Dodatak

Roca, Sunčica

Supplement / Prilog

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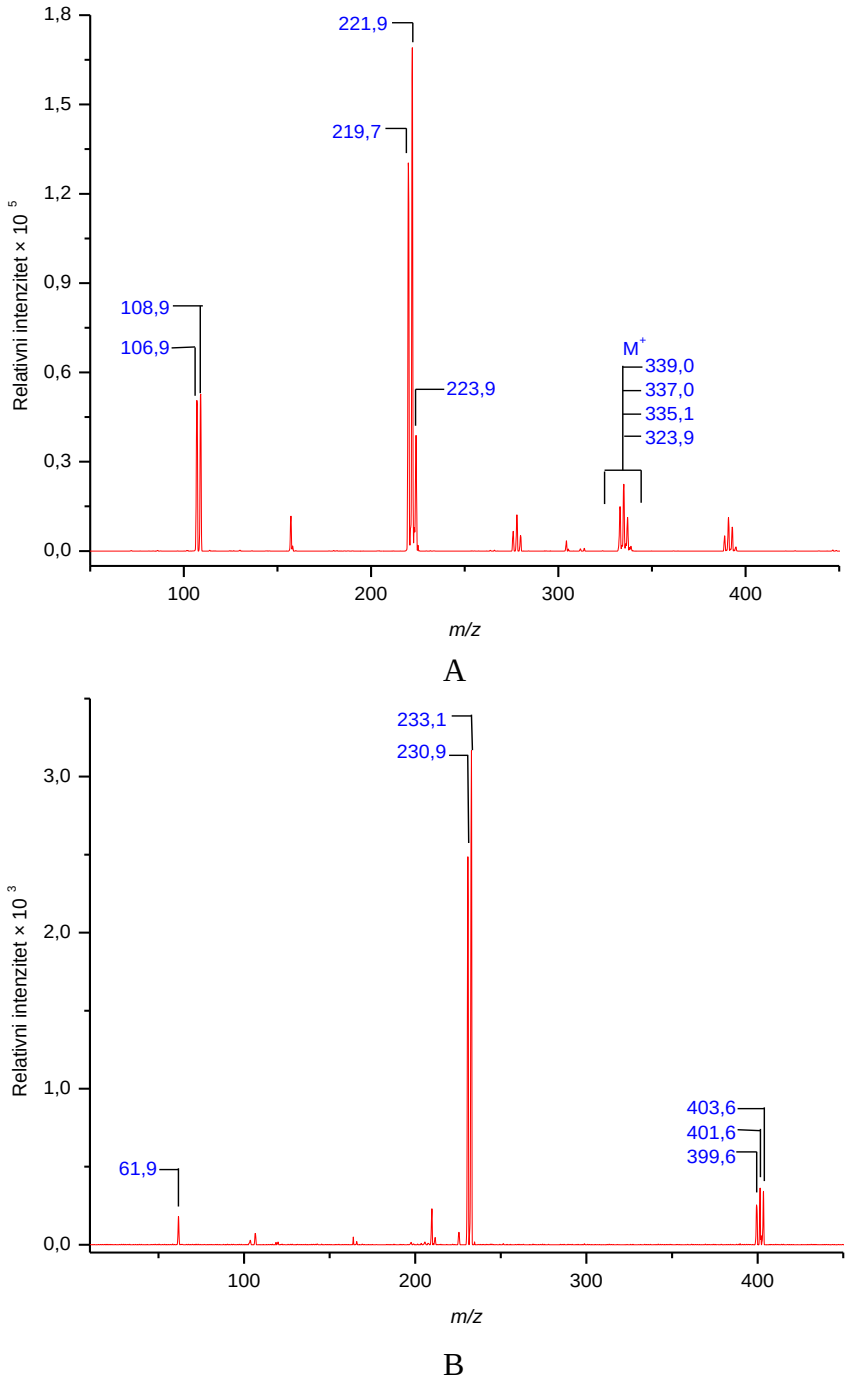
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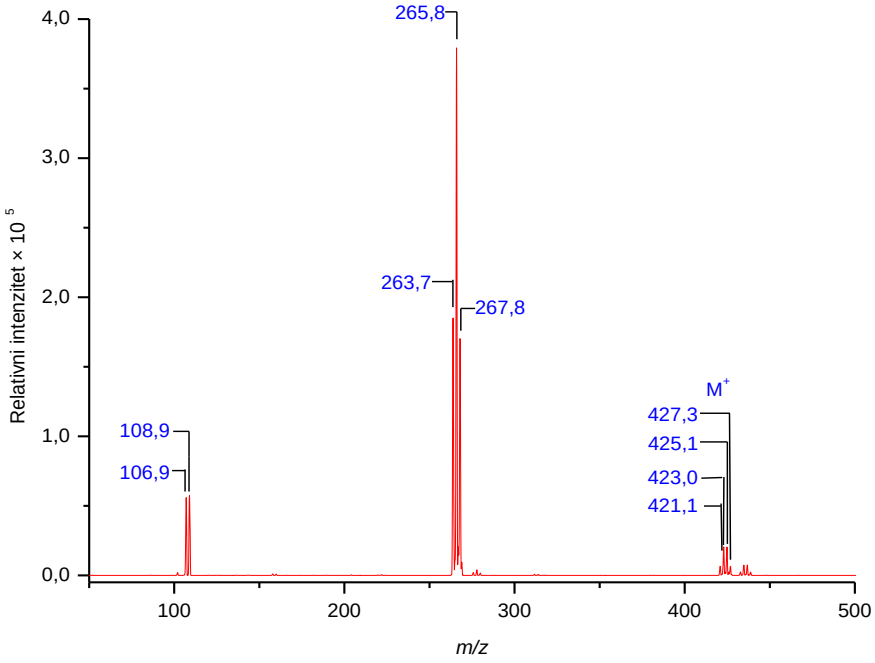


§ 8. DODATAK

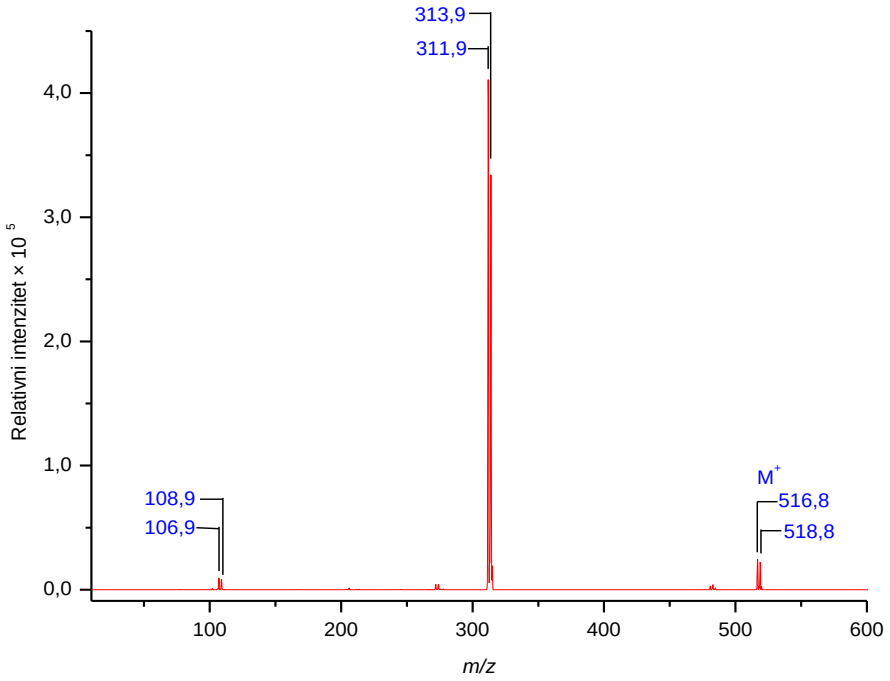
8.1. Spektri spektrometrije masa



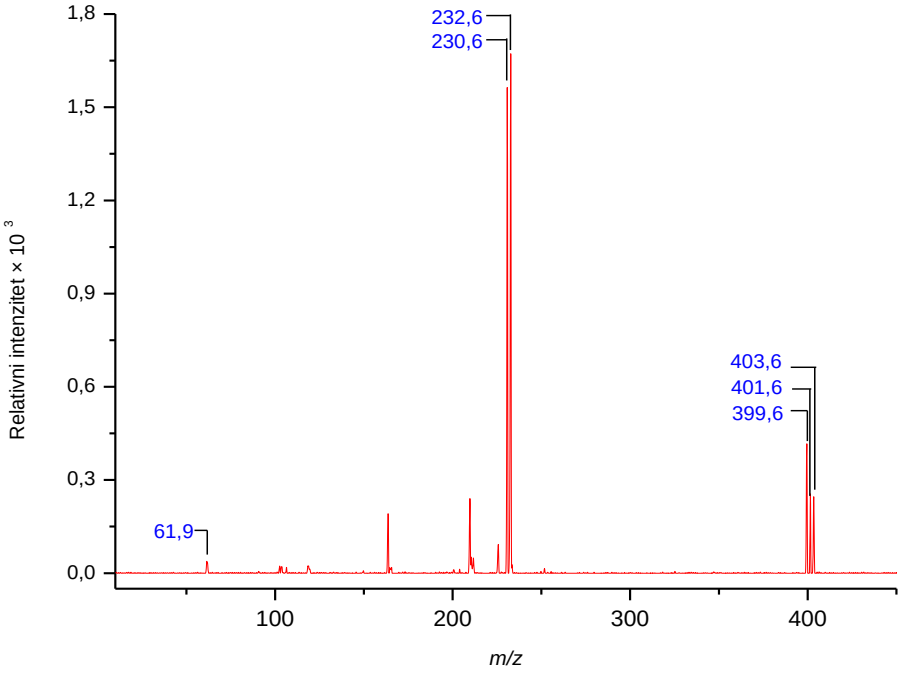
Slika D1. *A) ESI⁺-MS i B) ESI⁻-MS spektri kompleksa [Ag(NO₃)(2-Clpy)₂],* ***K1****.*



Slika D2. *A) ESI⁺-MS i B) ESI⁻-MS spektri kompleksa [Ag(NO₃)(2-Brpy)₂],* ***K2****.*

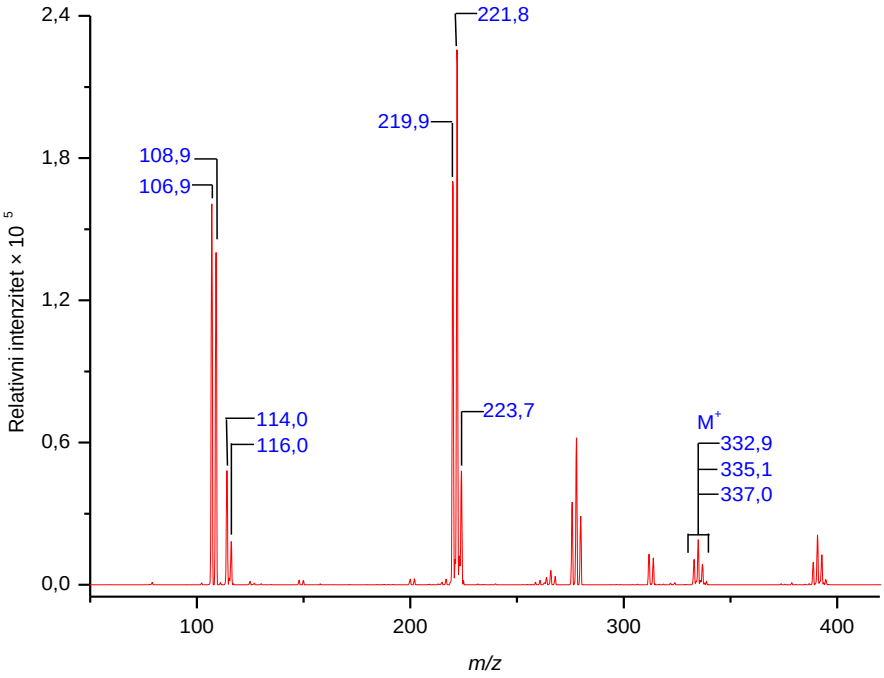


A

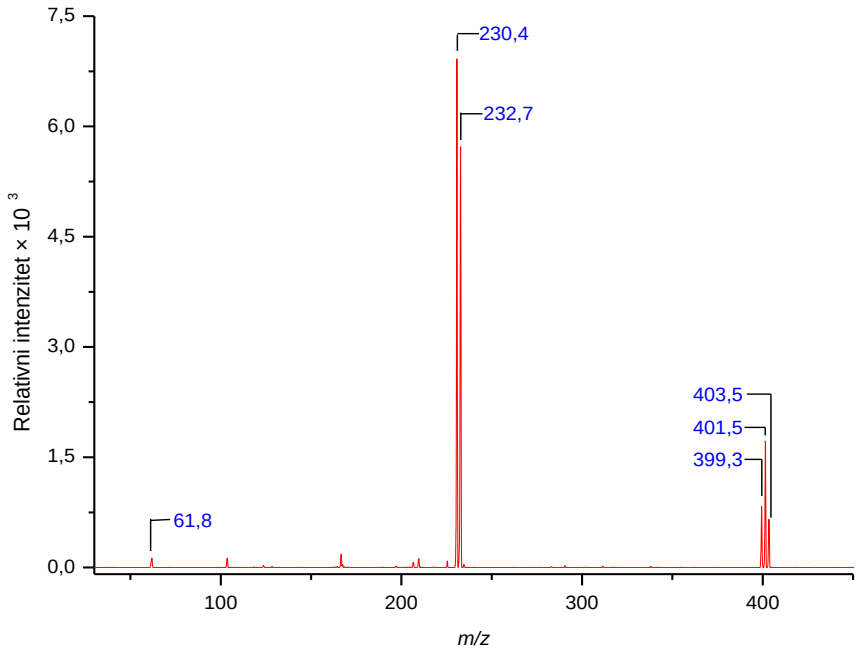


B

Slika D3. *A) ESI⁺-MS i B) ESI⁻-MS spektri kompleksa [Ag(NO₃)(2-Ipy)₂],* ***K3****.*

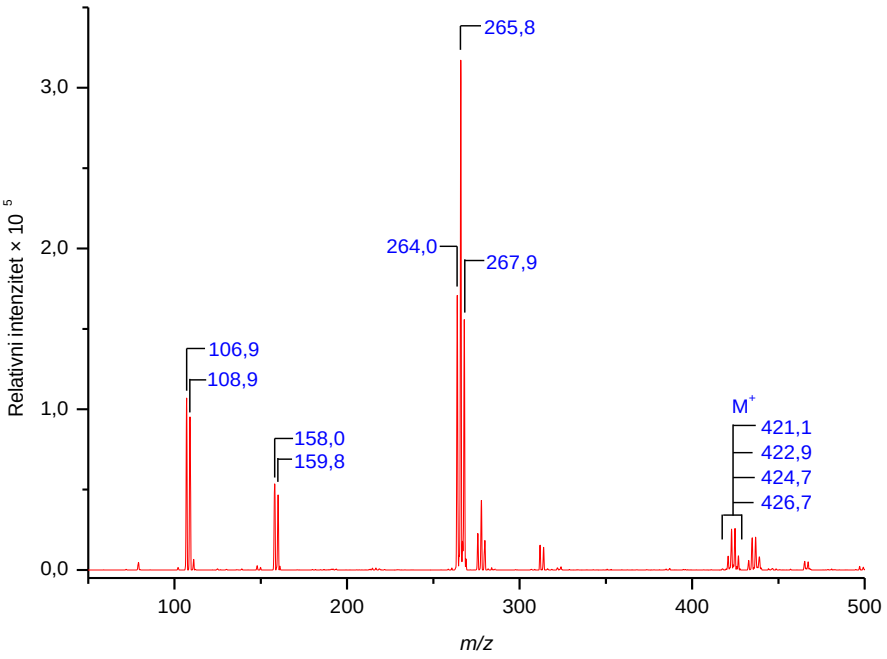


A

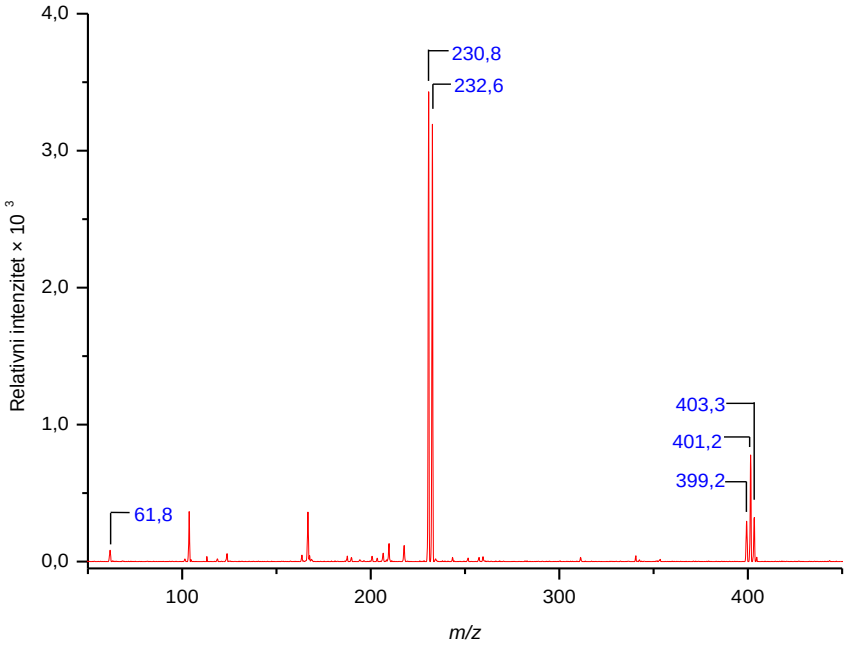


B

Slika D4. *A) ESI⁺-MS i B) ESI⁻-MS spektri kompleksa [Ag(NO₃)(3-Clpy)₂],* ***K4****.*

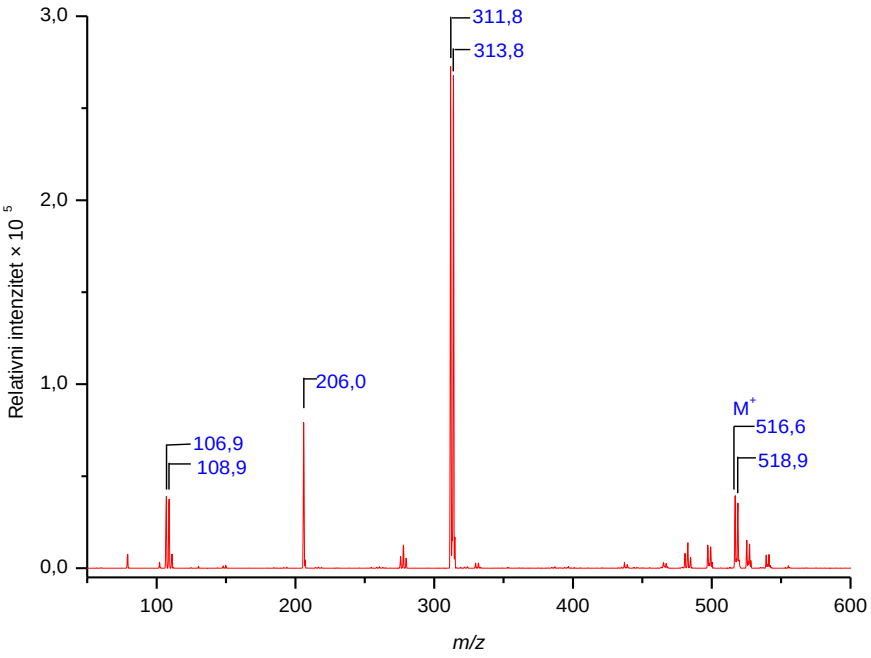


A

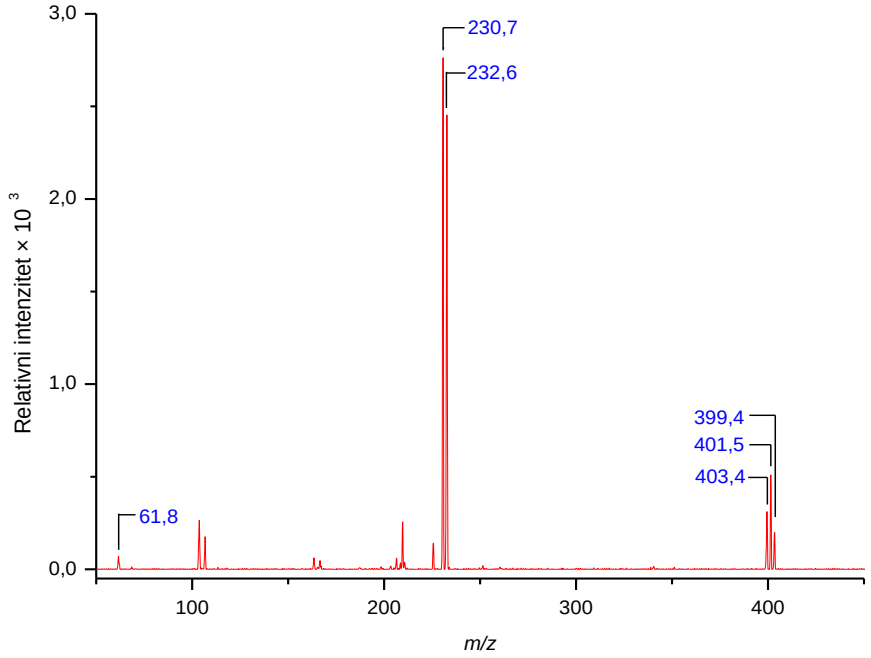


B

Slika D5. *A) ESI⁺-MS i B) ESI⁻-MS spektri kompleksa* $[Ag(NO_3)(3\text{-Brpy})_2]$, ***K5.***

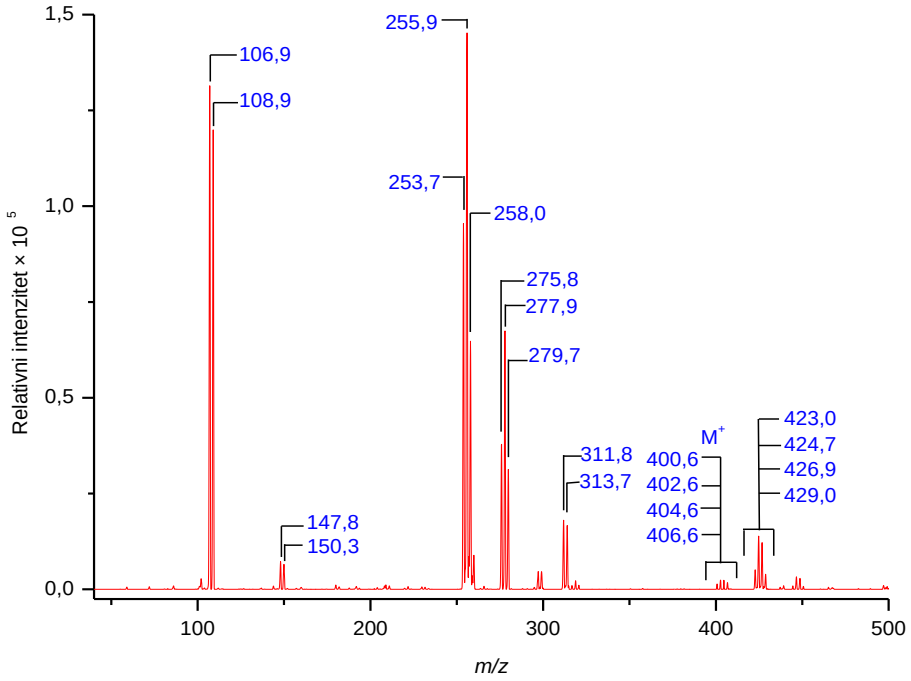


A

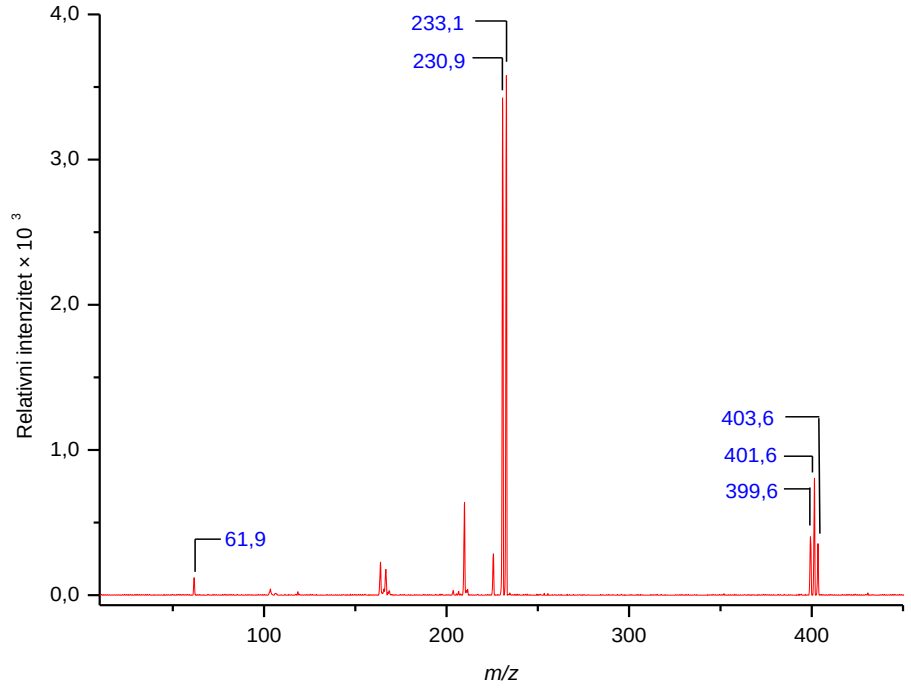


B

Slika D6. *A) ESI⁺-MS i B) ESI⁻-MS spektri kompleksa* $[Ag(NO_3)(3\text{-Ipy})_{2,}]$, ***K6.***

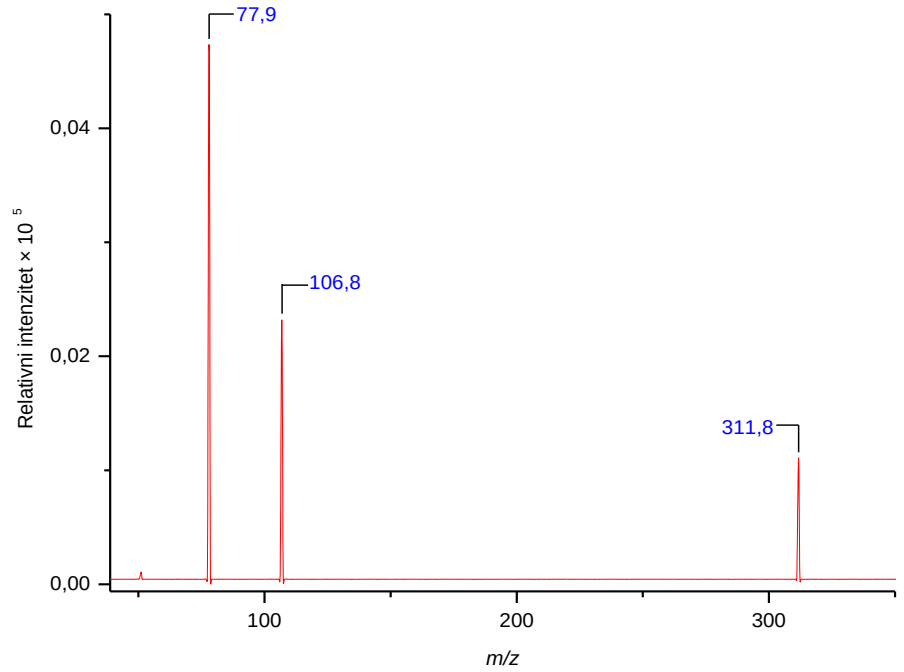


A

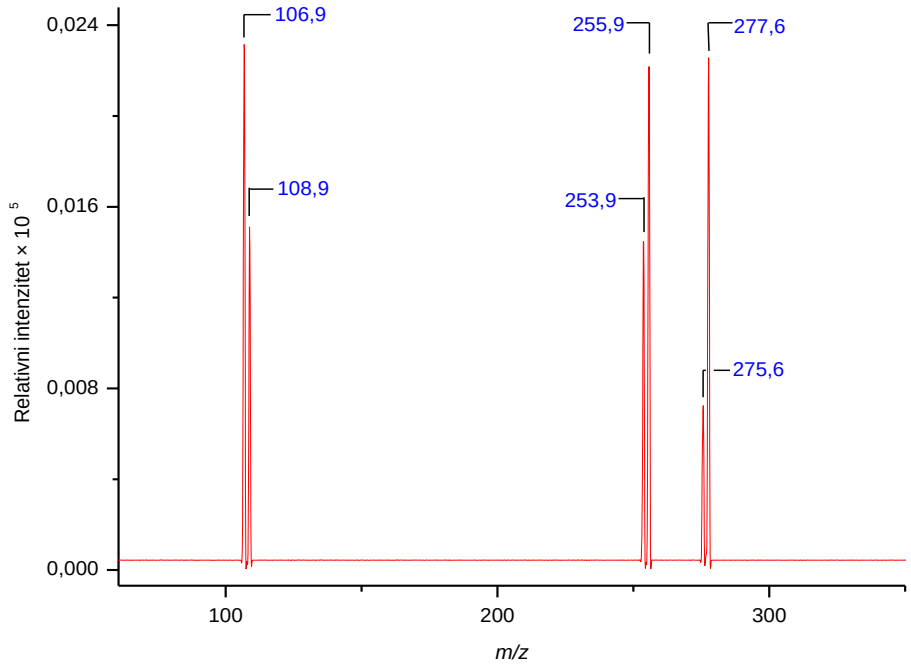


B

Slika D7. *A) ESI⁺-MS i B) ESI⁻-MS spektri kompleksa [Ag(NO₃)(2,5-Cl₂py)₂],* ***K7****.*

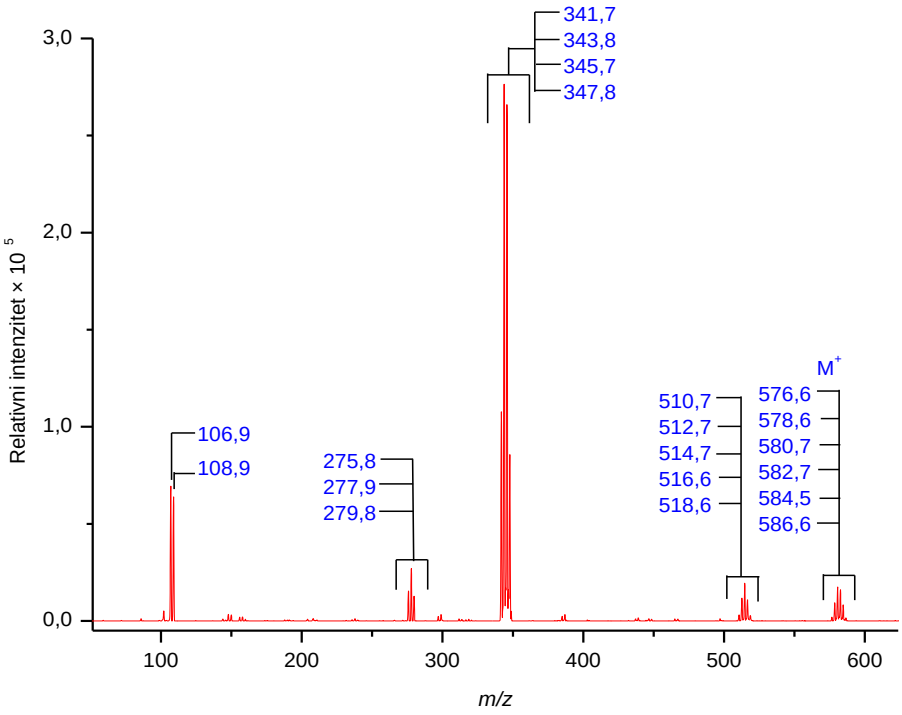


A

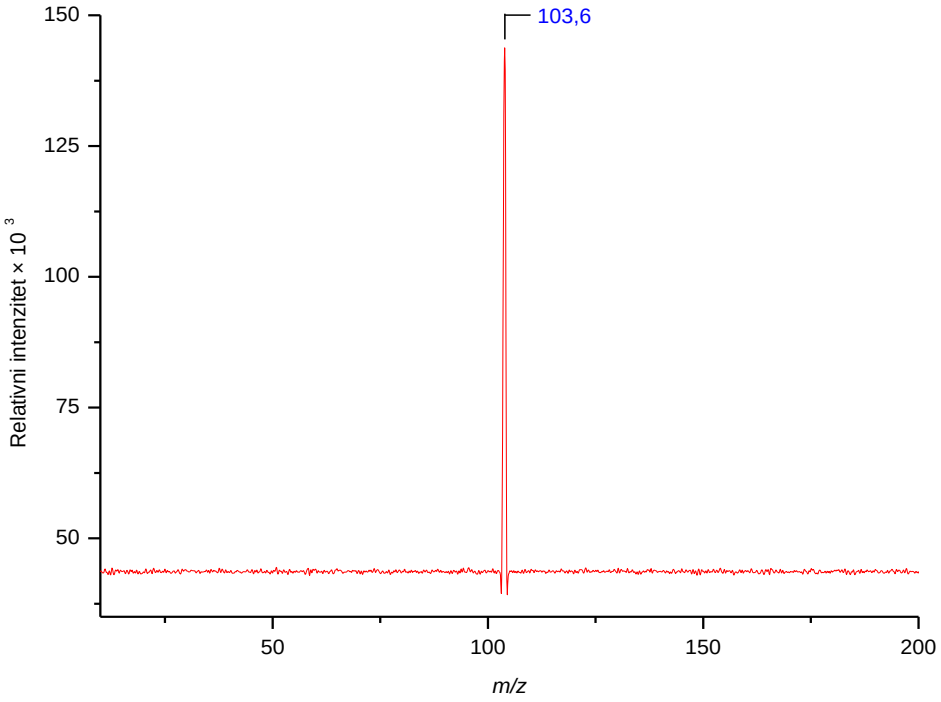


B

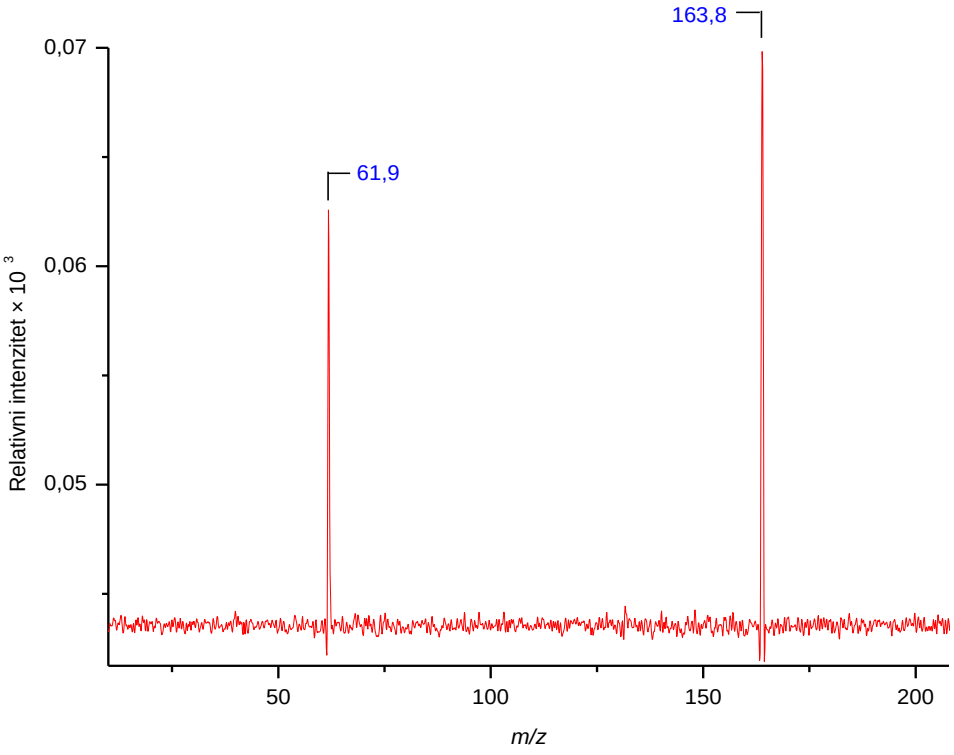
Slika D8. *ESI$^+$-MS/MS spektri dobiveni fragmentacijom iona A) m/z 311,8 i B) m/z 424,7 kod kompleksa [Ag(NO$_3$)(2,5-Cl$_2$py)$_2$],* ***K7****.*



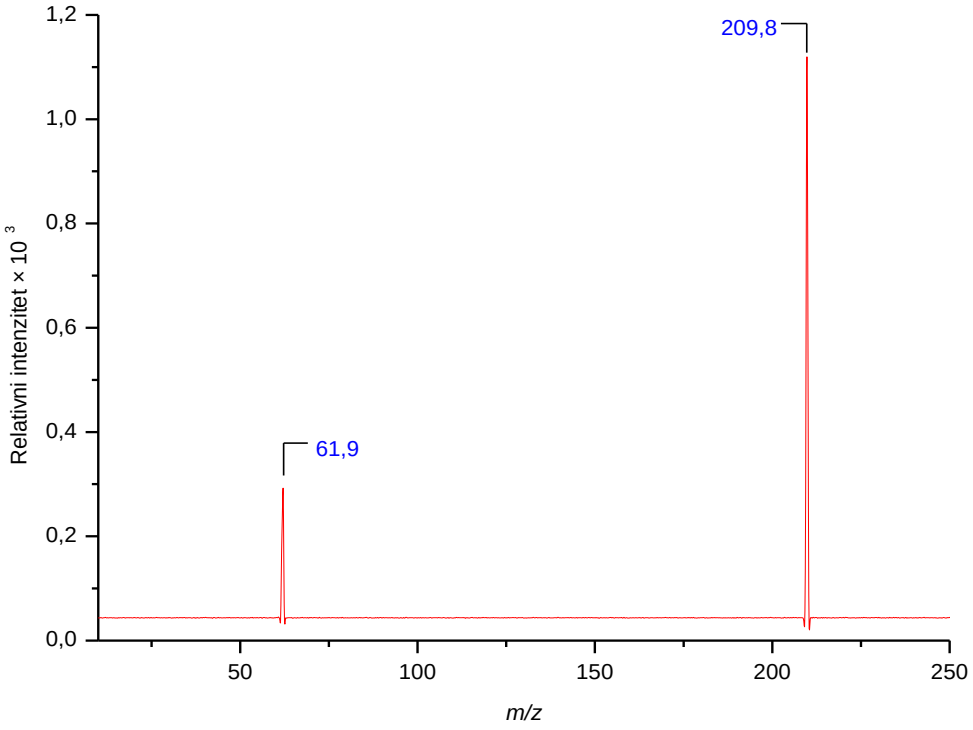
Slika D9. *A) ESI⁺-MS i B) ESI⁻-MS spektri kompleksa* $[Ag(NO_3)(2,5\text{-}Br_2py)_2]$, ***K8***.


103,6
150
125
100
75
50
Relativni intenzitet × 10 3
50
100
150
200
m/z

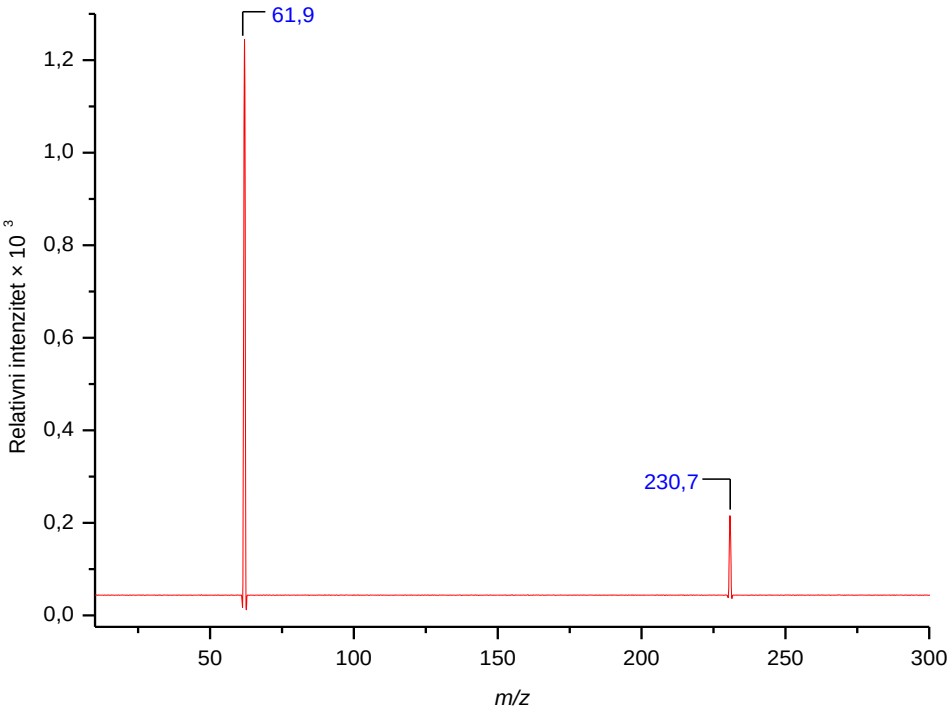
A


163,8
61,9
0,07
0,06
0,05
Relativni intenzitet × 10 3
50
100
150
200
m/z

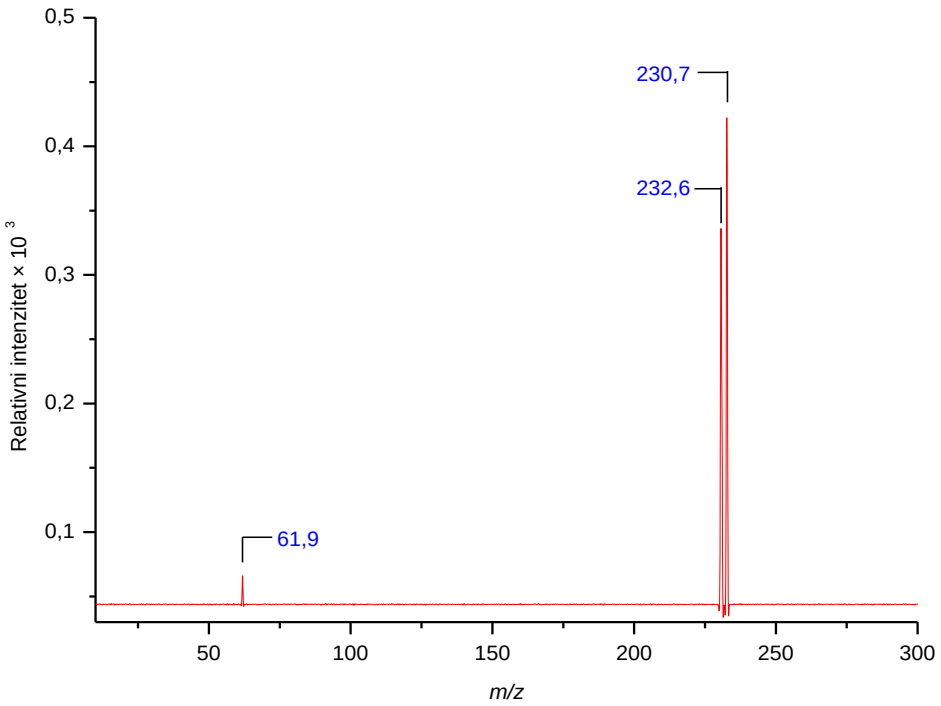
B


209,8
61,9
Relativni intenzitet × 10 3
m/z

C

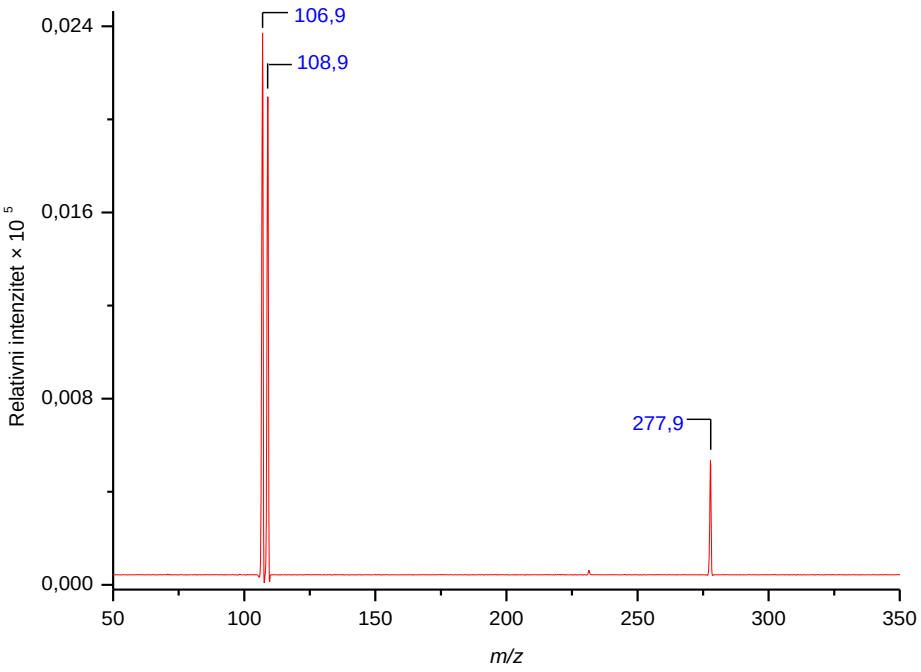

61,9
230,7
Relativni intenzitet × 10 3
m/z

D

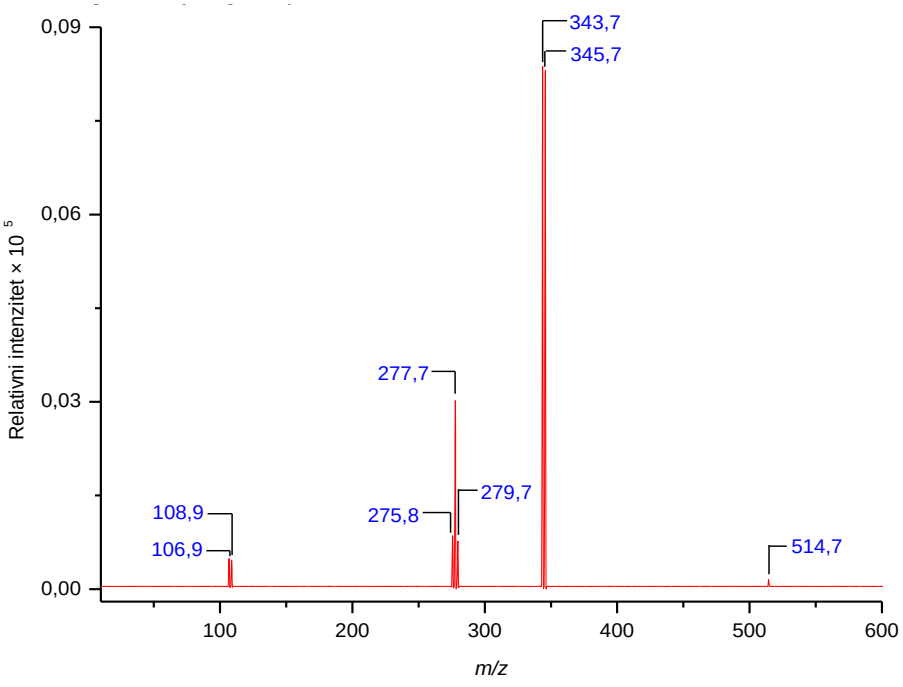


E

Slika D10. *ESI⁻-MS/MS spektri dobiveni fragmentacijom iona A) m/z 103,6, B) m/z 163,8, C) m/z* 209,8, D) *m/z* 230,7 i E) *m/z* 401,3 *kod kompleksa* $[Ag(NO_3)(2,5\text{-}Br_2py)_2]$, ***K8***.

