Supporting information

2,5-[C_4+C_2] Ringtransformation of Pyrylium Salts with α-Sulfinylacetaldehydes

Dominik Bauer[1], Kathrin Hofmann[2] and Michael Reggelin[1,*]

Technische Universität Darmstadt, Clemens-Schöpf-Institut für organische Chemie und Biochemie, 64287 Darmstadt, Germany; db@chemie.tu-darmstadt.de
[2] Technische Universität Darmstadt, Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, 64287 Darmstadt, Germany
* Correspondence: re@chemie.tu-darmstadt.de

Table of contents

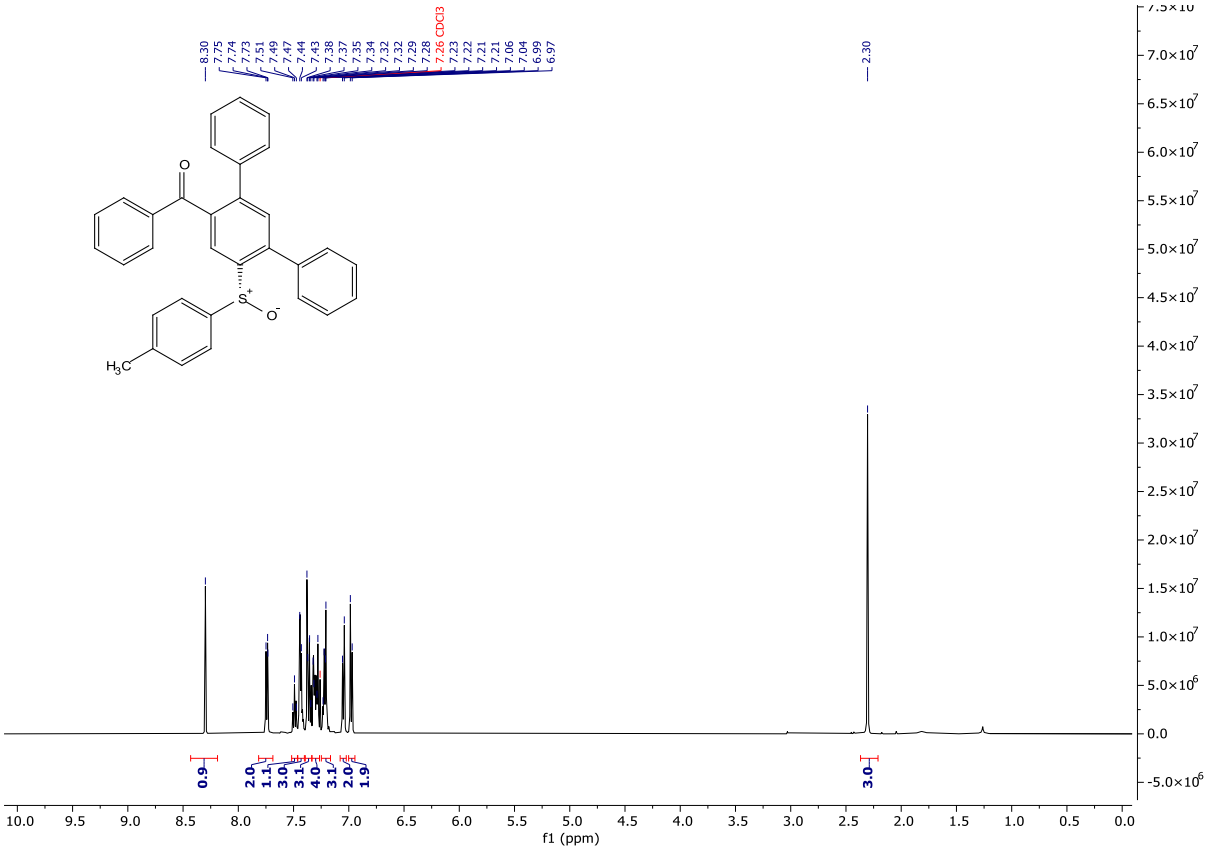

Figure 1. [1]H NMR (500 MHz, Chloroform-*d*) of compound **10a**.

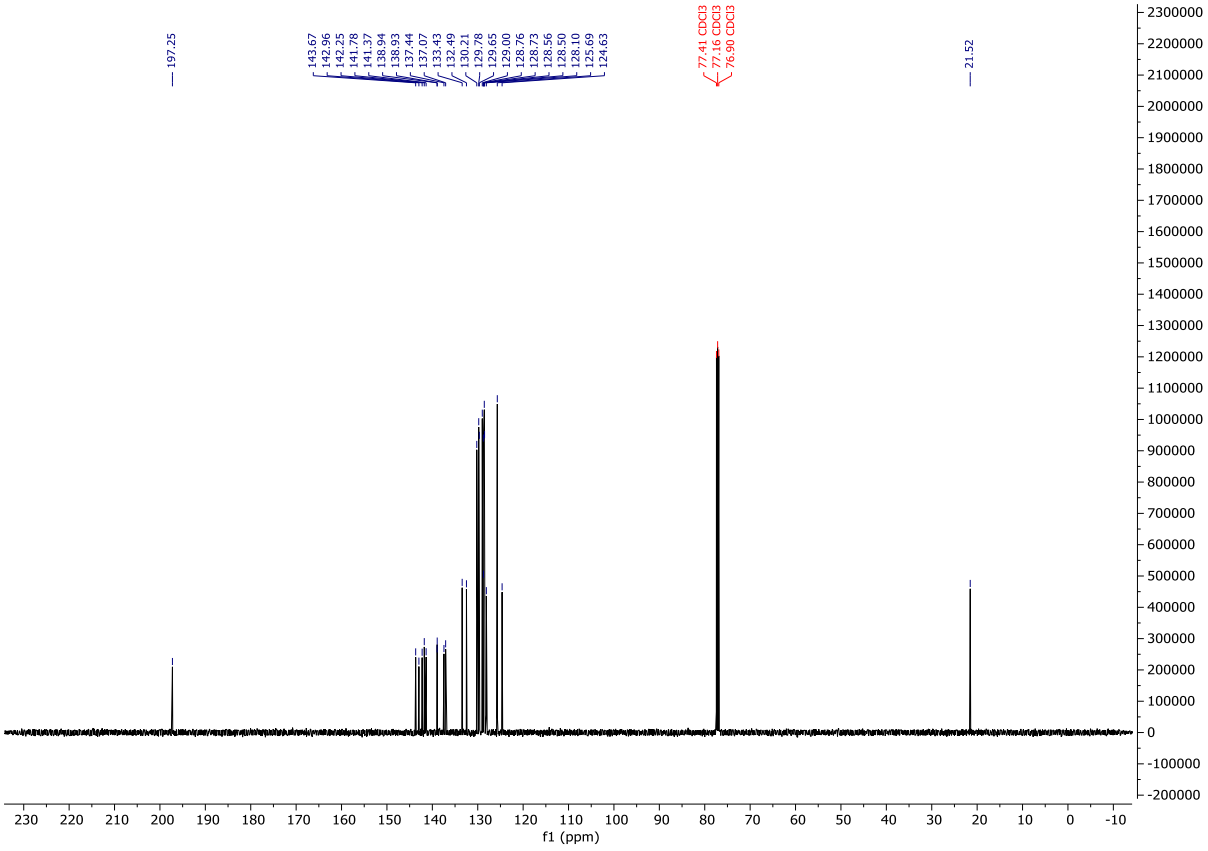

Figure 2. [13]C NMR (126 MHz, Chloroform-*d*) of compound **10a**.

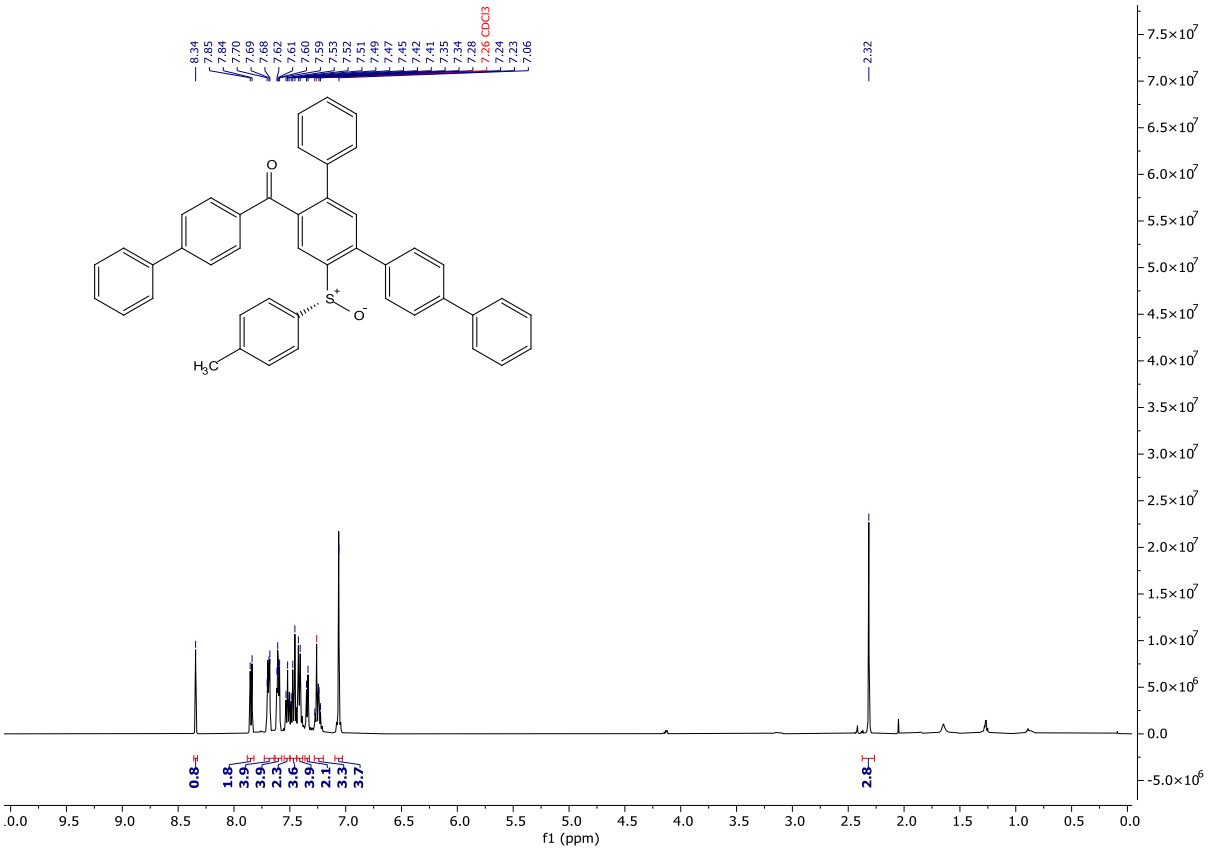

Figure 3. [1]H NMR (500 MHz, Chloroform-*d*) of compound **10b**.

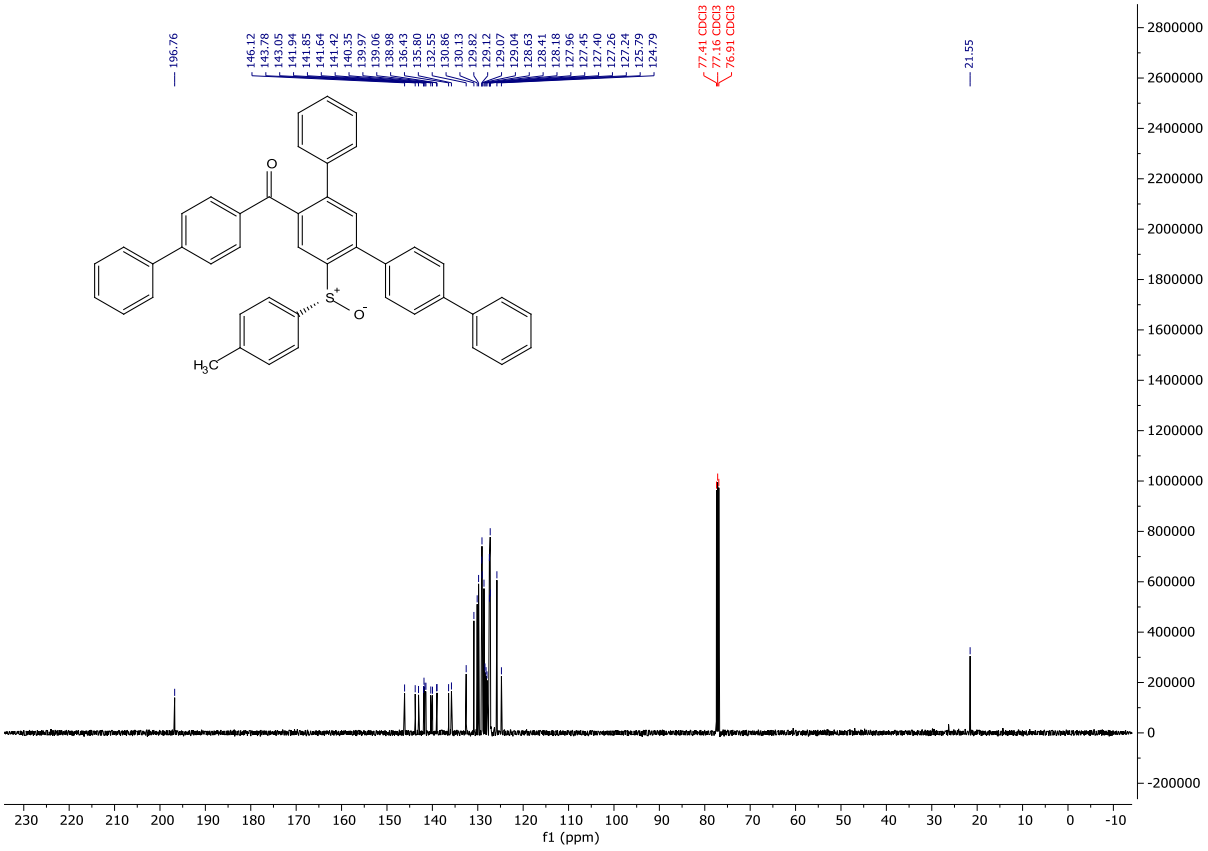

Figure 4. [13]C NMR (126 MHz, Chloroform-*d*) of compound **10b**.

