Supplementary Materials

Synthesis of Iodinated Cobalt Bis(dicarbollide) Conjugates with Acridine and Their Biological Studies

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NMR, IR, and mass spectra of compound **7** (S17-S24) 12

NMR, IR, and mass spectra of compound **8** (S25-S31) 17

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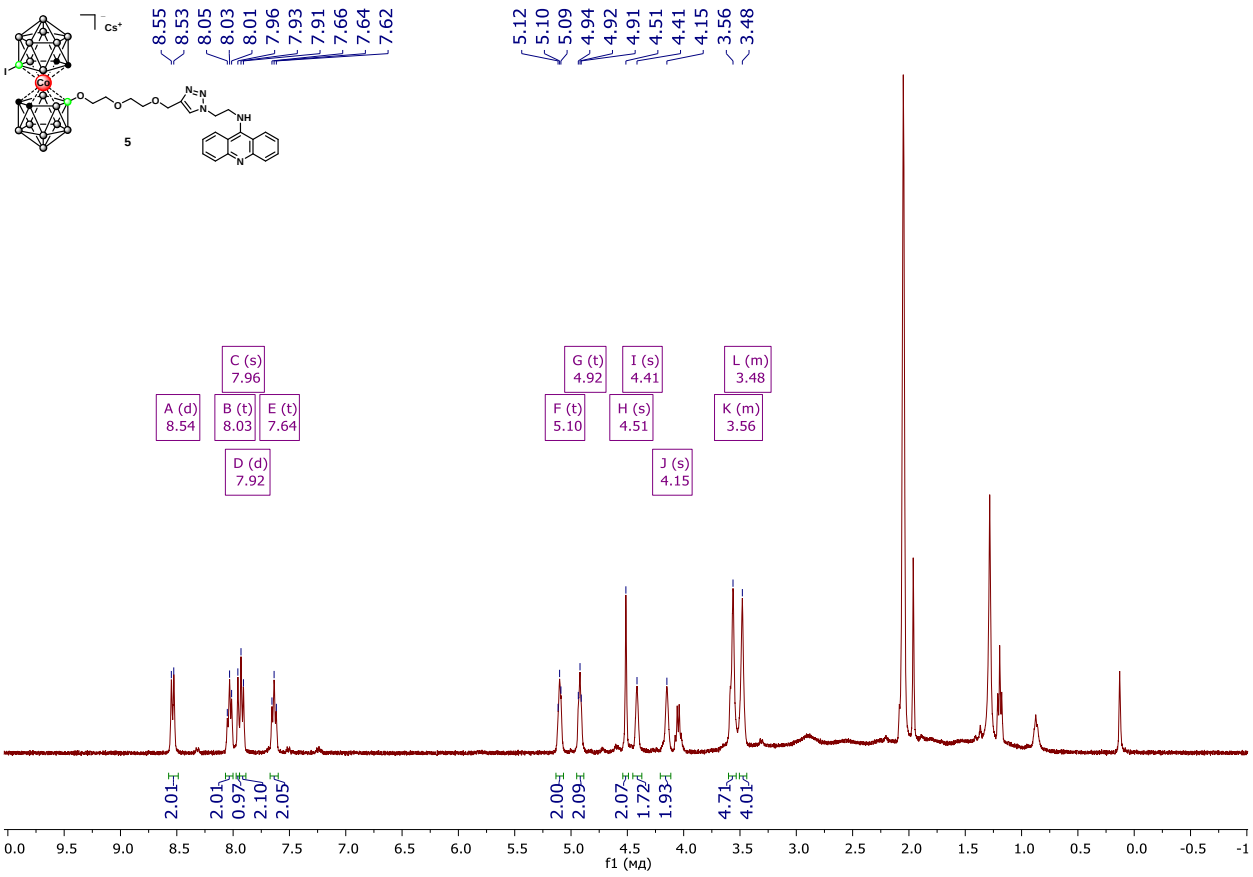


Figure S1. NMR ^{1}H spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$O(CH$_2$CH$_2$O)$_2$-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**5**)

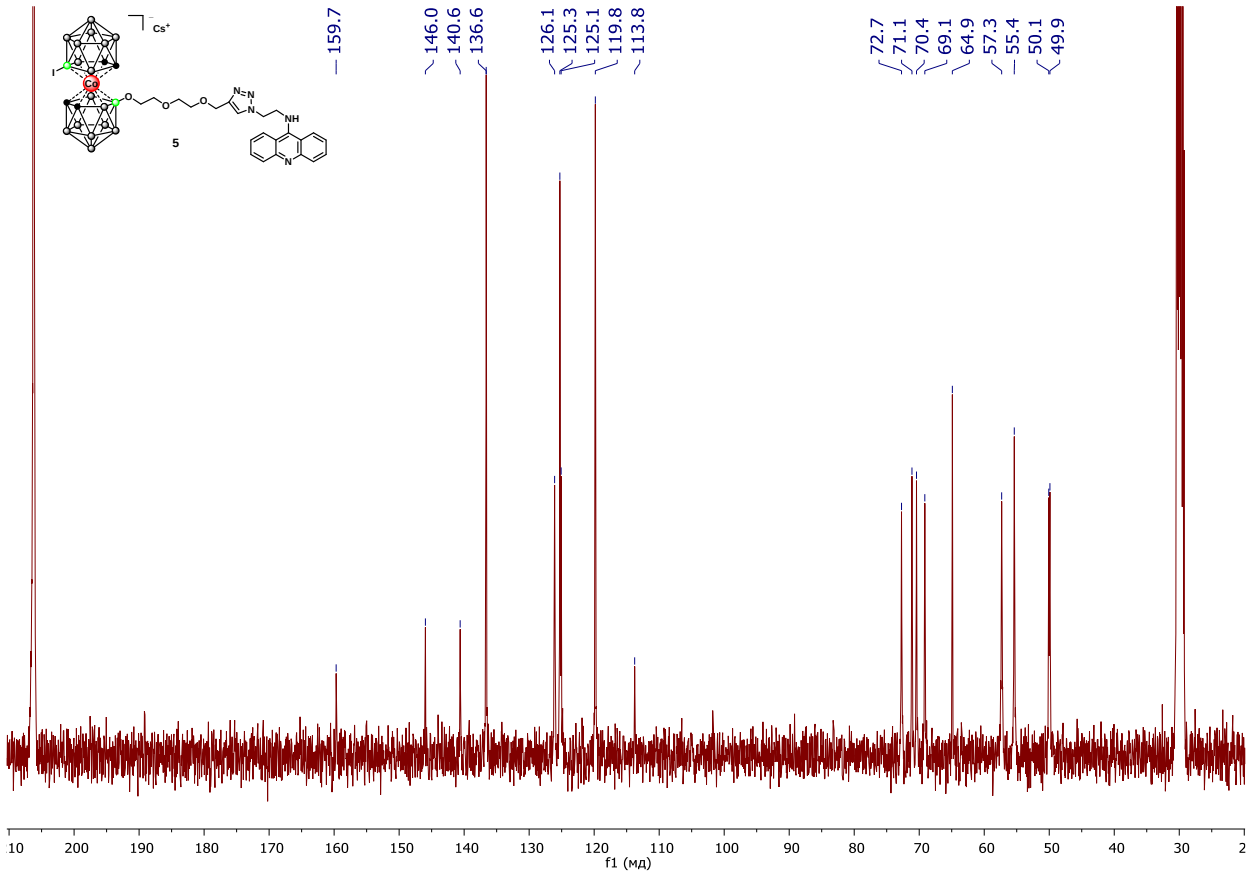


Figure S2. NMR ^{13}C{^{1}H} spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$O(CH$_2$CH$_2$O)$_2$-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**5**)

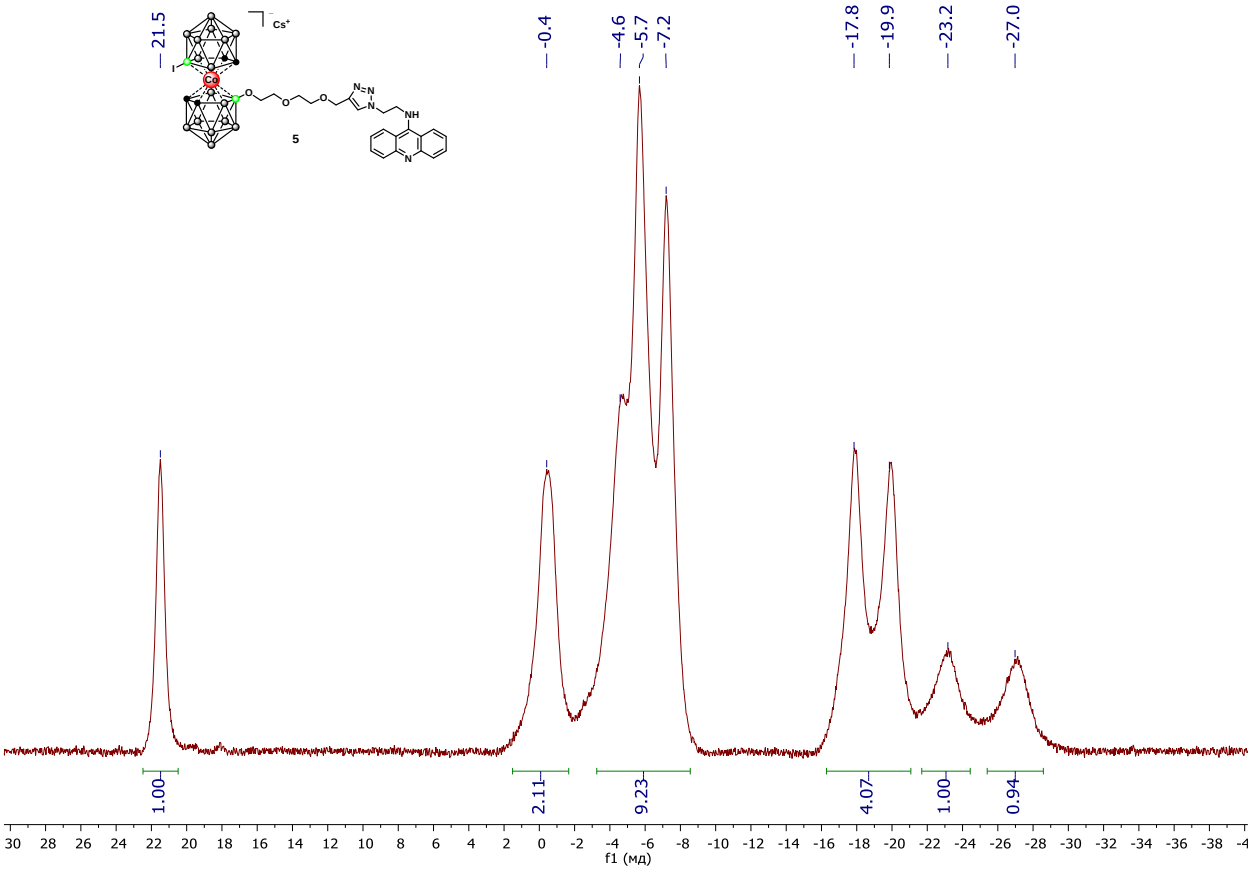


Figure S3. NMR $^{11}B\{^{1}H\}$ spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$O(CH$_2$CH$_2$O)$_2$-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**5**)

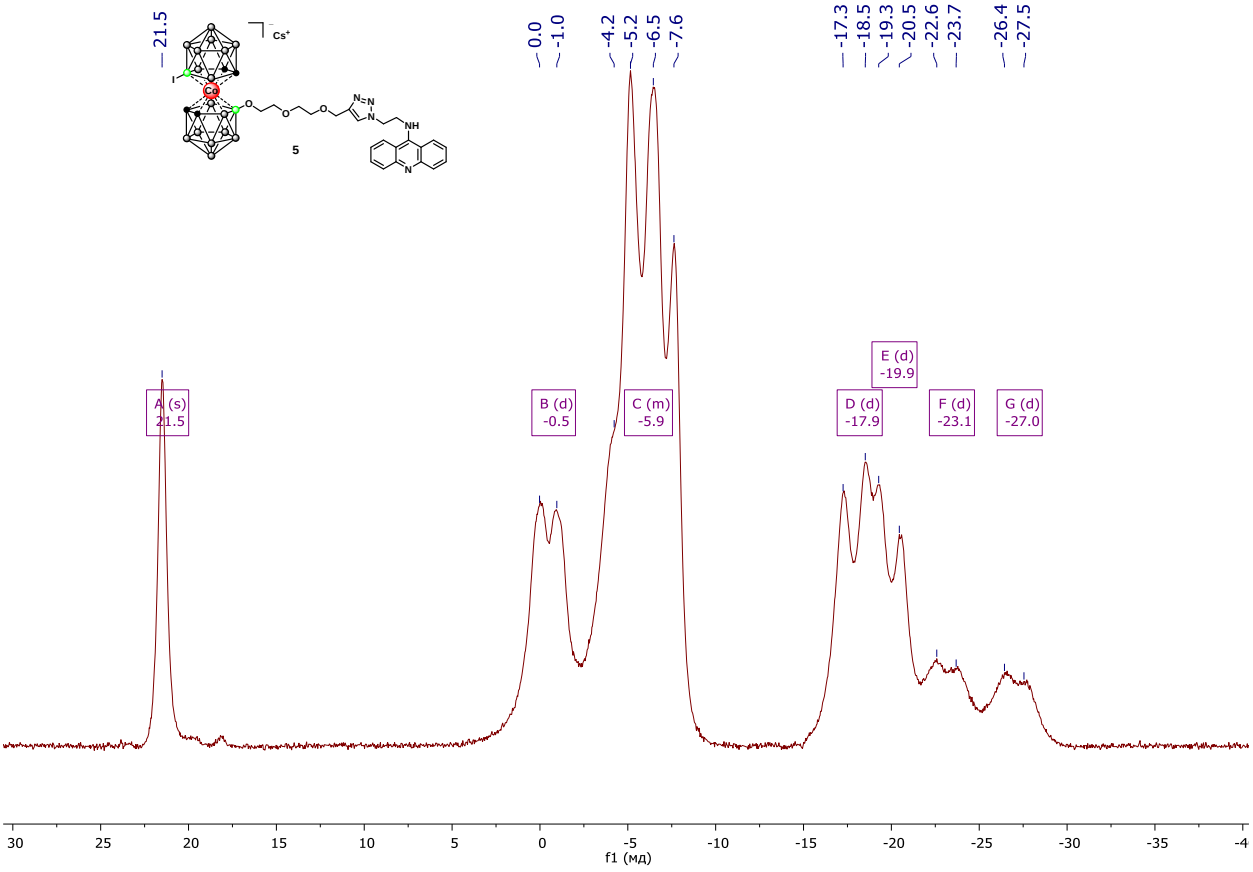


Figure S4. NMR ^{11}B spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$O(CH$_2$CH$_2$O)$_2$-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**5**)

