Supporting Information

Self-assembled organometallic arene-ruthenium-based metalla-rectangles bearing azodipyridyl ligands: Synthesis, Characterization and antitumor activities

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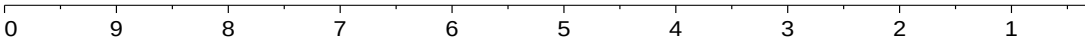

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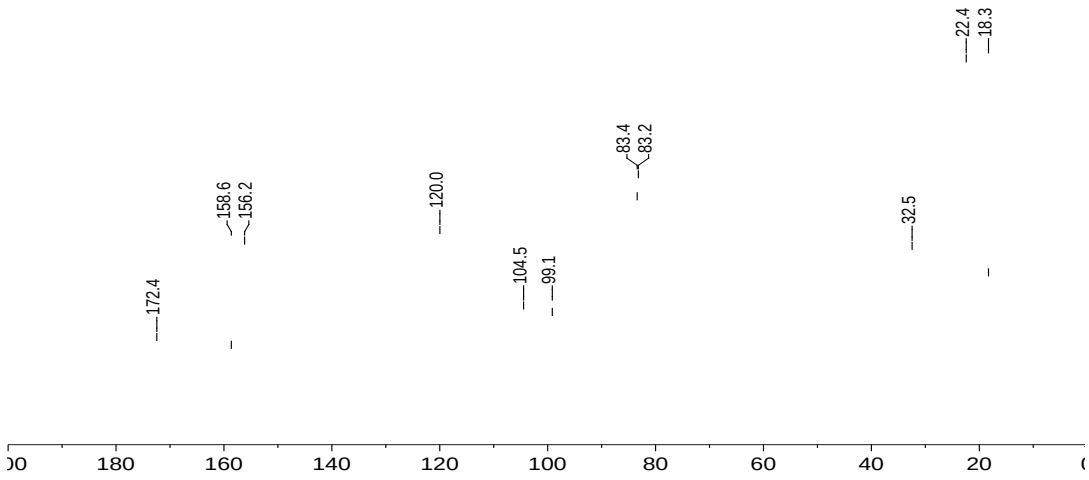

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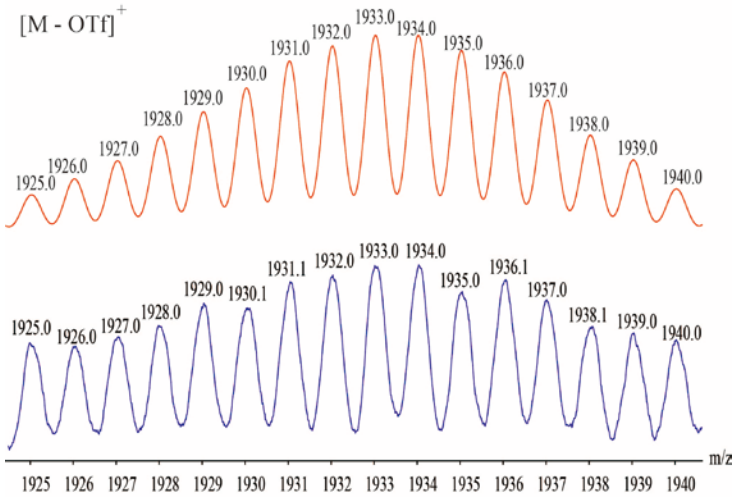
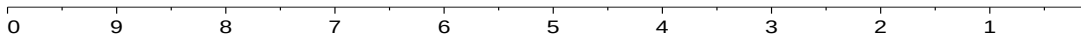


Figure 1. ^{1}H (a), ^{13}C NMR (b) and HR-ESI-MS (c) spectra of the molecular-rectangle **1a**.

(a)



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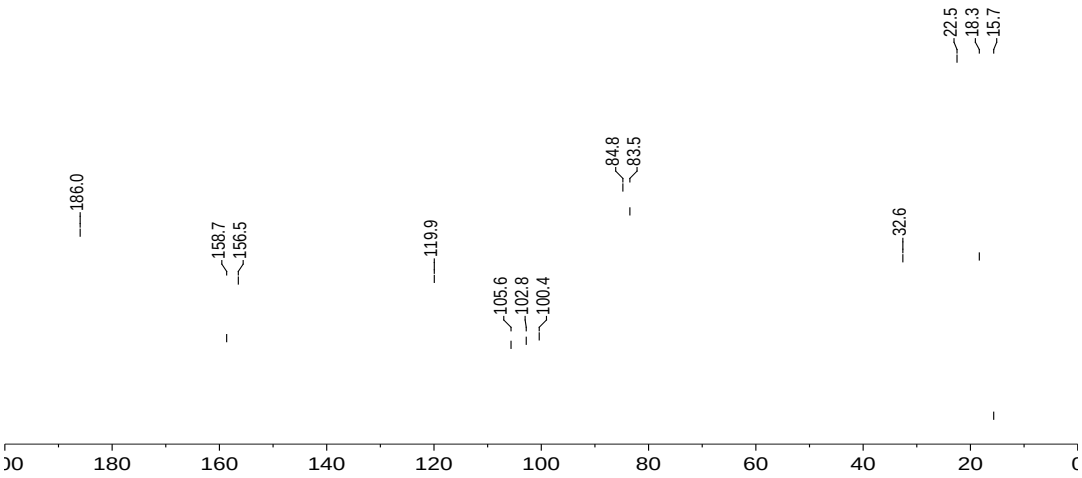

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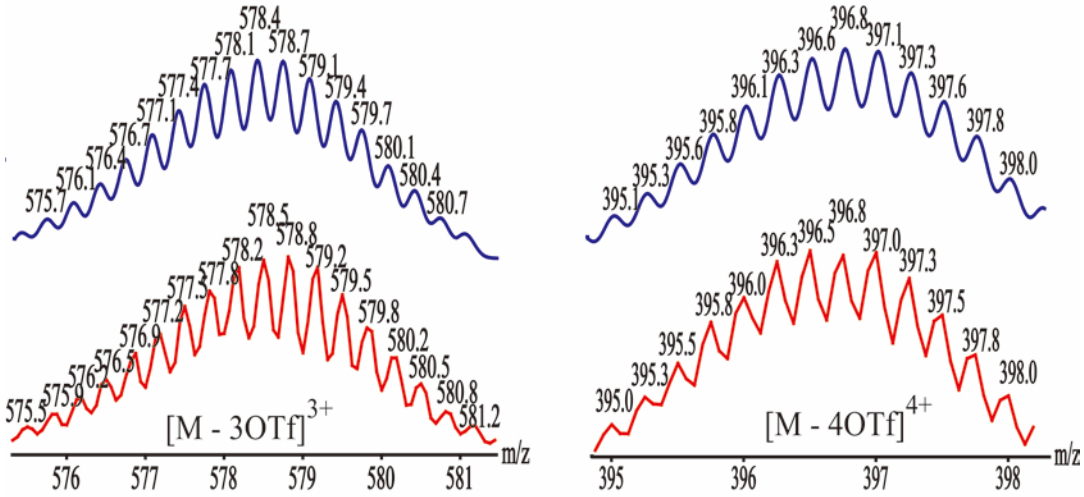

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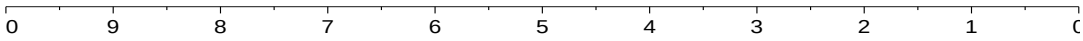
(a)



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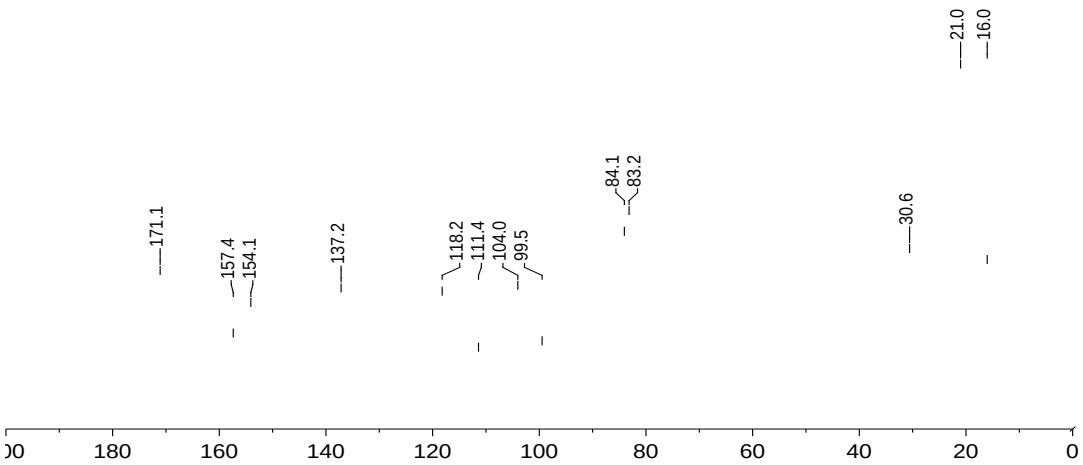