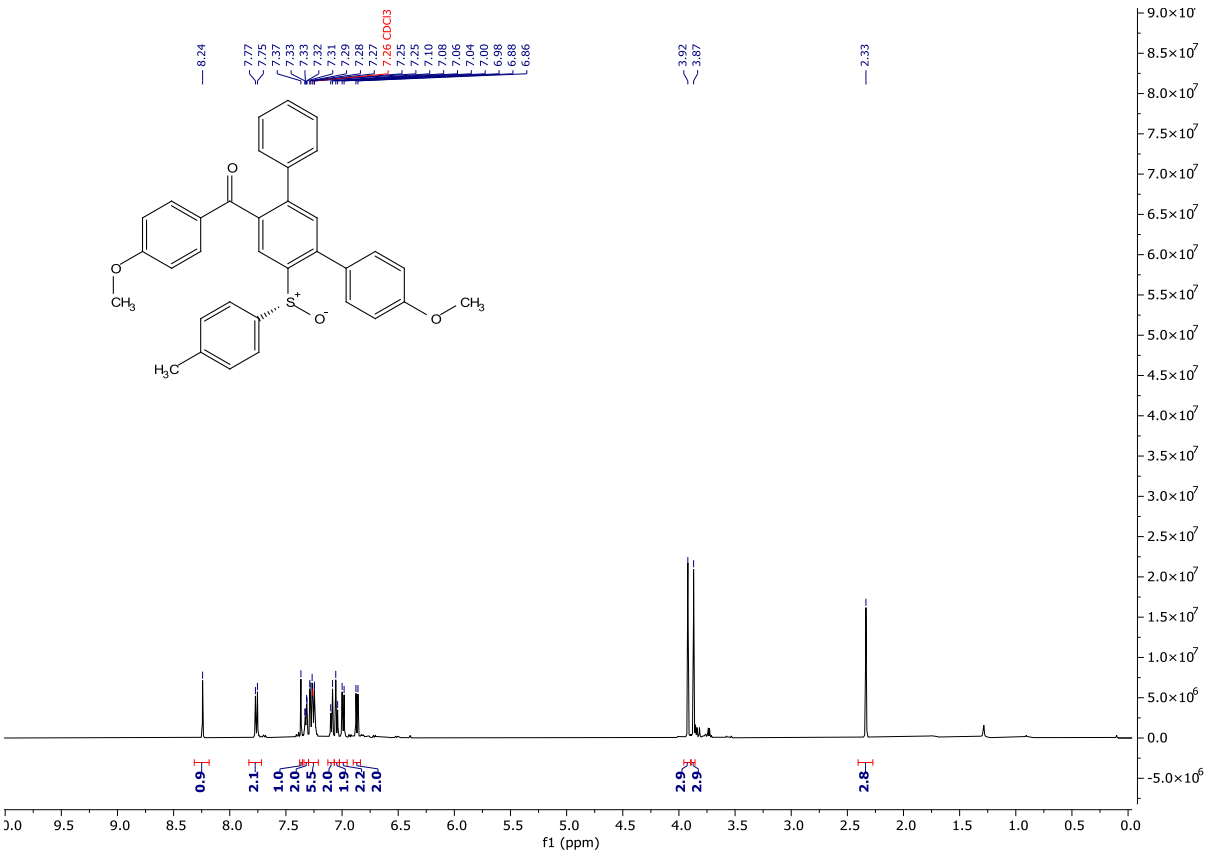

Figure 5. [1]H NMR (500 MHz, Chloroform-*d*) of compound **10c**.

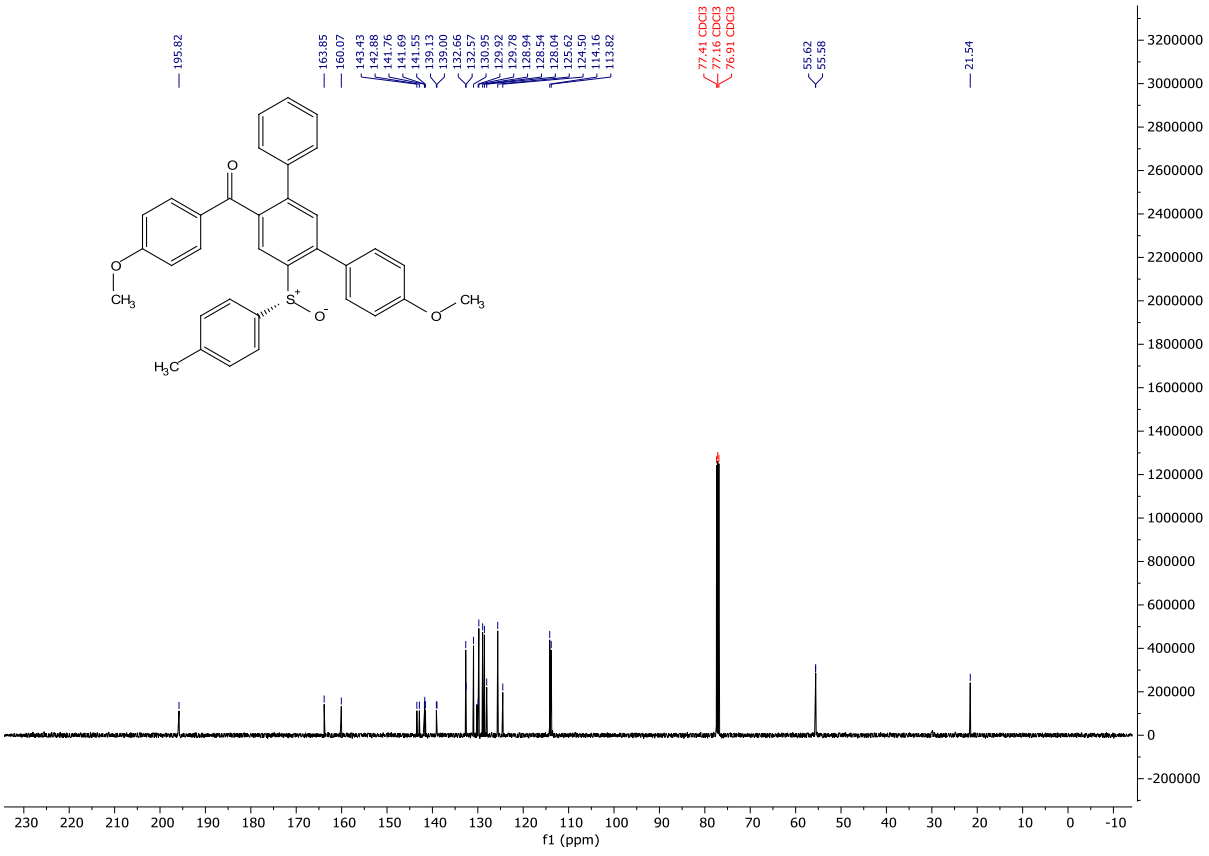

Figure 6. [13]C NMR (126 MHz, Chloroform-*d*) of compound **10c**.

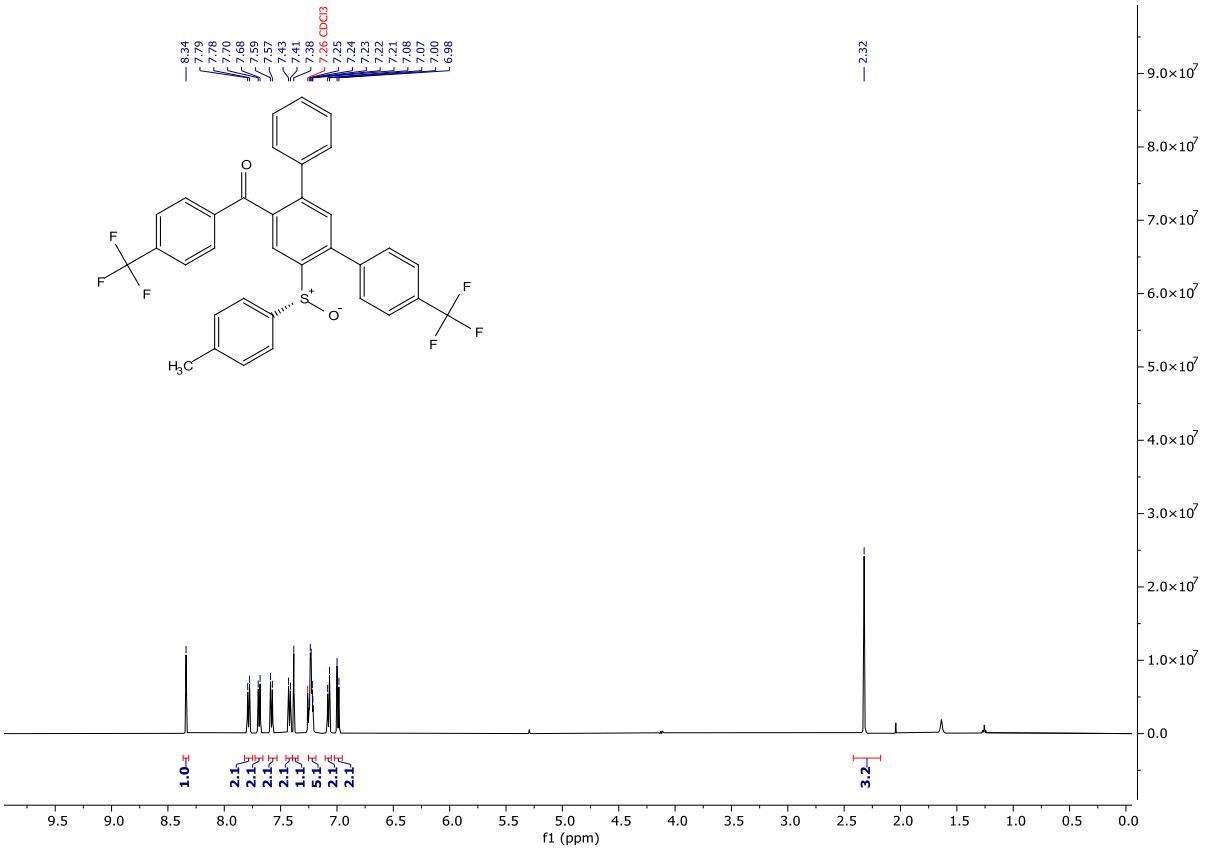

Figure 7. [1]H NMR (500 MHz, Chloroform-*d*) of compound **10d**.

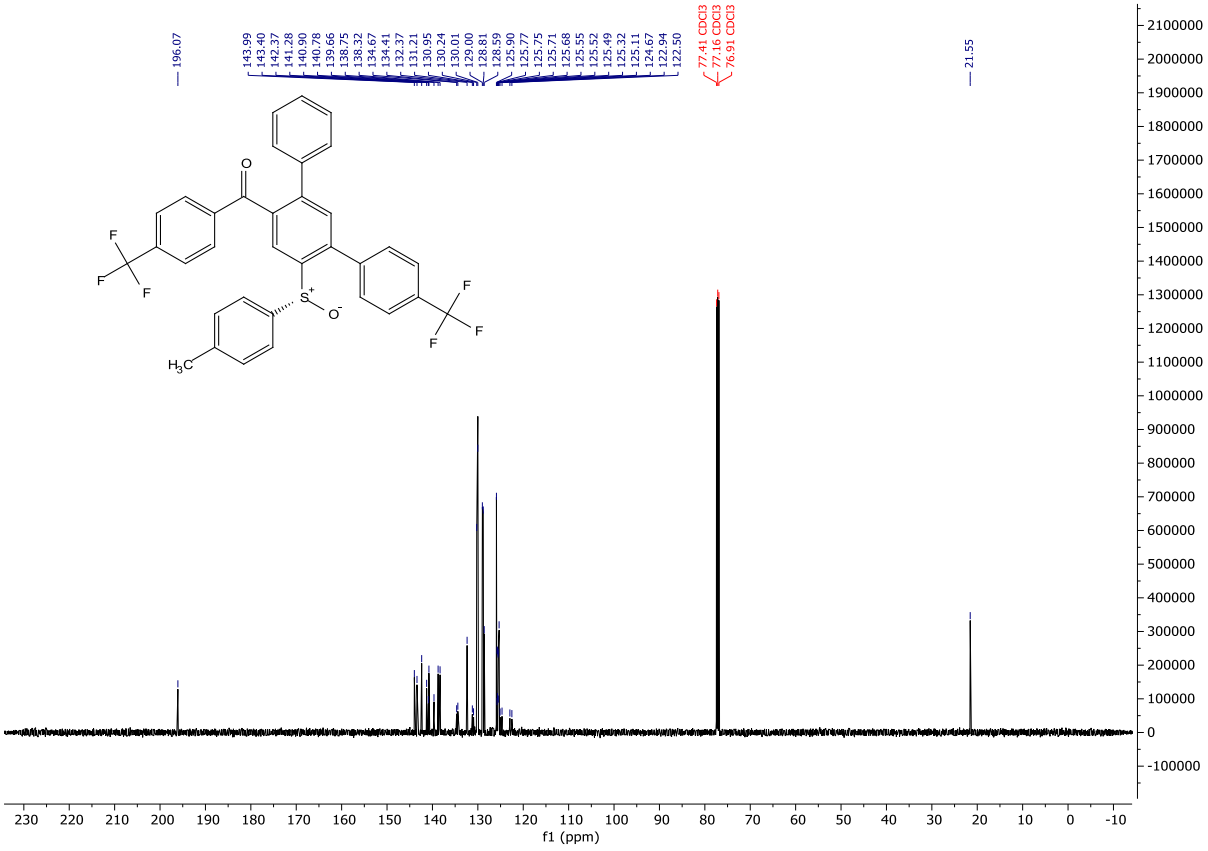

Figure 8. [13]C NMR (126 MHz, Chloroform-*d*) of compound **10d**.

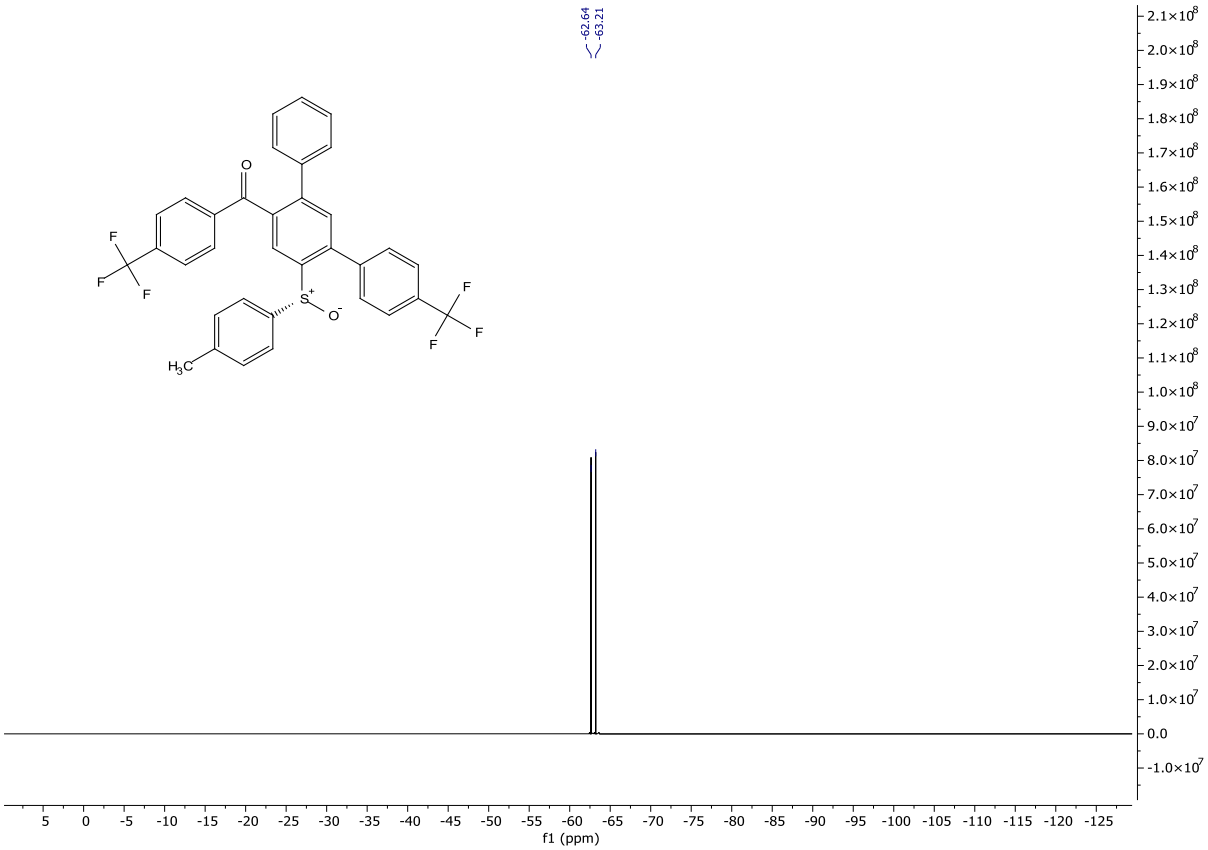

Figure 9. ^{19}F NMR (471 MHz, Chloroform-*d*) of compound **10d**.