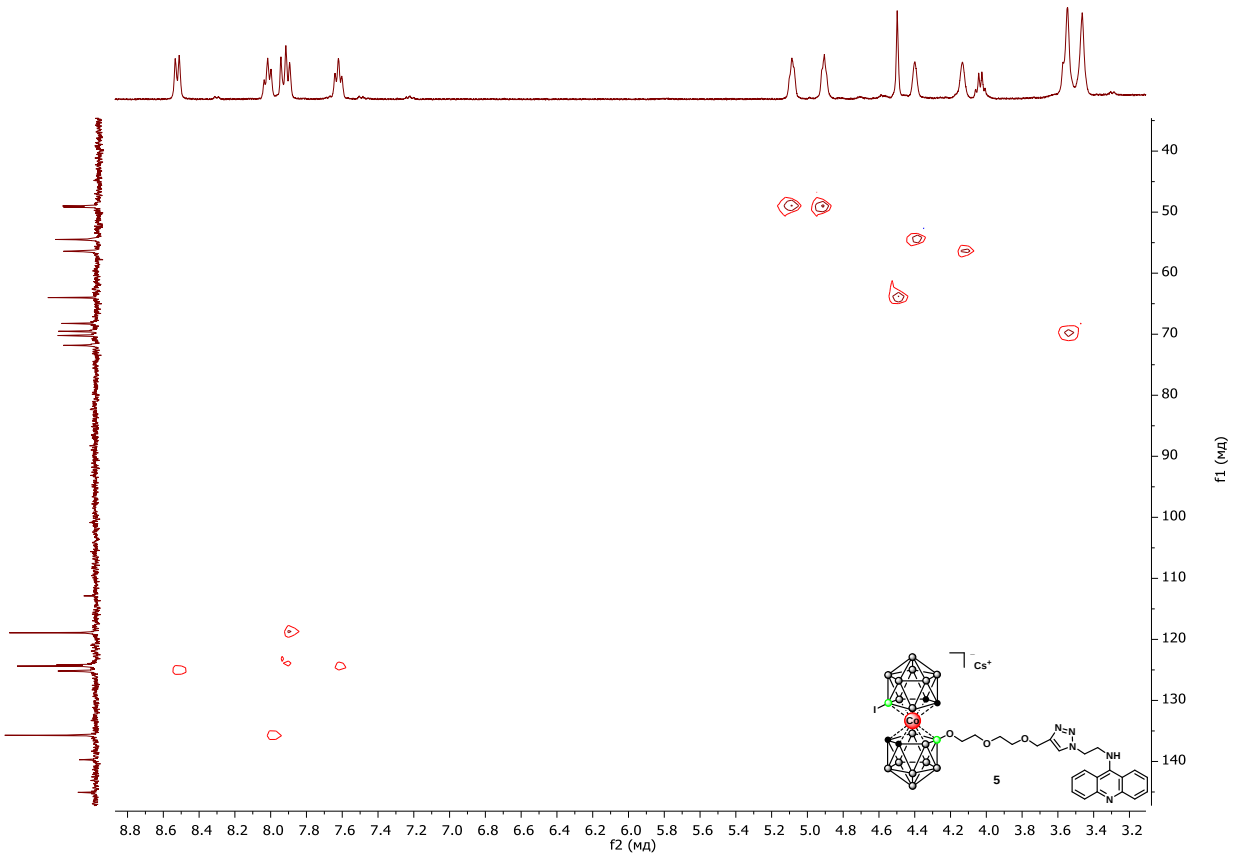


Figure S5. 2D NMR ^{1}H-^{13}C HMQC spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$O(CH$_2$CH$_2$O)$_2$-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**5**)

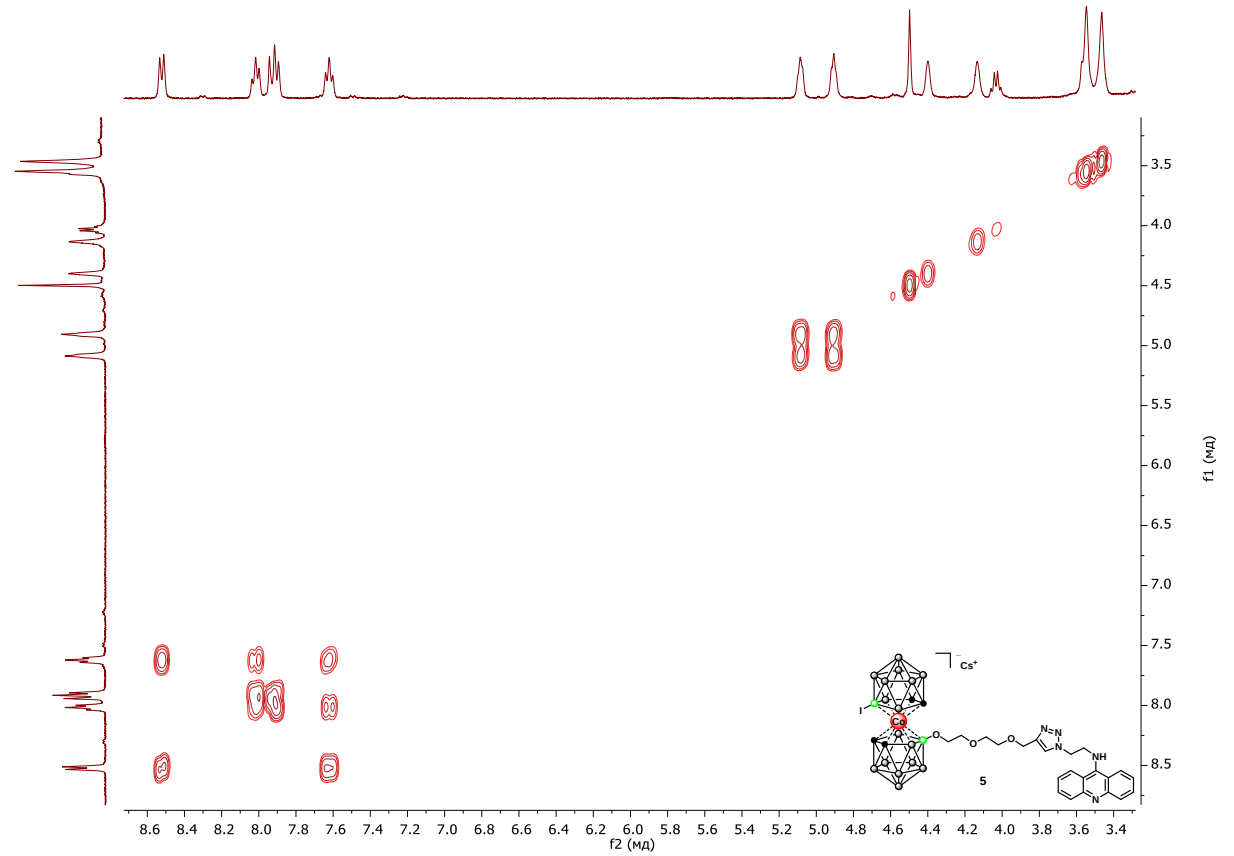


Figure S6. 2D NMR ^{1}H-^{1}H COSY spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$O(CH$_2$CH$_2$O)$_2$-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**5**)

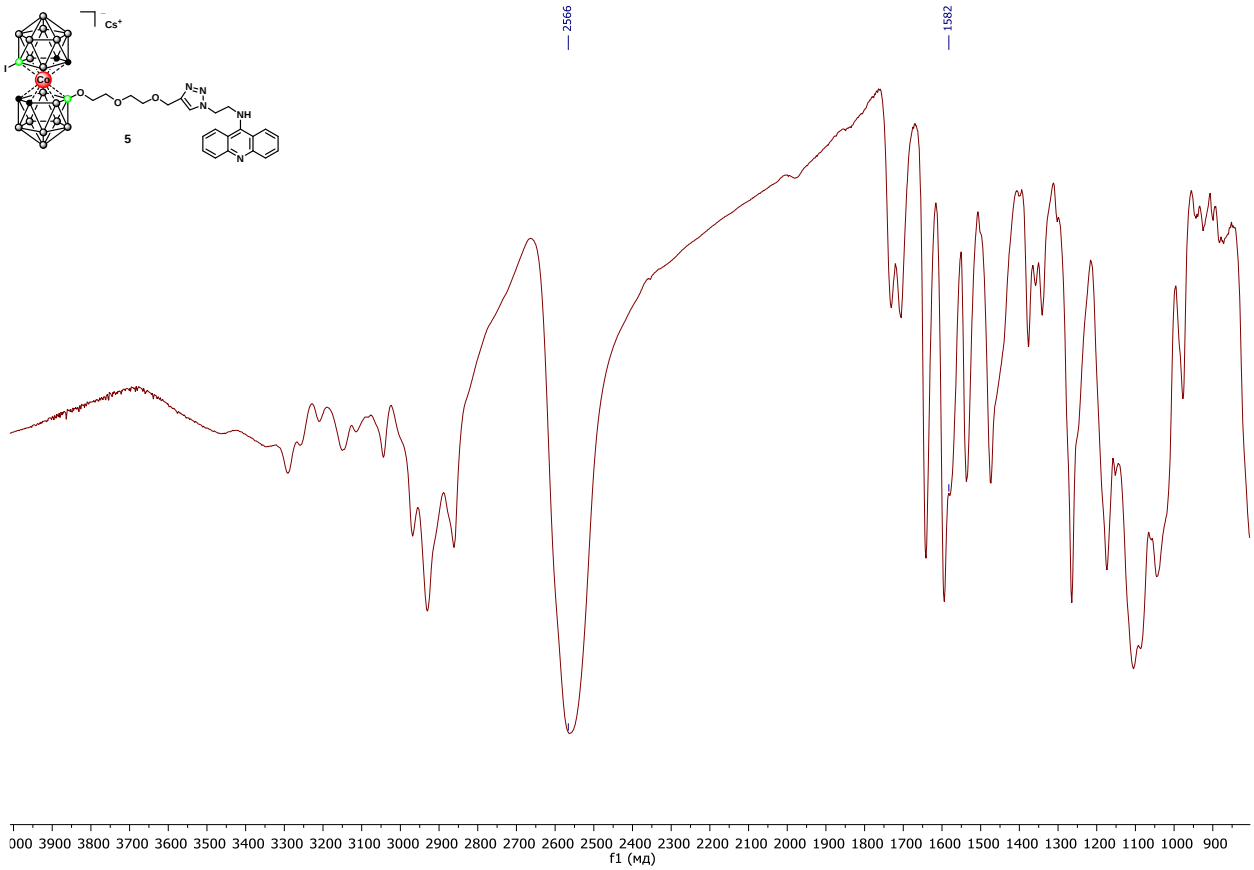


Figure S7. IR spectrum of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$O(CH$_2$CH$_2$O)$_2$-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**5**)

Display Report

Analysis Info

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Sample Name	/CHIZ DA-038	Instrument / Ser#	maXis 43
Comment	CH3CN 100 %, dil. 200, calibrant added		

Acquisition Parameter

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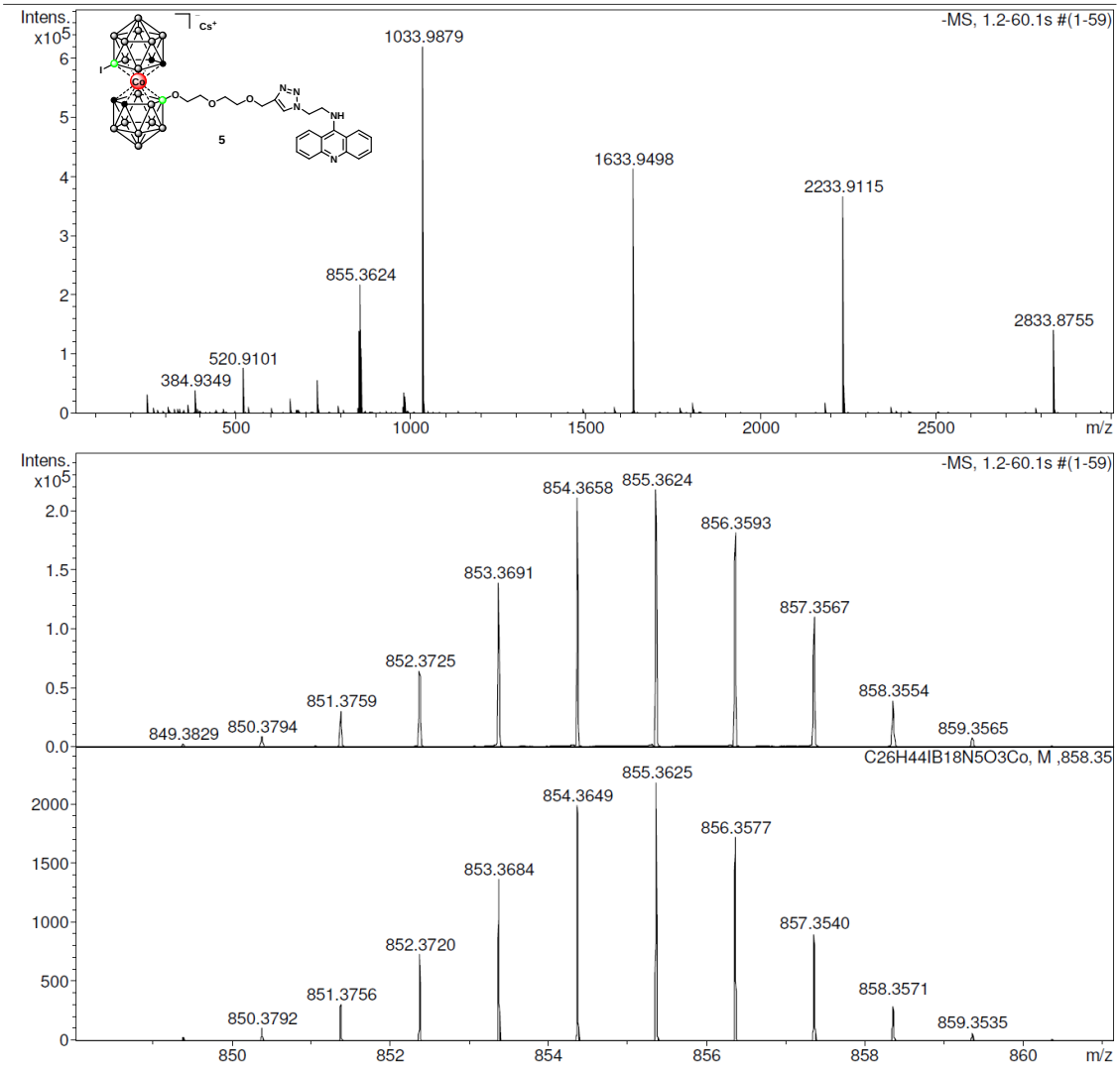


Figure S8. HRMS (ESI) of $C_{26}H_{44}B_{18}CoIN_5O_3$, *m/z*: calcd for $[M]^-$ 855.3625, found: 855.3624