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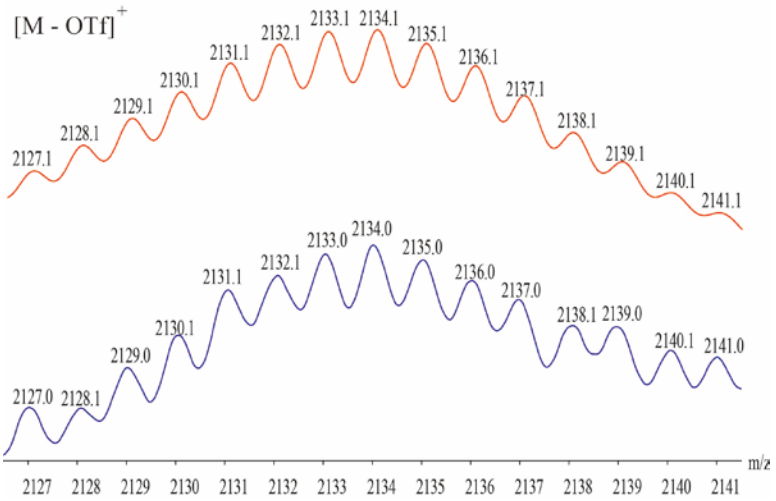
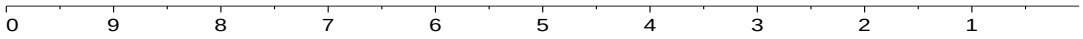


Figure 3. ^{1}H (a), ^{13}C NMR (b) and HR-ESI-MS (c) spectra of the molecular-rectangle **1c**.

(a)



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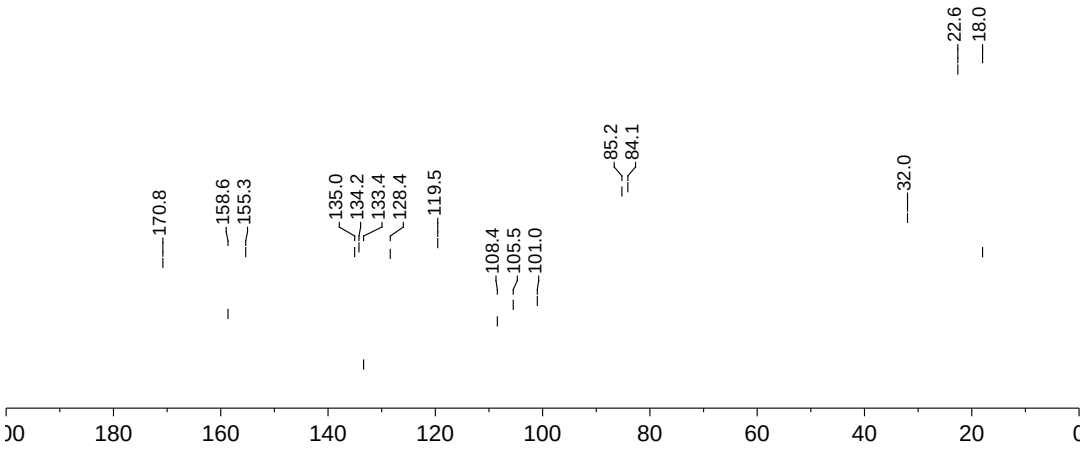

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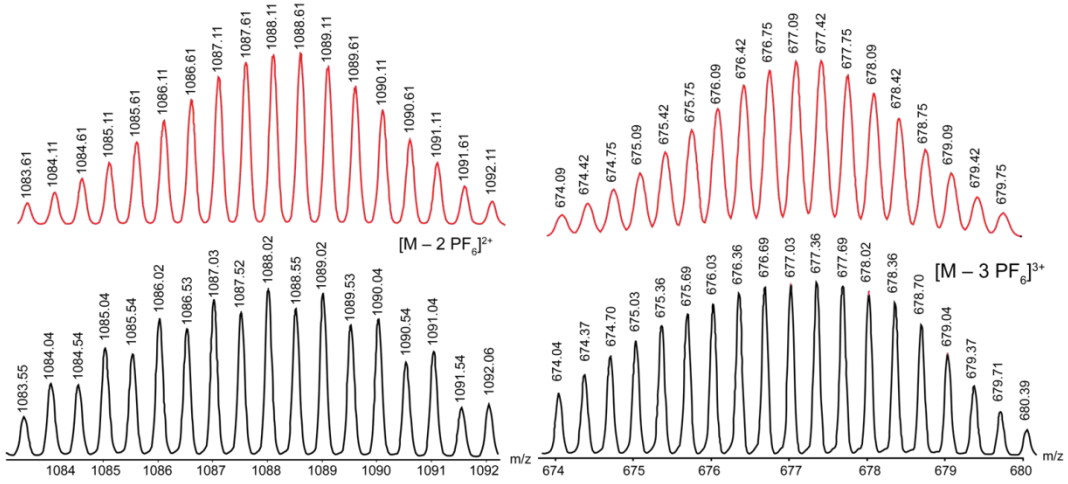

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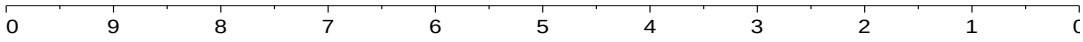
(a)



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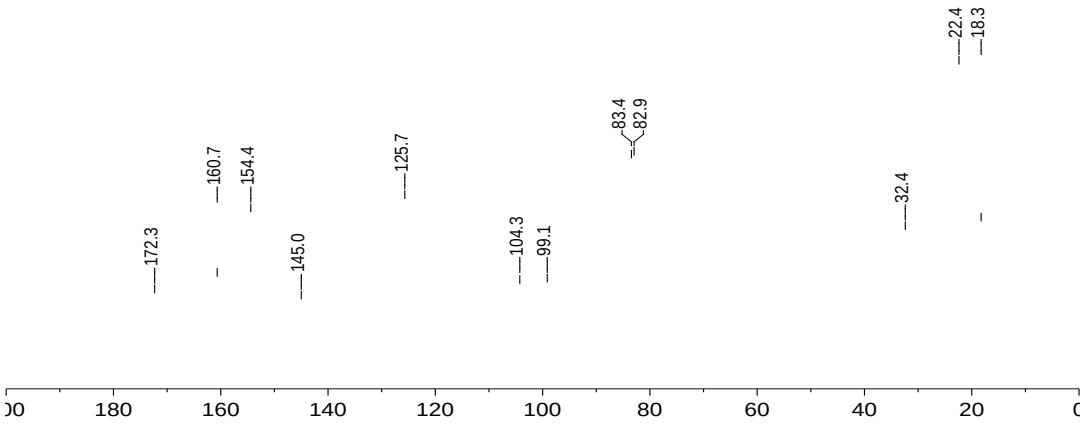

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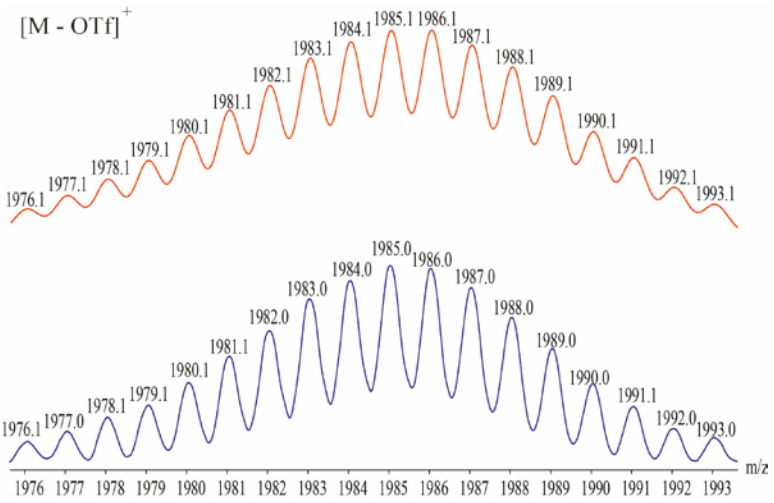
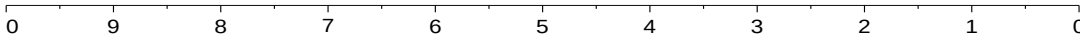


Figure 5. ^{1}H (a), ^{13}C NMR (b) and HR-ESI-MS (c) spectra of the molecular-rectangle **2a**.

