Dibenzo[*d,d'*]benzo[2,1-*b*:3,4-*b'*]difurans with extended π-conjugated chains: the synthetic approach and some properties

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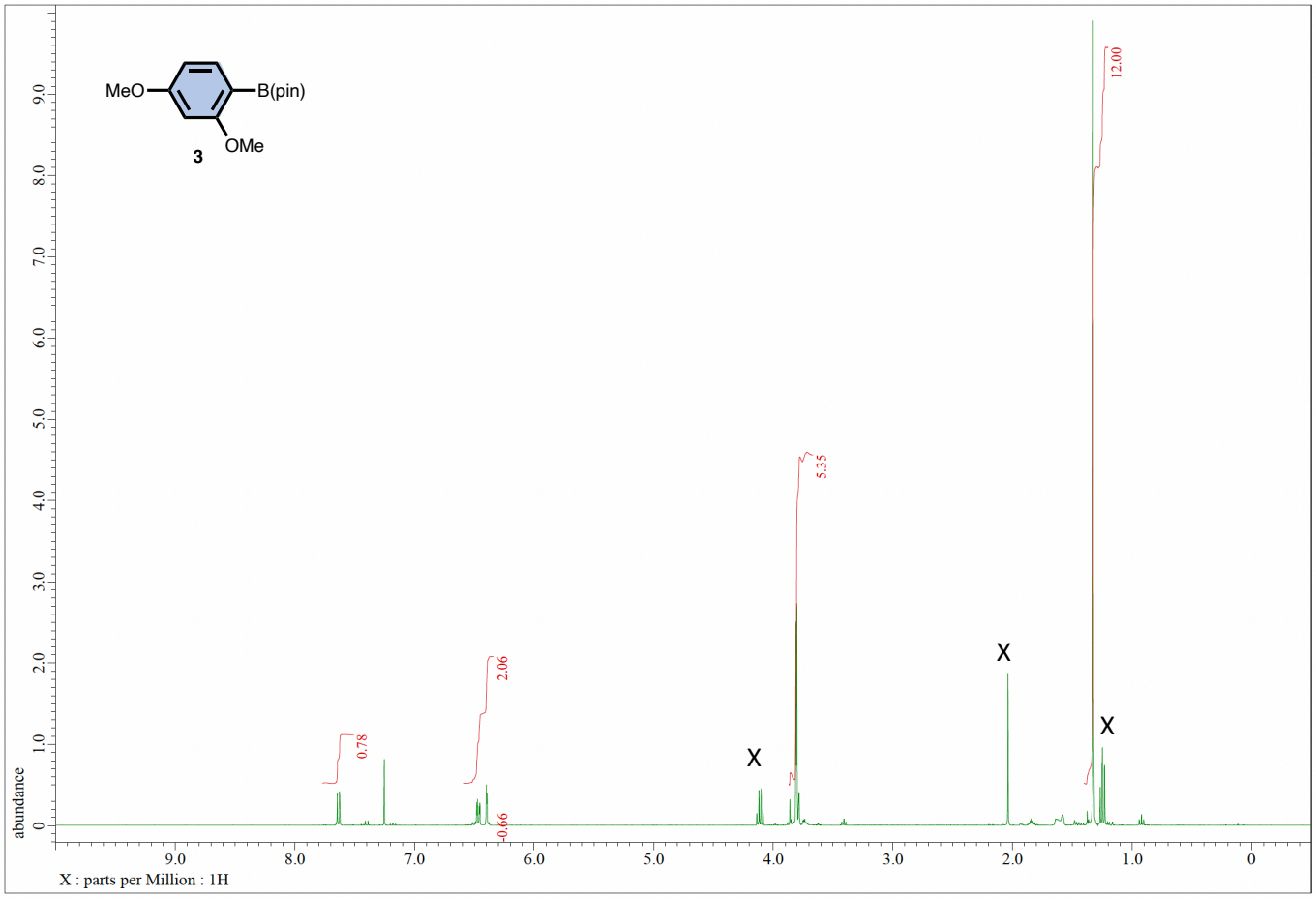

Figure S1. ^{1}H NMR Spectrum of 2-(2,4-dimethoxyphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**3**) (400 MHz, $CDCl_3$, r.t.). Xs indicate incorporated ethyl acetate.

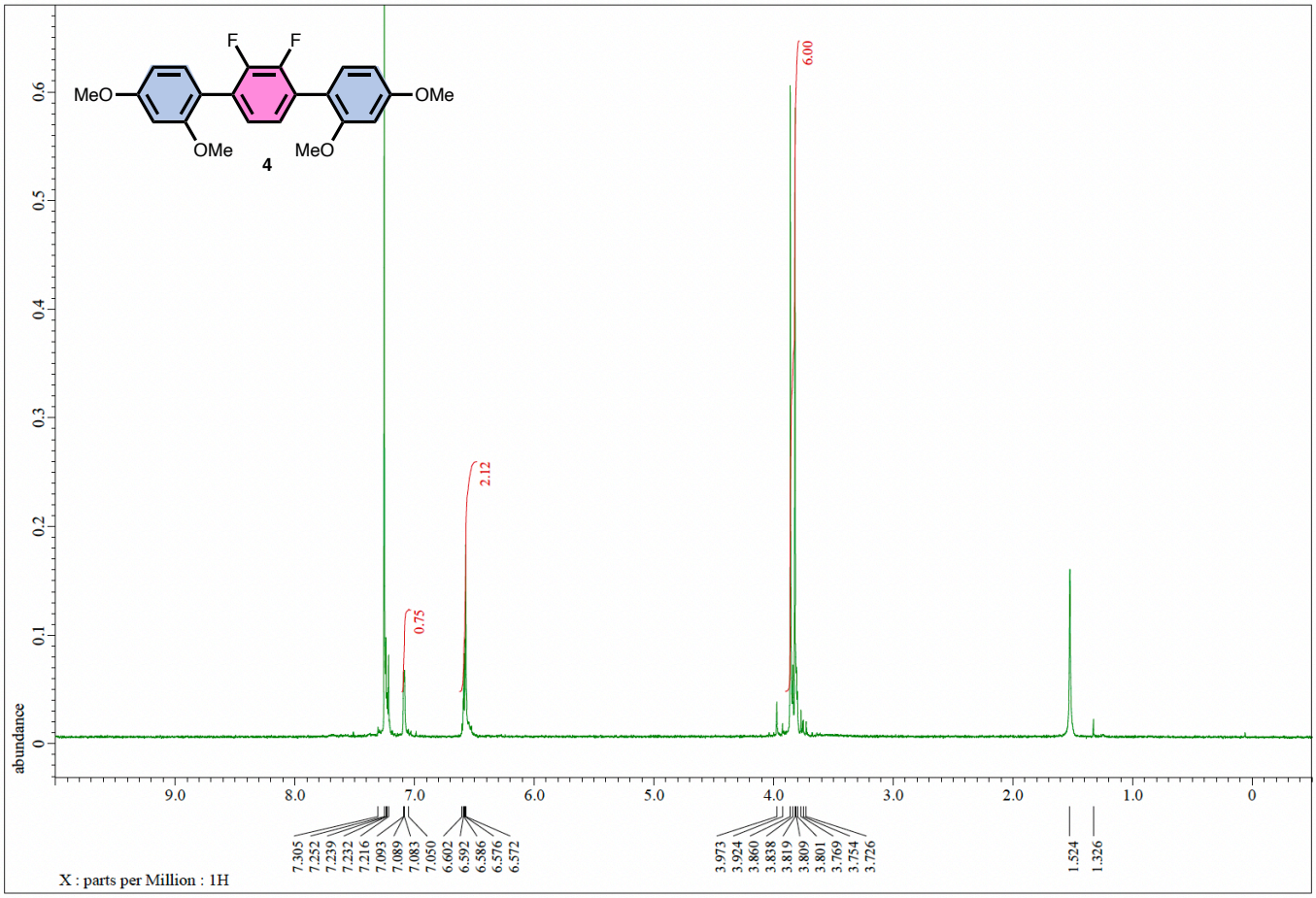

Figure S2. ^{1}H NMR Spectrum of 2,3-difluoro-1,4-bis(2,4-dimethoxyphenyl)benzene (**4**) (400 MHz, $CDCl_3$, r.t.).

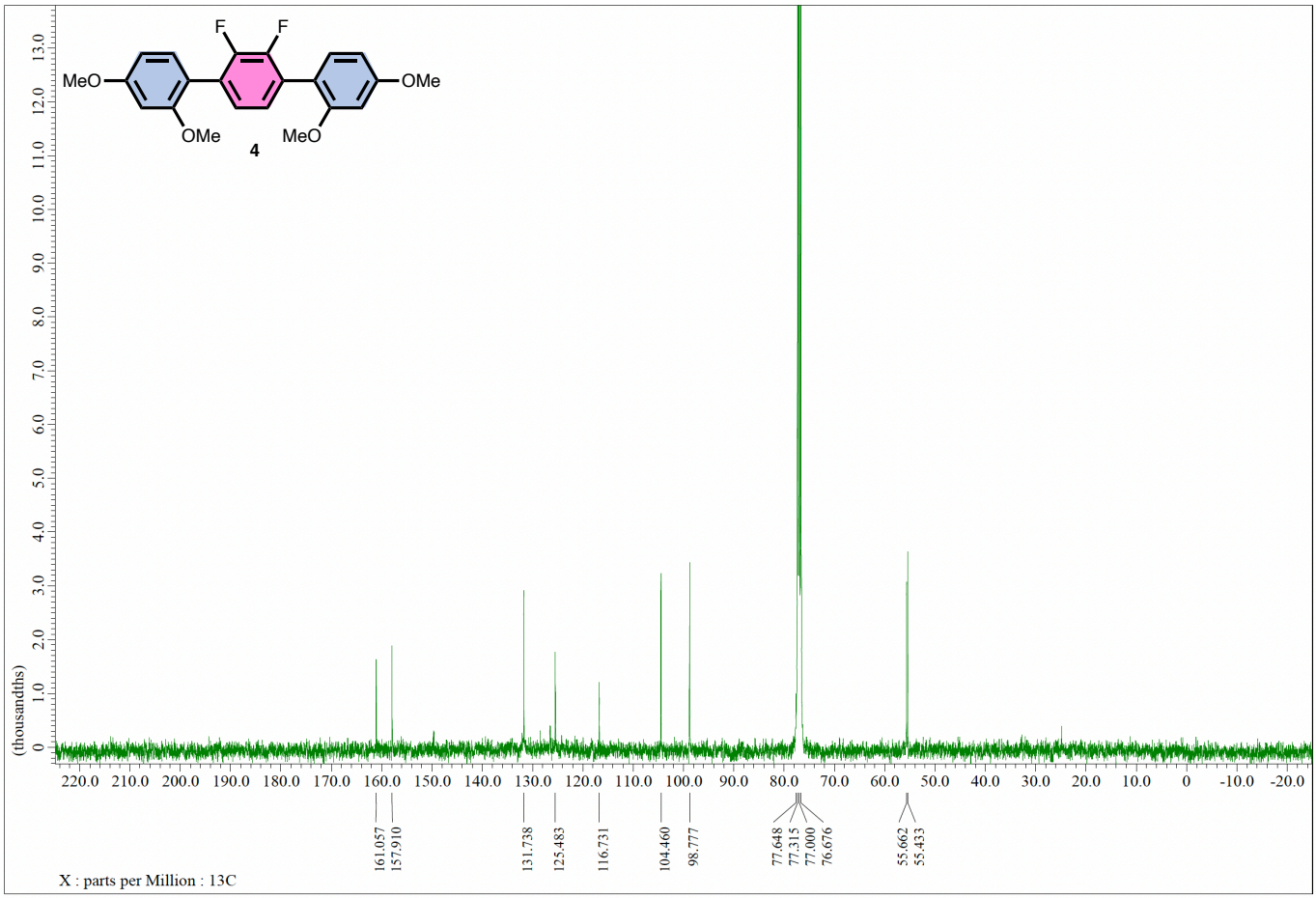

Figure S3. $^{13}C\{^{1}H\}$ NMR Spectrum of 2,3-difluoro-1,4-bis(2,4-dimethoxyphenyl)benzene (**4**) (100 MHz, $CDCl_3$, r.t.).

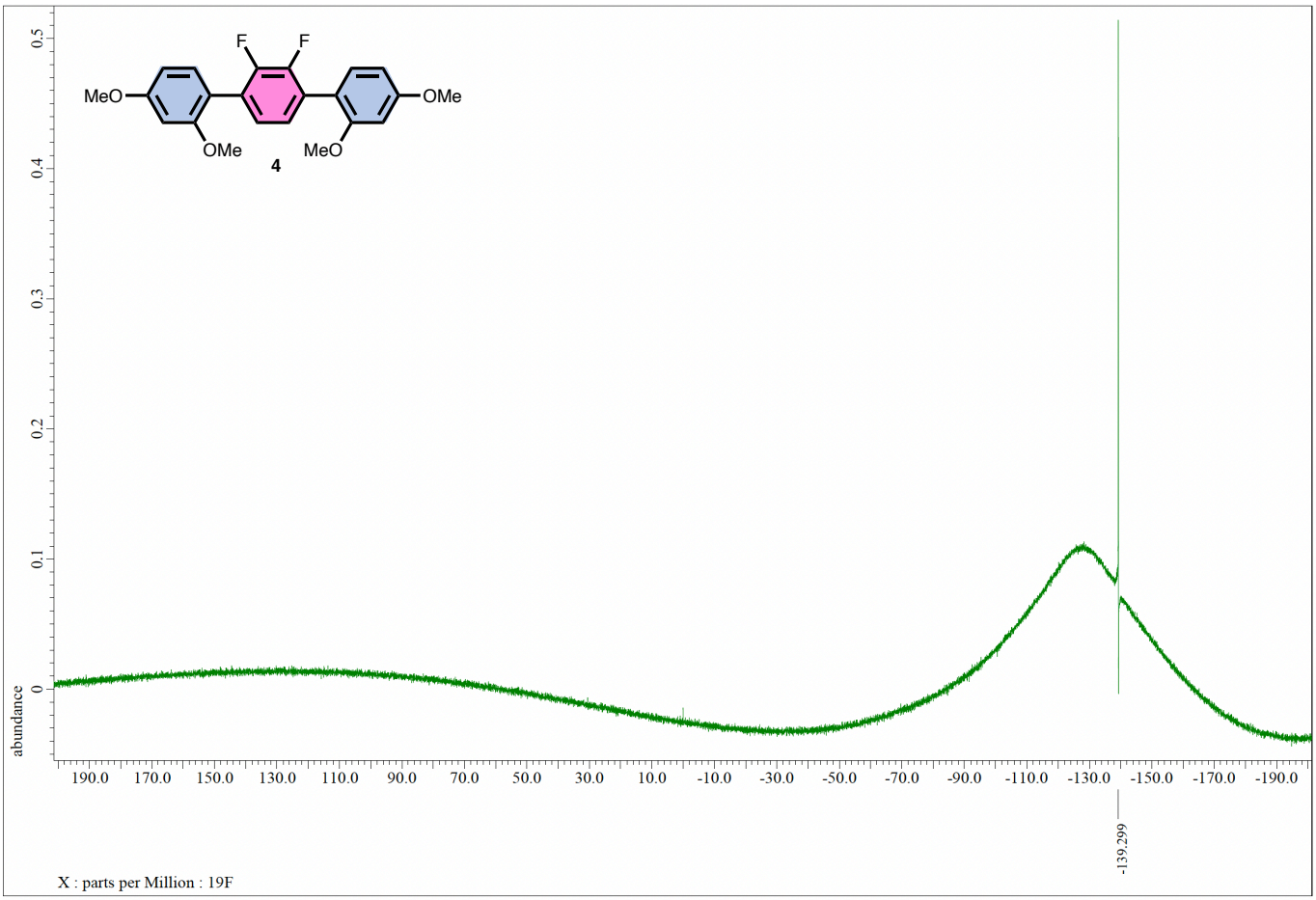

Figure S4. ^{19}F NMR Spectrum of 2,3-difluoro-1,4-bis(2,4-dimethoxyphenyl)benzene (**4**) (376 MHz, $CDCl_3$, r.t.).

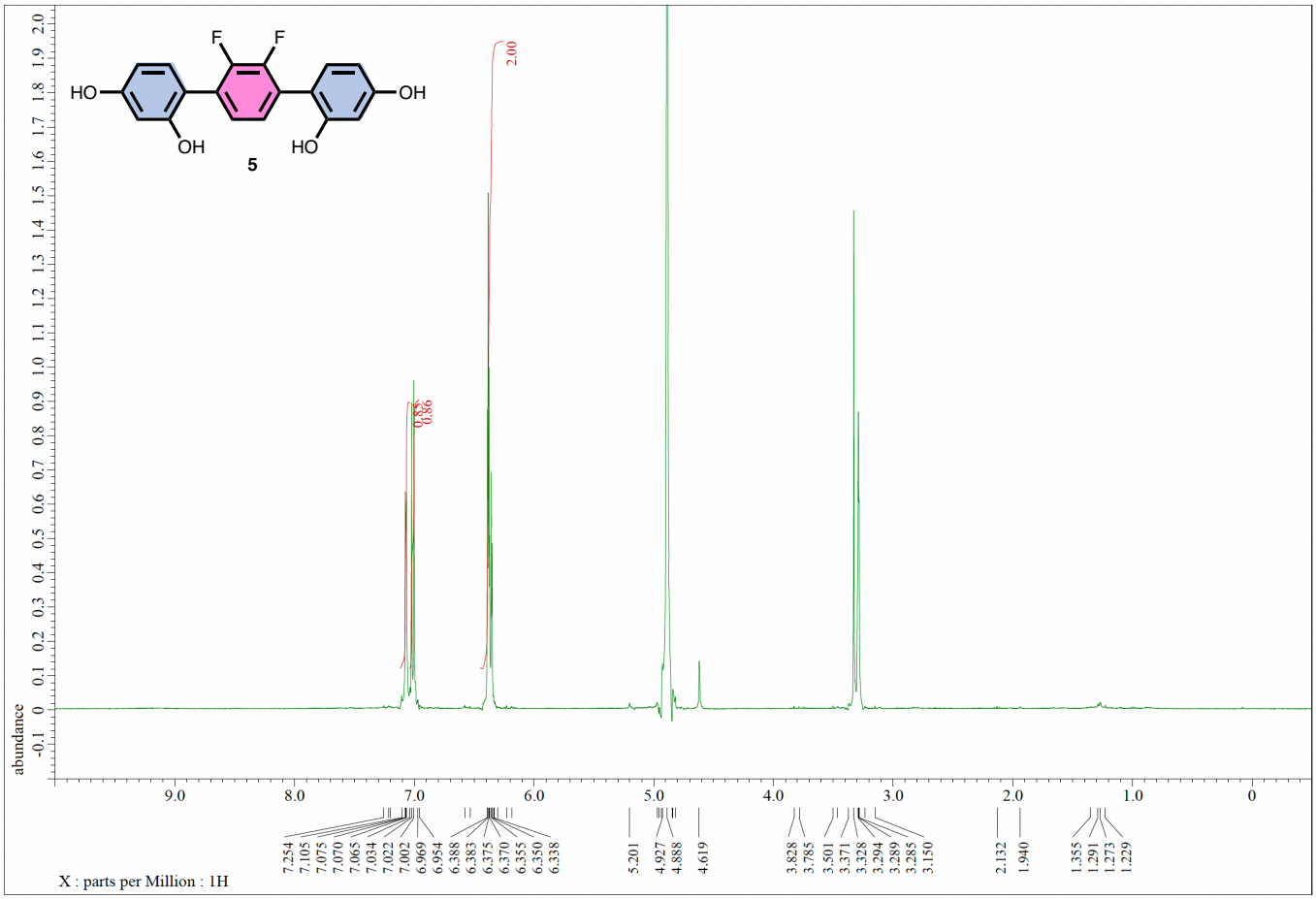

Figure S5. ^{1}H NMR Spectrum of 2,3-difluoro-1,4-bis(2,4-dihydroxyphenyl)benzene (**5**) (400 MHz, CD_3OD, r.t.).

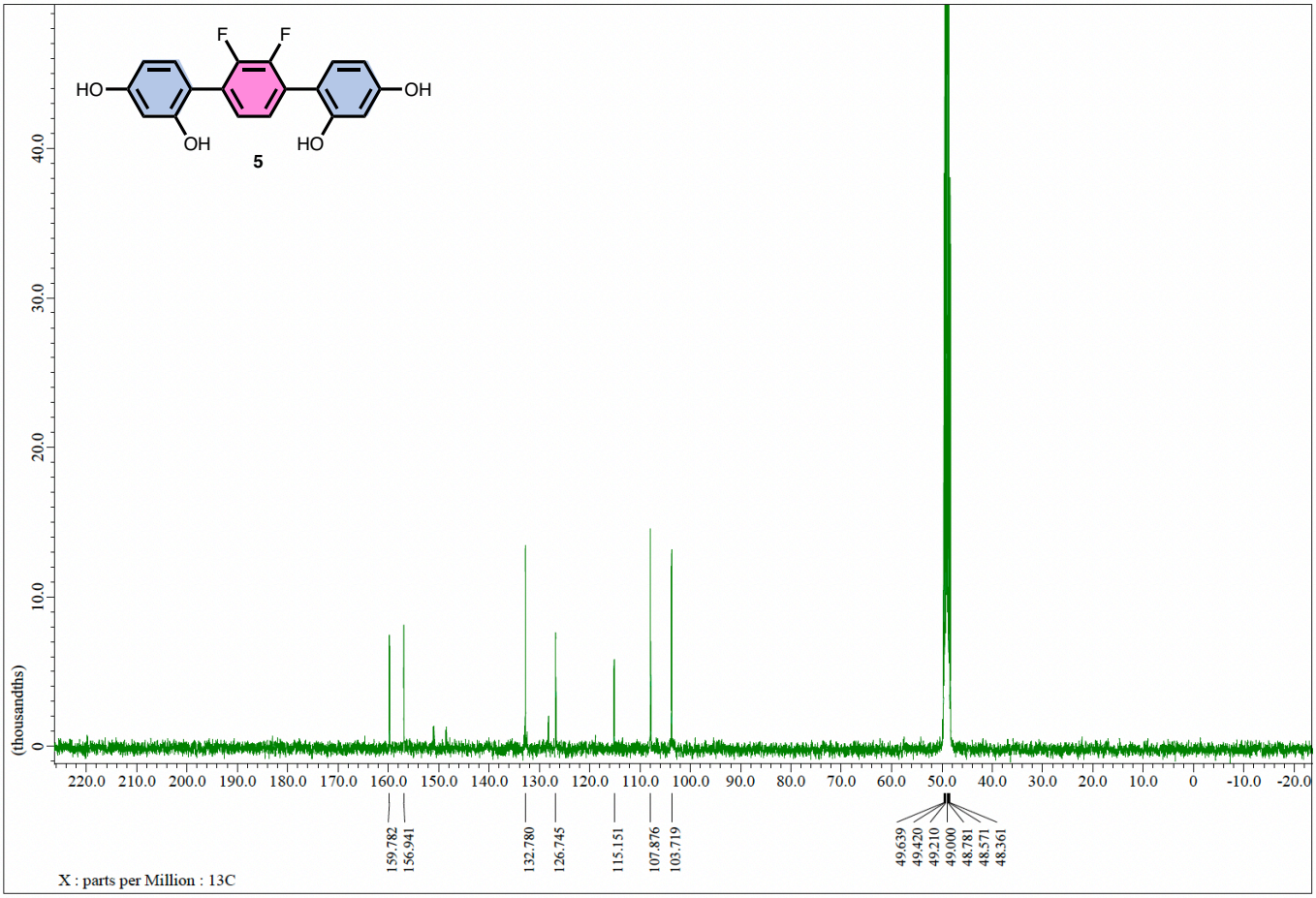

Figure S6. $^{13}C\{^{1}H\}$ NMR Spectrum of 2,3-difluoro-1,4-bis(2,4-dihydroxyphenyl)benzene (**5**) (100 MHz, CD_3OD, r.t.).

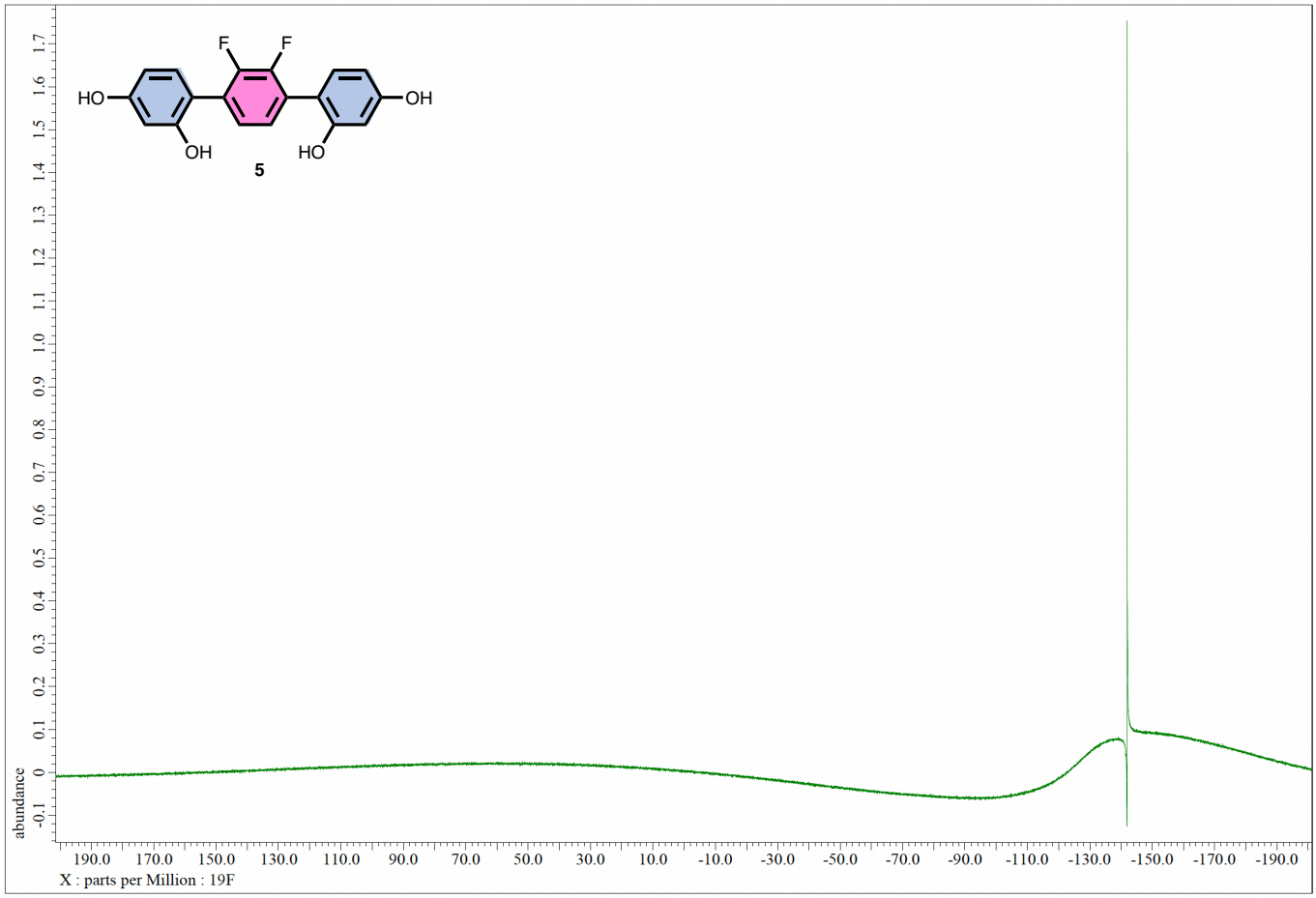

Figure S7. ^{19}F NMR Spectrum of 2,3-difluoro-1,4-bis(2,4-dihydroxyphenyl)benzene (**5**) (376 MHz, CD_3OD, r.t.).

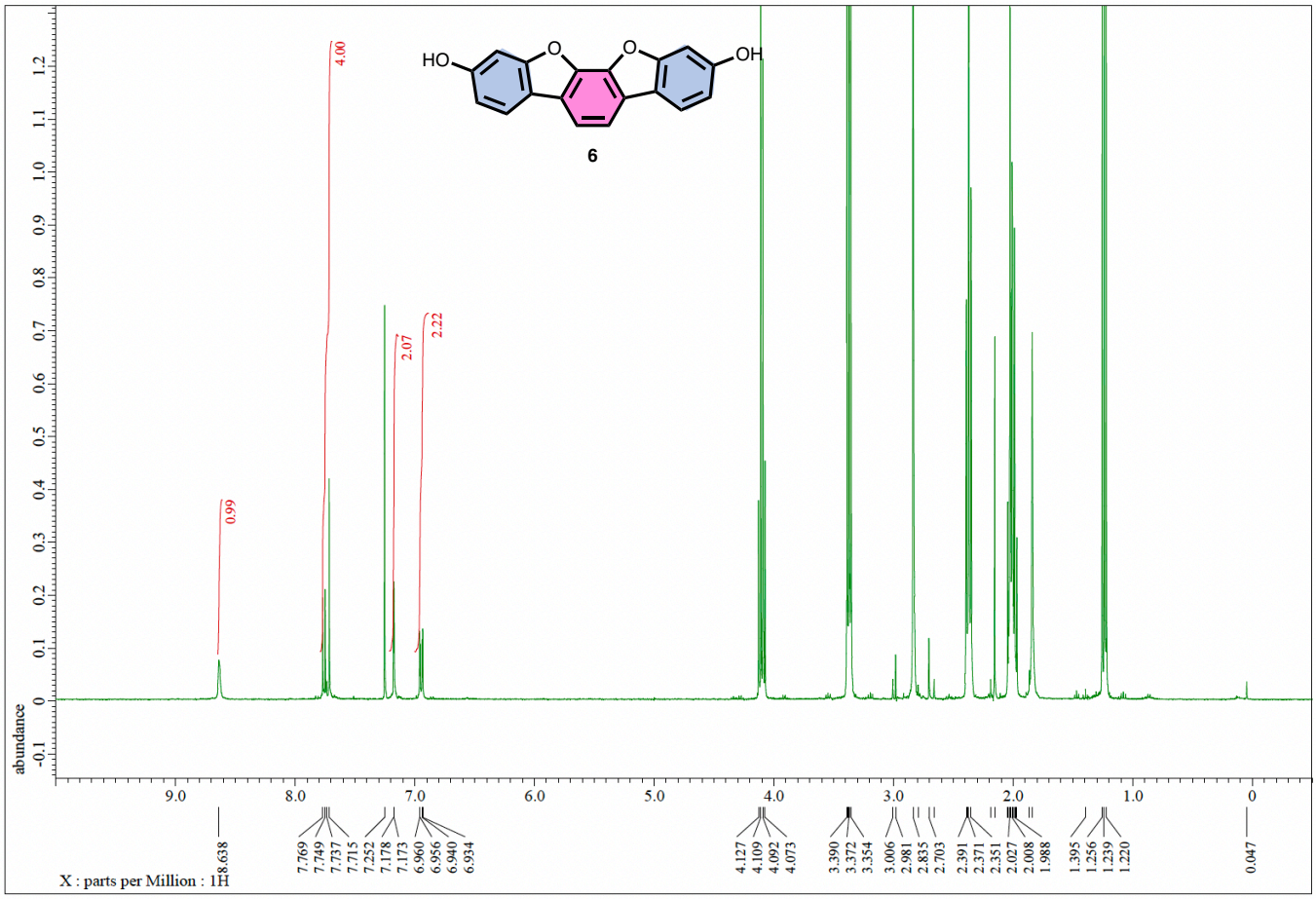

Figure S8. ^{1}H NMR Spectrum of dibenzo[*d,d'*]benzo[2,1-*b*:3,4-*b'*]difuran-3,8-diol (**6**) (400 MHz, $CDCl_3$, r.t.).

Because of low solubility, the incorporated solvent resonances were also observed.

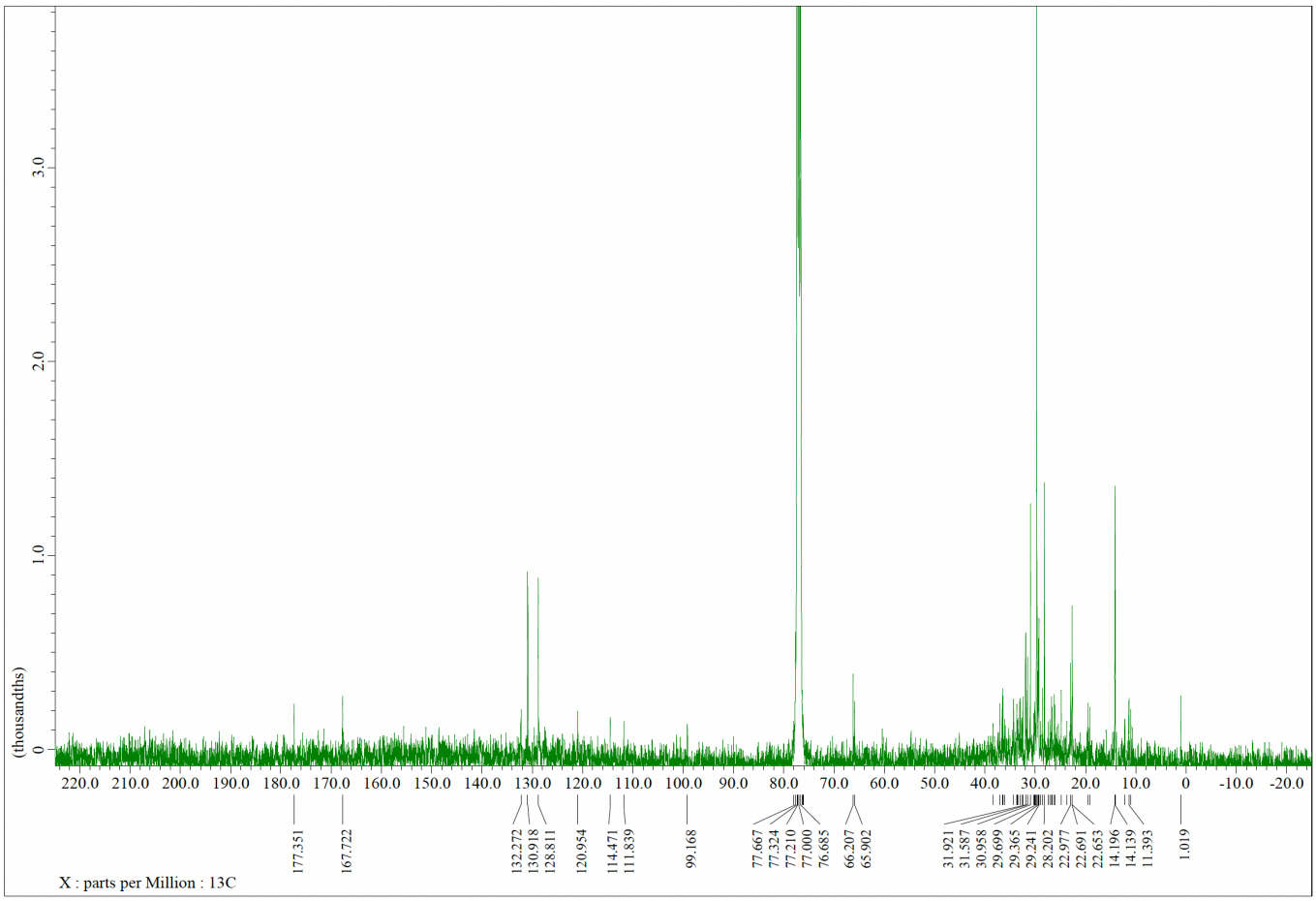

Figure S9. $^{13}C\{^{1}H\}$ NMR Spectrum of dibenzo[*d,d'*]benzo[2,1-*b*:3,4-*b'*]difuran-3,8-diol (**6**) (100 MHz, $CDCl_3$, r.t.).

Because compound shows low solubility to the solvent, impurities were found in the aliphatic region.

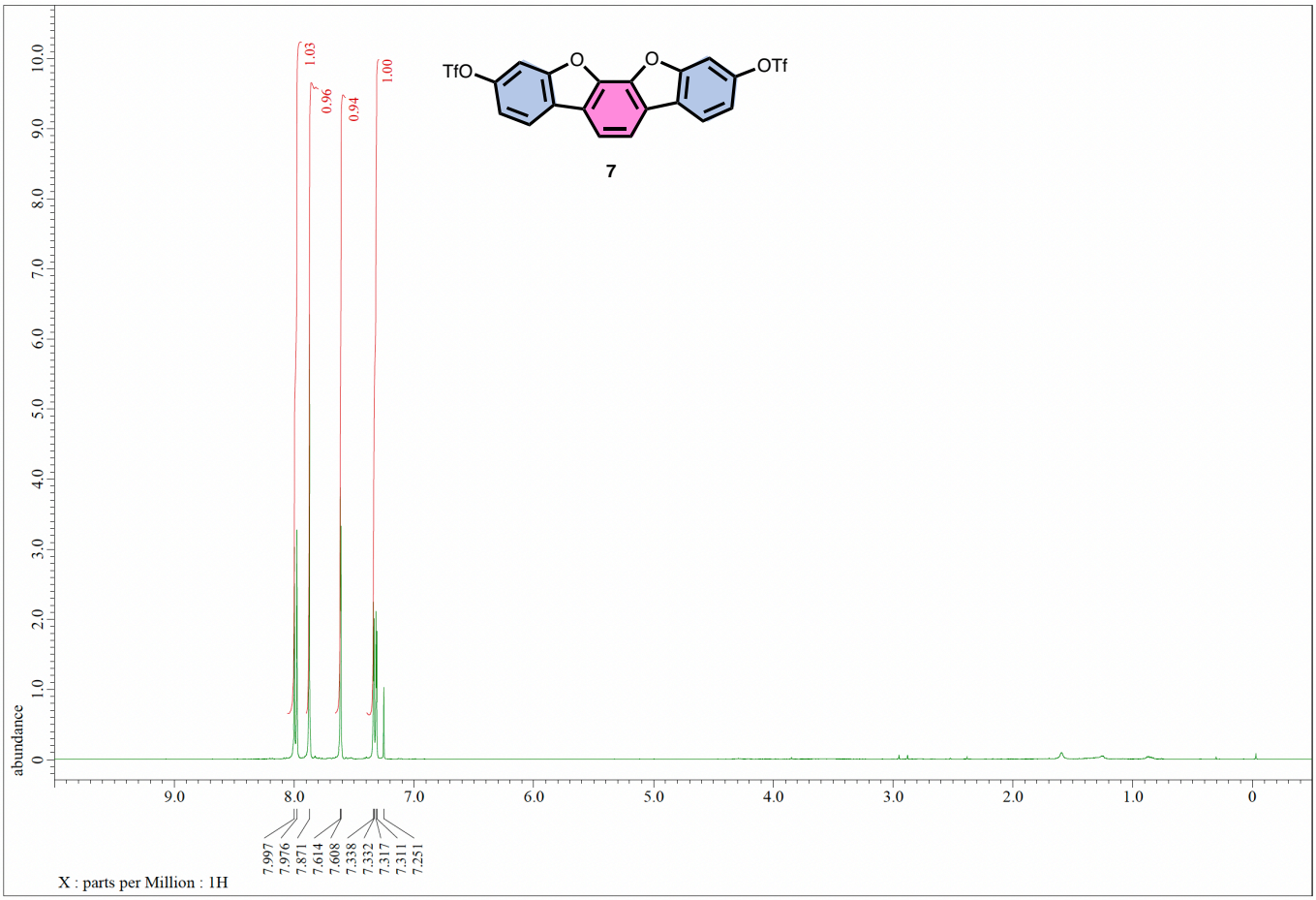

Figure S10. ^{1}H NMR Spectrum of dibenzo[*d,d'*]benzo[2,1-*b*:3,4-*b'*]difuran-3,8-diyltrifluoromethanesulfonate (**7**) (400 MHz, $CDCl_3$, r.t.).

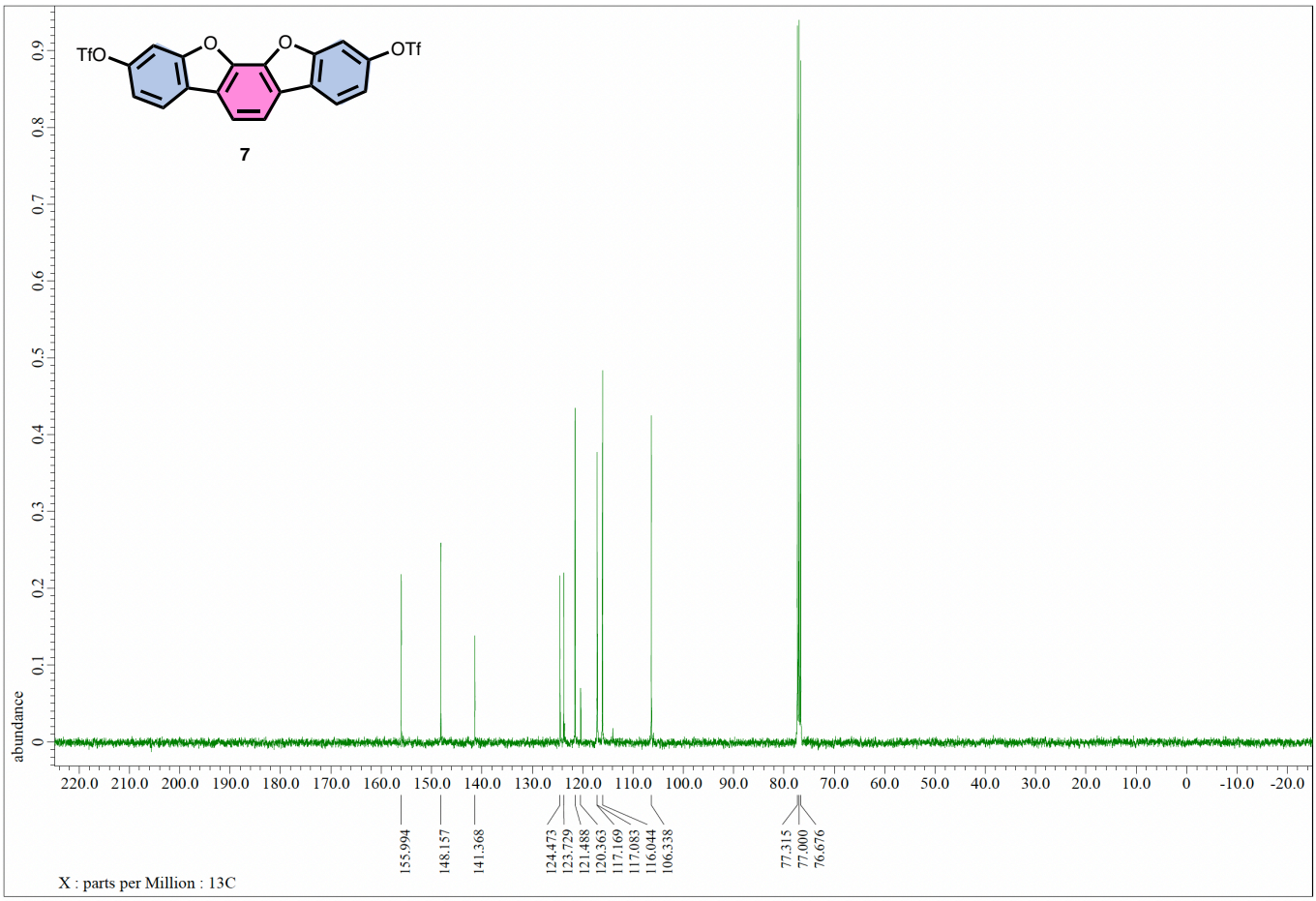

Figure S11. $^{13}C\{^{1}H\}$ NMR Spectrum of dibenzo[*d,d'*]benzo[2,1-*b*:3,4-*b'*]difuran-3,8-diyltrifluoromethanesulfonate (**7**) (100 MHz, $CDCl_3$, r.t.).

