CHEMISTRY
A EUROPEAN JOURNAL

Supporting Information

„Chemical Ligation" – A Versatile Method for Nucleoside Modification With Boron Clusters

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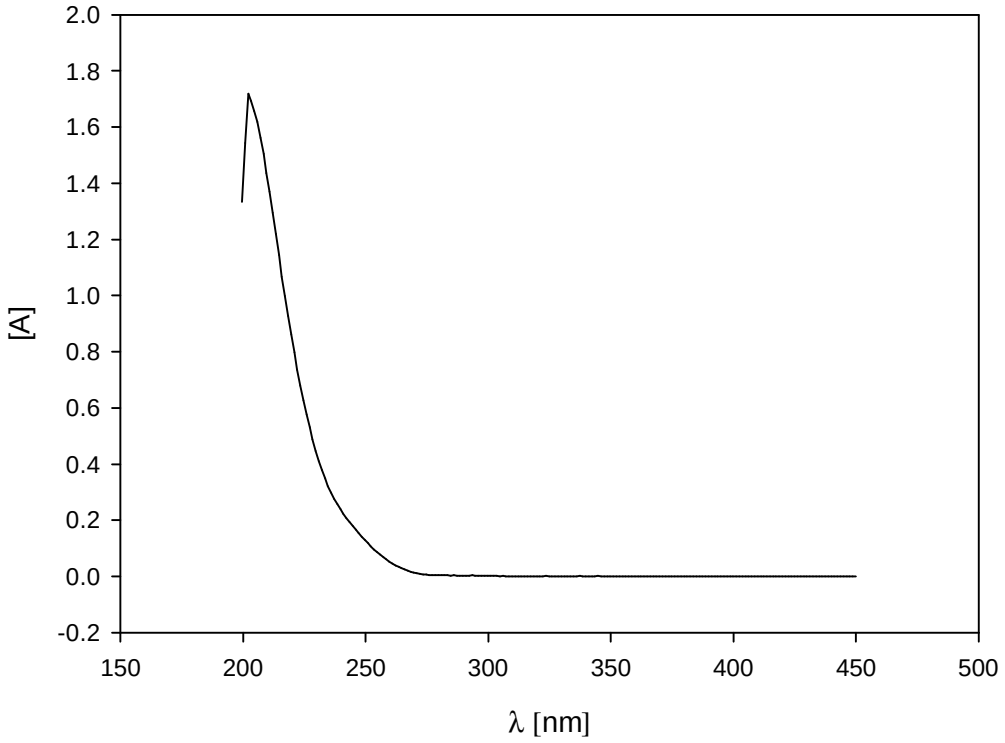
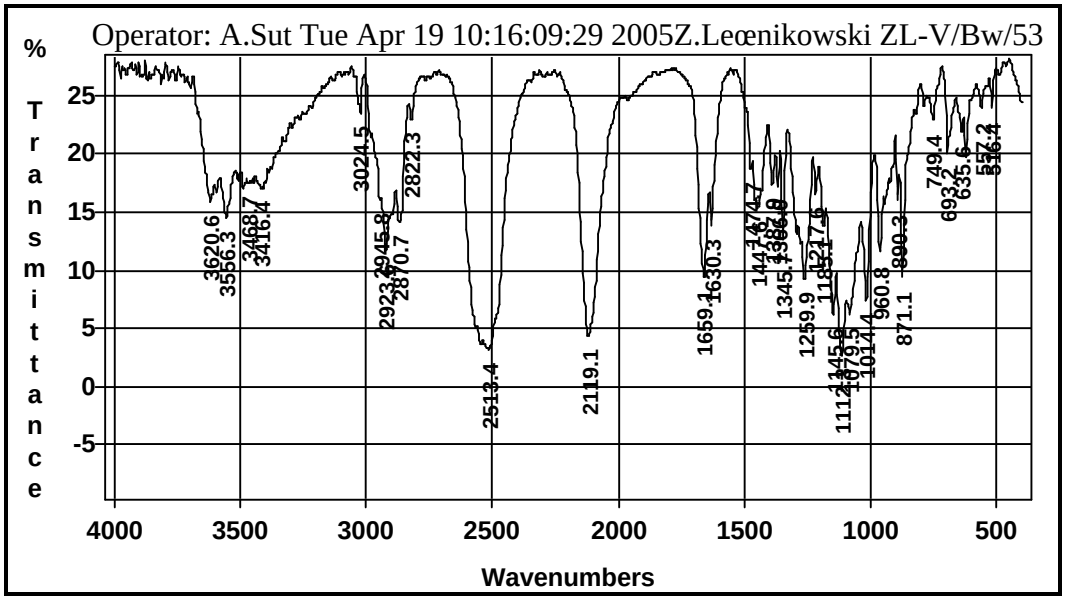
[b] Institute of Inorganic Chemistry, Academy of Sciences of the Czech Republic, 250-68 Rež, Czech Republic



UV/Vis (96% EtOH) spectrum of 10-(5-azido-3-oxa-pentoxy)-7,8-dikarba-*nido*-undekaborane (2).



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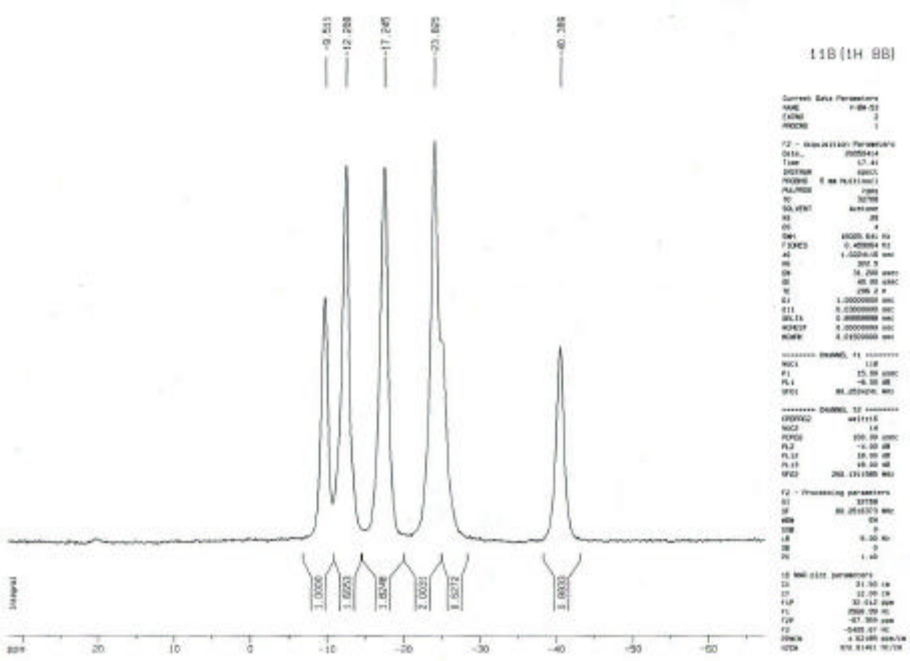
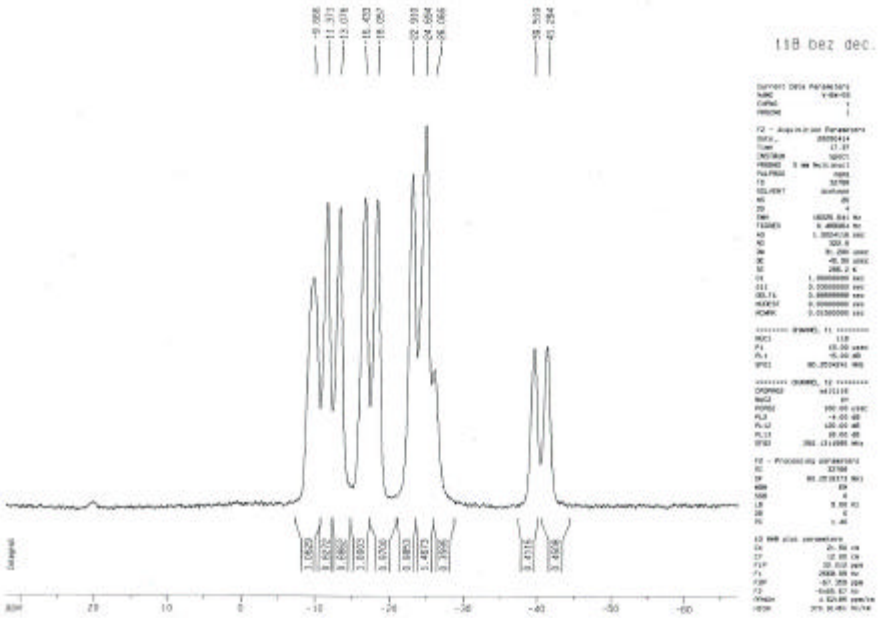


^{11}B {^{1}H BB} NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of 10-(5-azido-3-oxa-pentoxy)-7,8-dikarba-*nido*-undekaborane (2).



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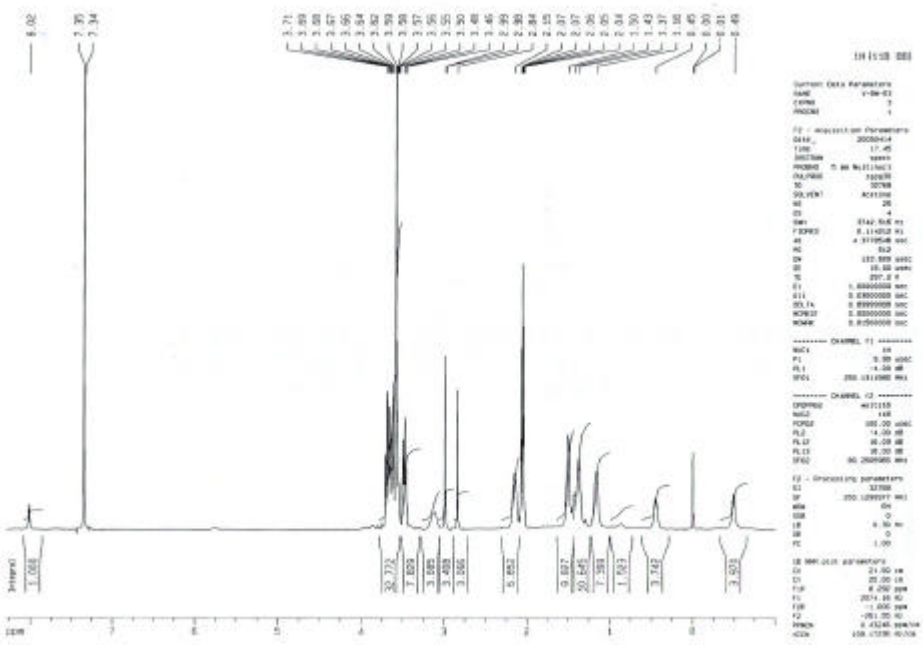

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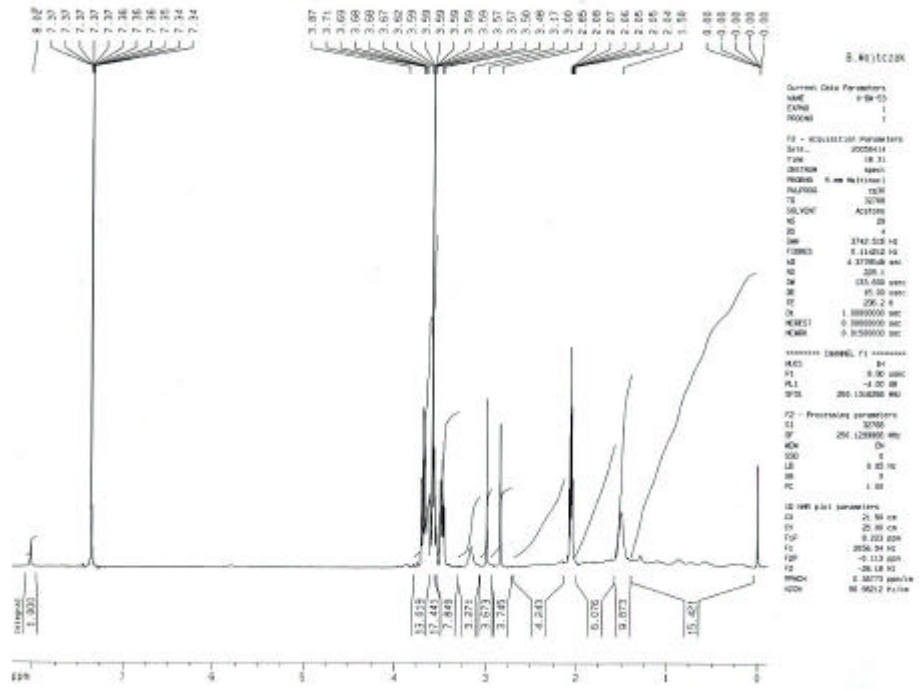

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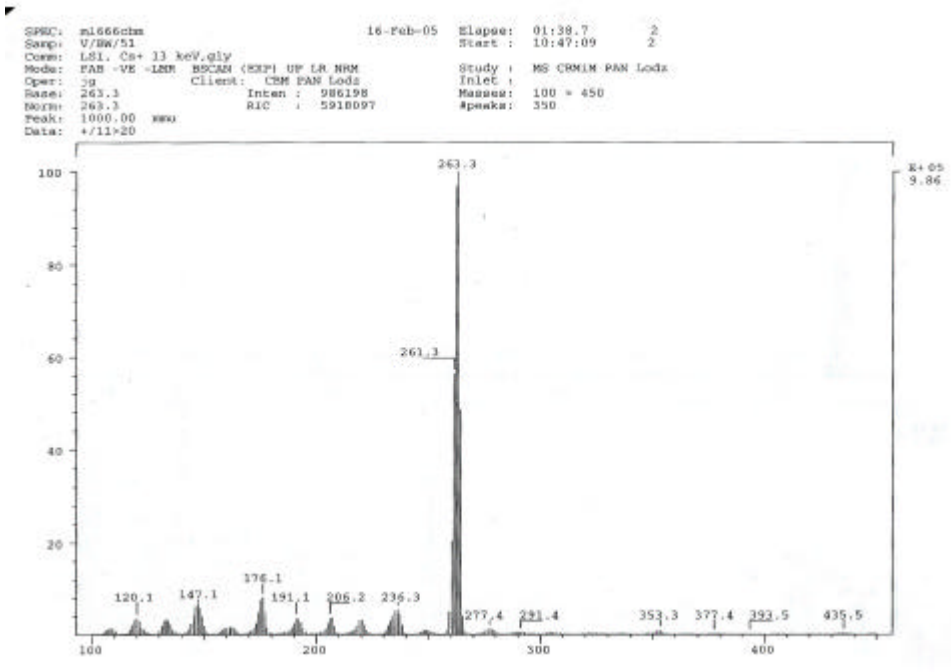
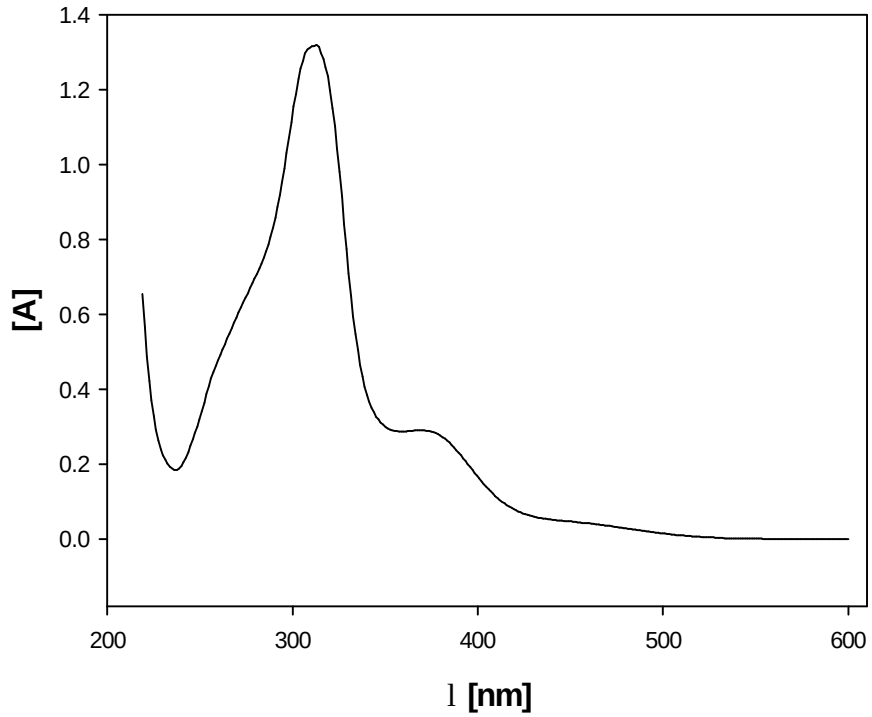
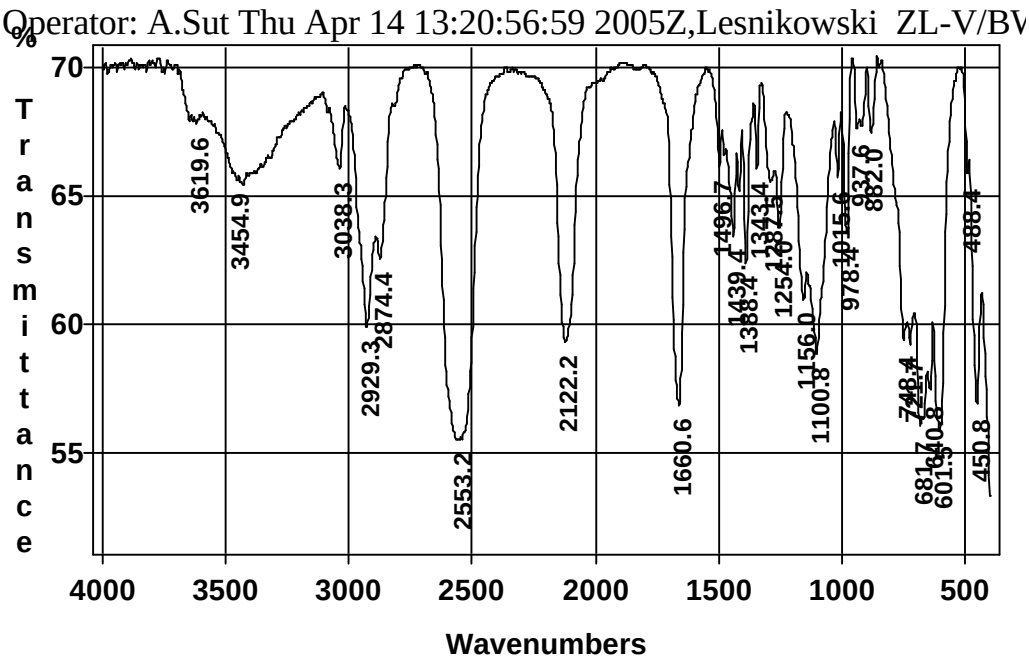


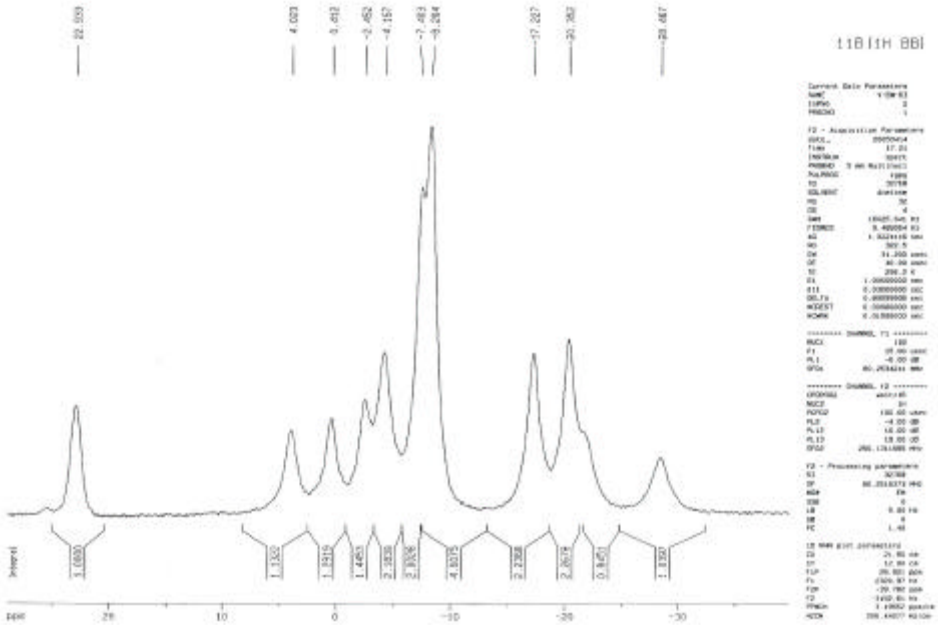
MS (Gly, FAB, -Ve): spectrum of 10-(5-azido-3-oxa-pentoxy)-7,8-dikarba-*nido*-undekaborane (2), m/z (%):molecular formula: $C_6H_{19}B_9N_3O_2$**; calculated average mass: 262.53, found 263.3 (100)** $[M+1H]^-$



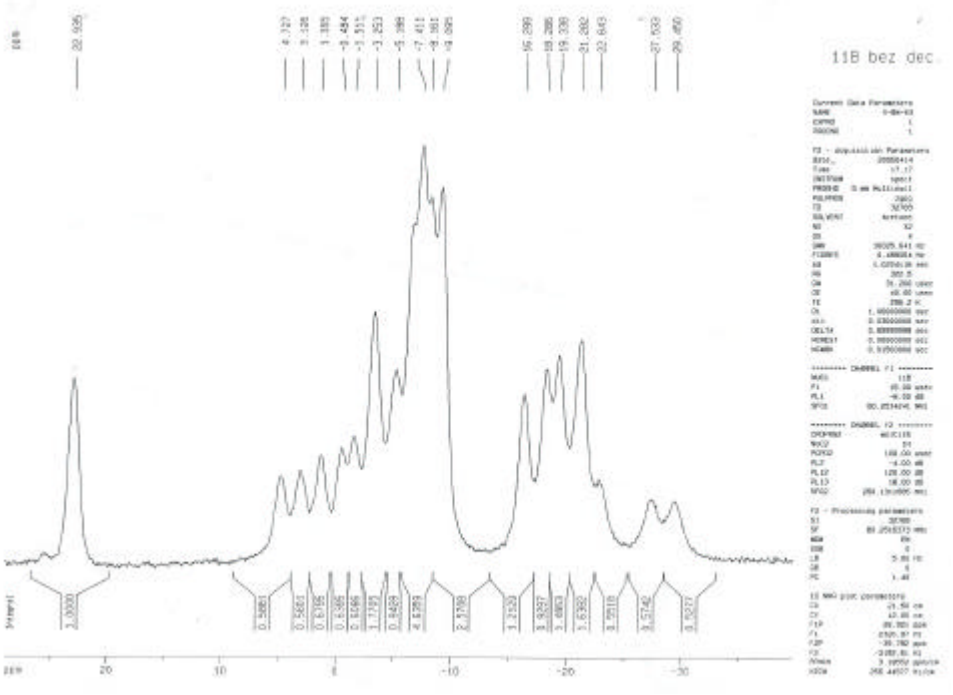
UV/Vis spectrum (96% EtOH) of 8-(5-azido-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) (5).



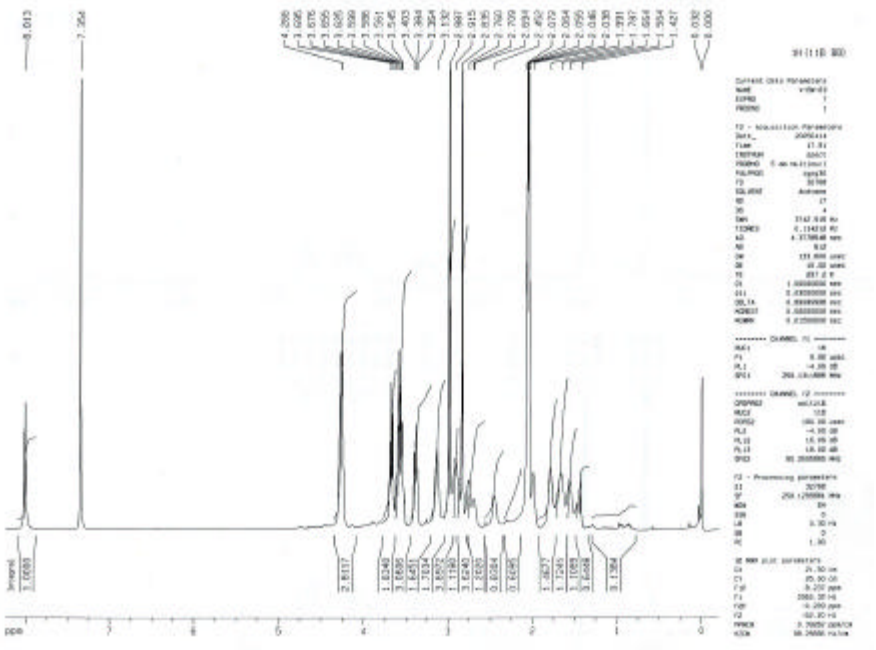
FT-IR (nujol) spectrum of 8-(5-azido-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) (5).



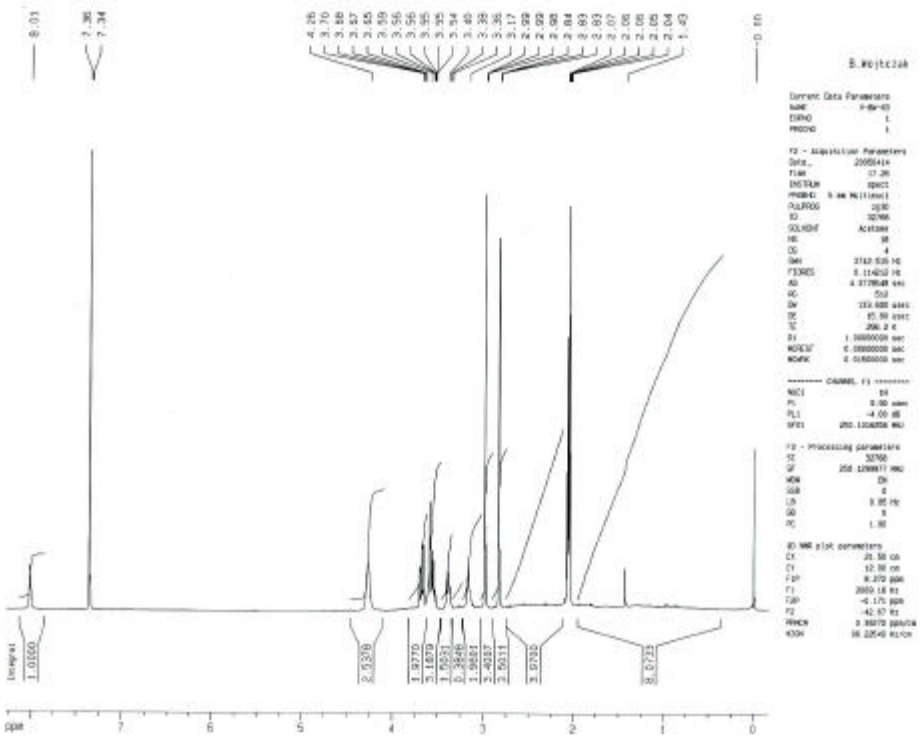
^{11}B {^{1}H BB} NMR (acetone-d*6*, 25°C, 80.25MHz, $BF_3{\cdot}Et_2O$) spectrum of 8-(5-azido-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) (5).



^{11}B NMR (acetone-d*6*, 25 °C, 80.25MHz, $BF_3{\cdot}Et_2O$) spectrum of 8-(5-azido-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) (5).



^{1}H {^{11}B BB} NMR (acetone-*d6*, 250.131MHz, 25°C, TMS) spectrum of 8-(5-azido-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) (5).



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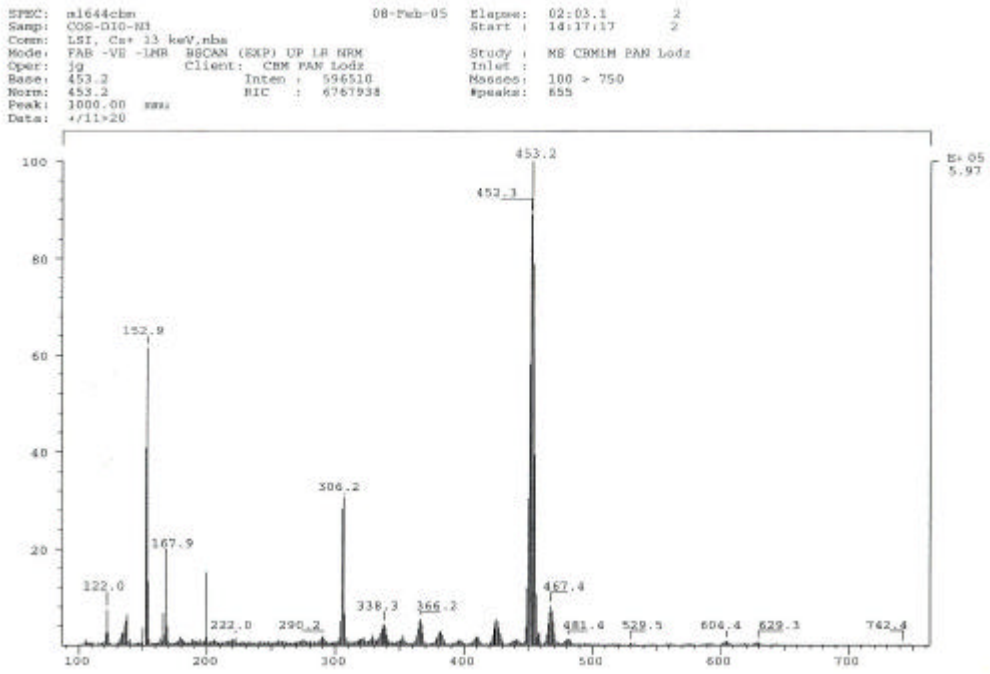
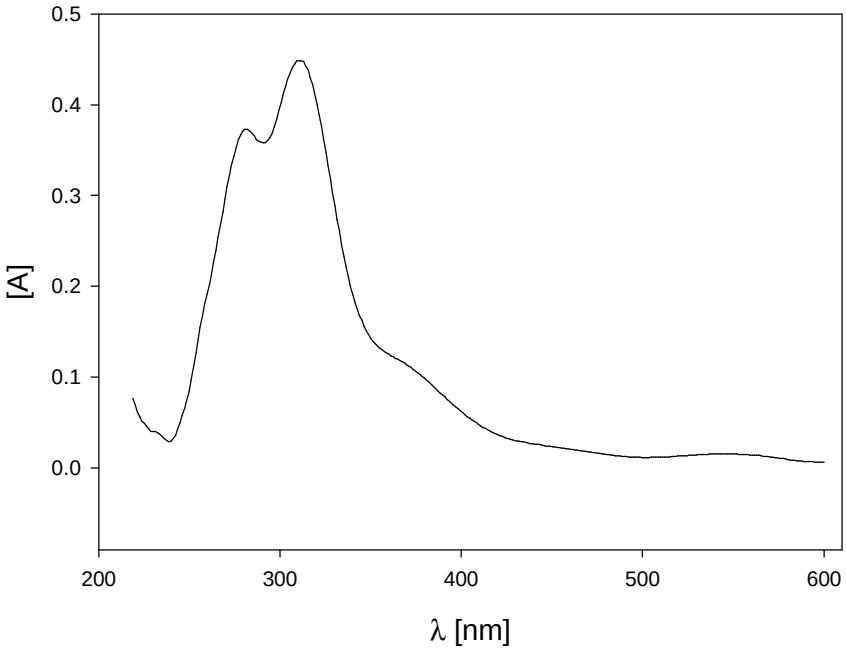
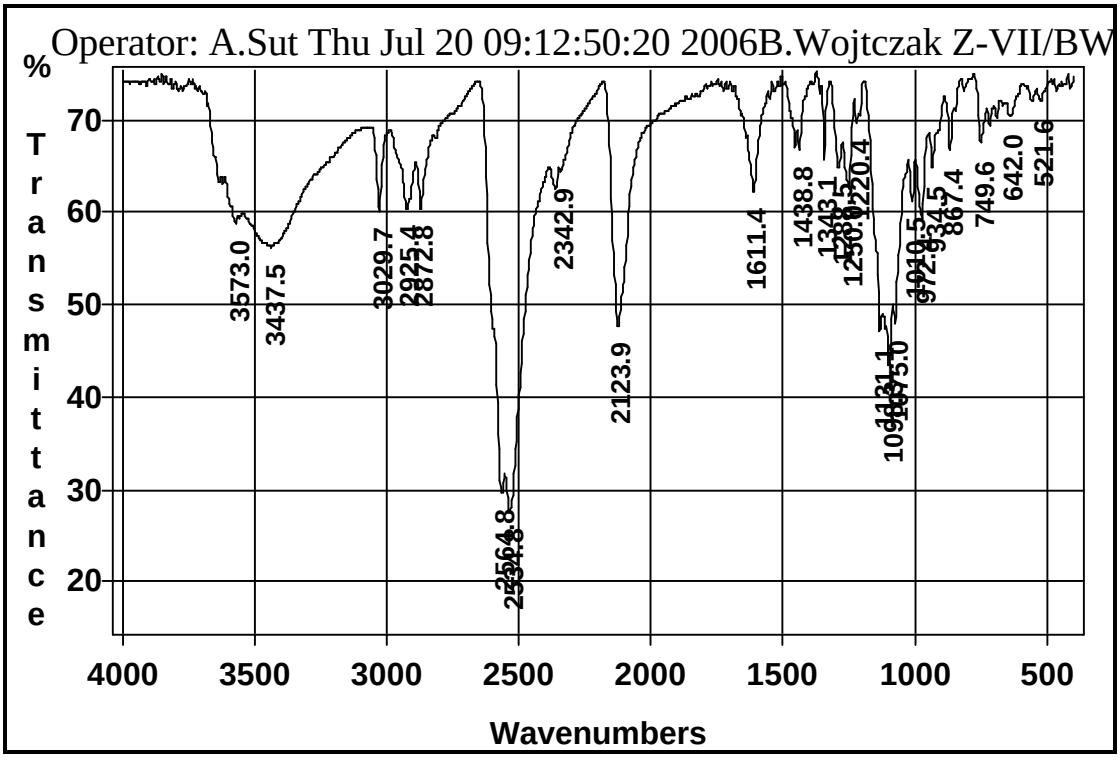


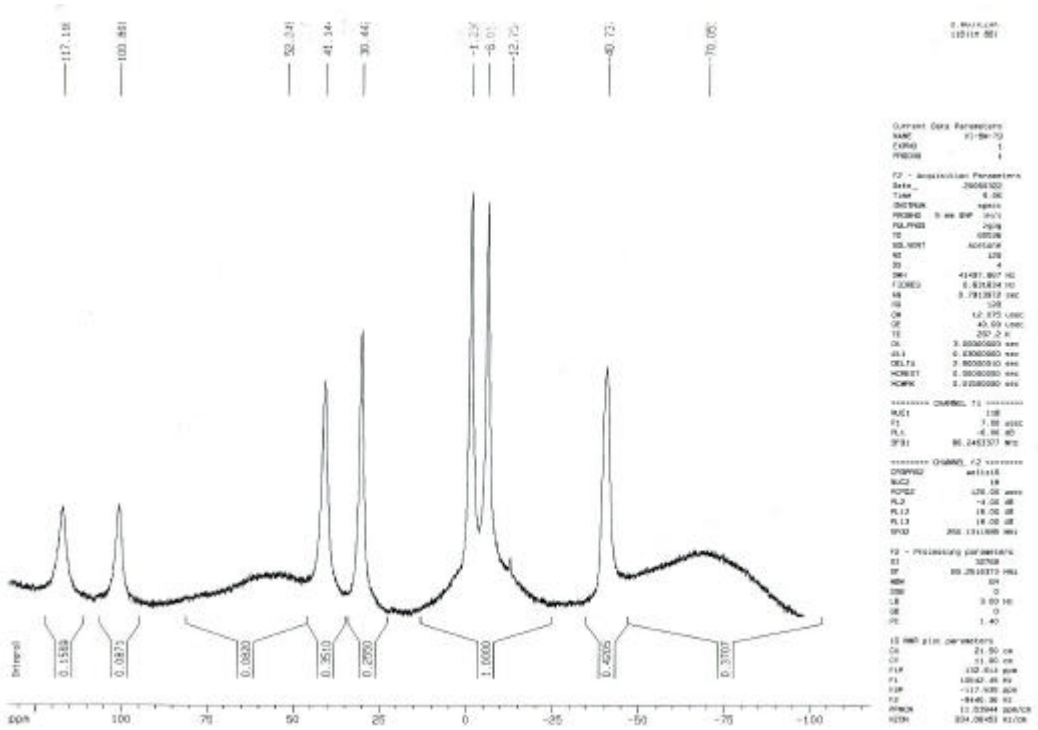
MS (Gly, FAB, -Ve) spectrum of 8-(5-azido-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) (5); m/z (%):molecular formula: $C_8H_{29}B_{18}CoN_3O_2$, calculated average mass: 452.87, found 453.2 (100) $[M]^-$



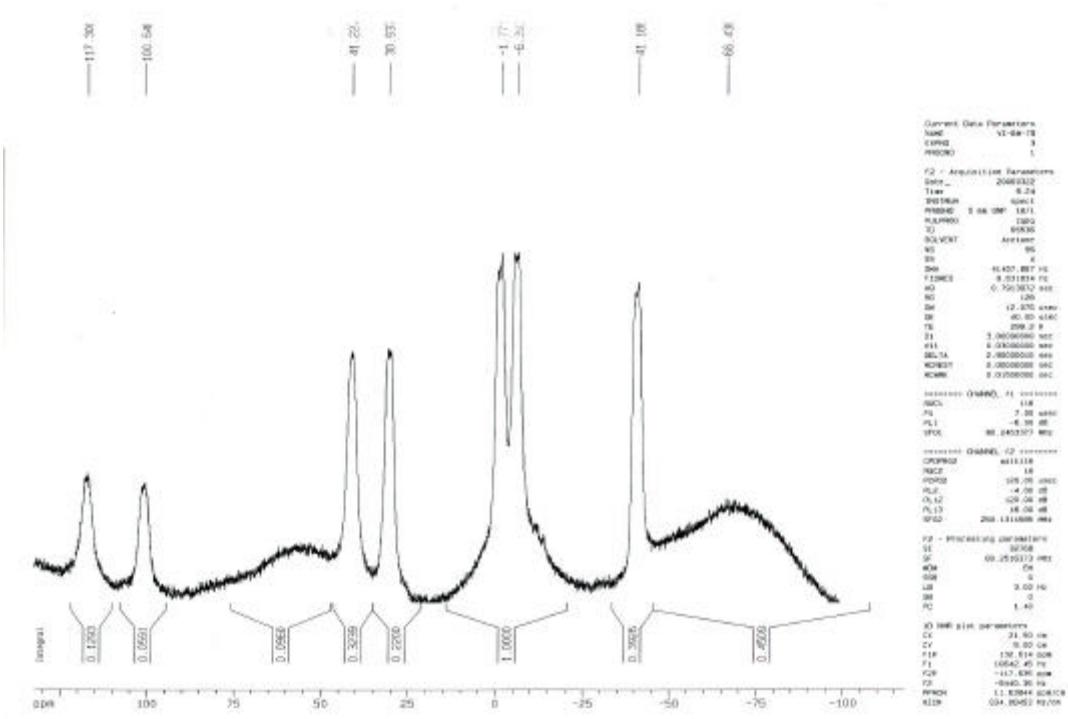
UV/Vis (96% EtOH) spectrum of 8-(5-azido-3-oxa-pentoxy)-3-iron bis(1,2-dicarbollide) (6).



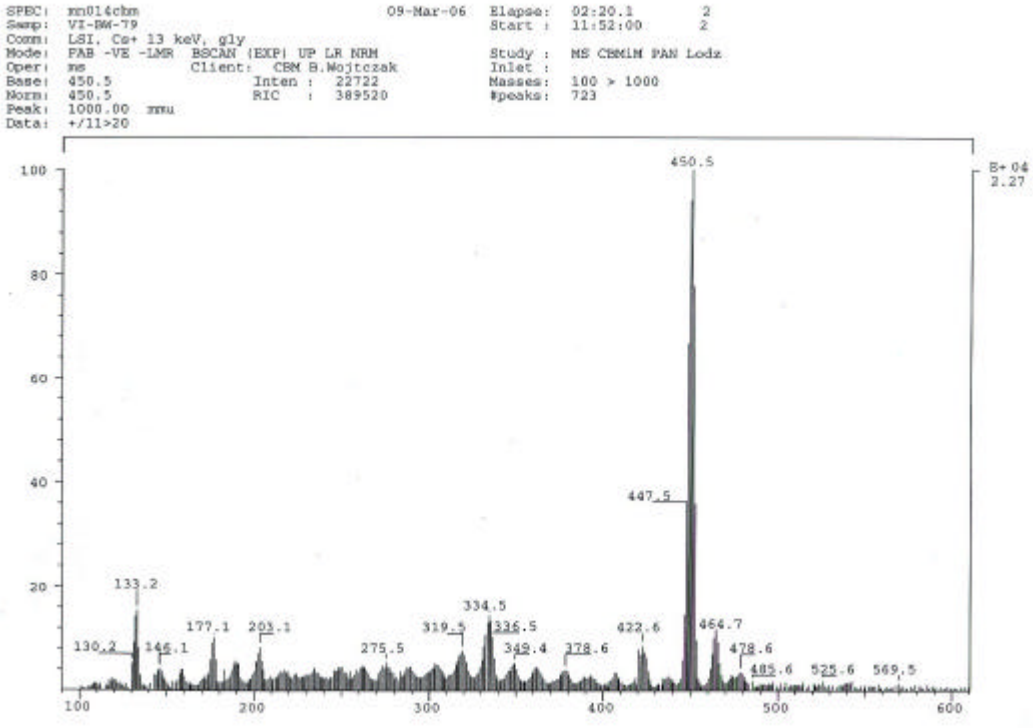
FT-IR (KBr) spectrum of 8-(5-azido-3-oxa-pentoxy)-3-iron bis(1,2-dicarbollide) (6).