(a)



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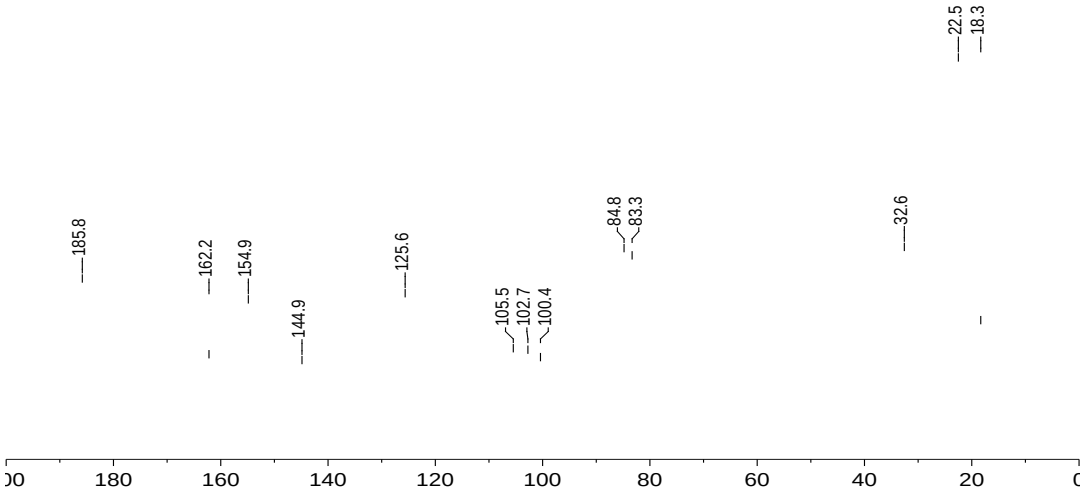

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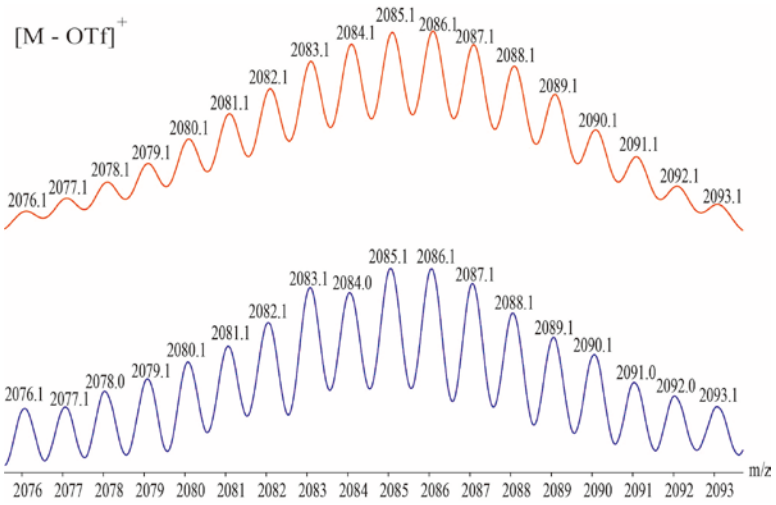
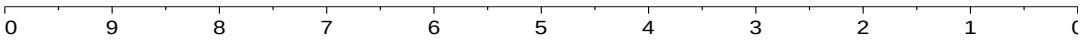


Figure 6. ^{1}H (a), ^{13}C NMR (b) and HR-ESI-MS (c) spectra of the molecular-rectangle **2b**.

(a)



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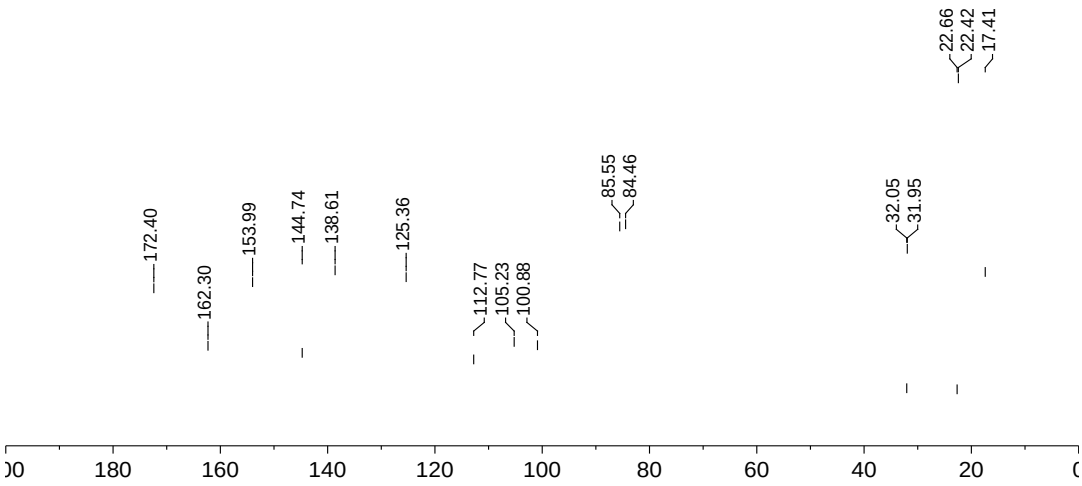

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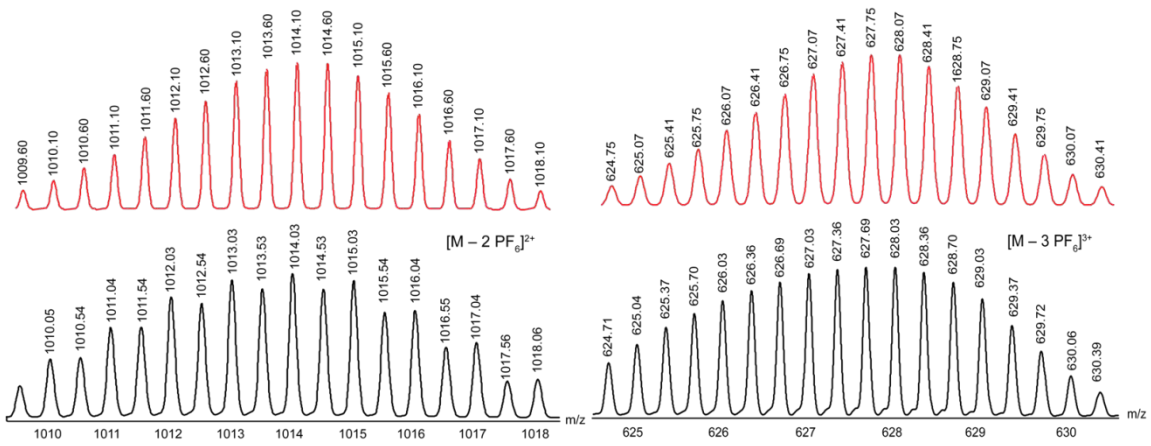
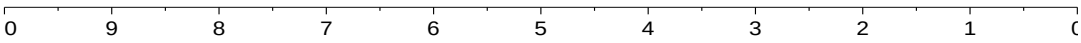


Figure 7. ^{1}H (a), ^{13}C NMR (b) and HR-ESI-MS (c) spectra of the molecular-rectangle **2c**.

(a)



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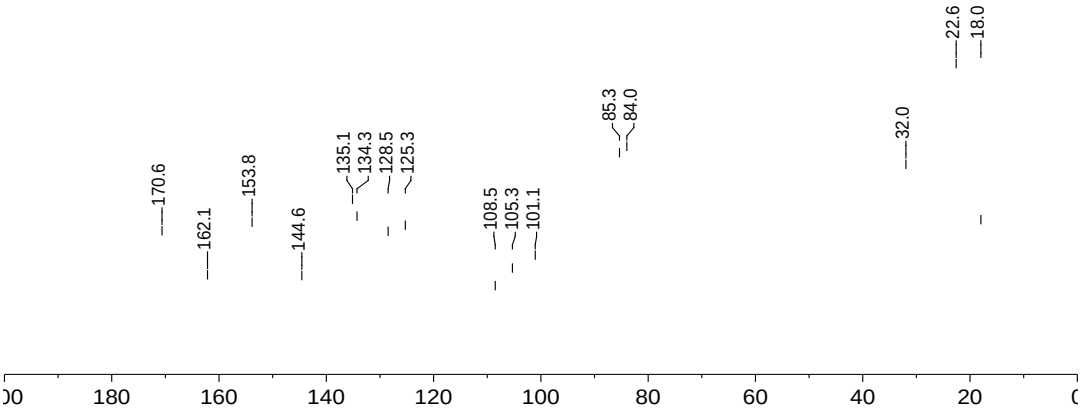