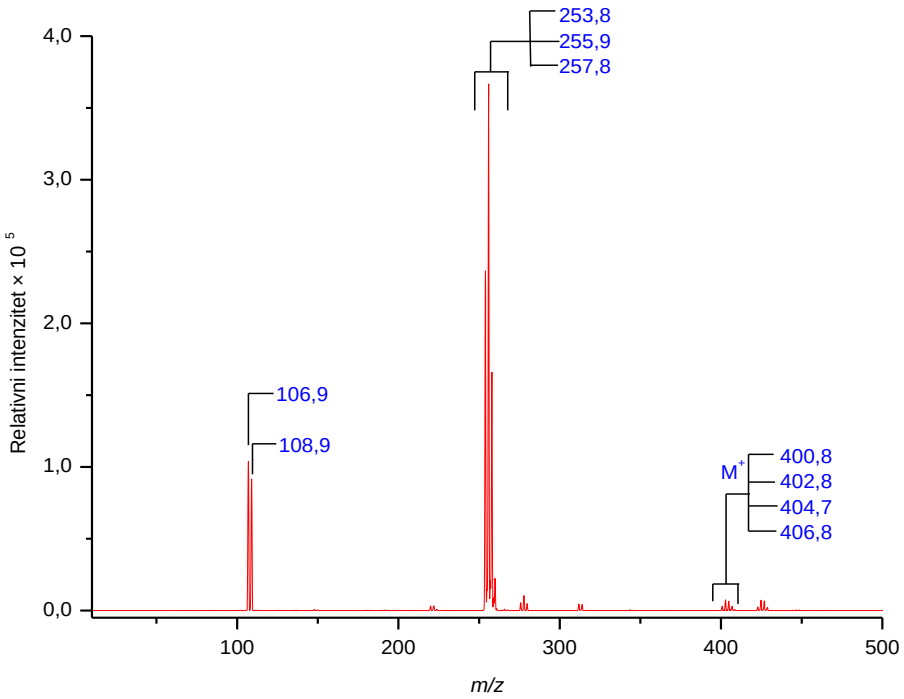


A

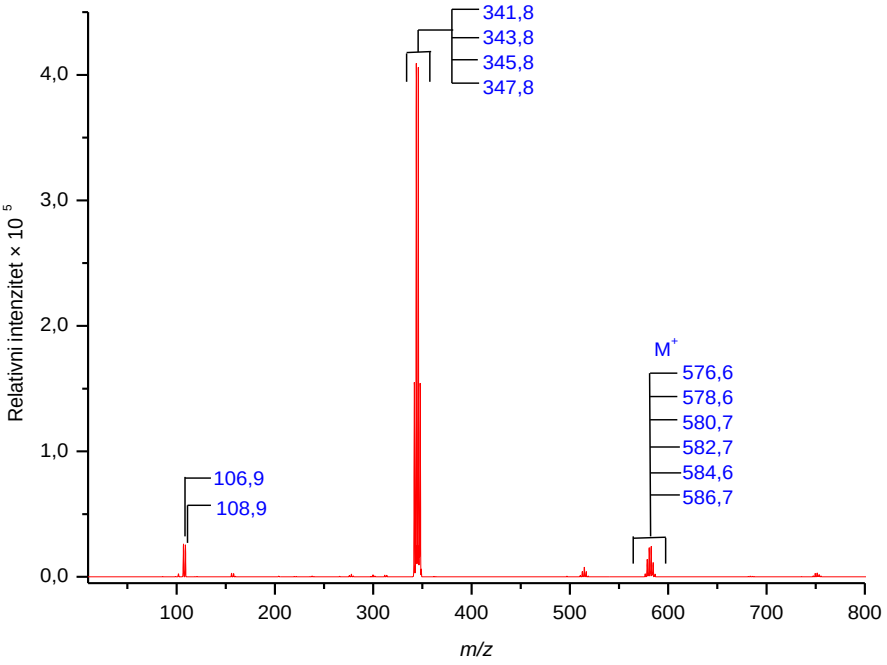


B

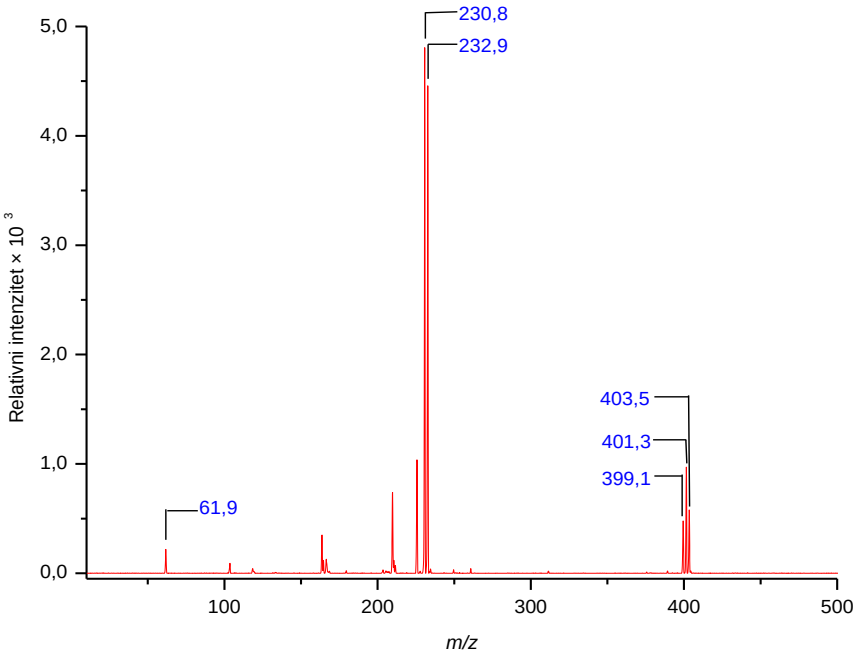
Slika D11. *ESI$^+$-MS/MS spektri dobiveni fragmentacijom iona A) m/z 277,9 i B) m/z 514,7 kod kompleksa [Ag(NO$_3$)(2,5-Br$_2$py)$_2$],* ***K8****.*



Slika D12. *A) ESI⁺-MS i B) ESI⁻-MS spektri kompleksa [Ag(NO₃)(2,6-Cl₂py)₂],* ***K9****.*

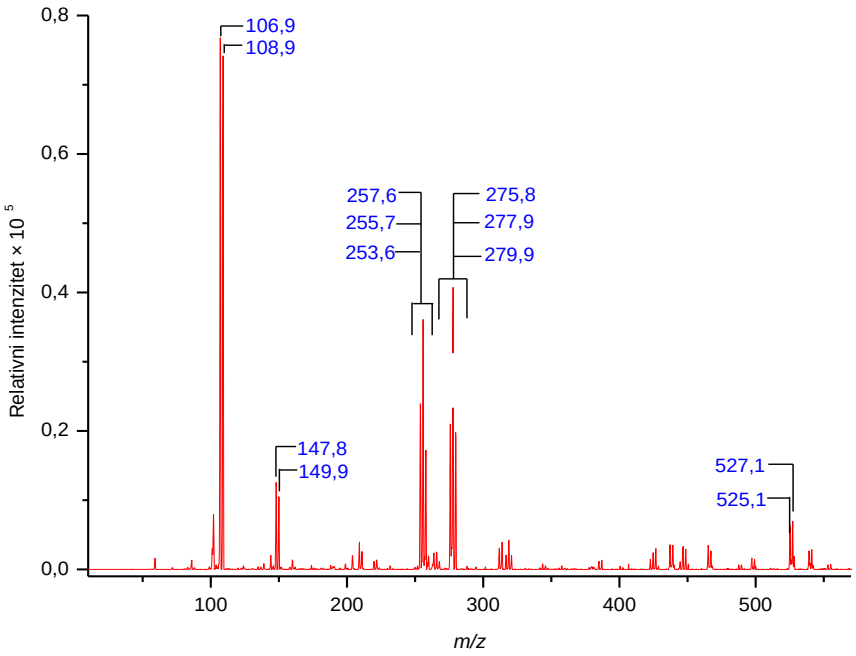


A

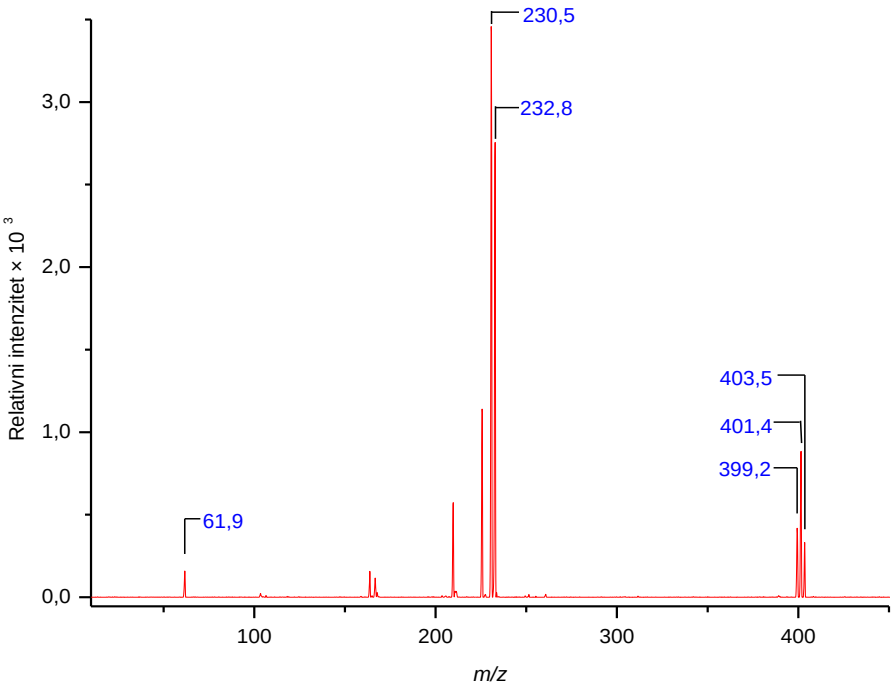


B

Slika D13. *A) ESI⁺-MS i B) ESI⁻-MS spektri kompleksa [Ag(NO₃)(2,6-Br₂py)₂],* ***K10****.*

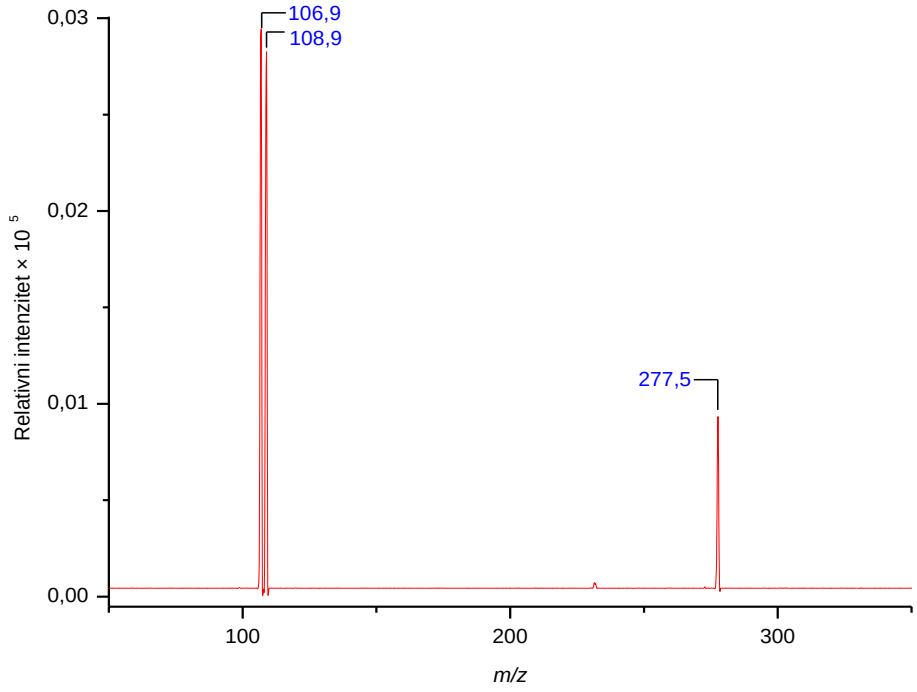


A

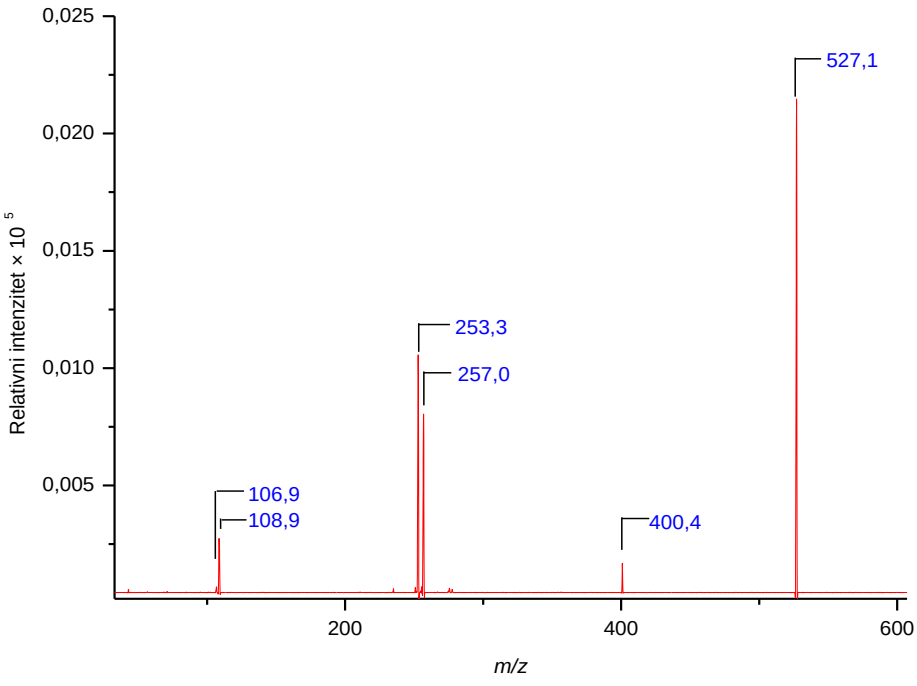


B

Slika D14. *A) ESI⁺-MS i B) ESI⁻-MS spektri kompleksa [Ag(NO₃)(3,5-Cl₂py)₂],* ***K11****. Molekulski ion u ESI⁺-MS spektru nije pronađen.*

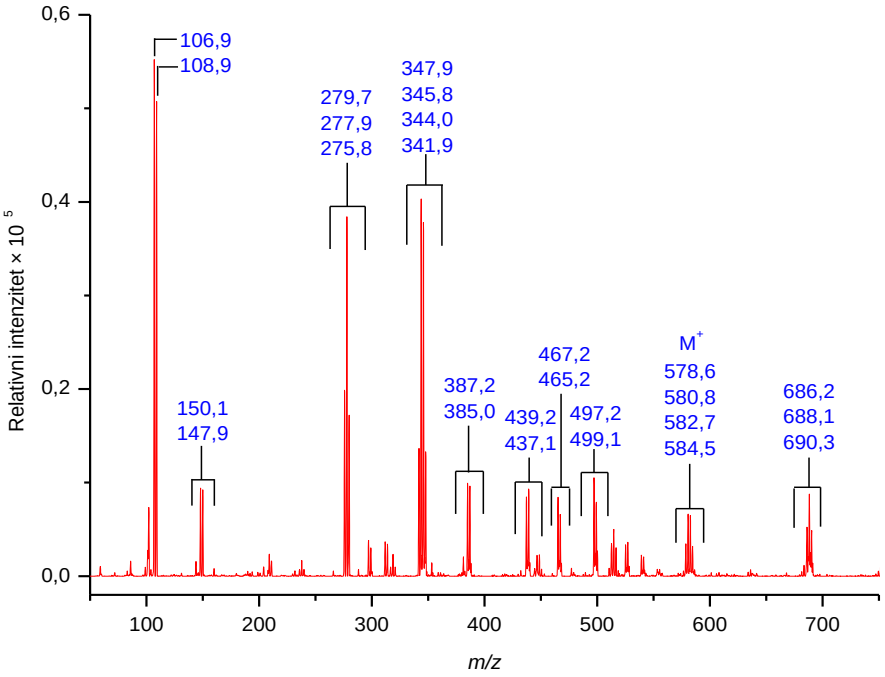


A

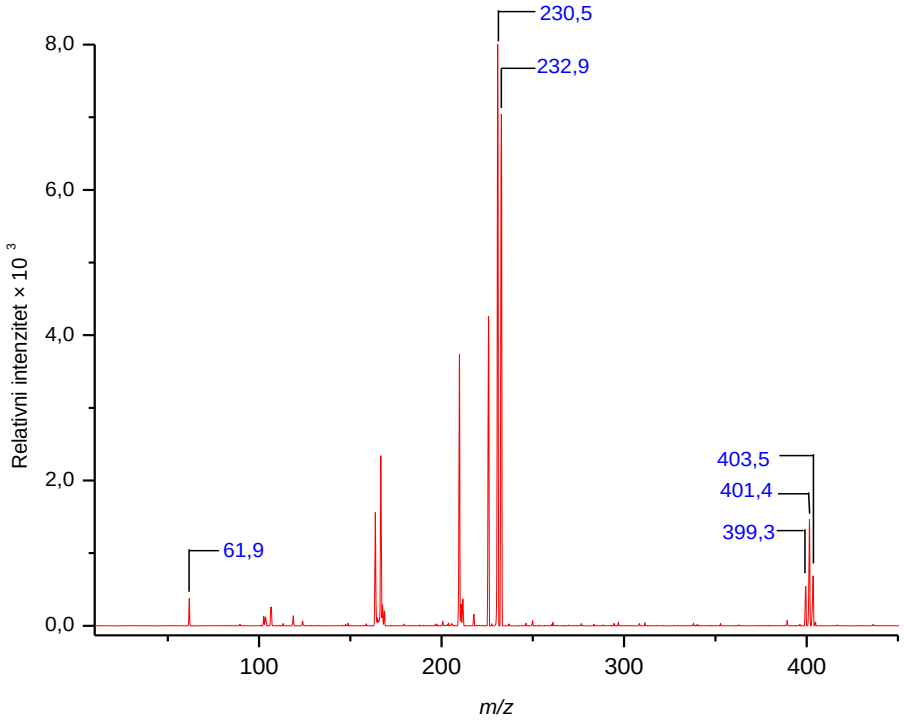


B

Slika D15. *ESI$^+$-MS/MS spektri dobiveni fragmentacijom iona A) m/z 277,5 i B) m/z 527,1 kod kompleksa [Ag(NO$_3$)(3,5-Cl$_2$py)$_2$],* ***K11****.*

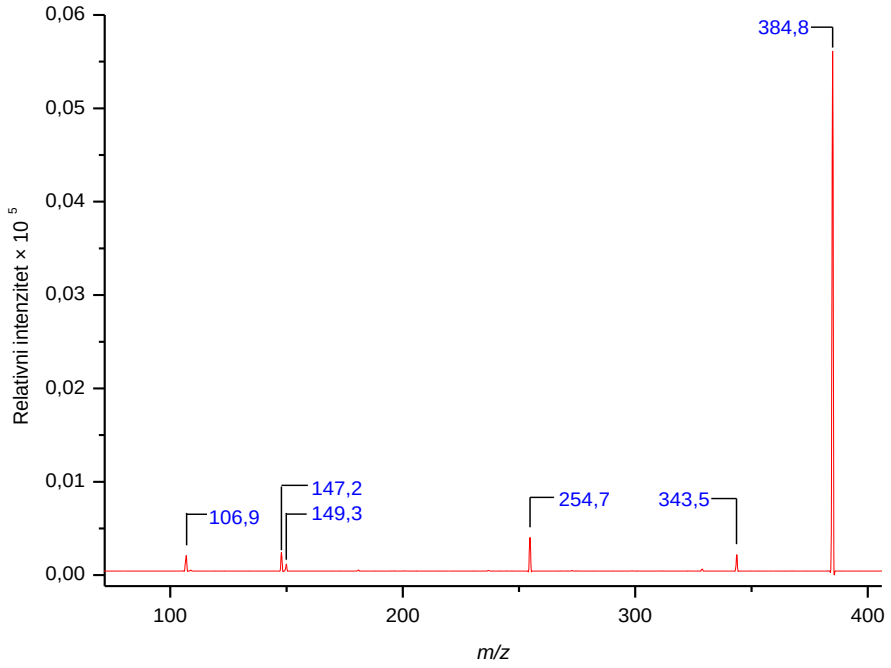


A

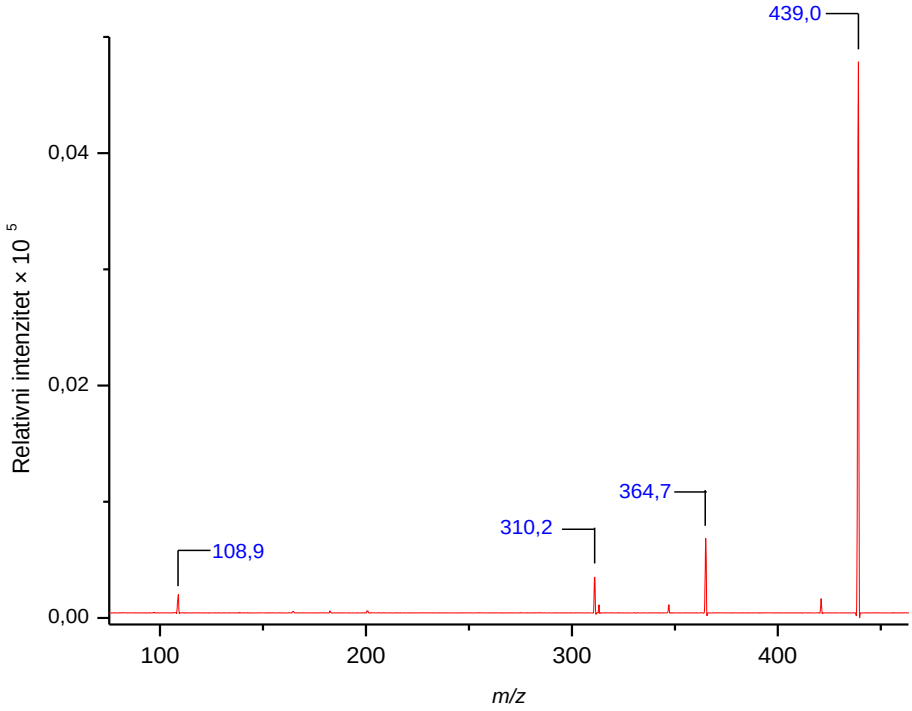


B

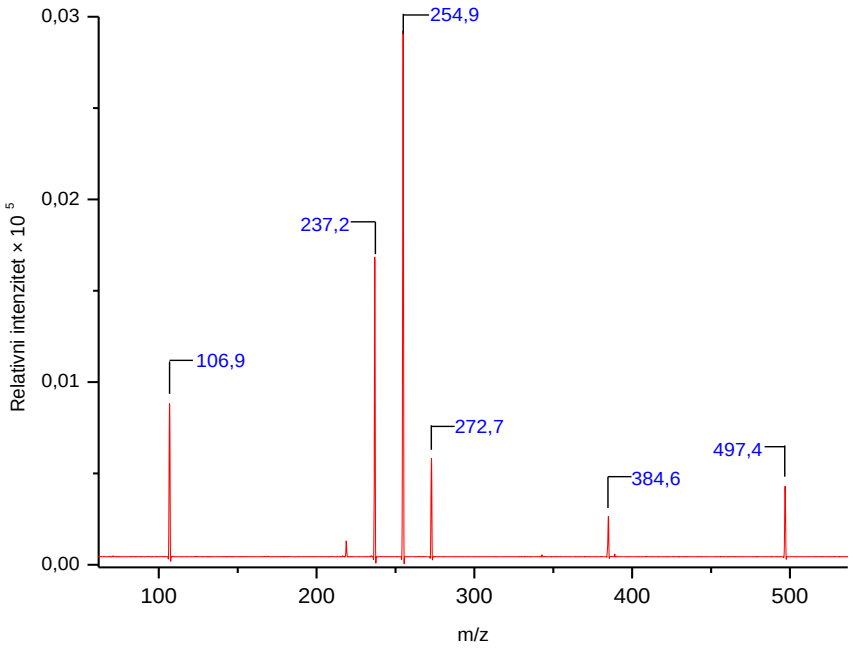
Slika D16. *A) ESI⁺-MS i B) ESI⁻-MS spektri kompleksa [Ag(NO₃)(3,5-Br₂py)₂],* ***K12****.*


0,06
0,05
0,04
0,03
0,02
0,01
0,00
Relativni intenzitet × 10 5
384,8
147,2
149,3
106,9
254,7
343,5
100
200
300
400
m/z

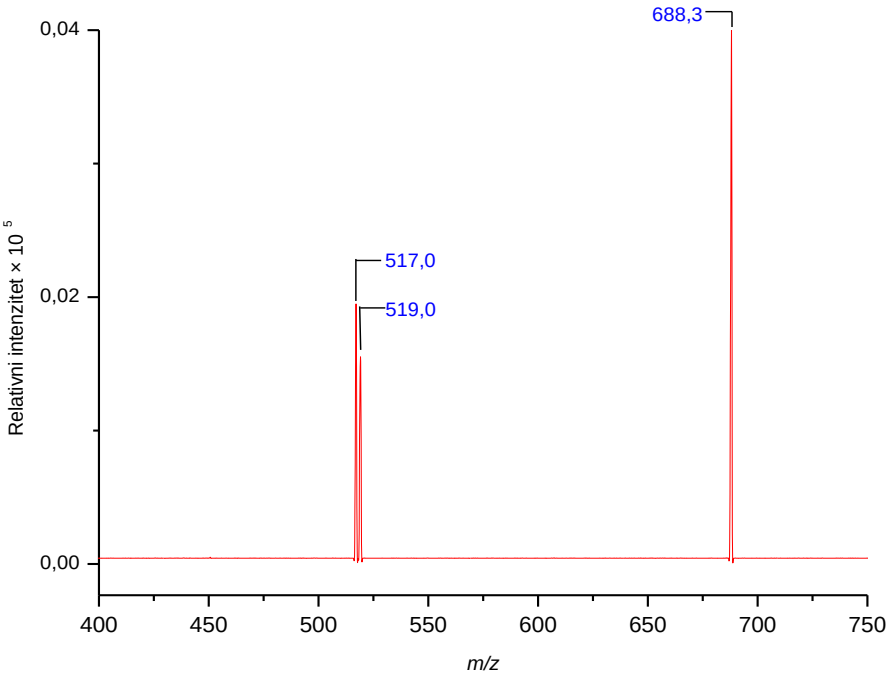
A


0,04
0,02
0,00
Relativni intenzitet × 10 5
439,0
364,7
310,2
108,9
100
200
300
400
m/z

B



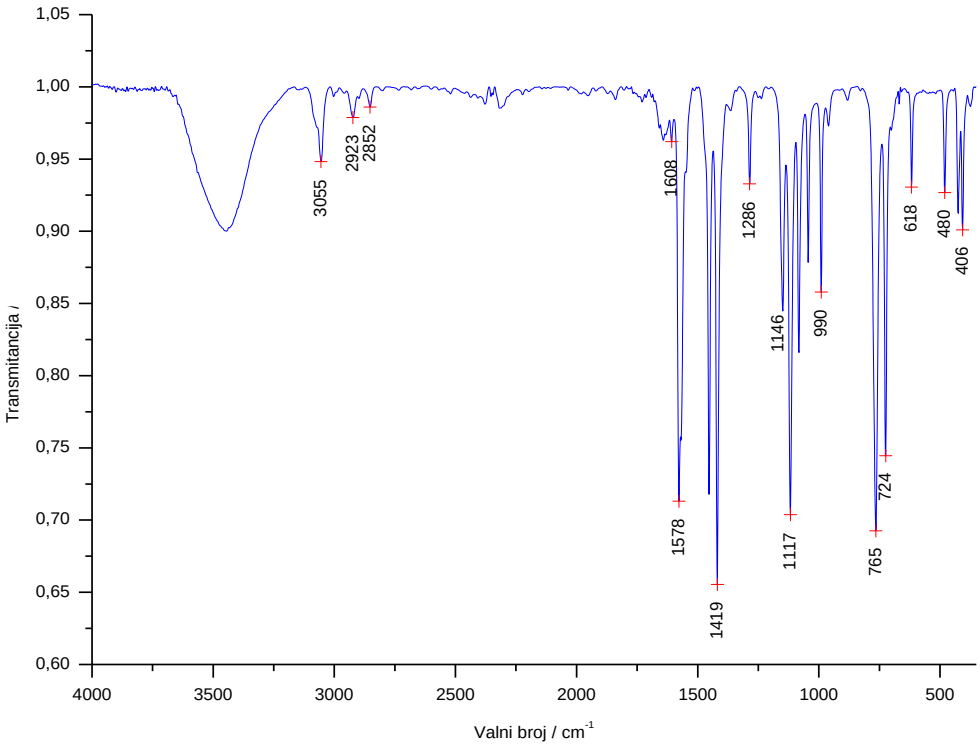
C



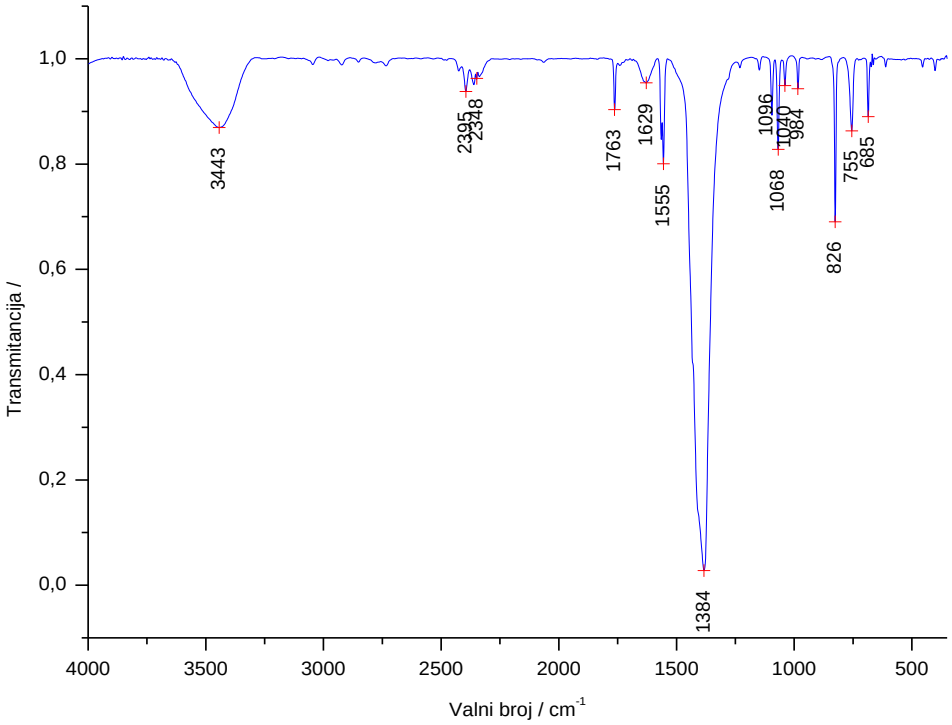
D

Slika D17. *ESI$^+$-MS/MS spektri dobiveni fragmentacijom iona A) m/z 385,0, B) m/z 439,0, C) m/z* 497,4 i D) *m/z* 688,3 *kod kompleksa [Ag(NO$_3$)(3,5-Br$_2$py)$_2$],* ***K12****.*

8.2. Infracrveni spektri

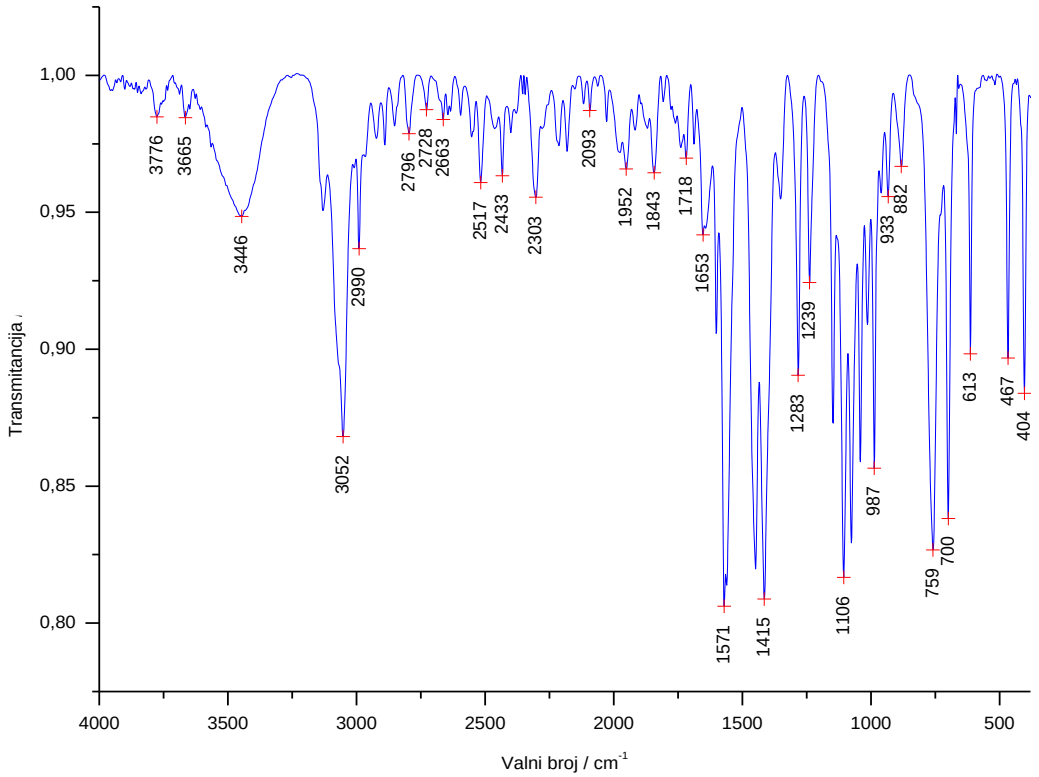


A

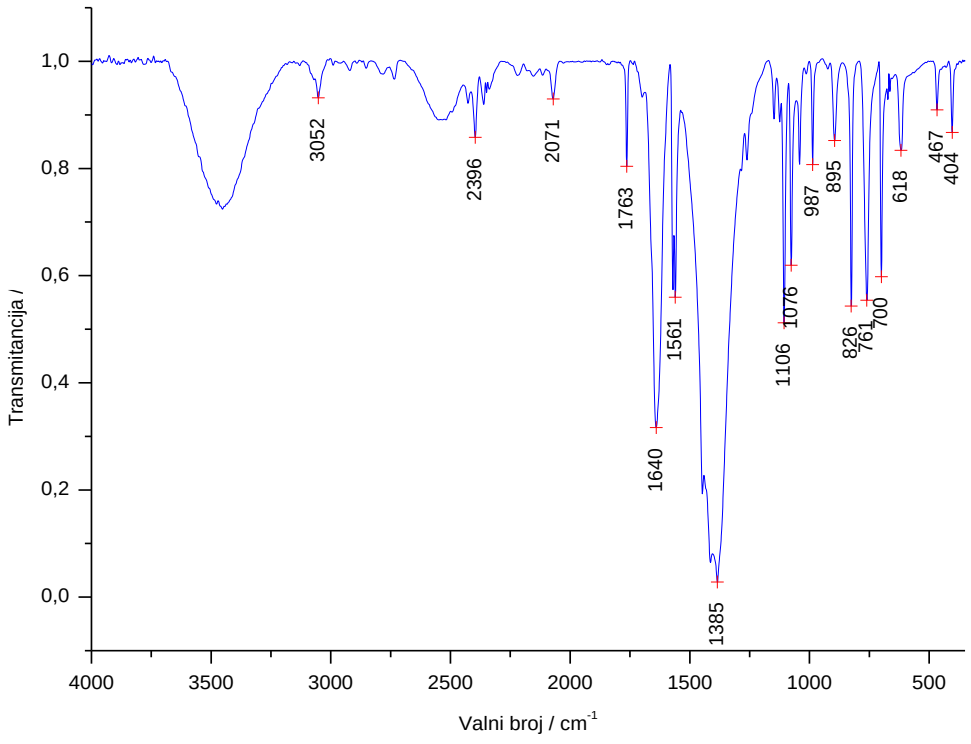


B

Slika D18. *Spektri IR A) 2-Clpy (**L1**)i B) [Ag(NO$_3$)(2-Clpy)$_2$] (**K1**).*

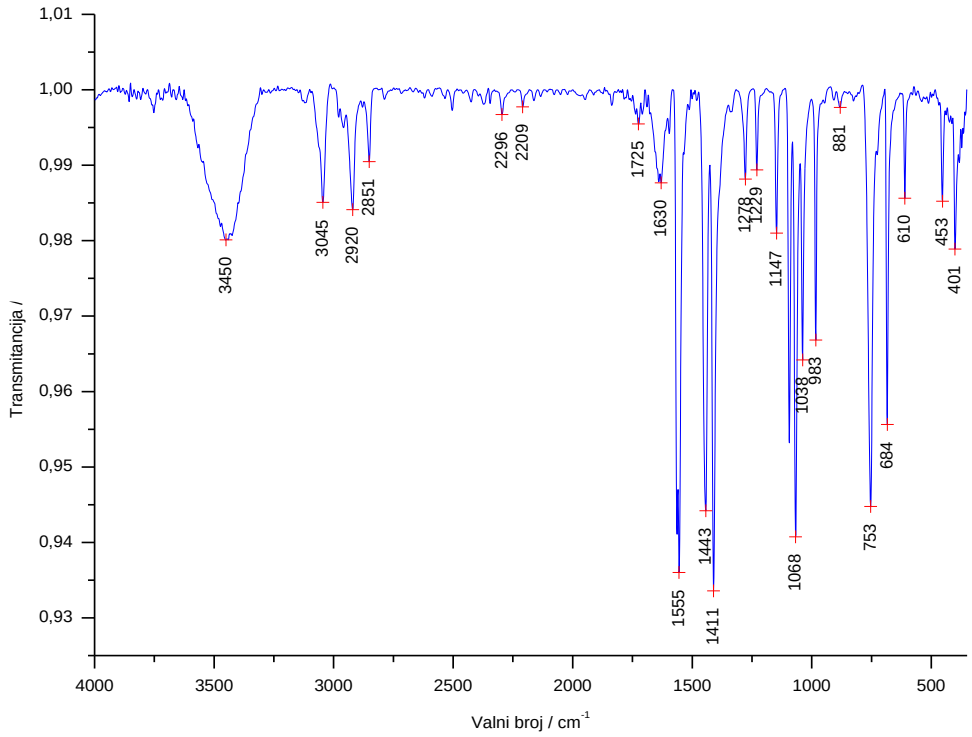


A

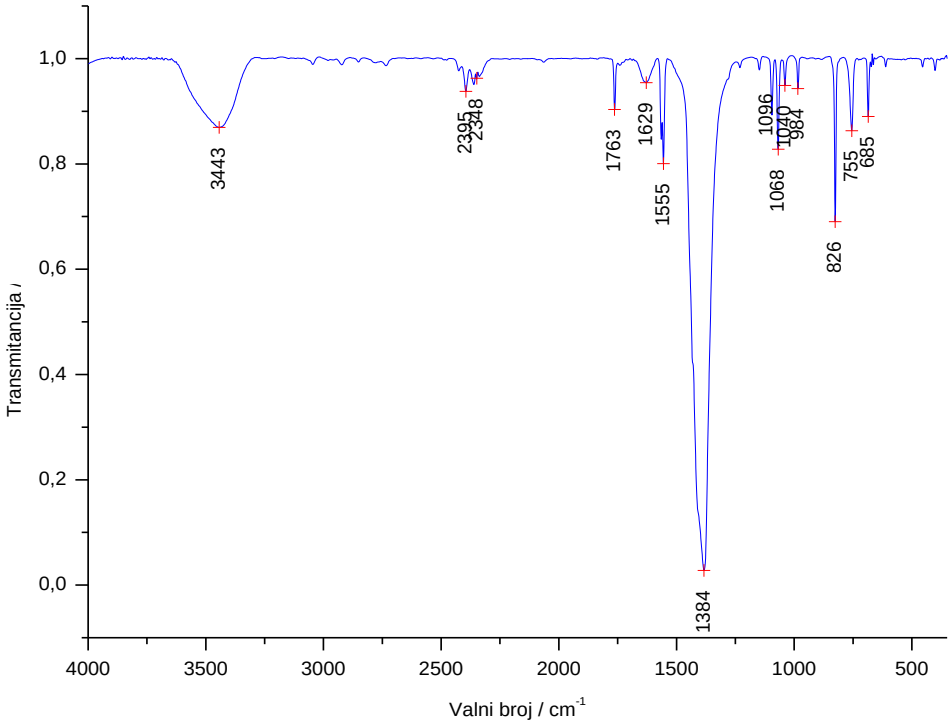


B

Slika D19. *Spektri IR A) 2-Brpy (**L2**) i B) [Ag(NO$_3$)(2-Brpy)$_2$] (**K2**).*

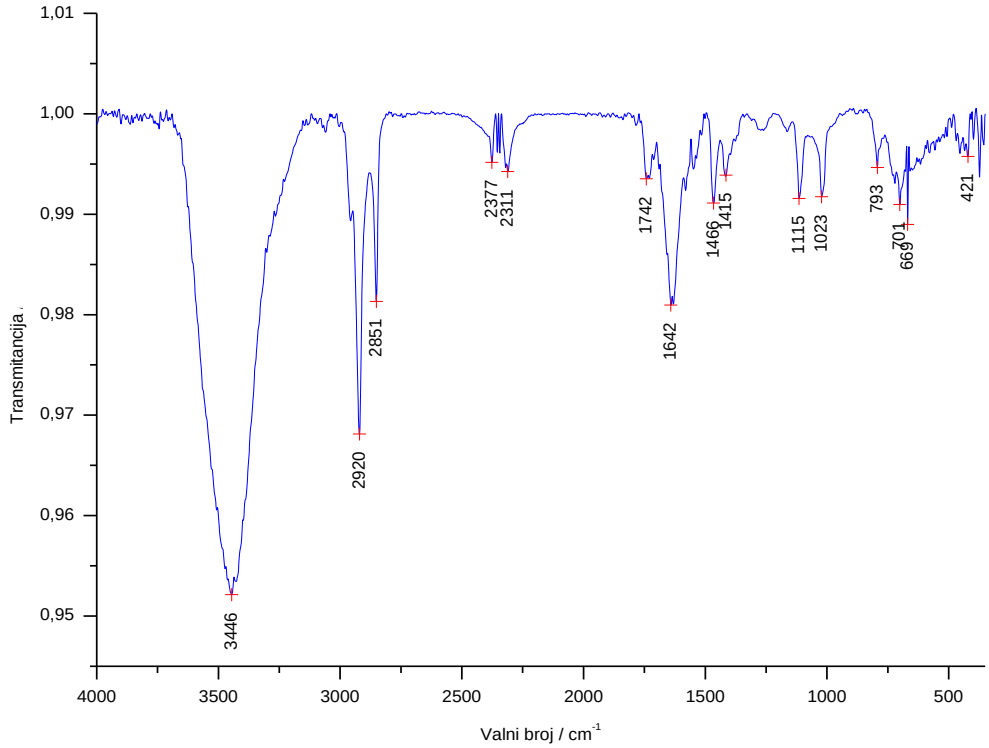


A

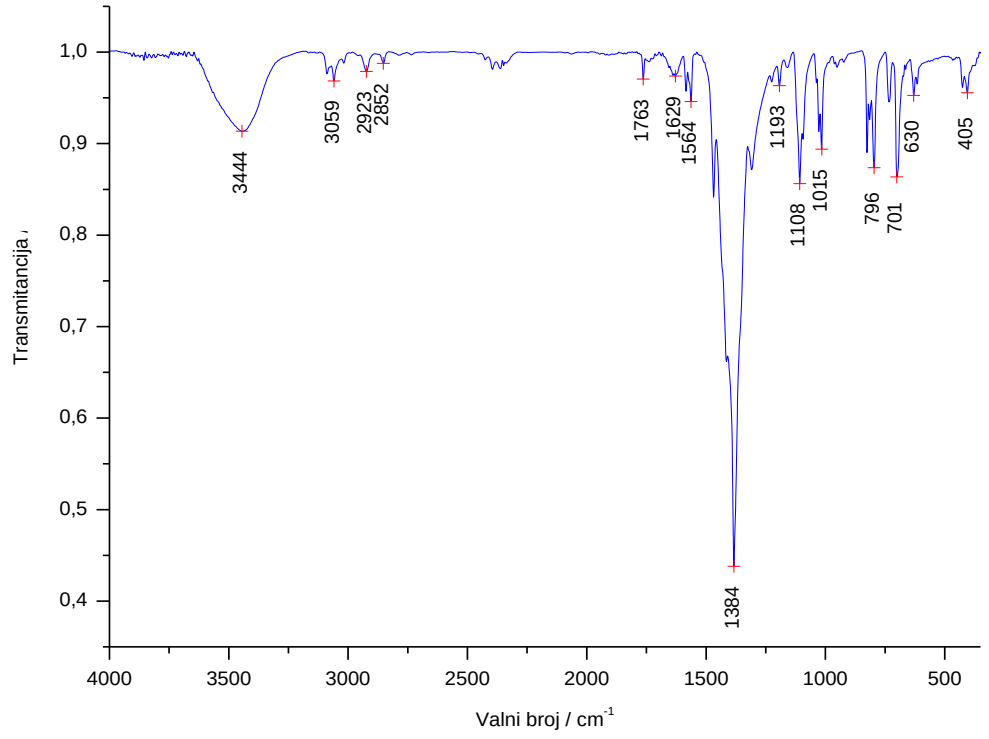


B

Slika D20. *Spektri IR A) 2-Ipy (**L3**) i B) [Ag(NO$_3$)(2-Ipy)$_2$] (**K3**).*

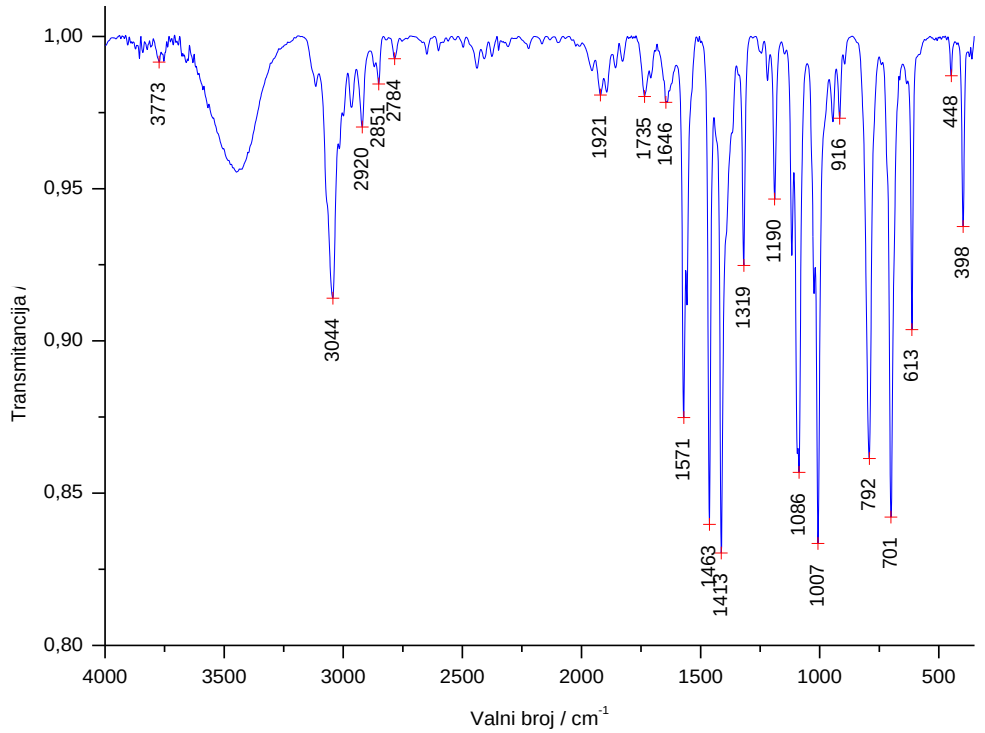


A

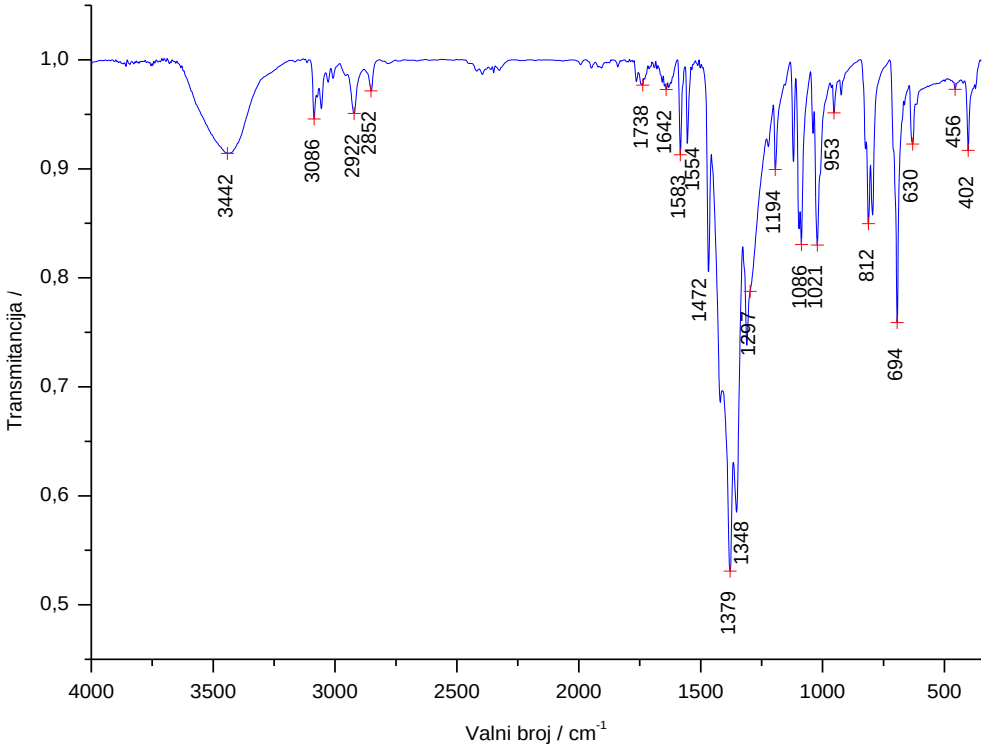


B

Slika D21. *Spektri IR A) 3-Clpy (**L4**) i B) [Ag(NO$_3$)(3-Clpy)$_2$] (**K4**).*