Figure S12. ^{19}F NMR Spectrum of dibenzo[*d,d'*]benzo[2,1-*b*:3,4-*b'*]difuran-3,8-diyltrifluoromethanesulfonate (**7**) (376 MHz, $CDCl_3$, r.t.).

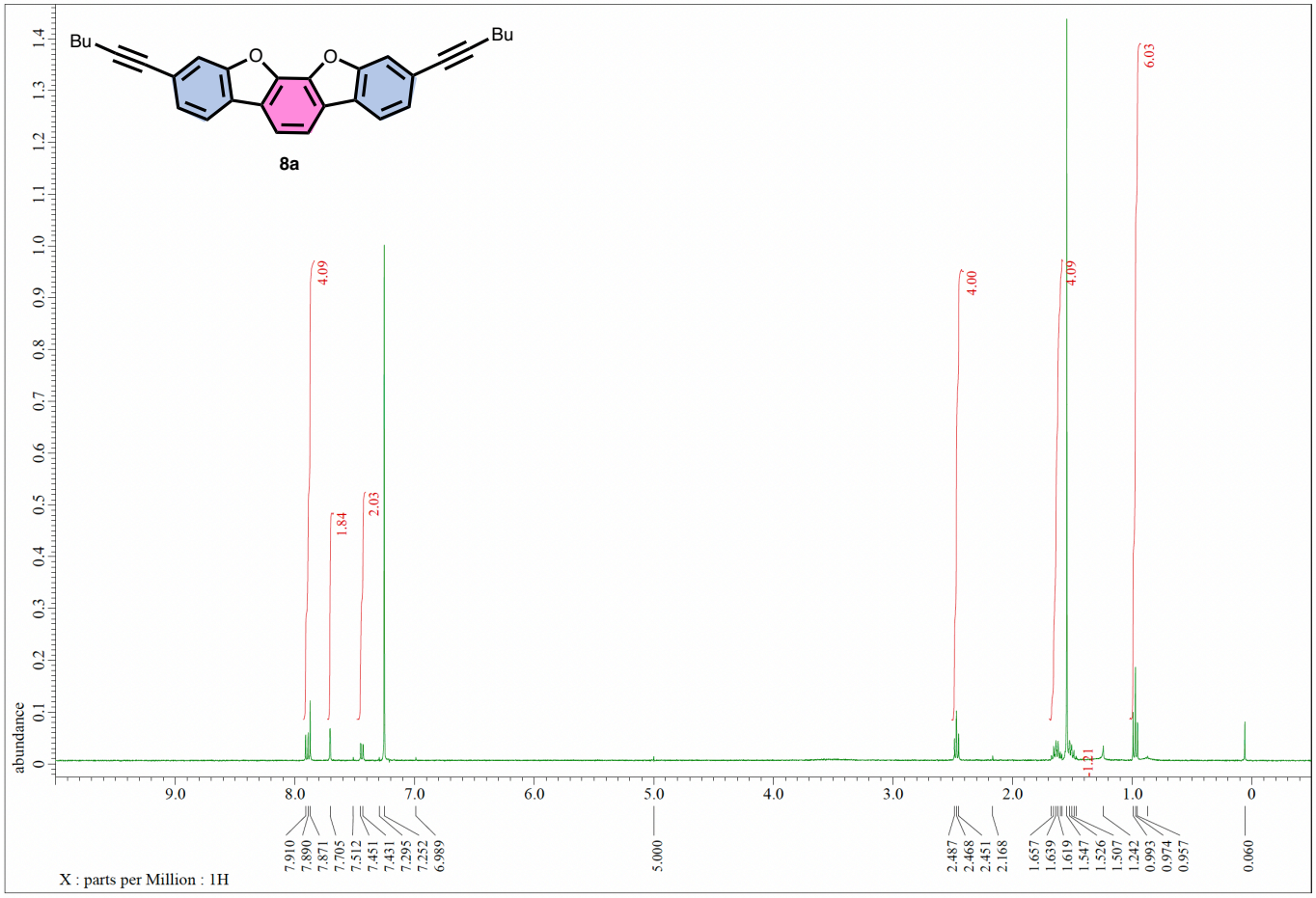

Figure S13. ^{1}H NMR Spectrum of 3,8-di(hex-1-yn-1-yl)dibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**8a**) (400 MHz, $CDCl_3$, r.t.).

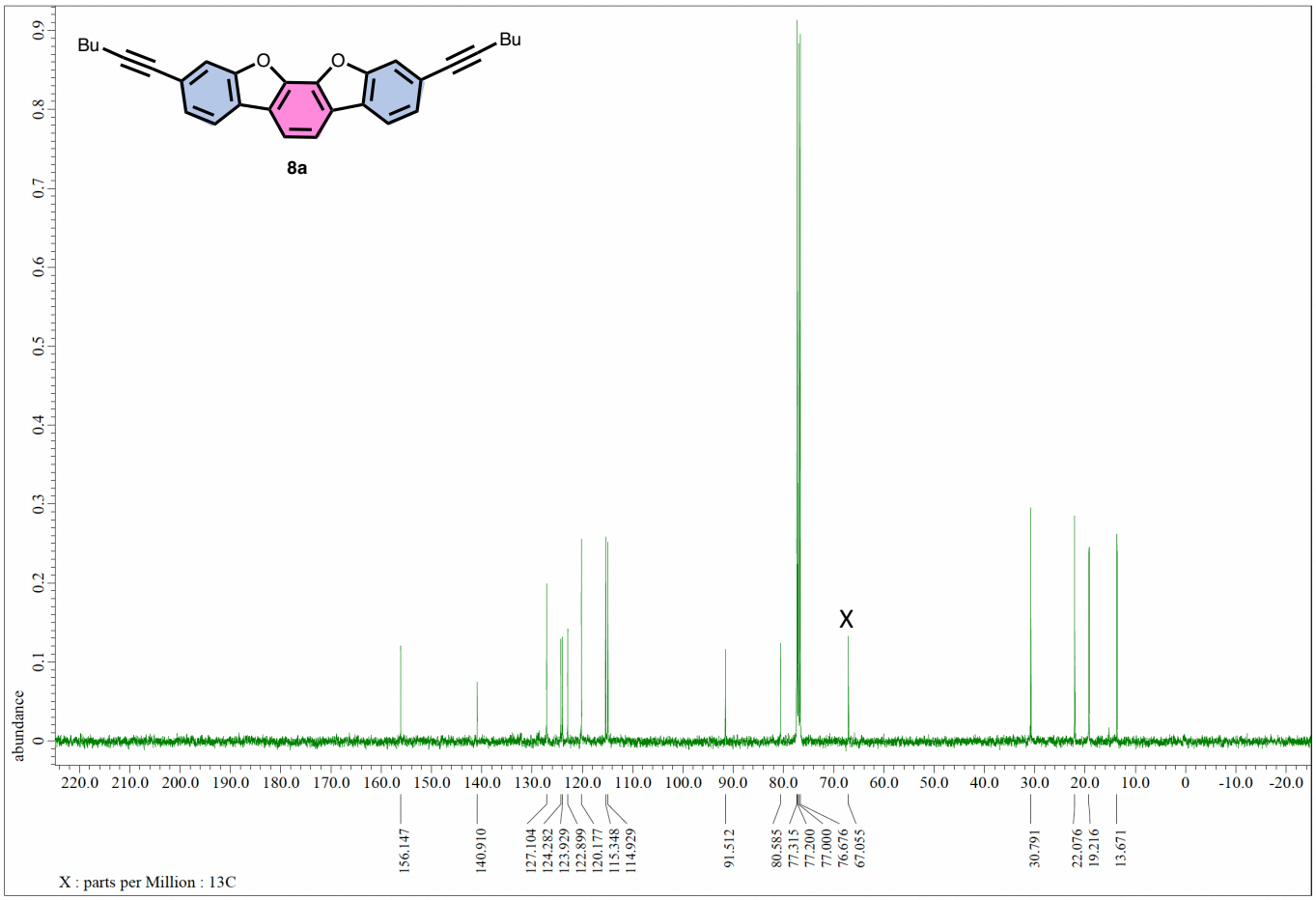

Figure S14. $^{13}C\{^{1}H\}$ NMR Spectrum of 3,8-di(hex-1-yn-1-yl)dibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**8a**) (100 MHz, $CDCl_3$, r.t.). X indicates incorporated 1,4-dioxane.

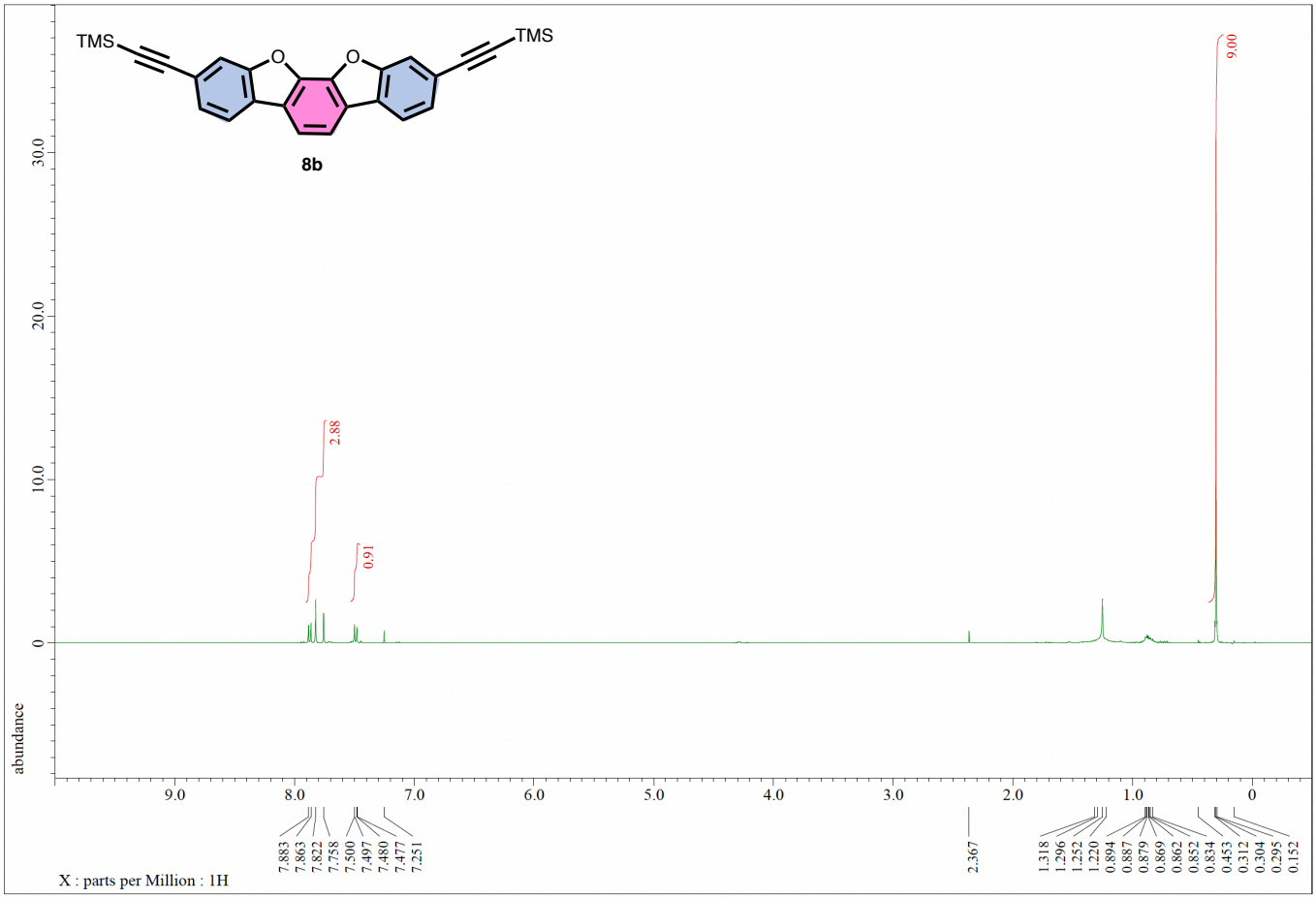

Figure S15. ^{1}H NMR Spectrum of 3,8-bis(trimethylsilylethynyl)dibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**8b**) (400 MHz, $CDCl_3$, r.t.).

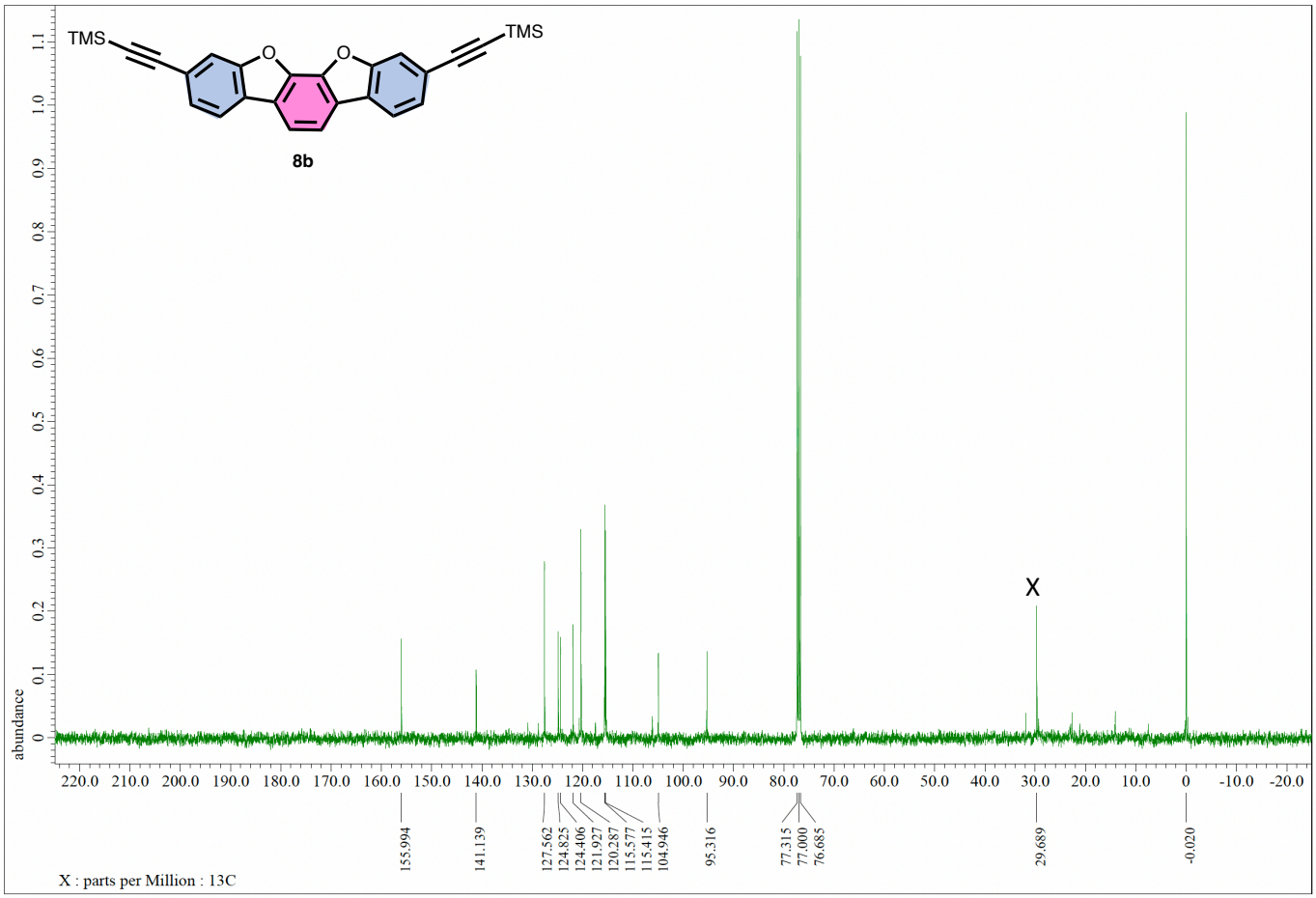

Figure S16. $^{13}C\{^{1}H\}$ NMR Spectrum of 3,8-bis(trimethylsilylethynyl)dibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**8b**) (100 MHz, $CDCl_3$, r.t.). X indicates an impurity.

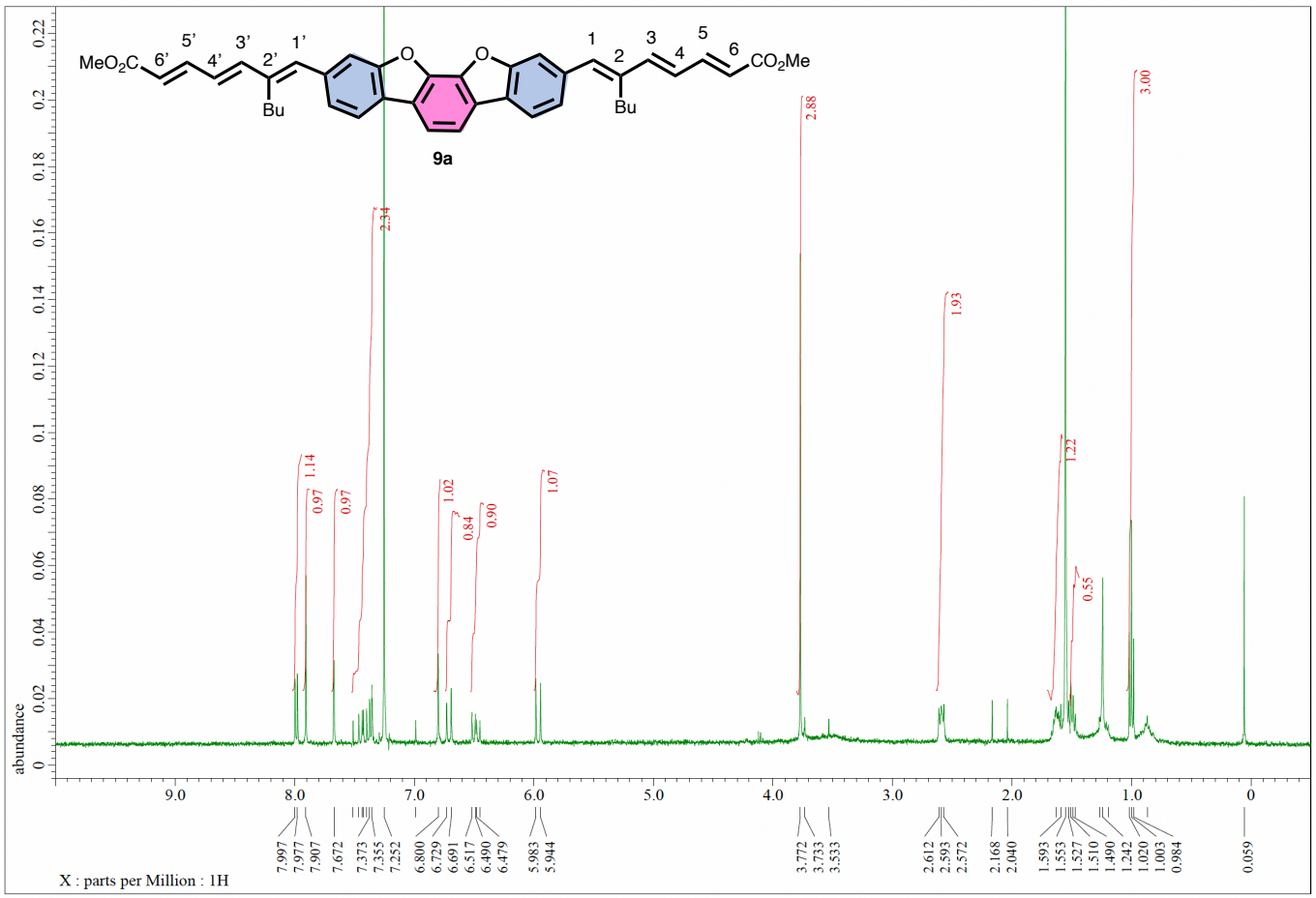

Figure S17. ^{1}H NMR Spectrum of 3,8-bis{(1*E*,3*E*,5*E*)-2-butyl-6-methoxycarbonylhepta-1,3,5-trien-1-yl}dibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**9a**) (400 MHz, $CDCl_3$, r.t.).

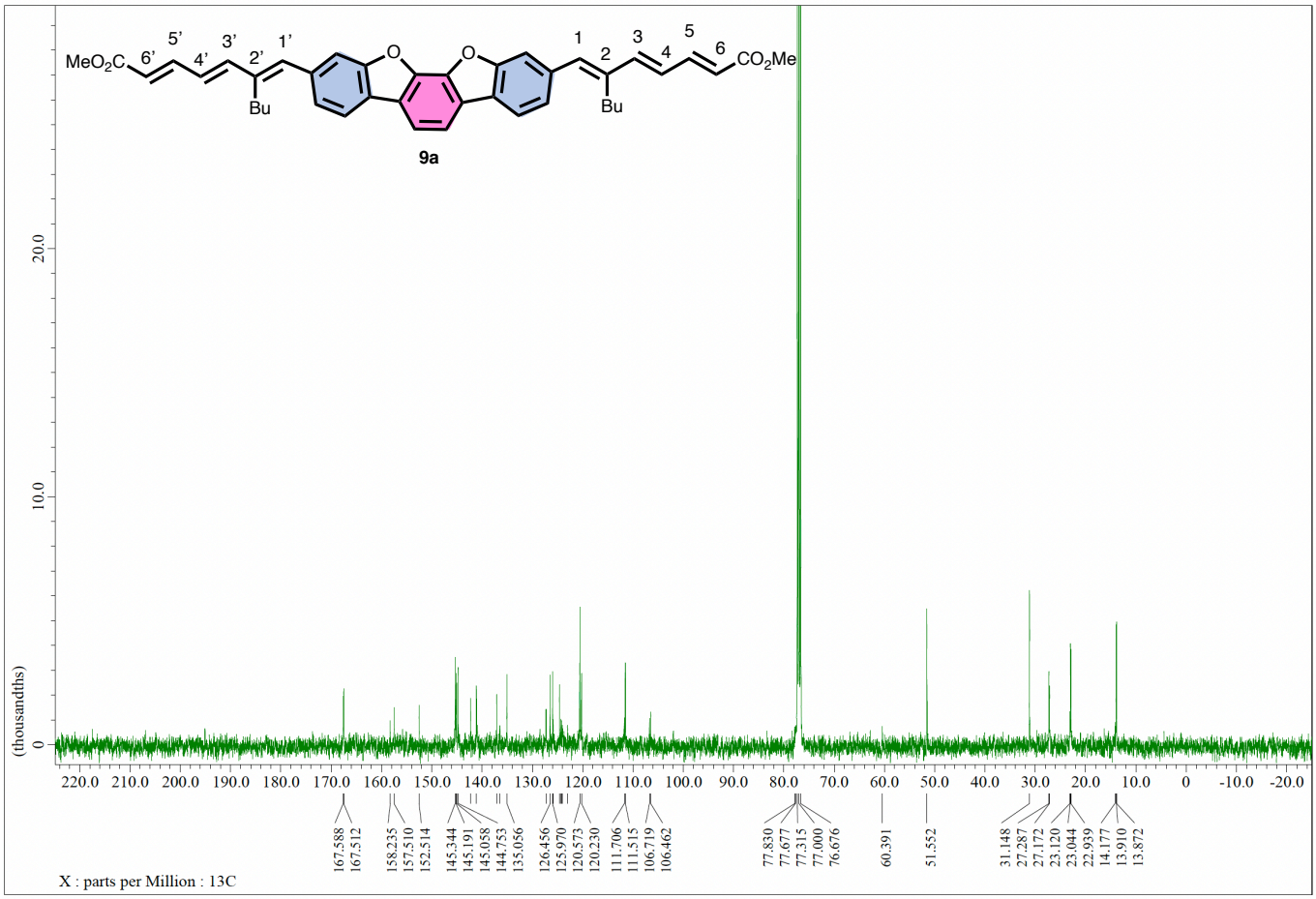

Figure S18. $^{13}C\{^{1}H\}$ NMR Spectrum of 3,8-bis{(1*E*,3*E*,5*E*)-2-butyl-6-methoxycarbonylhepta-1,3,5-trien-1-yl}dibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**9a**) (100 MHz, $CDCl_3$, r.t.).

Mass Spectrum SmartFormula Report

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Comment			

Acquisition Parameter

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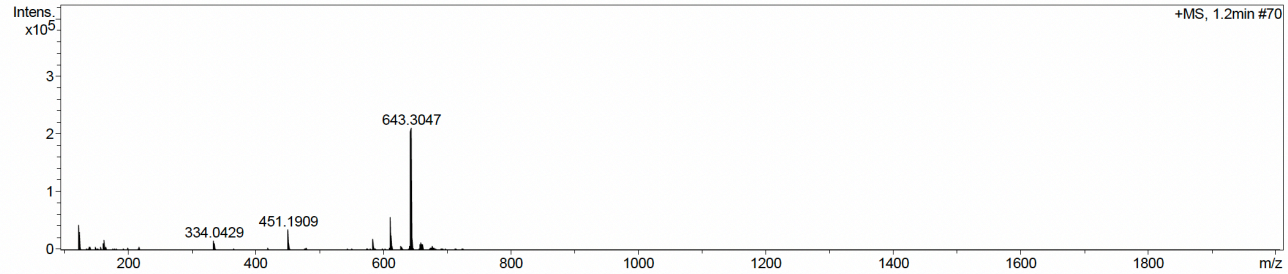

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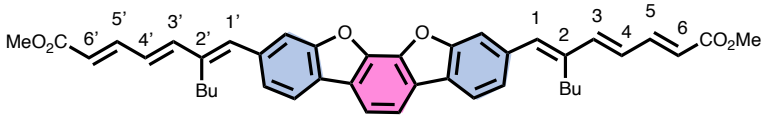


9a

Figure S19. High resolution mass spectrum (APCI) of 3,8-bis{(1*E*,3*E*,5*E*)-2-butyl-6-methoxycarbonylhepta-1,3,5-trien-1-yl}dibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**9a**).

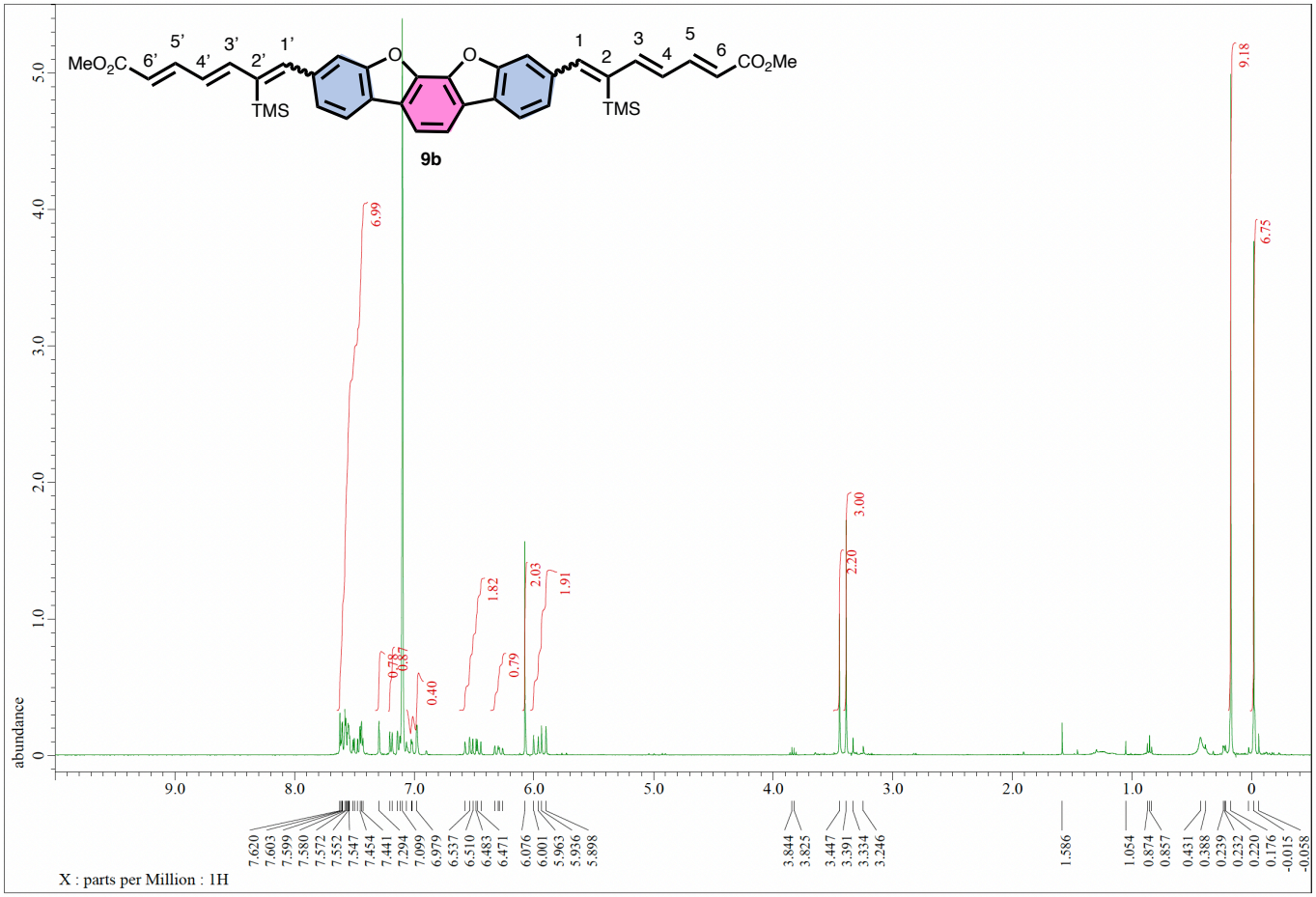


Figure S20. ^{1}H NMR Spectrum of 3,8-bis(6-methoxycarbonyl-2-trimethylsilylhepta-1,3,5-trien-1-yl)dibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**9b**) (400 MHz, $CDCl_3$, r.t.). This compound contained (1*E*,3*E*,5*E*)-**9b** and (1*Z*,3*E*,5*E*)-**9b**.

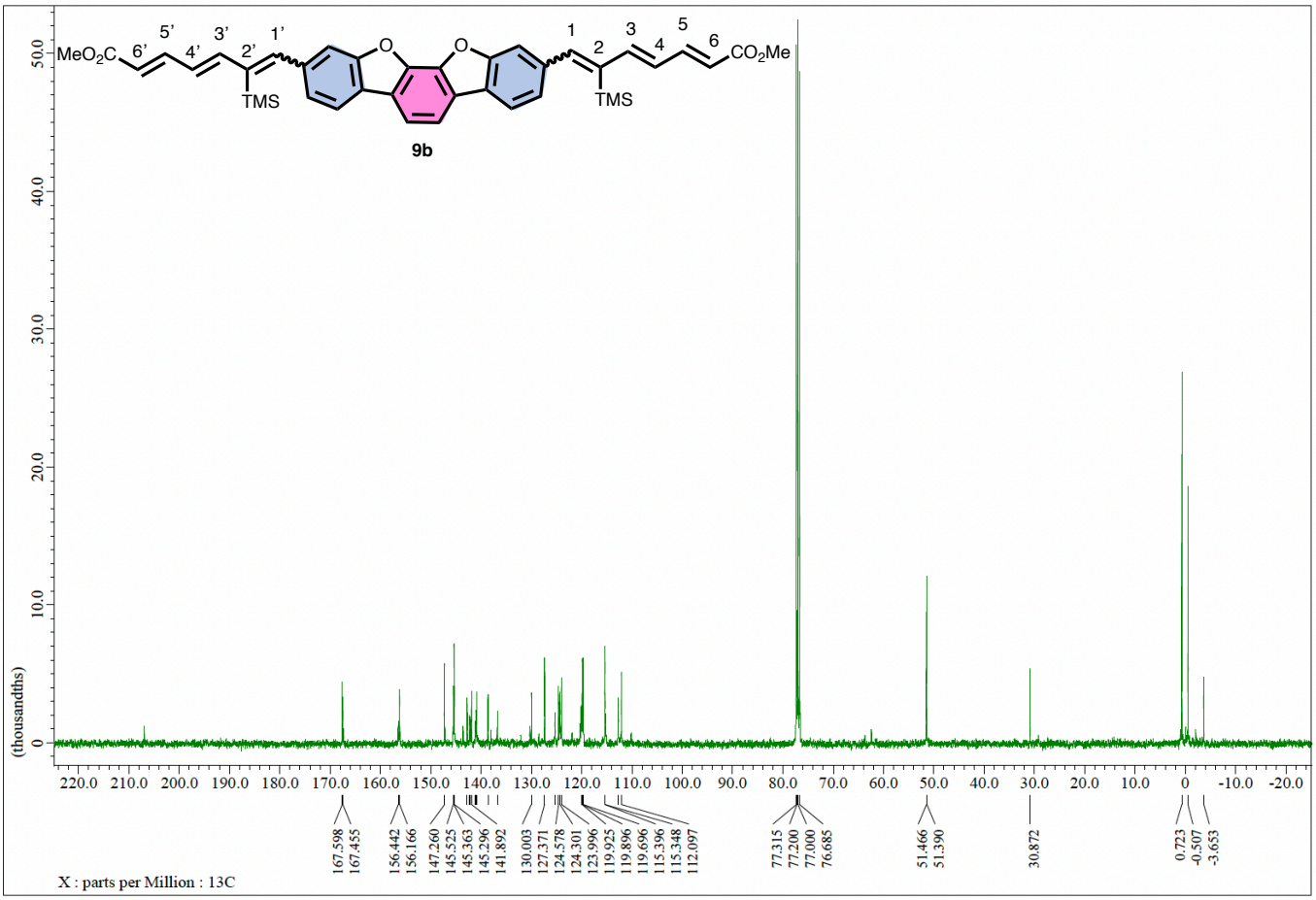
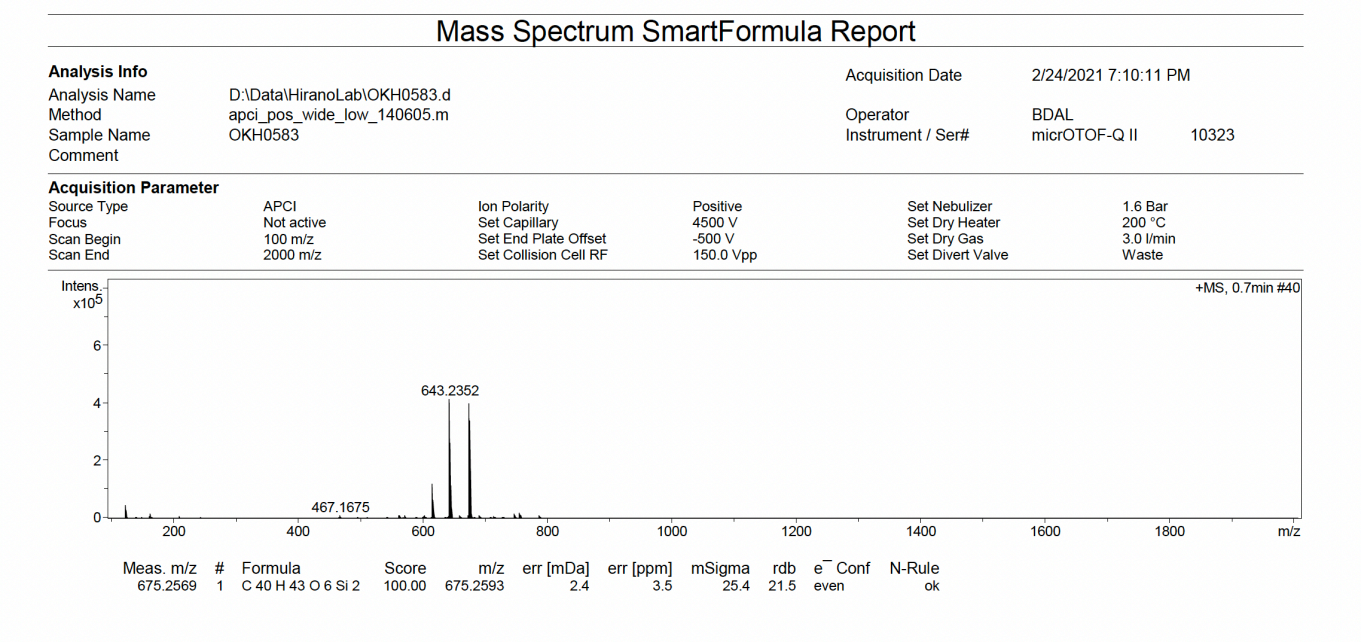


Figure S21. $^{13}C\{^{1}H\}$ NMR Spectrum of 3,8-bis(6-methoxycarbonyl-2-trimethylsilylhepta-1,3,5-trien-1-yl)dibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**9b**) (100 MHz, $CDCl_3$, r.t.).



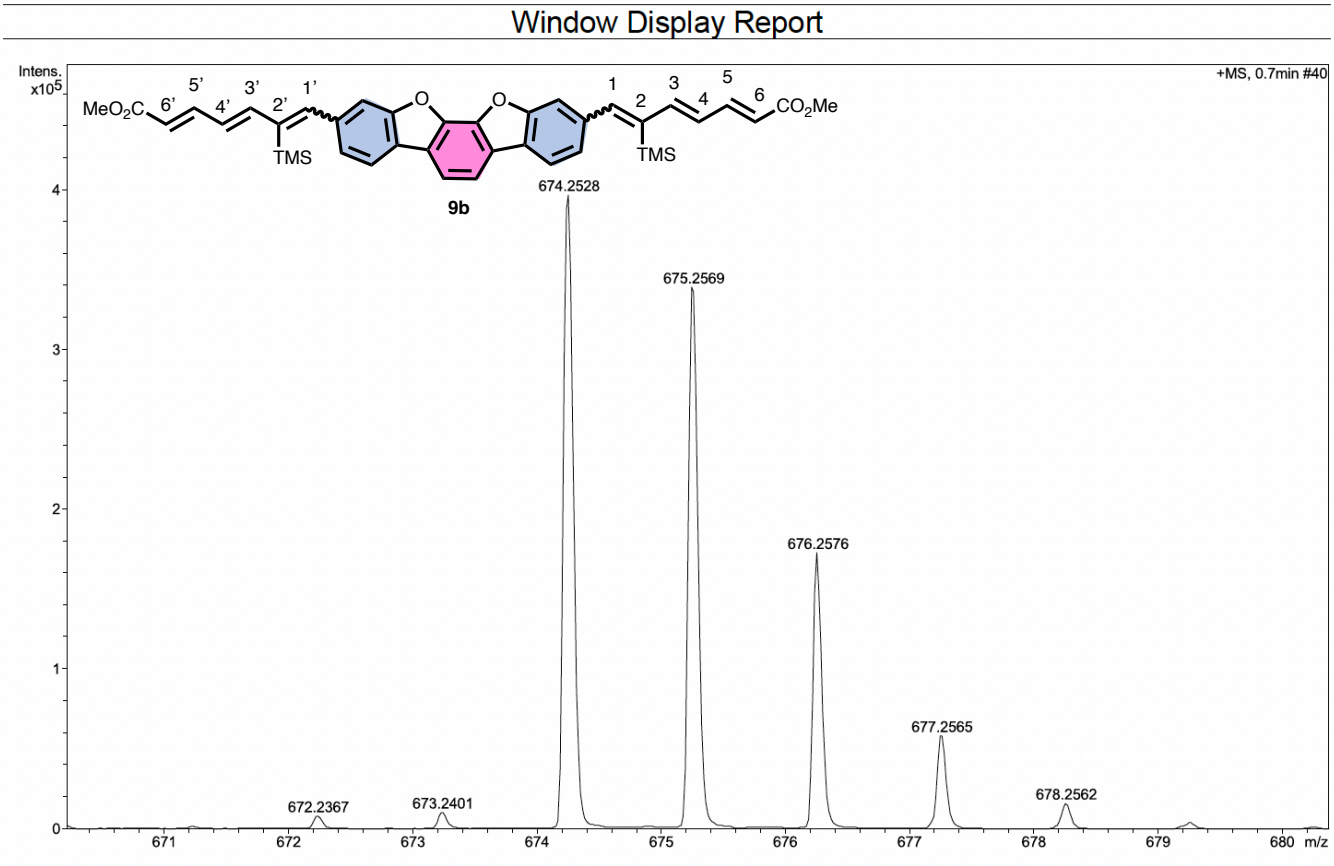


Figure S22. High resolution mass spectrum (APCI) of 3,8-bis(6-methoxycarbonyl-2-trimethylsilylhepta-1,3,5-trien-1-yl)dibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**9b**).

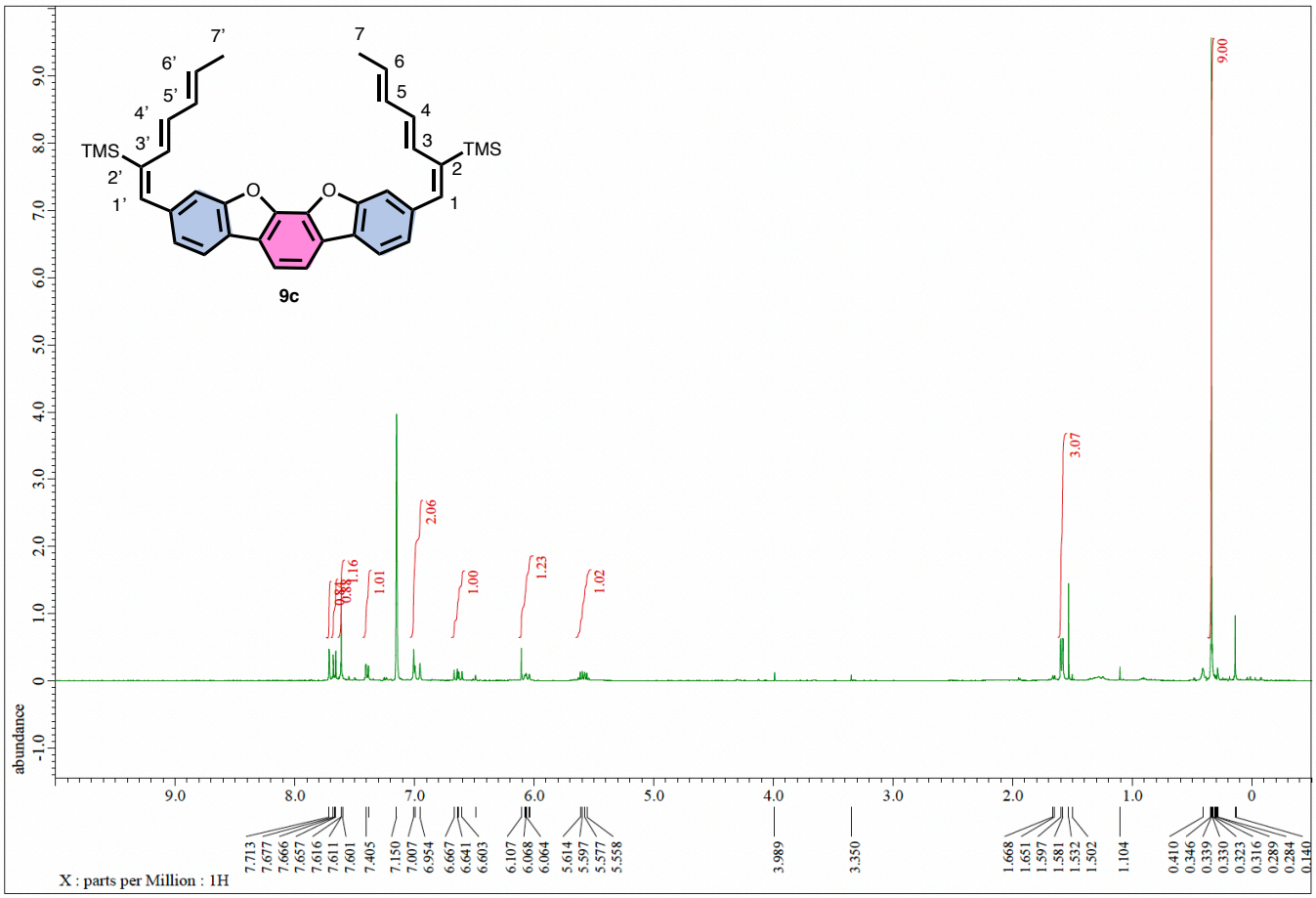


Figure S23. ^{1}H NMR Spectrum of 3,8-bis{(1*E*,3*E*,5*E*)-2-trimethylsilylhepta-1,3,5-trien-1-yl}dibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**9c**) (400 MHz, C_6D_6, r.t.).