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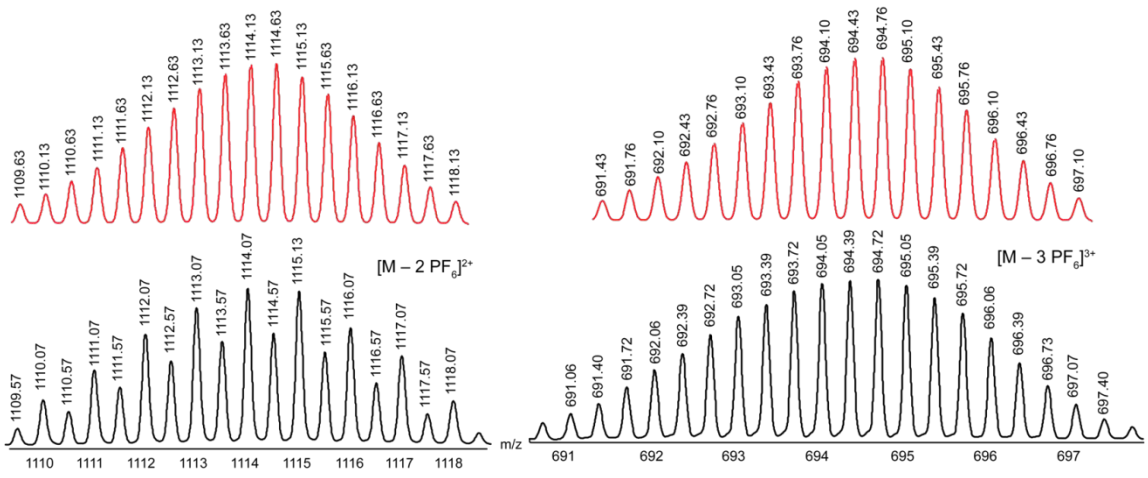
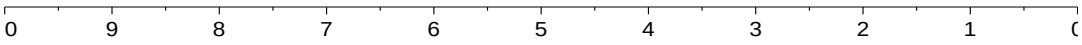


Figure 8. ^{1}H (a), ^{13}C NMR (b) and HR-ESI-MS (c) spectra of the molecular-rectangle **2d**.

(a)



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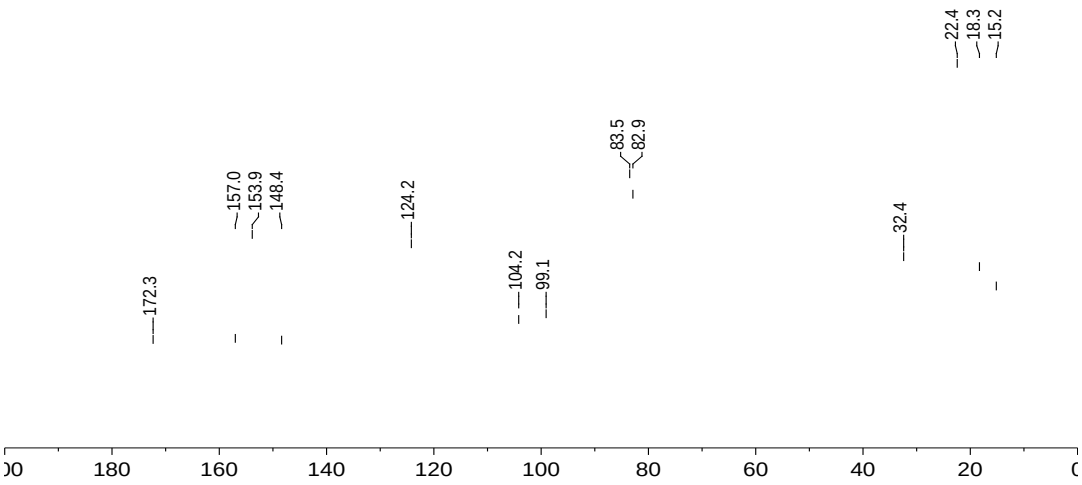
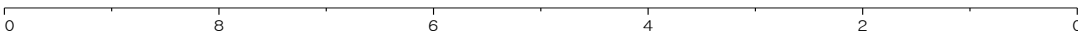


(c)

Figure 9. ^{1}H (a), ^{13}C NMR (b) and HR-ESI-MS (c) spectra of the molecular-rectangle **3a**.

(a)



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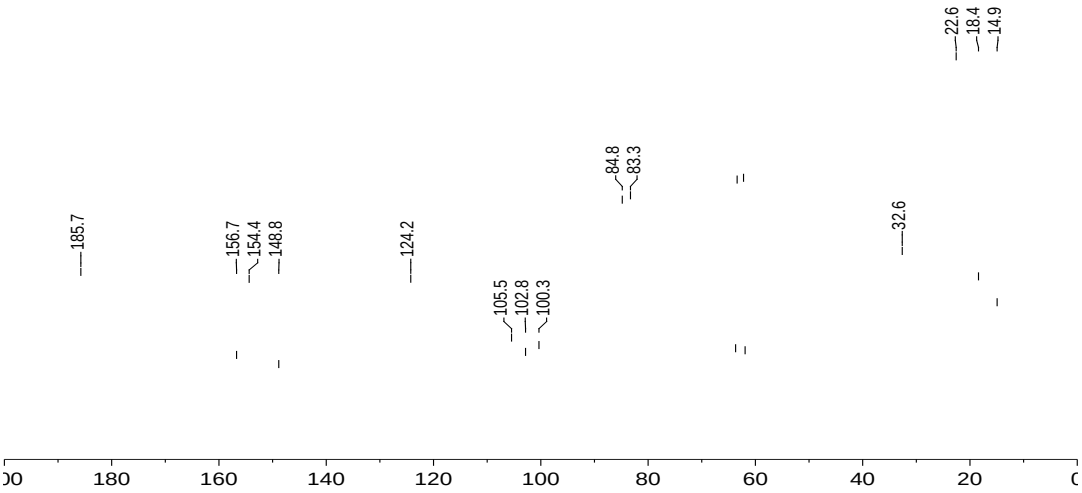

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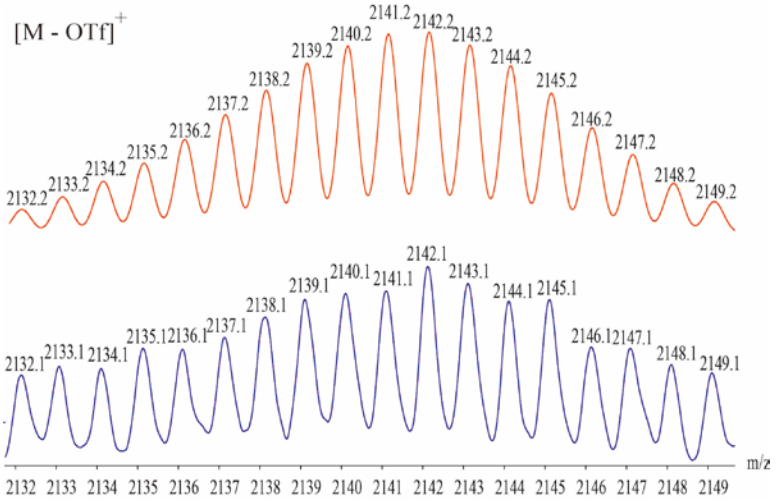
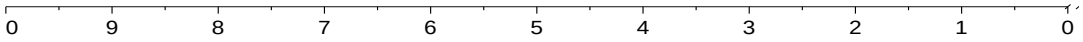


Figure 10. ^{1}H (a), ^{13}C NMR (b) and HR-ESI-MS (c) spectra of the molecular-rectangle **3b**.

(a)



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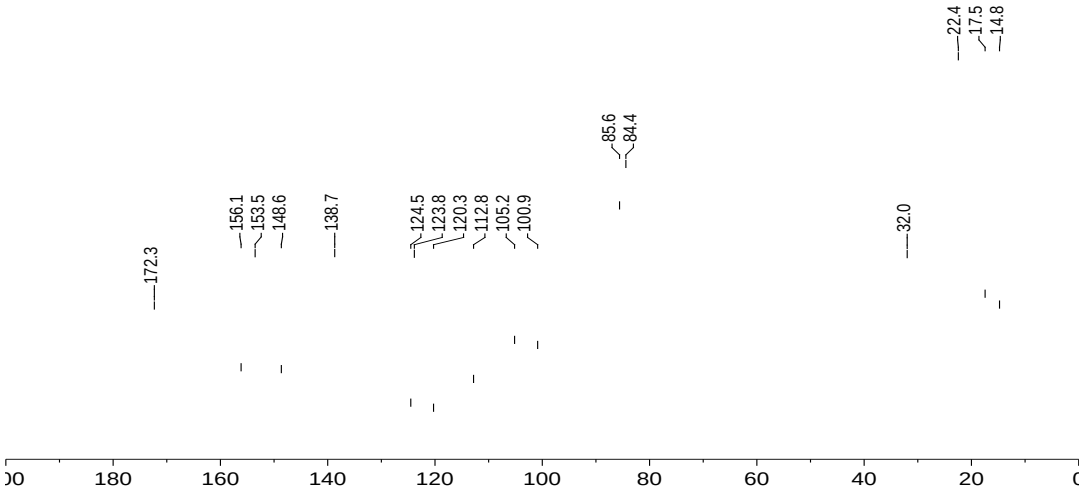