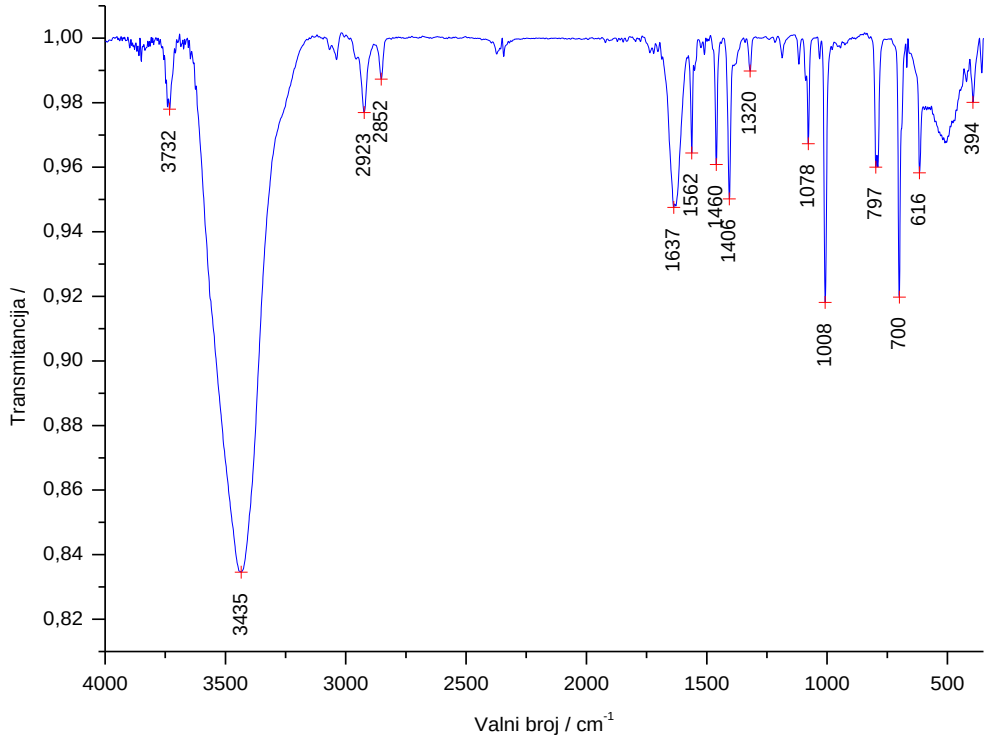


A

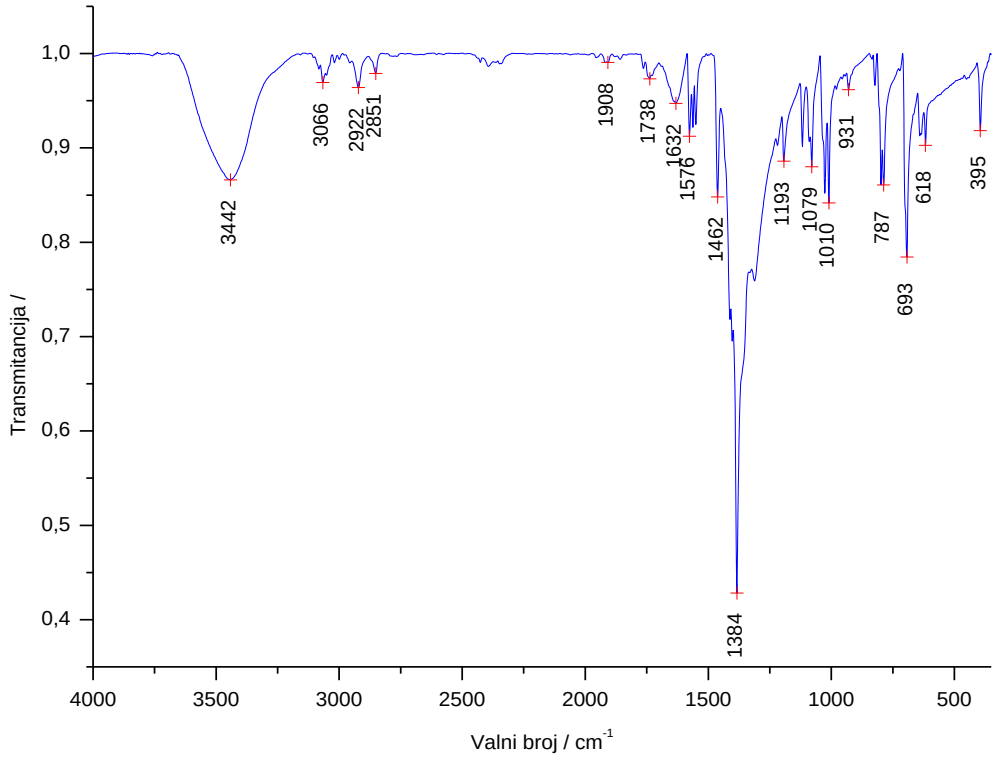


B

Slika D22. *Spektri IR A) 3-Brpy (**L5**) i B) [Ag(NO$_3$)(3-Brpy)$_2$] (**K5**).*

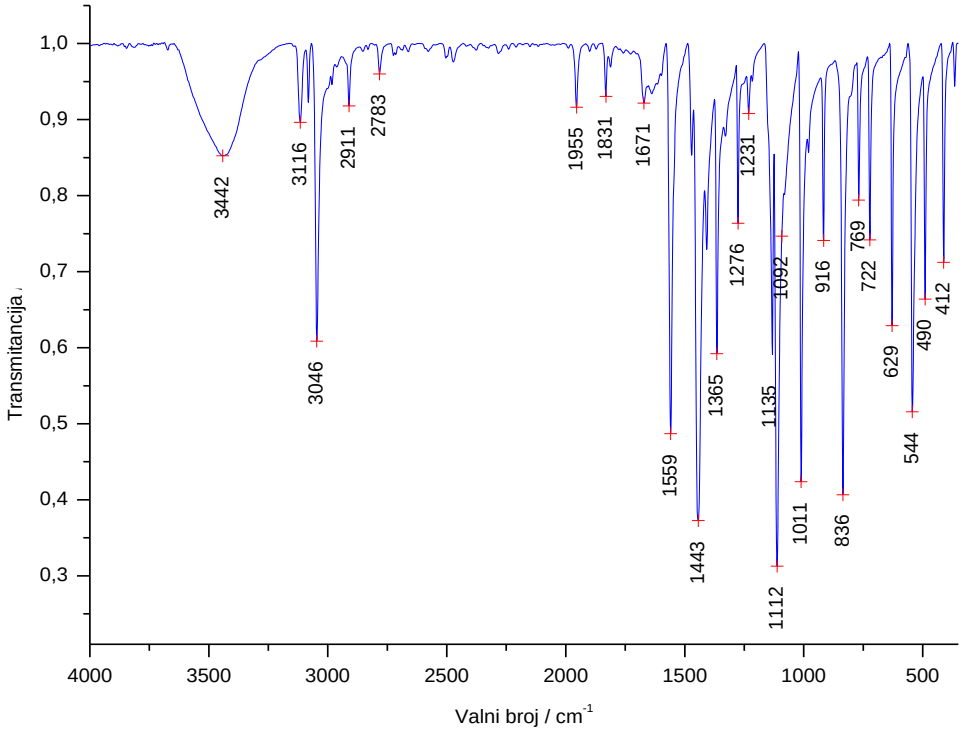


A

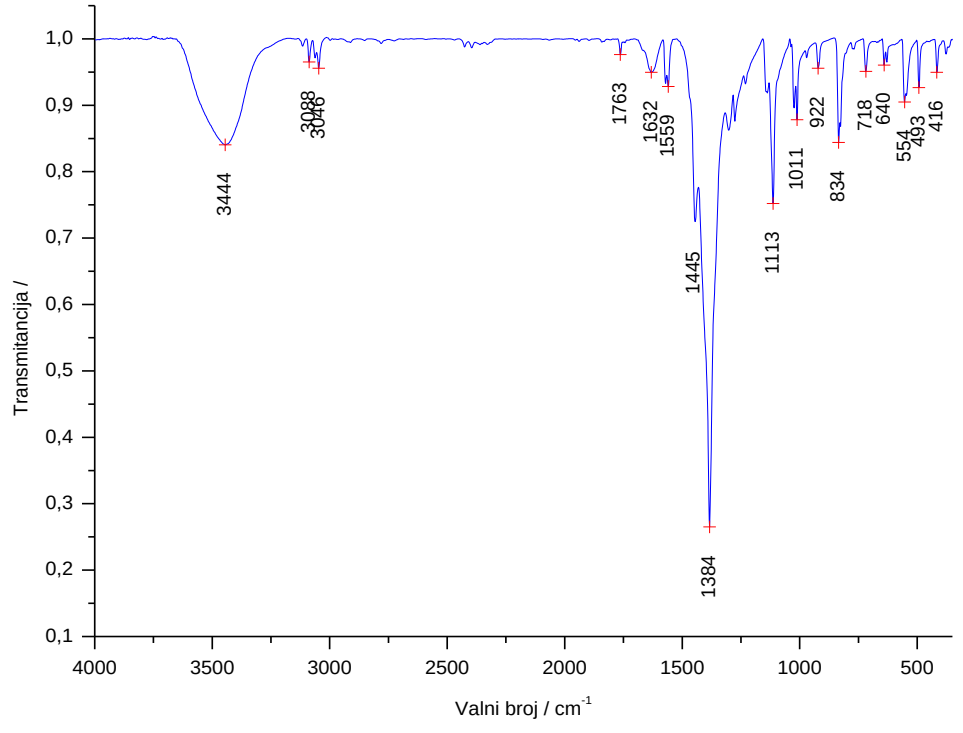


B

Slika D23. *Spektri IR A) 3-Ipy (**L6**) i B) [Ag(NO$_3$)(3-Ipy)$_2$] (**K6**).*

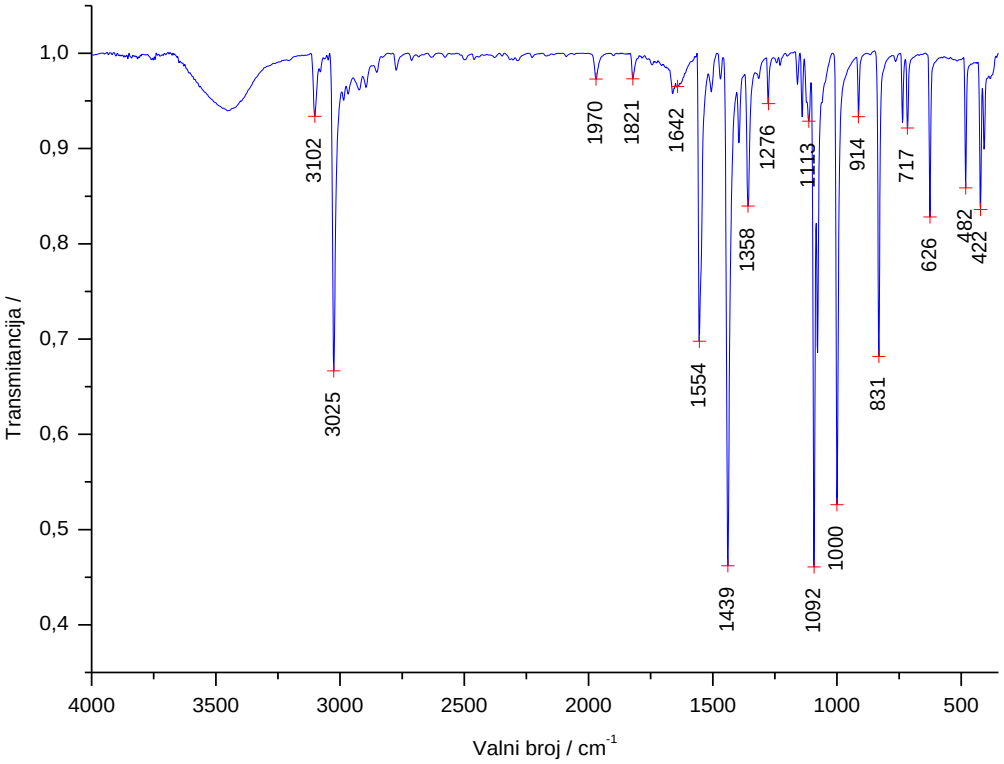


A

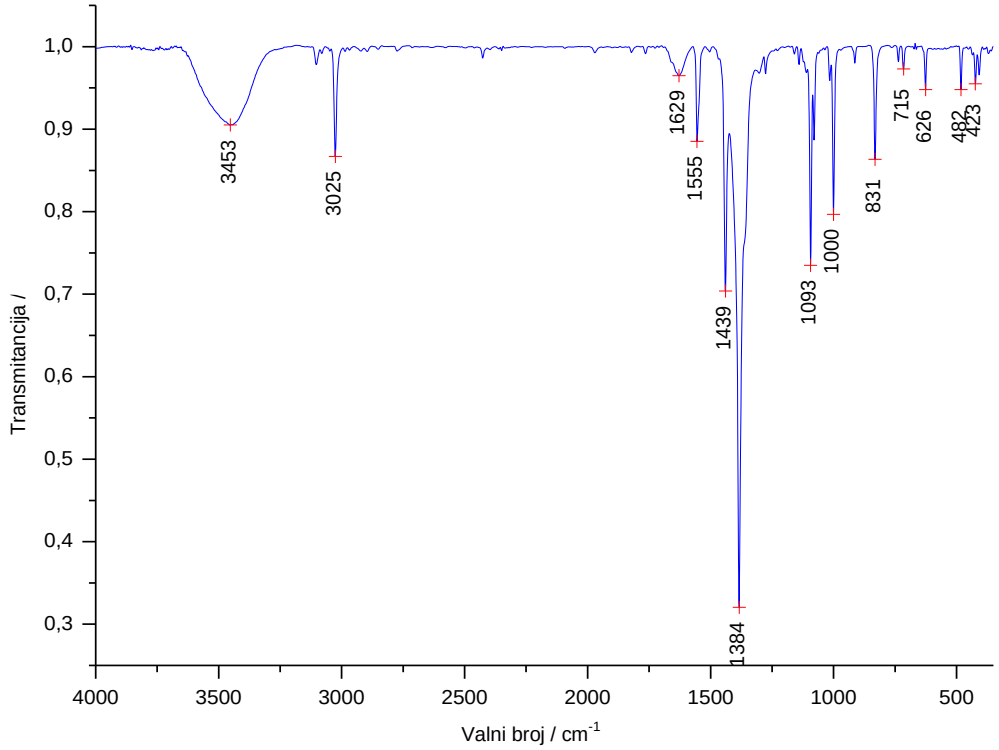


B

Slika D24. *Spektri IR A) 2,5-Cl_2py (**L7**) i B) [Ag(NO_3)(2,5-Cl_2py)$_2$] (**K7**).*

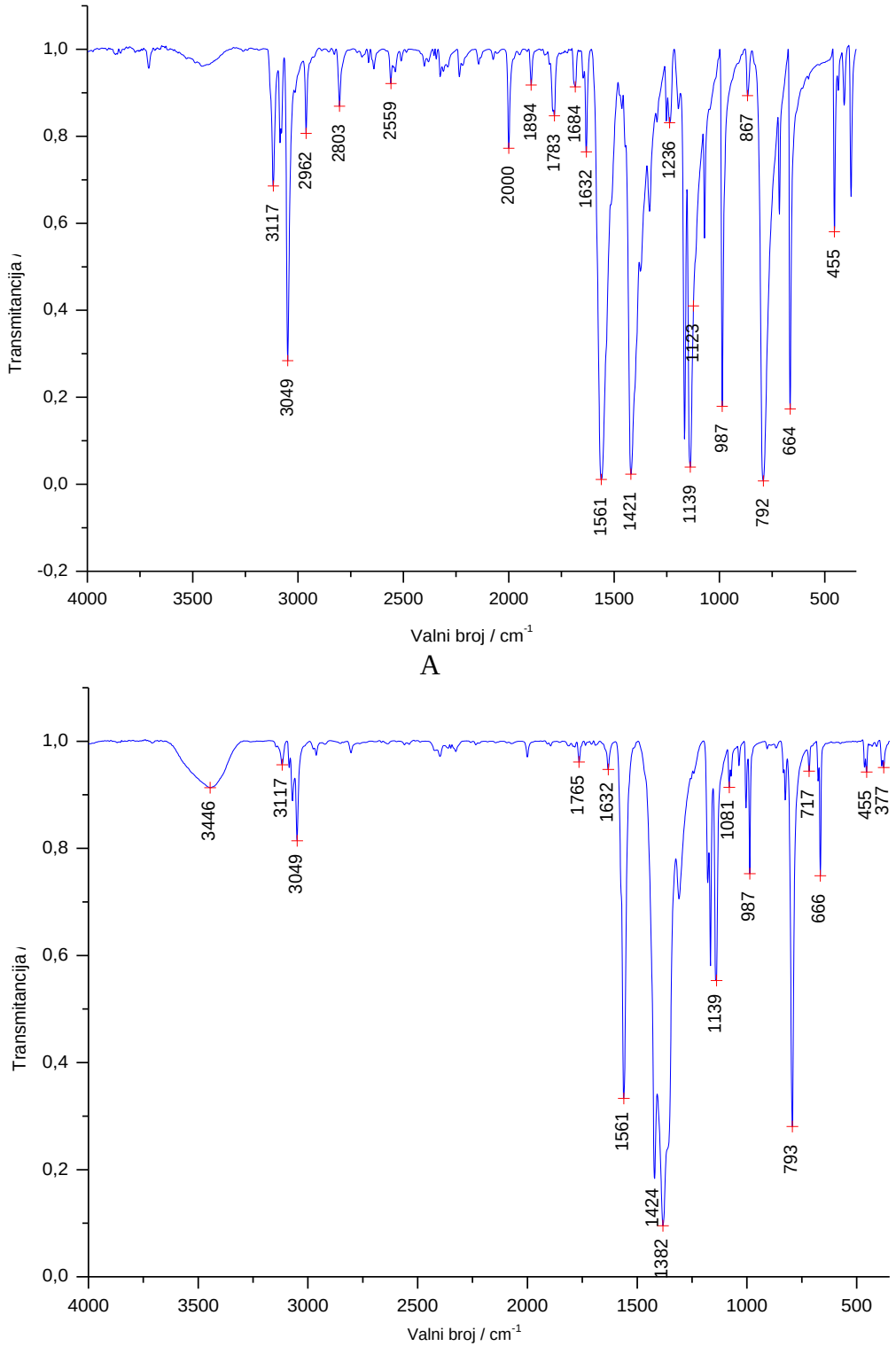


A

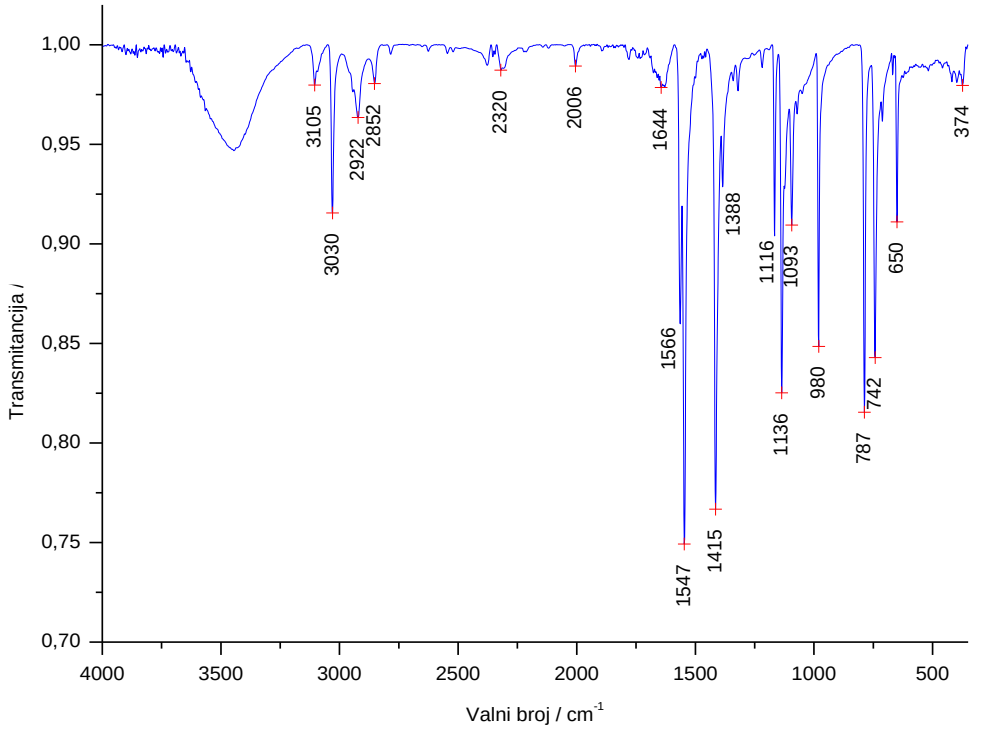


B

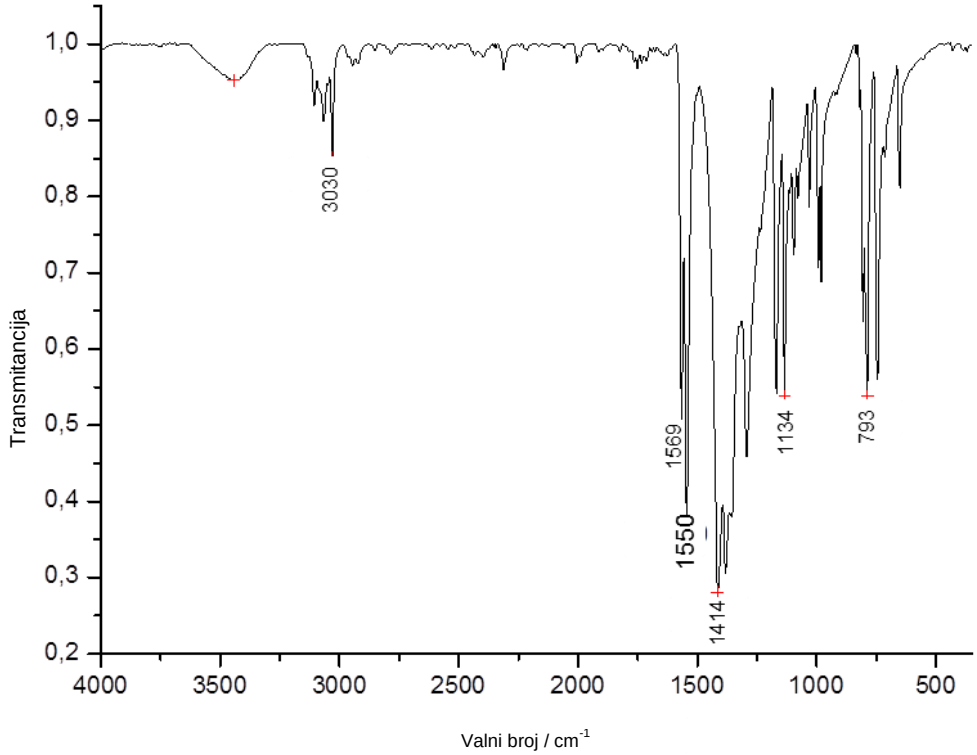
Slika D25. *Spektri IR A) 2,5-Br_2py (**L8**) i B) [Ag(NO_3)(2,5-Br_2py)$_2$] (**K8**).*



Slika D26. *Spektri IR A) 2,6-Cl_2py (**L9**) i B) [Ag(NO_3)(2,6-Cl_2py)$_2$] (**K9**).*

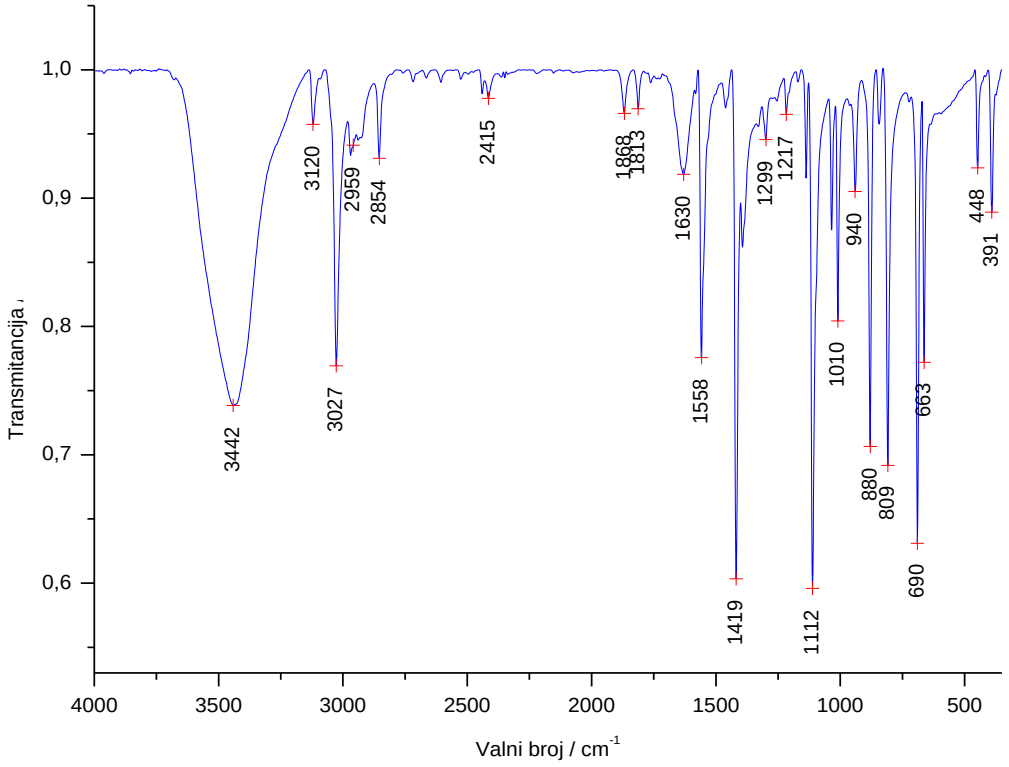


A

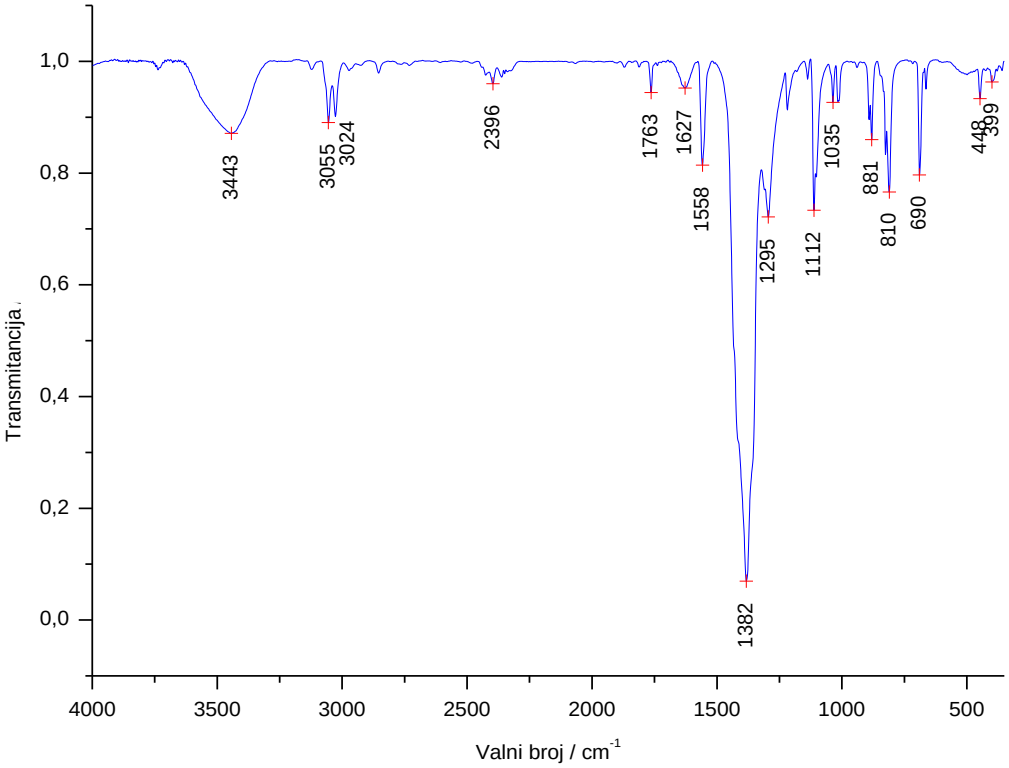


B

Slika D27. *Spektri IR A) 2,6-Br_2py* ***(L10)*** *i B) [Ag(NO_3)(2,6-Br_2py)$_2$]* ***(K10).***

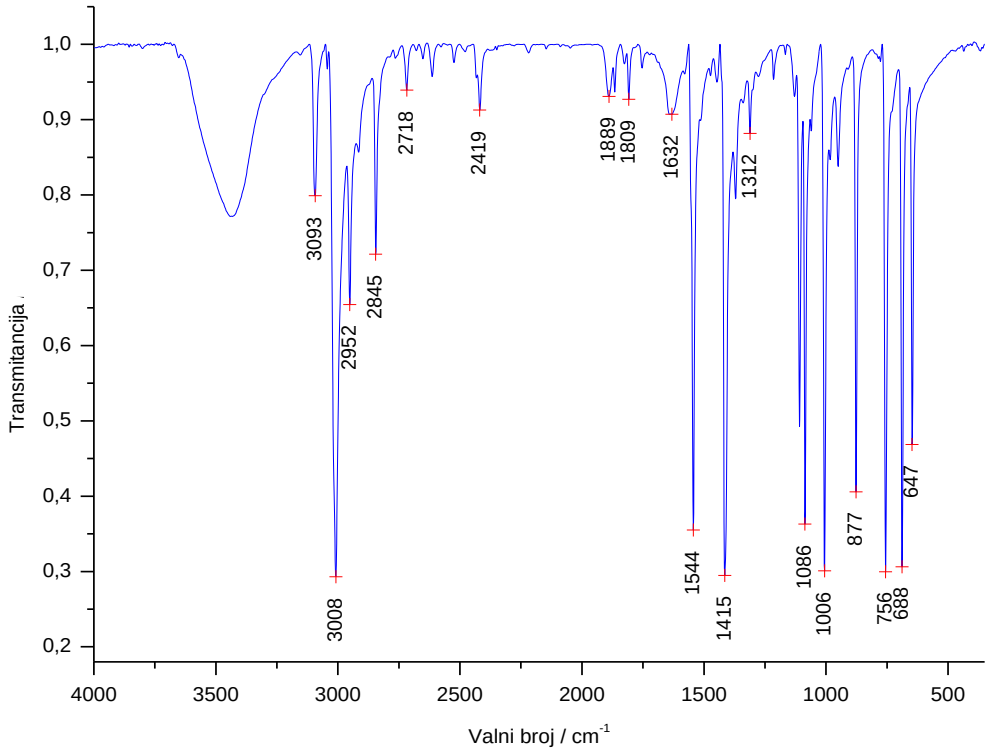


A

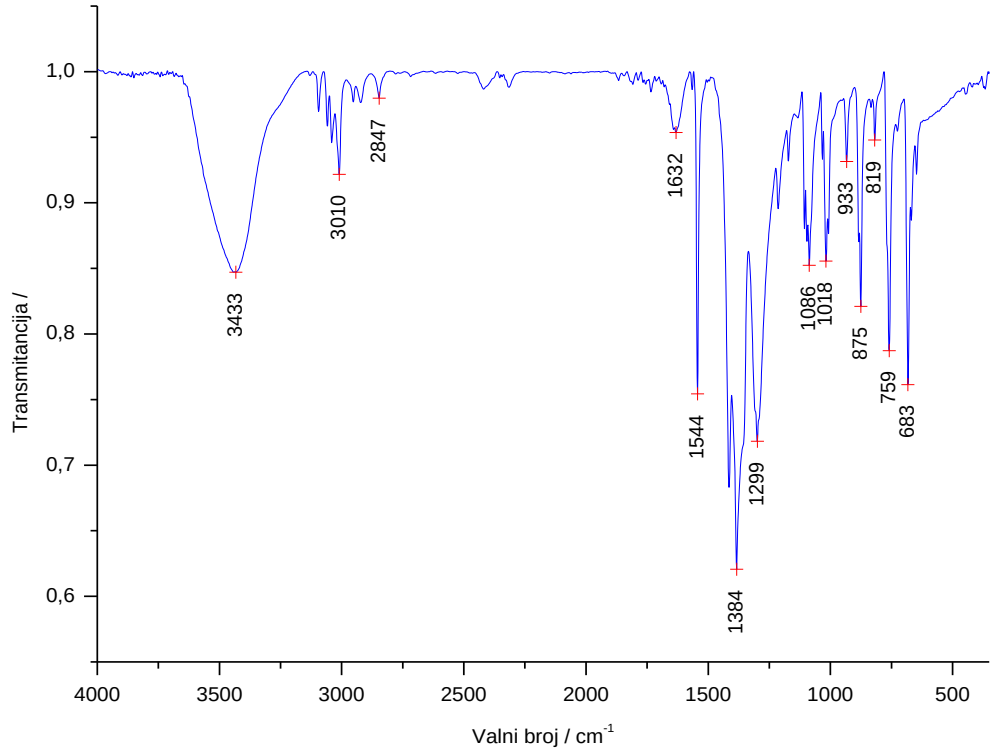


B

Slika D28. *Spektri IR A) 3,5-Cl_2py (**L11**) i B) [$Ag(NO_3)$(3,5-Cl_2py)$_2$] (**K11**).*



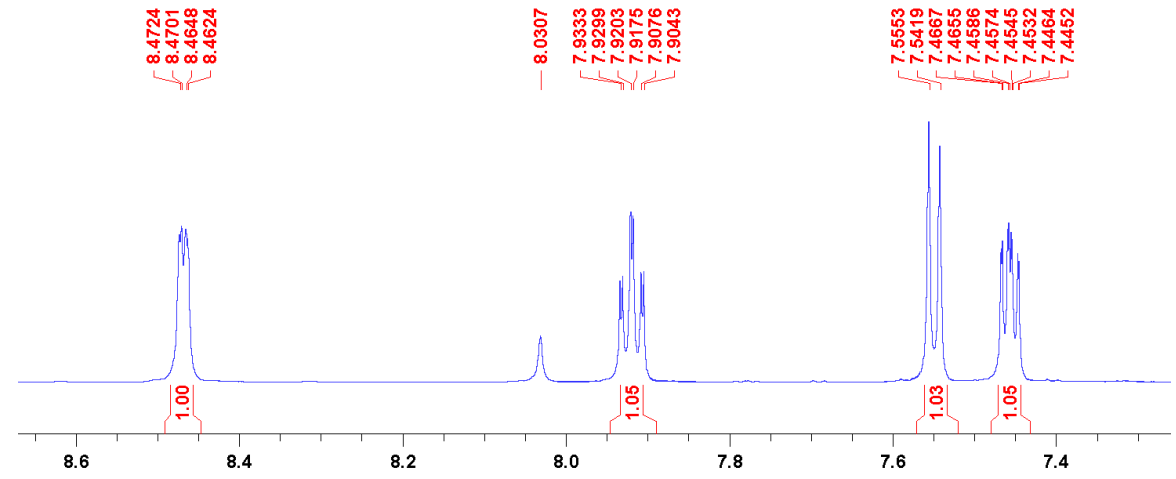
A



B

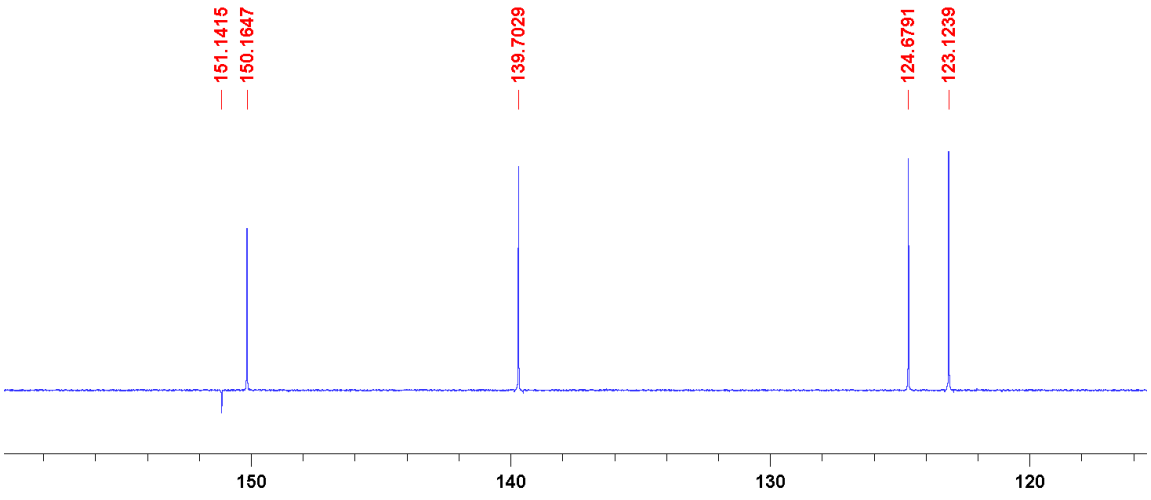
Slika D29. *Spektri IR A) 3,5-Br_2py (**L12**) i B) [$Ag(NO_3)$(3,5-Br_2py)$_2$] (**K12**).*

8.3. Slike spektara i drugi odabrani podaci dobiveni spektroskopijom NMR



δ / ppm

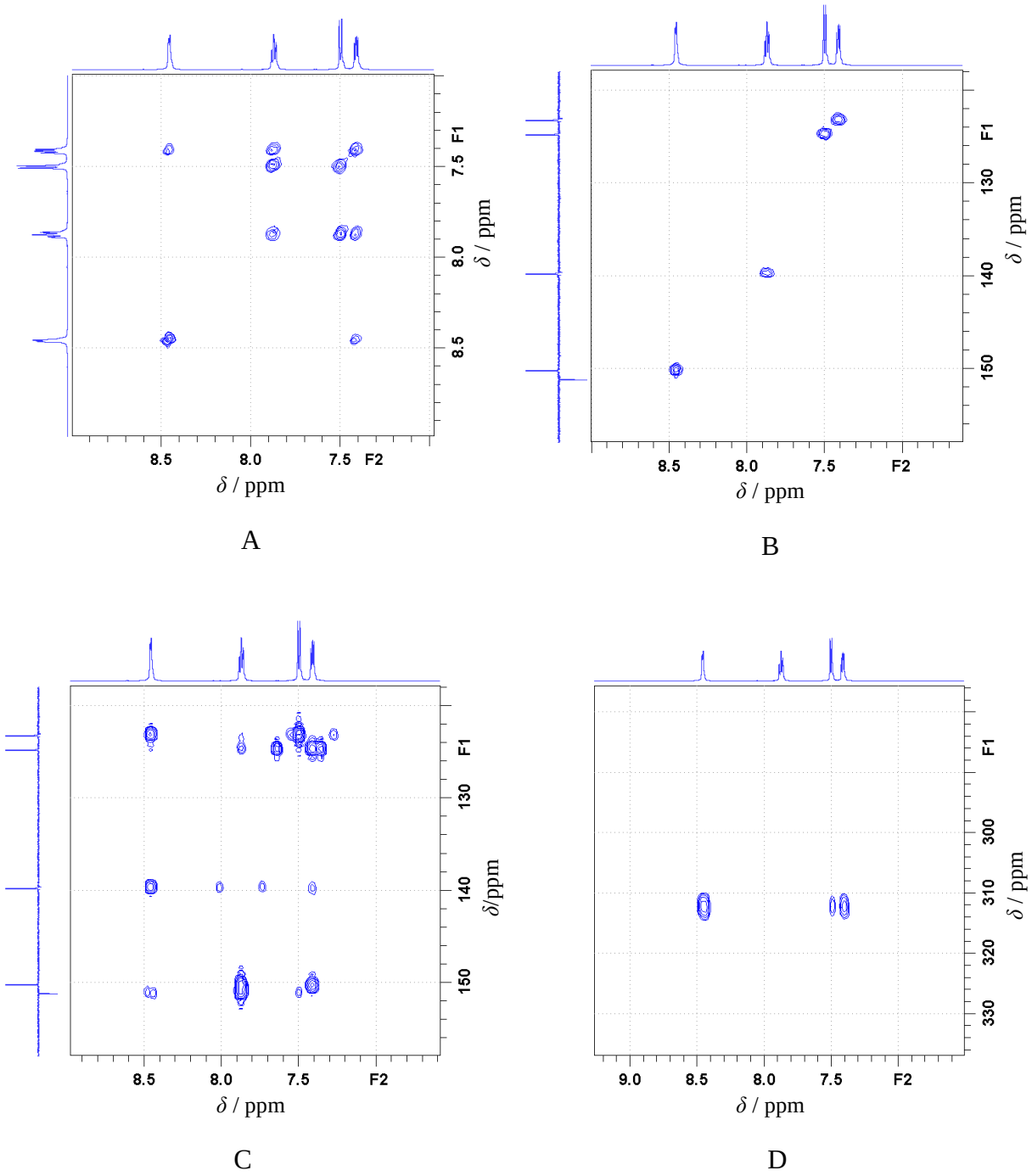
A



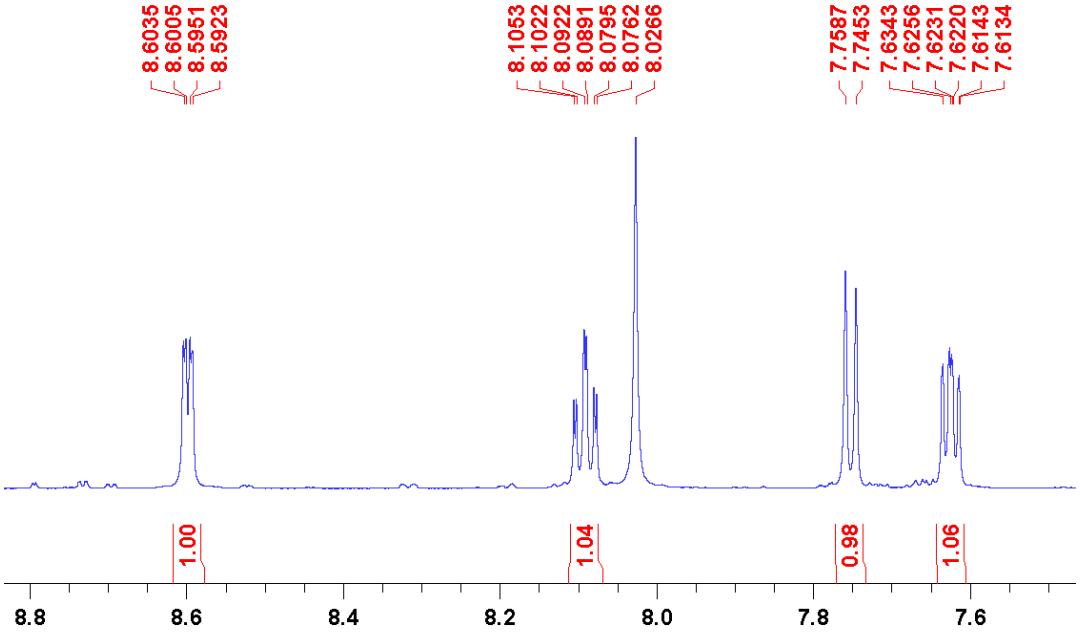
δ / ppm

B

Slika D30. *A) ^{1}H i B) ^{13}C spektri spoja 2-Clpy, (**L1**).*

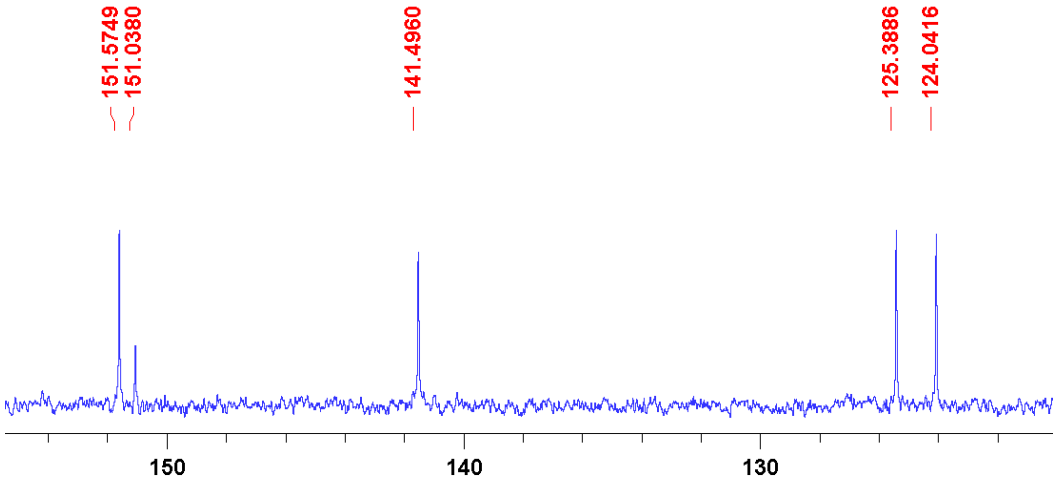


Slika D31. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR spoja 2-Clpy,* ***(L1)****.*