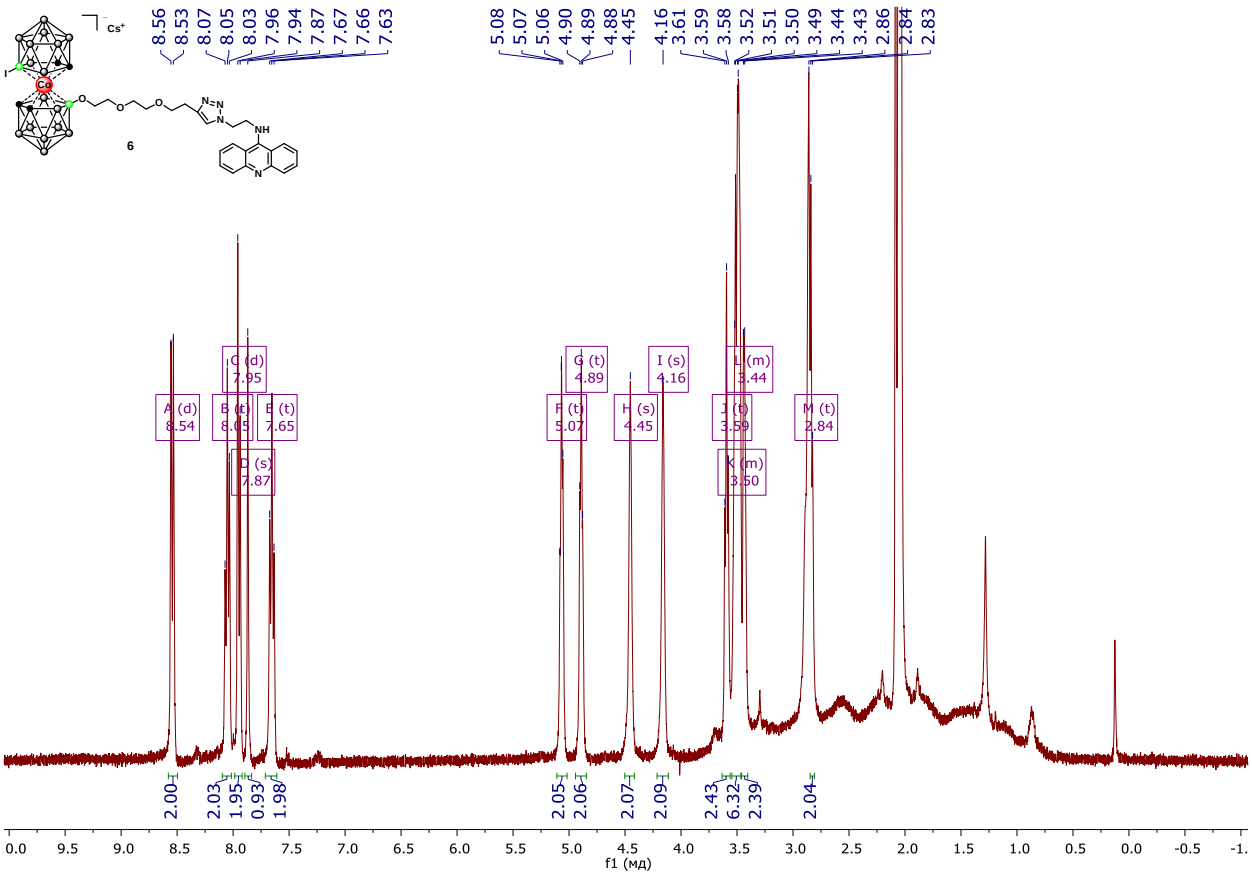


Figure S9. NMR ^{1}H spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$CH$_2$O(CH$_2$CH$_2$O)$_2$-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**6**)

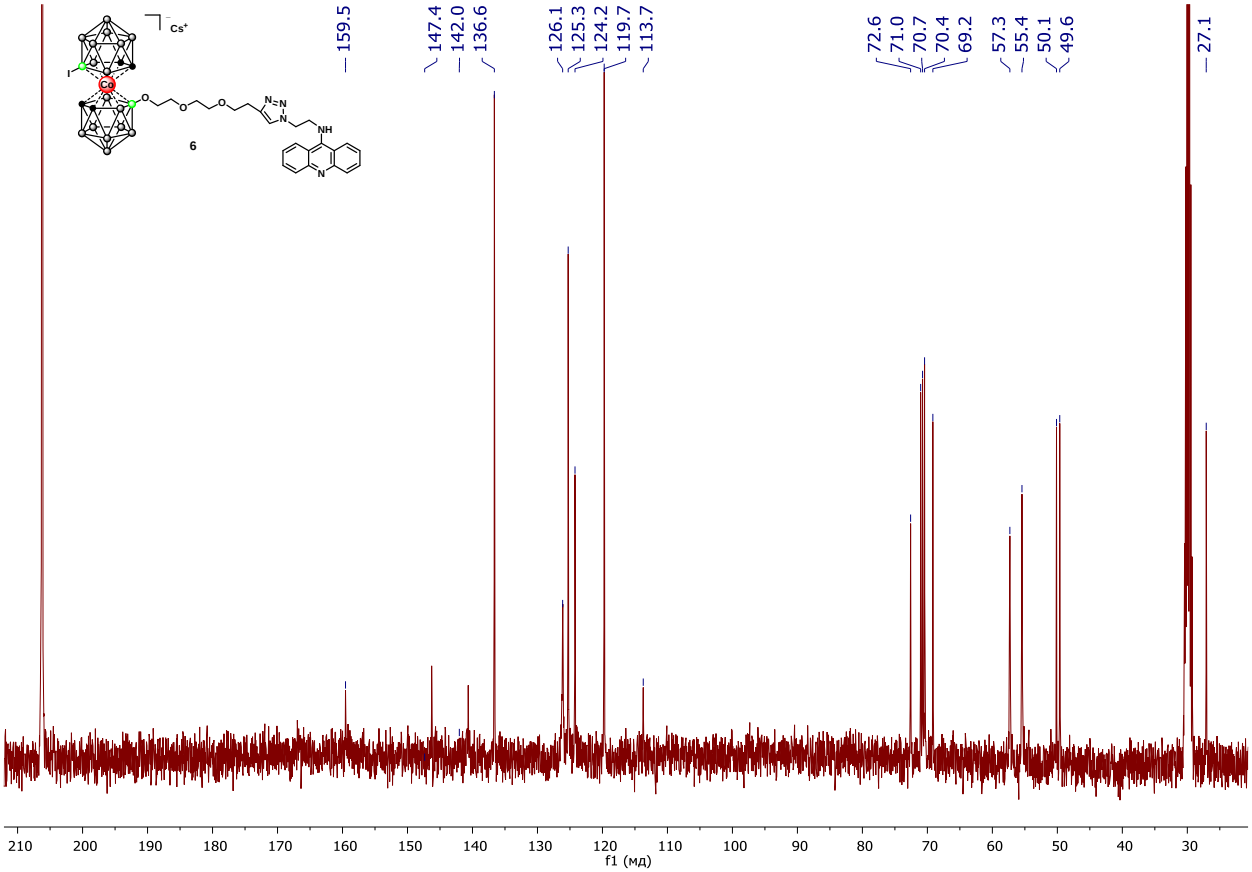


Figure S10. NMR $^{13}C\{^{1}H\}$ spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$CH$_2$O(CH$_2$CH$_2$O)$_2$-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**6**)

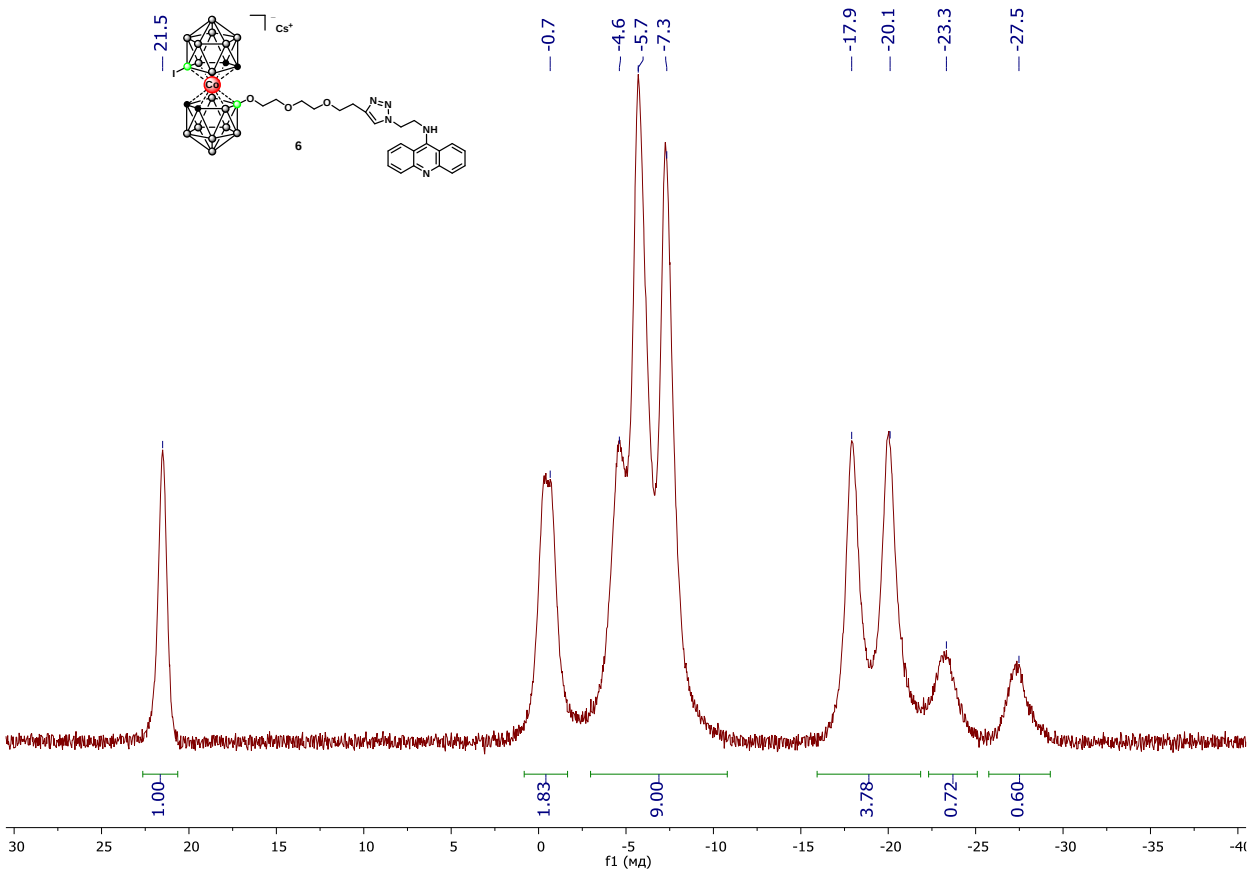


Figure S11. NMR $^{11}B\{^{1}H\}$ spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$CH$_2$O(CH$_2$CH$_2$O)$_2$-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**6**)

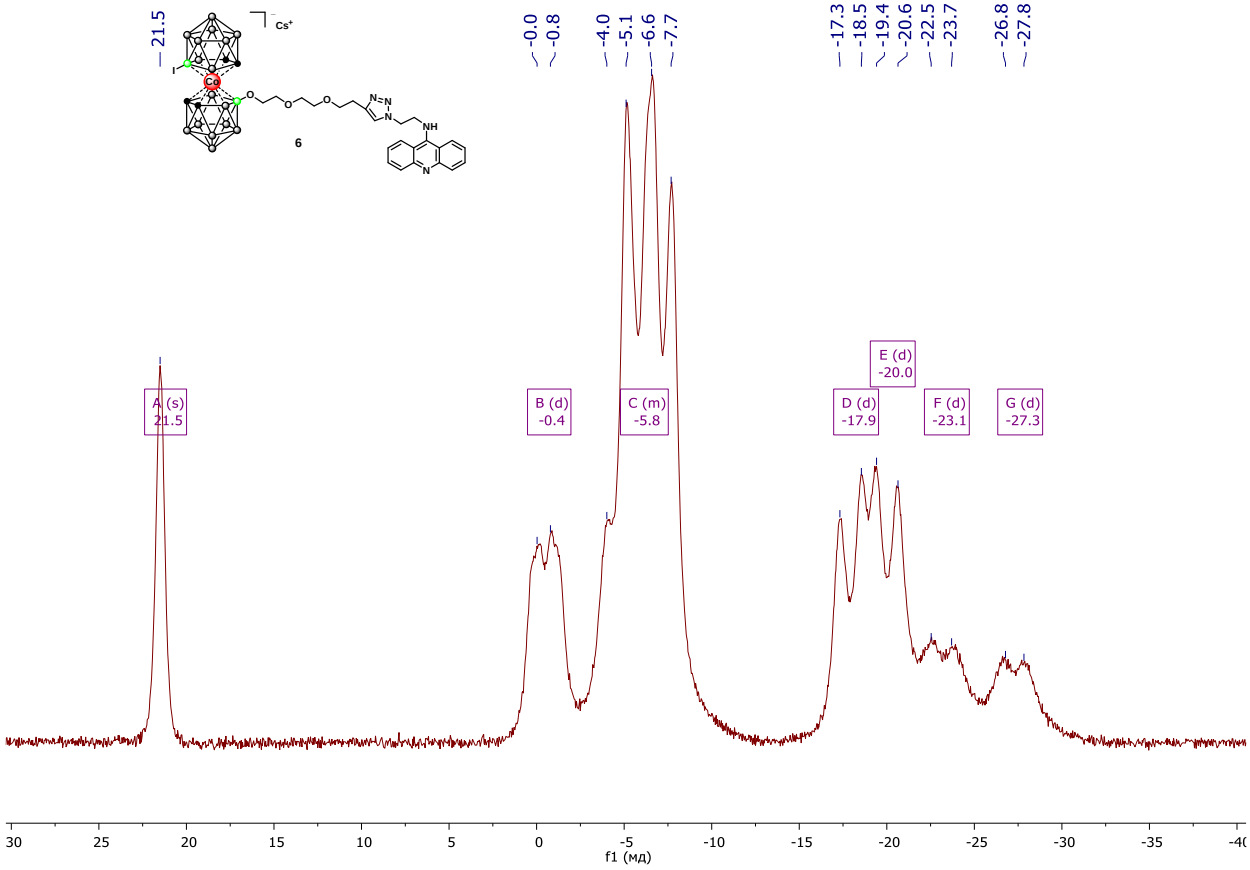


Figure S12. NMR ^{11}B spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$CH$_2$O(CH$_2$CH$_2$O)$_2$-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**6**)