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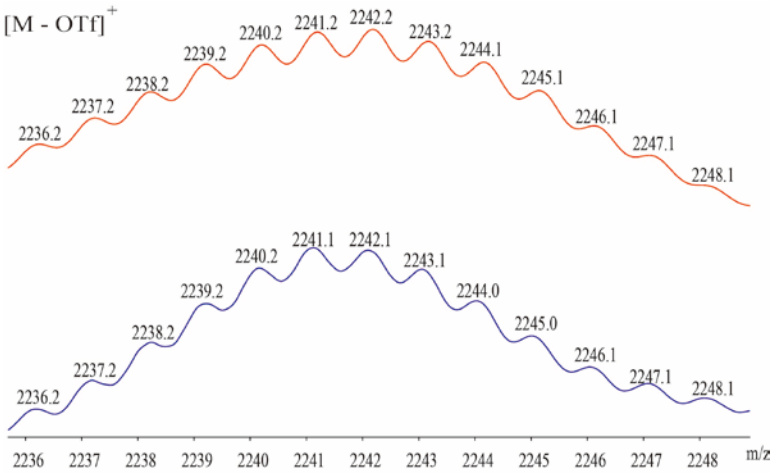
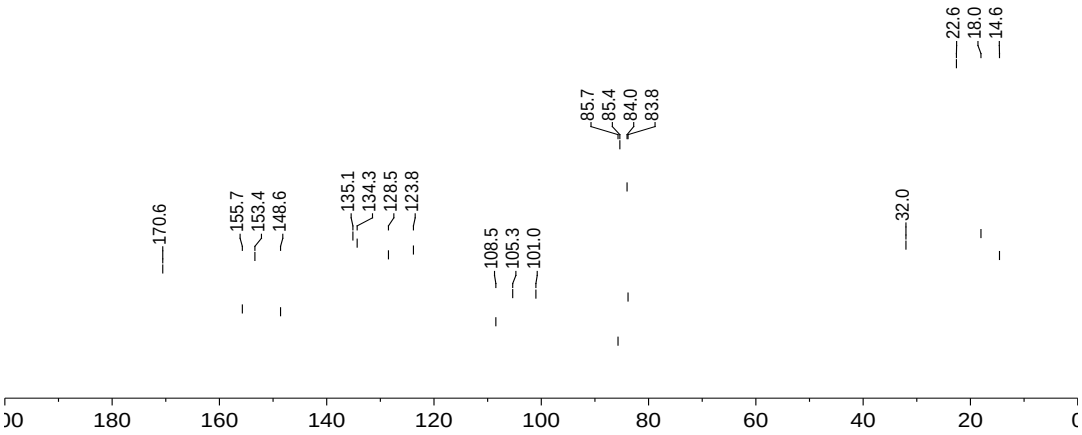


Figure 11. ^{1}H (a), ^{13}C NMR (b) and HR-ESI-MS (c) spectra of the molecular-rectangle **3c**.

(a)

(b)



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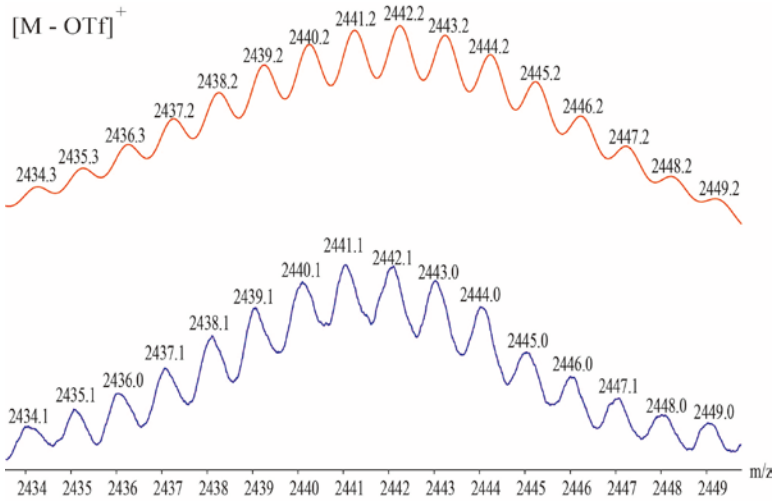

Figure 12. ^{1}H (a), ^{13}C NMR (b) and HR-ESI-MS (c) spectra of the molecular-rectangle **3d**.

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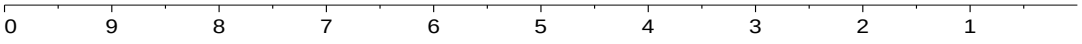

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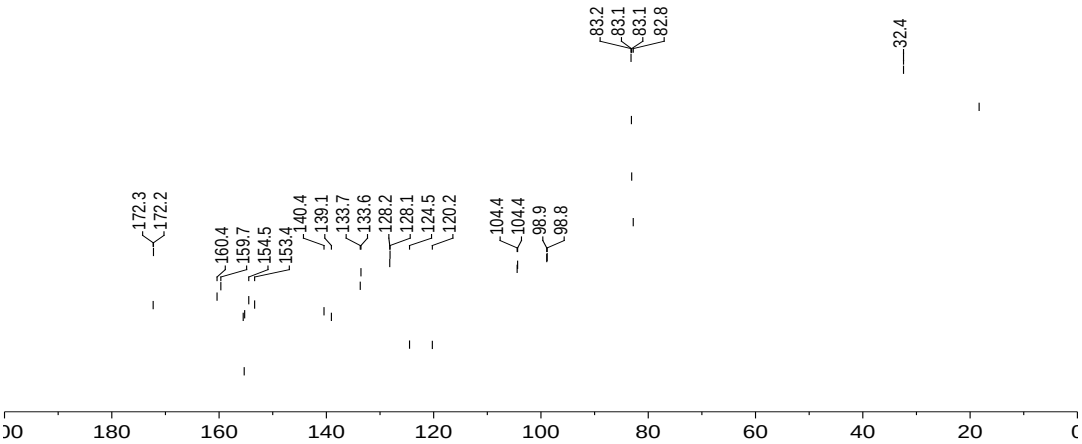

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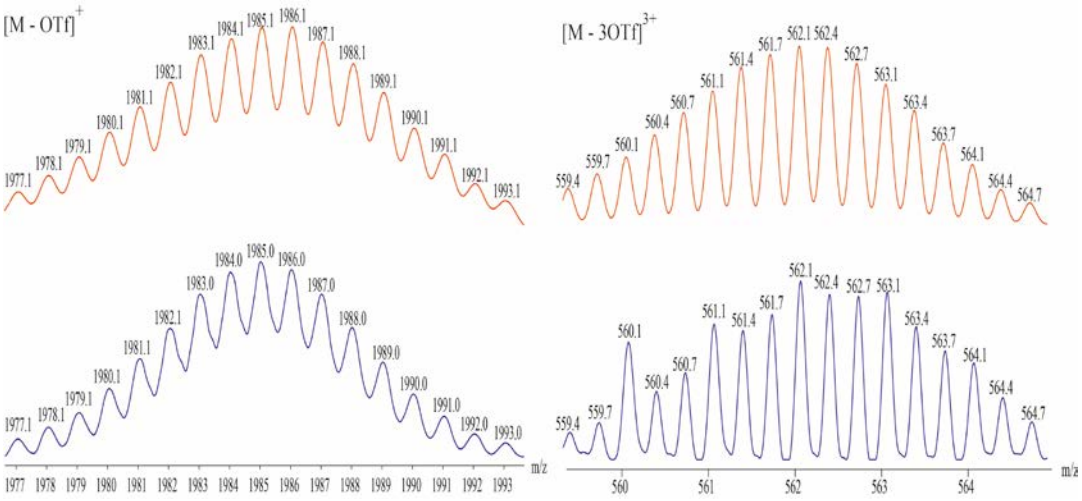
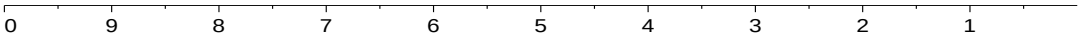


Figure 13. ^{1}H (a), ^{13}C NMR (b) and HR-ESI-MS (c) spectra of the molecular-rectangle **4a**.

