

Enantioselectivity of Chiral Derivatives of Xanthones in Virulence Effects of Resistant Bacteria

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Table S1. Minimum inhibitory concentrations of the compounds in the antibacterial and antifungal activity assays and synergy with antibiotics.

Compound	Antibacterial activity						Synergy with antimicrobials		Antifungal activity		
	Minimum Inhibitory Concentration (MIC) (μM)										
	<i>E. coli</i> ATCC 25922	<i>P. aeruginosa</i> ATCC 27853	<i>E. faecalis</i> ATCC 29212	<i>S. aureus</i> ATCC 29213	<i>S. aureus</i> 272123	SE03	<i>E. coli</i> SA/2	<i>E. faecalis</i> B3/101	<i>C. albicans</i> ATCC 10231	<i>A. fumigatus</i> ATCC 204305	<i>T. rubrum</i> FF5
							CTX MIC = 562 (256 μg/mL)	VAN MIC = 707 (1024 μg/mL)			
							CTX + Compound ¹	VAN + Compound ¹			
5	>100	>100	>100	>100	>100	>100	562 (256 μg/mL)	707 (1024 μg/mL)	>100	>100	>100
6	>100	>100	>100	>100	>100	>100	141 (64 μg/mL)	707 (1024 μg/mL)	>100	>100	>100
7	>100	>100	>100	>100	>100	>100	562 (256 μg/mL)	707 (1024 μg/mL)	>100	>100	>100
(S,S)-8	>100	>100	>100	>100	>100	>100	562 (256 μg/mL)	707 (1024 μg/mL)	>100	>100	>100
(R,R)-8	>100	>100	>100	>100	>100	>100	562 (256 μg/mL)	707 (1024 μg/mL)	>100	>100	>100
9	>100	>100	>100	>100	>100	>100	562 (256 μg/mL)	707 (1024 μg/mL)	>100	>100	>100
10	>100	>100	>100	>100	>100	>100	562 (256 μg/mL)	707 (1024 μg/mL)	>100	>100	>100
(S)-11	>100	>100	>100	>100	>100	>100	141 (64 μg/mL)	707 (1024 μg/mL)	>100	>100	>100
(R)-11	>100	>100	>100	>100	>100	>100	562 (256 μg/mL)	707 (1024 μg/mL)	>100	>100	>100
12	>100	>100	>100	>100	>100	>100	562	707	>100	>100	>100

							(256 µg/mL) 562	(1024 µg/mL) 707			
(S)-16	>100	>100	>100	>100	>100	>100	(256 µg/mL) 562	(1024 µg/mL) 707	>100	>100	>100
(R)-16	>100	>100	>100	>100	>100	>100	(256 µg/mL) 562	(1024 µg/mL) 707	>100	>100	>100
(S)-17	>100	>100	>100	>100	>100	>100	(256 µg/mL) 562	(1024 µg/mL) 707	>100	>100	>100
(R)-17	>100	>100	>100	>100	>100	>100	(256 µg/mL) 562	(1024 µg/mL) 707	>100	>100	>100
(S,R)-18	>100	>100	>100	>100	>100	>100	(256 µg/mL) 562	(1024 µg/mL) 707	>100	>100	>100
(R,S)-18	>100	>100	>100	>100	>100	>100	(256 µg/mL) 562	(1024 µg/mL) 707	>100	>100	>100

¹ All compounds were kept at the highest concentration tested in the antibacterial activity (64 µg/mL), considering that none showed a direct inhibitory effect on *E. coli* and *E. faecalis*. **CTX**: cefotaxime; **VAN**: vancomycin. **SE03**: *Salmonella enterica* serovar Typhimurium SL1344 (SE03).

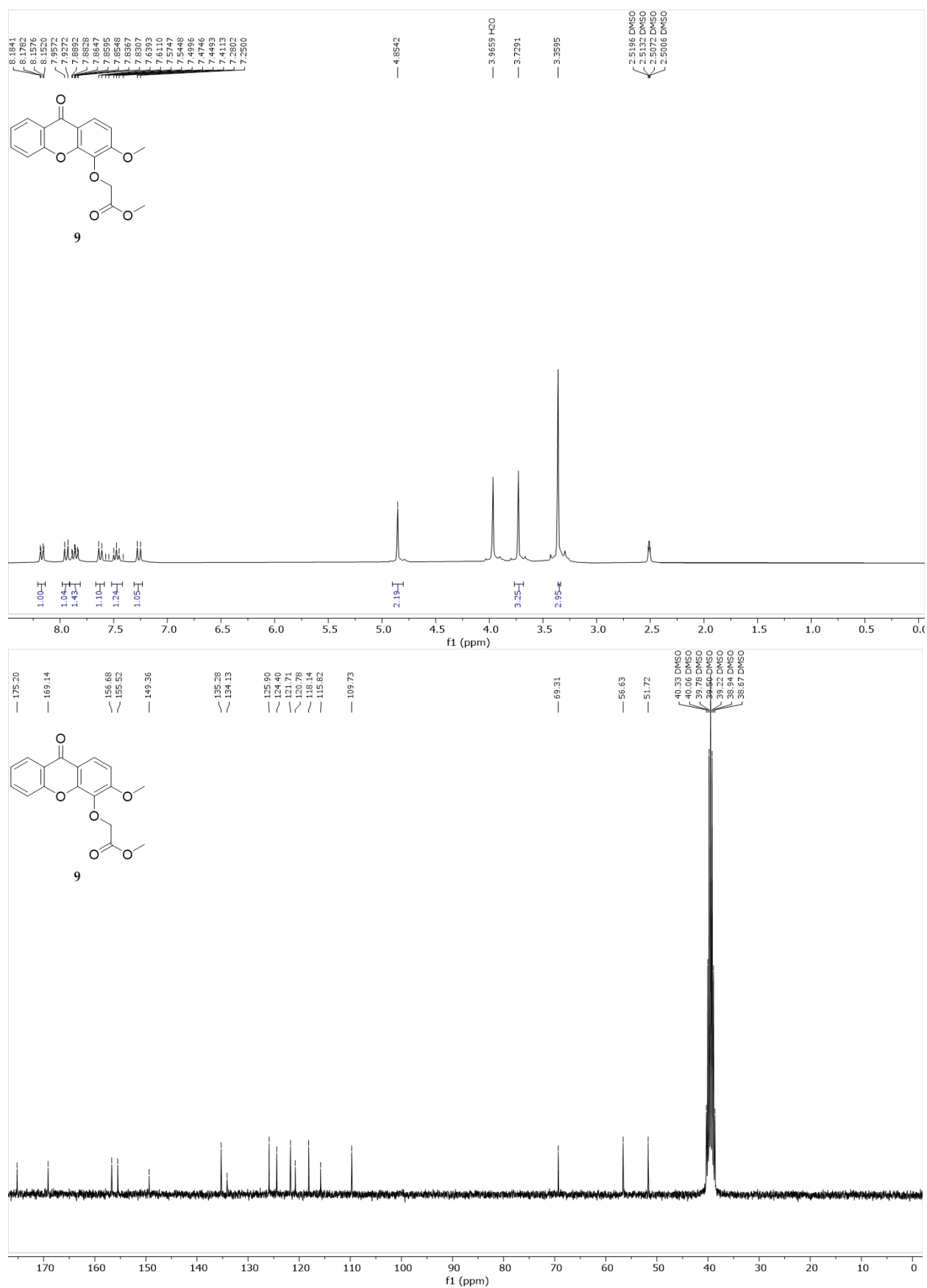
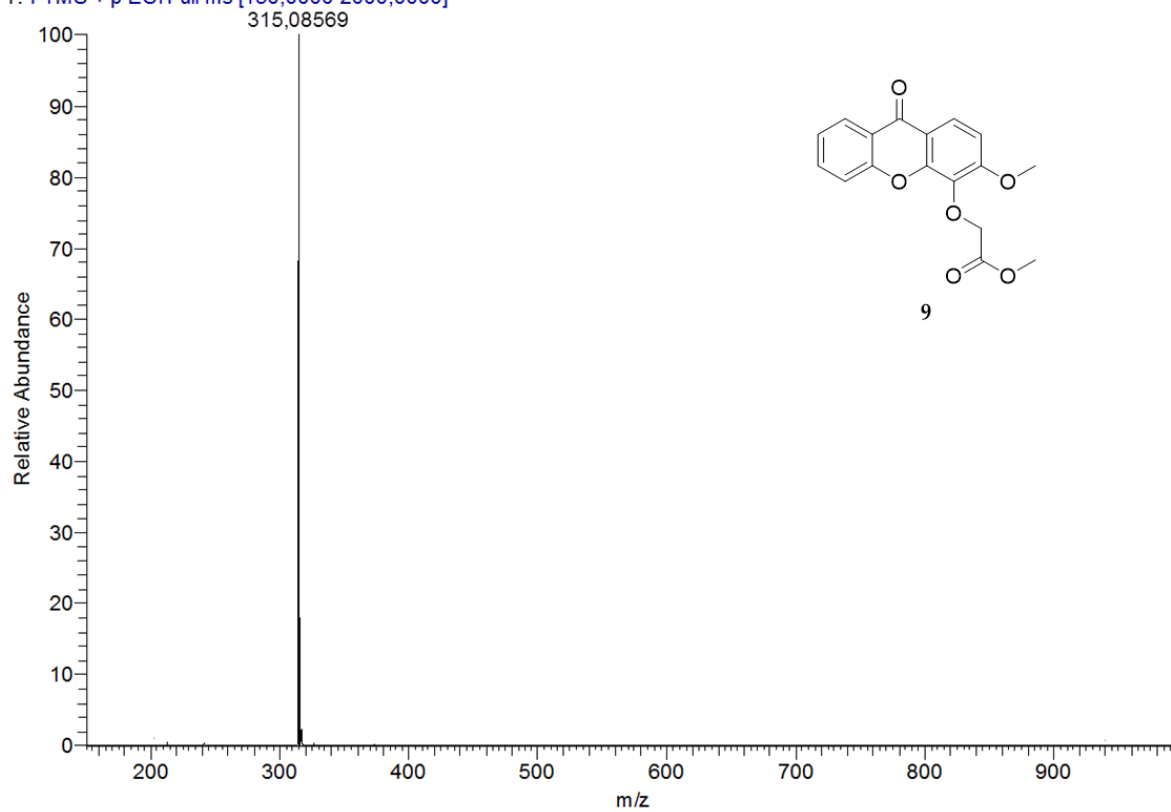