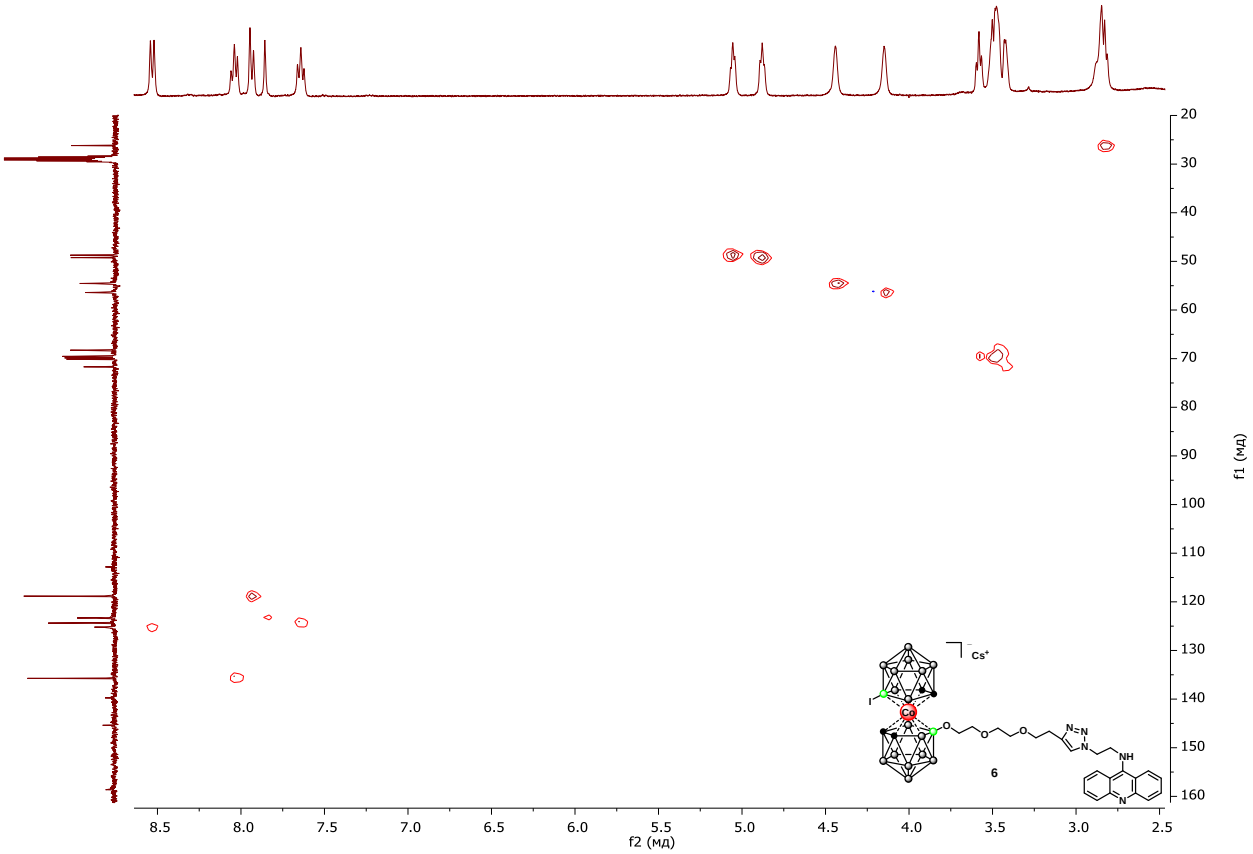


Figure S13. 2D NMR ^{1}H-^{13}C HMQC spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$CH$_2$O(CH$_2$CH$_2$O)$_2$-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**6**)

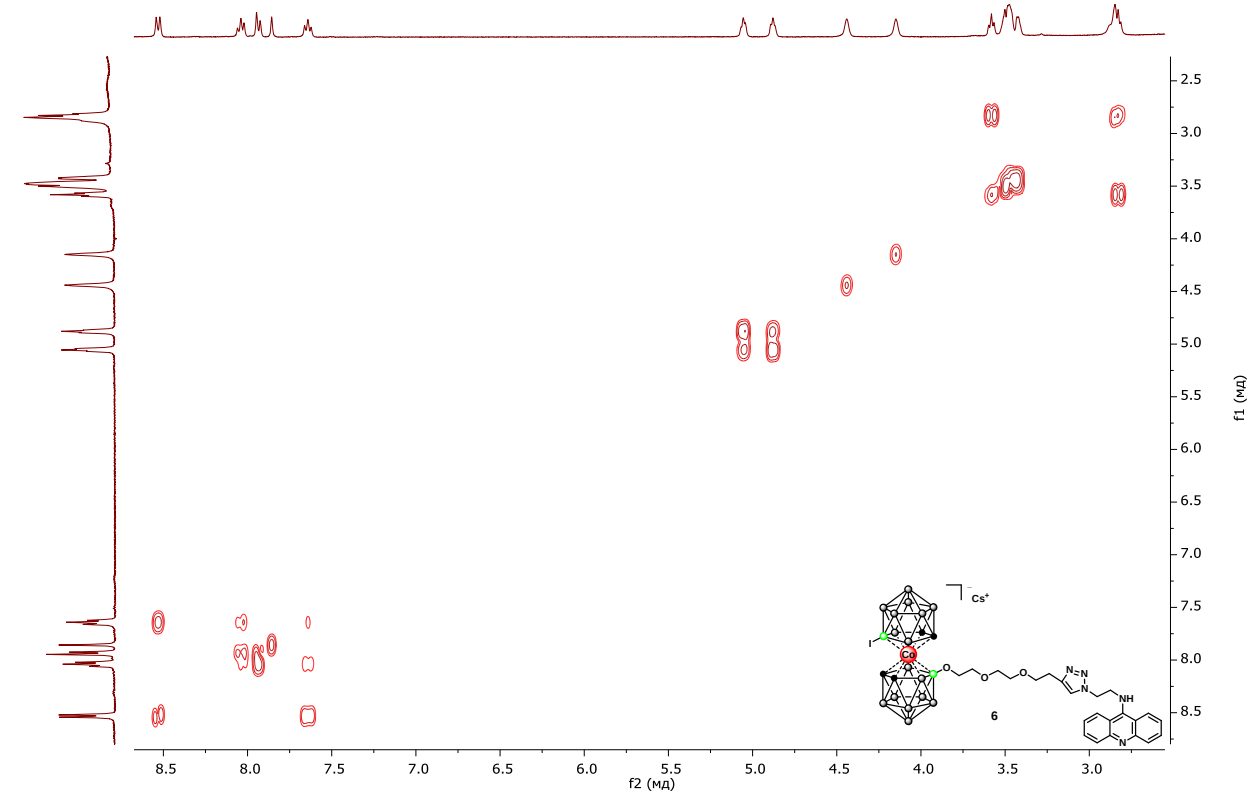


Figure S14. 2D NMR ^{1}H-^{1}H COSY spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$CH$_2$O(CH$_2$CH$_2$O)$_2$-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**6**)

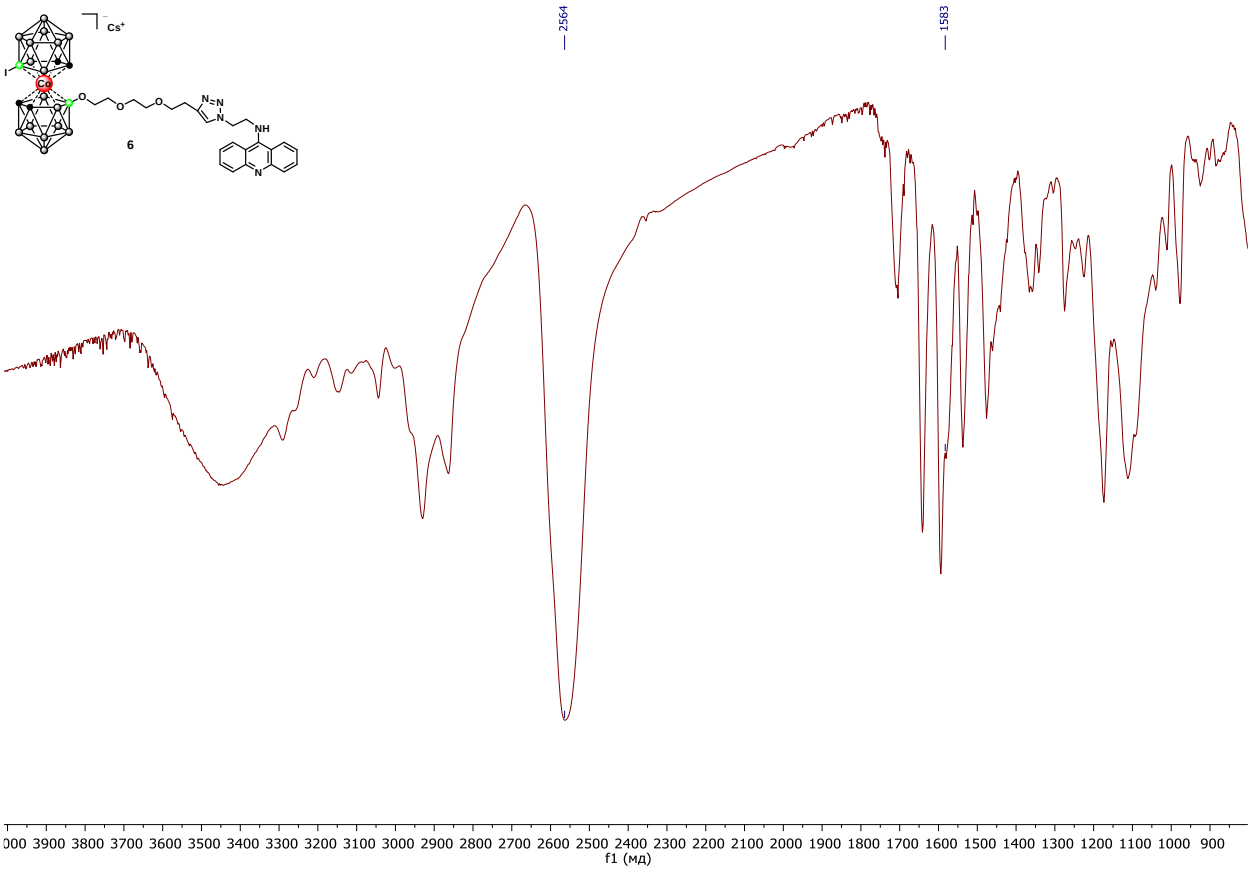


Figure S15. IR spectrum of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$CH$_2$O(CH$_2$CH$_2$O)$_2$-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs(**6**)

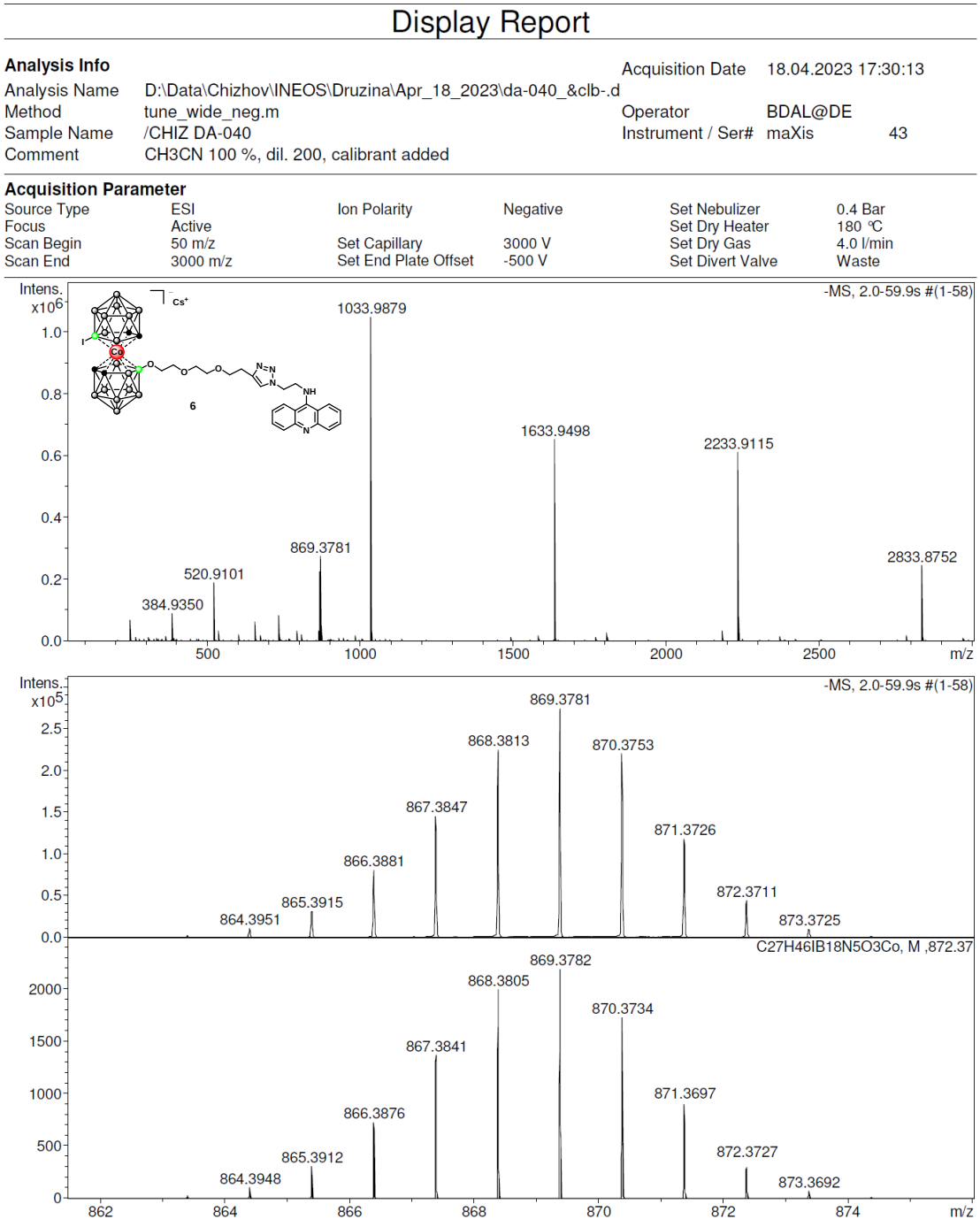


Figure S16. HRMS (ESI) of $C_{27}H_{46}IB_{18}CoN_5O_3$, *m/z*: calcd for $[M]^-$ 869.3782, found: 869.3781