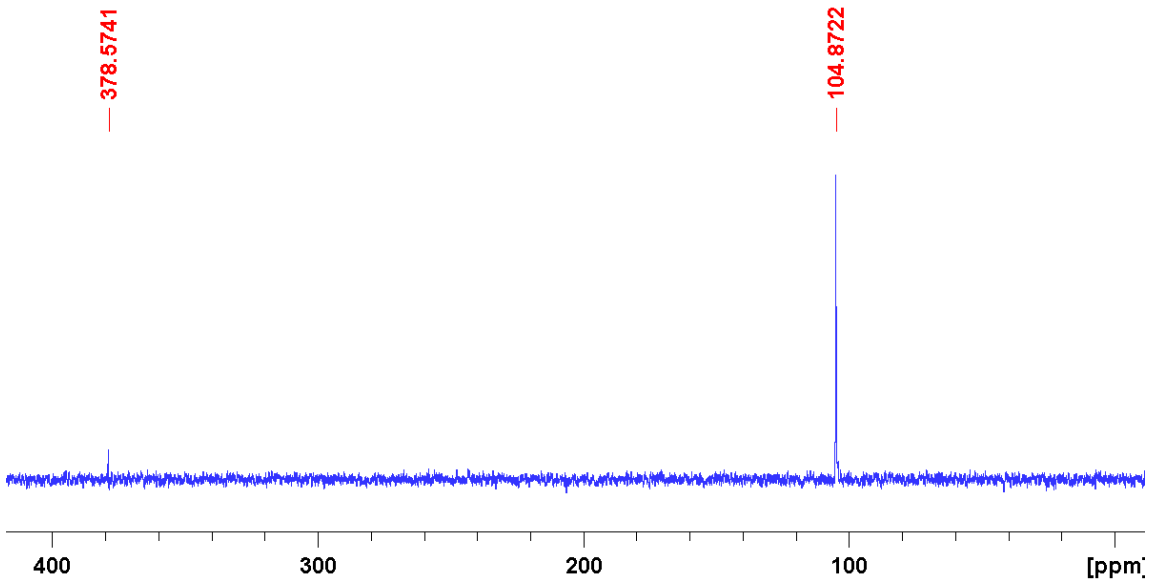
δ / ppm

A



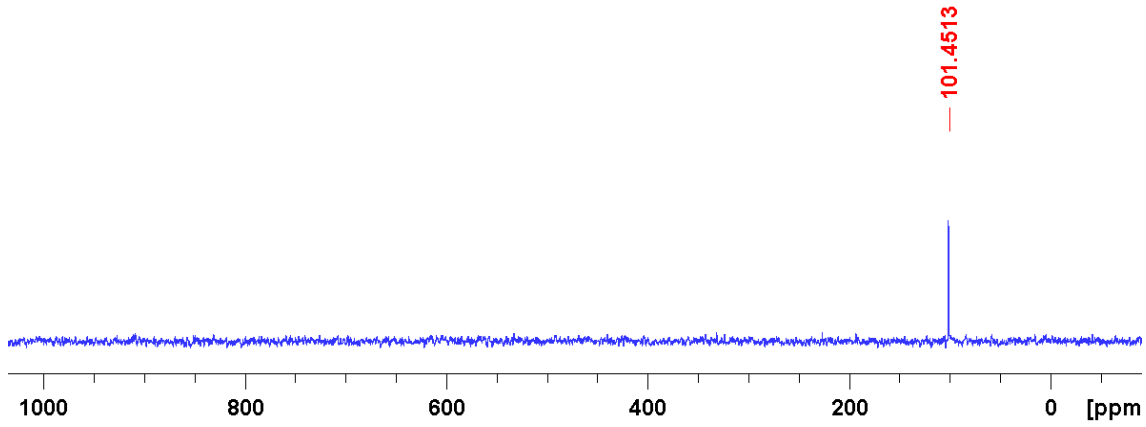
δ / ppm

B



δ / ppm

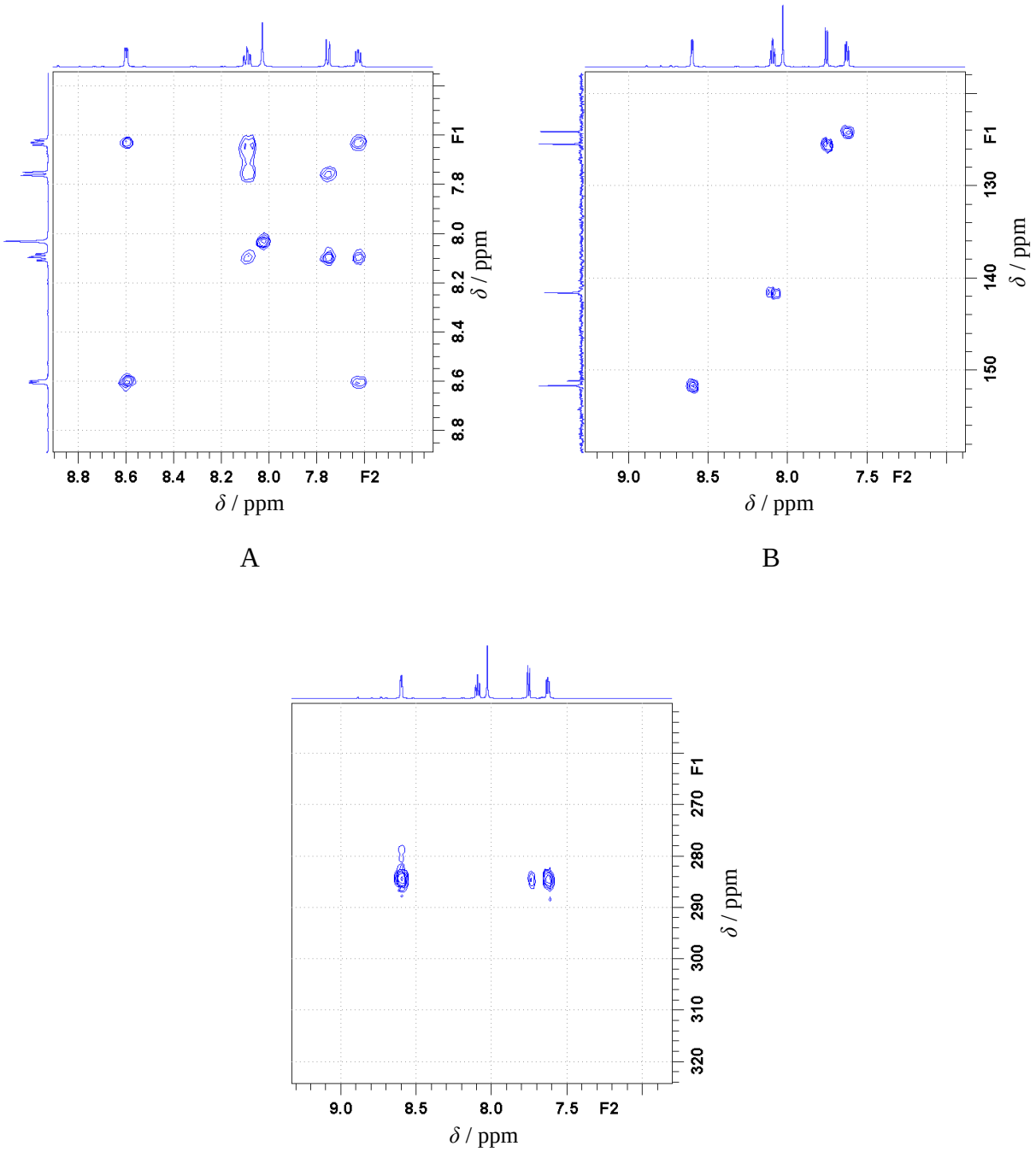
C



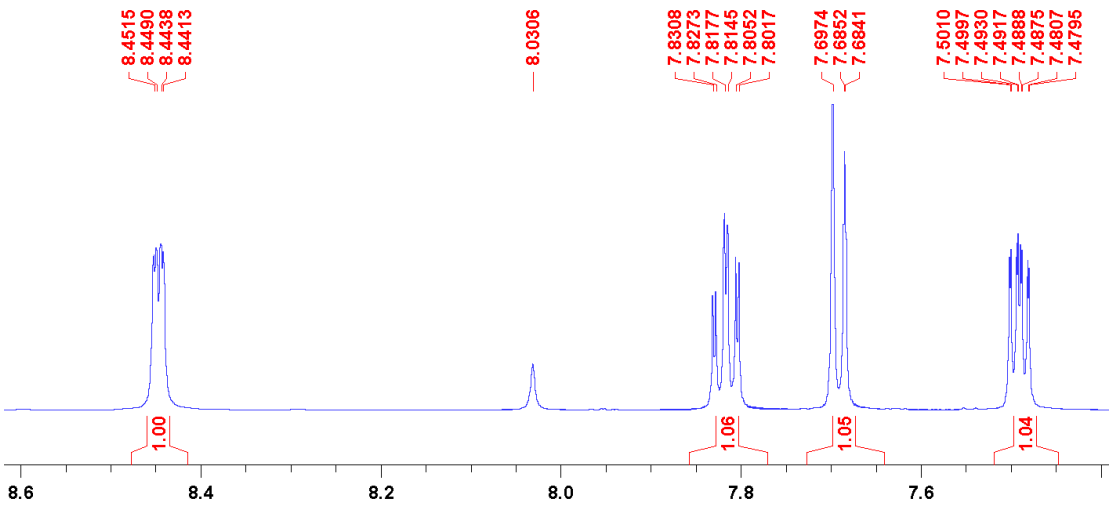
δ / ppm

D

Slika D32. *A) ^{1}H, B) ^{13}C, C) ^{15}N i D) ^{109}Ag spektri spoja $[Ag(NO_3)(2\text{-}Clpy)_2]$, (**K1**).*

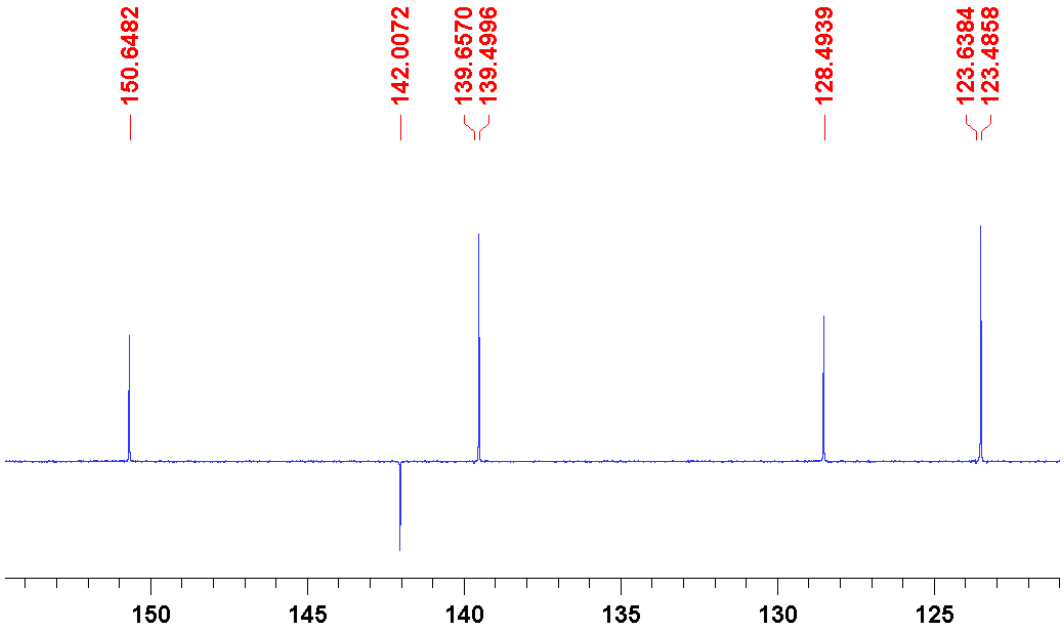


Slika D33. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC i C) ^{1}H-^{15}N HMBC spektara NMR kompleksa $[Ag(NO_3)(2\text{-Clpy})_2]$, (**K1**).*



δ / ppm

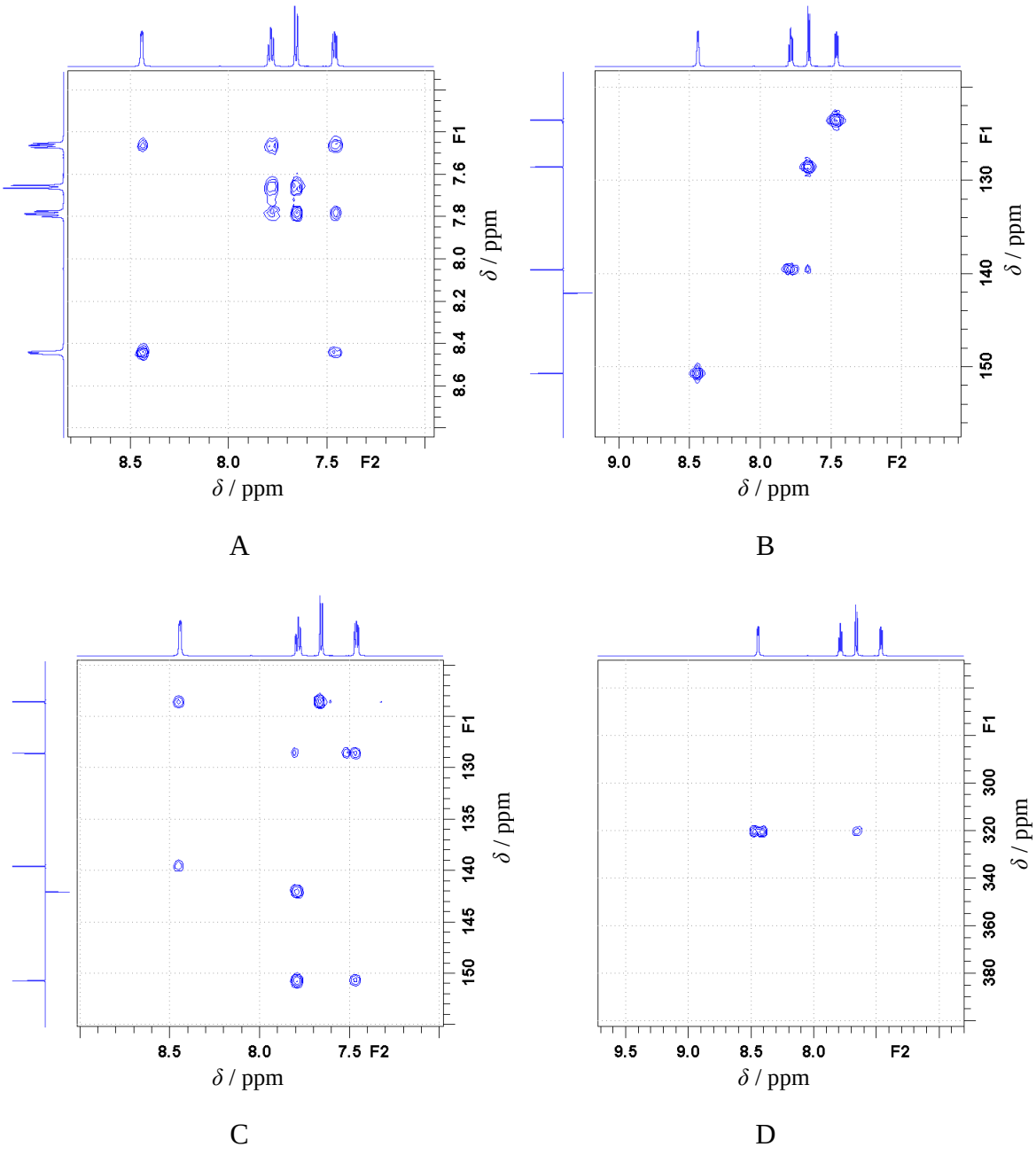
A



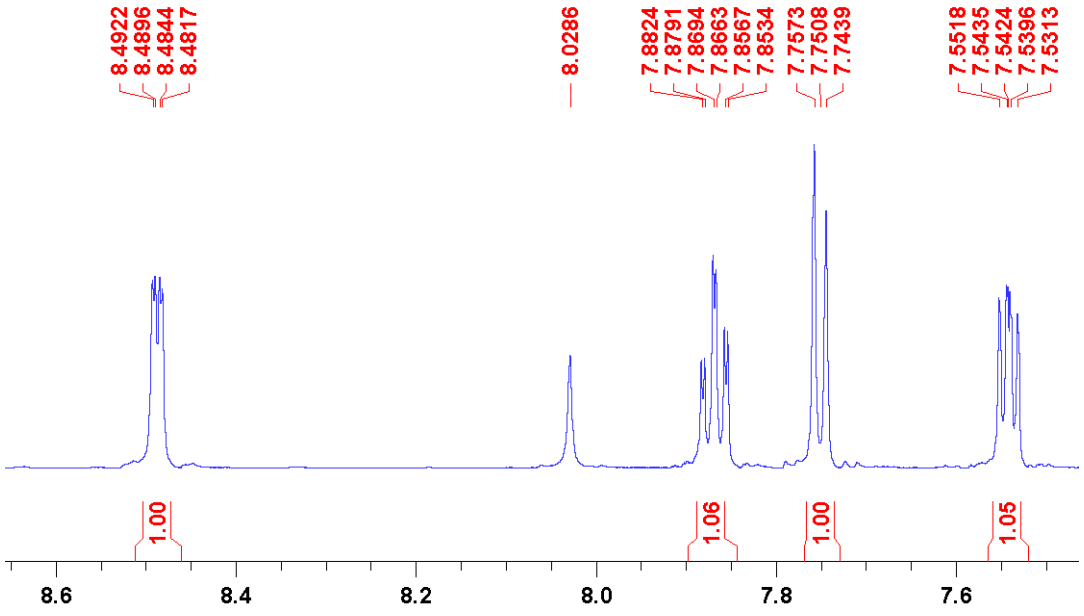
δ / ppm

B

Slika D34. *A) ^{1}H i B) ^{13}C spektri spoja 2-Brpy, (**L2**).*

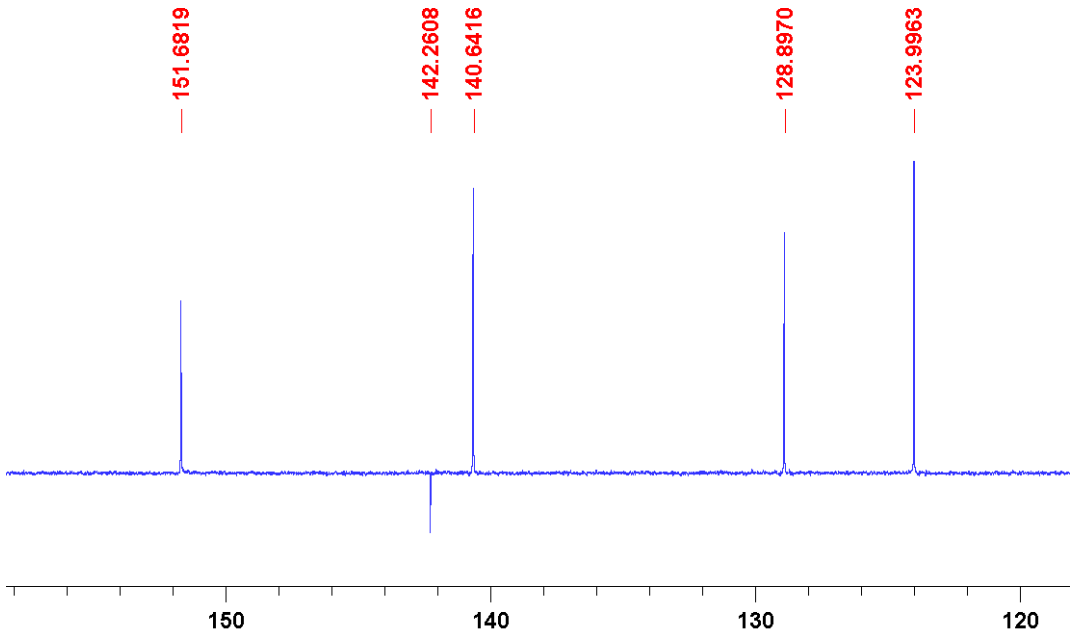


Slika D35. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR spoja 2-Brpy, (**L2**).*



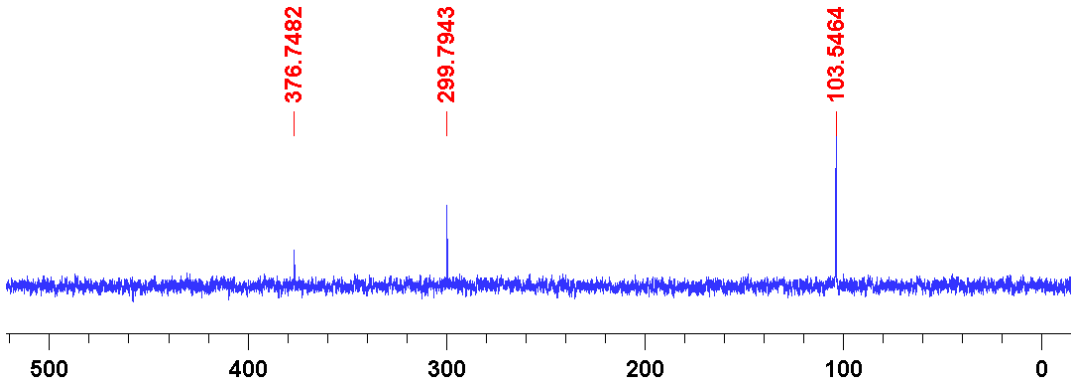
δ / ppm

A



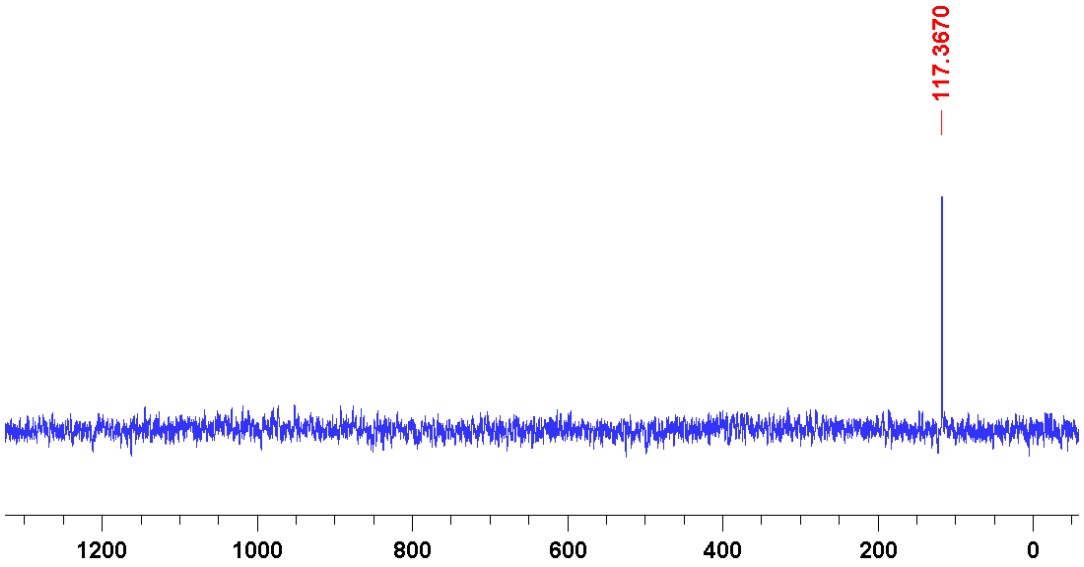
δ / ppm

B



δ / ppm

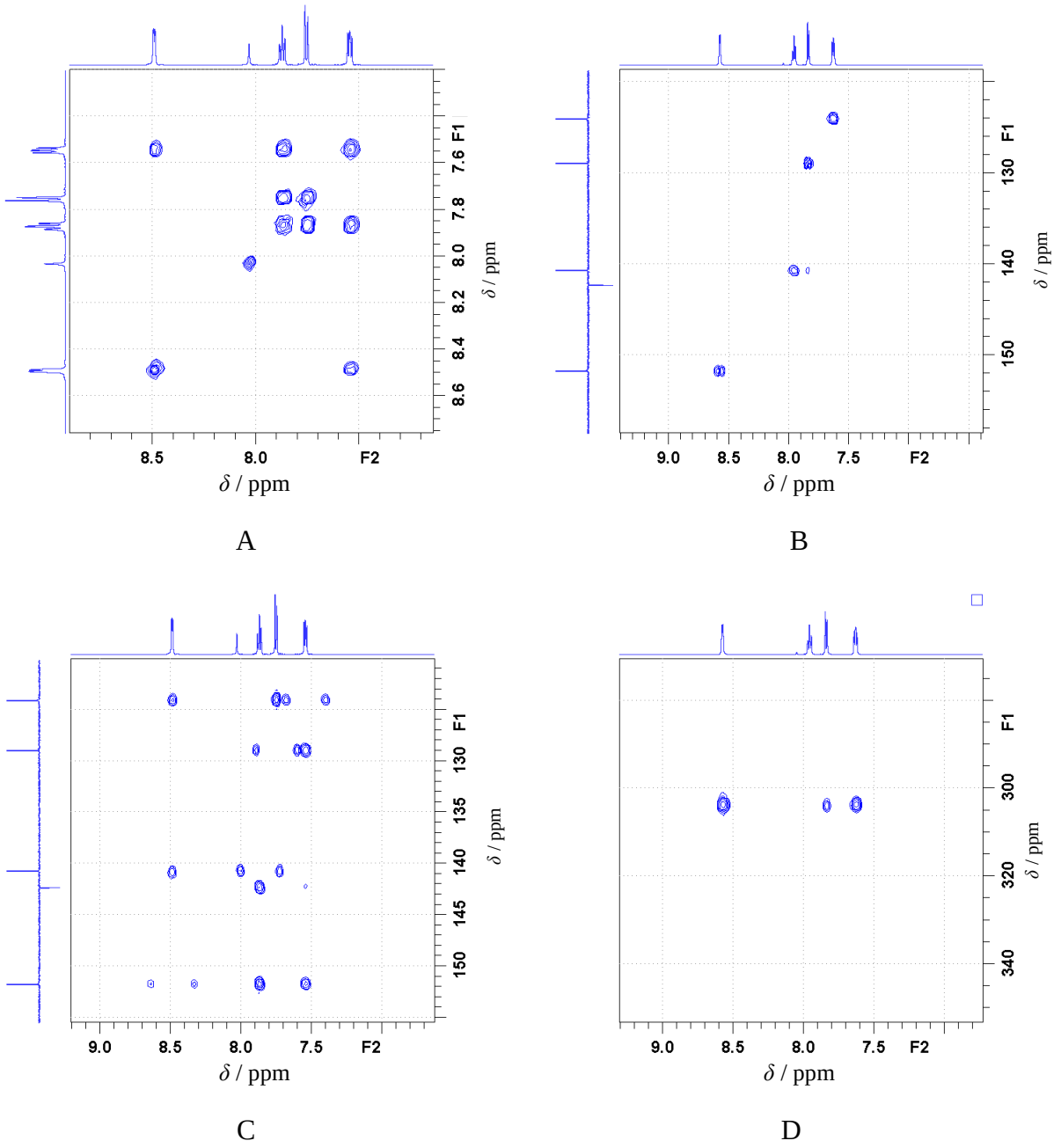
C



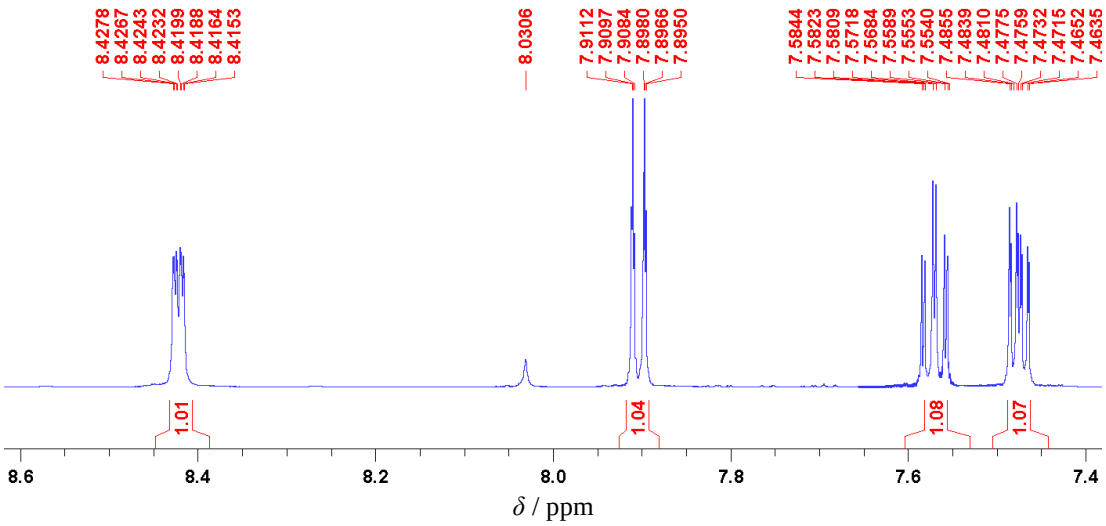
δ / ppm

D

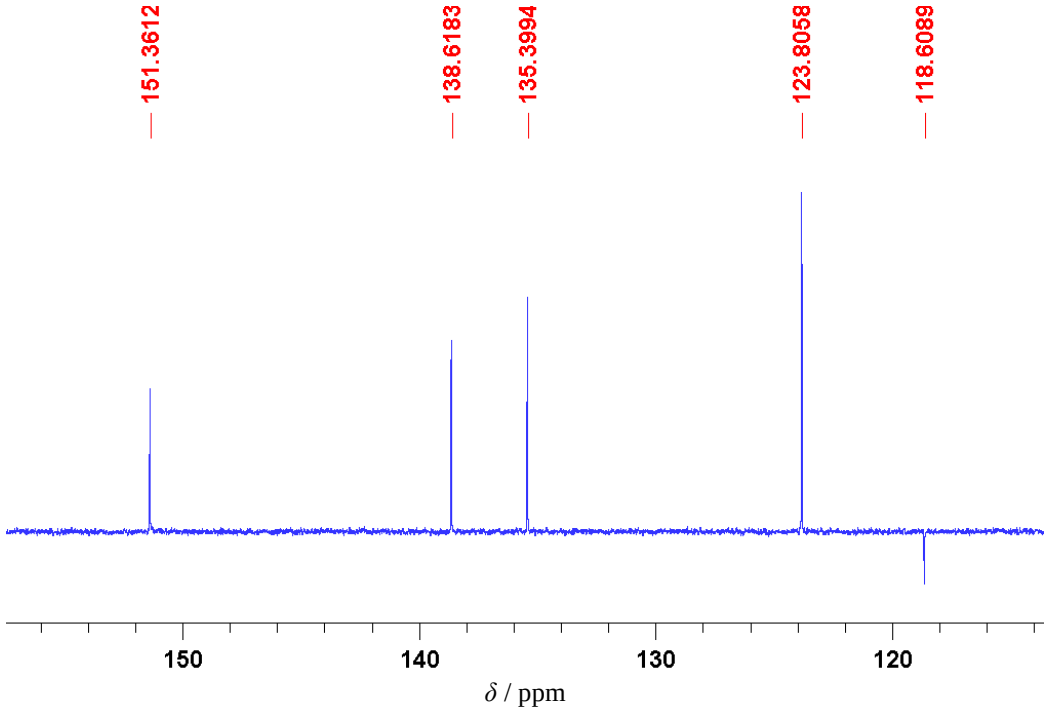
Slika D36. *A) ^{1}H, B) ^{13}C, C) ^{15}N i D) ^{109}Ag spektri spoja $[Ag(NO_3)(2\text{-}Brpy)_2]$, (**K2**).*



Slika D37. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR spoja $[Ag(NO_3)(2\text{-}Brpy)_2]$, (**K2**).*

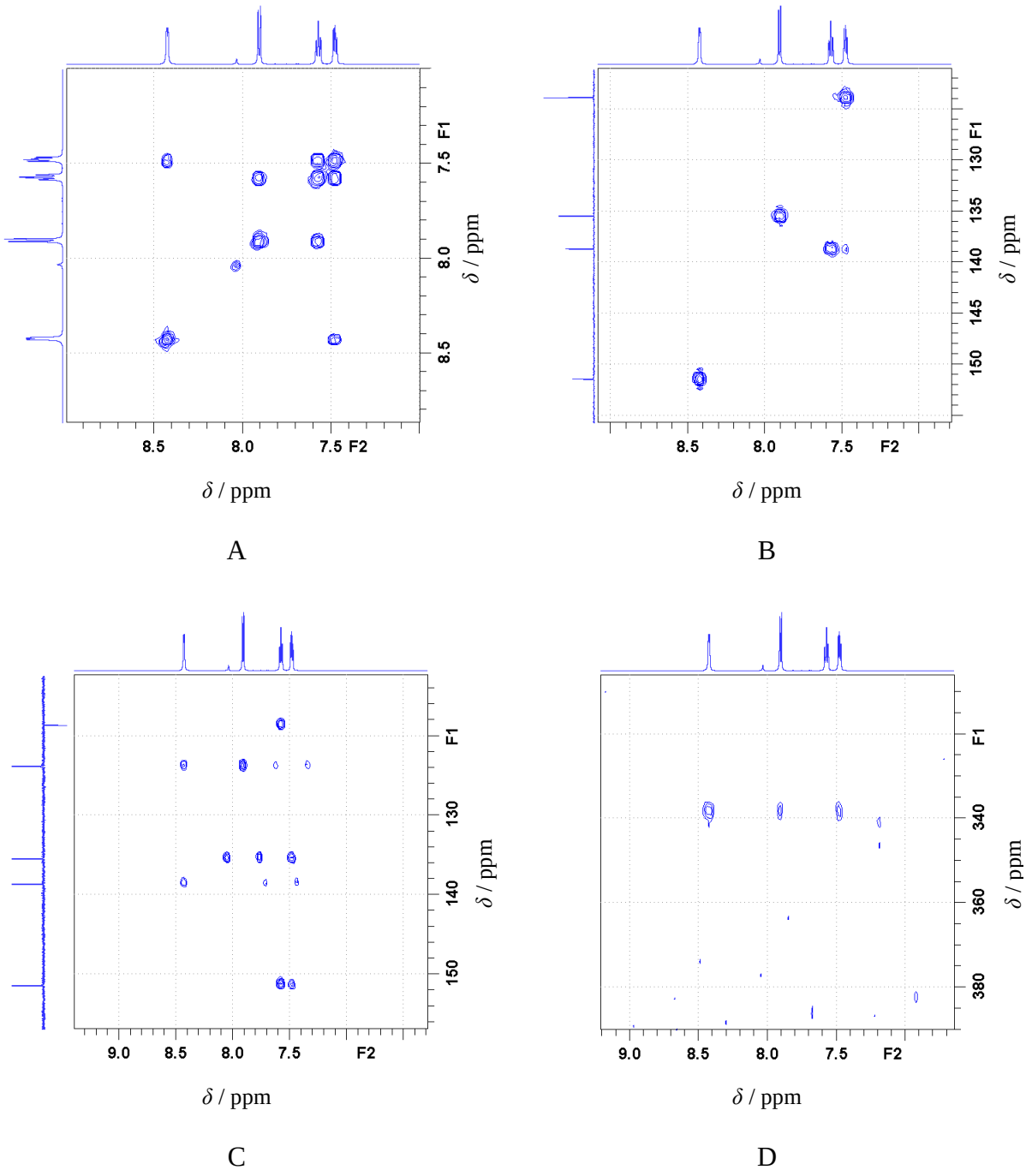


A

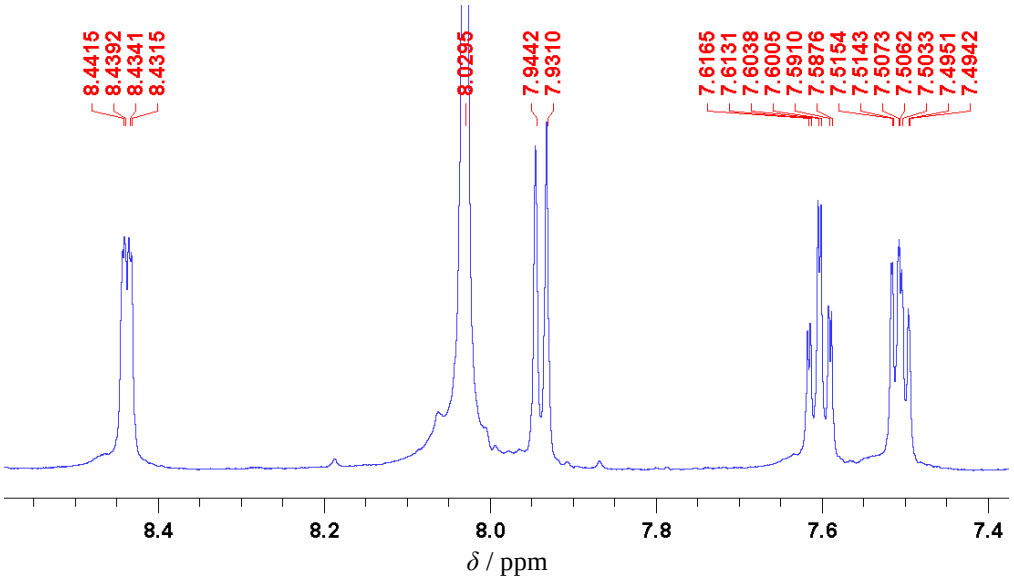


B

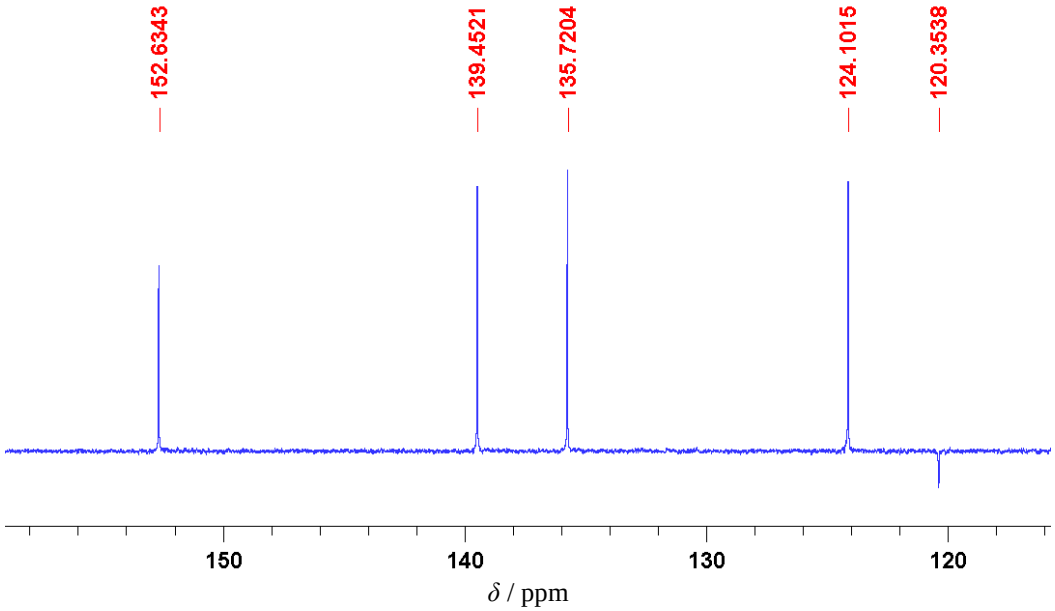
Slika D38. *A) ^{1}H i B) ^{13}C spektri spoja 2-Ipy, (**L3**).*



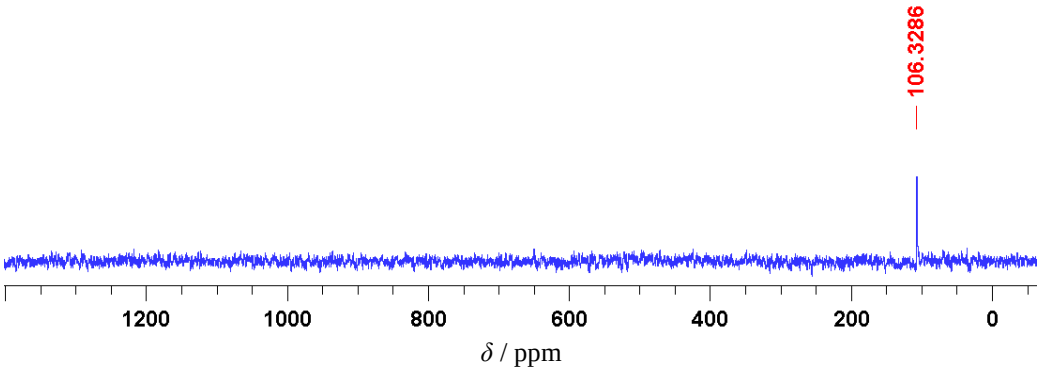
Slika D39. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR liganda 2-Ipy,* ***(L3)****.*


8.4415
8.4392
8.4341
8.4315
8.0295
7.9442
7.9310
7.6165
7.6131
7.6038
7.6005
7.5910
7.5876
7.5154
7.5143
7.5073
7.5062
7.5033
7.4951
7.4942
8.4
8.2
8.0
7.8
7.6
7.4
δ / ppm

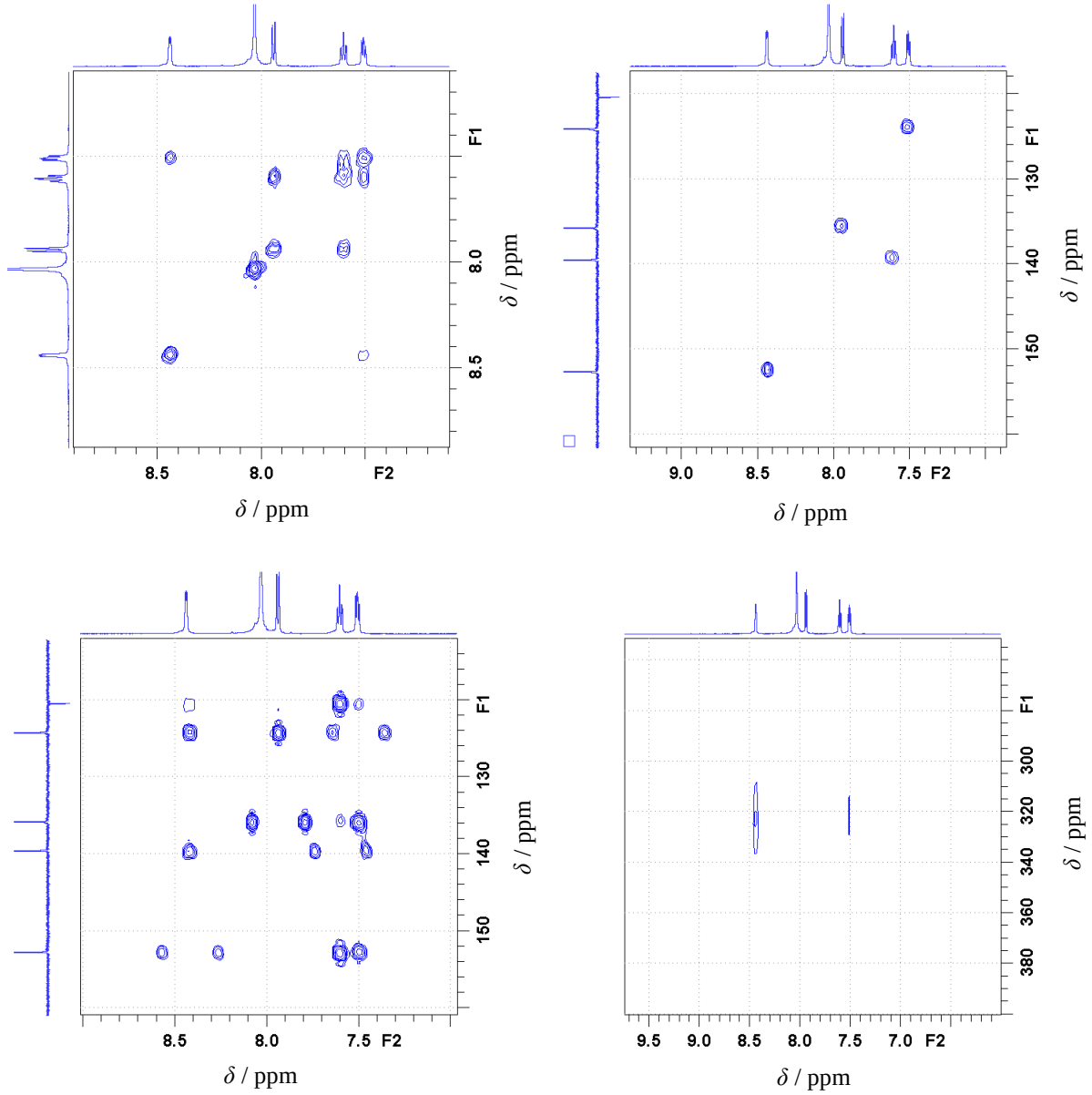
A


152.6343
139.4521
135.7204
124.1015
120.3538
150
140
130
120
δ / ppm

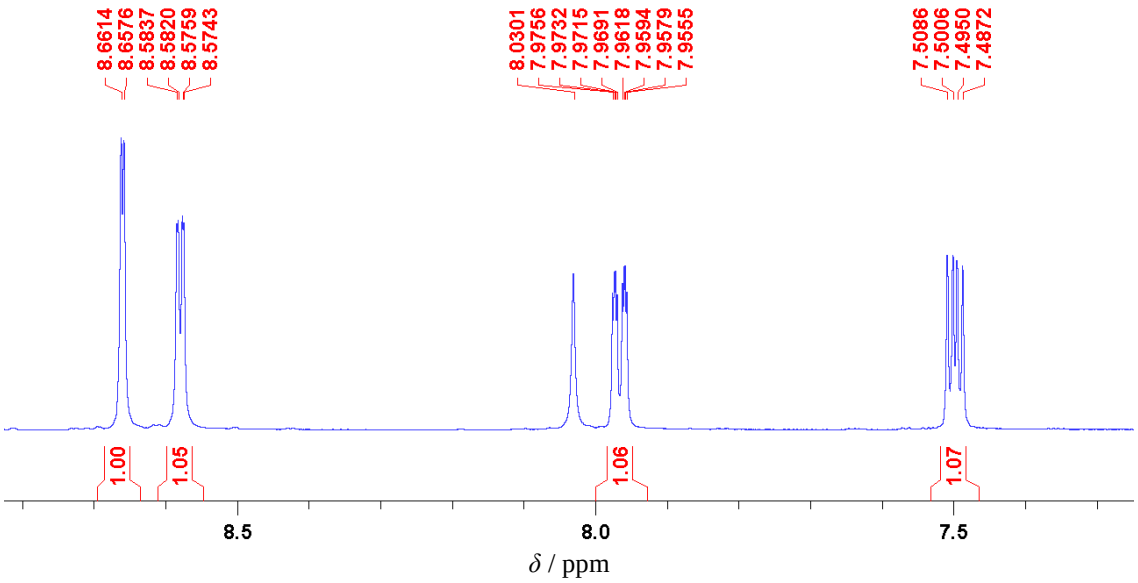
B



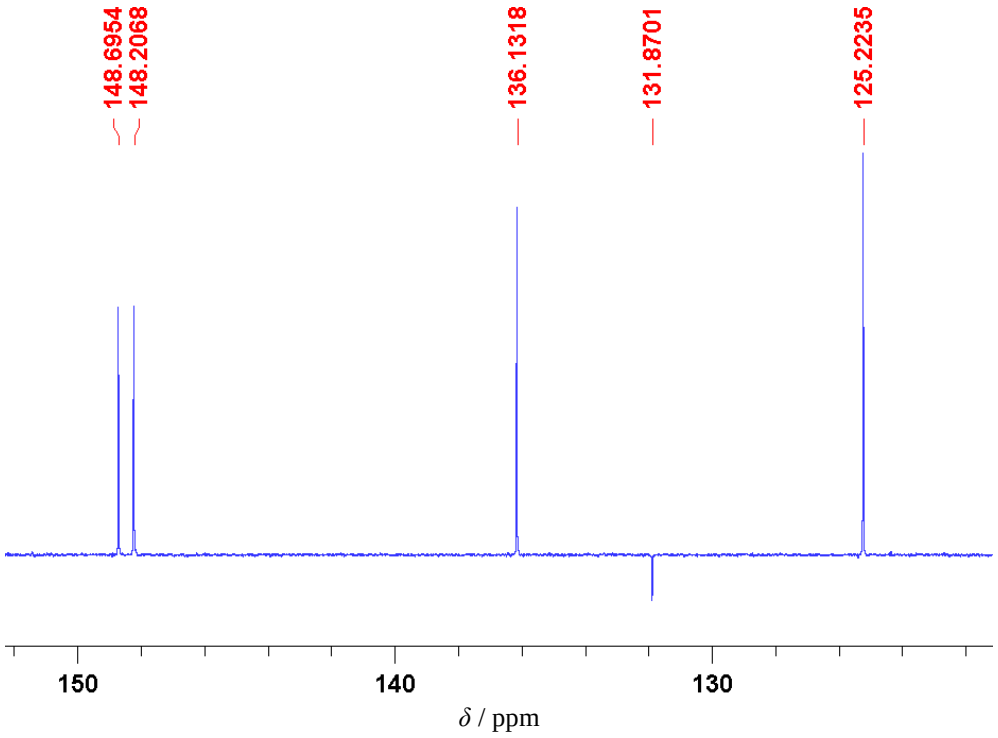
Slika D40. *A) ^{1}H, B) ^{13}C i C) ^{109}Ag spektri spoja $[Ag(NO_3)(2\text{-}Ipy)_2]$, (**K3**).*



Slika D41. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR kompleksa $[Ag(NO_3)(2\text{-}Ipy)_2]$, (**K3**).*