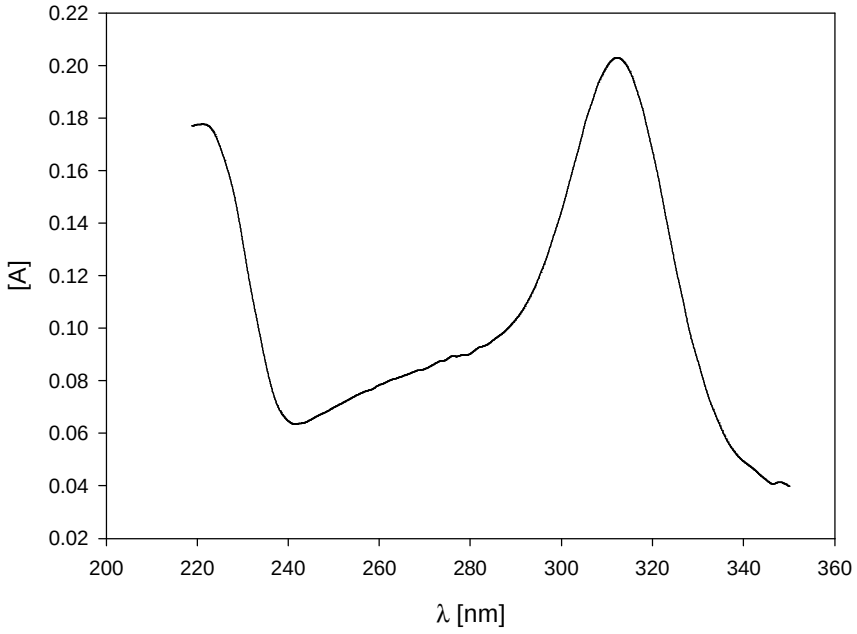
^{11}B {^{1}H BB} NMR (acetone-*d6*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of 8-(5-azido-3-oxa-pentoxy)-3-iron bis(1,2-dicarbollide) (6).



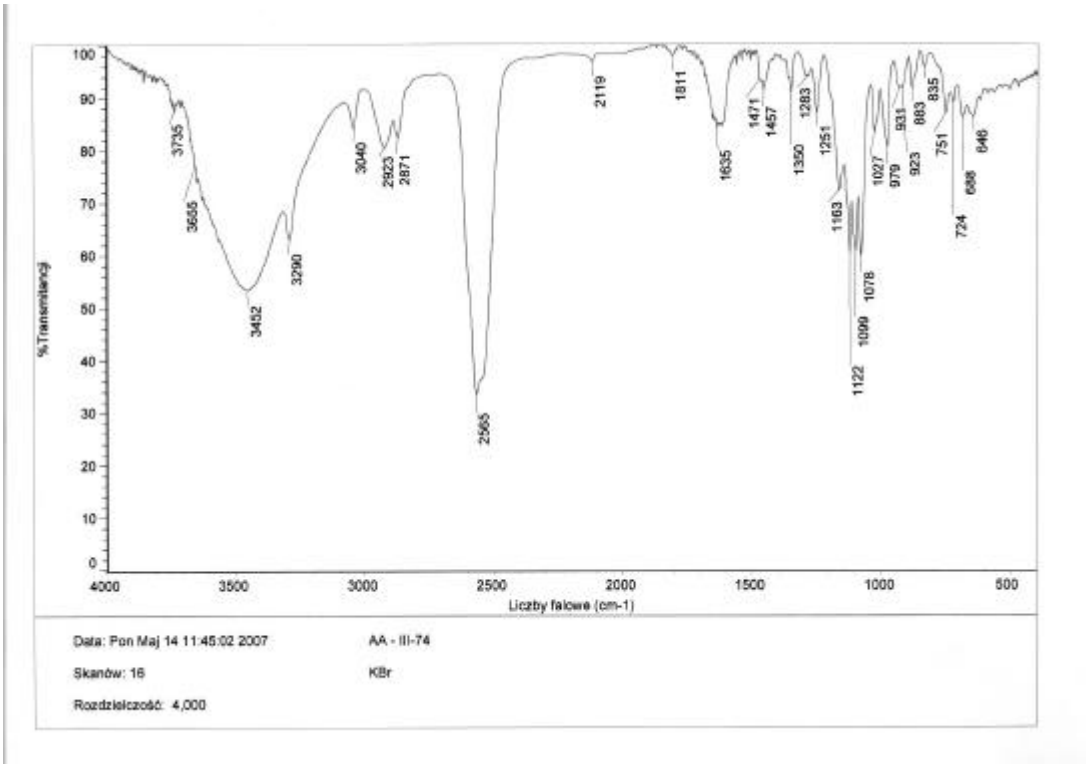
^{11}B NMR (acetone-*d6*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of 8-(5-azido-3-oxa-pentoxy)-3-iron bis(1,2-dicarbollide) (6).



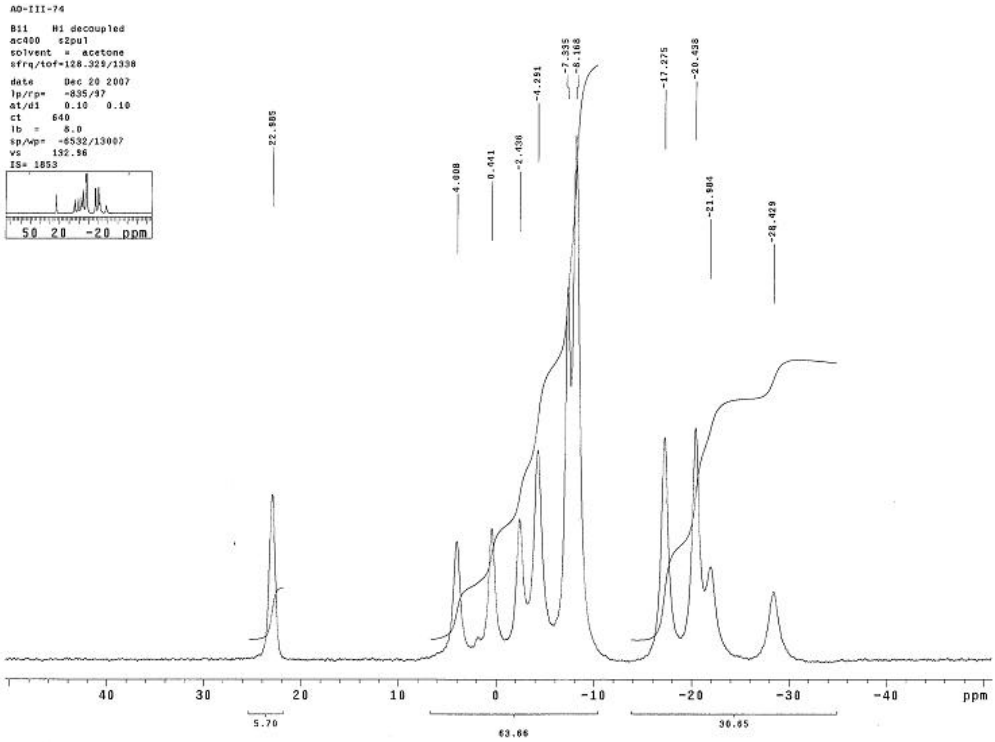
MS (Gly, FAB, -Ve) spectrum of 8-(5-azido-3-oxa-pentoxy)-3-iron bis(1,2-dicarbollide) (6). m/z (%): molecular formula: $C_8H_{29}B_{18}FeN_3O_2$, calculated average mass: 449.78, found 450.5 (100) [M+1H]



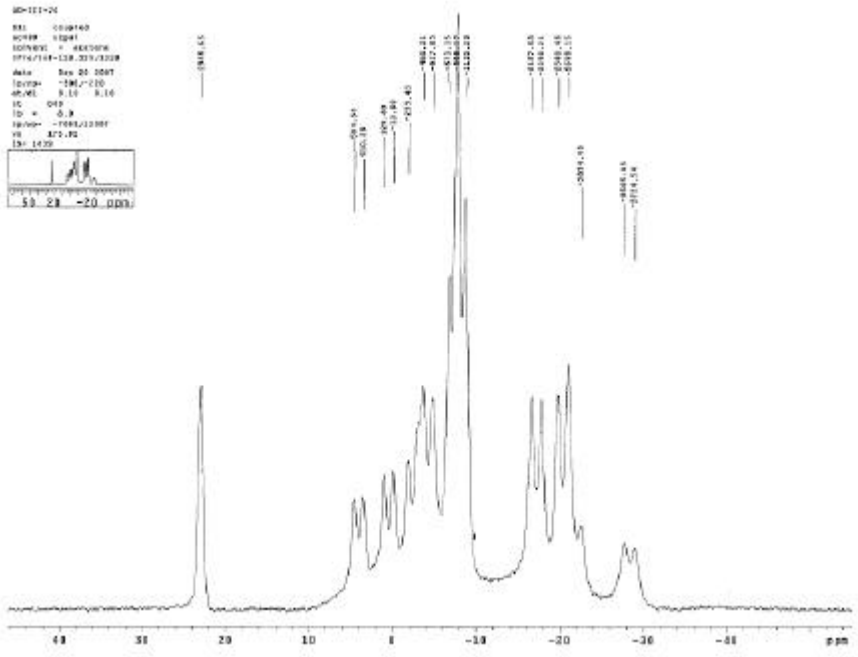
UV/Vis (96% EtOH) spectrum of 10-8-(5-propargyl-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) (7)



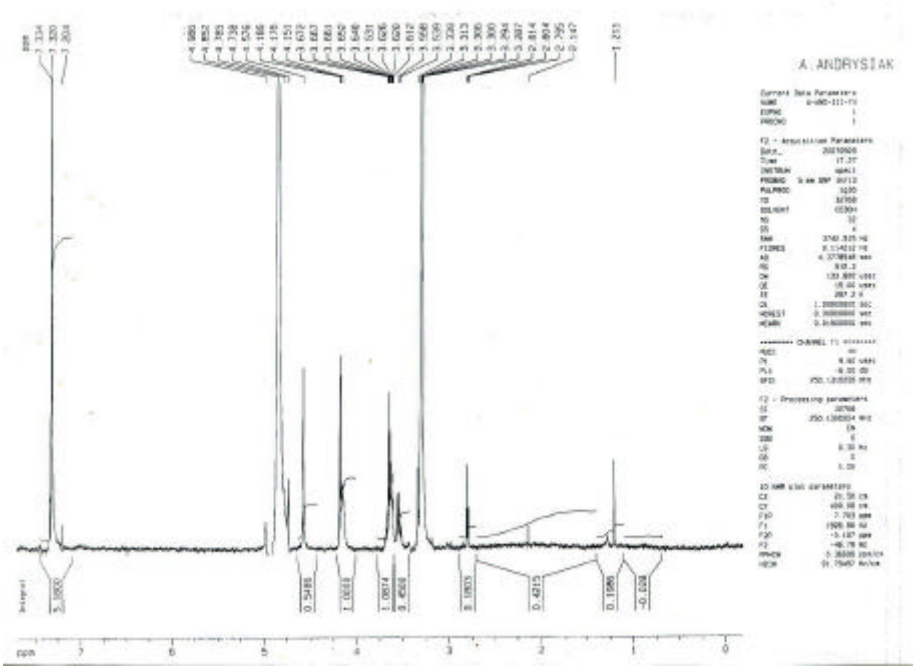
FT-IR (KBr) spectrum of 10-8-(5-propargyl-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) (7).



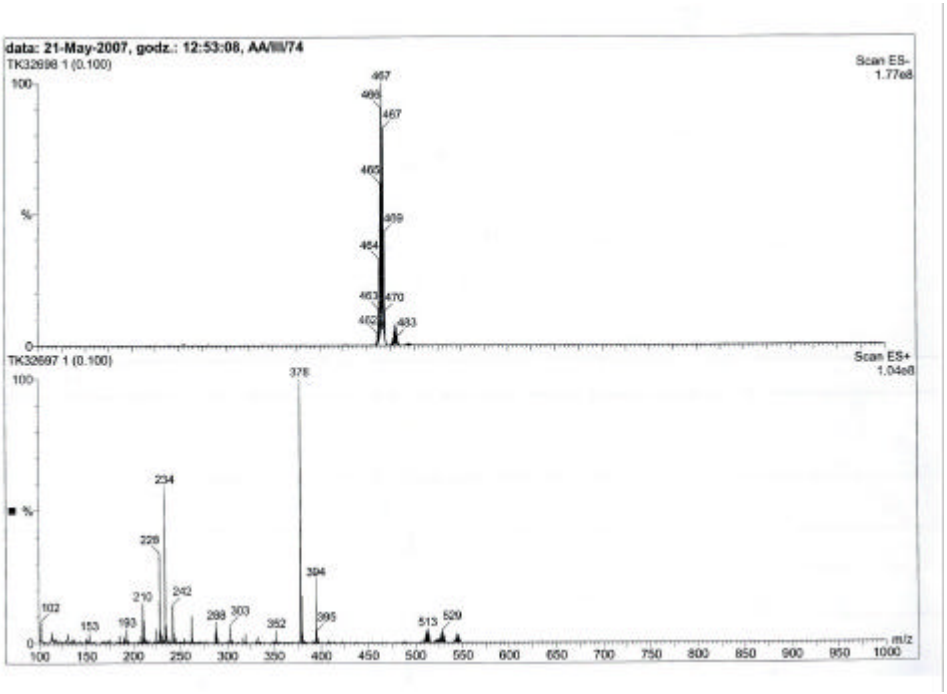
^{11}B {^{1}H BB} NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3 \cdot Et_2O$) spectrum of -8-(5-propargyl-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) (7).



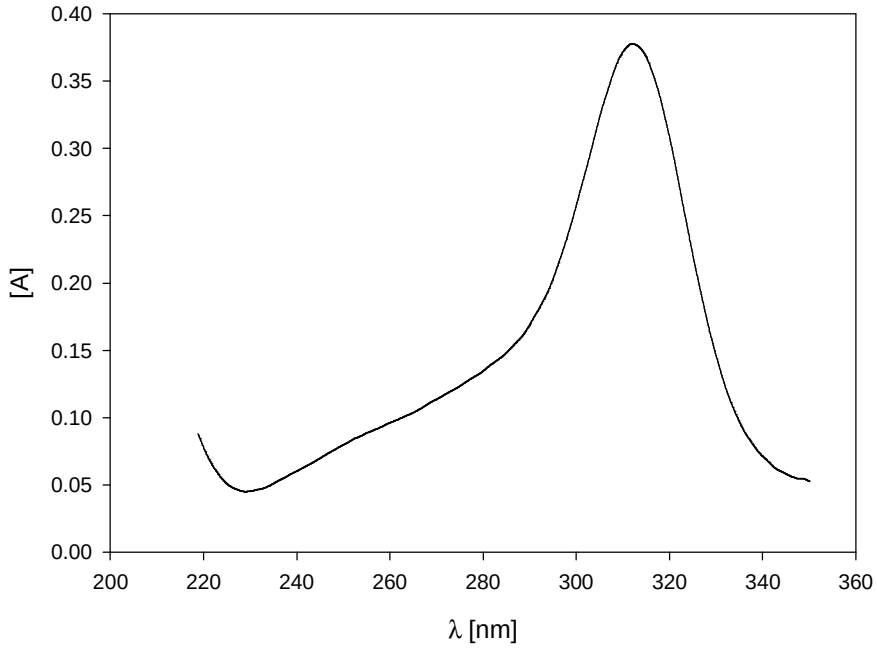
^{11}B NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3 \cdot Et_2O$) spectrum of -8-(5-propargyl-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) (7).



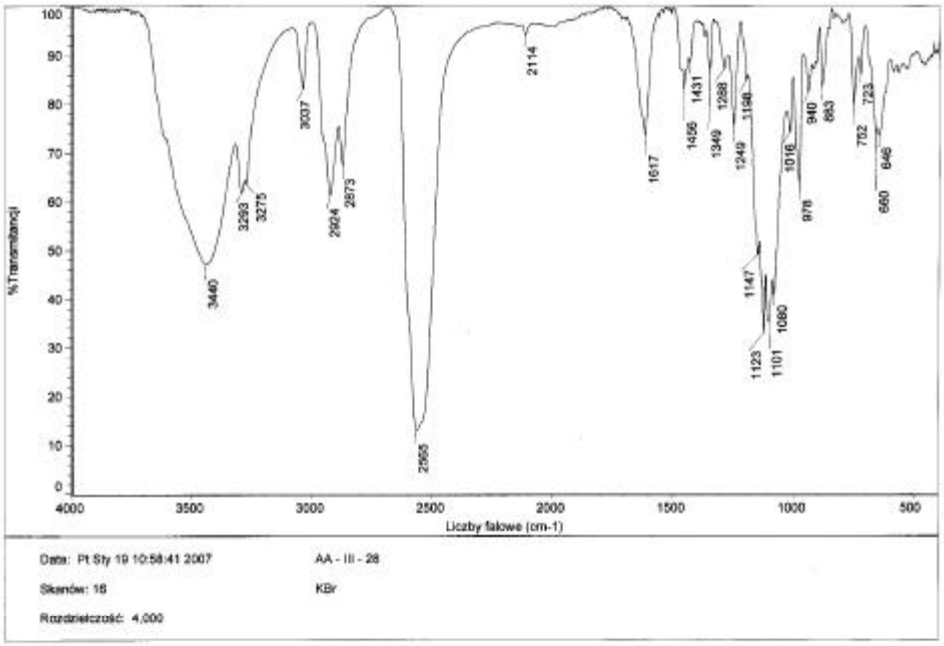
^{1}H NMR (acetone-*d6*, 250.131MHz, 25°C, TMS) spectrum of 10-8-(5-propargyl-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) (7).



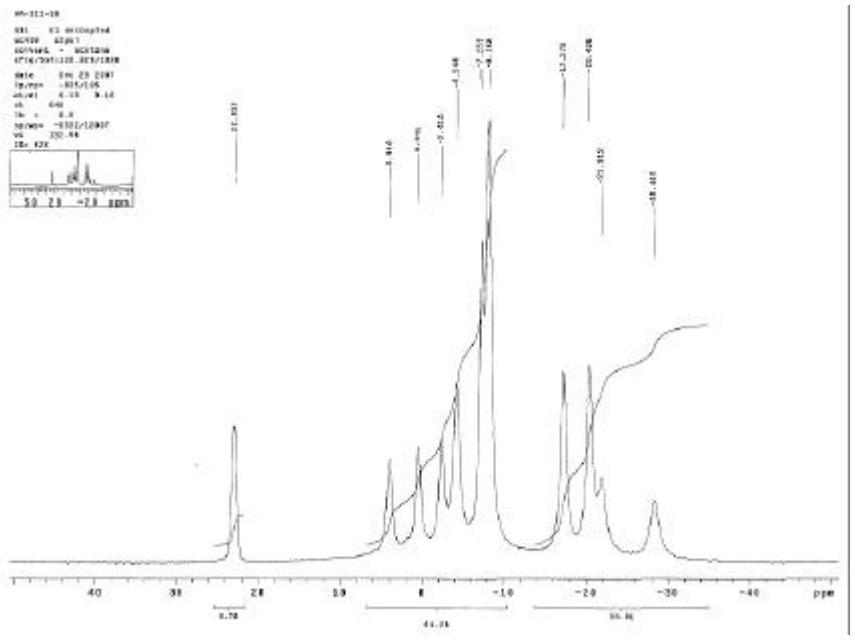
MS (ESI) spectrum of 10-8-(5-propargyl-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) (7), m/z (100): molecular formula: $C_{11}H_{32}B_{18}CoO_3$, calculated average mass: 465.90, found 467.0 (100) $[M+1H]^-$



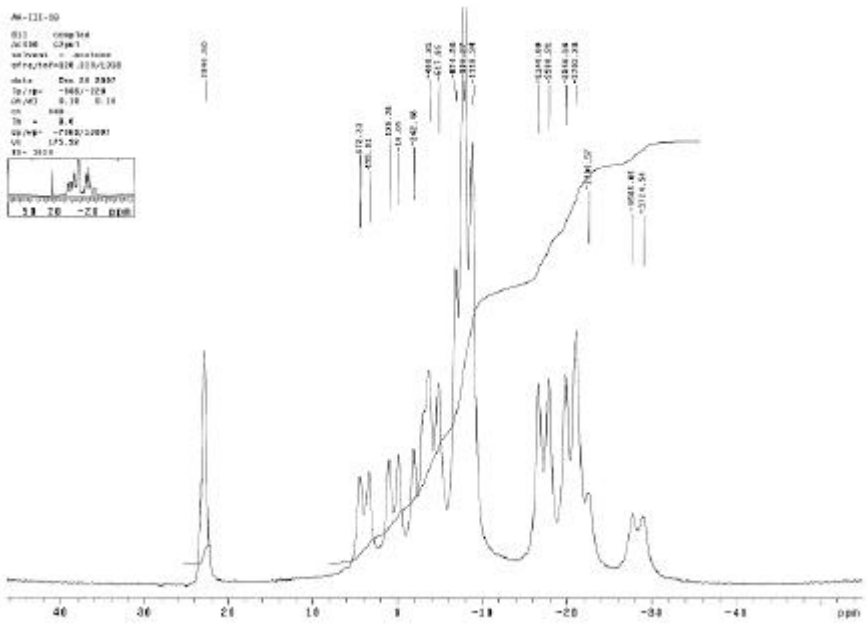
UV/Vis (96% EtOH) spectrum of 8-[5-(4-pentyn-1-yl)-3-oxa-pentoxy]-3-cobalt bis(1,2-dicarbollide) (8).



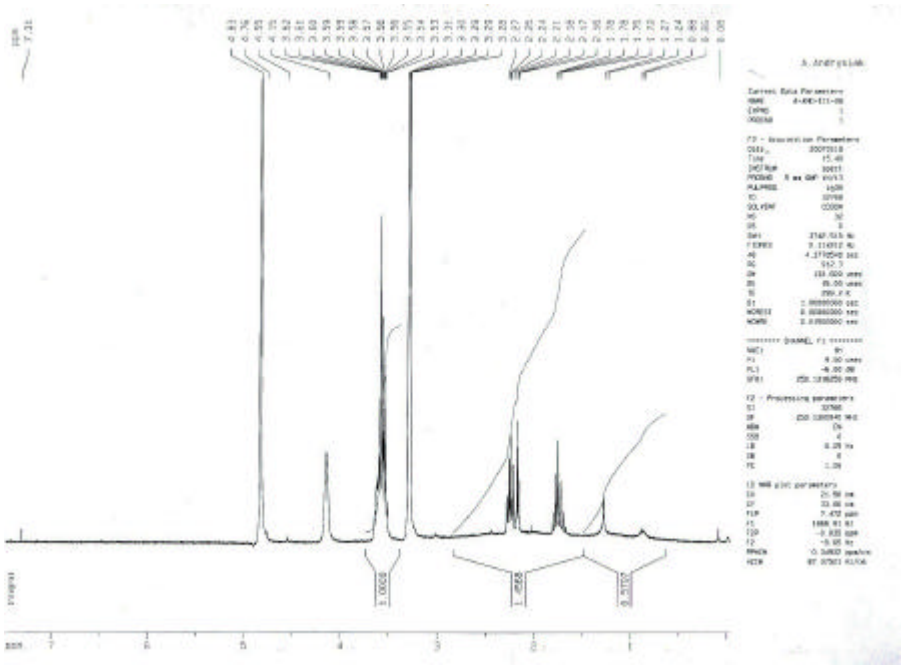
FT-IR (KBr) spectrum of 8-[5-(4-pentyn-1-yl)-3-oxa-pentoxy]-3-cobalt bis(1,2-dicarbollide) (8).



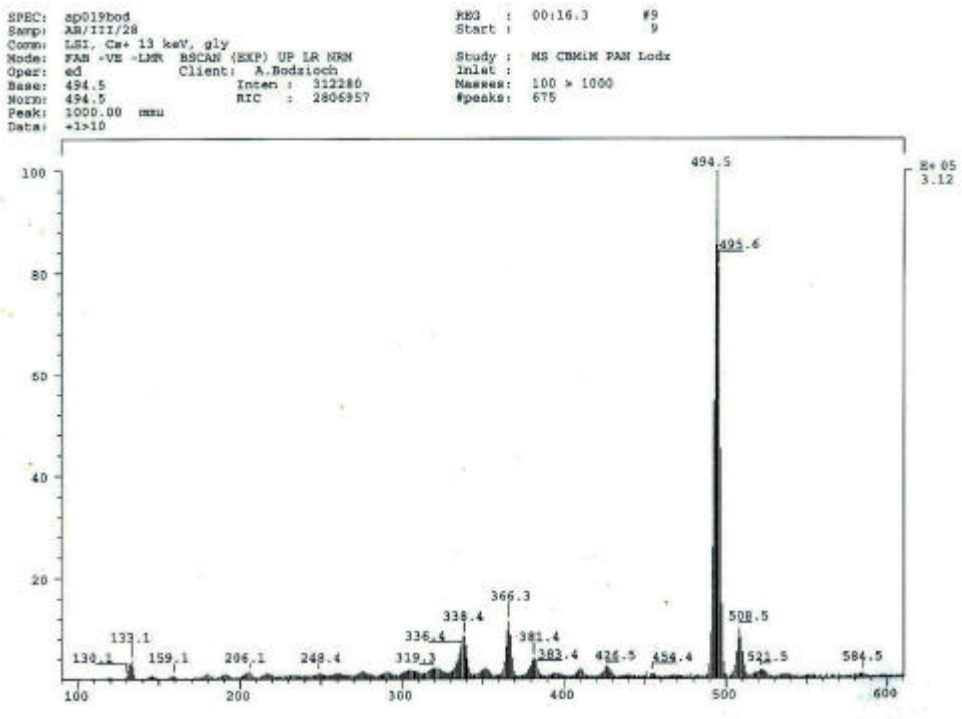
^{11}B {^{1}H BB} NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3 \cdot Et_2O$) spectrum of 8-[5-(4-pentyn-1-yl)-3-oxa-pentoxy]-3-cobalt bis(1,2-dicarbollide) (8).



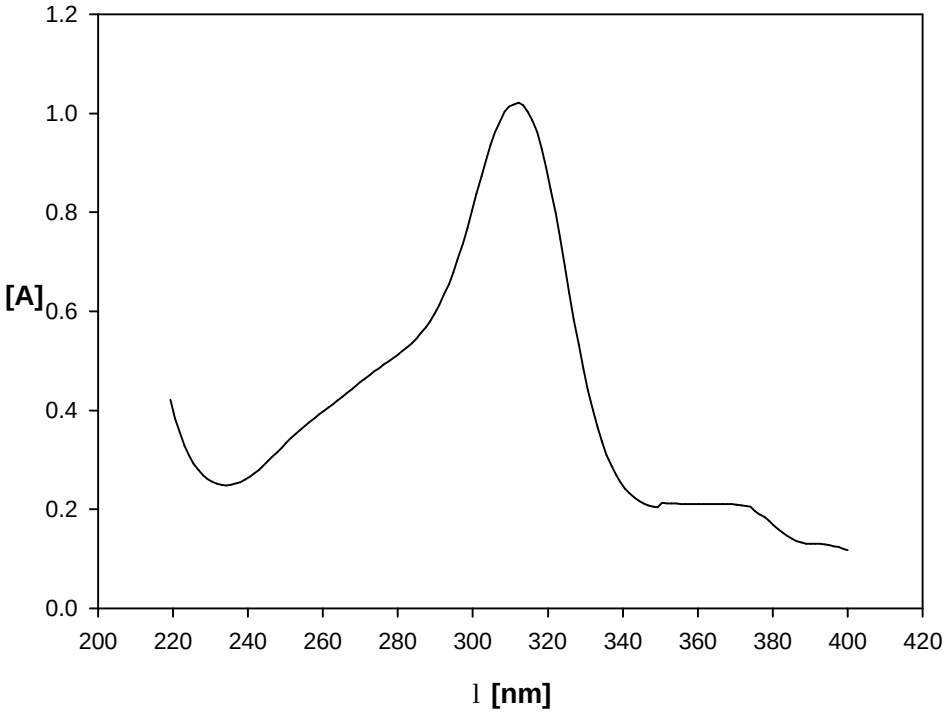
^{11}B NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of 8-[5-(4-pentyn-1-yl)-3-oxa-pentoxy]-3-cobalt bis(1,2-dicarbollide) (8).



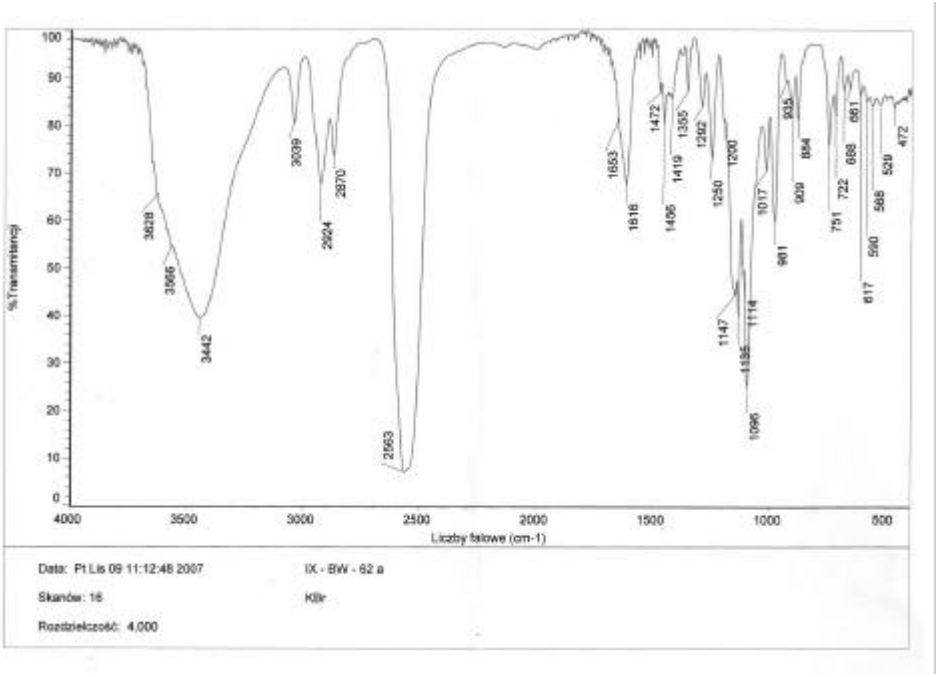
^{1}H NMR (acetone-*d6*, 250.131MHz, 25°C, TMS) spectrum of 8-[5-(4-pentyn-1-yl)-3-oxa-pentoxy]-3-cobalt bis(1,2-dicarbollide) (8).



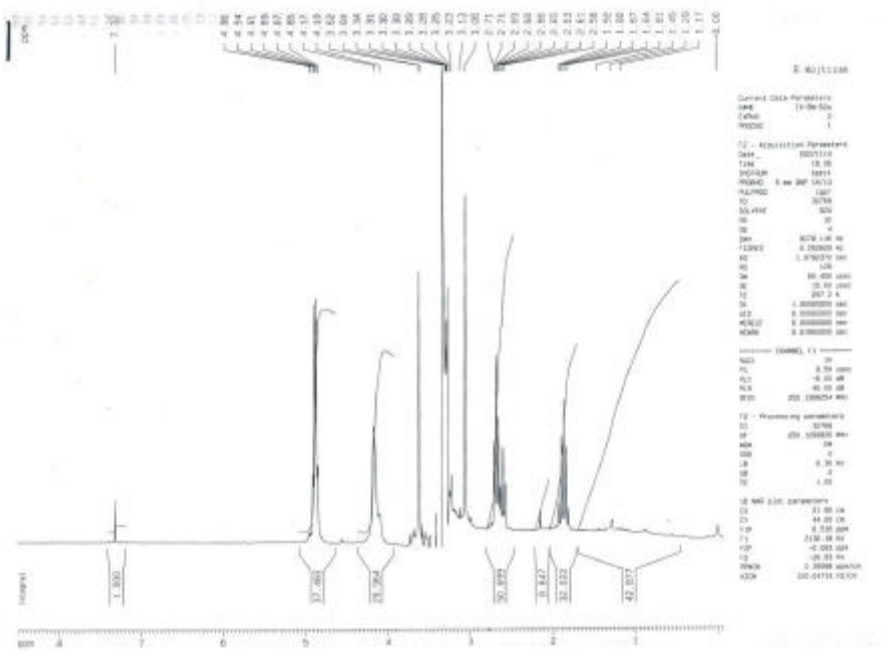
MS (Gly, FAB, -Ve) spectrum of 8-[5-(4-pentyn-1-yl)-3-oxa-pentoxy]-3-cobalt bis(1,2-dicarbollide) (8), m/z (%): molecular formula: $C_{13}H_{36}B_{18}CoO_3$, calculated average mass: 493.95, found 494.5 (100) $[M+1H]^-$



UV/Vis (96% EtOH) spectrum of 8-[(5-thia-(3-thiolo-propan-1-yl)-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) [(8-HS(CH_2)3S-(CH_2CH_2O)$_2$-1,2-$C_2B_9H_{10}$)(1',2'-$C_2B_9H_{11}$-3,3'-Co]Na (9).



FT-IR (KBr) spectrum of 8-[(5-thia-(3-thiolo-propan-1-yl)-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) [(8-HS(CH_2)3S-(CH_2CH_2O)$_2$-1,2-$C_2B_9H_{10}$)(1',2'-$C_2B_9H_{11}$-3,3'-Co]Na (9).



^{1}H NMR (D_2O, 250.131MHz, 25°C, TMS) spectrum of 8-[(5-thia-(3-thiolo-propan-1-yl)-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) [(8-HS(CH_2)3S-(CH_2CH_2O)$_2$-1,2-$C_2B_9H_{10}$)(1',2'-$C_2B_9H_{11}$-3,3'-Co]Na (9).

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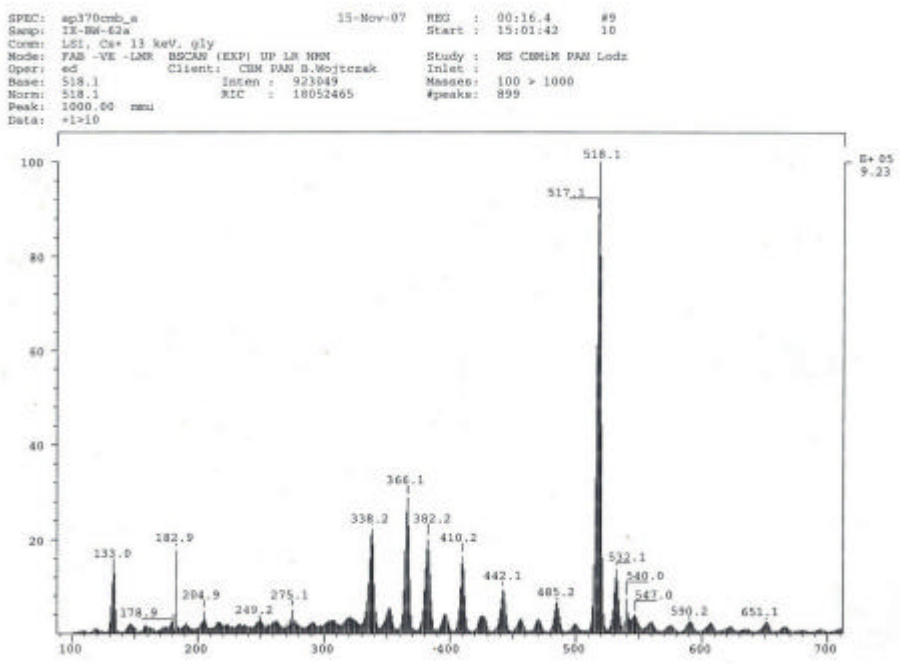
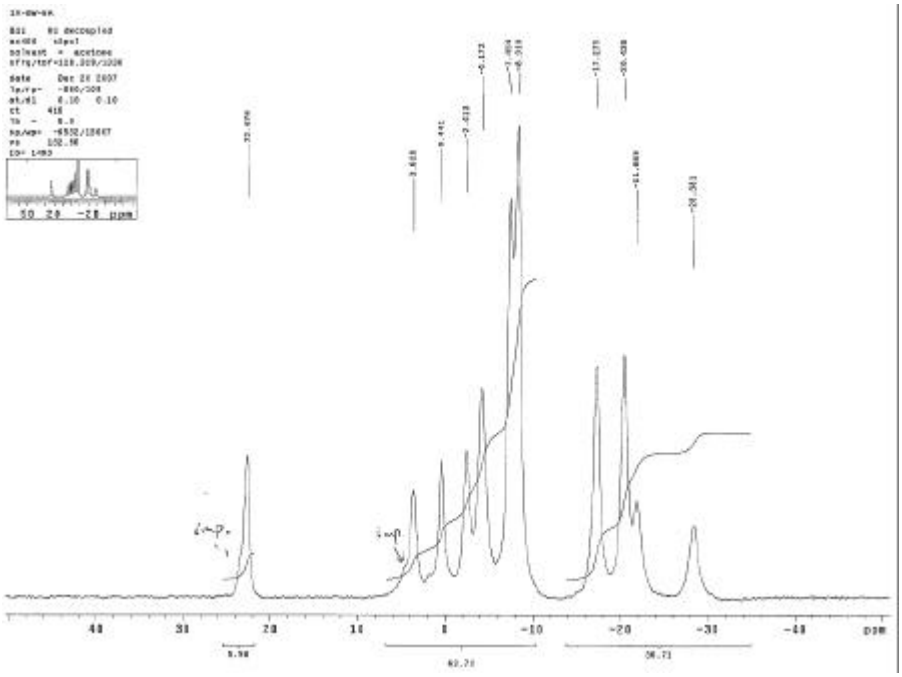
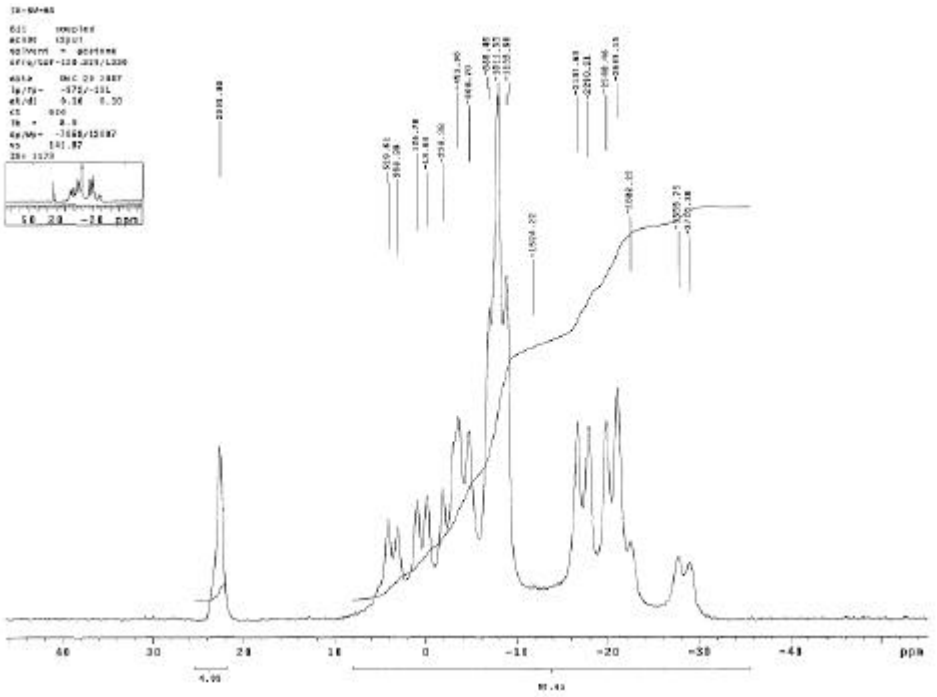


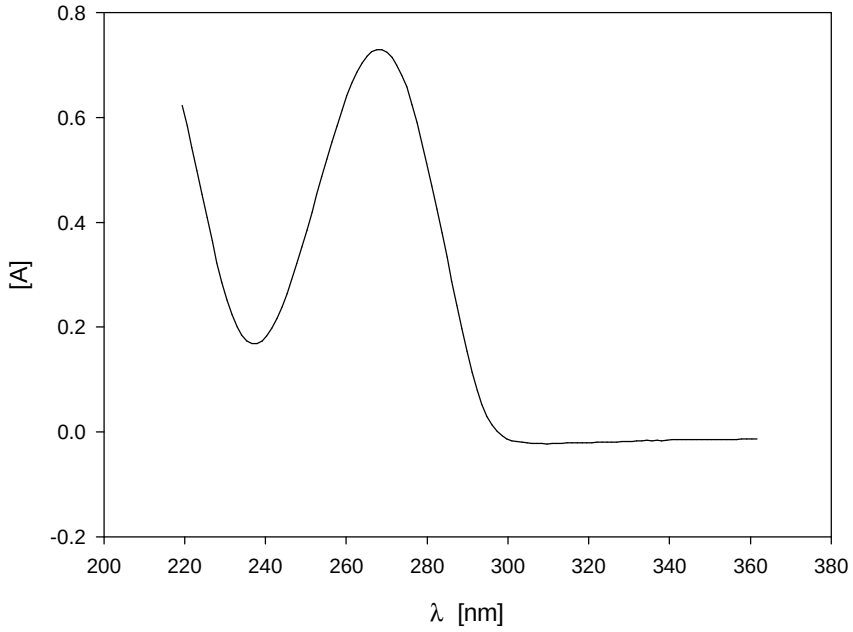
MS (FAB, Gly, -Ve) spectrum of 8-[(5-thia-(3-thiolo-propan-1-yl)-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) [(8-HS(CH_2)3S-(CH_2CH_2O)$_2$-1,2-$C_2B_9H_{10}$)(1',2'-$C_2B_9H_{11}$-3,3'-Co]Na (9), m/z (%): molecular formula:$C_{11}H_{36}B_{18}O_2S_2Co$, calculated average mass: 518.06, found 518.1 (100) $[M]^-$