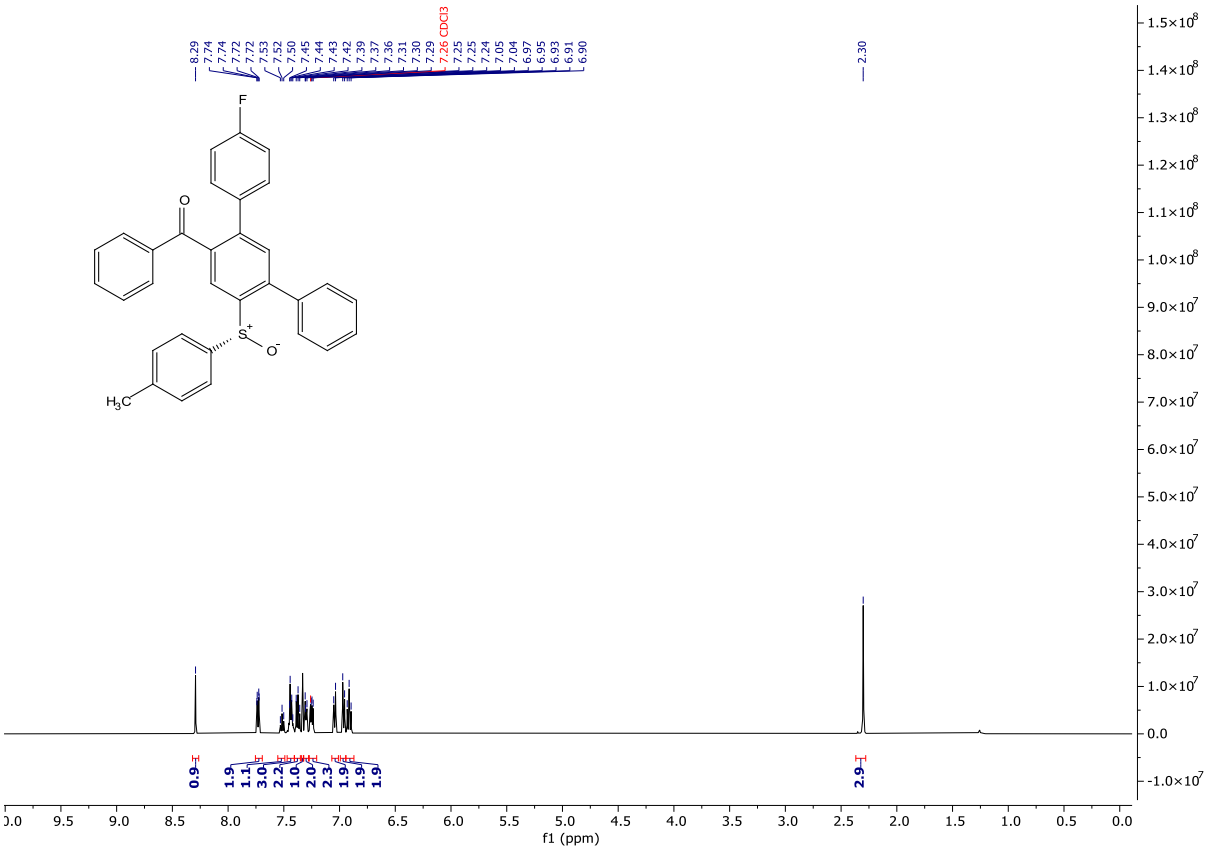

Figure 10. [1]H NMR (500 MHz, Chloroform-*d*) of compound **10e**.

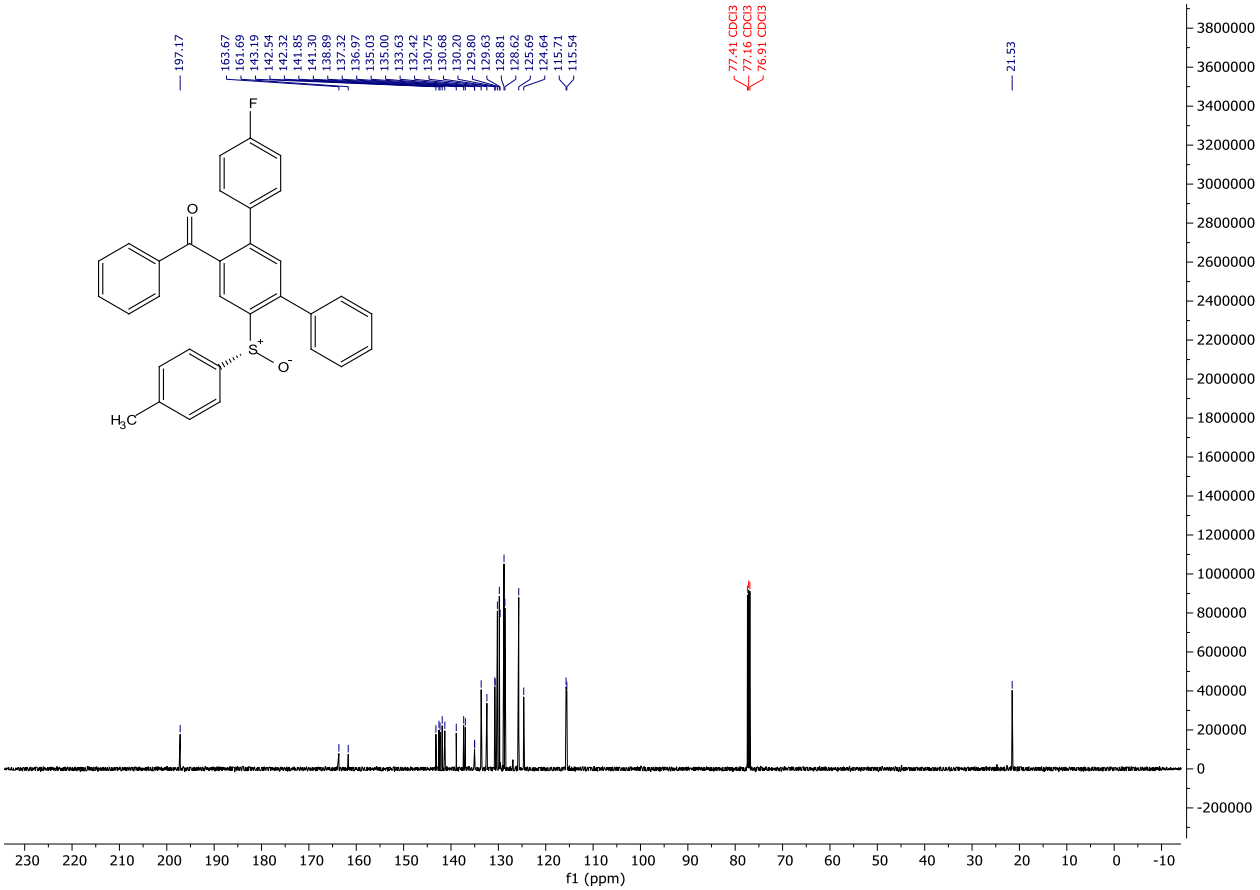

Figure 11. [13]C NMR (126 MHz, Chloroform-*d*) of compound **10e**.

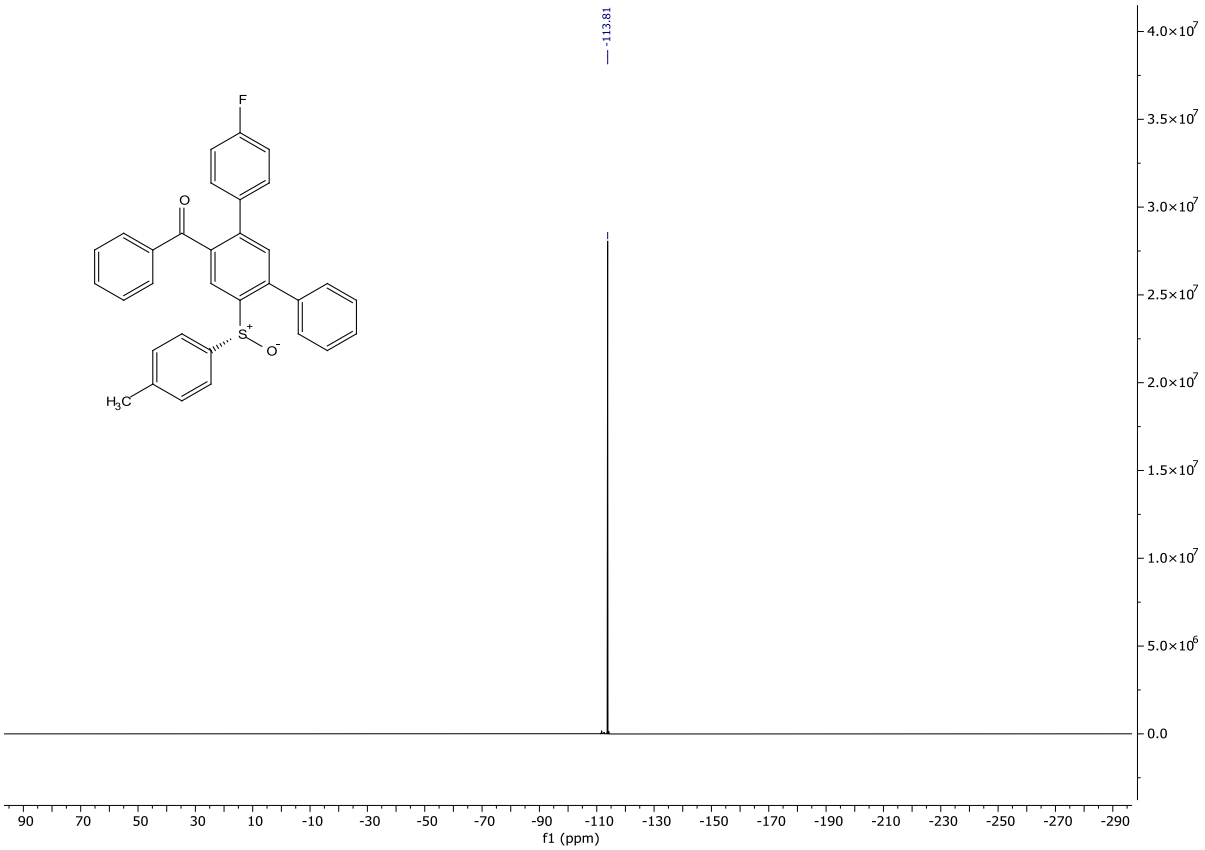

Figure 12. ^{19}F NMR (471 MHz, Chloroform-*d*) of compound **10e**.

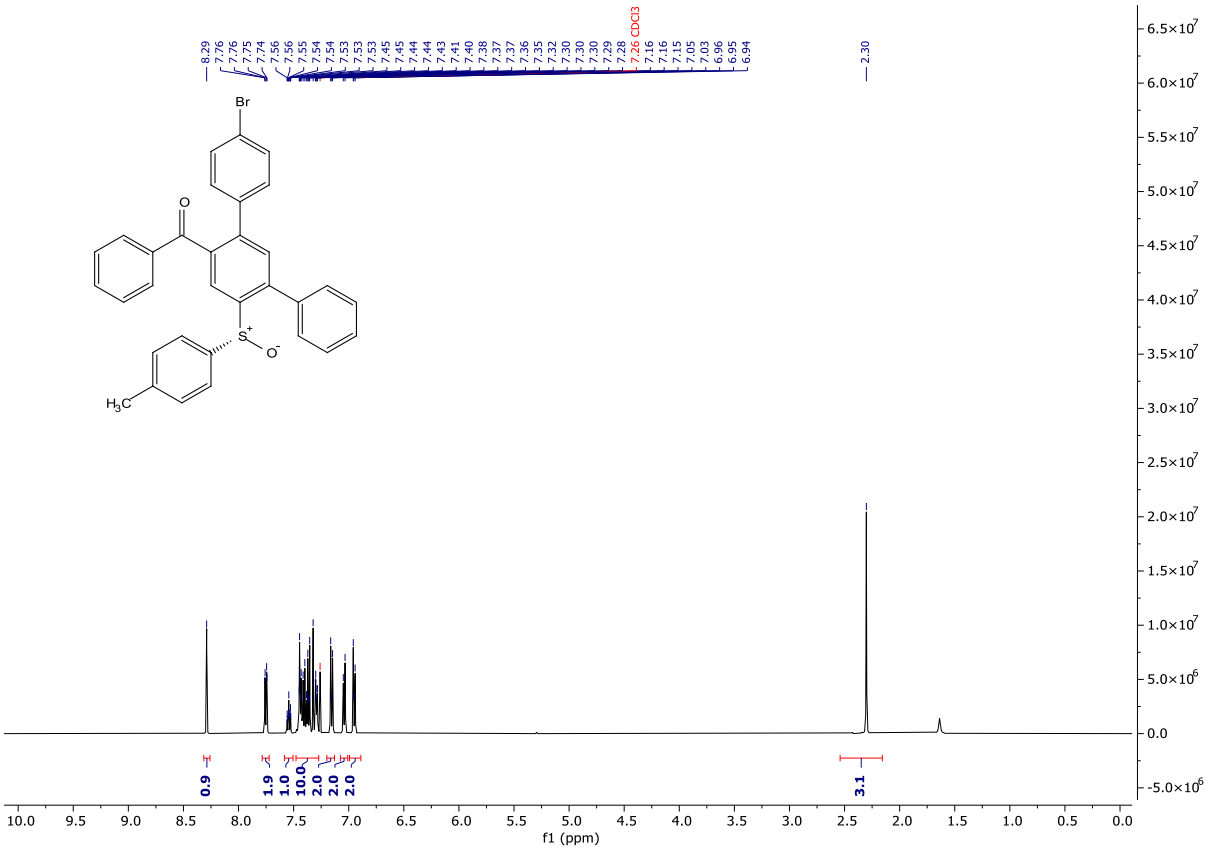

Figure 13. [1]H NMR (500 MHz, Chloroform-*d*) of compound **10f**.

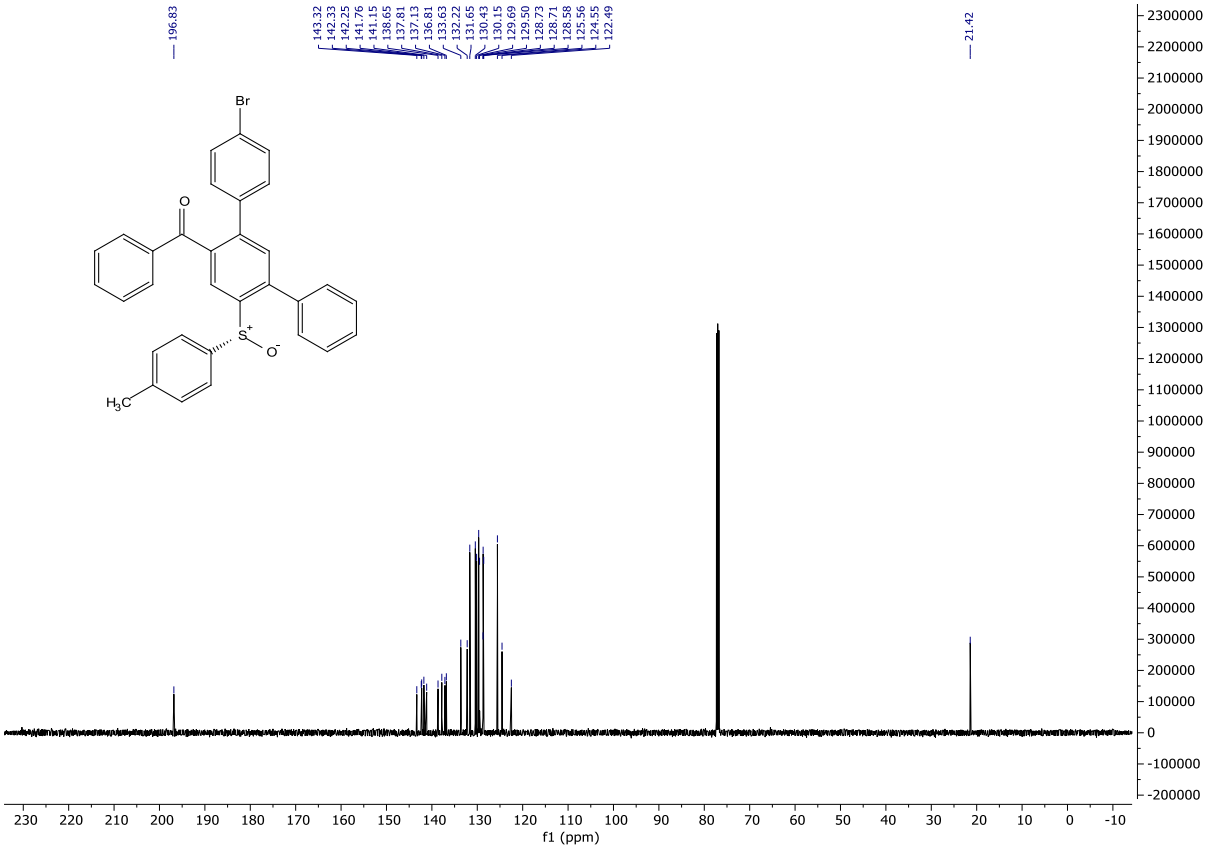

Figure 14. [13]C NMR (126 MHz, Chloroform-*d*) of compound **10f**.