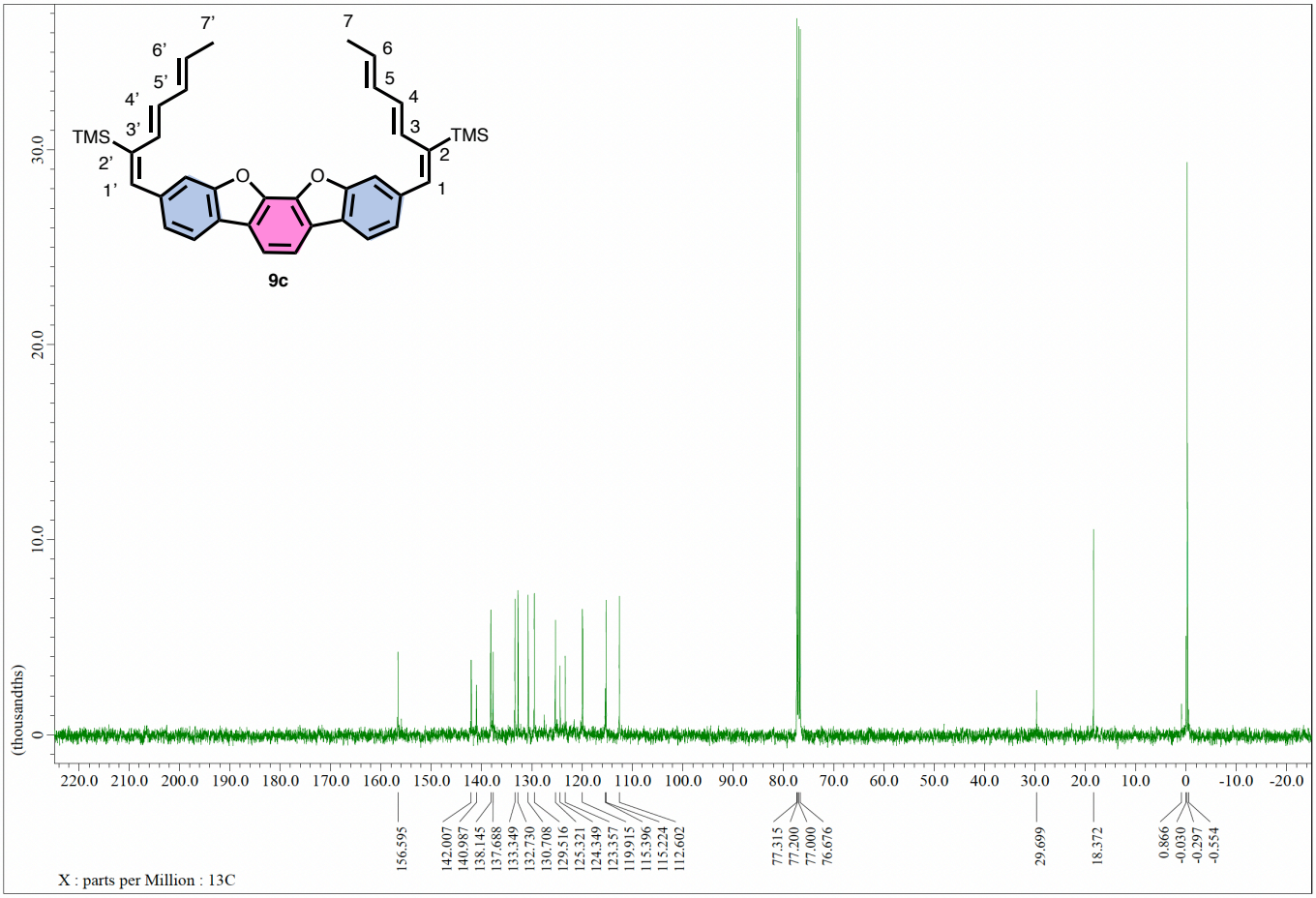


Figure S24. $^{13}C\{^{1}H\}$ NMR Spectrum of 3,8-bis{(1*E*,3*E*,5*E*)-2-trimethylsilylhepta-1,3,5-trien-1-yl}dibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**9c**) (100 MHz, $CDCl_3$, r.t.).

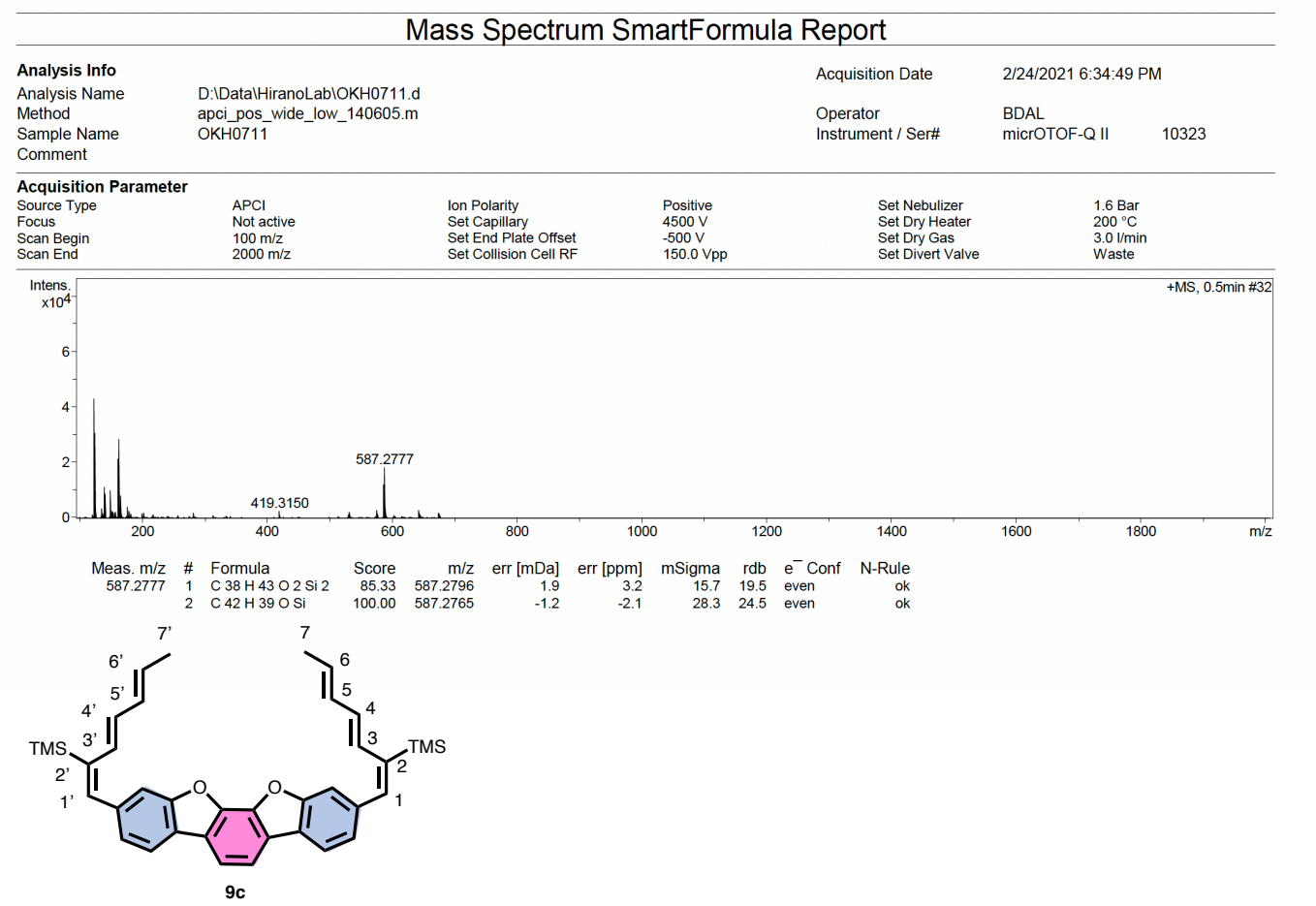


Figure S25. High resolution mass spectrum (APCI) of 3,8-bis{(1*E*,3*E*,5*E*)-2-trimethylsilylhepta-1,3,5-trien-1-yl}dibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**9c**).

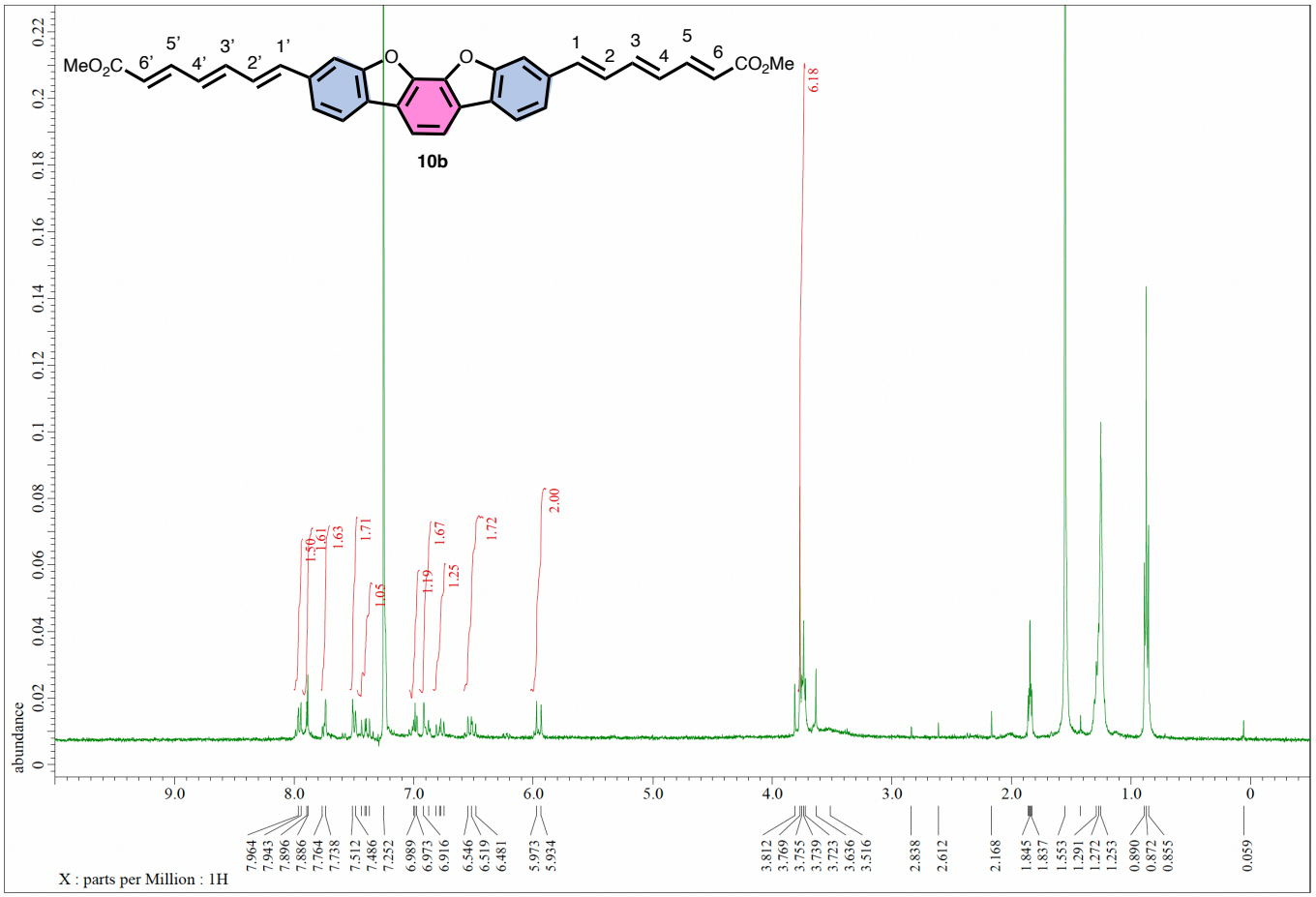


Figure S26. ^{1}H NMR Spectrum of 3,8-bis{(1*E*,3*E*,5*E*)-6-methoxycarbonylhepta-1,3,5-trien-1-yl}dibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**10b**) (400 MHz, $CDCl_3$, r.t.).

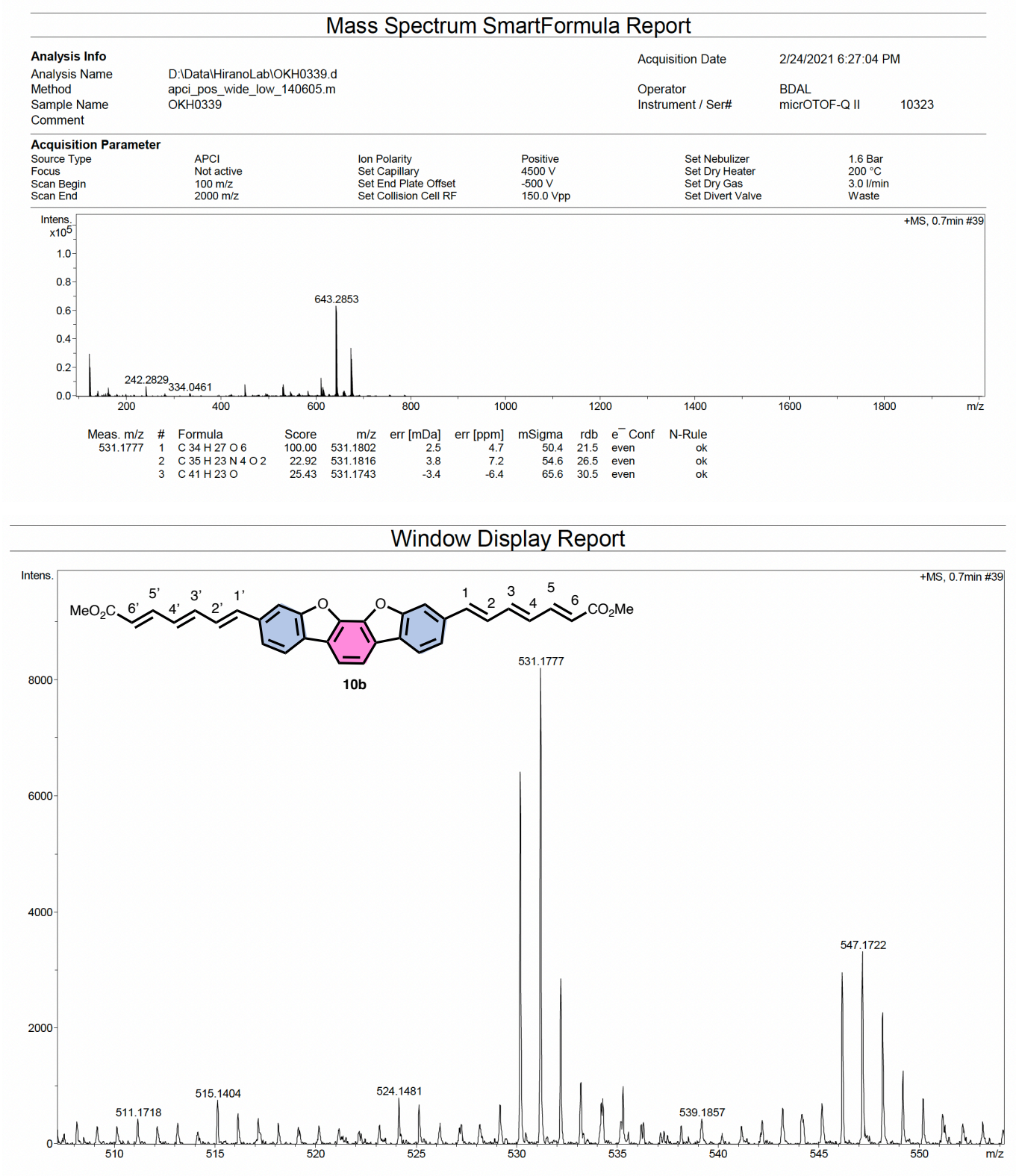


Figure S27. High resolution mass spectrum (APCI) of 3,8-bis{(1*E*,3*E*,5*E*)-6-methoxycarbonylhepta-1,3,5-trien-1-yl}dibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**10b**).

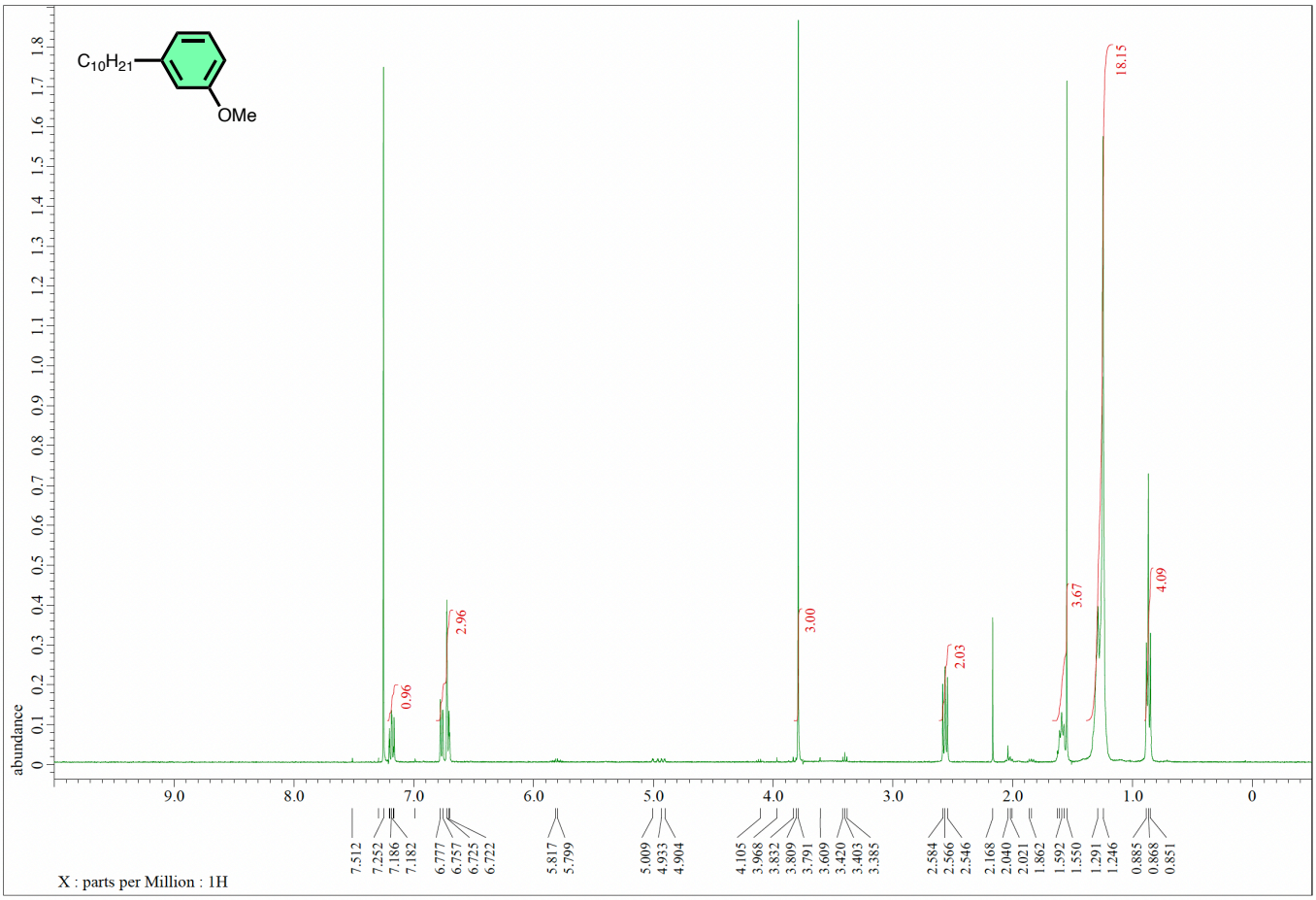


Figure S28. ^{1}H NMR Spectrum of 3-decylanisole (400 MHz, $CDCl_3$, r.t.).

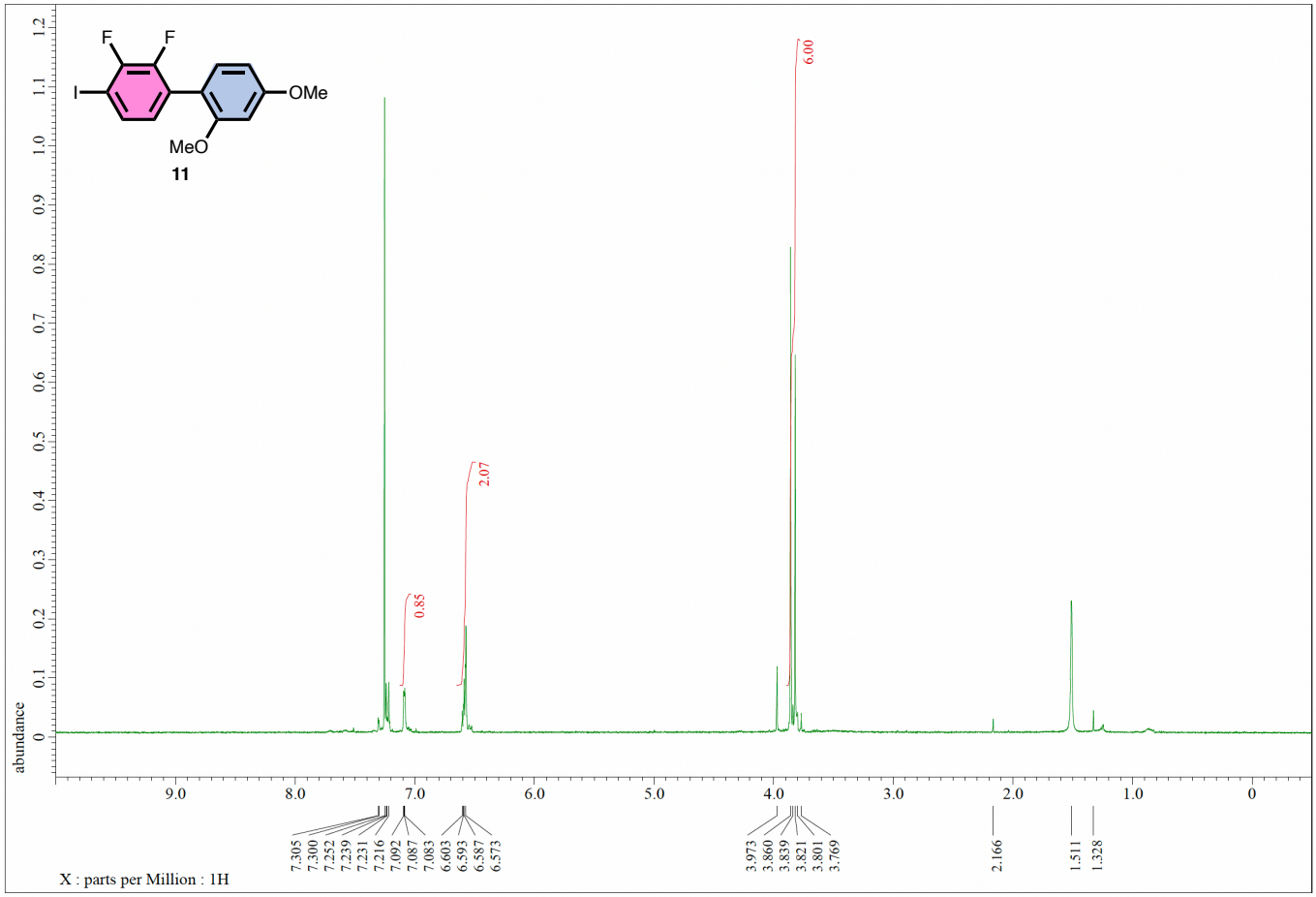


Figure S29. ^{1}H NMR Spectrum of 2,3-difluoro-4-iodo-2',4'-dimethoxy-1,1'-biphenyl (**11**) (400 MHz, $CDCl_3$, r.t.).

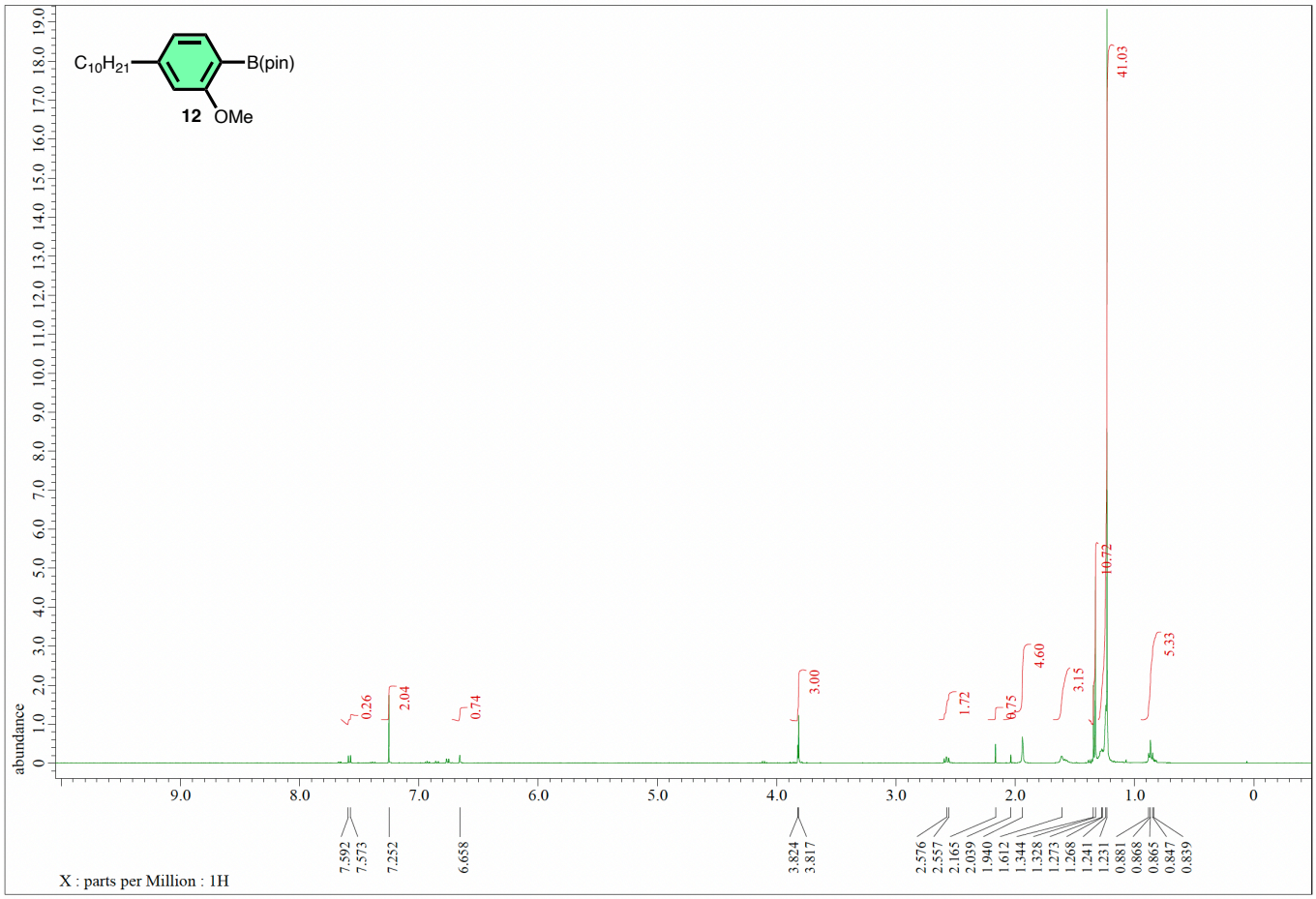


Figure S30. ^{1}H NMR Spectrum of 2-(4-decyl-2-methoxyphenyl)-4,4-5,5-tetramethyl-1,3,2-dioxaborolane (**12**) (400 MHz, $CDCl_3$, r.t.).

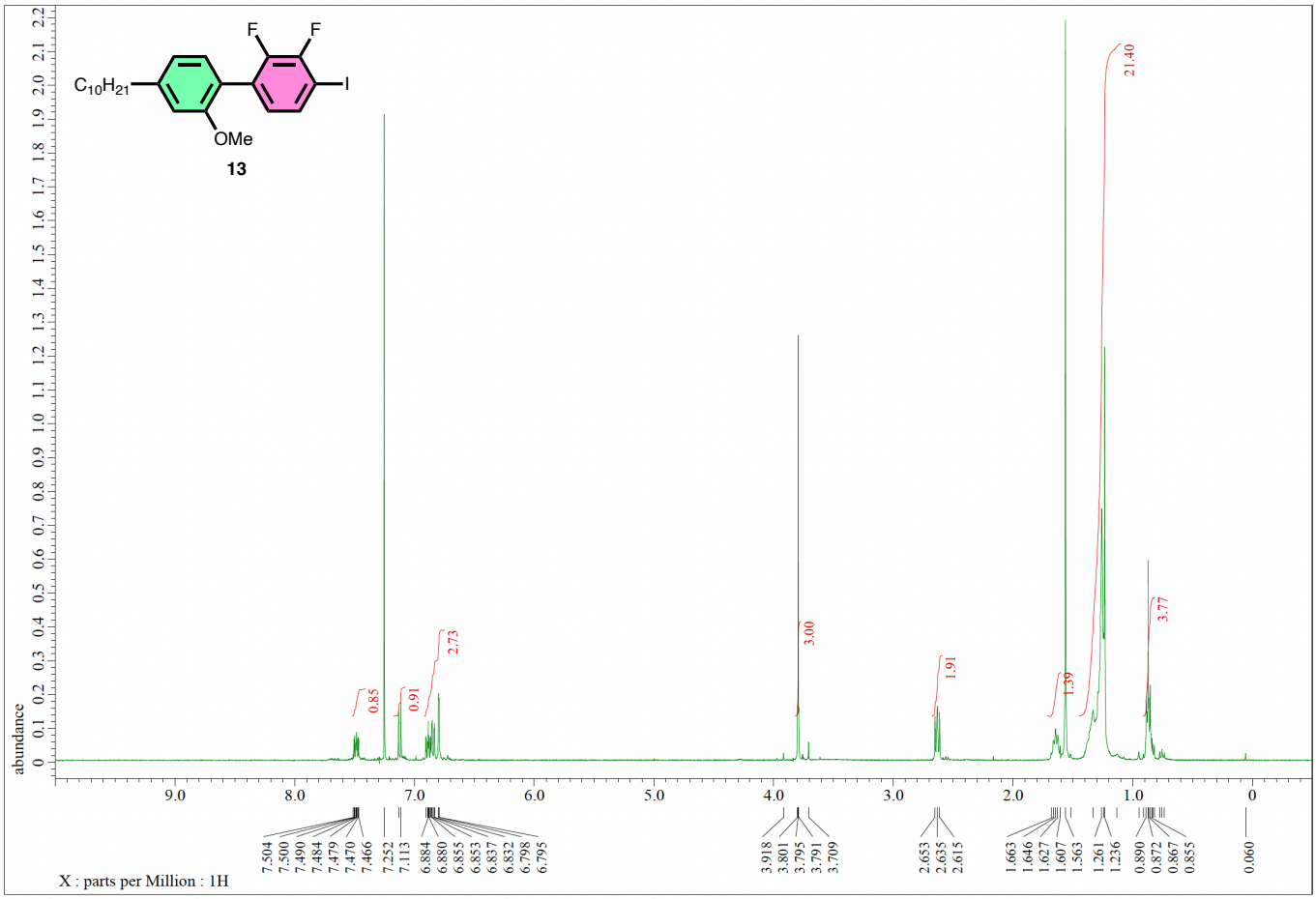


Figure S31. ^{1}H NMR Spectrum of 4-decyl-2,3-difluoro-4-iodo-2'-methoxy-1,1'-biphenyl (**13**) (400 MHz, $CDCl_3$, r.t.).

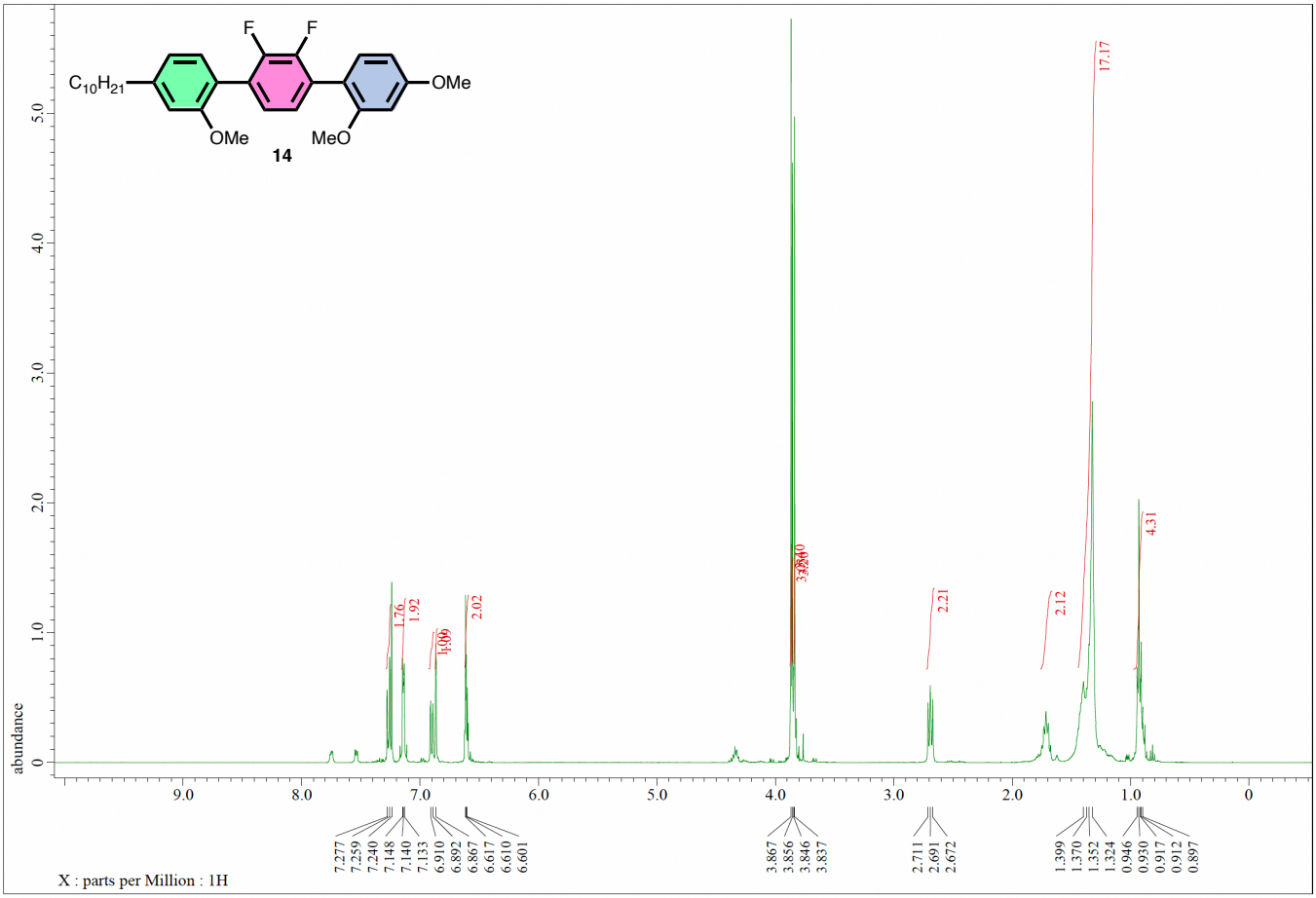


Figure S32. ^{1}H NMR Spectrum of 4-decyl-2',3'-difluoro-2,2",4"-trimethoxy-1,1':4',1"-terphenyl (**14**) (400 MHz, $CDCl_3$, r.t.).

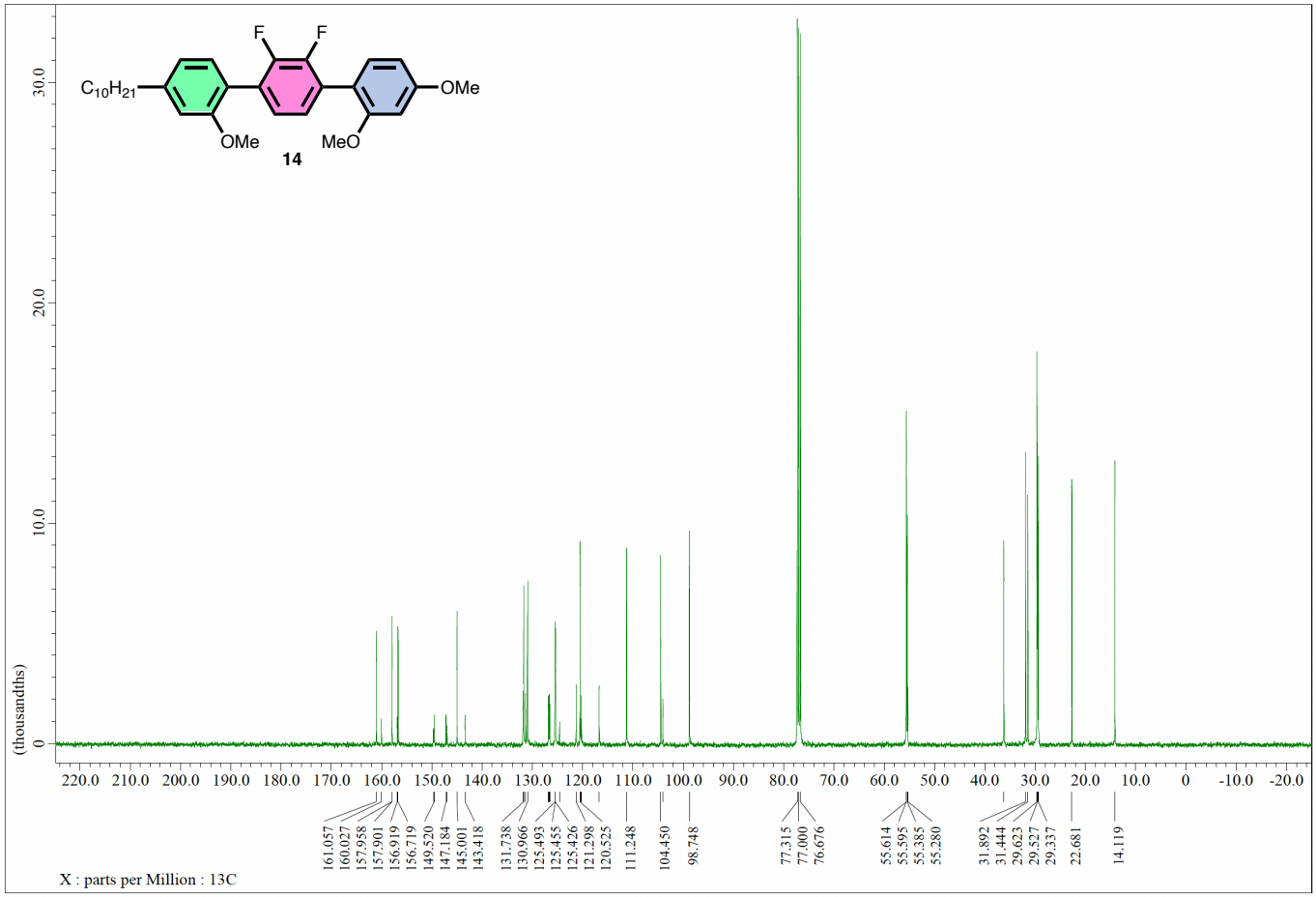


Figure S33. $^{13}C\{^{1}H\}$ NMR Spectrum of 4-decyl-2',3'-difluoro-2,2",4"-trimethoxy-1,1':4',1"-terphenyl (**14**) (100 MHz, $CDCl_3$, r.t.).