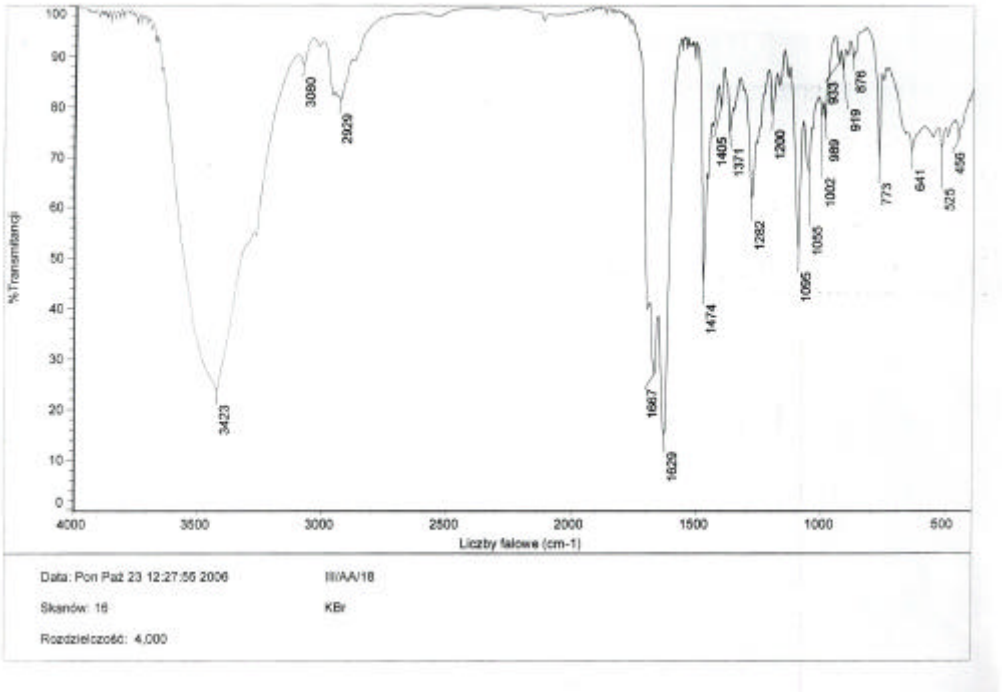
^{11}B {^1H BB} NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of -[(5-thia-(3-thiolo-propan-1-yl)-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) [(8-HS(CH_2)3S-(CH_2CH_2O)$_2$-1,2-$C_2B_9H_{10}$)(1',2'-$C_2B_9H_{11}$-3,3'-Co]Na (9),



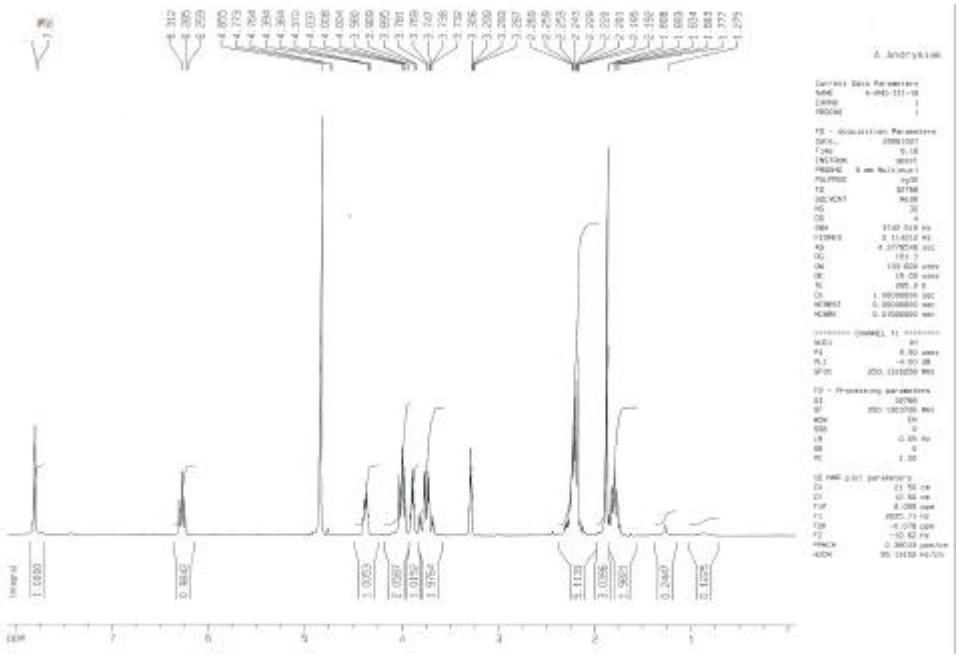
^{11}B NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of -[(5-thia-(3-thiolo-propan-1-yl)-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) [(8-HS(CH_2)3S-(CH_2CH_2O)$_2$-1,2-$C_2B_9H_{10}$)(1',2'-$C_2B_9H_{11}$-3,3'-Co]Na (9),



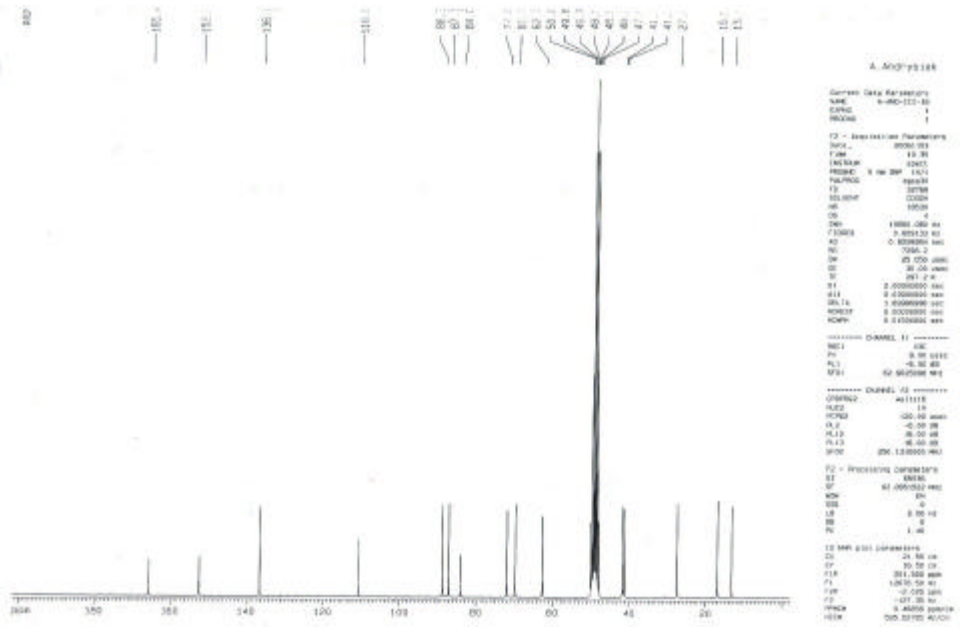
UV/Vis (96% EtOH) spectrum of 3N-(4-pentyn-1-yl)thymidine (12).



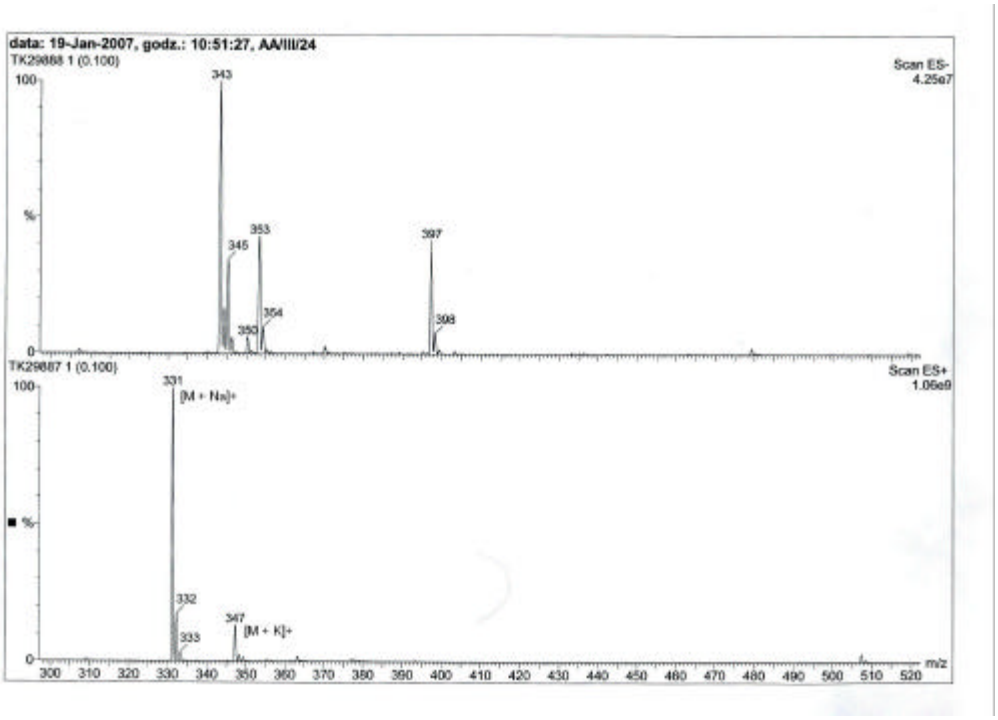
FT-IR (KBr) spectrum of 3N-(4-pentyn-1-yl)thymidine (12).



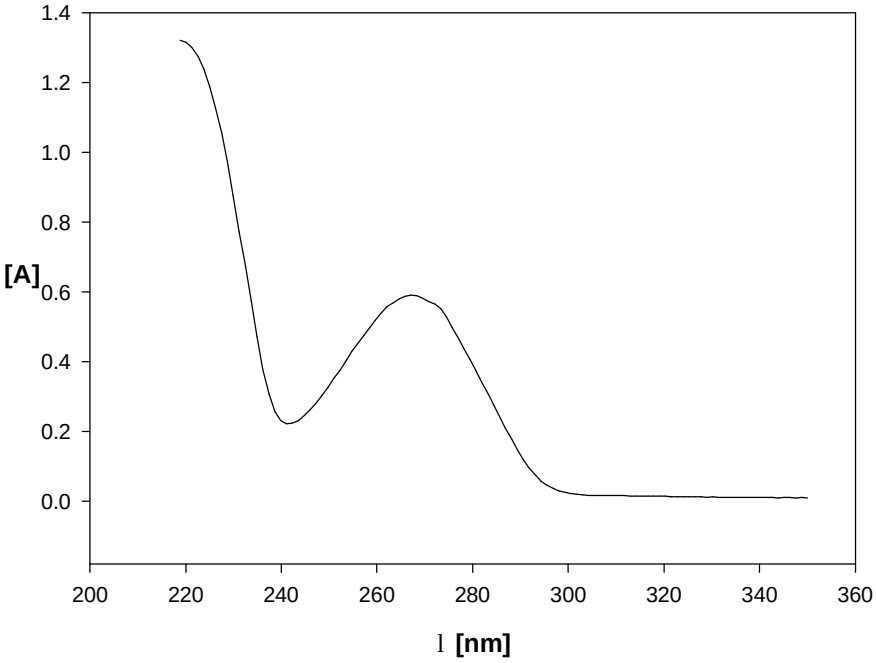
^{1}H NMR (MeOD, 250.131MHz, 25°C, TMS) spectrum of 3*N*-(4-pentyn-1-yl)thymidine (12).



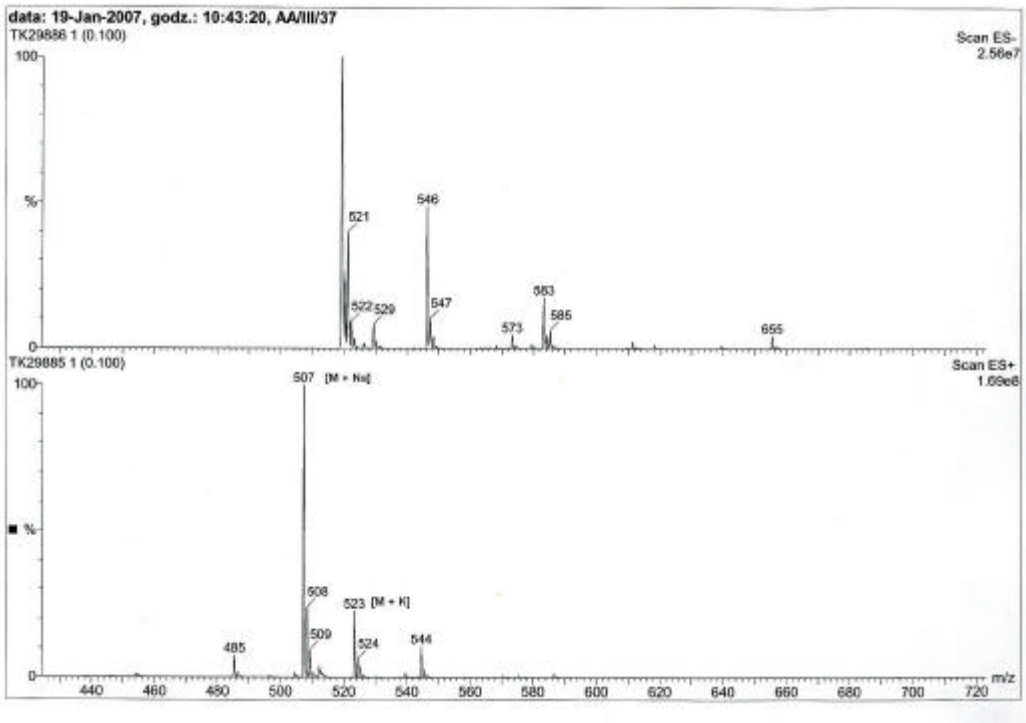
^{13}C NMR (62.90 MHz, CD_3OH, 25°C, TMS) spectrum of 3*N*-(4-pentyn-1-yl)thymidine (12).



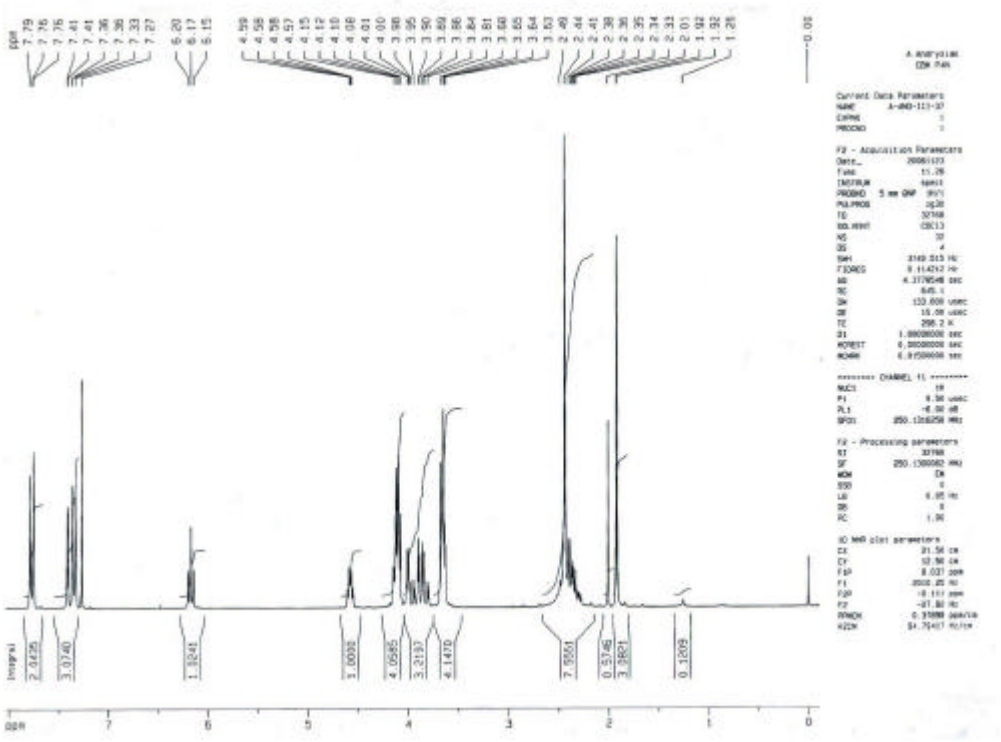
MS-ESI spectrum of 3*N*-(4-pentyn-1-yl)thymidine (12), molecular formula: $C_{15}H_{20}N_2O_5$; calculated average mass 308.33, found 331.0 (100) $[M+Na]^-$



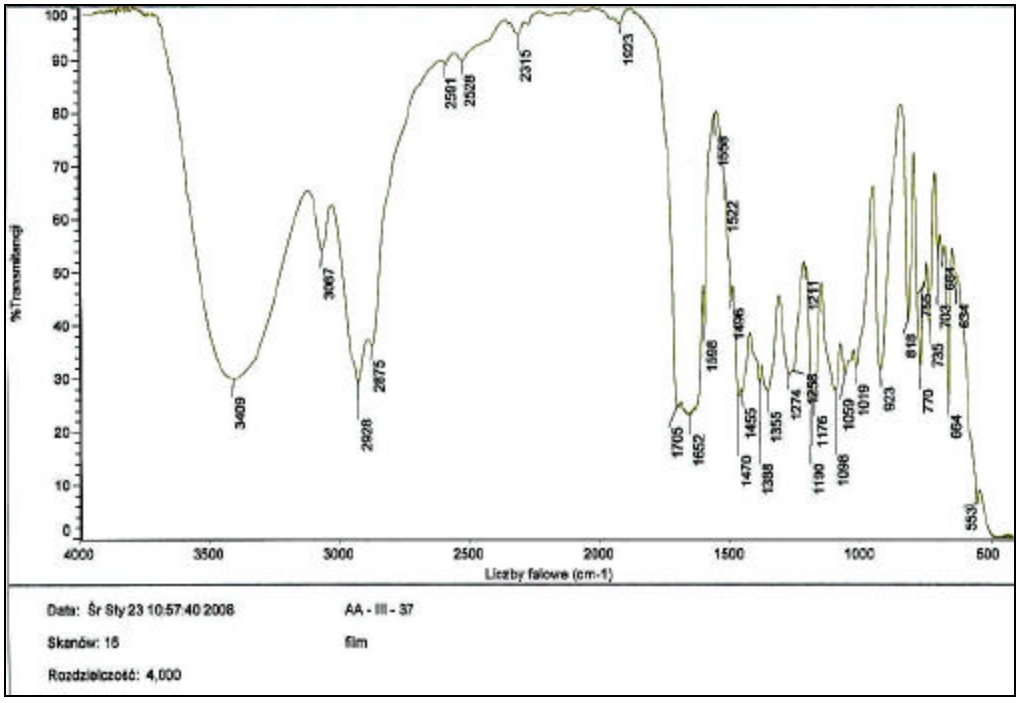
UV/Vis (96% EtOH) spectrum of 3*N*-[1-*para*-toluensulphonyl)-3-oxa-pentoxy)]thymidine (14).



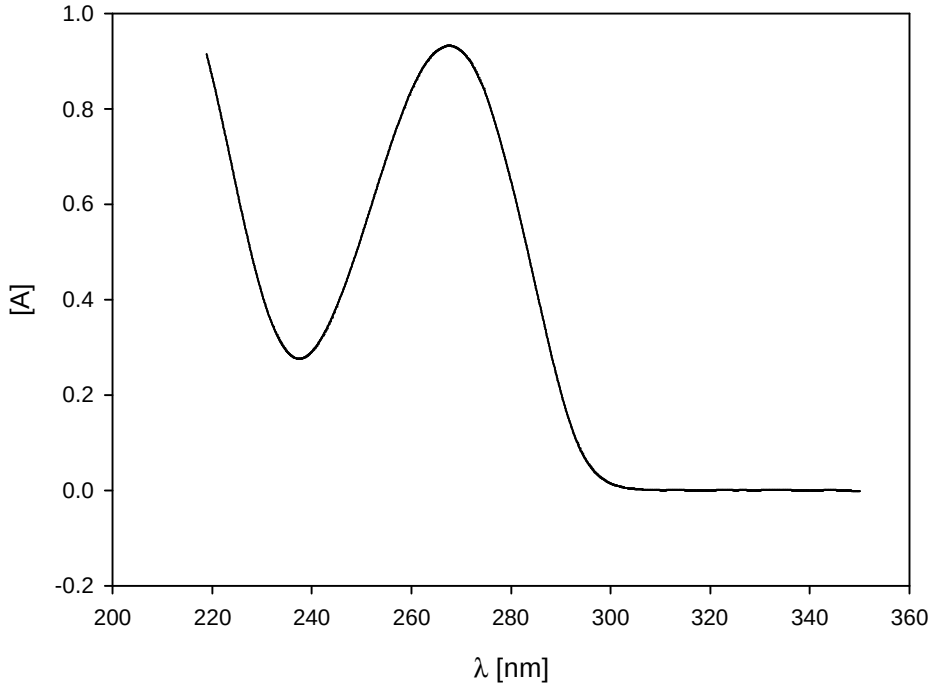
MS-ESI spectrum of 3*N*-[1-*para*-toluensulphonyl)-3-oxa-pentoxy)]thymidine (14), m/z (%): molecular formula: $C_{21}H_{28}N_2O_9S$**; calculated average mass:484.52, found 485.0 (10) [M+1H]$^-$**



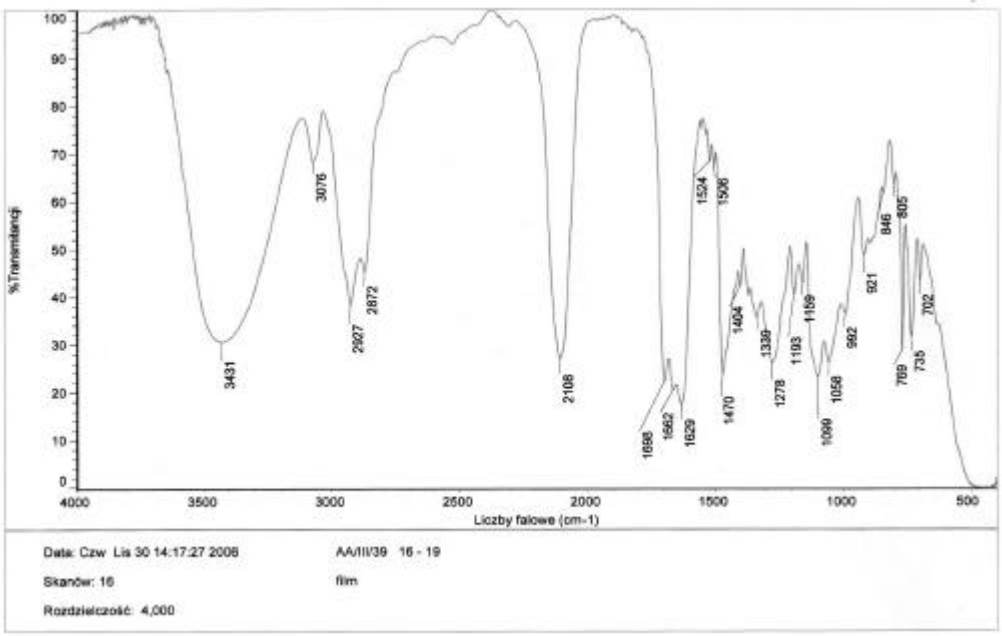
^{1}H NMR ($CDCl_3$, 250.131MHz, 25°C, TMS) spectrum of 3*N*-[1-*para*-toluensulphonyl)-3-oxa-pentoxy)]thymidine (14)



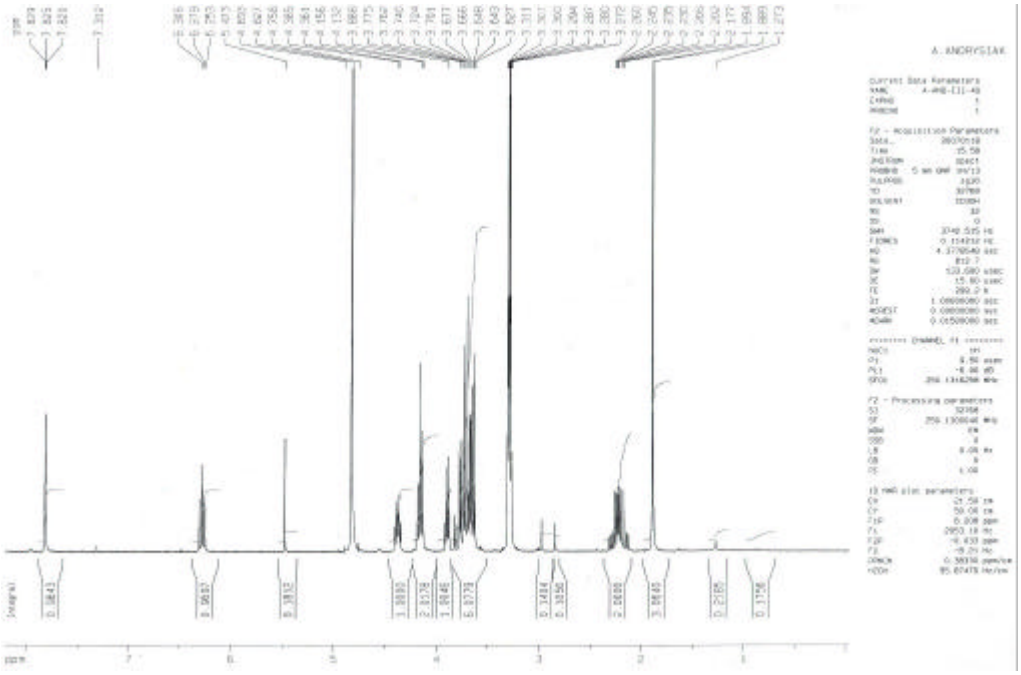
FT-IR (film) spectrum of 3*N*-[1-*para*-toluensulphonyl)-3-oxa-pentoxy)]thymidine (14).



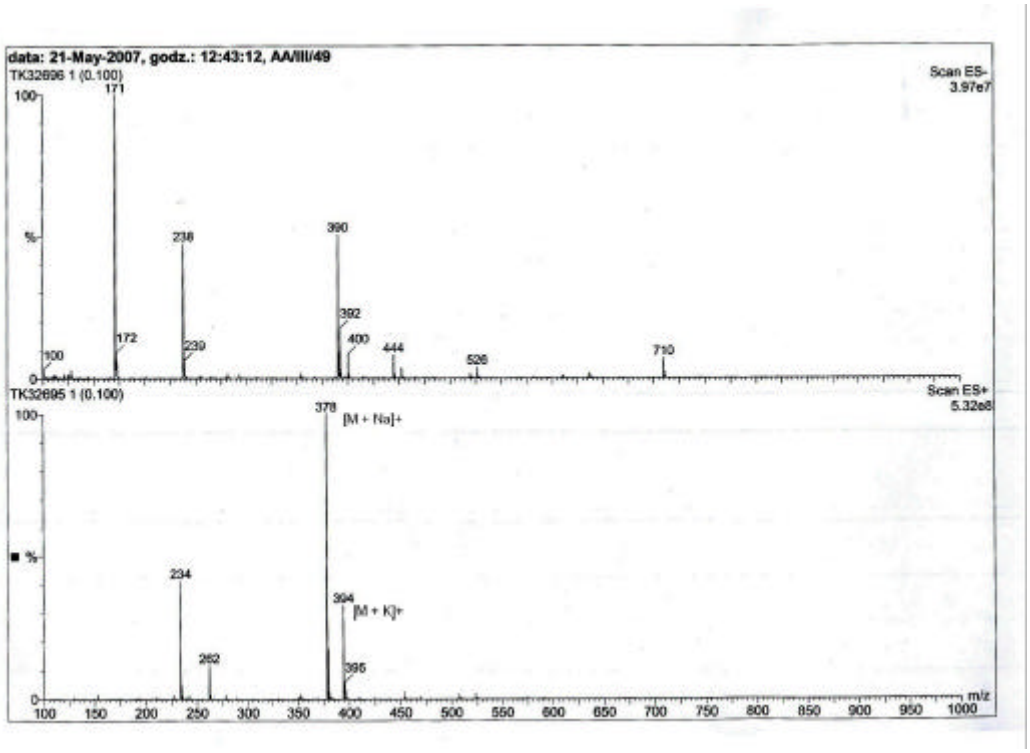
UV/Vis (96% EtOH) spectrum of 3*N*-[5-azide-3-oxa-pentoxy)]thymidine (15).



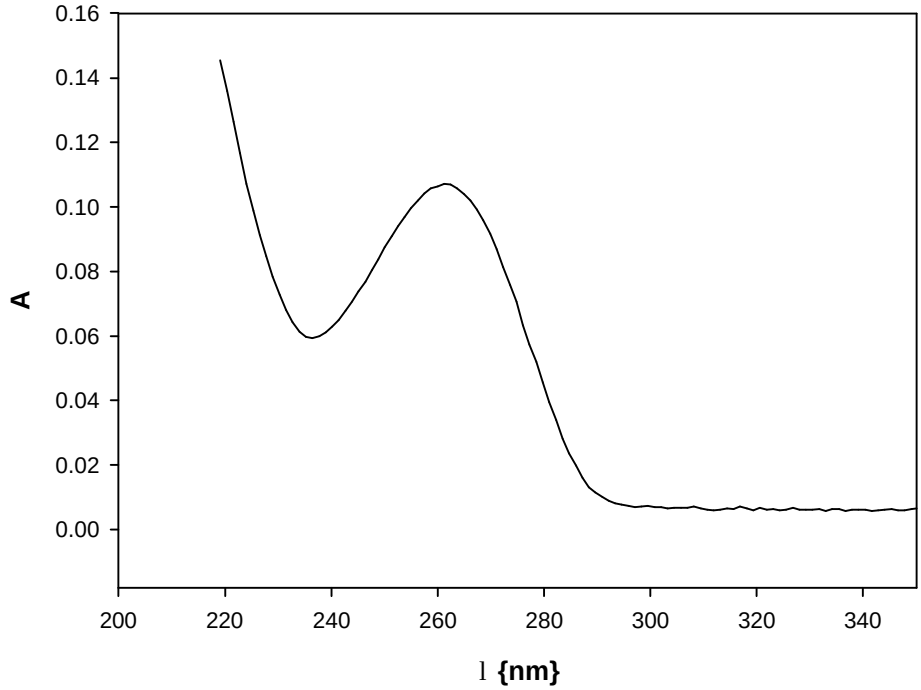
FT-IR (film) spectrum of 3*N*-[5-azide-3-oxa-pentoxy)]thymidine (15).



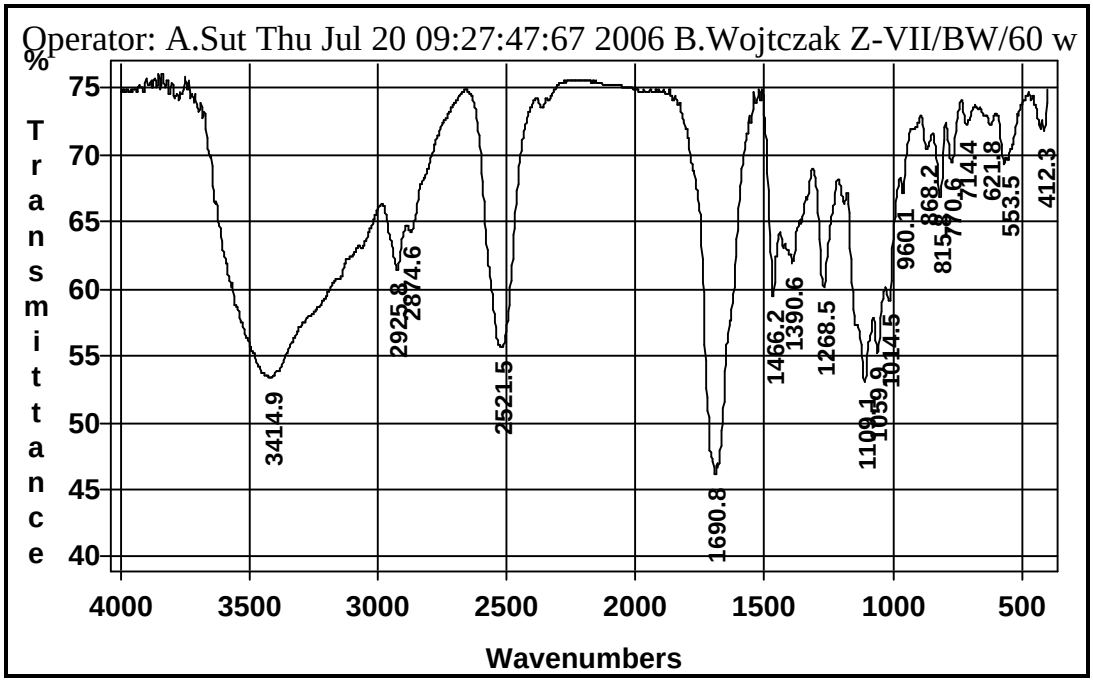
^{1}H NMR (acetone-*d6*, 250.131MHz, 25°C, TMS) spectrum of 3*N*-[5-azide-3-oxa-pentoxy)]thymidine (15).



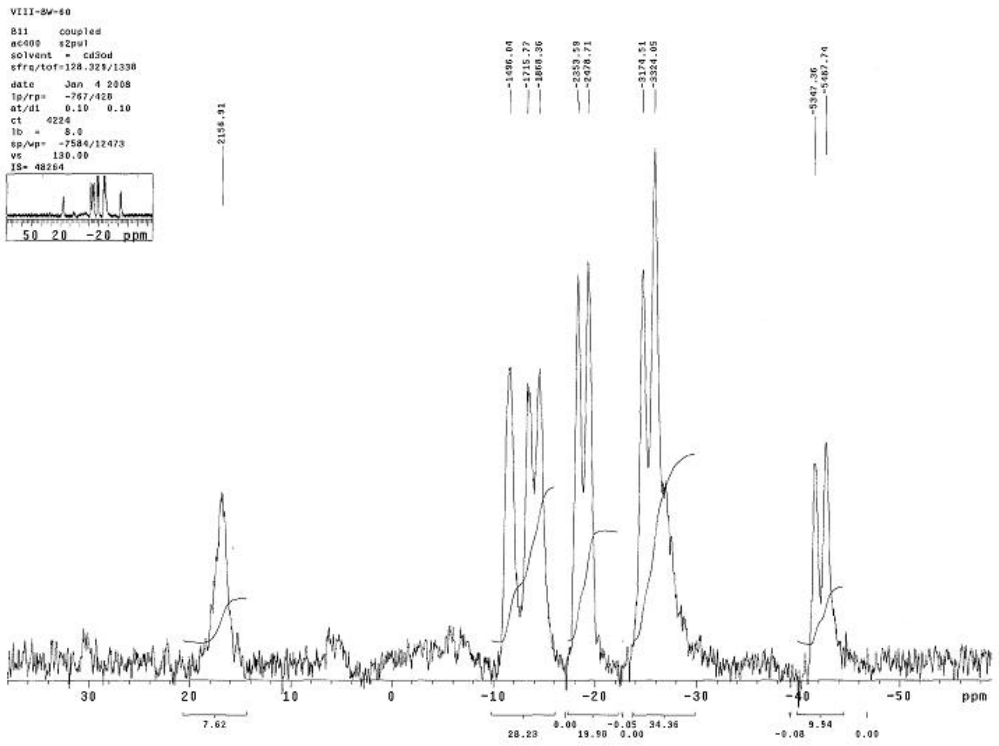
MS-ESI spectrum of 3*N*-[5-azide-3-oxa-pentoxy)]thymidine (15), m/z (%): molecular formula: $C_{14}H_{21}N_5O_6$ **,calculated average mass: 355.35, found 378.0 (100) [M+Na]$^{-}$**



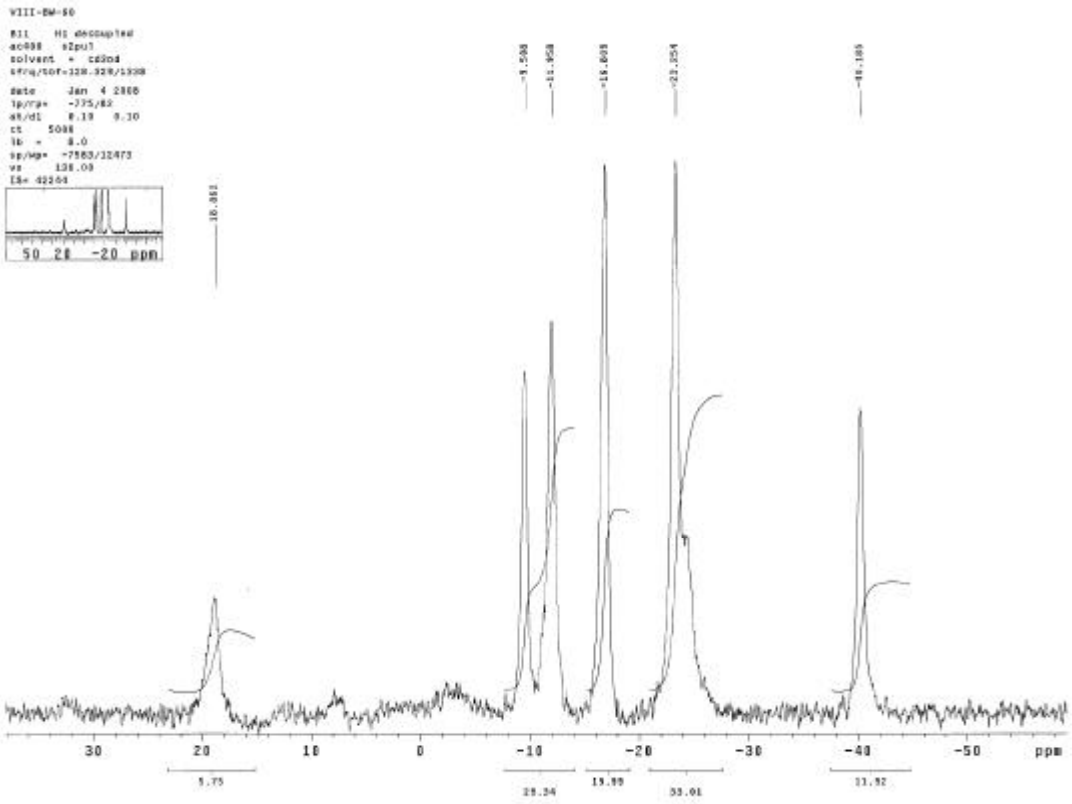
UV/Vis (96% EtOH) spectrum of 2'-*O*-{[5-(7,8-dikarba-nido-undekaborane-10-yl)-3-oxa-pentoxy]-1*N*-1,2,3-triazole-4-yl}methyluridine (17).



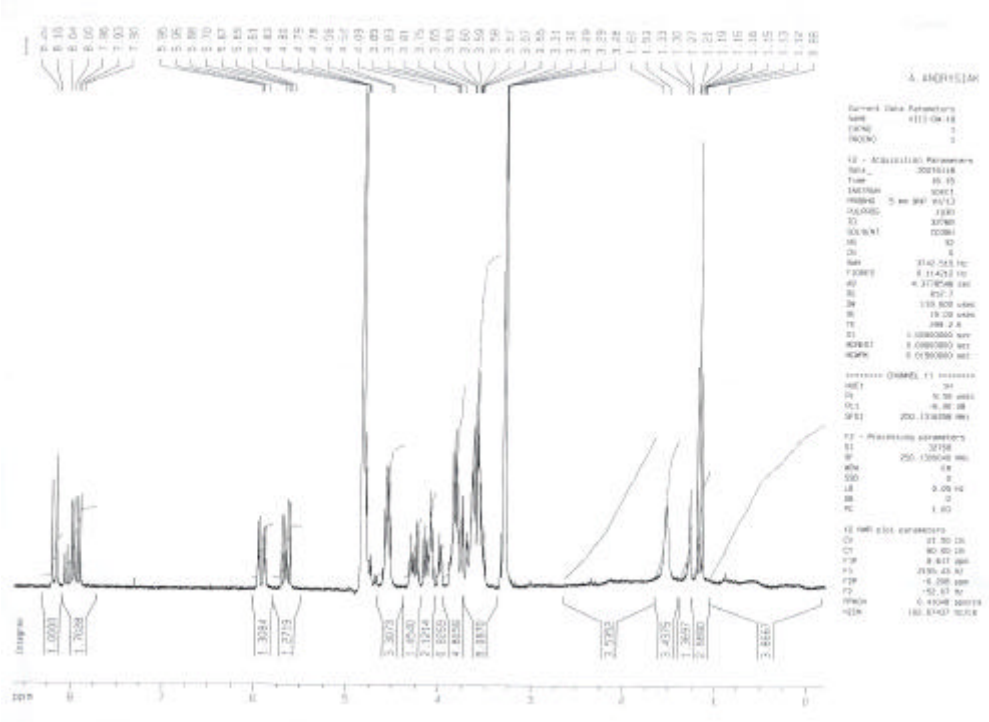
FT-IR (nujol) spectra of 2'-*O*-{[5-(7,8-dikarba-nido-undekaborane-10-yl)-3-oxa-pentoxy]-1*N*-1,2,3-triazole-4-yl}methyluridine (17).