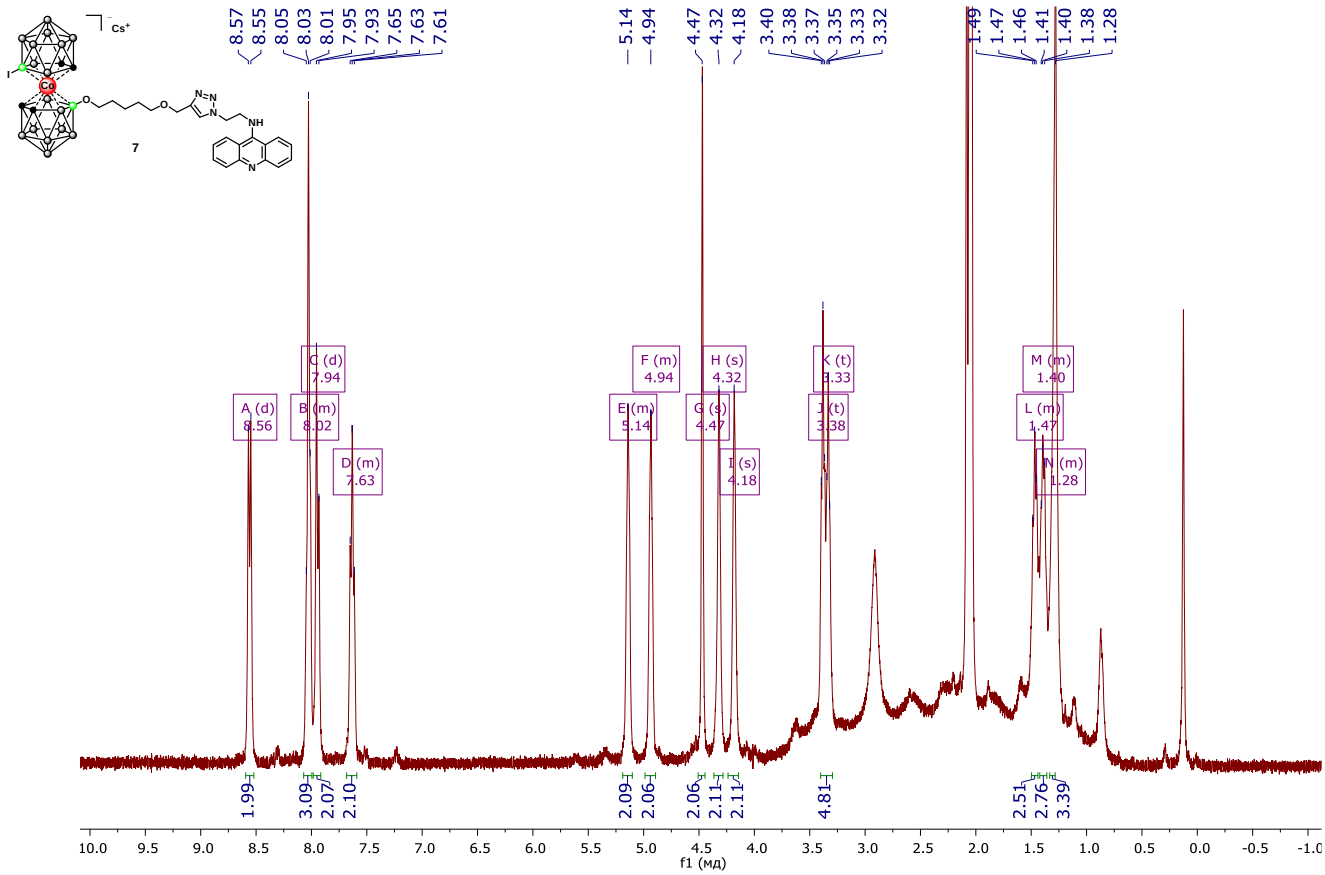


Figure S17. NMR ^{1}H spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$O(CH$_2$)5O-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**7**)

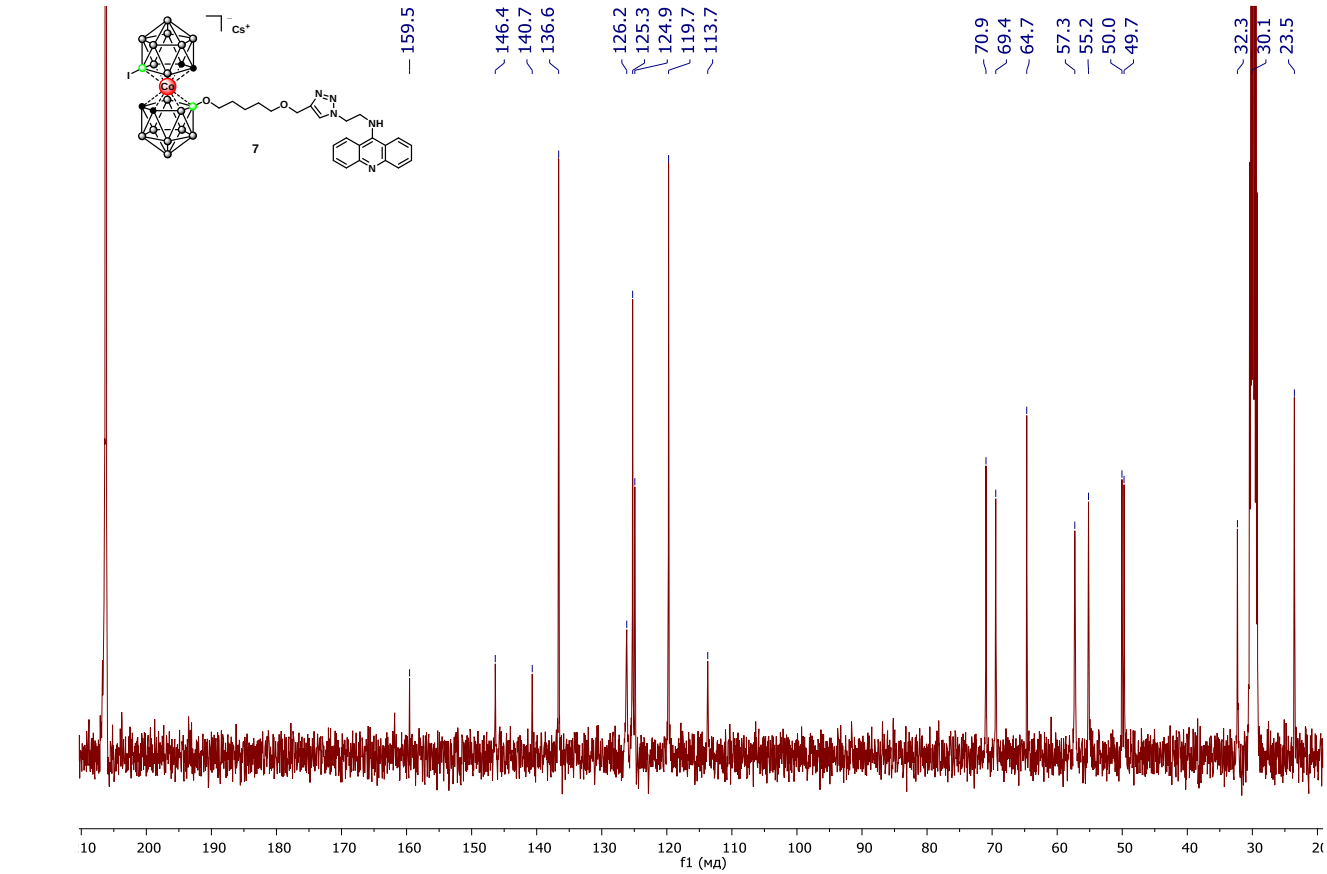


Figure S18. NMR ^{13}C{^{1}H} spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$O(CH$_2$)5O-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**7**)

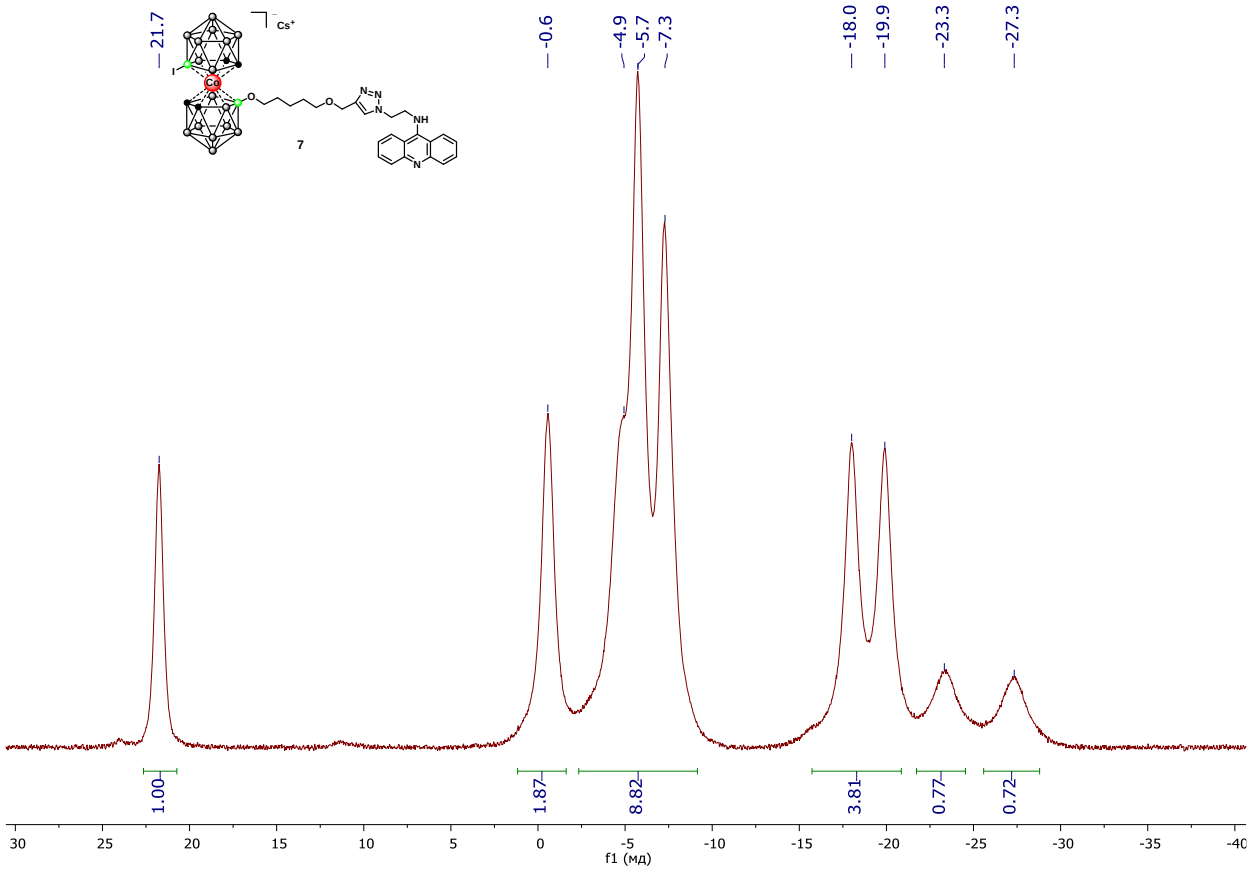


Figure S19. NMR $^{11}B\{^{1}H\}$ spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$O(CH$_2$)5O-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**7**)

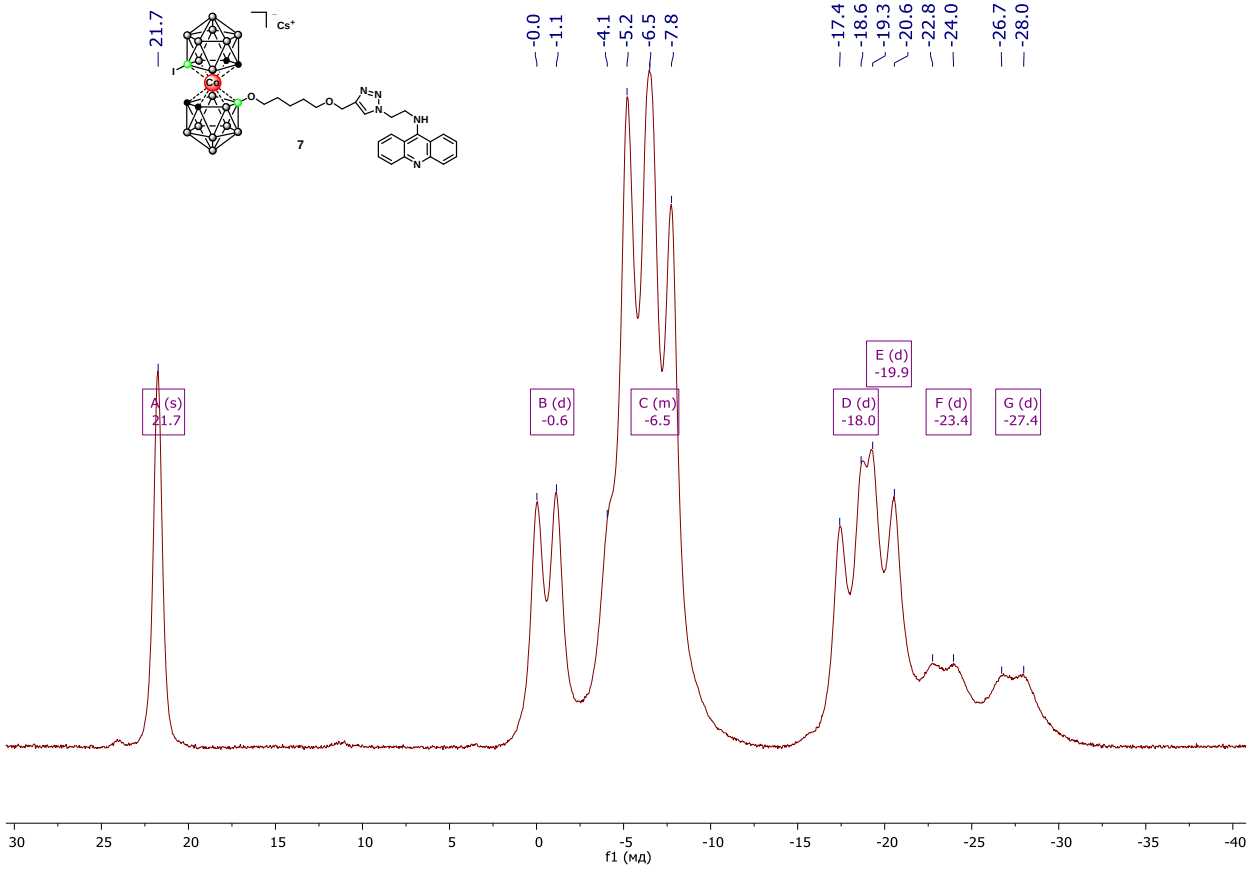


Figure S20. NMR ^{11}B spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$O(CH$_2$)5O-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**7**)