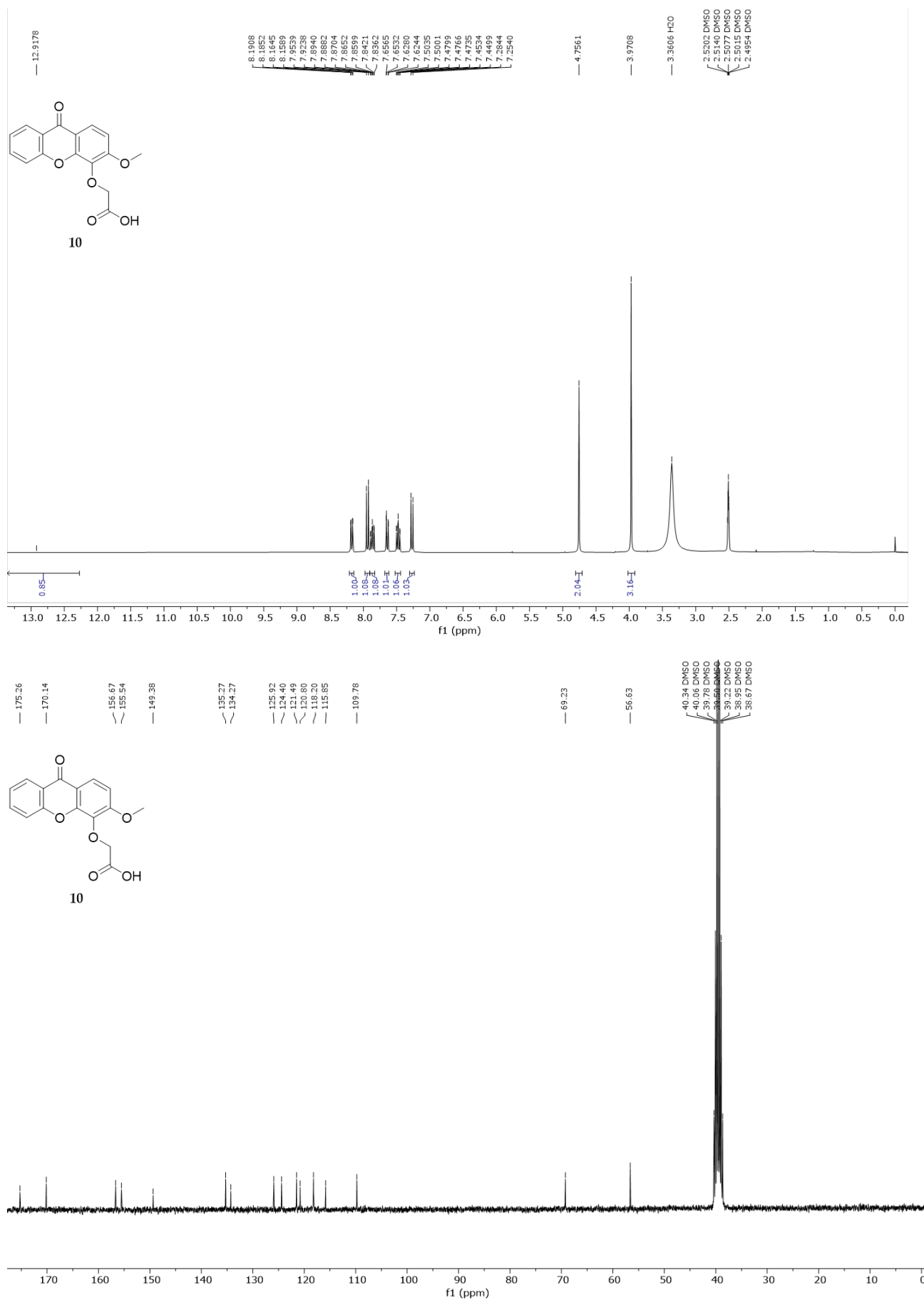
Figure S1. ^1H NMR (300.13 MHz, $\text{DMSO}-d_6$) and ^{13}C NMR (75.48 MHz, $\text{DMSO}-d_6$) for compound **9**.

T: FTMS + p ESI Full ms [150,0000-2000,0000]