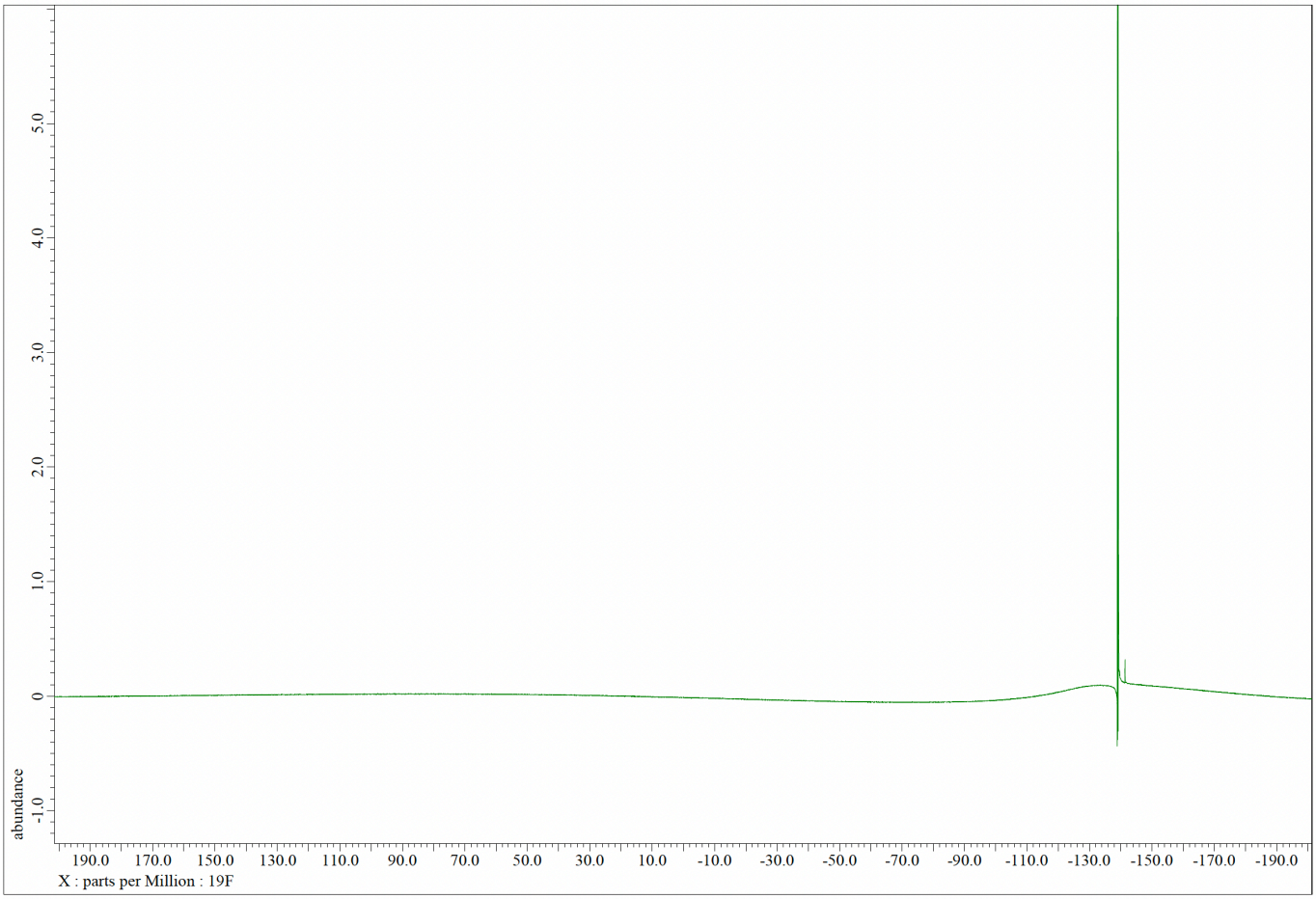


Figure S34. ^{19}F NMR Spectrum of 4-decyl-2',3'-difluoro-2,2",4"-trimethoxy-1,1':4',1"-terphenyl (**14**) (376 MHz, $CDCl_3$, r.t.).

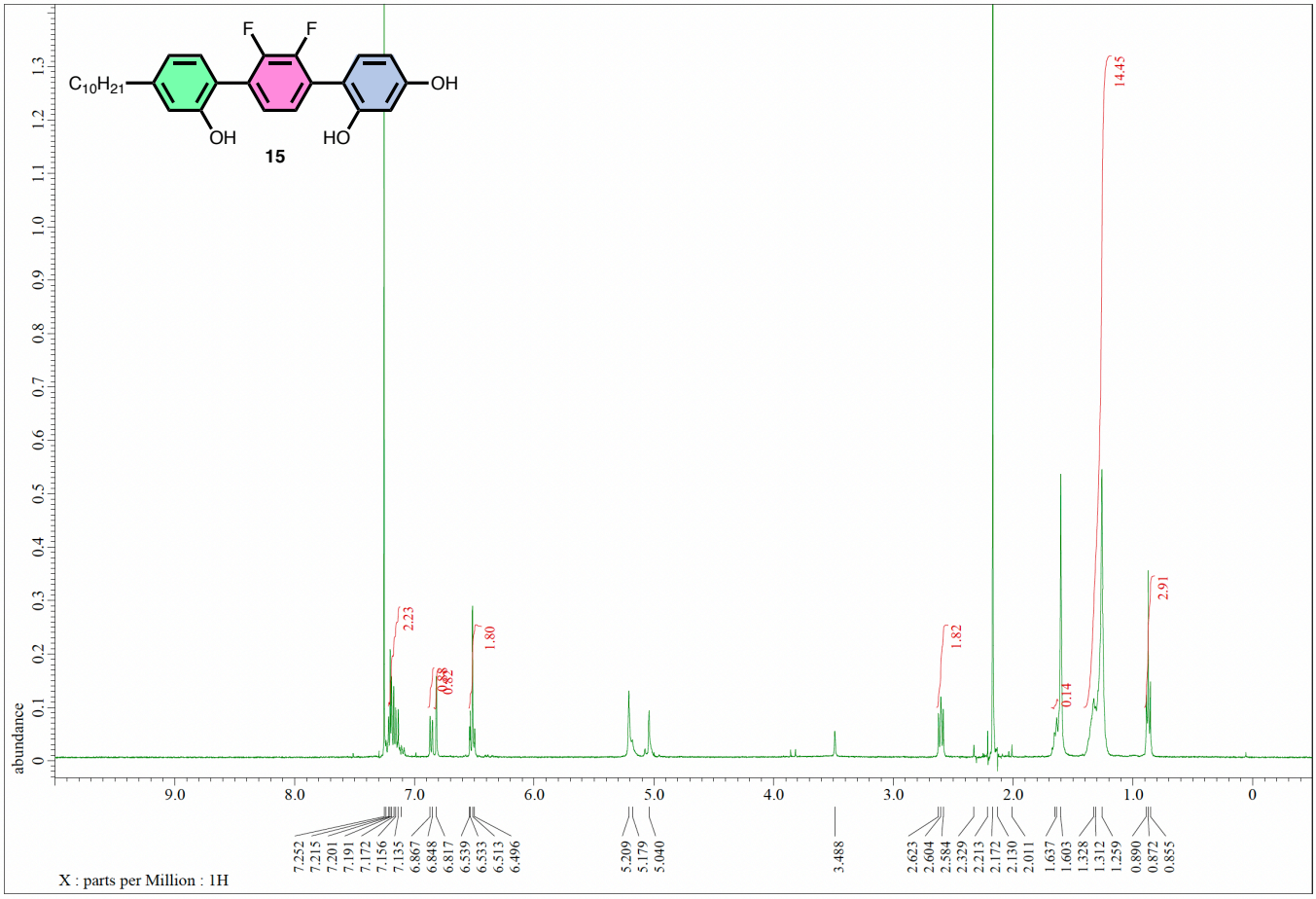


Figure S35. ^{1}H NMR Spectrum of 4”-decyl-2’,3’-difluoro[1,1’:4’,1”-terphenyl]-2,2”,4-triol (**15**) (400 MHz, $CDCl_3$, r.t.).

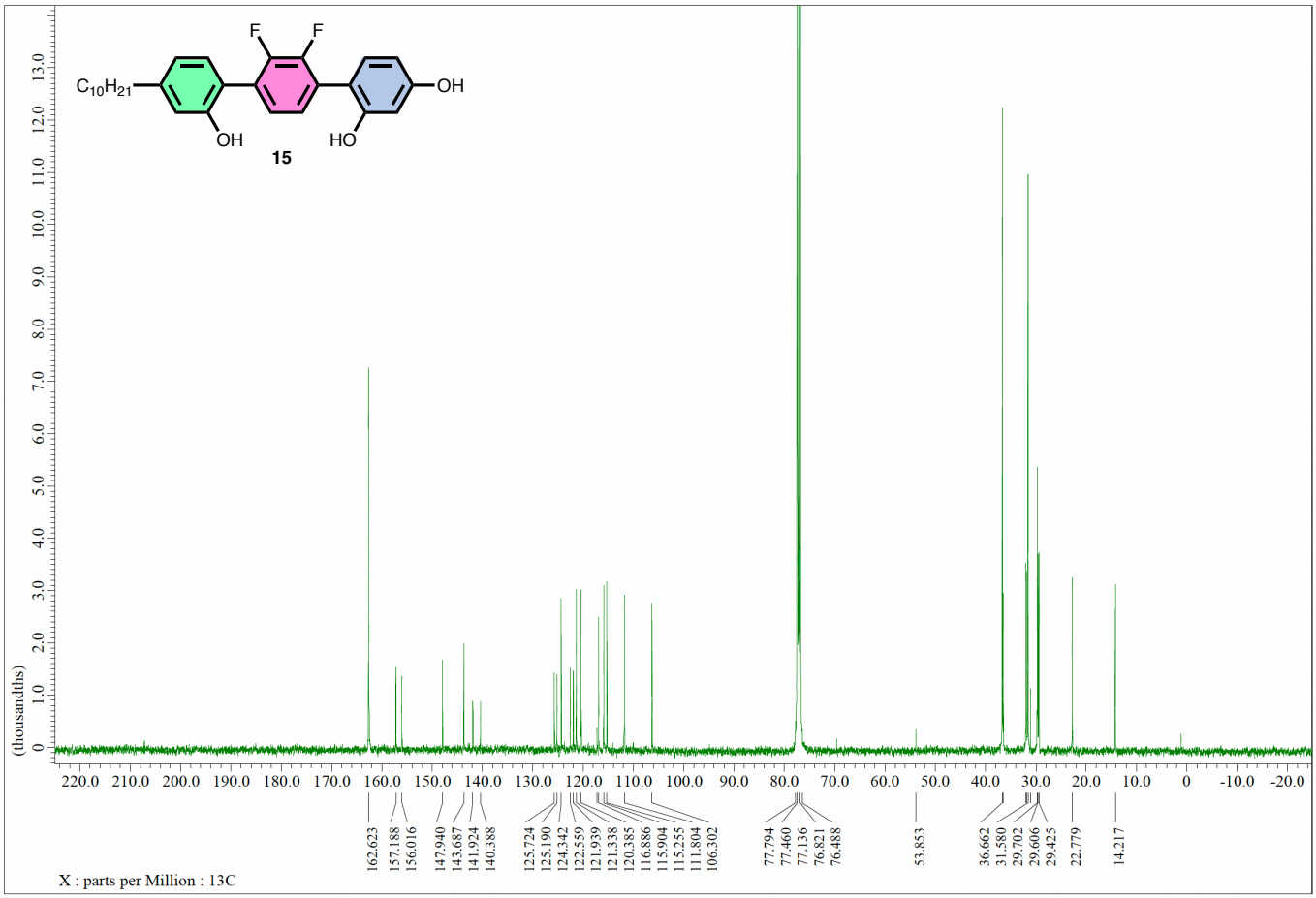


Figure S36. $^{13}C\{^{1}H\}$ NMR Spectrum of 4”-decyl-2’,3’-difluoro[1,1’:4’,1”-terphenyl]-2,2”,4-triol (**15**) (100 MHz, $CDCl_3$, r.t.).

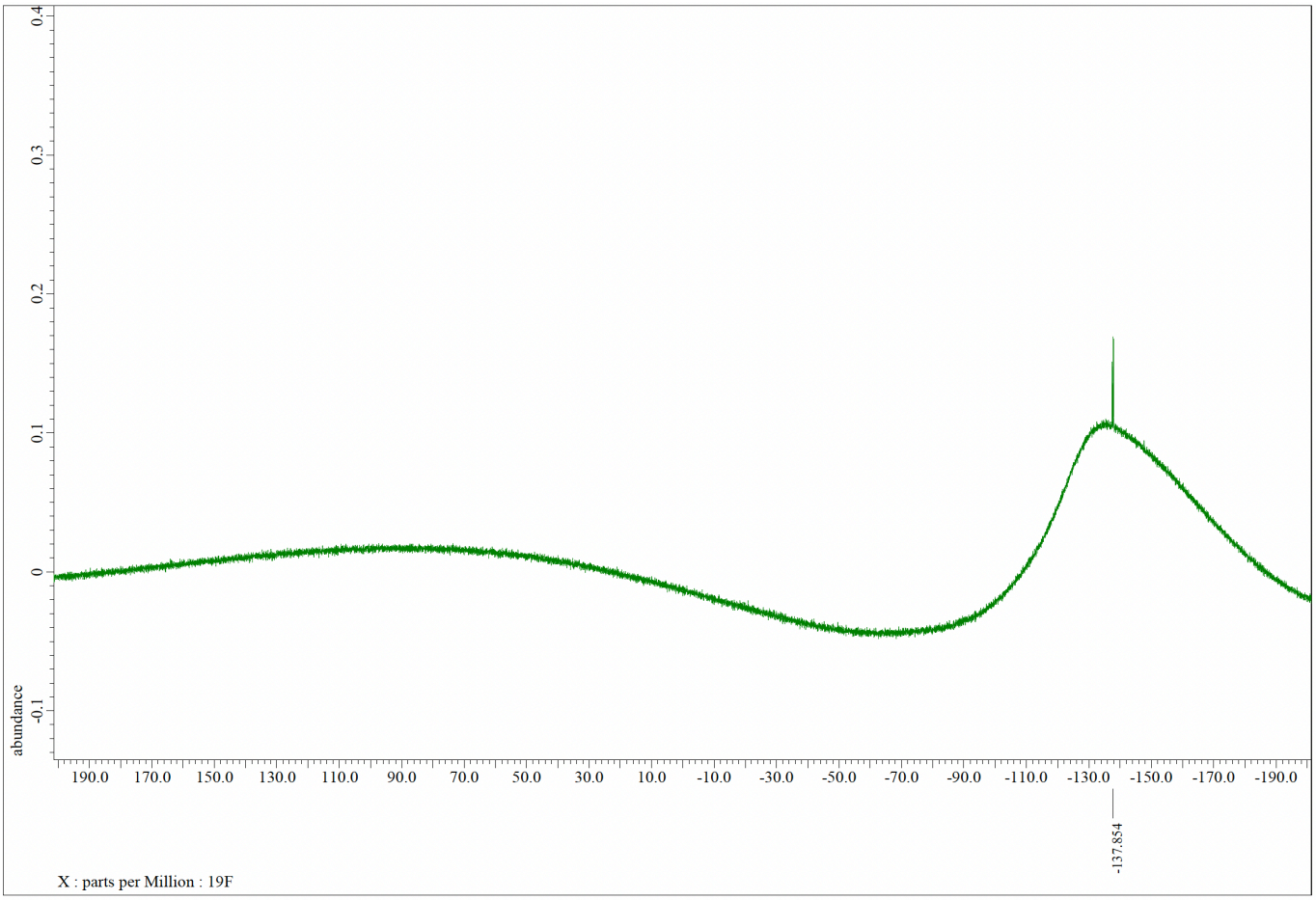


Figure S37. ^{19}F NMR Spectrum of 4”-decyl-2’,3’-difluoro[1,1’:4’,1”-terphenyl]-2,2”,4-triol (**15**) (376 MHz, $CDCl_3$, r.t.).

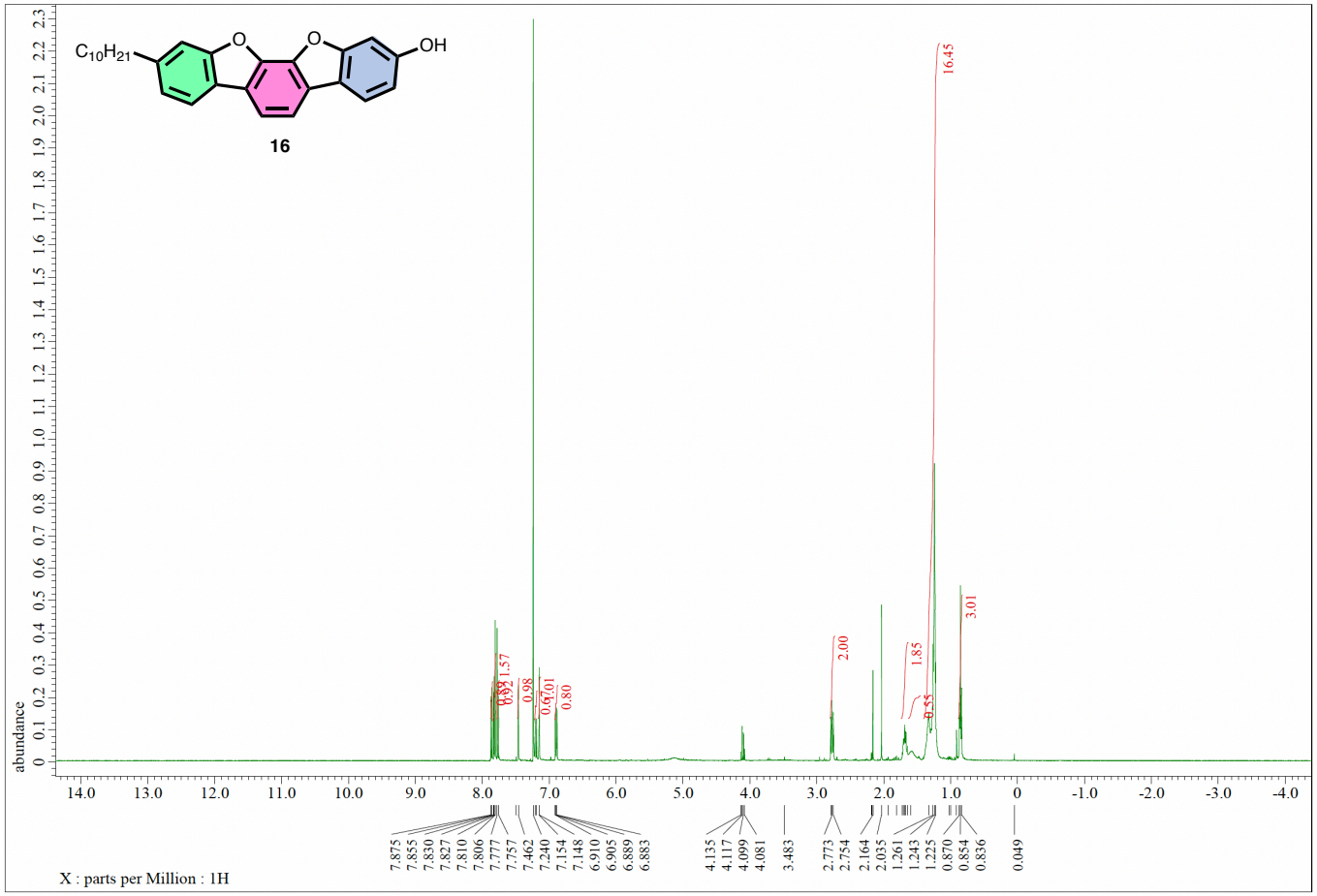


Figure S38. ^{1}H NMR Spectrum of 8-decyldibenzo[*d,d'*]benzo[2,1-*b*:3,4-*b'*]difuran-3-ol (**16**) (400 MHz, $CDCl_3$, r.t.).

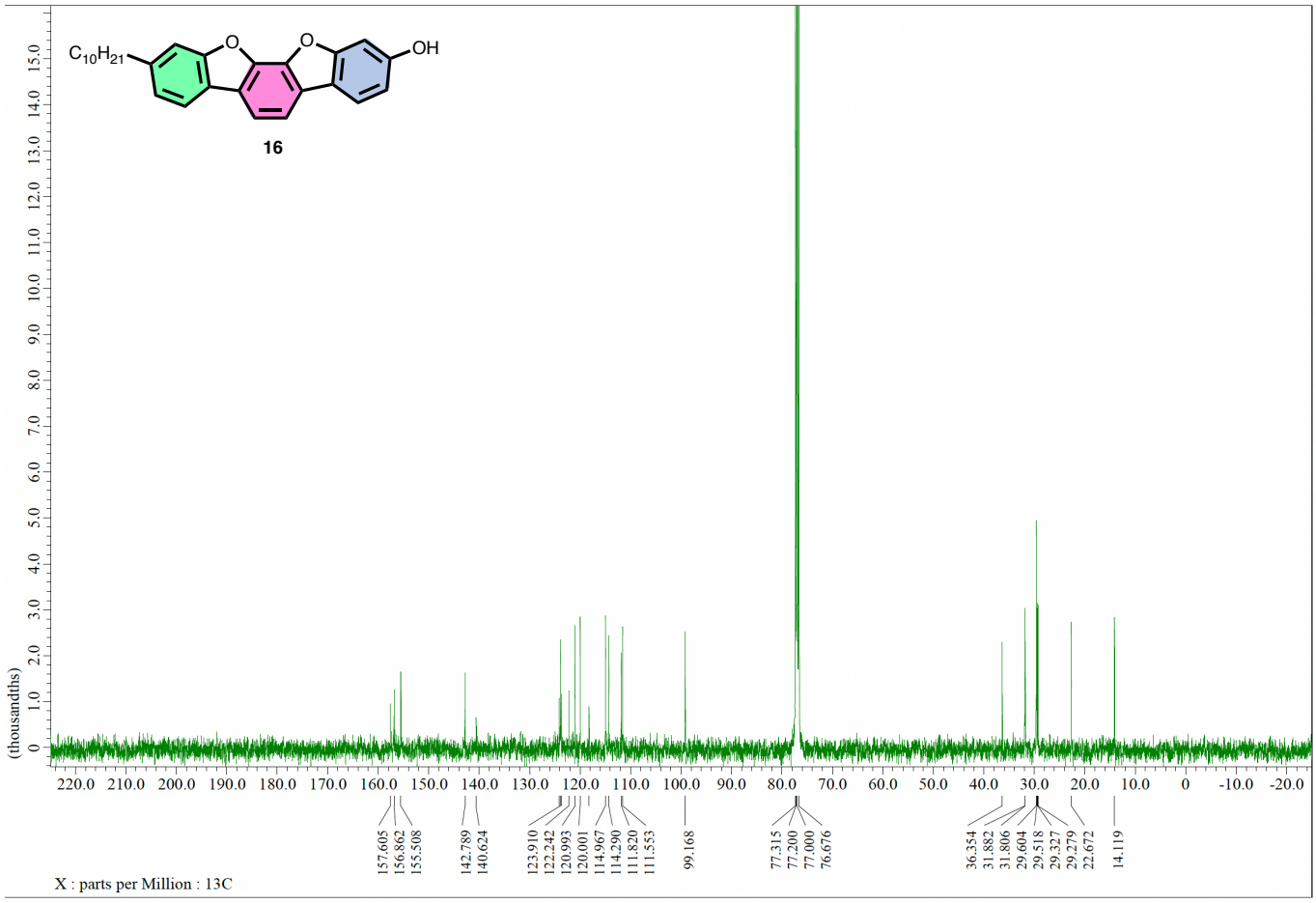


Figure S39. $^{13}C\{^{1}H\}$ NMR Spectrum of 8-decyldibenzo[*d,d'*]benzo[2,1-*b*:3,4-*b'*]difuran-3-ol (**16**) (100 MHz, $CDCl_3$, r.t.).

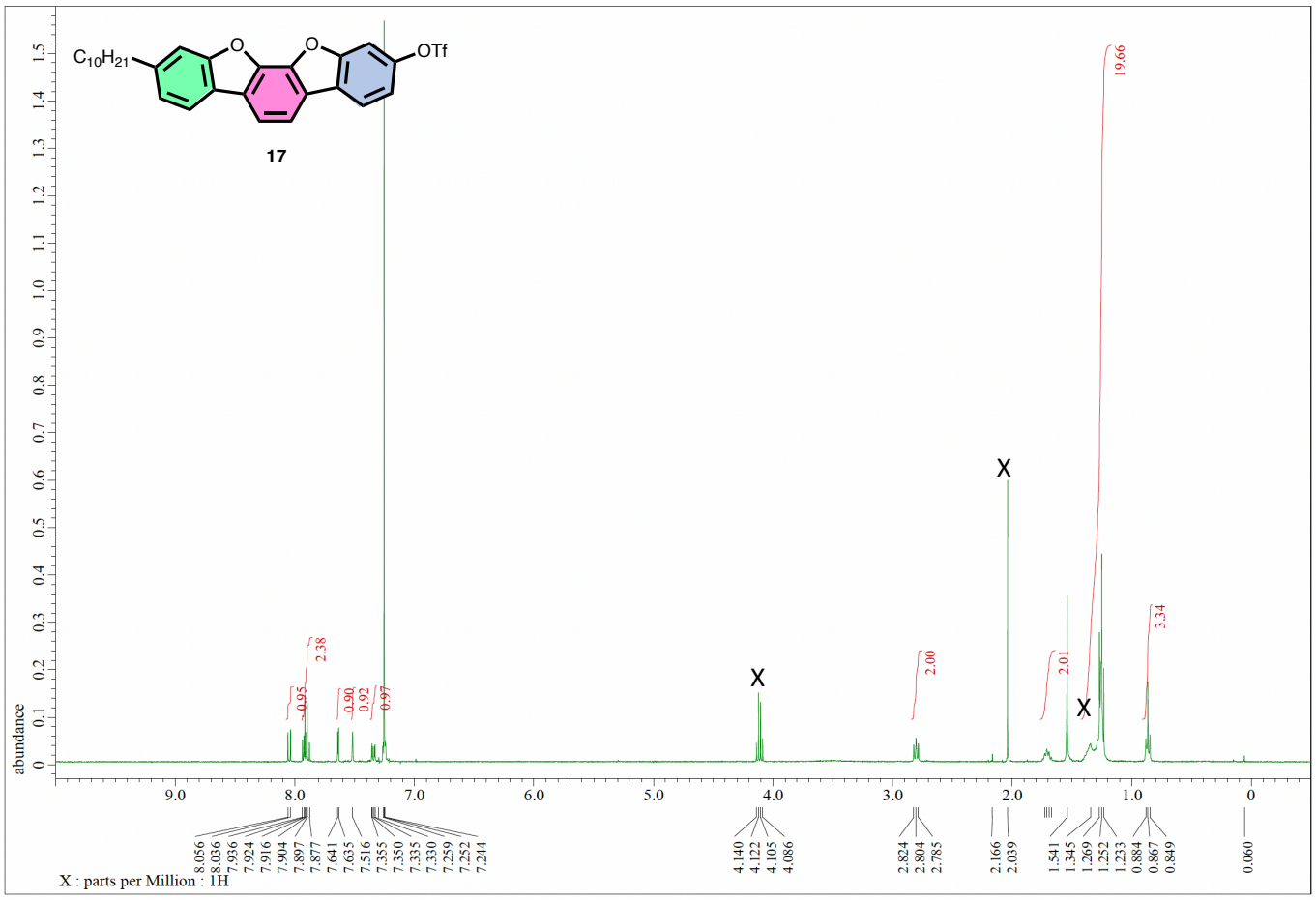


Figure S40. ^{1}H NMR Spectrum of 8-decyldibenzo[*d,d'*]benzo[2,1-*b*:3,4-*b'*]difuran-3-yltrifluoromethanesulfonate (**17**) (400 MHz, $CDCl_3$, r.t.). Xs indicate incorporated ethyl acetate.

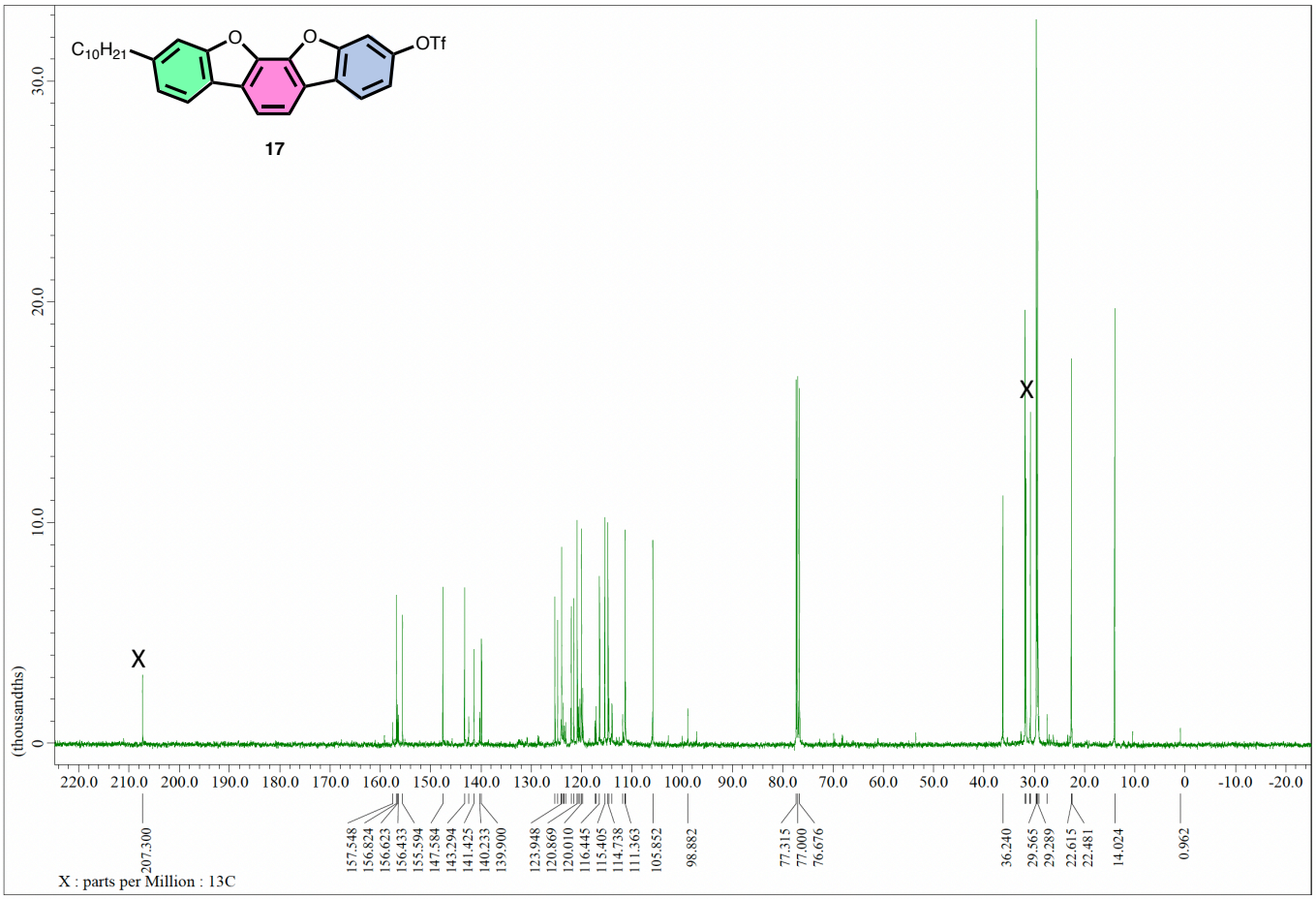


Figure S41. $^{13}C\{^{1}H\}$ NMR Spectrum of 8-decyldibenzo[*d,d'*]benzo[2,1-*b*:3,4-*b'*]difuran-3-yltrifluoromethanesulfonate (**17**) (100 MHz, $CDCl_3$, r.t.). Xs indicate incorporated acetone.

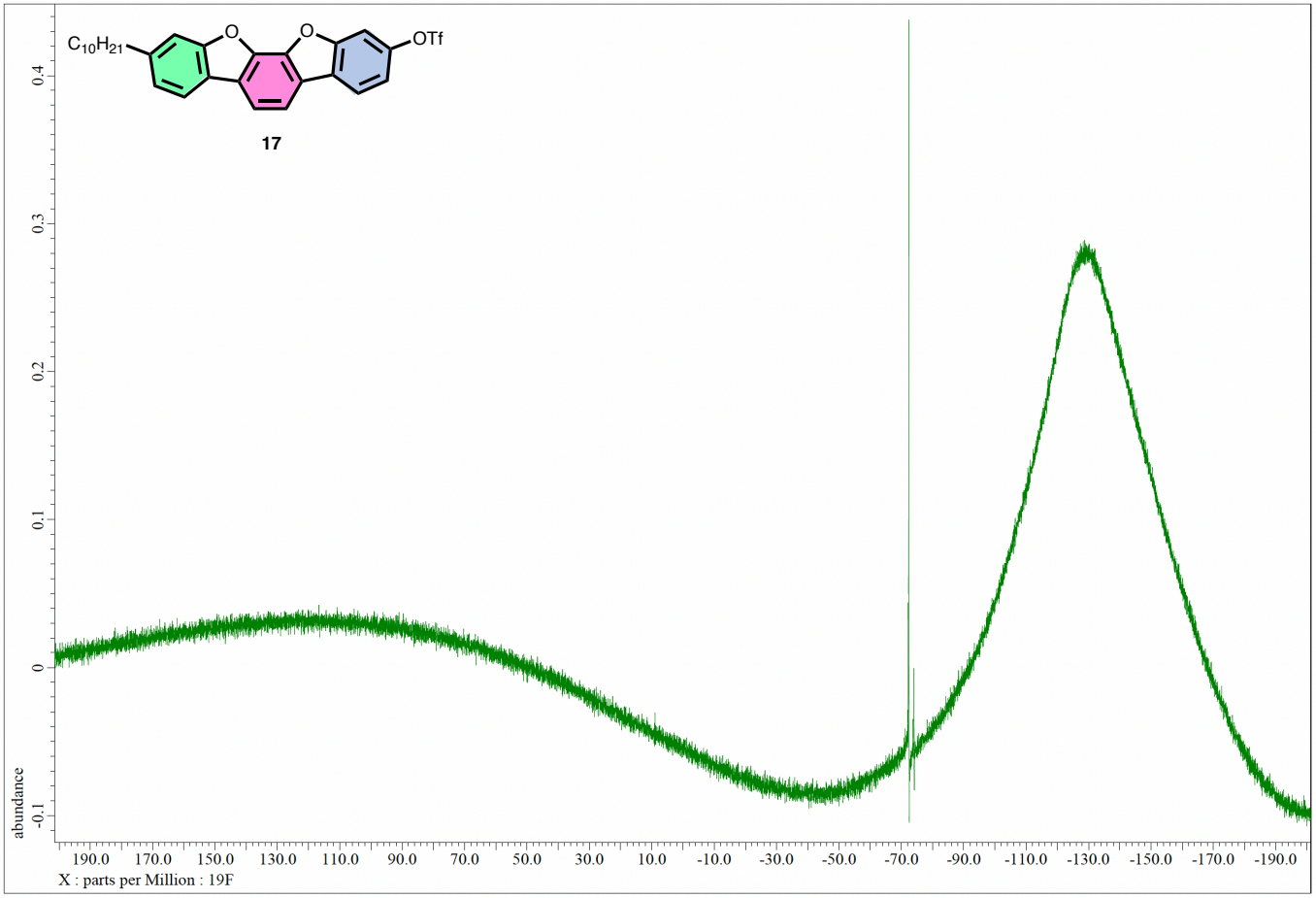


Figure S42. ^{19}F NMR Spectrum of 8-decyldibenzo[*d,d'*]benzo[2,1-*b*:3,4-*b'*]difuran-3-yltrifluoromethanesulfonate (**17**) (376 MHz, $CDCl_3$, r.t.).

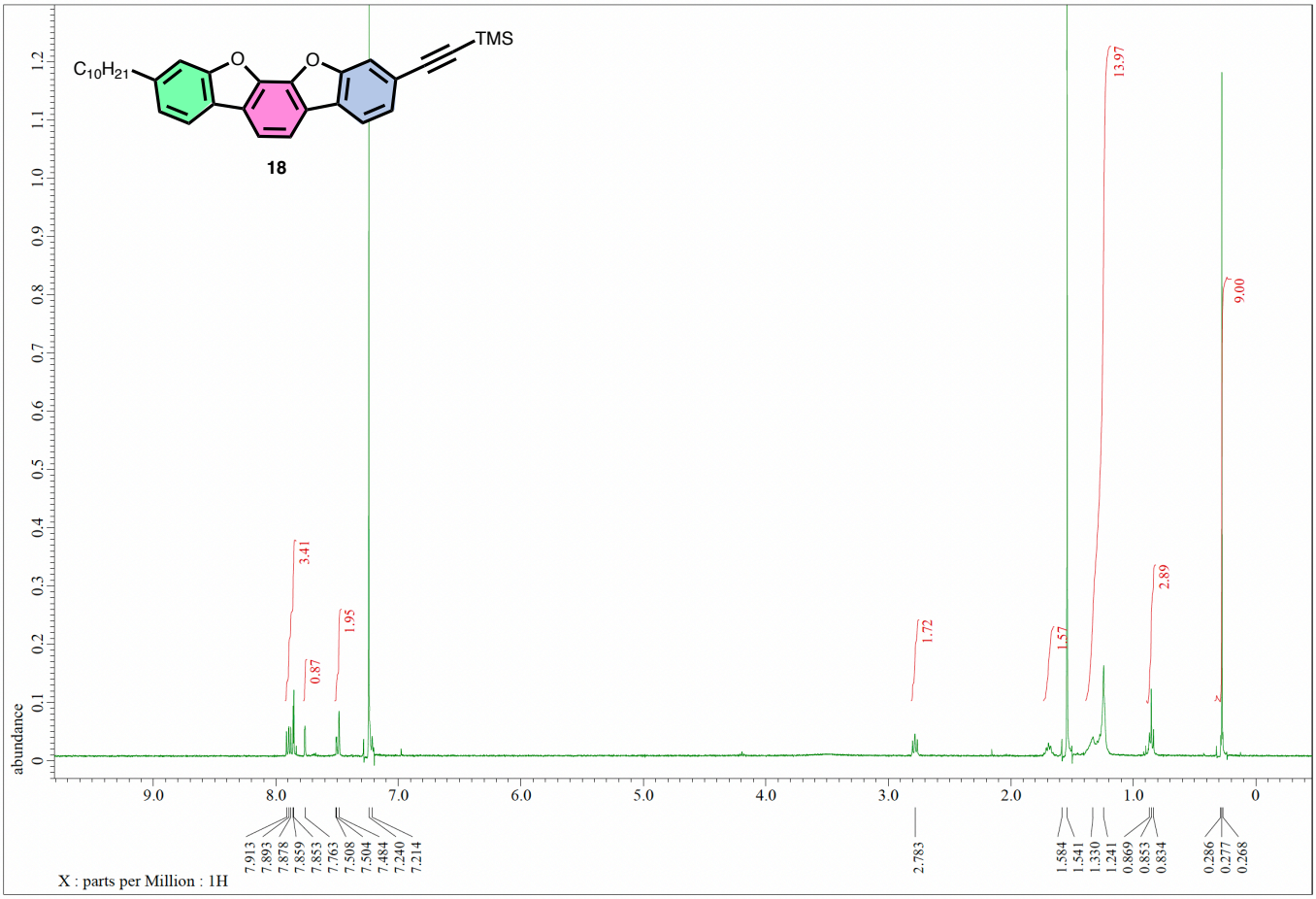


Figure S43. ^{1}H NMR Spectrum of 3-(trimethylsilylethynyl)-8-decyldibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**18**) (400 MHz, $CDCl_3$, r.t.).

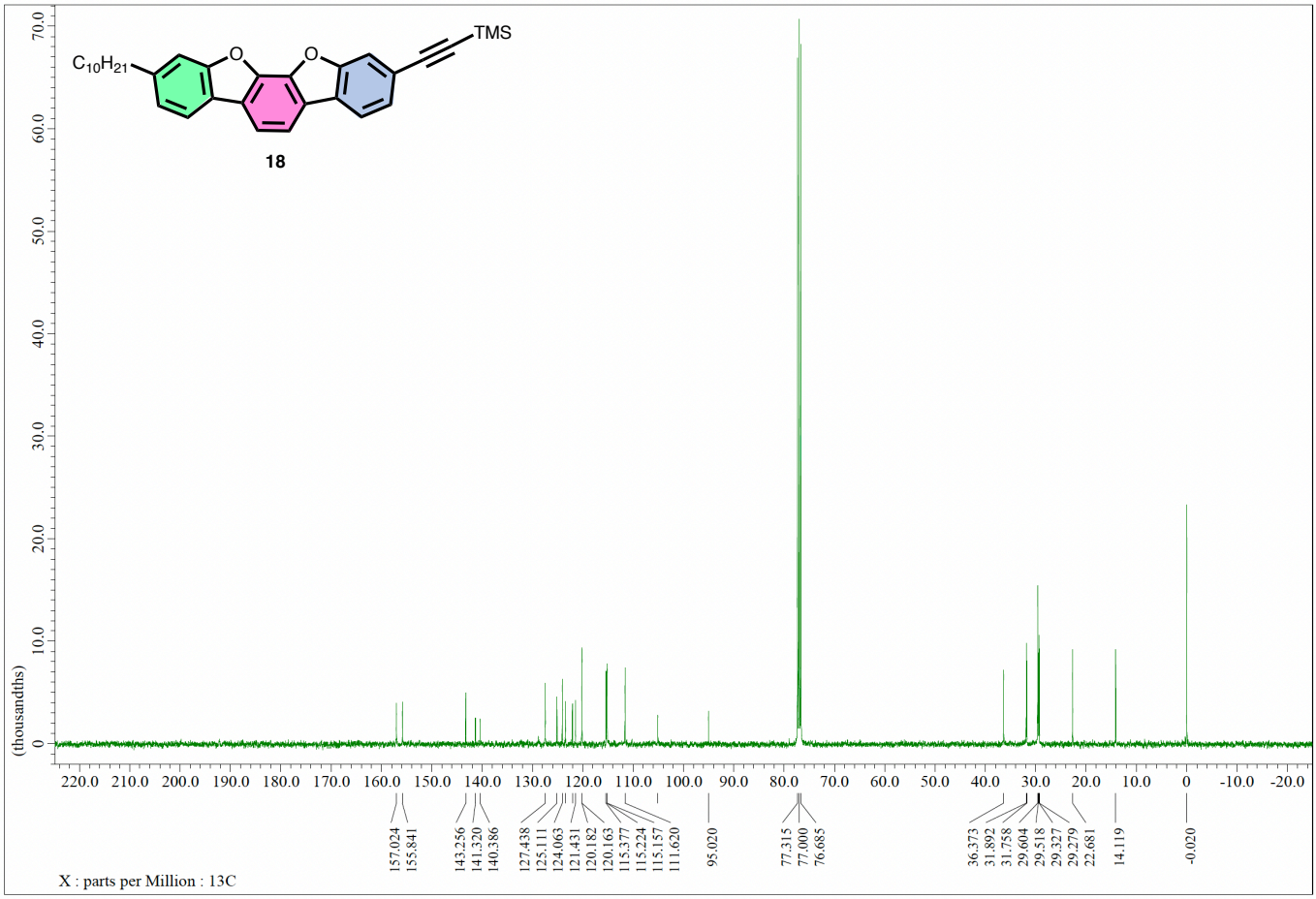


Figure S44. $^{13}C\{^{1}H\}$ NMR Spectrum of 3-(trimethylsilylethynyl)-8-decyldibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**18**) (100 MHz, $CDCl_3$, r.t.).