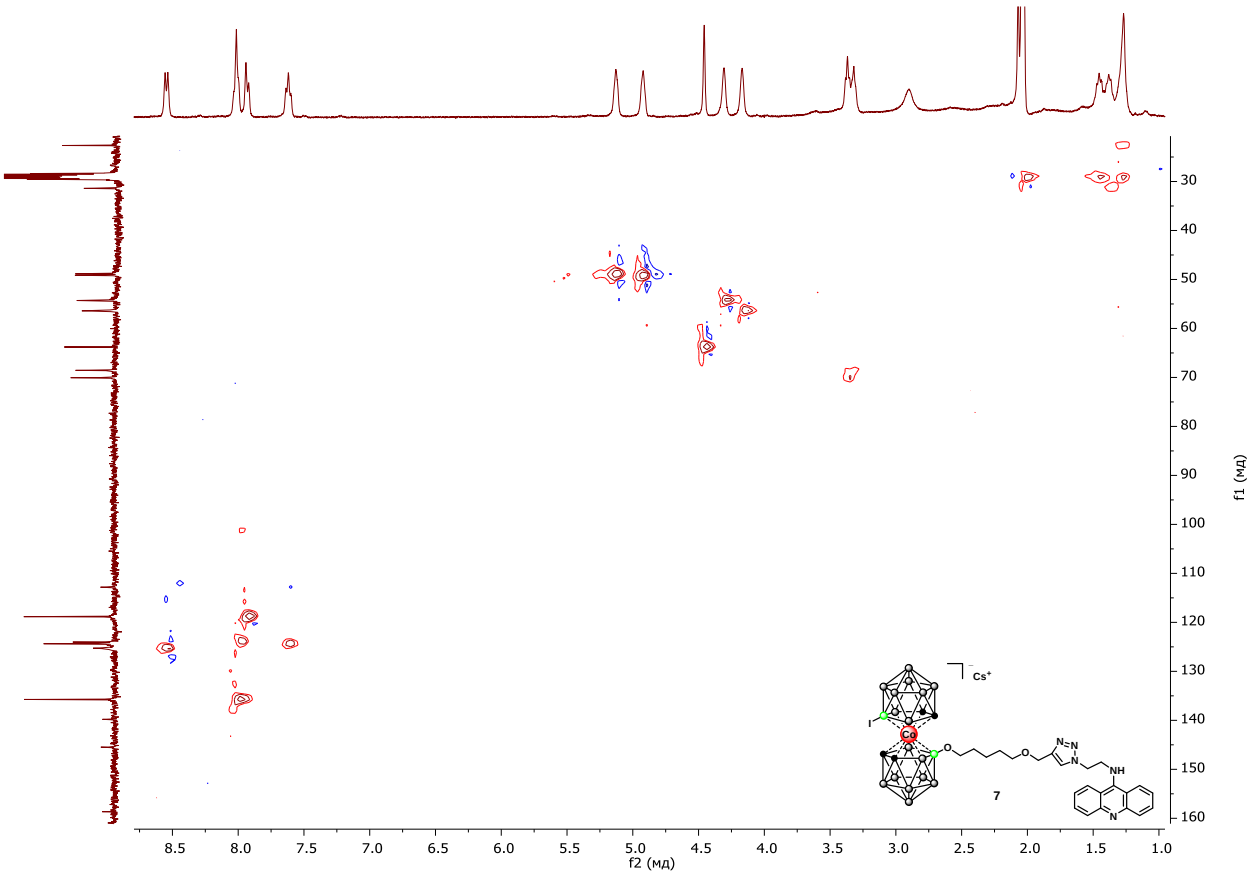


Figure S21. 2D NMR ^{1}H-^{13}C HMQC spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$O(CH$_2$)5O-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**7**)

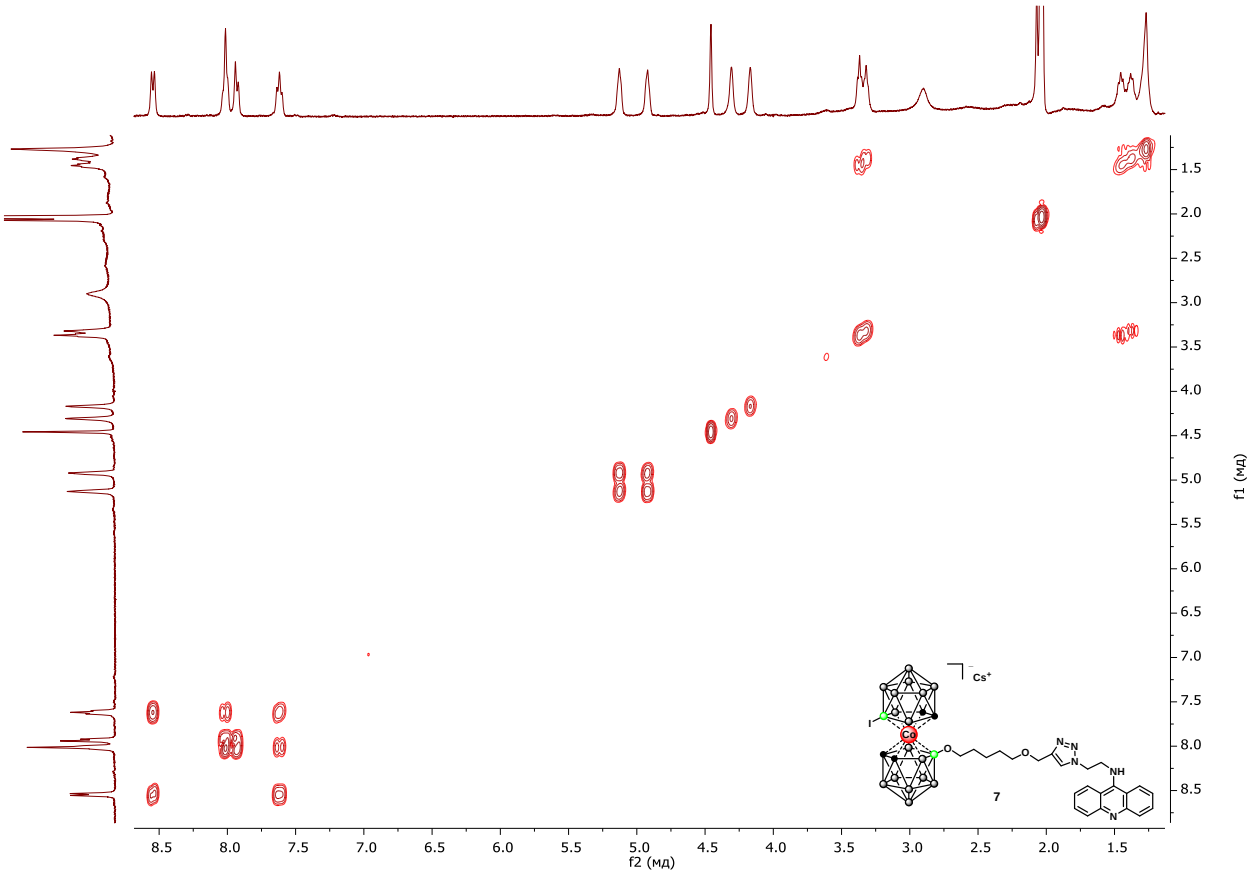


Figure S22. 2D NMR ^{1}H-^{1}H COSY spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$O(CH$_2$)5O-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**7**)

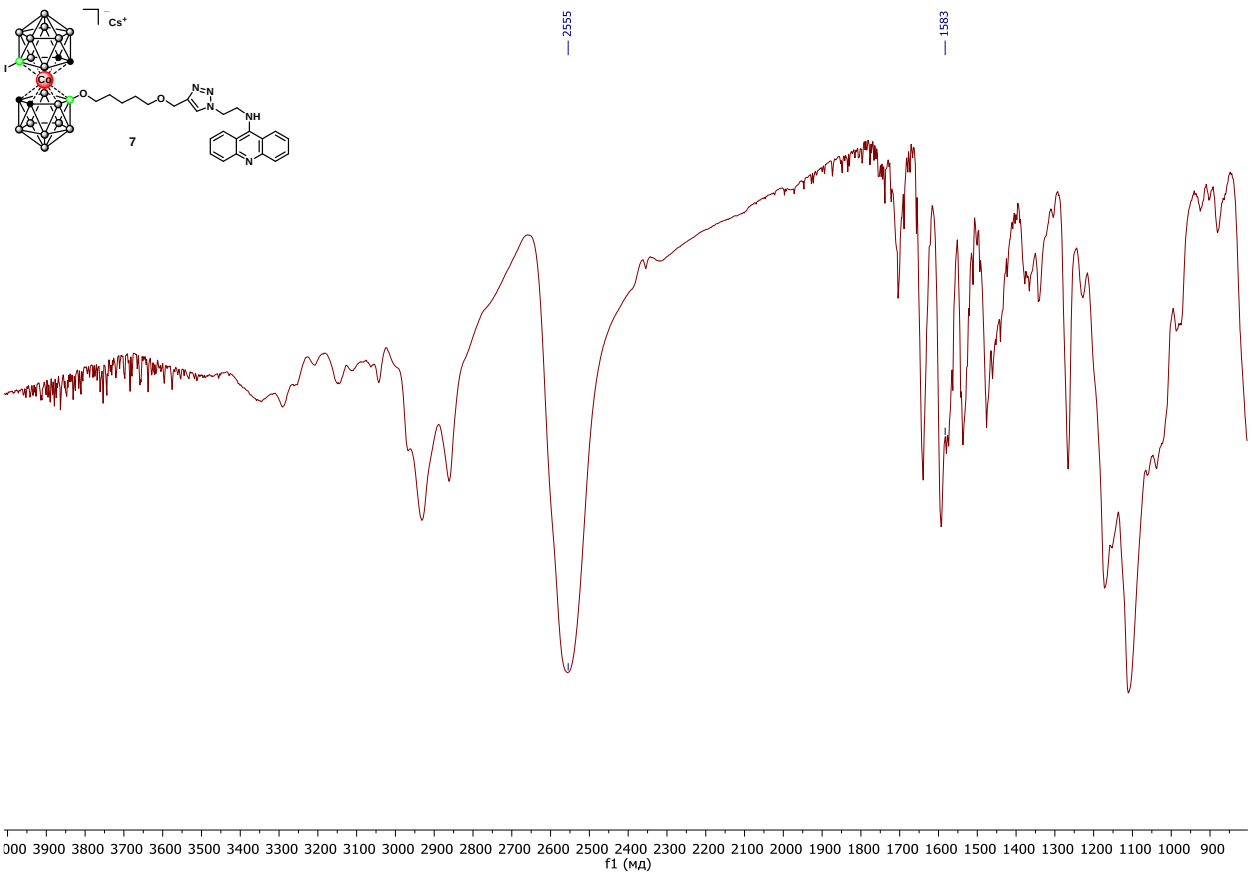


Figure S23. IR spectrum of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$O(CH$_2$)5O-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**7**)

Display Report

Analysis Info

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Sample Name	/CHIZ DA-041	Instrument / Ser#	maXis 43
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Acquisition Parameter

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Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

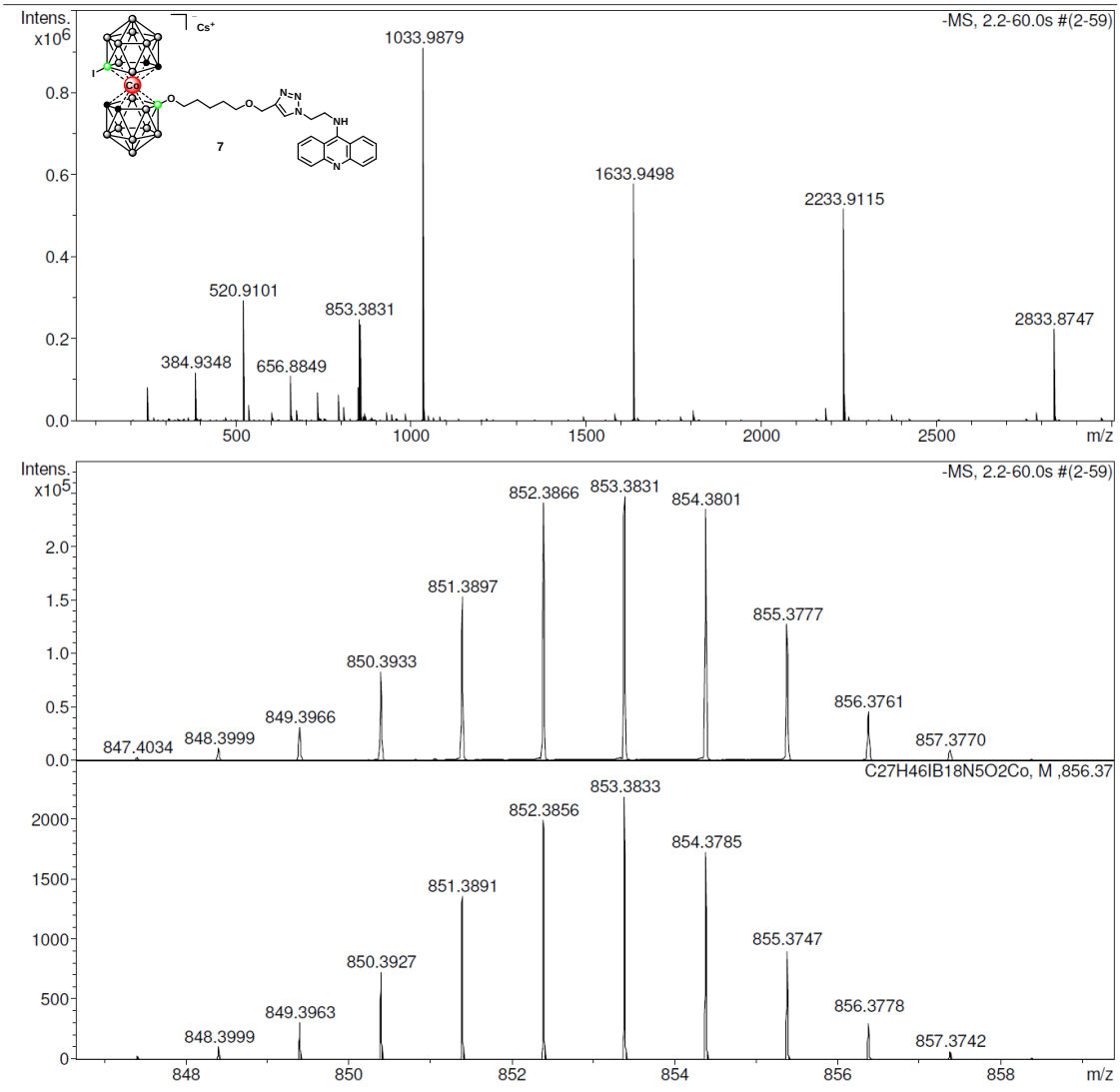


Figure S24. HRMS (ESI) of $C_{27}H_{46}IB_{18}CoN_5O_2$, *m/z*: calcd for $[M]^-$ 853.3833, found: 853.3831