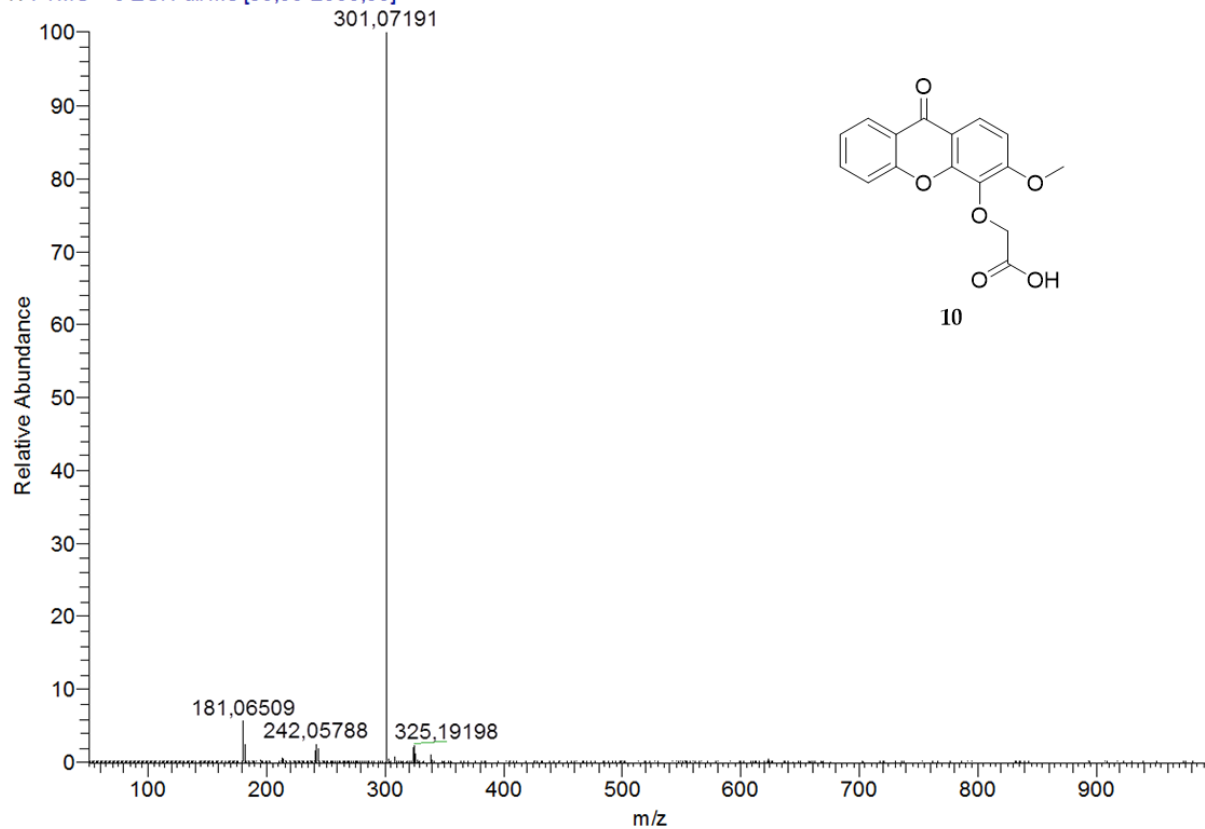


Meas. m/z	Formula	m/z	err [ppm]
314.07904	C ₁₇ H ₁₅ O ₆	315.08569	1.982

Figure S2. Electrospray ESI data for compound 9.



T: FTMS + c ESI Full ms [50,00-2000,00]



Meas. m/z	Formula	m/z	err [ppm]
301.07122	C ₁₆ H ₁₃ O ₆	301.07191	4.137

Figure S4. Electrospray ESI data for compound 10.

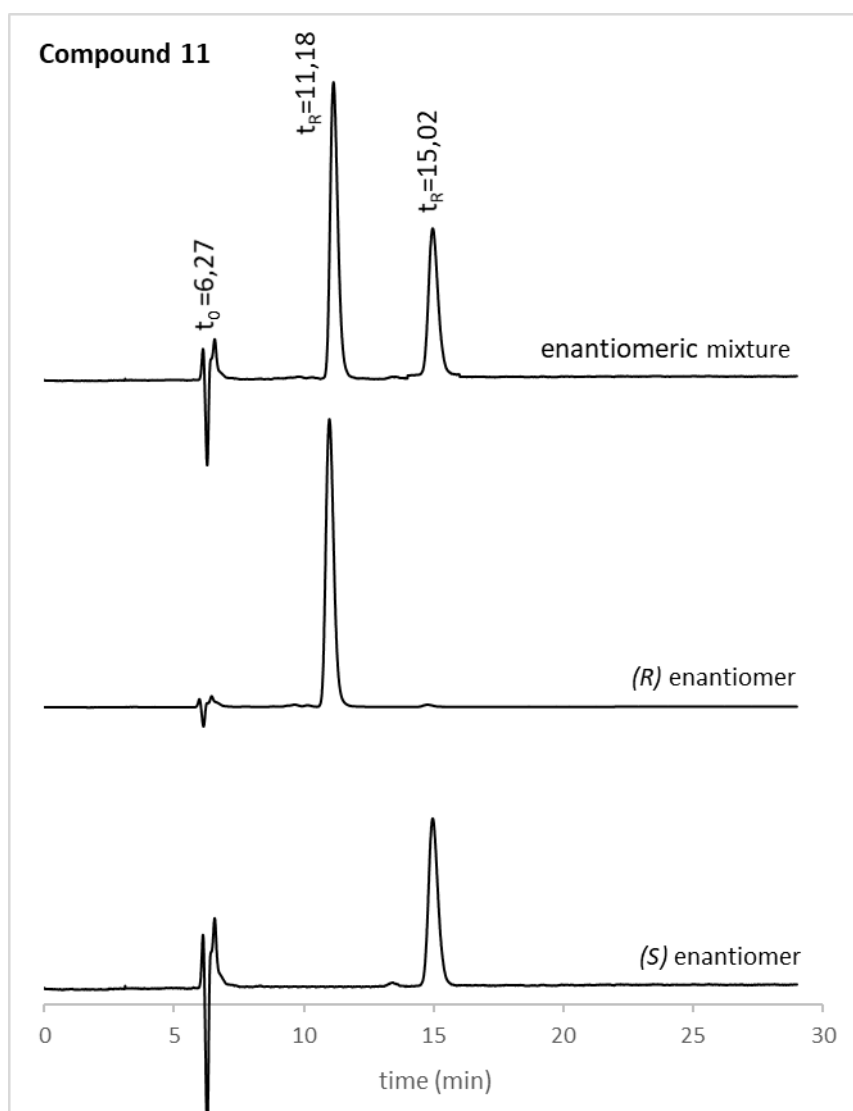


Figure S5. Chromatograms for the enantioseparation of the enantiomeric pair **11**, at optimized chromatographic conditions.