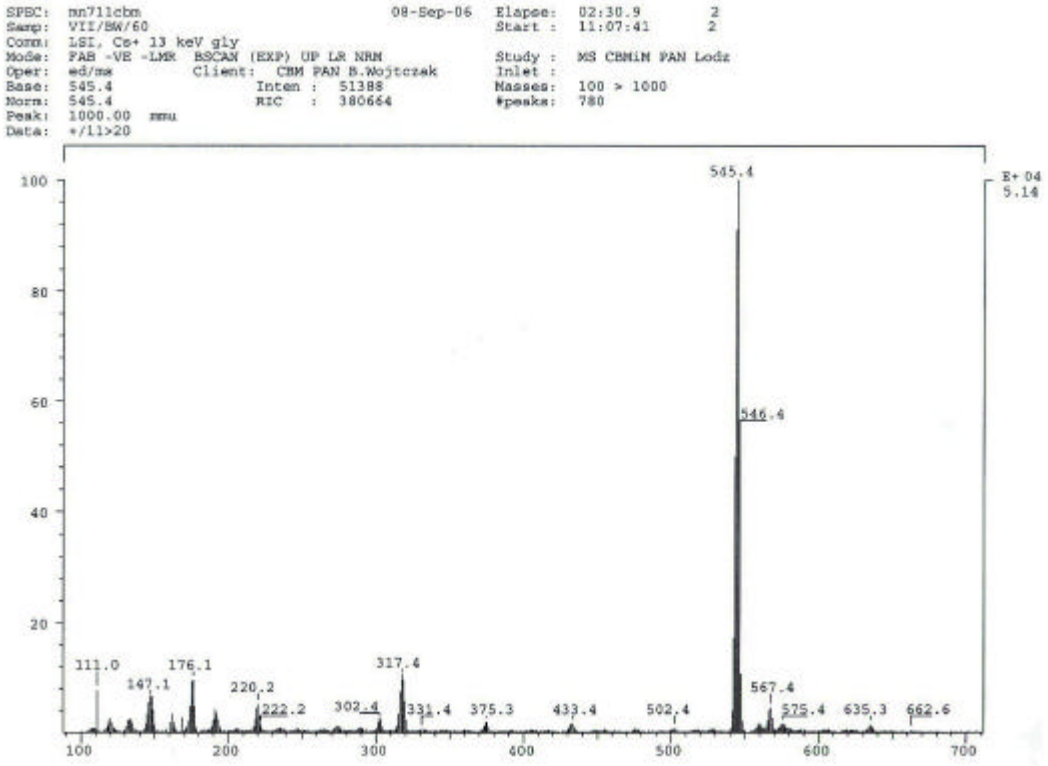
^{11}B NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of 2'-*O*-{[5-(7,8-dikarba-*nido*-undekaborane-10-yl)-3-oxa-pentoxy]-1*N*-1,2,3-triazole-4-yl}methyluridine (17).



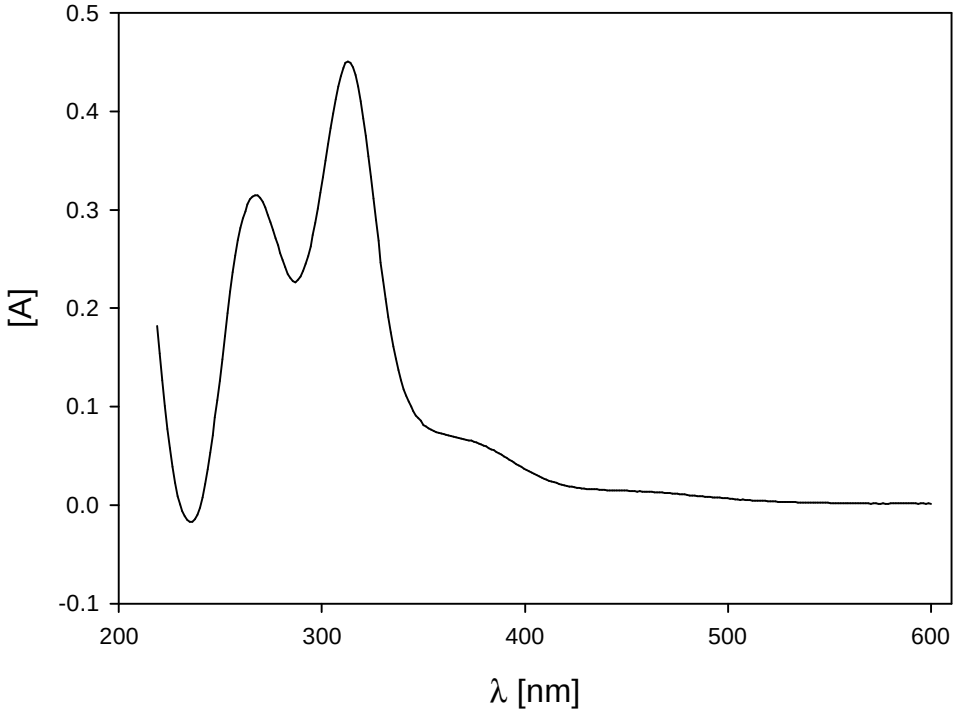
^{11}B {^{1}H BB} NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of 2'-*O*-{[5-(7,8-dikarba-*nido*-undekaborane-10-yl)-3-oxa-pentoxy]-1*N*-1,2,3-triazole-4-yl}methyluridine (17).



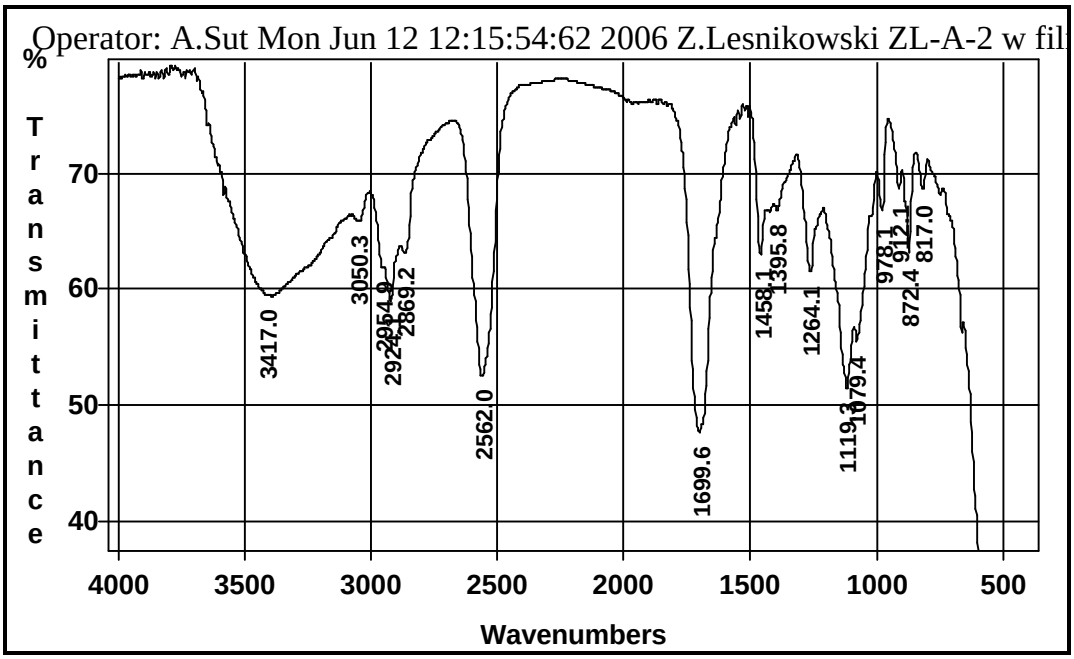
^{1}H NMR (CD_3OH, 250.131MHz, 25°C, TMS) spectrum of 2'-*O*-{[5-(7,8-dikarba-nido-undekaborane-10-yl)-3-oxa-pentoxy]-1*N*-1,2,3-triazole-4-yl}methyluridine (17).



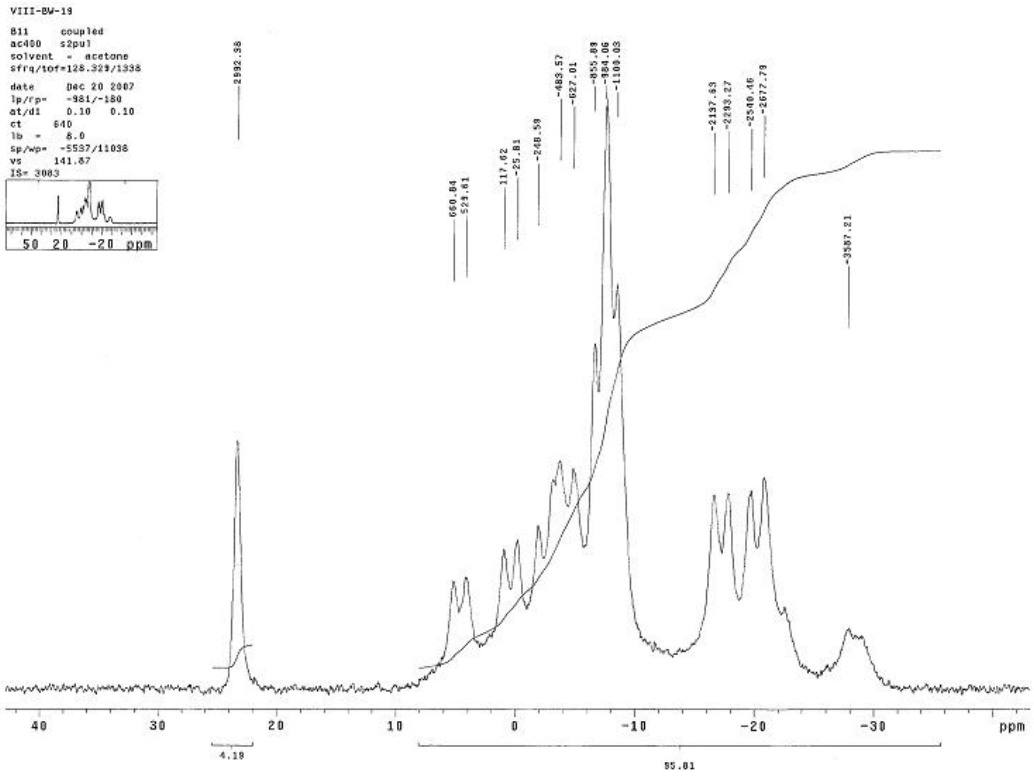
MS (FAB, Gly, -Ve) spectrum of 2'-*O*-{[5-(7,8-dikarba-nido-undekaborane-10-yl)-3-oxa-pentoxy]-1*N*-1,2,3-triazole-4-yl}methyluridine (17),m/z (%): molecular formula: $C_{18}H_{31}B_9N_5O_8$, calculated average mass: 542.77, found 545.4 (100) $[M+3H]^-$



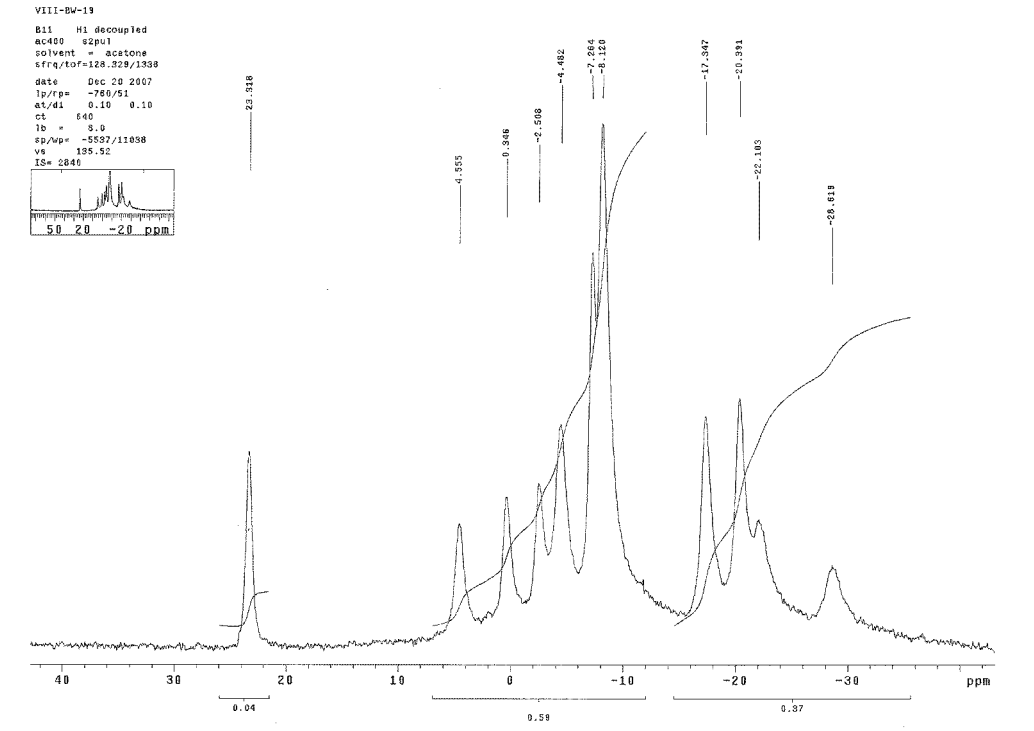
UV/VIS (96% EtOH) spectrum of 2'-*O*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}methyluridine (18).



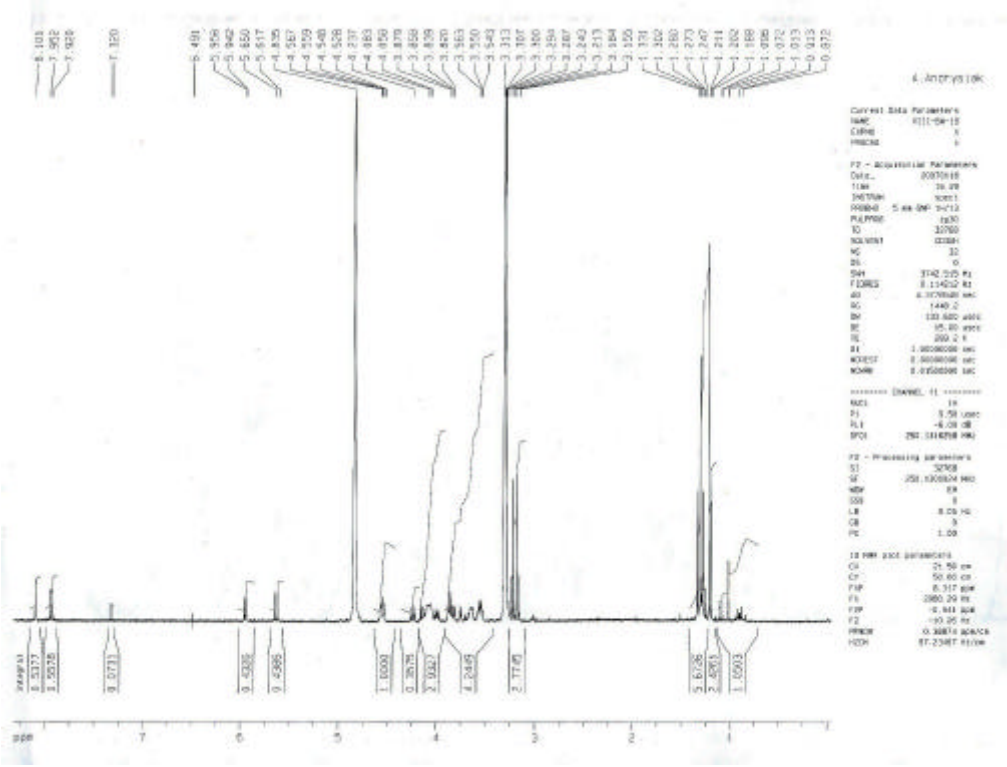
FT-IR (film) spectra of 2'-*O*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}methyluridine (18).



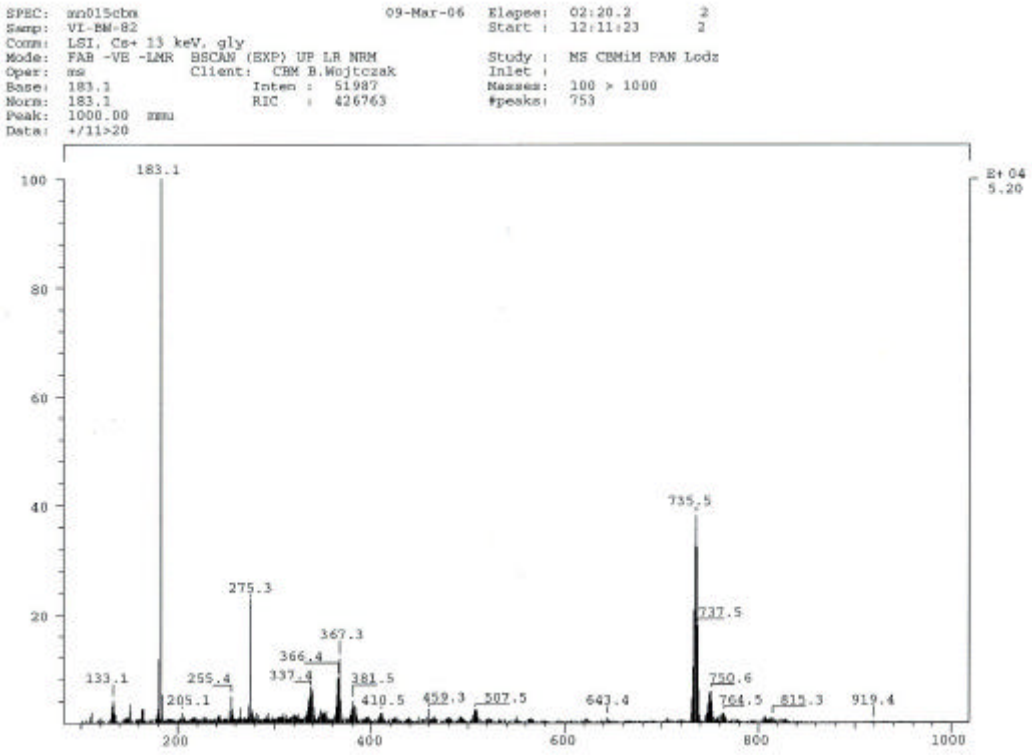
^{11}B NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of 2'-*O*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}methyluridine (18).



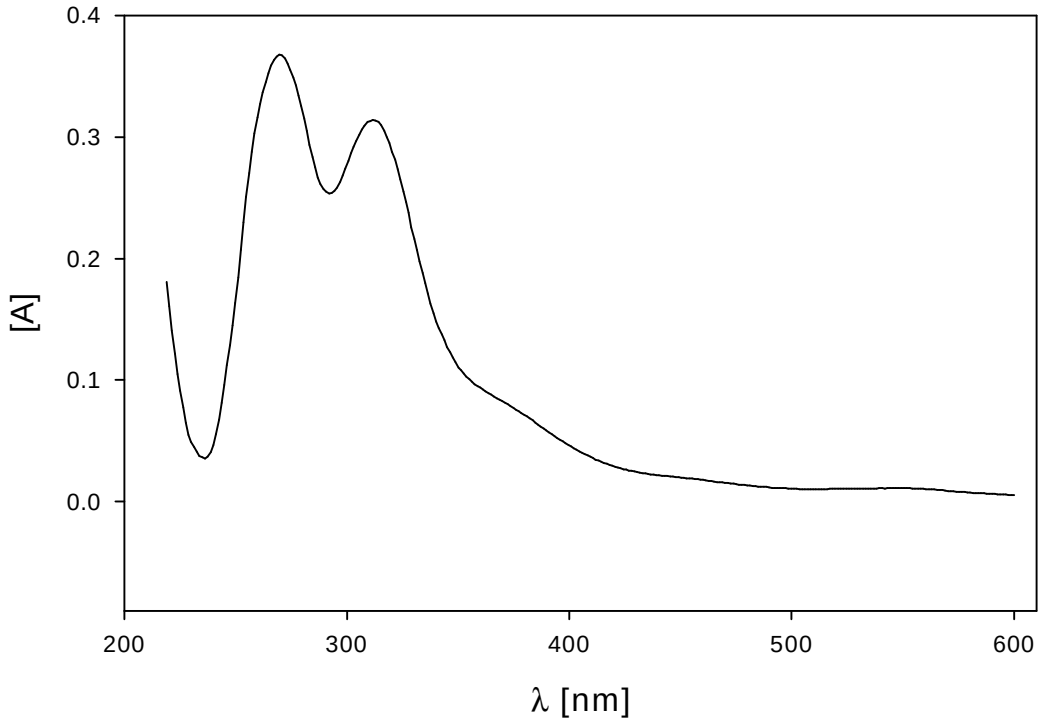
^{11}B {^{1}H BB} NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of 2'-*O*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}methyluridine (18).



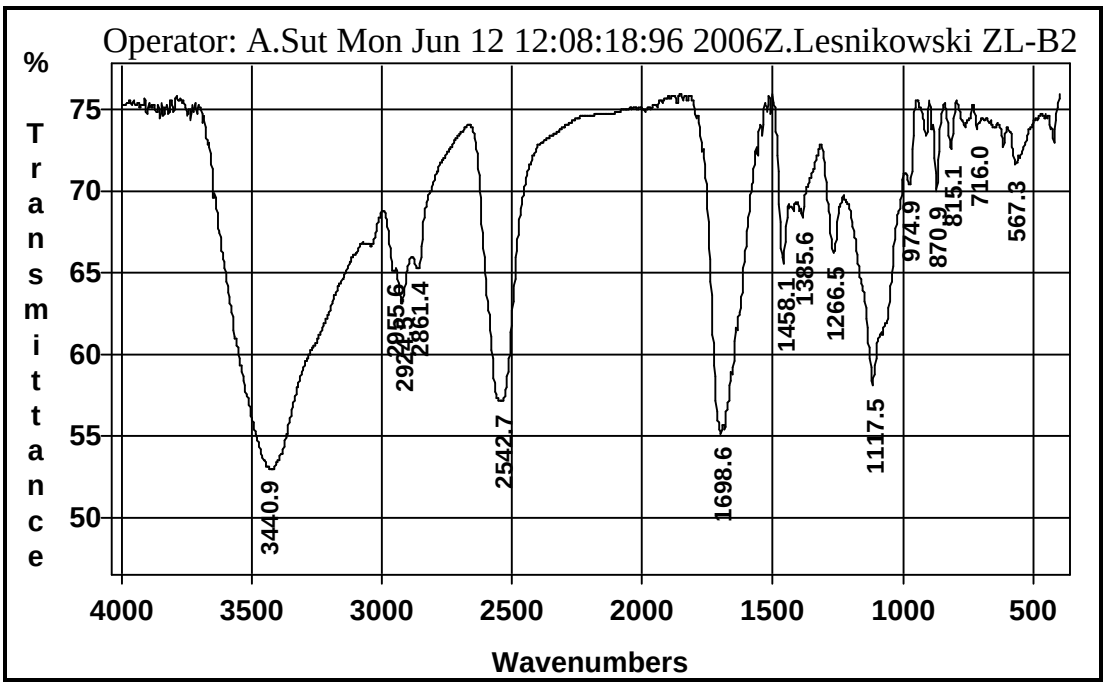
^{1}H NMR (CD_3OH, 250.131MHz, 25°C, TMS) spectrum of 2'-*O*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}methyluridine (18).



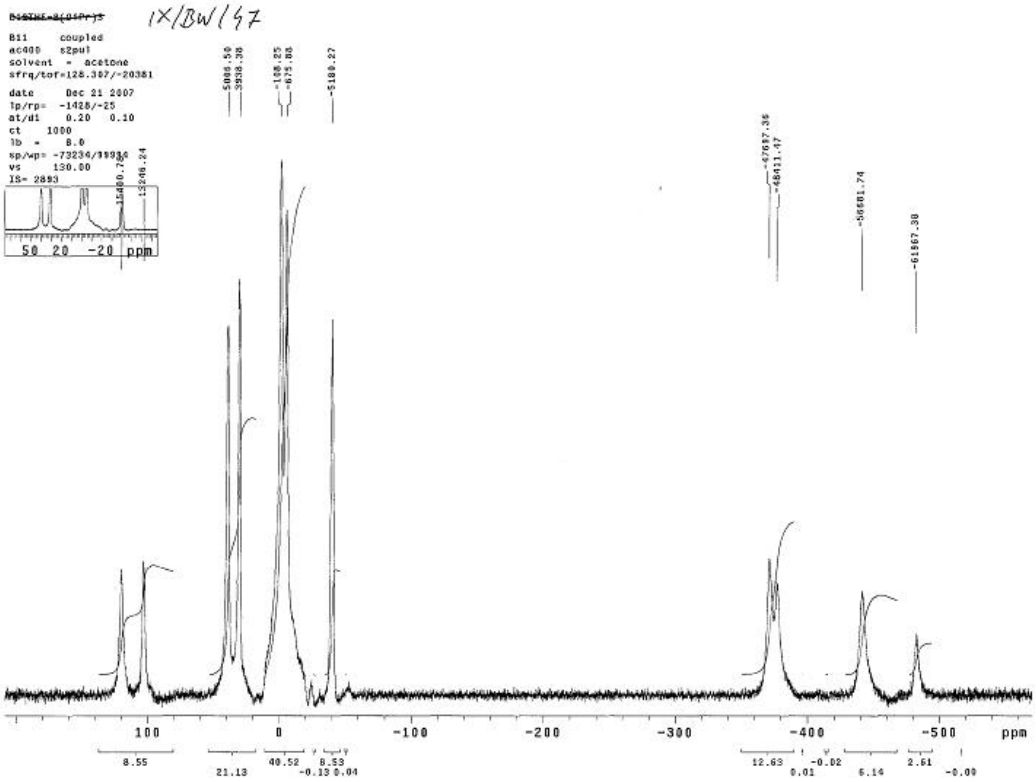
MS (FAB, Gly, -Ve) spectrum of 2'-*O*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}methyluridine (18), m/z (%): molecular formula: $C_{20}H_{43}B_{18}CoN_5O_8$, calculated average mass: 735.11, fund 735.5 (36) $[M]^-$



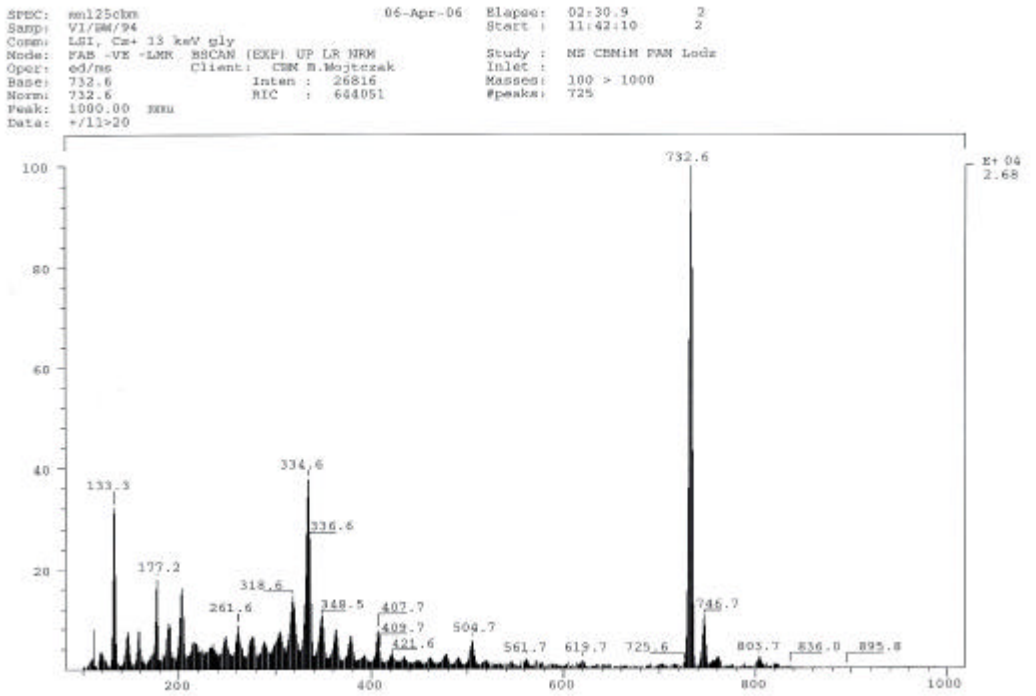
UV/Vis (96% EtOH) spectrum of 2'-*O*-{{5-[3-iron bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}methyluridine (19).



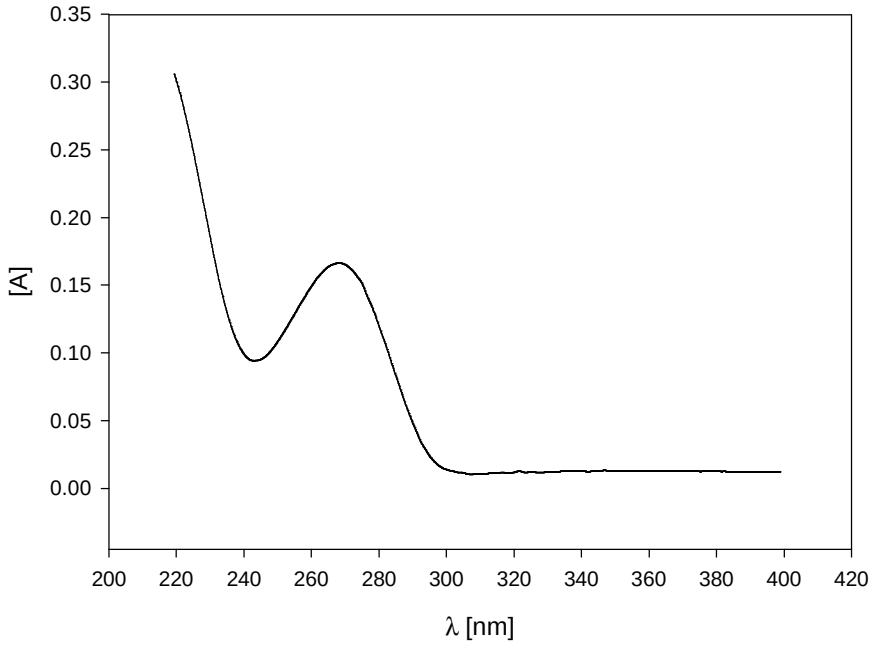
FT-IR (KBr) spectrum of 2'-*O*-{{5-[3-iron bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}methyluridine (19).



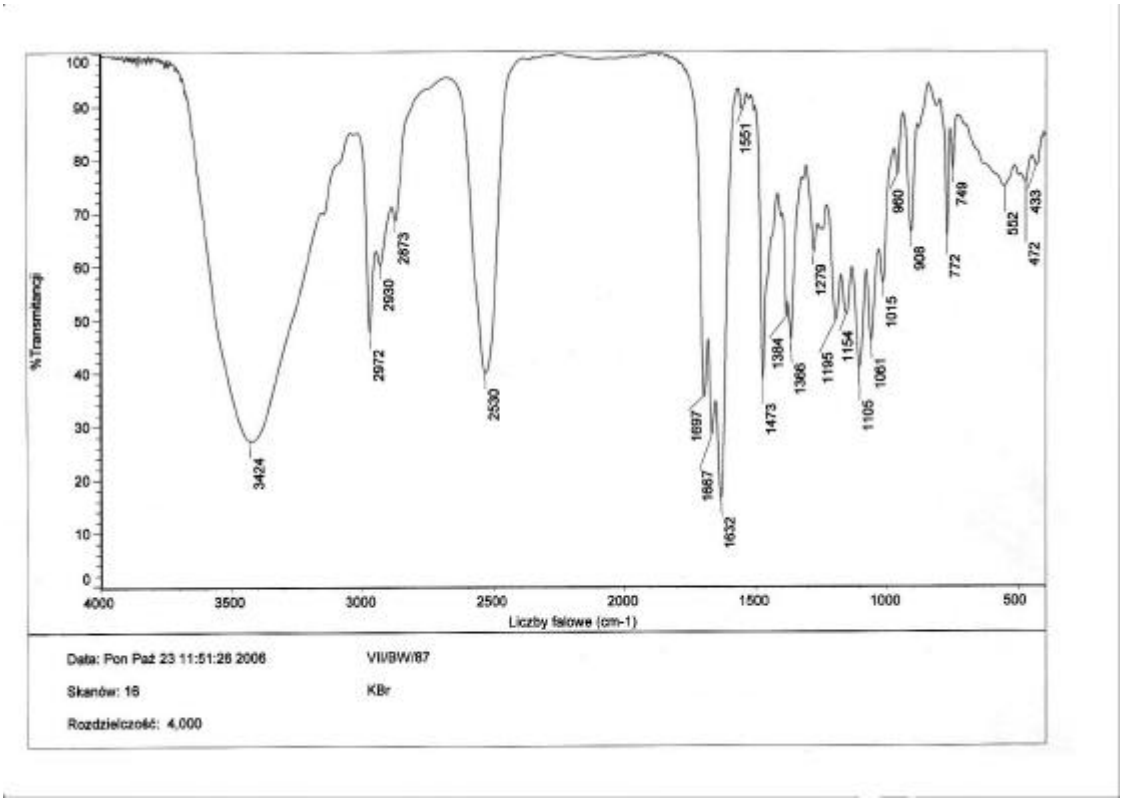
^{11}B NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of 2'-*O*-{{5-[3-iron bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}methyluridine (19).



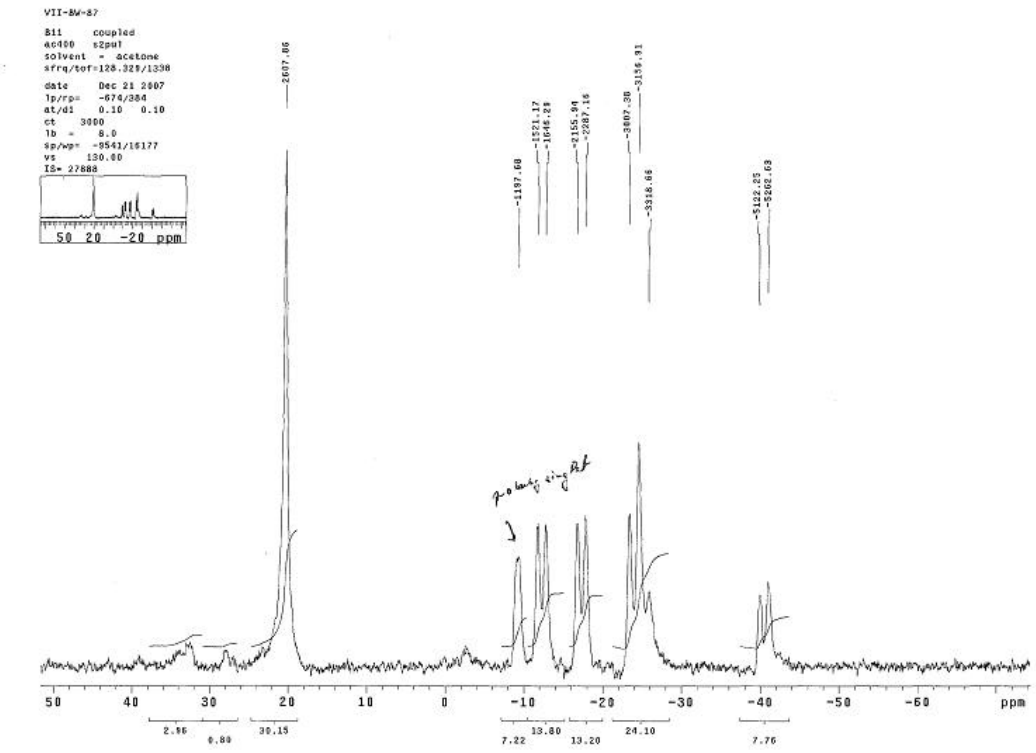
MS (FAB, Gly, -Ve) spectrum of 2'-*O*-{{5-[3-iron bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}methyluridine (19), m/z (%): molecular formula: $C_{20}H_{43}B_{18}FeN_5O_8$, calculated average mass: 732.03, found 732.6 (100) $[M]^-$



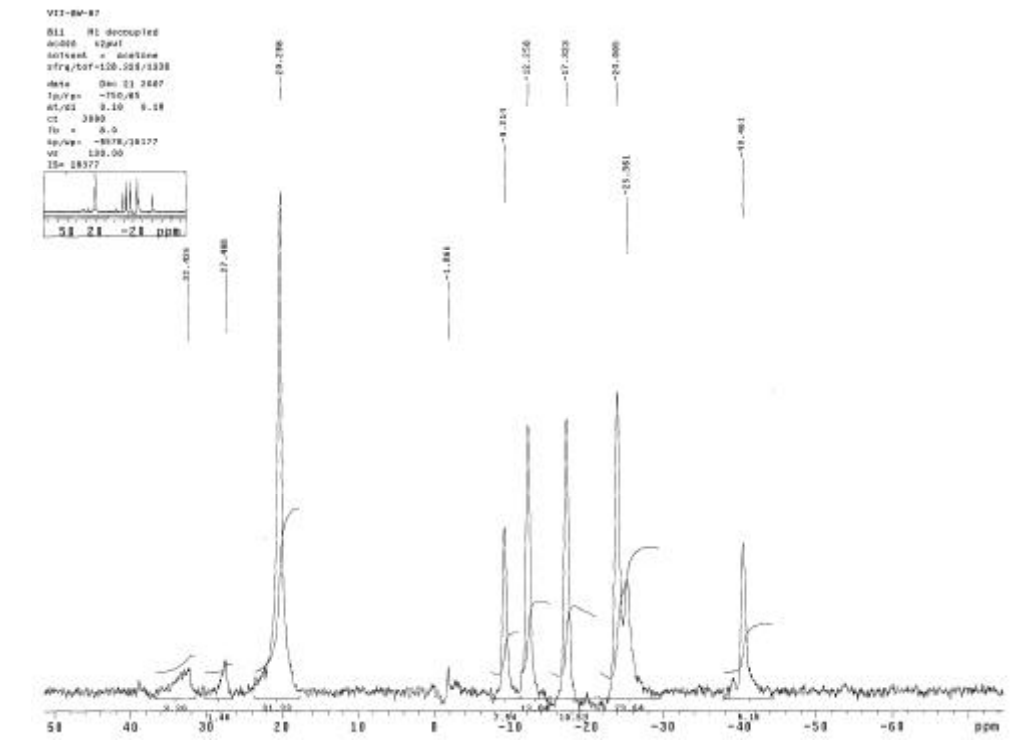
UV/Vis (96% EtOH) spectrum of 3-*N*-{[5-(7,8-dikarba-*nido*-undekaborane-10-yl)-3-oxa-pentoxy]-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (20).



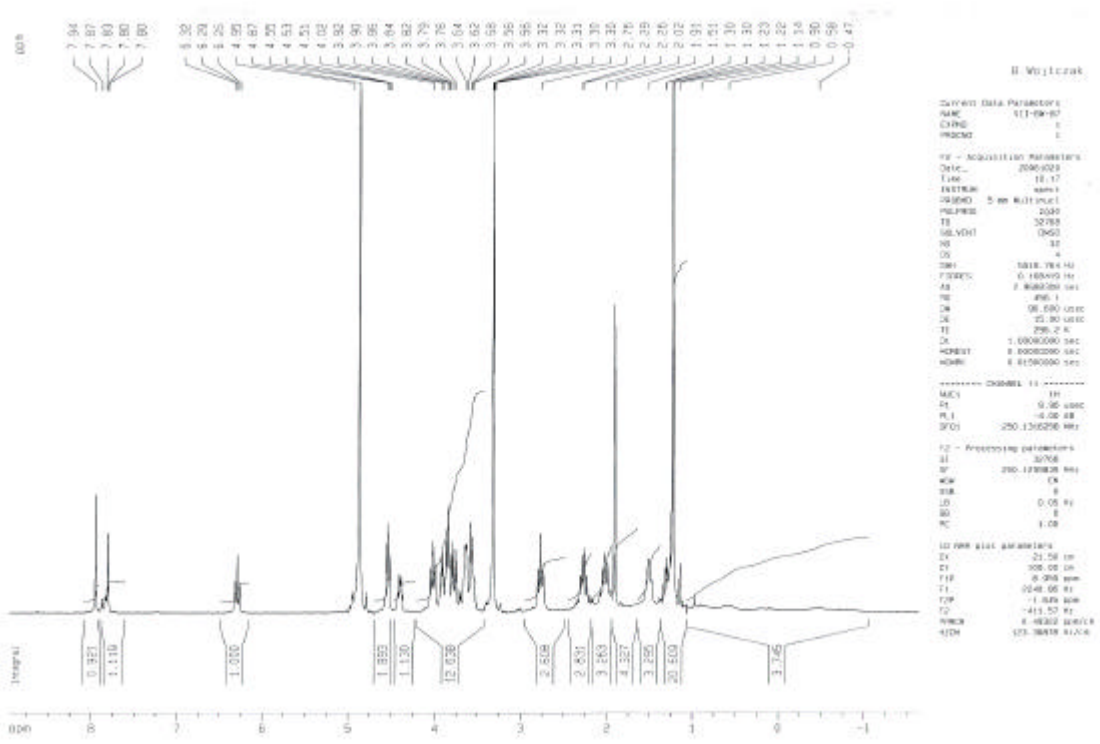
FT-IR (KBr) spectrum of 3-*N*-{[5-(7,8-dikarba-*nido*-undekaborane-10-yl)-3-oxa-pentoxy]-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (20).



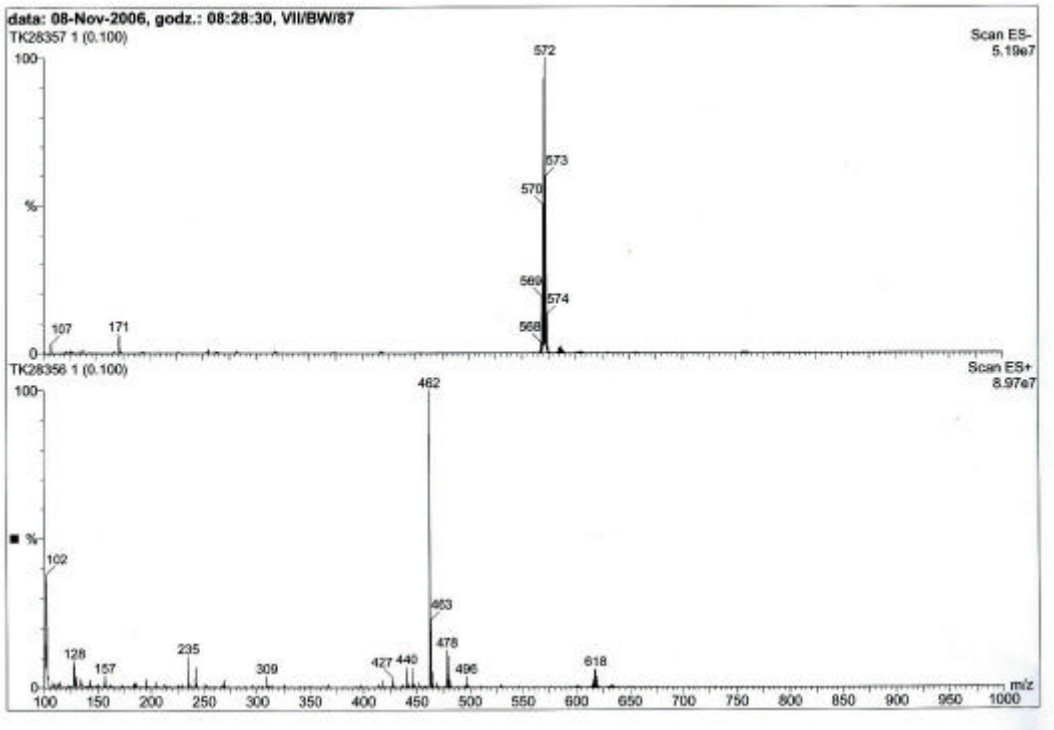
^{11}B NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of 3-*N*-{[5-(7,8-dikarba-*nido*-undekaborane-10-yl)-3-oxa-pentoxy]-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (20).



