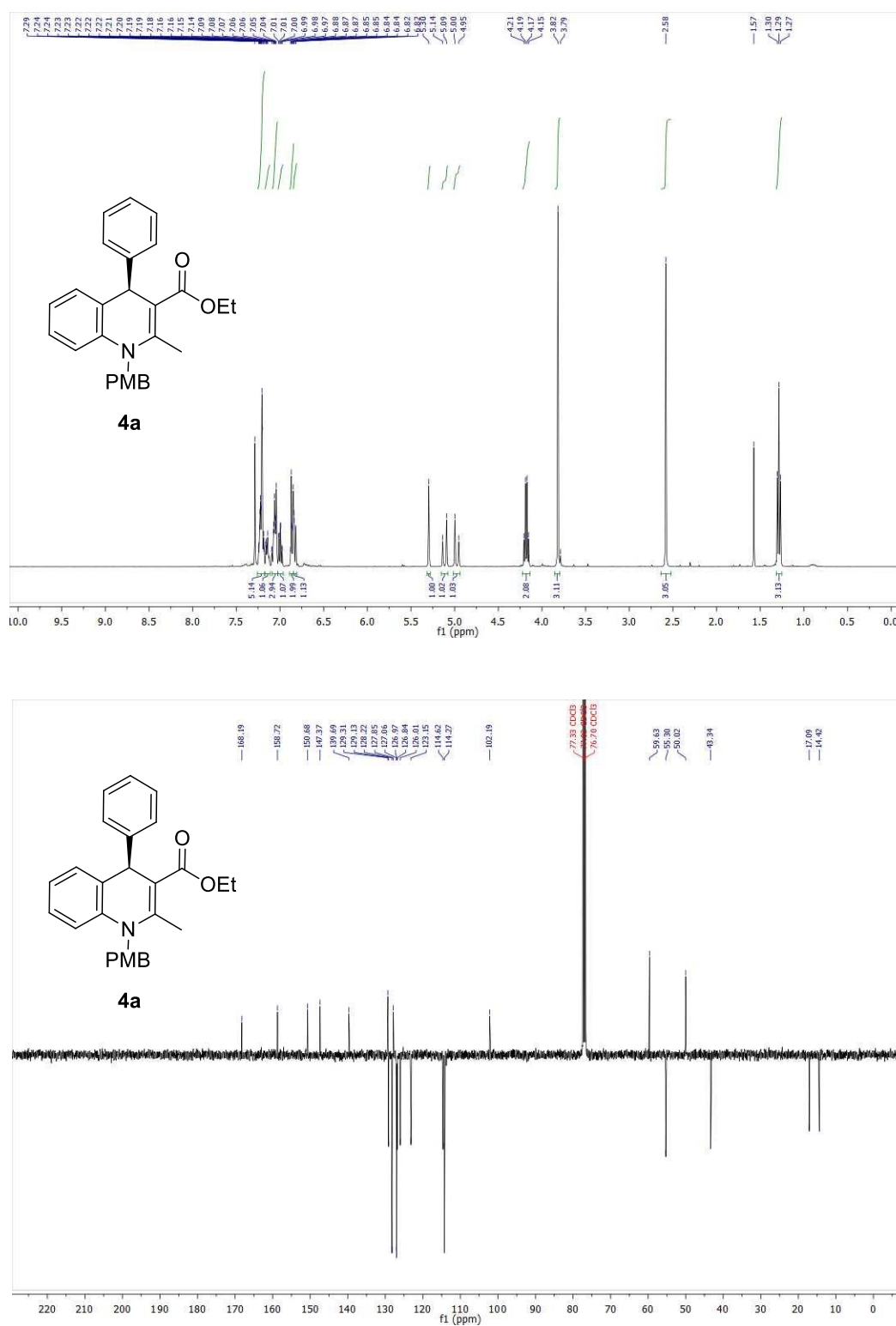


Figure 1.1. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**4a**).

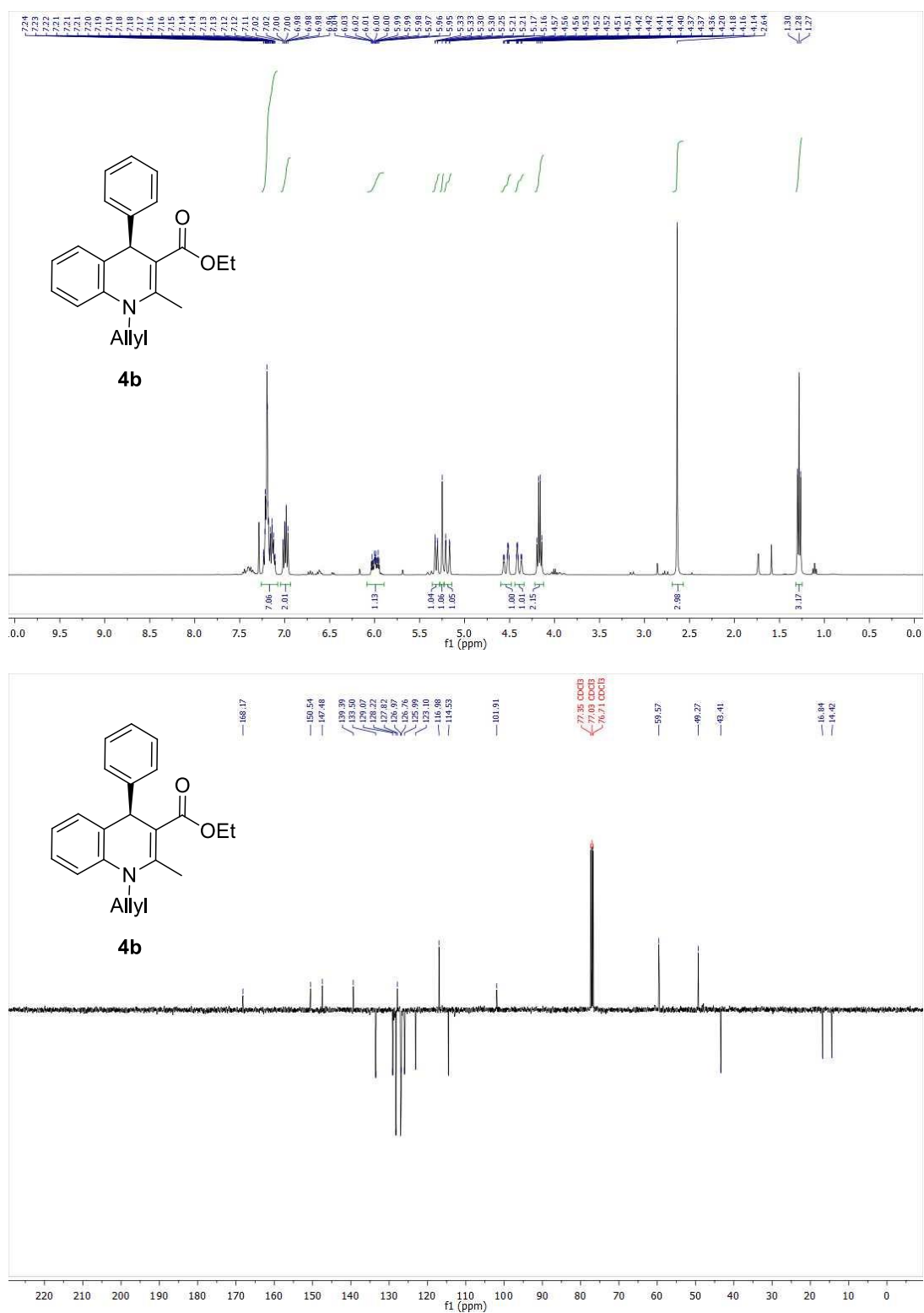


Figure 1.2. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of *(R)*-ethyl 1-allyl-2-methyl-4-phenyl-1,4-carboxylate (**4b**).

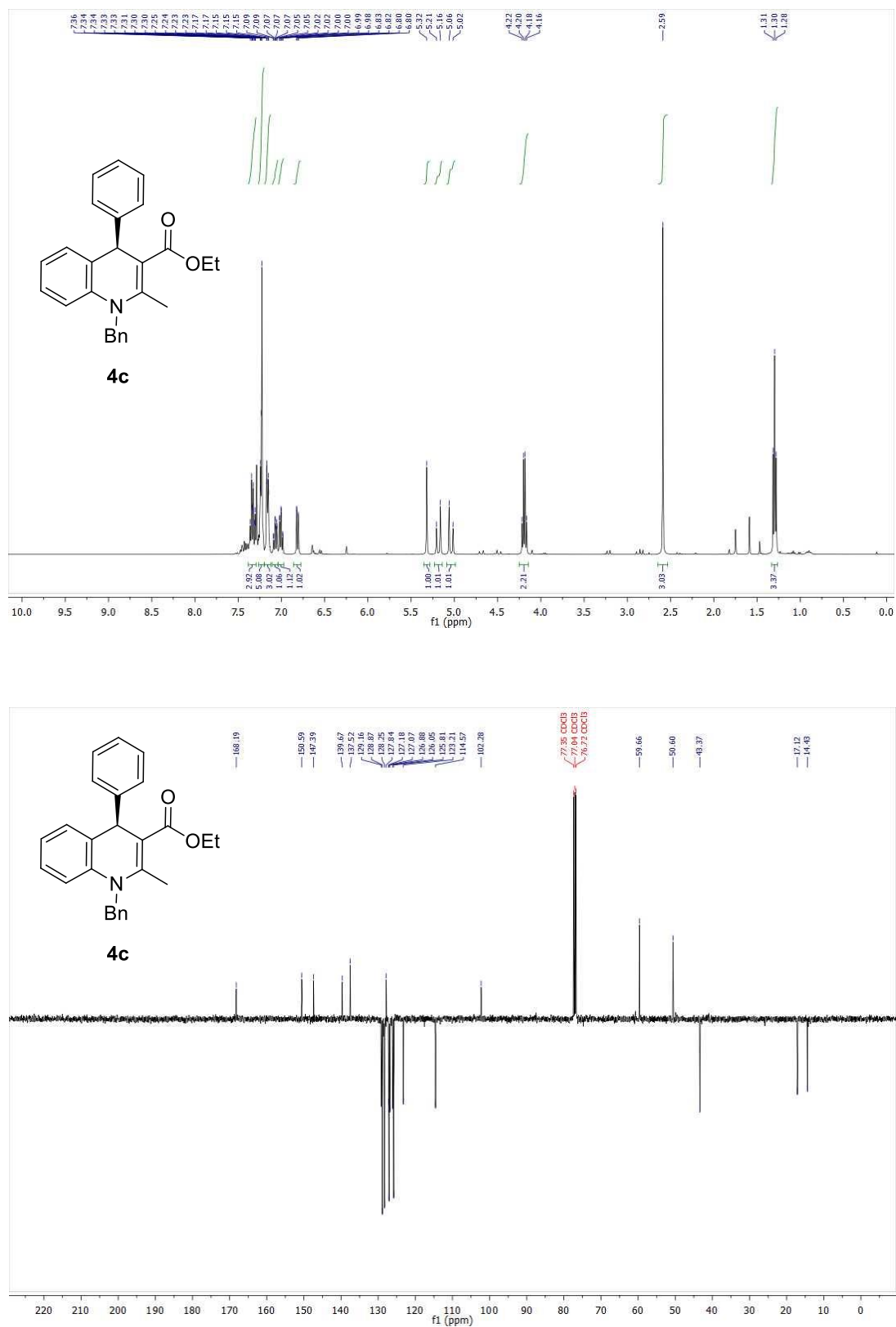


Figure 1.3. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 1-benzyl-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**4c**).

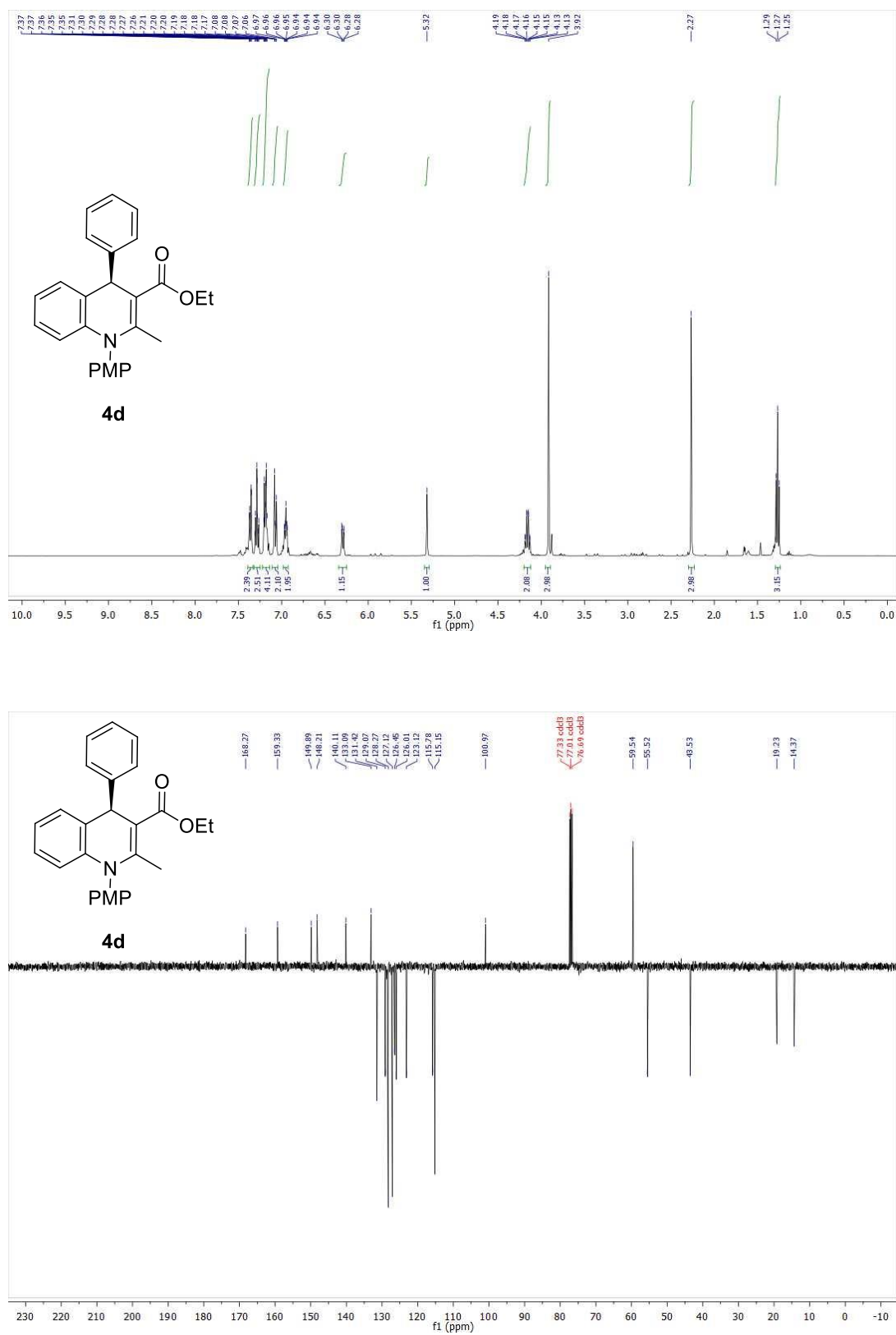


Figure 1.4. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 1-(4-methoxyphenyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**4d**).

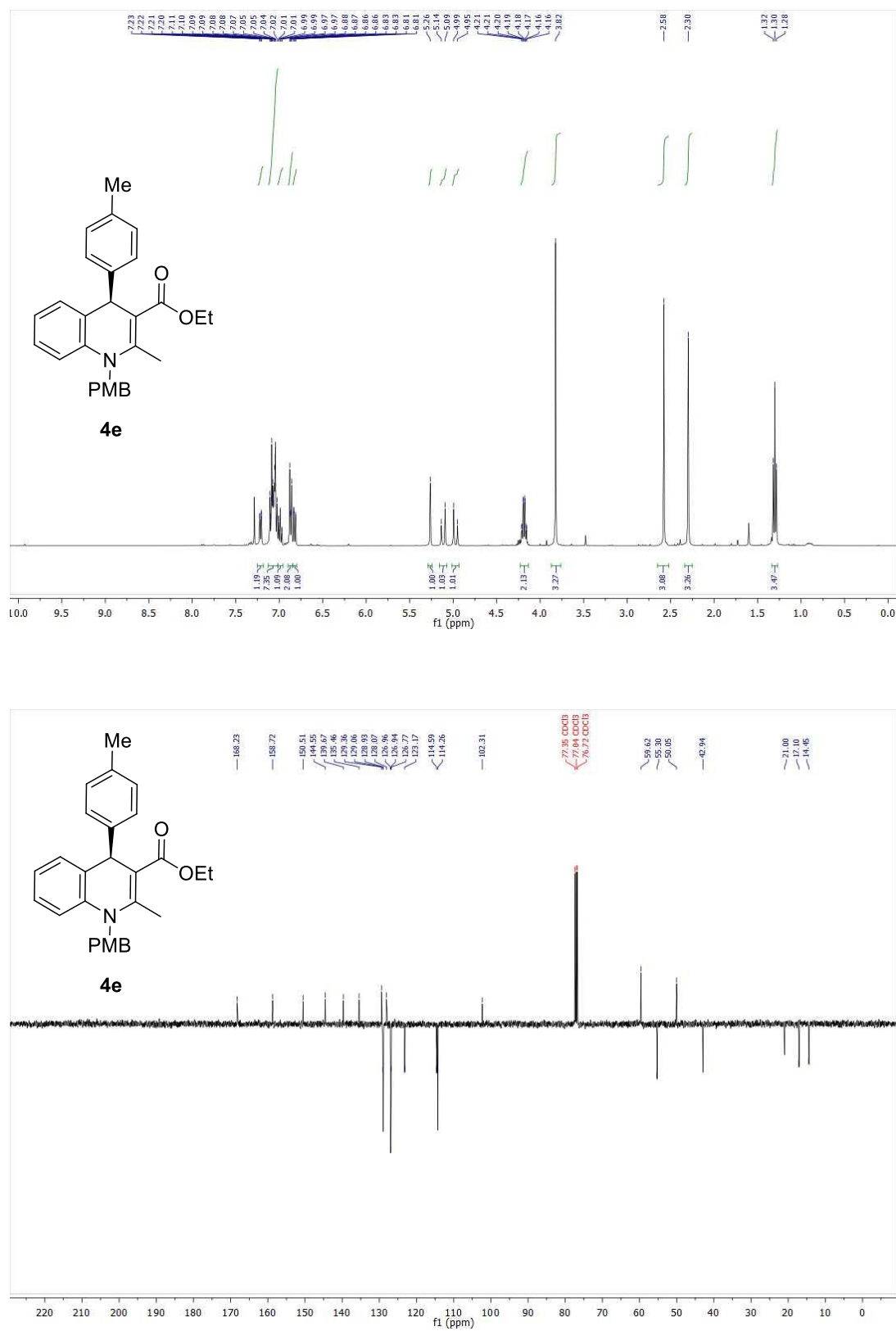


Figure 1.5. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 1-(4-methoxybenzyl)-2-methyl-4-(*p*-tolyl)-1,4-dihydroquinoline-3-carboxylate (**4e**).

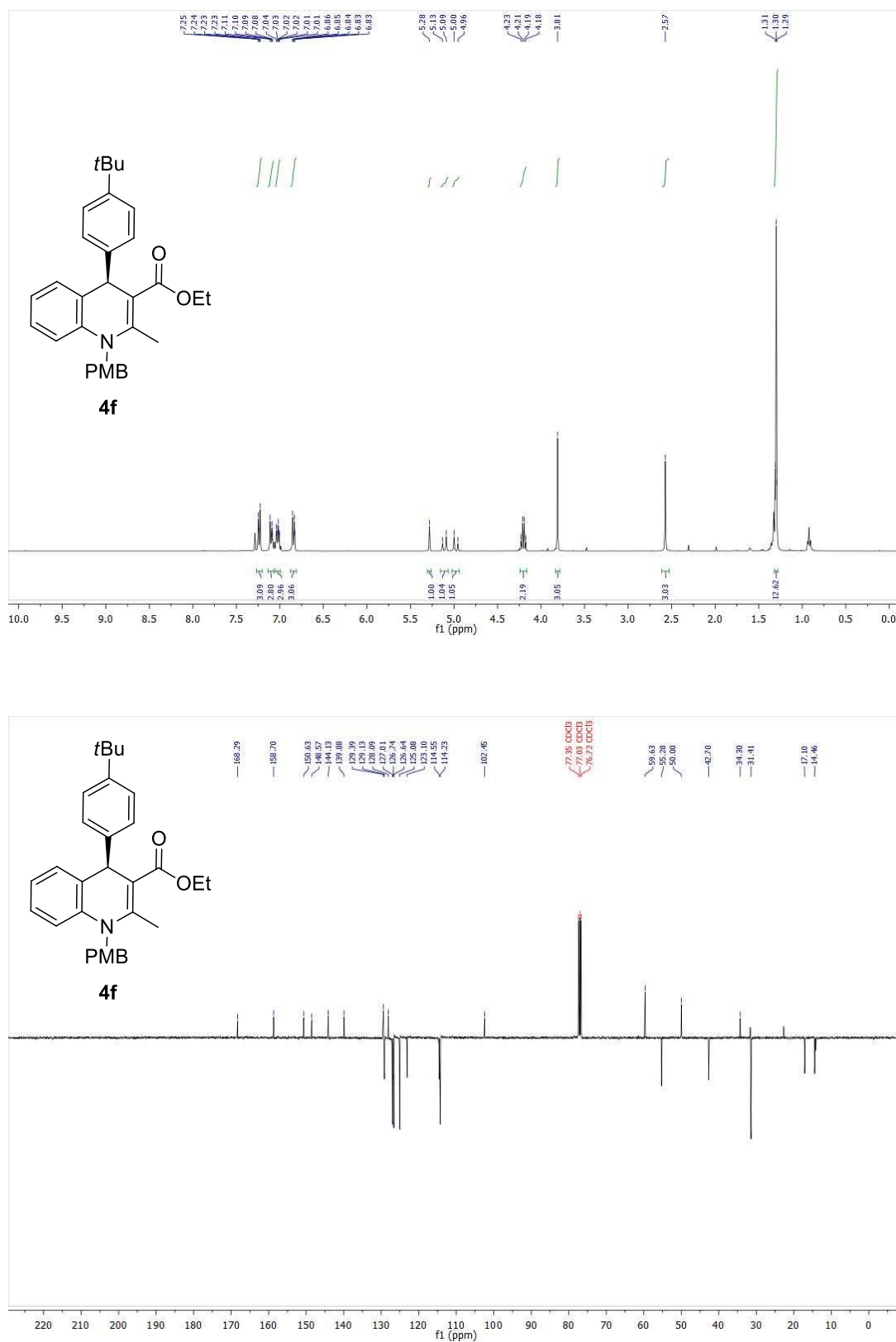


Figure 1.6. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 4-[4-(*tert*-butyl)phenyl]-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**4f**).

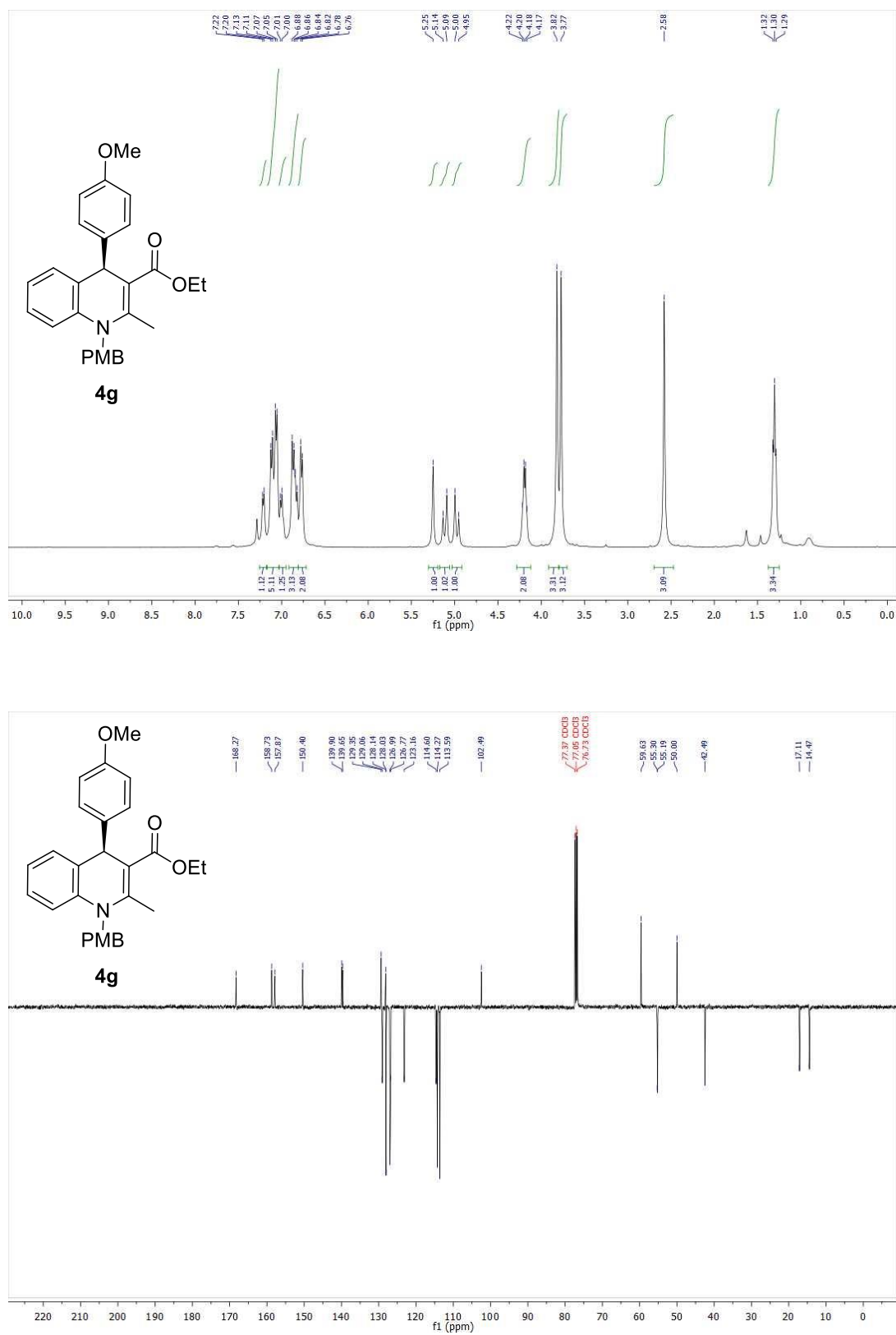


Figure 1.7. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 1-(4-methoxybenzyl)-4-(4-methoxyphenyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**4g**).

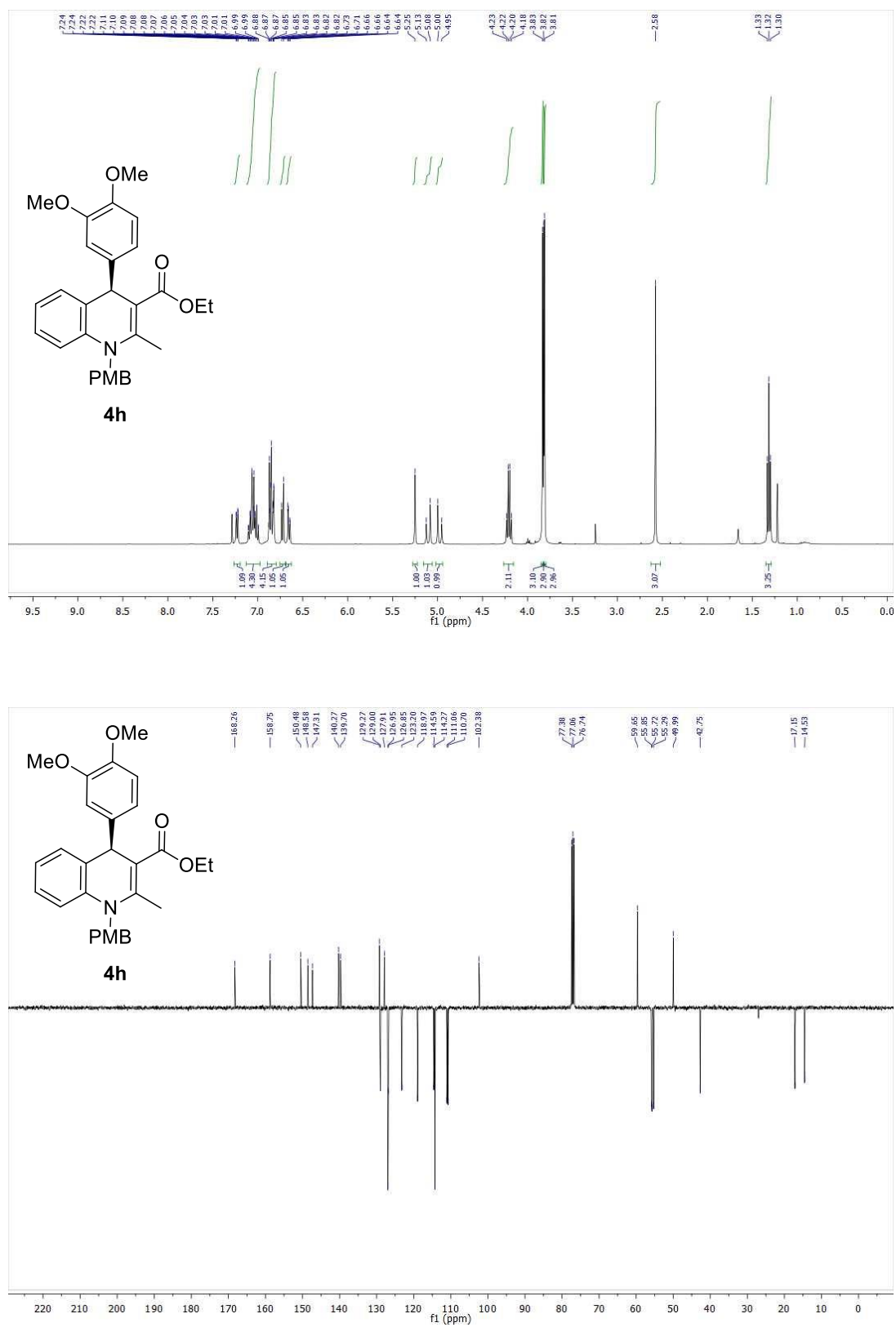


Figure 1.8. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 4-(3,4-dimethoxyphenyl)-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**4h**).

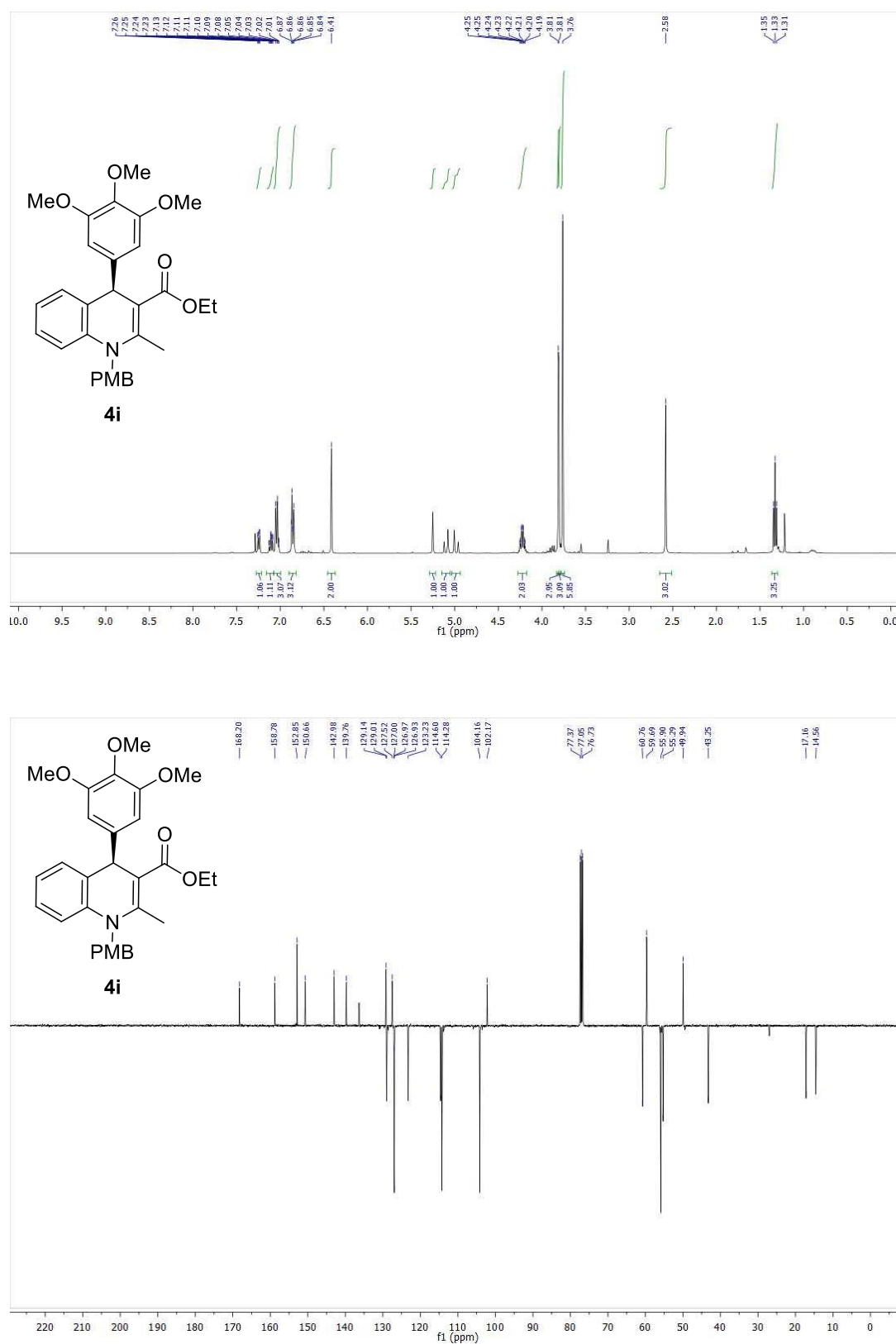


Figure 1.9. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 1-(4-methoxybenzyl)-2-methyl-4-(3,4,5-trimethoxyphenyl)-1,4-dihydroquinoline-3-carboxylate (**4i**).

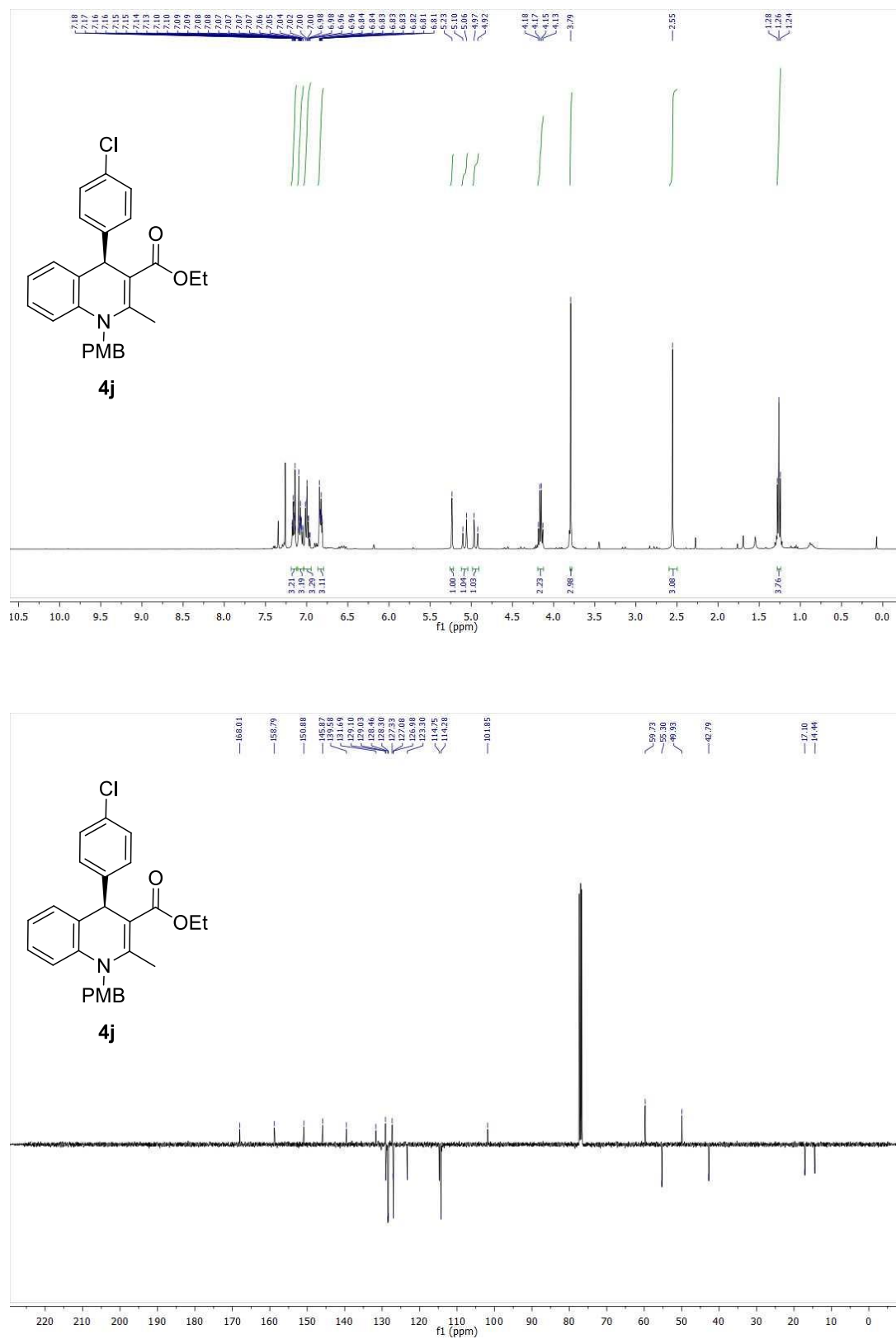


Figure 1.10. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of *(R)*-ethyl 4-(4-chlorophenyl)-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**4j**).

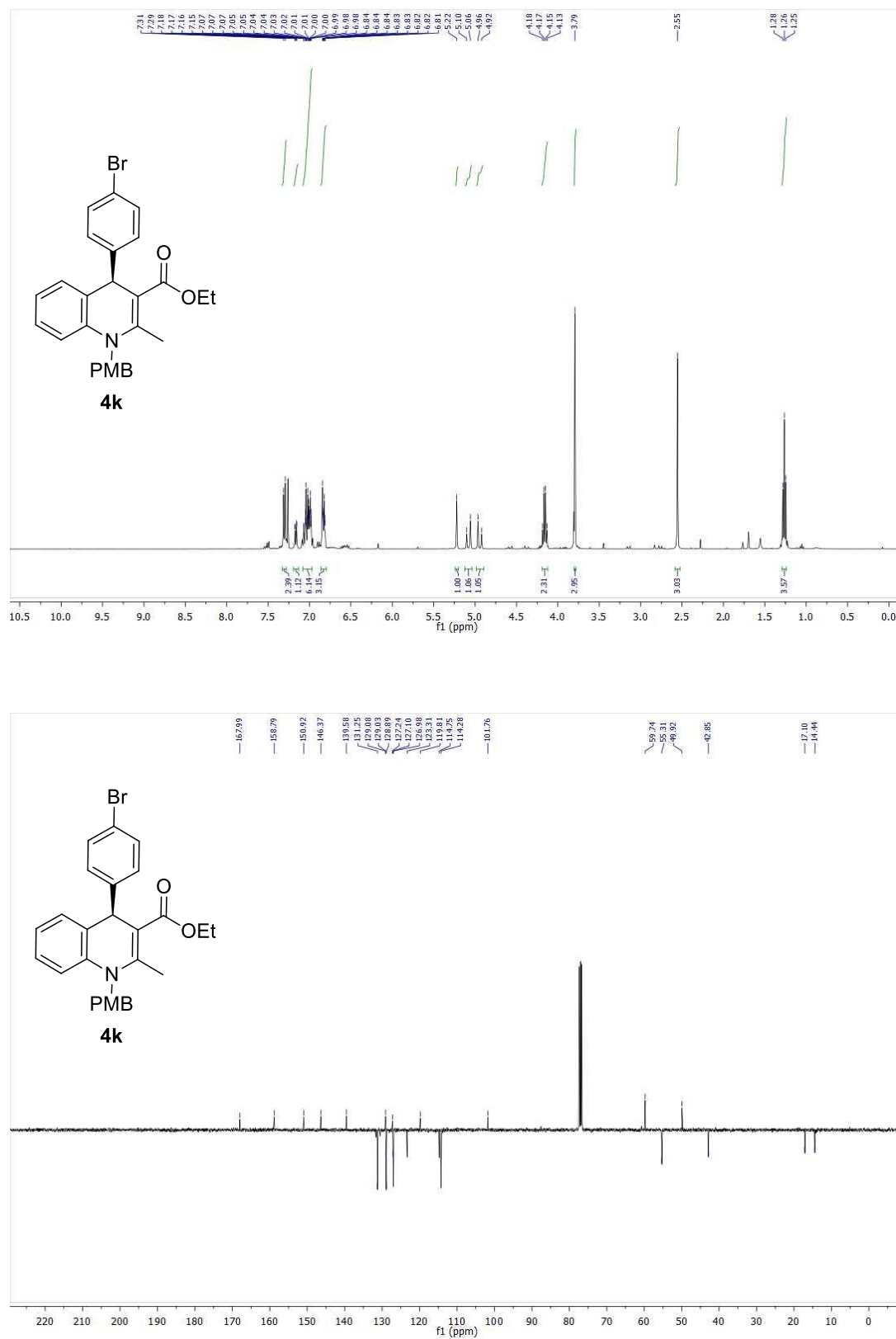


Figure 1.11. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of *(R)*-ethyl 4-(4-bromophenyl)-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**4k**).