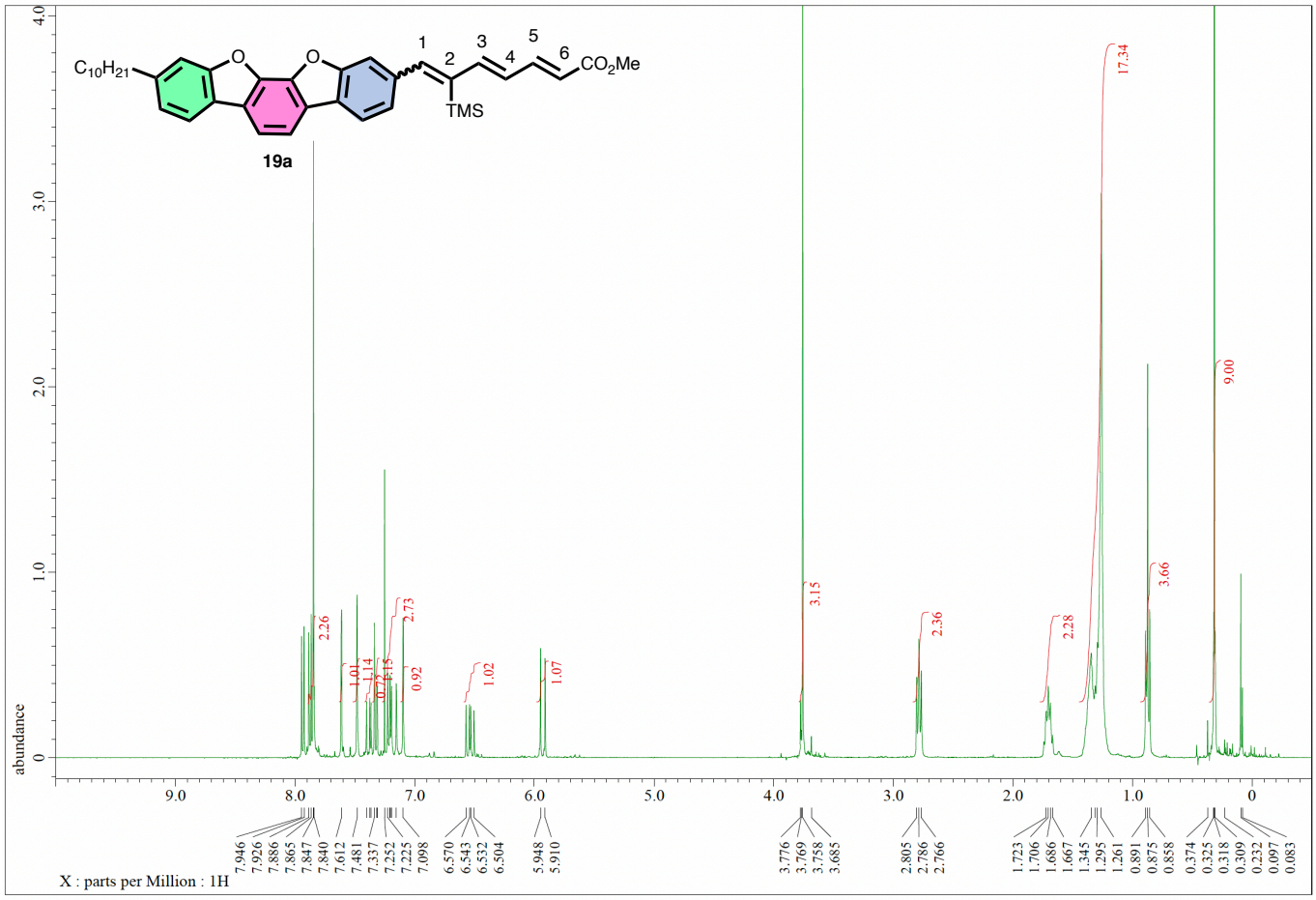


Figure S45. ^{1}H NMR Spectrum of 3-(6-methoxycarbonyl-2-trimethylsilylhexa-1,3,5-trien-1-yl)-8-decyldibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**19a**) (400 MHz, $CDCl_3$, r.t.).

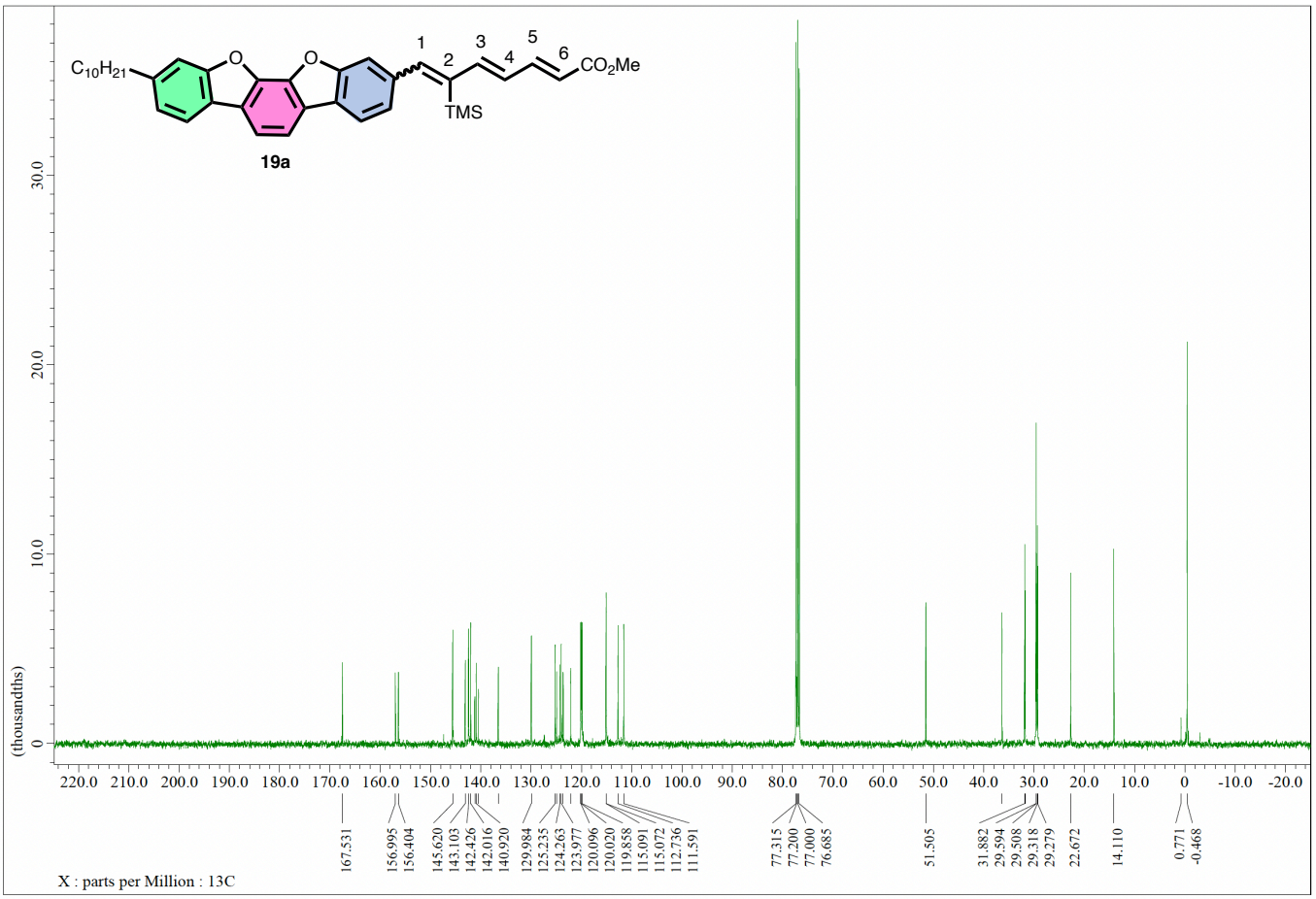
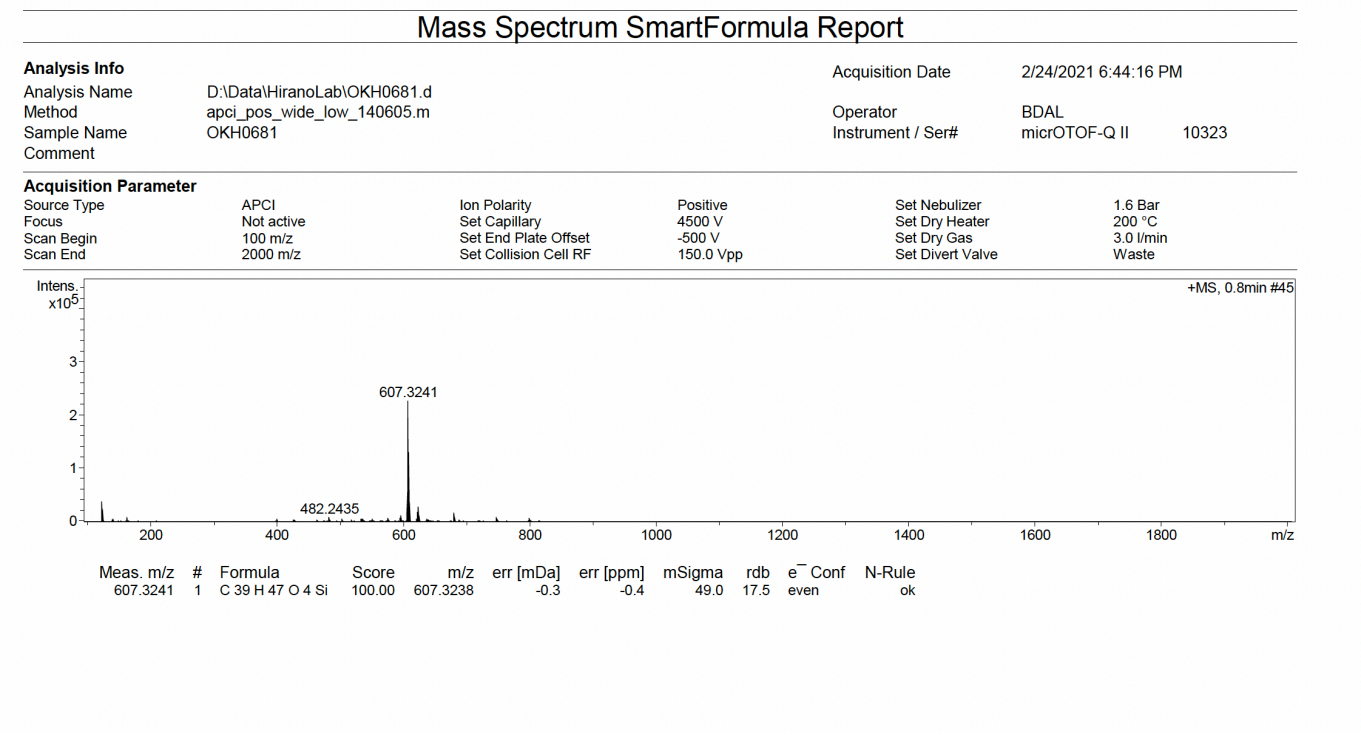
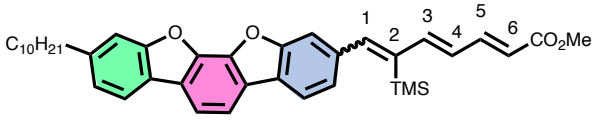


Figure S46. $^{13}C\{^{1}H\}$ NMR Spectrum of 3-(6-methoxycarbonyl-2-trimethylsilylhexa-1,3,5-trien-1-yl)-8-decyldibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**19a**) (100 MHz, $CDCl_3$, r.t.).





19a

Figure S47. High resolution mass spectrum (APCI) of 3-(6-methoxycarbonyl-2-trimethylsilylhexa-1,3,5-trien-1-yl)-8-decyldibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**19a**).

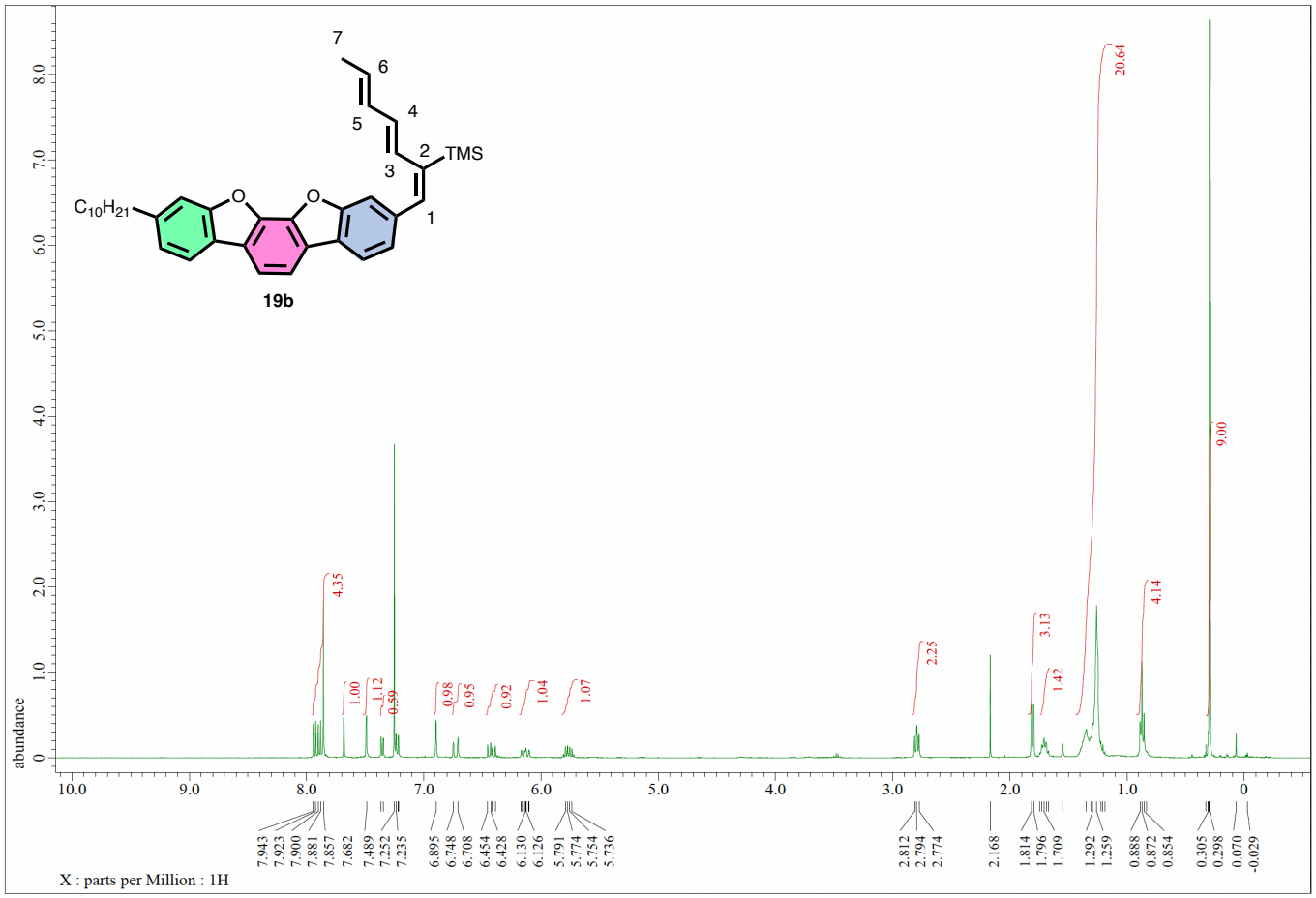


Figure S48. ^{1}H NMR Spectrum of 3-{(1*E*,3*E*,5*E*)-2-trimethylsilylhepta-1,3,5-trien-1-yl}-8-decyldibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**19b**) (400 MHz, $CDCl_3$, r.t.).

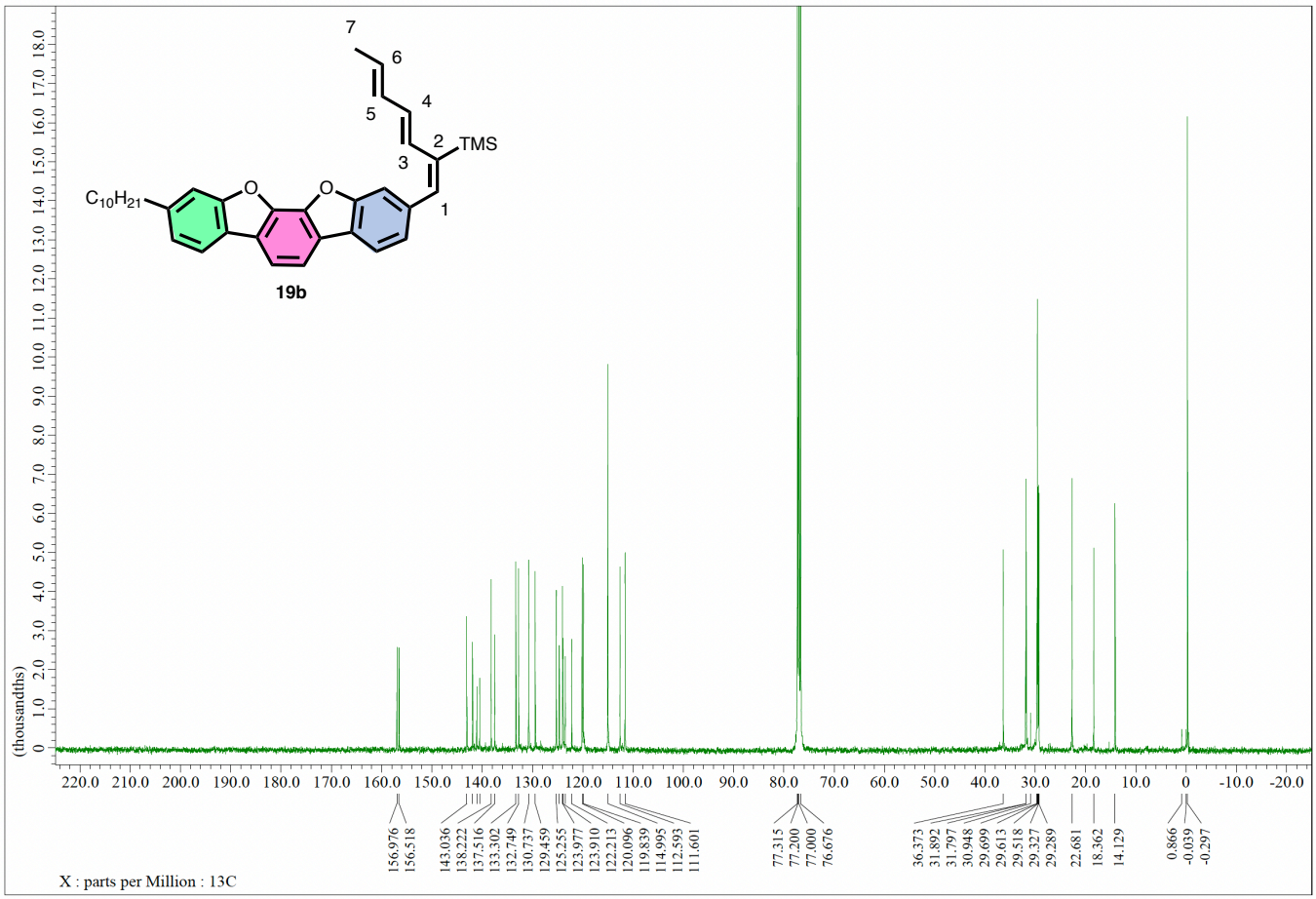
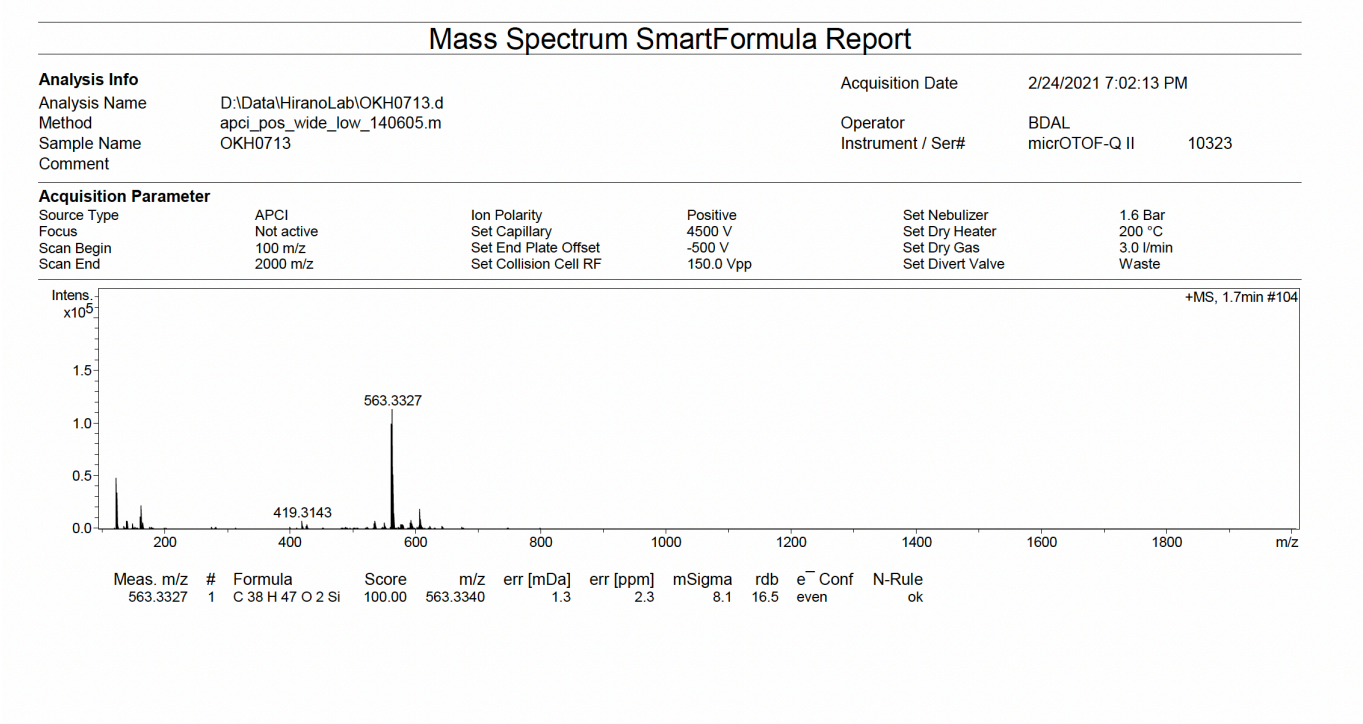
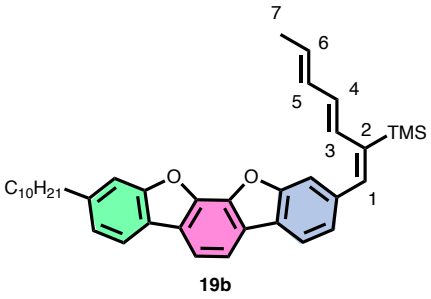


Figure S49. $^{13}C\{^{1}H\}$ NMR Spectrum of 3-{(1*E*,3*E*,5*E*)-2-trimethylsilylhepta-1,3,5-trien-1-yl}-8-decyldibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**19b**) (100 MHz, $CDCl_3$, r.t.).





19b

Figure S50. High resolution mass spectrum (APCI) of 3-{(1*E*,3*E*,5*E*)-2-trimethylsilylhepta-1,3,5-trien-1-yl}-8-decyldibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**19b**).

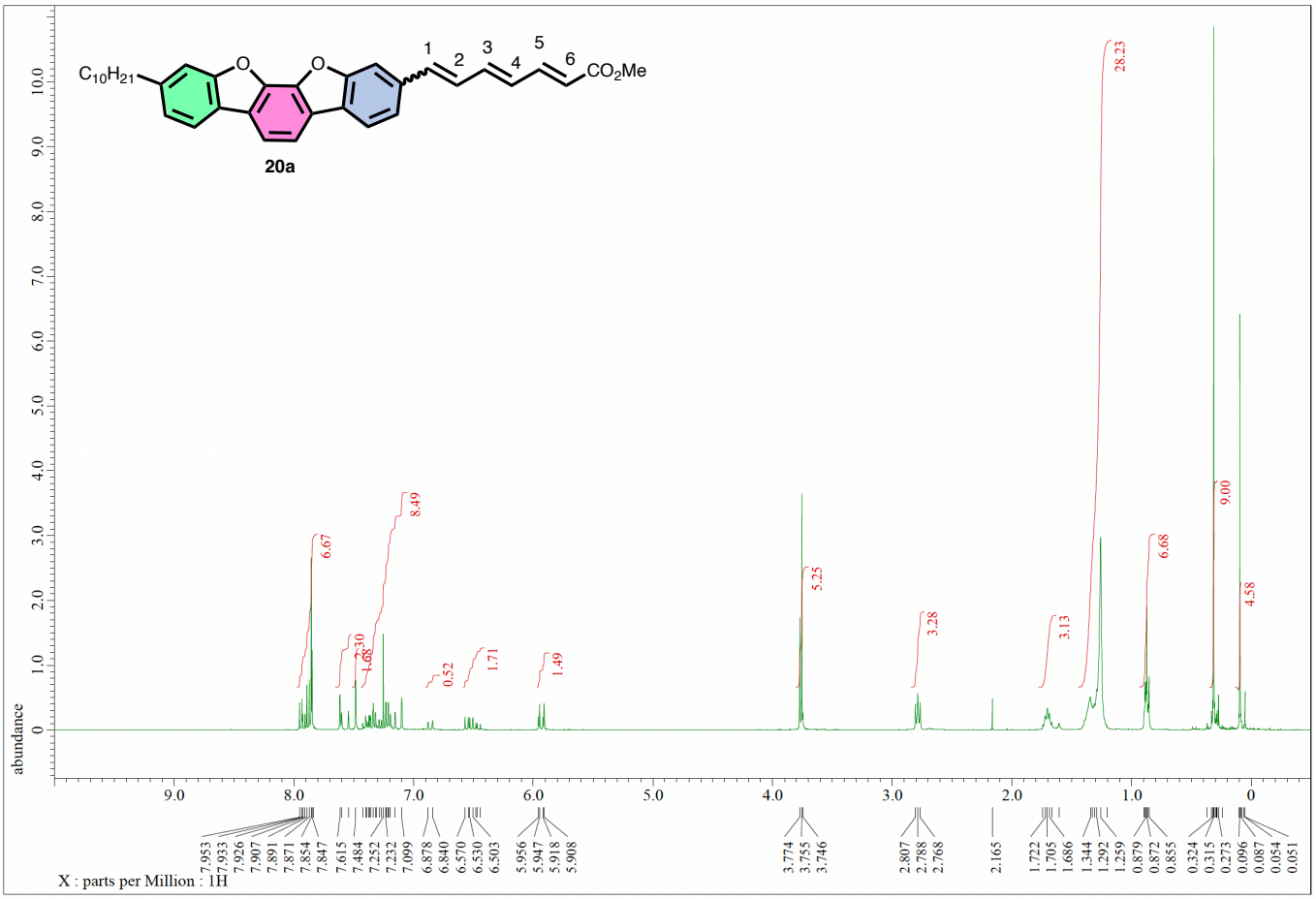


Figure S51. ^{1}H NMR Spectrum of 3-{(1*E*,3*E*,5*E*)-6-methoxycarbonylhepta-1,3,5-trien-1-yl}-8-decyldibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**20a**) (400 MHz, $CDCl_3$, r.t.).

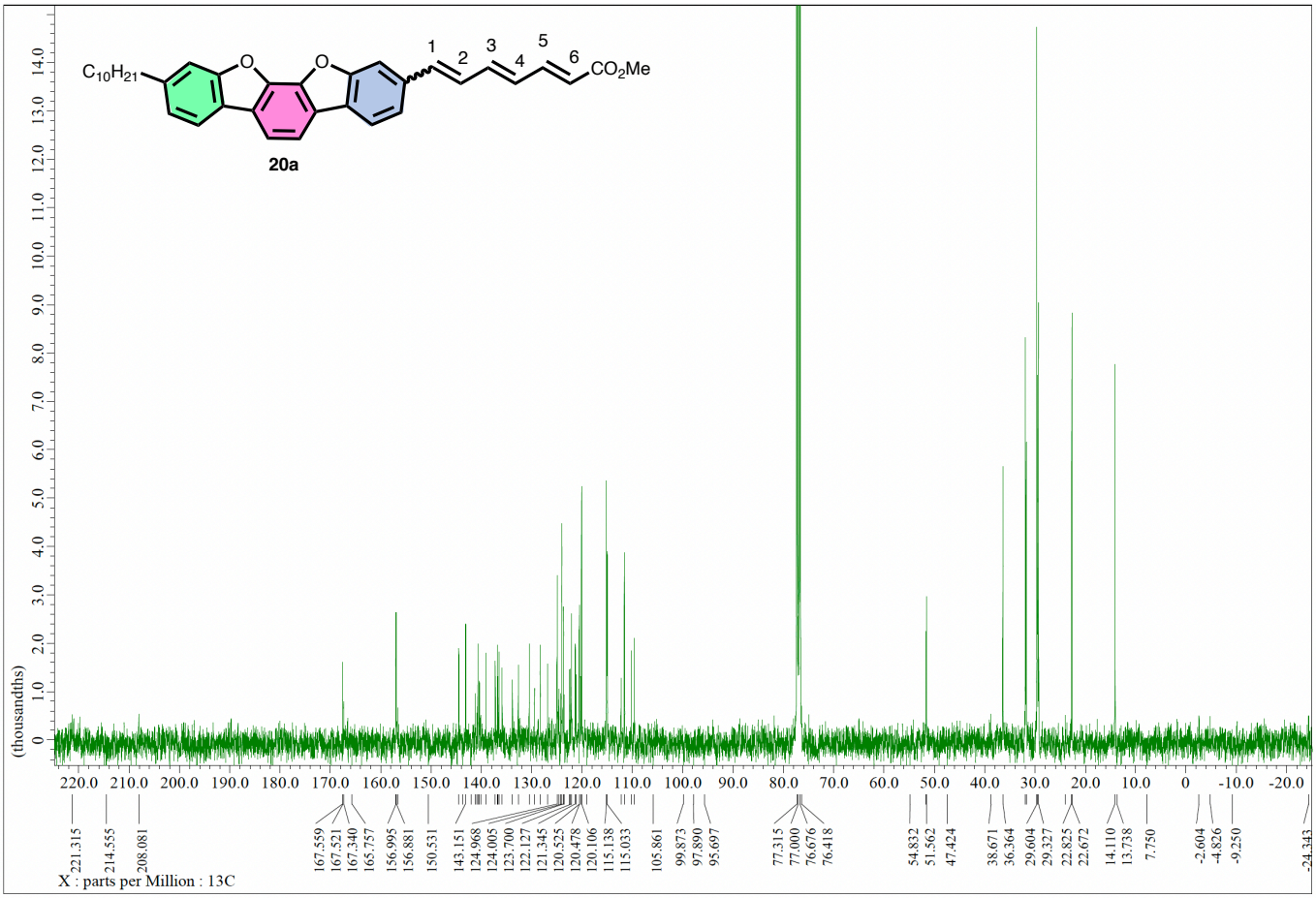


Figure S52. $^{13}C\{^{1}H\}$ NMR Spectrum of 3-{(1*E*,3*E*,5*E*)-6-methoxycarbonylhepta-1,3,5-trien-1-yl}-8-decyldibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**20a**) (100 MHz, $CDCl_3$, r.t.).

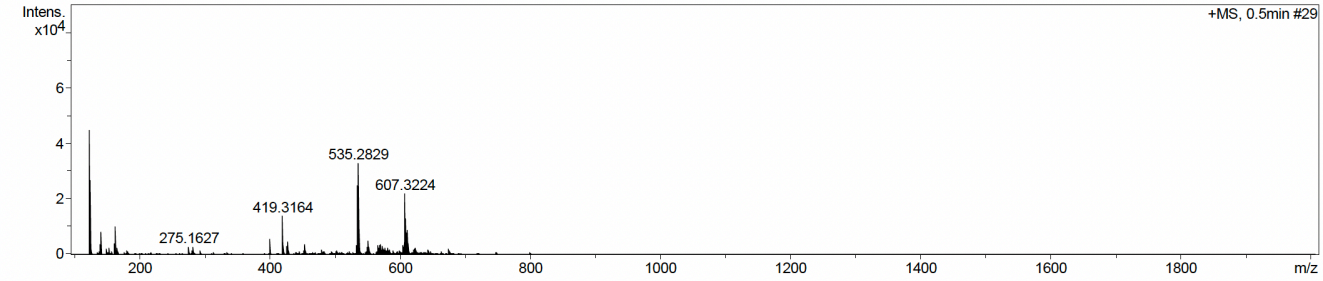
Mass Spectrum SmartFormula Report

Analysis Info

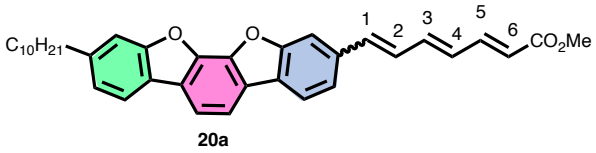
Analysis Name	D:\Data\HiranoLab\OKH0715.d	Acquisition Date	2/24/2021 6:55:02 PM
Method	apci_pos_wide_low_140605.m	Operator	BDAL
Sample Name	OKH0715	Instrument / Ser#	micrOTOF-Q II 10323
Comment			

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
535.2829	1	C 36 H 39 O 4	100.00	535.2843	1.3	2.5	30.5	17.5	even	ok
	2	C 37 H 35 N 4	34.65	535.2856	2.7	5.0	32.0	22.5	even	ok
	3	C 32 H 35 N 6 O 2	80.99	535.2816	-1.3	-2.5	38.7	18.5	even	ok
	4	C 31 H 39 N 2 O 6	24.86	535.2803	-2.7	-5.0	44.3	13.5	even	ok



20a

Figure S53. High resolution mass spectrum (APIC) of 3-{(1*E*,3*E*,5*E*)-6-methoxycarbonylhepta-1,3,5-trien-1-yl}-8-decyldibenzo[*d*,*d'*]benzo[2,1-*b*:3,4-*b'*]difuran (**20a**).

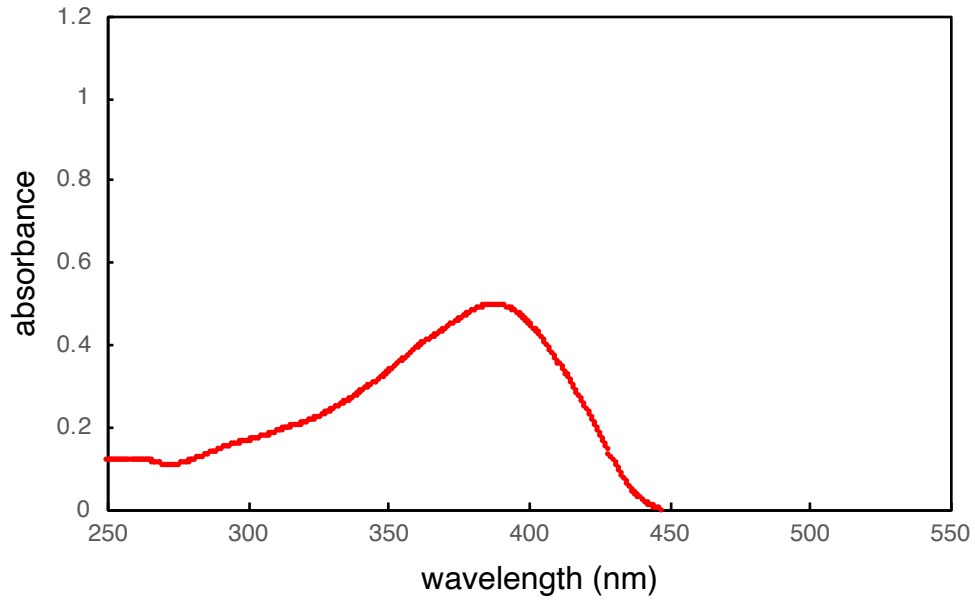


Figure S54. UV-vis spectrum of **9a** (1.00 x 10^{-5} M) in chloroform.

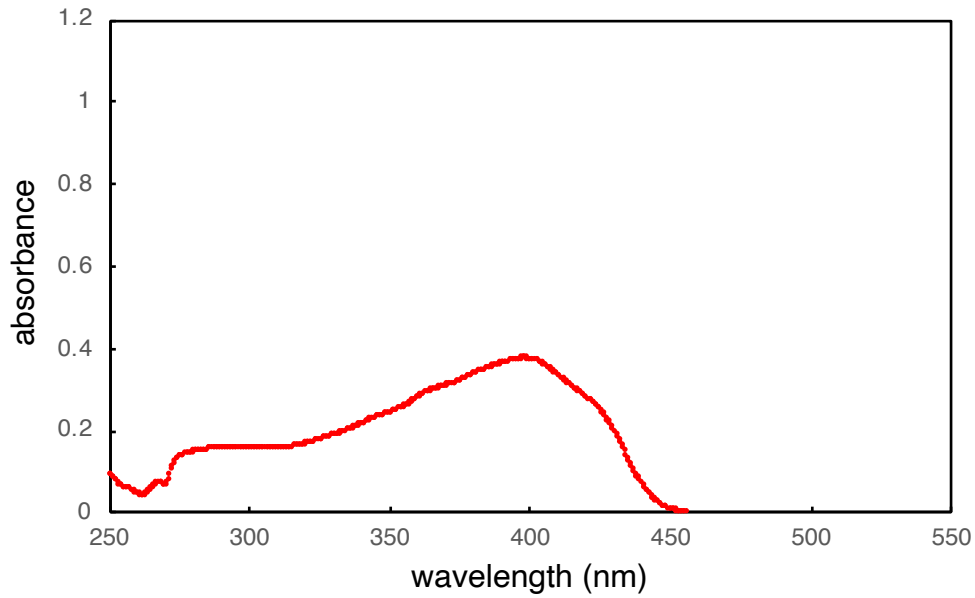


Figure S55. UV-vis spectrum of **10b** (1.00 x 10^{-5} M) in chloroform.

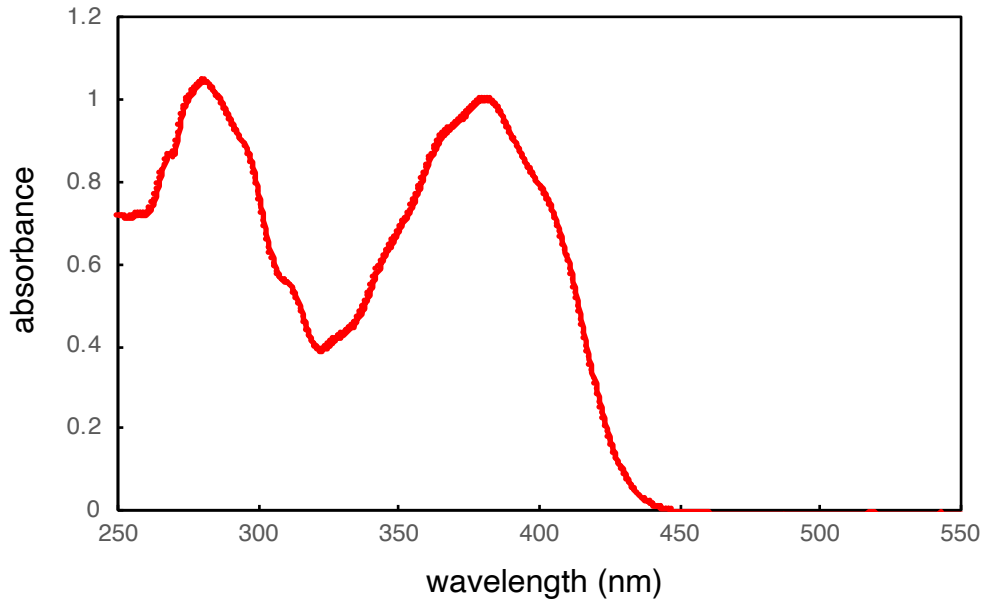


Figure S56. UV-vis spectrum of **20a** (1.00 x 10^{-5} M) in chloroform.

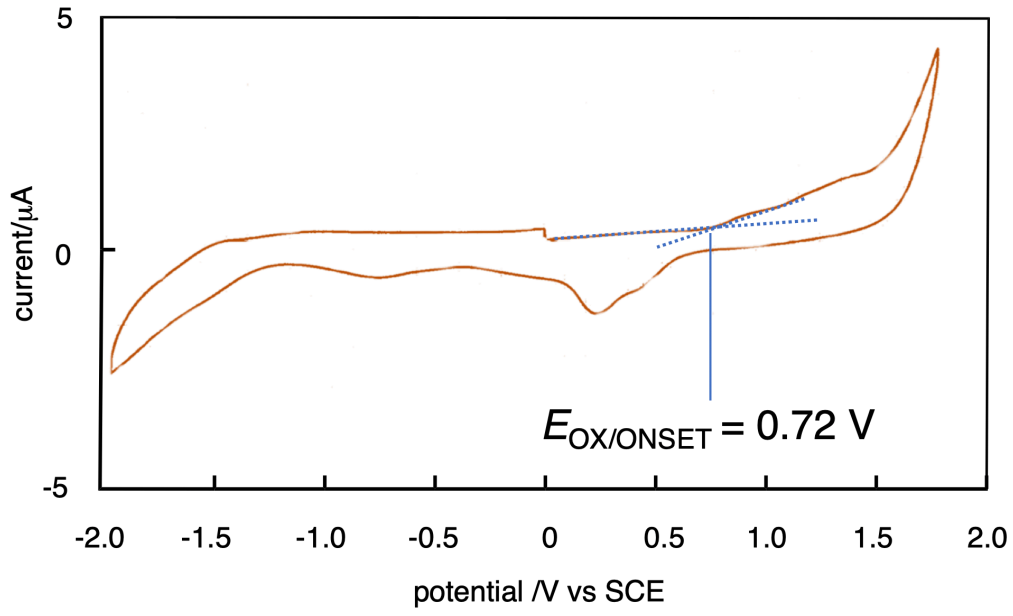


Figure S57. Cyclic voltammogram of **9a** in a dichloromethane solution at the Pt electrodes with $[Bu_4N][ClO_4]$ (0.1 M) as the supporting electrolyte at a sweep rate of 50 m Vs^{-1}. Platinum was employed as the working electrode, and the potential scale was corrected with the standard redox potential of ferrocene (E = +0.380 V).

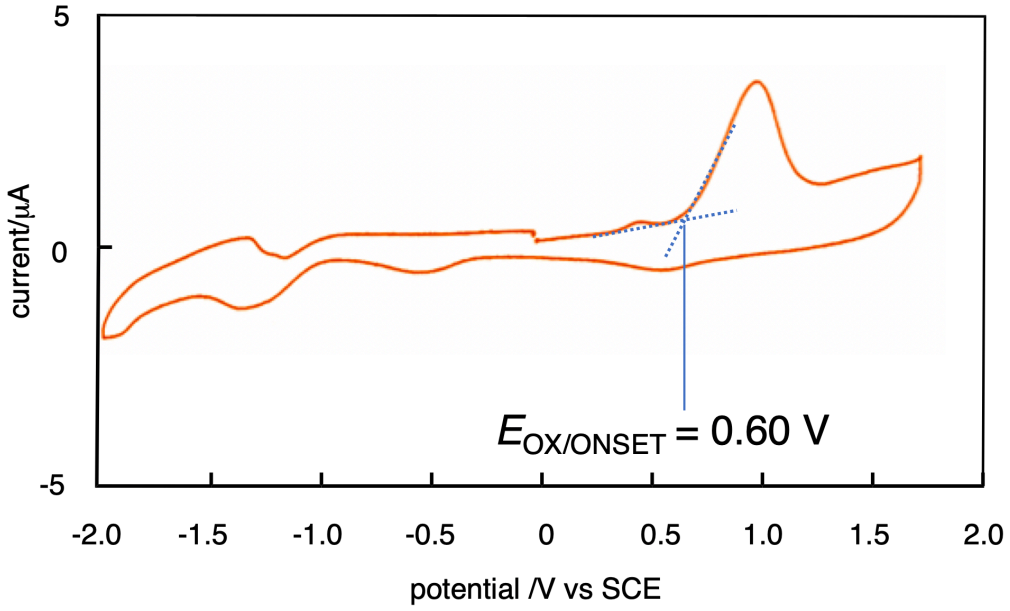


Figure S58. Cyclic voltammogram of **10b** in a dichloromethane solution at the Pt electrodes with $[Bu_4N][ClO_4]$ (0.1 M) as the supporting electrolyte at a sweep rate of 50 m Vs^{-1}. Platinum was employed as the working electrode, and the potential scale was corrected with the standard redox potential of ferrocene (*E* = +0.380 V).