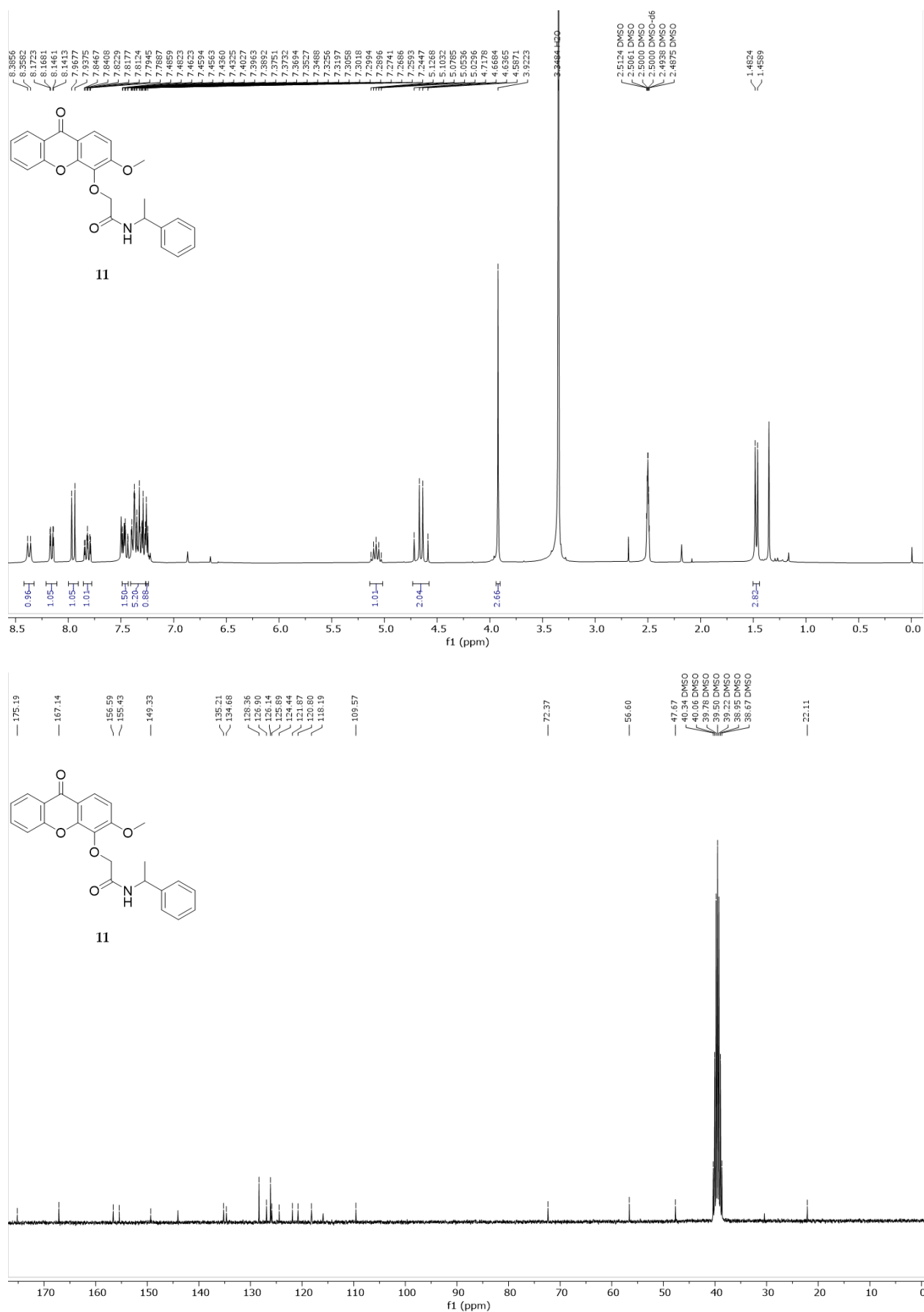
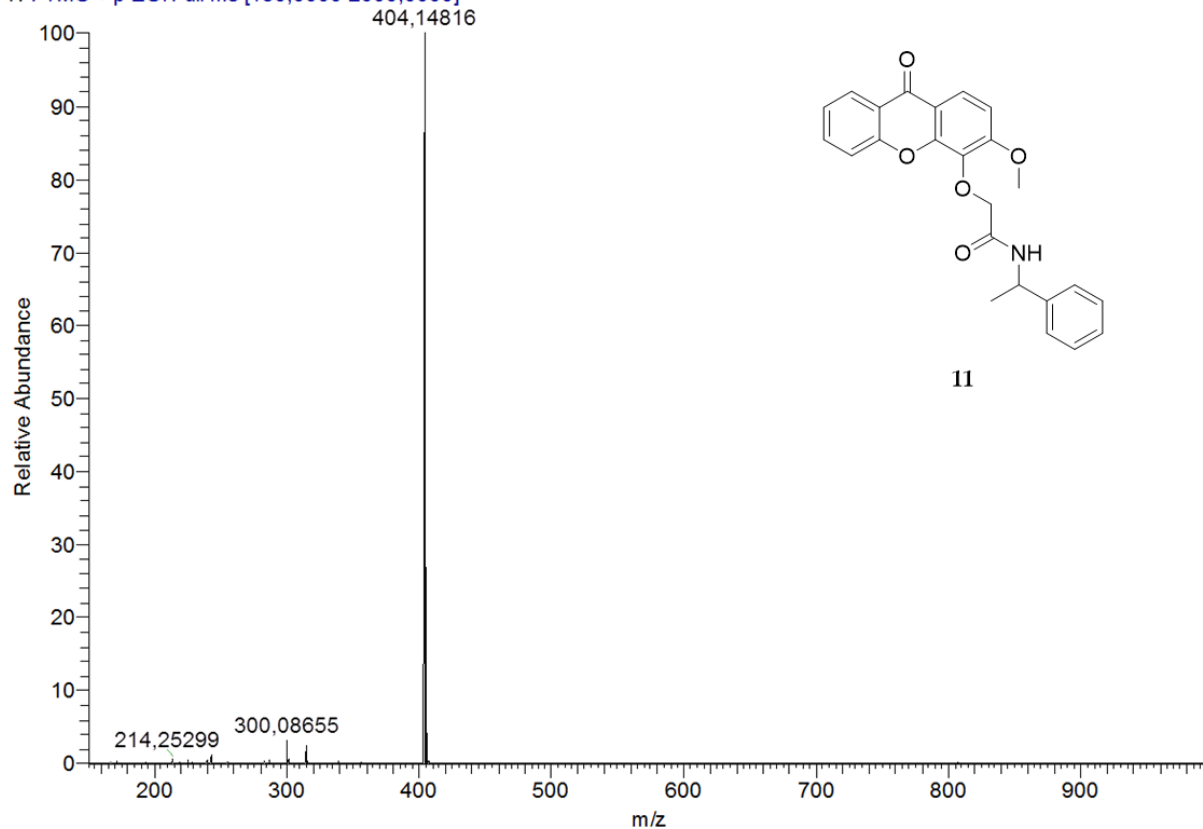


Figure S6. ¹H NMR (300.13 MHz, DMSO-*d*₆) and ¹³C NMR (75.48 MHz, DMSO-*d*₆) for the enantiomeric pair **11**.

T: FTMS + p ESI Full ms [150,0000-2000,0000]



Meas. m/z	Formula	m/z	err [ppm]
404.14980	C ₂₄ H ₂₂ NO ₅	404.14816	2.695

Figure S7. Electrospray ESI data for the enantiomeric pair 11.

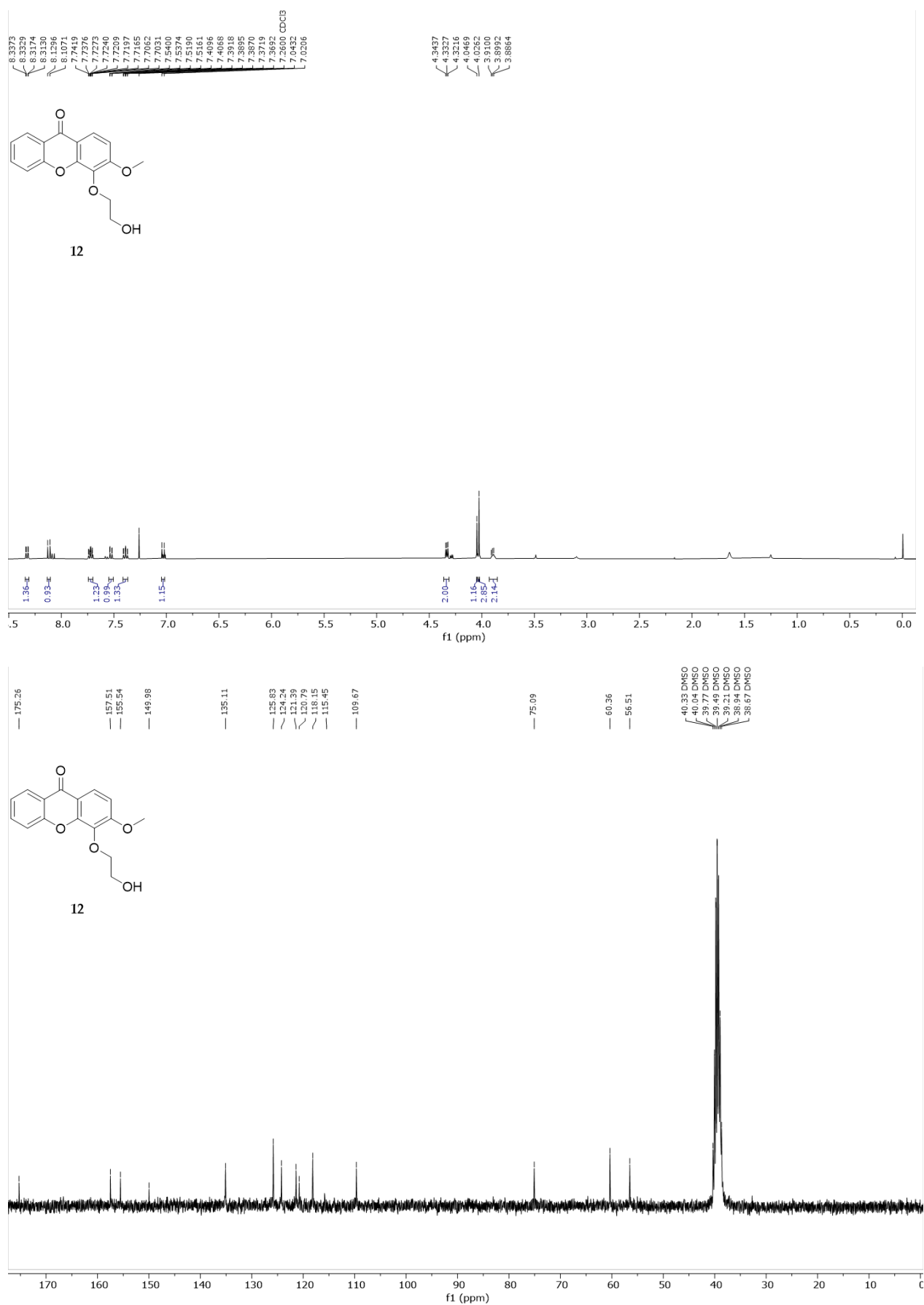
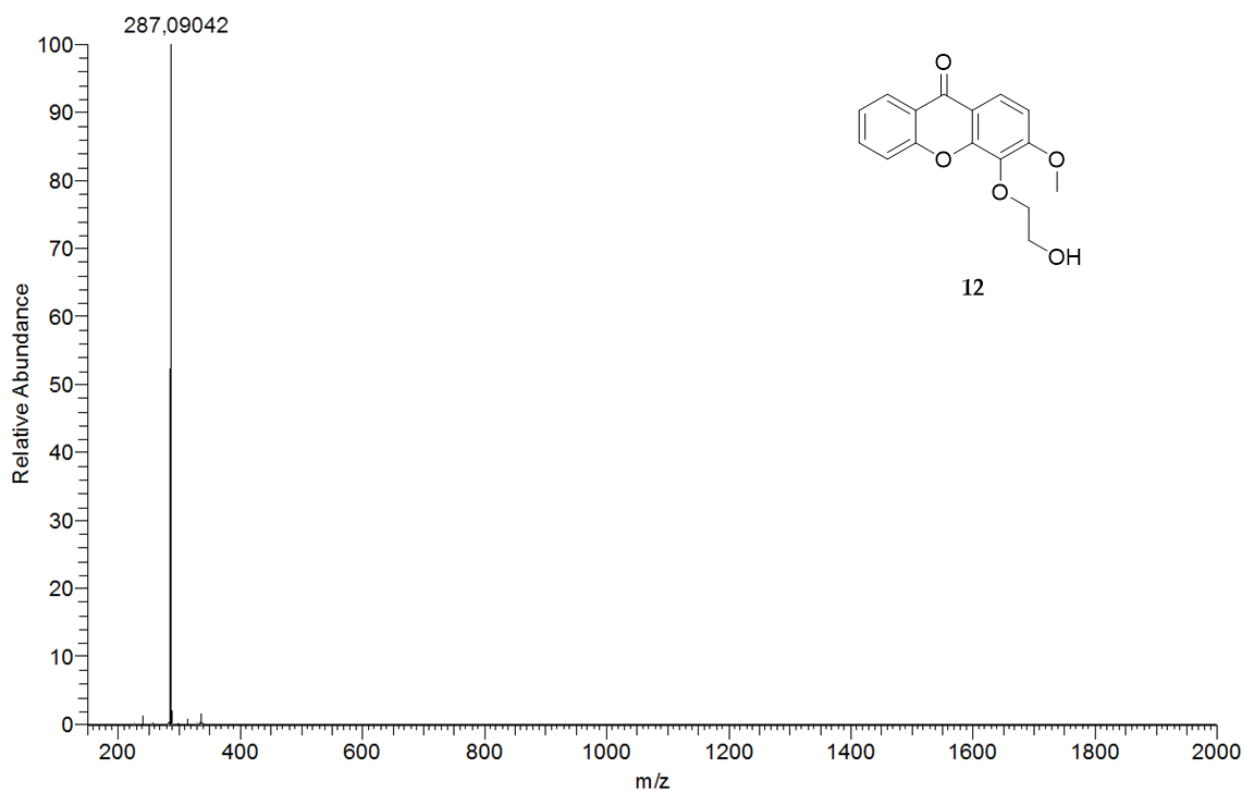