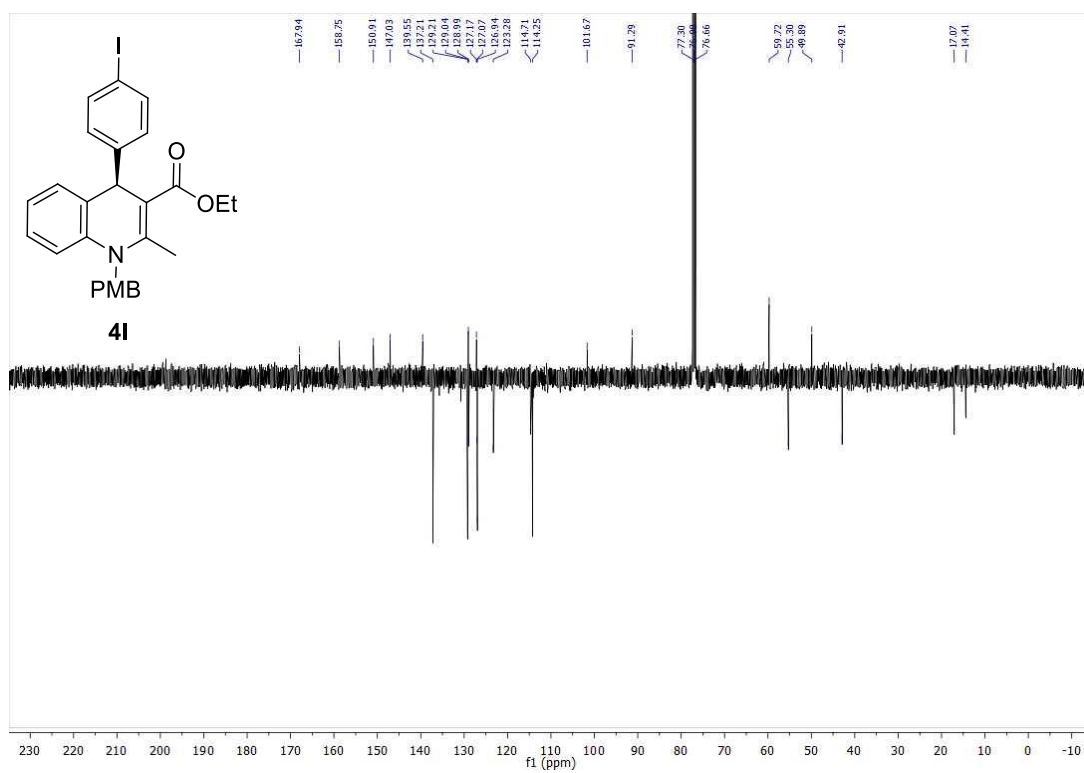
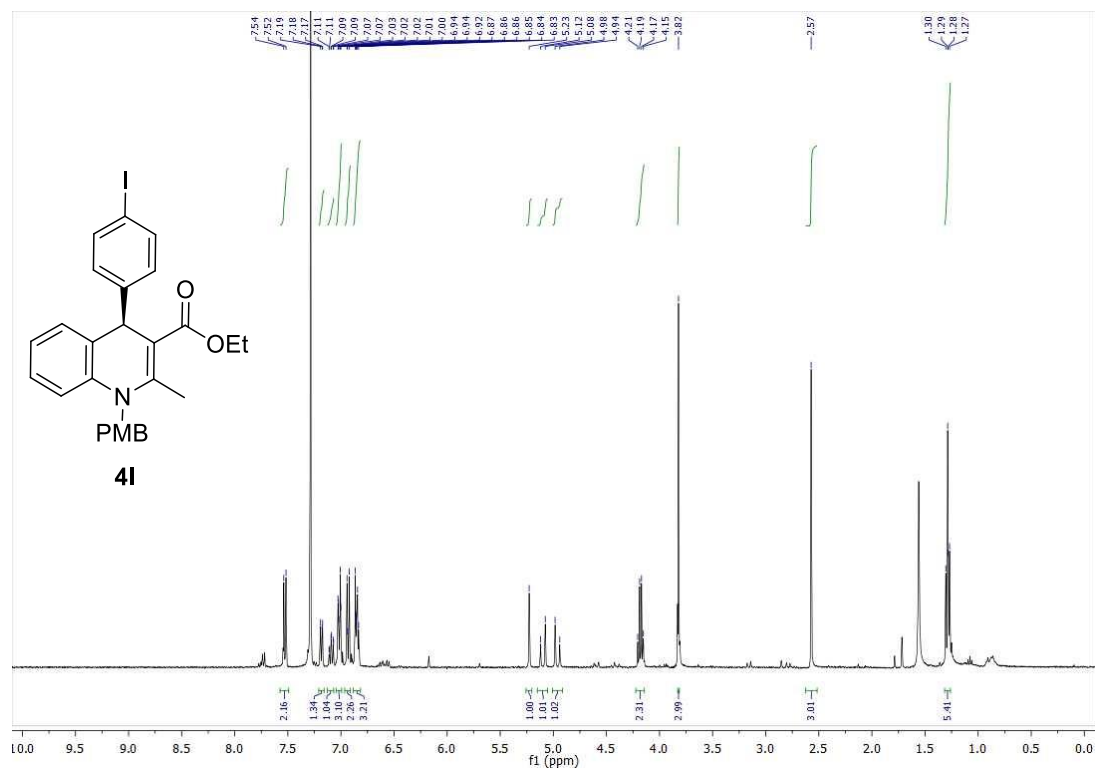


Figure 1.12. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 4-(4-iodophenyl)-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**4I**).

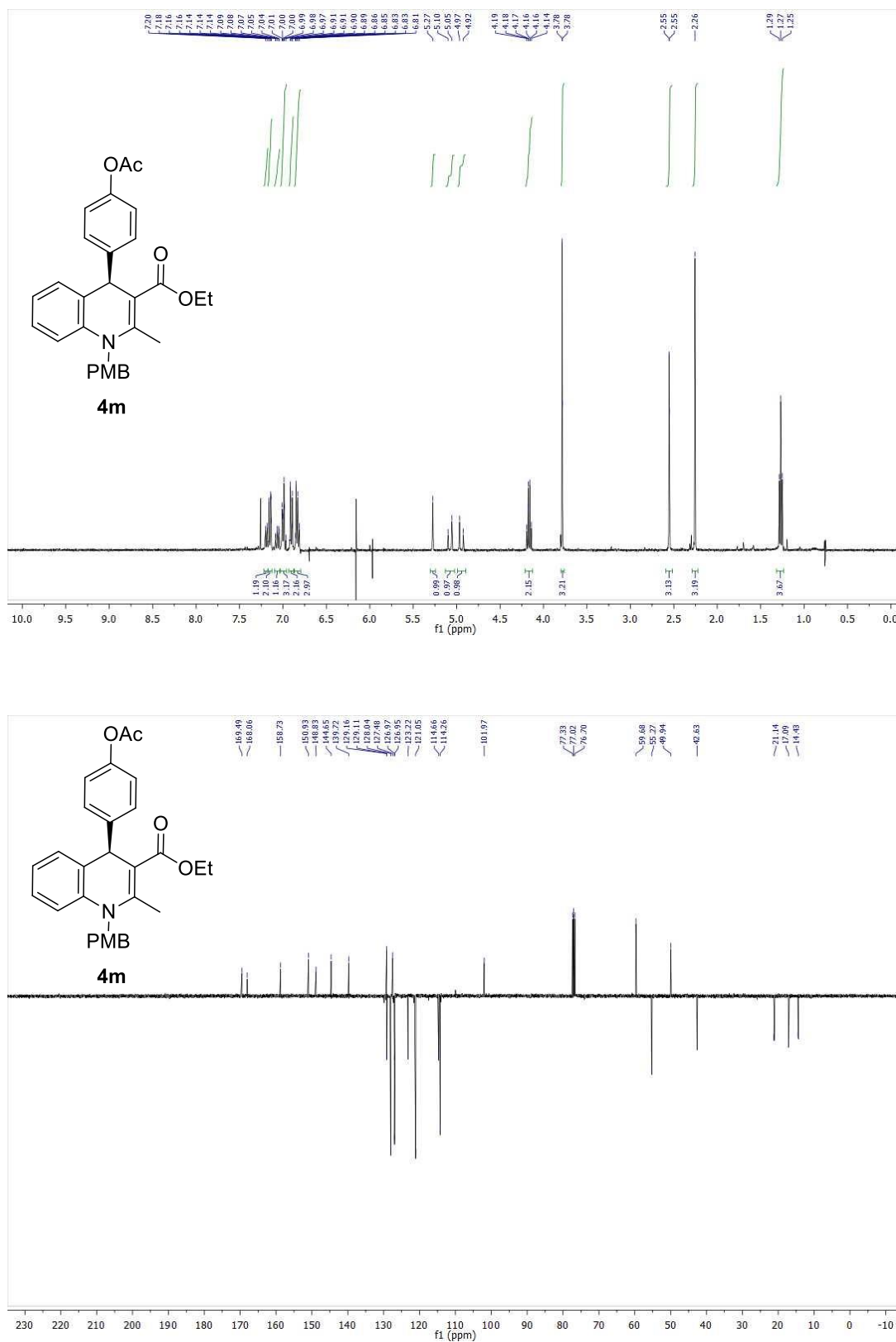


Figure 1.13. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 4-(4-acetoxyphenyl)-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**4m**).

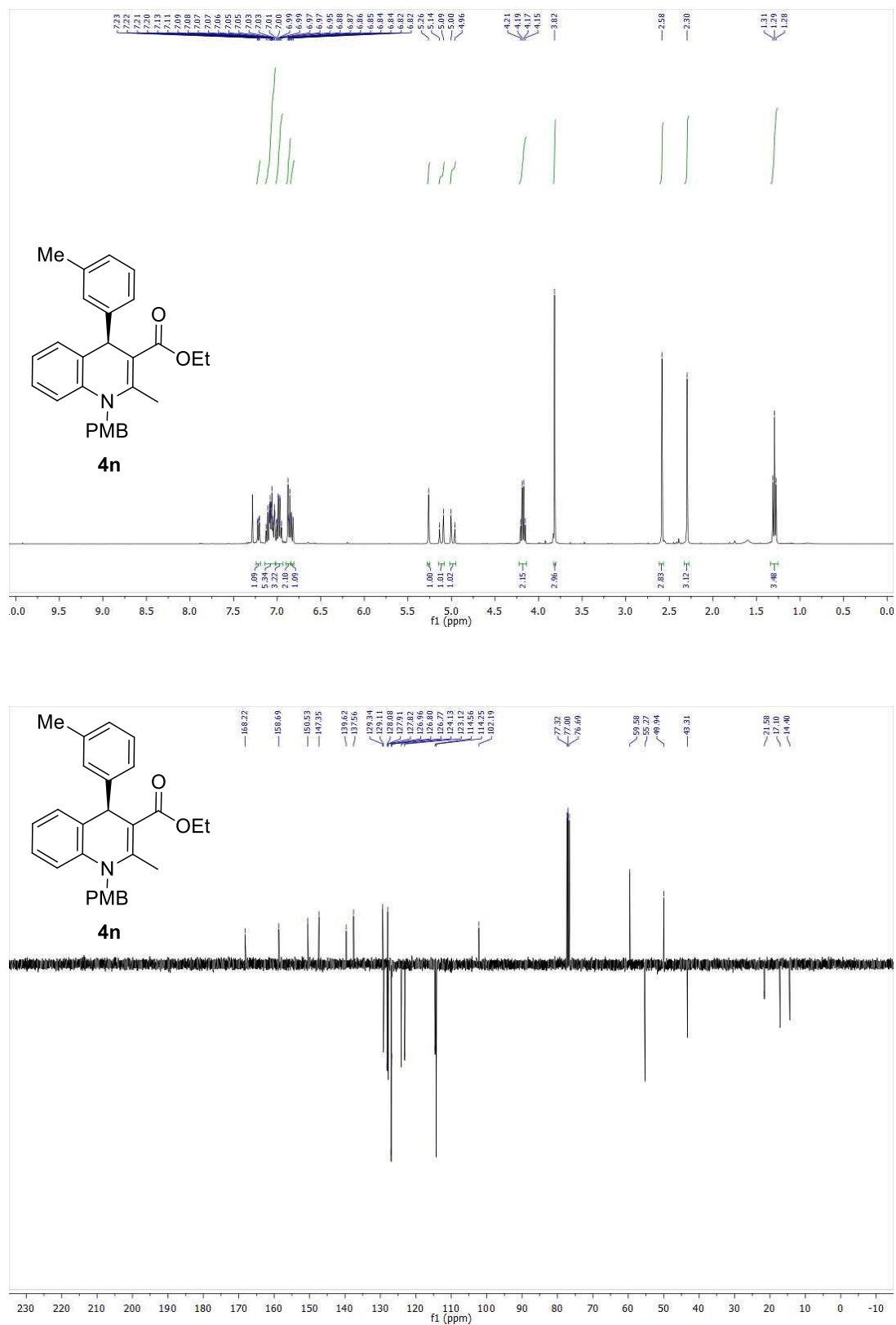


Figure 1.14. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 1-(4-methoxybenzyl)-2-methyl-4-(*m*-tolyl)-1,4-dihydroquinoline-3-carboxylate (**4n**).

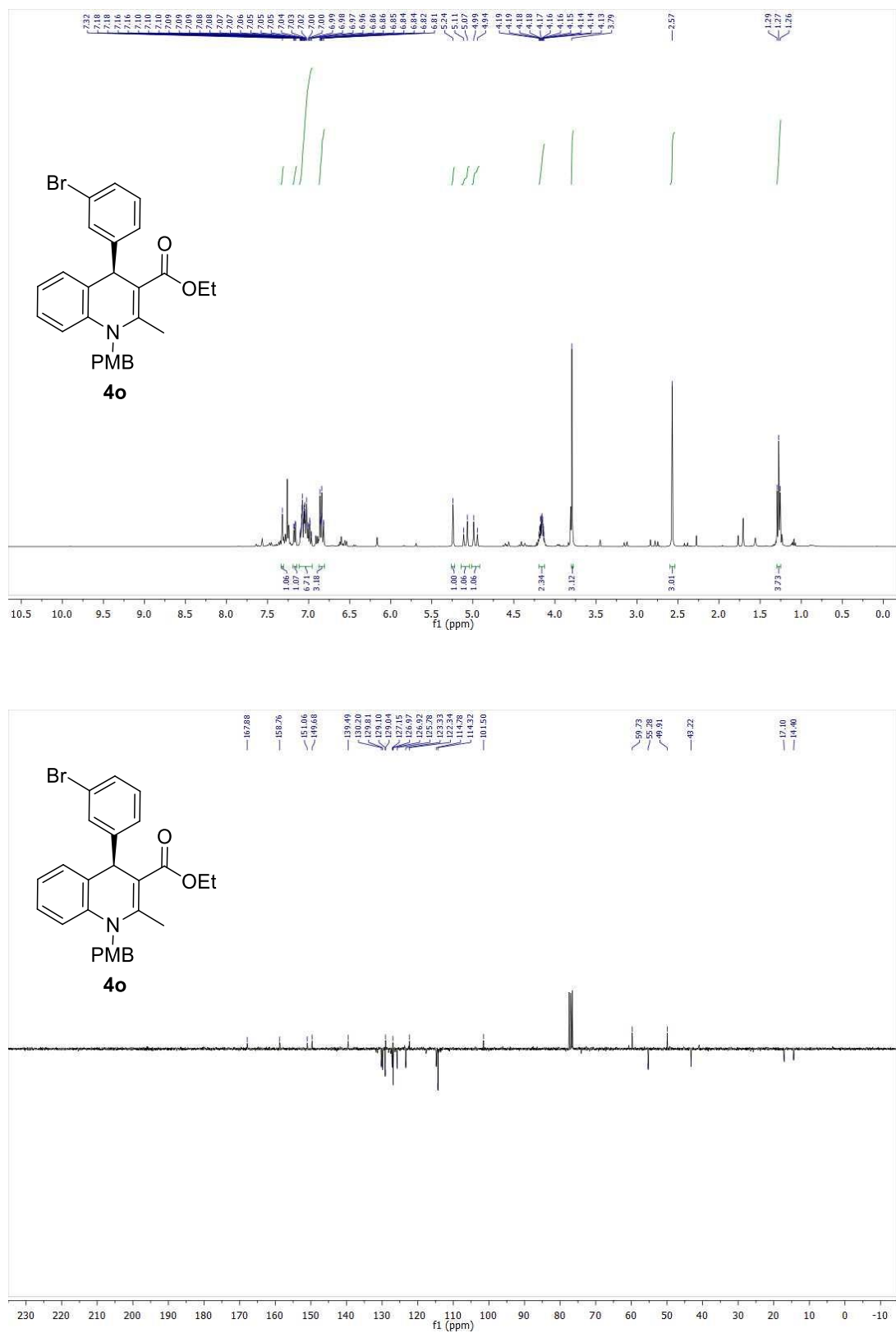


Figure 1.15. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 4-(3-bromophenyl)-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**4o**).

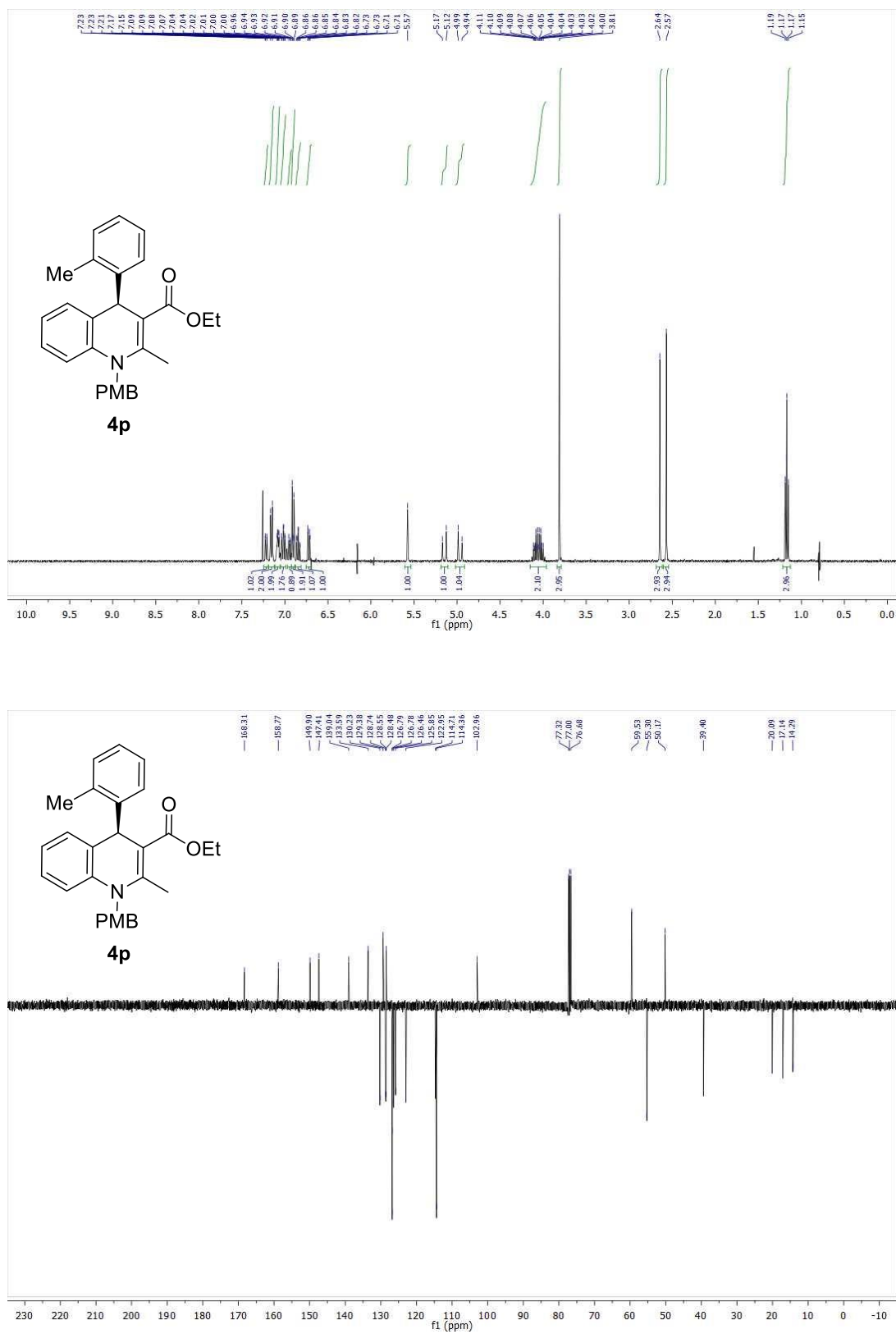


Figure 1.16. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 1-(4-methoxybenzyl)-2-methyl-4-(*o*-tolyl)-1,4-dihydroquinoline-3-carboxylate (**4p**).

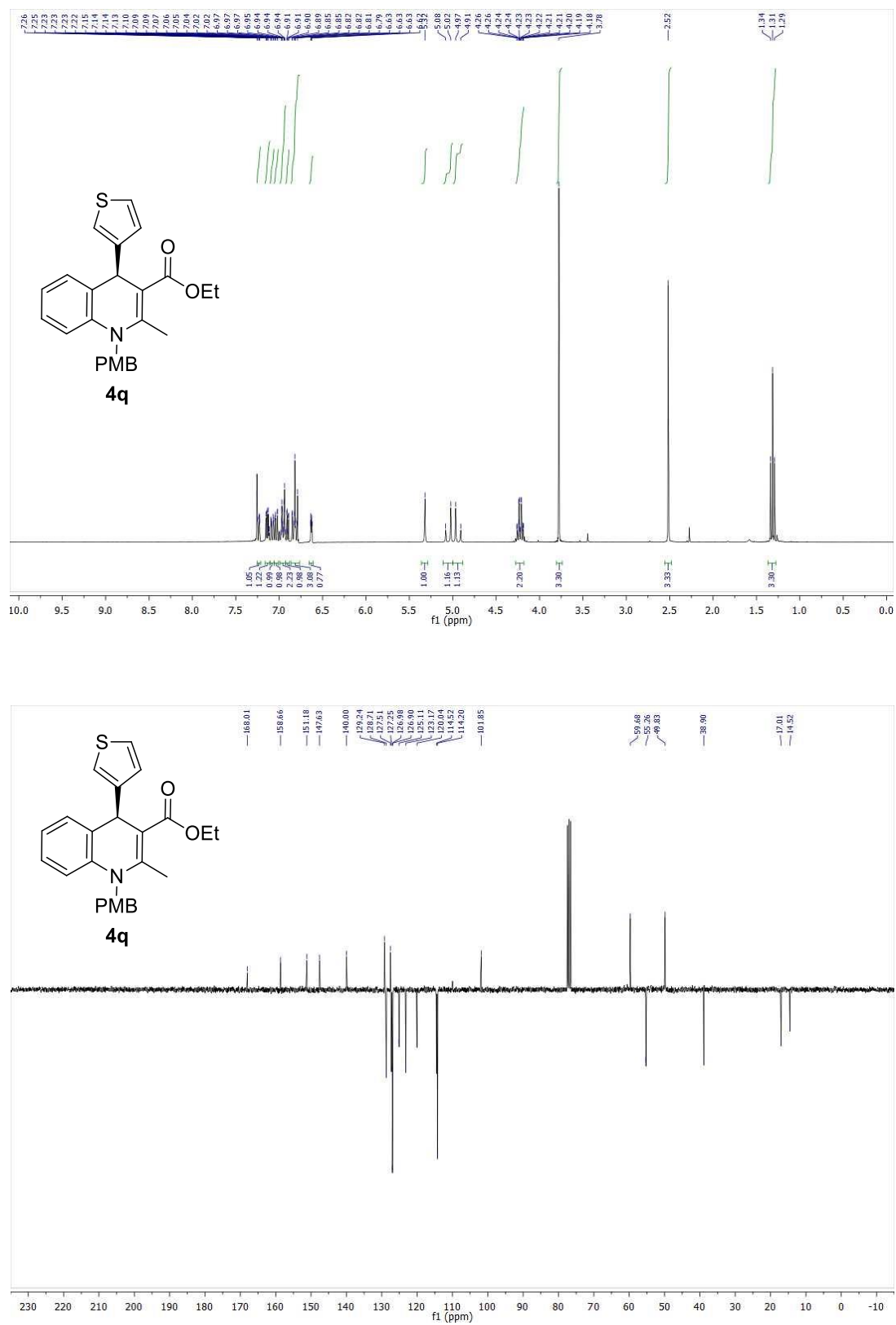


Figure 1.17. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 1-(4-methoxybenzyl)-2-methyl-4-(thiophen-3-yl)-1,4-dihydroquinoline-3-carboxylate (**4q**).

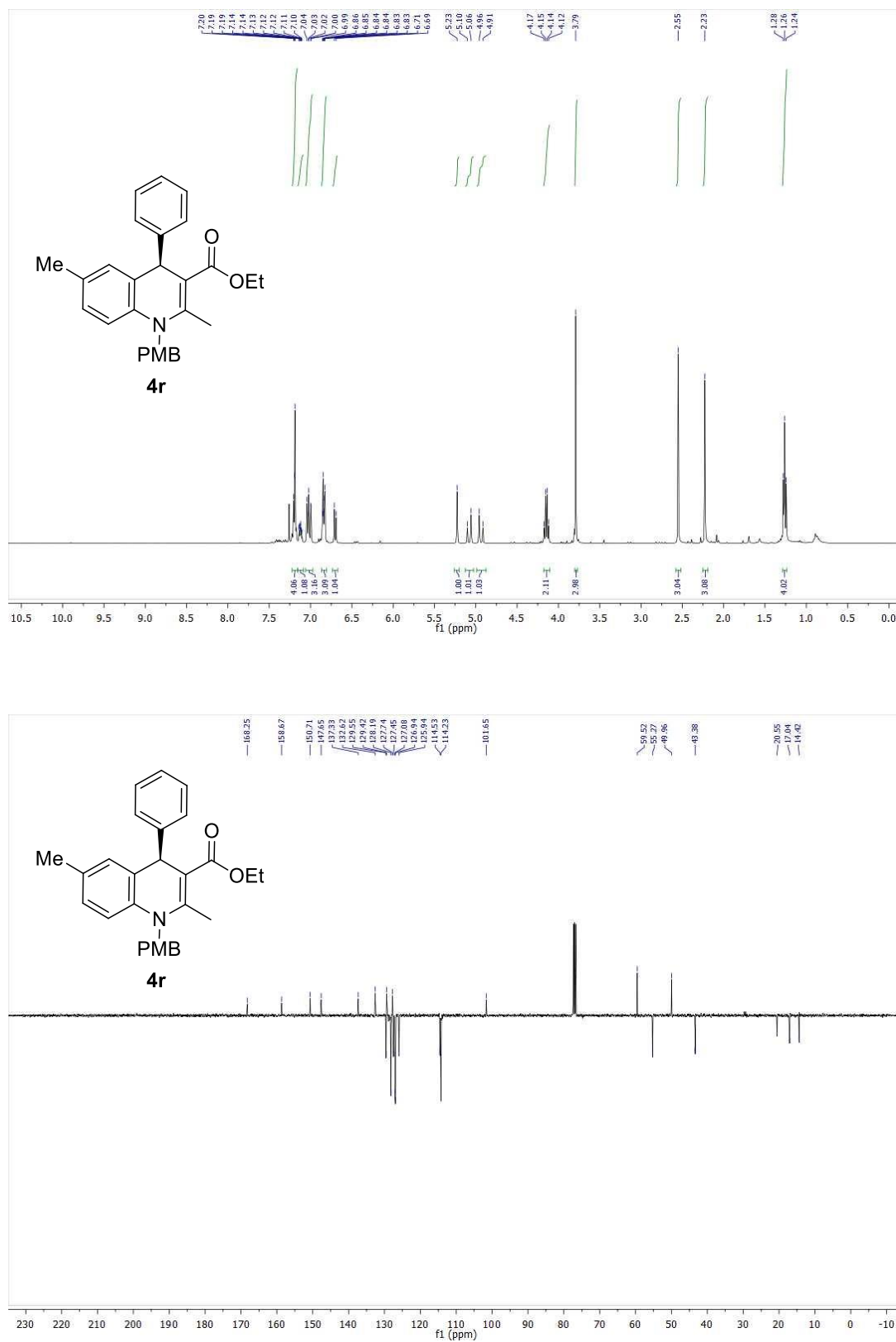


Figure 1.18. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 1-(4-methoxybenzyl)-2,6-dimethyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**4r**).

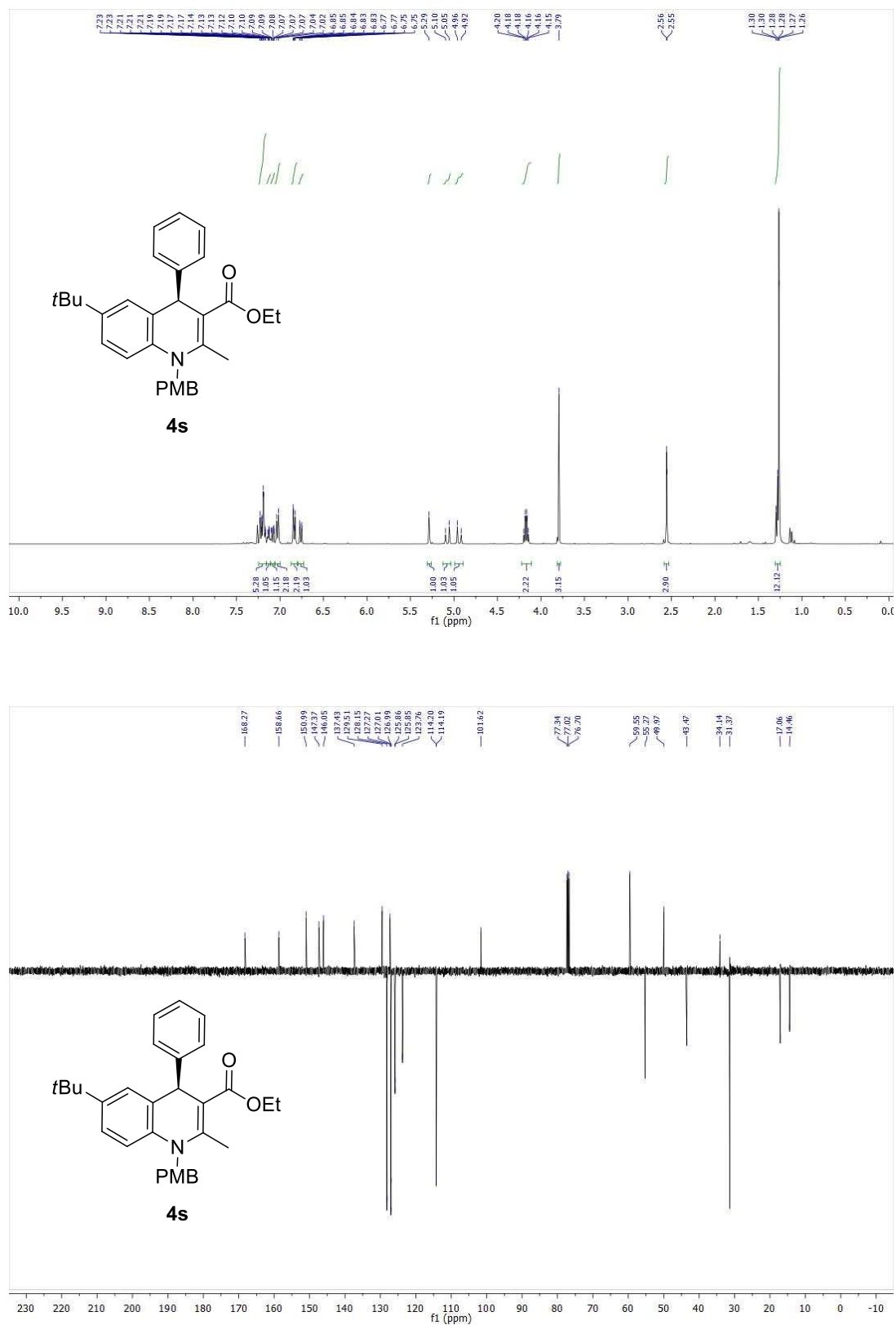


Figure 1.19. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 6-(*tert*-butyl)-1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**4s**).

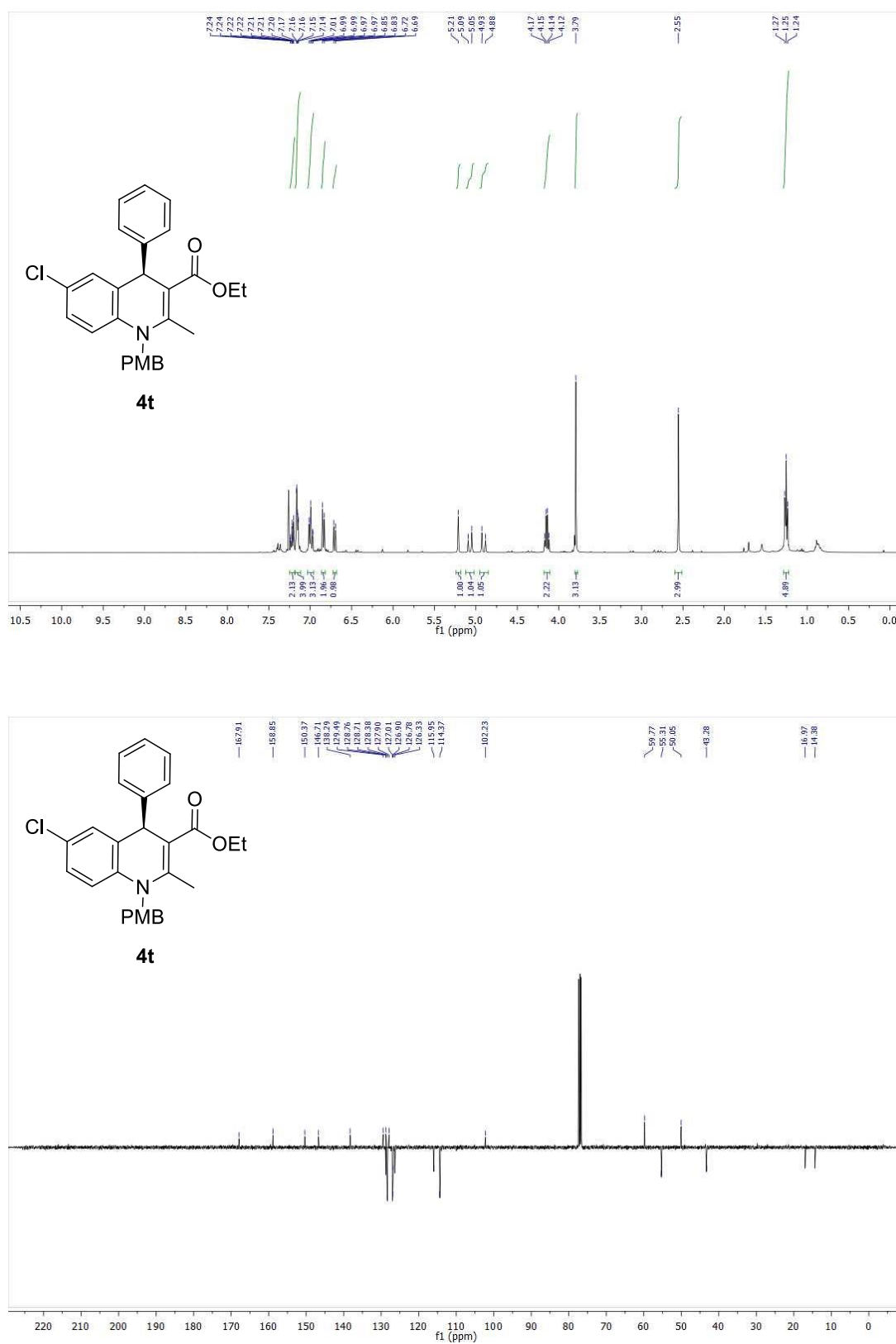


Figure 1.20. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 6-chloro-1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**4t**).

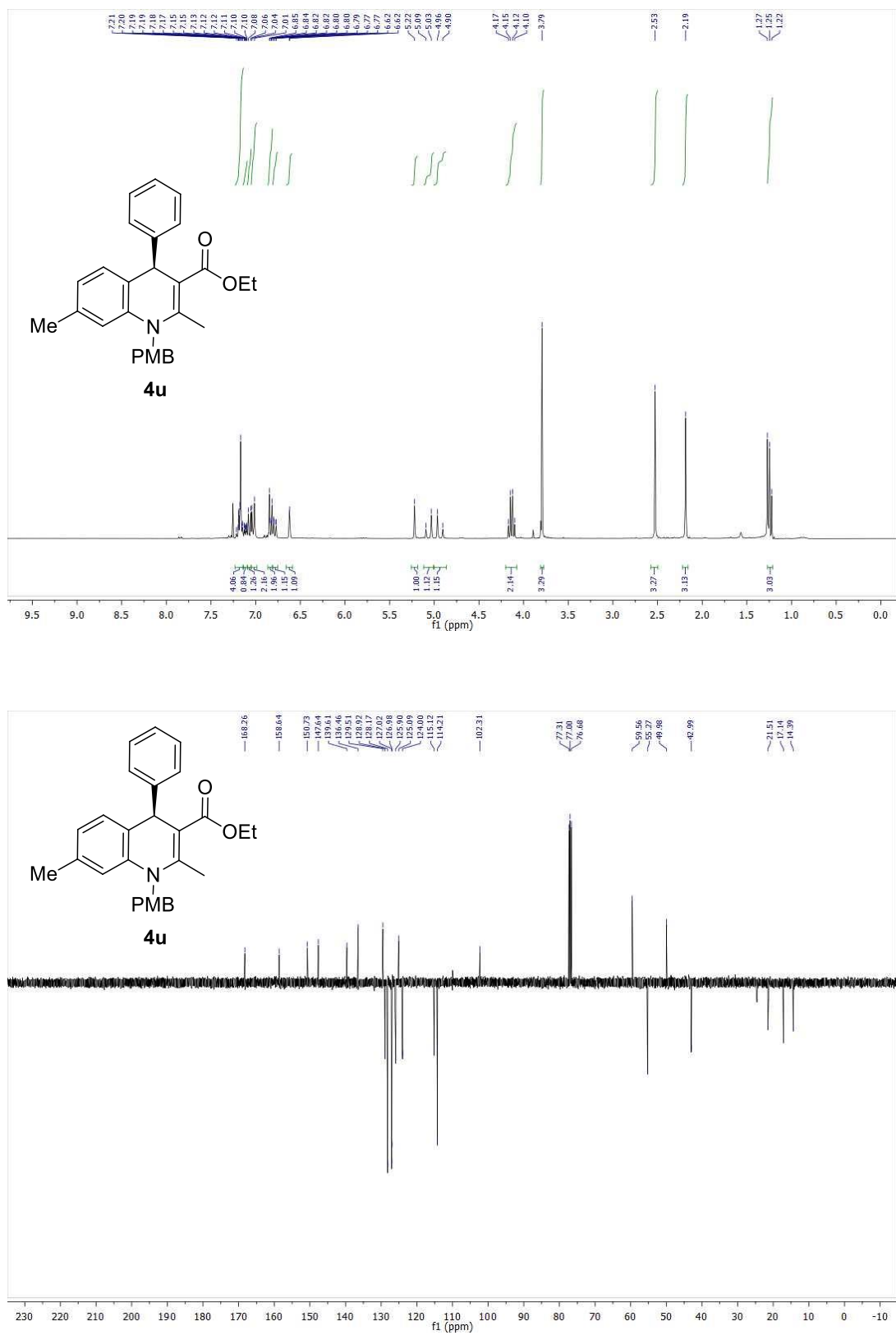


Figure 1.21. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 1-(4-methoxybenzyl)-2,7-dimethyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**4u**).