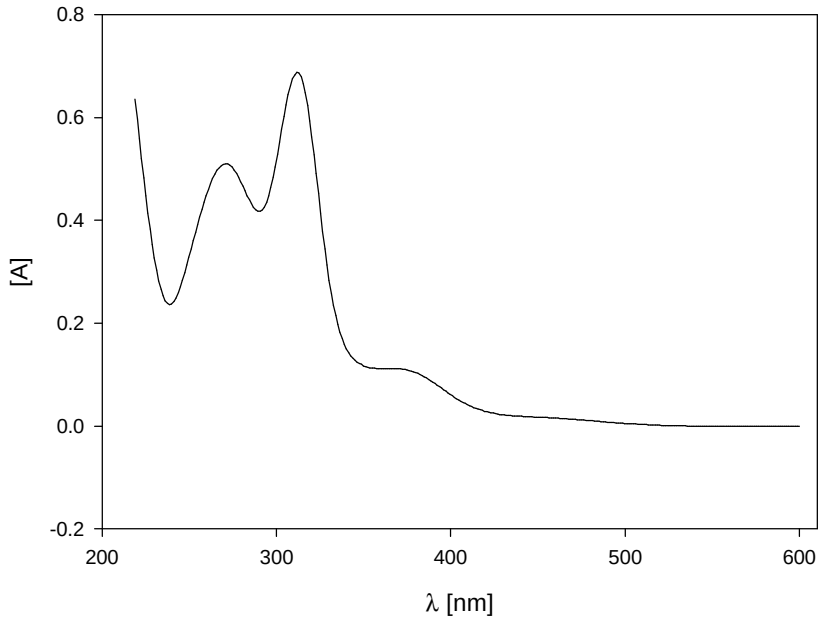
^{11}B {^{1}H BB} NMR (acetone-d*6?*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of 3-*N*-{[5-(7,8-dikarba-*nido*-undekaborane-10-yl)-3-oxa-pentoxy]-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (20).



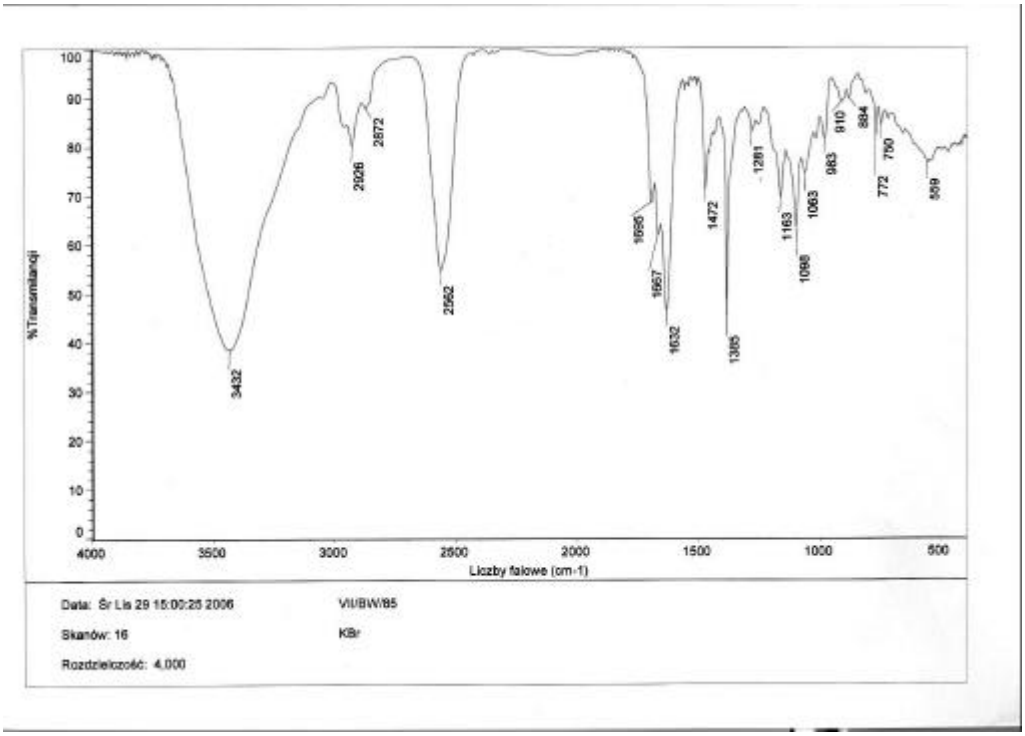
^{1}H NMR (CD_3OH, 250.131MHz, 25°C, TMS) spectrum of 3-*N*-{[5-(7,8-dikarba-*nido*-undekaborane-10-yl)-3-oxa-pentoxy]-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (20).



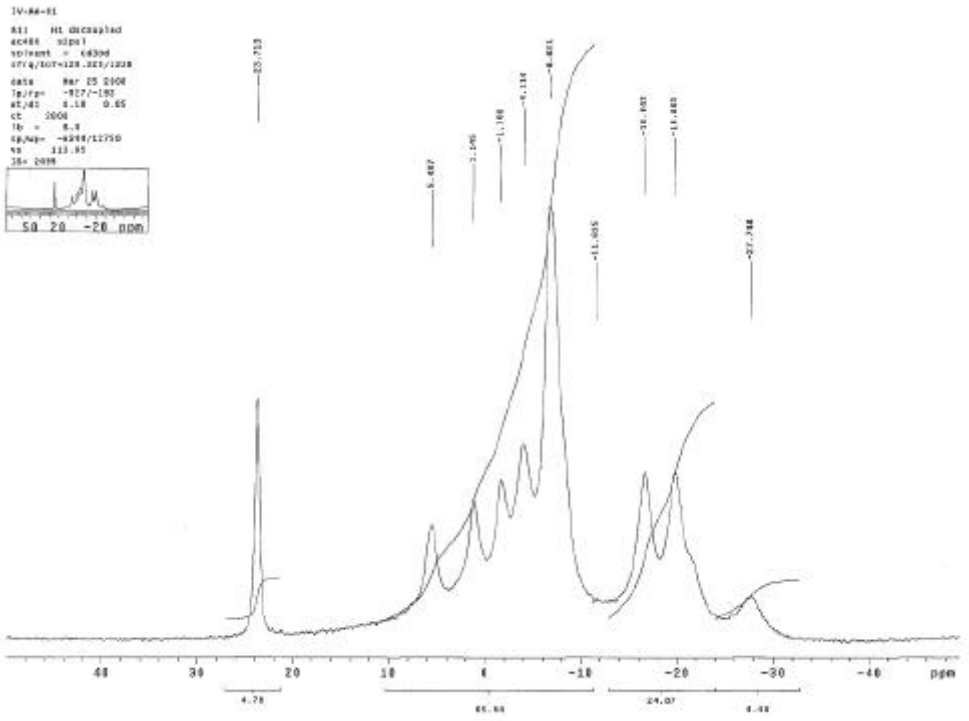
MS-ESI spectrum of 3-*N*-{[5-(7,8-dikarba-*nido*-undekaborane-10-yl)-3-oxa-pentoxy]-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (20), m/z (%): molecular formula: $C_{21}H_{38}B_9N_5O_7$**, calculated average mass**: **569.85, found 572.0 (100) [M+2H]$^-$**



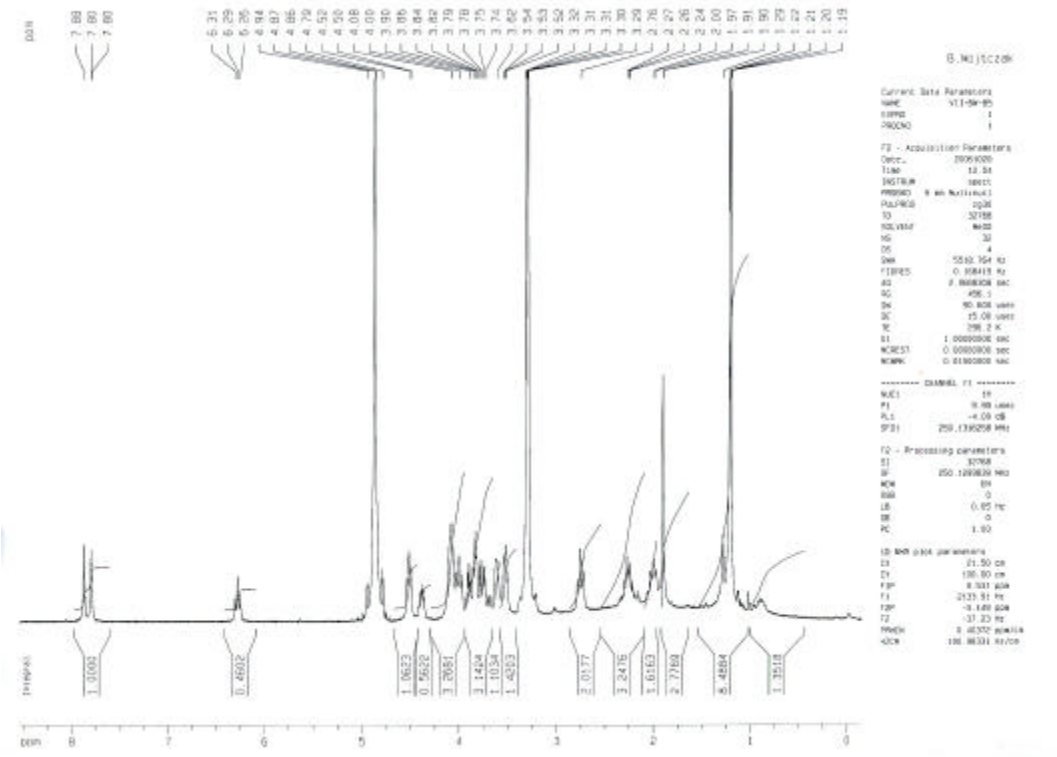
UV/Vis (96% EtOH) spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (21).



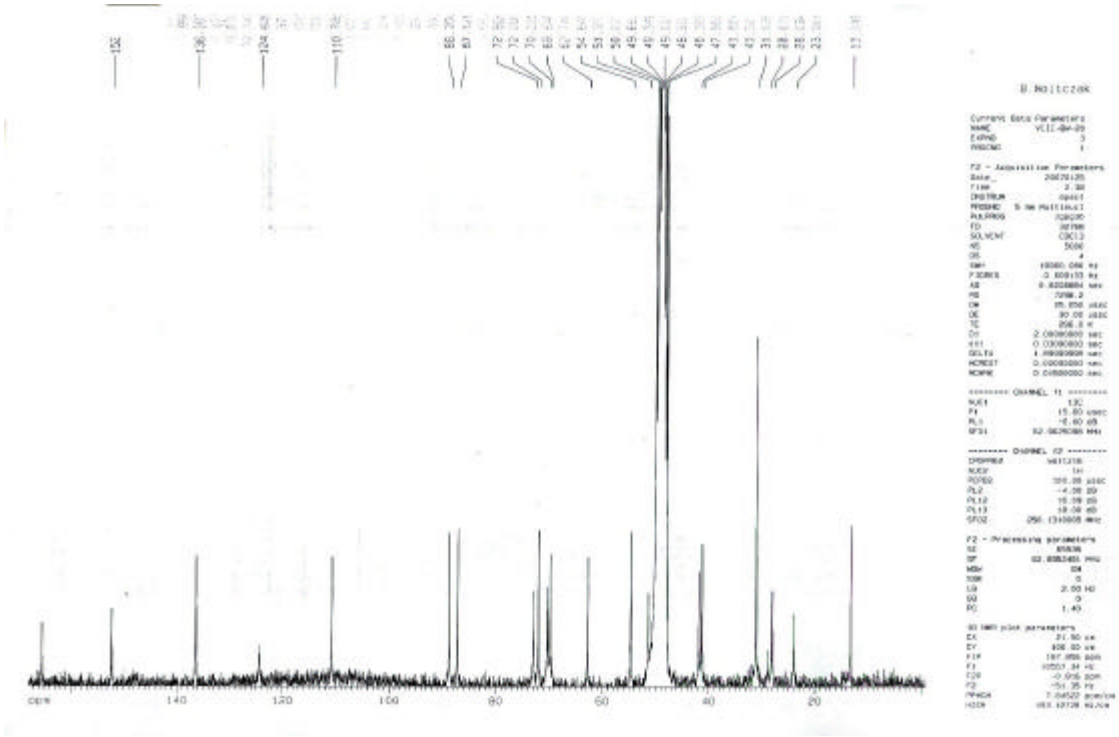
FT-IR (KBr) spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (21).



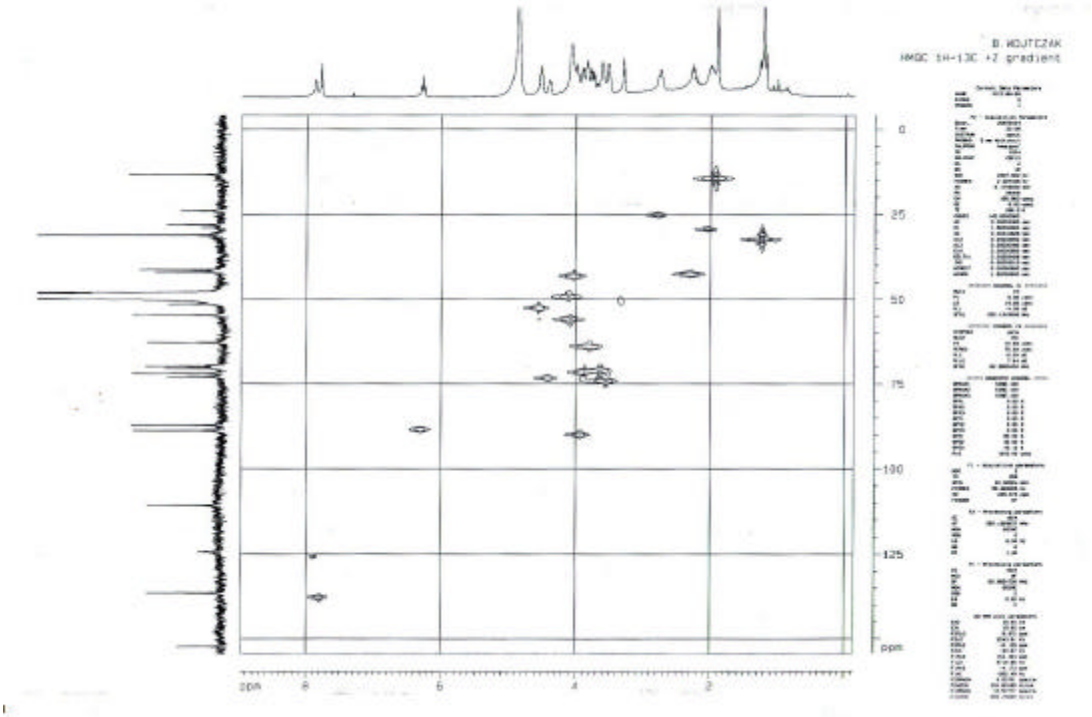
^{11}B {^{1}H BB} NMR (acetone-d*6?*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (21).



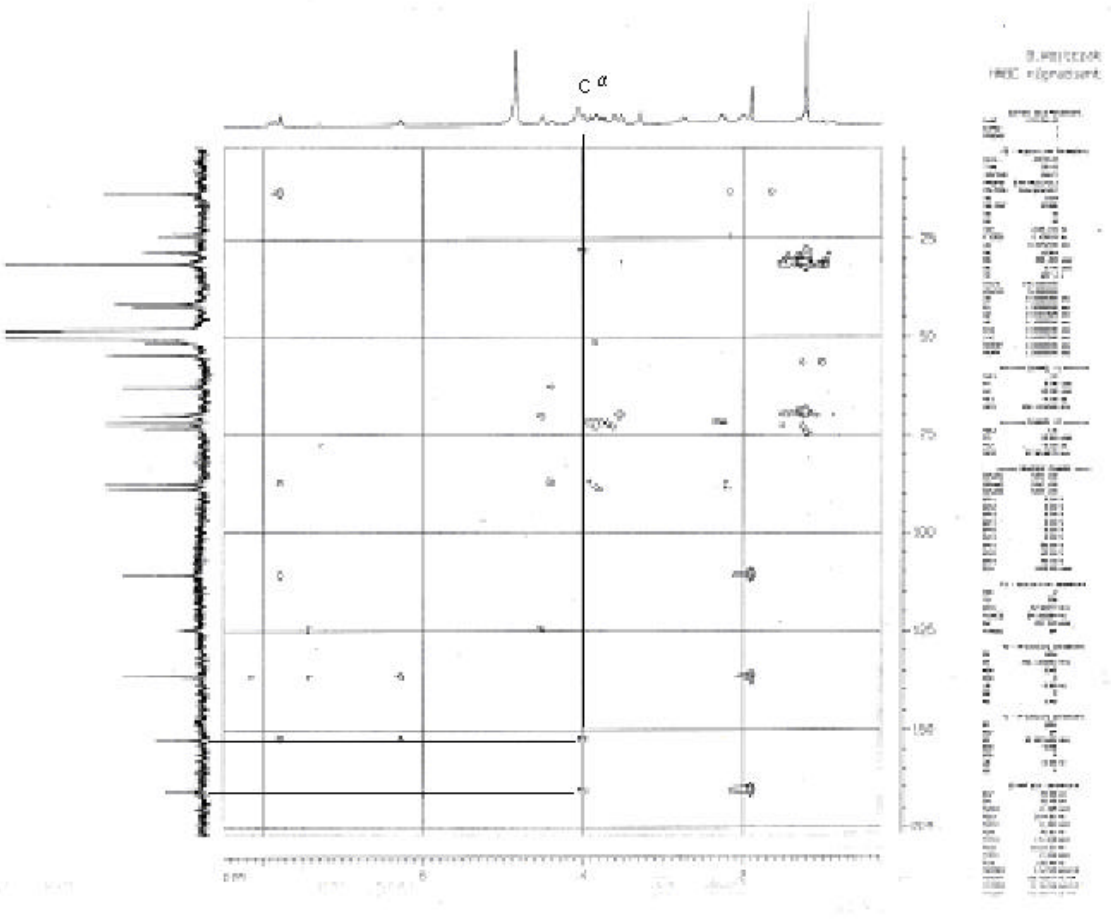
^{1}H NMR (CD_3OH, 250.131MHz, 25°C, TMS) spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (21).



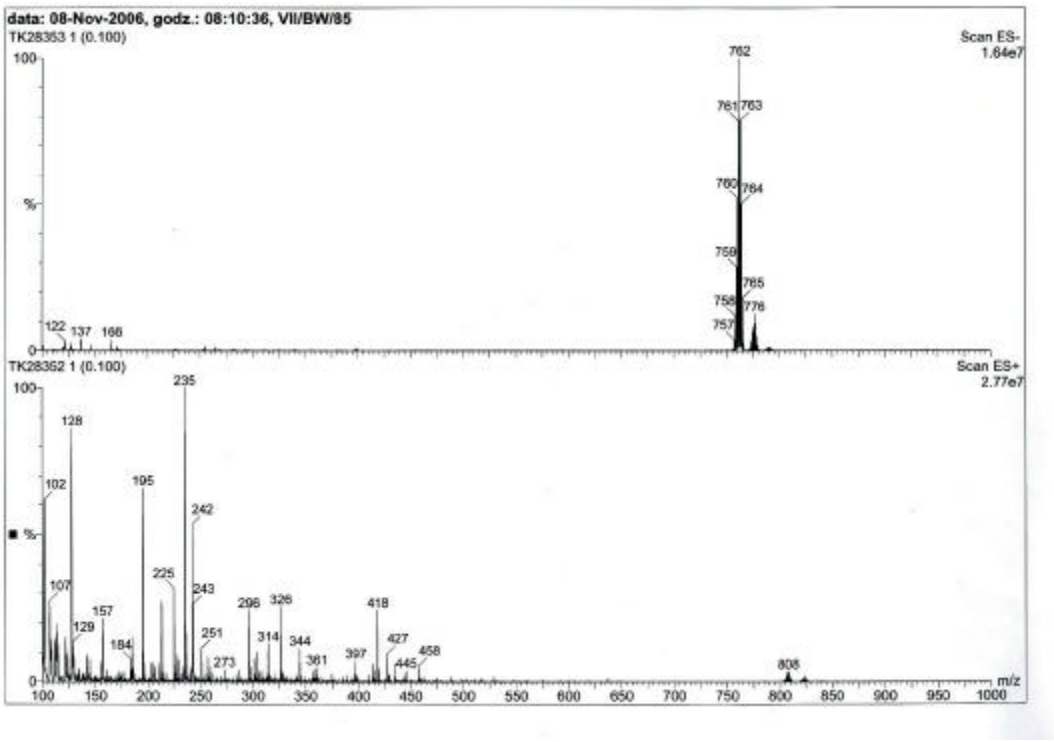
^{13}C NMR (62.90 MHz, CD_3OH, 25°C, TMS) spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (21).



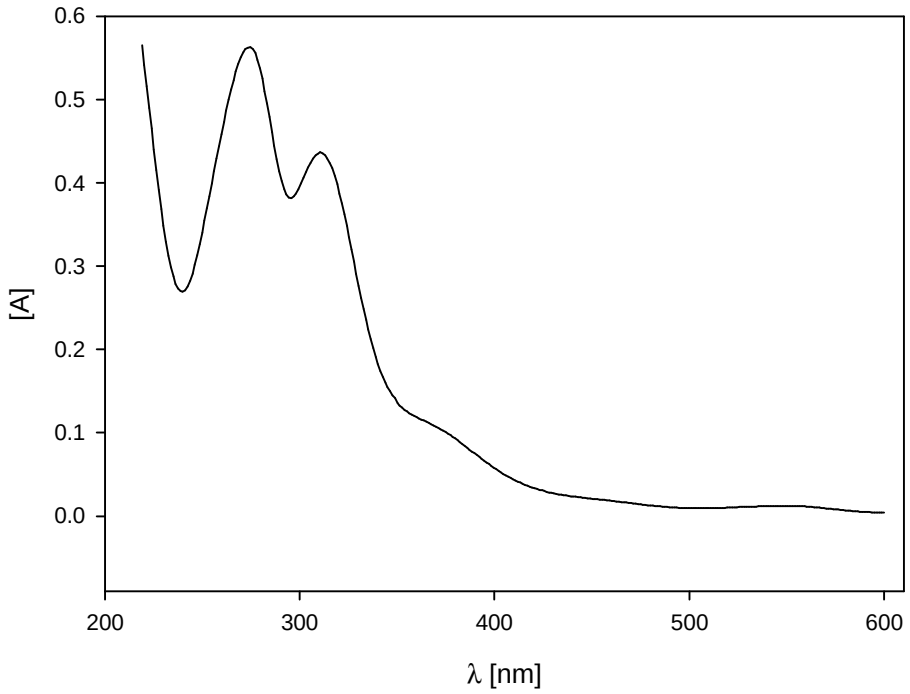
250 MHz ^{1}H-^{13}C correlation (CD_3OH) spectrum (HMQC) of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (21).



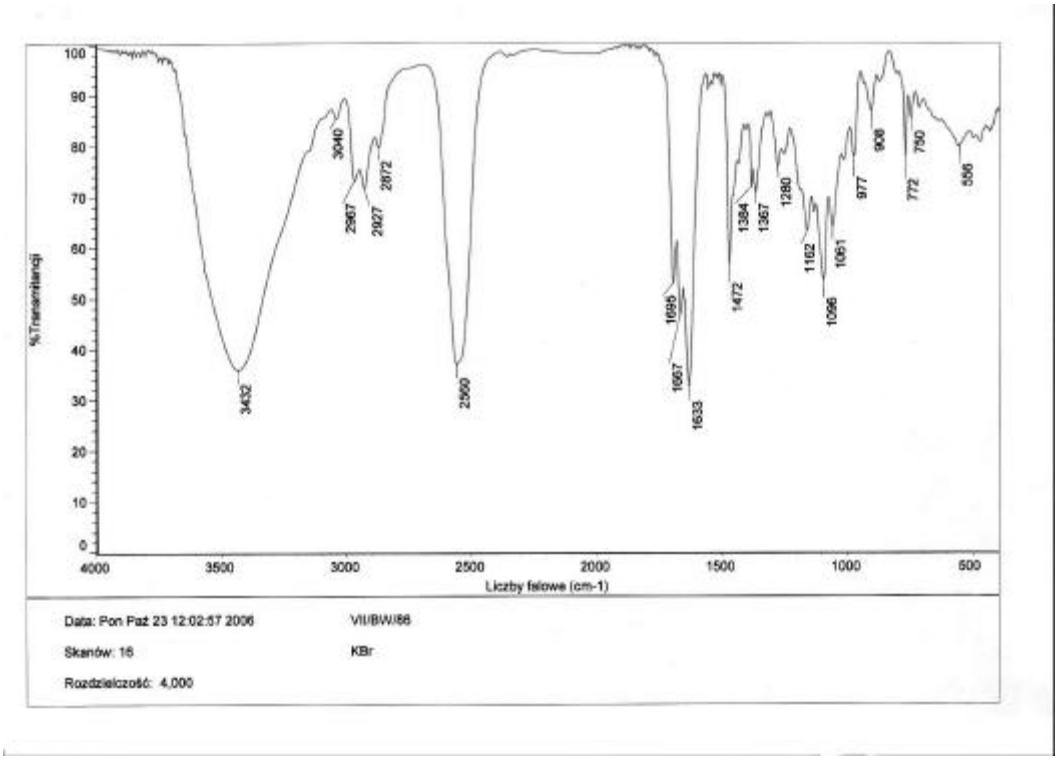
250 MHz ^{1}H-^{13}C Heteronuclear Multiple Bond Correlation (HMBC) (CD_3OH) experiments for analysis of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (21). Observable on the HMBC spectrum two connectivities, C-2/a-H and C-4/ a -H, allow assignment of the alkylation site in thymine nucleobase to 3N.



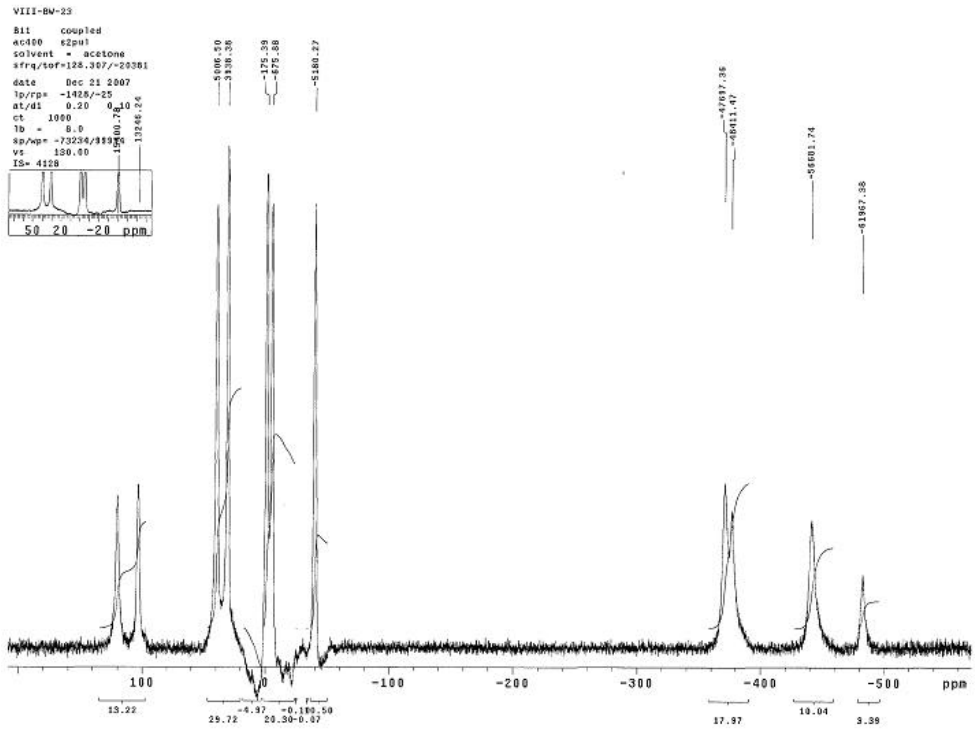
MS-ESI spectrum of of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (21), m/z (%): molecular formula: $C_{23}H_{49}B_{18}CoN_5O_7$, calculated average mass: 761.20, found 762.0 (100) $[M+1H]^-$



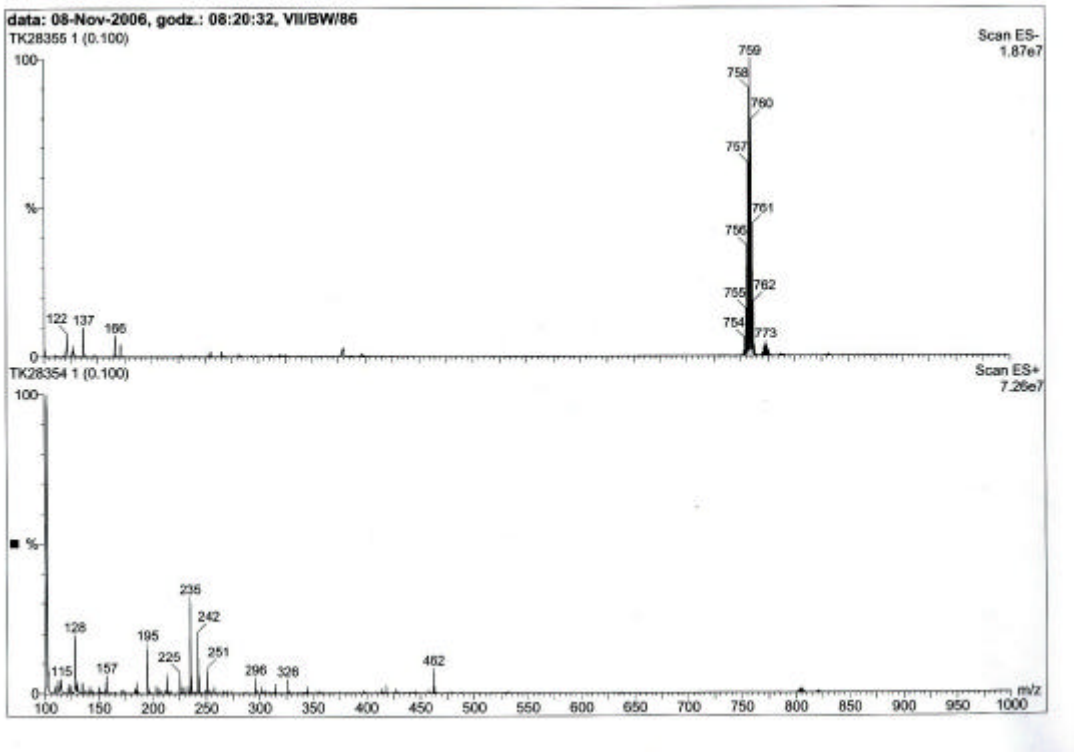
UV/Vis (96% EtOH) spectrum of 3-*N*-{{5-[3-iron bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (22).



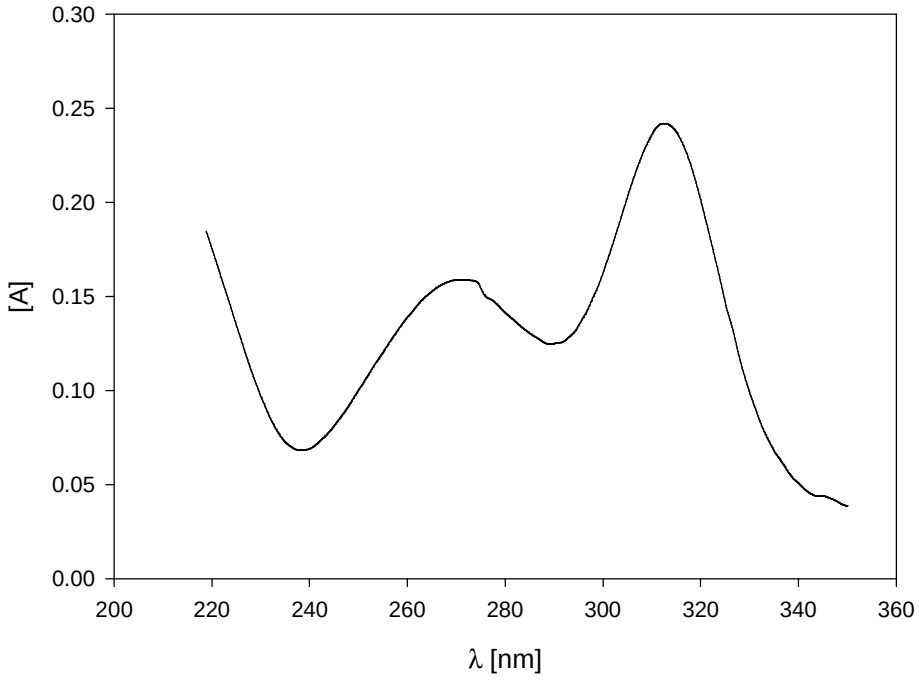
FT-IR (KBr) spectrum of 3-*N*-{{5-[3-iron bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (22).



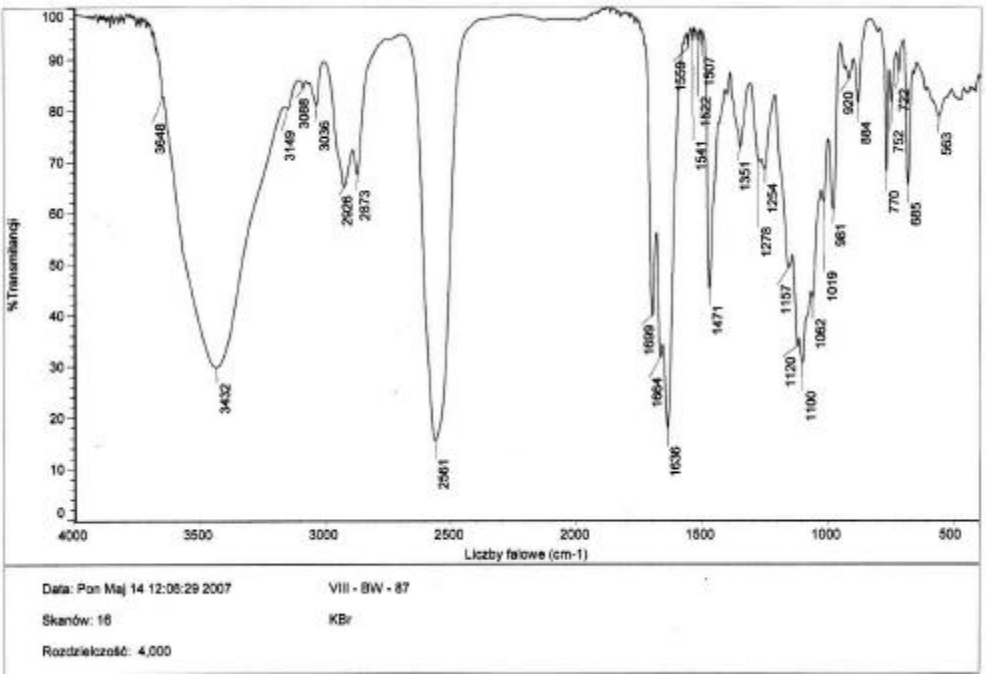
^{11}B NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of 3-*N*-{{5-[3-iron bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (22).



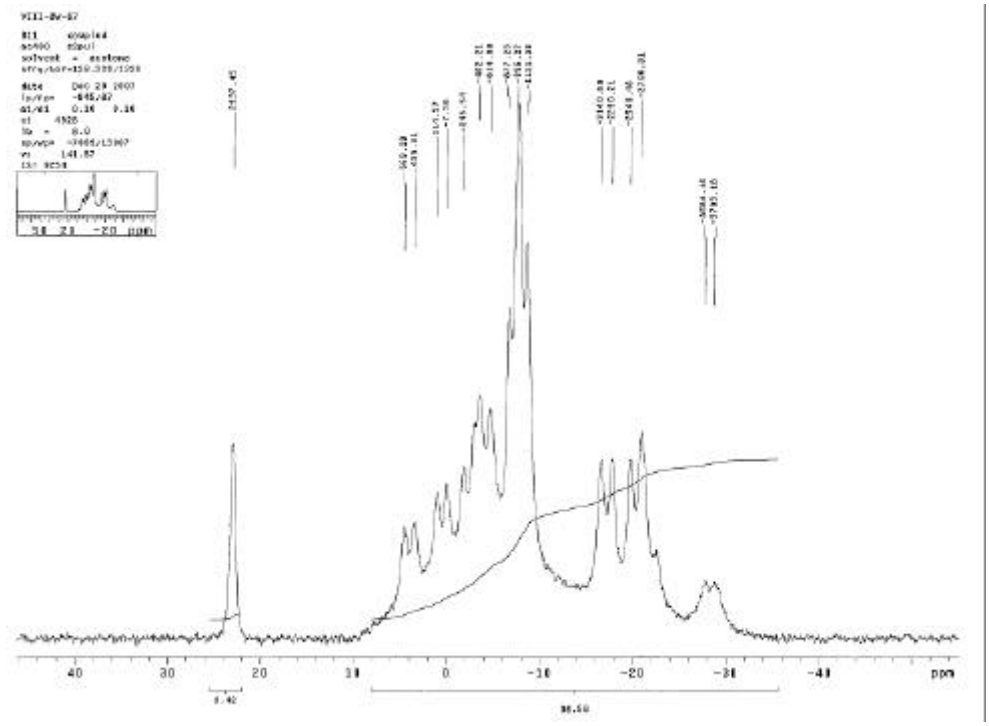
MS-ESI spectrum of 3-*N*-{{5-[3-iron bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (22). m/z (%): molecular formula: $C_{23}H_{49}B_{18}FeN_5O_7$, calculated average mass: 758.11, found 759.0 (100) $[M+1H]^-$



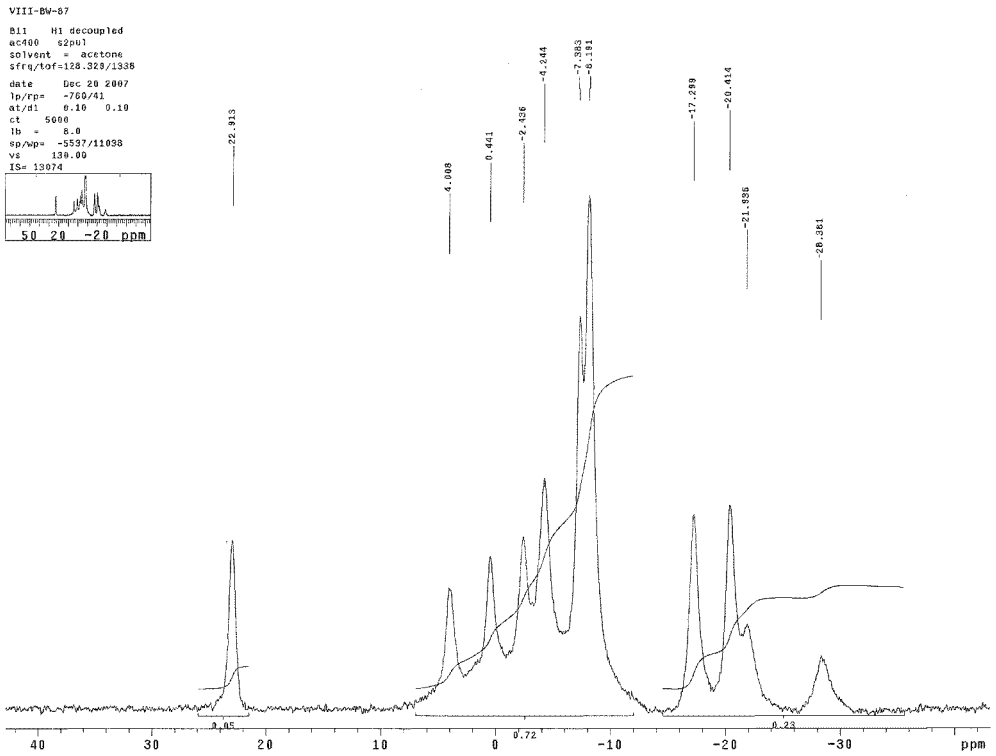
UV/Vis (96% EtOH) spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}methyl-(4-1,2,3-triazole-1*N*-yl}} (1-ethoxyethan-4-yl)thymidine (23).