(a)



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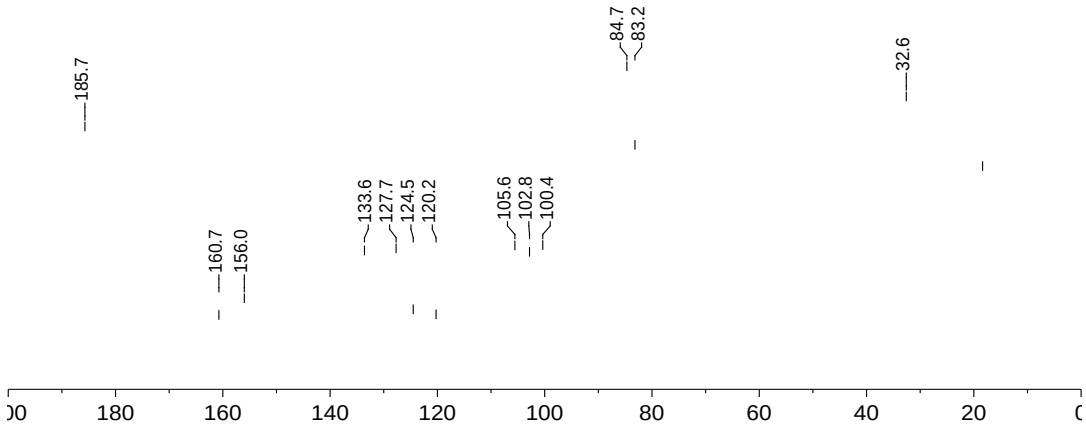

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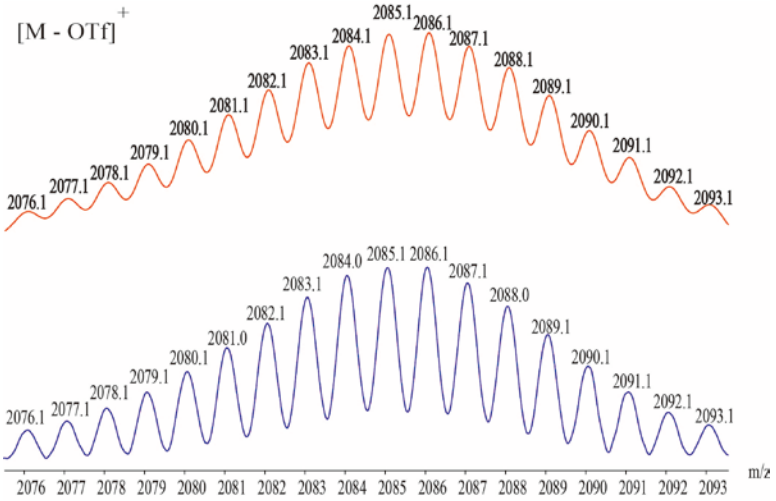
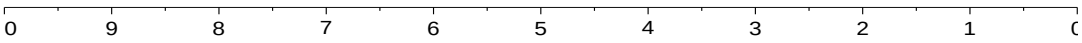


Figure 14. ^{1}H (a), ^{13}C NMR (b) and HR-ESI-MS (c) spectra of the molecular-rectangle **4b**.

(a)



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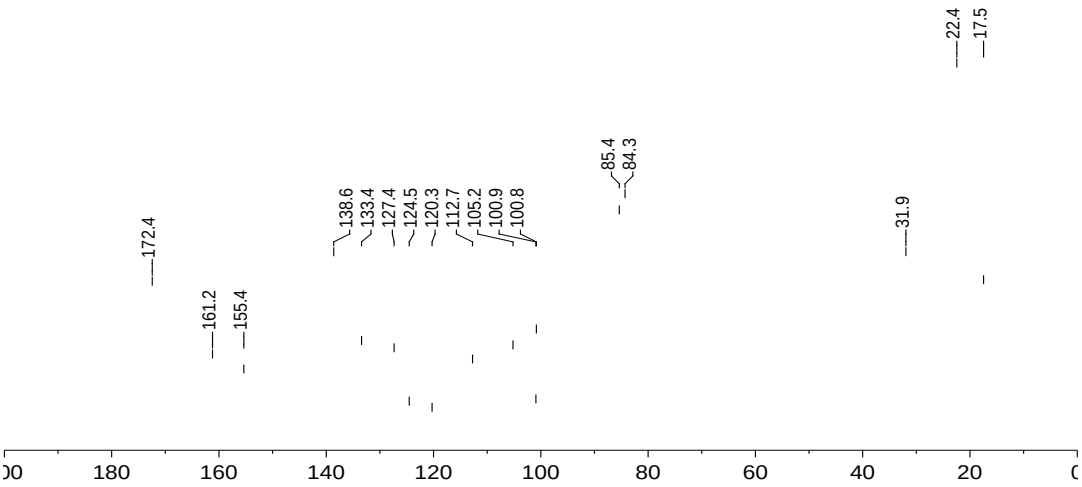

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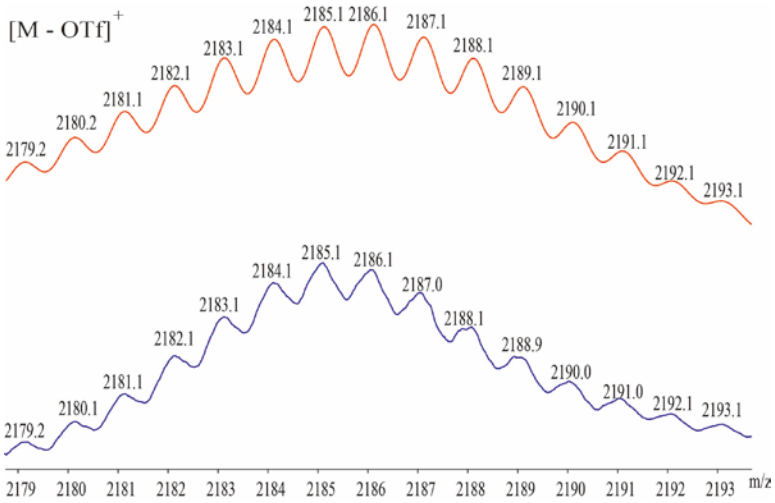
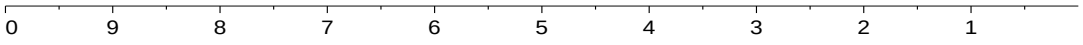


Figure 15. ^{1}H (a), ^{13}C NMR (b) and HR-ESI-MS (c) spectra of the molecular-rectangle **4c**.

(a)



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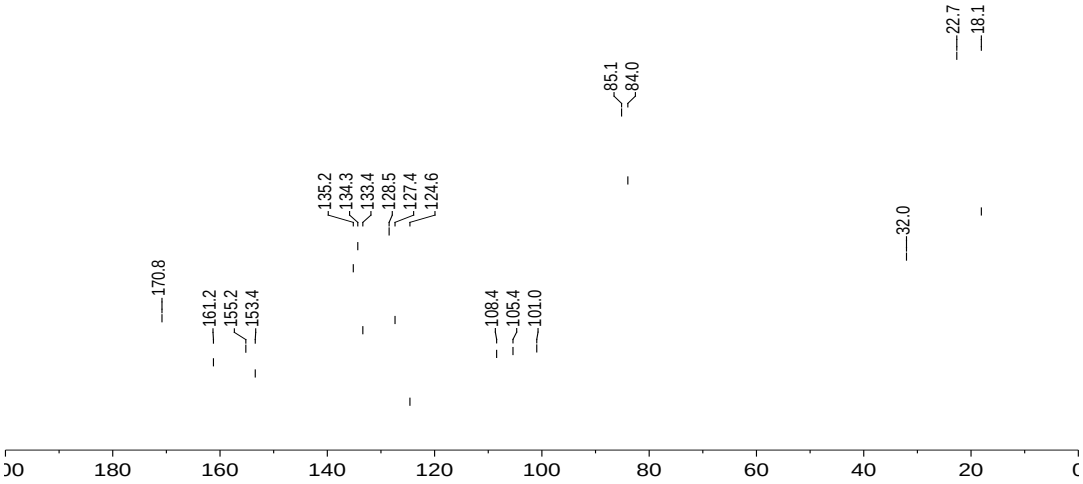

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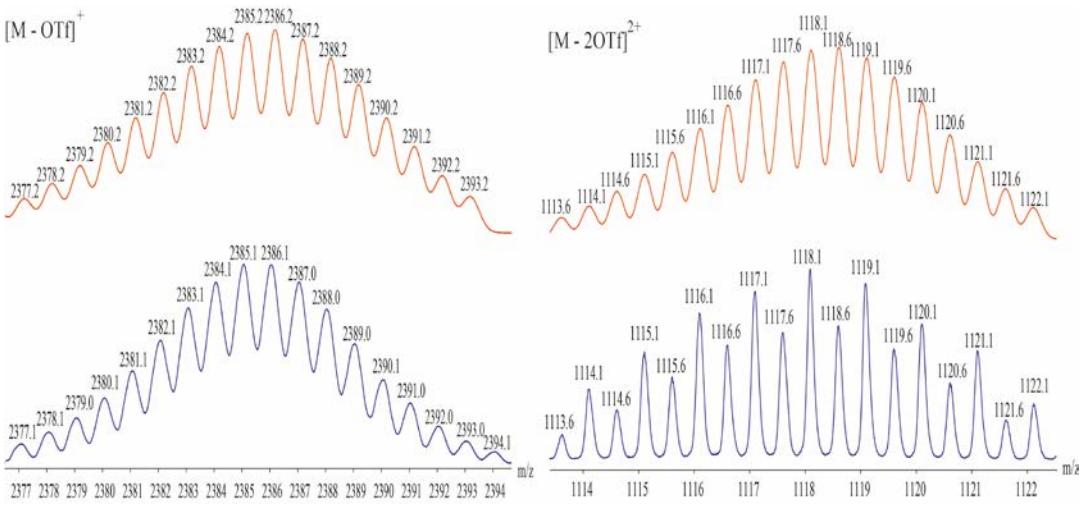

Figure 16. ^{1}H (a), ^{13}C NMR (b) and HR-ESI-MS (c) spectra of the molecular-rectangle **4d**.