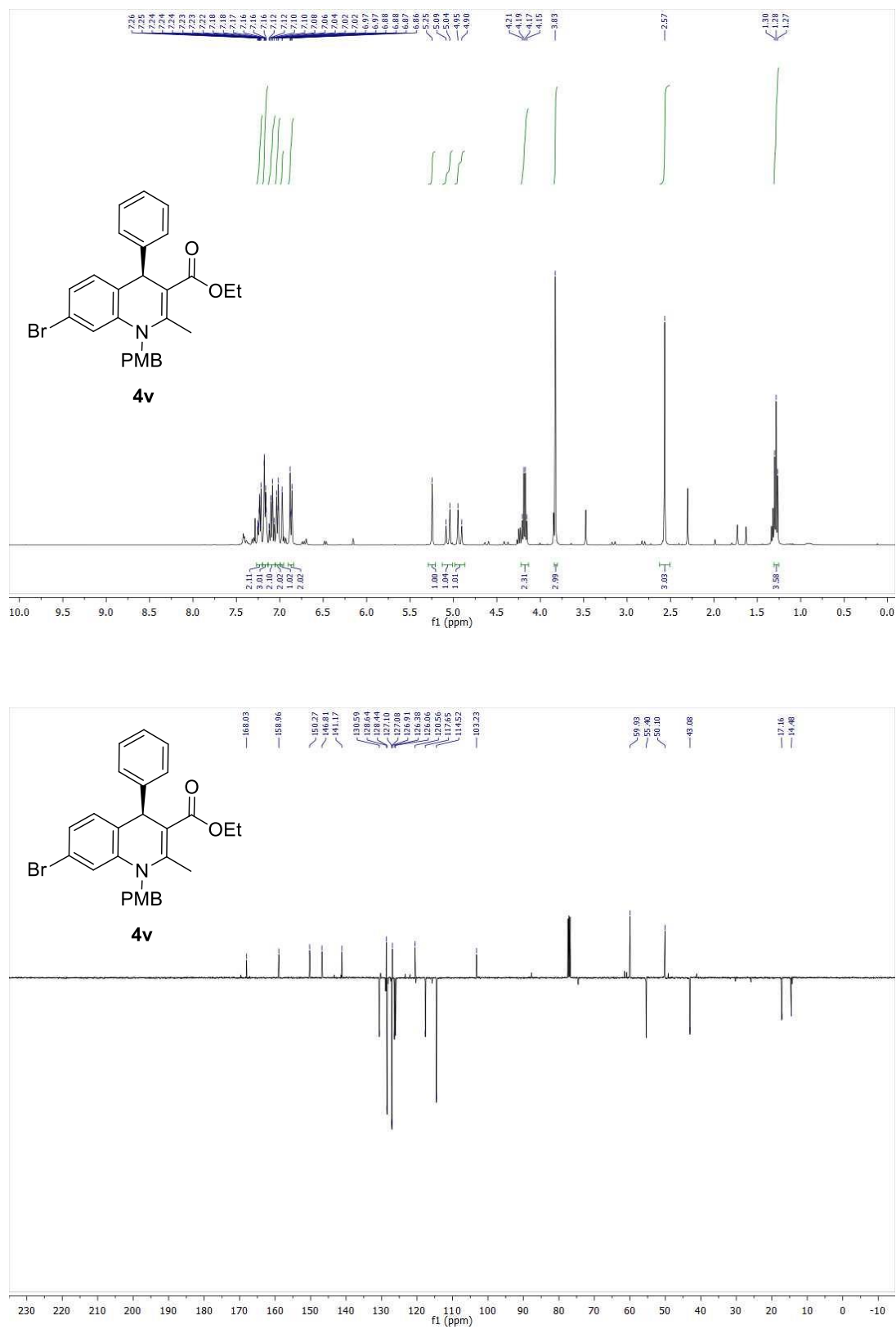


Figure 1.22. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 7-bromo-1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**4v**).

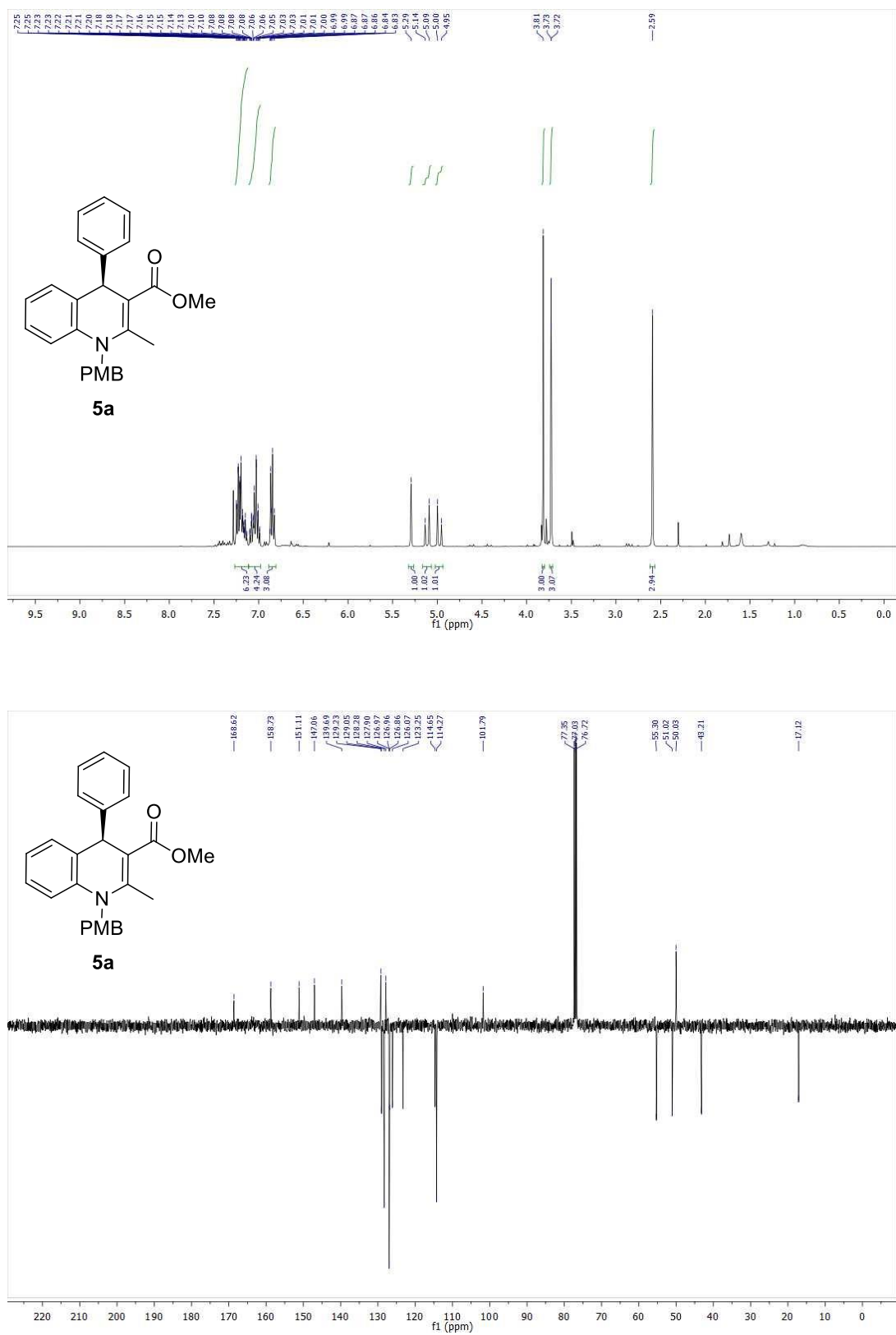


Figure 1.23. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-methyl 1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**5a**).

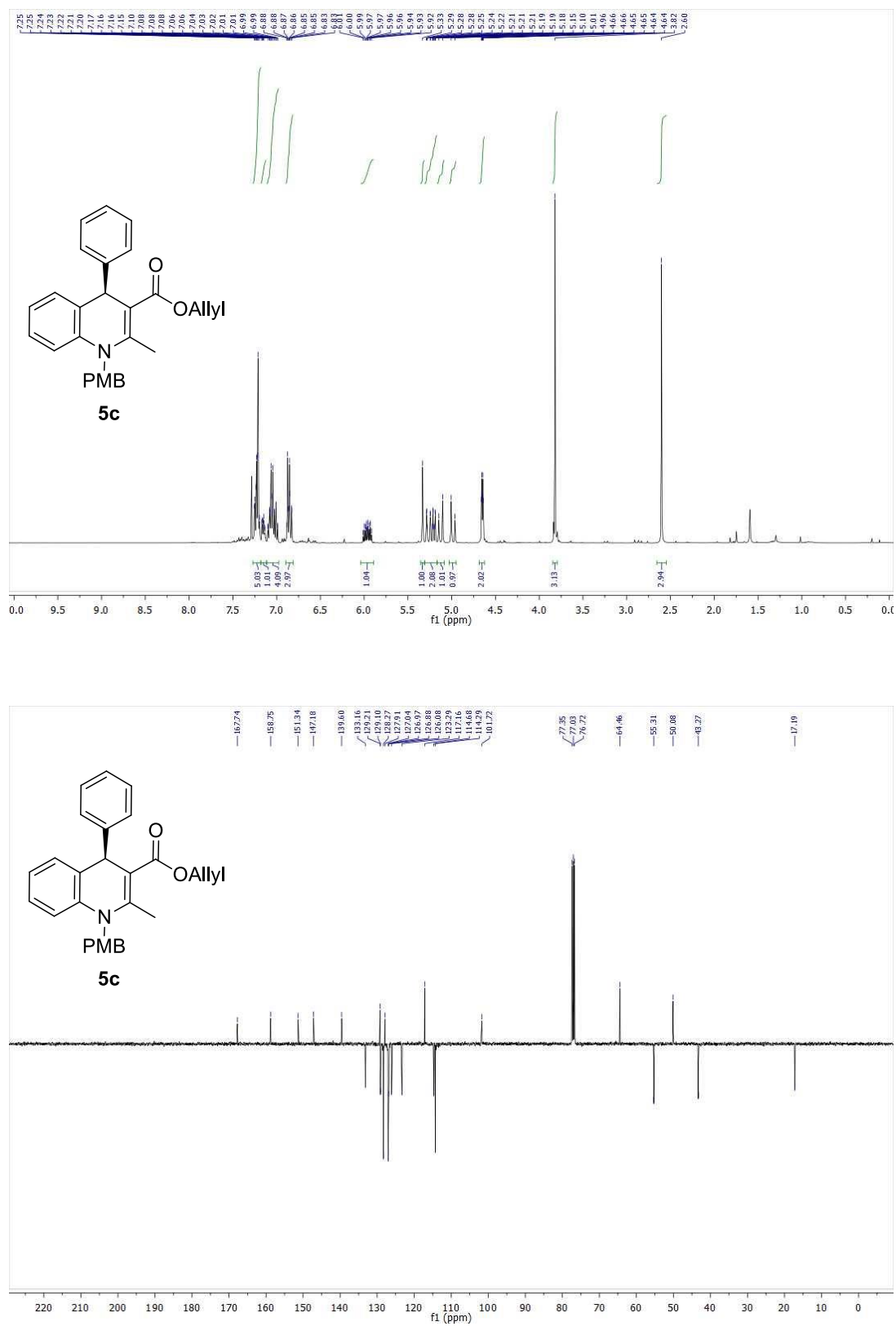


Figure 1.25. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-allyl 1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**5c**).

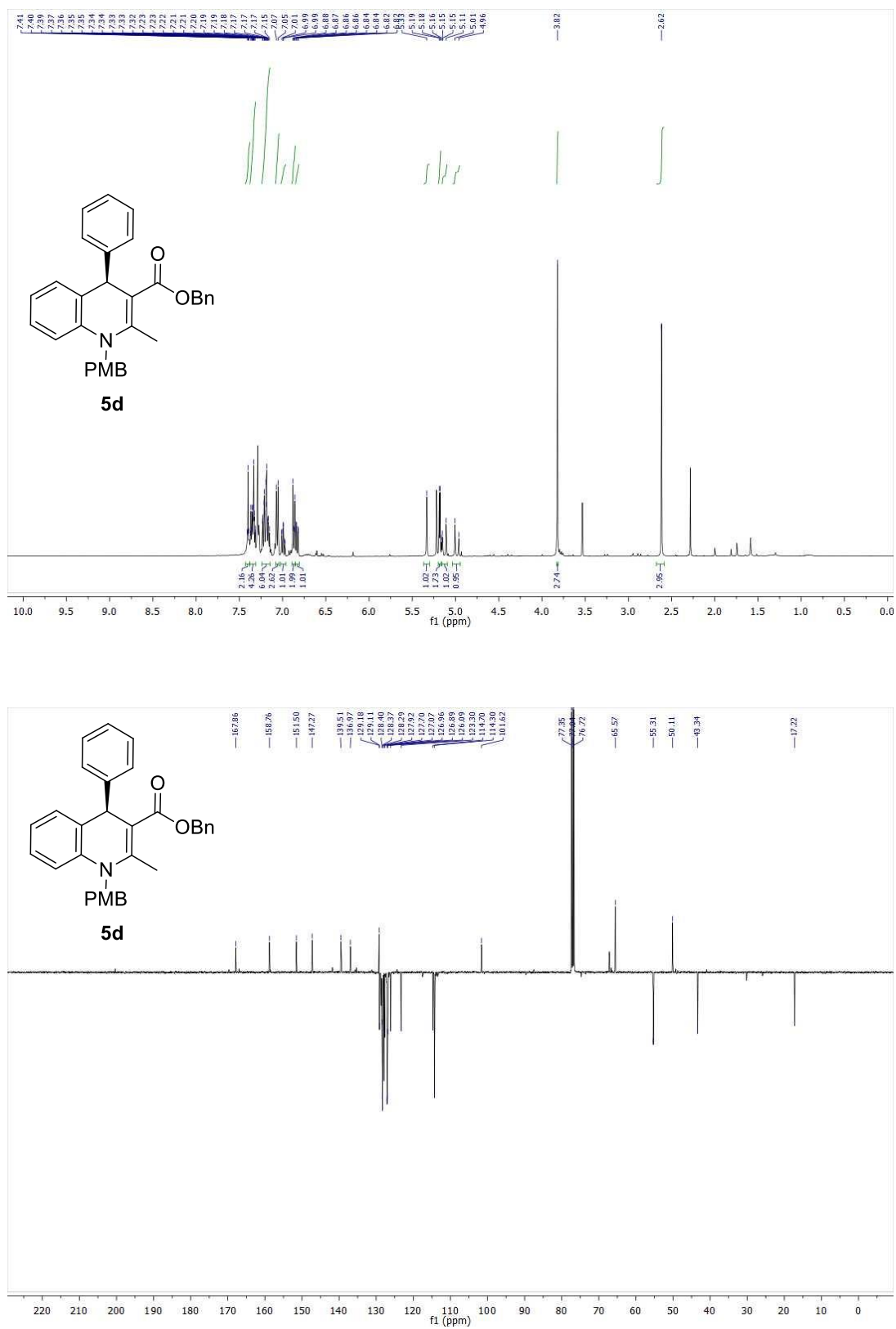


Figure 1.26. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-benzyl 1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**5d**).

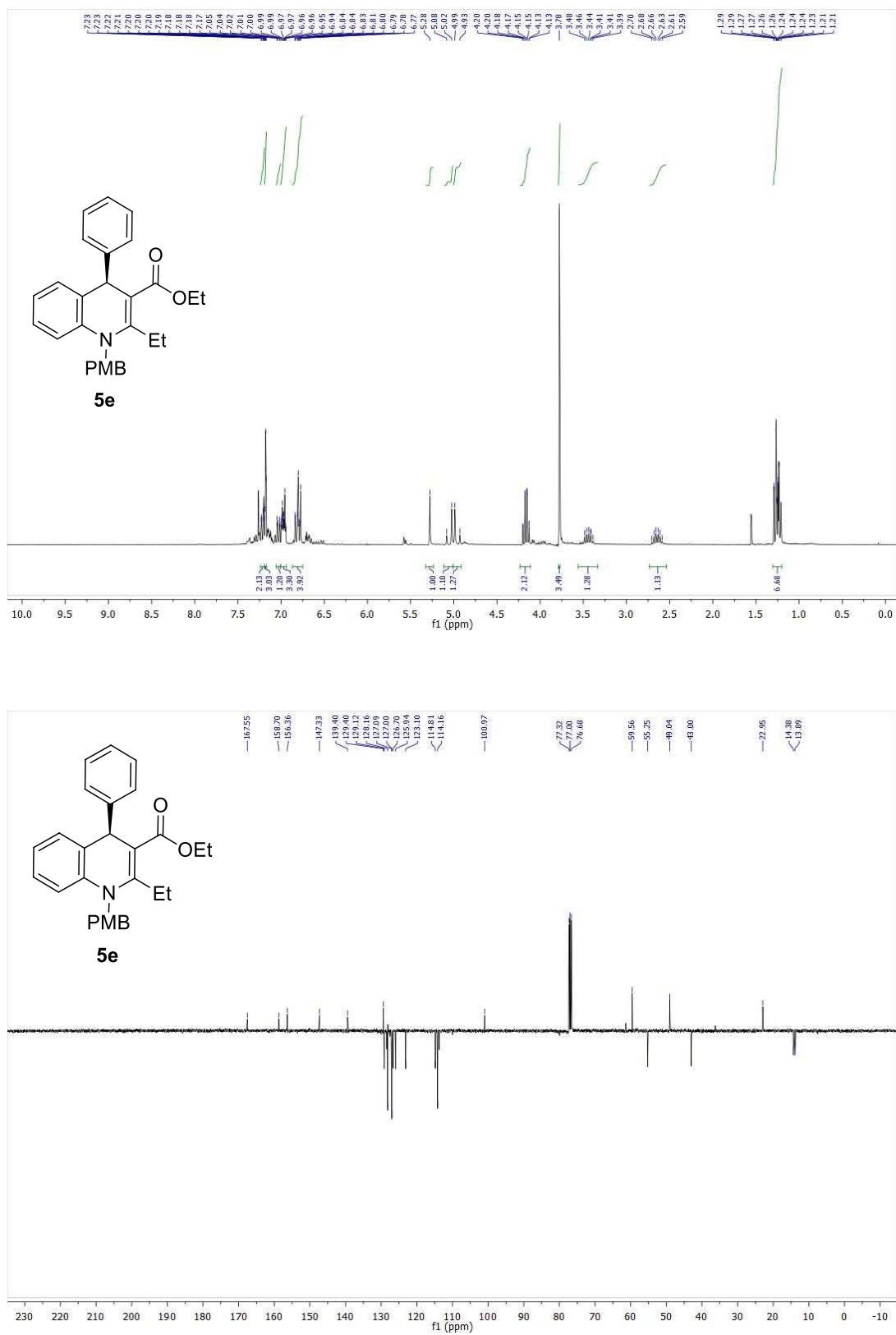


Figure 1.27. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-ethyl 2-ethyl-1-(4-methoxybenzyl)-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**5e**).

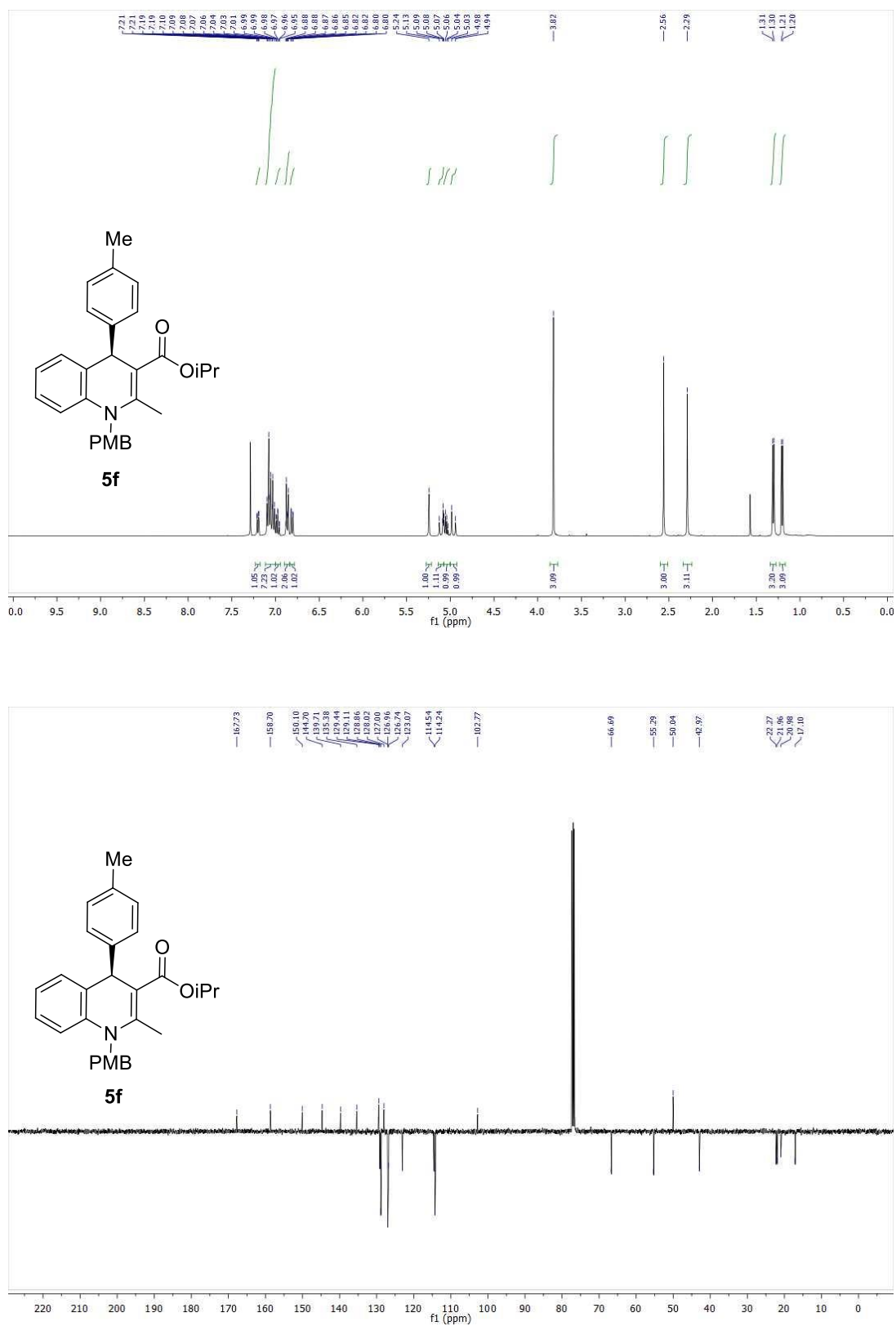


Figure 1.28. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-isopropyl 1-(4-methoxybenzyl)-2-methyl-4-(*p*-tolyl)-1,4-dihydroquinoline-3-carboxylate (**5f**).

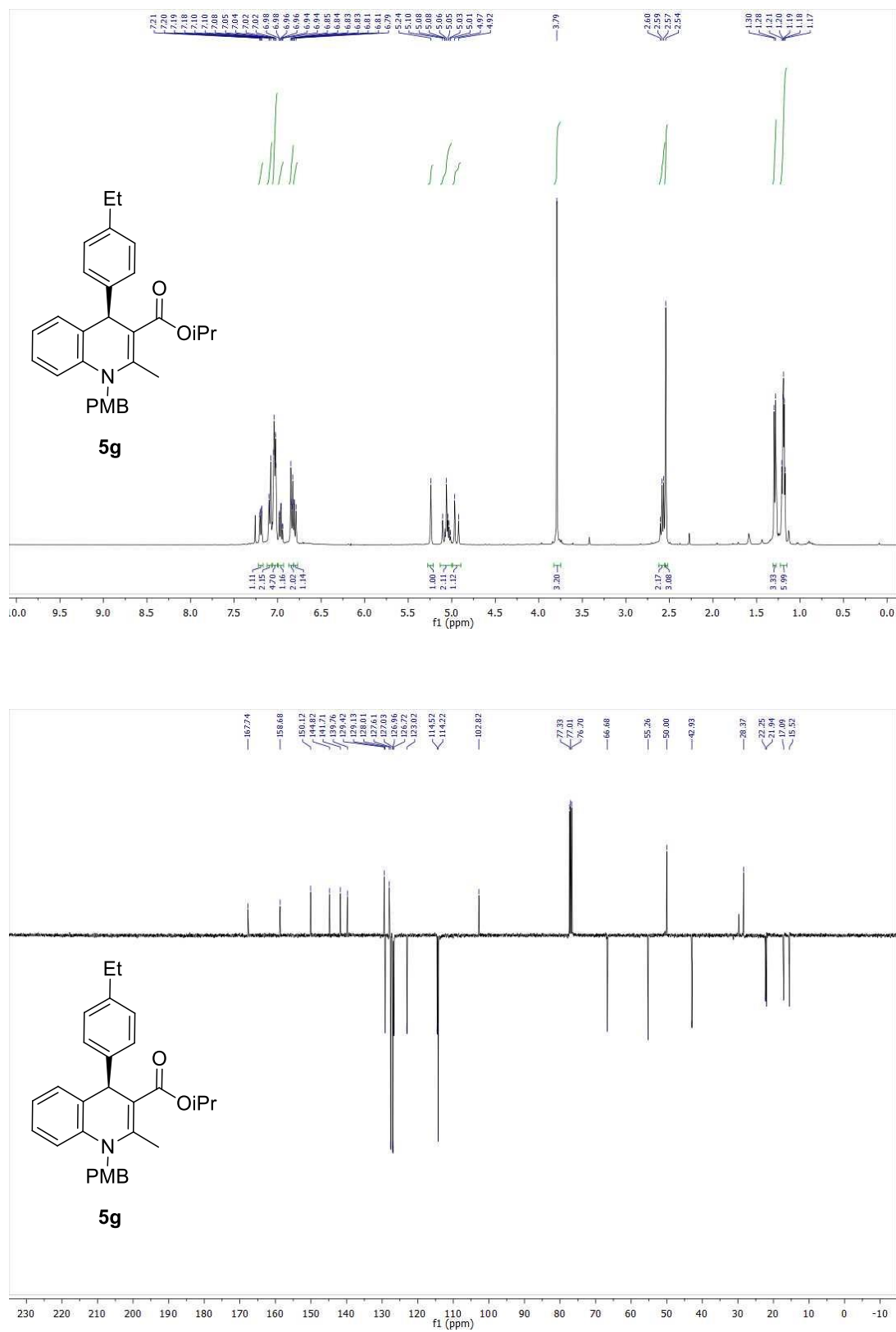


Figure 1.29. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-isopropyl 4-(4-ethylphenyl)-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**5g**).

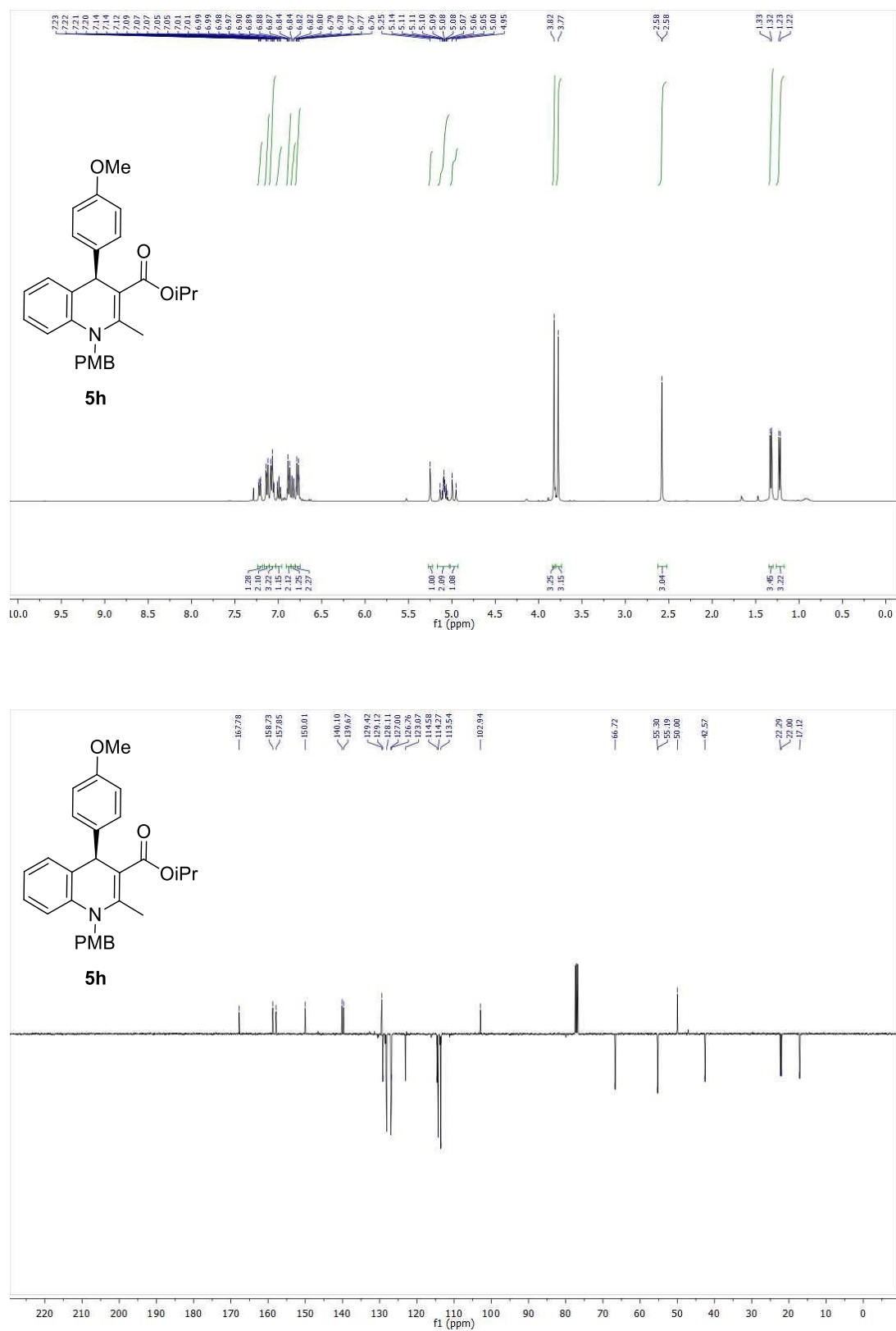


Figure 1.30. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-isopropyl 1-(4-methoxybenzyl)-4-(4-methoxyphenyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**5h**).

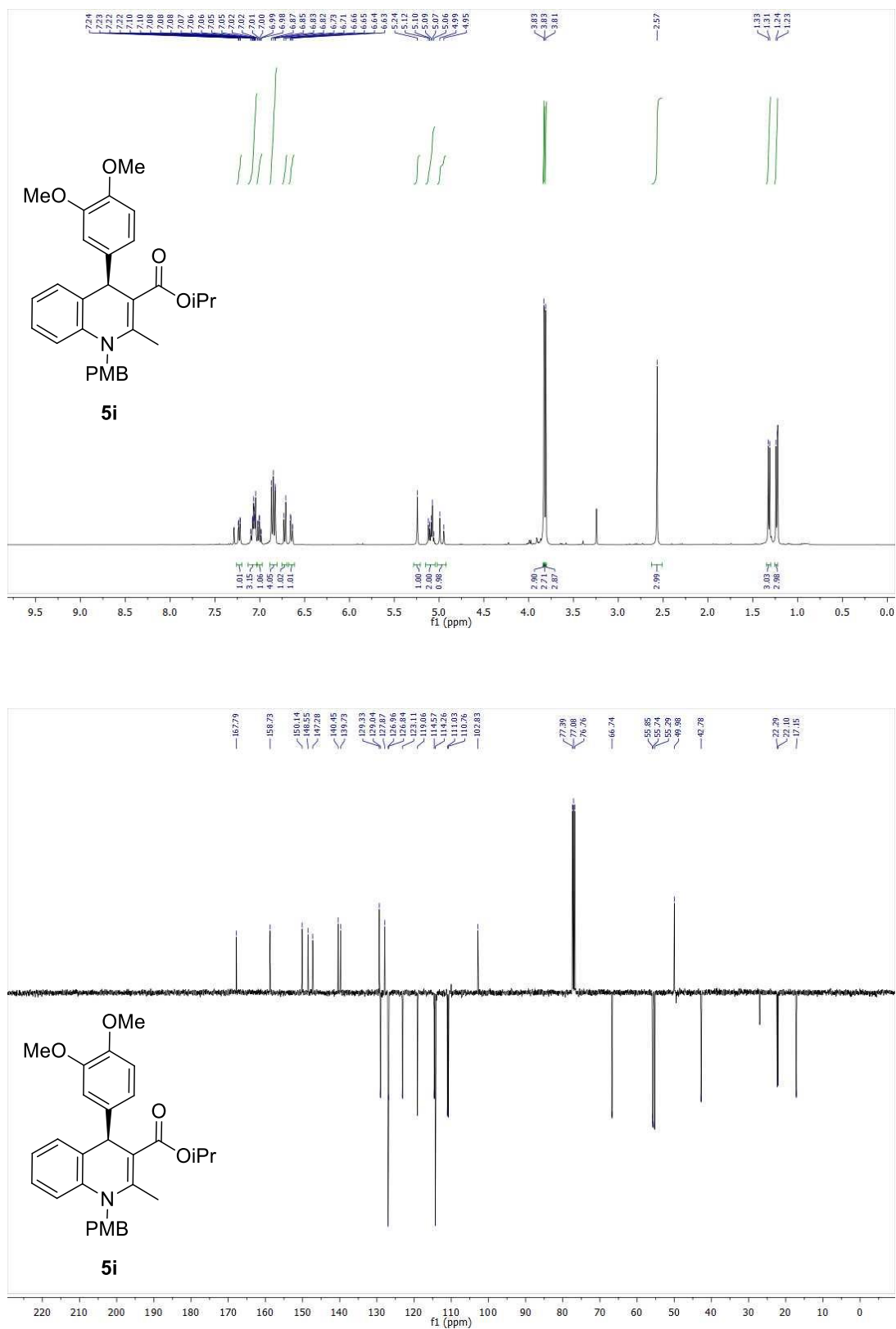


Figure 1.31. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-isopropyl 4-(3,4-dimethoxyphenyl)-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**5i**).

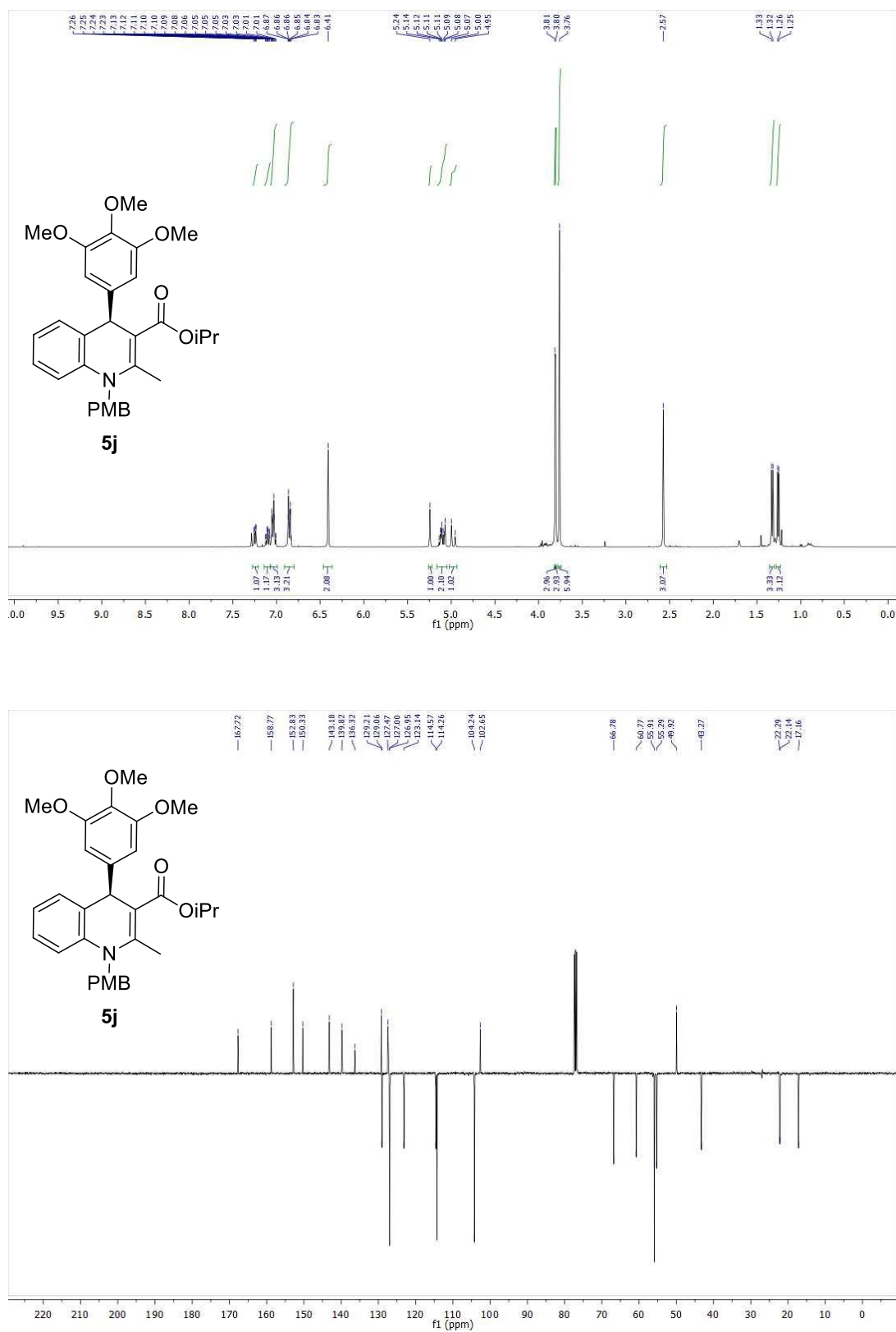


Figure 1.32. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-isopropyl 1-(4-methoxybenzyl)-2-methyl-4-(3,4,5-trimethoxyphenyl)-1,4-dihydroquinoline-3-carboxylate (**5j**).