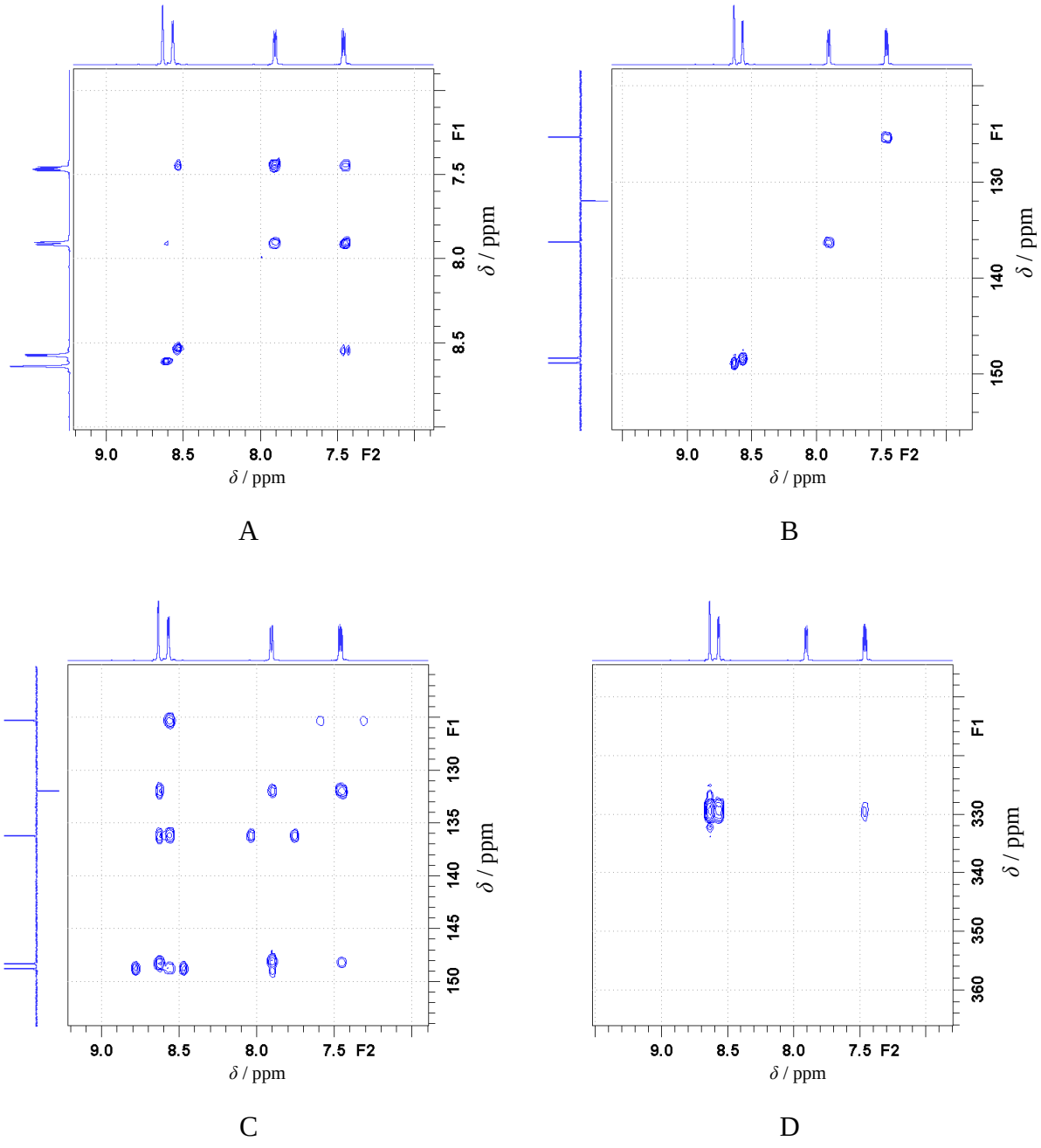


A

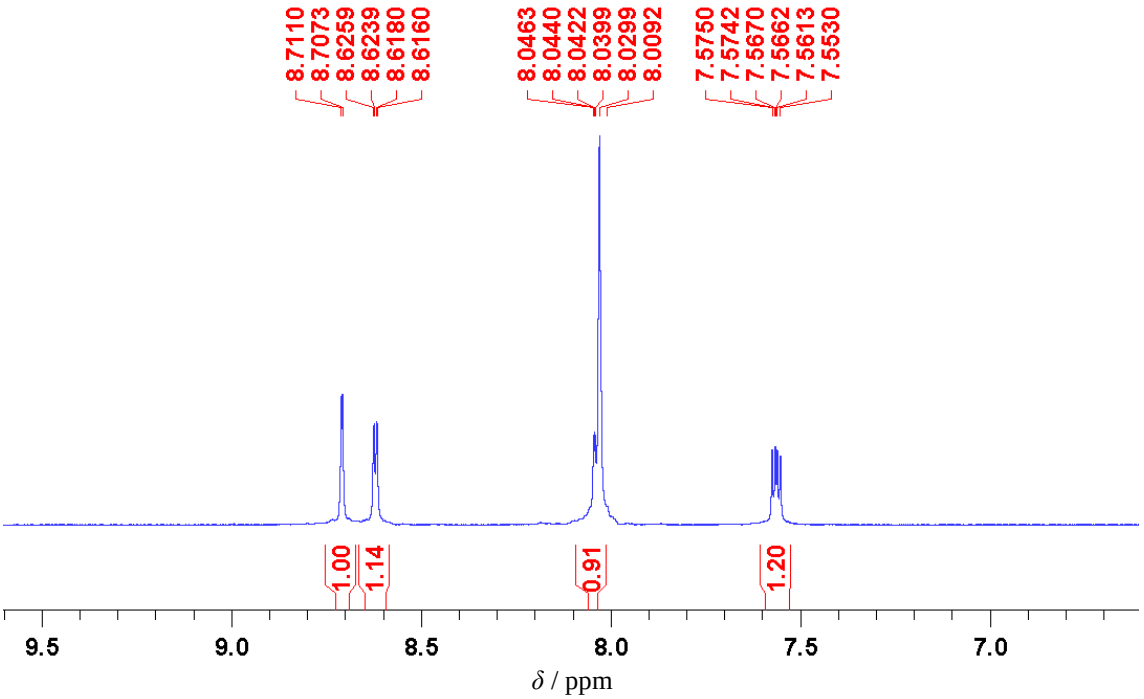


B

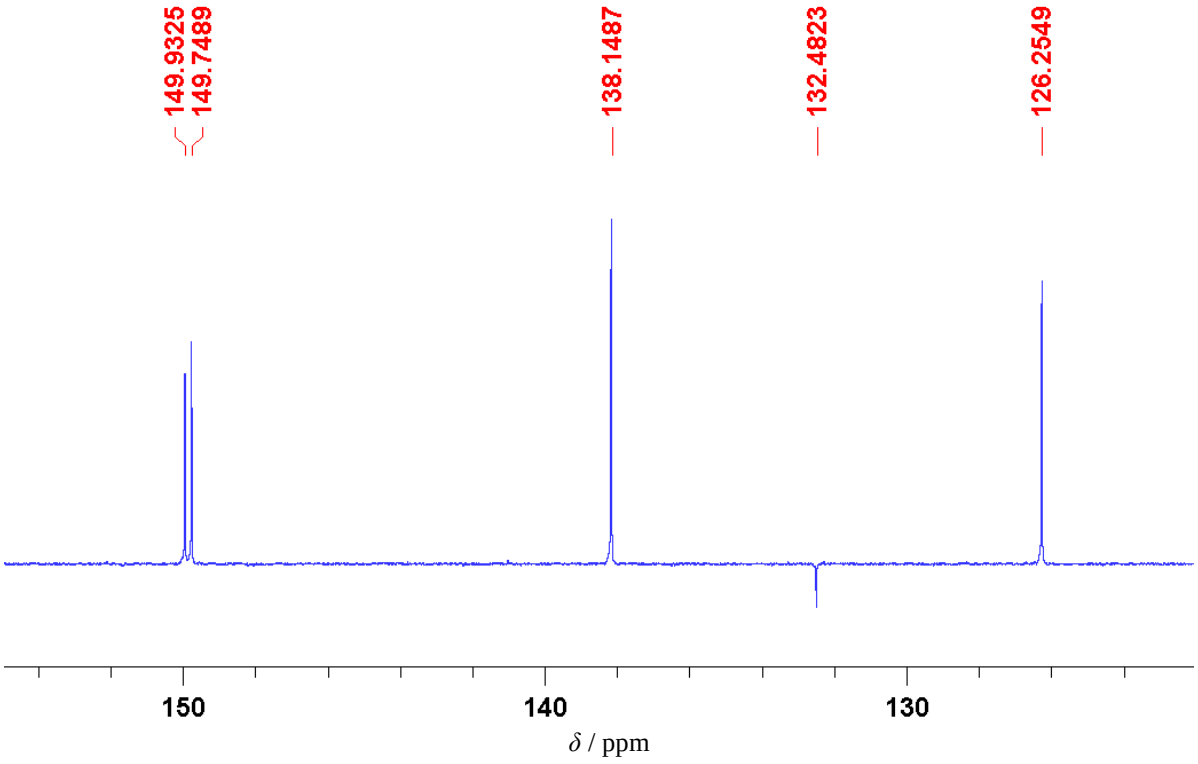
Slika D42. *A) ^{1}H i B) ^{13}C spektri spoja 3-Clpy, (**L4**).*



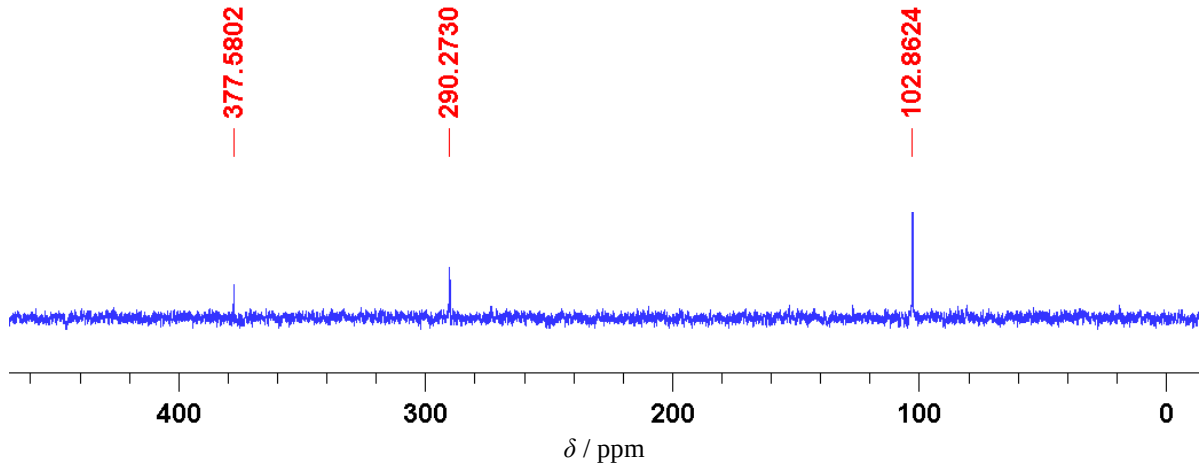
Slika D43. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR liganda 3-Clpy, (**L4**).*


8.7110
8.7073
8.6259
8.6239
8.6180
8.6160
8.0463
8.0440
8.0422
8.0399
8.0299
8.0092
7.5750
7.5742
7.5670
7.5662
7.5613
7.5530
1.00
1.14
0.91
1.20
9.5
9.0
8.5
8.0
7.5
7.0
δ / ppm

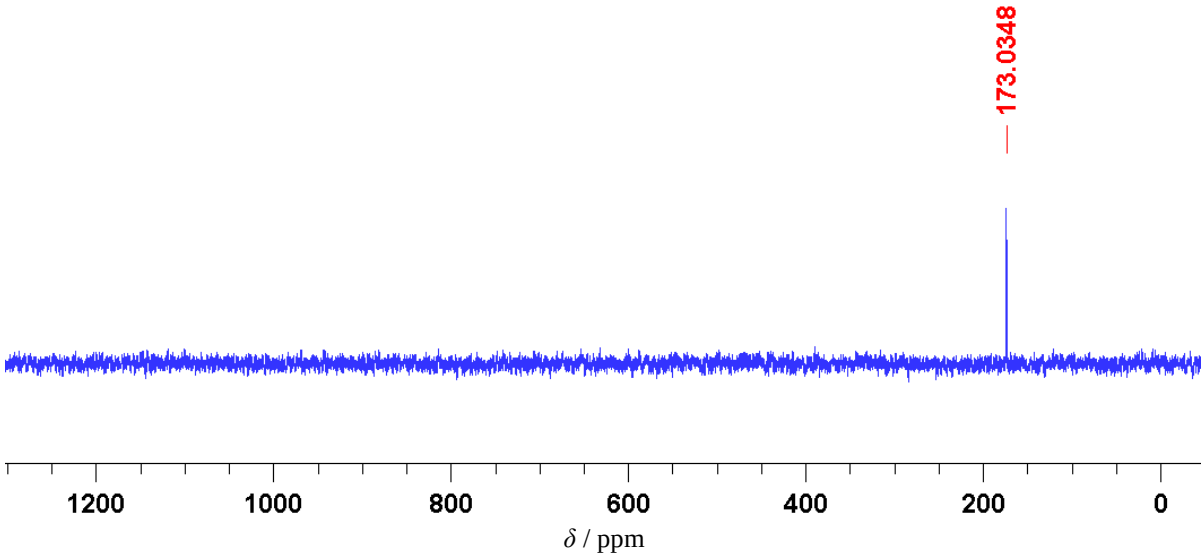
A


149.9325
149.7489
138.1487
132.4823
126.2549
150
140
130
δ / ppm

B

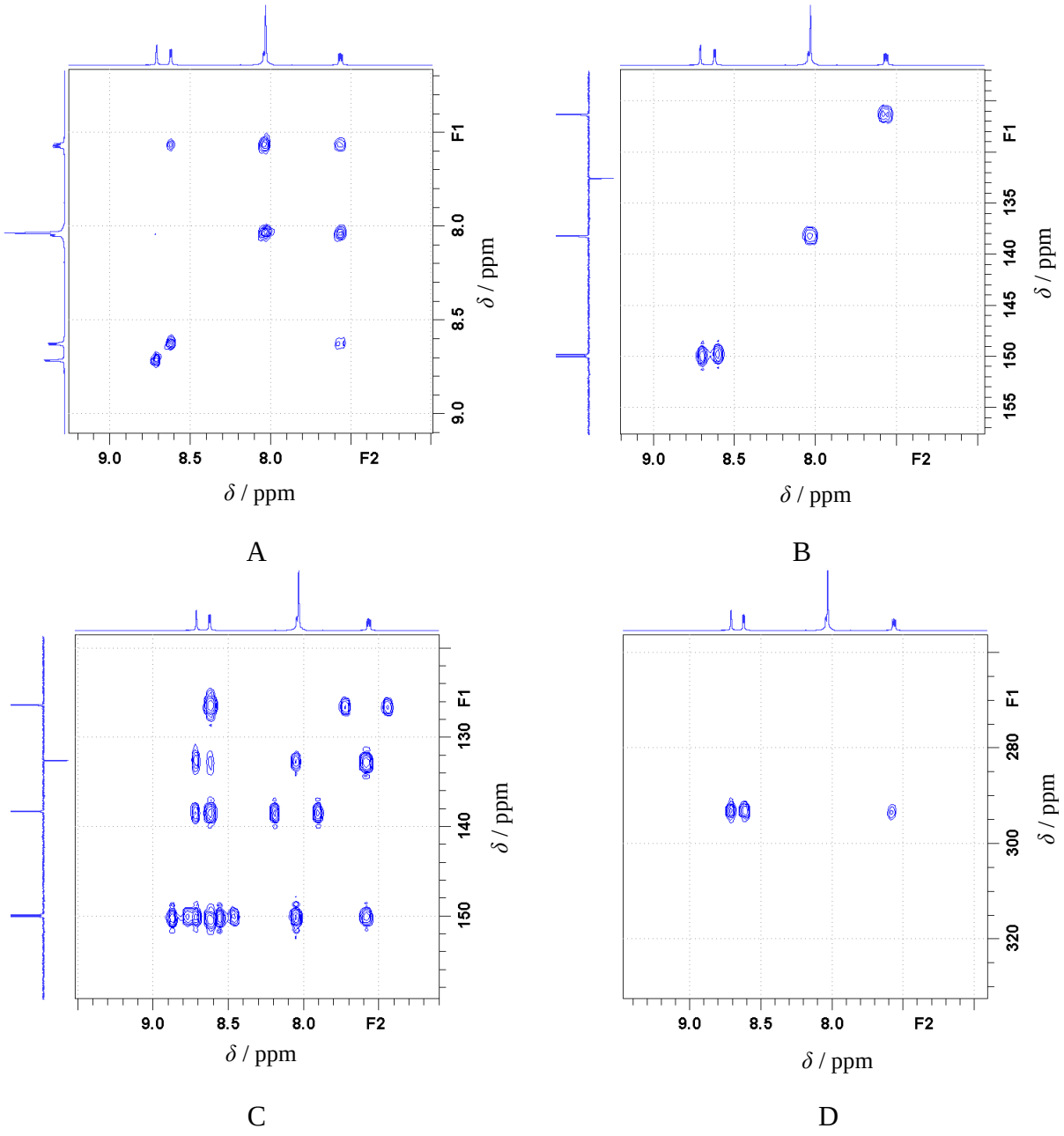


C

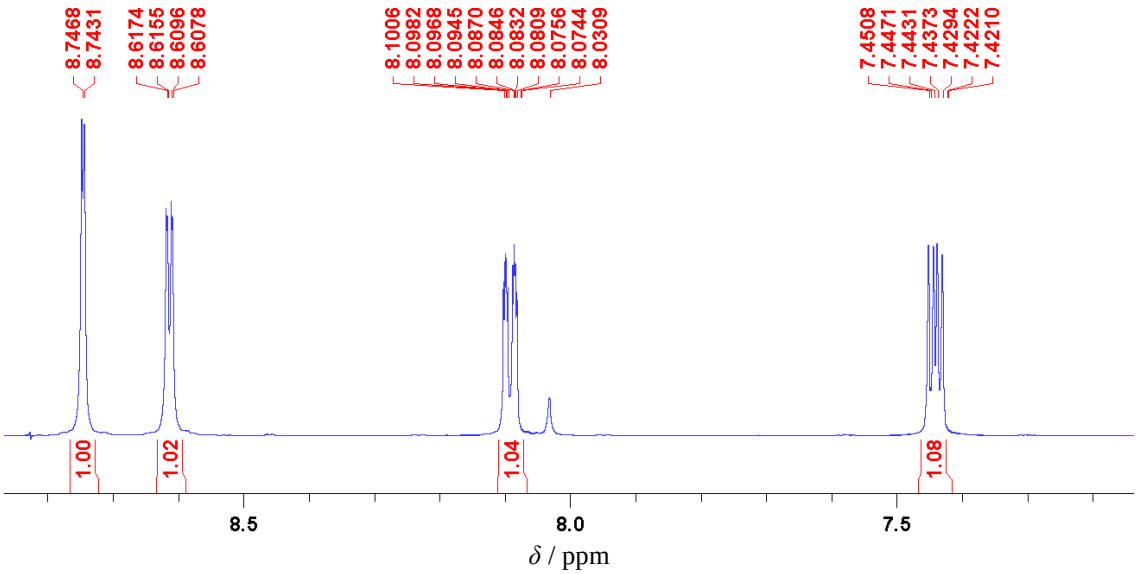


D

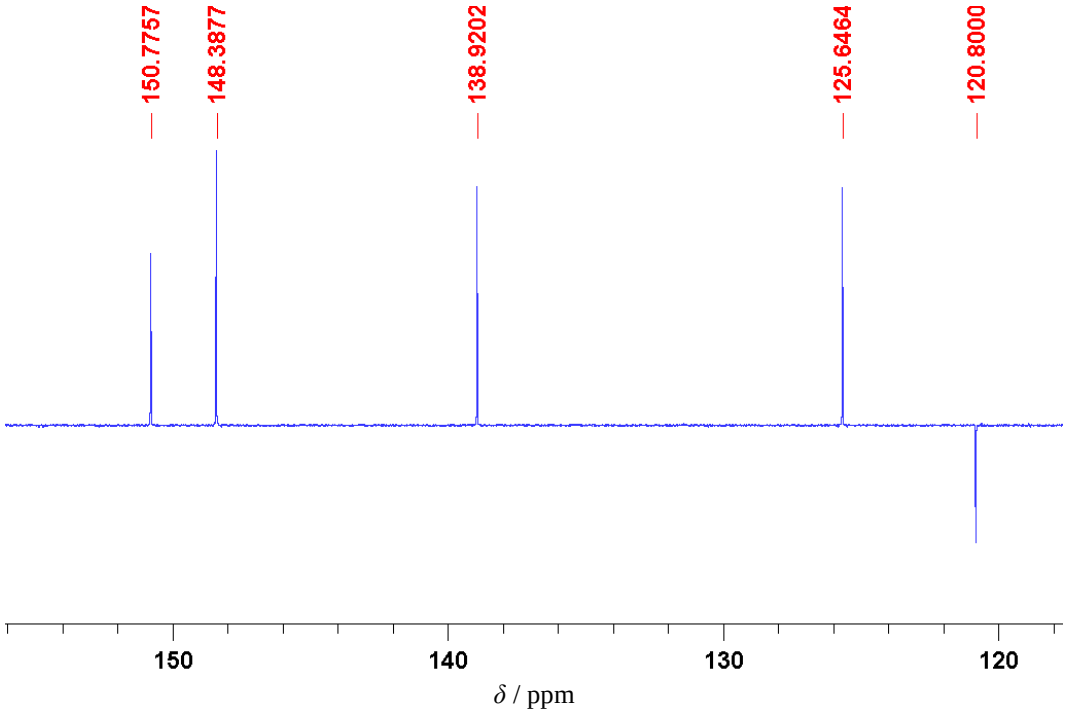
Slika D44. *A) ^{1}H, B) ^{13}C, C) ^{15}N i D) ^{109}Ag spektri kompleksa $[Ag(NO_3)(3\text{-}Clpy)_2]$, (**K4**).*



Slika D45. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR kompleksa [Ag(NO$_3$)(3-Clpy)$_2$], (**K4**).*

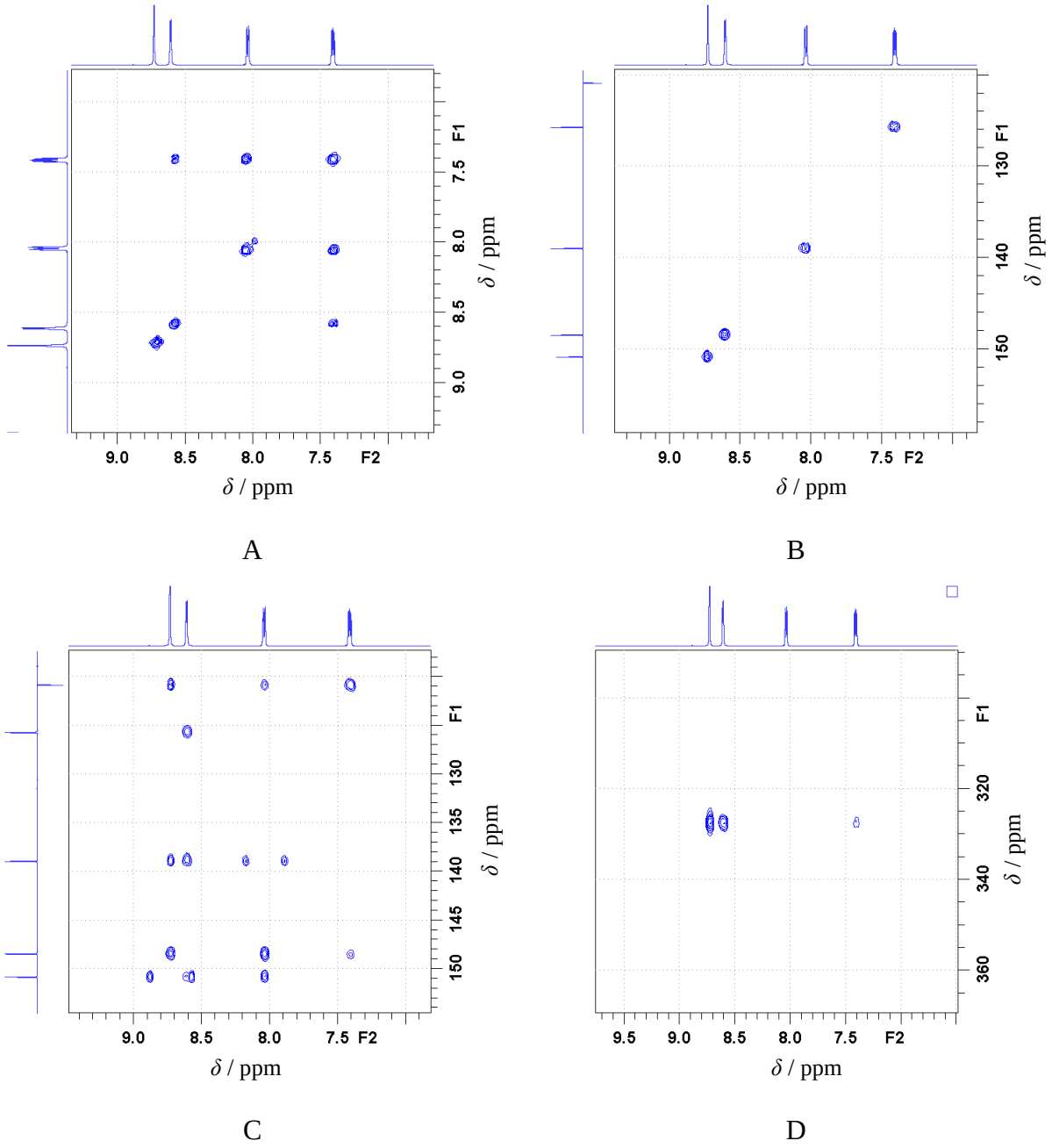


A

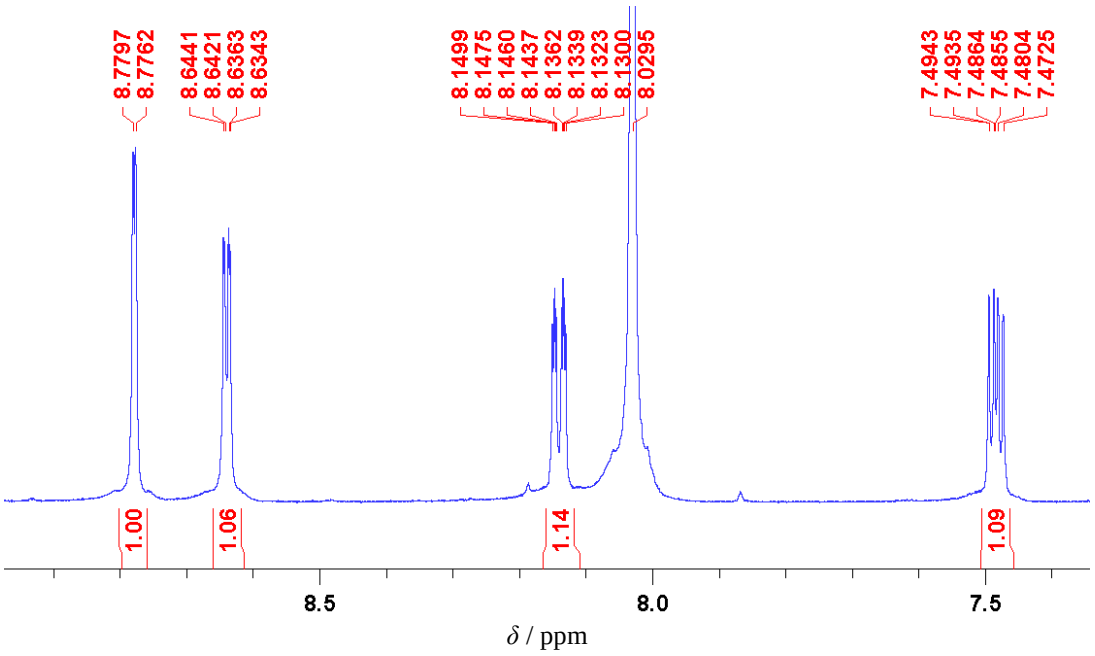


B

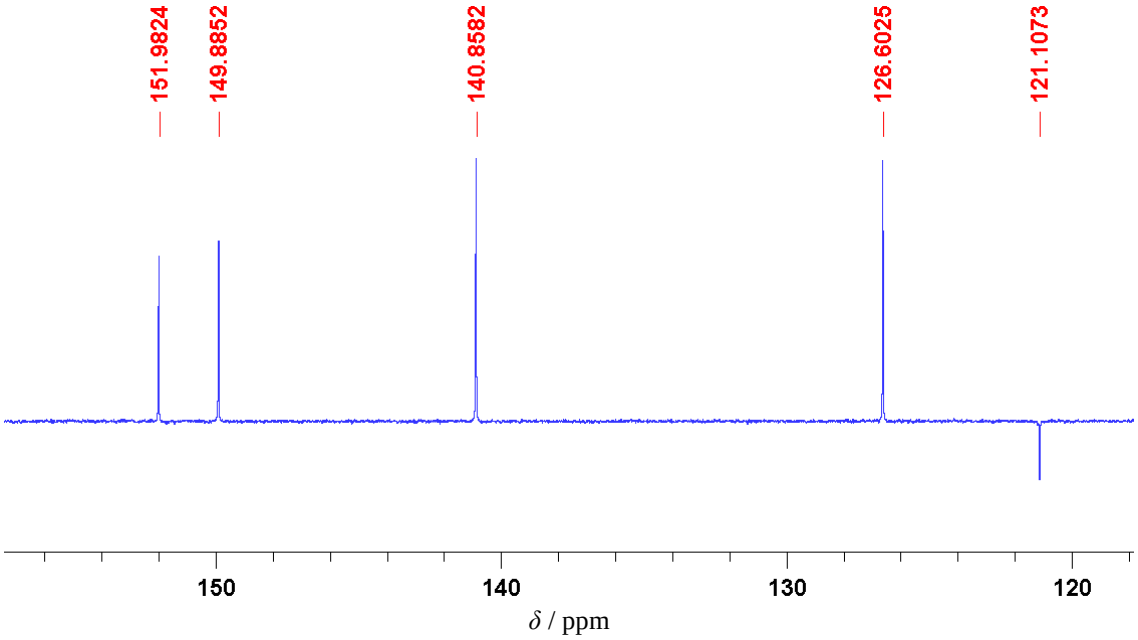
Slika D46. *A) ^{1}H i B) ^{13}C spektri spoja 3-Brpy,* ***(L5).***



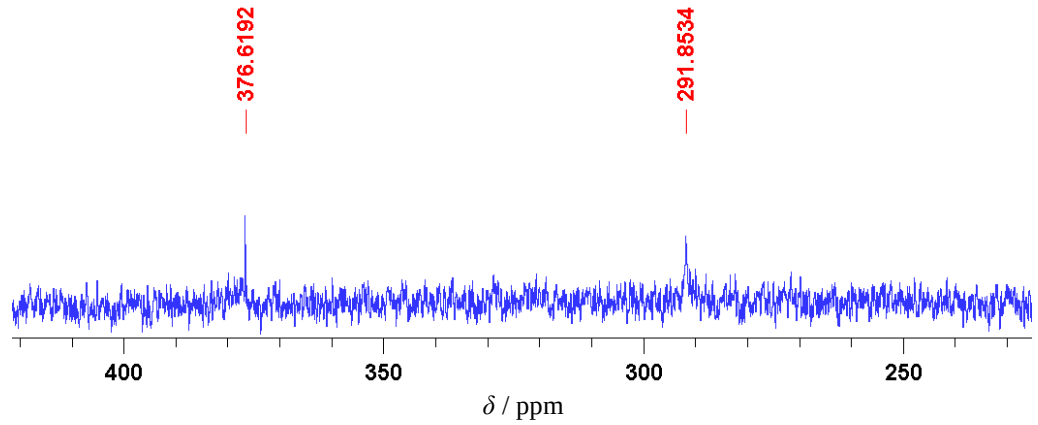
Slika D47. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR spoja 3-Brpy, (**L5**).*


8.7797
8.7762
8.6441
8.6421
8.6363
8.6343
8.1499
8.1475
8.1460
8.1437
8.1362
8.1339
8.1323
8.1300
8.0295
7.4943
7.4935
7.4864
7.4855
7.4804
7.4725
1.00
1.06
1.14
1.09
8.5
8.0
7.5
δ / ppm

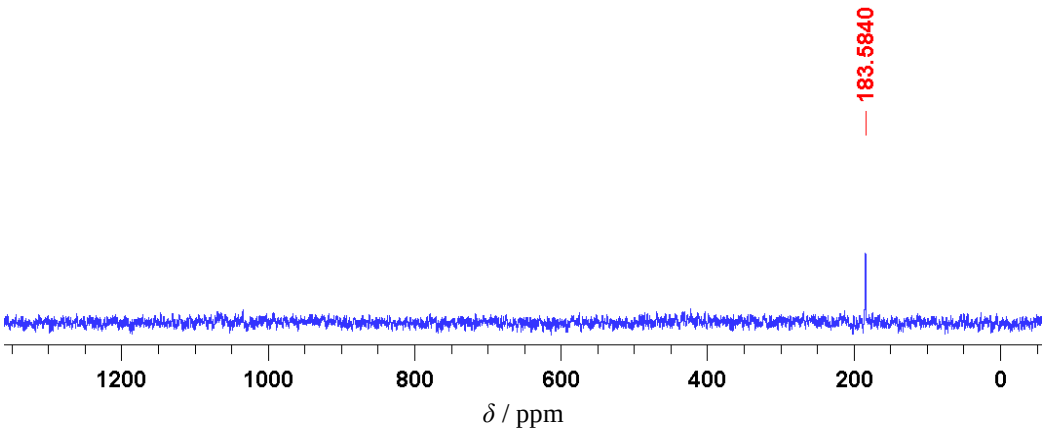
A


151.9824
149.8852
140.8582
126.6025
121.1073
150
140
130
120
δ / ppm

B

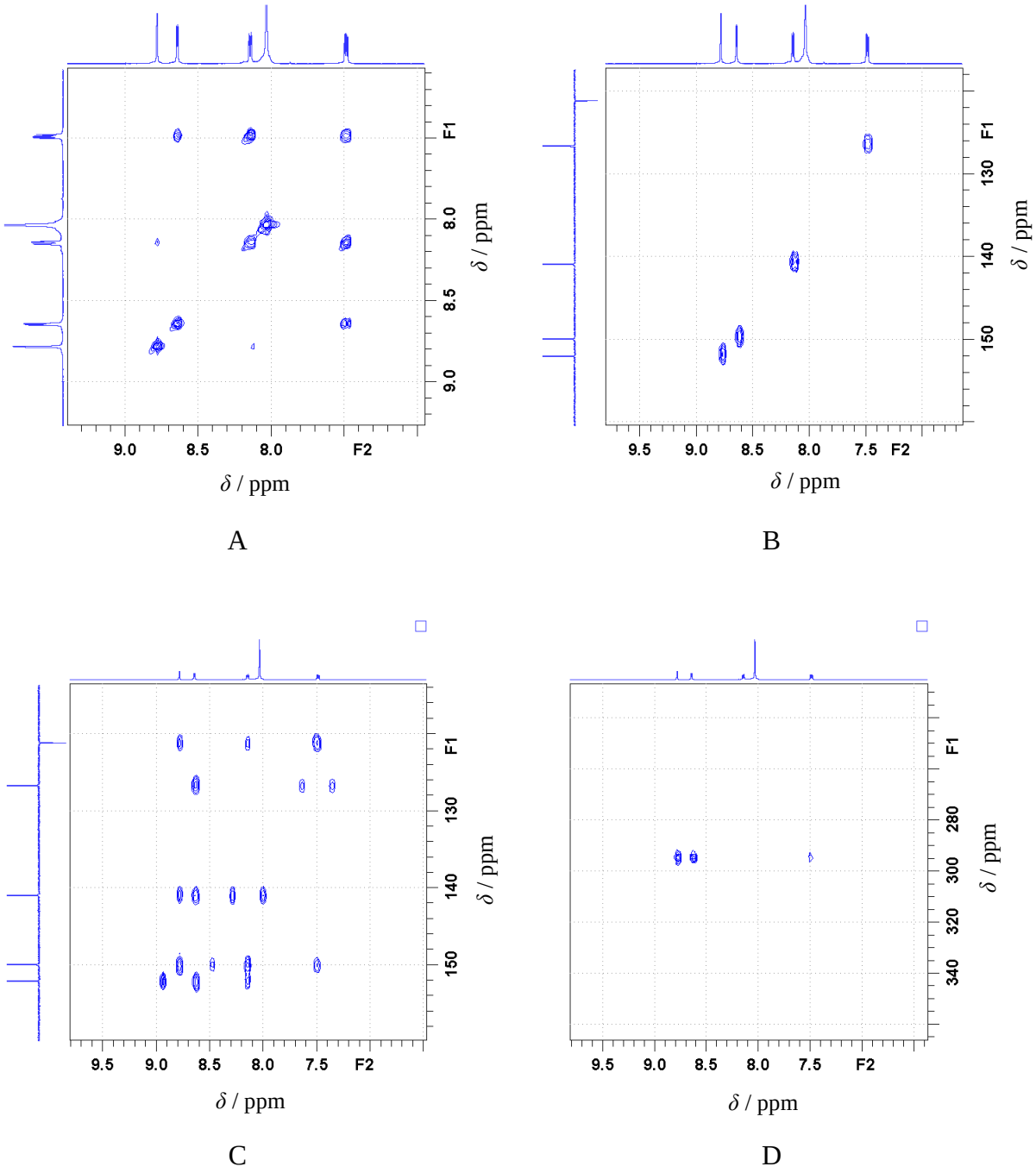


C

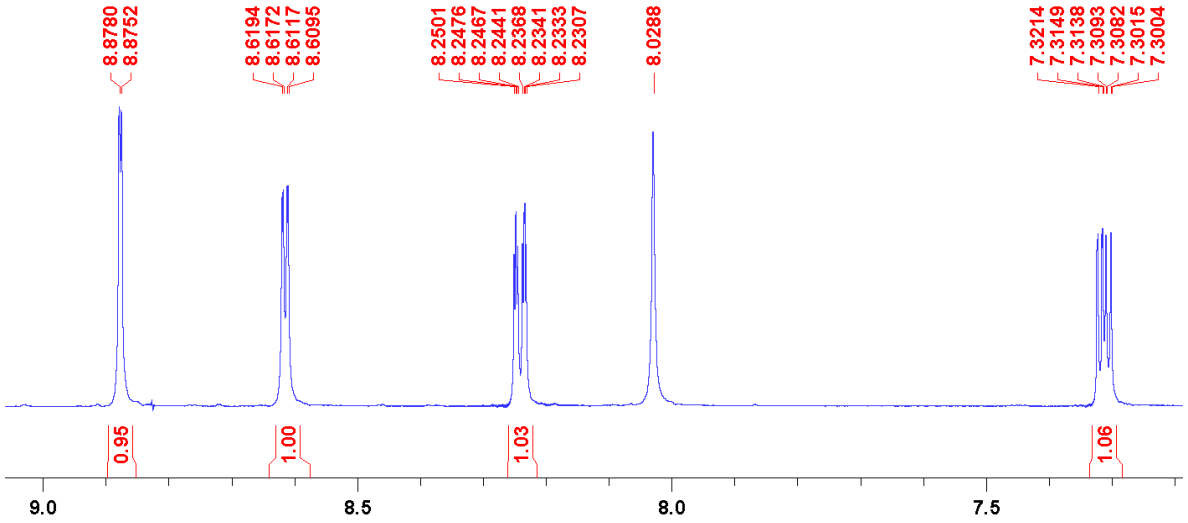


D

Slika D48. *A) ^{1}H, B) ^{13}C, C) ^{15}N i D) ^{109}Ag spektri spoja $[Ag(NO_3)(3\text{-}Brpy)_2]$, (**K5**).*

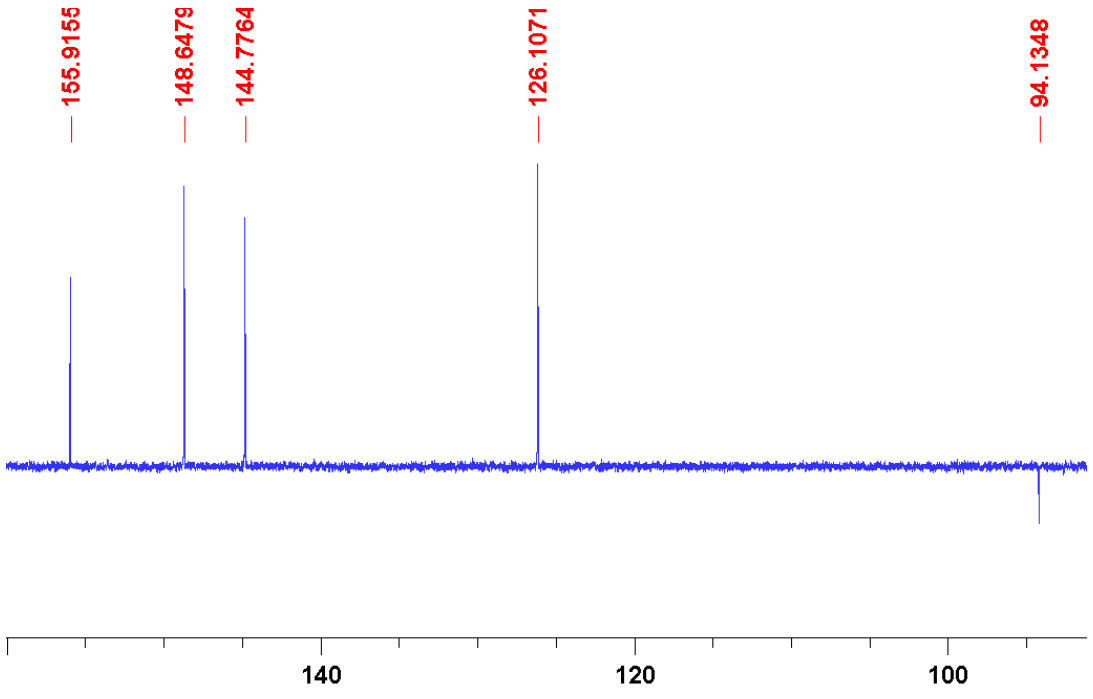


Slika D49. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR kompleksa $[Ag(NO_3)(3\text{-}Brpy)_2]$, (**K5**).*



δ / ppm

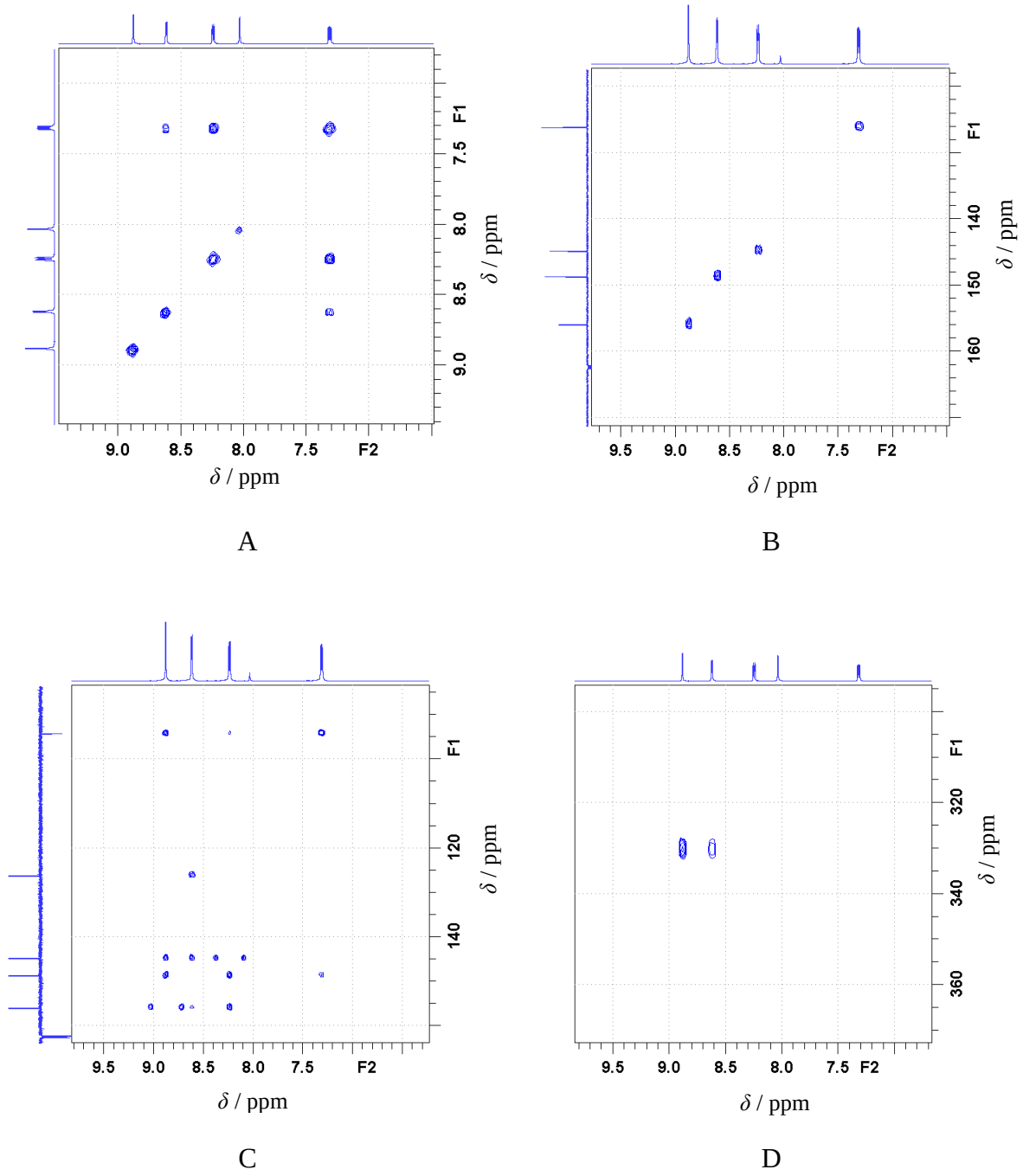
A



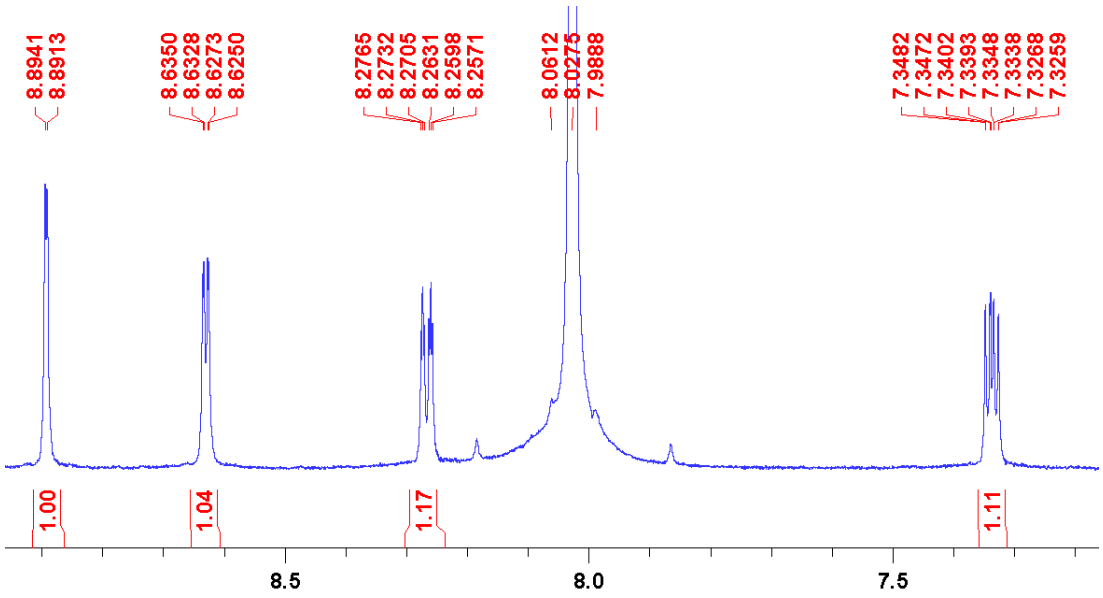
δ / ppm

B

Slika D50. *A)* ^{1}H *i B)* ^{13}C *spektri spoja 3-Ipy,* ***(L6)****.*

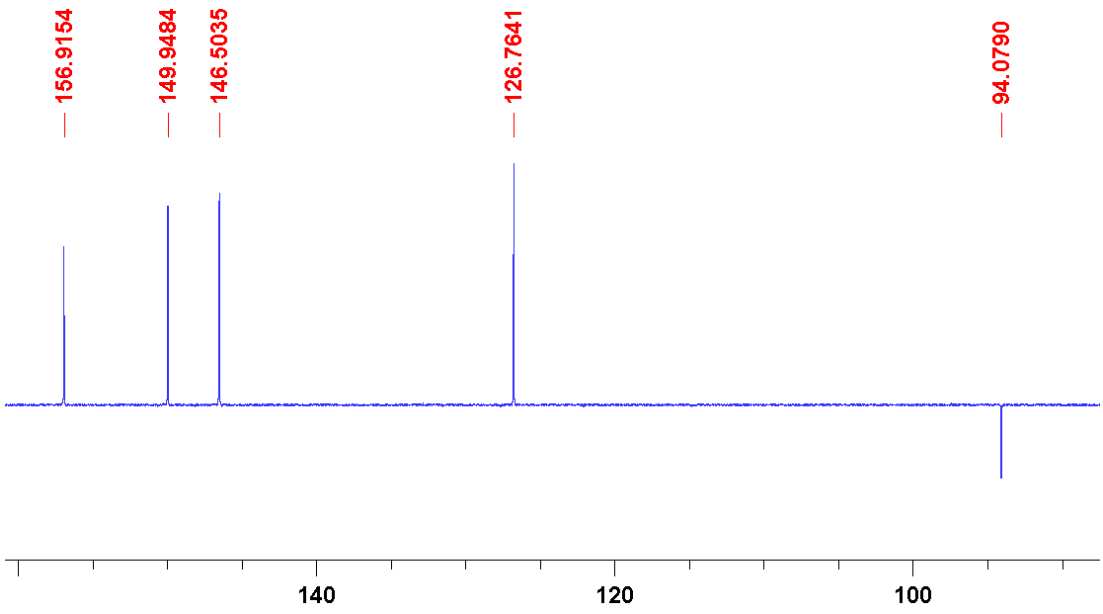


Slika D51. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR spoja 3-Ipy, (**L6**).*