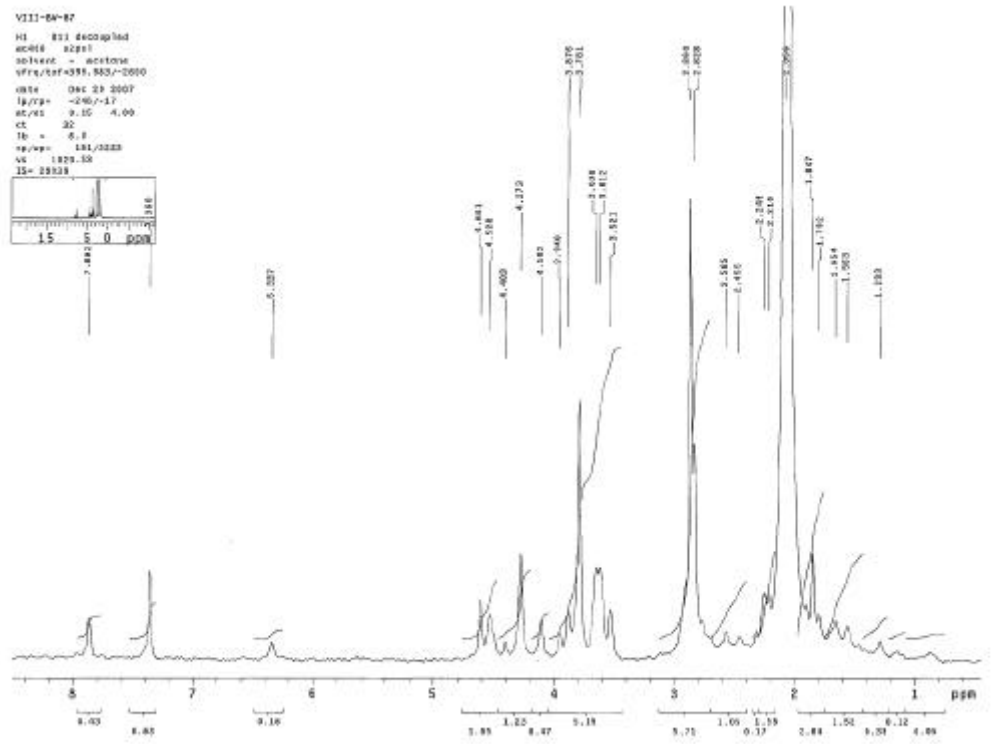
FT-IR (KBr) spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}methyl-(4-1,2,3-triazole-1*N*-yl)} (1-ethoxyethan-4-yl)thymidine (23).



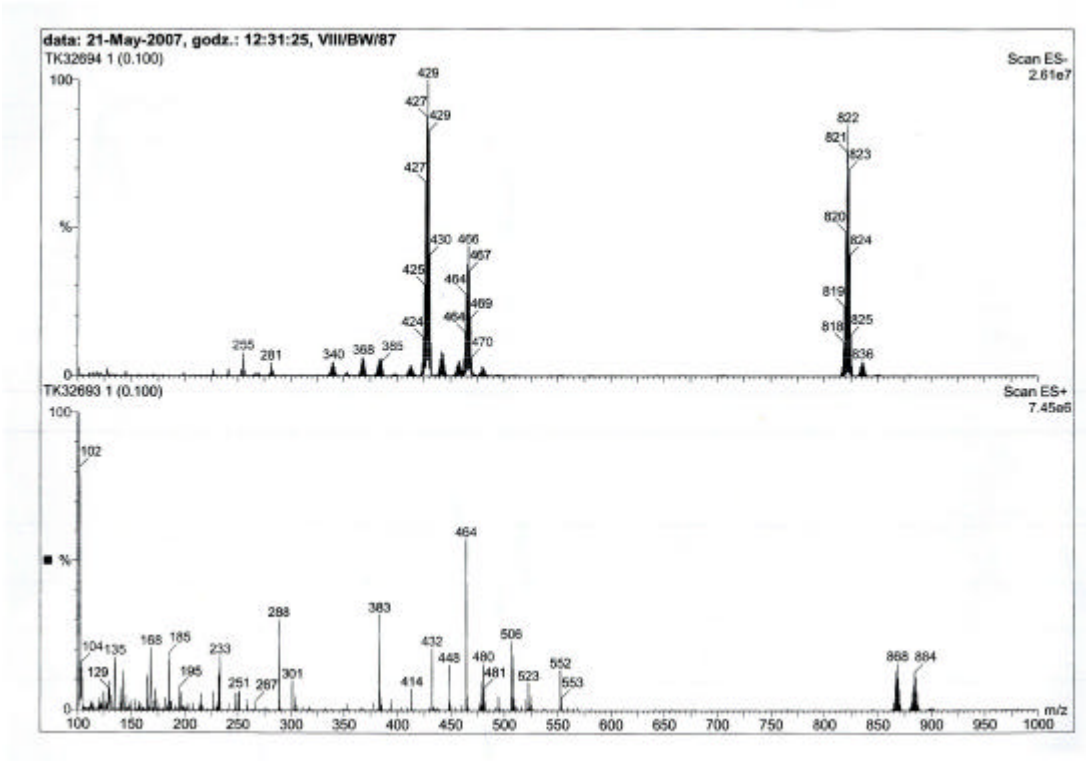
^{11}B NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}methyl-(4-1,2,3-triazole-1*N*-yl)} (1-ethoxyethan-4-yl)thymidine (23).



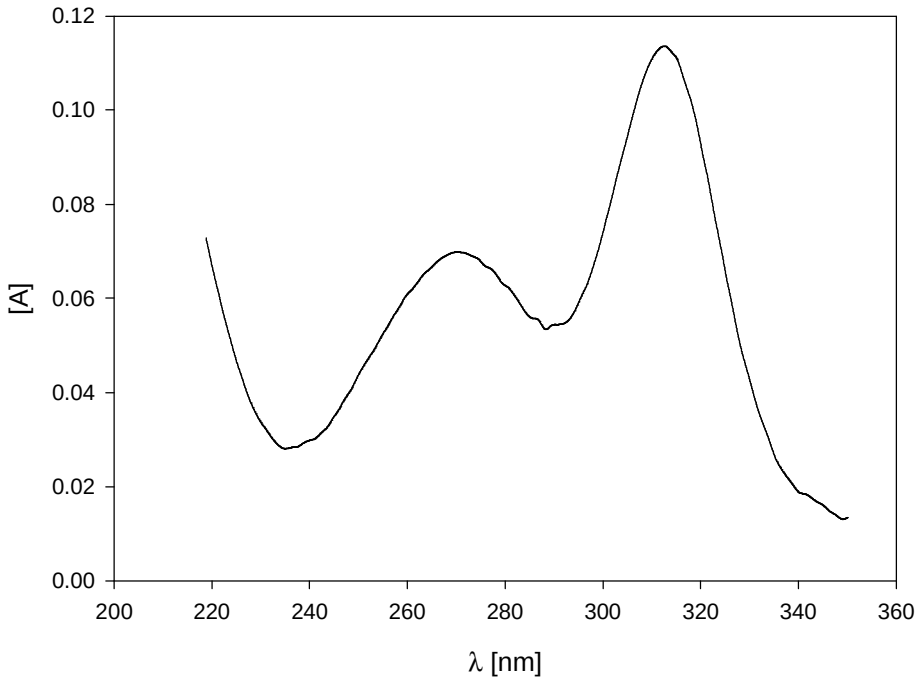
^{11}B {^{1}H BB} NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}methyl-(4-1,2,3-triazole-1*N*-yl}} (1-ethoxyethan-4-yl)thymidine (23).



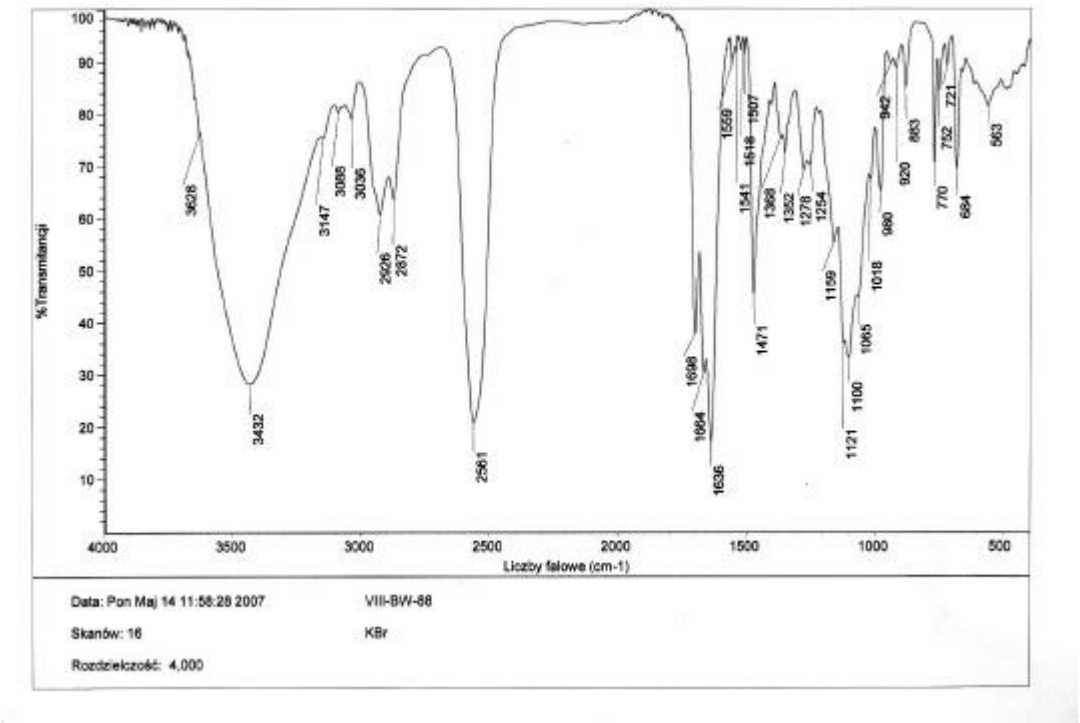
^{1}H NMR {^{11}B BB} (CD_3OH, 250.131MHz, 25°C, TMS) spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}methyl-(4-1,2,3-triazole-1*N*-yl}} (1-ethoxyethan-4-yl)thymidine (23).



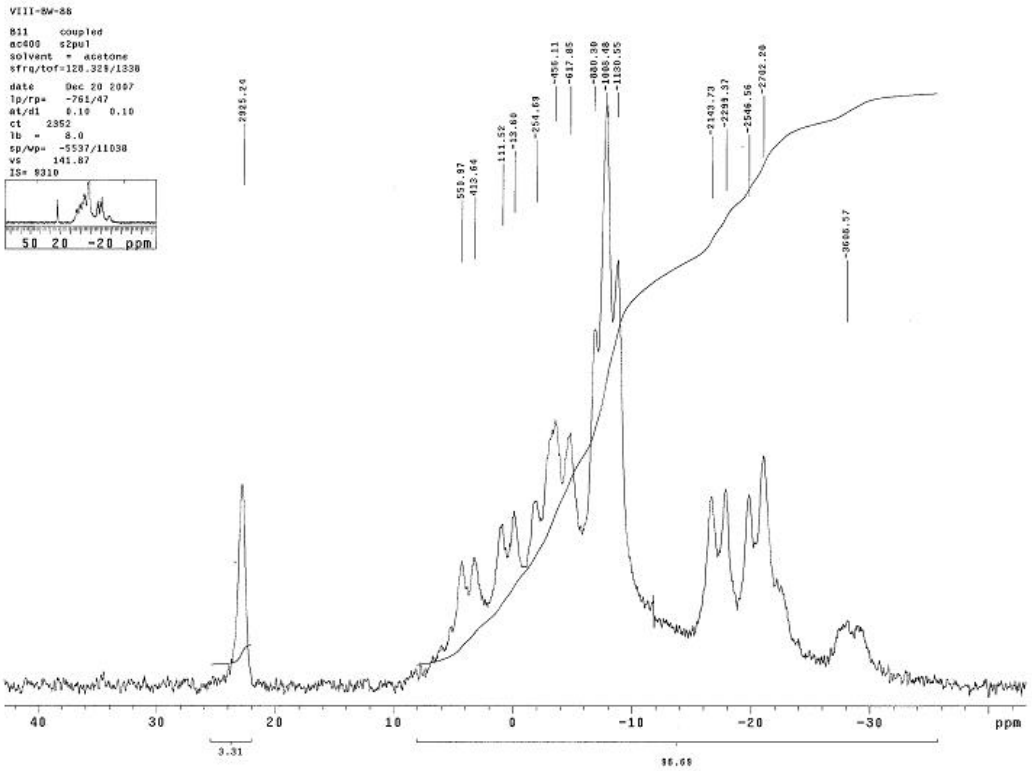
MS-ESI spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}methyl-(4-1,2,3-triazole-1*N*-yl)} (1-ethoxyethan-4-yl)thymidine (23), m/z (%): molecular formula: $C_{25}H_{53}B_{18}CoN_5O_9$, calculated average mass: 821.25, found 822.0 (90) $[M+1H]^-$



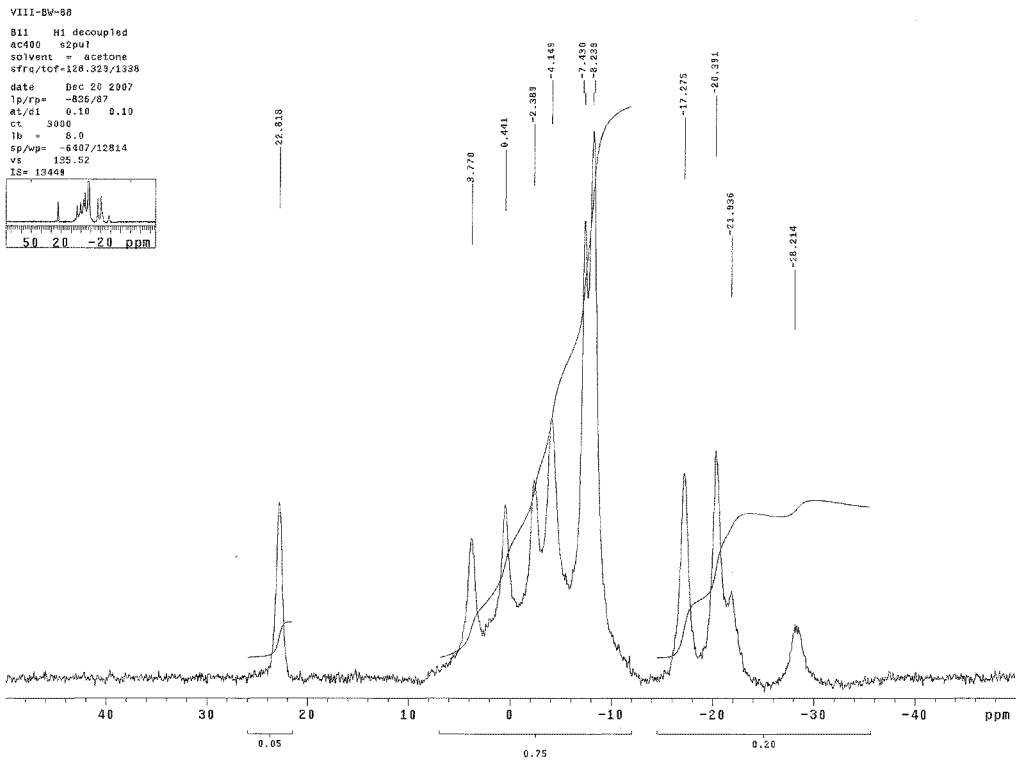
UV/Vis (96% EtOH) spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}propyl-(4-1,2,3-triazole-1*N*-yl)} (1-ethoxyethan-4-yl)thymidine (24).



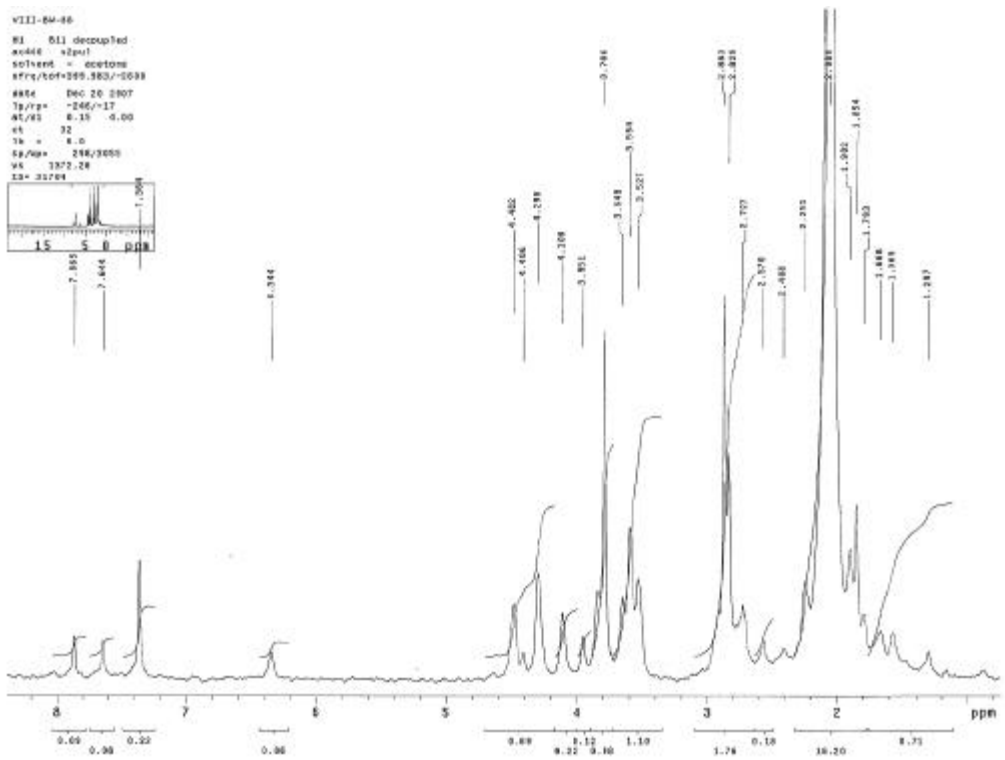
FT-IR (KBr) spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}propyl-(4-1,2,3-triazole-1*N*-yl}} (1-ethoxyethan-4-yl)thymidine (24).



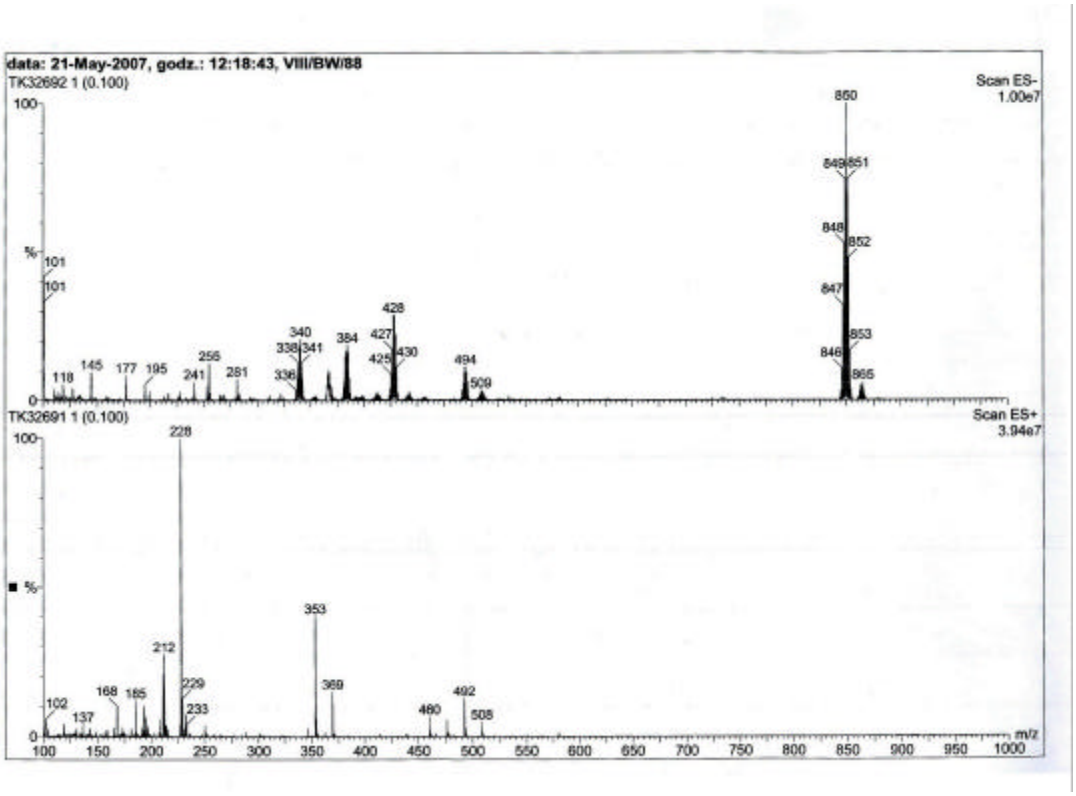
^{11}B NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}propyl-(4-1,2,3-triazole-1*N*-yl}} (1-ethoxyethan-4-yl)thymidine (24).



^{11}B {^{1}H BB} NMR (acetone-d*6*, 25°C, 80.253MHz, $BF_3{\cdot}Et_2O$) spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}propyl-(4-1,2,3-triazole-1*N*-yl}} (1-ethoxyethan-4-yl)thymidine (24).

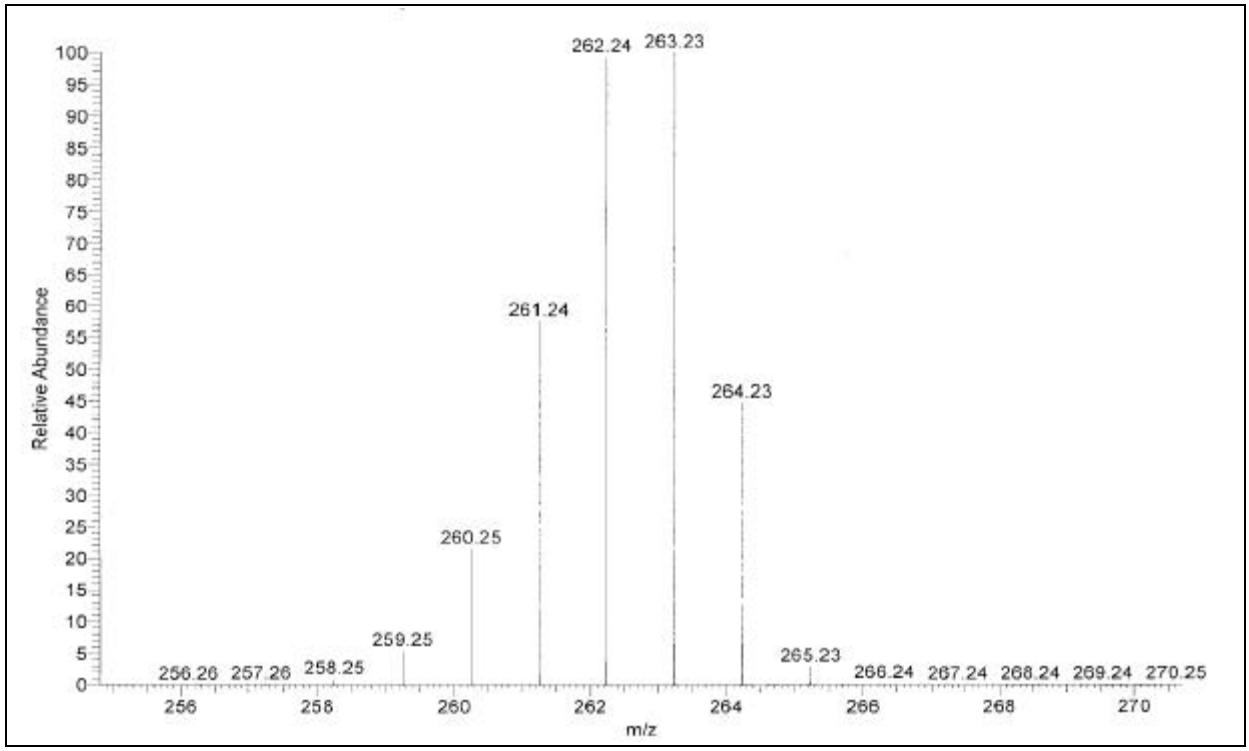


^{1}H NMR {^{11}B BB} (CD_3OH, 250.131MHz, 25°C, TMS) spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}propyl-(4-1,2,3-triazole-1*N*-yl}} (1-ethoxyethan-4-yl)thymidine (24).

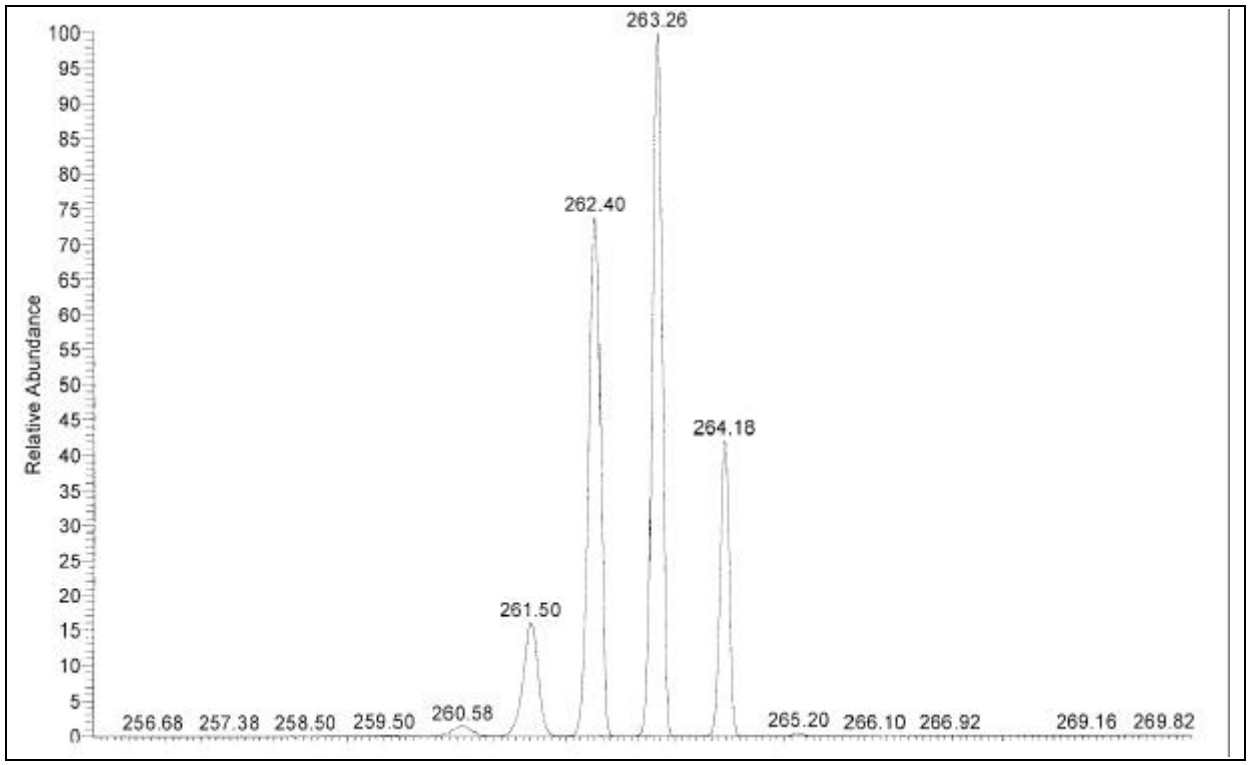


MS-ESI spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}propyl-(4-1,2,3-triazole-1*N*-yl)} (1-ethoxyethan-4-yl)thymidine (24), m/z (%): molecular formula: $C_{27}H_{57}B_{18}CoN_5O_9$, calculated average mass: 849.30, found 850.0 (100) $[M+1H]^-$

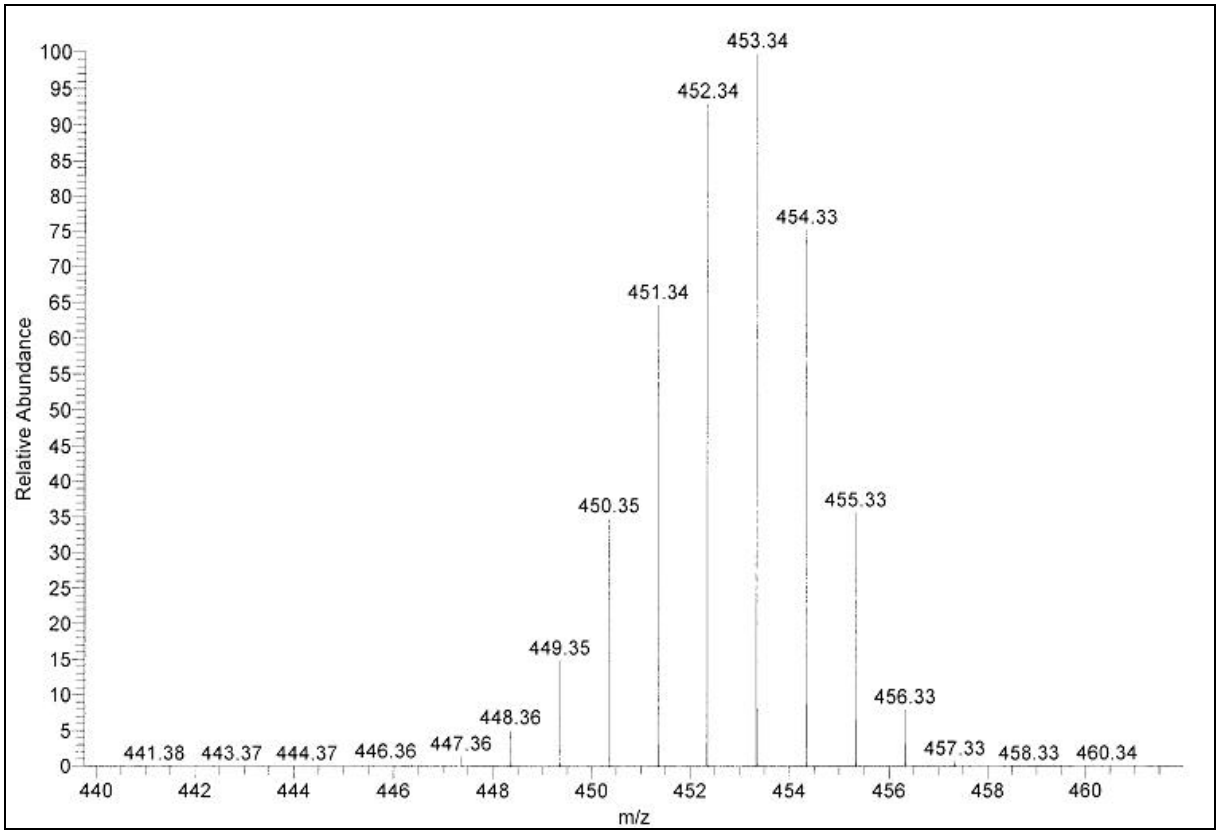
Comparison of high resolution experimental spectra with simulated spectra within the range of molecular ion m/z.



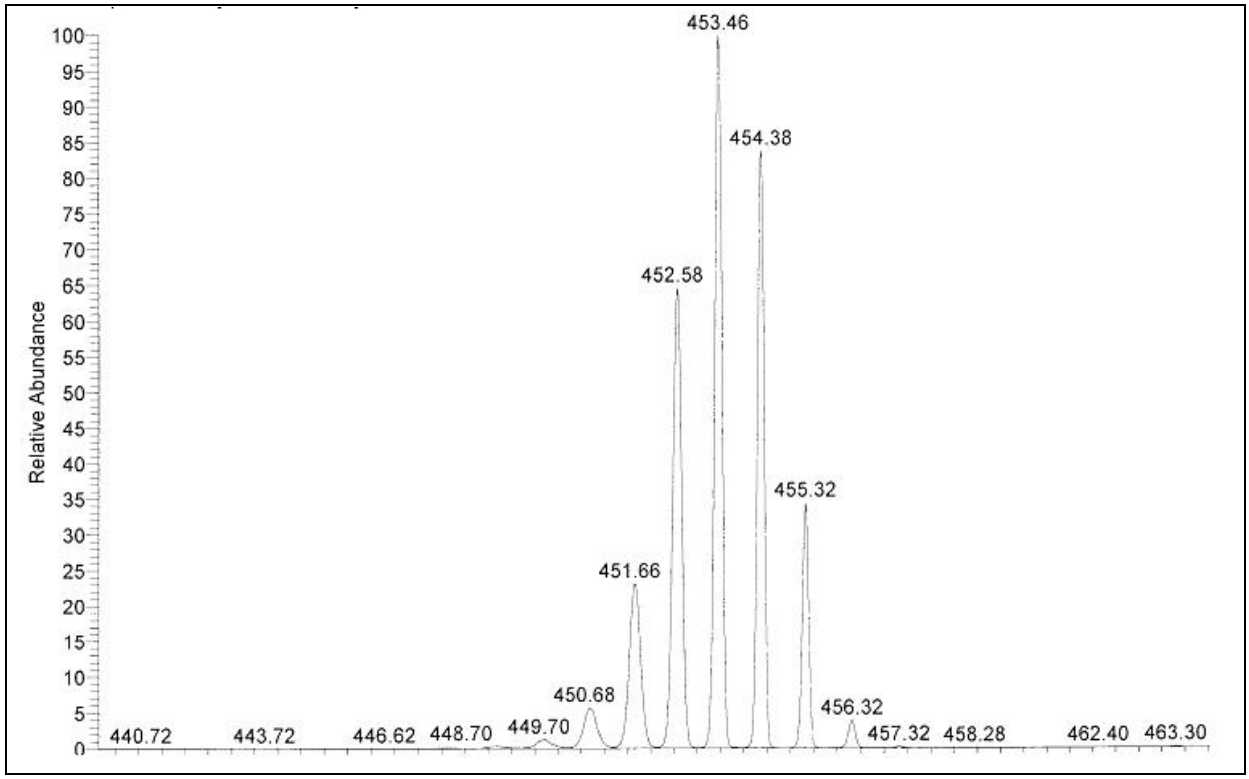
Simulated spectrum of the molecular ion of 10-(5-azido-3-oxa-pentoxy)-7,8-dikarba-*nido*-undekaborane (2), calculated exact mass for $C_6H_{19}B_9N_3O_2$: 264.23



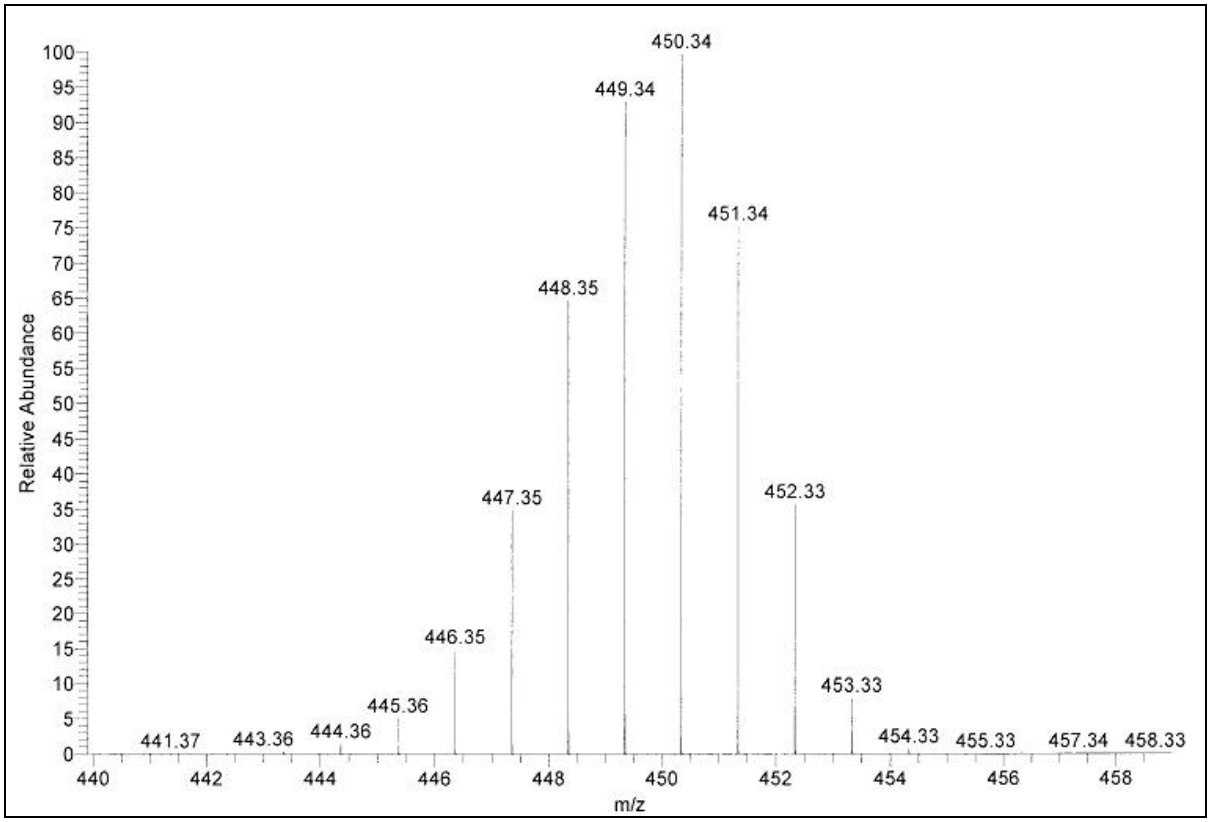
Fragment of the MS ESI spectrum of 10-(5-azido-3-oxa-pentoxy)-7,8-dikarba-*nido*-undekaborane (2) corresponding to molecular ion range, m/z (%): 263.26 (100%), 264.18 (42%), calculated exact mass for $C_6H_{19}B_9N_3O_2$: 264.23



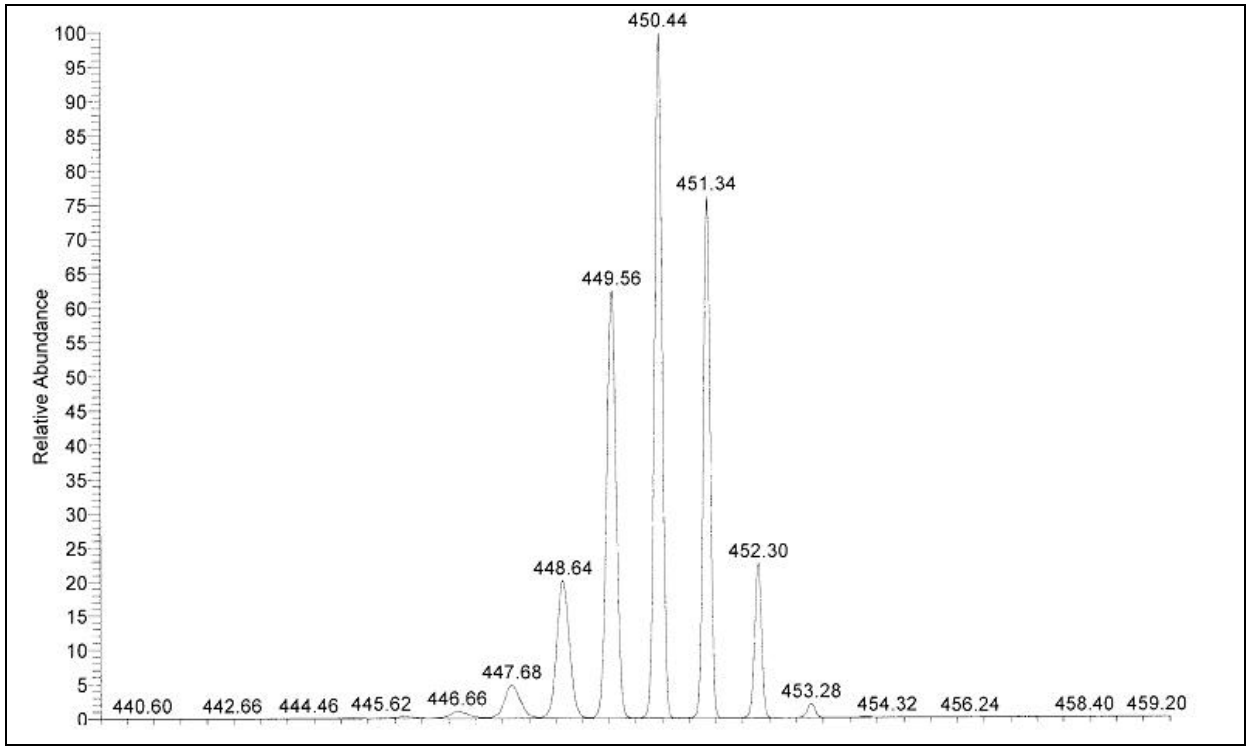
Simulated spectrum of the molecular ion of 8-(5-azido-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) (5), calculated exact mass for $C_8H_{29}B_{18}CoN_3O_2$: 456.33



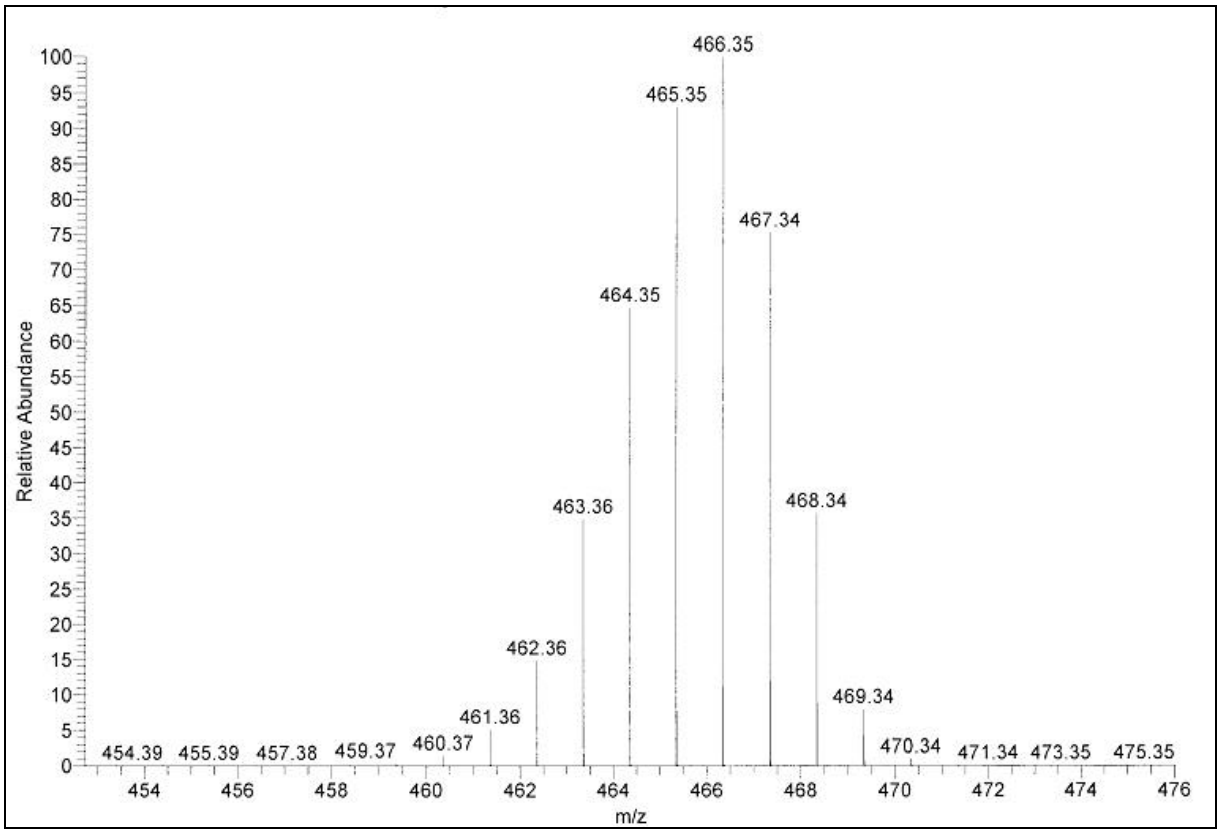
Fragment of the MS ESI spectrum of 8-(5-azido-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) (5) corresponding to molecular ion range, m/z (%): 453.46 (100%), 456.32 (5%), calculated exact mass for $C_8H_{29}B_{18}CoN_3O_2$: 456.33