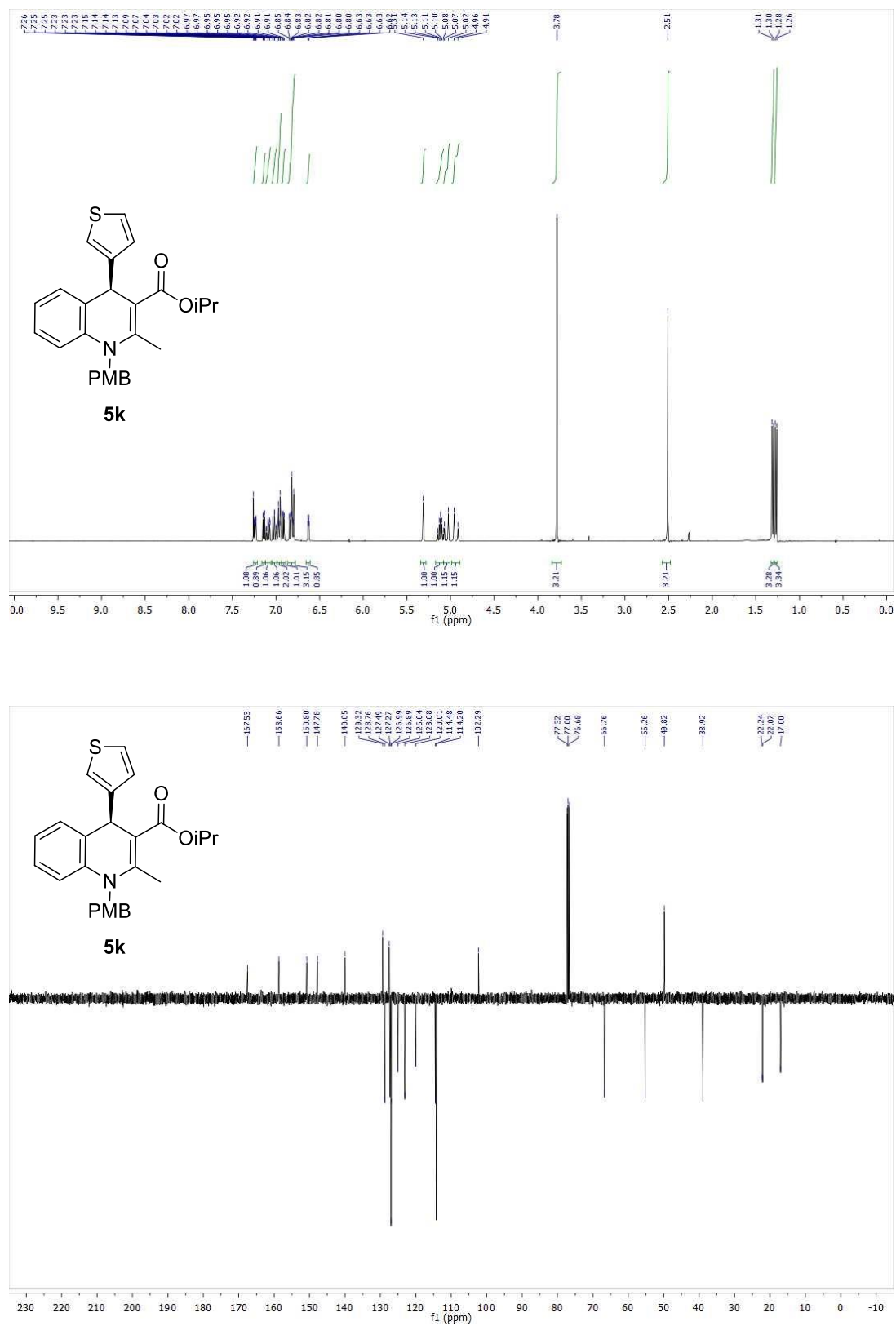


Figure 1.33. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-isopropyl 1-(4-methoxybenzyl)-2-methyl-4-(thiophen-3-yl)-1,4-dihydroquinoline-3-carboxylate (**5k**).

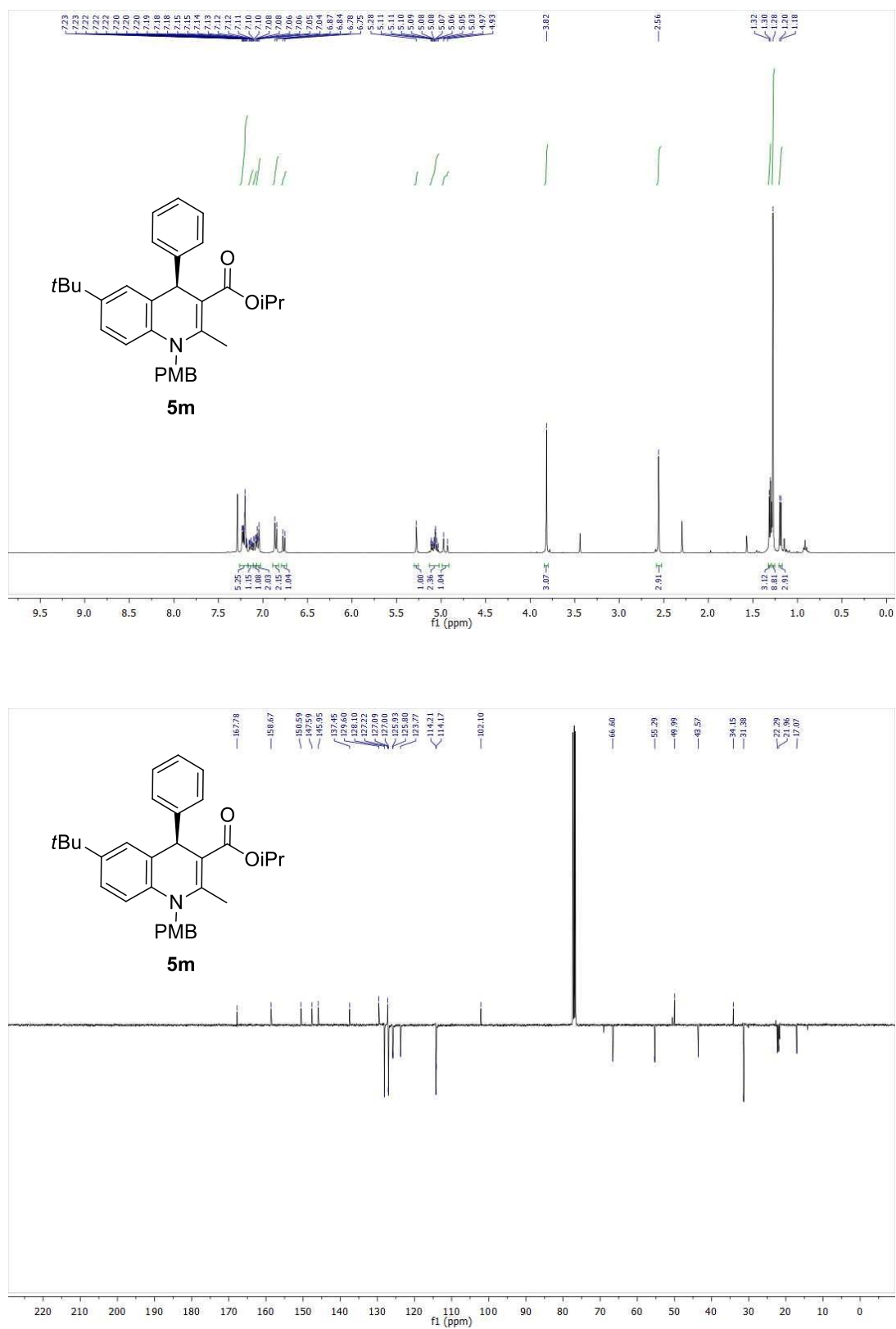


Figure 1.35. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-isopropyl 6-(*tert*-butyl)-1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**5m**).

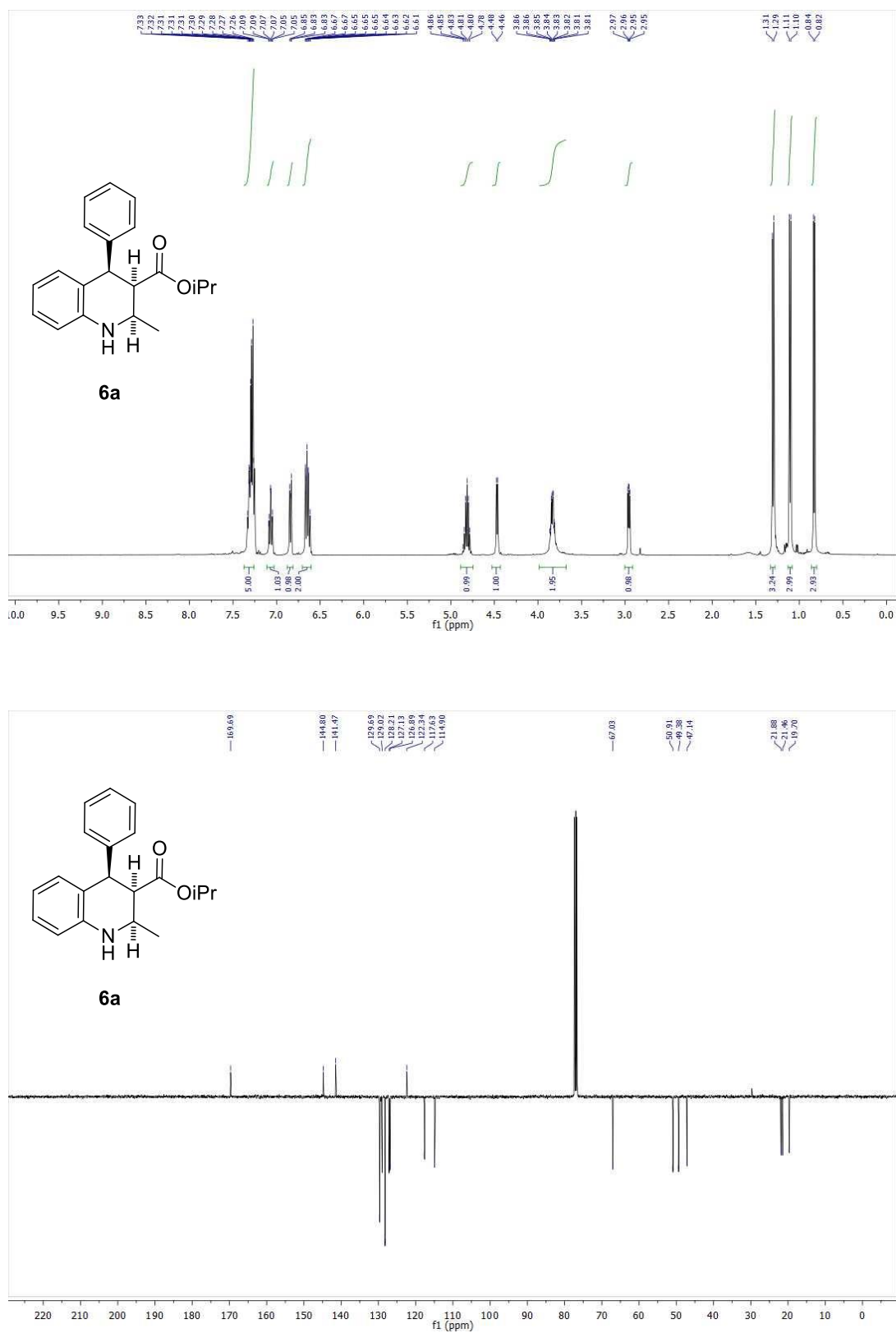


Figure 1.36. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (2*R*,3*R*,4*R*)-isopropyl 2-methyl-4-phenyl-1,2,3,4-tetrahydroquinoline-3-carboxylate (**6a**).

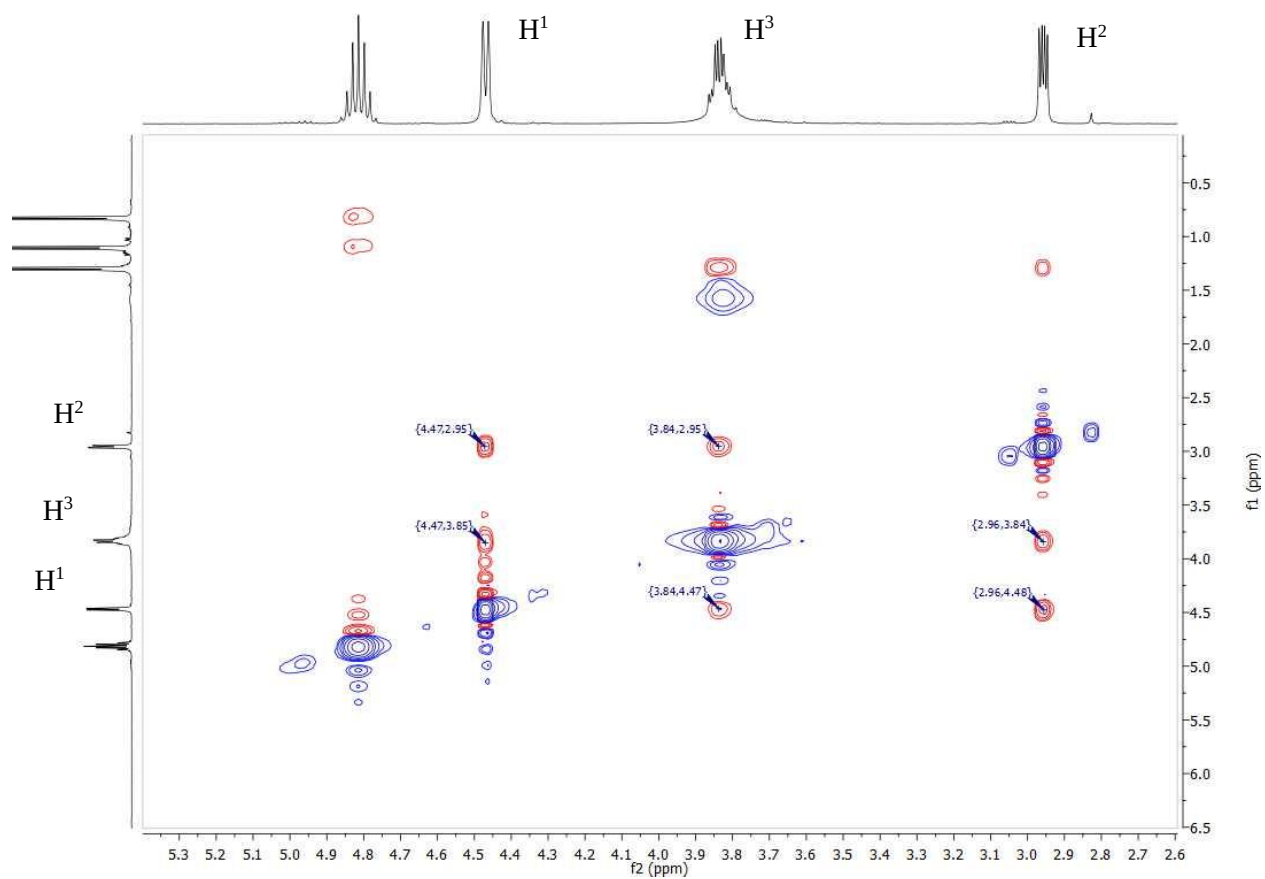
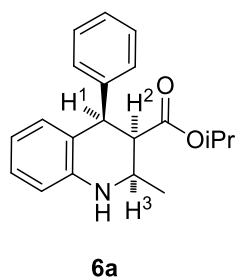


Figure 1.37. NOESY of (2*R*,3*R*,4*R*)-isopropyl 2-methyl-4-phenyl-1,2,3,4-tetrahydroquinoline-3-carboxylate (**6a**).

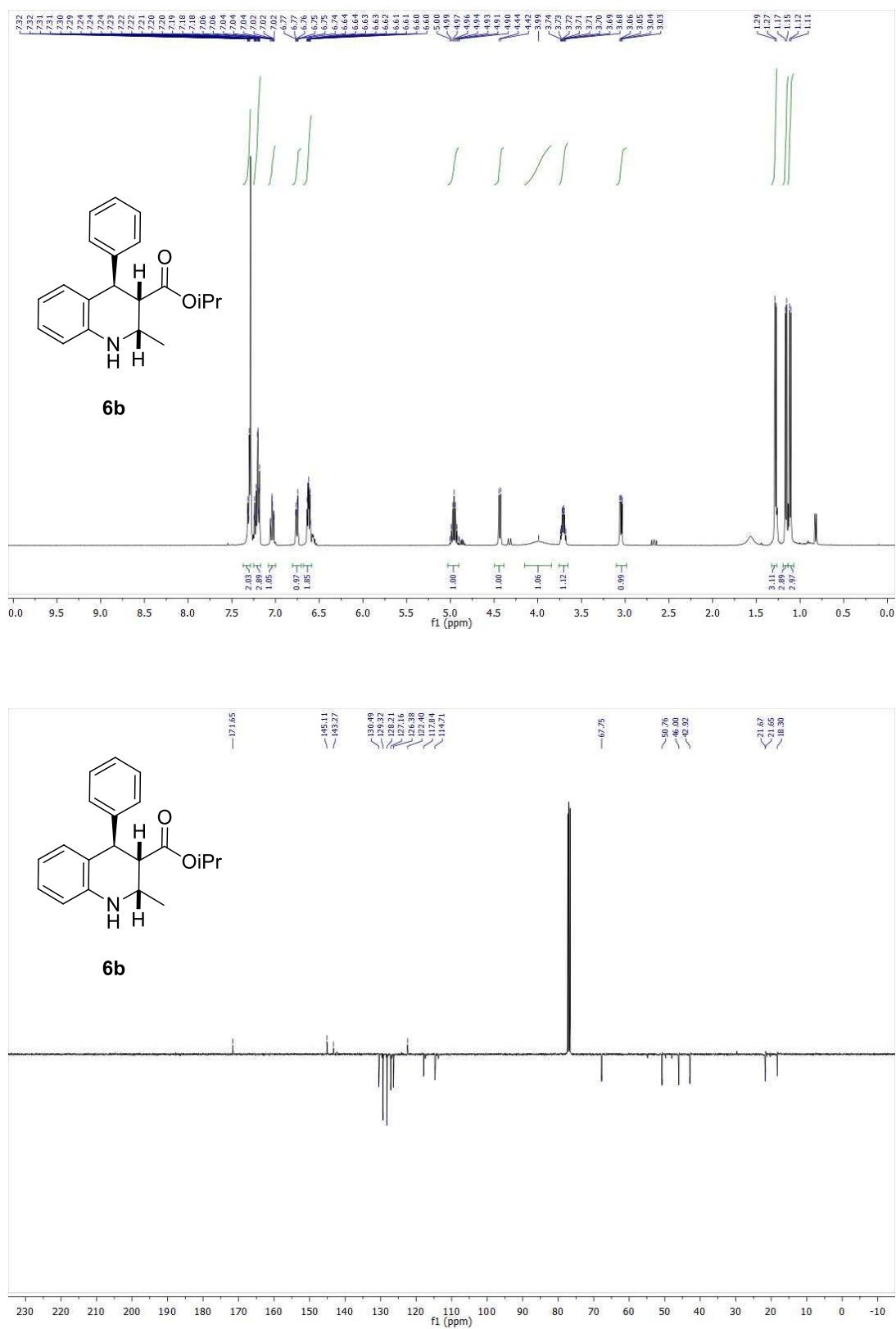


Figure 1.38. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (2S,3S,4R)-isopropyl 2-methyl-4-phenyl-1,2,3,4-tetrahydroquinoline-3-carboxylate (**6b**).

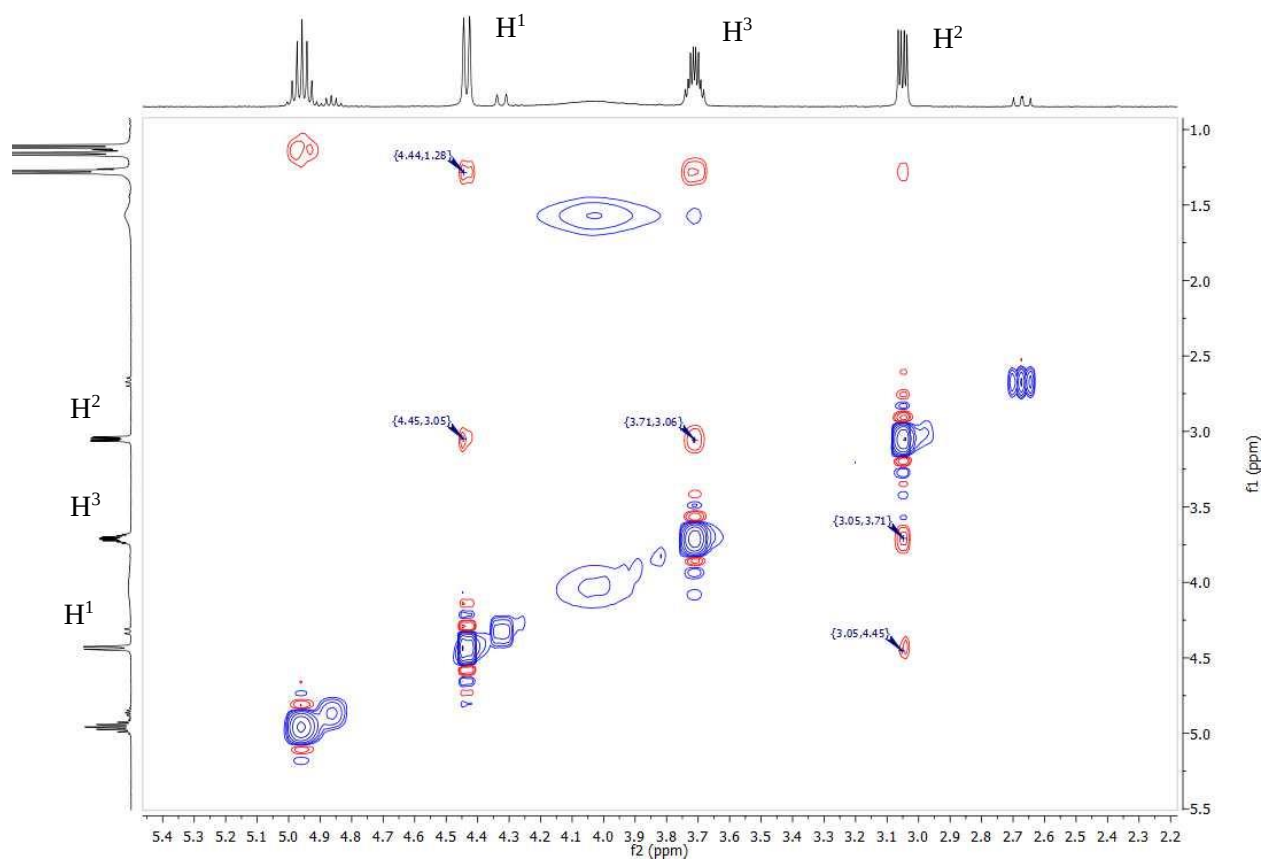
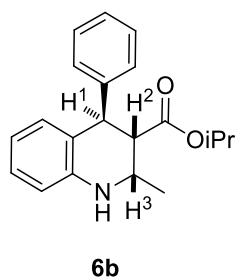


Figure 1.39. NOESY of (2*S*,3*S*,4*R*)-isopropyl 2-methyl-4-phenyl-1,2,3,4-tetrahydroquinoline-3-carboxylate (**6b**).

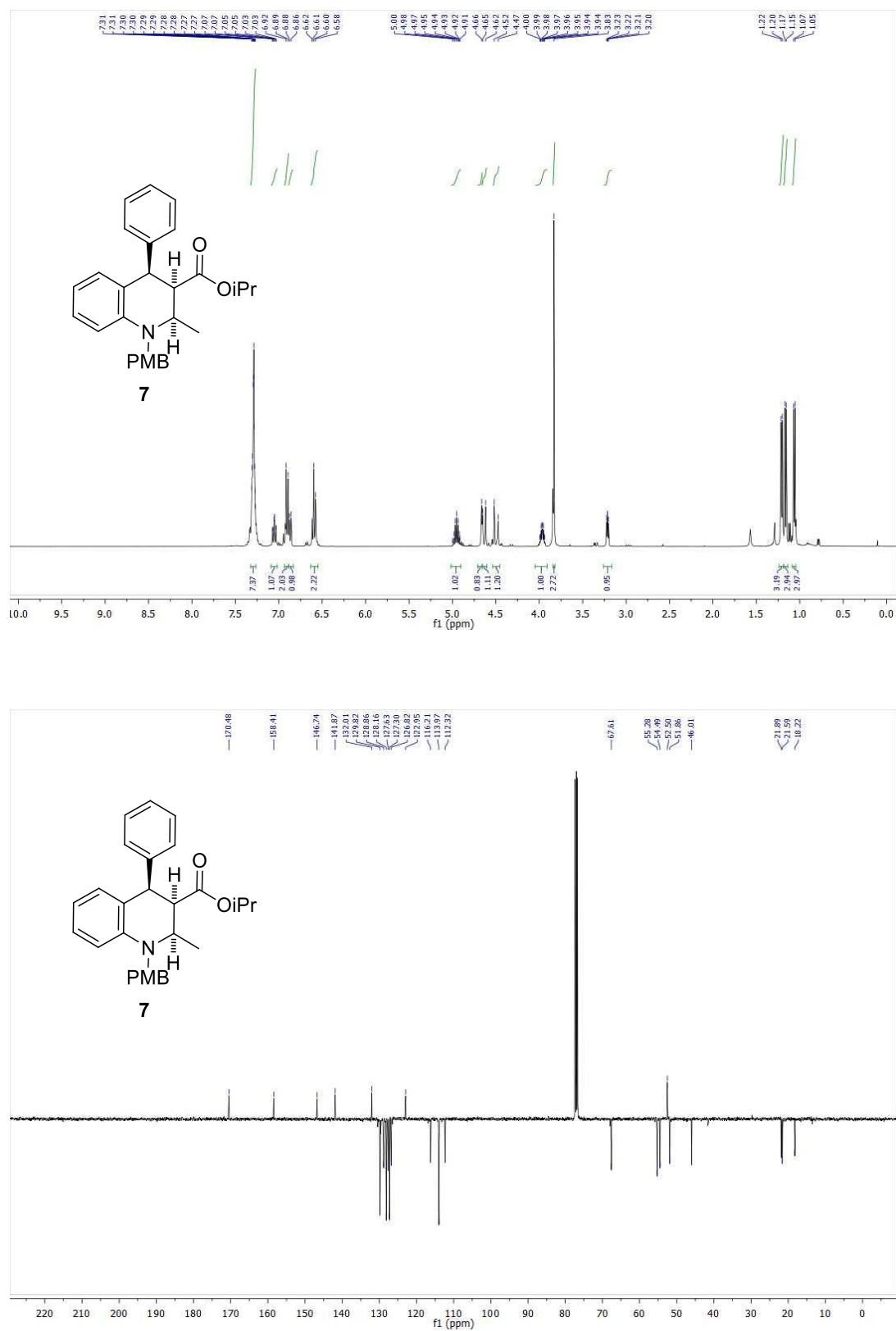


Figure 1.40. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (2*R*,3*R*,4*R*)-isopropyl 1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,2,3,4-tetrahydroquinoline-3-carboxylate (**7**).

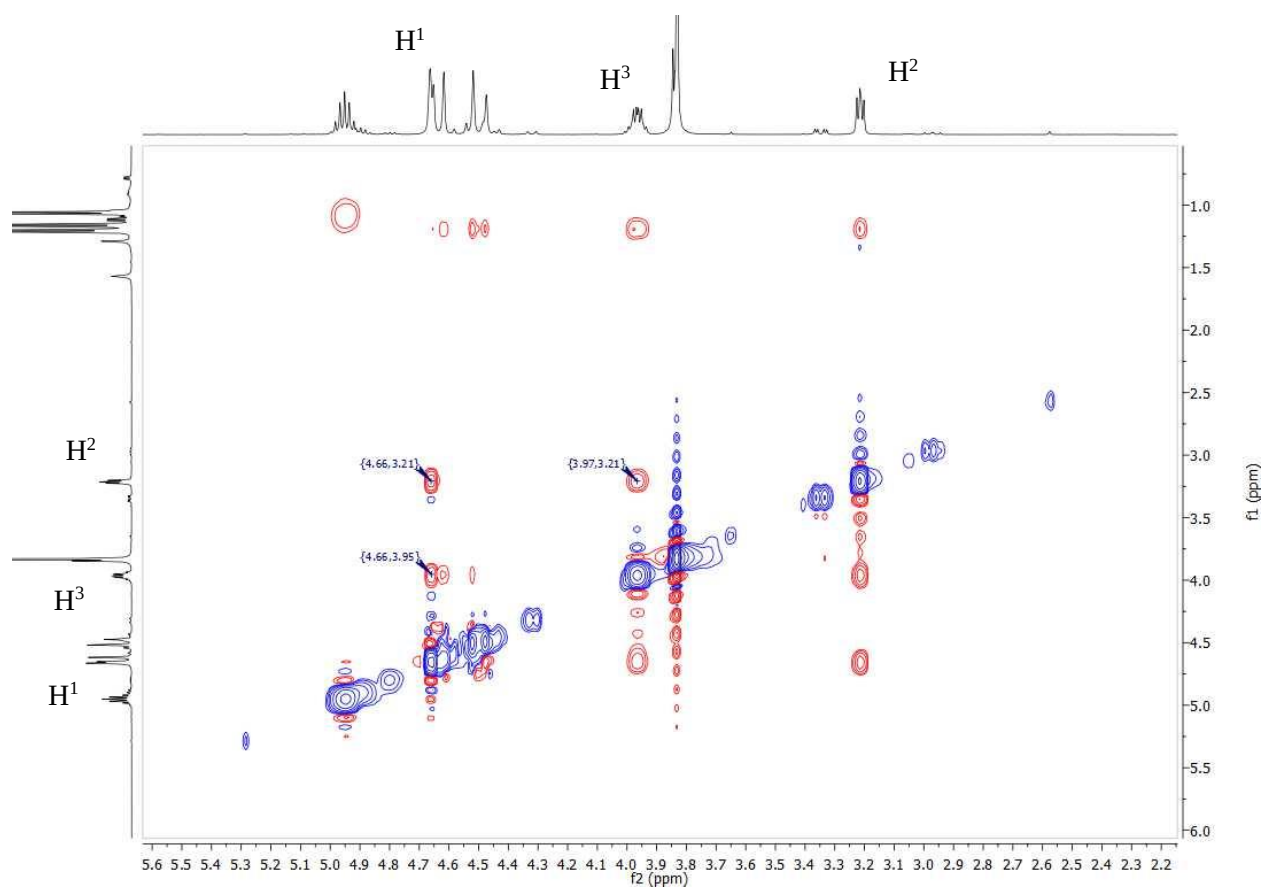
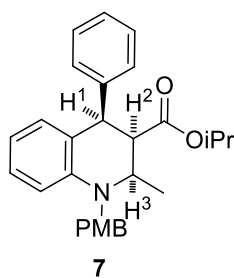


Figure 1.41. NOESY of (2*R*,3*R*,4*R*)-isopropyl 1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,2,3,4-tetrahydroquinoline-3-carboxylate (**7**).

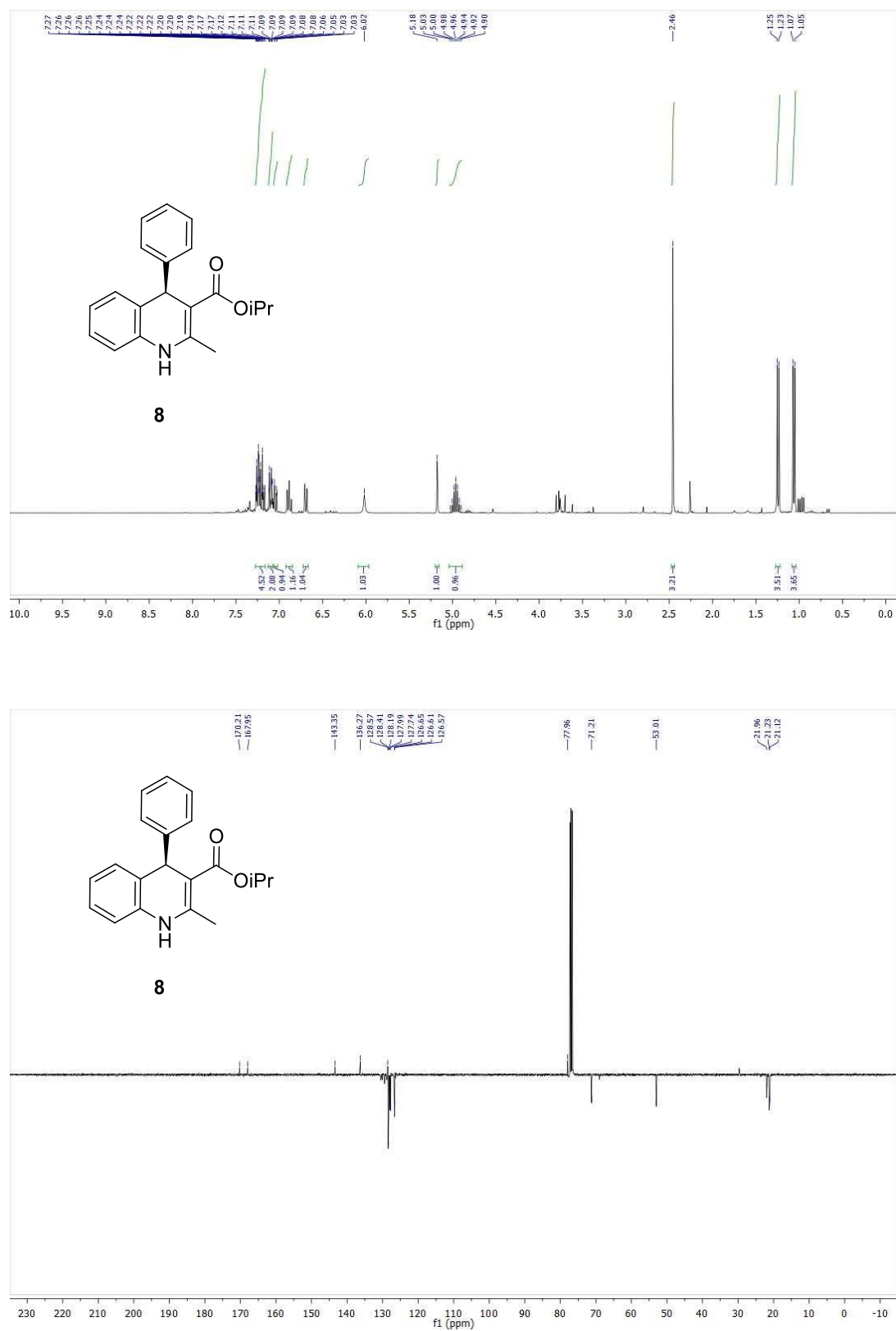
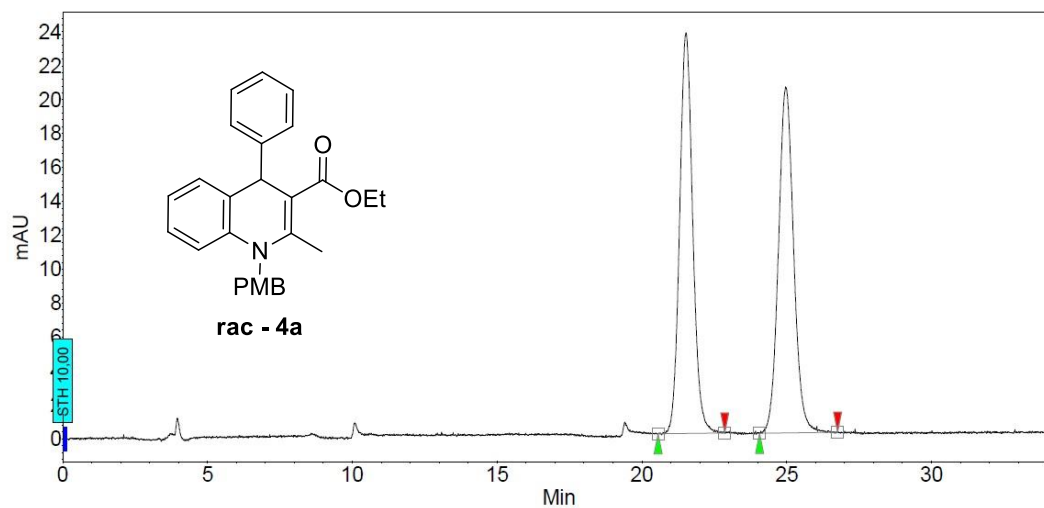


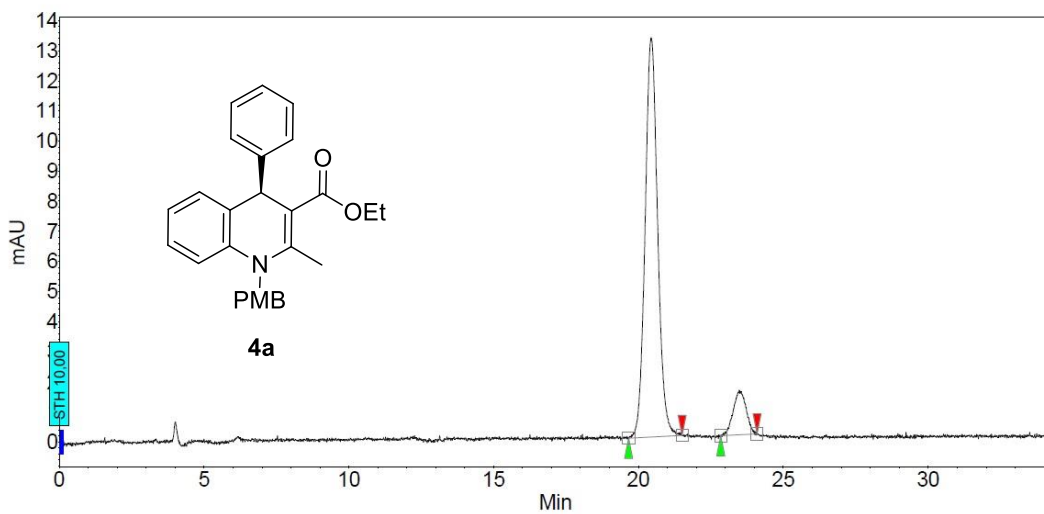
Figure 1.42. ¹H (400 MHz, CDCl₃) and ¹³C APT (100 MHz, CDCl₃) NMR of (*R*)-isopropyl-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**8**).

HPLC Chromatograms of the Racemic and Enantioenriched Products



Peak results :

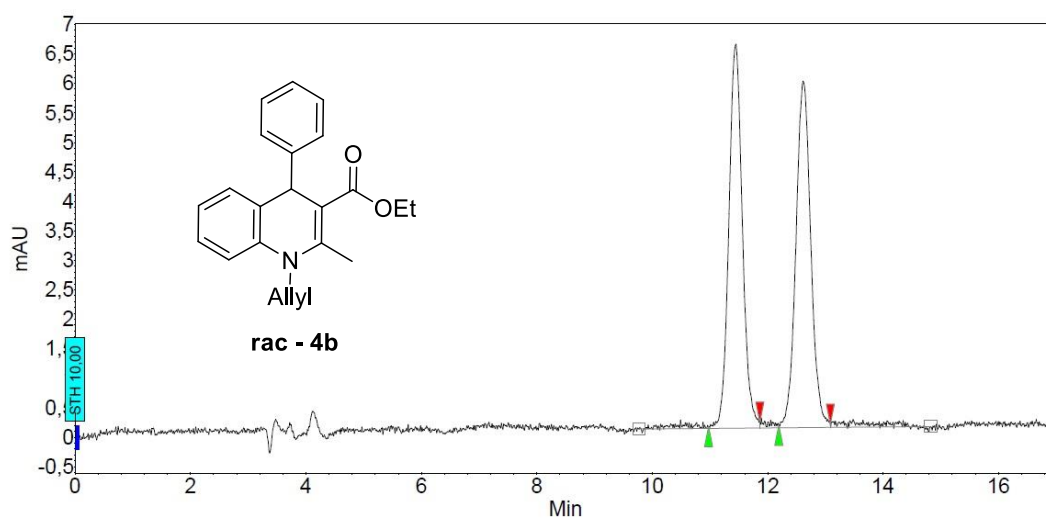
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	21.518	49.98	23.6	12.4	49.976
2	UNKNOWN	24.972	50.02	20.3	12.4	50.024
Total			100.00	44.0	24.8	100.000



Peak results :

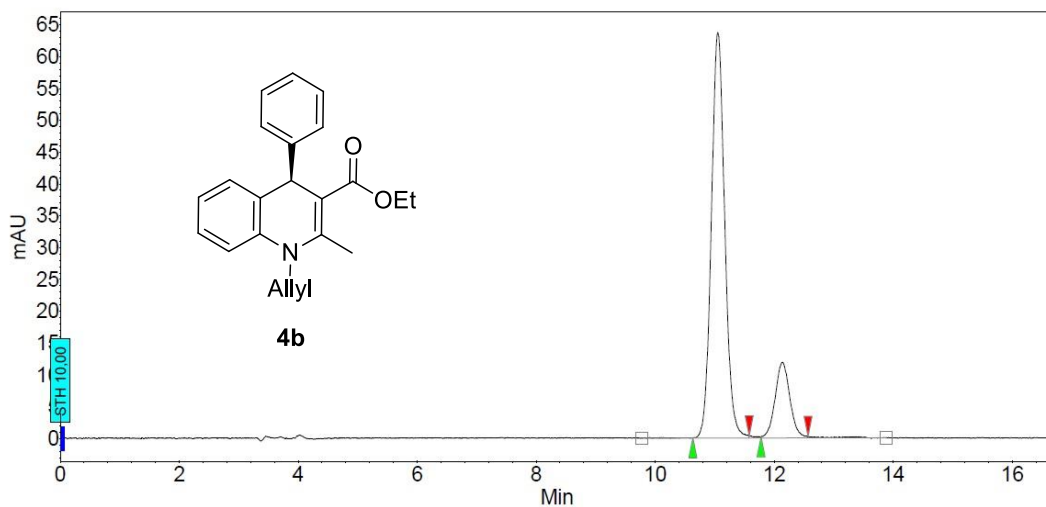
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	20.439	89.86	13.3	6.6	89.860
2	UNKNOWN	23.492	10.14	1.5	0.7	10.140
Total			100.00	14.7	7.4	100.000

Figure 2.1. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-ethyl 1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**4a**).