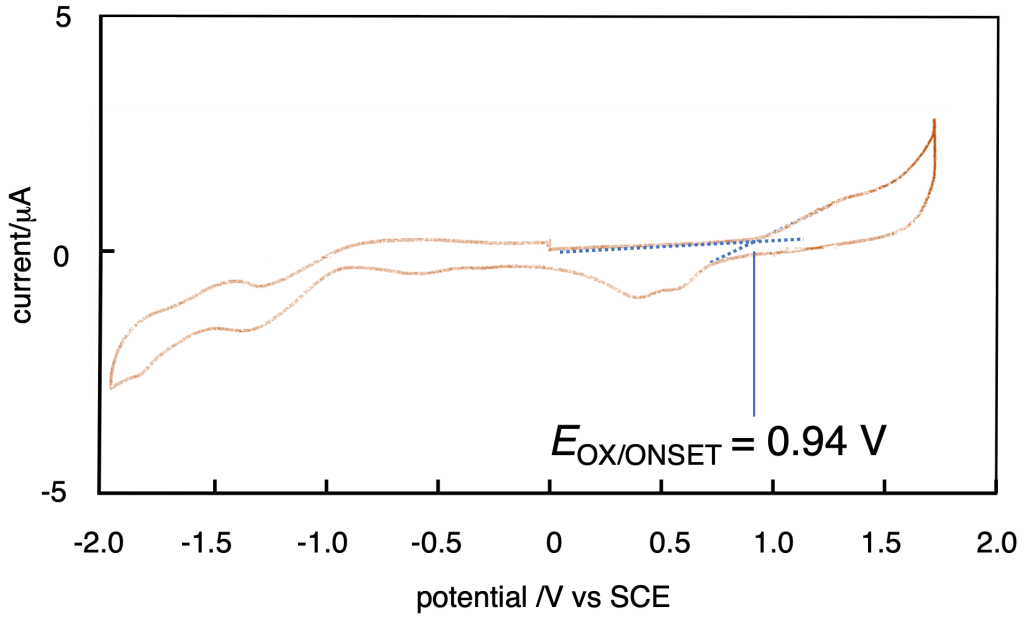


Figure S59. Cyclic voltammogram of **20a** in a dichloromethane solution at the Pt electrodes with $[Bu_4N][ClO_4]$ (0.1 M) as the supporting electrolyte at a sweep rate of 50 m Vs^{-1}. Platinum was employed as the working electrode, and the potential scale was corrected with the standard redox potential of ferrocene (*E* = +0.380 V).

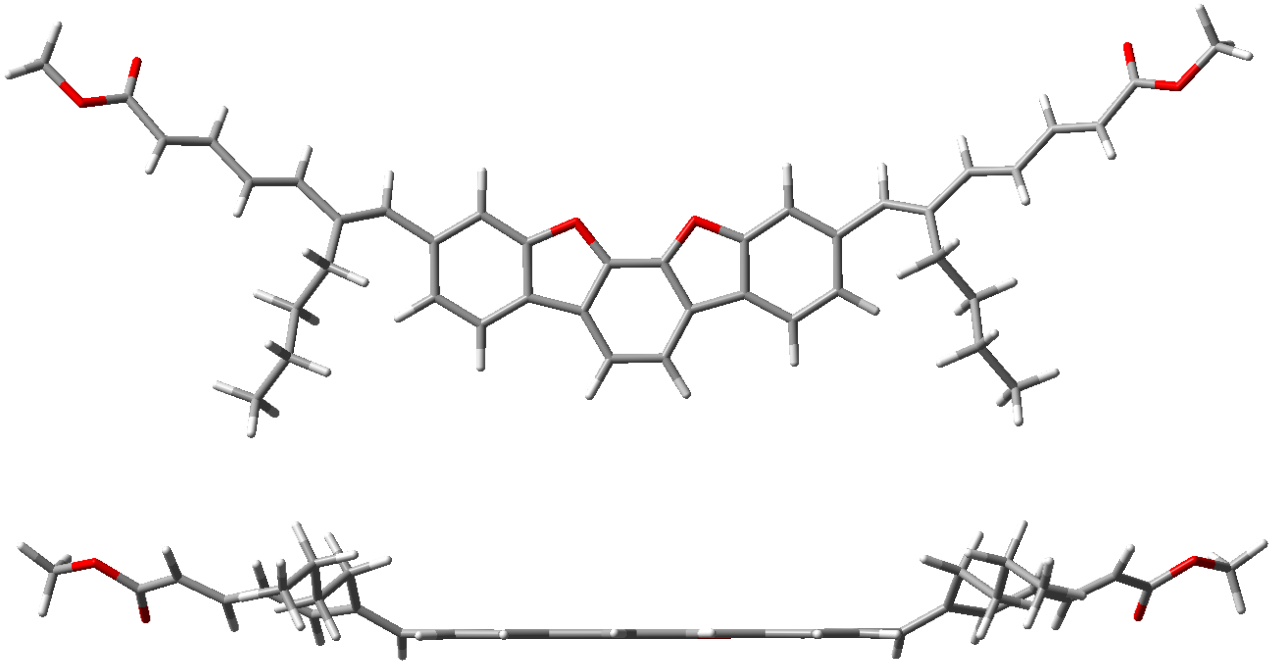


Figure S60. Top and side views of TD-DFT calculations of **9a** of isomer A (the most stable isomer). ΔH° = 0 kcal mol^{-1}, ΔG° = 0 kcal mol^{-1}.

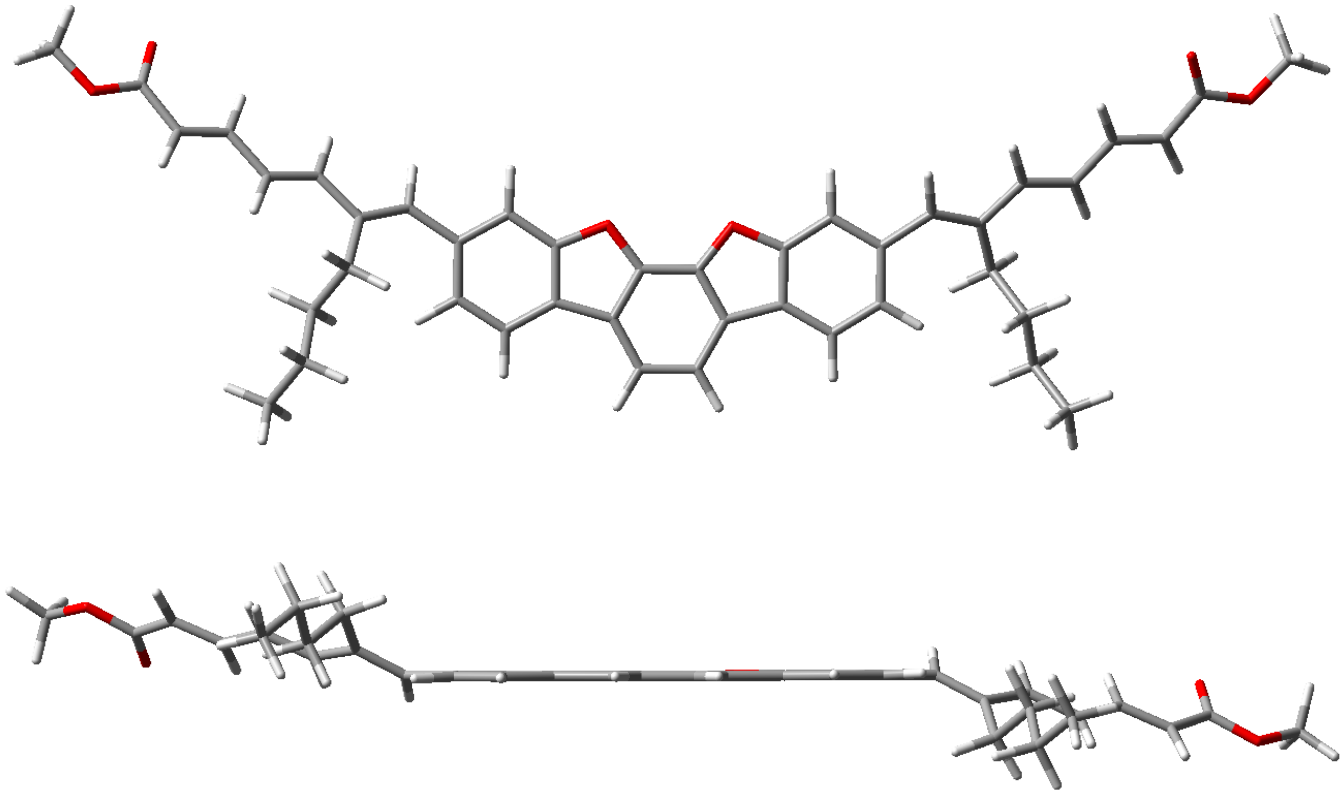
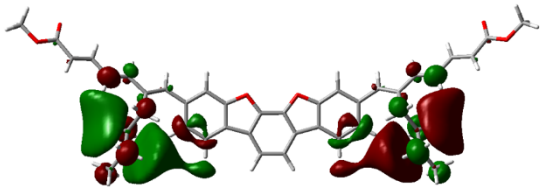
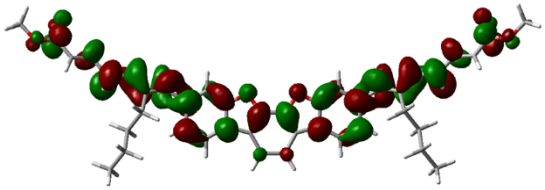


Figure S61. Top and side views of TD-DFT calculations of **9a** of isomer B (the second stable isomer).ΔH° = 0.064 kcal mol^{-1}, ΔG° = 0.087 kcal mol^{-1}.

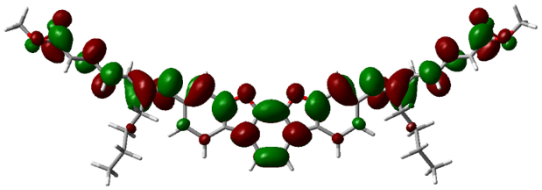
LUMO+9 (181) 2.9646 eV



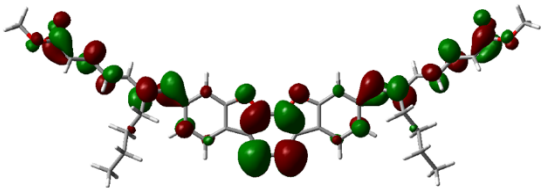
LUMO+8 (180) 2.7073 eV



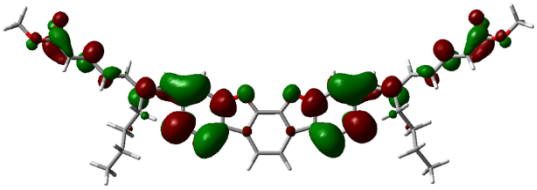
LUMO+7 (179) 2.1212 eV



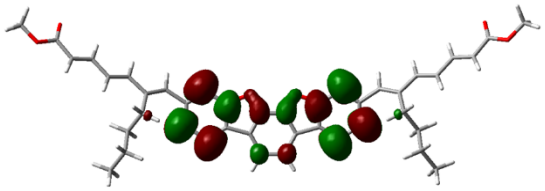
LUMO+6 (178) 1.7727 eV



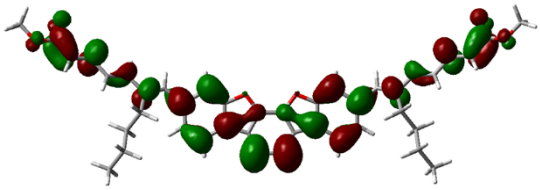
LUMO+5 (177) 1.5053 eV



LUMO+4 (176) 1.4693 eV



LUMO+3 (175) 1.0007 eV



LUMO+2 (174) 0.3062 eV

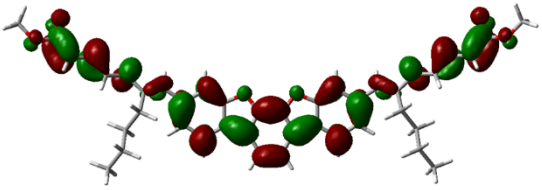
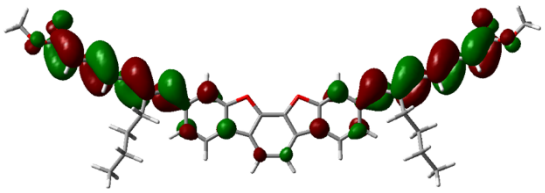
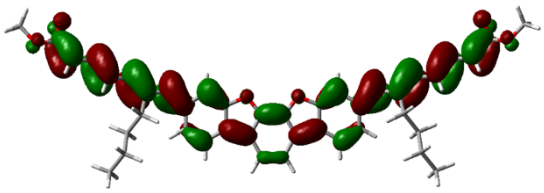


Figure S62. Selected orbitals by TD-DFT calculations of isomer A of **9a** in chloroform. Orbital numbers in parenthesis and orbital energy in eV.

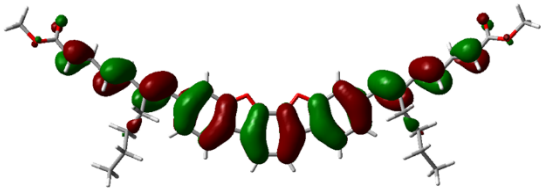
LUMO+1 (173) -0.5349 eV



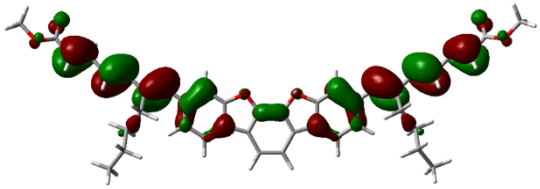
LUMO (172) -0.7634 eV



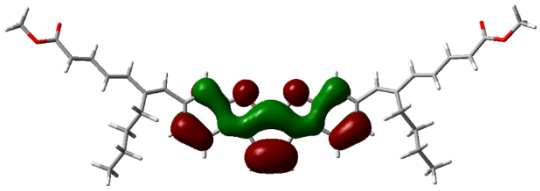
HOMO (171) -7.4018 eV



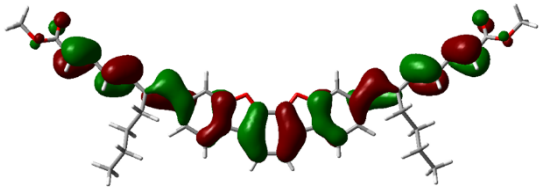
HOMO-1 (170) -7.8474 eV



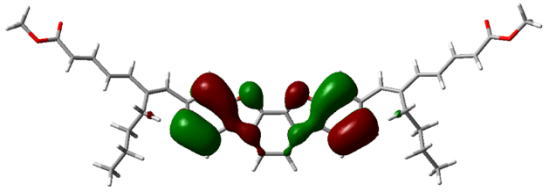
HOMO-2 (169) -8.3348 eV



HOMO-3 (168) -8.5436 eV



HOMO-4 (167) -9.0632 eV



HOMO-5 (166) -9.4058 eV

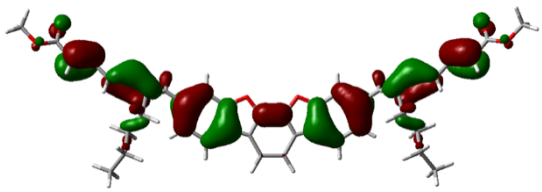
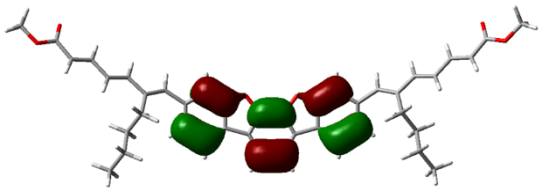
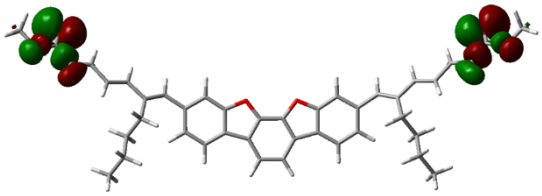


Figure S62. continued.

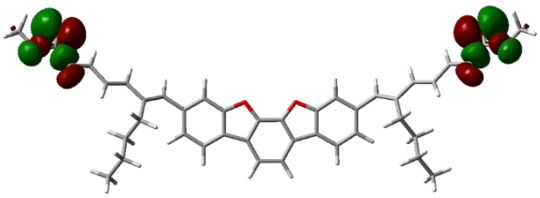
HOMO-6 (165) -9.6846 eV



HOMO-7 (164) -9.9937 eV



HOMO-8 (163) -9.9943 eV



HOMO-9 (162) -10.0257 eV

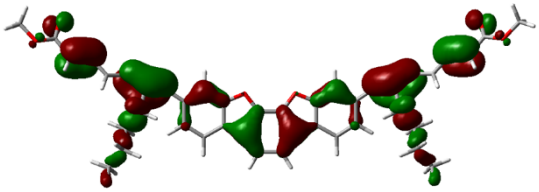
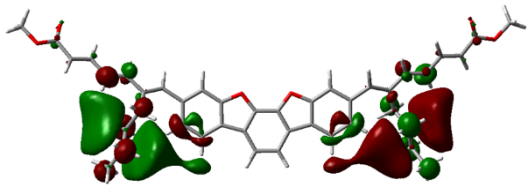
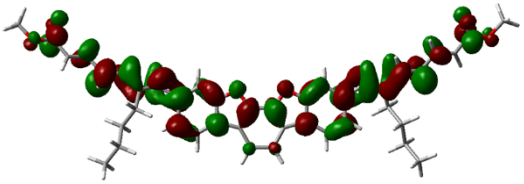


Figure S62. continued.

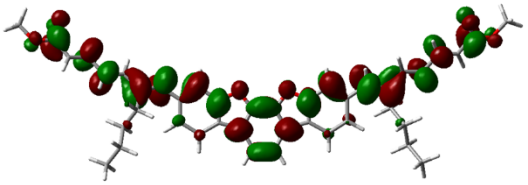
LUMO+9 (181) 2.9633 eV



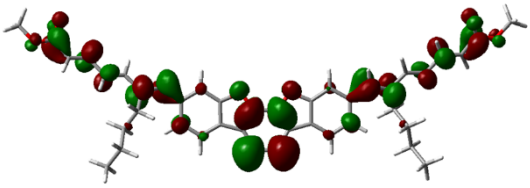
LUMO+8 (180) 2.7182 eV



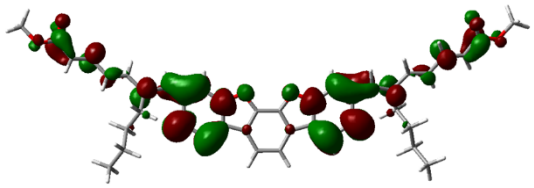
LUMO+7 (179) 2.1252 eV



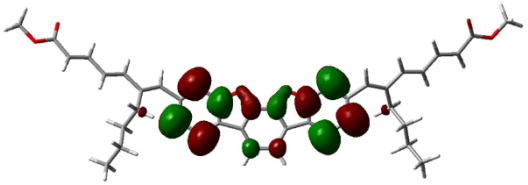
LUMO+6 (178) 1.7709 eV



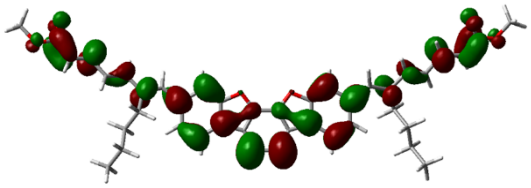
LUMO+5 (177) 1.5007 eV



LUMO+4 (176) 1.4681 eV



LUMO+3 (175) 1.0000 eV



LUMO+2 (174) 0.3102 eV

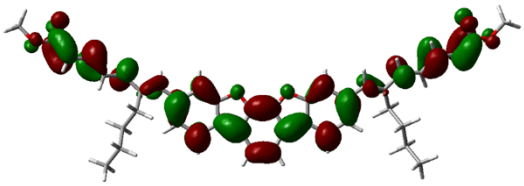
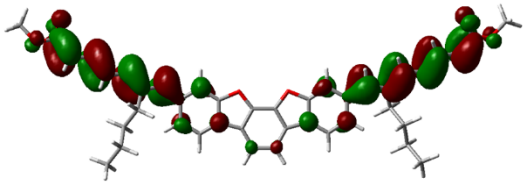
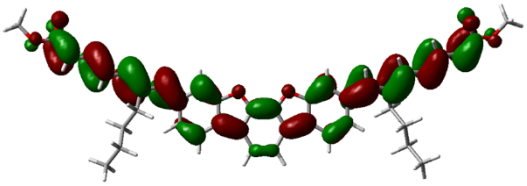


Figure S63. Selected orbitals by TD-DFT calculations of isomer B of **9a** in chloroform. Orbital numbers in parenthesis and orbital energy in eV.

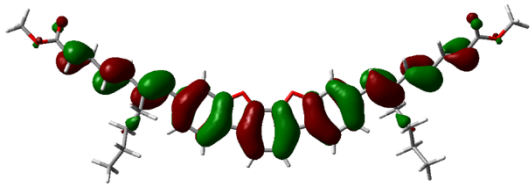
LUMO+1 (173) -0.5380 eV



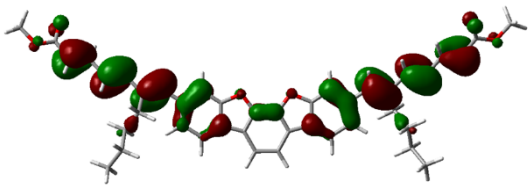
LUMO (172) -0.7704 eV



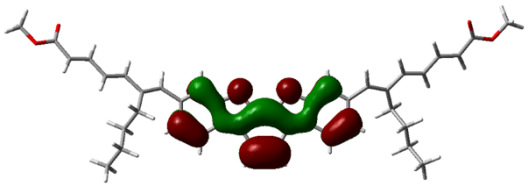
HOMO (171) -7.3948 eV



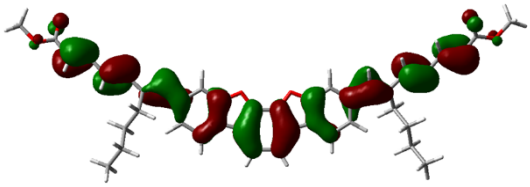
HOMO-1 (170) -7.8418 eV



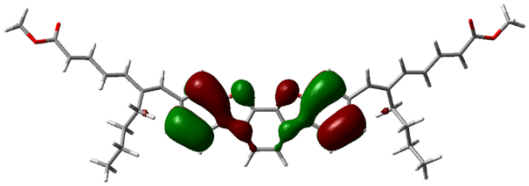
HOMO-2 (169) -8.3352 eV



HOMO-3 (168) -8.5480 eV



HOMO-4 (167) -9.0639 eV



HOMO-5 (166) -9.4065 eV

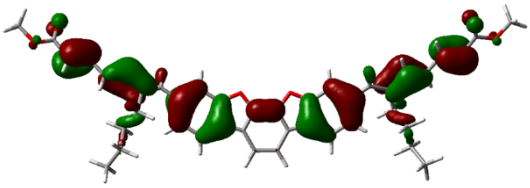
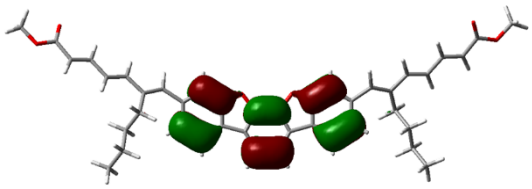
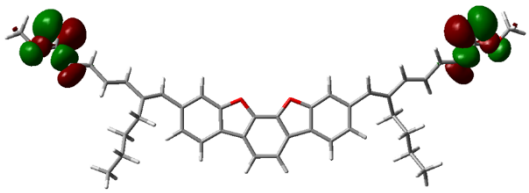


Figure S63. continued.

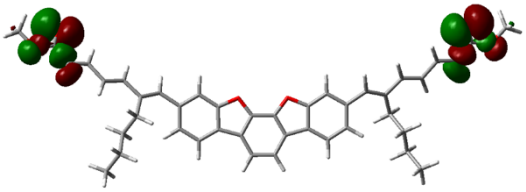
HOMO-6 (165) -9.6852 eV



HOMO-7 (164) -9.9927 eV



HOMO-8 (163) -9.9932 eV



HOMO-9 (162) -10.0237 eV

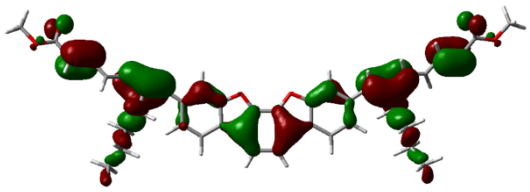


Figure S63. continued.

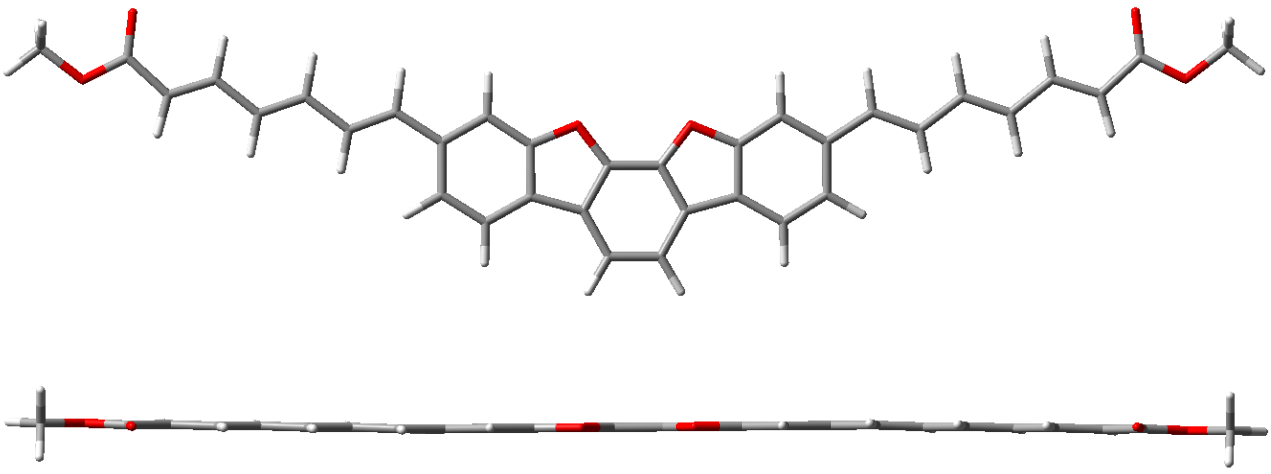
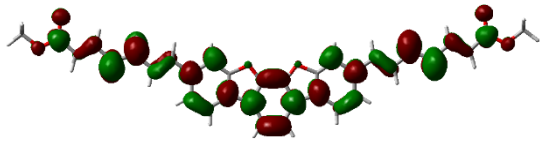
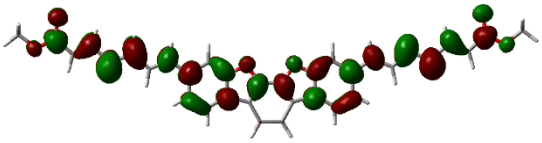


Figure S64. Top and side views of TD-DFT calculations of **10b**.

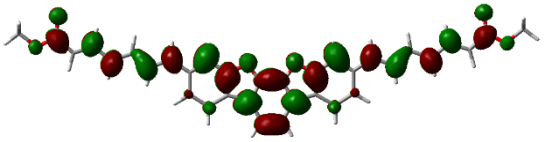
LUMO+9 (149) 3.2453 eV



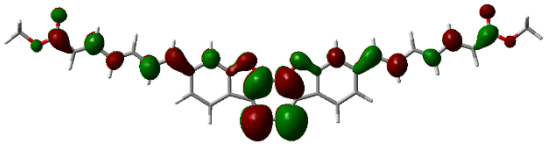
LUMO+8 (148) 2.9459 eV



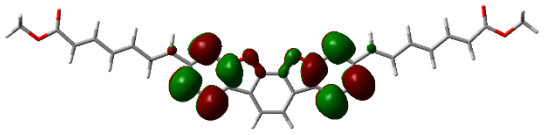
LUMO+7 (147) 2.2357 eV



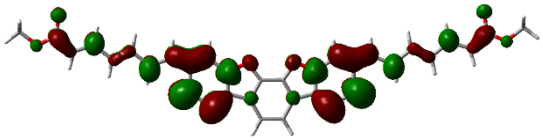
LUMO+6 (146) 1.7459 eV



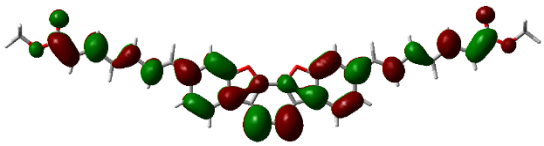
LUMO+5 (145) 1.4278 eV



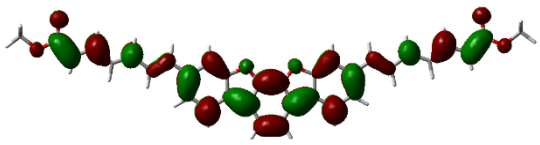
LUMO+4 (144) 1.3611 eV



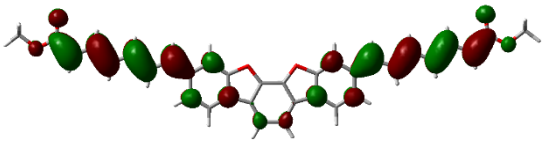
LUMO+3 (143) 0.9935 eV



LUMO+2 (142) 0.3801 eV



LUMO+1 (141) -0.6928 eV



LUMO (140) -0.9546 eV

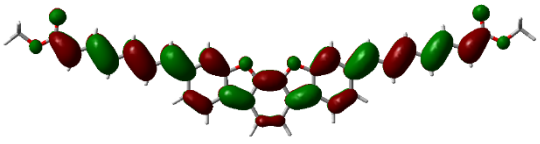
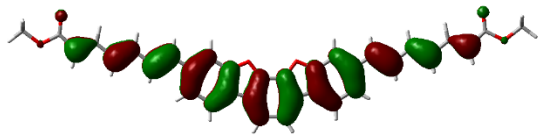
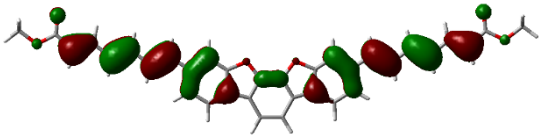


Figure S65. Selected orbitals by TD-DFT calculations of **10b** in chloroform. Orbital numbers in parenthesis and orbital energy in eV.

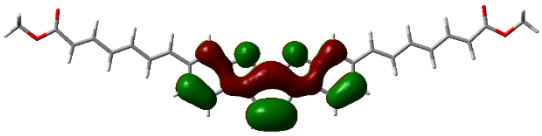
HOMO (139) -7.3104 eV



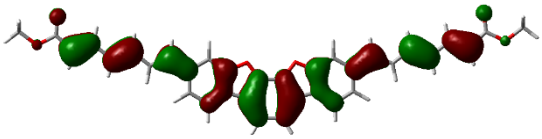
HOMO-1 (138) -7.8057 eV



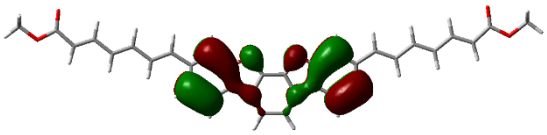
HOMO-2 (137) -8.3659 eV



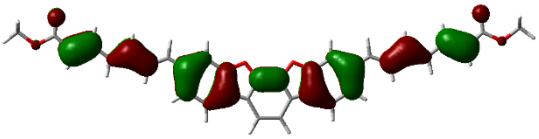
HOMO-3 (136) -8.6947 eV



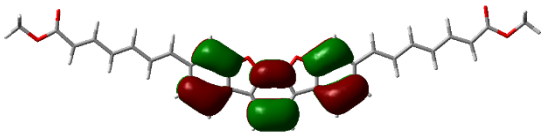
HOMO-4 (135) -9.1159 eV



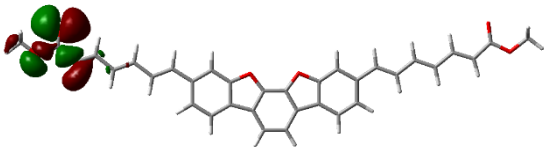
HOMO-5 (134) -9.5633 eV



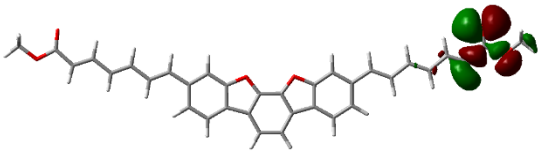
HOMO-6 (133) -9.7273 eV



HOMO-7 (132) -10.0087 eV



HOMO-8 (131) -10.0087 eV



HOMO-9 (130) -10.2688 eV

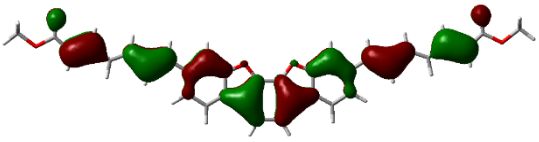


Figure S65. continued.

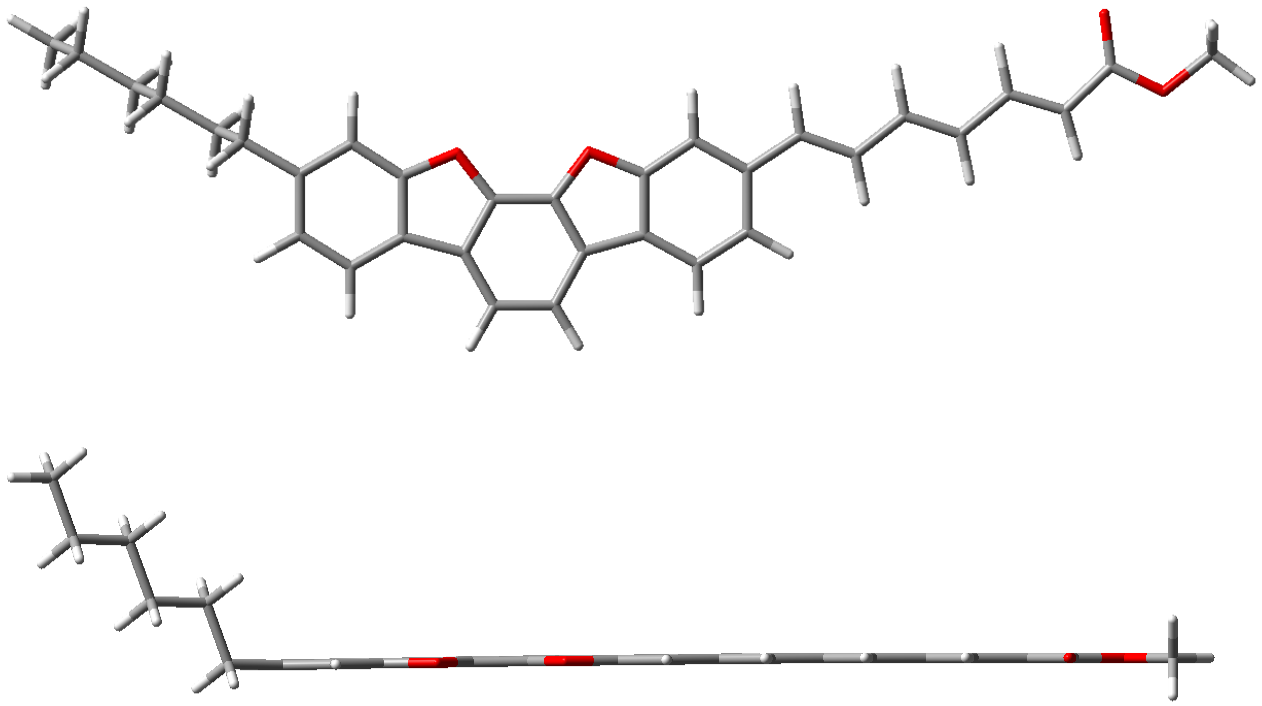
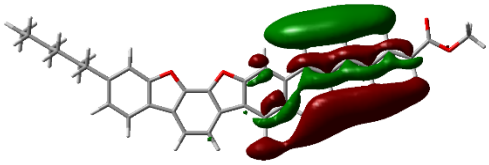
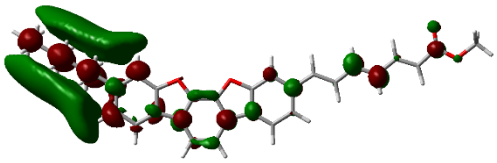


Figure S66. Top and side views of TD-DFT calculations of **21a**.

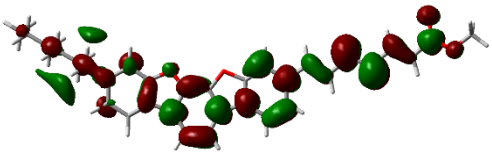
LUMO+9 (137) 3.2963 eV



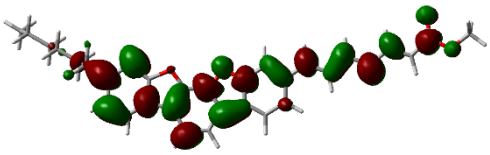
LUMO+8 (136) 3.2657 eV



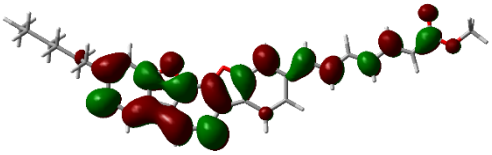
LUMO+7 (135) 3.2011 eV



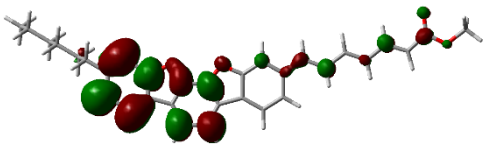
LUMO+6 (134) 2.6539 eV



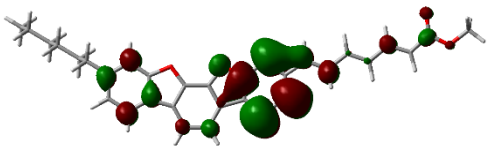
LUMO+5 (133) 1.9789 eV



LUMO+4 (132) 1.6174 eV



LUMO+3 (131) 1.4461 eV



LUMO+2 (130) 1.0913 eV

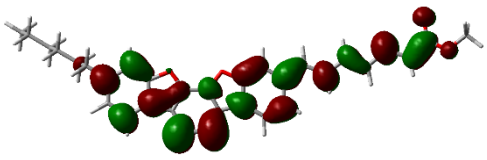
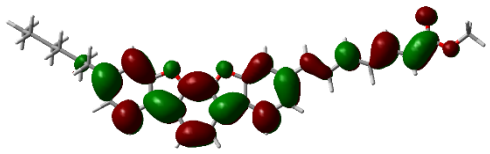
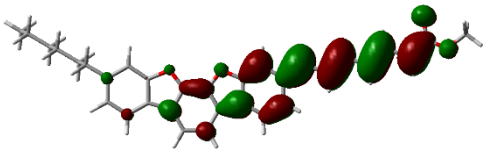


Figure S67. Selected orbitals by TD-DFT calculations of **21a** in chloroform. Orbital numbers in parenthesis and orbital energy in eV.

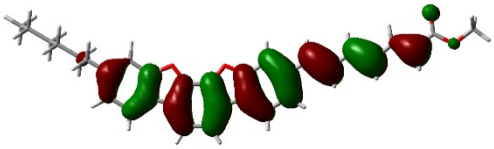
LUMO+1 (129) 0.3315 eV



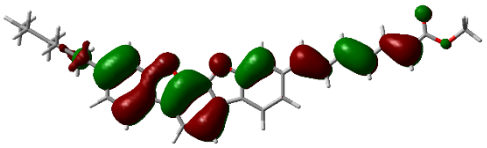
LUMO (128) -0.8205 eV



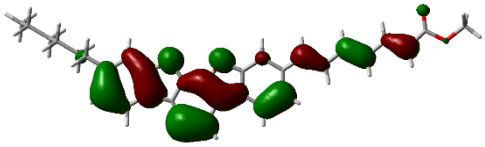
HOMO (127) -7.3991 eV



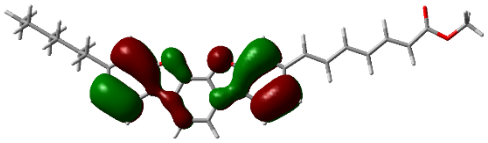
HOMO-1 (126) -8.2316 eV



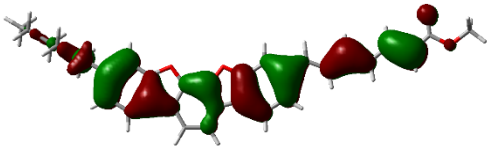
HOMO-2 (125) -8.2895 eV



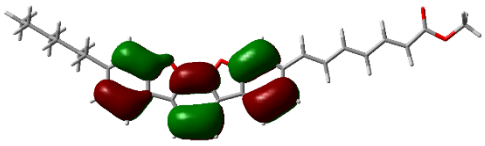
HOMO-3 (124) -9.0030 eV



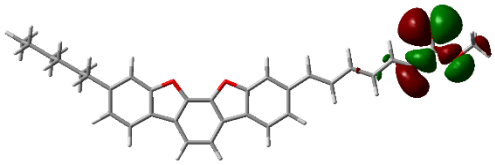
HOMO-4 (123) -9.3671 eV



HOMO-5 (122) -9.6339 eV



HOMO-6 (121) -10.0037 eV



HOMO-7 (120) -10.2793 eV

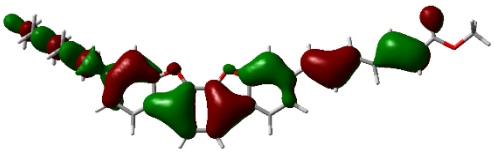
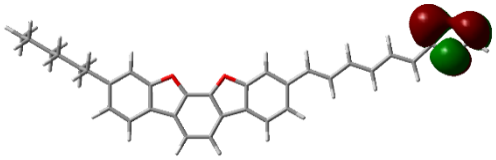


Figure S67. continued.

HOMO-8 (119) -10.6376 eV



HOMO-9 (118) - -10.7496 eV

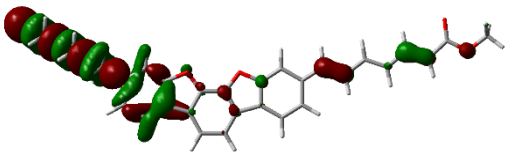


Figure S67. continued.