Figure S8. ¹H NMR (300.13 MHz, CDCl₃) and ¹³C NMR (75.48 MHz, DMSO-*d*₆) for compound 12.

T: FTMS + p ESI Full ms [150,0000-2000,0000]



Meas. m/z	Formula	m/z	err [ppm]
287.09195	C ₁₆ H ₁₅ O ₅	287.09042	-3.414

Figure S9. Electrospray ESI data for compound 12.

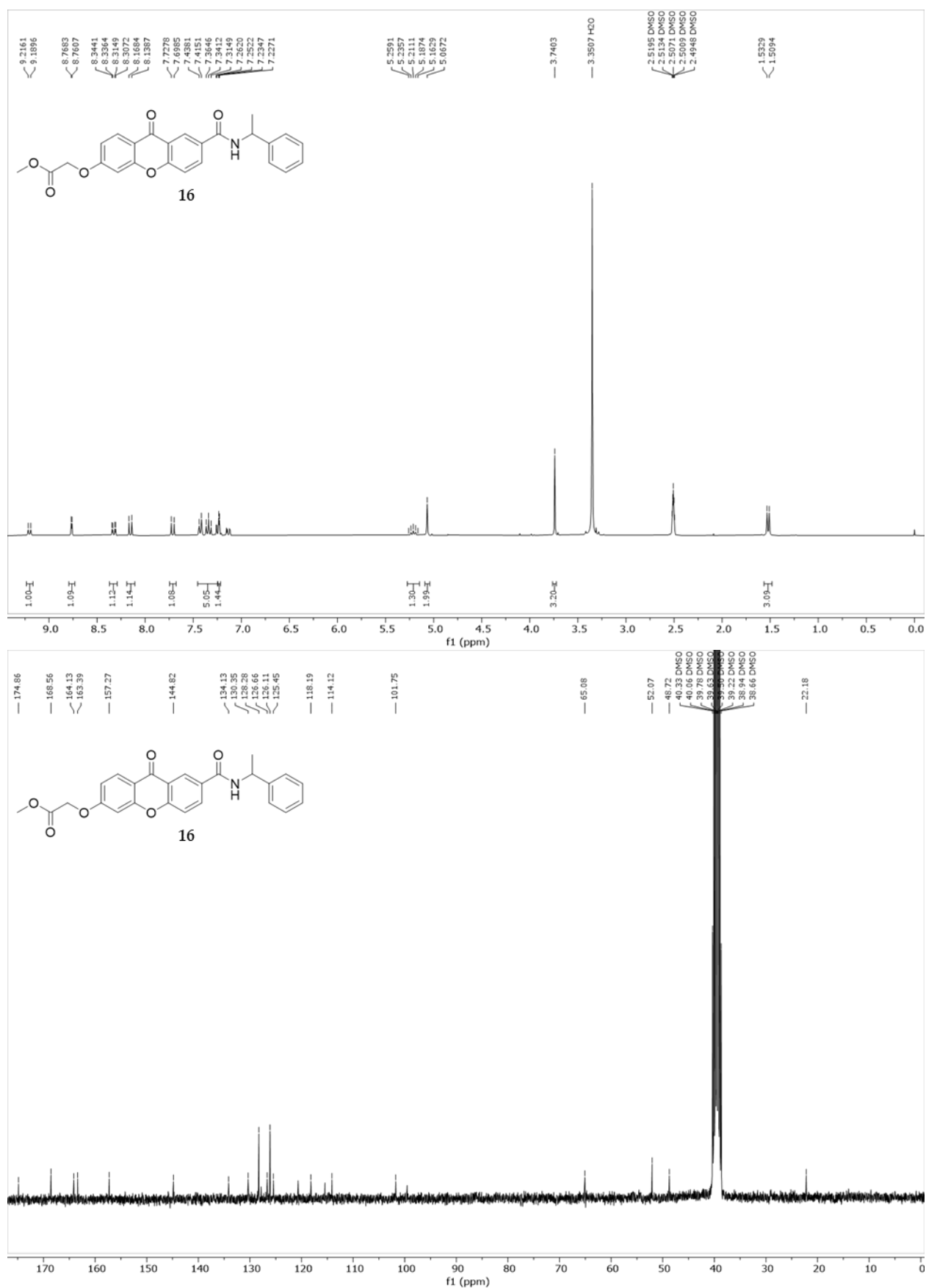
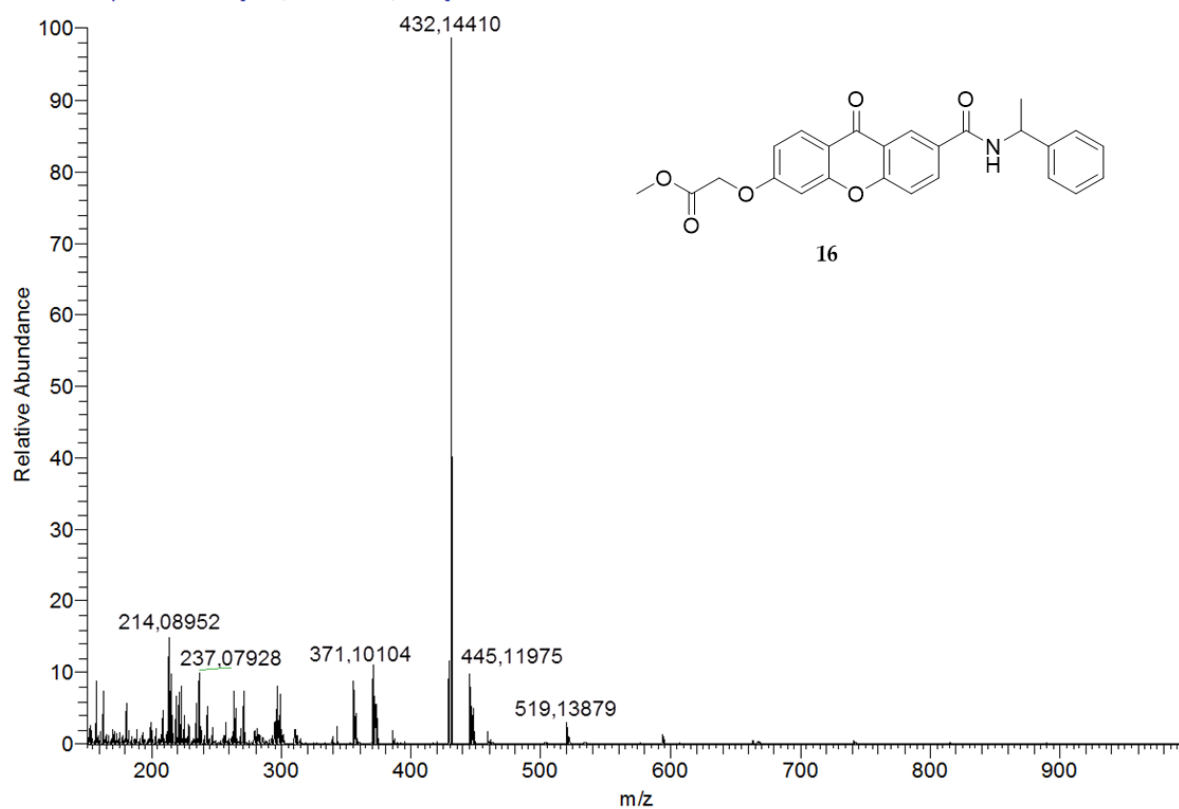