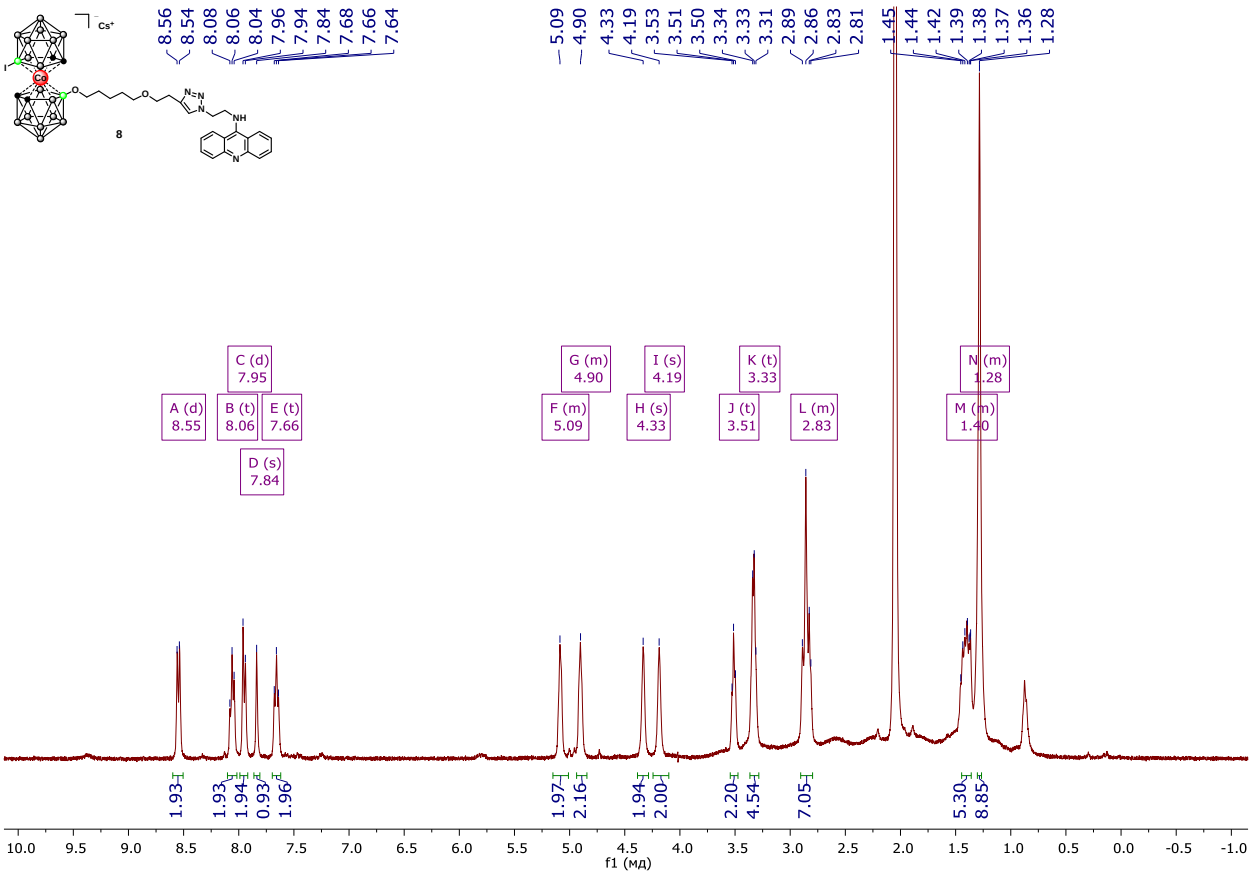


Figure S25. NMR ^{1}H spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$CH$_2$O(CH$_2$)$_5$O-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**8**)

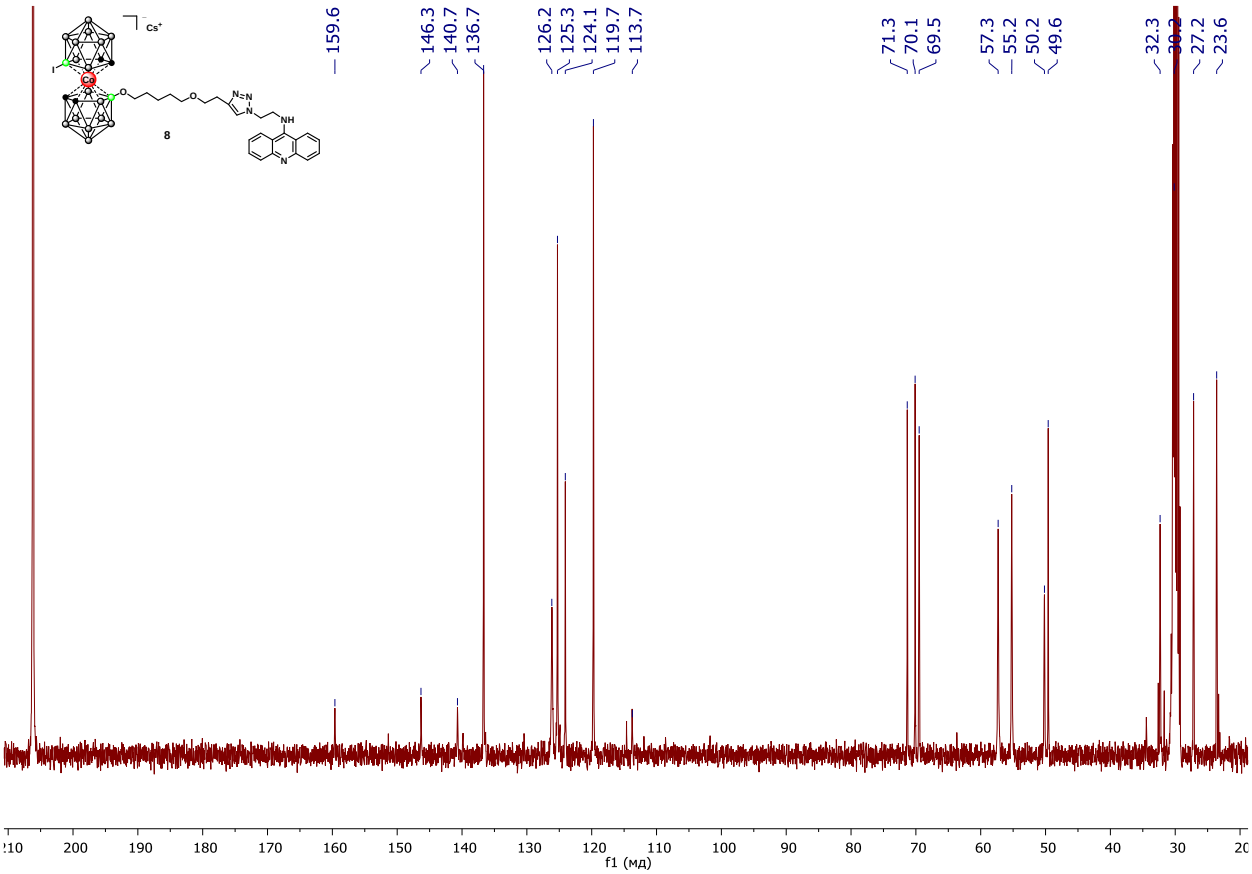


Figure S26. NMR ^{13}C{^{1}H} spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$CH$_2$O(CH$_2$)$_5$O-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**8**)

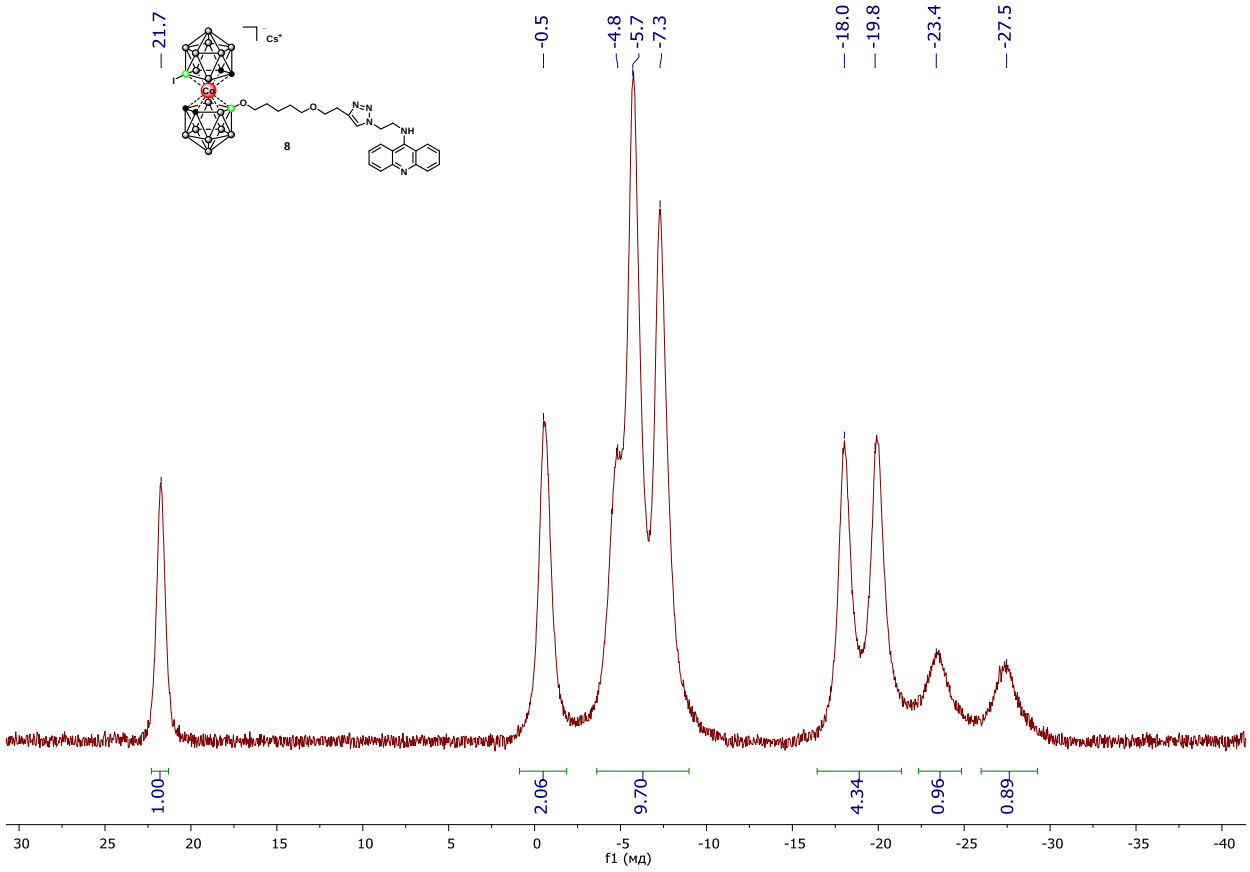


Figure S27. NMR $^{11}B\{^{1}H\}$ spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$CH$_2$O(CH$_2$)$_5$O-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**8**)

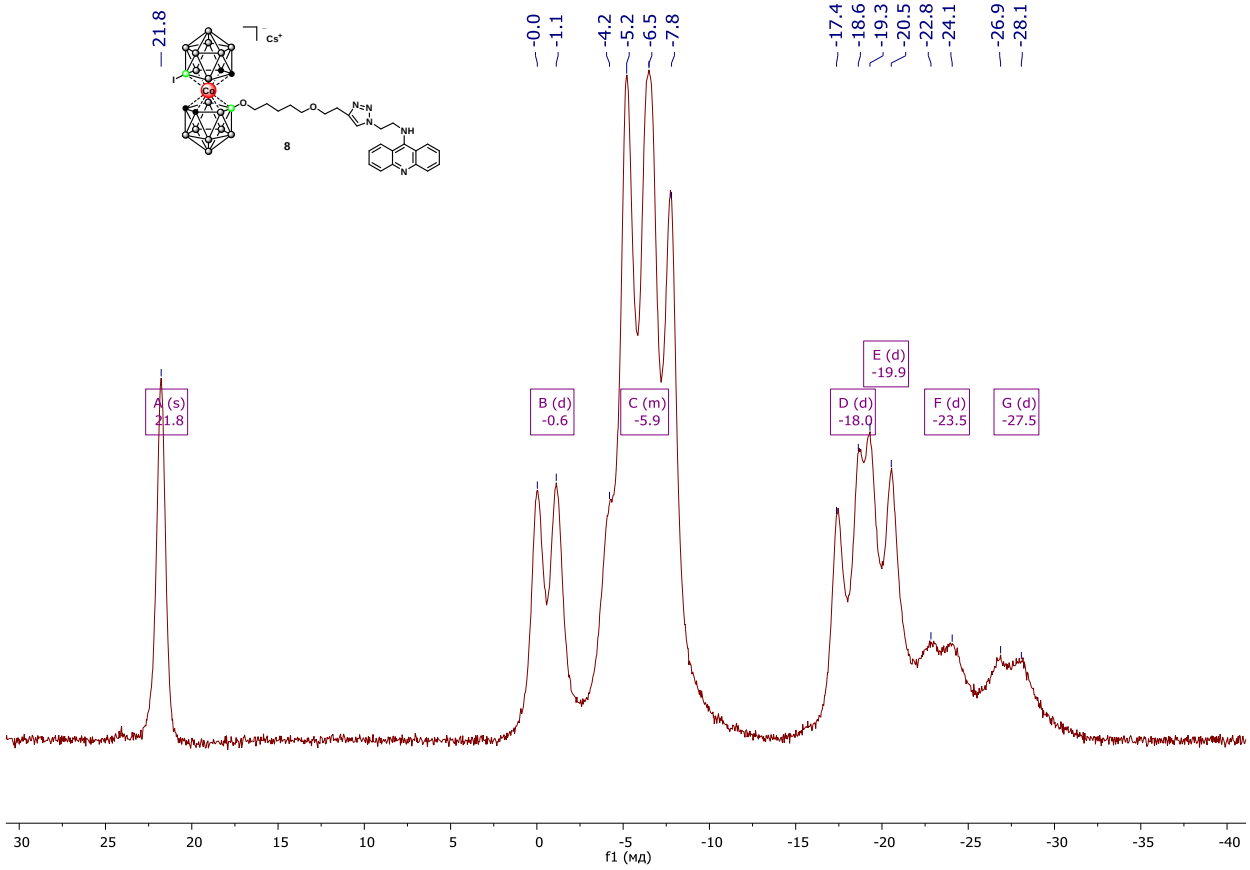


Figure S28. NMR ^{11}B spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$CH$_2$O(CH$_2$)$_5$O-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**8**)