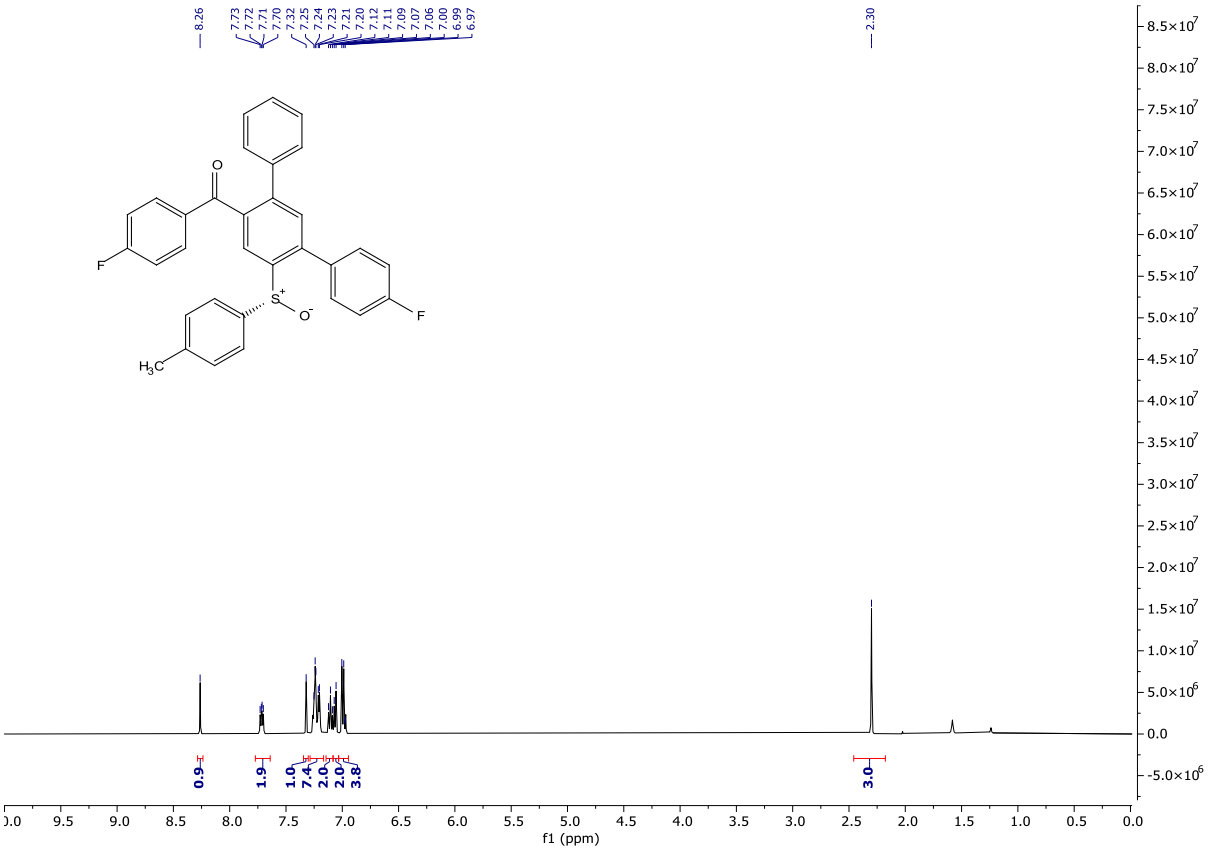

Figure 15. [1]H NMR (500 MHz, Chloroform-*d*) of compound **10g**.

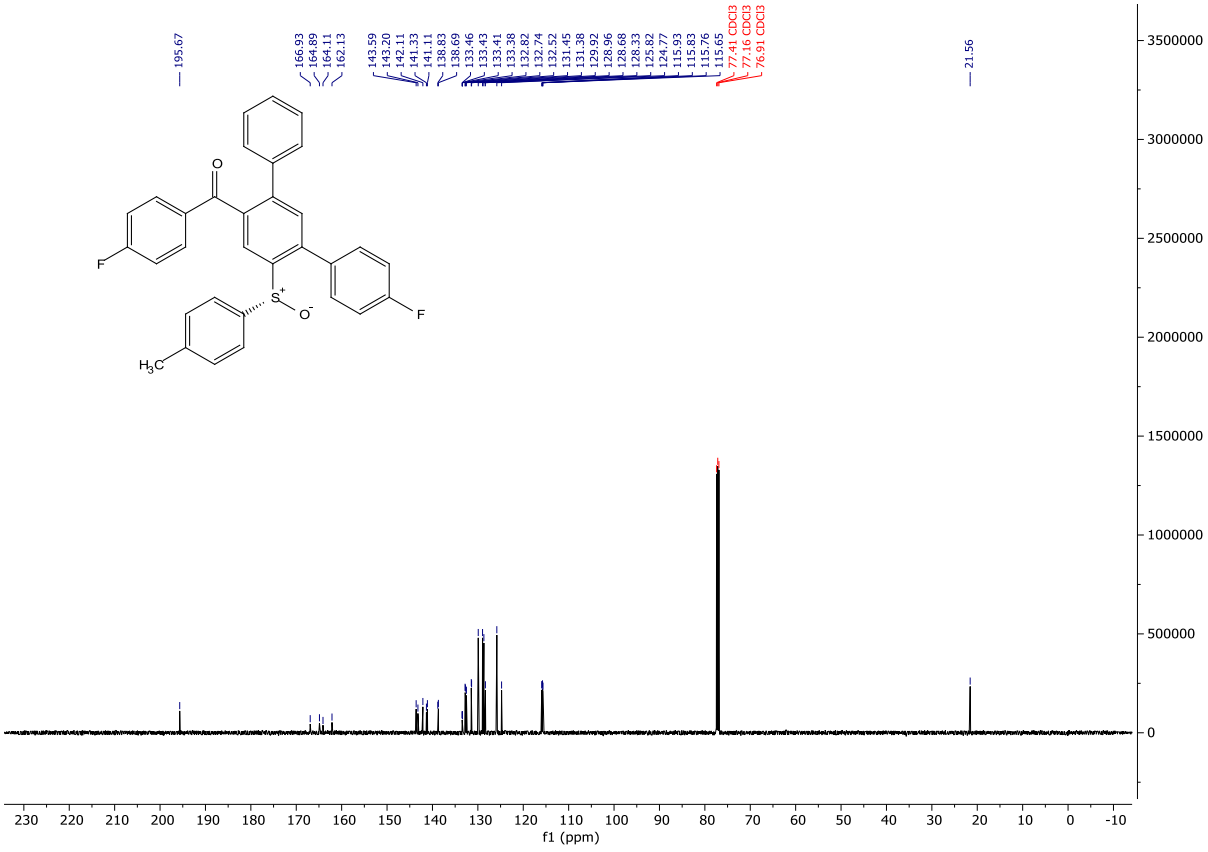

Figure 16. [13]C NMR (126 MHz, Chloroform-*d*) of compound **10g**.

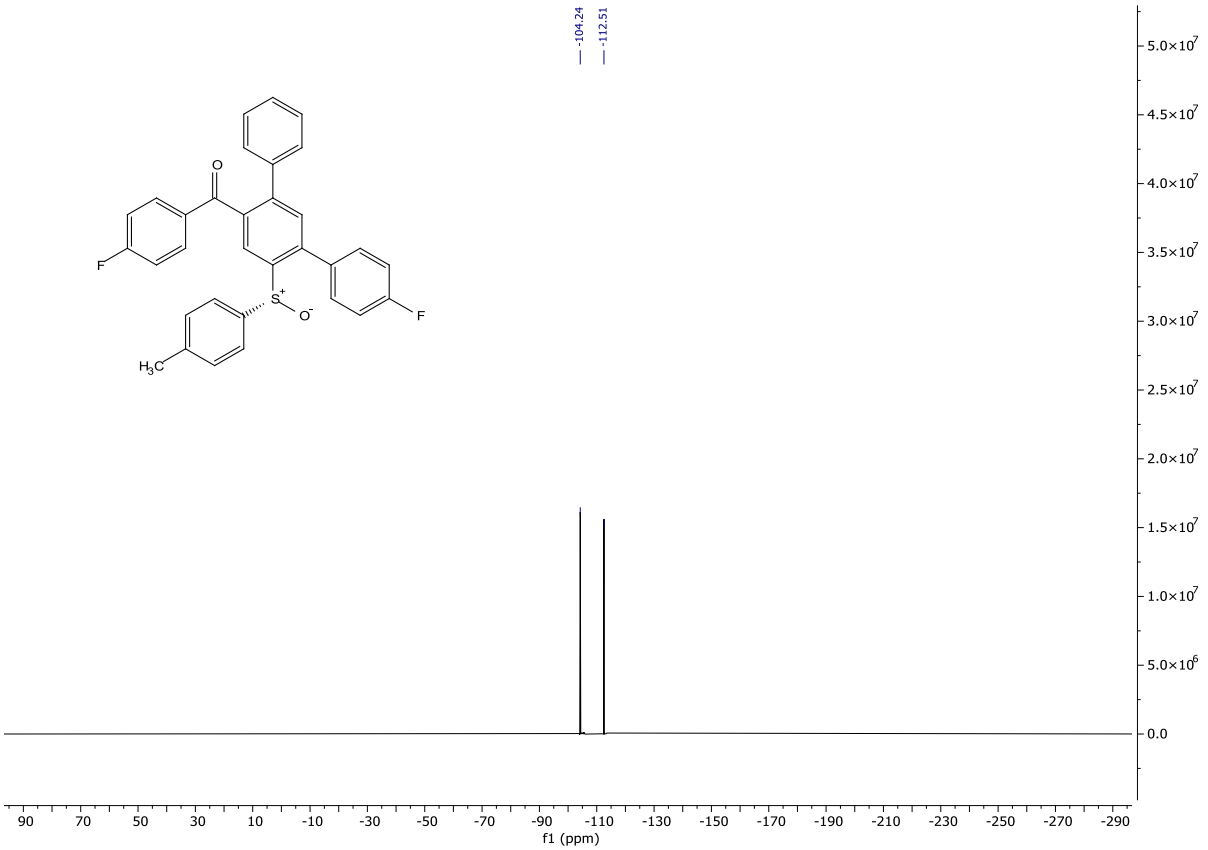

Figure 17. ^{19}F NMR (471 MHz, Chloroform-*d*) of compound **10g**.

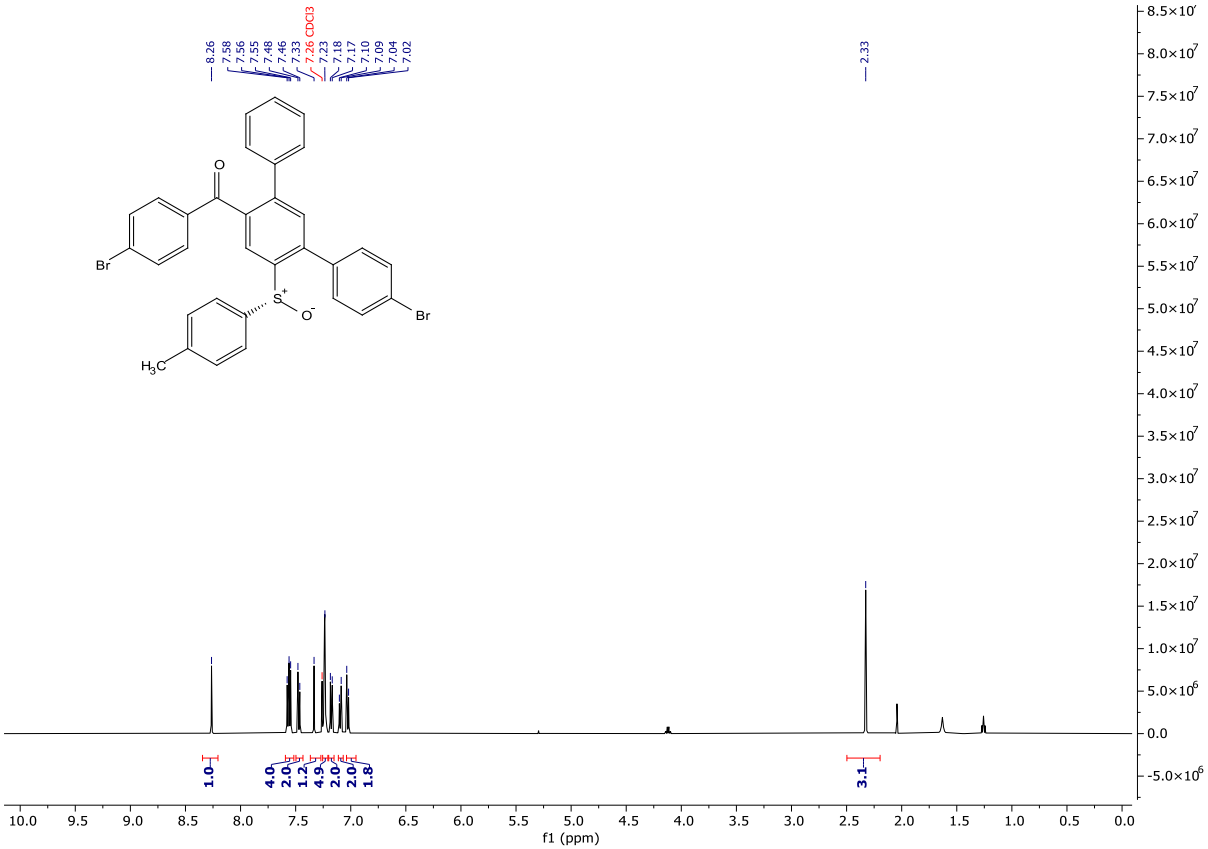

Figure 18. [1]H NMR (500 MHz, Chloroform-*d*) of compound **10h**.