Peak results :

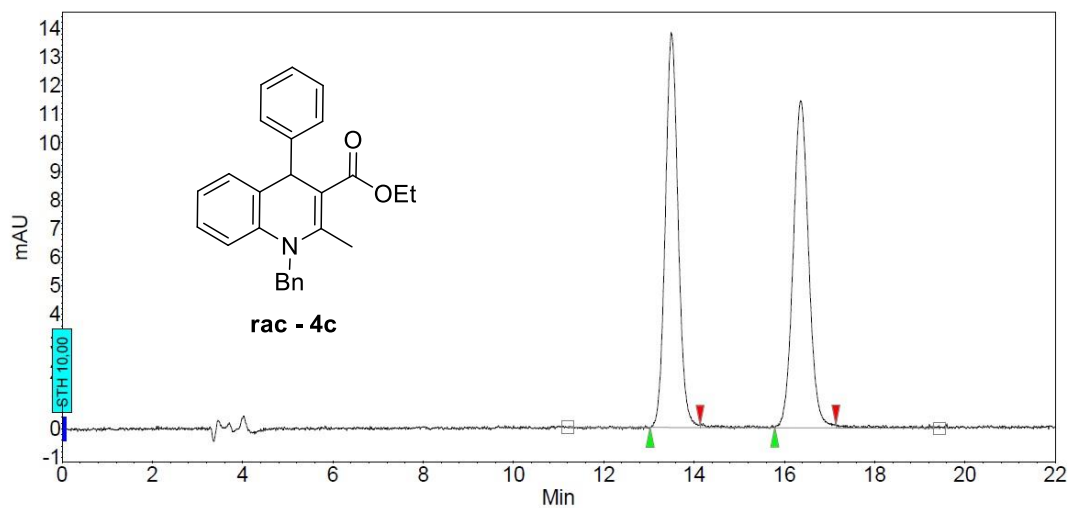
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	11.439	50.18	6.5	1.8	50.177
2	UNKNOWN	12.626	49.82	5.8	1.8	49.823
Total			100.00	12.3	3.5	100.000



Peak results :

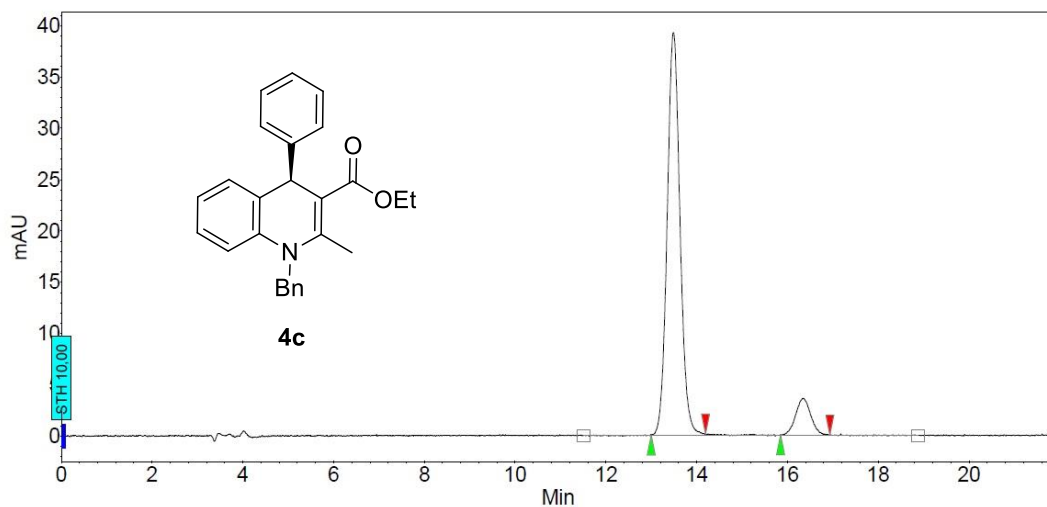
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	11.053	83.04	63.7	16.6	83.041
2	UNKNOWN	12.132	16.96	11.9	3.4	16.959
Total			100.00	75.6	20.0	100.000

Figure 2.2. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-ethyl 1-allyl-2-methyl-4-phenyl-1,4-carboxylate (**4b**).



Peak results :

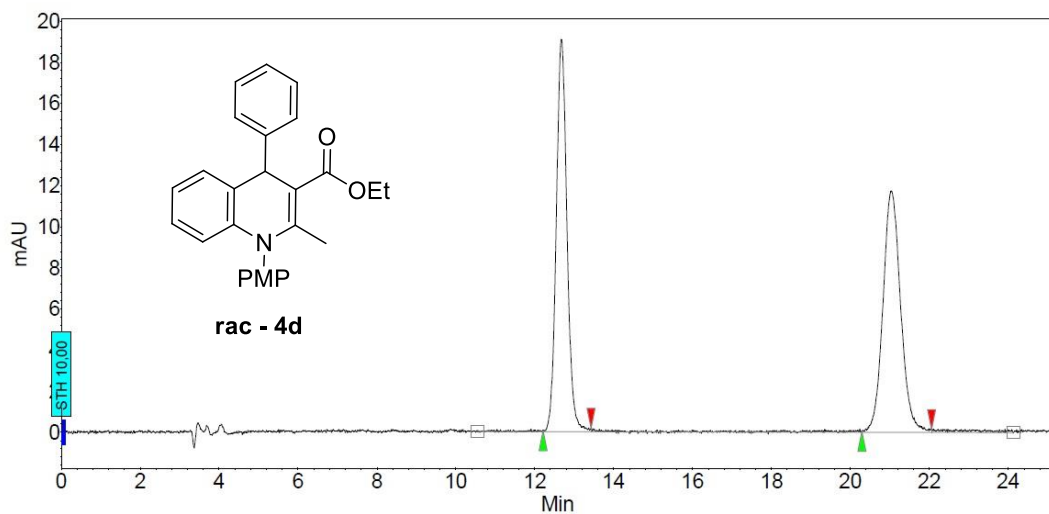
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	13.506	49.84	13.7	4.5	49.836
2	UNKNOWN	16.359	50.16	11.4	4.5	50.164
Total			100.00	25.2	9.1	100.000



Peak results :

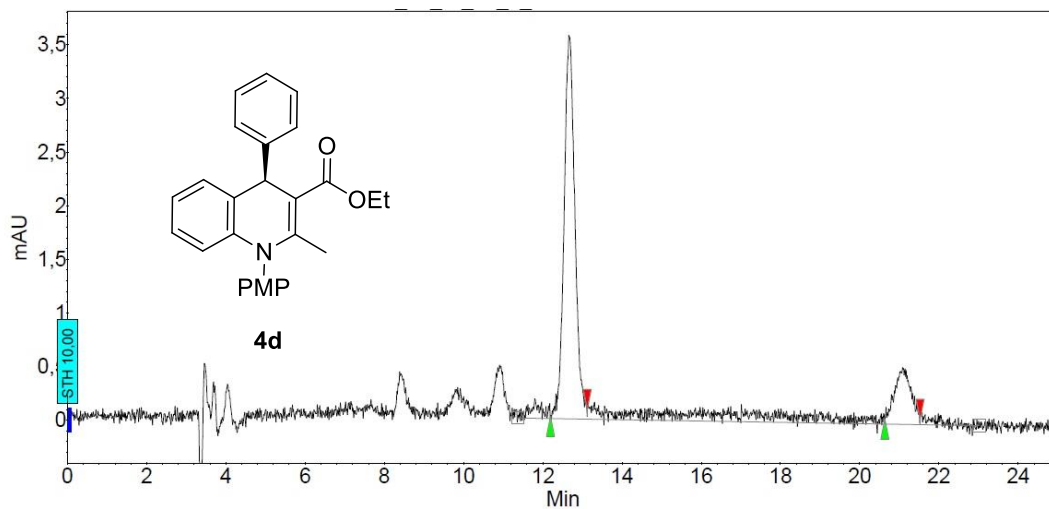
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	13.492	90.07	39.2	12.9	90.068
2	UNKNOWN	16.345	9.93	3.6	1.4	9.932
Total			100.00	42.9	14.3	100.000

Figure 2.3. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-ethyl 1-benzyl-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**4c**).



Peak results :

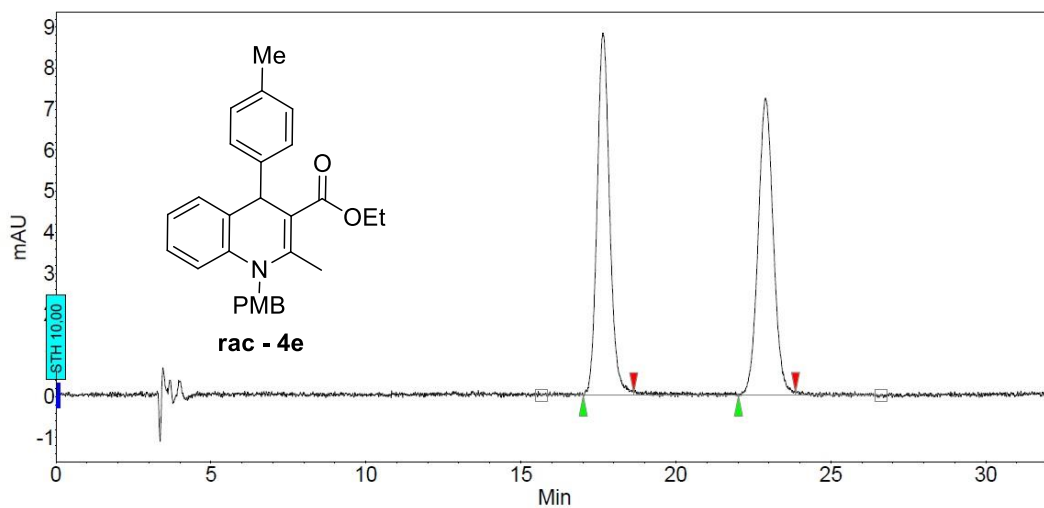
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	12.679	49.56	19.1	6.0	49.560
2	UNKNOWN	21.038	50.44	11.8	6.1	50.440
Total			100.00	30.8	12.1	100.000



Peak results :

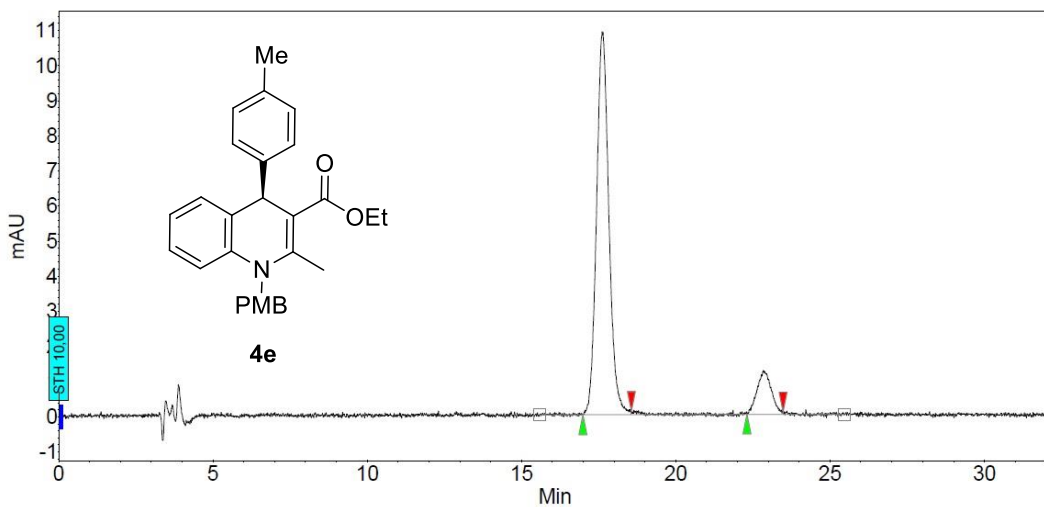
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	12.666	81.47	3.6	1.1	81.466
2	UNKNOWN	21.105	18.53	0.5	0.3	18.534
Total			100.00	4.1	1.4	100.000

Figure 2.4. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 328 nm) of (*R*)-ethyl 1-(4-methoxyphenyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**4d**).



Peak results :

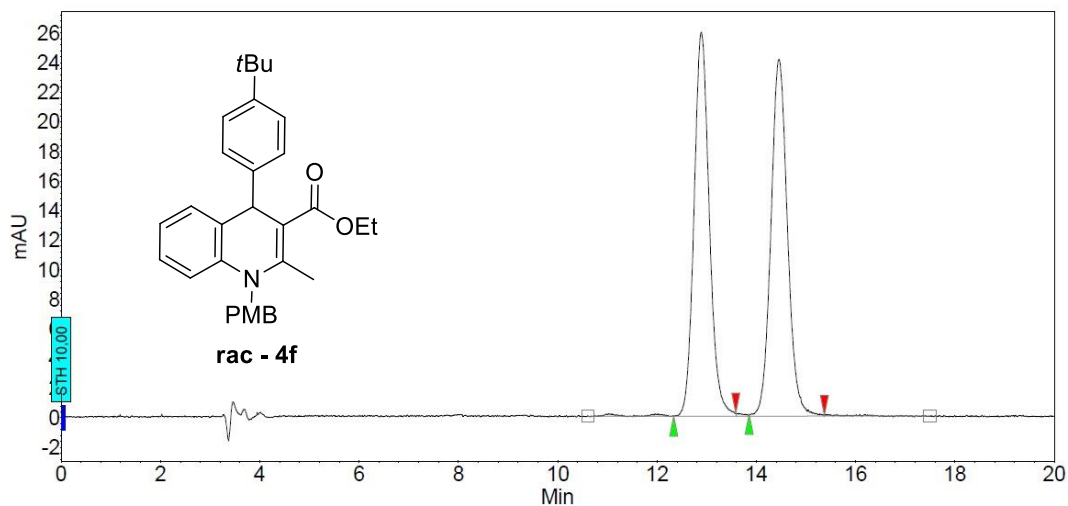
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	17.652	50.05	8.8	4.1	50.049
2	UNKNOWN	22.892	49.95	7.2	4.1	49.951
Total			100.00	16.1	8.2	100.000



Peak results :

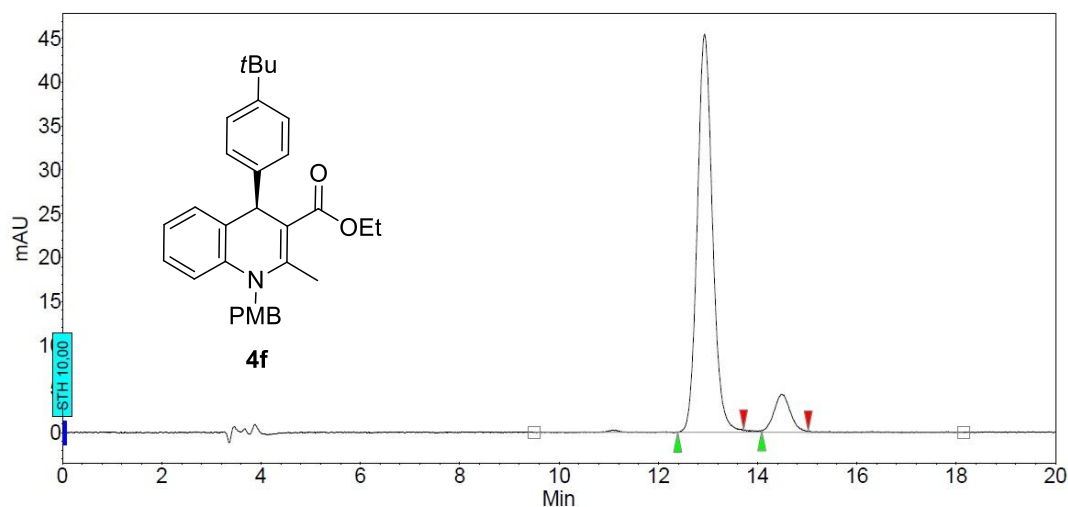
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	17.625	88.26	10.8	5.0	88.265
2	UNKNOWN	22.865	11.74	1.2	0.7	11.735
Total			100.00	12.0	5.7	100.000

Figure 2.5. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-ethyl 1-(4-methoxybenzyl)-2-methyl-4-(*p*-tolyl)-1,4-dihydroquinoline-3-carboxylate (**4e**).



Peak results :

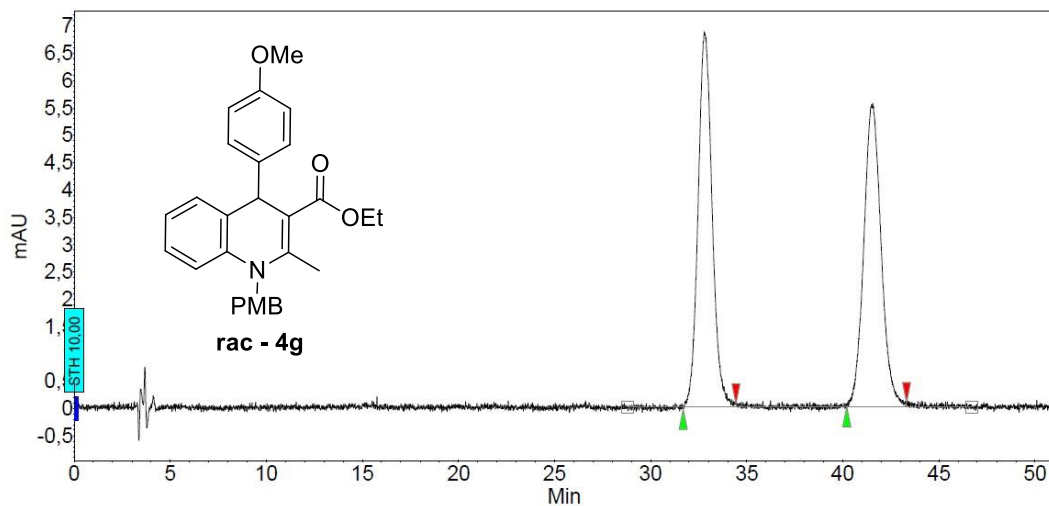
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	12.892	49.81	25.9	9.2	49.808
2	UNKNOWN	14.452	50.19	24.1	9.3	50.192
Total			100.00	50.1	18.5	100.000



Peak results :

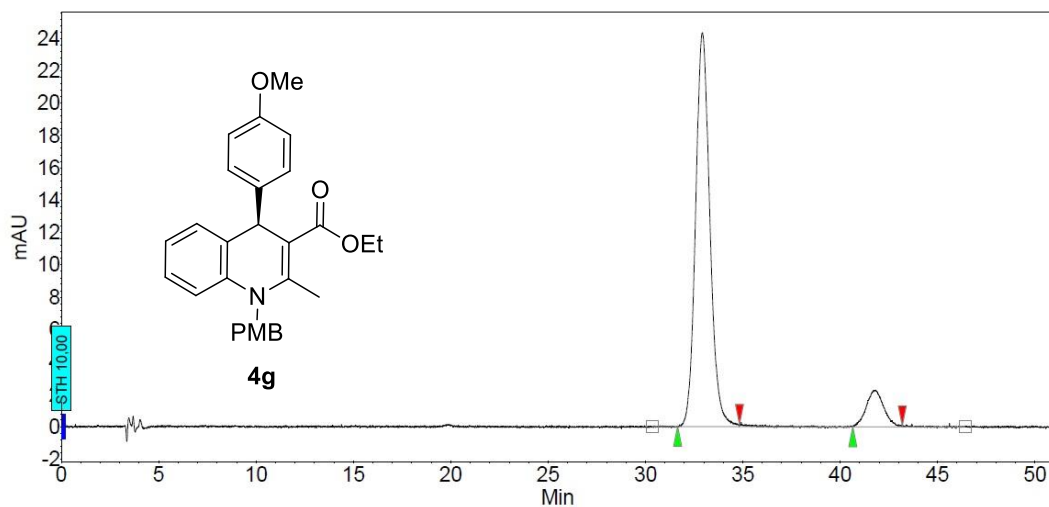
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	12.932	90.57	45.5	16.1	90.570
2	UNKNOWN	14.492	9.43	4.3	1.7	9.430
Total			100.00	49.8	17.8	100.000

Figure 2.6. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-ethyl 4-[4-(*tert*-butyl)phenyl]-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**4f**).



Peak results :

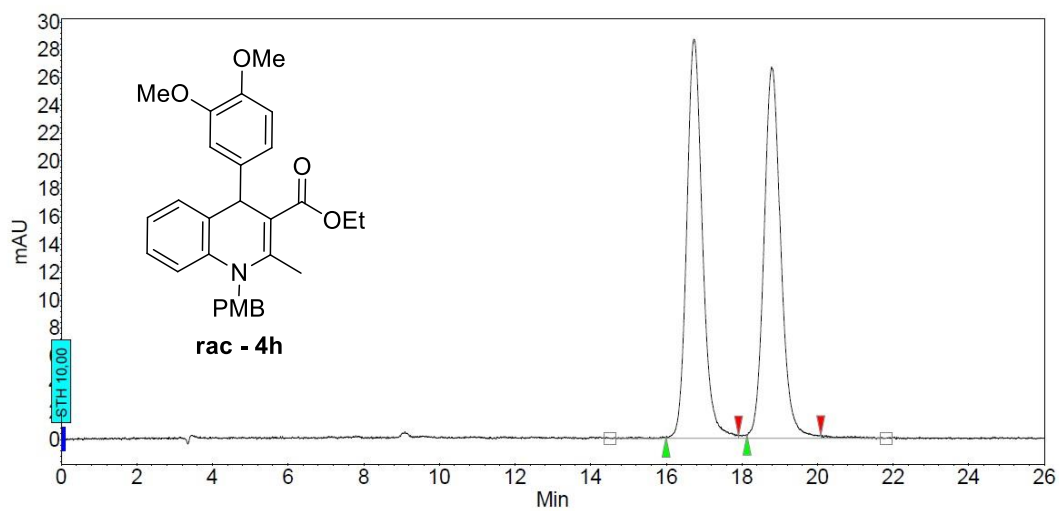
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	32.811	49.99	6.8	5.8	49.990
2	UNKNOWN	41.530	50.01	5.5	5.8	50.010
Total			100.00	12.3	11.6	100.000



Peak results :

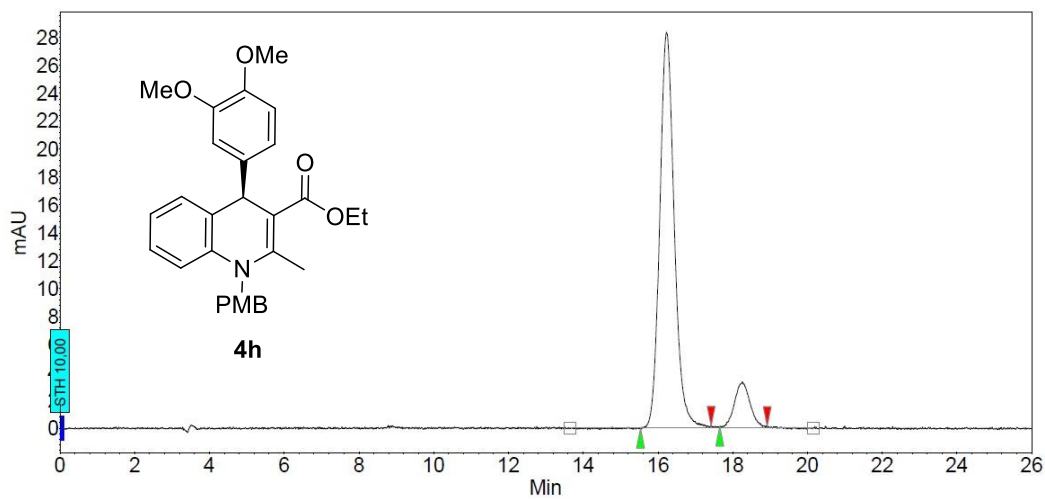
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	32.918	89.82	24.4	20.7	89.823
2	UNKNOWN	41.770	10.18	2.2	2.3	10.177
Total			100.00	26.6	23.0	100.000

Figure 2.7. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-ethyl 1-(4-methoxybenzyl)-4-(4-methoxyphenyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**4g**).



Peak results :

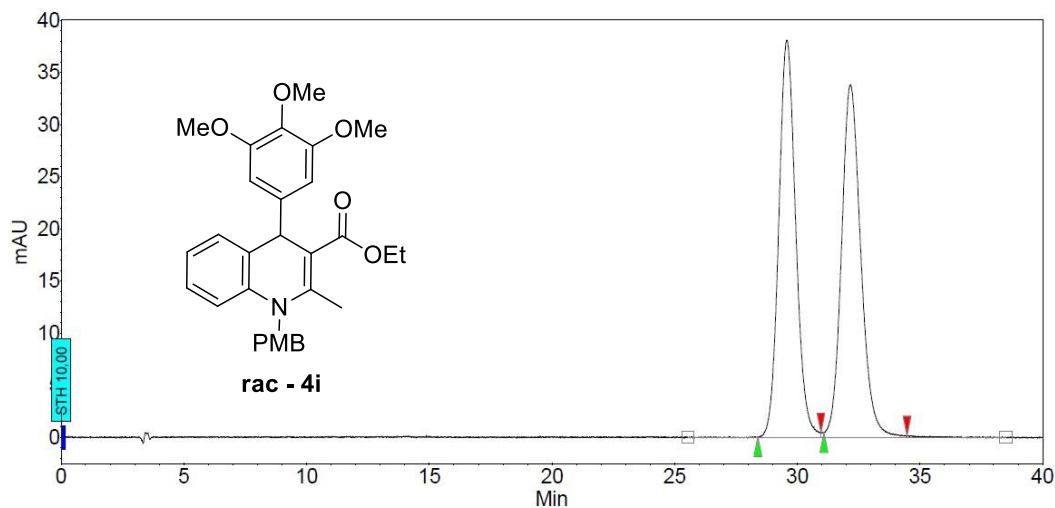
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	16.732	49.95	28.7	13.7	49.949
2	UNKNOWN	18.799	50.05	26.6	13.7	50.051
Total			100.00	55.3	27.5	100.000



Peak results :

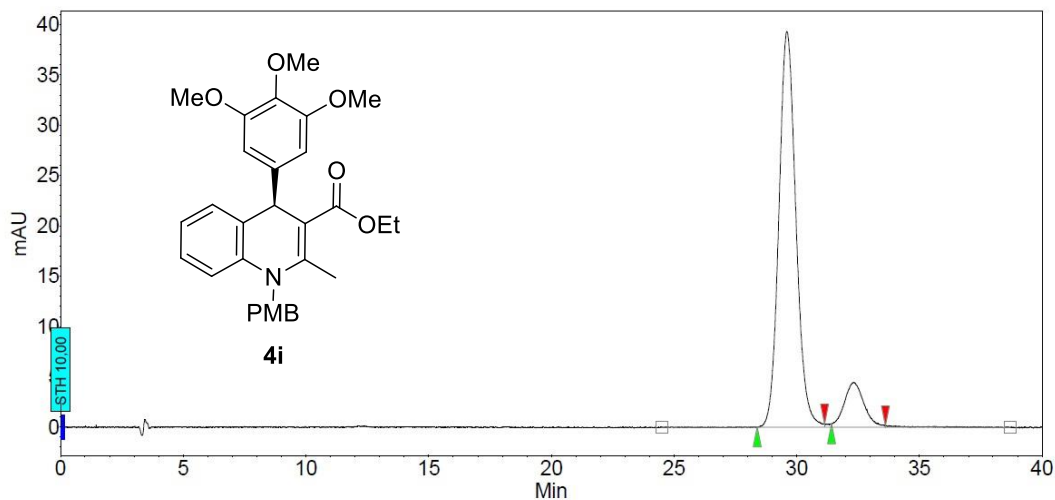
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	16.225	88.96	28.4	12.8	88.955
2	UNKNOWN	18.252	11.04	3.3	1.6	11.045
Total			100.00	31.6	14.4	100.000

Figure 2.8. HPLC analysis (IA Column; 90% hexane/10% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-ethyl 4-(3,4-dimethoxyphenyl)-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**4h**).



Peak results :

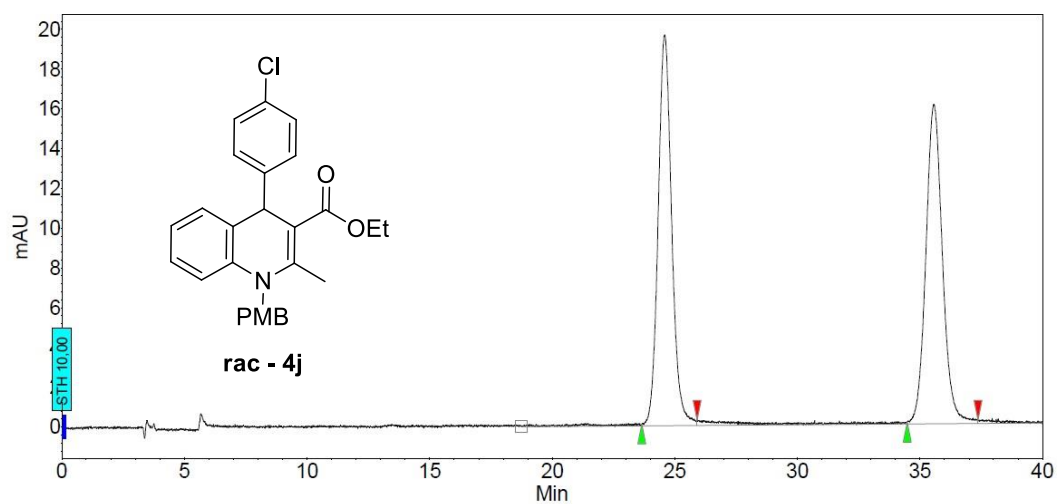
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	29.571	49.76	38.1	30.6	49.760
2	UNKNOWN	32.158	50.24	33.8	30.9	50.240
Total			100.00	71.9	61.5	100.000



Peak results :

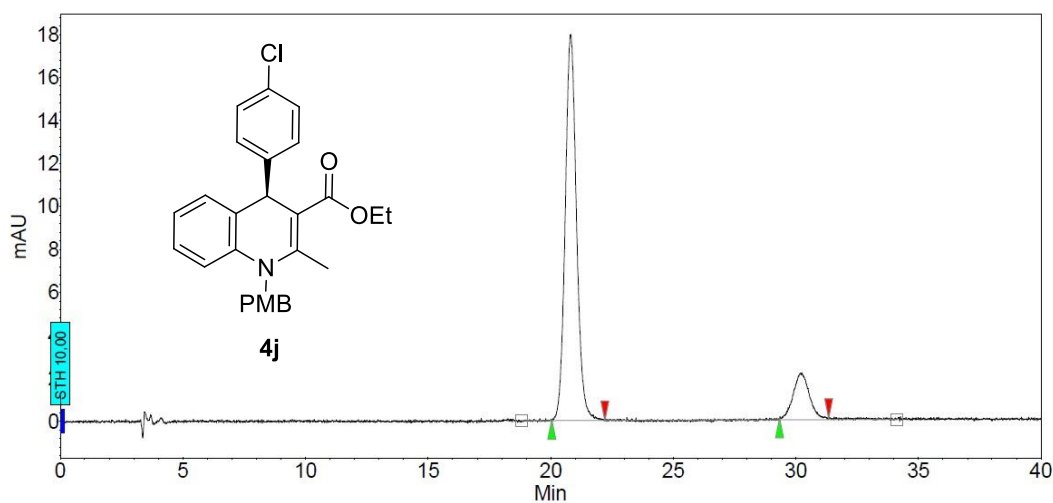
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	29.603	88.42	39.3	31.7	88.416
2	UNKNOWN	32.322	11.58	4.5	4.1	11.584
Total			100.00	43.8	35.8	100.000

Figure 2.9. HPLC analysis (IA Column; 90% hexane/10% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-ethyl 1-(4-methoxybenzyl)-2-methyl-4-(3,4,5-trimethoxyphenyl)-1,4-dihydroquinoline-3-carboxylate (**4i**).



Peak results :

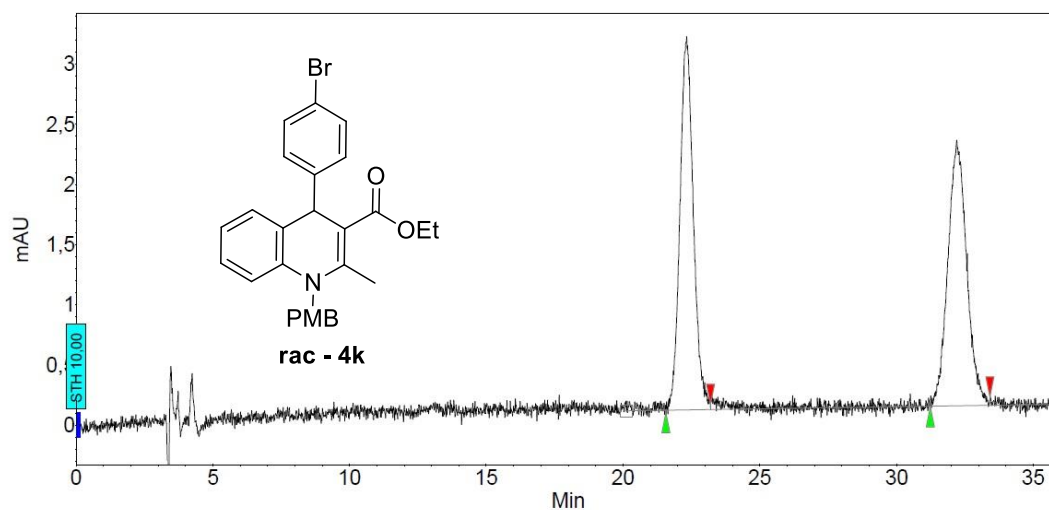
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	24.585	49.94	19.7	12.6	49.935
2	UNKNOWN	35.557	50.06	16.0	12.6	50.065
Total			100.00	35.7	25.2	100.000



Peak results :

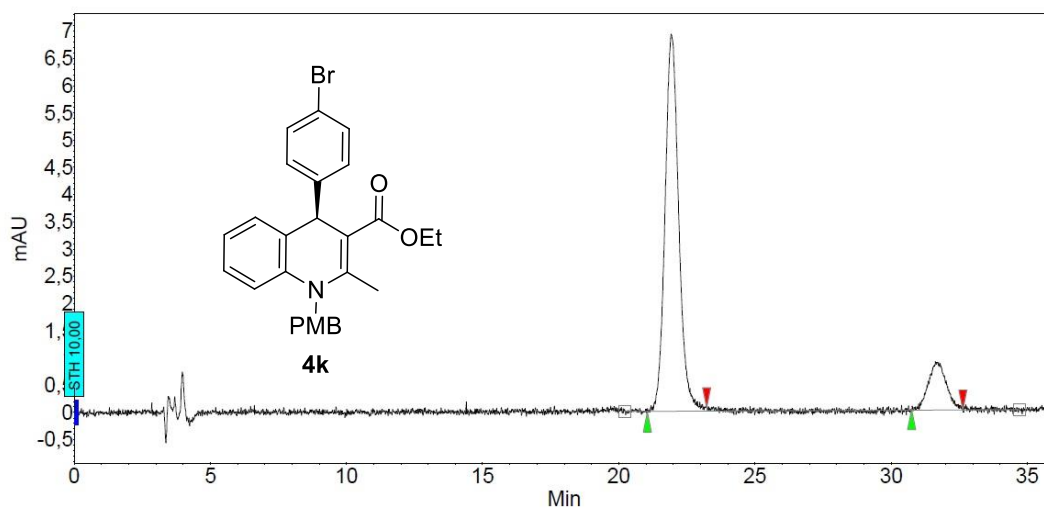
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	20.812	85.10	17.9	9.6	85.100
2	UNKNOWN	30.224	14.90	2.1	1.7	14.900
Total			100.00	20.0	11.3	100.000

Figure 2.10. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-ethyl 4-(4-chlorophenyl)-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**4j**).



Peak results :

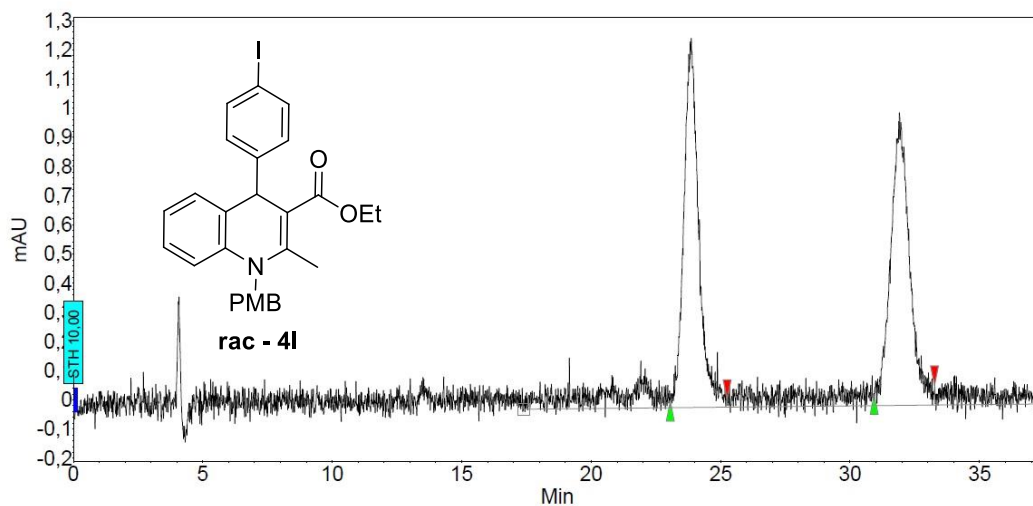
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	22.318	50.14	3.1	1.8	50.139
2	UNKNOWN	32.211	49.86	2.2	1.8	49.861
Total			100.00	5.3	3.5	100.000



Peak results :

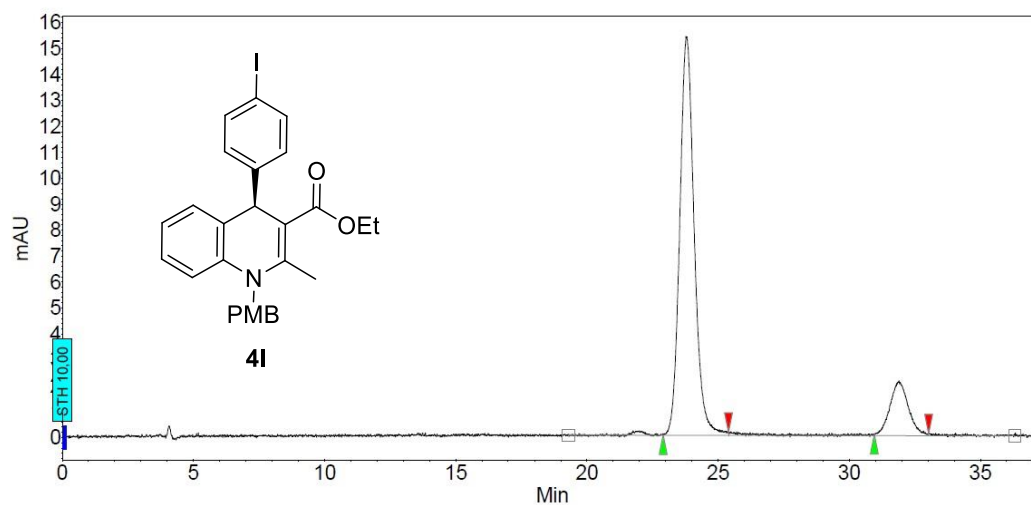
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	21.932	85.65	6.9	4.0	85.648
2	UNKNOWN	31.704	14.35	0.9	0.7	14.352
Total			100.00	7.8	4.7	100.000

Figure 2.11. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-ethyl 4-(4-bromophenyl)-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**4k**).