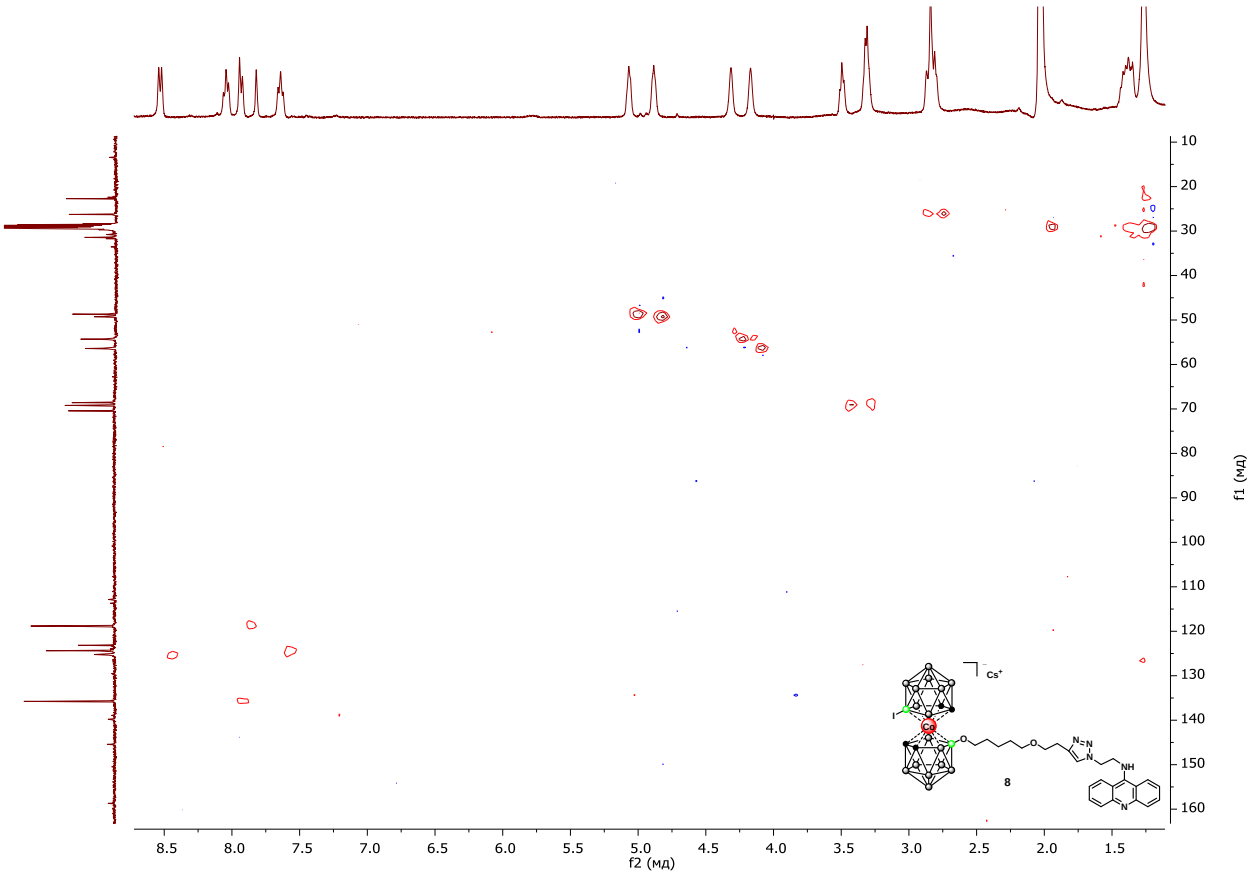


Figure S29. 2D NMR ^{1}H-^{13}C HMQC spectrum (acetone-d_6) of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$CH$_2$O(CH$_2$)$_5$O-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**8**)

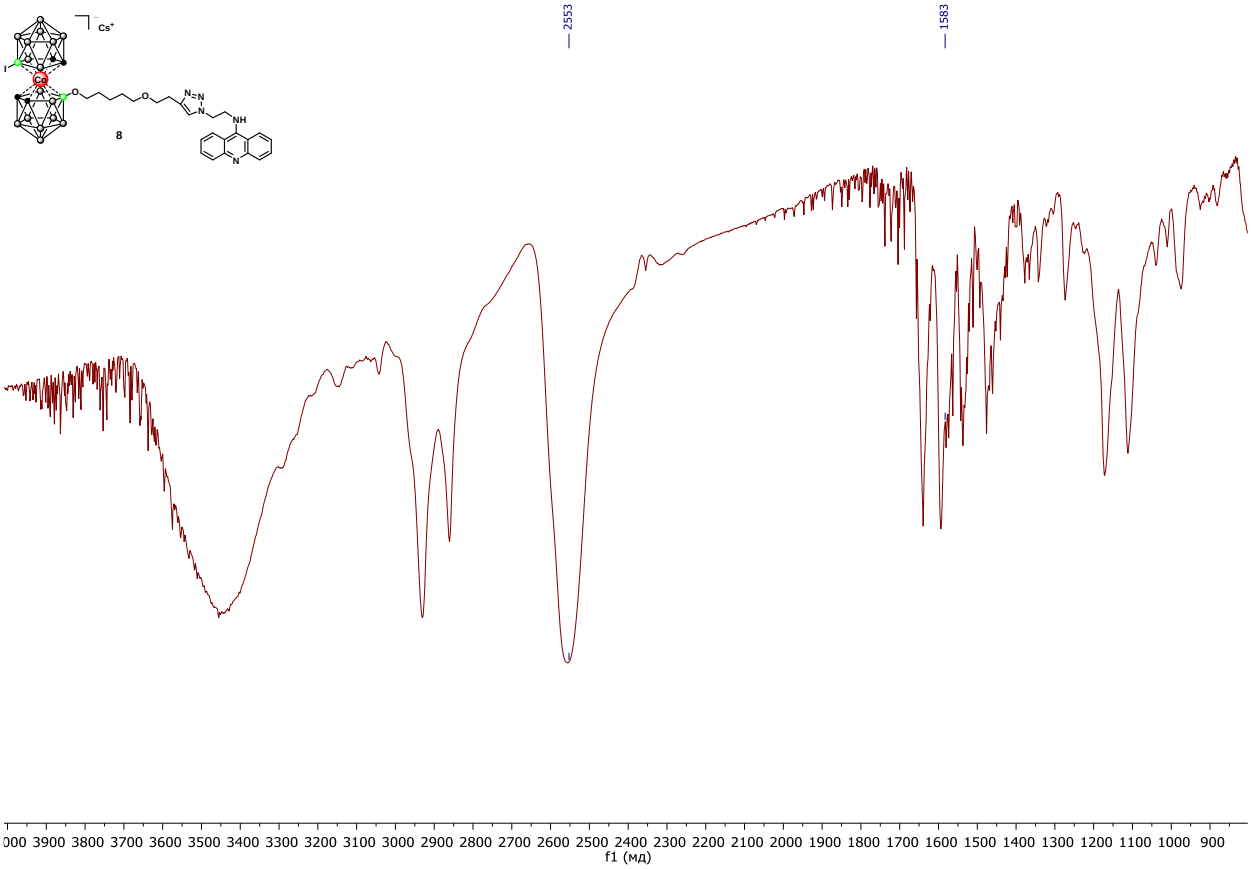


Figure S30. IR spectrum of [p-{8-NHCH$_2$CH$_2$-N$_3$CHC-CH$_2$CH$_2$O(CH$_2$)$_5$O-8′-I-3,3′-Co(1,2-C$_2$B$_9$H$_{10}$)(1′,2′-C$_2$B$_9$H$_{10}$)}-(C$_6$H$_4$)$_2$[b,e]pyridinate]Cs (**8**)

Display Report

Analysis Info

Analysis Name	D:\Data\Chizhov\INEOS\Druzina\Apr_18_2023\da-055_&clb-.d	Acquisition Date	18.04.2023 18:06:18
Method	tune_wide_neg.m	Operator	BDAL@DE
Sample Name	/CHIZ DA-055	Instrument / Ser#	maXis 43
Comment	CH3CN 100 %, dil. 200, calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3000 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

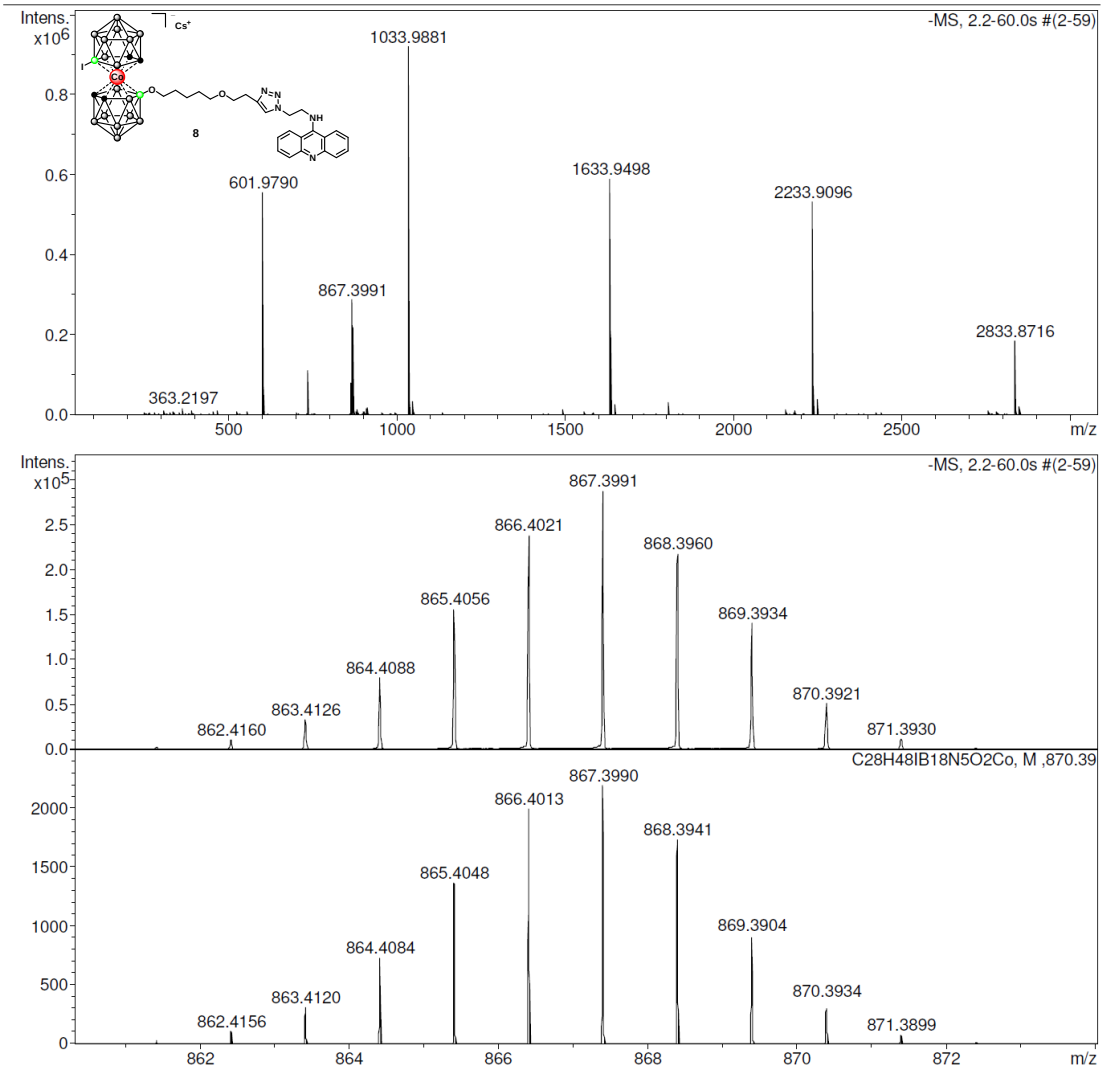


Figure S31. HRMS (ESI) of $C_{28}H_{48}IB_{18}CoN_5O_2$, *m/z*: calcd for $[M]^-$ 867.3990, found: 867.3991

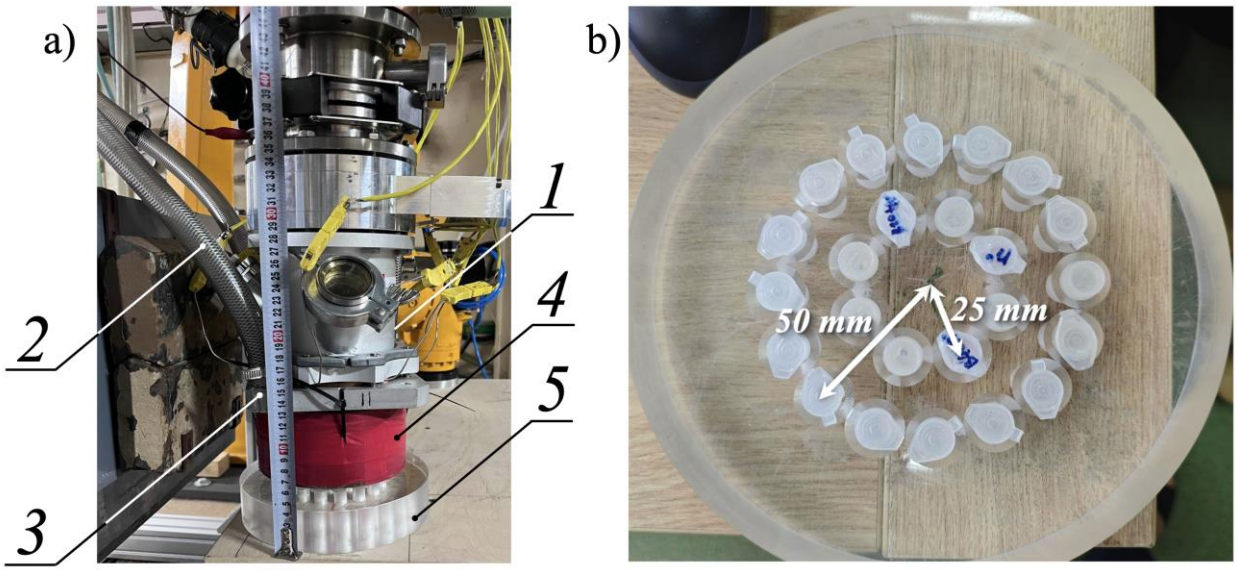


Figure S32. Experimental setup for *in vitro* studies at the VITA accelerator-based neutron source: a) General view of the setup: 1 — high-energy proton beam transport line, 2 — pipes of the target unit cooling system, 3 — target unit, 4 — Poly-Biz neutron moderator, 5 — phantom with cryotubes; b) PMMA phantom holder loaded with cryotubes at the inner (25 mm) and outer (50 mm) radii.

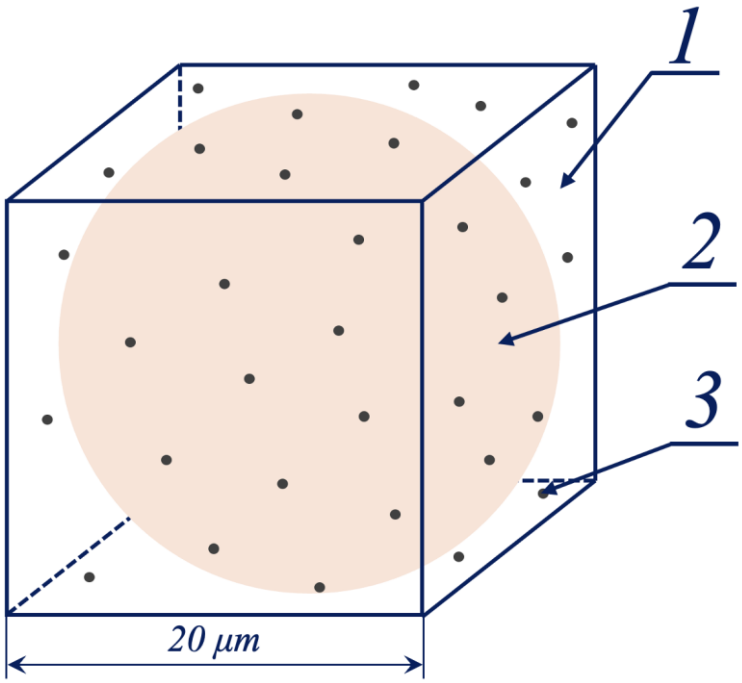


Figure S33. Schematic representation of the approximation used to calculate the volume of boron-loaded cells sedimented at the bottom of the cryotube: 1 — water; 2 — soft tissue; 3 — ^{10}B atoms.