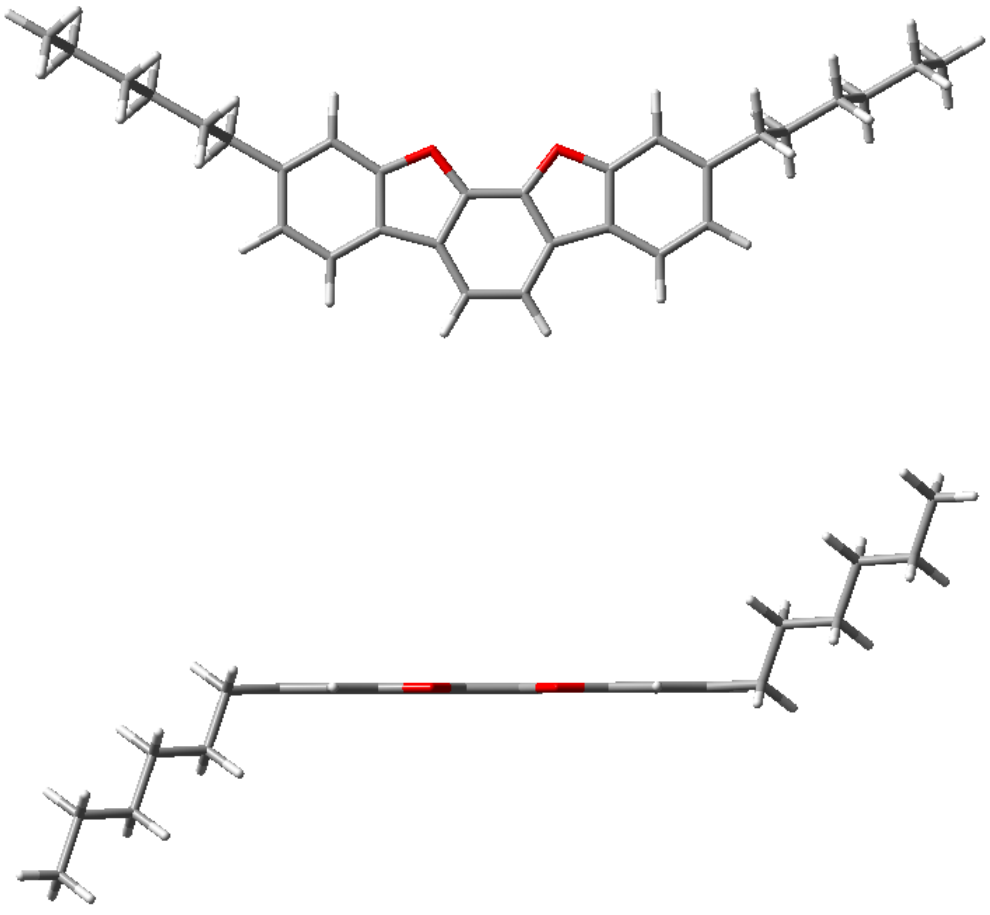


Figure S68. Top and side views of TD-DFT calculations of **22** of isomer A (The most stable isomer). ΔH° =0 kcal mol^{-1}, ΔG° = 0 kcal mol^{-1}.

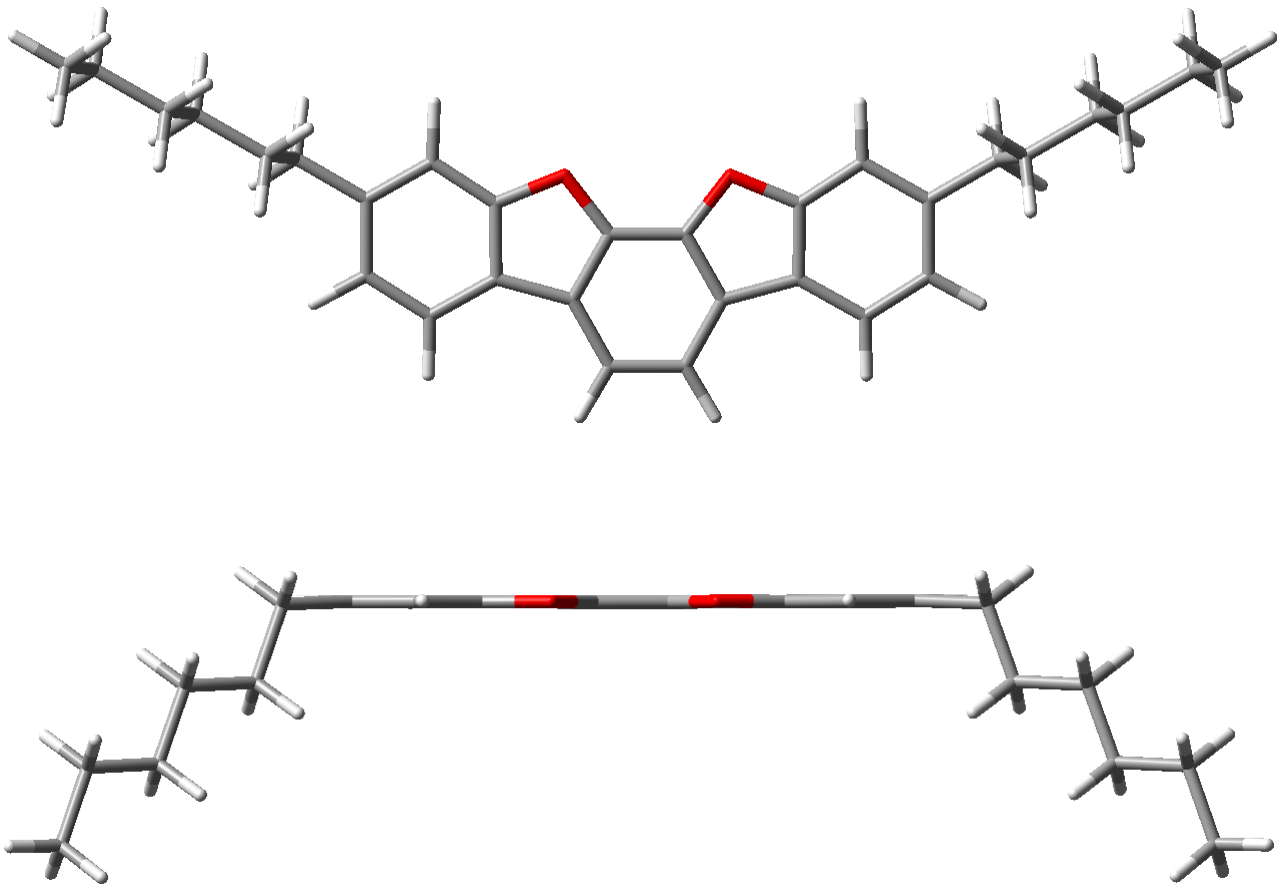
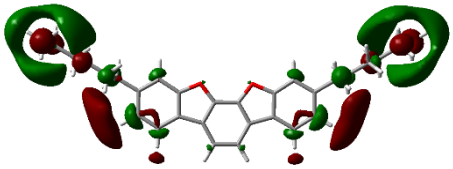
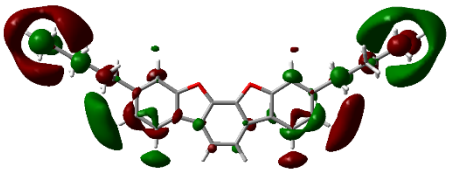


Figure S69. Top and side views of TD-DFT calculations of **22** of isomer B (The second stable isomer). ΔH° = 0.0446 kcal mol^{-1}, ΔG° = 0.612 kcal mol^{-1}.

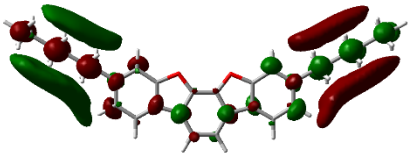
LUMO+9 (125) 3.5540 eV



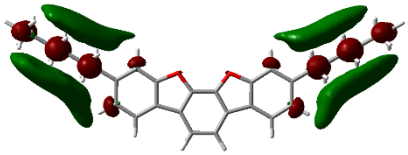
LUMO+8 (124) 3.5516 eV



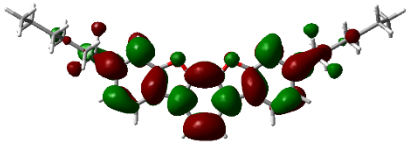
LUMO+7 (123) 3.2787 eV



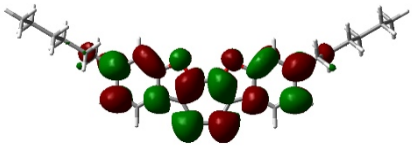
LUMO+6 (122) 3.2663 eV



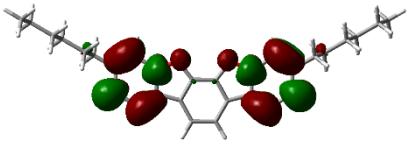
LUMO+5 (121) 3.0771 eV



LUMO+4 (120) 2.3346 eV



LUMO+3 (119) 1.7792 eV



LUMO+2 (118) 1.6189 eV

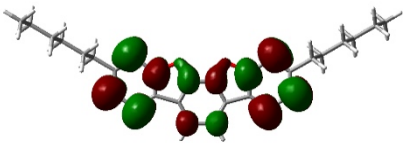
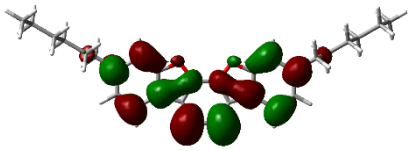
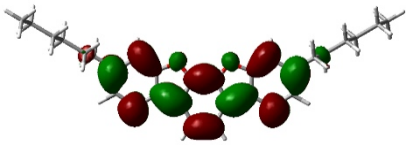


Figure S70. Selected orbitals by TD-DFT calculations of **22** (isomer A) in chloroform. Orbital numbers in parenthesis and orbital energy in eV.

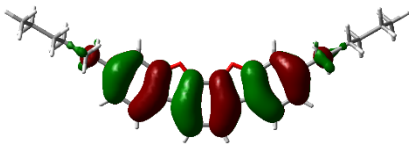
LUMO+1 (117) 1.2561 eV



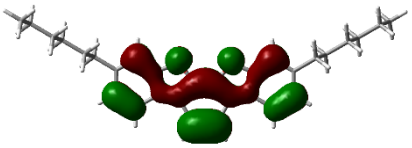
LUMO (116) 0.2730 eV



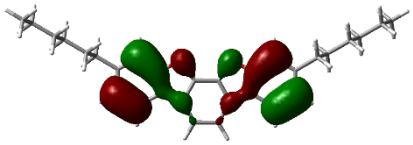
HOMO (115) -7.6477 eV



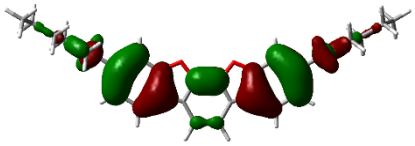
HOMO-1 (114) -8.1785 eV



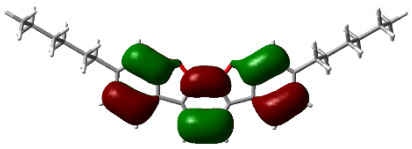
HOMO-2 (113) -8.8864 eV



HOMO-3 (112) -9.0080 eV



HOMO-4 (111) -9.5223 eV



HOMO-5 (110) -10.2894 eV

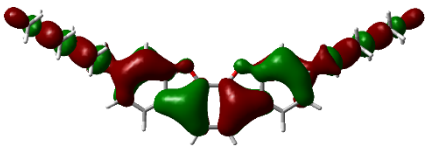
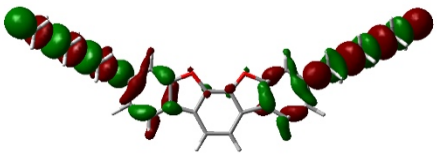


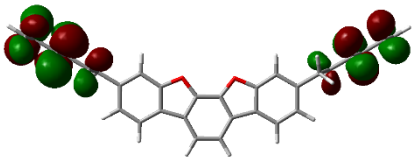
Figure S70. continued.

HOMO-6 (109) -10.7111 eV



HOMO-7 (108) -10.8010 eV

HOMO-8 (107) -10.9070 eV



HOMO-9 (106) - -10.9070 eV

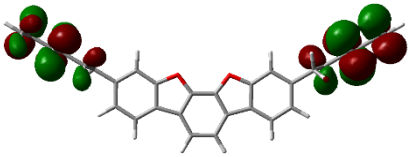
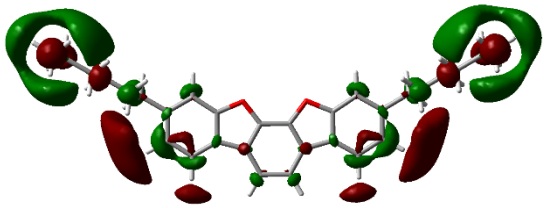
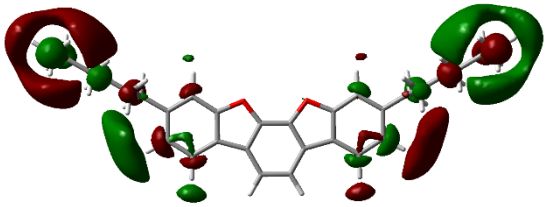


Figure S70. continued.

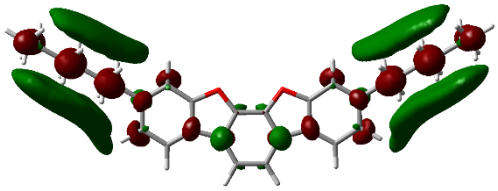
LUMO+9 (125) 3.5603 eV



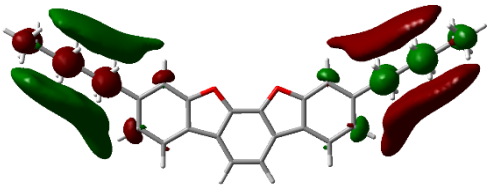
LUMO+8 (124) 3.5449 eV



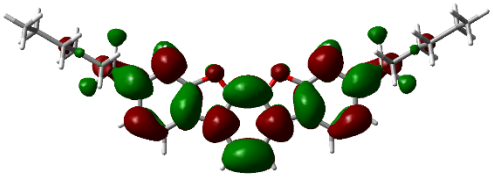
LUMO+7 (123) 3.2808 eV



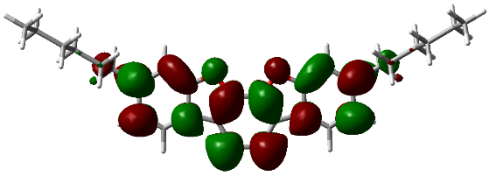
LUMO+6 (122) 3.2637 eV



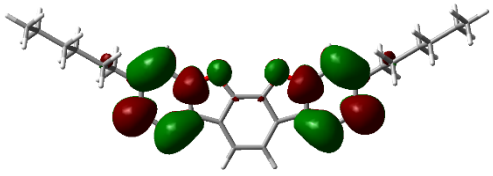
LUMO+5 (121) 3.0771 eV



LUMO+4 (120) 2.3346 eV



LUMO+3 (119) 1.7798 eV



LUMO+2 (118) 1.6192 eV

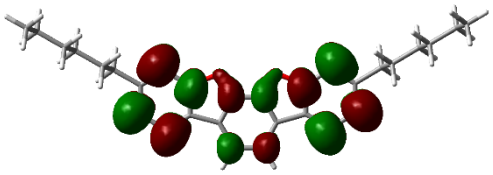
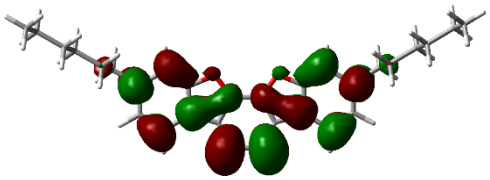
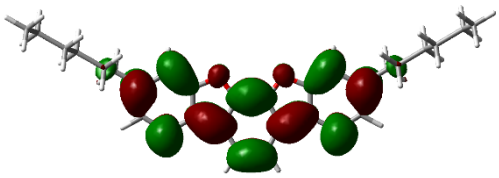


Figure S71. Selected orbitals by TD-DFT calculations of **22** (isomer B) in chloroform. Orbital numbers in parenthesis and orbital energy in eV.

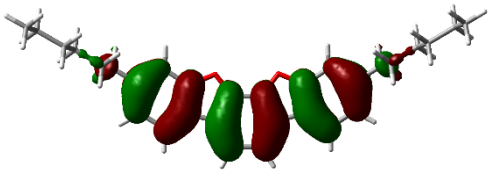
LUMO+1 (117) 1.2561 eV



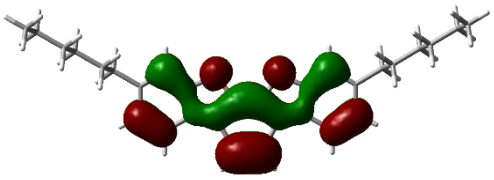
LUMO (116) 0.2727 eV



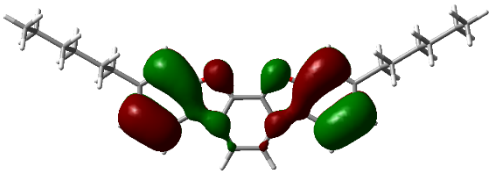
HOMO (115) -7.6479 eV



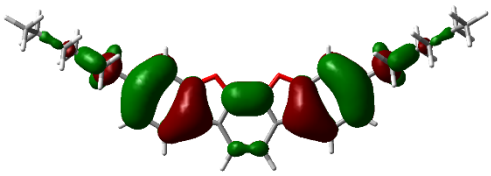
HOMO-1 (114) -8.1784 eV



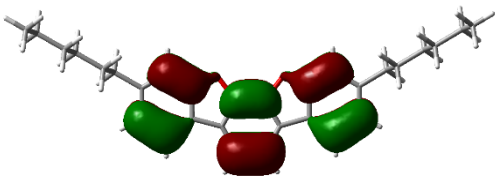
HOMO-2 (113) -8.8863 eV



HOMO-3 (112) -9.0079 eV



HOMO-4 (111) -9.5222 eV



HOMO-5 (110) -10.2887 eV

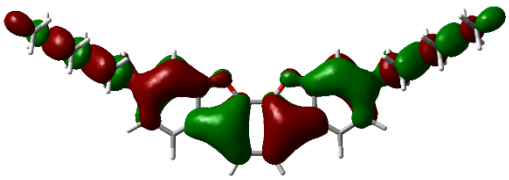
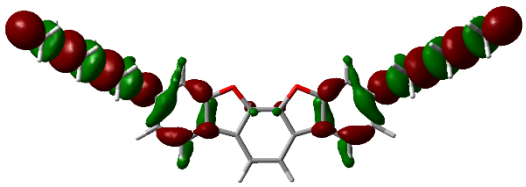
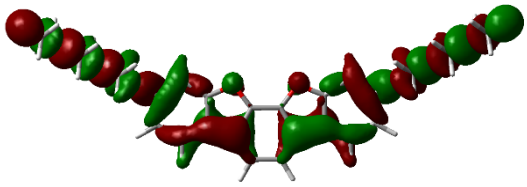


Figure S71. continued.

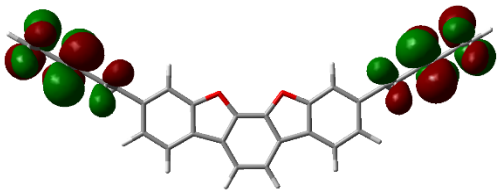
HOMO-6 (109) -10.7156 eV



HOMO-7 (108) -10.7965 eV



HOMO-8 (107) -10.9070 eV



HOMO-9 (106) -10.9070 eV

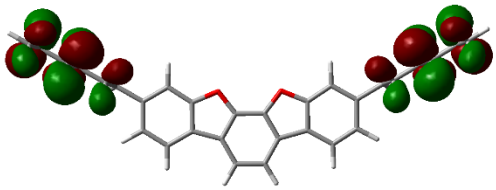


Figure S71. continued.

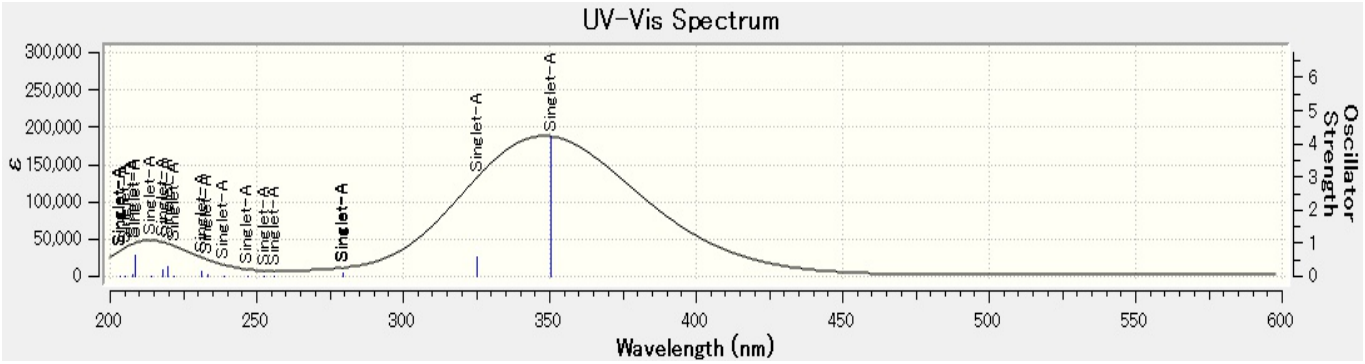


Figure S72. Calculated Uv-vis spectrum of isomer A of **9a** in chloroform by TD-DFT.

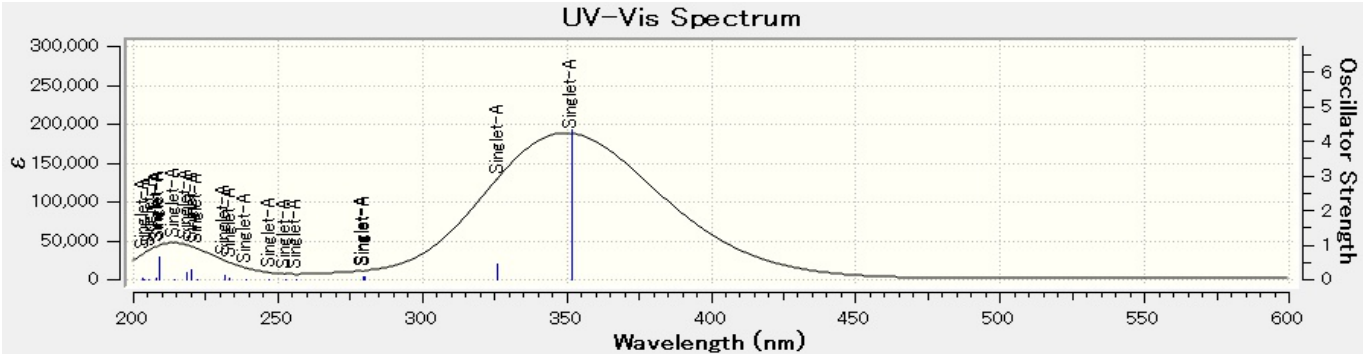


Figure S73. Calculated Uv-vis spectrum of isomer B of **9a** in chloroform by TD-DFT.

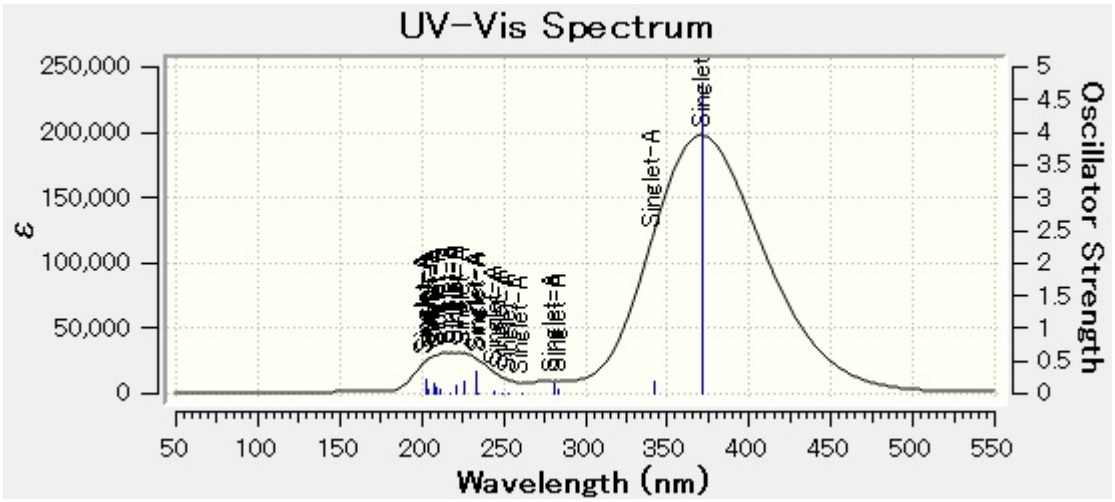


Figure S74. Calculated Uv-vis spectrum of **10b** in chloroform by TD-DFT.

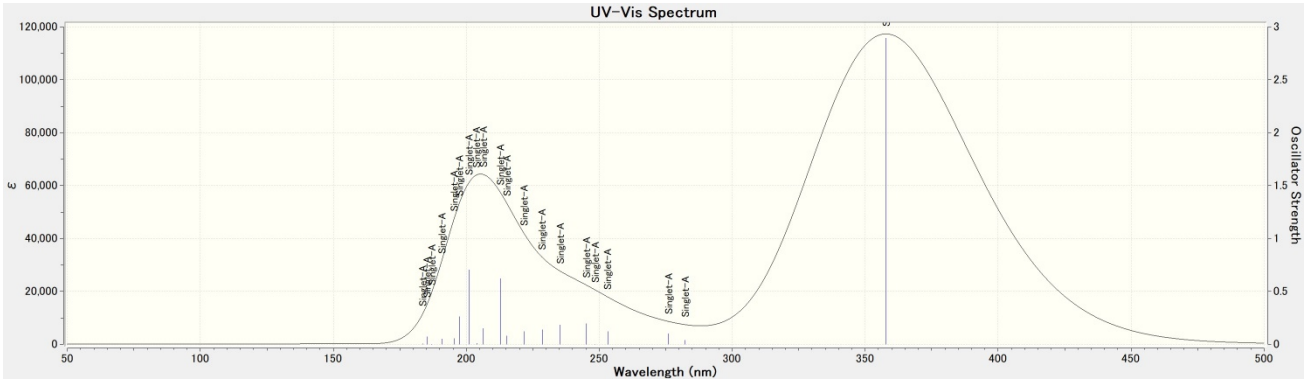


Figure S75. Calculated Uv-vis spectrum of **21a** in chloroform by TD-DFT.

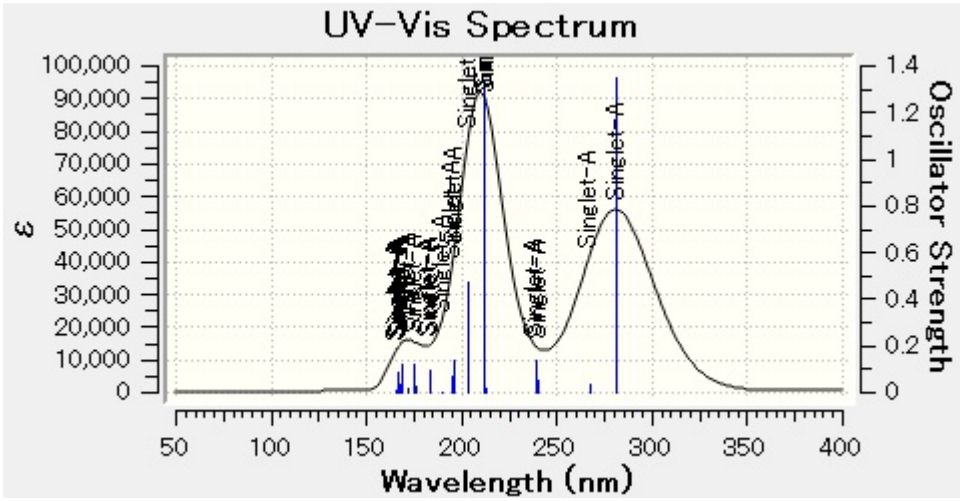


Figure S76. Calculated Uv-vis spectrum of isomer A of **22** in chloroform by TD-DFT.

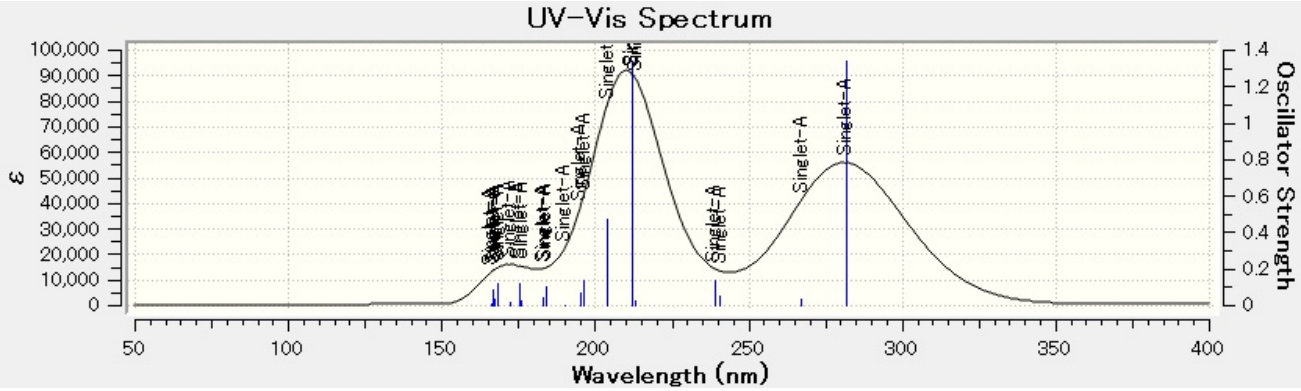


Figure S77. Calculated Uv-vis spectrum of isomer B of **22** in chloroform by TD-DFT.

Table S1. TD-DFT results for **9a** (isomer A) in chloroform.

Excited State 1: 3.5379 eV 350.64 nm f=4.2221

168 → 174 0.15609

170 → 173 0.35610

171 → 172 0.56382

171 → 174 -0.10574

Excited State 2: 3.8103 eV 325.39 nm f=0.5790

168 → 173 0.16727

170 → 172 0.46452

171 → 173 0.46927

Excited State 3: 4.4334 eV 279.66 nm f=0.0922

167 → 173 0.13847

167 → 175 -0.13052

169 → 172 0.48832

169 → 174 -0.35418

171 → 176 -0.18041

Excited State 4: 4.4392 eV 279.29 nm f=0.0609

166 → 173 0.10254

167 → 172 0.11671

168 → 172 0.34349

169 → 175 -0.11723

170 → 173 0.30507

171 → 174 0.42207

Excited State 5: 4.8419 eV 256.06 nm f=0.0038

165 → 173 -0.12192

166 → 176 -0.10575

167 → 172 0.38201

Table S1. continued.

167 → 174	-0.20274
168 → 172	-0.18305
169 → 173	0.26417
169 → 175	-0.18196
170 → 176	0.11602
171 → 177	-0.22812

Excited State 6: 4.9087 eV 252.58 nm f=0.0181

165 → 172	-0.15338
166 → 172	0.21967
167 → 173	0.13396
168 → 173	0.27203
170 → 174	0.26366
171 → 175	0.35763
171 → 176	0.15791

Excited State 7: 5.0206 eV 246.95 nm f=0.0002

163 → 172	-0.24948
163 → 173	-0.30009
163 → 174	-0.18365
163 → 175	-0.14125
164 → 172	0.26123
164 → 173	0.29368
164 → 174	0.19224
164 → 175	0.13347

Excited State 8: 5.0207 eV 246.95 nm f=0.0002

163 → 172	-0.26354
163 → 173	0.28625
163 → 174	-0.19401

Table S1. continued.

163 → 175 0.13475

163 → 179 -0.10010

164 → 172 -0.24727

164 → 173 0.29735

164 → 174 -0.18198

164 → 175 0.13990

Excited State 9: 5.1937 eV 238.72 nm f=0.0113

165 → 172 -0.10813

166 → 172 -0.15400

166 → 174 -0.13325

168 → 173 -0.30529

170 → 172 -0.28870

170 → 174 0.21884

171 → 173 0.35037

171 → 176 0.14552

Excited State 10: 5.3162 eV 233.22 nm f=0.0424

162 → 173 0.10955

165 → 172 0.22881

165 → 174 -0.15081

166 → 172 0.17196

167 → 173 -0.13867

168 → 175 0.18629

169 → 174 -0.12682

170 → 172 -0.18937

170 → 174 0.31380

170 → 177 0.16748

171 → 173 0.11032

171 → 176 -0.10365

Table S1. continued.

171 → 178 0.23435

Excited State 11: 5.3596 eV 231.33 nm f=0.1345

166 → 173 -0.23913

167 → 172 -0.11778

168 → 172 -0.36329

169 → 173 -0.11854

170 → 175 0.19174

171 → 172 0.11058

171 → 174 0.40499

Excited State 12: 5.5851 eV 221.99 nm f=0.0140

162 → 172 0.23650

165 → 175 0.10014

166 → 173 0.24321

167 → 172 0.15021

167 → 174 -0.10791

168 → 174 0.28713

169 → 173 -0.11851

169 → 175 0.16127

169 → 176 -0.12245

169 → 178 -0.17881

170 → 175 0.28445

171 → 179 0.19392

Excited State 13: 5.6404 eV 219.82 nm f=0.3002

166 → 176 0.11302

168 → 172 -0.13076

168 → 174 0.15242

169 → 173 0.36688

Table S1. continued.

169 → 175 -0.21167

169 → 176 0.10456

170 → 175 0.13003

170 → 176 -0.16057

170 → 178 0.12354

171 → 177 0.36679

Excited State 14: 5.6869 eV 218.02 nm f=0.2181

162 → 173 0.10320

166 → 172 0.20204

168 → 178 -0.16425

169 → 172 -0.26610

170 → 177 -0.20147

171 → 175 -0.30581

171 → 176 0.36729

171 → 178 0.13134

Excited State 15: 5.7949 eV 213.95 nm f=0.0001

162 → 173 0.10705

165 → 172 -0.25009

166 → 172 0.17251

167 → 173 0.29844

169 → 172 0.11933

169 → 174 0.21731

169 → 177 -0.10336

170 → 172 -0.10259

170 → 177 0.11256

171 → 173 0.10242

171 → 175 -0.23204

171 → 176 -0.25980

Table S1. continued.

171 → 178 0.11915

Excited State 16: 5.9410 eV 208.69 nm f=0.6529

162 → 172 -0.17585
166 → 173 -0.15060
167 → 172 0.24130
167 → 174 -0.22827
167 → 177 0.14487
168 → 174 -0.14238
169 → 173 -0.16087
169 → 175 0.10215
169 → 176 -0.24285
170 → 176 -0.23070
171 → 177 0.26862
171 → 179 -0.12959

Excited State 17: 5.9641 eV 207.88 nm f=0.0335

161 → 172 -0.15452
162 → 173 -0.24740
165 → 174 -0.10408
166 → 172 -0.24380
167 → 173 0.12264
167 → 176 0.17261
168 → 178 -0.11458
169 → 174 0.20820
169 → 177 -0.20545
170 → 172 0.14318
170 → 174 0.10358
171 → 173 -0.13450
171 → 178 0.27393

Table S1. continued.

171 → 180 0.11525

Excited State 18: 6.0440 eV 205.14 nm f=0.0012

162 → 172 -0.11998

166 → 173 -0.17251

168 → 172 -0.13428

168 → 174 0.18887

169 → 175 0.12252

169 → 178 -0.12580

170 → 173 0.40293

171 → 172 -0.34965

171 → 174 -0.12939

Excited State 19: 6.0902 eV 203.58 nm f=0.0221

161 → 172 0.13576

165 → 172 -0.20427

165 → 174 0.17596

166 → 172 -0.12400

166 → 174 0.15889

167 → 175 -0.11172

167 → 176 -0.16777

168 → 175 0.21619

169 → 172 -0.19066

169 → 174 -0.12442

169 → 177 0.17656

170 → 177 0.16336

170 → 179 0.18051

171 → 173 -0.13707

171 → 178 0.23007

Table S1. continued.

Excited State 20: 6.0970 eV 203.35 nm f=0.0148

161 → 173	-0.18095
162 → 172	-0.20633
165 → 173	-0.18467
166 → 175	-0.10297
167 → 172	0.14504
167 → 174	0.18755
167 → 177	-0.20855
169 → 175	0.26820
169 → 176	0.27108
169 → 178	-0.17000
170 → 173	-0.10458
171 → 172	0.10462

Table S2. TD-DFT results for **9a** (isomer B) in chloroform.

Excited State 1: 3.5256 eV 351.66 nm f=4.3226

168 → 174 -0.15513

170 → 173 0.35567

171 → 172 0.56494

171 → 174 -0.10405

Excited State 2: 3.8016 eV 326.14 nm f=0.4673

168 → 173 -0.16495

170 → 172 0.46455

171 → 173 0.47020

Excited State 3: 4.4295 eV 279.91 nm f=0.0908

167 → 173 0.13982

167 → 175 0.13003

169 → 172 0.49051

169 → 174 -0.35138

171 → 176 0.17977

Excited State 4: 4.4374 eV 279.41 nm f=0.0857

166 → 173 0.10227

167 → 172 0.11871

168 → 172 -0.34283

169 → 175 0.11755

170 → 173 0.30511

171 → 174 0.42105

Excited State 5: 4.8368 eV 256.34 nm f=0.0063

165 → 173 -0.12231

166 → 176 -0.10473

167 → 172 0.38250

Table S2. continued.

167 → 174	-0.20036
168 → 172	0.18484
169 → 173	0.26510
169 → 175	0.18028
170 → 176	0.11663
171 → 177	-0.22755

Excited State 6: 4.9063 eV 252.70 nm f=0.0146

165 → 172	0.15488
166 → 172	-0.21888
167 → 173	-0.13483
168 → 173	0.27210
170 → 174	-0.26404
171 → 175	0.35658
171 → 176	-0.15935

Excited State 7: 5.0206 eV 246.95 nm f=0.0002

163 → 172	0.24811
163 → 173	0.26992
163 → 174	0.18371
163 → 175	-0.12850
164 → 172	0.26628
164 → 173	0.31200
164 → 174	0.19416
164 → 175	-0.14848
164 → 178	-0.10035

Excited State 8: 5.0206 eV 246.95 nm f=0.0002

Table S2. continued.

163 → 172	-0.26393
163 → 173	0.31398
163 → 174	-0.19541
163 → 175	-0.14948
163 → 178	-0.10104
164 → 172	0.24623
164 → 173	-0.26775
164 → 174	0.18226
164 → 175	0.12178

Excited State 9: 5.1881 eV 238.98 nm f=0.0099

165 → 172	-0.10611
166 → 172	-0.15102
166 → 174	-0.13252
168 → 173	0.30399
170 → 172	-0.29345
170 → 174	0.22119
171 → 173	0.35160
171 → 176	0.14528

Excited State 10: 5.3114 eV 233.43 nm f=0.0412

162 → 173	-0.11115
165 → 172	0.22973
165 → 174	-0.15007
166 → 172	0.17480
167 → 173	-0.13876
168 → 175	0.18446
169 → 174	-0.12715

Table S2. continued.

170 → 172	-0.18686
170 → 174	0.31052
170 → 177	0.17004
171 → 173	0.10825
171 → 176	-0.10837
171 → 178	-0.23458

Excited State 11: 5.3571 eV 231.44 nm f=0.1375

166 → 173	-0.23800
167 → 172	-0.11730
168 → 172	0.36364
169 → 173	-0.11969
170 → 175	0.19337
171 → 172	0.10796
171 → 174	0.40521

Excited State 12: 5.5830 eV 222.07 nm f=0.0156

162 → 172	0.23843
166 → 173	-0.24544
167 → 172	-0.15390
167 → 174	0.10715
168 → 174	0.28547
169 → 173	0.11534
169 → 175	0.15832
169 → 176	0.11889
169 → 178	-0.17911
170 → 175	0.28519
171 → 179	-0.19236

Excited State 13: 5.6348 eV 220.03 nm f=0.2995

Table S2. continued.

166 → 176	0.11280
168 → 172	0.13064
168 → 174	-0.14675
169 → 173	0.36773
169 → 175	0.21238
169 → 176	0.10385
170 → 175	-0.12805
170 → 176	-0.16401
170 → 178	-0.12210
171 → 177	0.36822

Excited State 14: 5.6823 eV 218.20 nm f=0.2135

162 → 173	-0.10619
166 → 172	0.20604
168 → 173	-0.10049
168 → 178	-0.16482
169 → 172	-0.26429
170 → 177	-0.20238
171 → 175	0.30733
171 → 176	0.36373
171 → 178	-0.13257

Excited State 15: 5.7909 eV 214.10 nm f=0.0002

162 → 173	-0.10906
165 → 172	-0.25139
166 → 172	0.17481
167 → 173	0.29699
169 → 172	0.11699
169 → 174	0.21384
169 → 177	-0.10224

Table S2. continued.

170 → 172	-0.10353
170 → 177	0.11353
171 → 173	0.10446
171 → 175	0.23056
171 → 176	-0.26419
171 → 178	-0.11497

Excited State 16: 5.9380 eV 208.80 nm f=0.6425

162 → 172	0.18128
166 → 173	-0.15492
167 → 172	0.24339
167 → 174	-0.22719
167 → 177	0.14346
168 → 174	0.14104
169 → 173	-0.16519
169 → 175	-0.10397
169 → 176	-0.23892
170 → 176	-0.22873
171 → 177	0.26558
171 → 179	-0.12871

Excited State 17: 5.9606 eV 208.01 nm f=0.0360

161 → 172	-0.14908
162 → 173	-0.24385
166 → 172	0.24364
167 → 173	-0.12573
167 → 176	-0.17043
168 → 178	0.11648
169 → 174	-0.20718
169 → 177	0.20362

Table S2. continued.

170 → 172	-0.14263
170 → 174	-0.10559
171 → 173	0.13587
171 → 178	0.28335
171 → 180	0.11321

Excited State 18: 6.0376 eV 205.35 nm f=0.0014

162 → 172	0.10412
166 → 173	-0.16603
168 → 172	0.14153
168 → 174	-0.19534
169 → 175	-0.11097
169 → 178	0.11934
170 → 173	0.40876
171 → 172	-0.35443
171 → 174	-0.13144

Excited State 19: 6.0876 eV 203.67 nm f=0.0096

161 → 172	0.13922
165 → 172	0.20596
165 → 174	-0.17738
166 → 172	0.11602
166 → 174	-0.15715
167 → 175	-0.11199
167 → 176	0.17148
168 → 175	-0.21383
169 → 172	0.19310
169 → 174	0.13170
169 → 177	-0.18170
170 → 177	-0.16368

Table S2. continued.

170 → 179	-0.17845
171 → 173	0.13270
171 → 178	0.22575

Excited State 20: 6.0963 eV 203.38 nm f=0.0206

161 → 173	0.18454
162 → 172	0.21351
165 → 173	-0.18612
167 → 172	0.14221
167 → 174	0.18968
167 → 177	-0.21051
169 → 175	-0.26742
169 → 176	0.27559
169 → 178	0.16998

Table S3. TD-DFT results for **10b** in chloroform.

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.3333 eV 371.96 nm f=4.7425

136→142 -0.13627

138→141 0.35574

139→140 0.57690

Excited State 2: Singlet-A 3.6286 eV 341.69 nm f=0.1848

136→141 0.13330

138→140 0.46108

139→141 0.48893

Excited State 3: Singlet-A 4.3650 eV 284.04 nm f=0.0590

135→141 -0.16767

135→143 0.11944

137→140 0.51112

137→142 0.31476

139→145 -0.15503

139→146 -0.10777

Excited State 4: Singlet-A 4.4203 eV 280.49 nm f=0.1393

135→140 -0.17526

136→140 -0.30675

Table S3. continued.