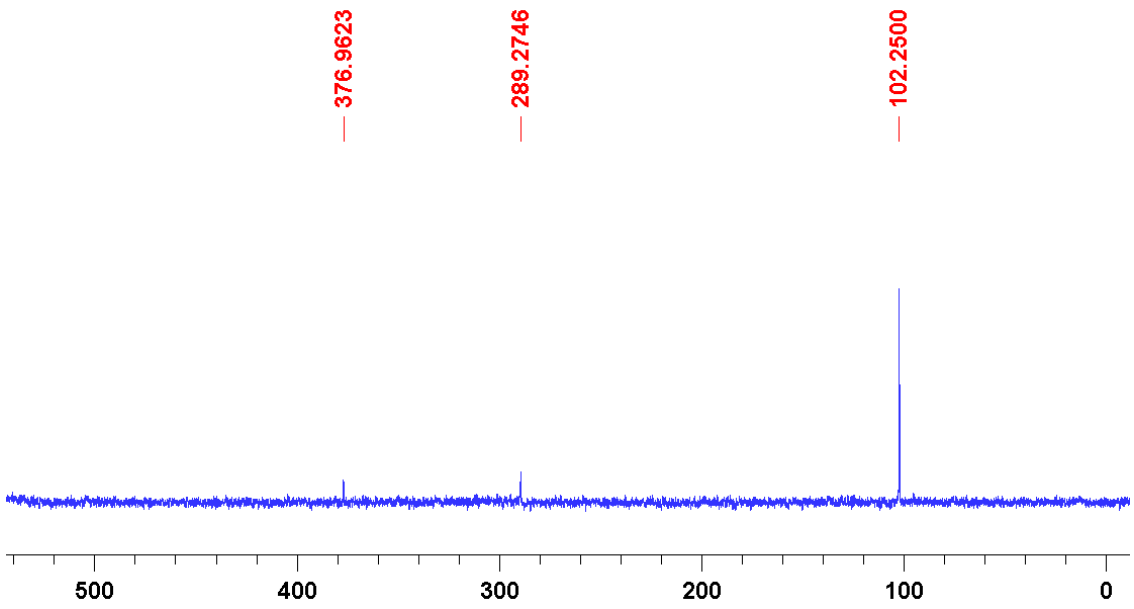
δ / ppm

A

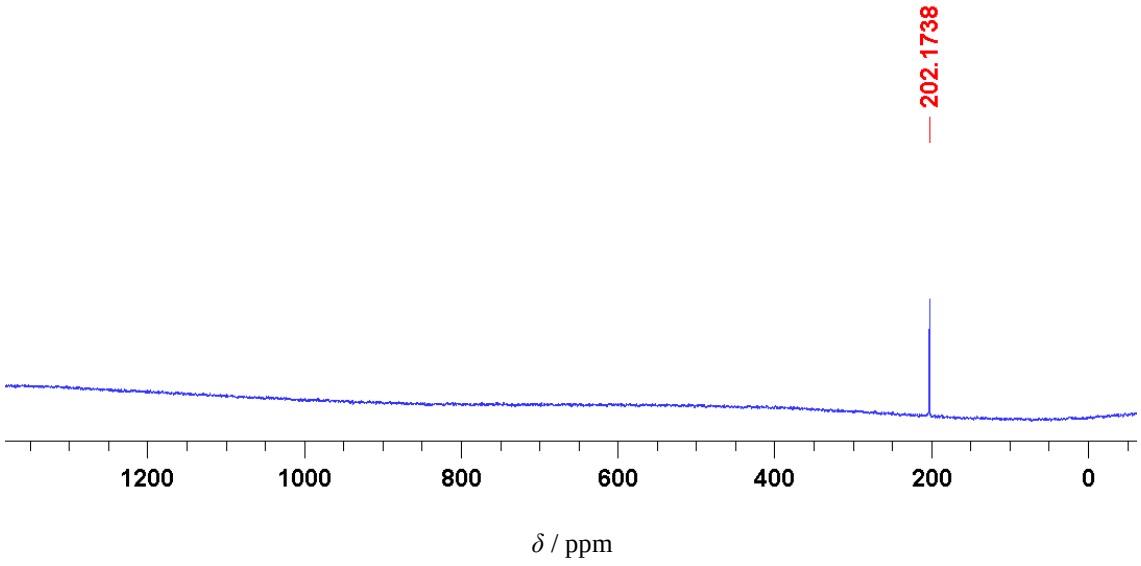


δ / ppm

B

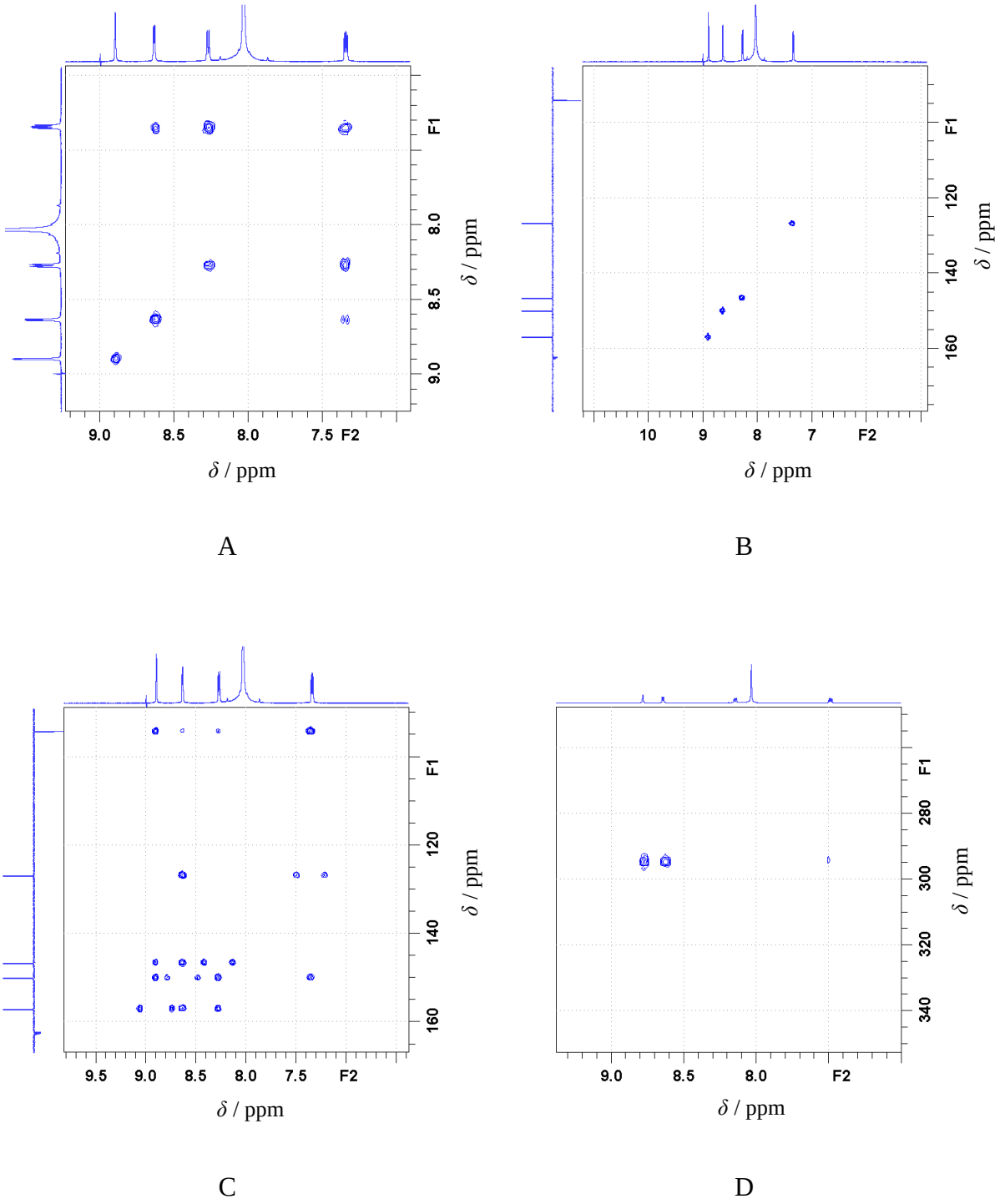


C

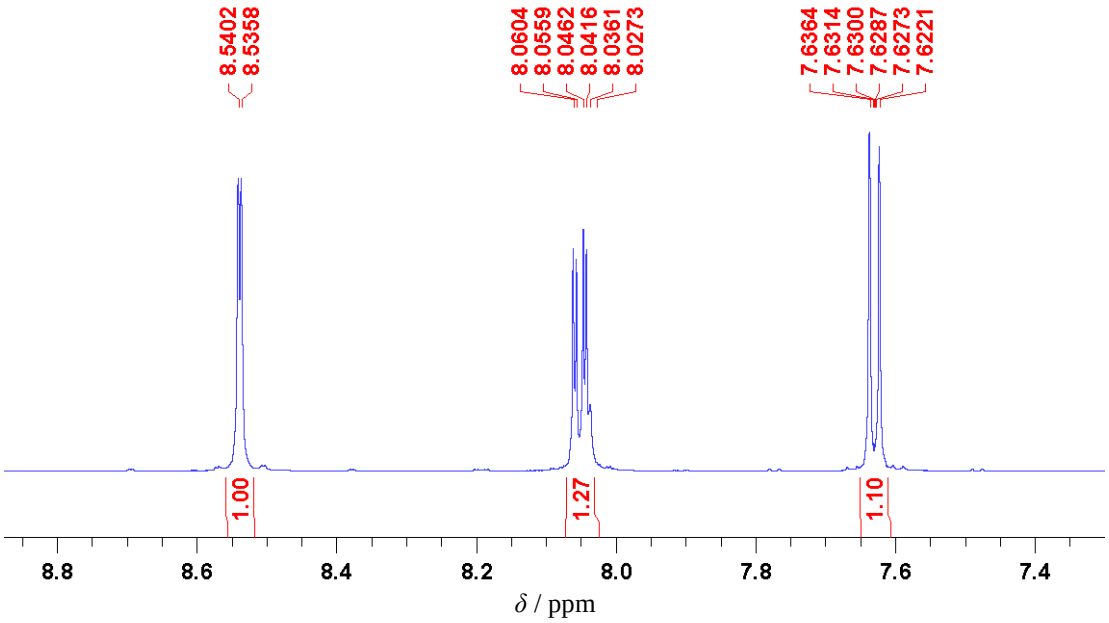


D

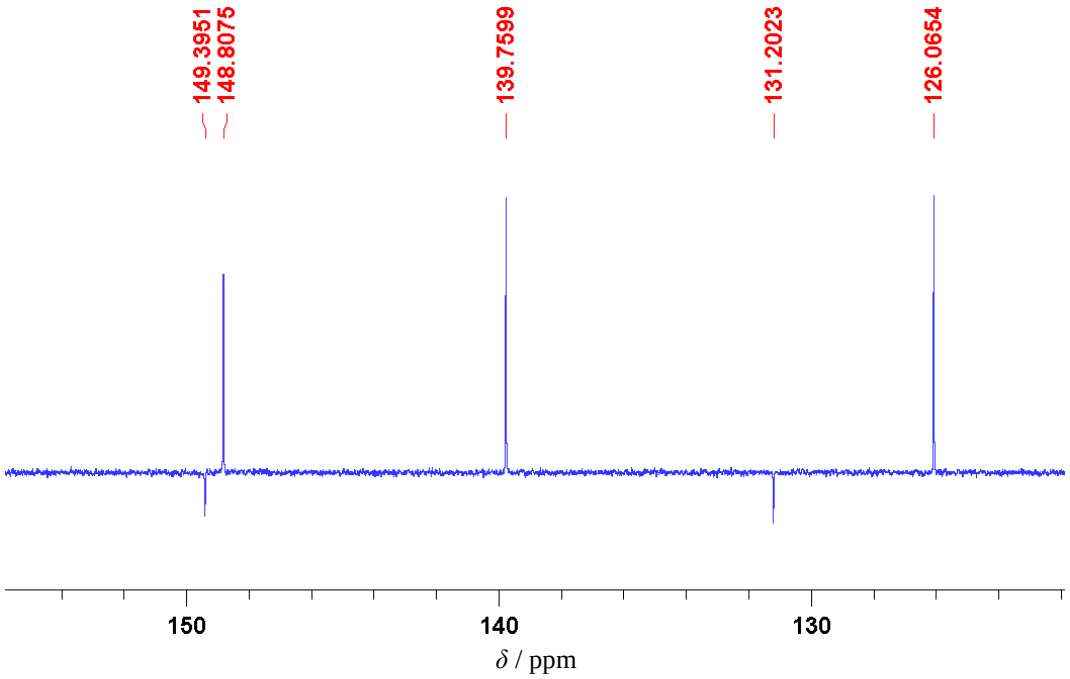
Slika D52. *A) ^{1}H, B) ^{13}C, C) ^{15}N i D) ^{109}Ag spektri kompleksa $[Ag(NO_3)(3\text{-}Ipy)_2]$, (**K6**).*



Slika D53. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR kompleksa $[Ag(NO_3)(3\text{-}Ipy)_2]$, (**K6**).*

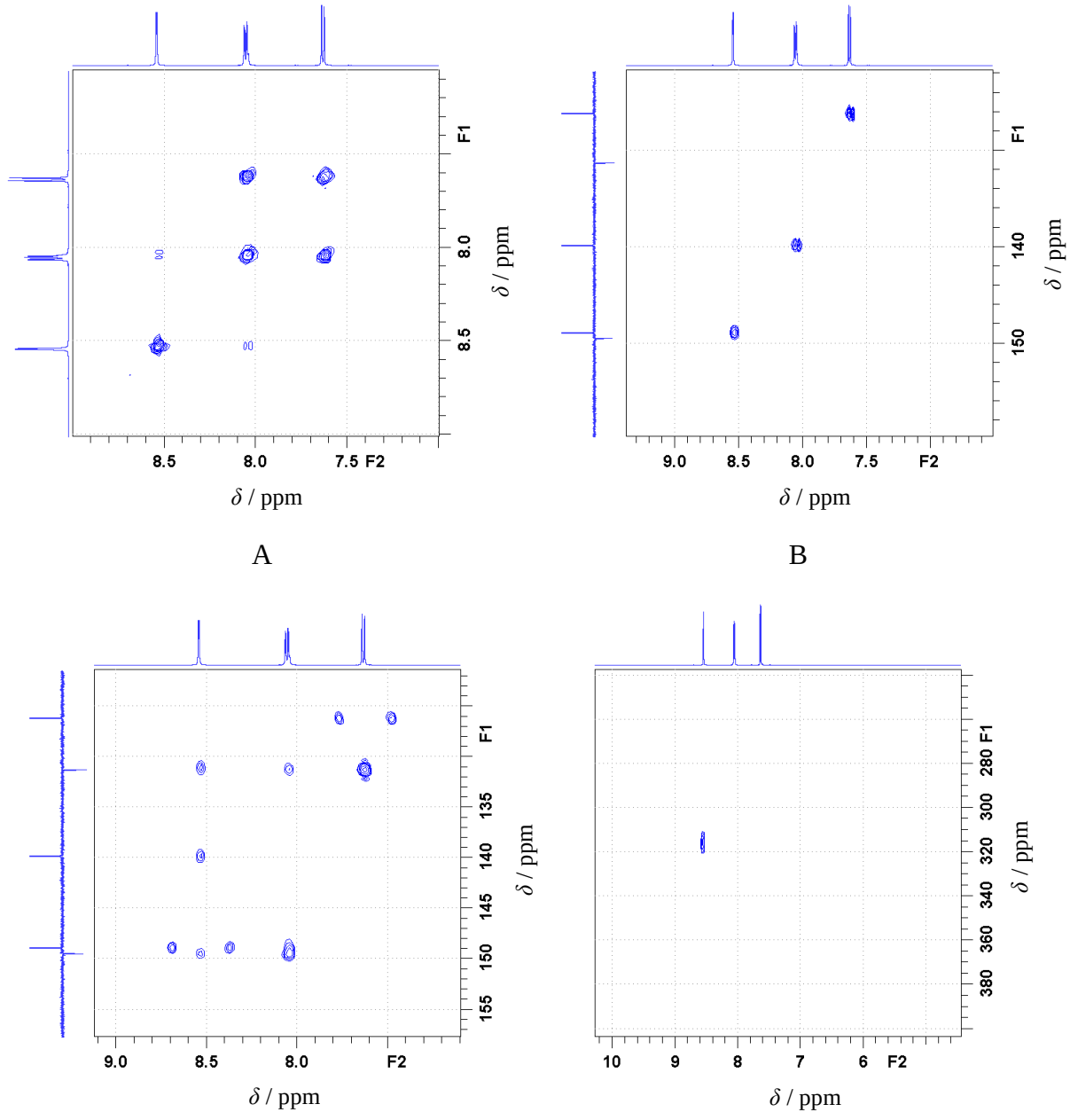


A

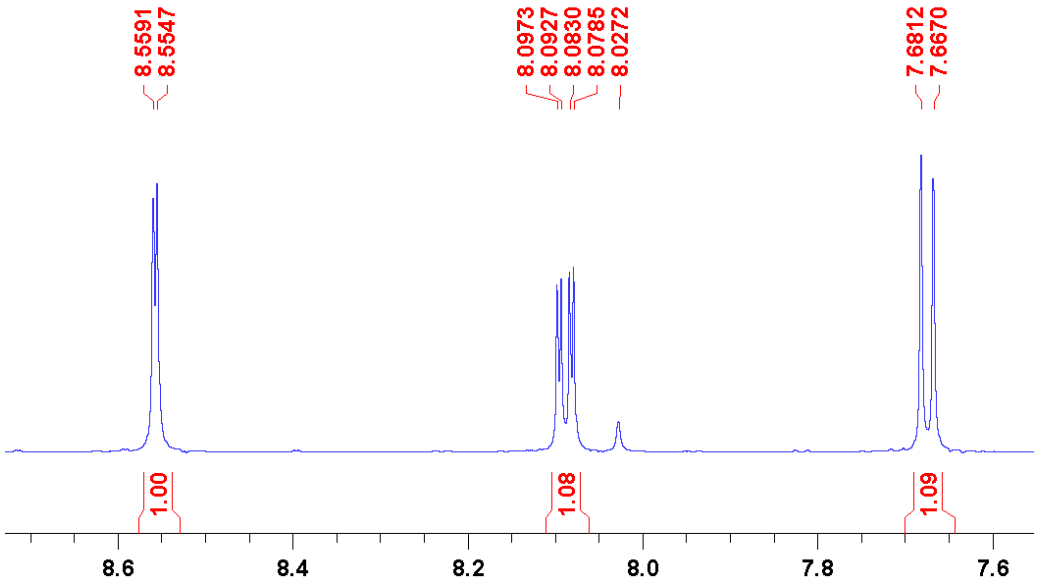


B

Slika D54. *A) ^{1}H i B) ^{13}C spektri spoja 2,5-Cl_2py, (**L7**).*

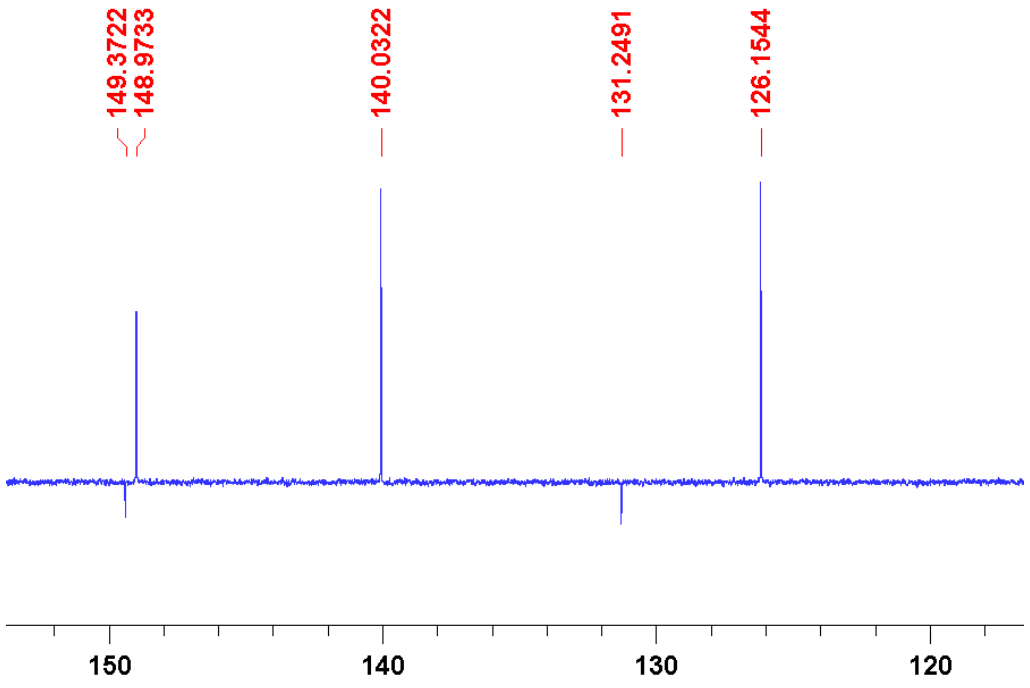


Slika D55. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR spoja 2,5-Cl$_2$py, (**L7**).*



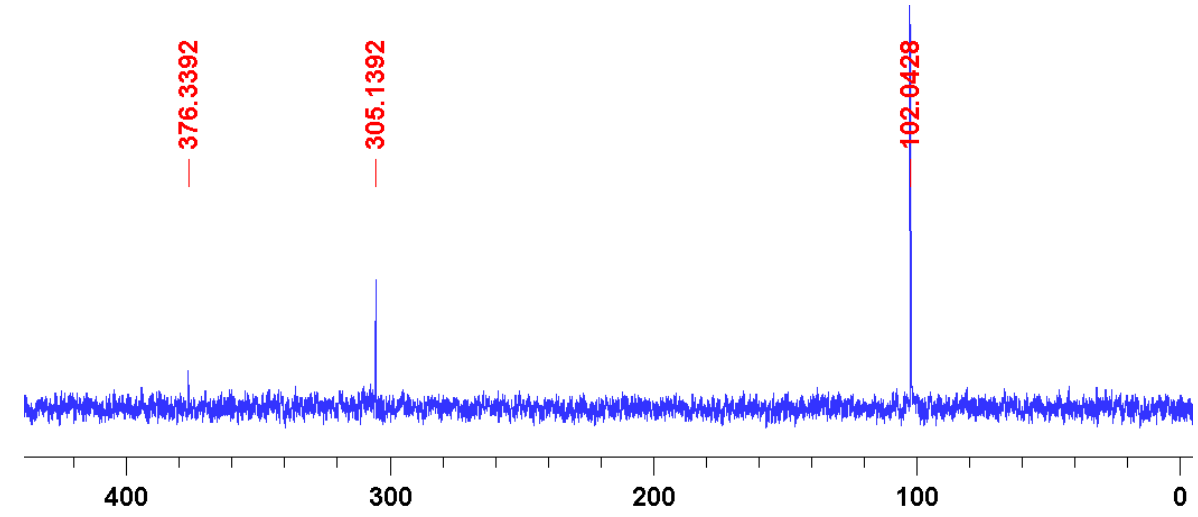
δ / ppm

A



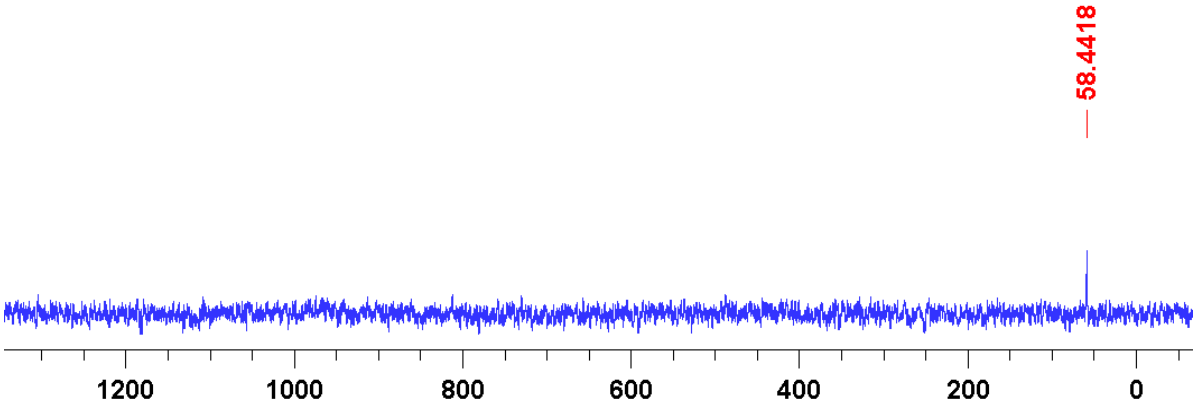
δ / ppm

B



δ / ppm

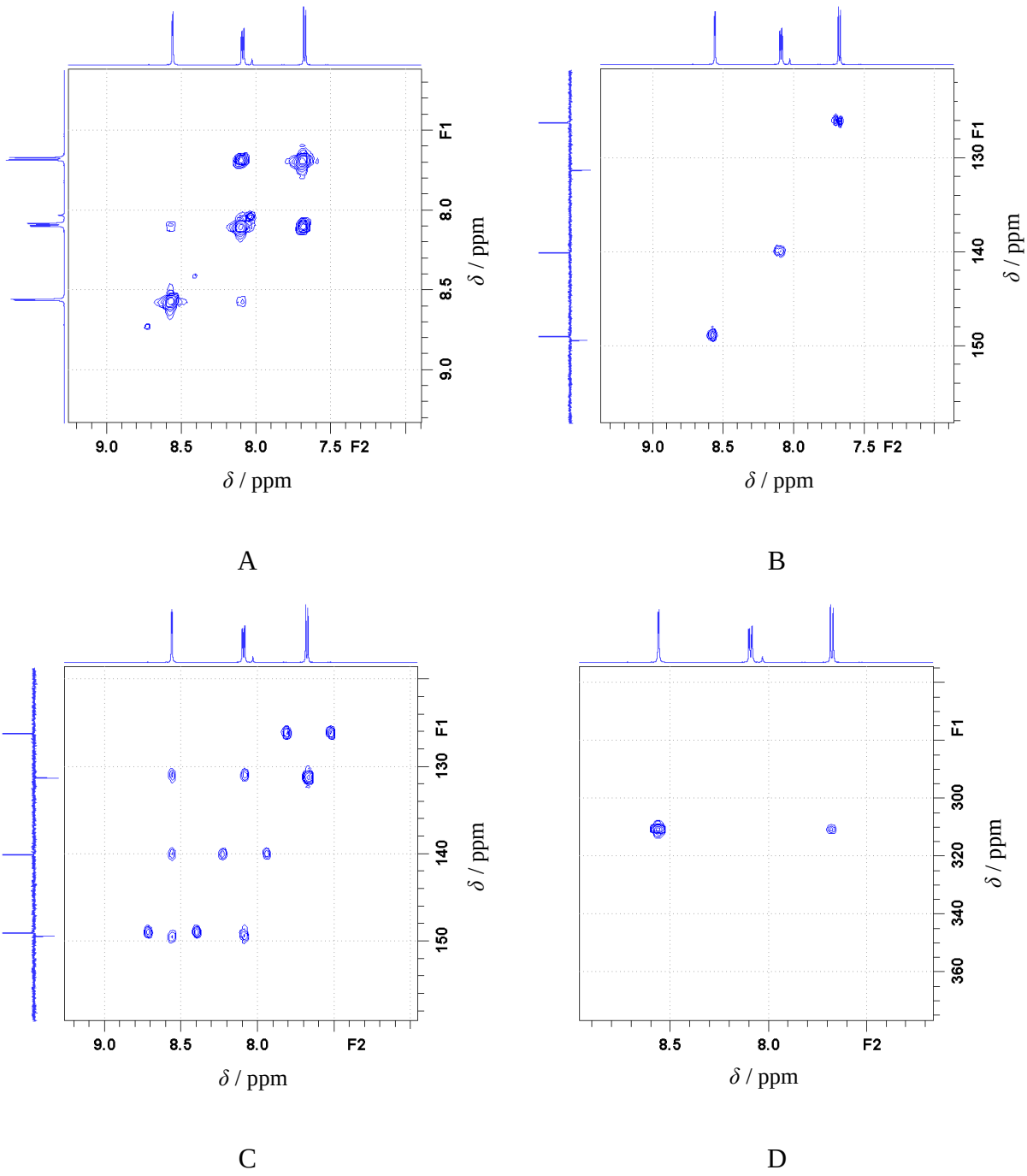
C



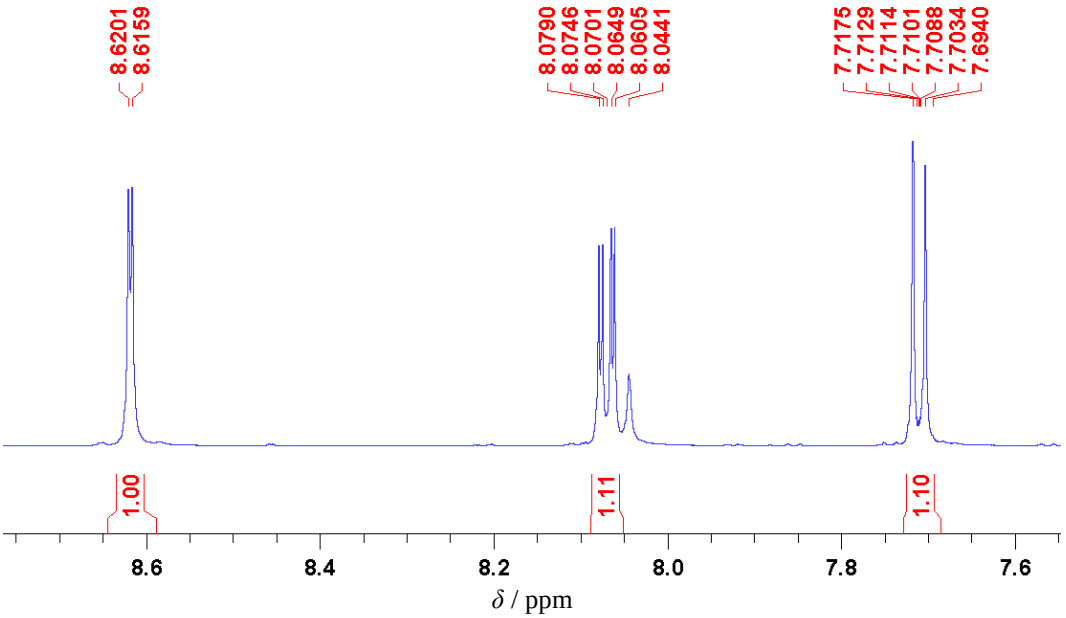
δ / ppm

D

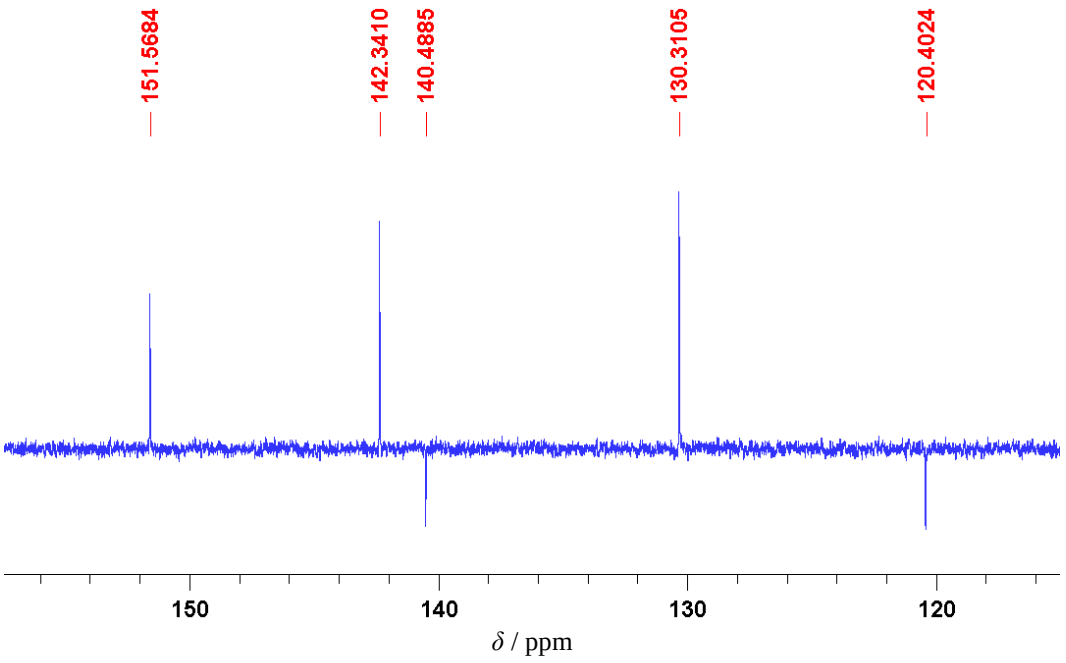
Slika D56. *A) ^{1}H, B) ^{13}C, C) ^{15}N i D) ^{109}Ag spektri NMR kompleksa $[Ag(NO_3)(2,5\text{-}Cl_2py)_2]$, (**K7**).*



Slika D57. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR kompleksa $[Ag(NO_3)(2,5\text{-}Cl_2py)_2]$, (**K7**).*

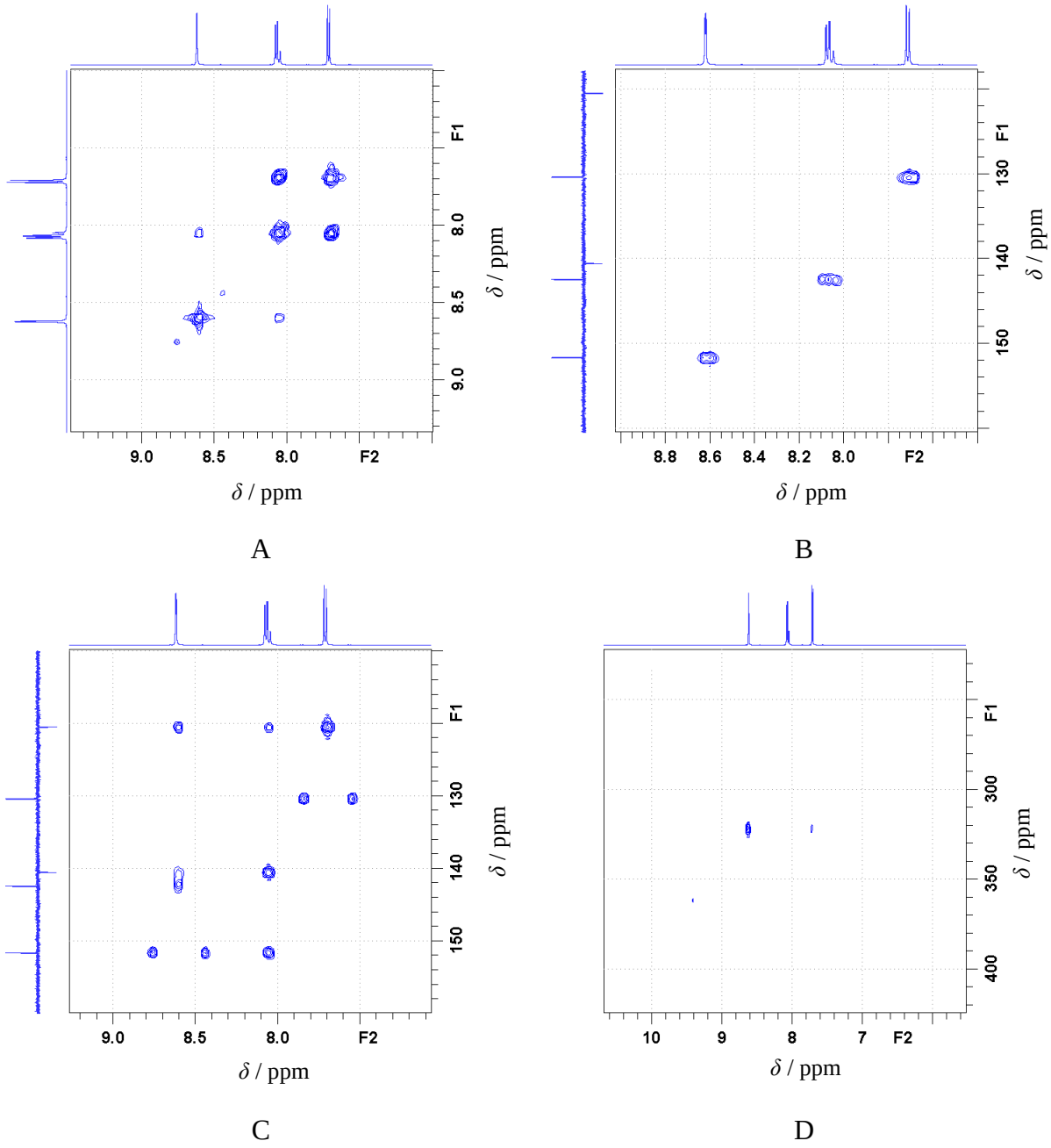


A

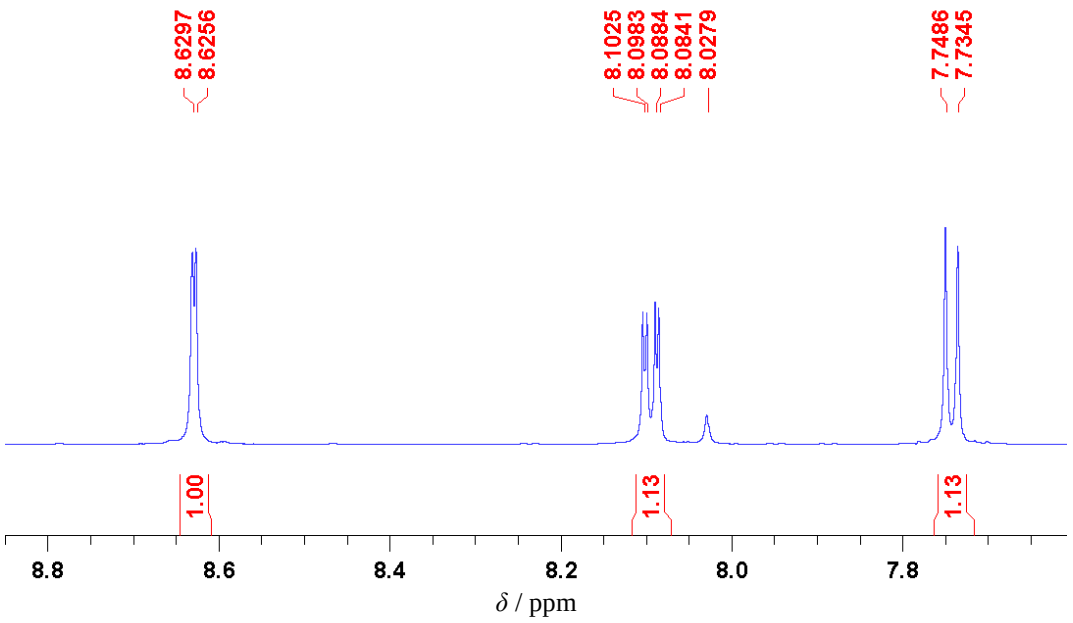


B

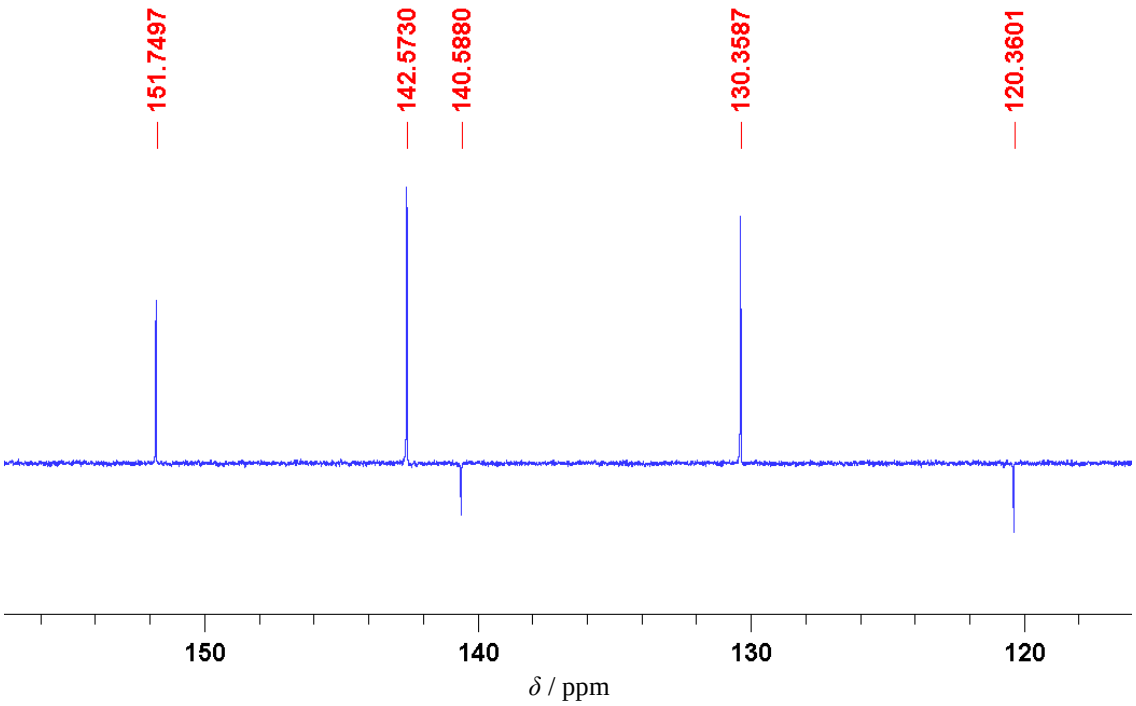
Slika D58. *A) ^{1}H i B) ^{13}C spektri spoja 2,5-Br_2py, (**L8**).*



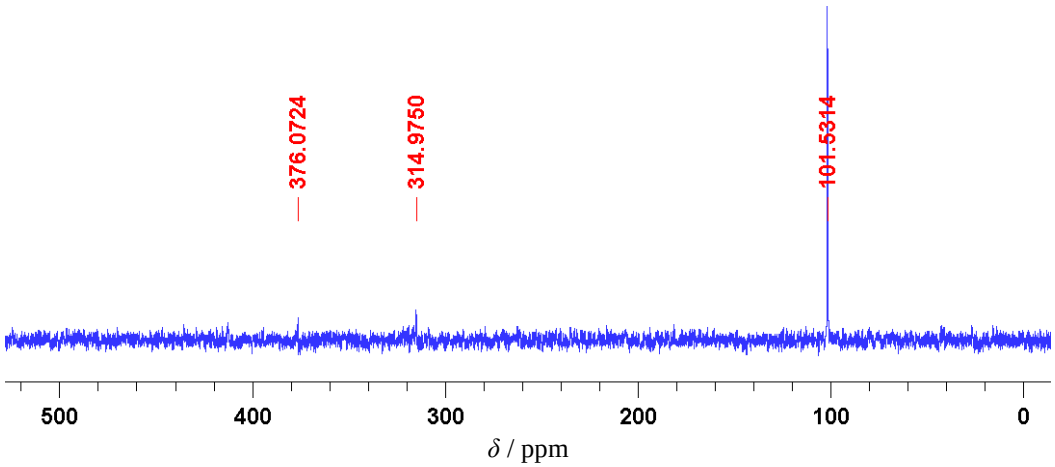
Slika D59. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR spoja 2,5-Br$_2$py,* ***(L8)****.*


8.6297
8.6256
8.1025
8.0983
8.0884
8.0841
8.0279
7.7486
7.7345
1.00
1.13
1.13
8.8
8.6
8.4
8.2
8.0
7.8
δ / ppm