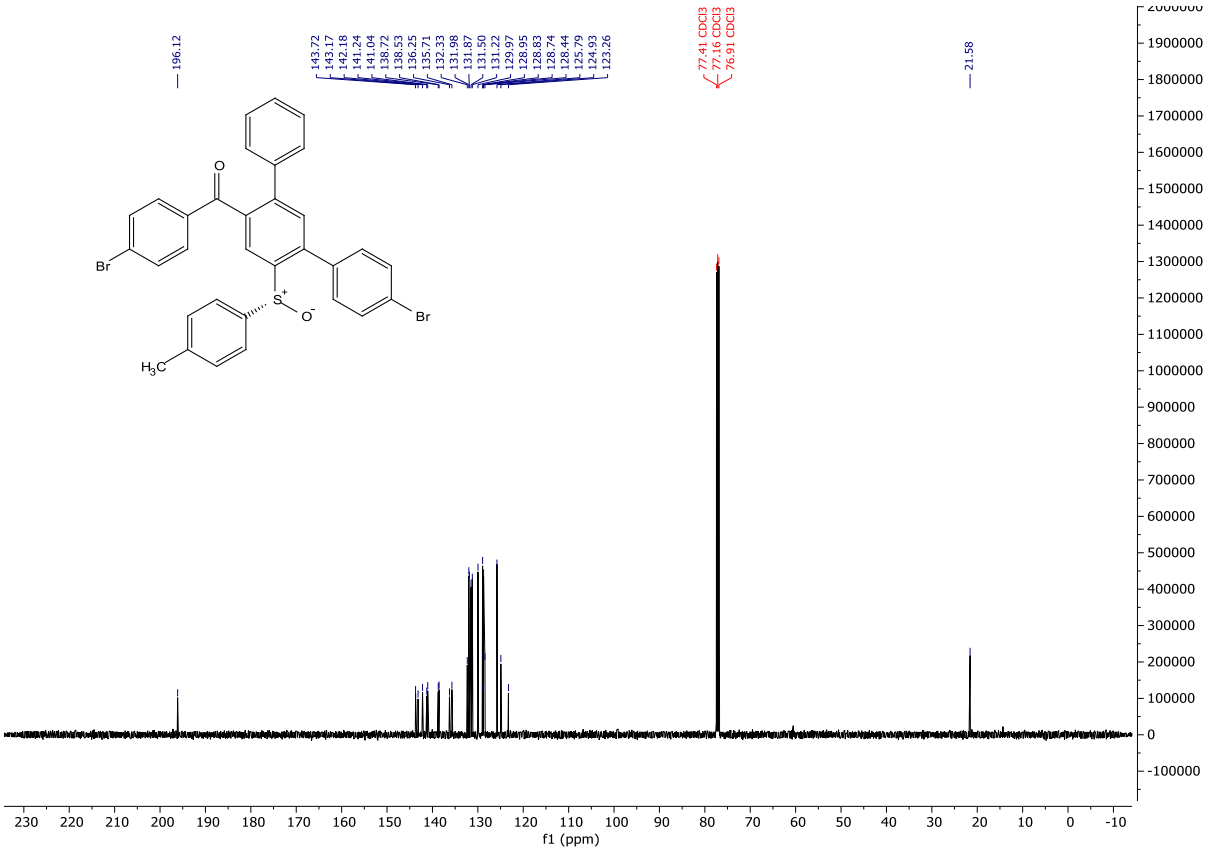

Figure 19. [13]C NMR (126 MHz, Chloroform-*d*) of compound **10h**.

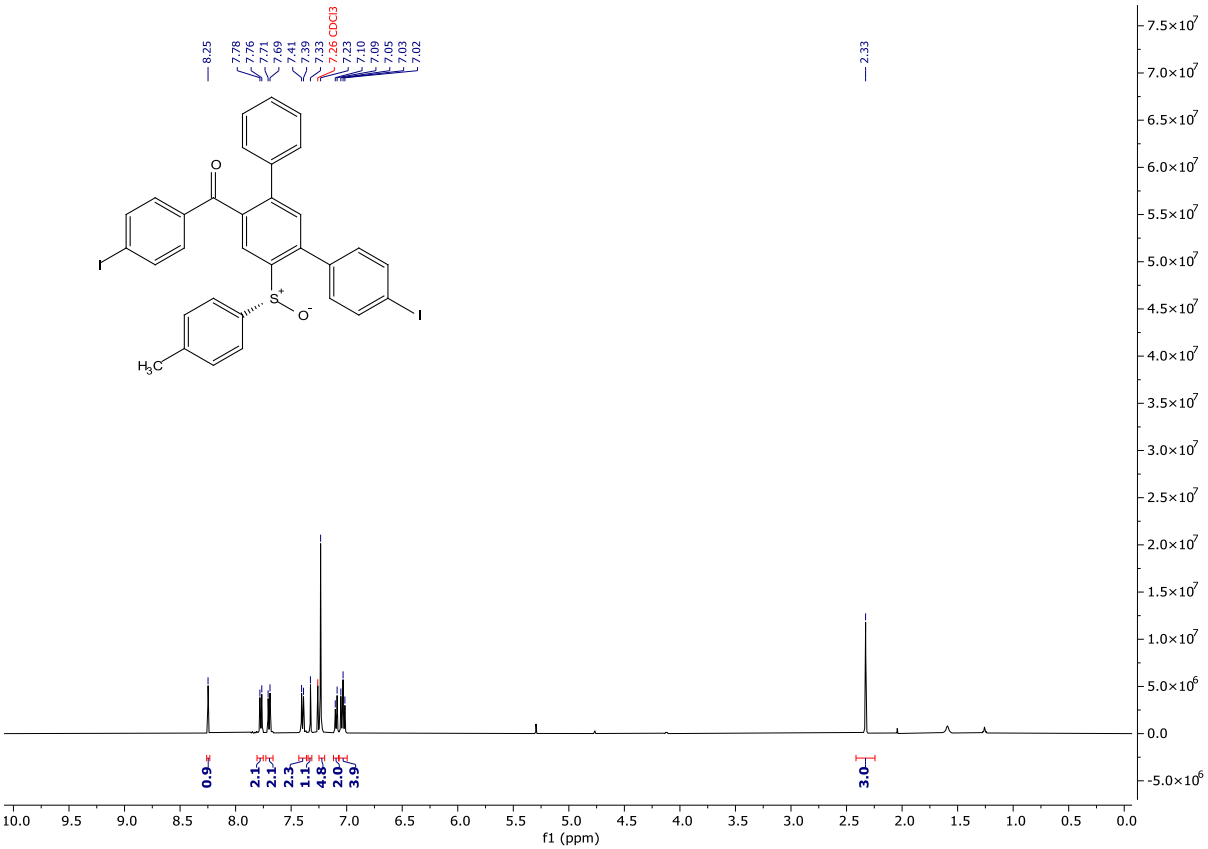

Figure 20. [1]H NMR (500 MHz, Chloroform-*d*) of compound **10i**.

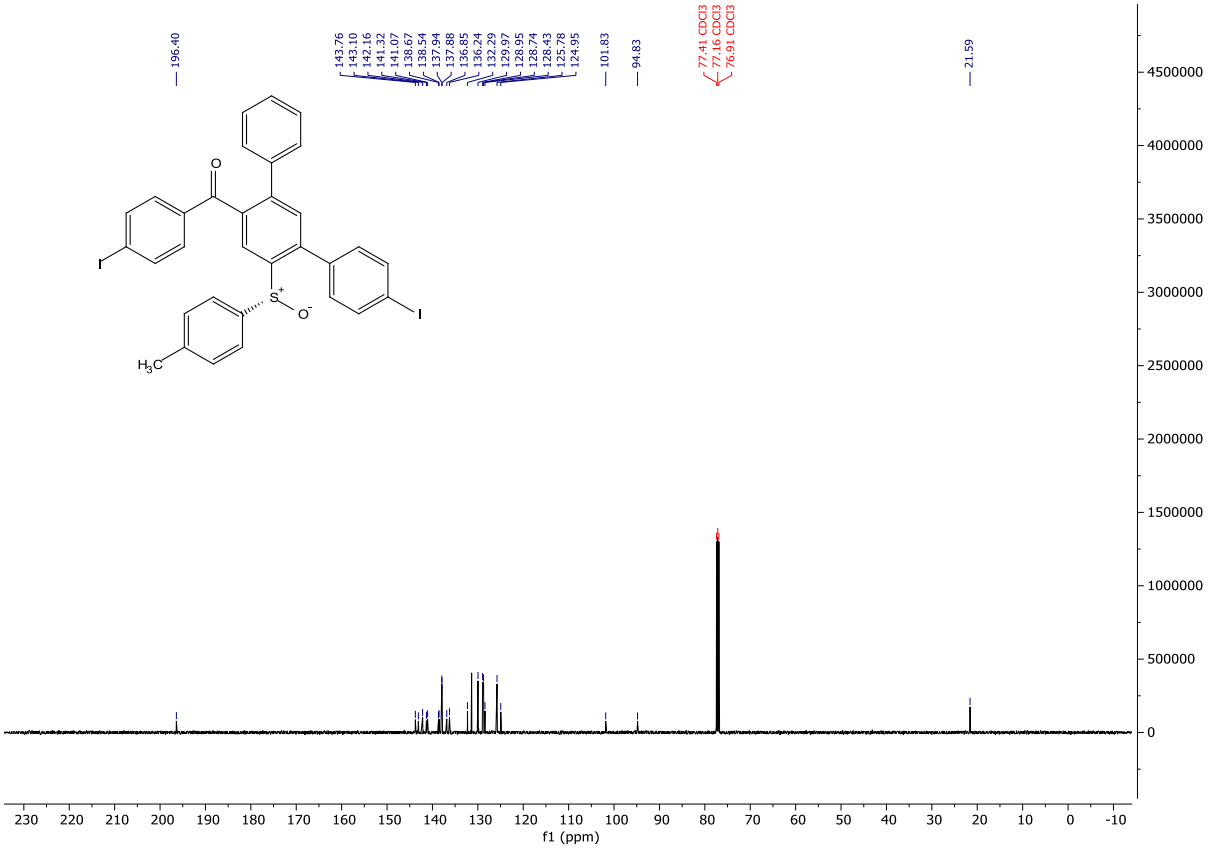

Figure 21. [13]C NMR (126 MHz, Chloroform-*d*) of compound **10i**.

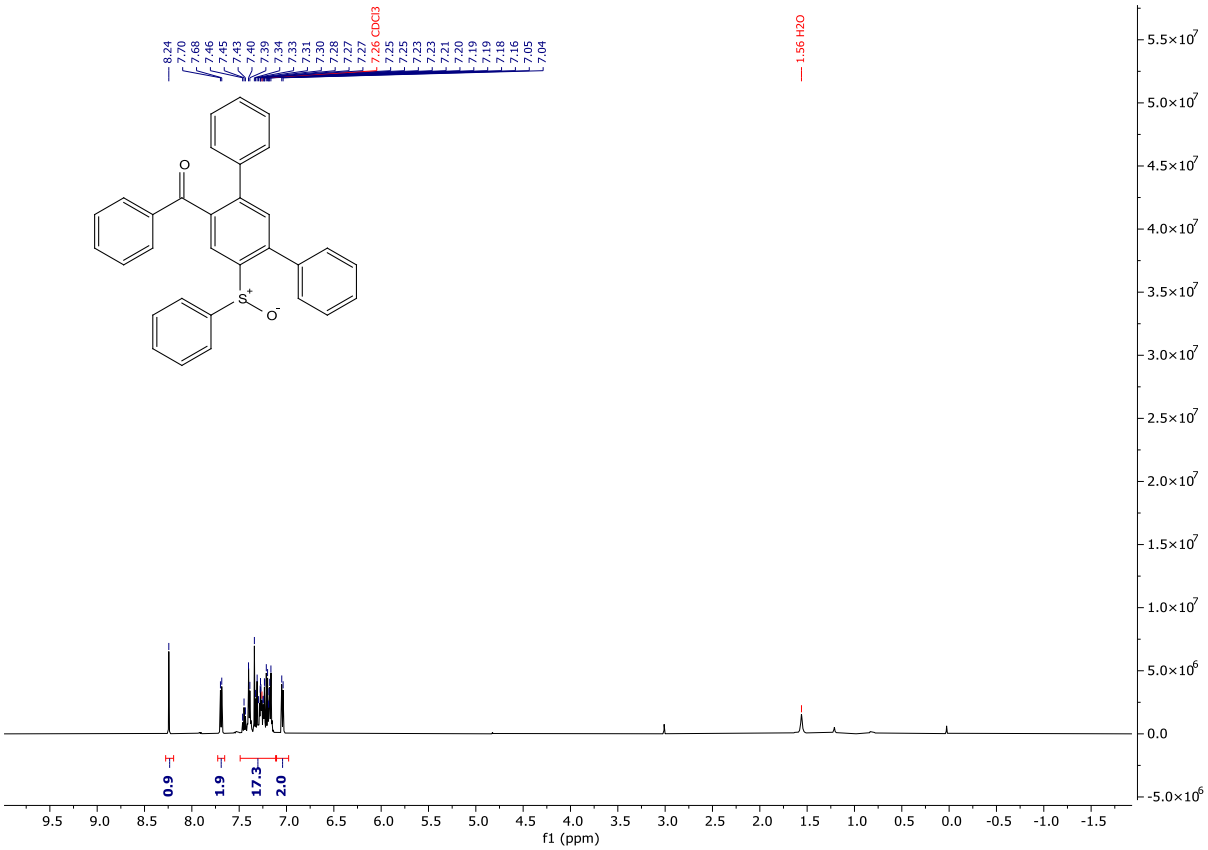

Figure 22. [1]H NMR (500 MHz, Chloroform-*d*) of compound **10j**.

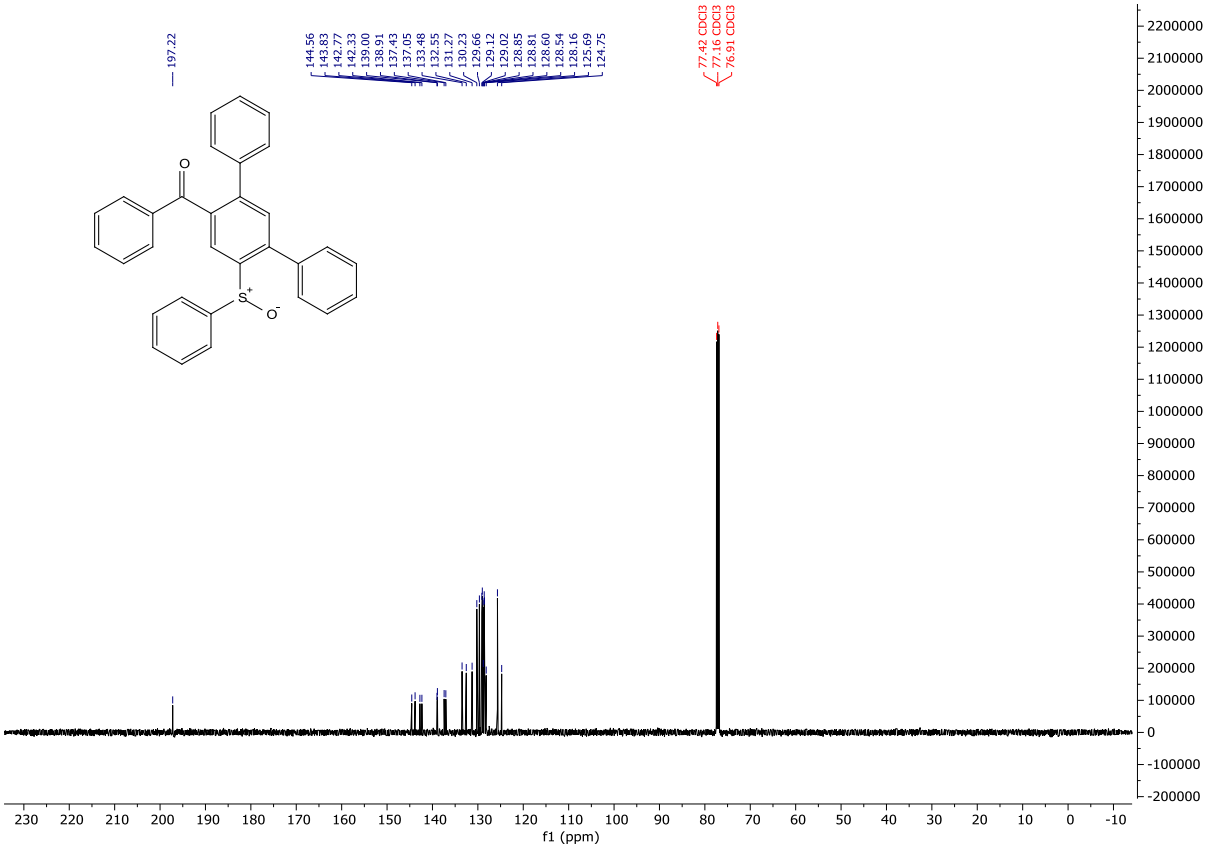

Figure 23. [13]C NMR (126 MHz, Chloroform-*d*) of compound **10j**.