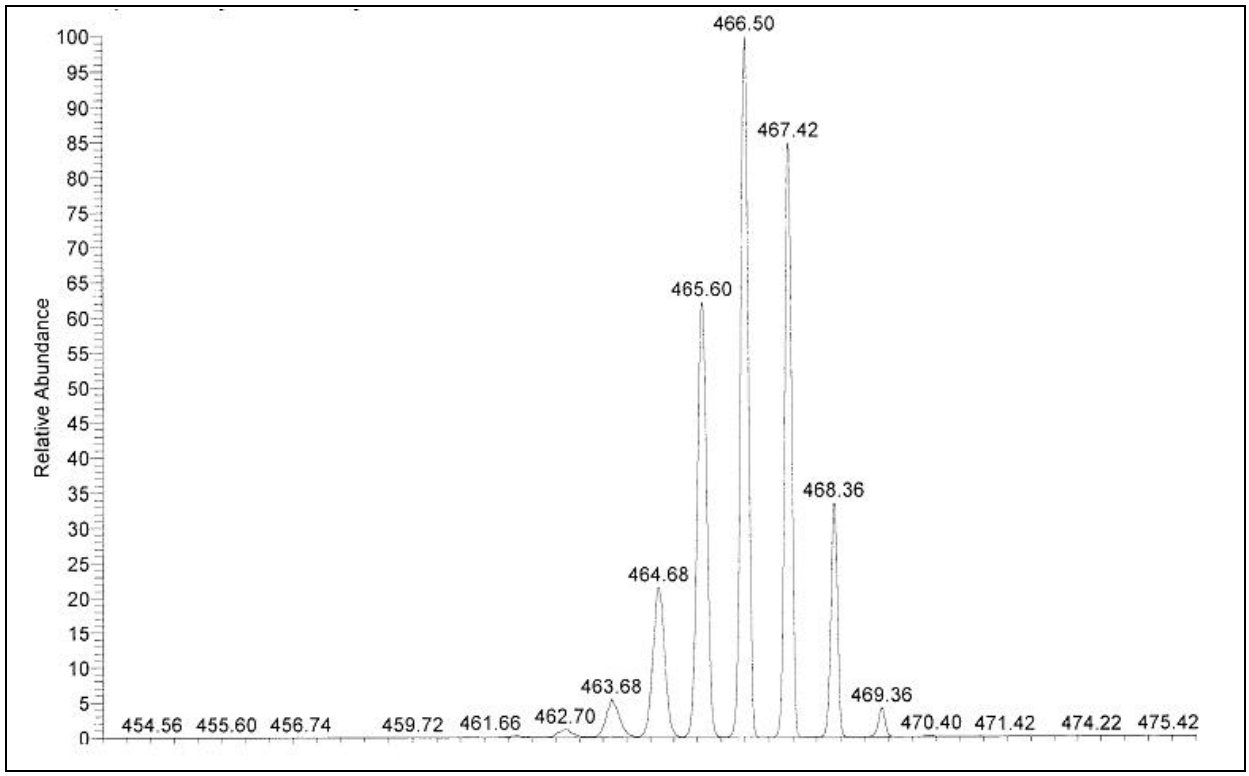
Simulated spectrum of the molecular ion of 8-(5-azido-3-oxa-pentoxy)-3-iron bis(1,2-dicarbollide) (6), calculated exact mass for $C_8H_{29}B_{18}FeN_3O_2$: 453.33



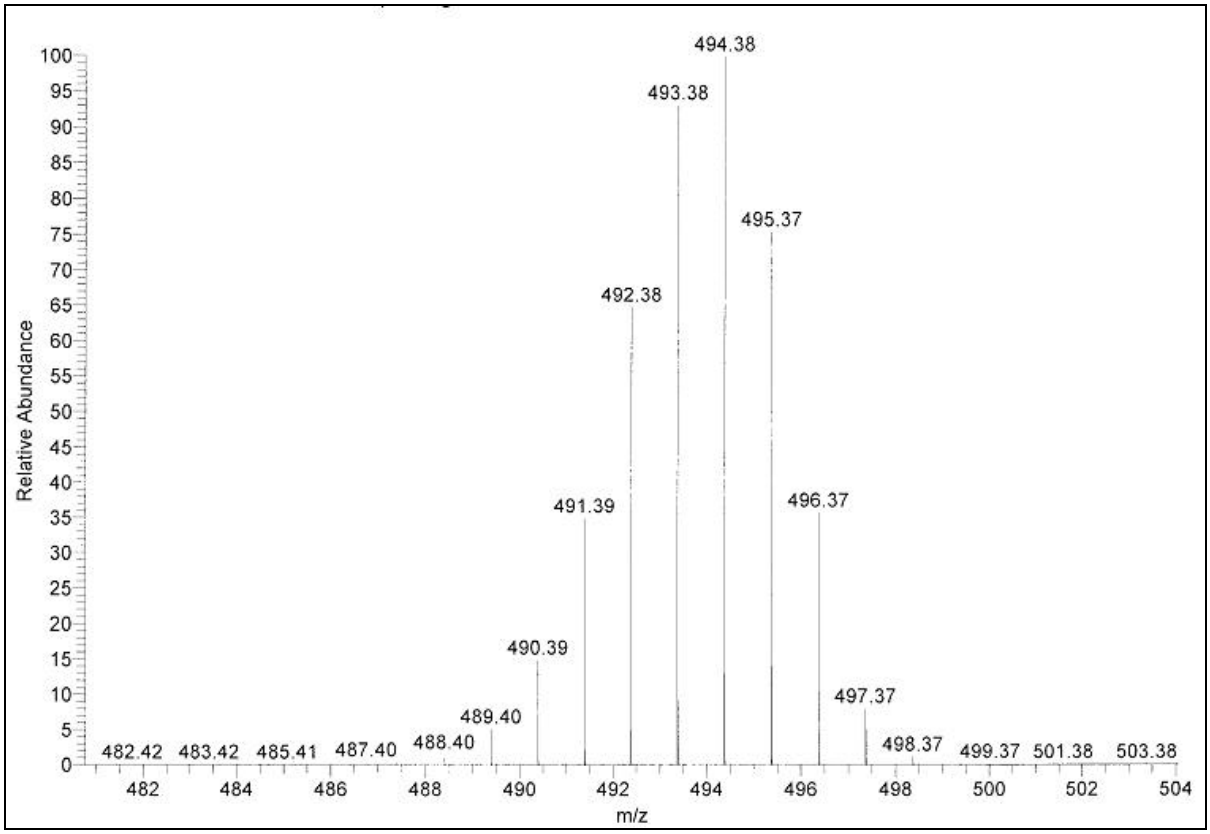
Fragment of the MS ESI spectrum of 8-(5-azido-3-oxa-pentoxy)-3-iron bis(1,2-dicarbollide) (6) corresponding to molecular ion range, m/z (%): 450.44 (100%), 453.28 (2%), calculated exact mass for $C_8H_{29}B_{18}FeN_3O_2$: 453.33



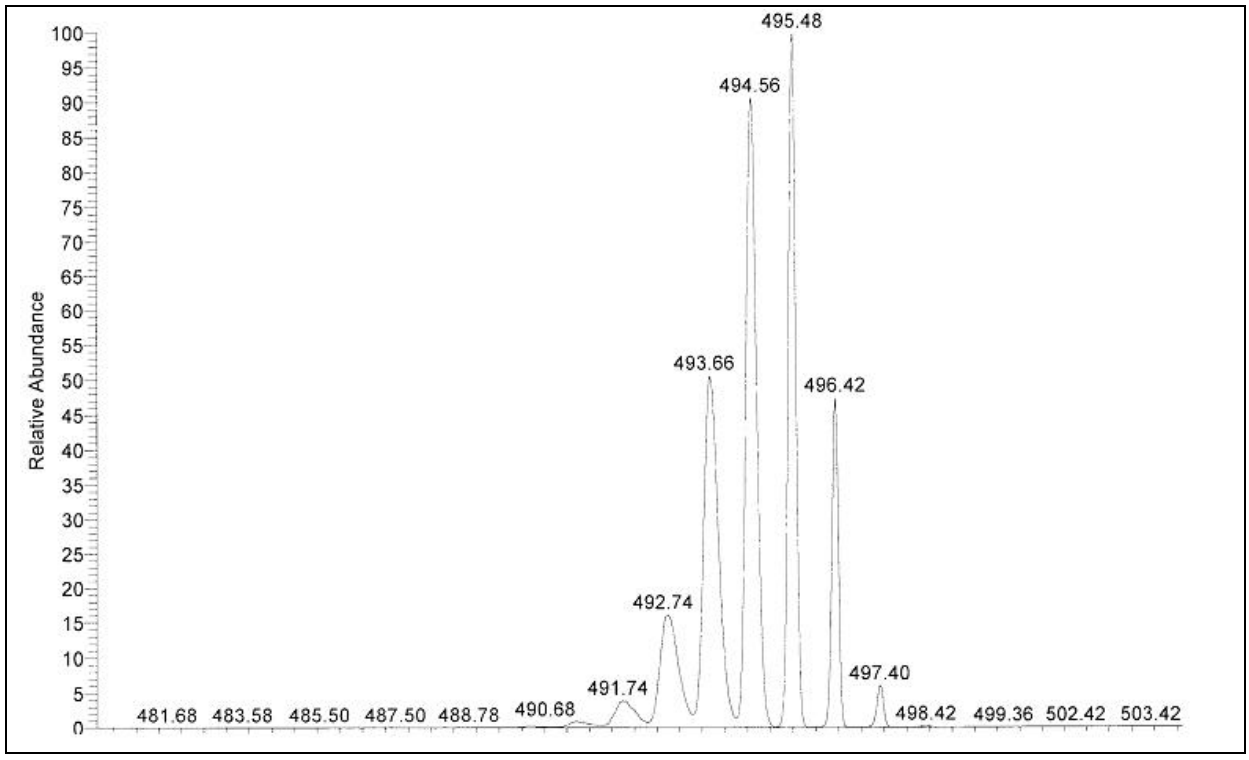
Simulated spectrum of the molecular ion of 10-8-(5-propargyl-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) (7), calculated exact mass for $C_{11}H_{32}B_{18}CoO_3$: 469.34



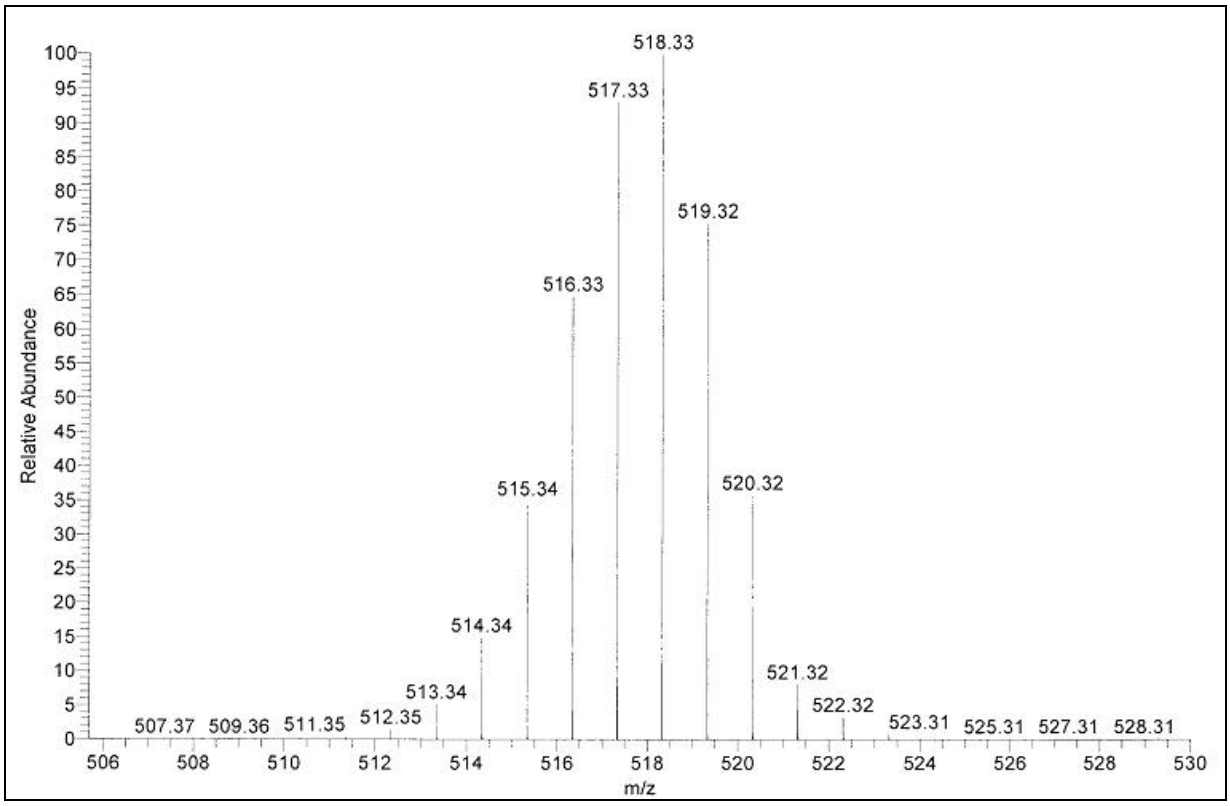
Fragment of the MS ESI spectrum of 10-8-(5-propargyl-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) (7) corresponding to molecular ion range, m/z (%): 466.50 (100%), 469.36 (5%), calculated exact mass for $C_{11}H_{32}B_{18}CoO_3$: 469.34



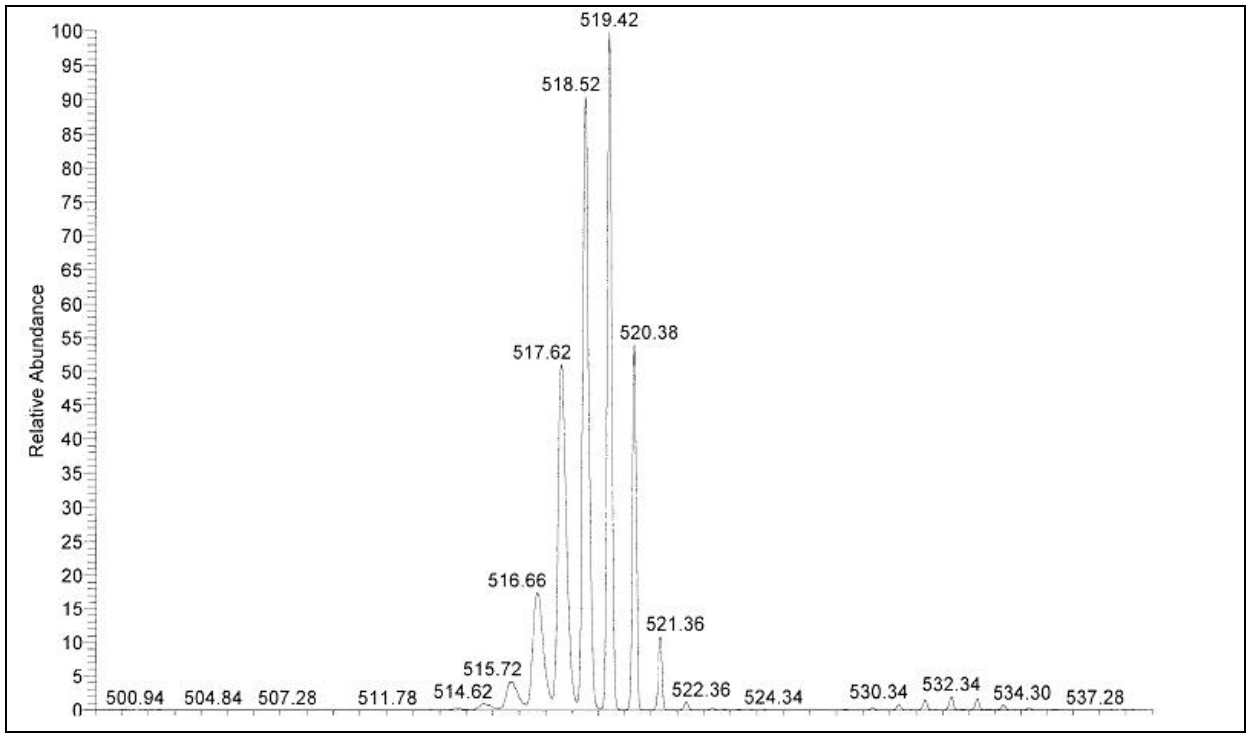
Simulated spectrum of the molecular ion of 8-[5-(4-pentyn-1-yl)-3-oxa-pentoxy]-3-cobalt bis(1,2-dicarbollide) (8), calculated exact mass for $C_{13}H_{36}B_{18}CoO_3$: 497.37



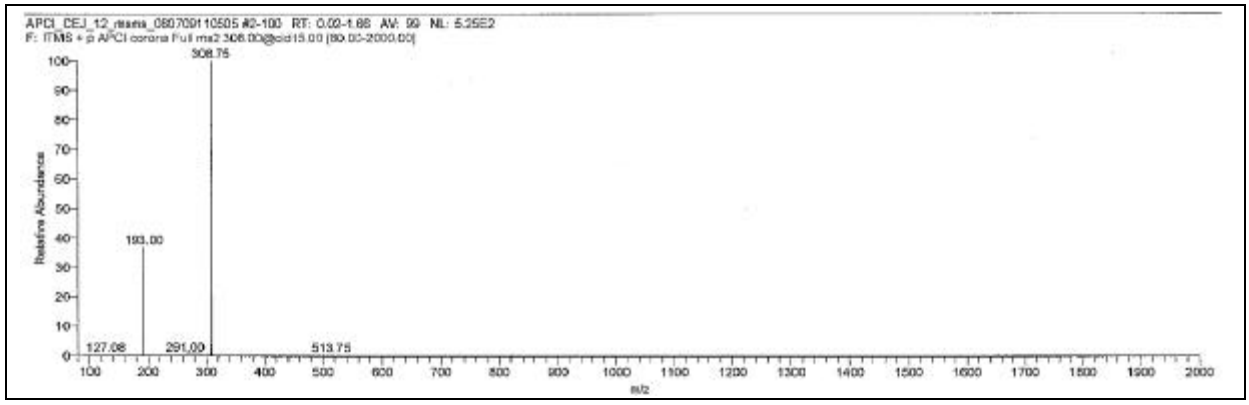
Fragment of the MS ESI spectrum of 8-[5-(4-pentyn-1-yl)-3-oxa-pentoxy]-3-cobalt bis(1,2-dicarbollide) (8), corresponding to molecular ion range, m/z (%): 495.48 (100%), 497.40 (6%), calculated exact mass for $C_{13}H_{36}B_{18}CoO_3$: 497.37



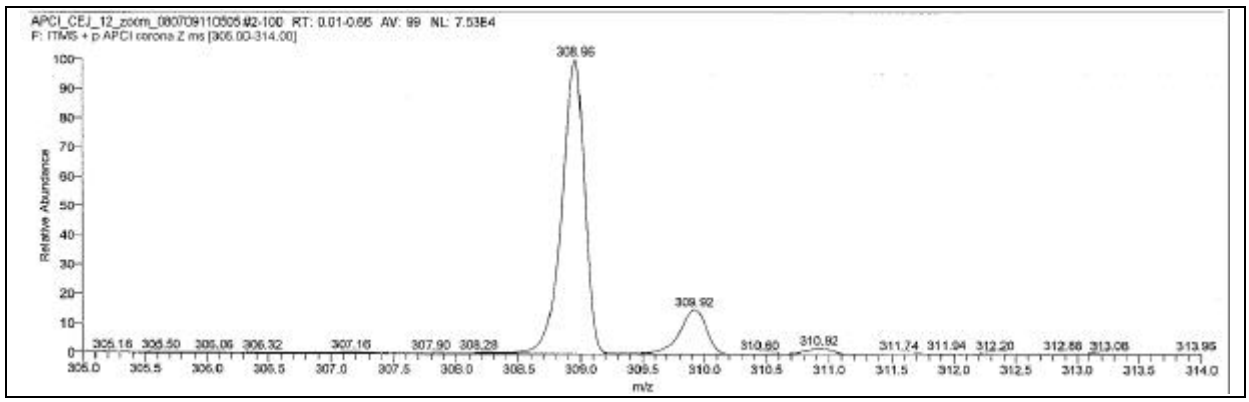
Simulated spectrum of the molecular ion of 8-[(5-thia-(3-thiolo-propan-1-yl)-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) [(8-HS(CH_2)3S-(CH_2CH_2O)$_2$-1,2-$C_2B_9H_{10}$)(1',2'-$C_2B_9H_{11}$-3,3'-Co]Na (9), calculated exact mass for $C_{11}H_{36}B_{18}O_2S_2Co$: 521.32



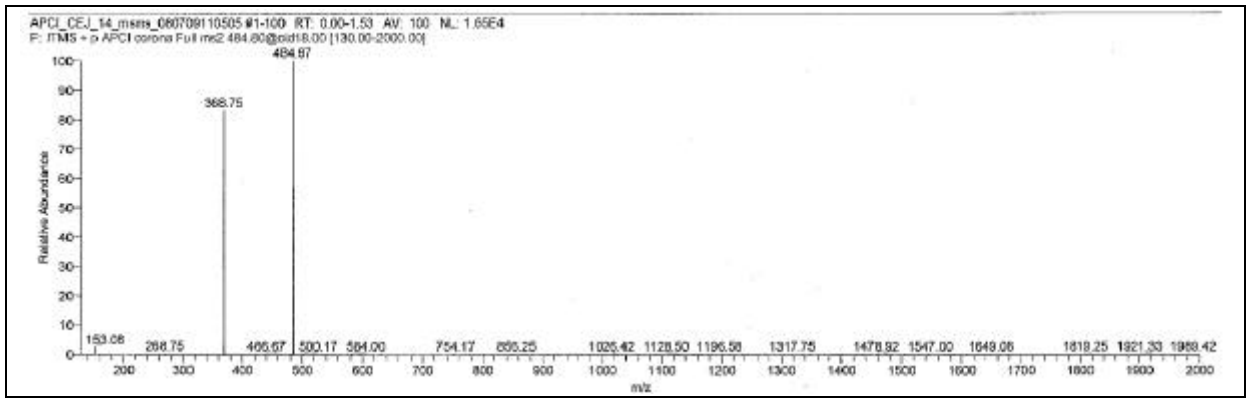
Fragment of the MS ESI spectrum of 8-[(5-thia-(3-thiolo-propan-1-yl)-3-oxa-pentoxy)-3-cobalt bis(1,2-dicarbollide) [(8-HS(CH_2)3S-(CH_2CH_2O)$_2$-1,2-$C_2B_9H_{10}$)(1',2'-$C_2B_9H_{11}$-3,3'-Co]Na (9) corresponding to molecular ion range, m/z (%): 519.42 (100%), 521.36 (10%), calculated exact mass for $C_{11}H_{36}B_{18}O_2S_2Co$: 521.32



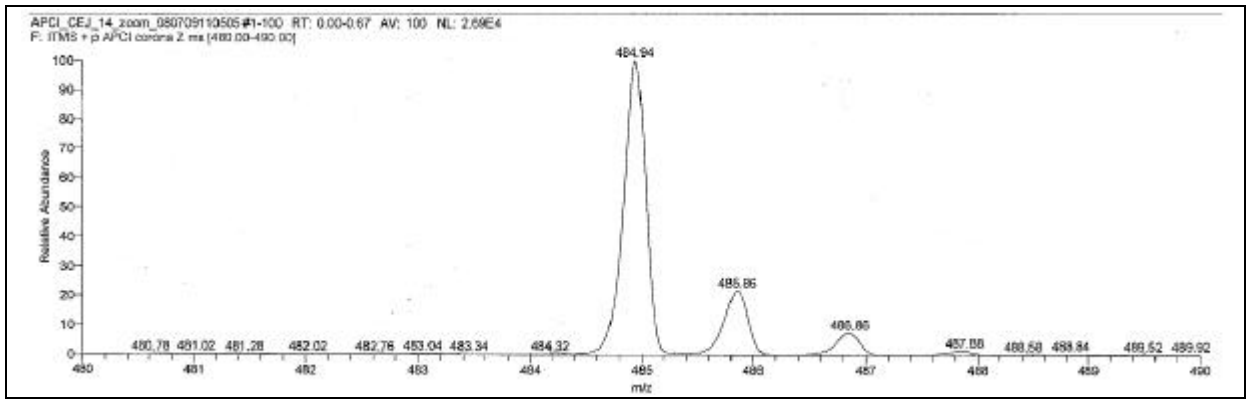
Simulated spectrum of the molecular ion of 3*N*-(4-pentyn-1-yl)thymidine (12), calculated exact mass for $C_{15}H_{20}N_2O_5$: 308.14



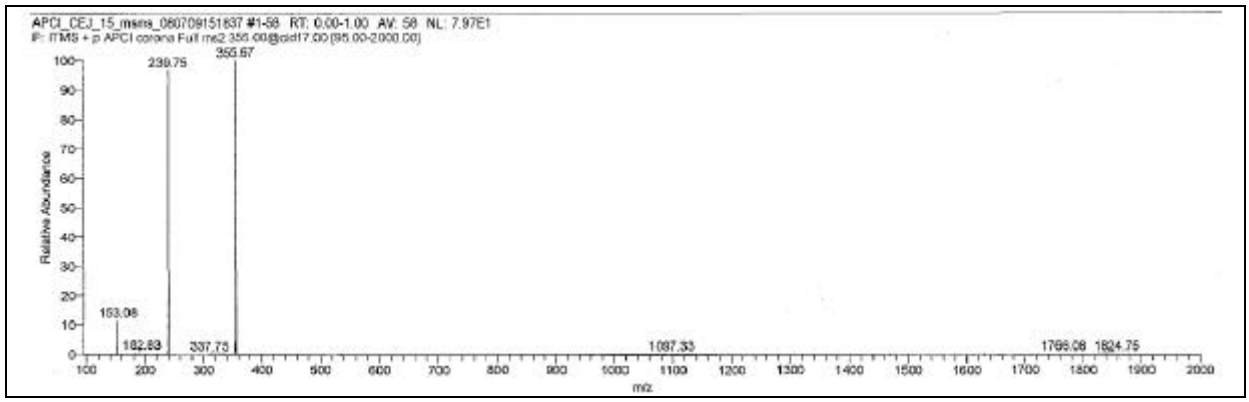
Fragment of the MS-APCI spectrum of 3*N*-(4-pentyn-1-yl)thymidine (12), corresponding to molecular ion range, m/z (%):308.96 (100%), 309.92 (15%), calculated exact mass for $C_{15}H_{20}N_2O_5$: 308.14



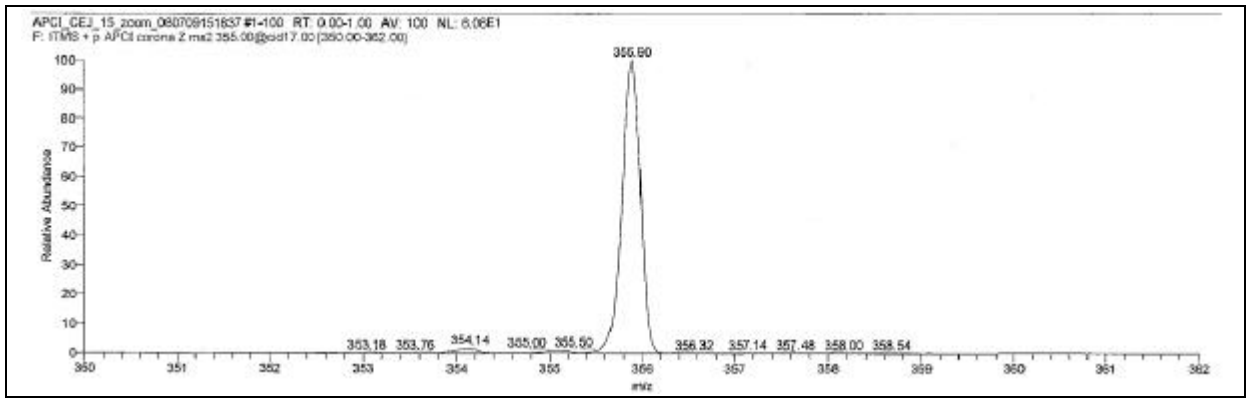
Simulated spectrum of the molecular ion of 3*N*-[1-*para*-toluensulphonyl)-3-oxa-pentoxy)]thymidine (14), calculated exact mass for $C_{21}H_{28}N_2O_9S$: 484.15



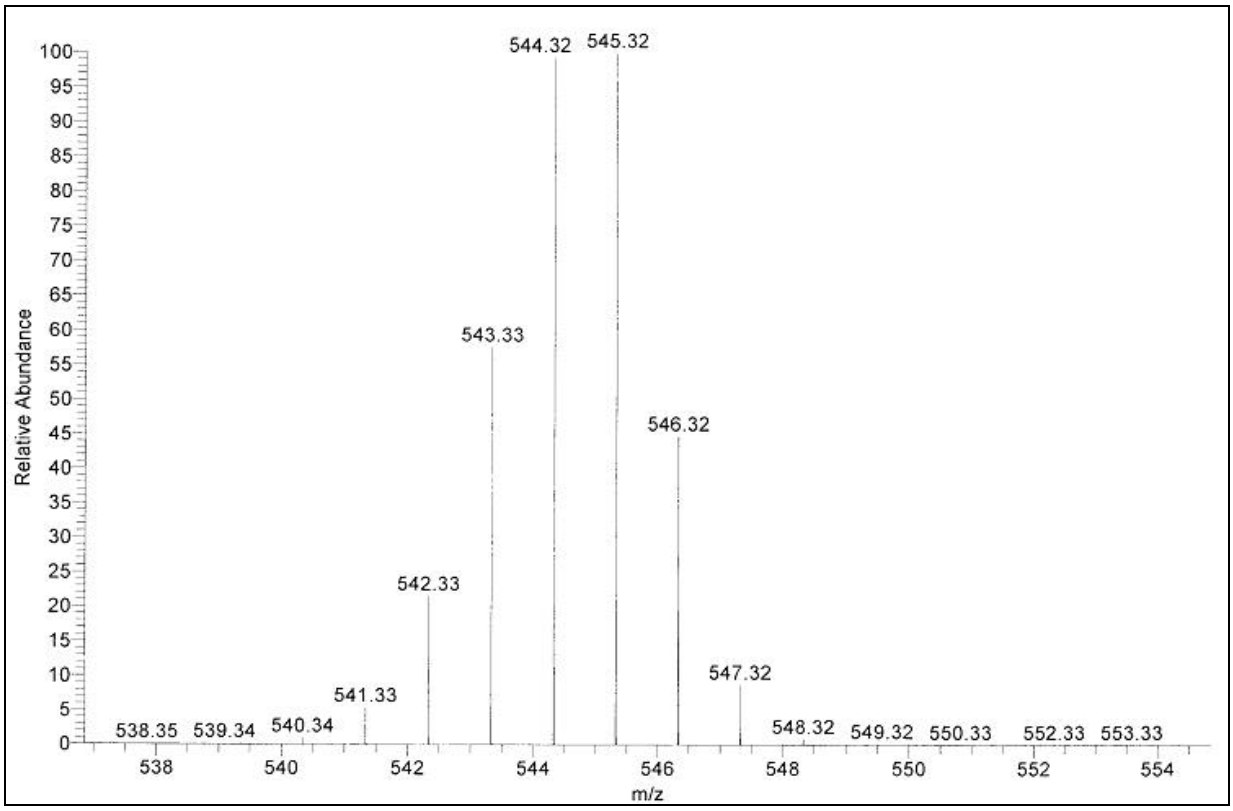
Fragment of the MS-APCI spectrum of 3*N*-[1-*para*-toluensulphonyl)-3-oxa-pentoxy)]thymidine (14) corresponding to molecular ion range, m/z (%): 484.94 (100%), 485.86 (22%), 486.86 (6%), calculated exact mass for $C_{21}H_{28}N_2O_9S$: 484.15



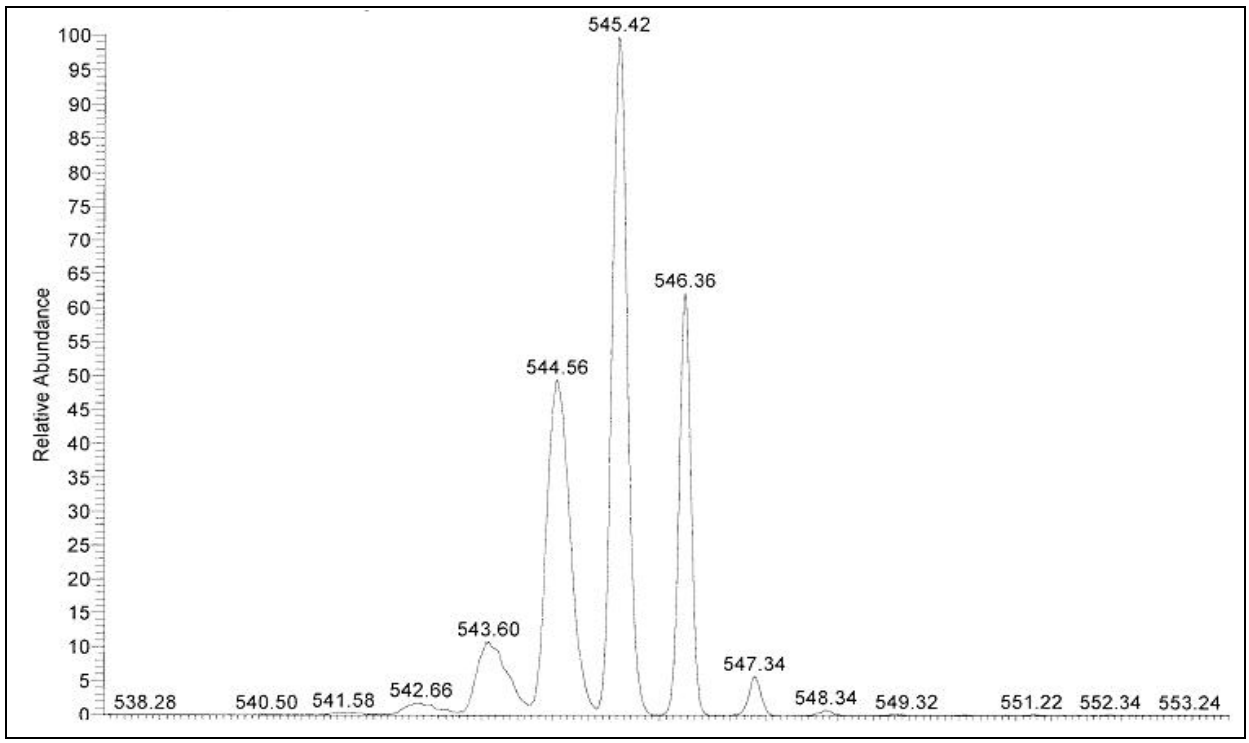
Simulated spectrum of the molecular ion of 3*N*-[5-azide-3-oxa-pentoxy)]thymidine (15), calculated exact mass for $C_{14}H_{21}N_5O_6$: 355.15



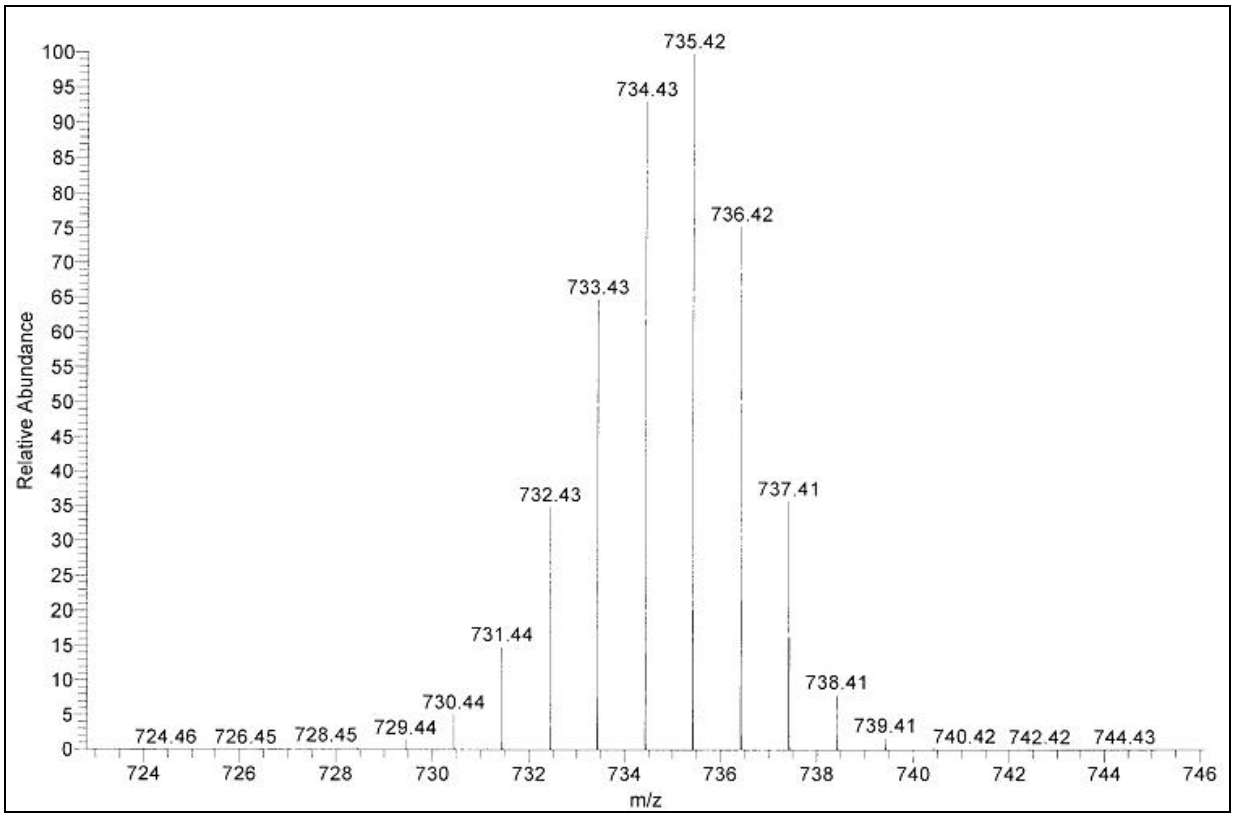
Fragment of the MS-APCI spectrum of 3*N*-[5-azide-3-oxa-pentoxy)]thymidine (15) corresponding to molecular ion range, m/z (%): 355.90 (100%), calculated exact mass for $C_{14}H_{21}N_5O_6$: 355.15



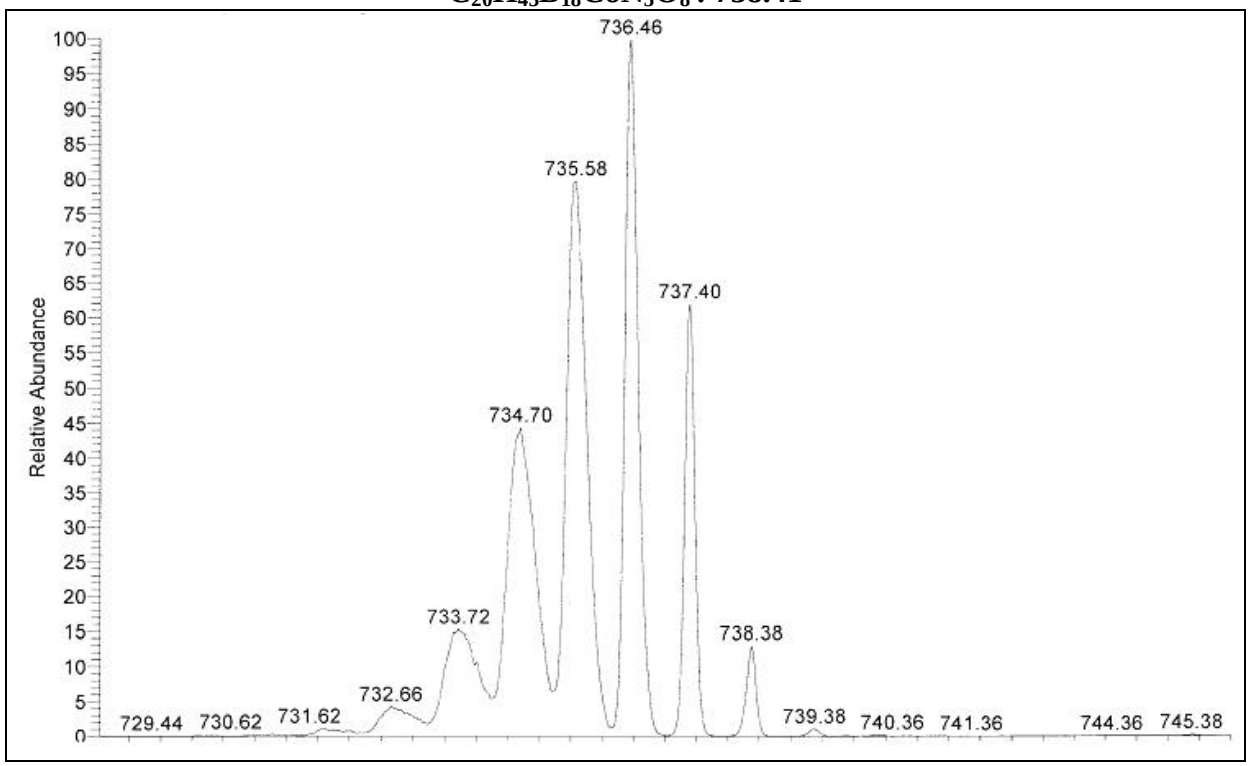
Simulated spectrum of the molecular ion of 2'-*O*-{[5-(7,8-dikarba-nido-undekaborane-10-yl)-3-oxa-pentoxy]-1*N*-1,2,3-triazole-4-yl}methyluridine (17), calculated exact mass for $C_{18}H_{31}B_9N_5O_8$: 544.30