Figure S10. ¹H NMR (300.13 MHz, DMSO-*d*₆) and ¹³C NMR (75.48 MHz, DMSO-*d*₆) for the enantiomeric pair **16**.

T: FTMS + p ESI Full ms [150,0000-2000,0000]



Meas. m/z	Formula	m/z	err [ppm]
432.14471	C ₂₅ H ₂₂ NO ₆	432.14410	-0.148

Figure S11. Electrospray ESI data for the enantiomeric pair **16**.

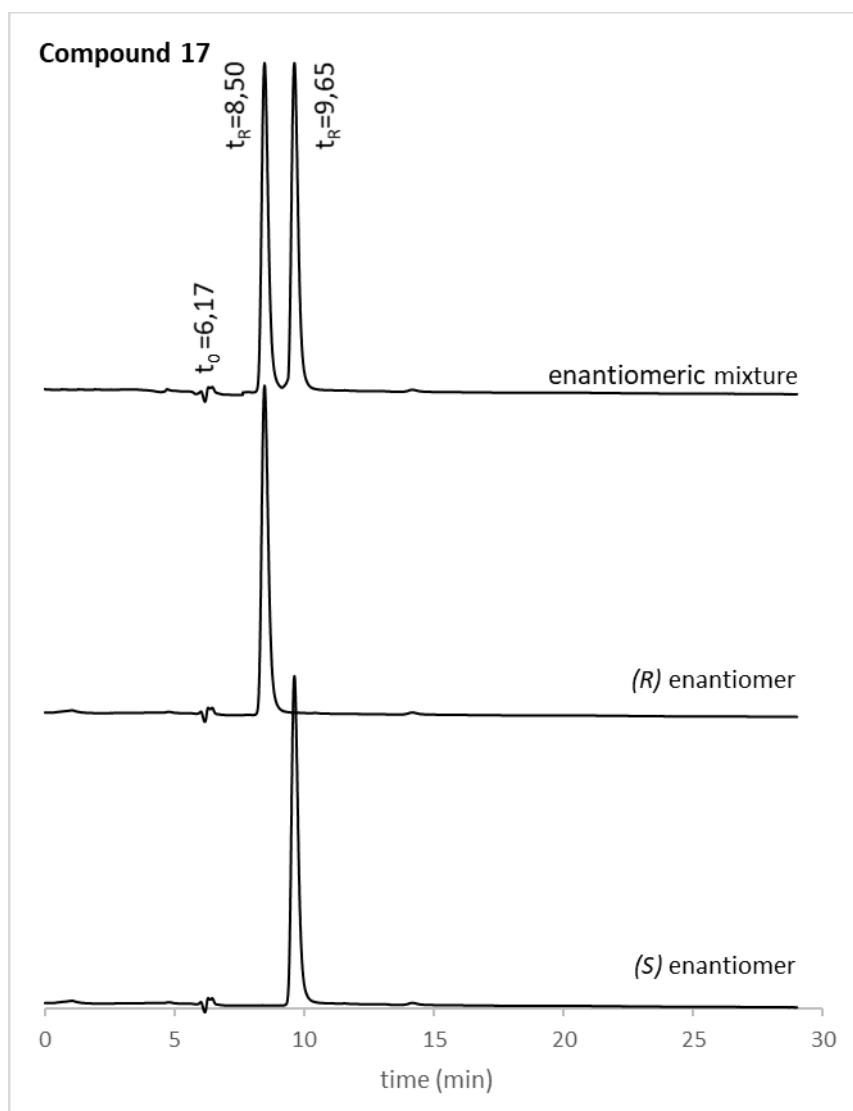


Figure S12. Chromatograms for the enantioseparation of the enantiomeric pair **17**, at optimized chromatographic conditions