Peak results :

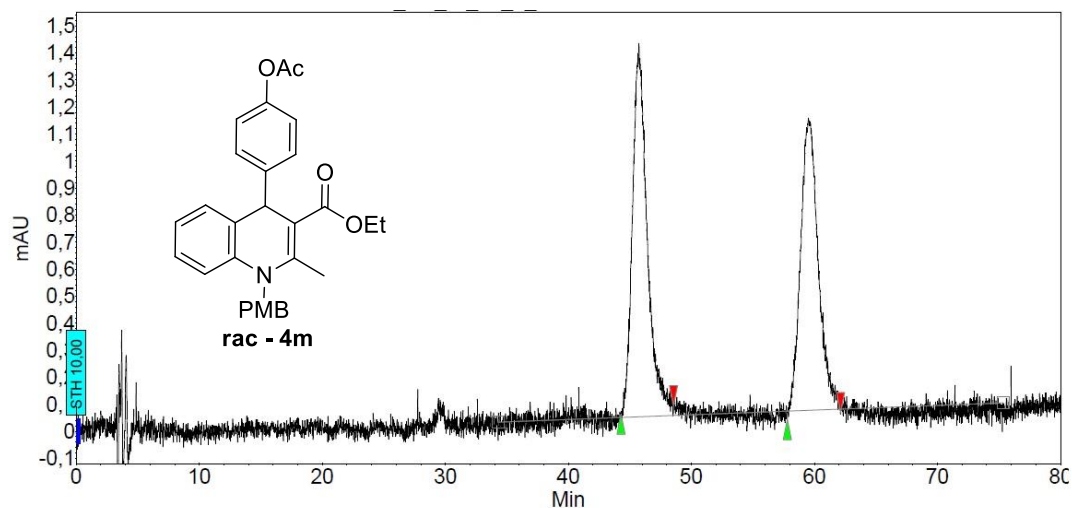
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	23.865	50.10	1.3	0.8	50.099
2	UNKNOWN	31.931	49.90	0.9	0.8	49.901
Total			100.00	2.2	1.7	100.000



Peak results :

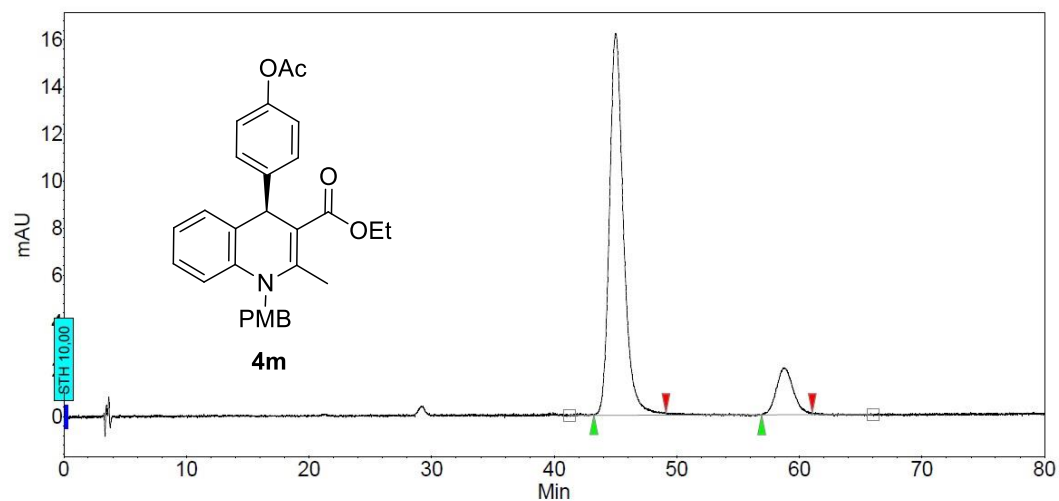
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	23.798	85.19	15.3	9.8	85.194
2	UNKNOWN	31.891	14.81	2.1	1.7	14.806
Total			100.00	17.5	11.5	100.000

Figure 2.12. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 320 nm) of (*R*)-ethyl 4-(4-iodophenyl)-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**4I**).



Peak results :

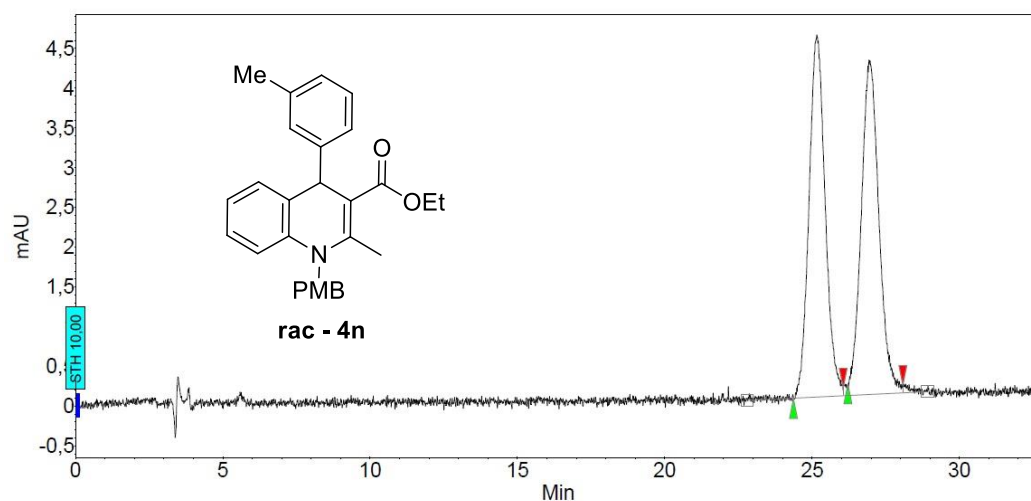
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	45.730	51.83	1.4	1.9	51.833
2	UNKNOWN	59.539	48.17	1.1	1.8	48.167
Total			100.00	2.4	3.7	100.000



Peak results :

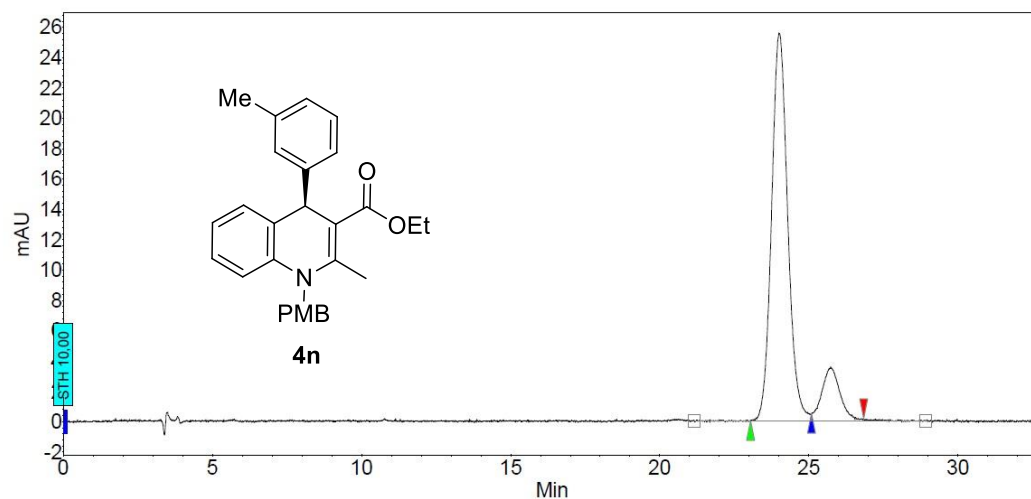
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	45.024	87.11	16.2	21.4	87.105
2	UNKNOWN	58.792	12.89	2.0	3.2	12.895
Total			100.00	18.2	24.6	100.000

Figure 2.13. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 320 nm) of (*R*)-ethyl 4-(4-acetoxyphe-1-yl)-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**4m**).



Peak results :

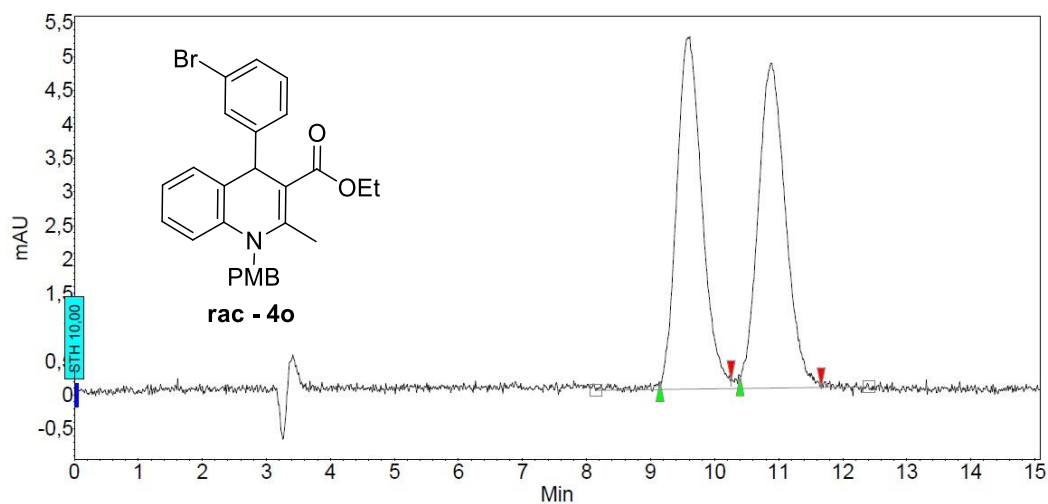
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	25.158	49.66	4.6	2.9	49.661
2	UNKNOWN	26.958	50.34	4.2	2.9	50.339
Total			100.00	8.8	5.8	100.000



Peak results :

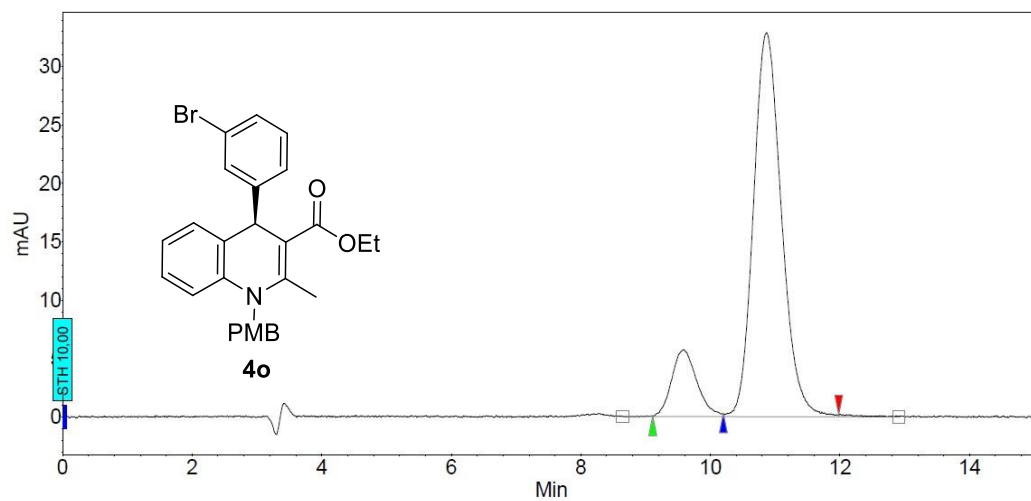
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	24.012	86.48	25.5	16.0	86.482
2	UNKNOWN	25.731	13.52	3.6	2.5	13.518
Total			100.00	29.1	18.6	100.000

Figure 2.14. HPLC analysis (IA Column; 99% hexane/1% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-ethyl 1-(4-methoxybenzyl)-2-methyl-4-(*m*-tolyl)-1,4-dihydroquinoline-3-carboxylate (**4n**).



Peak results :

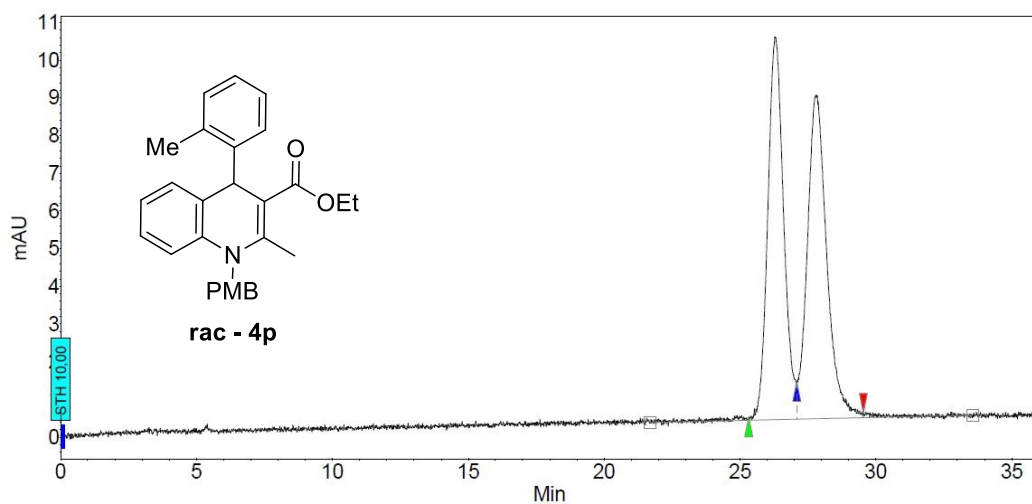
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	9.587	49.93	5.2	2.4	49.928
2	UNKNOWN	10.880	50.07	4.8	2.4	50.072
Total			100.00	10.0	4.7	100.000



Peak results :

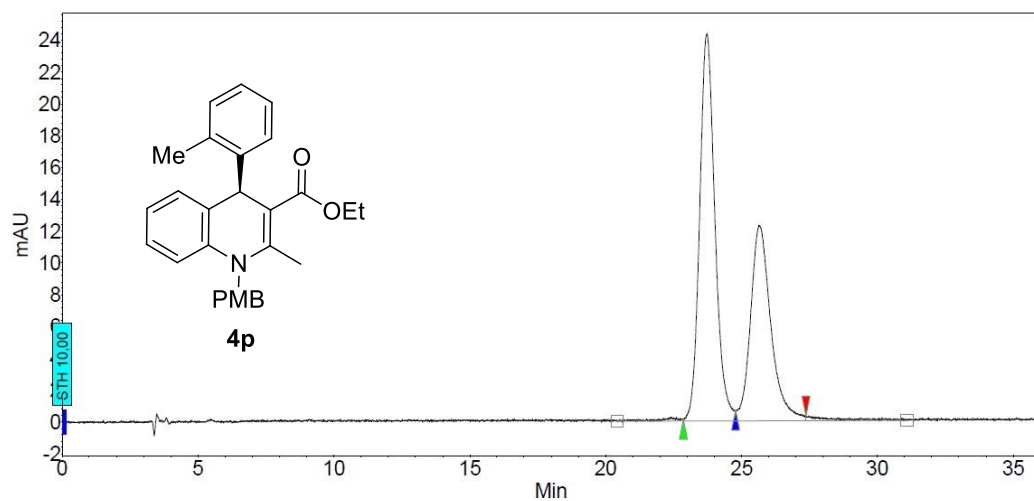
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	9.573	13.47	5.7	2.6	13.472
2	UNKNOWN	10.866	86.53	32.9	16.5	86.528
Total			100.00	38.6	19.0	100.000

Figure 2.15. HPLC analysis (OD-H Column; 90% hexane/10% *i*-propanol; 1 mL/min; 328 nm) of (*R*)-ethyl 4-(3-bromophenyl)-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**4o**).



Peak results :

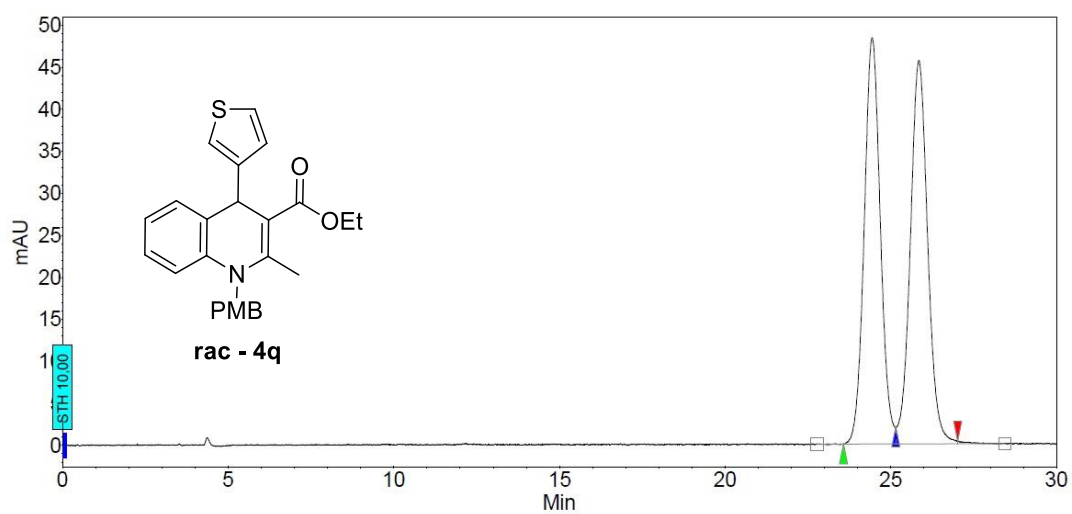
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	26.305	49.26	10.1	6.9	49.257
2	UNKNOWN	27.798	50.74	8.6	7.1	50.743
Total			100.00	18.7	14.0	100.000



Peak results :

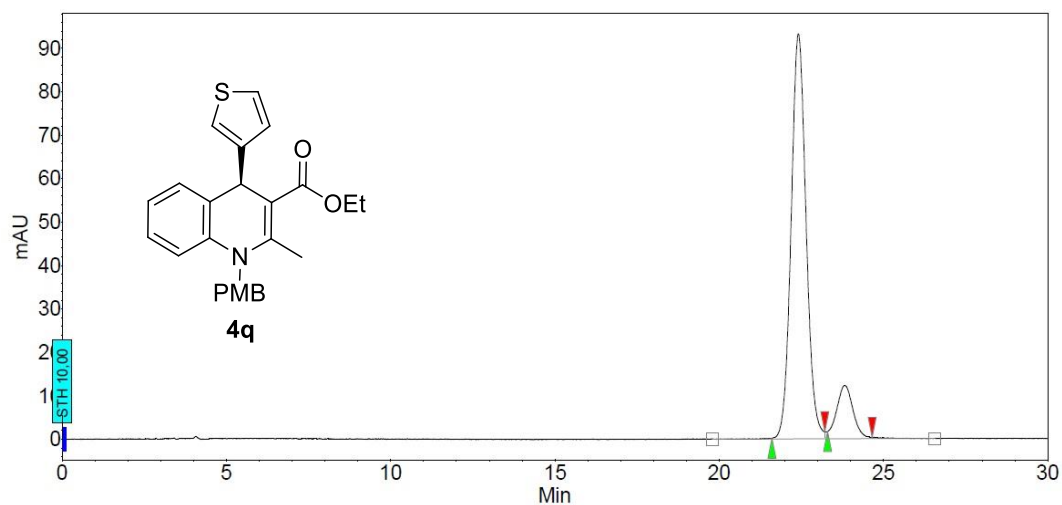
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	23.718	59.90	24.3	15.9	59.897
2	UNKNOWN	25.665	40.10	12.3	10.6	40.103
Total			100.00	36.5	26.5	100.000

Figure 2.16. HPLC analysis (IA Column; 99% hexane/1% *i*-propanol; 1 mL/min; 328 nm) of (*R*)-ethyl 1-(4-methoxybenzyl)-2-methyl-4-(*o*-tolyl)-1,4-dihydroquinoline-3-carboxylate (**4p**).



Peak results :

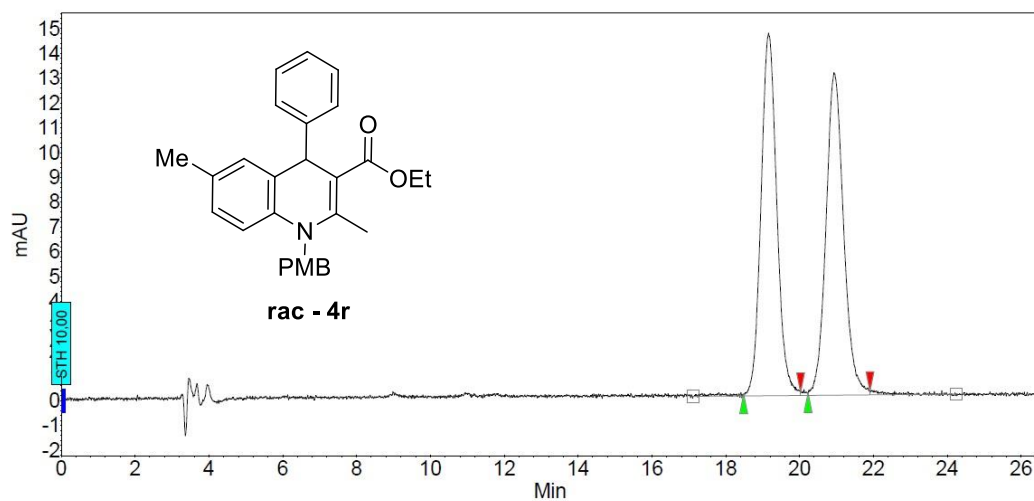
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	24.438	49.53	48.3	27.2	49.532
2	UNKNOWN	25.851	50.47	45.6	27.7	50.468
Total			100.00	93.9	55.0	100.000



Peak results :

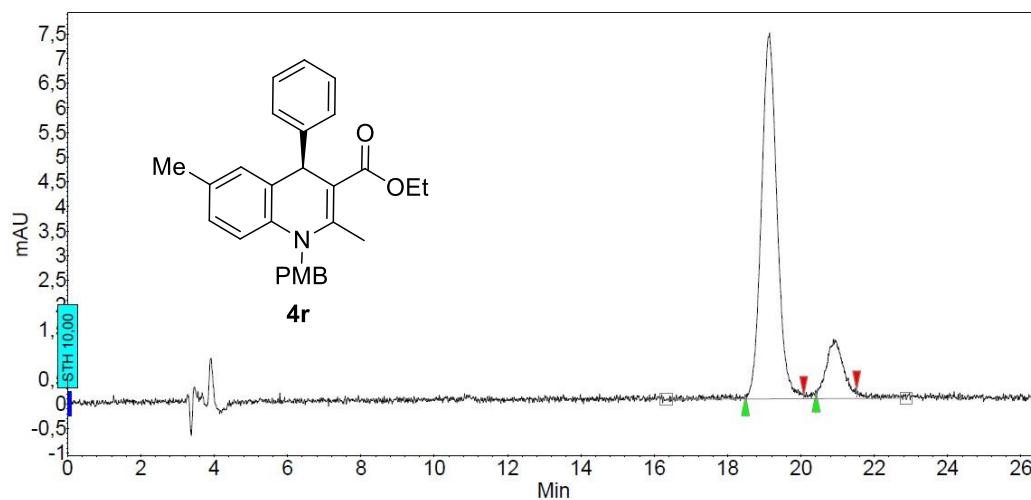
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	22.412	87.37	93.3	49.1	87.365
2	UNKNOWN	23.825	12.63	12.3	7.1	12.635
Total			100.00	105.5	56.2	100.000

Figure 2.17. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 320 nm) of (*R*)-ethyl 1-(4-methoxybenzyl)-2-methyl-4-(thiophen-3-yl)-1,4-dihydroquinoline-3-carboxylate (**4q**).



Peak results :

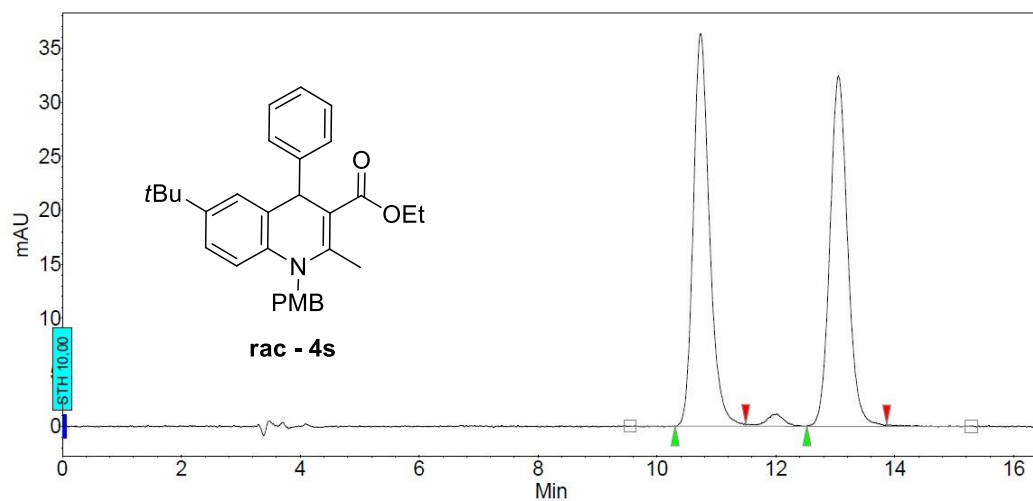
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	19.159	49.98	14.6	7.2	49.975
2	UNKNOWN	20.945	50.02	12.9	7.2	50.025
Total			100.00	27.6	14.4	100.000



Peak results :

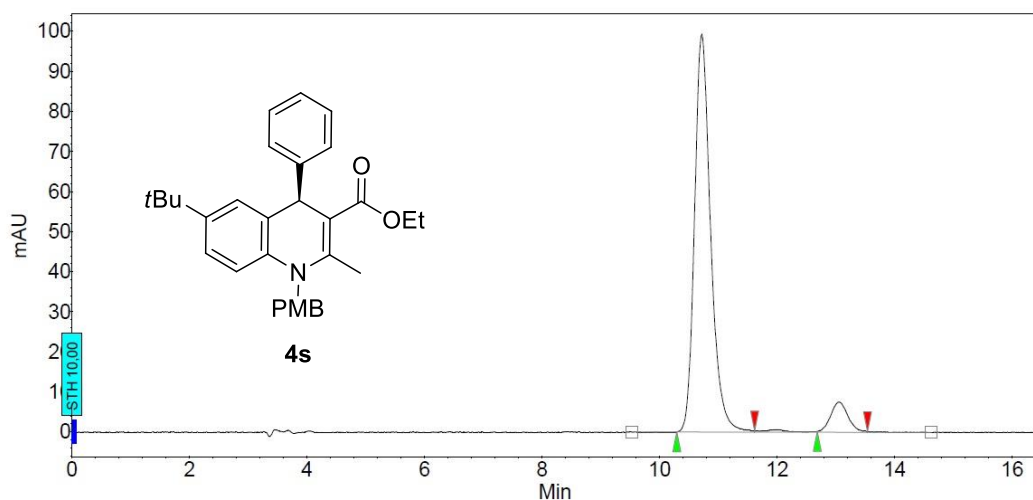
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	19.132	85.03	7.3	3.6	85.033
2	UNKNOWN	20.918	14.97	1.2	0.6	14.967
Total			100.00	8.5	4.3	100.000

Figure 2.18. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 328 nm) of (*R*)-ethyl 1-(4-methoxybenzyl)-2,6-dimethyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**4r**).



Peak results :

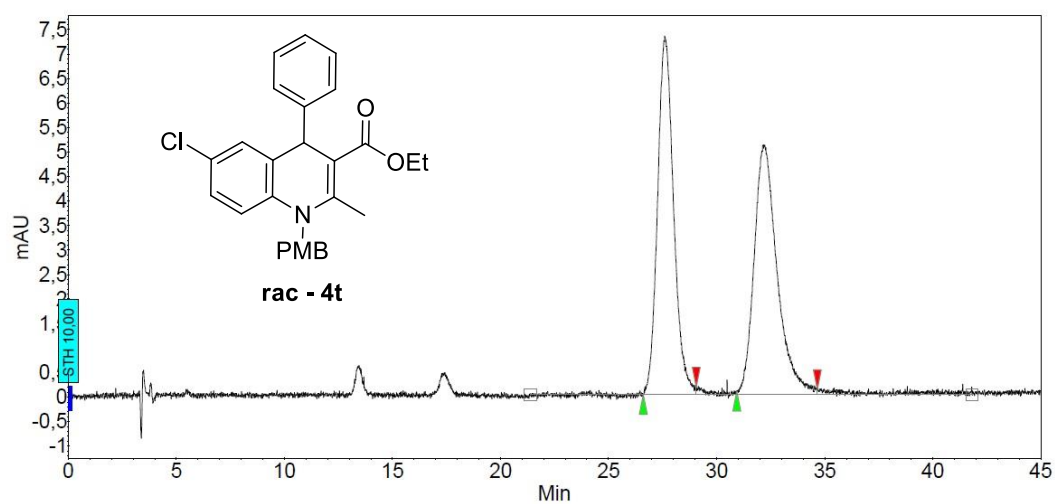
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	10.733	50.57	36.3	11.4	50.570
2	UNKNOWN	13.052	49.43	32.4	11.2	49.430
Total			100.00	68.8	22.6	100.000



Peak results :

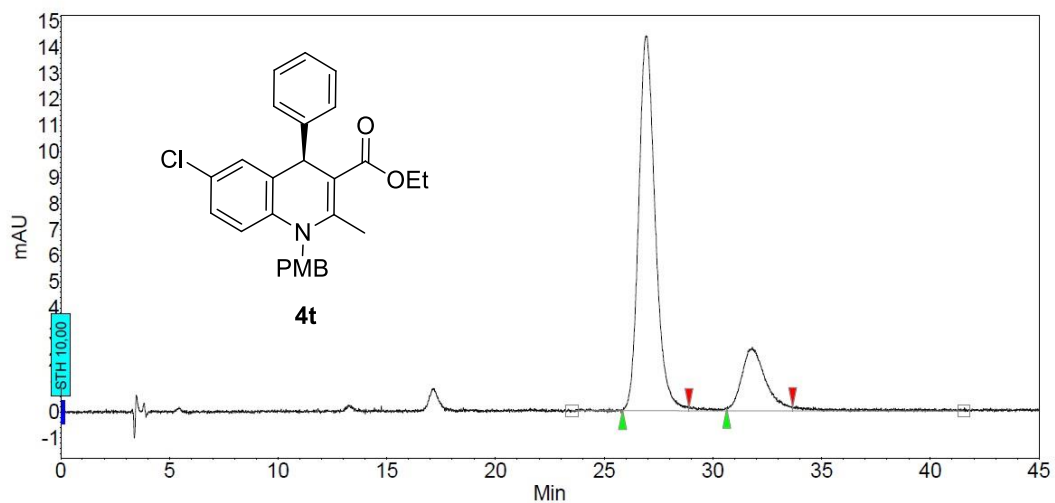
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	10.719	92.40	99.3	31.5	92.399
2	UNKNOWN	13.052	7.60	7.5	2.6	7.601
Total			100.00	106.9	34.1	100.000

Figure 2.19. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-ethyl 6-(*tert*-butyl)-1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**4s**).



Peak results :

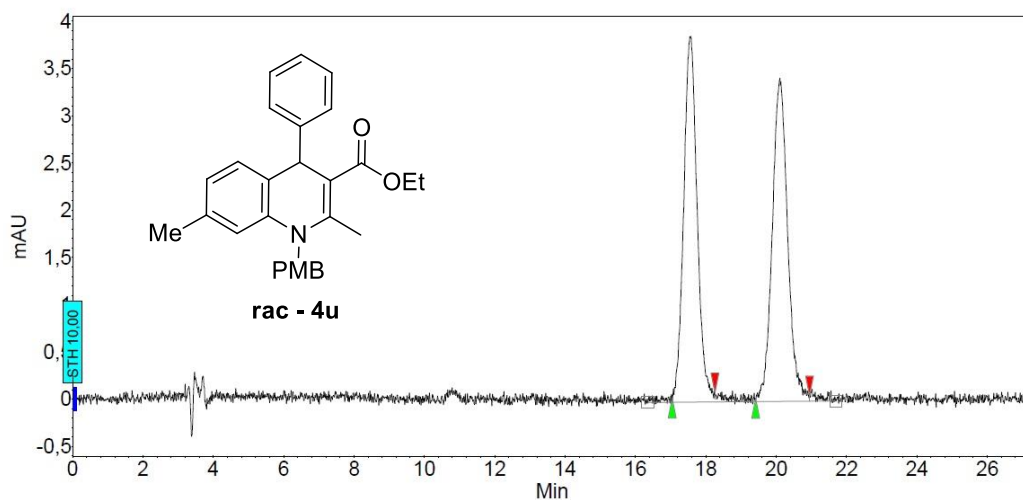
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	27.611	50.00	7.3	6.3	50.004
2	UNKNOWN	32.184	50.00	5.1	6.3	49.996
Total			100.00	12.4	12.6	100.000



Peak results :

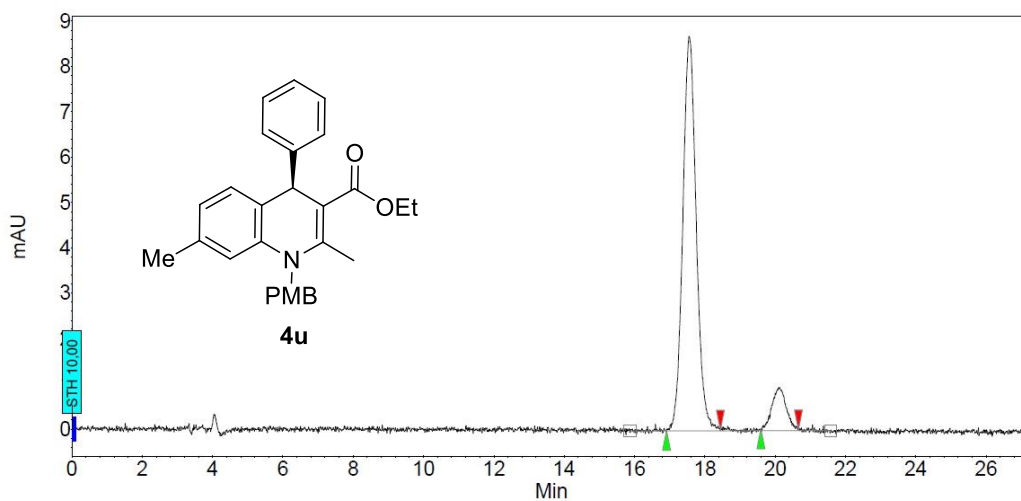
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	26.931	80.66	14.4	12.7	80.665
2	UNKNOWN	31.784	19.34	2.4	3.0	19.335
Total			100.00	16.8	15.8	100.000

Figure 2.20. HPLC analysis (IA Column; 99% hexane/1% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-ethyl 6-chloro-1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**4t**).



Peak results :

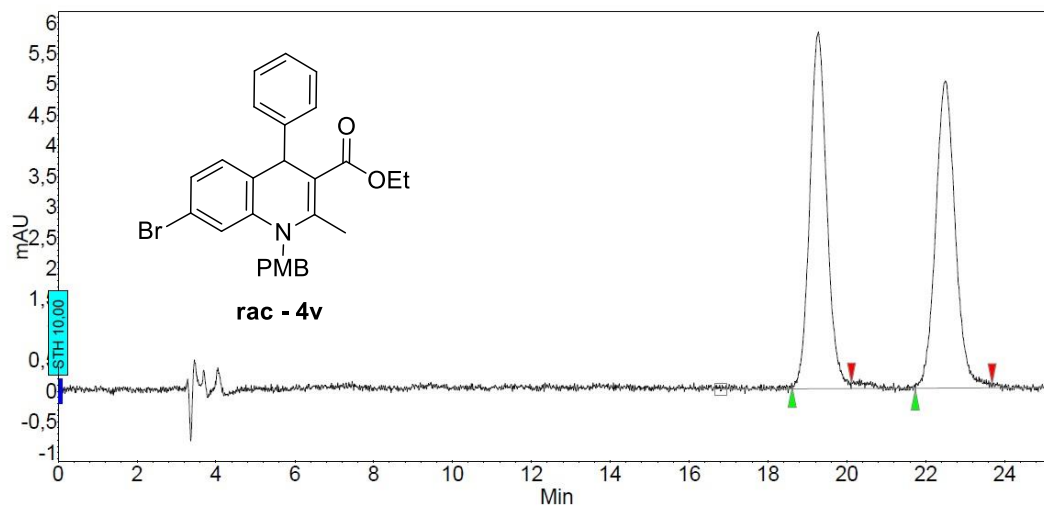
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	17.559	49.75	3.9	1.7	49.748
2	UNKNOWN	20.105	50.25	3.4	1.7	50.252
Total			100.00	7.3	3.4	100.000



Peak results :

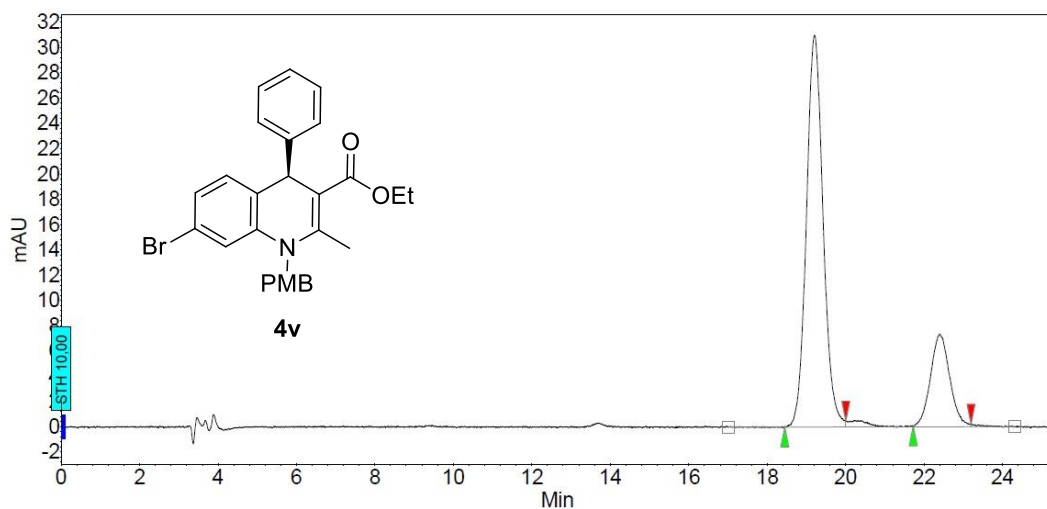
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	17.559	89.51	8.7	3.9	89.509
2	UNKNOWN	20.105	10.49	0.9	0.5	10.491
Total			100.00	9.6	4.3	100.000

Figure 2.21. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-ethyl 1-(4-methoxybenzyl)-2,7-dimethyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**4u**).



Peak results :

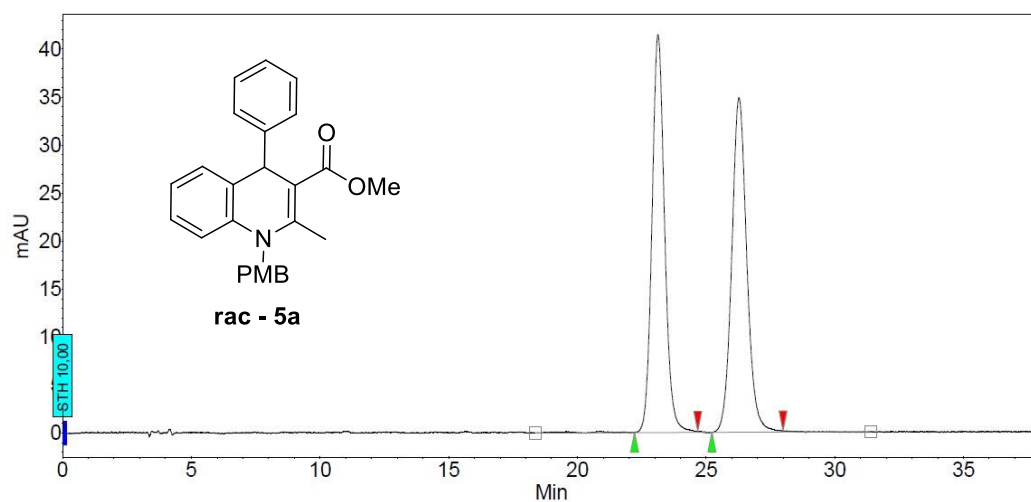
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	19.265	50.07	5.8	2.9	50.068
2	UNKNOWN	22.492	49.93	5.0	2.9	49.932
Total			100.00	10.8	5.8	100.000



Peak results :

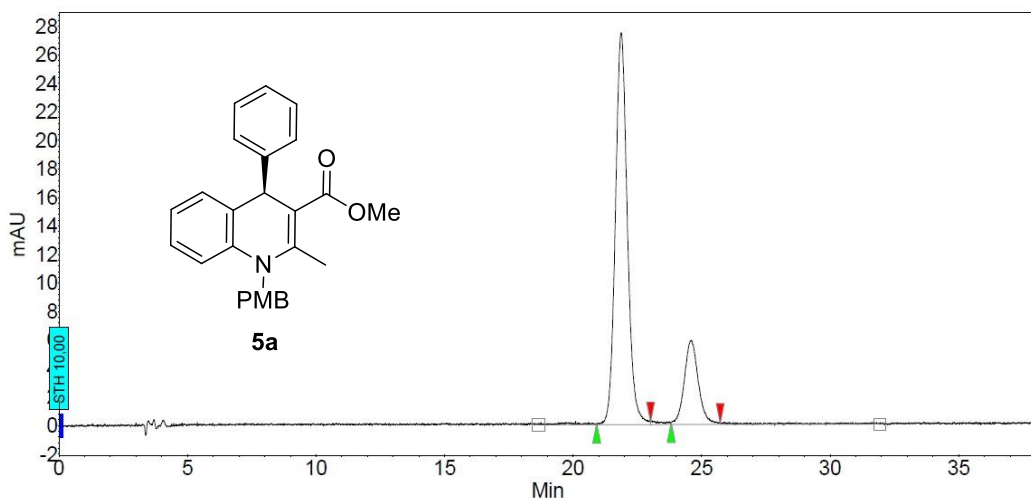
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	19.199	78.61	31.0	15.3	78.611
2	UNKNOWN	22.398	21.39	7.3	4.2	21.389
Total			100.00	38.3	19.5	100.000

Figure 2.22. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-ethyl 7-bromo-1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**4v**).