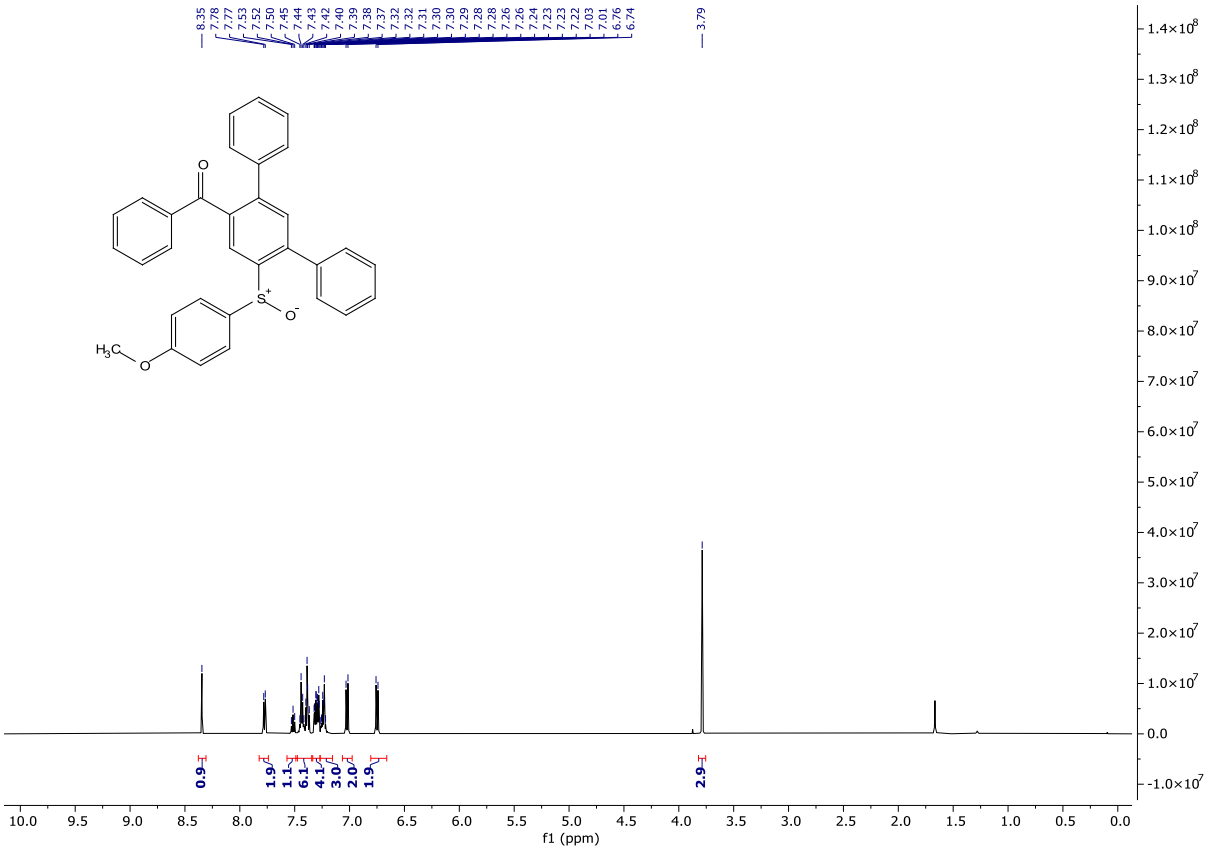

Figure 24. [1]H NMR (500 MHz, Chloroform-*d*) of compound **10k**.

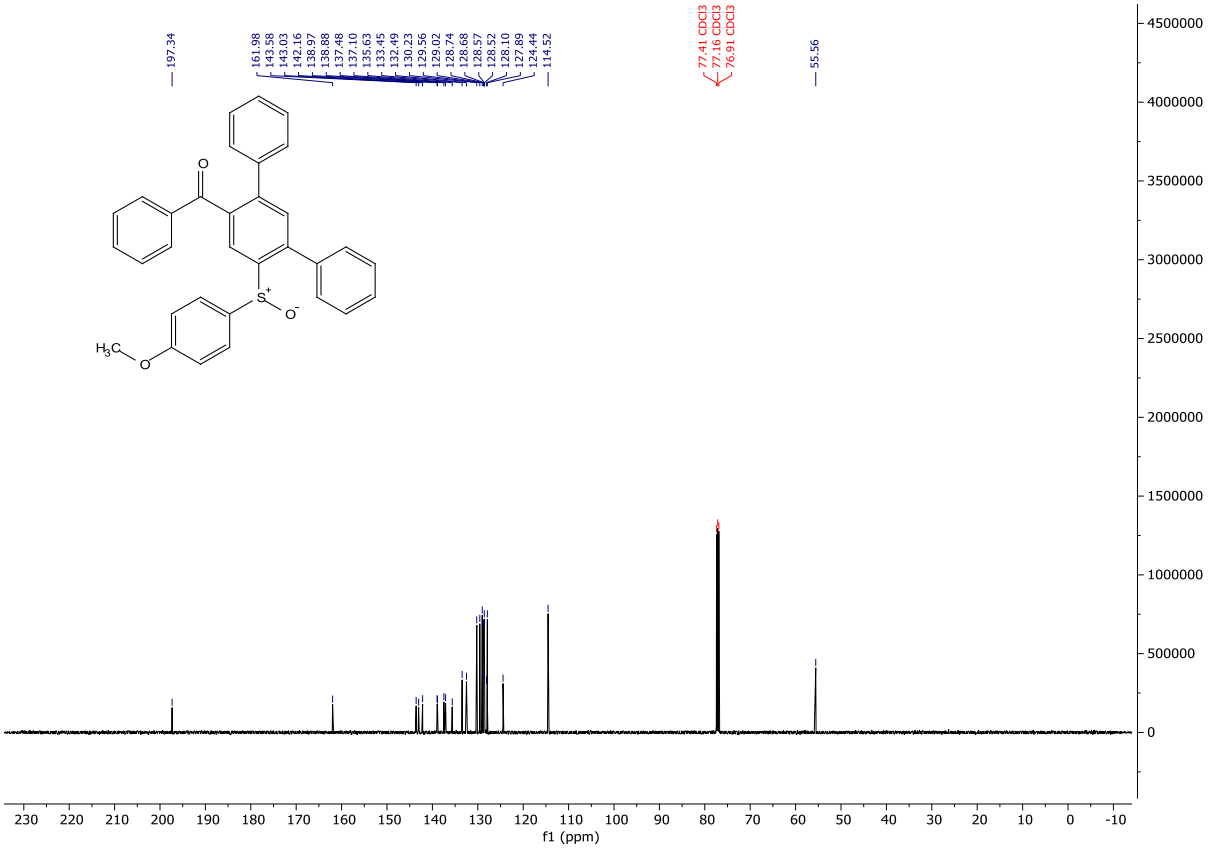

Figure 25. [13]C NMR (126 MHz, Chloroform-*d*) of compound **10k**.

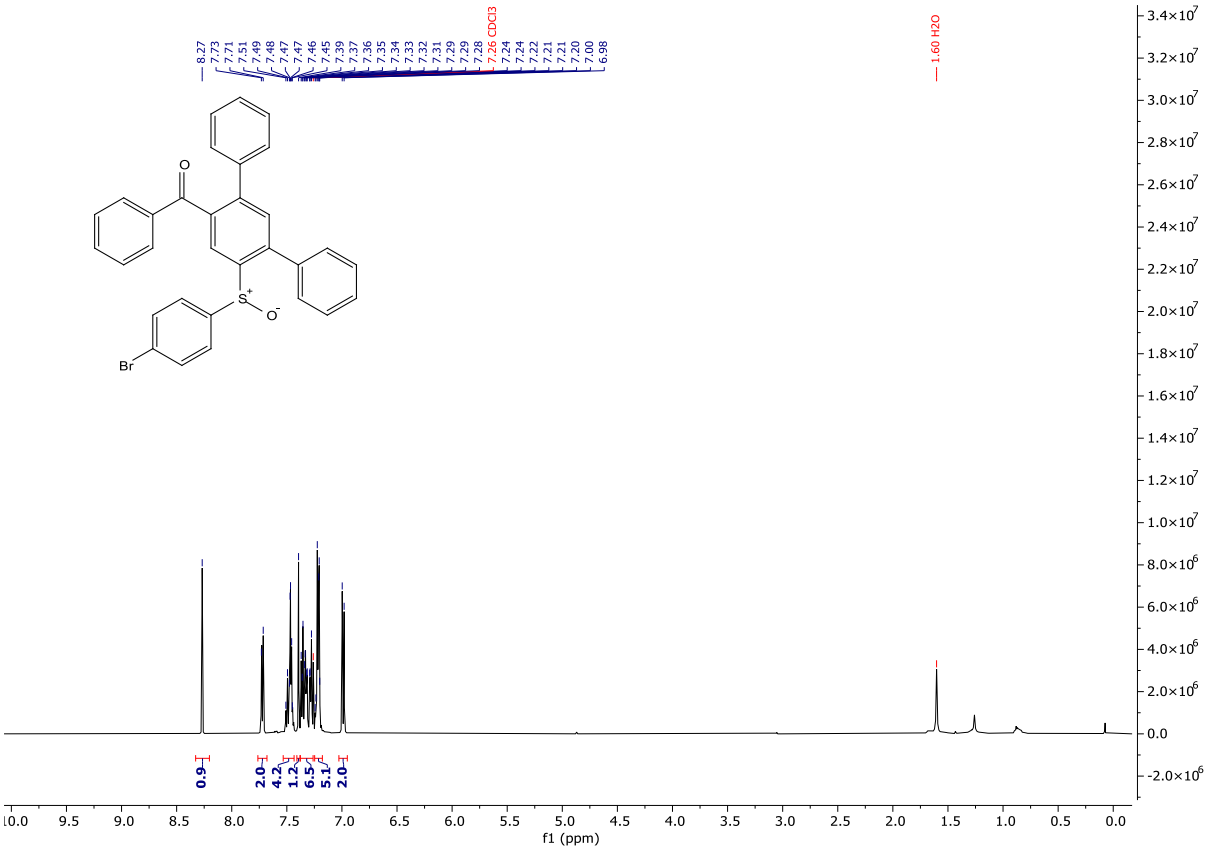

Figure 26. [1]H NMR (500 MHz, Chloroform-*d*) of compound **10l**.

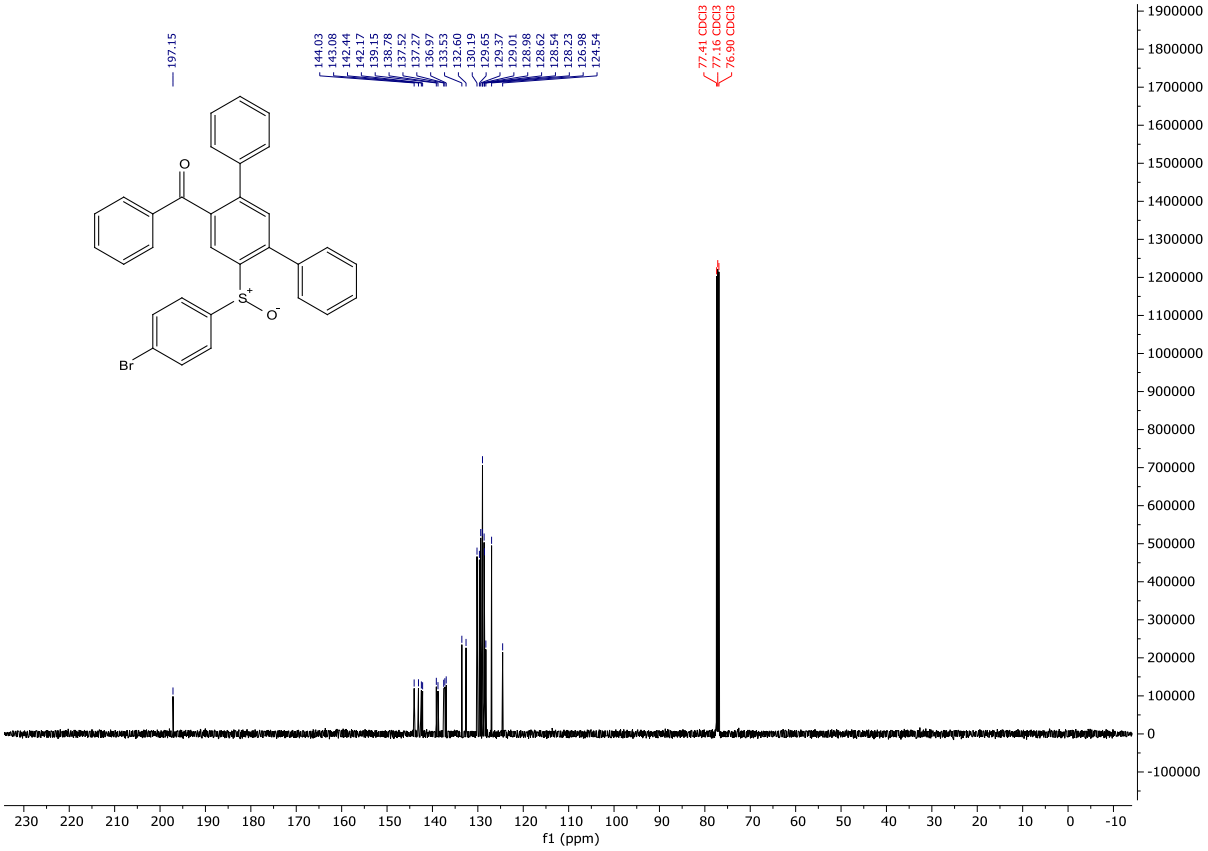

Figure 27. [13]C NMR (126 MHz, Chloroform-*d*) of compound **10l**.