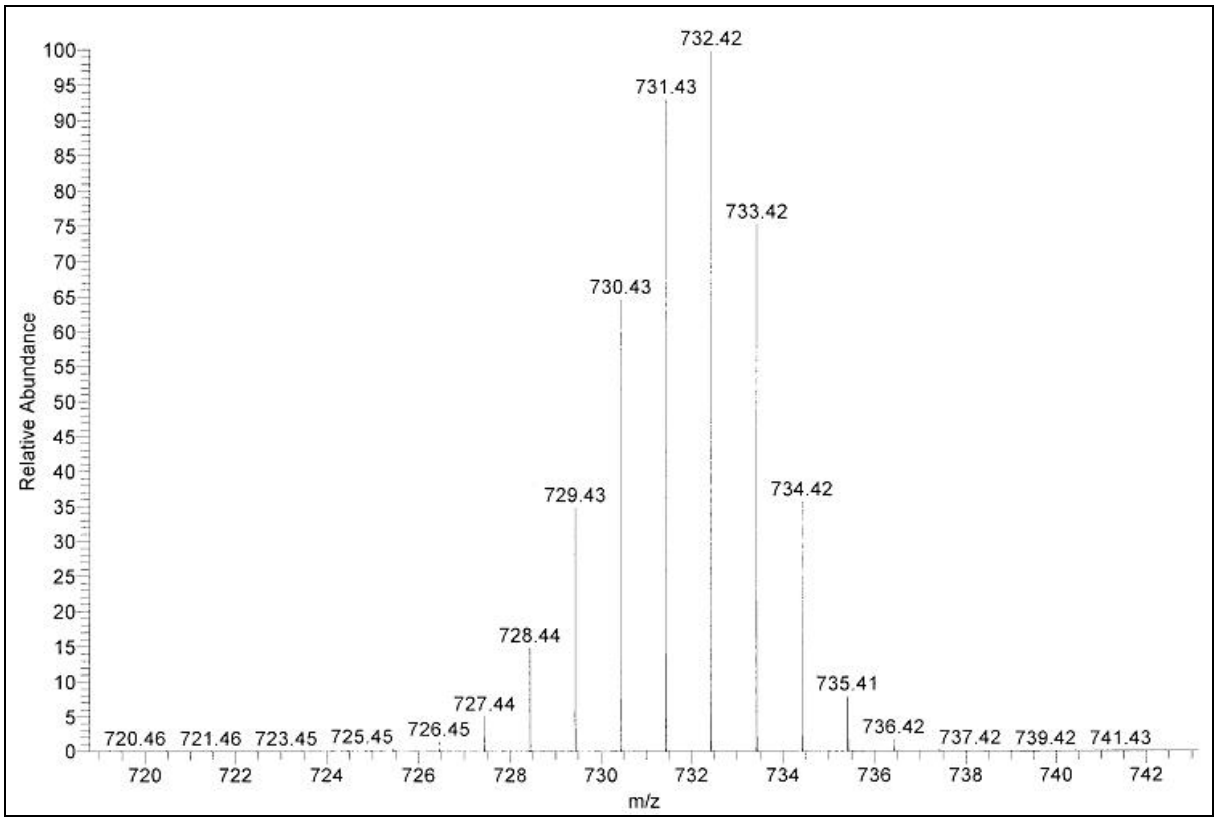
Fragment of the MS ESI spectrum of 2'-*O*-{[5-(7,8-dikarba-nido-undekaborane-10-yl)-3-oxa-pentoxy]-1*N*-1,2,3-triazole-4-yl}methyluridine (17), corresponding to molecular ion range, m/z (%): 545.42 (100%), 547.34 (5%), calculated exact mass for $C_{18}H_{31}B_9N_5O_8$: 544.30



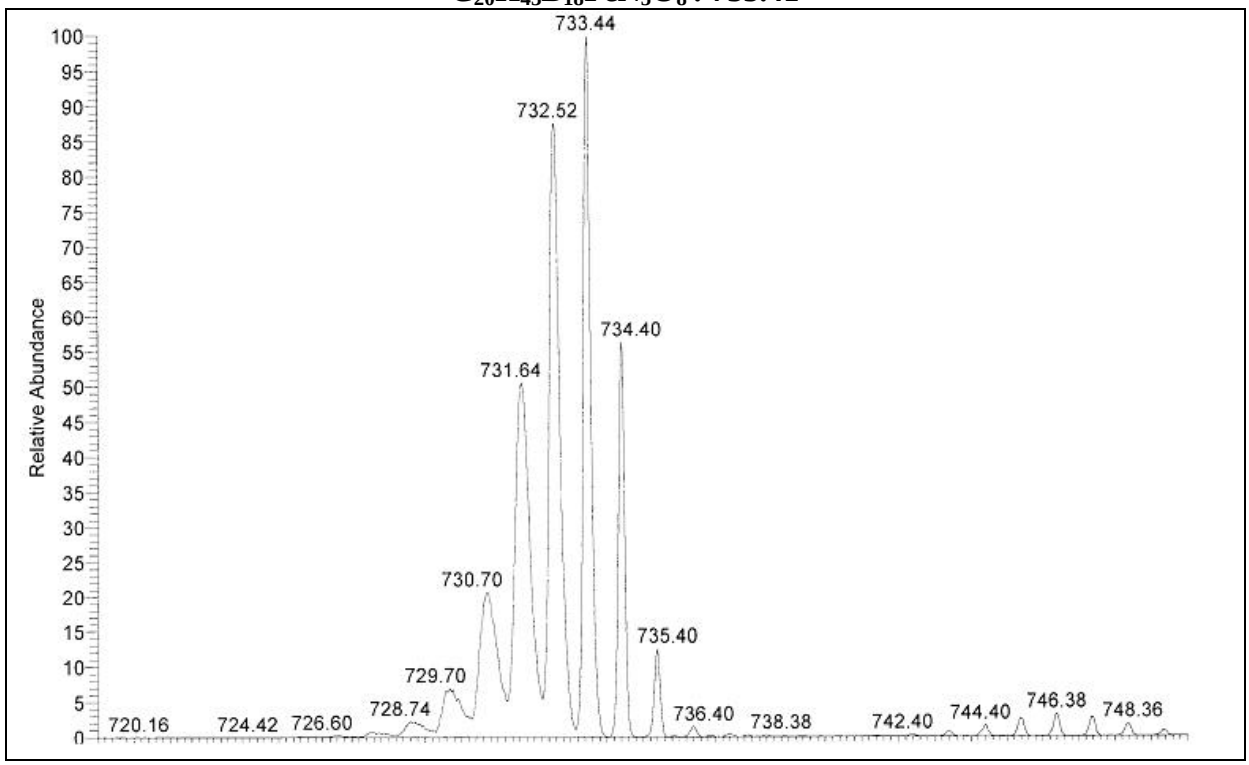
Simulated spectrum of the molecular ion of 2'-*O*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}methyluridine (18), calculated exact mass for $C_{20}H_{43}B_{18}CoN_5O_8$: 738.41



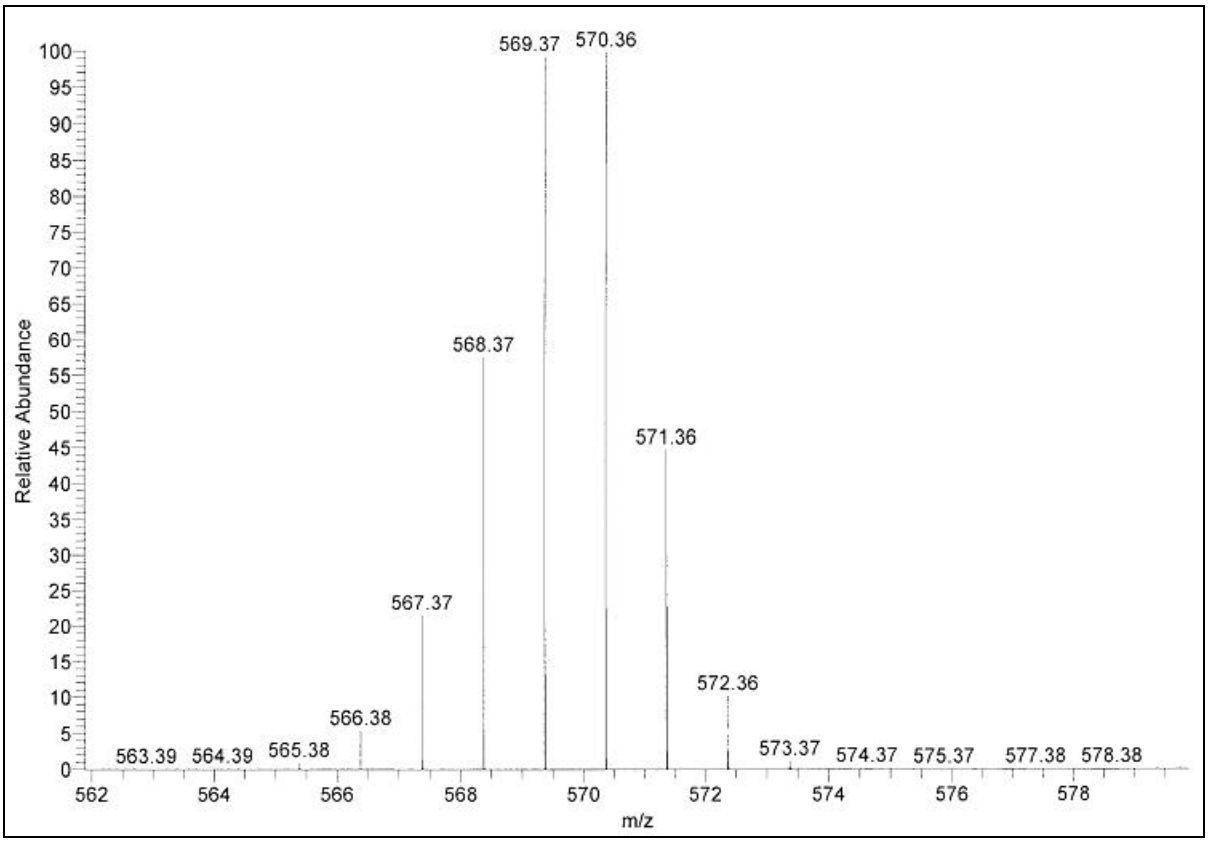
Fragment of the MS ESI spectrum of 2'-*O*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}methyluridine (18)corresponding to molecular ion range, m/z (%):736.46 (100%), 738.38 (12%), calculated exact mass for $C_{20}H_{43}B_{18}CoN_5O_8$: 738.41



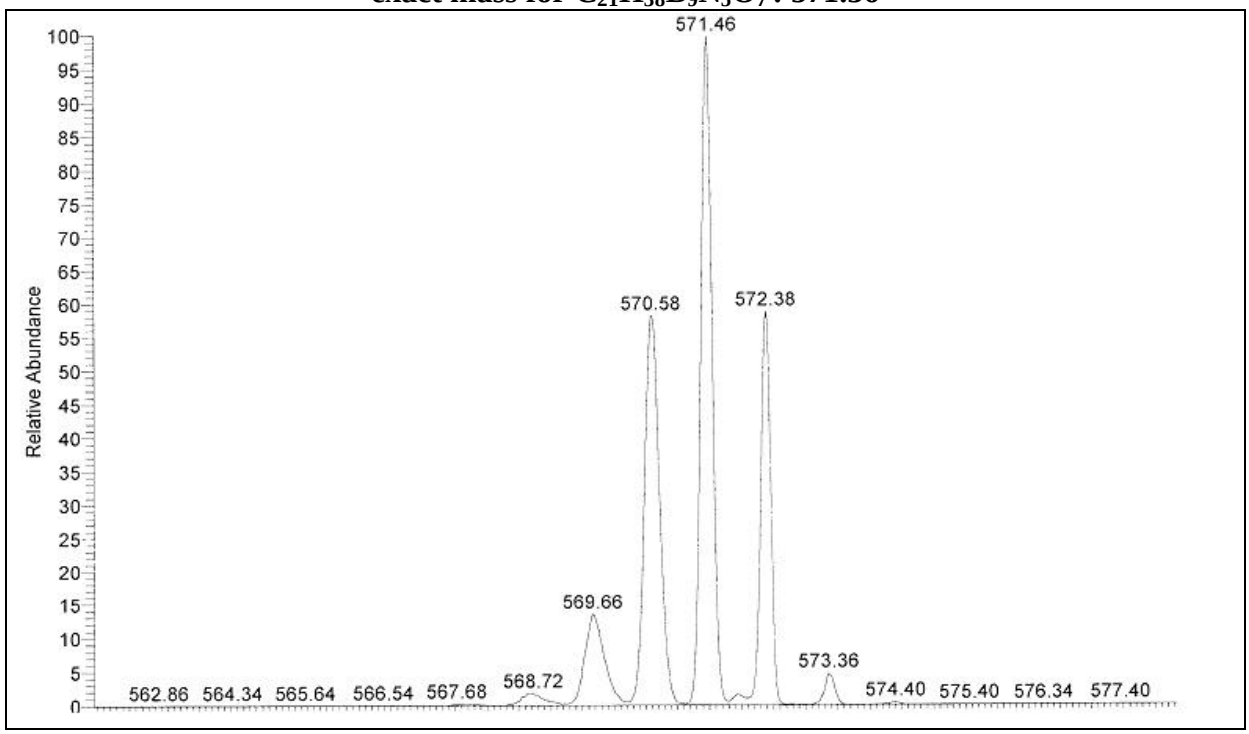
Simulated spectrum of the molecular ion of 2'-*O*-{{5-[3-iron bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}methyluridine (19), calculated exact mass for $C_{20}H_{43}B_{18}FeN_5O_8$: 735.41



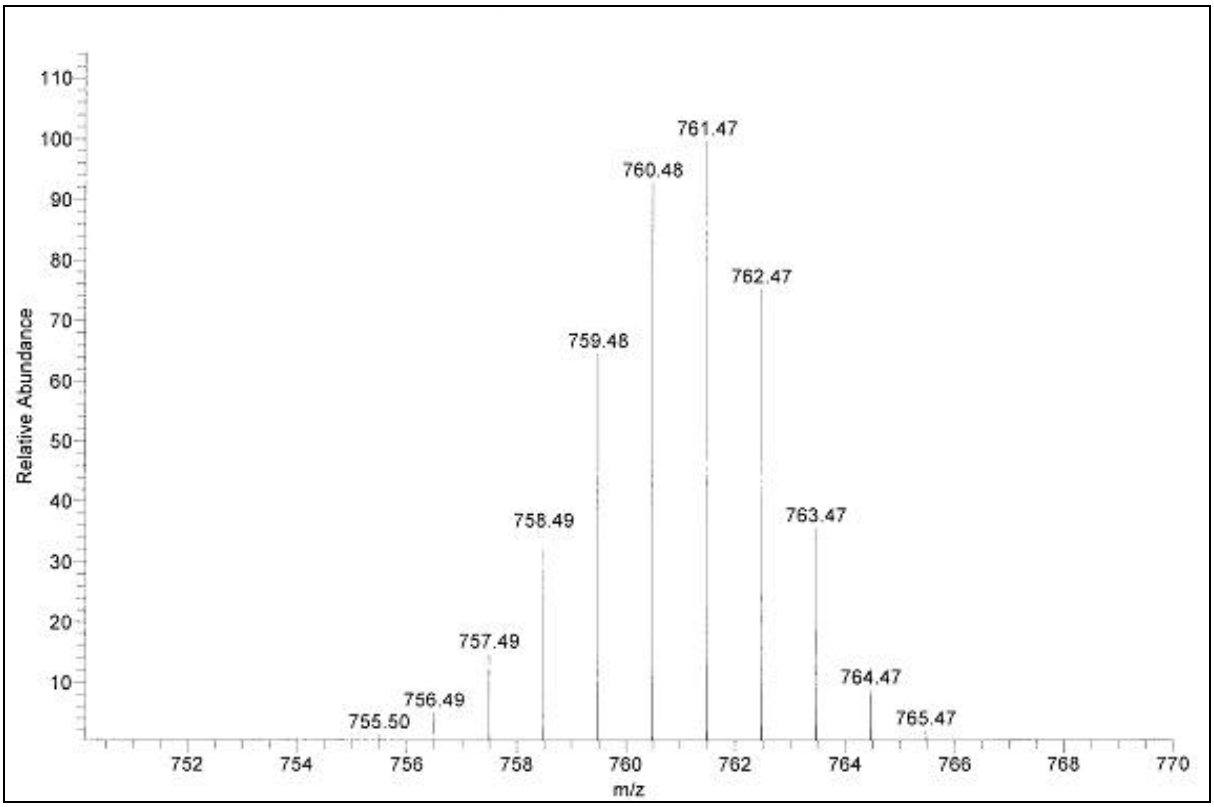
Fragment of the MS ESI spectrum of 2'-*O*-{{5-[3-iron bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}methyluridine (19), corresponding to molecular ion range, m/z (%):733.44 (100%), 735.40 (12%), calculated exact mass for $C_{20}H_{43}B_{18}FeN_5O_8$: 735.41



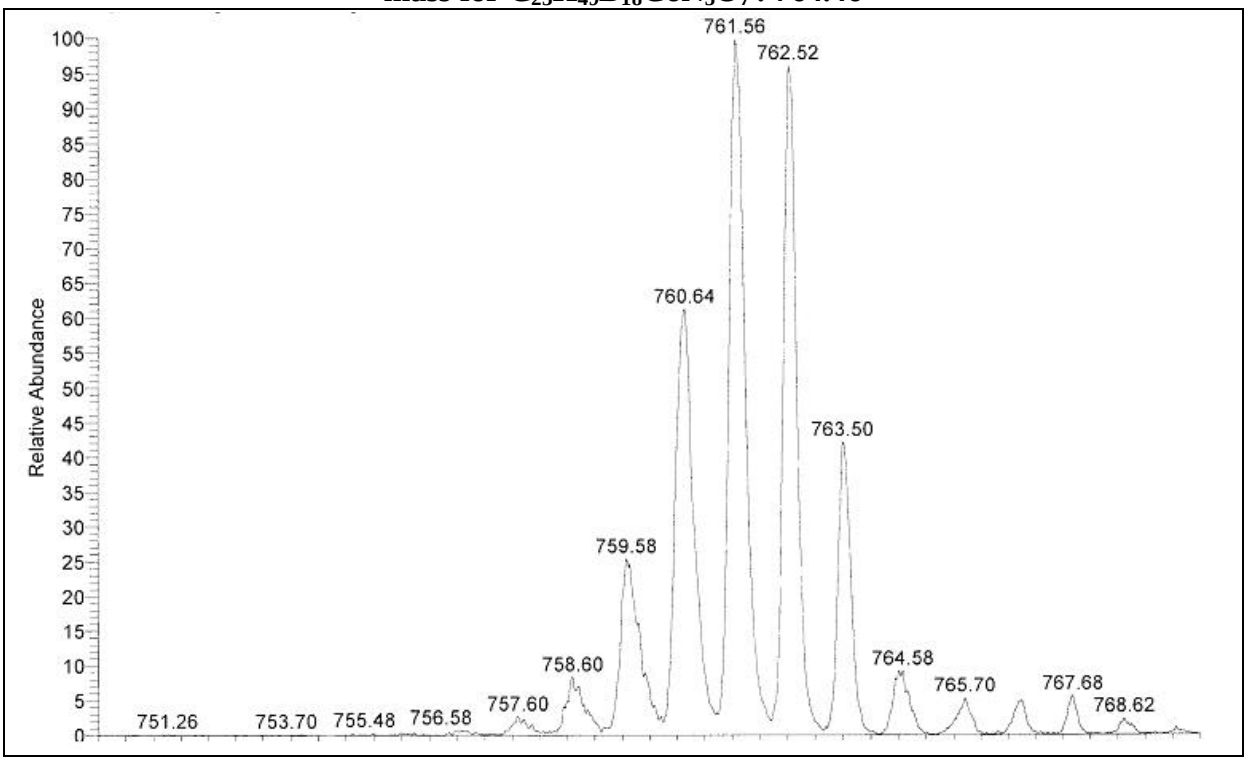
Simulated spectrum of the molecular ion of 3-*N*-{[5-(7,8-dikarba-*nido*-undekaborane-10-yl)-3-oxa-pentoxy]-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (20), calculated exact mass for $C_{21}H_{38}B_9N_5O_7$: 571.36



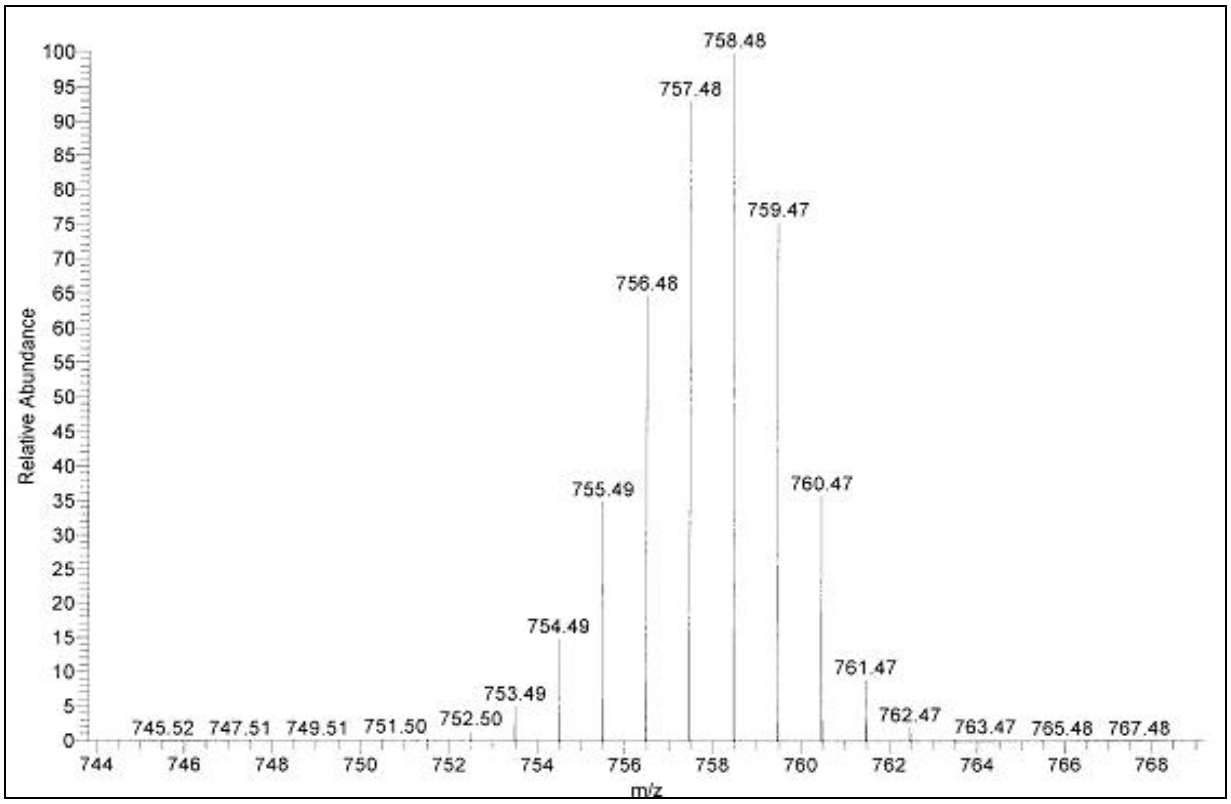
Fragment of the MS ESI spectrum of 3-*N*-{[5-(7,8-dikarba-*nido*-undekaborane-10-yl)-3-oxa-pentoxy]-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (20) corresponding to molecular ion range, m/z $[M+2H]^-$: 571.46 (100%), 573.36 (5%), calculated exact mass for $C_{21}H_{38}B_9N_5O_7$: 571.36



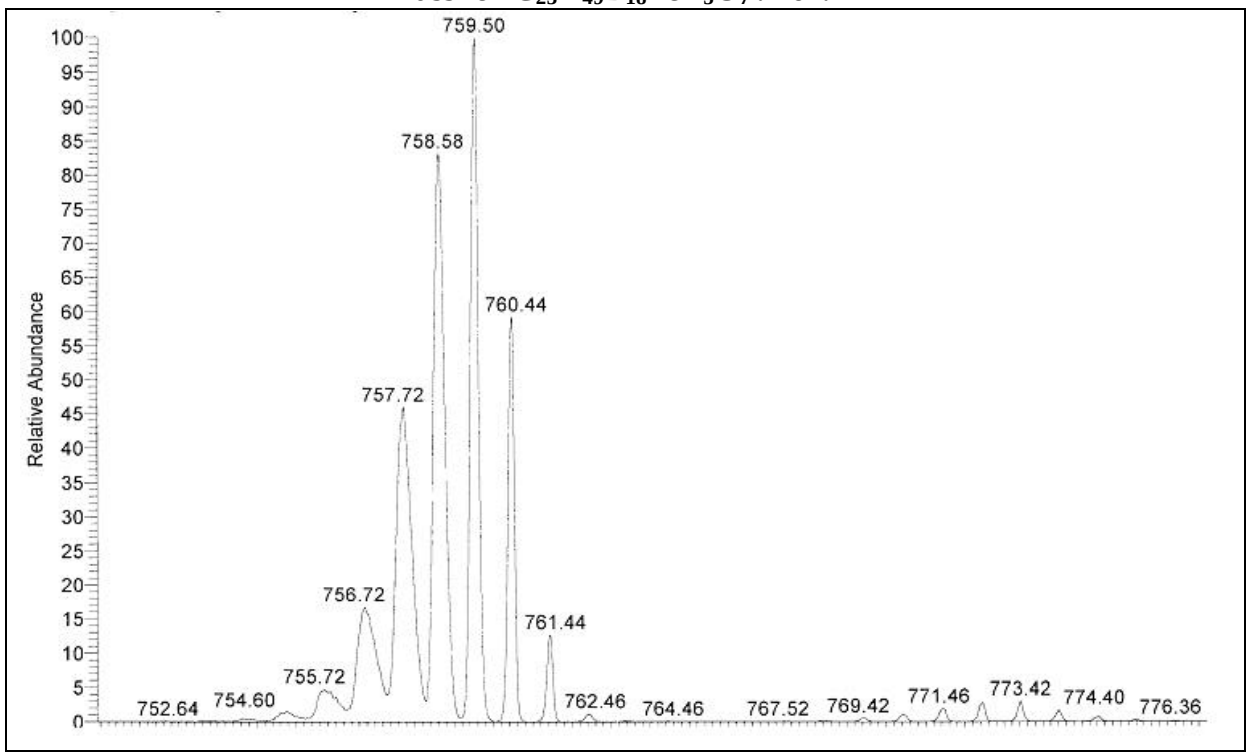
Simulated spectrum of the molecular ion of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (21), calculated exact mass for $C_{23}H_{49}B_{18}CoN_5O_7$: 764.46



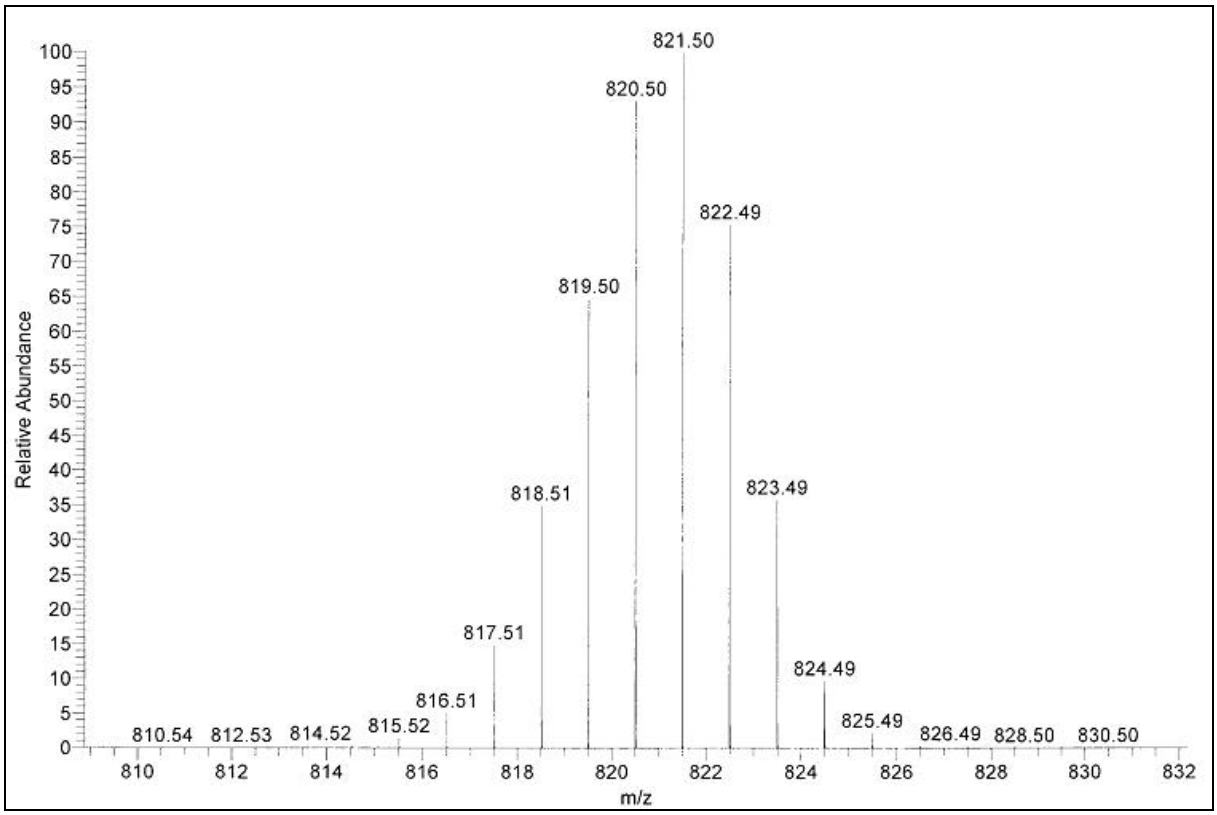
Fragment of the MS ESI spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (21), corresponding to molecular ion range, m/z (%):761.56 (100%), 764.58 (7%), calculated exact mass for $C_{23}H_{49}B_{18}CoN_5O_7$: 764.46



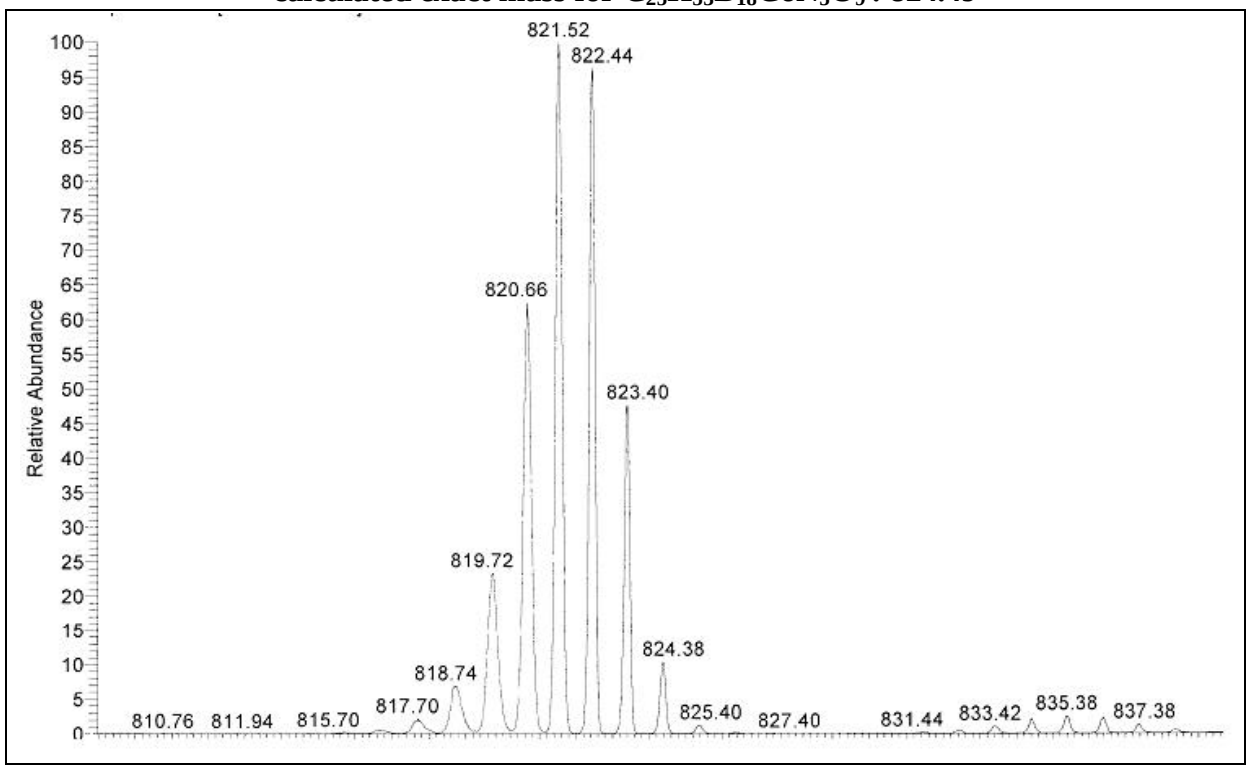
Simulated spectrum of the molecular ion of 3-*N*-{{5-[3-iron bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (22), calculated exact mass for $C_{23}H_{49}B_{18}FeN_5O_7$: 761.47



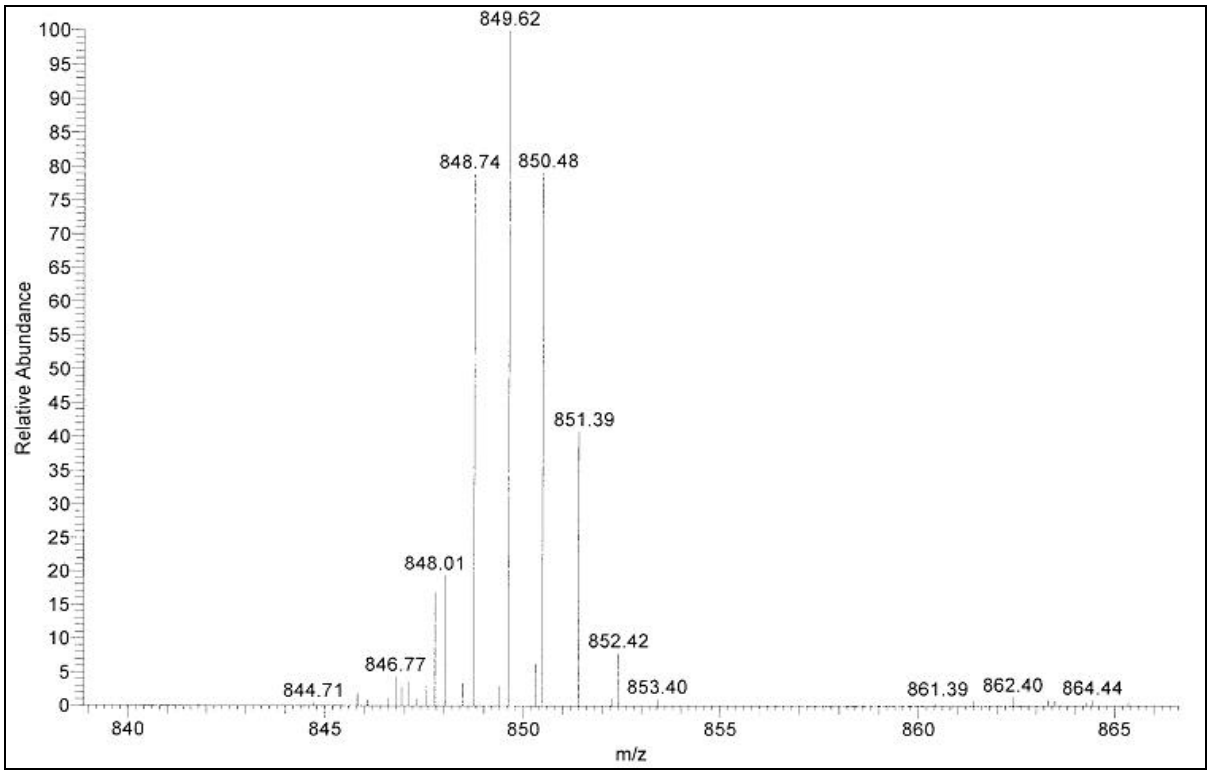
Fragment of the MS ESI spectrum of 3-*N*-{{5-[3-iron bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}-1*N*-1,2,3-triazole-4-yl}(4-propan-1-yl)thymidine (22) corresponding to molecular ion range, m/z (%):759.50 (100%), 761.44 (12%), calculated exact mass for $C_{23}H_{49}B_{18}FeN_5O_7$: 761.47



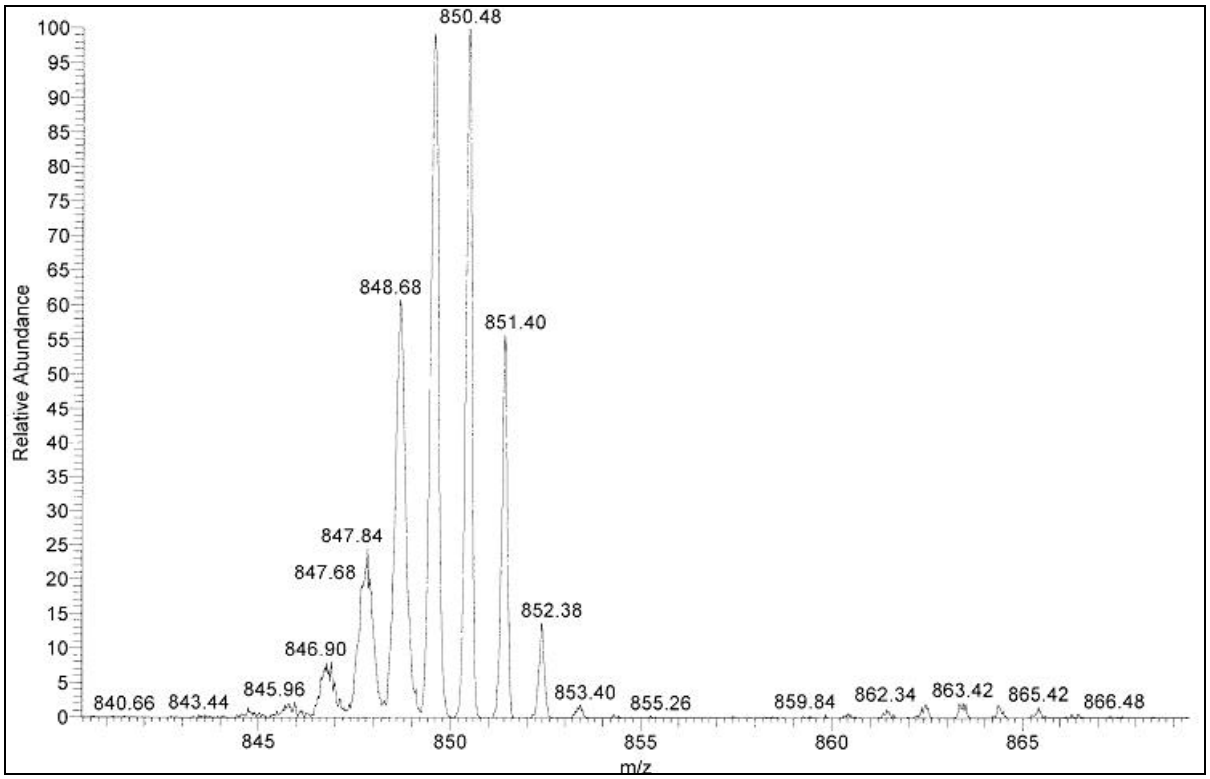
Simulated spectrum of the molecular ion of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}methyl-(4-1,2,3-triazole-1*N*-yl)} (1-ethoxyethan-4-yl)thymidine (23), calculated exact mass for $C_{25}H_{53}B_{18}CoN_5O_9$: 824.49



Fragment of the MS ESI spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}methyl-(4-1,2,3-triazole-1*N*-yl)} (1-ethoxyethan-4-yl)thymidine (23), corresponding to molecular ion range, m/z (%): 821.52 (100%), 824.38 (10%) calculated exact mass for $C_{25}H_{53}B_{18}CoN_5O_9$: 824.49



Simulated spectrum of the molecular ion of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}propyl-(4-1,2,3-triazole-1*N*-yl}} (1-ethoxyethan-4-yl)thymidine (24), calculated exact mass for $C_{27}H_{57}B_{18}CoN_5O_9$: 852.52



Fragment of the MS ESI spectrum of 3-*N*-{{5-[3-cobalt bis(1,2-dicarbollide)-8-yl]-3-oxa-pentoxy}propyl-(4-1,2,3-triazole-1*N*-yl}} (1-ethoxyethan-4-yl)thymidine (24) corresponding to molecular ion range, m/z (%): 850.48 (100%), 852.38 (12%), calculated exact mass for $C_{27}H_{57}B_{18}CoN_5O_9$: 852.52