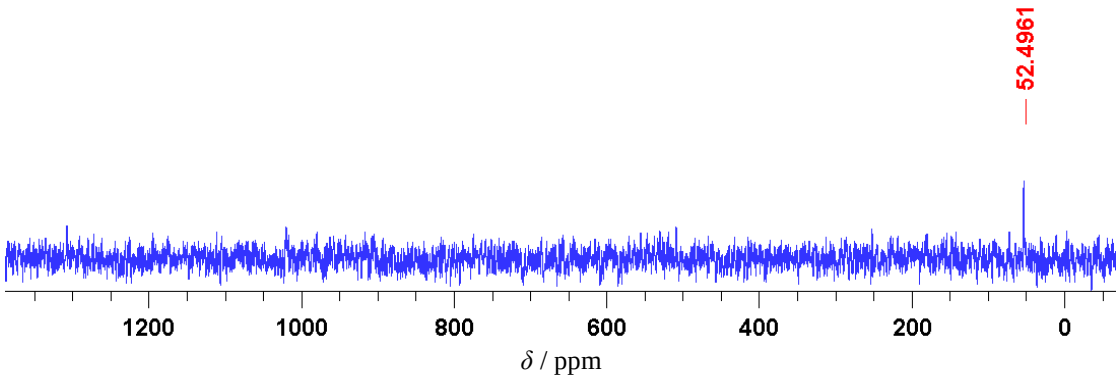
A


151.7497
142.5730
140.5880
130.3587
120.3601
150
140
130
120
δ / ppm

B

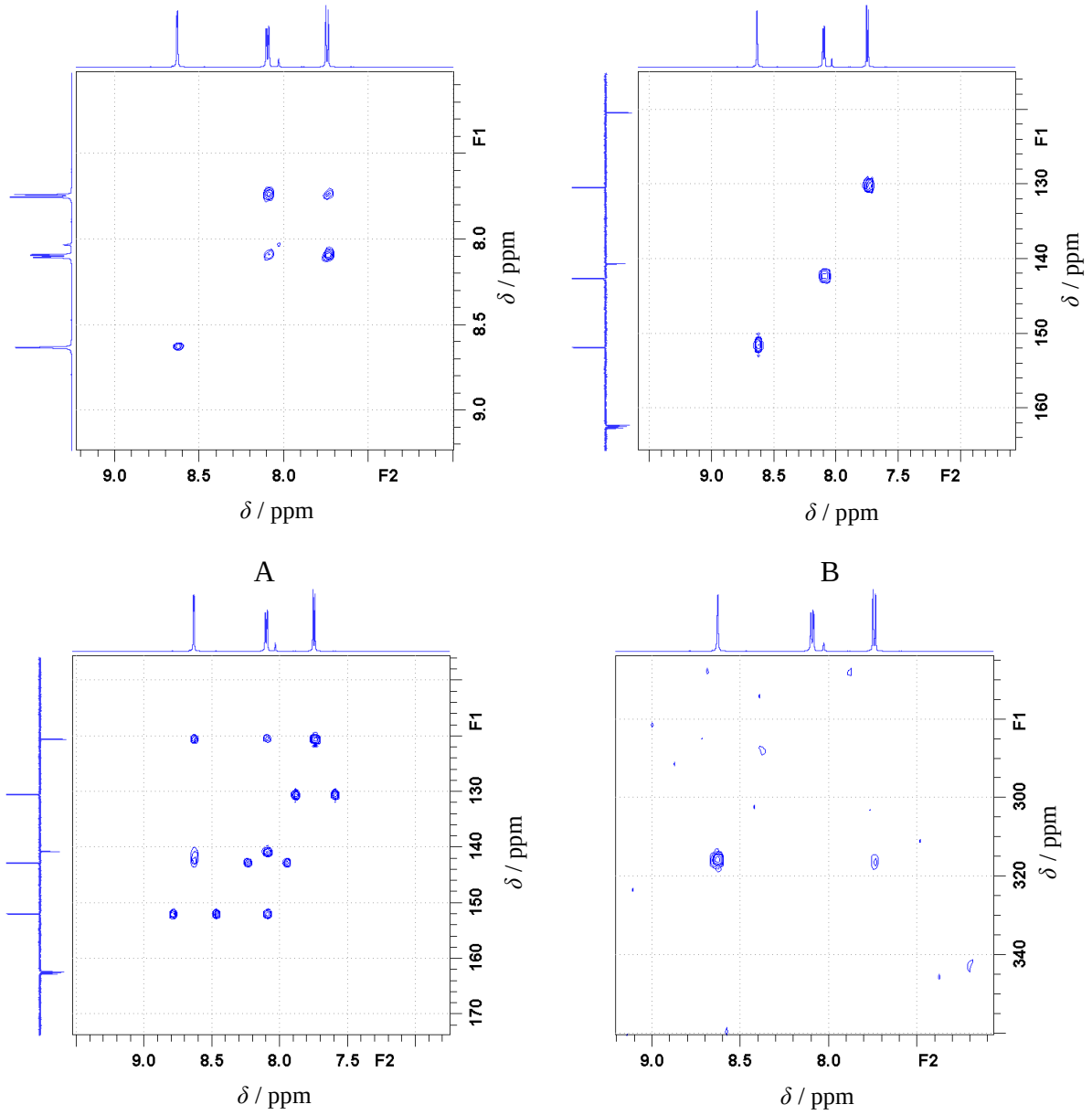


C

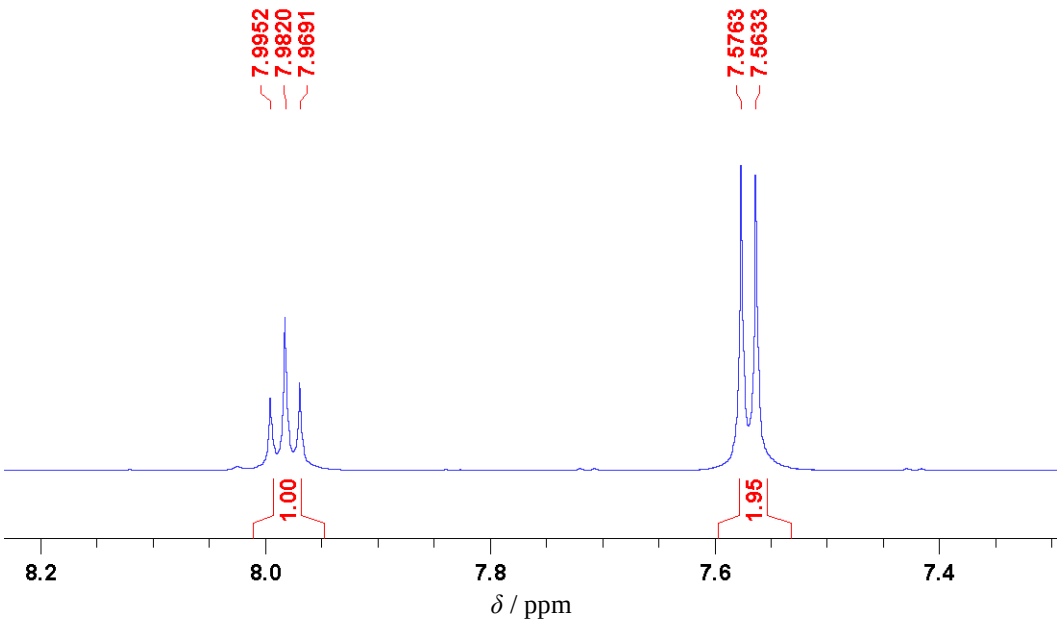


D

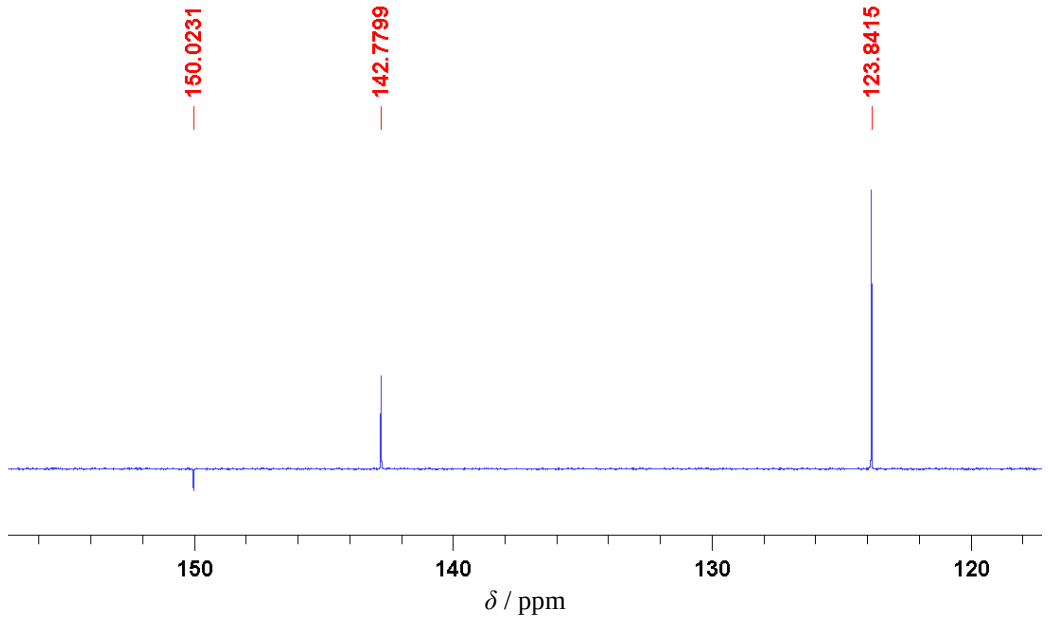
Slika D60. *A) ^{1}H, B) ^{13}C, C) ^{15}N i D) ^{109}Ag spektri kompleksa $[Ag(NO_3)(2,5\text{-}Br_2py)_2]$, (**K8**).*



Slika D61. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR kompleksa $[Ag(NO_3)(2,5\text{-}Br_2py)_2]$,* ***(K8)****.*

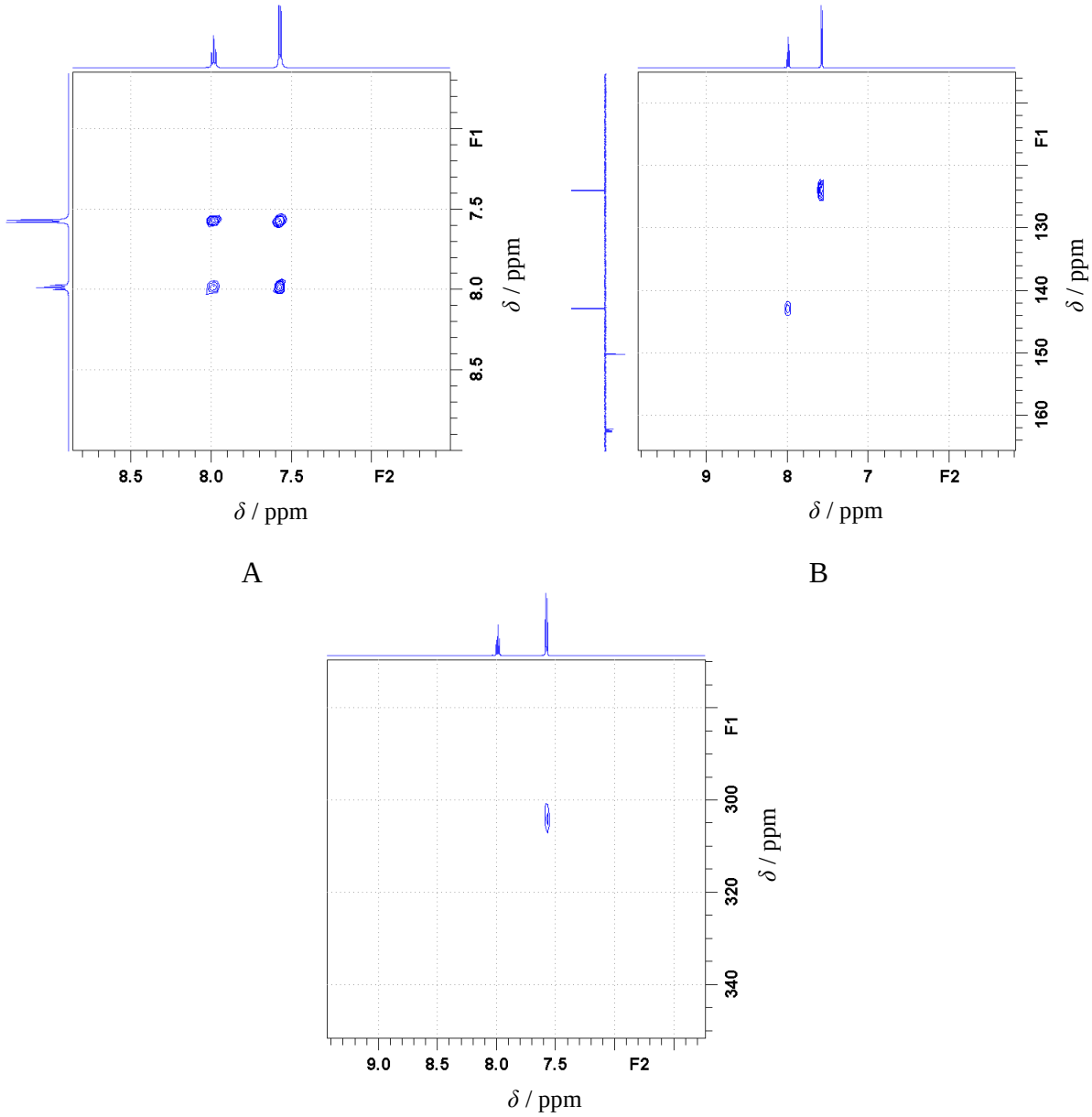


A

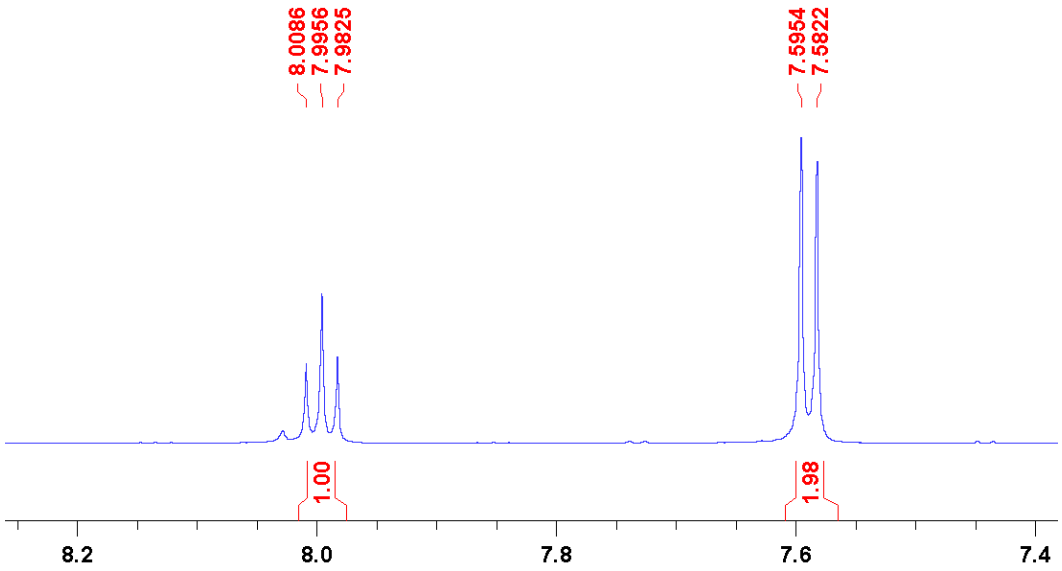


B

Slika D62. *A) ^{1}H i B) ^{13}C spektri spoja 2,6-Cl_2py, (**L9**).*

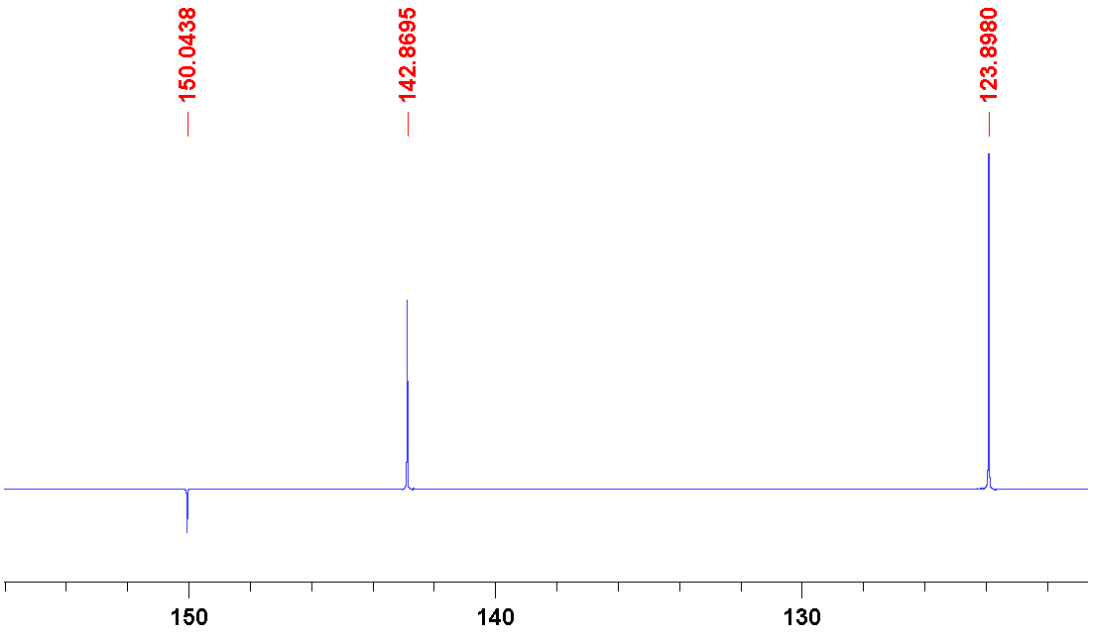


Slika D63. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC i C) ^{1}H-^{15}N HMBC spektara NMR spoja 2,6-Cl$_2$py, (**L9**).*



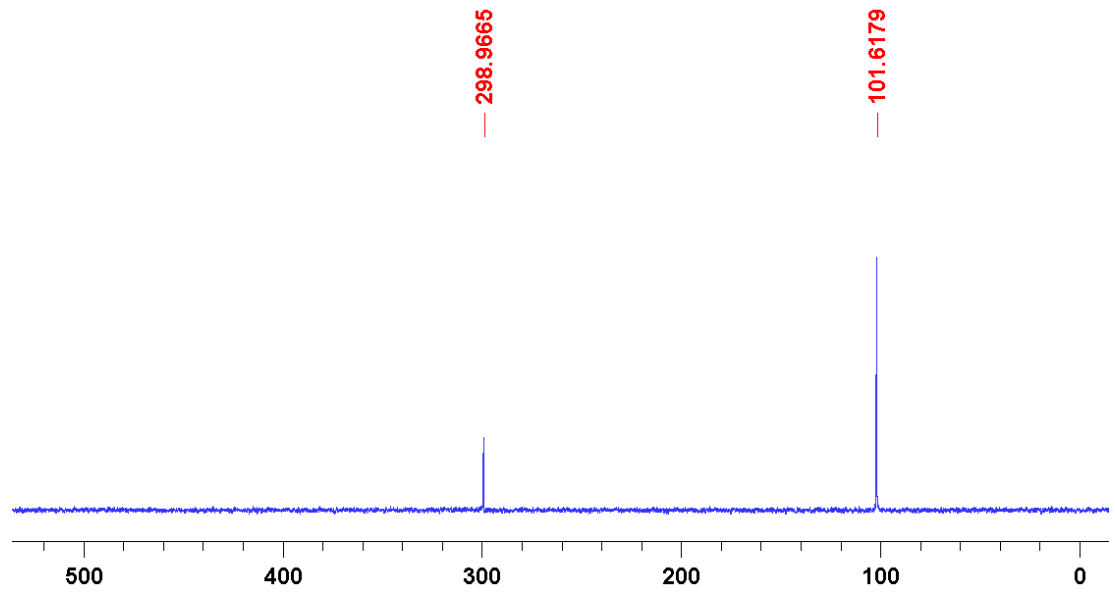
δ / ppm

A



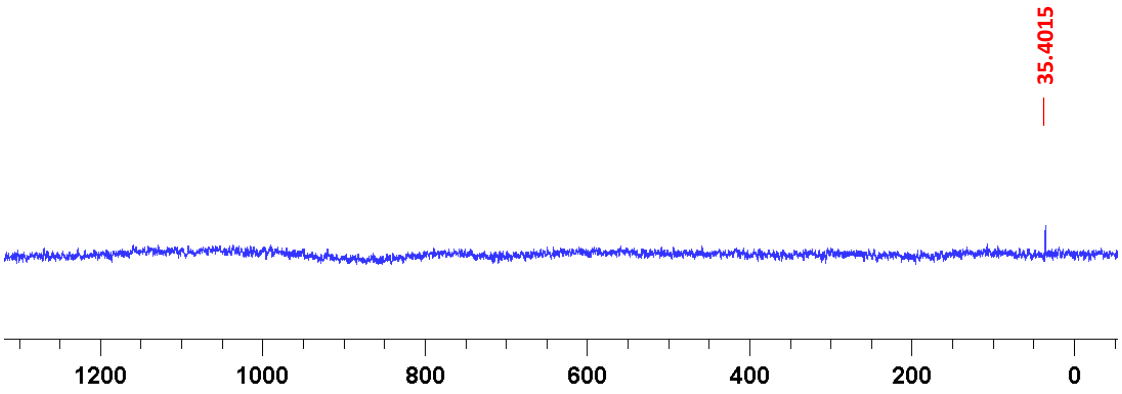
δ / ppm

B



δ / ppm

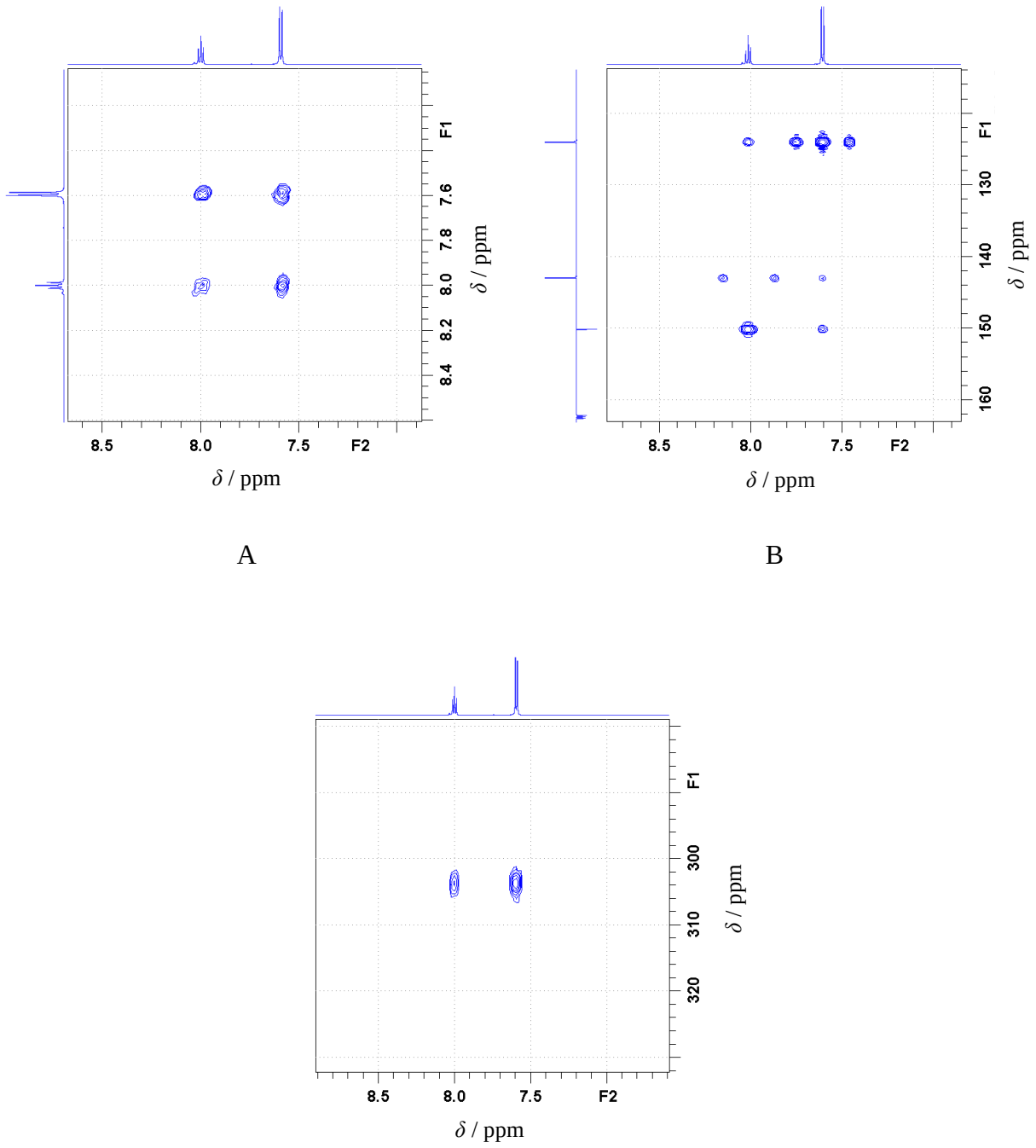
C



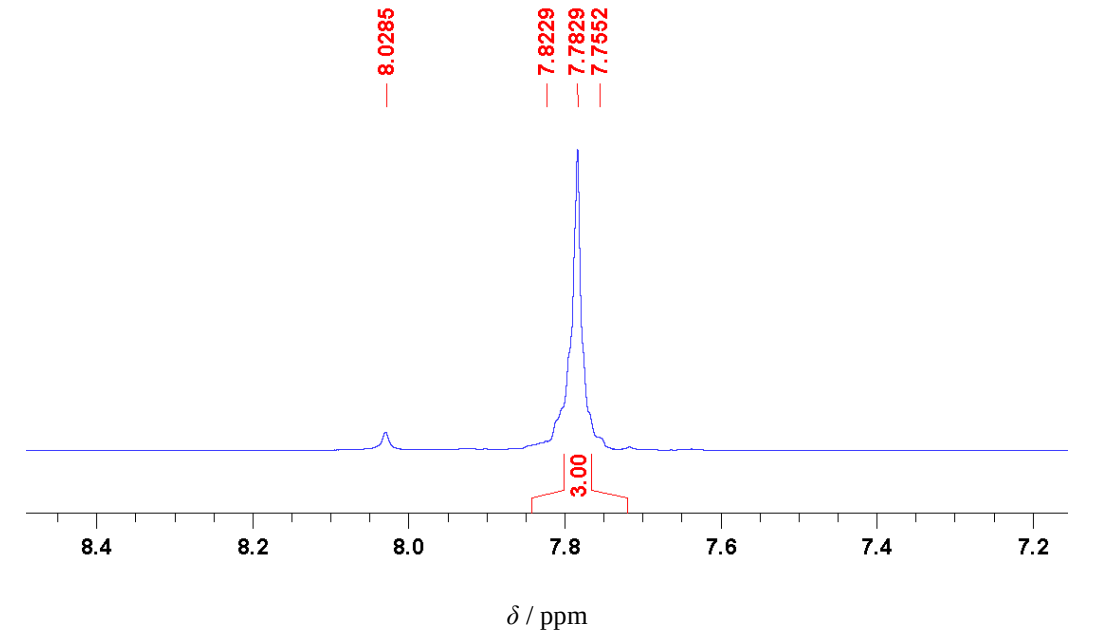
δ / ppm

D

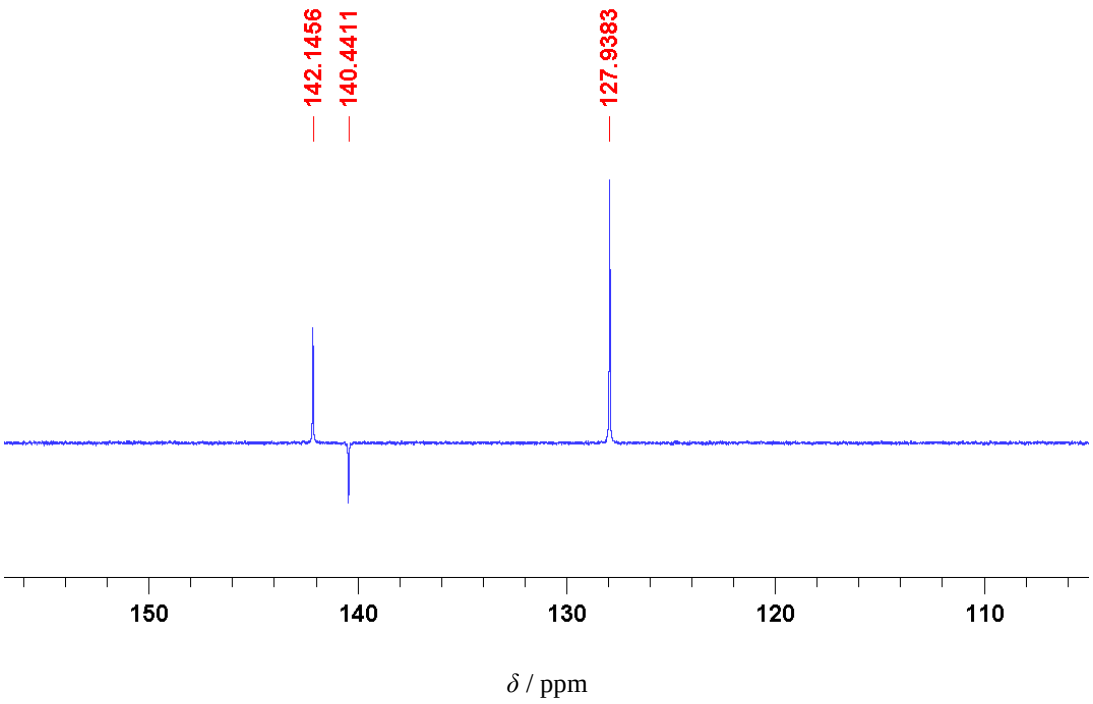
Slika D64. *A) ^{1}H, B) ^{13}C, C) ^{15}N i D) ^{109}Ag spektri kompleksa $[Ag(NO_3)(2,6\text{-}Cl_2py)_2]$, (**K9**).*



Slika D65. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMBC i C) ^{1}H-^{15}N HMBC spektara NMR kompleksa $[Ag(NO_3)(2,6\text{-}Cl_2py)_2]$, (**K9**).*

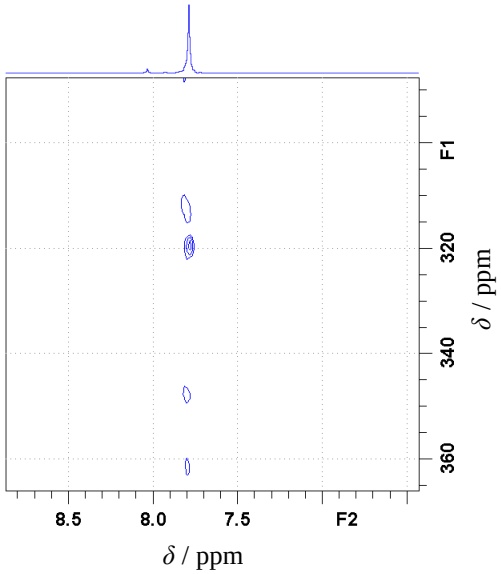


A

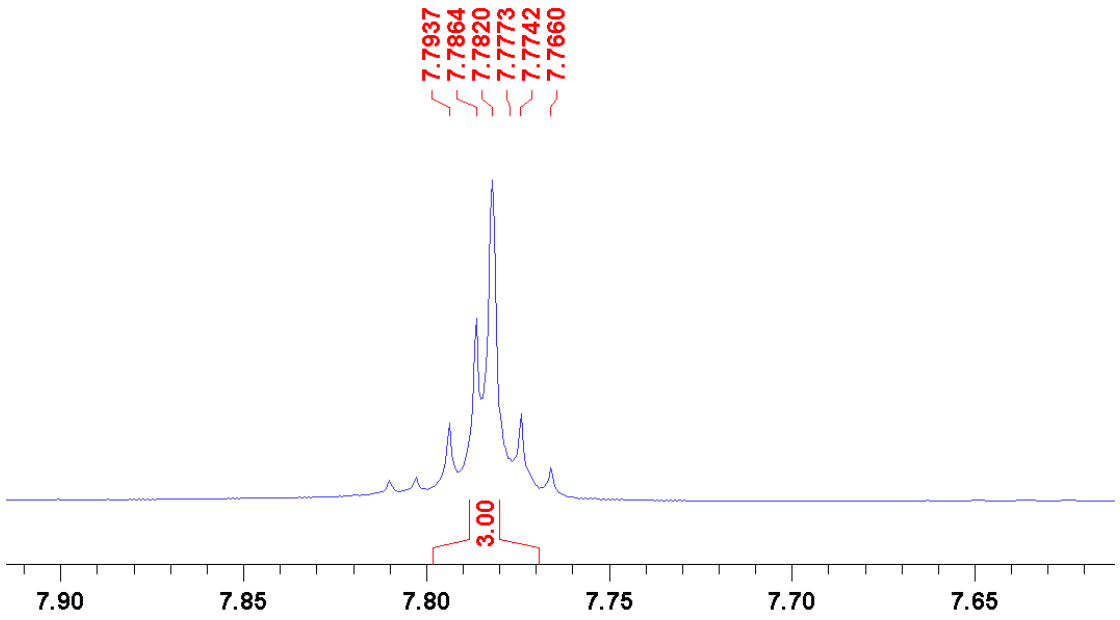


B

Slika D66. *A) ^{1}H i B) ^{13}C spektri spoja 2,6-Br_2py, (**L10**).*

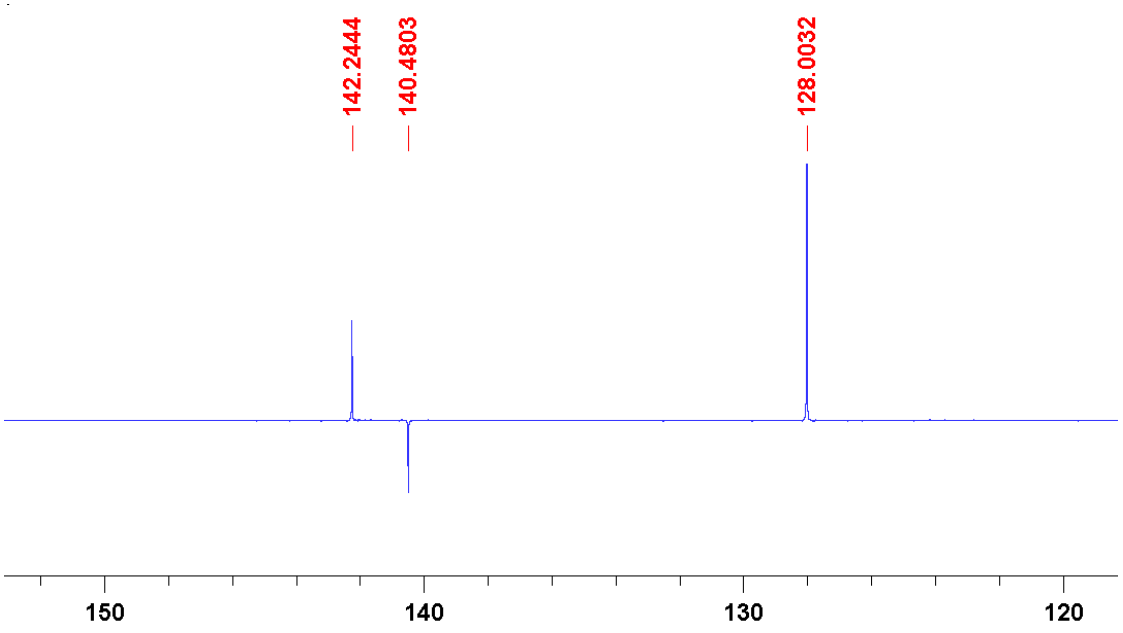


Slika D67. *Uvećani prikaz ^{1}H-^{15}N HMBC spektra NMR spoja 2,6-Br_2py (**L10**).*



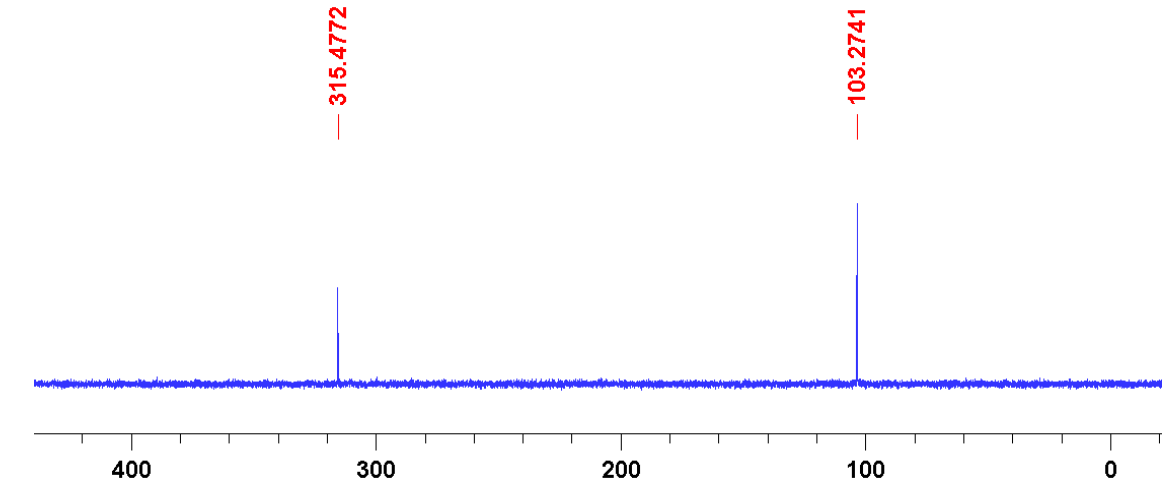
δ / ppm

A

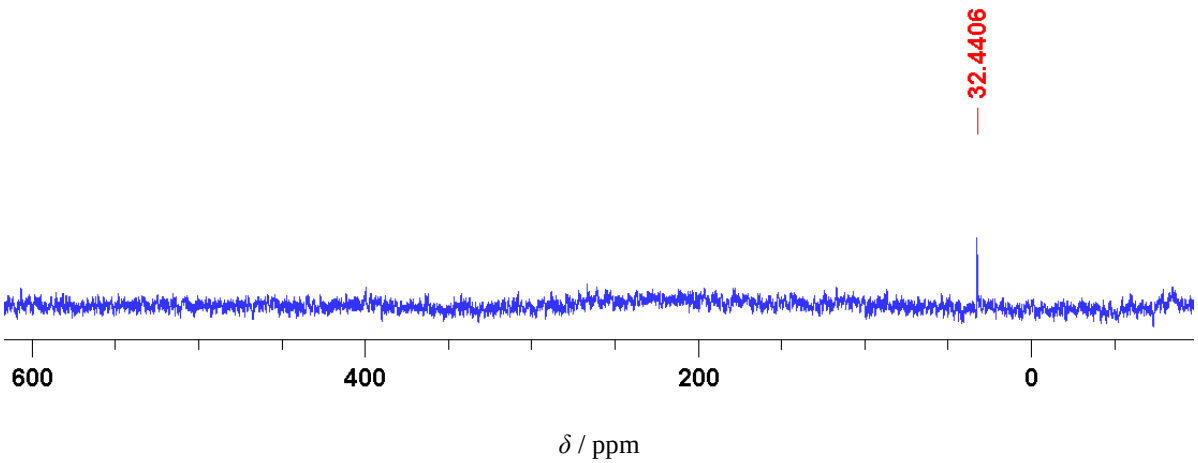


δ / ppm

B

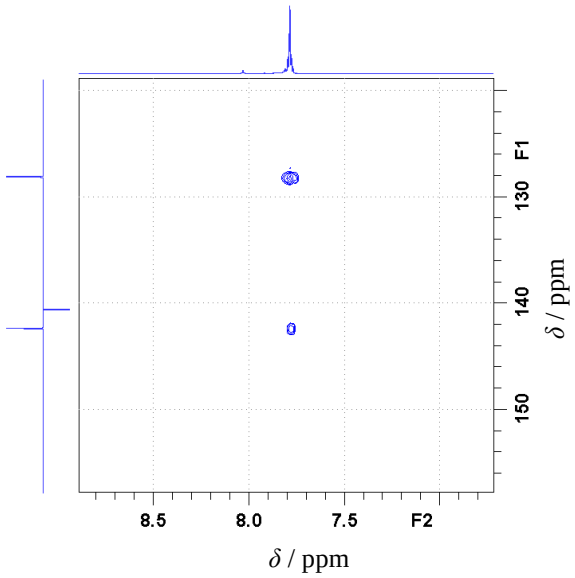


C

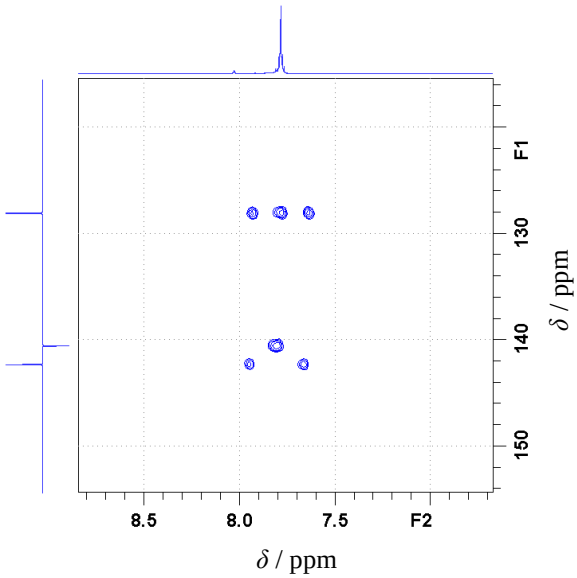


D

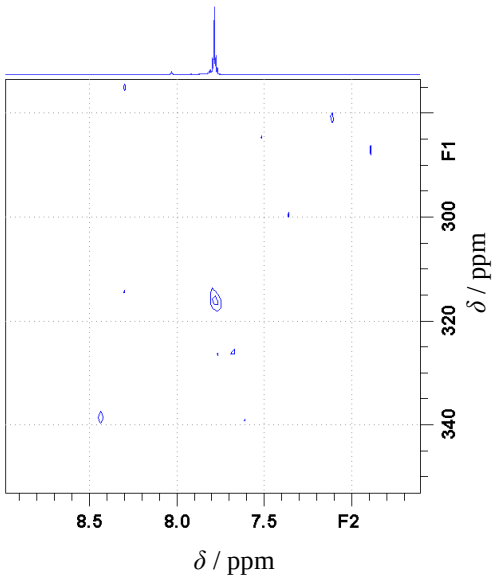
Slika D68. *A) ^{1}H, B) ^{13}C, C) ^{15}N i D) ^{109}Ag spektri kompleksa $[Ag(NO_3)(2,6\text{-}Br_2py)_2]$, (**K10**).*



A

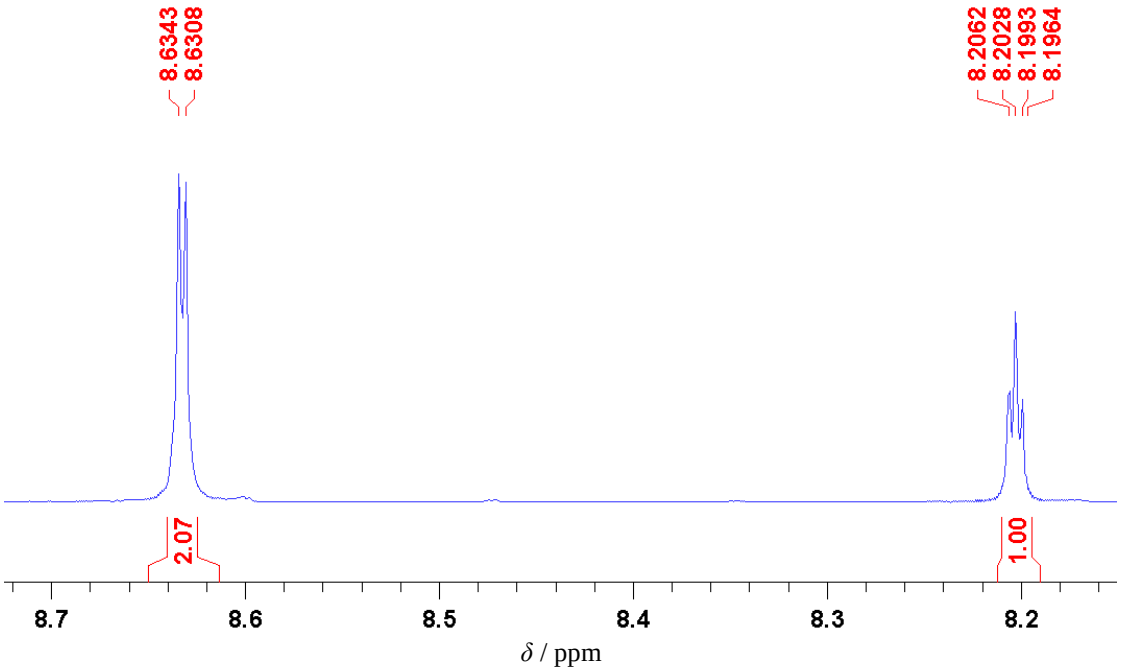


B

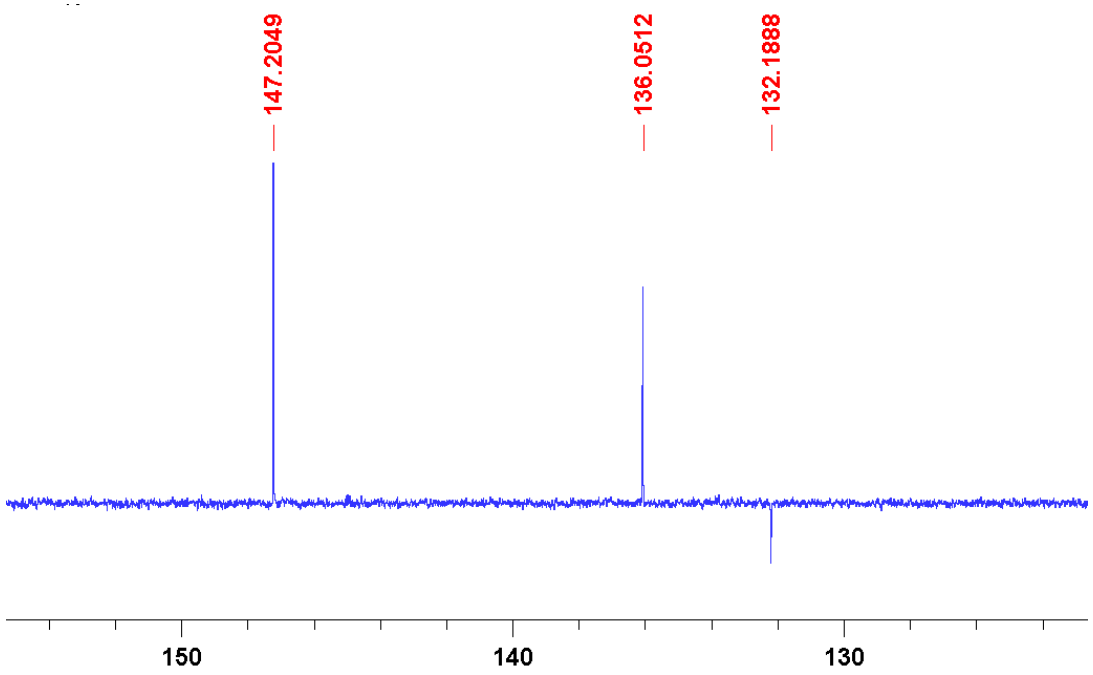


C

Slika D69. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMBC i C) ^{1}H-^{15}N HMBC spektara NMR kompleksa [Ag(NO$_3$)(2,6-Br$_2$py)$_2$],* ***(K10)****.*