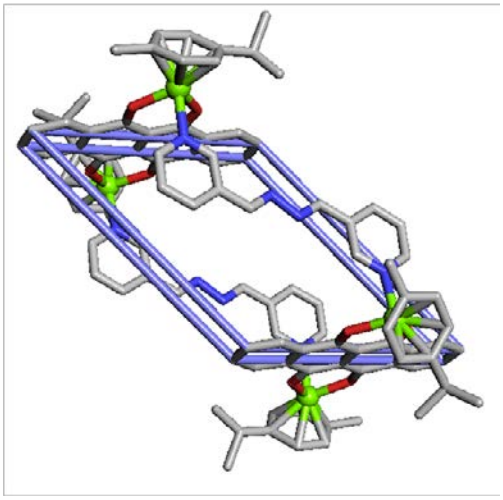

Figure 17. X-ray crystal structure of and **4d** emphasizing a rhombohedral molecular cavity.

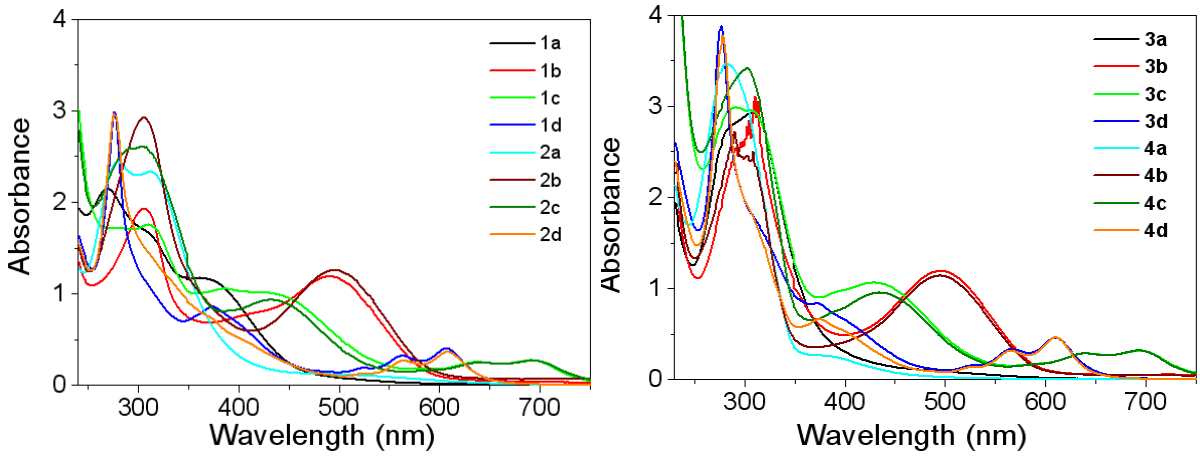

Figure 17. UV-Visible spectra of molecular- rectangles.

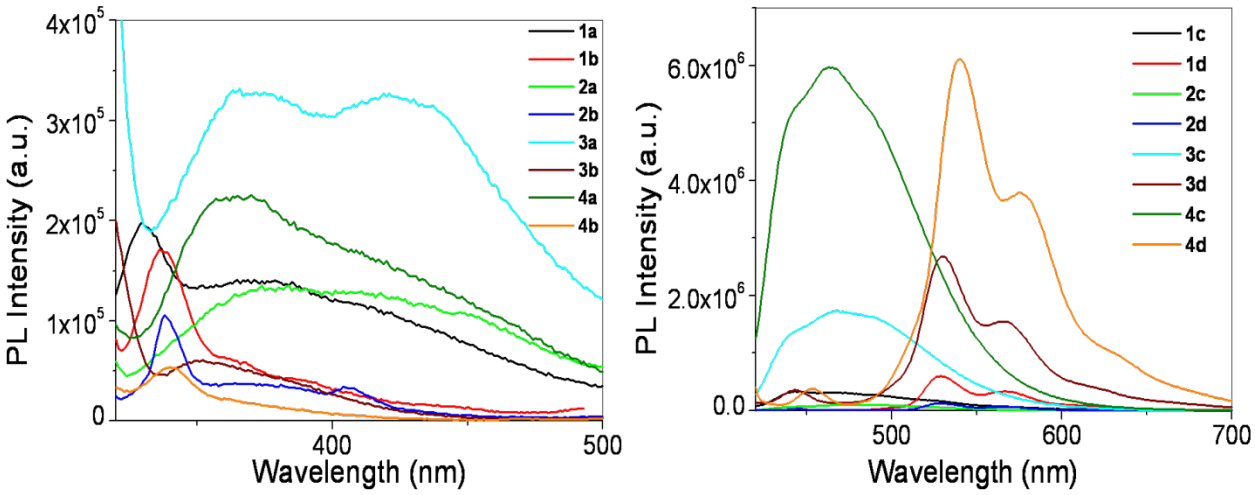

Figure 18. Fluorescence spectra of molecular- rectangles.

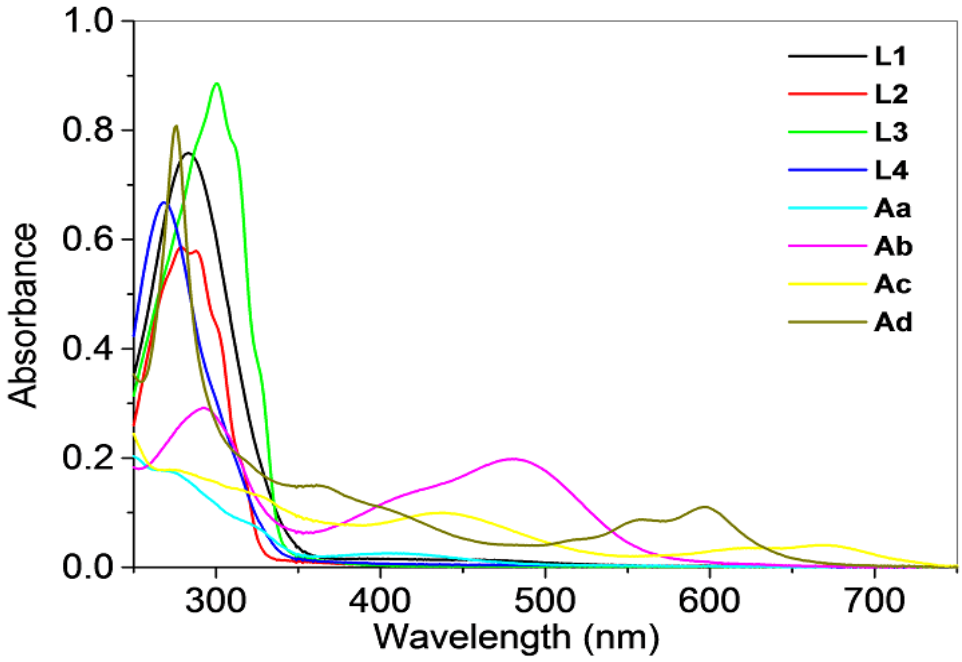

Figure 19. UV-visible spectra of acceptors and donors.