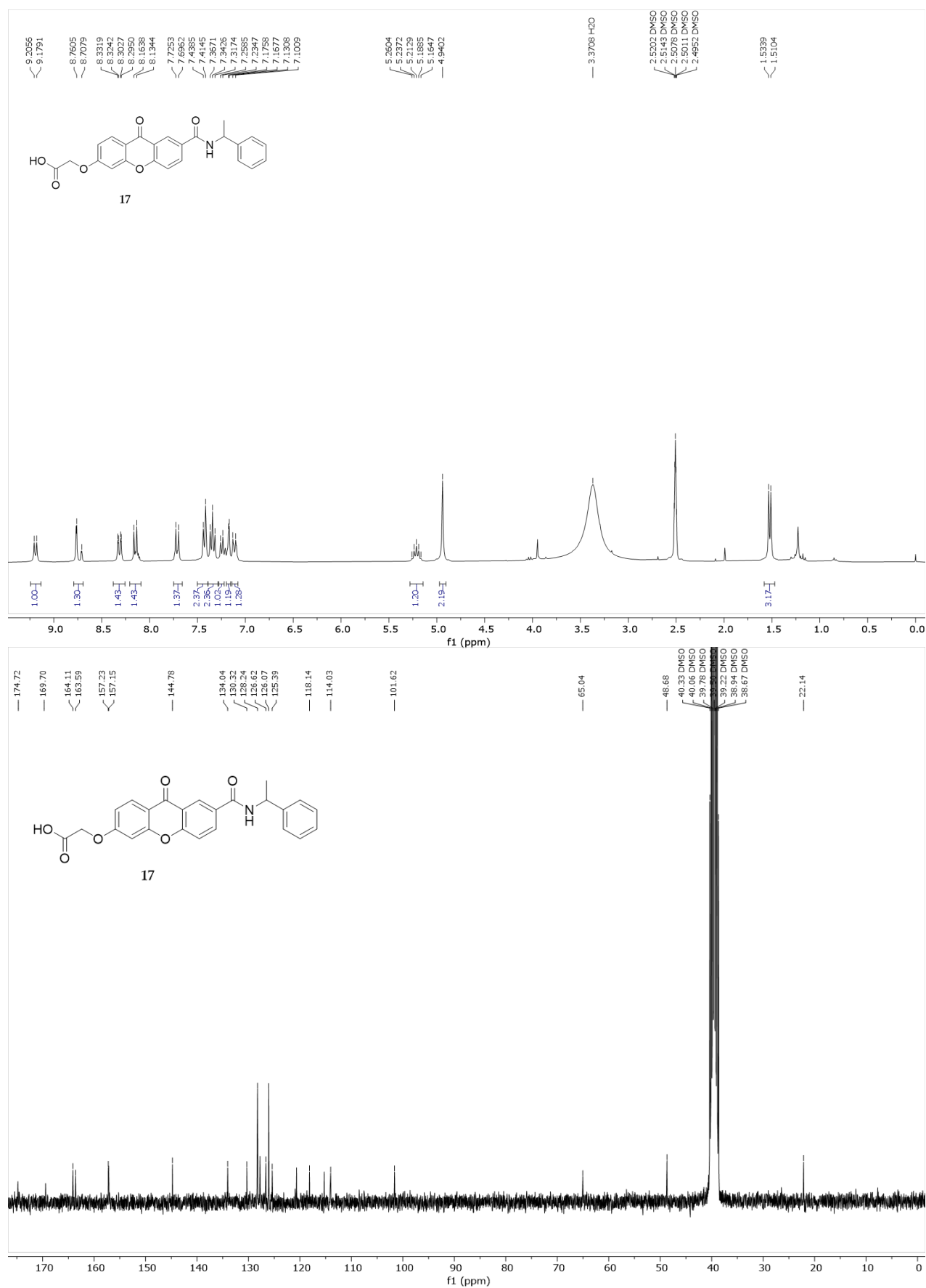
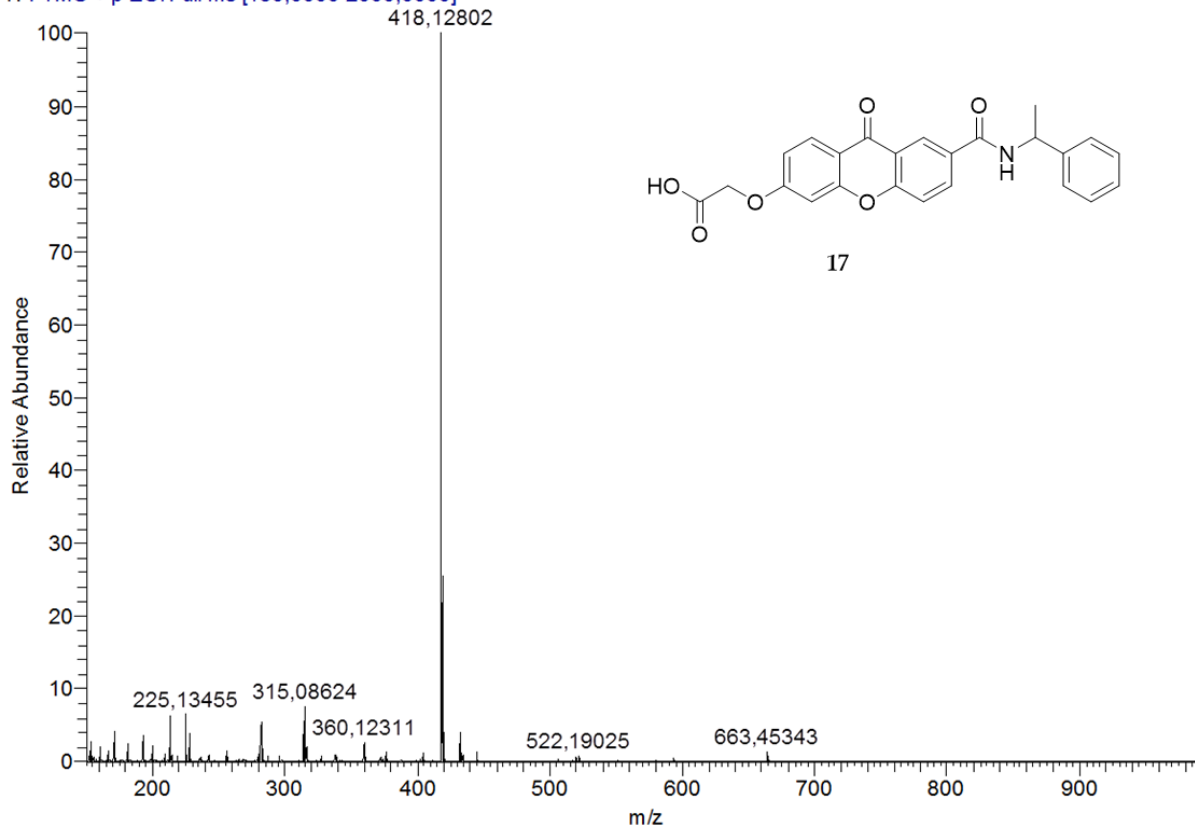


Figure S13. ^1H NMR (300.13 MHz, DMSO- d_6) and ^{13}C NMR (75.48 MHz, DMSO- d_6) for the enantiomeric pair 17.

T: FTMS + p ESI Full ms [150,0000-2000,0000]



Meas. m/z	Formula	m/z	err [ppm]
418.12906	C ₂₄ H ₂₀ NO ₆	418.12802	-1.191

Figure S14. Electrospray ESI data for the enantiomeric pair 17.

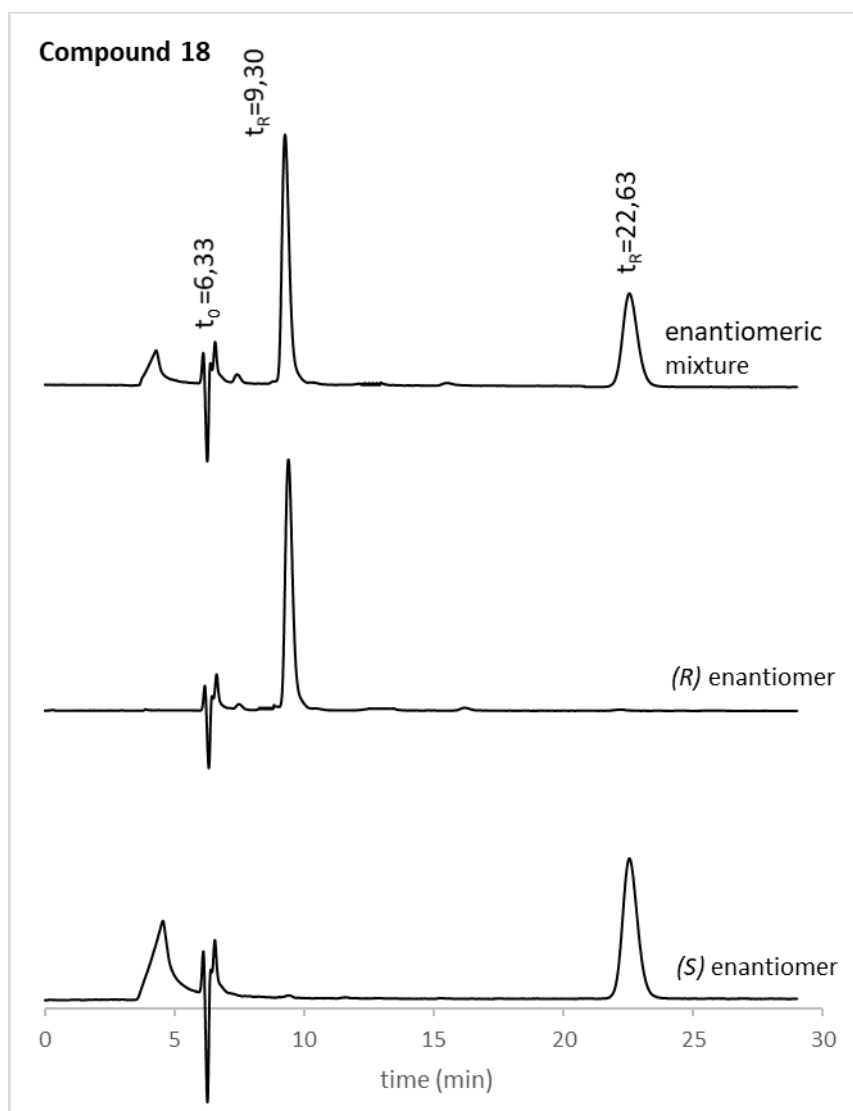


Figure S15. Chromatograms for the enantioseparation of the enantiomeric pair **18**, at optimized chromatographic conditions.