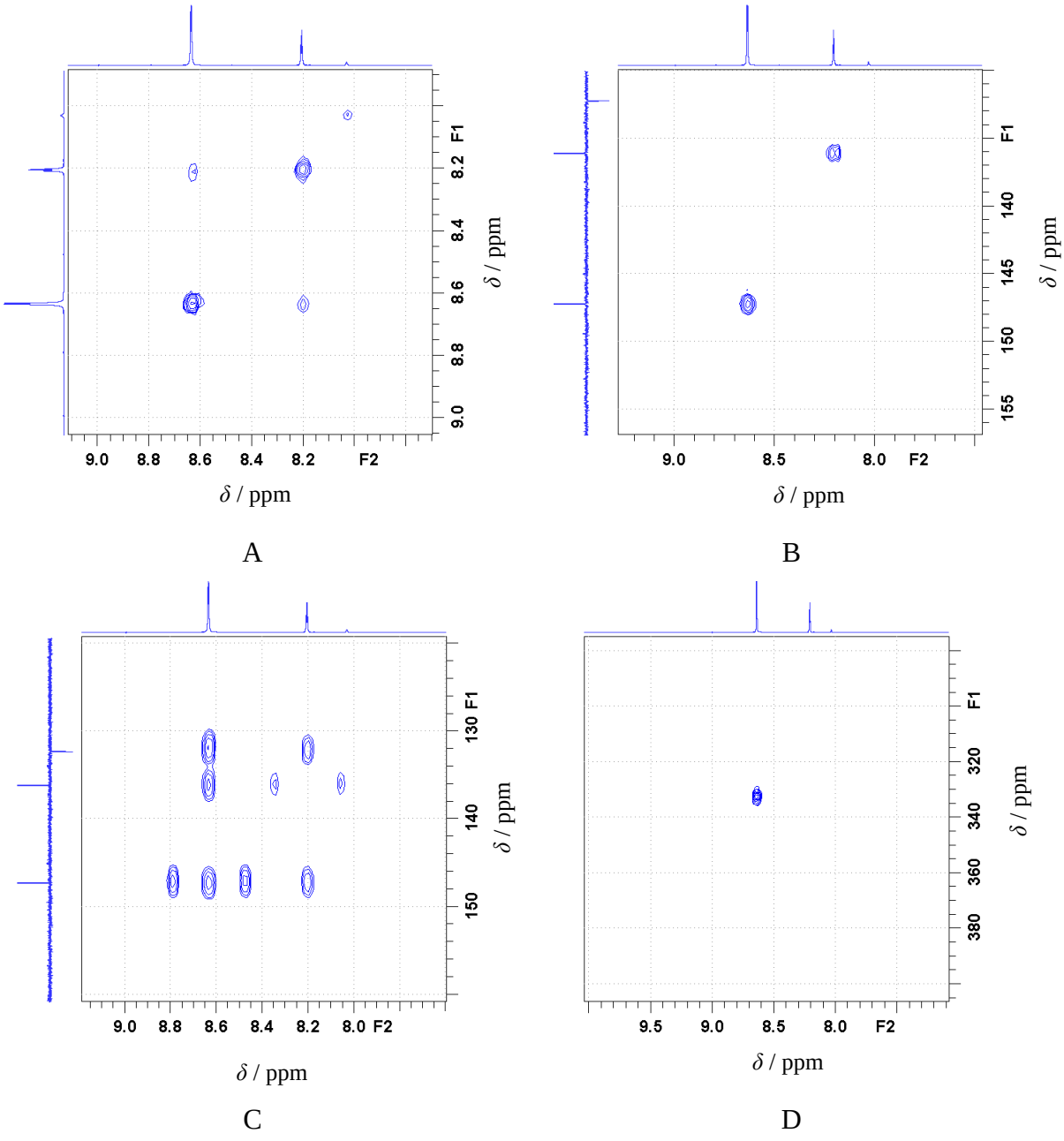


A

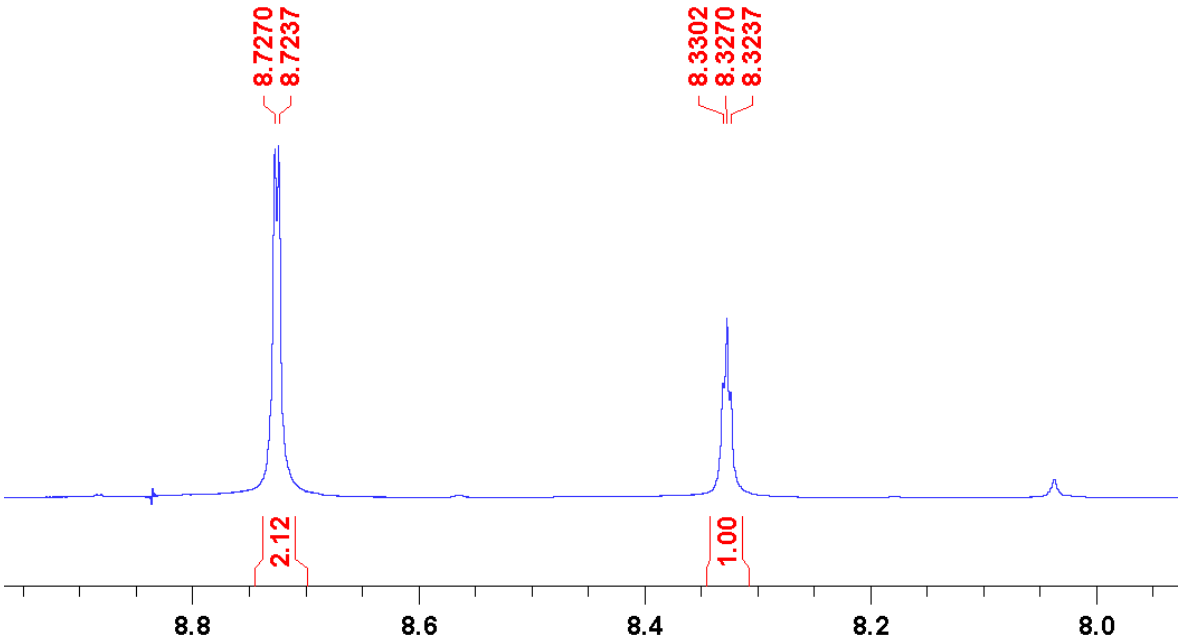


B

Slika D70. *A) ^{1}H i B) ^{13}C spektri spoja 3,5-Cl_2py,* ***(L11)****.*

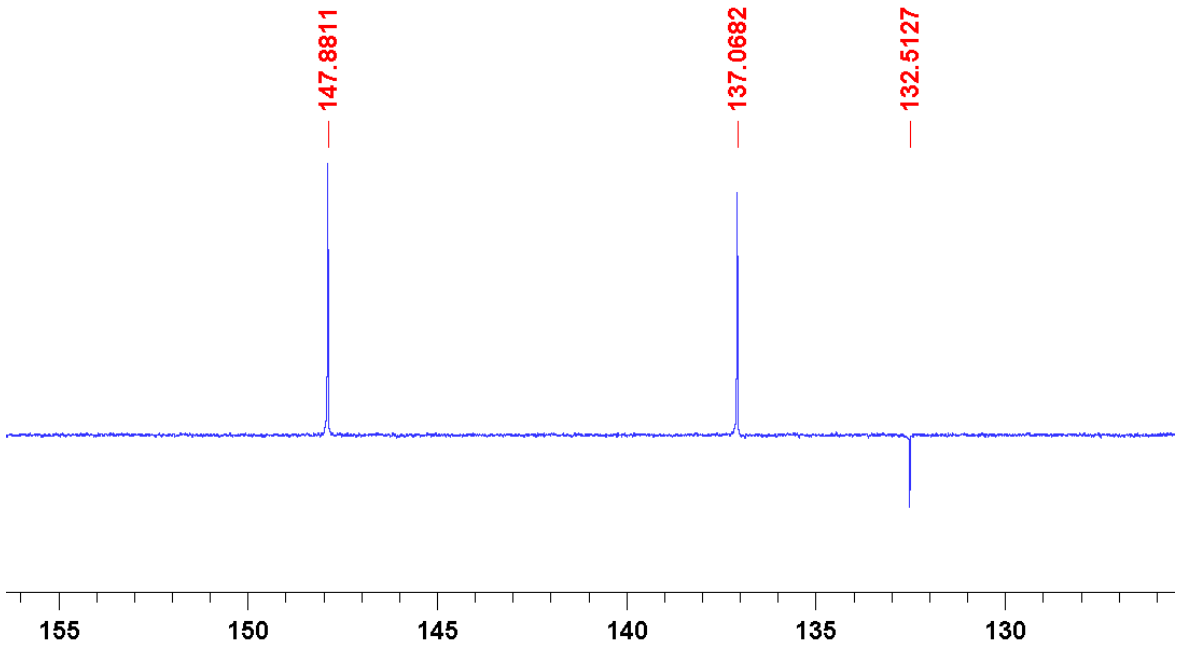


Slika D71. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR spoja 3,5-Cl$_2$py, (**L11**).*



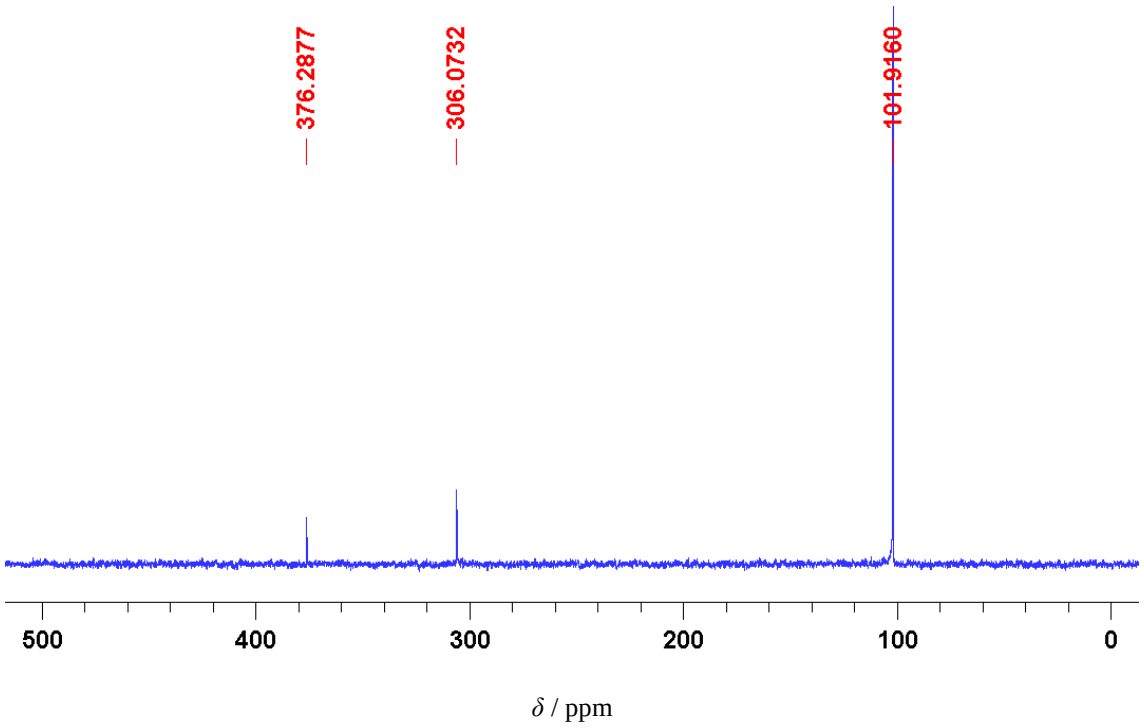
δ / ppm

A

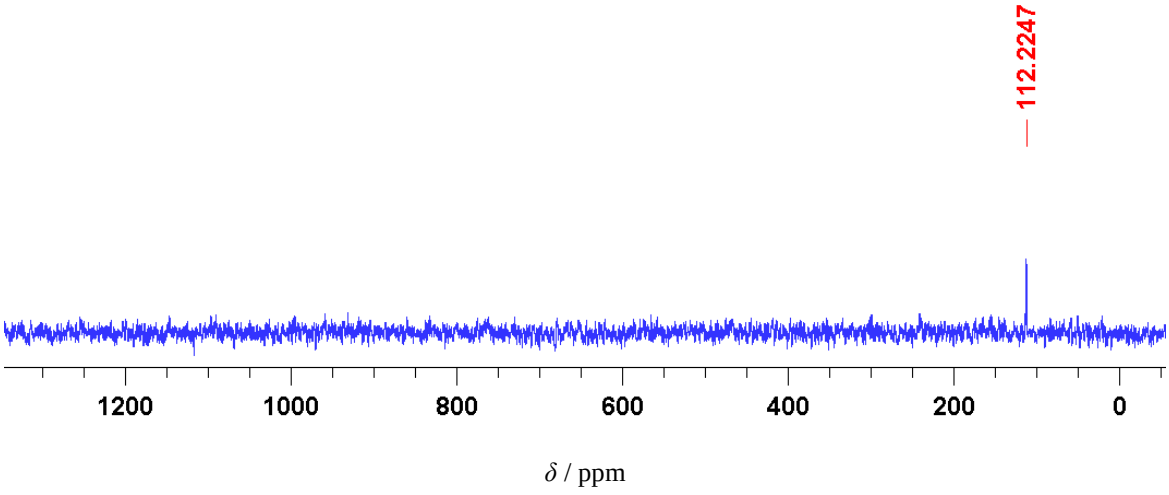


δ / ppm

B

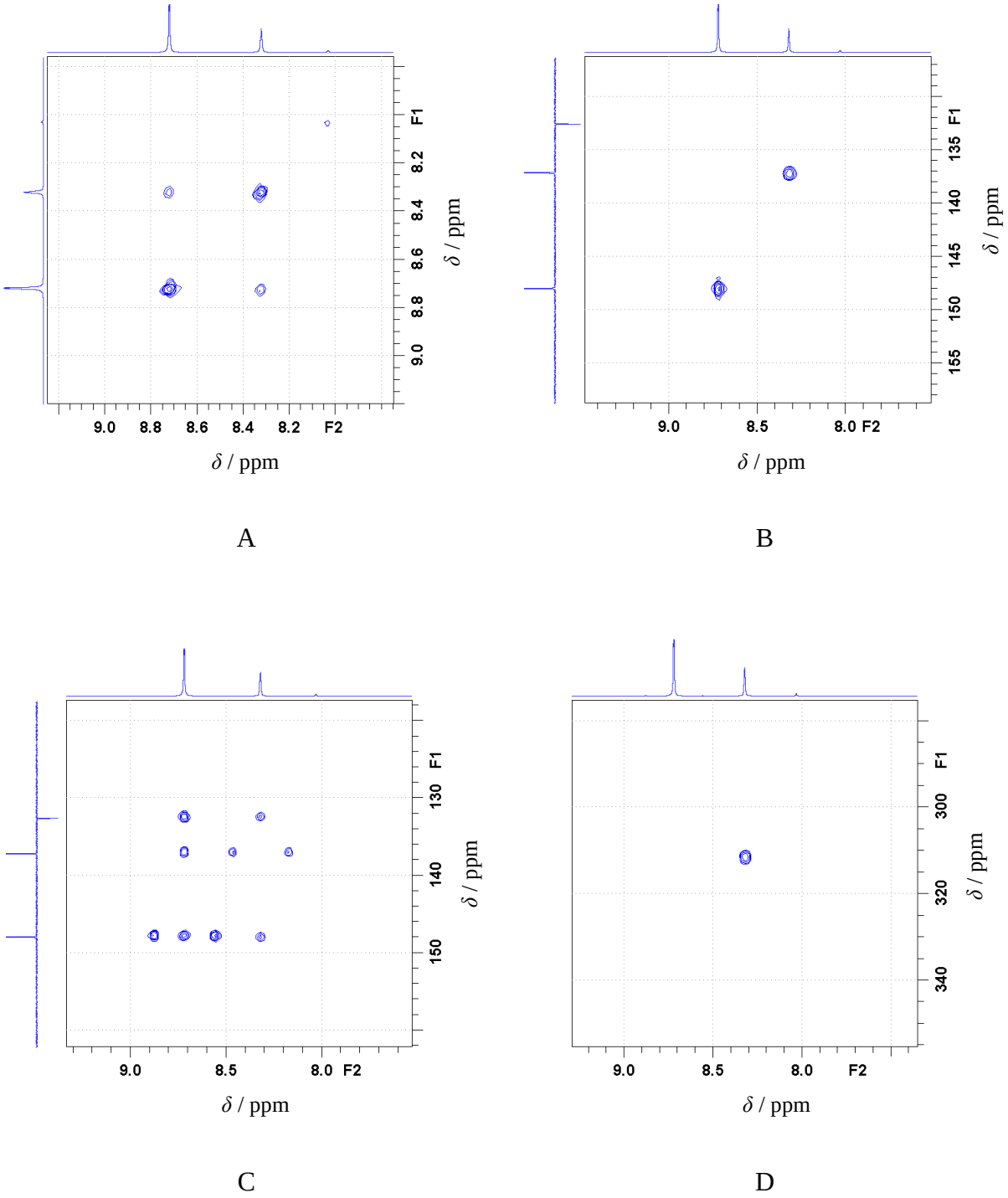


C

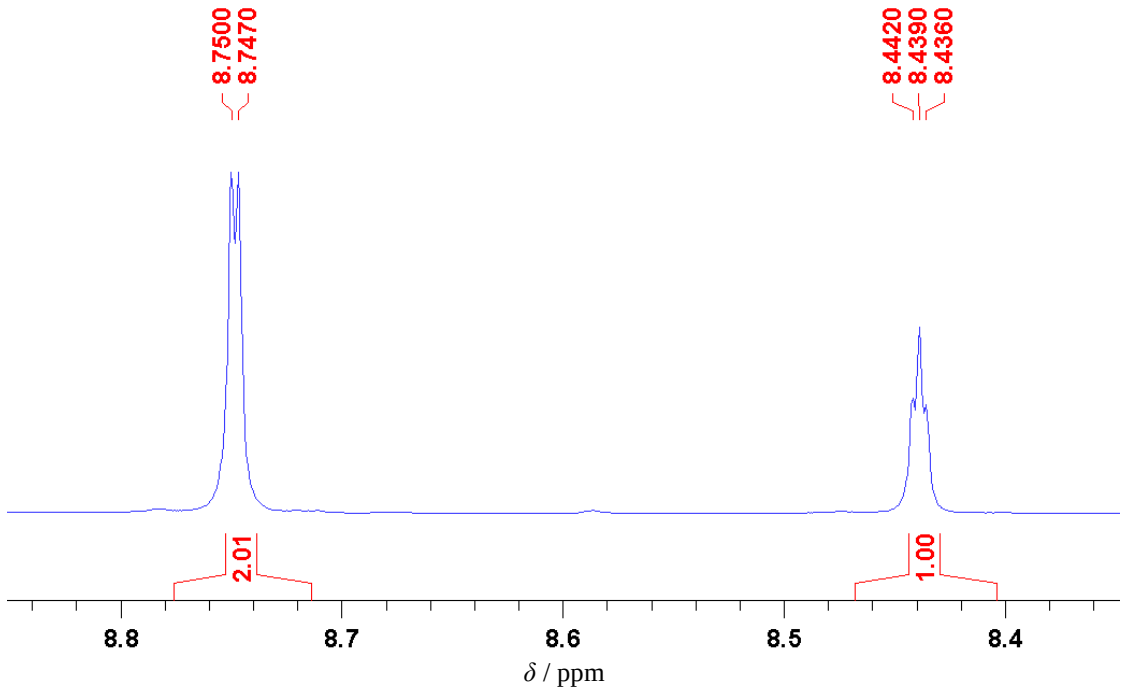


D

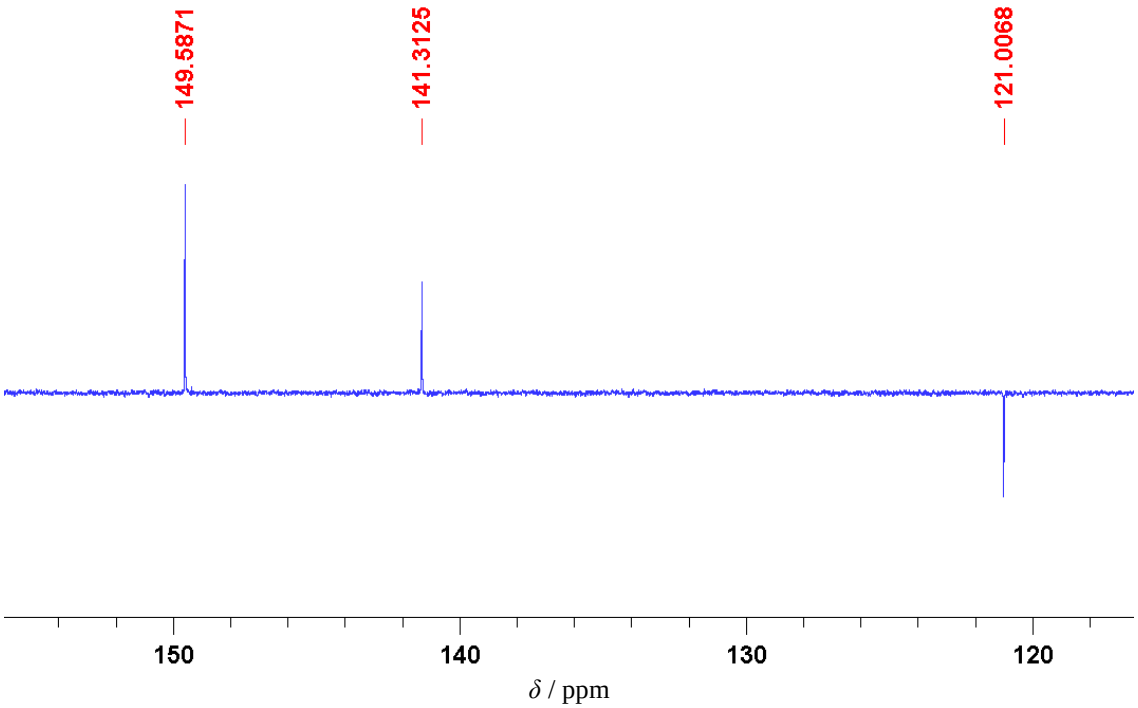
Slika D72. *A) ^{1}H, B) ^{13}C, C) ^{15}N i D) ^{109}Ag spektri kompleksa $[Ag(NO_3)(3,5\text{-}Cl_2py)_2]$, (**K11**).*



Slika D73. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR kompleksa $[Ag(NO_3)(3,5\text{-}Cl_2py)_2]$, (**K11**).*

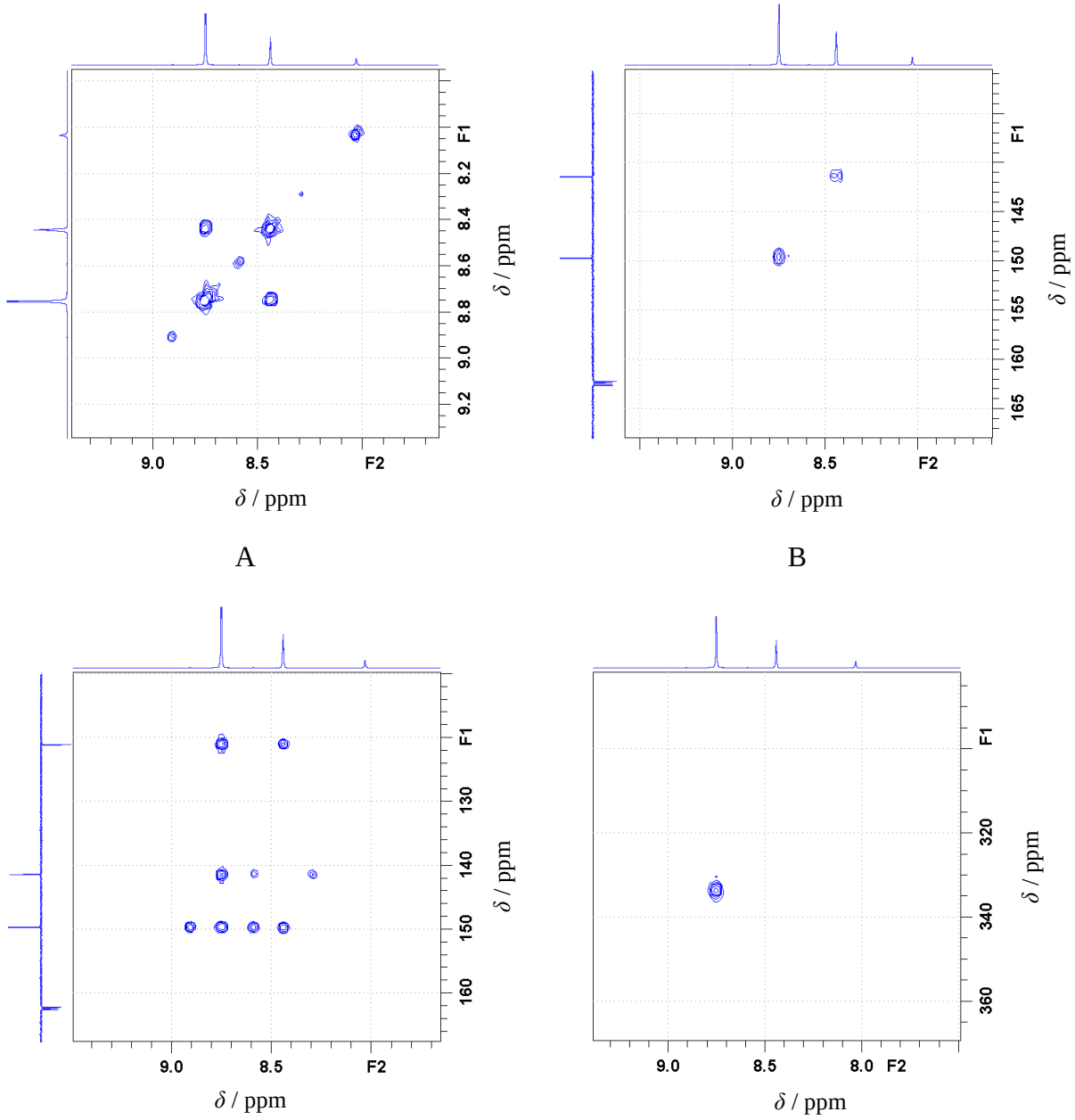


A

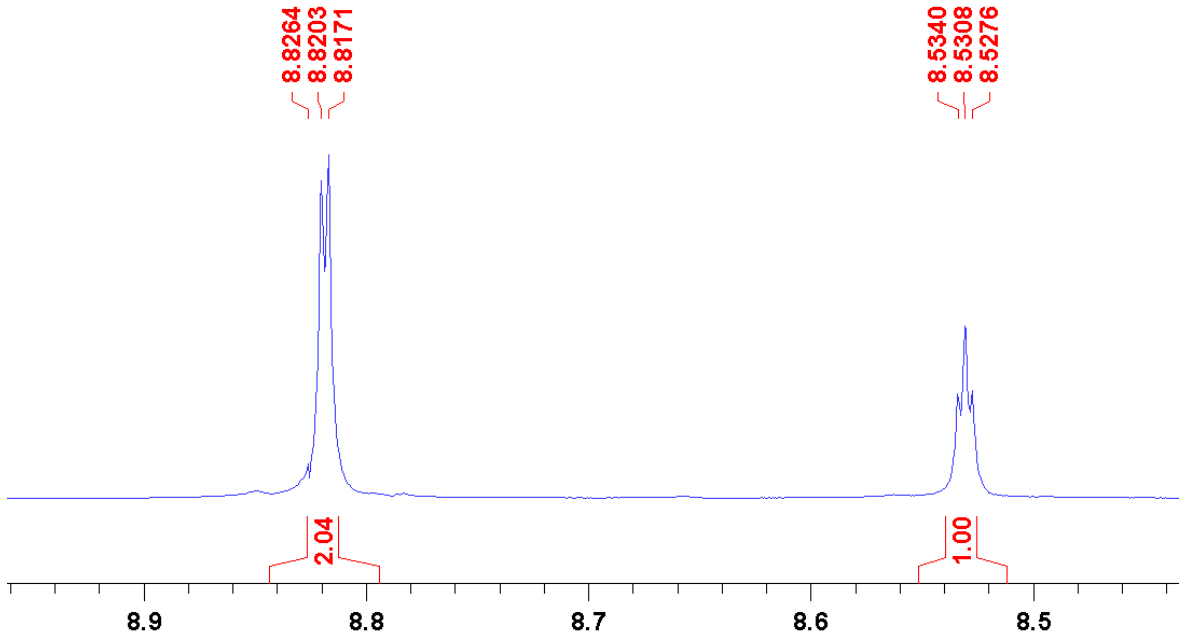


B

Slika D74. *A) ^{1}H i B) ^{13}C spektri spoja 3,5-Br_2py, (**L12**).*

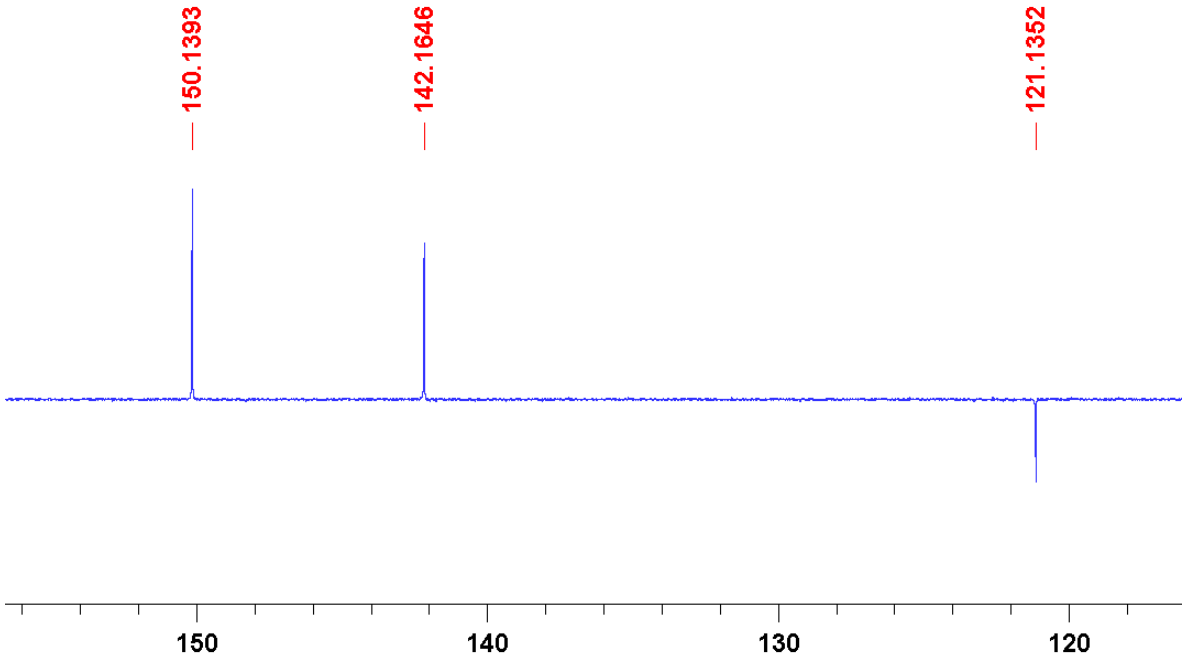


Slika D75. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC, C) ^{1}H-^{13}C HMBC i D) ^{1}H-^{15}N HMBC spektara NMR spoja 3,5-Br$_2$py (**L12**).*



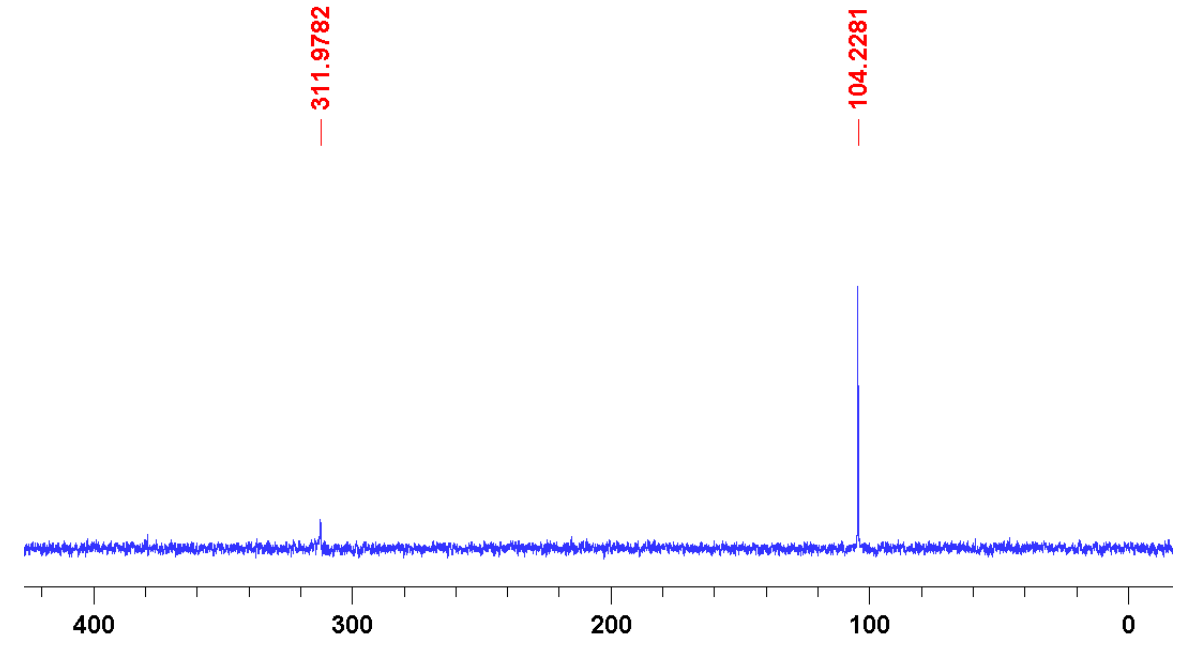
δ / ppm

A

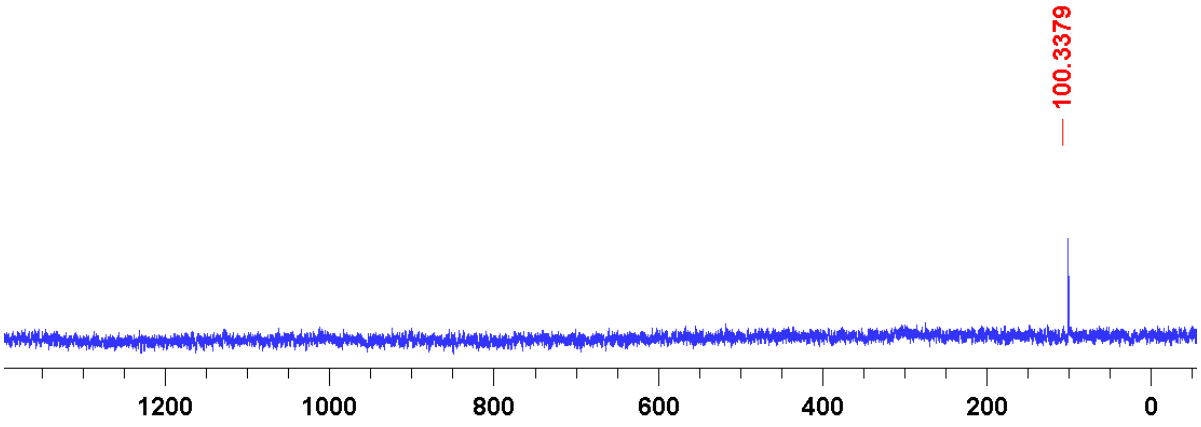


δ / ppm

B

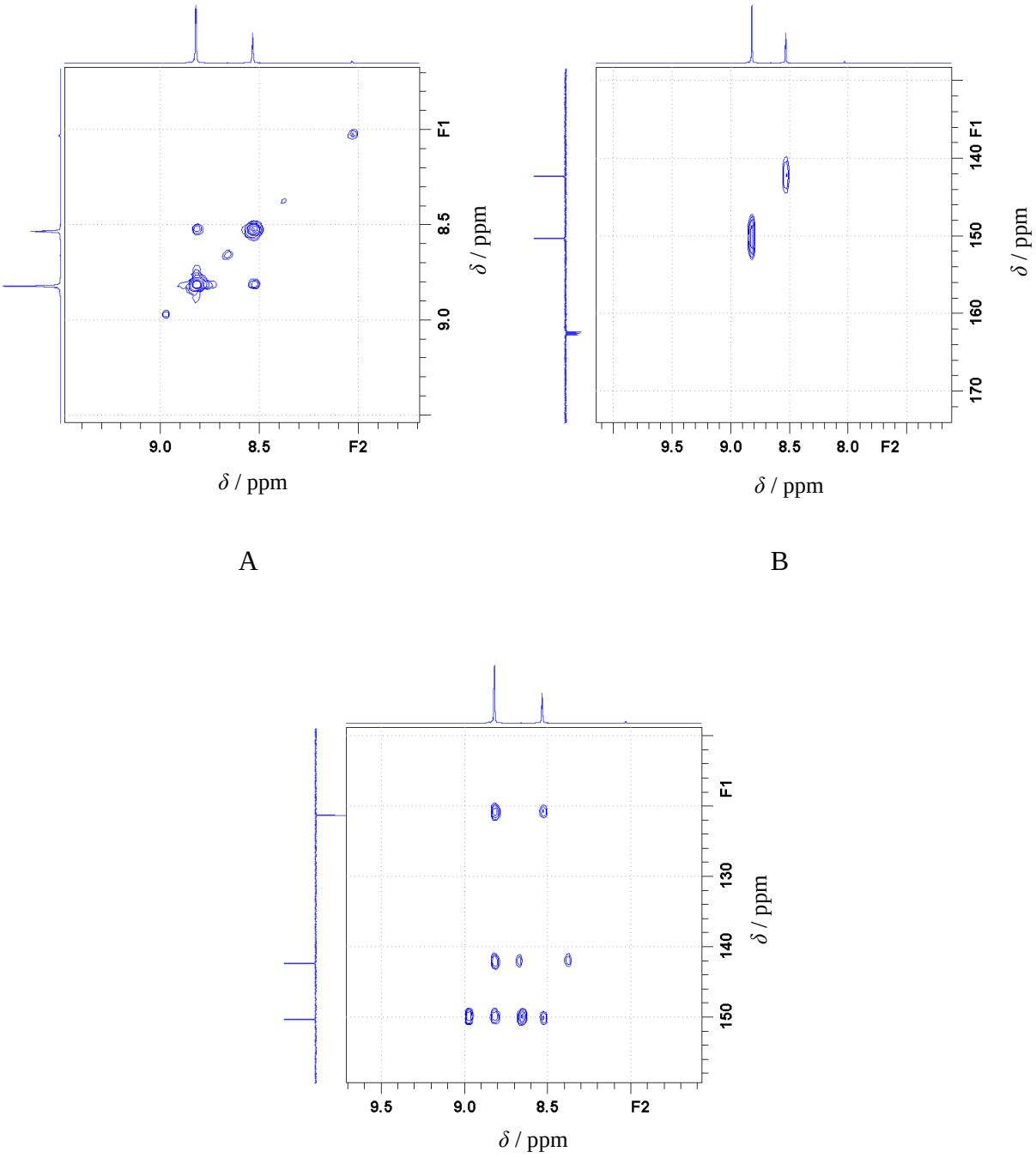


C



D

Slika D76. *A) ^{1}H, B) ^{13}C, C) ^{15}N i D) ^{109}Ag spektri kompleksa $[Ag(NO_3)(3,5\text{-}Br_2py)_2]$,* ***(K12).***



Slika D77. *Uvećani prikaz A) ^{1}H-^{1}H COSY, B) ^{1}H-^{13}C HMQC i C) ^{1}H-^{13}C HMBC spektara NMR kompleksa [Ag(NO$_3$)(3,5-Br$_2$py)$_2$], (**K12**).*

Tablica D1. *Kemijski pomaci (δ / ppm) i konstante sprege ($^{n}J_{H,H}$ / Hz) signala jezgri ^{1}H-atoma kod spojeva* ***K1*** *–* ***K6*** *te razlike u njihovom kemijskom pomaku nakon kompleksiranja ($\Delta\delta_{koord}$ / ppm) izračunate prema relaciji $\Delta\delta_{koord} = \delta_{kompleksa} - \delta_{liganda}$. (podaci u zagradi).*

Spoj	H-atom (δ / ppm, $\Delta\delta_{koord}$ / ppm, $^{n}J_{H,H}$ / Hz)				
	2	3	4	5	6
K1	/	7,75 (+0,20)[a] $^{3}J_{3,4}$ = 8,03 $^{4}J_{3,5}$ = 1,05 $^{5}J_{3,6}$ = 0,70	8,09 (+0,17) $^{3}J_{3,4}$ = 8,03 $^{3}J_{4,5}$ = 7,39 $^{4}J_{4,6}$ = 1,89	7,62 (+0,17) $^{3}J_{4,5}$ = 7,39 $^{3}J_{5,6}$ = 5,12 $^{4}J_{3,5}$ = 1,05	8,60 (+0,13) $^{3}J_{5,6}$ = 5,12 $^{4}J_{4,6}$ = 1,89
K2	/	7,75 (+0,06) $^{3}J_{3,4}$ = 8,07 $^{4}J_{3,5}$ = 0,81 $^{5}J_{3,6}$ = 0,60	7,87 (+0,06) $^{3}J_{3,4}$ = 8,07 $^{3}J_{4,5}$ = 7,31 $^{4}J_{4,6}$ = 2,10	7,54 (+0,05) $^{3}J_{4,5}$ = 7,31 $^{3}J_{5,6}$ = 4,85 $^{4}J_{3,5}$ = 0,81	8,49 (+0,05) $^{3}J_{5,6}$ = 4,85 $^{4}J_{4,6}$ = 2,10 $^{5}J_{3,6}$ = 0,60
K3	/	7,94 (+0,04) $^{3}J_{3,4}$ = 7,94 $^{4}J_{3,5}$ = 0,99 $^{5}J_{3,6}$ = 0,95	7,60 (+0,03) $^{3}J_{3,4}$ = 7,94 $^{3}J_{4,5}$ = 7,49 $^{4}J_{4,6}$ = 2,09	7,50 (+0,03) $^{3}J_{4,5}$ = 7,49 $^{3}J_{5,6}$ = 4,82 $^{4}J_{3,5}$ = 0,99	8,44 (+0,02) $^{3}J_{5,6}$ = 4,82 $^{4}J_{4,6}$ = 2,09 $^{5}J_{3,6}$ = 0,95
K4	8,71 (+0,05) $^{4}J_{2,4}$ = 2,53 $^{5}J_{2,5}$ = 0,60	/	8,04 (+0,08) $^{3}J_{4,5}$ = 8,14 $^{4}J_{2,4}$ = 2,53 $^{4}J_{4,6}$ = 1,36	7,56 (+0,06) $^{3}J_{4,5}$ = 8,14 $^{3}J_{5,6}$ = 4,80 $^{5}J_{2,5}$ = 0,60	8,62 (+0,04) $^{3}J_{5,6}$ = 4,80 $^{4}J_{4,6}$ = 1,36
K5	8,78 (+0,04) $^{4}J_{2,4}$ = 2,33 $^{5}J_{2,5}$ = 0,76	/	8,14 (+0,05) $^{3}J_{4,5}$ = 8,16 $^{4}J_{2,4}$ = 2,33 $^{4}J_{4,6}$ = 1,44	7,48 (+0,04) $^{3}J_{4,5}$ = 8,16 $^{3}J_{5,6}$ = 4,77 $^{5}J_{2,5}$ = 0,76	8,64 (+0,03) $^{3}J_{5,6}$ = 4,77 $^{4}J_{4,6}$ = 1,44
K6	8,97 (+0,09) $^{4}J_{2,4}$ = 2,18 $^{5}J_{2,5}$ = 0,75	/	8,36 (+0,12) $^{3}J_{4,5}$ = 8,03 $^{4}J_{2,4}$ = 2,18 $^{4}J_{4,6}$ = 1,48	7,43 (+0,12) $^{3}J_{4,5}$ = 8,03 $^{3}J_{5,6}$ = 4,75 $^{5}J_{2,5}$ = 0,75	8,70 (+0,09) $^{3}J_{5,6}$ = 4,75 $^{4}J_{4,6}$ = 1,48

Tablica D2. *Kemijski pomaci (δ / ppm) i konstante sprege ($^{n}J_{H,H}$ / Hz) signala jezgri ^{1}H-atoma kod spojeva* ***K7*** *–* ***K12*** *te razlike u njihovom kemijskom pomaku nakon kompleksiranja ($\Delta\delta_{koord}$ / ppm) izračunate prema relaciji $\Delta\delta_{koord} = \delta_{kompleksa} - \delta_{liganda}$ (podaci u zagradi).*

Spoj	H-atom (δ / ppm, $\Delta\delta_{koord}$ / ppm, $^{n}J_{H,H}$ / Hz)				
	2	3	4	5	6
K7	/	7,69 (+0,15) $^{3}J_{3,4}$ = 8,62	8,10 (+0,13) $^{3}J_{3,4}$ = 8,56 $^{4}J_{4,6}$ = 2,75	/	8,57 (+0,11) $^{4}J_{4,6}$ = 2,63
K8	/	7,74 (+0,12) $^{3}J_{3,4}$ = 8,81	8,09 (+0,10) $^{3}J_{3,4}$ = 8,81 $^{4}J_{4,6}$ = 2,64	/	8,63 (+0,09) $^{4}J_{4,6}$ = 2,20
K9	/	7,59 (+0,02) $^{3}J_{3,4}$ = 7,83	7,99 (+0,01) $^{3}J_{3(5),4}$ = 8,14	7,59 (+0,02) $^{3}J_{4,5}$ = 7,83	/
K10	/		7,80-7,77 (+0,01) m[a]		/
K11	8,73 (+0,14) $^{3}J_{2(6),4}$ = 1,90	/	8,33 (+0,14) $^{3}J_{4,4(6)}$ = 1,73	/	8,73 (+0,14) $^{3}J_{2(6),4}$ = 1,90
K12	8,82 (+0,12) $^{3}J_{2(6),4}$ = 1,94	/	8,53 (+0,11) $^{3}J_{4,4(6)}$ = 1,92	/	8,82 (+0,12) $^{3}J_{2(6),4}$ = 1,94

[a]multiplet

Tablica D3. *Kemijski pomaci (δ / ppm) signala jezgri ^{13}C-atoma kod spojeva* ***K1*** *–* ***K12*** *te razlika u njihovom kemijskom pomaku nakon kompleksiranja ($\Delta\delta_{koord}$ / ppm) izračunata prema relaciji $\Delta\delta_{koord} = \delta_{kompleksa} - \delta_{liganda}$ (podaci u zagradi).*

C-atom	Spoj (δ / ppm, $\Delta\delta_{koord}$ / ppm)											
	K1	**K2**	**K3**	**K4**	**K5**	**K6**	**K7**	**K8**	**K9**	**K10**	**K11**	**K12**
2	151,0	142,3	120,3	149,9	152,0	156,9	149,4	140,6	150,0	140,5	147,9	150,1
	a	+0,3	+1,7	+1,2	+1,2	+1,0	+0,9	+0,7	*a*	+0,1	+1,2	+1,1
3	125,4	128,9	135,7	132,5	121,1	94,1	126,1	130,3	123,9	128,0	132,5	121,1
	+0,7	+0,4	+0,3	+0,6	+0,3	*a*	+0,5	+0,5	+0,1	+0,1	+1,1	+0,5
4	141,5	140,6	139,4	138,1	140,8	146,5	140,0	142,6	142,9	142,2	137,1	142,2
	+1,7	+1,1	+0,8	+2,0	+1,9	+1,7	+0,7	+0,7	+0,1	+0,1	+1,4	+1,4
5	124,0	124,0	124,1	126,2	126,7	126,7	131,2	120,4	123,9	128,0	132,5	121,1
	+0,9	+0,5	+0,3	+1,0	+1,1	+0,6	+0,8	+0,5	+0,1	+0,1	+1,1	+0,5
6	151,6	151,7	152,6	149,7	149,9	149,9	149,0	151,7	150,0	140,5	147,9	150,1
	+1,4	+1,1	+1,2	+1,5	+1,5	+1,3	+0,8	+0,7	*a*	+0,1	+1,2	+1,1

[a]Nema promjene u kemijskom pomaku signala u spektru.

Tablica D4. *Kemijski pomaci (δ / ppm) signala jezgri ^{15}N-py-atoma kod spojeva **L1 – L12** te razlika istih u odnosu na one u jezgri piridina ($\Delta\delta_{koord}$ / ppm) izračunata prema relaciji $\Delta\delta_{koord} = \delta_{liganda} - \delta_{piridina}$ (podaci u zagradi).*

Jezgra	Spoj (δ / ppm, $\Delta\delta_{koord}$ / ppm)											
	L1	**L2**	**L3**	**L4**	**L5**	**L6**	**L7**	**L8**	**L9**	**L10**	**L11**	**L12**
^{15}N-py	307,6 (-9,8)	316,3 (-1,1)	332,0 (+14,6)	322,3 (+4,9)	323,6 (+6,2)	323,2 (+5,8)	312,2 (-5,2)	321,3 (+3,9)	301,2 (-16,2)	319,4 (+2,0)	325,3 (+7,9)	326,0 (+8,6)

Tablica D5. *Kemijski pomaci (δ / ppm) signala jezgri ^{15}N-atoma kod spojeva **K1 – K12** te razlika u pomacima tih signala nakon kompleksiranja ($\Delta\delta_{koord}$ / ppm) izračunata prema relaciji $\Delta\delta_{koord} = \delta_{kompleksa} - \delta_{liganda}$ (podaci u zagradi).*

Jezgra	Spoj (δ / ppm, $\Delta\delta_{koord}$ / ppm)											
	K1	**K2**	**K3**	**K4**	**K5**	**K6**	**K7**	**K8**	**K9**	**K10**	**K11**	**K12**
^{15}N-py	284,2 (-23,4)	299,2 (-17,1)	322,2 (-9,8)	289,0 (-33,3)	291,8 (-31,8)	289,3 (-33,9)	305,1 (-7,1)	315,7 (-5,6)	299,3 (-1,9)	315,7 (-3,7)	306,1 (-19,2)	312,0 (-14,0)
$^{15}NO_3^-$	378,6 (+2,4)	376,1 (-0,1)	*a*	376,3 (+0,1)	376,6 (+0,4)	376,9 (+0,7)	376,3 (+0,1)	376,8 (+0,6)	*a*	371,5 (-4,7)	376,3 (+0,1)	378,8 (+2,6)

[a]Signal u spektru nije detektiran.

Tablica D6. *Kemijski pomaci (δ / ppm) signala jezgri ^{109}Ag-atoma u spektrima spojeva* ***K1*** *–* ***K12*** *te razlika u pomaku njihovih signala ($\Delta\delta_{koord}$ / ppm) u odnosu prema pomaku srebrova(I) iona u srebrovom nitratu ($AgNO_3$) izračunata prema relaciji $\Delta\delta_{koord} = \delta_{kompleks} - \delta_{AgNO3}$ (podaci u zagradi).*

Jezgra	Spoj (δ / ppm, $\Delta\delta_{koord}$ / ppm)											
	K1	**K2**	**K3**	**K4**	**K5**	**K6**	**K7**	**K8**	**K9**	**K10**	**K11**	**K12**
^{109}Ag	101,4 (+95,2)	116,7 (+110,5)	106,3 (+100,1)	173,0 (+166,8)	181,6 (+175,4)	201,1 (+194,9)	58,4 (+52,2)	52,5 (+46,3)	36,6 (+30,4)	26,9 (+20,7)	112,2 (+106,0)	100,3 (+94,1)