137→141 0.14346

137→143 -0.13131

138→141 -0.29414

138→145 -0.10559

139→140 0.10402

139→142 0.40067

139→144 0.12385

Excited State 5: Singlet-A 4.7492 eV 261.06 nm f=0.0004

133→141 0.13635

135→140 0.36359

135→142 0.16399

136→140 -0.24615

137→141 -0.27174

137→143 0.13815

138→141 -0.14668

138→145 0.11808

139→142 0.11777

139→144 -0.21239

Excited State 6: Singlet-A 4.8915 eV 253.47 nm f=0.0074

133→140 0.17590

Table S3. continued.

134→140	-0.20060
135→141	0.17338
136→141	0.28076
137→142	0.10332
137→144	0.10470
138→140	0.10542
138→142	-0.20377
139→141	-0.13503
139→143	0.30434
139→145	0.20884

Excited State 7: Singlet-A 4.9846 eV 248.73 nm f=0.0001

131→140	-0.36374
131→141	0.40155
131→142	0.26029
131→143	0.21710
131→144	-0.13790
131→146	0.11627
131→147	-0.12390
131→148	0.10825

Excited State 8: Singlet-A 4.9846 eV 248.73 nm f=0.0002

Table S3. continued.

132→140 0.36368

132→141 0.40160

132→142 -0.26029

132→143 0.21710

132→144 0.13791

132→146 0.11628

132→147 0.12390

132→148 0.10825

Excited State 9: Singlet-A 5.0646 eV 244.81 nm f=0.0372

133→140 0.12207

134→142 -0.12549

136→141 -0.25462

137→140 0.11762

138→140 -0.34328

138→142 -0.23167

139→141 0.35450

139→145 0.17775

Excited State 10: Singlet-A 5.2807 eV 234.79 nm f=0.0110

133→140 0.19645

133→142 0.11669

Table S3. continued.

134→140	0.17626
136→141	-0.12859
136→143	-0.13412
138→140	0.16494
138→142	0.31092
138→144	-0.22795
139→141	-0.11185
139→143	-0.21524
139→145	0.20526
139→146	-0.17475

Excited State 11: Singlet-A 5.3123 eV 233.39 nm f=0.3229

134→141	-0.22100
135→140	0.14364
136→140	0.32239
137→141	-0.20914
138→143	-0.13799
138→145	-0.11489
139→142	0.39900
139→144	0.16563

Excited State 12: Singlet-A 5.4887 eV 225.89 nm f=0.1821

Table S3. continued.

136→140	-0.17203
136→142	-0.12911
137→141	-0.28581
137→143	0.13535
138→143	0.26247
138→145	-0.18618
138→146	0.10240
139→142	-0.14791
139→144	0.39784

Excited State 13: Singlet-A 5.6015 eV 221.34 nm f=0.0533

130→140	-0.16355
133→143	-0.12122
134→141	-0.23685
135→140	0.22634
135→142	0.13140
136→142	-0.17613
137→141	0.24969
137→143	-0.22871
137→146	0.20854
138→143	0.23575
139→147	0.16342

Table S3. continued.

Excited State 14: Singlet-A 5.6155 eV 220.79 nm f=0.1101

130→141	-0.12021
133→140	-0.13205
134→140	-0.23633
135→141	-0.11899
136→141	0.17283
136→146	-0.15220
137→140	0.23653
138→144	-0.21095
139→143	-0.27518
139→145	0.29604
139→146	0.18356

Excited State 15: Singlet-A 5.7052 eV 217.32 nm f=0.0031

133→140	0.23934
134→140	-0.21578
135→141	0.29443
137→142	0.21156
137→144	0.11987
139→141	0.10045
139→143	-0.26063

Table S3. continued.

139→145	-0.25990
139→146	0.10998

Excited State 16: Singlet-A 5.8699 eV 211.22 nm f=0.0508

134→141	0.20315
135→140	0.12630
135→142	0.11125
136→140	-0.18019
136→142	-0.11095
137→143	-0.10035
137→145	0.12175
137→146	0.10200
138→141	0.41371
139→140	-0.30710
139→142	0.10134
139→144	0.11542

Excited State 17: Singlet-A 5.9217 eV 209.37 nm f=0.1068

130→141	0.15889
134→140	0.24320
135→141	0.10402
136→141	-0.11191

Table S3. continued.

136→143	0.15383
136→146	-0.12556
137→140	0.13603
137→142	0.10301
137→144	0.11048
138→140	0.16209
138→142	-0.13483
139→141	-0.15995
139→146	0.39524

Excited State 18: Singlet-A 5.9750 eV 207.51 nm f=0.1586

130→140	0.18602
134→141	0.11052
135→140	0.22028
135→142	0.21113
135→144	0.10182
136→140	0.14178
136→142	0.25641
137→141	0.19699
137→145	0.13479
138→141	-0.14955
138→145	-0.20401

Table S3. continued.

139→140	0.15652
139→144	0.16609
139→147	-0.19135

Excited State 19: Singlet-A 6.0813 eV 203.88 nm f=0.0557

130→141	0.10540
133→140	-0.23049
133→142	-0.19672
135→145	0.24198
136→143	-0.13213
137→140	-0.21186
137→142	0.27246
137→144	0.30491
138→144	-0.15073
138→147	-0.10478

Excited State 20: Singlet-A 6.1238 eV 202.46 nm f=0.2043

127→141	0.12851
130→140	-0.20451
133→141	-0.22150
134→141	-0.10516
135→140	-0.14453

Table S3. continued.

135→142	0.16808
135→144	0.25851
137→141	-0.11049
137→143	0.12861
137→145	0.42303

Table S4. TD-DFT results for **21a** in chloroform.

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.4642 eV 357.90 nm f=2.8925

125→128 0.11195

126→128 0.16253

126→129 -0.11183

127→128 0.64639

Excited State 2: Singlet-A 4.3907 eV 282.38 nm f=0.0353

124→128 -0.18887

125→128 0.12178

125→130 0.13628

126→128 -0.37766

126→129 -0.21591

127→129 0.38332

127→131 -0.14798

Excited State 3: Singlet-A 4.4909 eV 276.08 nm f=0.0983

123→128 -0.10149

124→128 -0.10400

125→128 0.43354

Table S4. continued.

125→129 0.32787

126→132 0.11301

127→129 -0.28977

127→130 -0.10938

Excited State 4: Singlet-A 4.8971 eV 253.18 nm f=0.1181

122→128 0.21401

124→128 0.29176

124→129 0.15434

125→129 0.14116

125→132 0.10686

126→129 -0.25939

126→130 0.19616

127→130 -0.13696

127→131 0.28287

127→132 -0.13189

Excited State 5: Singlet-A 4.9886 eV 248.53 nm f=0.0002

121→128 0.54072

121→129 -0.28354

Table S4. continued.

121→130	-0.23934
121→133	-0.12925
121→134	0.11620
121→135	-0.10015

Excited State 6: Singlet-A 5.0563 eV 245.21 nm f=0.1959

123→128	0.26692
124→129	0.18754
124→130	-0.10399
125→129	0.20163
125→130	-0.14327
125→131	0.12269
126→128	-0.21979
126→129	0.14782
126→132	0.12973
126→133	0.11472
127→130	0.32122
127→132	-0.12409

Excited State 7: Singlet-A 5.2676 eV 235.37 nm f=0.1835

Table S4. continued.

123→128	-0.16888
123→129	0.12252
124→128	0.14725
124→129	0.11522
126→128	0.34266
126→130	0.13567
126→133	0.10639
127→128	-0.10742
127→129	0.37870
127→131	-0.19326

Excited State 8: Singlet-A 5.4258 eV 228.51 nm f=0.1345

122→129	0.12539
125→128	0.20555
125→129	0.10356
125→130	0.16820
126→129	0.21904
126→130	0.10165
127→129	0.16009
127→130	0.26724

Table S4. continued.

127→131	0.34344
127→133	0.12932

Excited State 9: Singlet-A 5.5927 eV 221.69 nm f=0.1212

120→128	0.14475
122→130	-0.10300
123→128	0.26238
124→129	-0.15179
125→128	-0.24220
125→129	0.15712
125→130	-0.12545
125→132	-0.13617
126→128	0.13513
126→130	0.18720
126→133	-0.13675
127→130	-0.13439
127→131	-0.18461
127→133	0.24556

Excited State 10: Singlet-A 5.7583 eV 215.31 nm f=0.0774

Table S4. continued.

122→128	0.30818
122→129	0.15097
124→128	0.24645
124→130	0.12783
125→129	0.16182
126→128	-0.10424
126→130	-0.18511
126→132	-0.15392
127→130	0.17942
127→131	-0.25435
127→132	0.21819

Excited State 11: Singlet-A 5.8244 eV 212.87 nm f=0.6192

122→128	0.12791
123→128	0.14003
123→129	0.14214
124→128	0.10094
124→129	0.11041
124→131	-0.14467
125→129	-0.13813

Table S4. continued.

125→130	0.24385
125→132	0.16432
125→133	-0.20671
126→129	0.20950
126→130	-0.21078
127→130	-0.22855
127→131	-0.10485
127→132	-0.13216
127→134	0.11051

Excited State 12: Singlet-A 6.0049 eV 206.47 nm f=0.1472

120→128	0.23485
123→128	0.26345
124→128	0.10432
124→129	0.20436
124→132	0.14057
125→128	0.17826
126→131	-0.13874
126→132	-0.24921
126→134	0.10283

Table S4. continued.

127→132	0.26901

Excited State 13: Singlet-A 6.0800 eV 203.92 nm f=0.0080

120→128	-0.18292
123→128	-0.19117
124→129	0.23777
124→131	-0.19356
125→130	-0.12164
125→131	0.22830
125→132	-0.12121
126→128	-0.14681
126→130	0.12168
126→131	-0.22313
126→133	-0.14780
127→133	0.21919

Excited State 14: Singlet-A 6.1644 eV 201.13 nm f=0.7027

123→129	-0.14577
124→132	0.17823
124→133	0.13074

Table S4. continued.

125→128	-0.19048
125→129	0.13014
125→130	0.18561
125→132	0.36566
126→132	-0.23230
127→129	-0.10663
127→130	0.13648
127→132	-0.12417
127→133	0.17172
127→134	-0.10658

Excited State 15: Singlet-A 6.2798 eV 197.43 nm f=0.2607

120→128	-0.18577
123→129	0.26025
124→128	-0.14273
125→128	-0.15265
125→129	0.18490
125→130	-0.14447
125→131	0.11164
125→133	-0.16746

Table S4. continued.

126→128	0.13085
126→129	-0.15893
126→130	-0.12102
126→132	-0.13951
127→131	0.13921
127→132	0.17658
127→134	0.14696

Excited State 16: Singlet-A 6.3425 eV 195.48 nm f=0.0539

122→128	-0.20586
122→129	-0.24875
123→130	-0.10983
124→128	0.19048
124→129	0.13256
124→131	0.15626
125→129	0.10767
125→130	0.12586
125→131	-0.19268
125→132	-0.10850
125→133	-0.13480

Table S4. continued.

126→131	0.12533
126→132	-0.11537
127→133	0.26063

Excited State 17: Singlet-A 6.4975eV 190.82nm f=0.0485

120→131	-0.10627
124→132	0.11632
125→129	0.18263
125→130	-0.12270
125→131	-0.21222
125→132	0.13089
125→133	0.18310
126→128	-0.11030
126→129	0.33891
126→131	-0.18234
127→128	0.13748
127→130	-0.18636
127→133	-0.11621

Excited State 18: Singlet-A 6.6286 eV 187.04 nm f=0.0015

Table S4. continued.

116→128	0.20713
119→128	0.39701
119→129	-0.16480
119→130	-0.11876
120→128	0.20644
123→128	-0.18081
123→129	-0.12372
125→133	-0.11056
127→134	0.14371

Excited State 19: Singlet-A 6.6918 eV 185.28 nm f=0.0685

116→128	-0.16273
118→128	-0.13030
119→128	0.43928
119→129	-0.19131
119→130	-0.14387
120→128	-0.16799
123→128	0.12866
123→129	0.14770
125→133	0.12261

Table S4. continued.

Excited State 20: Singlet-A 6.7482 eV 183.73 nm f=0.0036

116→128	0.12105
120→129	-0.11484
122→129	0.26123
124→128	-0.20034
124→129	0.26336
124→131	0.10466
125→129	-0.12780
125→130	-0.15755
125→132	0.12315
125→134	-0.14487
126→131	0.27246
126→132	-0.11454
126→133	-0.12608
127→133	0.10904

Table S5. TD-DFT results for **22** (isomer A) in chloroform.

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 4.4024 eV 281.63 nm f=1.3452

112 →117 0.12192

115 →116 0.66773

Excited State 2: Singlet-A 4.6410 eV 267.15 nm f=0.0314

113→117 -0.13420

114 →116 0.58331

115 →117 -0.21964

115 →118 -0.22345

Excited State 3: Singlet-A 5.1524 eV 240.63 nm f=0.0493

112→116 0.27299

112→119 0.15416

113→117 -0.14184

113→120 -0.11538

115→117 0.47228

115→118 -0.22921

115→120 -0.10476

Table S5. continued.

Excited State 4: Singlet-A 5.1887 eV 238.95 nm f=0.1347 <S**2>=0.000

111→117	0.12867
112→118	0.20877
113→116	0.44781
114→117	-0.23271
114→120	-0.11803
115→116	0.11596
115→119	-0.35314

Excited State 5: Singlet-A 5.8148 eV 213.22 nm f=0.0202 <S**2>=0.000

110→117	-0.10237
111→116	0.32459
112→116	0.34470
112→119	0.16799
113→117	0.11052
113→118	-0.20538
114→119	-0.18049
115→117	0.11191
115→120	0.32537

Table S5. continued.

Excited State 6: Singlet-A 5.8436 eV 212.17 nm f=1.3427

111→117	0.14007
113→119	0.10547
114→117	0.53907
114→118	0.30053
114→120	-0.15552
115→119	-0.14770

Excited State 7: Singlet-A 5.8495 eV 211.96 nm f=0.4722

111→116	0.10680
112→116	-0.11283
112→119	-0.10750
113→118	0.10121
114→116	0.34267
114→119	0.14622
115→117	0.33976
115→118	0.40601
115→120	-0.12868

Excited State 8: Singlet-A 6.0807 eV 203.90 nm f=0.4708

Table S5. continued.

112→118 -0.14876

113→116 0.30527

113→119 0.21760

114→117 -0.10559

114→118 0.37398

115→119 0.38044

115→121 -0.11593

Excited State 9: Singlet-A 6.3174 eV 196.26 nm f=0.1394

111→116 0.36203

112→116 -0.30336

112→119 0.12616

113→117 0.21627

115→117 0.21463

115→118 -0.35875

Excited State 10: Singlet-A 6.3535 eV 195.14 nm f=0.0701

110→116 0.12177

111→117 0.10663

112→117 -0.13287

Table S5. continued.

112→120	-0.10798
113→116	0.32315
113→119	-0.26366
114→117	0.18066
114→118	-0.29231
114→120	-0.14512
115→119	0.30320
115→121	0.10826

Excited State 11: Singlet-A 6.5262 eV 189.98 nm f=0.0003

111→116	0.16932
112→116	0.37999
113→117	0.10913
113→118	0.24376
114→119	0.41948
115→120	-0.14874

Excited State 12: Singlet-A 6.7425 eV 183.89 nm f=0.0955

111→116	-0.14124
112 →116	-0.11480

Table S5. continued.

112→121	-0.11424
113→117	-0.11033
113→118	0.14680
114→119	0.33240
115→117	0.13412
115→120	0.50714

Excited State 13: Singlet-A 6.7705 eV 183.12 nm f=0.0444

110→116	-0.24437
111→118	-0.20525
112→117	0.33272
113→116	0.18335
114→117	0.24913
114→118	-0.27158
114→120	0.14200
115→121	-0.20355

Excited State 14: Singlet-A 7.0452 eV 175.98 nm f=0.0290

111→116	0.27906
113→117	0.52163

Table S5. continued.

113→118 0.17899

113→120 -0.14758

114→119 -0.12843

114→121 0.12078

Excited State 15: Singlet-A 7.0802 eV 175.11 nm f=0.1226

111→117 -0.12543

112→117 0.41864

112→118 0.13154

112→120 -0.14208

113→119 -0.15521

114→120 -0.41365

115→121 -0.12931

Excited State 16: Singlet-A 7.2074 eV 172.02 nm f=0.0151

108→116 -0.19165

110→116 0.42877

111→117 -0.25161

113→121 0.14859

114→120 0.13695

Table S5. continued.

115→119 -0.11297

115→121 -0.30091

Excited State17: Singlet-A 7.3653 eV 168.34 nm f=0.1189

110→118 0.16069

111→119 0.42509

113→117 0.18594

113→118 -0.24637

113→120 -0.26292

114→119 0.22800

114→121 -0.15663

Excited State18: Singlet-A 7.4126 eV 167.26 nm f=0.0315

110→119 0.10248

111→118 0.23107

111→120 0.14034

112→117 0.22621

112→118 0.22606

112→120 -0.17424

113→119 -0.14987

Table S5. continued.

114→118 0.12459

114→120 0.43393

115→121 0.14854

Excited State 19: Singlet-A 7.4365 eV 166.72 nm f=0.0861

110→116 0.24281

110→119 0.11904

111→117 0.34145

111→118 -0.16497

112→118 0.28770

113→116 -0.10841

113→119 0.25631

113→121 -0.13100

114→118 -0.18156

115→119 0.16416

Excited State 20: Singlet-A 7.4651 eV 166.09 nm f=0.0098

110→118 0.18945

111→116 0.21303

111→119 -0.14453

Table S5. continued.

112→119	0.23583
113→118	0.31095
113→120	-0.21648
114→119	-0.19999
114→121	-0.27629
115→118	0.14850
115→120	0.14251

Table S6. TD-DFT results for **22** (isomer B) in chloroform.

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 4.4024 eV 281.63 nm f=1.3422

112→117 -0.12202

115→116 0.66772

Excited State 2: Singlet-A 4.6409 eV 267.15 nm f=0.0315

113→117 0.13420

114→116 0.58339

115→117 -0.21941

115→118 -0.22349

Excited State 3: Singlet-A 5.1525 eV 240.63 nm f=0.0509

111→116 -0.19794

112→116 -0.27309

112→119 -0.15412

113→117 0.14187

113→120 0.11536

115→117 0.47236

115→118 -0.22891

115→120 -0.10483

Table S6. continued.

Excited State 4: Singlet-A 5.1888 eV 238.95 nm f=0.1343

111→117	-0.12868
112→118	0.20866
113→116	0.44796
114→117	0.23280
114→120	0.11800
115→116	-0.11605
115→119	0.35292

Excited State 5: Singlet-A 5.8148 eV 213.22 nm f=0.0227

110→117	0.10238
111→116	-0.32446
112→116	0.34507
112→119	-0.16756
113→117	0.11055
113→118	-0.20566
114→119	0.18083
115→117	-0.11077
115→120	-0.32571

Table S6. continued.

Excited State 6: Singlet-A 5.8435 eV 212.1 8 nm f=1.3410

111→117	0.14014
113→119	-0.10542
114→117	0.53894
114→118	0.30074
114→120	-0.15552
115→119	-0.14760

Excited State 7: Singlet-A 5.8496 eV 211.95 nm f=0.4734

111→116	0.10808
112→116	0.11166
112→119	0.10803
113→118	-0.10051
114→116	0.34258
114→119	0.14565
115→117	0.34009
115→118	0.40632
115→120	-0.12752

Excited State 8: Singlet-A 6.0810 eV 203.89 nm f=0.4698

Table S6. continued.

112→118	0.14874
113→116	-0.30490
113→119	-0.21780
114→117	-0.10575
114→118	0.37410
115→119	0.38033
115→121	-0.11611

Excited State 9: Singlet-A 6.3177 eV 196.25 nm f=0.1406

111→116	0.36164
112→116	0.30382
112→119	-0.12626
113→117	-0.21599
115→117	0.21478
115→118	-0.35880

Excited State 10: Singlet-A 6.3539 eV 195.13 nm f=0.0693

110→116	-0.12152
111→117 -	0.10650
112→117	-0.13263

Table S6. continued.

112→120	-0.10799
113→116	0.32344
113→119	-0.26354
114→117	-0.18069
114→118	0.29211
114→120	0.14498
115→119	-0.30348
115→121	-0.10807

Excited State 11: Singlet-A 6.5263 eV 189.98 nm f=0.0023

111→116	0.16959
112→116	-0.37959
113→117	-0.10919
113→118	-0.24391
114→119	0.41945
115→120	-0.14891

Excited State 12: Singlet-A 6.7426eV 183.88nm f=0.0999

111→116	-0.14136
112→116	0.11467

Table S6. continued.

112→121	0.11429
113→117	0.11037
113→118	-0.14686
114→119	0.33235
115→117	0.13412
115→120	0.50714

Excited State 13 :Singlet-A 6.7705 eV 183.12 nm f=0.0405

110→116	0.24437
111→118	0.20527
112→117	0.33267
113→116	0.18322
114→117	-0.24925
114→118	0.27135
114→120	-0.14215
115→121	0.20349

Excited State 14: Singlet-A 7.0451 eV 175.99 nm f=0.0294

111→116	0.27906
113→117	0.52162

Table S6. continued.

113→118	0.17909
113→120	-0.14753
114→119	0.12841
114→121	-0.12100

Excited State 15: Singlet-A 7.0801 eV 175.12nm f=0.1206

111→117	0.12558
112→117	0.41862
112→118	0.13156
112→120	-0.14203
113→119	-0.15520
114→120	0.41357
115→121	0.12965

Excited State 16: Singlet-A 7.2074 eV 172.02nm f=0.0146

108→116	-0.19211
110→116	0.42848
111→117	-0.25144
113→121	-0.14870
114→120	0.13735

Table S6. continued.

115→119 -0.11305

115→121 -0.30092

Excited State 17: Singlet-A 7.3655 eV 168.33n mf=0.1209

110→118 0.16047

111→119 0.42499

113→117 -0.18592

113→118 0.24599

113→120 0.26309

114→119 0.22801

114→121 -0.15704

ExcitedState18: Singlet-A 7.4127 eV 167.26 nm f=0.0309

110→119 0.10287

111→118 0.23022

111→120 0.13996

112→117 -0.22641

112→118 -0.22756

112→120 0.17449

113→119 0.14864

Table S6. continued.

114→118 0.12365

114→120 0.43396

115→121 0.14846

Excited State 19: Singlet-A 7.4367 eV 166.72 nm f=0.0844

110→116 0.24228

110→119 0.11843

111→117 0.34266

111→118 -0.16589

112→118 -0.28686

113→116 0.10882

113→119 -0.25725

113→121 0.13167

114→118 -0.18244

115→119 0.16427

Excited State 20: Singlet-A 7.4652 eV 166.08 nm f=0.0100

110→118 -0.18904

111→116 -0.21296

111→119 0.14468

Table S6. continued.

112→119	0.23517
113→118	0.31115
113→120	-0.21660
114→119	0.20020
114→121	0.27657
115→118	-0.14826
115→120	-0.14248

Table S7. Cartesian coordinates of isomer A of **9a** by TD-DFT calculations

C	1.37895	-2.23886	-0.50485
C	2.77803	-1.86050	-0.53161
C	0.69103	-1.02703	-0.60193
C	0.69104	-3.45785	-0.40724
C	-0.69113	-3.45782	-0.40725
C	-0.69105	-1.02701	-0.60195
C	-1.37901	-2.23882	-0.50489
H	1.24100	-4.38790	-0.33165
H	-1.24113	-4.38786	-0.33168
C	-2.77807	-1.86042	-0.53168
C	2.79048	-0.46691	-0.64282
C	3.99339	-2.53956	-0.48813
C	5.16803	-1.80772	-0.53717
C	3.94774	0.28113	-0.70416
C	5.16735	-0.40065	-0.62769
H	4.02396	-3.62092	-0.42738
H	6.11065	-2.33791	-0.53856
O	1.52132	0.04732	-0.68651
H	3.90975	1.35998	-0.79438
C	6.39885	0.40222	-0.68487
C	-3.99345	-2.53944	-0.48821
C	-2.79047	-0.46682	-0.64288
C	-3.94772	0.28126	-0.70425
C	-5.16807	-1.80756	-0.53728
C	-5.16734	-0.40049	-0.62782
O	-1.52130	0.04737	-0.68655
H	-3.90969	1.36010	-0.79447
H	-4.02405	-3.62080	-0.42745
H	-6.11072	-2.33771	-0.53866

Table S7. continued.

C	-6.39884	0.40238	-0.68502
C	7.56254	0.22778	-0.02449
C	7.82752	-0.88615	0.95570
C	-7.56251	0.22789	-0.02463
C	-7.82740	-0.88607	0.95554
H	8.32156	-0.47085	1.84102
H	6.87965	-1.30044	1.30685
C	8.69709	-2.01497	0.38532
H	-6.87949	-1.30031	1.30665
H	-8.32145	-0.47082	1.84089
C	-8.69691	-2.01494	0.38517
H	8.25340	-2.38607	-0.54630
H	9.68155	-1.62219	0.10877
C	8.86532	-3.17286	1.36515
C	9.73850	-4.29405	0.80971
H	9.29896	-2.79472	2.29835
H	7.87638	-3.56934	1.62459
H	-9.68136	-1.62220	0.10853
H	-8.25314	-2.38607	-0.54641
C	-8.86518	-3.17279	1.36504
H	-7.87624	-3.56921	1.62460
H	-9.29892	-2.79462	2.29818
C	-9.73825	-4.29404	0.80958
C	8.61564	1.21264	-0.26685
H	6.32163	1.28525	-1.31611
C	9.82038	1.26086	0.32770
H	8.38320	1.98050	-1.00267
H	10.10685	0.51961	1.06825
C	10.79044	2.28844	0.02077
C	12.00057	2.38150	0.58803

Table S7. continued.

H	10.51571	3.03529	-0.72140
H	12.34121	1.67354	1.33517
C	12.92358	3.46590	0.21208
O	14.07164	3.37908	0.89946
O	12.70402	4.33235	-0.60288
C	15.04738	4.38448	0.61723
H	15.34315	4.34760	-0.43243
H	14.65272	5.37612	0.84417
H	15.89610	4.15862	1.25812
C	-8.61566	1.21270	-0.26695
H	-6.32164	1.28539	-1.31629
C	-9.82037	1.26089	0.32766
H	-8.38331	1.98056	-1.00281
H	-10.10676	0.51965	1.06826
C	-10.79050	2.28842	0.02075
C	-12.00060	2.38144	0.58808
H	-10.51585	3.03524	-0.72147
H	-12.34116	1.67349	1.33527
C	-12.92368	3.46577	0.21214
O	-14.07170	3.37893	0.89959
O	-12.70422	4.33221	-0.60286
C	-15.04750	4.38426	0.61737
H	-14.65289	5.37593	0.84426
H	-15.34334	4.34732	-0.43227
H	-15.89618	4.15838	1.25832
H	-10.74167	-3.92779	0.57230
H	-9.30925	-4.70532	-0.10931
H	-9.84102	-5.11220	1.52669
H	9.30960	-4.70530	-0.10924
H	10.74192	-3.92774	0.57255

Table S7. continued.

H	9.84123	-5.11224	1.52679

Table S8. Cartesian coordinates of isomer B of **9a** by TD-DFT calculations

C	-1.37351	-2.18606	-0.12129
C	-2.76723	-1.80709	-0.24318
C	-0.68835	-0.97021	-0.06116
C	-0.68838	-3.40899	-0.06078
C	0.68839	-3.40898	0.06080
C	0.68835	-0.97021	0.06123
C	1.37352	-2.18605	0.12134
H	-1.23620	-4.34211	-0.10921
H	1.23622	-4.34210	0.10921
C	2.76723	-1.80708	0.24323
C	-2.77995	-0.40909	-0.24567
C	-3.97635	-2.48783	-0.36399
C	-5.14707	-1.75502	-0.46424
C	-3.93239	0.34083	-0.35462
C	-5.14894	-0.34501	-0.44505
H	-4.00427	-3.57065	-0.39037
H	-6.08073	-2.28475	-0.59488
O	-1.51574	0.10730	-0.13445
H	-3.89457	1.42342	-0.35777
C	-6.37410	0.46137	-0.55710
C	3.97636	-2.48781	0.36401
C	2.77995	-0.40907	0.24573
C	3.93238	0.34085	0.35468
C	5.14707	-1.75500	0.46425
C	5.14893	-0.34499	0.44508
O	1.51573	0.10731	0.13453
H	3.89456	1.42344	0.35784
H	4.00428	-3.57063	0.39037
H	6.08073	-2.28472	0.59487

Table S8. continued.

C	6.37410	0.46139	0.55712
C	-7.60039	0.23204	-0.04266
C	-7.96210	-0.96362	0.80071
C	7.60039	0.23205	0.04267
C	7.96208	-0.96363	-0.80068
H	-7.05555	-1.40704	1.21900
H	-8.55613	-0.62790	1.65783
C	-8.75127	-2.03768	0.03967
H	7.05553	-1.40706	-1.21894
H	8.55609	-0.62793	-1.65782
C	8.75127	-2.03766	-0.03962
H	-9.69900	-1.61955	-0.31649
H	-8.19926	-2.33041	-0.86147
C	-9.02564	-3.27329	0.89228
C	-9.81735	-4.34215	0.14482
H	-8.07158	-3.69213	1.23410
H	-9.57044	-2.97372	1.79524
H	9.69900	-1.61953	0.31650
H	8.19927	-2.33037	0.86154
C	9.02561	-3.27330	-0.89220
H	8.07154	-3.69216	-1.23398
H	9.57039	-2.97376	-1.79518
C	9.81735	-4.34214	-0.14473
C	-8.62873	1.23618	-0.31078
H	-6.23714	1.39690	-1.09580
C	-9.89436	1.22939	0.14268
H	-8.32210	2.06860	-0.94175
H	-10.25672	0.42301	0.77395
C	-10.83388	2.27969	-0.18173
C	-12.10402	2.31821	0.24271

Table S8. continued.

H	-10.48252	3.09194	-0.81484
H	-12.52232	1.54397	0.87597
C	-12.98953	3.43039	-0.14214
O	-14.21107	3.27784	0.38952
O	-12.68509	4.36885	-0.84197
C	-15.15880	4.30260	0.08252
H	-14.80688	5.27052	0.44284
H	-15.32588	4.35979	-0.99424
H	-16.07531	4.01820	0.59362
C	8.62873	1.23619	0.31075
H	6.23715	1.39693	1.09580
C	9.89435	1.22940	-0.14271
H	8.32211	2.06863	0.94171
H	10.25671	0.42299	-0.77396
C	10.83388	2.27969	0.18167
C	12.10402	2.31820	-0.24279
H	10.48253	3.09196	0.81475
H	12.52232	1.54394	-0.87604
C	12.98954	3.43039	0.14203
O	14.21108	3.27781	-0.38963
O	12.68512	4.36885	0.84184
C	15.15882	4.30256	-0.08266
H	14.80692	5.27048	-0.44301
H	15.32588	4.35978	0.99411
H	16.07533	4.01813	-0.59373
H	10.78801	-3.95502	0.17968
H	9.27835	-4.67598	0.74721
H	9.99877	-5.21722	-0.77363
H	-10.78801	-3.95505	-0.17963
H	-9.27834	-4.67603	-0.74710

Table S8. continued.

H	-9.99879	-5.21721	0.77375

Table S9. Cartesian coordinates of **10b** by TD-DFT calculations

C	-1.37924	2.24994	-0.01693
C	-2.77722	1.87019	-0.03343
C	-0.69100	1.03418	-0.00811
C	-0.69083	3.47318	-0.00858
C	0.69084	3.47318	0.00861
C	0.69101	1.03418	0.00815
C	1.37925	2.24994	0.01697
H	-1.24055	4.40642	-0.01527
H	1.24055	4.40642	0.01530
C	2.77722	1.87019	0.03349
C	-2.78946	0.47355	-0.03215
C	-3.99507	2.55187	-0.05094
C	-5.16732	1.82057	-0.06392
C	-3.94807	-0.27718	-0.04481
C	-5.16599	0.40895	-0.05844
H	-4.02381	3.63493	-0.05627
H	-6.10999	2.35317	-0.08259
O	-1.52127	-0.04307	-0.01705
H	-3.91001	-1.35970	-0.04210
C	-6.40002	-0.38160	-0.06668
C	3.99507	2.55186	0.05105
C	2.78946	0.47355	0.03224

Table S9. continued.

C	3.94807	-0.27718	0.04495
C	5.16732	1.82056	0.06408
C	5.16599	0.40895	0.05861
O	1.52127	-0.04307	0.01712
H	3.91001	-1.35971	0.04225
H	4.02381	3.63493	0.05639
H	6.10999	2.35316	0.08281
C	6.40002	-0.38160	0.06689
C	-7.65989	0.08010	-0.02581
H	-7.86036	1.14729	0.02114
C	7.65988	0.08009	0.02575
H	7.86034	1.14727	-0.02152
C	-8.81340	-0.79206	-0.03719
H	-6.25631	-1.45969	-0.10604
C	-10.08601	-0.35796	0.00336
H	-8.62320	-1.86317	-0.08128
H	-10.28948	0.70981	0.04716
C	-11.21858	-1.25504	-0.00825
C	-12.49895	-0.86208	0.03053
H	-11.01421	-2.32284	-0.05123
H	-12.77863	0.18445	0.07401
C	-13.58746	-1.85468	0.01572

Table S9. continued.

O	-14.78522	-1.25404	0.06003
O	-13.44963	-3.05547	-0.02969
C	-15.92126	-2.12129	0.05215
H	-15.93573	-2.72614	-0.85586
H	-15.90671	-2.77969	0.92217
H	-16.78977	-1.46815	0.08618
C	8.81340	-0.79205	0.03723
H	6.25632	-1.45969	0.10653
C	10.08600	-0.35796	-0.00356
H	8.62321	-1.86315	0.08160
H	10.28946	0.70979	-0.04765
C	11.21858	-1.25503	0.00817
C	12.49894	-0.86208	-0.03080
H	11.01421	-2.32282	0.05144
H	12.77862	0.18444	-0.07456
C	13.58746	-1.85467	-0.01582
O	14.78521	-1.25405	-0.06037
O	13.44963	-3.05545	0.02990
C	15.92125	-2.12129	-0.05237
H	15.93581	-2.72590	0.85580
H	15.90662	-2.77993	-0.92221
H	16.78976	-1.46816	-0.08666

Table S10. Cartesian coordinates of **21a** by TD-DFT calculations

C	2.36078	-1.04842	-0.26418
C	0.98511	-1.05457	-0.13140
O	0.11546	-0.05819	-0.45188
C	-1.12658	-0.54278	-0.13918
C	-2.30953	0.14874	-0.30710
C	-3.49538	-0.49313	0.06248
C	-4.75412	0.23586	-0.11507
C	-5.99273	-0.19846	0.16675
C	-7.17179	0.60927	-0.05360
C	-8.42611	0.20208	0.21222
C	-9.58325	1.03451	-0.02325
C	-10.84753	0.66626	0.22450
C	-11.96327	1.58765	-0.05139
O	-13.13917	1.02600	0.26393
C	-14.29794	1.83087	0.03559
C	0.34739	-2.18521	0.38542
O	3.14443	-0.04542	-0.74374
C	4.42941	-0.51853	-0.67305
C	5.55340	0.18373	-1.06752
C	6.78598	-0.44984	-0.93261
C	8.05631	0.27815	-1.29264
C	-3.44141	-1.80307	0.58539

Table S10. continued.

C	-2.24525	-2.47650	0.74517
C	-1.05947	-1.83876	0.37745
C	1.08110	-3.31634	0.77382
C	2.45713	-3.30969	0.64131
C	3.09410	-2.17283	0.12117
C	4.47288	-1.81430	-0.15317
C	5.70983	-2.44293	-0.02042
C	6.84652	-1.75369	-0.41047
H	3.04149	-4.17287	0.93583
H	0.57130	-4.18439	1.17357
H	5.47294	1.18757	-1.46784
H	5.78189	-3.44936	0.37522
H	-2.31422	1.15342	-0.71229
H	-2.23137	-3.48198	1.14859
H	7.81657	-2.23044	-0.31553
H	-4.35886	-2.30194	0.87193
H	-4.65067	1.23918	-0.52389
H	-6.15505	-1.19191	0.57644
H	-7.01779	1.60659	-0.46225
H	-8.59479	-0.79207	0.62036
H	-9.41258	2.02866	-0.43100
H	-11.09382	-0.30852	0.63007

Table S10. continued.

O	-11.86317	2.70582	-0.50170
H	-14.38322	2.08850	-1.02127
H	-14.25056	2.74739	0.62582
H	-15.14399	1.22302	0.34670
H	8.78433	-0.43295	-1.69721
H	7.85193	1.00727	-2.08338
C	8.67334	0.99984	-0.08819
H	7.93975	1.70577	0.31928
H	8.87183	0.26873	0.70467
C	9.96086	1.74125	-0.43612
H	10.68822	1.03072	-0.84926
H	9.75629	2.46921	-1.23154
C	10.58057	2.46049	0.75911
H	9.85196	3.16912	1.17347
H	10.78571	1.73201	1.55418
C	11.86827	3.20636	0.41601
H	12.59468	2.49754	0.00113
H	11.66151	3.93400	-0.37770
C	12.47987	3.92067	1.61802
H	11.78293	4.65573	2.03247
H	12.72340	3.20954	2.41347
H	13.39874	4.44671	1.34664

Table S11. Cartesian coordinates of isomer A of **22** by TD-DFT calculations

O	1.47736	-0.21115	-0.36646
C	0.67066	0.86664	-0.16667
C	-0.67066	0.86664	0.16669
O	-1.47737	-0.21115	0.36648
C	-1.33924	2.08181	0.33275
C	1.33924	2.08181	-0.33274
C	2.71038	0.30505	-0.67131
C	3.83545	-0.44807	-0.95289
C	2.69864	1.70185	-0.66906
C	5.01049	0.23853	-1.24808
C	6.28690	-0.52038	-1.50968
C	5.01491	1.64414	-1.24980
C	0.67116	3.30367	-0.16671
C	-2.71038	0.30505	0.67132
C	-3.83545	-0.44807	0.95290
C	-2.69864	1.70186	0.66907
C	-5.01050	0.23853	1.24808
C	-6.28691	-0.52038	1.50968
C	-5.01492	1.64414	1.24980
C	-7.11584	-0.71895	0.23474
C	3.87777	2.38313	-0.96558
C	-0.67117	3.30367	0.16673

Table S11. continued.

C	-3.87777	2.38314	0.96558
C	-8.41439	-1.48096	0.48282
C	-9.24302	-1.68215	-0.78320
C	-10.54410	-2.44420	-0.54097
C	-11.36458	-2.63926	-1.81295
C	7.11584	-0.71895	-0.23475
C	8.41439	-1.48096	-0.48284
C	9.24303	-1.68215	0.78318
C	10.54411	-2.44420	0.54094
C	11.36460	-2.63925	1.81292
H	3.79897	-1.53118	-0.94490
H	3.90496	3.46655	-0.97721
H	1.20481	4.23707	-0.29904
H	7.34164	0.26127	0.20204
H	8.18245	-2.45881	-0.92392
H	6.05239	-1.49823	-1.94271
H	5.94004	2.16036	-1.48462
H	-1.20481	4.23707	0.29905
H	-3.79898	-1.53117	0.94491
H	6.88874	0.01800	-2.24945
H	9.01428	-0.94229	-1.22755
H	6.50937	-1.25445	0.50548

Table S11. continued.

H	9.47394	-0.70403	1.22458
H	-3.90497	3.46655	0.97721
H	8.64238	-2.22013	1.52788
H	10.31187	-3.42091	0.10015
H	10.79779	-3.20112	2.56176
H	-6.88875	0.01801	2.24944
H	-5.94004	2.16036	1.48462
H	-7.34164	0.26127	-0.20204
H	11.14270	-1.90592	-0.20350
H	11.63462	-1.67561	2.25592
H	-6.05239	-1.49822	1.94271
H	-6.50936	-1.25445	-0.50548
H	12.28937	-3.18659	1.61312
H	-9.01428	-0.94229	1.22753
H	-9.47393	-0.70404	-1.22461
H	-8.18245	-2.45881	0.92391
H	-8.64237	-2.22014	-1.52789
H	-11.14270	-1.90593	0.20346
H	-10.31187	-3.42091	-0.10017
H	-11.63459	-1.67562	-2.25596
H	-10.79777	-3.20114	-2.56178
H	-12.28935	-3.18660	-1.61316

Table S12. Cartesian coordinates of isomer B of **22** by TD-DFT calculations

O	-1.52213	-0.44880	-0.89668
C	-0.69109	-1.29264	-0.22615
C	0.69109	-1.29264	-0.22615
O	1.52213	-0.44880	-0.89668
C	1.38008	-2.24402	0.52974
C	-1.38008	-2.24402	0.52974
C	-2.79231	-0.85240	-0.57497
C	-3.95192	-0.26482	-1.04637
C	-2.78051	-1.94604	0.29397
C	-5.16357	-0.80485	-0.62267
C	-6.46536	-0.17929	-1.05587
C	-5.16843	-1.90485	0.25235
C	-0.69154	-3.20052	1.28990
C	2.79231	-0.85240	-0.57496
C	3.95192	-0.26482	-1.04637
C	2.78051	-1.94604	0.29398
C	5.16357	-0.80485	-0.62267
C	6.46536	-0.17929	-1.05586
C	5.16843	-1.90485	0.25236
C	6.96561	0.87229	-0.05790
C	-3.99648	-2.48170	0.71468
C	0.69154	-3.20052	1.28990

Table S12. continued.

C	3.99648	-2.48171	0.71468
C	8.28480	1.51190	-0.48107
C	8.78707	2.56157	0.50679
C	10.10706	3.20506	0.08757
C	10.59968	4.25327	1.08145
C	-6.96561	0.87229	-0.05790
C	-8.28480	1.51190	-0.48108
C	-8.78707	2.56157	0.50678
C	-10.10706	3.20506	0.08756
C	-10.59968	4.25327	1.08144
H	-3.91424	0.58198	-1.72166
H	-4.02630	-3.33246	1.38557
H	-1.24102	-3.93121	1.87085
H	-7.08204	0.40478	0.92721
H	-8.16343	1.97283	-1.46969
H	-6.34114	0.28738	-2.03847
H	-6.12295	-2.31232	0.56915
H	1.24102	-3.93121	1.87085
H	3.91424	0.58198	-1.72166
H	-7.22684	-0.95818	-1.16889
H	-9.04592	0.72981	-0.59795
H	-6.19943	1.64832	0.05726

Table S12. continued.

H	-8.90765	2.10066	1.49565
H	4.02630	-3.33246	1.38557
H	-8.02518	3.34297	0.62391
H	-9.98510	3.66433	-0.90056
H	-9.86945	5.06088	1.19223
H	6.34114	0.28738	-2.03846
H	6.12295	-2.31232	0.56915
H	6.19943	1.64832	0.05727
H	-10.86705	2.42335	-0.02894
H	-10.75758	3.81126	2.07010
H	7.22684	-0.95818	-1.16889
H	7.08204	0.40478	0.92722
H	-11.54450	4.69827	0.75902
H	8.16343	1.97283	-1.46969
H	8.02518	3.34297	0.62392
H	9.04592	0.72981	-0.59794
H	8.90765	2.10066	1.49566
H	9.98510	3.66434	-0.90055
H	10.86705	2.42335	-0.02893
H	9.86945	5.06088	1.19224
H	10.75758	3.81126	2.07011
H	11.54450	4.69827	0.75902