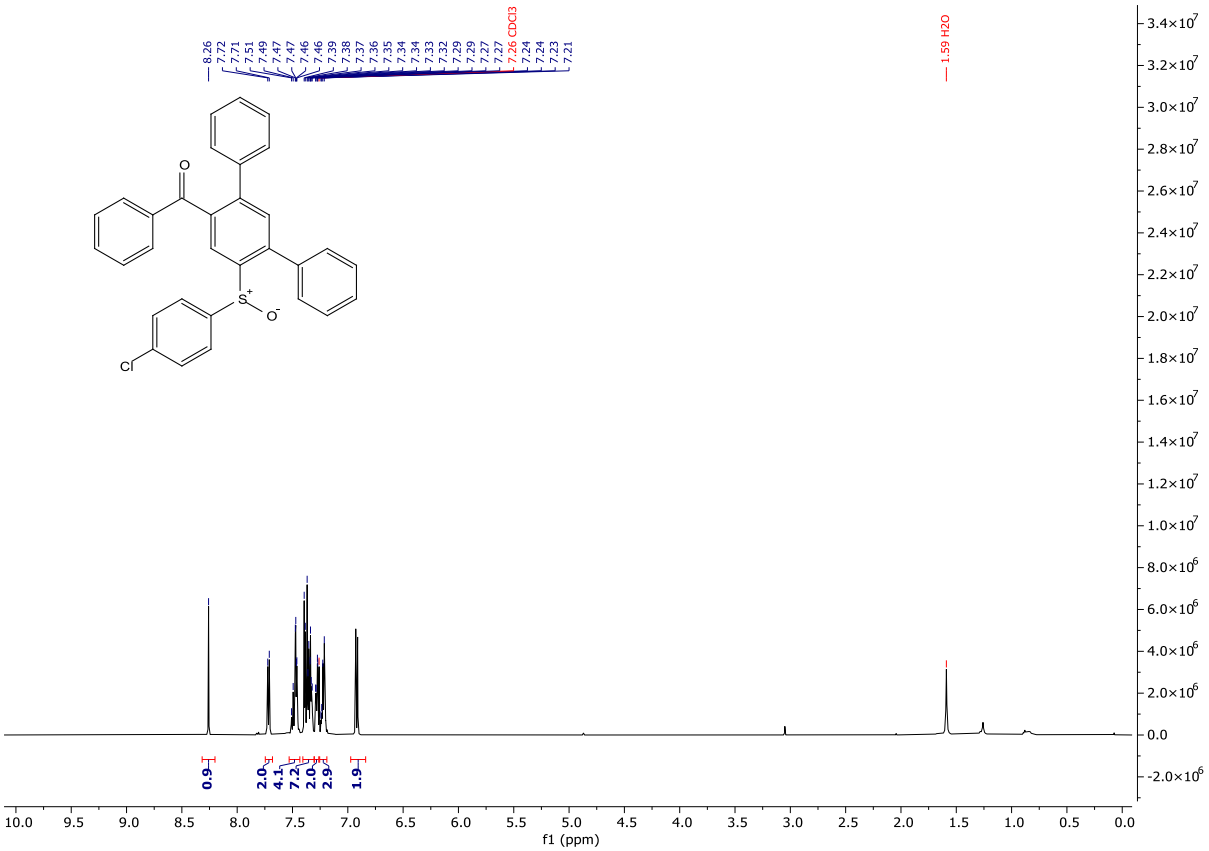

Figure 28. [1]H NMR (500 MHz, Chloroform-*d*) of compound **10m**.

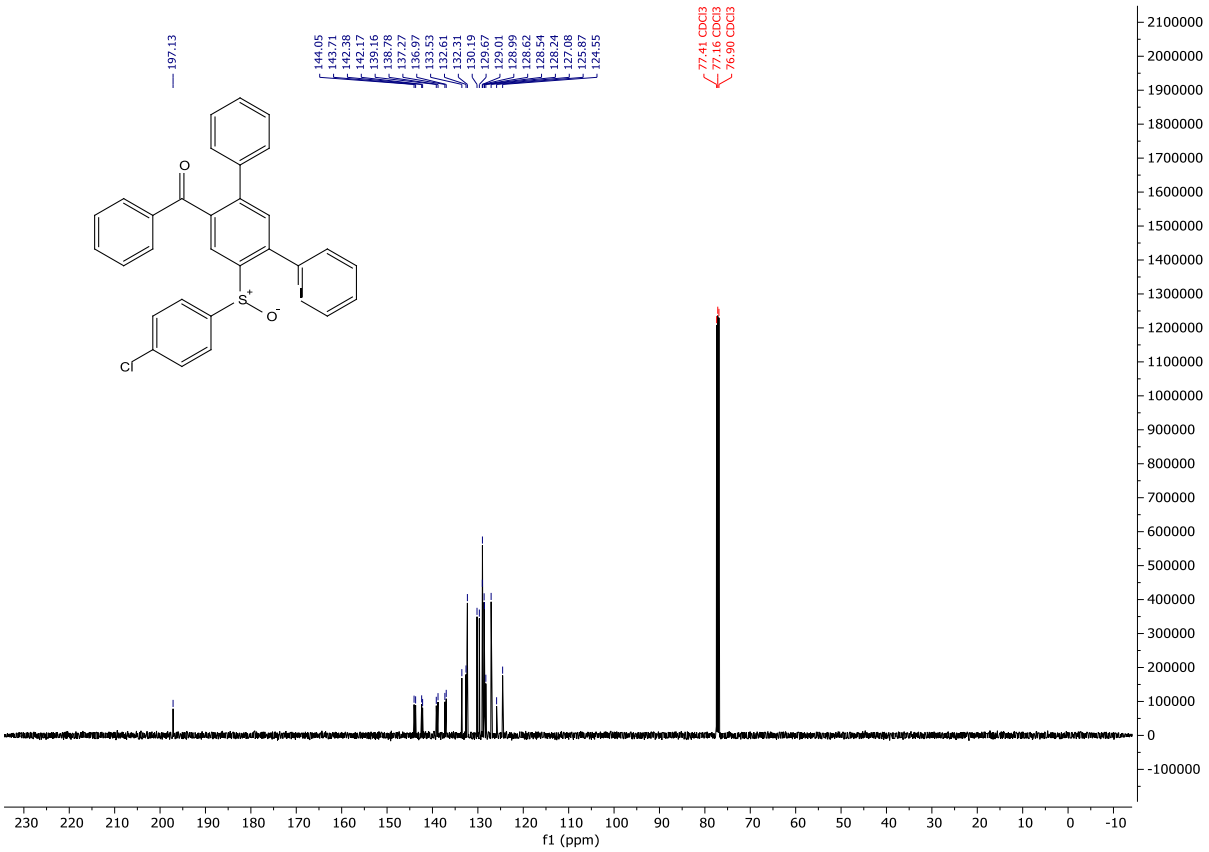

Figure 29. [13]C NMR (126 MHz, Chloroform-*d*) of compound **10m**.

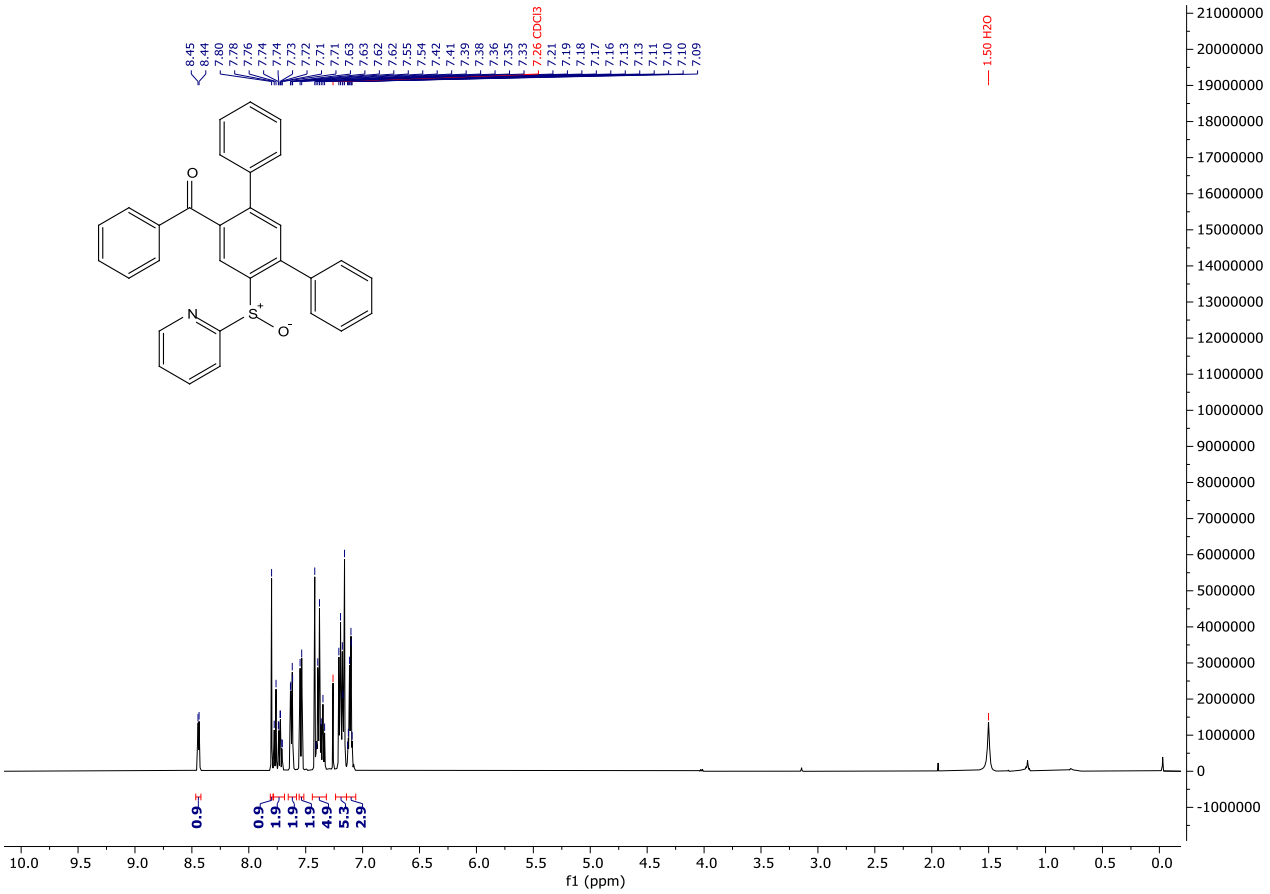

Figure 30. [1]H NMR (500 MHz, Chloroform-*d*) of compound **10n**.

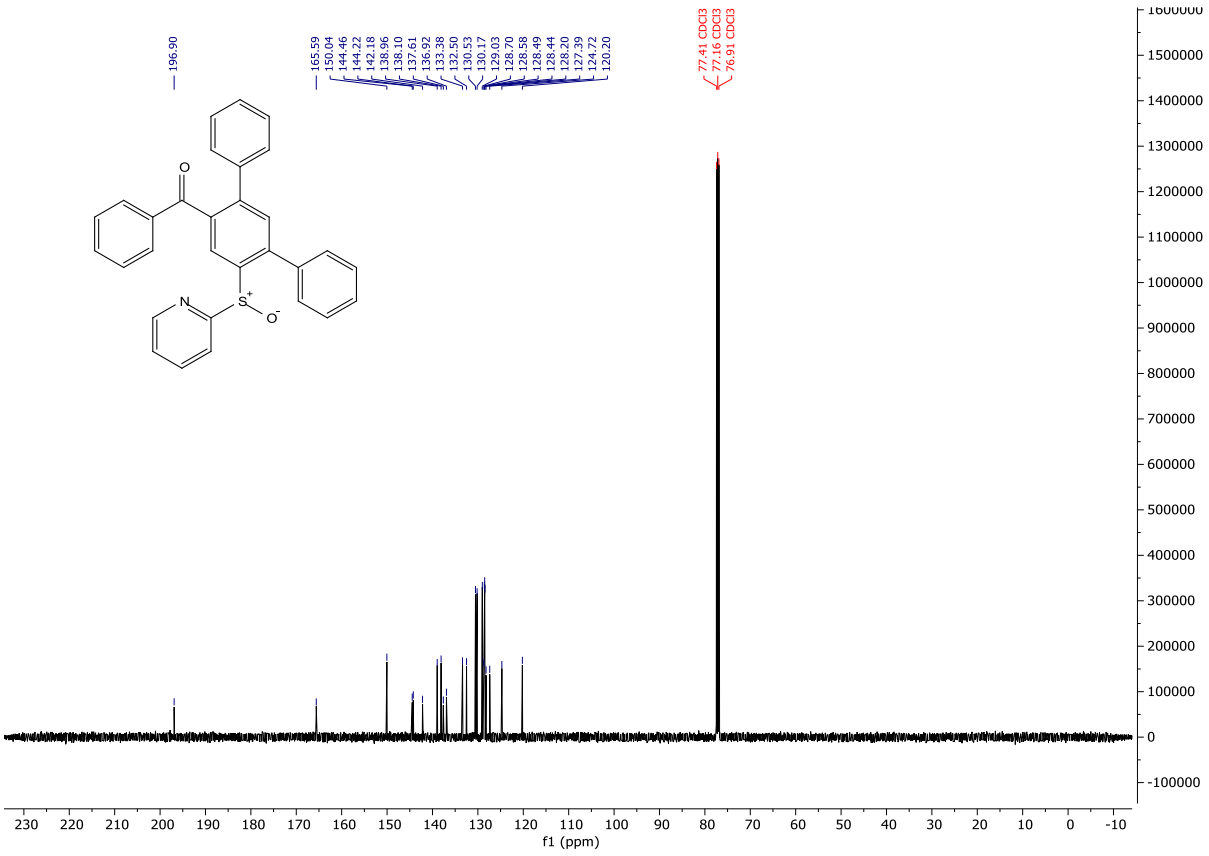

Figure 31. [13]C NMR (126 MHz, Chloroform-*d*) of compound **10n**.

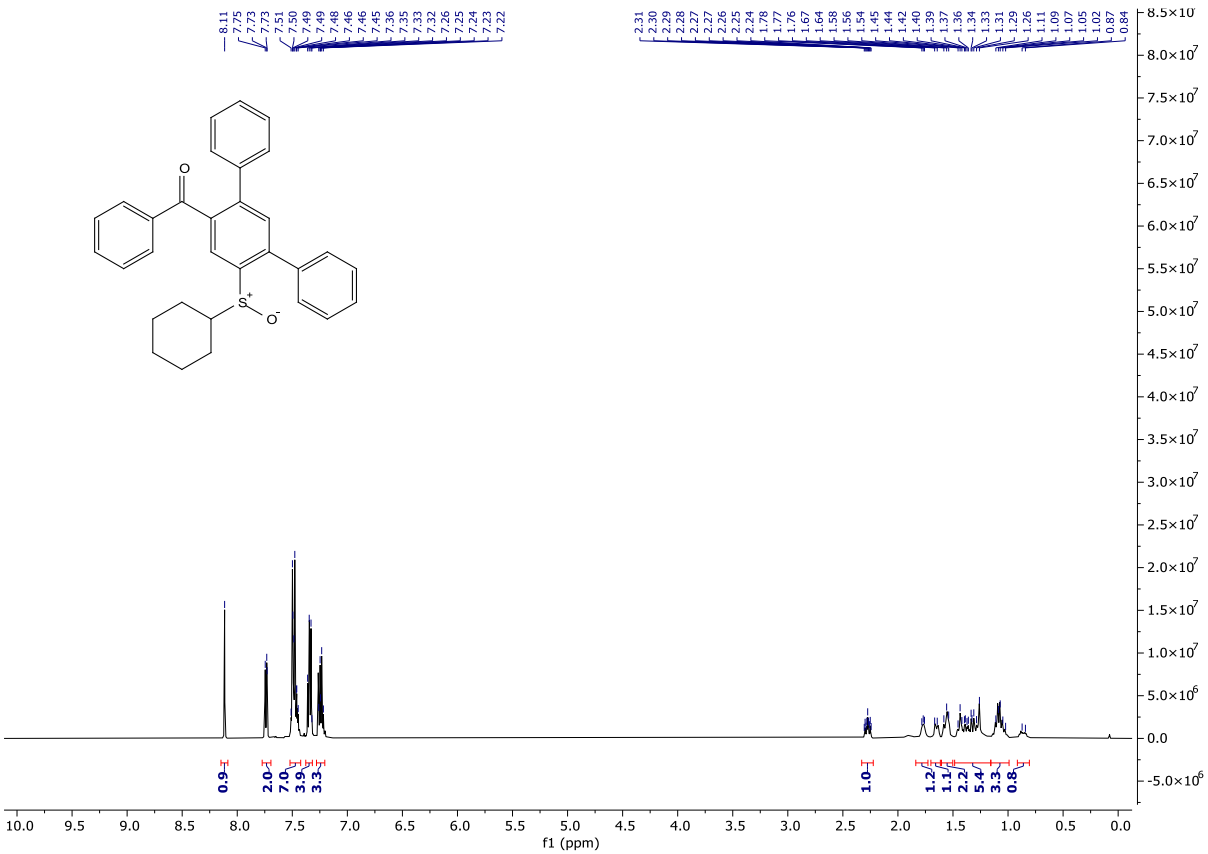

Figure 32. [1]H NMR (500 MHz, Chloroform-*d*) of compound **10o**.