Peak results :

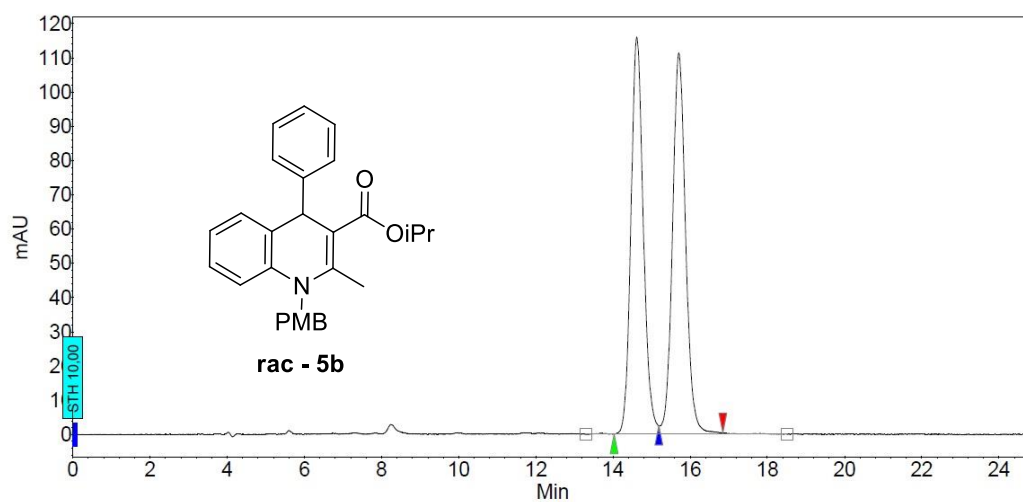
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	23.125	49.95	41.4	23.6	49.949
2	UNKNOWN	26.271	50.05	34.8	23.6	50.051
Total			100.00	76.3	47.2	100.000



Peak results :

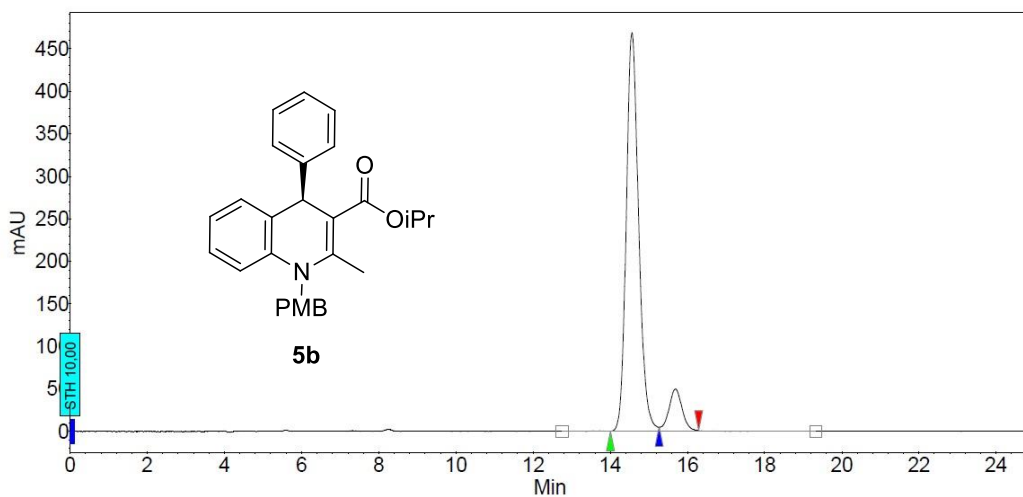
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	21.865	79.92	27.5	14.8	79.915
2	UNKNOWN	24.585	20.08	5.9	3.7	20.085
Total			100.00	33.3	18.5	100.000

Figure 2.23. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-methyl 1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**5a**).



Peak results :

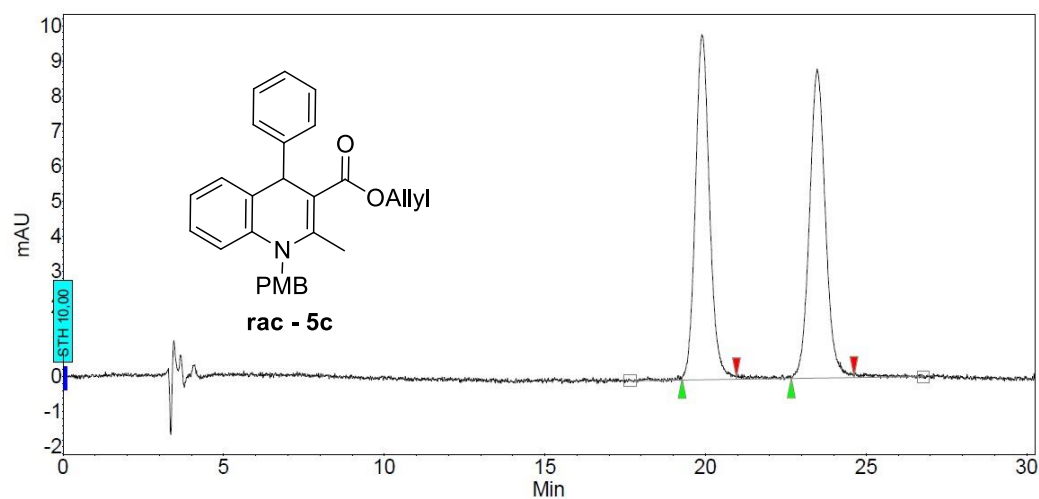
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	14.612	49.47	115.9	43.1	49.470
2	UNKNOWN	15.706	50.53	111.3	44.0	50.530
Total			100.00	227.2	87.1	100.000



Peak results :

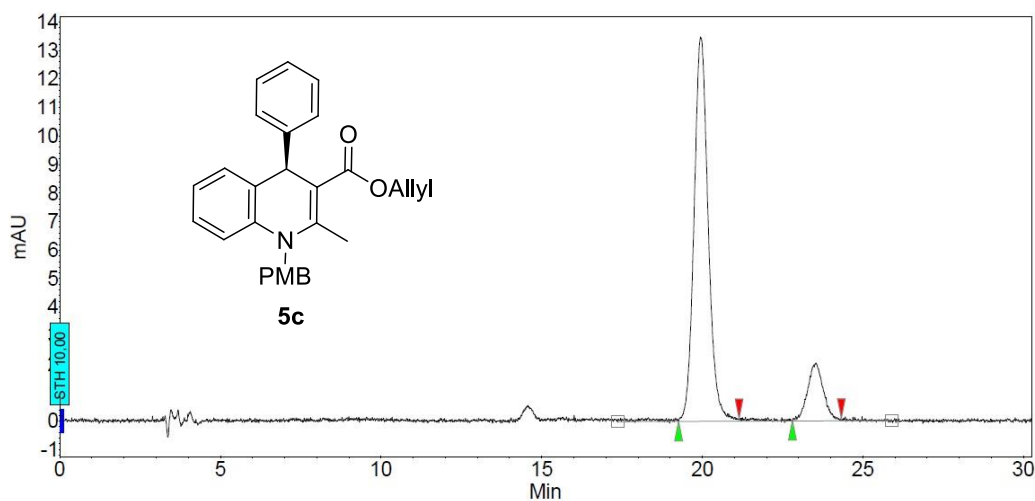
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	14.559	89.71	468.9	174.8	89.708
2	UNKNOWN	15.692	10.29	49.9	20.1	10.292
Total			100.00	518.8	194.9	100.000

Figure 2.24. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-isopropyl 1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**5b**).



Peak results :

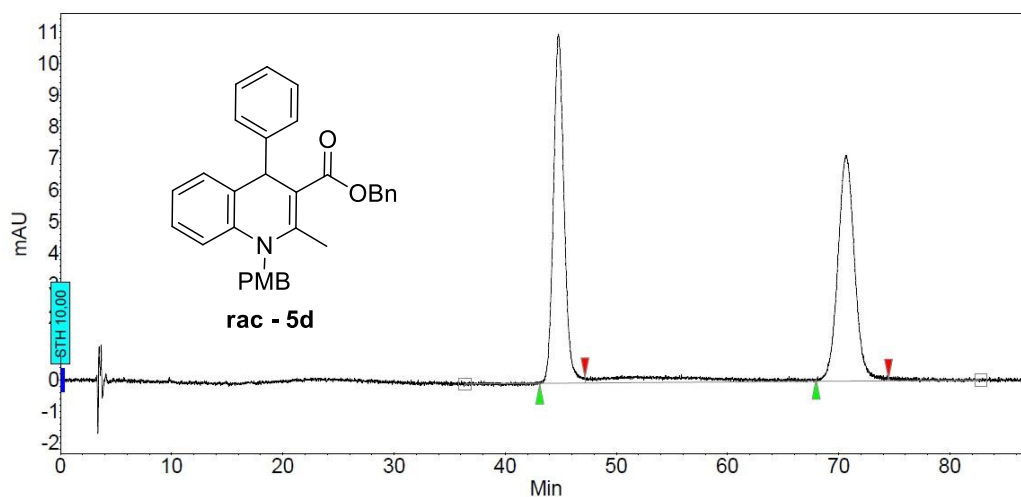
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	19.892	49.85	9.8	5.0	49.850
2	UNKNOWN	23.478	50.15	8.8	5.1	50.150
Total			100.00	18.7	10.1	100.000



Peak results :

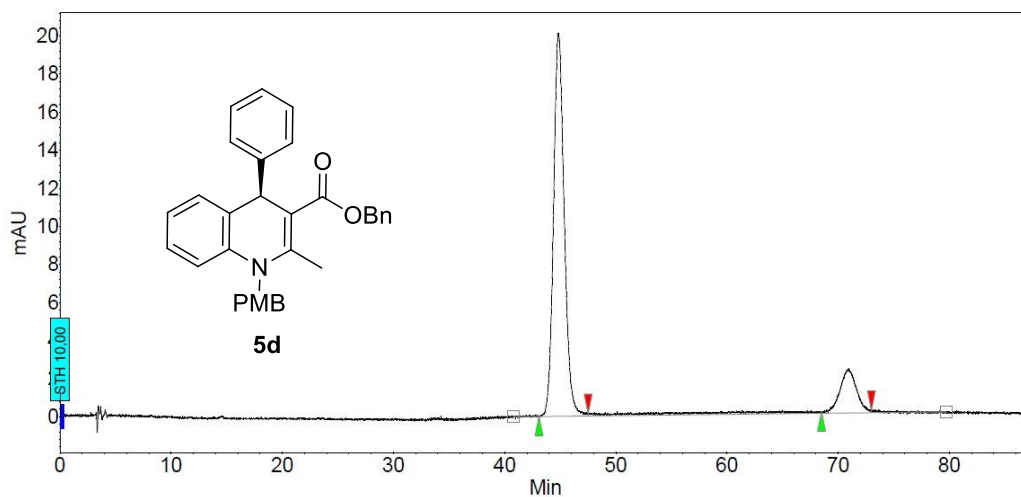
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	19.959	85.60	13.4	6.9	85.603
2	UNKNOWN	23.518	14.40	2.0	1.2	14.397
Total			100.00	15.4	8.0	100.000

Figure 2.25. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-allyl 1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**5c**).



Peak results :

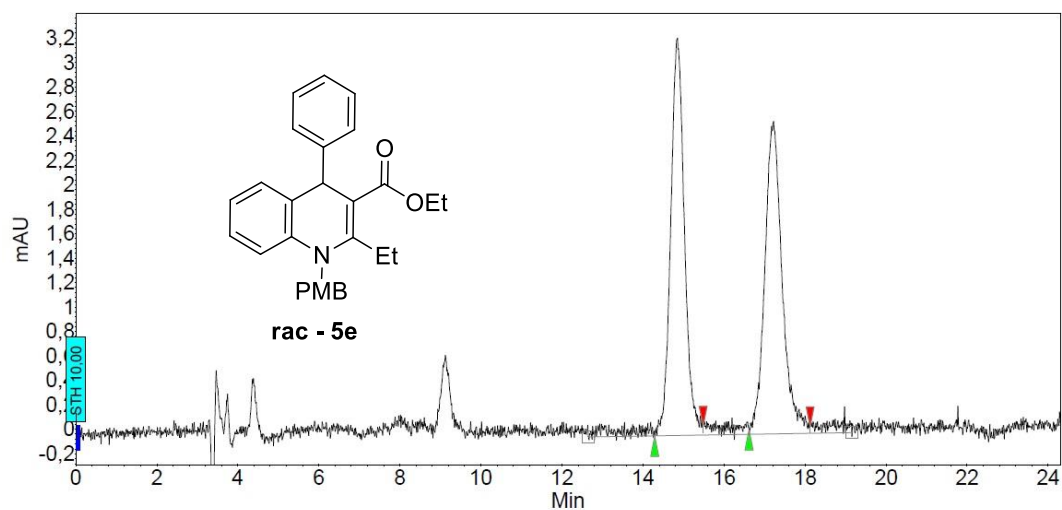
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	44.797	49.57	11.0	12.2	49.566
2	UNKNOWN	70.681	50.43	7.1	12.5	50.434
Total			100.00	18.2	24.7	100.000



Peak results :

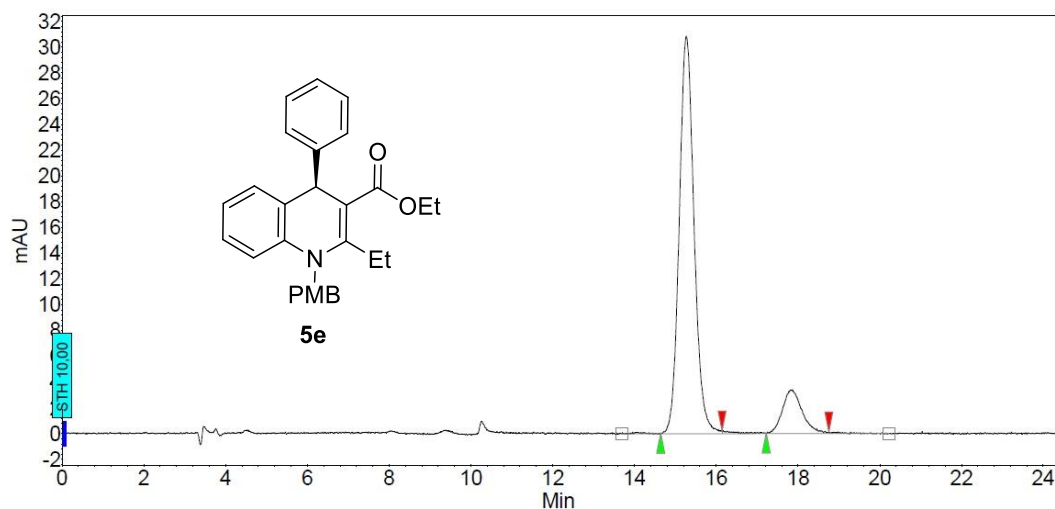
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	44.851	84.90	20.1	22.5	84.905
2	UNKNOWN	70.921	15.10	2.3	4.0	15.095
Total			100.00	22.4	26.5	100.000

Figure 2.26. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-benzyl 1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**5d**).



Peak results :

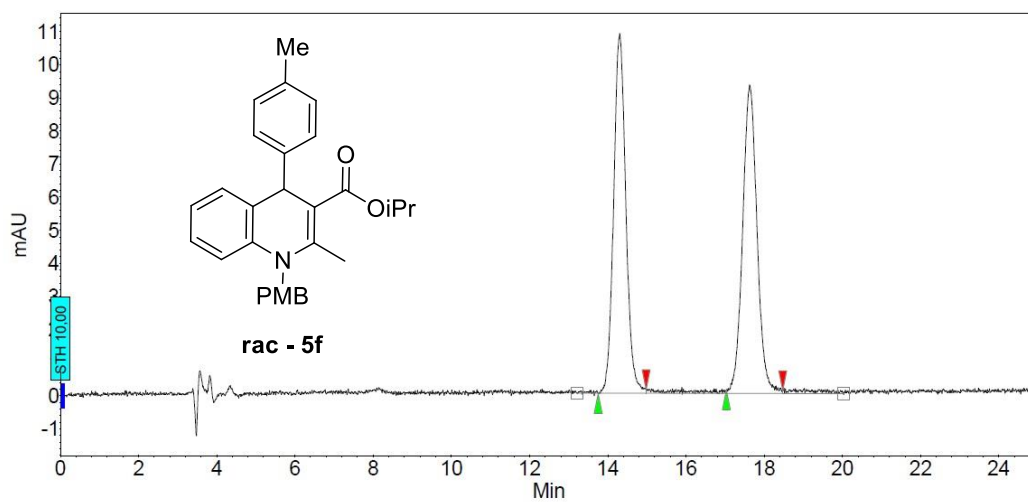
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	14.852	50.12	3.2	1.3	50.118
2	UNKNOWN	17.212	49.88	2.5	1.3	49.882
Total			100.00	5.8	2.5	100.000



Peak results :

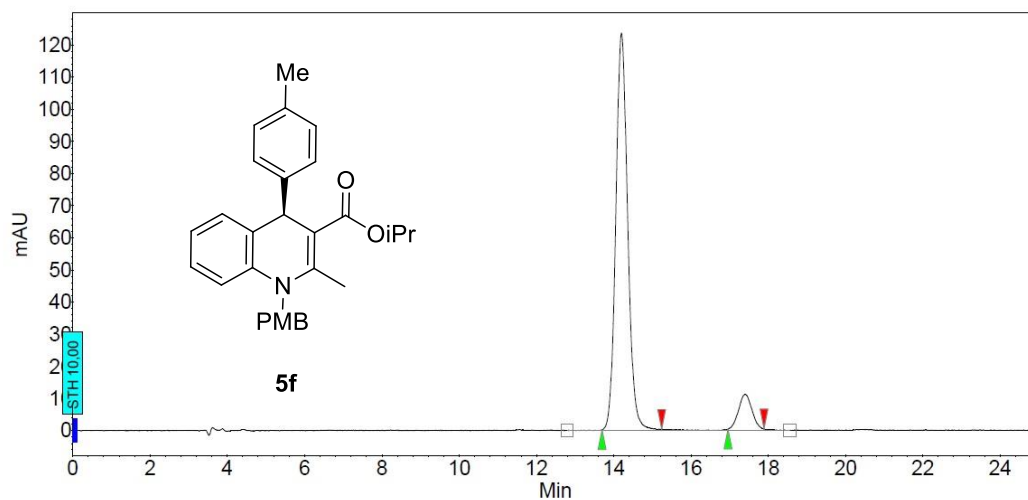
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	15.266	87.17	30.9	13.0	87.169
2	UNKNOWN	17.839	12.83	3.4	1.9	12.831
Total			100.00	34.2	14.9	100.000

Figure 2.27. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-ethyl 2-ethyl-1-(4-methoxybenzyl)-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**5e**).



Peak results :

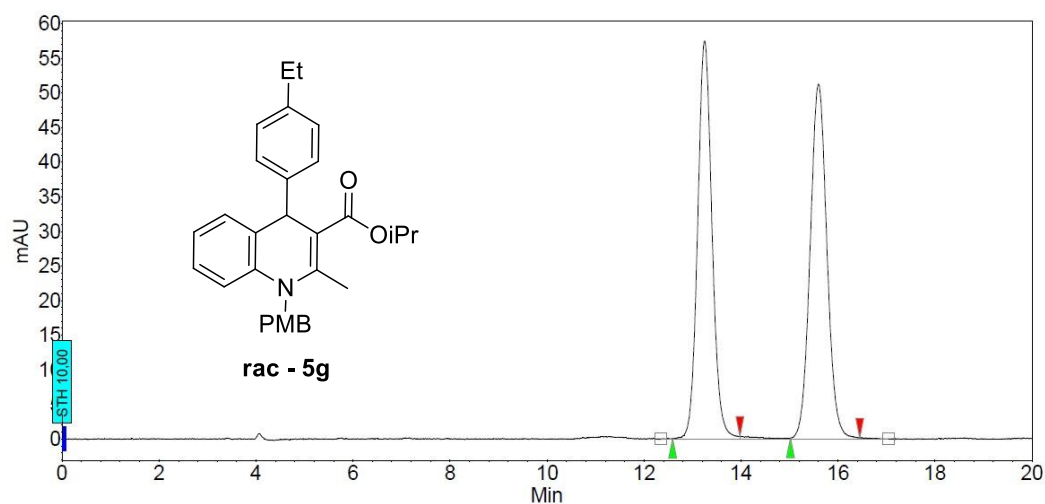
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	14.306	49.56	10.9	3.9	49.555
2	UNKNOWN	17.625	50.44	9.3	4.0	50.445
Total			100.00	20.2	7.9	100.000



Peak results :

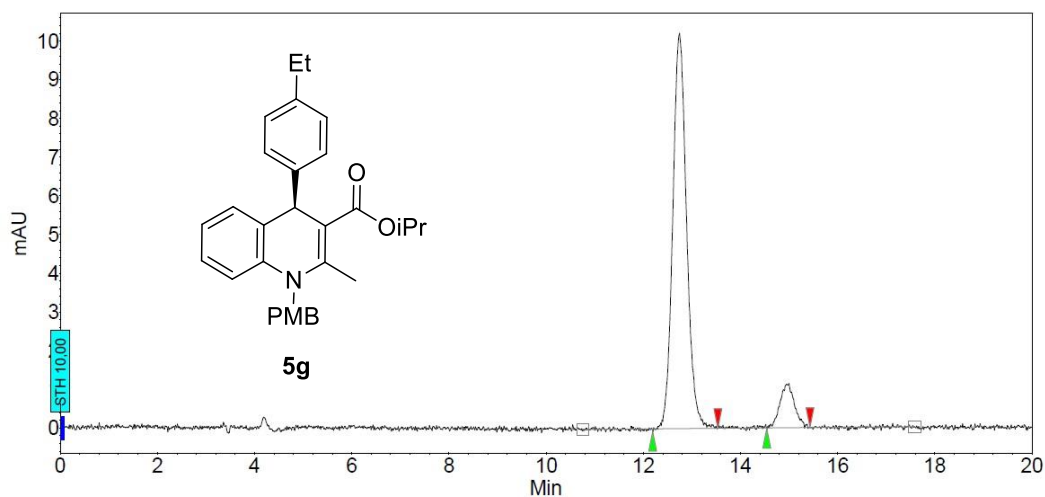
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	14.199	90.47	123.7	44.1	90.468
2	UNKNOWN	17.399	9.53	11.1	4.6	9.532
Total			100.00	134.8	48.8	100.000

Figure 2.28. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-isopropyl 1-(4-methoxybenzyl)-2-methyl-4-(*p*-tolyl)-1,4-dihydroquinoline-3-carboxylate (**5f**).



Peak results :

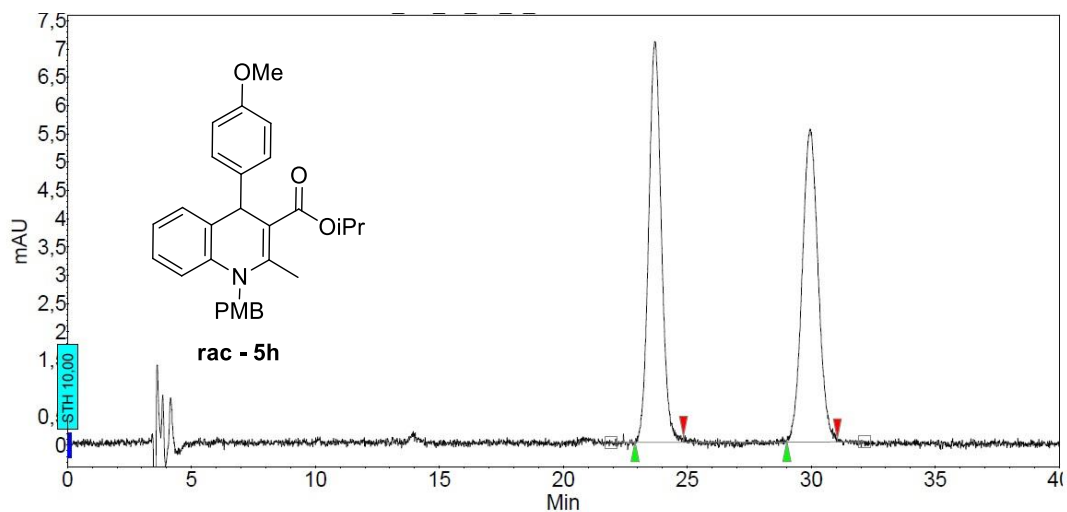
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	13.252	49.05	57.5	19.8	49.050
2	UNKNOWN	15.599	50.95	51.3	20.6	50.950
Total			100.00	108.7	40.3	100.000



Peak results :

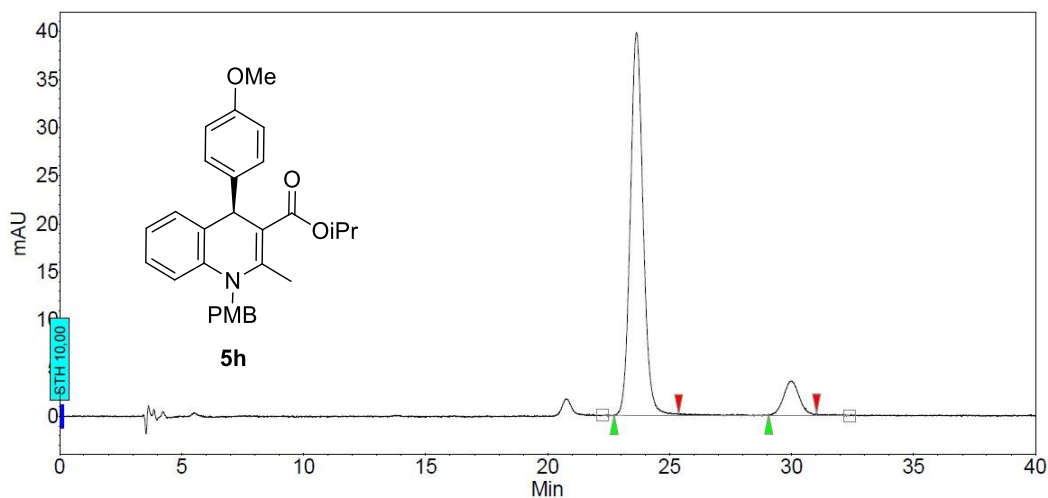
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	12.746	89.45	10.2	3.4	89.447
2	UNKNOWN	14.959	10.55	1.1	0.4	10.553
Total			100.00	11.3	3.8	100.000

Figure 2.29. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-isopropyl 4-(4-ethylphenyl)-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**5g**).



Peak results :

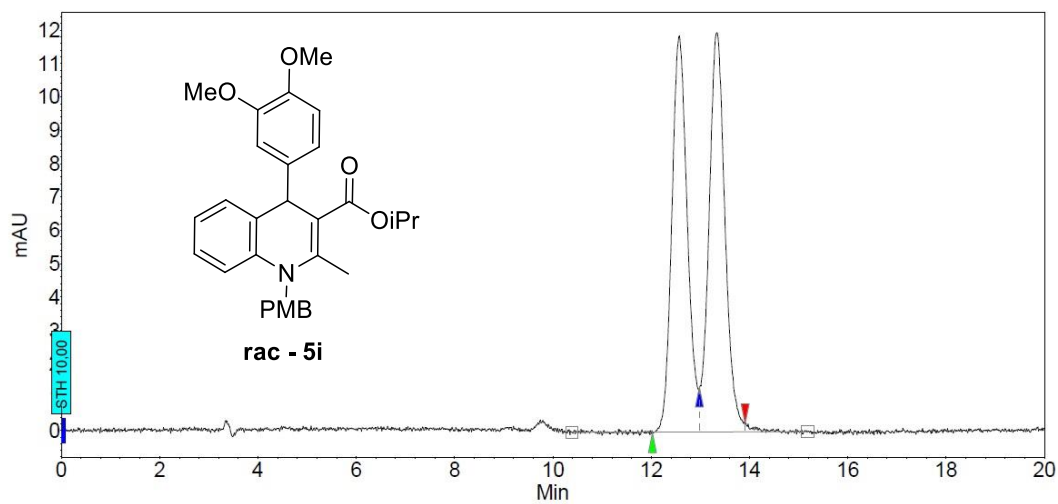
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	23.692	50.46	7.1	4.2	50.459
2	UNKNOWN	29.944	49.54	5.5	4.1	49.541
Total			100.00	12.6	8.3	100.000



Peak results :

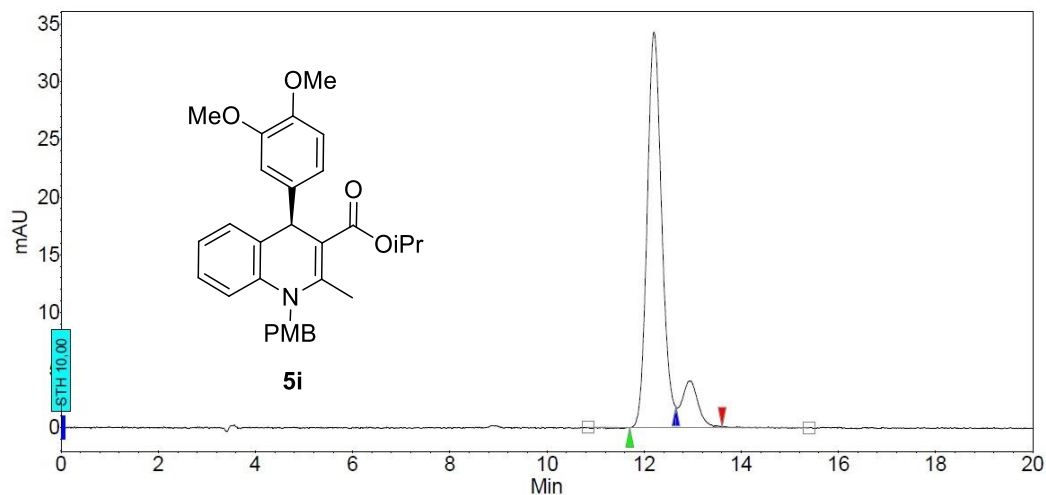
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	23.638	89.85	39.8	24.1	89.846
2	UNKNOWN	29.984	10.15	3.6	2.7	10.154
Total			100.00	43.4	26.9	100.000

Figure 2.30. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-isopropyl 1-(4-methoxybenzyl)-4-(4-methoxyphenyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**5h**).



Peak results :

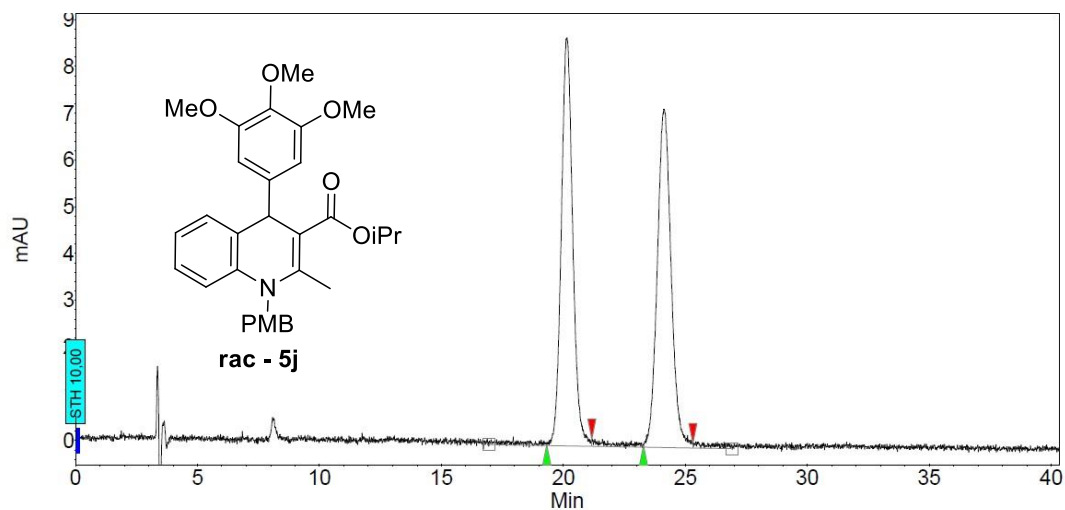
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	No. Peaks	2D View Area [mAU.Min]	Area % [%]
1	UNKNOWN	12.559	48.97	11.8		4.3	48.972
2	UNKNOWN	13.332	51.03	12.0		4.5	51.028
Total			100.00	23.8		8.8	100.000



Peak results :

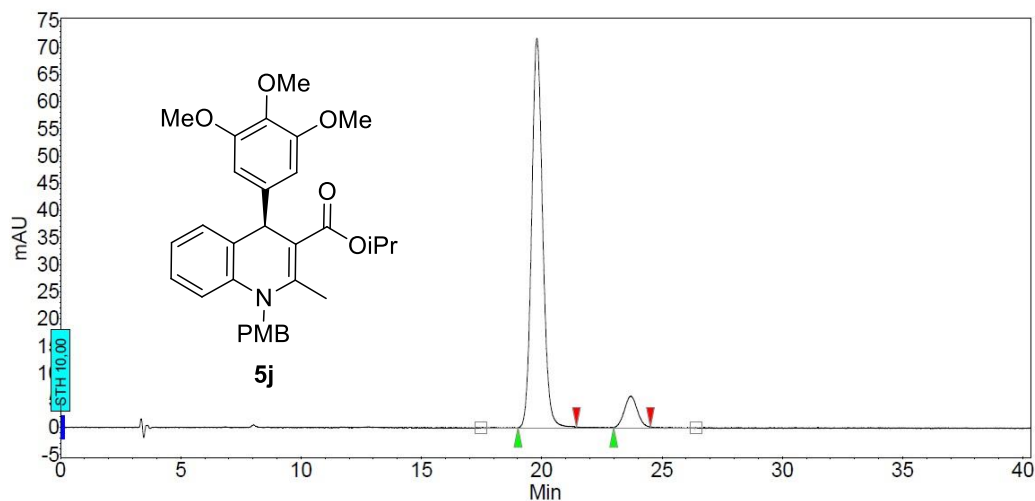
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	No. Peaks	2D View Area [mAU.Min]	Area % [%]
1	UNKNOWN	12.209	88.18	34.3		11.9	88.179
2	UNKNOWN	12.942	11.82	4.0		1.6	11.821
Total			100.00	38.3		13.5	100.000

Figure 2.31. HPLC analysis (IA Column; 90% hexane/10% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-isopropyl 4-(3,4-dimethoxyphenyl)-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate (**5i**).



Peak results :

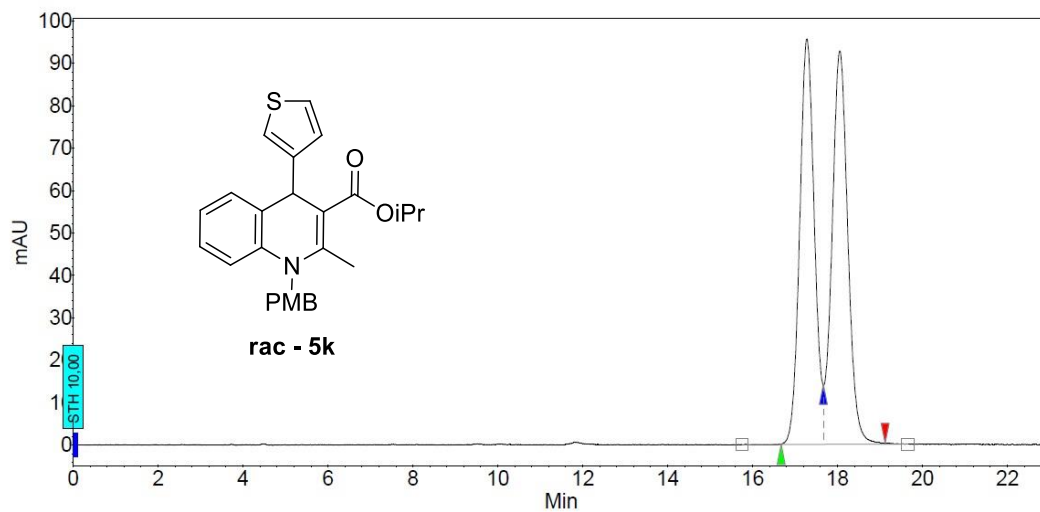
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	20.145	49.97	8.7	4.7	49.968
2	UNKNOWN	24.132	50.03	7.2	4.8	50.032
Total			100.00	16.0	9.5	100.000



Peak results :

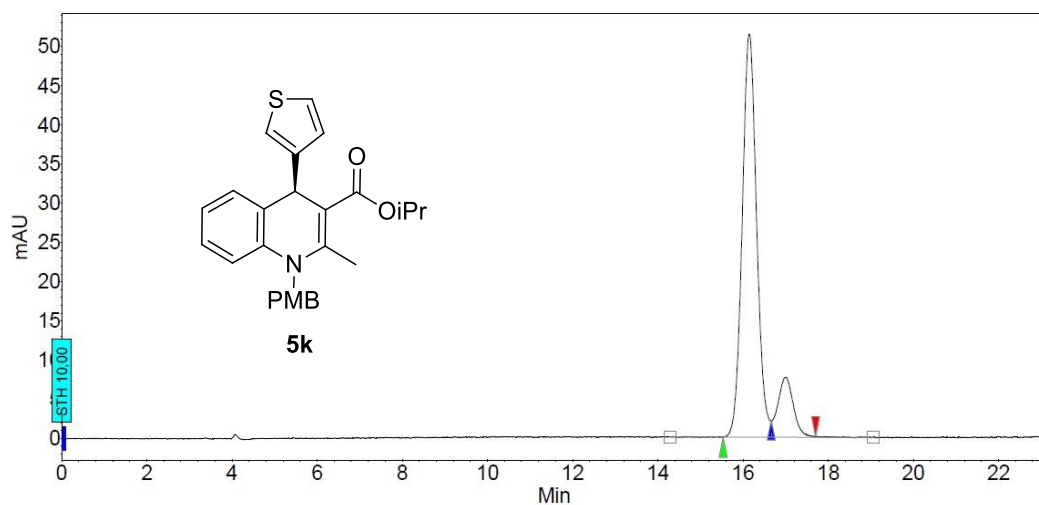
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	19.799	91.17	71.8	38.2	91.173
2	UNKNOWN	23.705	8.83	5.8	3.7	8.827
Total			100.00	77.6	41.9	100.000

Figure 2.32. HPLC analysis (IA Column; 90% hexane/10% *i*-propanol; 1 mL/min; 324 nm) of (*R*)-isopropyl 1-(4-methoxybenzyl)-2-methyl-4-(3,4,5-trimethoxyphenyl)-1,4-dihydroquinoline-3-carboxylate (**5j**).