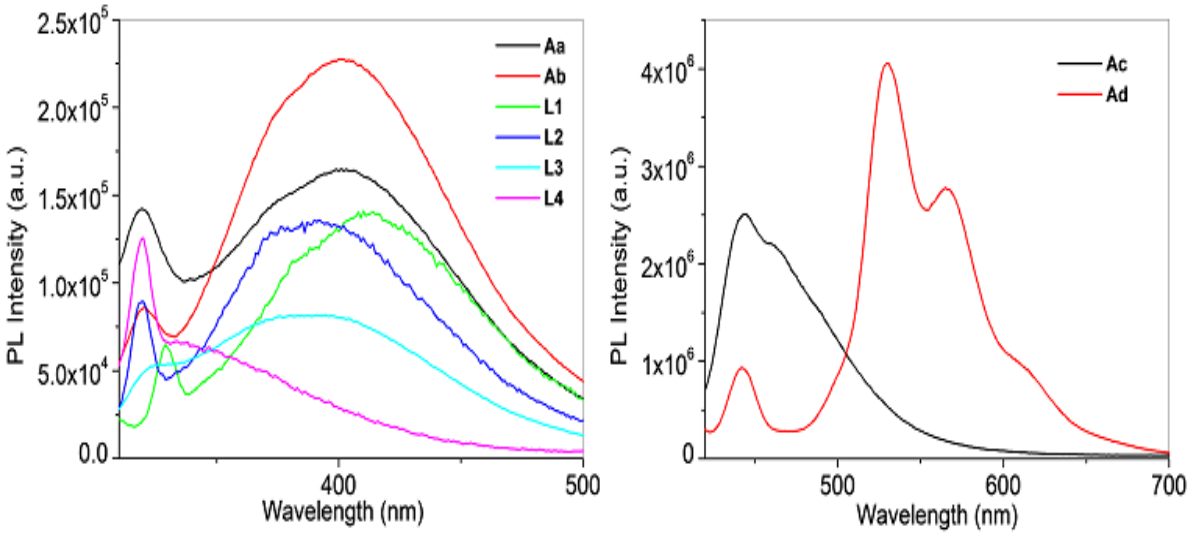

Figure 20. Fluorescence spectra of acceptors and donors (left, excited at 298 nm) and acceptors (right, excited at 390 nm).

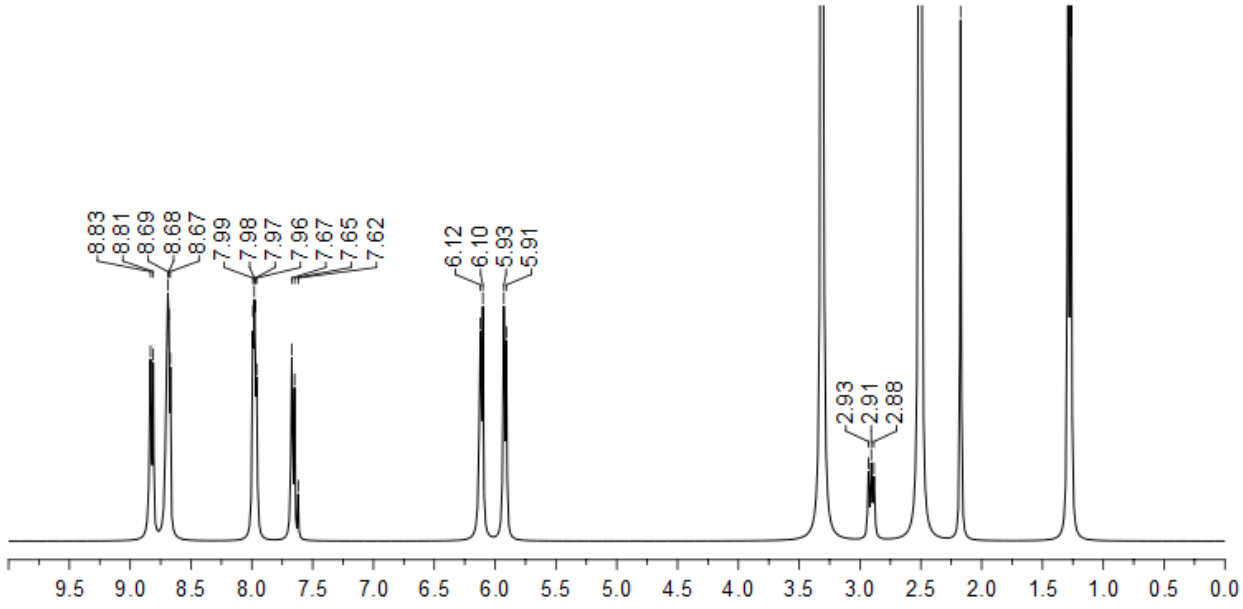

Figure 21. ^{1}H NMR Spectra of **1d** in DMSO after 48 h dissolution.

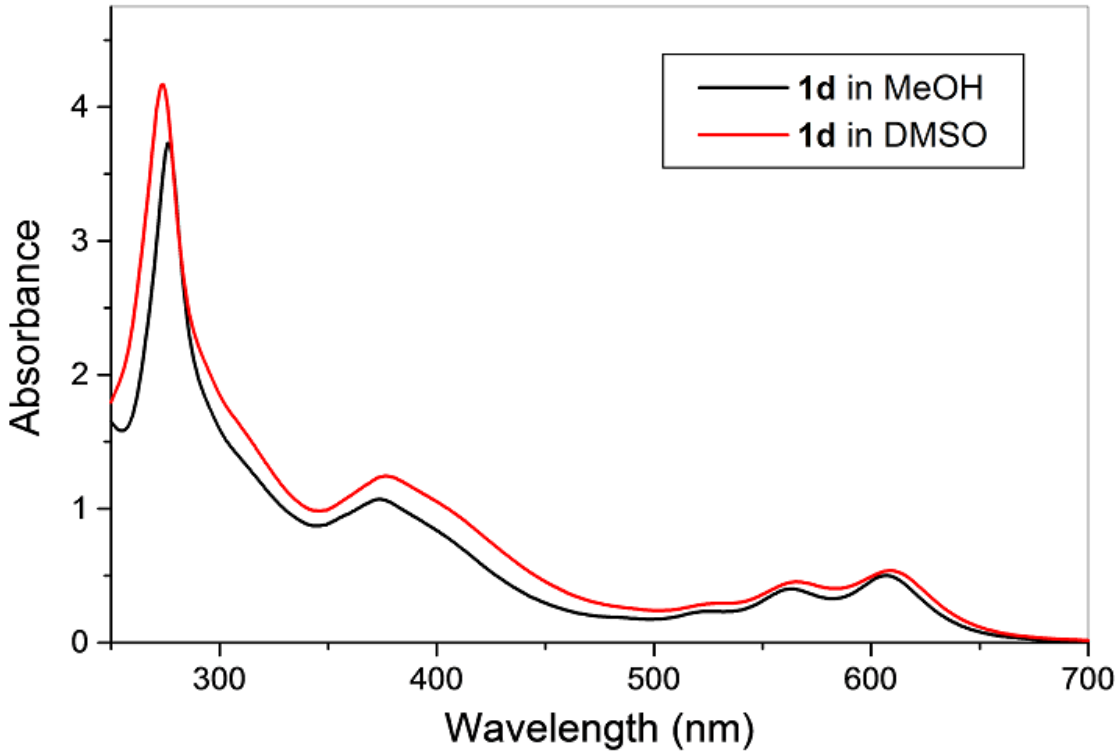

Figure 22. Compared UV-Visible Spectra of **1d after** 48 h dissolution.

Table 1. Crystal data and structure refinement for **1b** and **4d**.

	1b	4d
Empirical formula	C_{76} H_{76} F_{12} N_8 O_{20} Ru_4 S_4	$C_{114}H_{112}F_{12}N_8O_{24}Ru_4S_4$
Formula weight	2181.97	2738.64
Temp.	100(2) K	173(2)
Wavelength	0.90000 Å	0.71073 Å
Crystal system	Triclinic	Monoclinic
Space group	*P*-1	$P2_1/c$
Unit cell Dimension	a = 10.472(2) Å, α = 97.98(3)° b =19.443(4) Å, β = 94.22(3)° c = 24.876(5) Å, γ = 91.94(3)°	a = 15.356(3) Å, α = 90° b = 23.897(5) Å, β = 108.7(3)° c = 17.071(3) Å, γ = 90°
Volume	4997.3(17) $Å^3$	5931(2) $Å^3$
Z	2	2
Density (calculated)	1.450 g/cm^3	1.534 Mg/m^3
Absorption coefficient	1.425 mm^{-1}	0.662 mm^{-1}
F(000)	2192	2784
Crystal size	0.41 x 0.25 x 0.20 mm^3	0.28 x 0.23 x 0.10 mm^3
Theta range for data collection	1.34 to 25.00°	2.99 to 27.48°
Independent reflections	7974 [R(int) = 0.0282]	13558 [R(int) = 0.1240]
Completeness to theta = 25.00°	92.1 %	99.7 %
Max. and min. transmission	0.8626 and 0.7453	0.9368 and 0.8364
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Goodness-of-fit on F^2	1.067	0.985
Final R indices	R1 = 0.0753, wR2 = 0.2389	R1 = 0.0677, wR2 = 0.1585
R indices (all data)	R1 = 0.084, wR2 = 0.246	R1 = 0.172, wR2 = 0.210
Largest diff. peak and hole	1.632 and -0.970 e.$Å^{-3}$	1.424 and -1.000 e.$Å^{-3}$