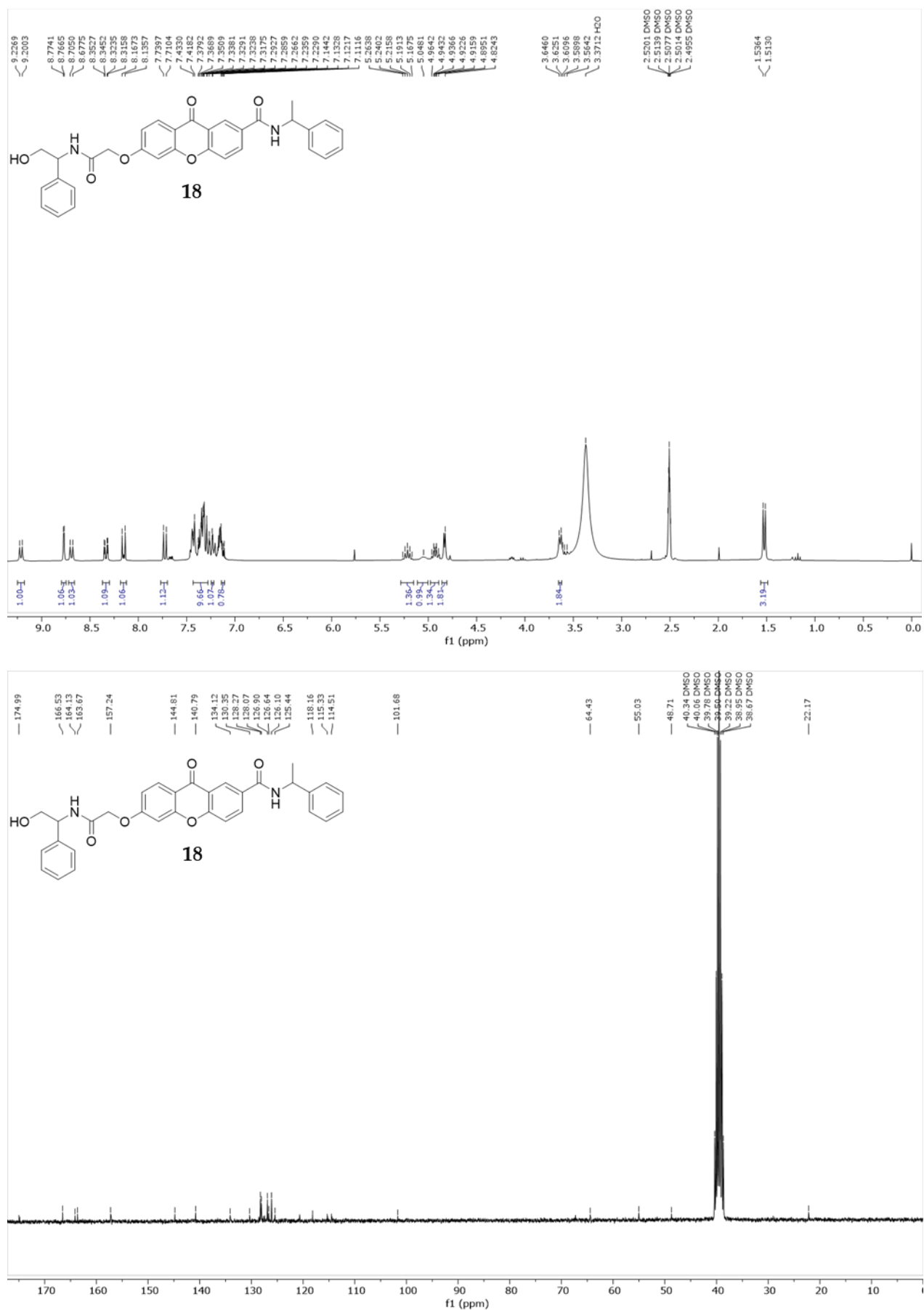
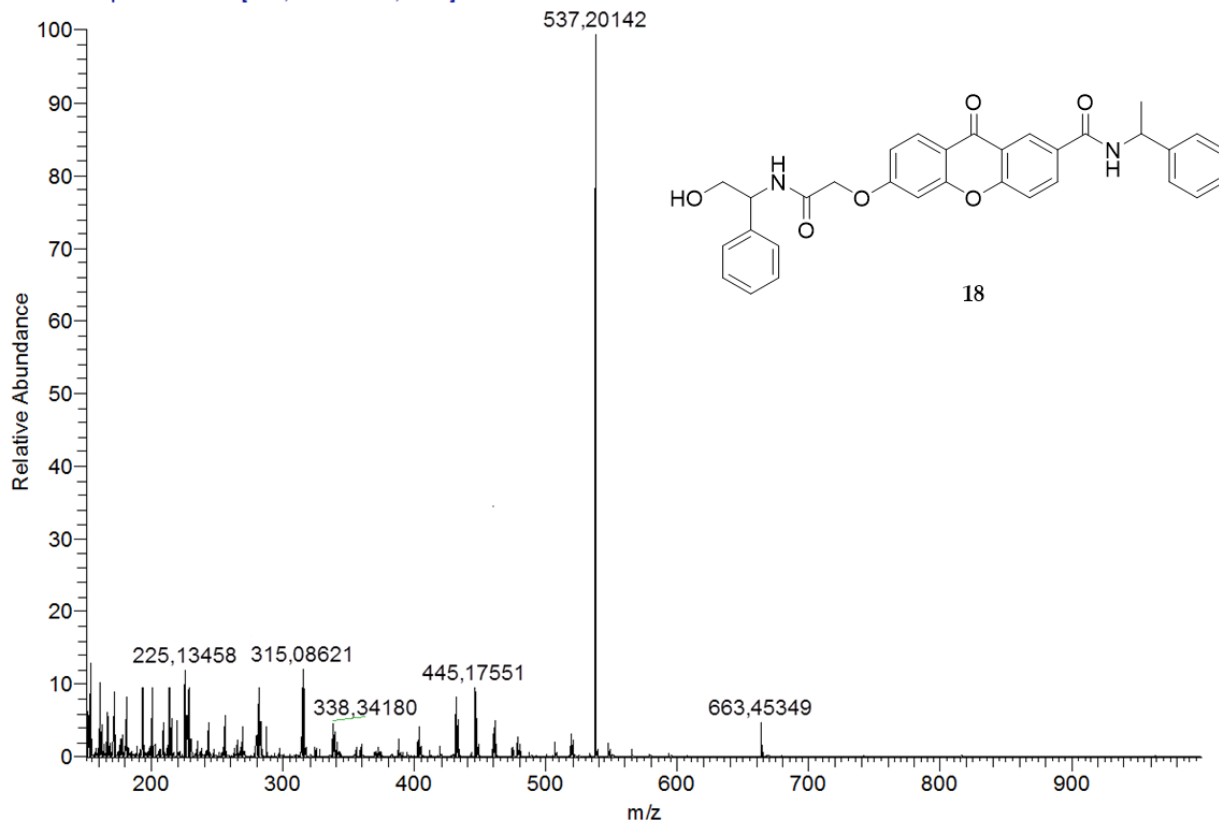


Figure S16. ¹H NMR (300.13 MHz, DMSO-*d*₆) and ¹³C NMR (75.48 MHz, DMSO-*d*₆) for the enantiomeric pair 18.

T: FTMS + p ESI Full ms [150,0000-2000,0000]



Meas. m/z	Formula	m/z	err [ppm]
537.20256	C ₃₂ H ₂₉ N ₂ O ₆	537.20142	-1.104

Figure S17. Electrospray ESI data for the enantiomeric pair **18**.