Peak results :

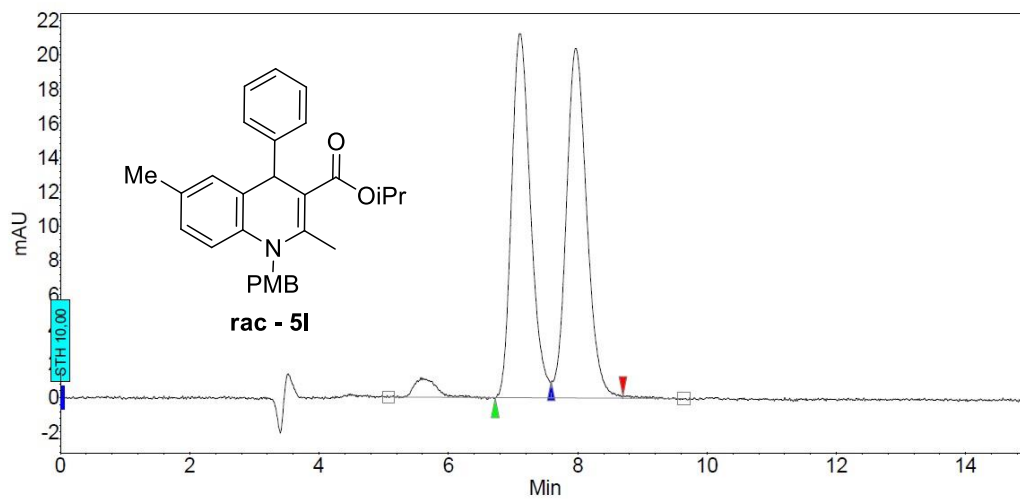
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	17.279	48.99	95.6	38.2	48.988
2	UNKNOWN	18.052	51.01	92.8	39.8	51.012
Total			100.00	188.4	78.0	100.000



Peak results :

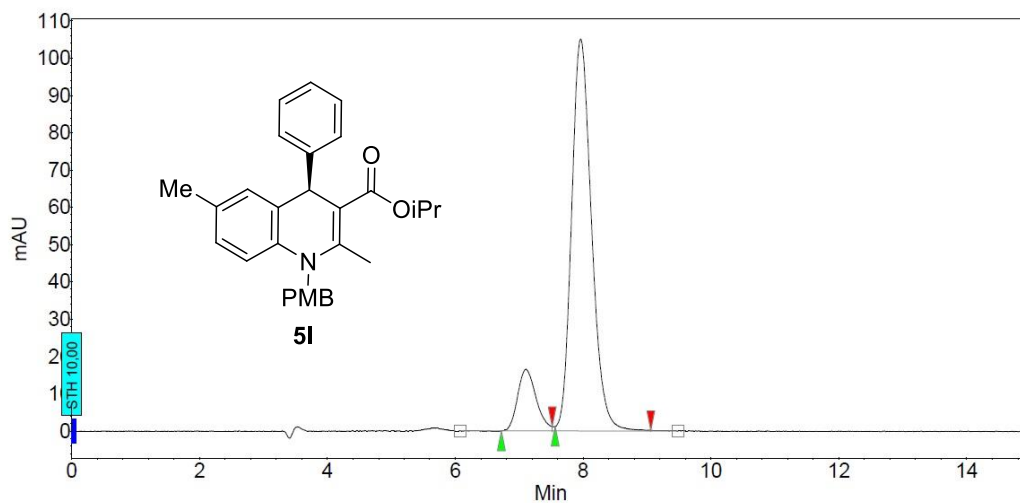
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	16.145	86.15	51.5	20.1	86.148
2	UNKNOWN	16.999	13.85	7.6	3.2	13.852
Total			100.00	59.1	23.4	100.000

Figure 2.33. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 320 nm) of (*R*)-isopropyl 1-(4-methoxybenzyl)-2-methyl-4-(thiophen-3-yl)-1,4-dihydroquinoline-3-carboxylate (**5k**).



Peak results :

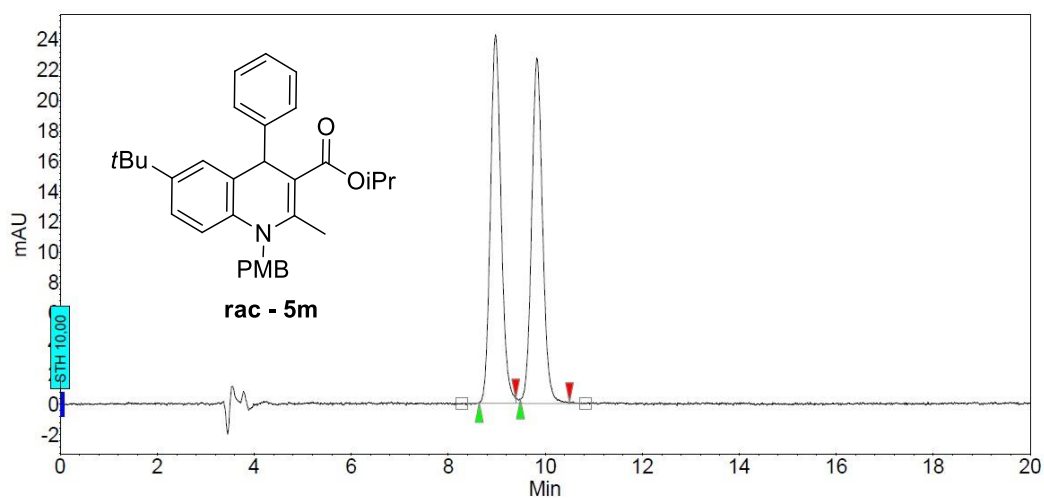
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	7.106	49.15	21.2	7.2	49.152
2	UNKNOWN	7.973	50.85	20.4	7.5	50.848
Total			100.00	41.6	14.7	100.000



Peak results :

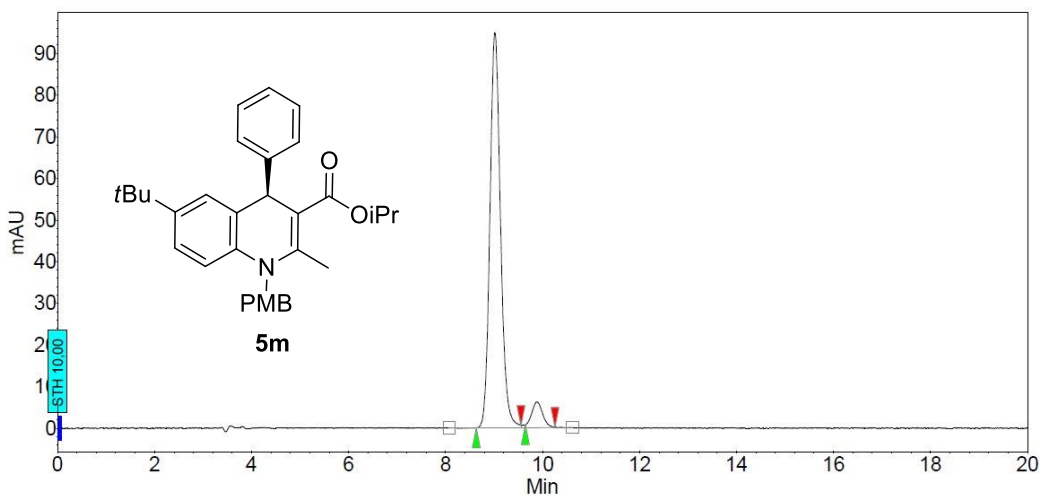
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	7.106	12.70	16.6	5.5	12.702
2	UNKNOWN	7.959	87.30	105.2	38.1	87.298
Total			100.00	121.8	43.7	100.000

Figure 2.34. HPLC analysis (ODH Column; 90% hexane/10% *i*-propanol; 1 mL/min; 328 nm) of (*R*)-isopropyl 1-(4-methoxybenzyl)-2,6-dimethyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**5I**).



Peak results :

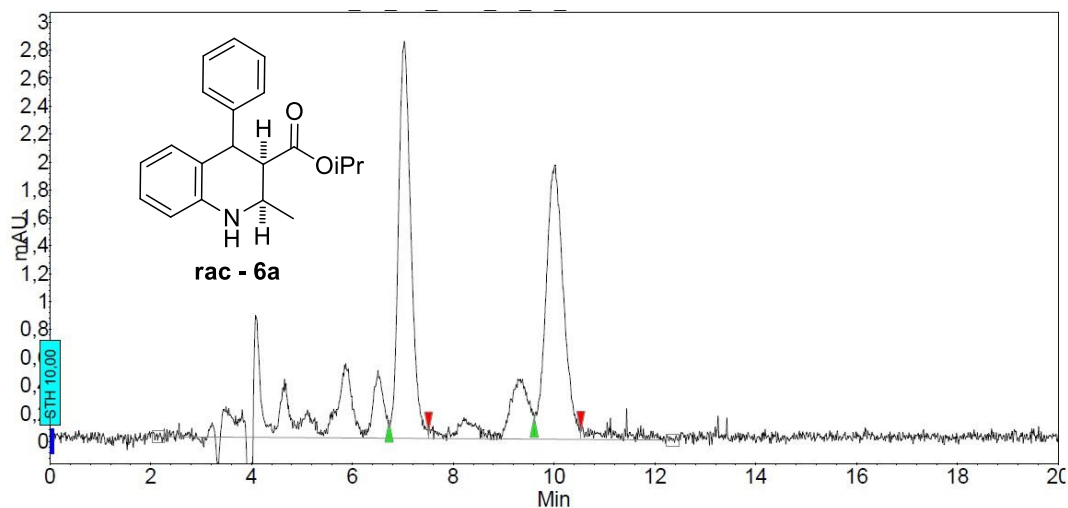
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	8.973	51.00	24.2	6.2	50.999
2	UNKNOWN	9.826	49.00	22.7	5.9	49.001
Total			100.00	47.0	12.1	100.000



Peak results :

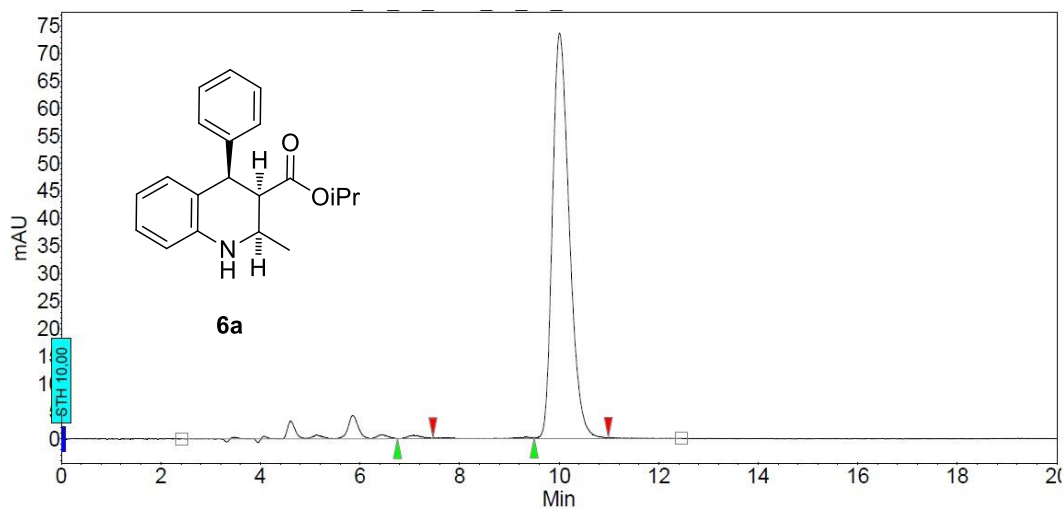
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	9.013	93.57	94.9	24.0	93.567
2	UNKNOWN	9.879	6.43	6.2	1.6	6.433
Total			100.00	101.1	25.6	100.000

Figure 2.35. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 328 nm) of (*R*)-isopropyl 6-(*tert*-butyl)- 1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**5m**).



Peak results :

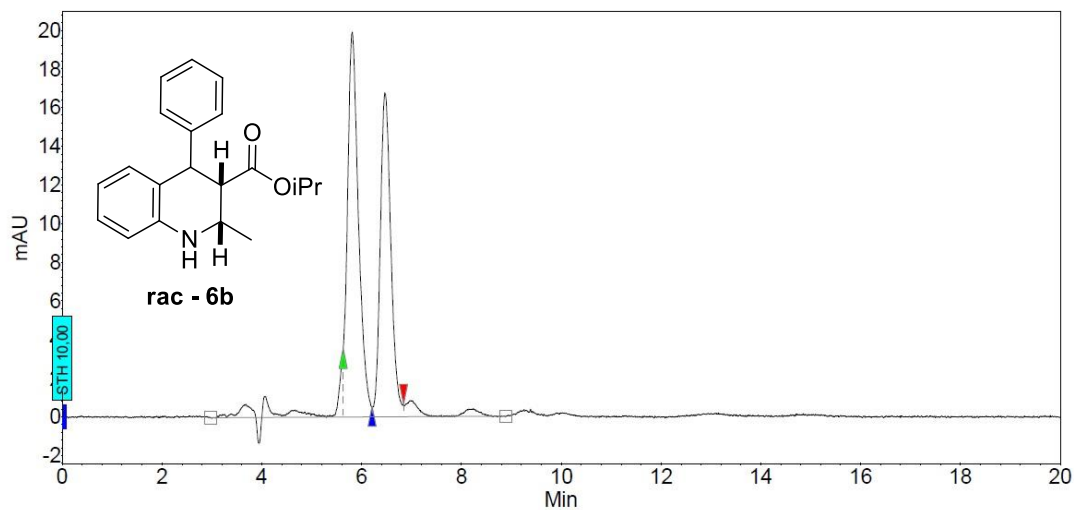
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	7.026	50.69	2.8	0.8	50.688
2	UNKNOWN	9.999	49.31	1.9	0.8	49.312
Total			100.00	4.8	1.6	100.000



Peak results :

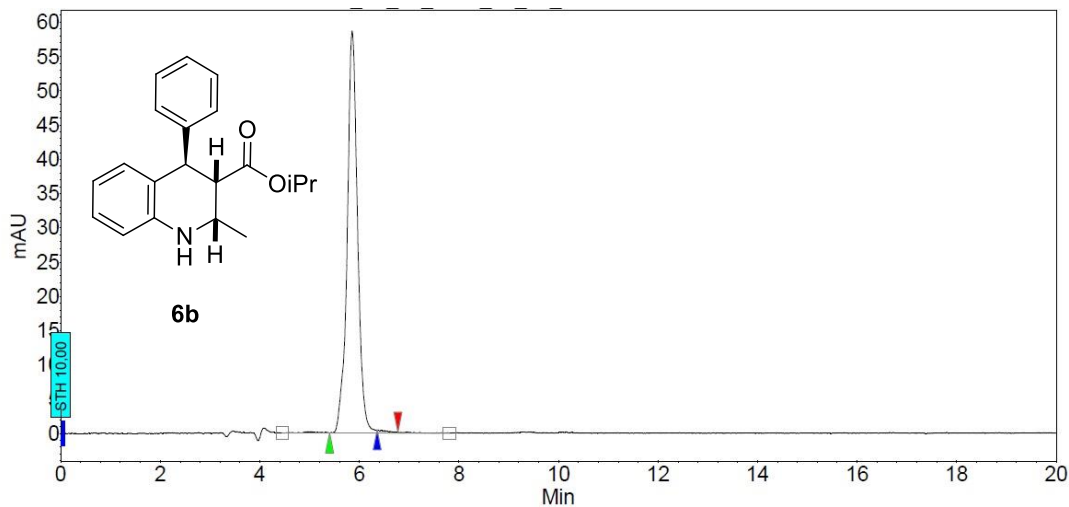
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
2	UNKNOWN	7.093	0.74	0.6	0.2	0.735
1	UNKNOWN	10.013	99.26	73.6	28.9	99.265
Total			100.00	74.2	29.1	100.000

Figure 2.36. HPLC analysis (ODH Column; 90% hexane/10% *i*-propanol; 1 mL/min; 300 nm) of (2*R*,3*R*,4*R*)-isopropyl 2-methyl-4-phenyl-1,2,3,4-tetrahydroquinoline-3-carboxylate (**6a**).



Peak results :

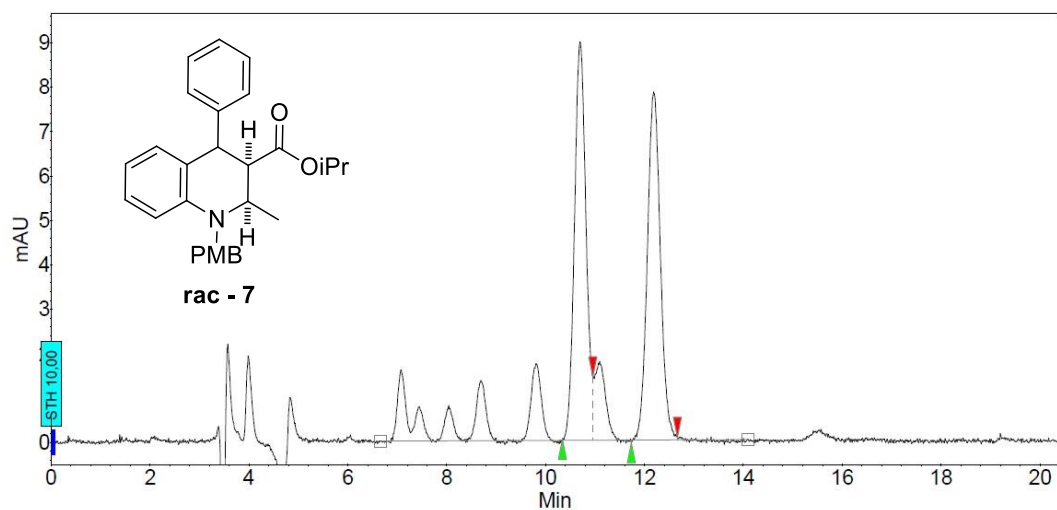
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
2	UNKNOWN	5.813	54.96	19.9	5.0	54.959
1	UNKNOWN	6.466	45.04	16.8	4.1	45.041
Total			100.00	36.7	9.2	100.000



Peak results :

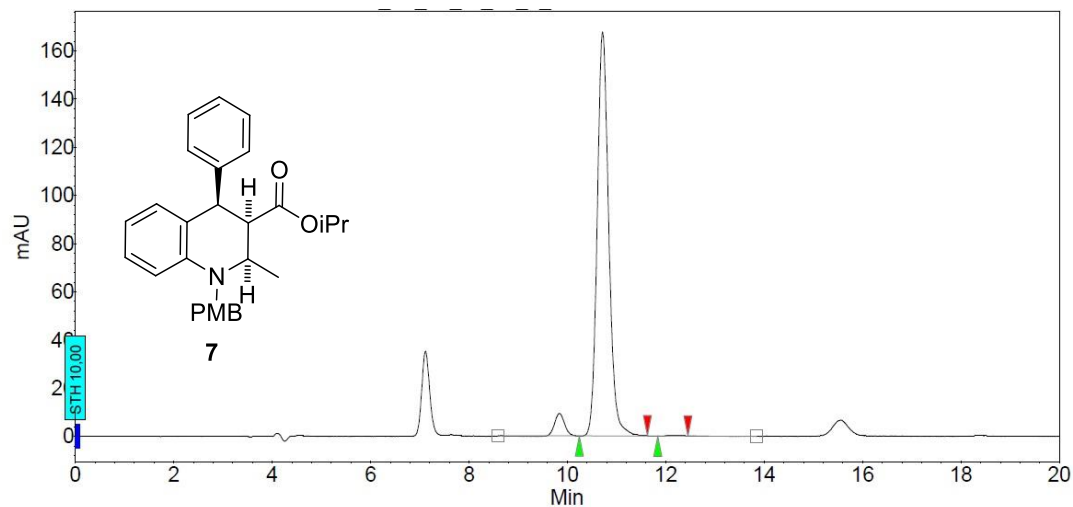
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	5.853	99.35	58.6	14.1	99.345
2	UNKNOWN	6.360	0.65	0.4	0.1	0.655
Total			100.00	59.0	14.2	100.000

Figure 2.37. HPLC analysis (ODH Column; 90% hexane/10% *i*-propanol; 1 mL/min; 300 nm) of (2*S*,3*S*,4*R*)-isopropyl 2-methyl-4-phenyl-1,2,3,4-tetrahydroquinoline-3-carboxylate (**6b**).



Peak results :

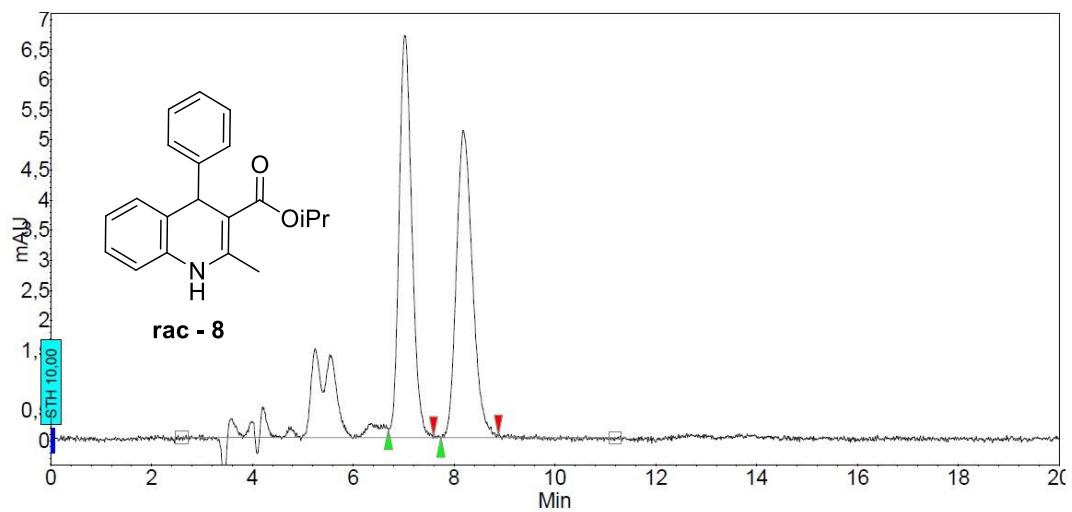
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	10.693	50.26	9.0	2.4	50.261
2	UNKNOWN	12.186	49.74	7.8	2.4	49.739
Total			100.00	16.8	4.8	100.000



Peak results :

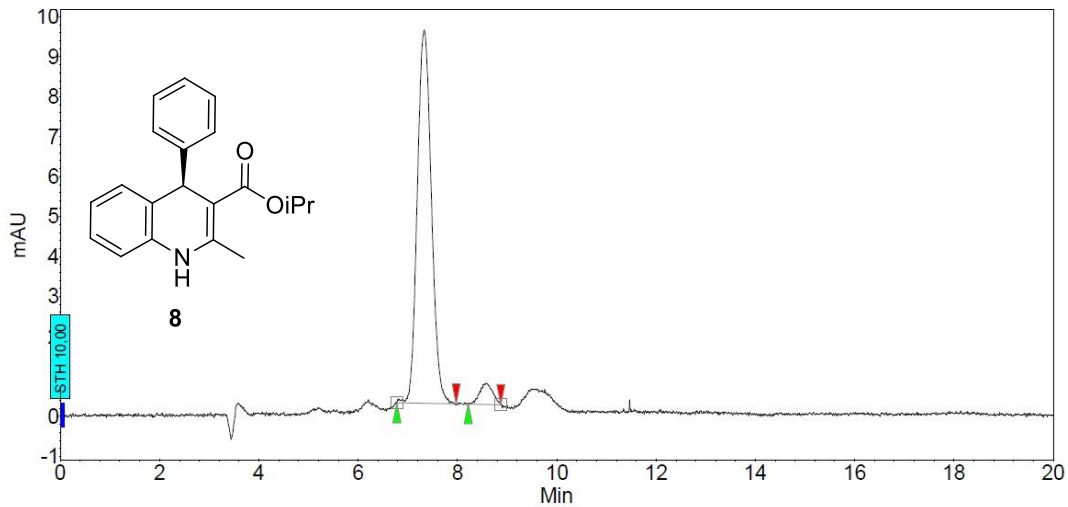
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	10.719	99.70	167.7	45.7	99.700
2	UNKNOWN	12.199	0.30	0.4	0.1	0.300
Total			100.00	168.1	45.8	100.000

Figure 2.38. HPLC analysis (IA Column; 98% hexane/2% *i*-propanol; 1 mL/min; 304 nm) of (2*R*,3*R*,4*R*)-isopropyl 1-(4-methoxybenzyl)-2-methyl-4-phenyl-1,2,3,4-tetrahydroquinoline-3-carboxylate (**7**).



Peak results :

Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	7.026	50.85	6.7	2.0	50.845
2	UNKNOWN	8.186	49.15	5.1	1.9	49.155
Total			100.00	11.8	3.8	100.000



Peak results :

Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area %
1	UNKNOWN	7.333	94.96	9.3	3.1	94.958
2	UNKNOWN	8.573	5.04	0.5	0.2	5.042
Total			100.00	9.9	3.2	100.000

Figure 2.39. HPLC analysis (IA Column; 90% hexane/10% *i*-propanol; 1 mL/min; 308 nm) of (*R*)-isopropyl 2-methyl-4-phenyl-1,4-dihydroquinoline-3-carboxylate (**11**).

X-ray Structure Determination

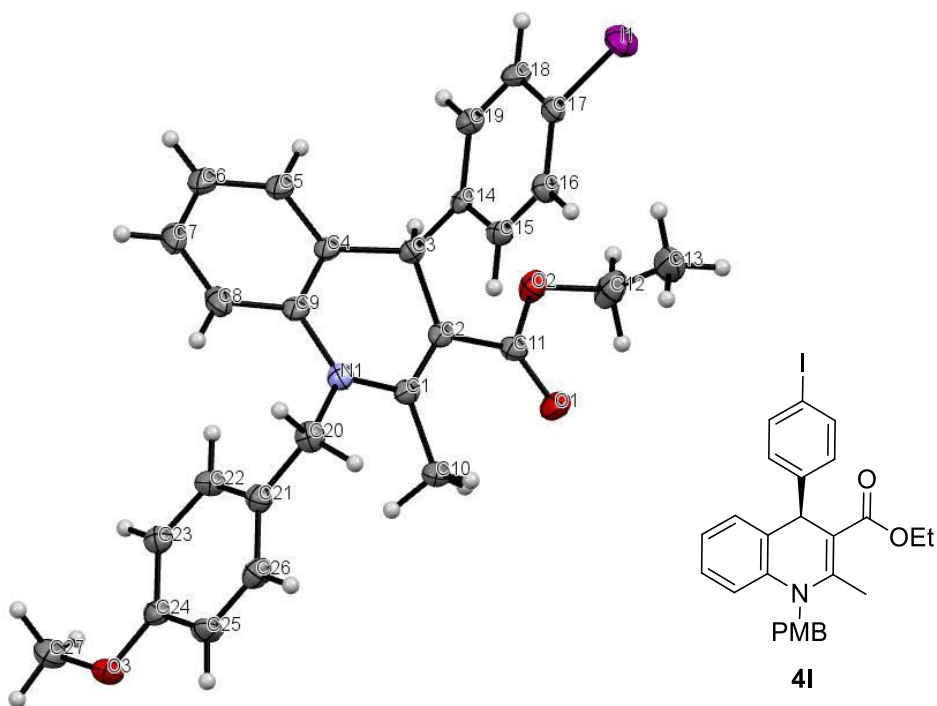


Table 1. Crystal data and structure refinement for **4I**.

Identification code	x2503fin	
Empirical formula	C ₂₇ H ₂₆ I N O ₃	
Formula weight	539.39	
Temperature	130(2) K	
Wavelength	71.073 μm	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 559.010(10) μm	α = 90°.
	b = 1012.07(2) μm	β = 90°.
	c = 4045.85(8) μm	γ = 90°.
Volume	2.28897(8) nm ³	
Z	4	
Density (calculated)	1.565 Mg/m ³	
Absorption coefficient	1.428 mm ⁻¹	
F(000)	1088	
Crystal size	0.33 x 0.09 x 0.03 mm ³	

Theta range for data collection	2.013 to 26.746°.
Index ranges	-6<= <i>h</i> <=6, -12<= <i>k</i> <=12, -50<= <i>l</i> <=45
Reflections collected	16514
Independent reflections	4527 [R(int) = 0.0318]
Completeness to theta = 25.350°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1 and 0.97842
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4527 / 0 / 296
Goodness-of-fit on F ²	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0262, wR2 = 0.0496
R indices (all data)	R1 = 0.0298, wR2 = 0.0509
Absolute structure parameter	-0.03(1)
Largest diff. peak and hole	0.403 and -0.421 e.Å ⁻³

Comments: Structure solution with SHELXT-2014 (dual-space method). Anisotropic refinement of all non-hydrogen atoms with SHELXL-2014. Excluding H(3) all hydrogen atoms were calculated on idealized positions.

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{pm}^2 \times 10^{-1}$) for **4l**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
I(1)	5250(1)	9766(1)	7524(1)	34(1)
O(1)	1277(6)	7788(3)	5717(1)	37(1)
O(2)	-1373(4)	7624(2)	6128(1)	27(1)
O(3)	5799(4)	-221(3)	4997(1)	33(1)
N(1)	4540(5)	4308(3)	6132(1)	22(1)
C(1)	3470(6)	5372(4)	5973(1)	21(1)
C(2)	1633(6)	6032(3)	6117(1)	20(1)
C(3)	843(6)	5718(4)	6465(1)	19(1)
C(4)	1452(6)	4307(3)	6553(1)	21(1)
C(5)	126(7)	3619(3)	6786(1)	27(1)
C(6)	746(9)	2352(4)	6885(1)	35(1)
C(7)	2751(8)	1781(4)	6748(1)	37(1)
C(8)	4068(8)	2418(4)	6509(1)	30(1)
C(9)	3391(6)	3684(3)	6401(1)	21(1)
C(10)	4474(6)	5699(3)	5640(1)	25(1)
C(11)	585(6)	7204(3)	5961(1)	23(1)
C(12)	-2280(7)	8904(4)	6026(1)	37(1)
C(13)	-818(8)	9978(4)	6183(1)	45(1)
C(14)	1897(6)	6677(3)	6717(1)	19(1)
C(15)	4092(6)	7282(3)	6667(1)	22(1)
C(16)	5035(7)	8163(3)	6894(1)	24(1)
C(17)	3796(6)	8446(3)	7179(1)	22(1)
C(18)	1581(7)	7857(4)	7238(1)	25(1)
C(19)	681(7)	6970(3)	7008(1)	22(1)
C(20)	6693(6)	3706(4)	5990(1)	25(1)
C(21)	6282(7)	2700(4)	5718(1)	23(1)
C(22)	4299(6)	1886(4)	5710(1)	24(1)
C(23)	4062(6)	890(4)	5472(1)	24(1)
C(24)	5831(6)	730(4)	5237(1)	24(1)
C(25)	7801(6)	1574(4)	5234(1)	28(1)
C(26)	8006(7)	2539(4)	5474(1)	27(1)

C(27)	3924(7)	-1176(4)	5012(1)	36(1)
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Table 3. Bond lengths [pm] and angles [°] for **4l**.

I(1)-C(17)	209.9(3)
O(1)-C(11)	121.1(4)
O(2)-C(11)	135.5(4)
O(2)-C(12)	145.1(4)
O(3)-C(24)	136.8(4)
O(3)-C(27)	142.7(4)
N(1)-C(1)	138.9(4)
N(1)-C(9)	141.4(4)
N(1)-C(20)	146.7(4)
C(1)-C(2)	135.7(5)
C(1)-C(10)	149.8(4)
C(2)-C(11)	146.6(5)
C(2)-C(3)	151.1(5)
C(3)-C(4)	151.0(5)
C(3)-C(14)	152.5(5)
C(3)-H(3)	95(3)
C(4)-C(5)	138.8(5)
C(4)-C(9)	139.5(5)
C(5)-C(6)	138.8(5)
C(5)-H(5)	95.00
C(6)-C(7)	137.8(6)
C(6)-H(6)	95.00
C(7)-C(8)	137.6(6)
C(7)-H(7)	95.00
C(8)-C(9)	140.5(5)
C(8)-H(8)	95.00
C(10)-H(10A)	98.00
C(10)-H(10B)	98.00
C(10)-H(10C)	98.00
C(12)-C(13)	150.0(6)
C(12)-H(12A)	99.00

C(12)-H(12B)	99.00
C(13)-H(13A)	98.00
C(13)-H(13B)	98.00
C(13)-H(13C)	98.00
C(14)-C(15)	138.7(5)
C(14)-C(19)	139.0(5)
C(15)-C(16)	138.5(5)
C(15)-H(15)	95.00
C(16)-C(17)	137.2(5)
C(16)-H(16)	95.00
C(17)-C(18)	139.6(5)
C(18)-C(19)	138.9(5)
C(18)-H(18)	95.00
C(19)-H(19)	95.00
C(20)-C(21)	151.6(5)
C(20)-H(20A)	99.00
C(20)-H(20B)	99.00
C(21)-C(22)	138.2(5)
C(21)-C(26)	139.0(5)
C(22)-C(23)	139.9(5)
C(22)-H(22)	95.00
C(23)-C(24)	138.1(5)
C(23)-H(23)	95.00
C(24)-C(25)	139.4(5)
C(25)-C(26)	138.2(5)
C(25)-H(25)	95.00
C(26)-H(26)	95.00
C(27)-H(27A)	98.00
C(27)-H(27B)	98.00
C(27)-H(27C)	98.00
C(11)-O(2)-C(12)	114.9(3)
C(24)-O(3)-C(27)	117.1(3)
C(1)-N(1)-C(9)	120.5(3)
C(1)-N(1)-C(20)	119.6(3)
C(9)-N(1)-C(20)	119.3(3)

C(2)-C(1)-N(1)	120.6(3)
C(2)-C(1)-C(10)	124.1(3)
N(1)-C(1)-C(10)	115.3(3)
C(1)-C(2)-C(11)	121.1(3)
C(1)-C(2)-C(3)	121.2(3)
C(11)-C(2)-C(3)	117.1(3)
C(4)-C(3)-C(2)	110.6(3)
C(4)-C(3)-C(14)	111.0(3)
C(2)-C(3)-C(14)	112.1(3)
C(4)-C(3)-H(3)	106(2)
C(2)-C(3)-H(3)	111(2)
C(14)-C(3)-H(3)	106(2)
C(5)-C(4)-C(9)	119.1(3)
C(5)-C(4)-C(3)	120.9(3)
C(9)-C(4)-C(3)	120.0(3)
C(6)-C(5)-C(4)	121.8(4)
C(6)-C(5)-H(5)	119.1
C(4)-C(5)-H(5)	119.1
C(7)-C(6)-C(5)	118.3(4)
C(7)-C(6)-H(6)	120.9
C(5)-C(6)-H(6)	120.9
C(8)-C(7)-C(6)	121.5(4)
C(8)-C(7)-H(7)	119.2
C(6)-C(7)-H(7)	119.2
C(7)-C(8)-C(9)	120.0(4)
C(7)-C(8)-H(8)	120.0
C(9)-C(8)-H(8)	120.0
C(4)-C(9)-C(8)	119.0(3)
C(4)-C(9)-N(1)	119.3(3)
C(8)-C(9)-N(1)	121.6(3)
C(1)-C(10)-H(10A)	109.5
C(1)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(1)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5

O(1)-C(11)-O(2)	120.7(3)
O(1)-C(11)-C(2)	128.1(3)
O(2)-C(11)-C(2)	111.2(3)
O(2)-C(12)-C(13)	109.7(3)
O(2)-C(12)-H(12A)	109.7
C(13)-C(12)-H(12A)	109.7
O(2)-C(12)-H(12B)	109.7
C(13)-C(12)-H(12B)	109.7
H(12A)-C(12)-H(12B)	108.2
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(15)-C(14)-C(19)	117.5(3)
C(15)-C(14)-C(3)	121.7(3)
C(19)-C(14)-C(3)	120.8(3)
C(16)-C(15)-C(14)	121.6(3)
C(16)-C(15)-H(15)	119.2
C(14)-C(15)-H(15)	119.2
C(17)-C(16)-C(15)	119.9(3)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(16)-C(17)-C(18)	120.3(3)
C(16)-C(17)-I(1)	119.7(3)
C(18)-C(17)-I(1)	120.0(3)
C(19)-C(18)-C(17)	118.7(4)
C(19)-C(18)-H(18)	120.6
C(17)-C(18)-H(18)	120.6
C(18)-C(19)-C(14)	122.0(3)
C(18)-C(19)-H(19)	119.0
C(14)-C(19)-H(19)	119.0
N(1)-C(20)-C(21)	116.1(3)
N(1)-C(20)-H(20A)	108.3
C(21)-C(20)-H(20A)	108.3

N(1)-C(20)-H(20B)	108.3
C(21)-C(20)-H(20B)	108.3
H(20A)-C(20)-H(20B)	107.4
C(22)-C(21)-C(26)	118.0(3)
C(22)-C(21)-C(20)	122.6(3)
C(26)-C(21)-C(20)	119.3(3)
C(21)-C(22)-C(23)	121.4(3)
C(21)-C(22)-H(22)	119.3
C(23)-C(22)-H(22)	119.3
C(24)-C(23)-C(22)	119.3(3)
C(24)-C(23)-H(23)	120.3
C(22)-C(23)-H(23)	120.3
O(3)-C(24)-C(23)	124.2(3)
O(3)-C(24)-C(25)	115.7(3)
C(23)-C(24)-C(25)	120.1(3)
C(26)-C(25)-C(24)	119.4(3)
C(26)-C(25)-H(25)	120.3
C(24)-C(25)-H(25)	120.3
C(25)-C(26)-C(21)	121.7(4)
C(25)-C(26)-H(26)	119.2
C(21)-C(26)-H(26)	119.2
O(3)-C(27)-H(27A)	109.5
O(3)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
O(3)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{pm}^2 \times 10^{-1}$) for **4l**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I(1)	42(1)	32(1)	28(1)	-9(1)	-6(1)	-2(1)
O(1)	54(2)	32(2)	24(2)	10(1)	8(2)	10(1)
O(2)	23(1)	27(2)	32(2)	8(1)	-1(1)	4(1)
O(3)	45(1)	30(1)	25(1)	-6(1)	11(1)	0(1)
N(1)	24(1)	22(2)	21(2)	0(1)	-3(1)	2(1)
C(1)	23(2)	22(2)	18(2)	-1(2)	-1(1)	-7(2)
C(2)	21(2)	20(2)	17(2)	0(1)	-4(2)	-4(2)
C(3)	16(2)	21(2)	19(2)	2(1)	0(1)	-1(1)
C(4)	27(2)	21(2)	14(2)	0(1)	-3(2)	-3(2)
C(5)	38(2)	26(2)	17(2)	-1(1)	0(2)	-5(2)
C(6)	59(3)	27(2)	18(2)	-1(2)	2(2)	-9(2)
C(7)	70(3)	20(2)	22(2)	1(2)	-5(2)	3(2)
C(8)	45(2)	23(2)	22(2)	-3(2)	-8(2)	7(2)
C(9)	27(2)	23(2)	14(2)	-2(1)	-5(2)	-3(2)
C(10)	31(2)	24(2)	20(2)	-2(1)	1(2)	0(2)
C(11)	26(2)	24(2)	18(2)	-3(1)	-1(2)	-1(2)
C(12)	28(2)	38(3)	45(3)	18(2)	4(2)	10(2)
C(13)	54(2)	30(3)	51(3)	3(2)	17(2)	9(2)
C(14)	23(2)	18(2)	15(2)	5(1)	-2(2)	5(2)
C(15)	23(2)	22(2)	21(2)	-2(1)	3(2)	0(2)
C(16)	24(2)	23(2)	25(2)	-1(1)	-2(2)	-1(2)
C(17)	30(2)	18(2)	19(2)	0(1)	-4(2)	3(2)
C(18)	31(2)	29(2)	14(2)	1(2)	2(2)	2(2)
C(19)	23(2)	24(2)	20(2)	2(1)	1(2)	-1(2)
C(20)	22(2)	27(2)	28(2)	0(2)	-2(2)	1(2)
C(21)	24(2)	23(2)	23(2)	0(2)	-2(2)	5(2)
C(22)	24(2)	29(2)	20(2)	-2(2)	2(2)	1(2)
C(23)	23(2)	26(2)	23(2)	1(2)	-1(2)	1(2)
C(24)	30(2)	23(2)	18(2)	2(1)	0(2)	5(2)
C(25)	27(2)	32(2)	25(2)	1(2)	10(2)	7(2)
C(26)	21(2)	29(2)	30(2)	6(2)	0(2)	-3(2)

C(27) 47(2) 34(2) 26(2) -7(2) 0(2) -4(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{pm}^2 \times 10^{-1}$) for **4I**.

	x	y	z	U(eq)
H(5)	-1243	4027	6881	32
H(6)	-188	1889	7044	42
H(7)	3234	928	6820	45
H(8)	5437	2002	6417	36
H(10A)	3242	6133	5506	37
H(10B)	4992	4885	5530	37
H(10C)	5846	6293	5665	37
H(12A)	-3973	8994	6094	44
H(12B)	-2200	8982	5783	44
H(13A)	-937	9913	6424	67
H(13B)	-1419	10841	6110	67
H(13C)	858	9883	6116	67
H(15)	4972	7088	6472	26
H(16)	6537	8571	6854	29
H(18)	706	8057	7433	30
H(19)	-809	6551	7050	27
H(20A)	7596	3271	6170	31
H(20B)	7716	4420	5900	31
H(22)	3071	2004	5869	29
H(23)	2698	330	5472	29
H(25)	8992	1487	5067	34
H(26)	9359	3107	5472	32
H(27A)	3964	-1622	5227	54
H(27B)	4142	-1828	4836	54
H(27C)	2378	-733	4984	54
H(3)	-850(60)	5790(30)	6485(8)	13(9)