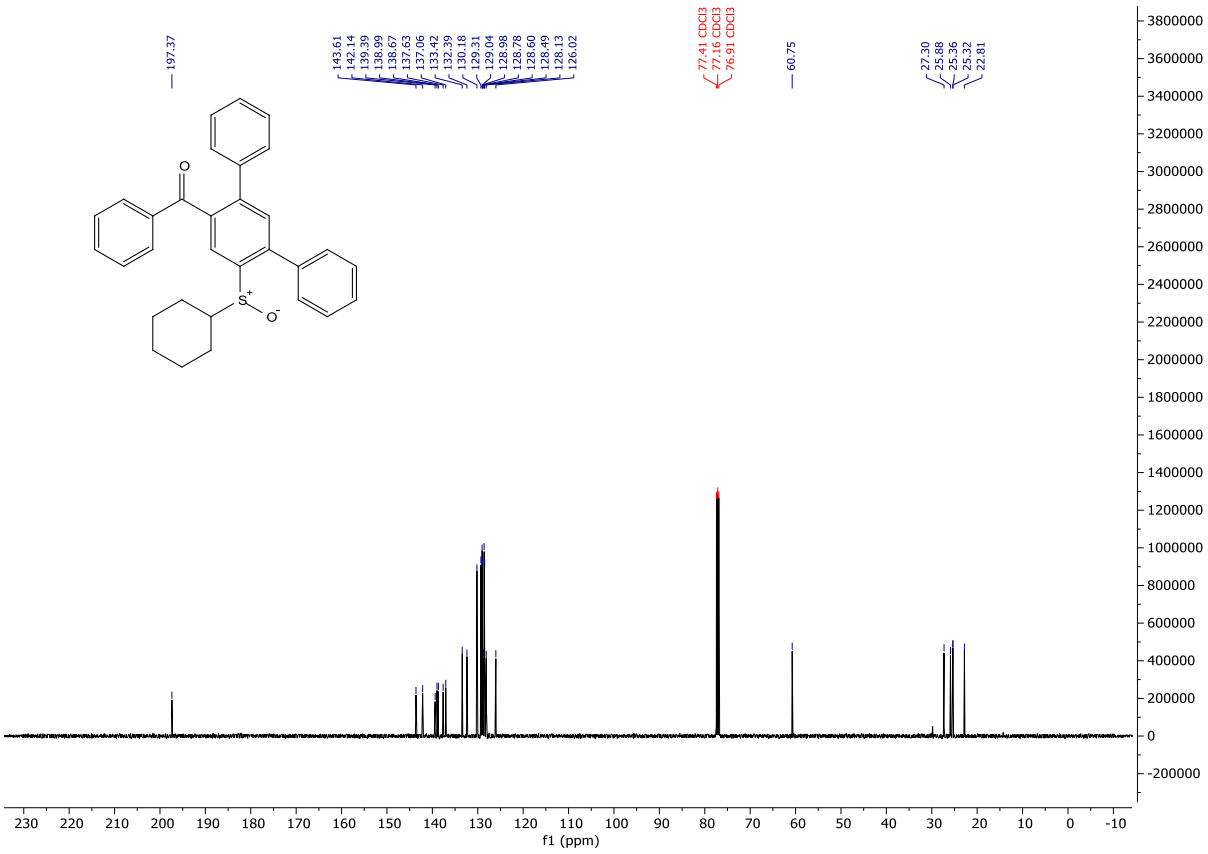

Figure 33. [13]C NMR (126 MHz, Chloroform-*d*) of compound **10o**.

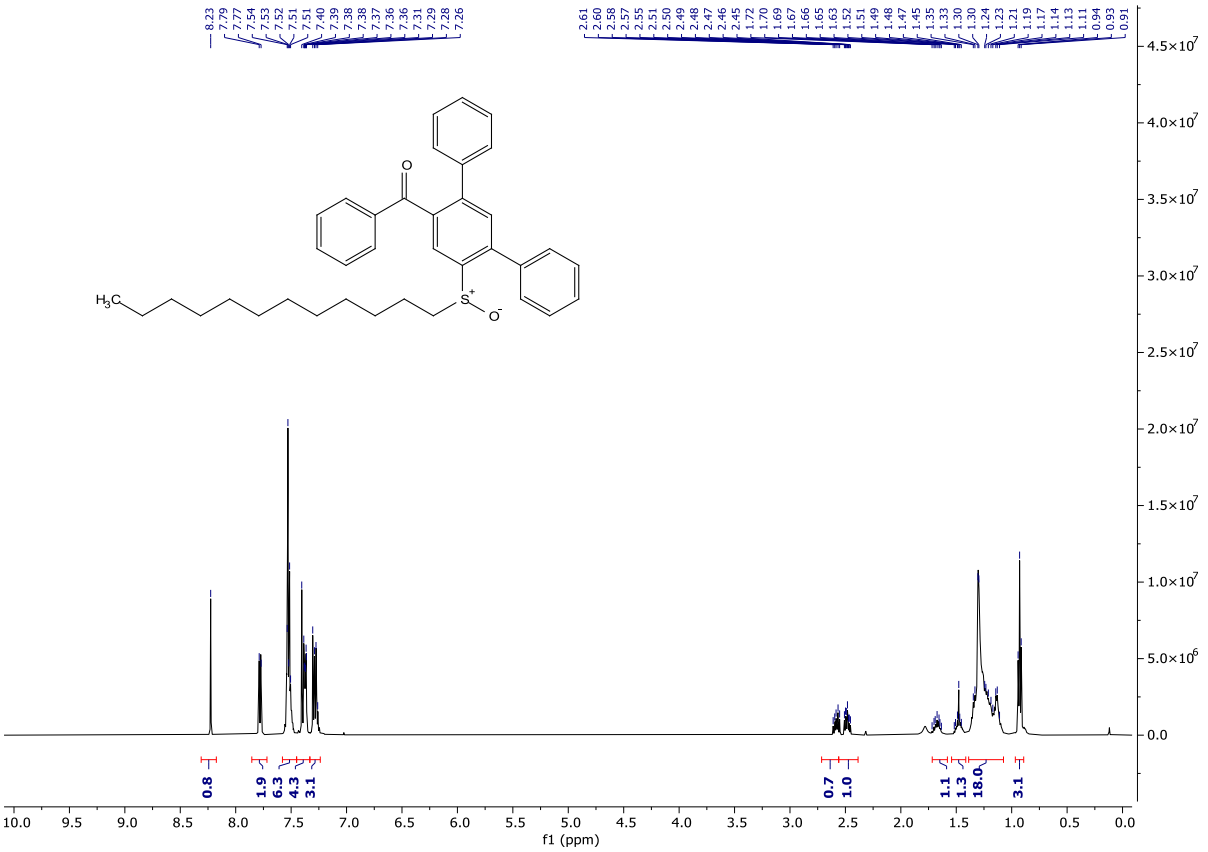

Figure 34. [1]H NMR (500 MHz, Chloroform-*d*) of compound **10p**.

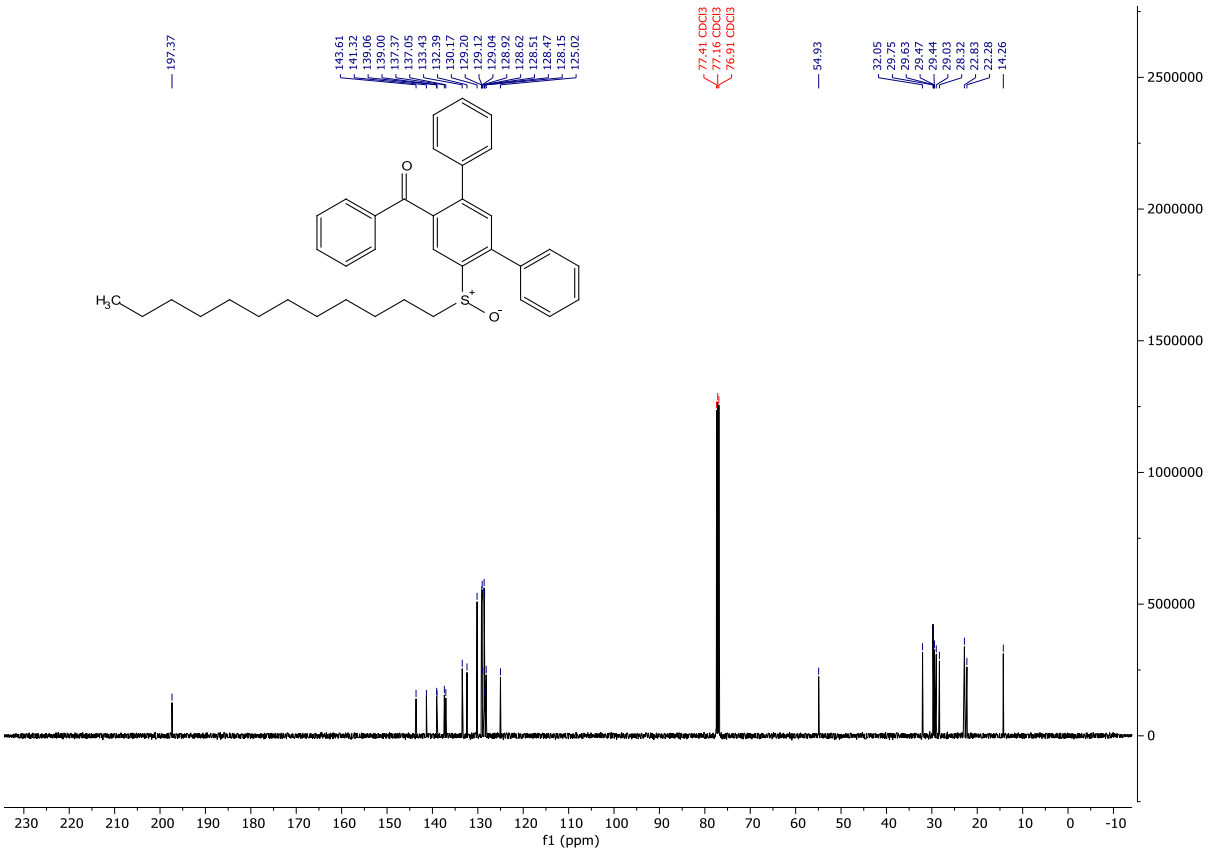

Figure 35. [13]C NMR (126 MHz, Chloroform-*d*) of compound **10p**.

Crystal structure data of compound 10a

Table 1: Crystallographic data

Molecular formula	$C_{32}H_{24}O_2S$
Space group	*P* $2_12_12_1$ (Nr. 19)
Crystal system	Orthorhombisch
Number of formula units, Z	4
Temperature/K	213,6(2)
a/pm	949,9(2)
b/pm	1464,9(3)
c/pm	1739,5(4)
$V/10^6$pm^3	2420,6(8)
Wave length/pm	71,073
Diffractometer	IPDS II, Fa. Stoe & Cie GmbH, Darmstadt
Number of measured reflexes	35706
Number of independent reflexes	6482
Number of refined parameters	319
$\delta_{min}/\delta_{max}$ (e/10^6pm^3)	-0,20/0,218
Absolute structure, flack parameter	1,09(10)
R_1 ($F_o > 4\ \sigma$)	0,0586
R_1 (all reflexes)	0,2697
wR_2	0,0728
GoF	0,753

Table 2: Position parameters and isotropic thermal deflection parameters. The standard deviations (in parentheses) refer to the last decimal place.

Atom	*x*/*a*	*y*/*b*	*z*/*c*	U_{iso}
S1	0,2774(2)	0,43277(7)	0,91833(8)	0,0464(4)
O2	0,4311(3)	0,4167(2)	0,9082(2)	0,060(1)
O3	0,4983(3)	0,7705(2)	0,0200(2)	0,064(1)
C1	0,1306(5)	0,5942(2)	0,0918(2)	0,034(1)
H1	0,0506	0,6006	0,1222	0,041
C4	0,2236(5)	0,5062(3)	0,8412(3)	0,038(1)
C5	0,2579(5)	0,5145(2)	0,9947(2)	0,032(1)
C6	0,2123(5)	0,8220(3)	0,1263(2)	0,039(1)
H6	0,2266	0,8328	0,0741	0,048
C7	0,4859(5)	0,7072(3)	0,0649(3)	0,040(1)
C8	0,2782(5)	0,5776(3)	0,7227(3)	0,050(2)
H8	0,3434	0,5909	0,6844	0,060
C9	0,2408(5)	0,6550(2)	0,1012(2)	0,029(1)
C10	0,7197(5)	0,7376(3)	0,1206(3)	0,046(2)
H10	0,7345	0,7795	0,0812	0,055
C11	0,1450(6)	0,6086(3)	0,7154(3)	0,043(1)
C12	0,2222(5)	0,7336(3)	0,1548(3)	0,035(1)
C13	0,0093(5)	0,4653(3)	0,0284(2)	0,033(1)
C14	0,1362(5)	0,5237(3)	0,0381(2)	0,033(1)
C15	0,3198(5)	0,5269(3)	0,7850(3)	0,044(2)
H15	0,4123	0,5068	0,7891	0,053
C16	0,8232(5)	0,7238(3)	0,1751(3)	0,0510(2)

H16	0,9078	0,7556	0,1720	0,061
C17	0,5951(5)	0,6901(3)	0,1239(3)	0,035(1)
C18	0,3630(5)	0,6434(3)	0,0591(2)	0,033(1)
C19	0,0181(5)	0,3703(3)	0,0264(2)	0,039(1)
H19	0,1049	0,3418	0,0323	0,047
C20	-0,1021(5)	0,3185(3)	0,0158(3)	0,049(2)
H20	-0,0956	0,2551	0,0144	0,058
C21	-0.1208(5)	0,05046(3)	0,0220(2)	0,043(1)
H21	-0,1288	0,5677	0,0253	0,052
C22	0,2015(5)	0,7192(3)	0,2319(3)	0,047(2)
H22	0,2054	0,6603	0,2517	0,056
C23	0,8007(5)	0,6631(3)	0,2339(3)	0,060(2)
H23	0,8692	0,6549	0,2716	0,072
C24	0,0480(5)	0,5900(3)	0,7729(3)	0,054(2)
H24	-0,0434	0,6124	0,7697	0,064
C25	0,1745(5)	0,7929(3)	0,2809(3)	0,057(2)
H25	0,1643	0,7829	0,3334	0,069
C26	0,1814(5)	0,8937(3)	0,1745(3)	0,055(2)
H26	0,1729	0,9524	0,1547	0,066
C27	0,0891(5)	0,5383(3)	0,8345(3)	0,048(2)
H27	0,0238	0,5246	0,8727	0,058
C28	-0,2402(5)	0,4527(3)	0,0108(3)	0,058(2)
H28	-0.3273	0,4810	0,0056	0,070
C29	0,6766(6)	0,6141(3)	0,2374(3)	0,065(2)
H29	0,6620	0,5721	0,2767	0,077
C30	0,3694(4)	0,5739(3)	0,0054(2)	0,035(1)
H30	0,4503	0,5669	0,9759	0,042
C31	0,5743(5)	0,6280(3)	0,1821(2)	0,048(2)
H31	0,4907	0,5951	0,1843	0,058
C32	0,0969(5)	0,6654(3)	0,6474(3)	0,075(2)
H32A	0,1448	0,6453	0,6018	0,112
H32B	0,1183	0,7285	0,6567	0,112
H32C	-0,0028	0,6583	0,6406	0,112
C33	-0,2303(6)	0,3598(3)	0,0074(3)	0,059(2)
H33	-0,3106	0,3246	0,9994	0,071
C34	0,1629(5)	0,8789(3)	0,2525(3)	0,054(2)
H34	0,1428	0,9275	0,2851	0,065