Electronic Supplementary Information (ESI)

New Journal of Chemistry

Silver(I) complexes with 2-acetylpyridinebenzoylhydrazones exhibit antimicrobial effects against yeast and filamentous fungi

Ane F. Santos,[a] Isabella P. Ferreira,[a] Jacqueline A. Takahashi,[a] Gabriel L. S. Rodrigues[a], Carlos B. Pinheiro[b], Letícia R. Teixeira[a], Willian R. Rocha[a], Heloisa Beraldo*[a]

[a] Departamento de Química, Universidade Federal de Minas Gerais, 31270-901, Belo Horizonte, MG, Brazil

[b] Departamento de Física, Universidade Federal de Minas Gerais, 31270-901, Belo Horizonte, MG, Brazil

*Corresponding author. Phone number: +55 (31) 3409-5740.

E-mail address: hberaldo@ufmg.br

heloisaberaldoufmg@gmail.com (H. Beraldo)

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*The chemical structures of 2-acetylpyridine derived hydrazones and their silver(I) complexes (**1-4**)*

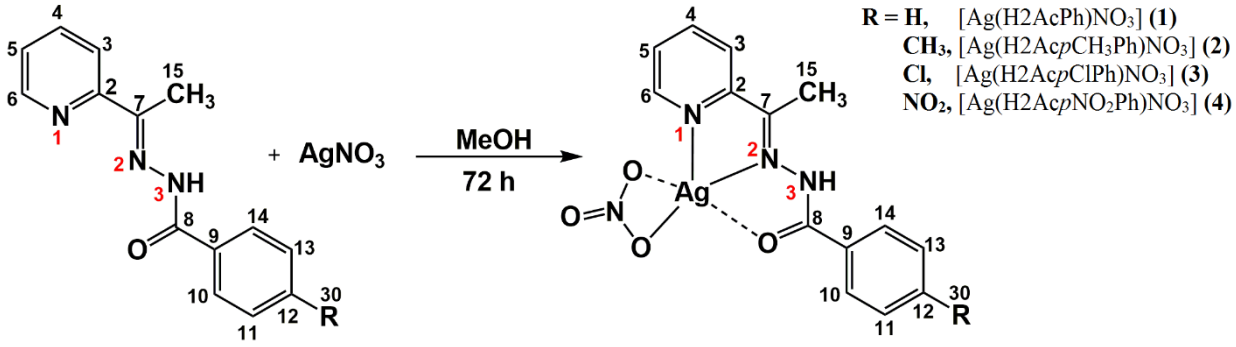

Fig. S1 Syntheses of the silver(I) complexes with 2-acetylpyridine derived hydrazones and carbon atoms numbering.

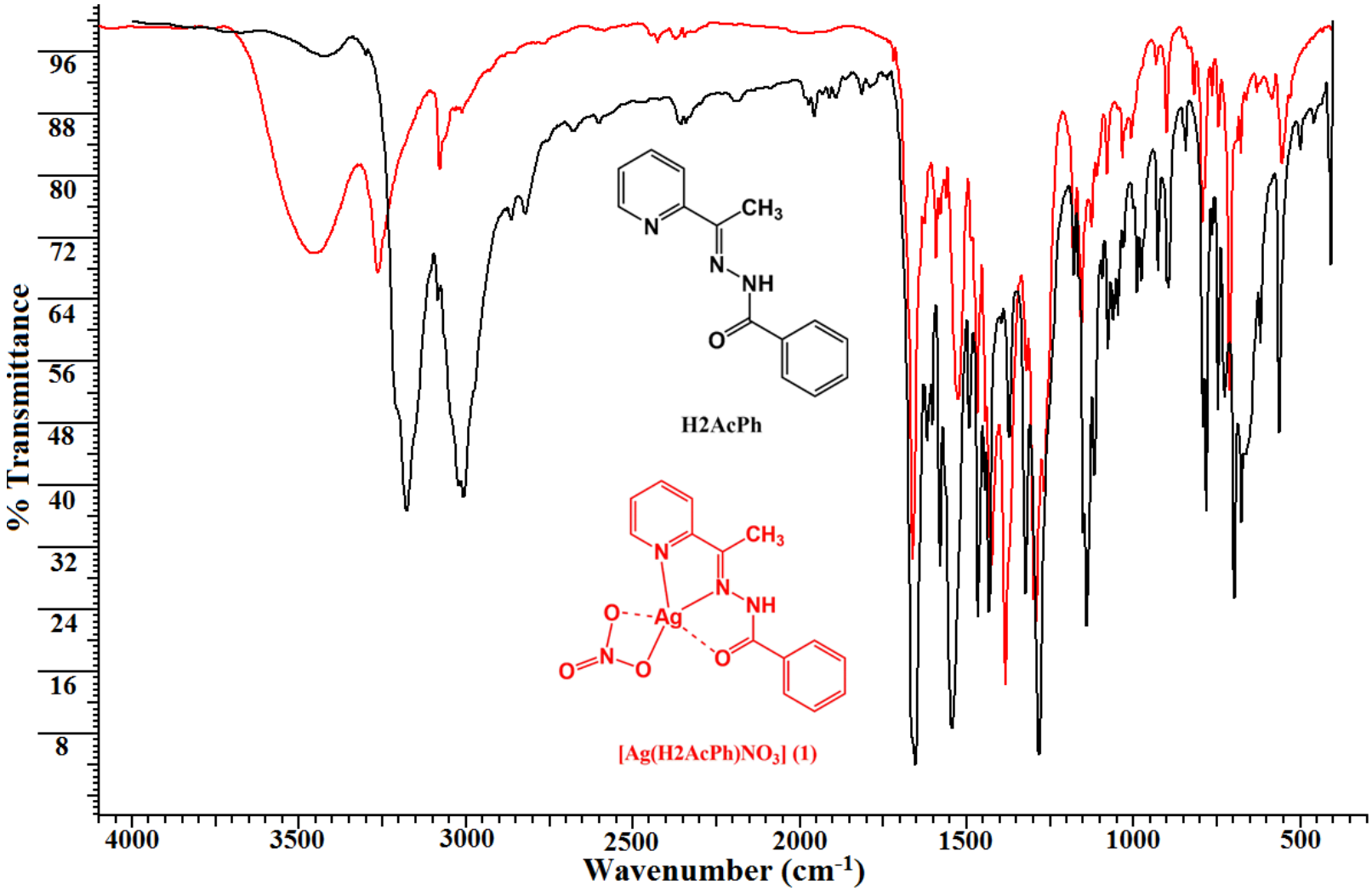

Fig. S2 IR spectrum of H2AcPh (black) and [Ag(H2AcPh)NO_3] (**1**) (red) obtained in KBr pellets (4000-400 cm^{-1}).

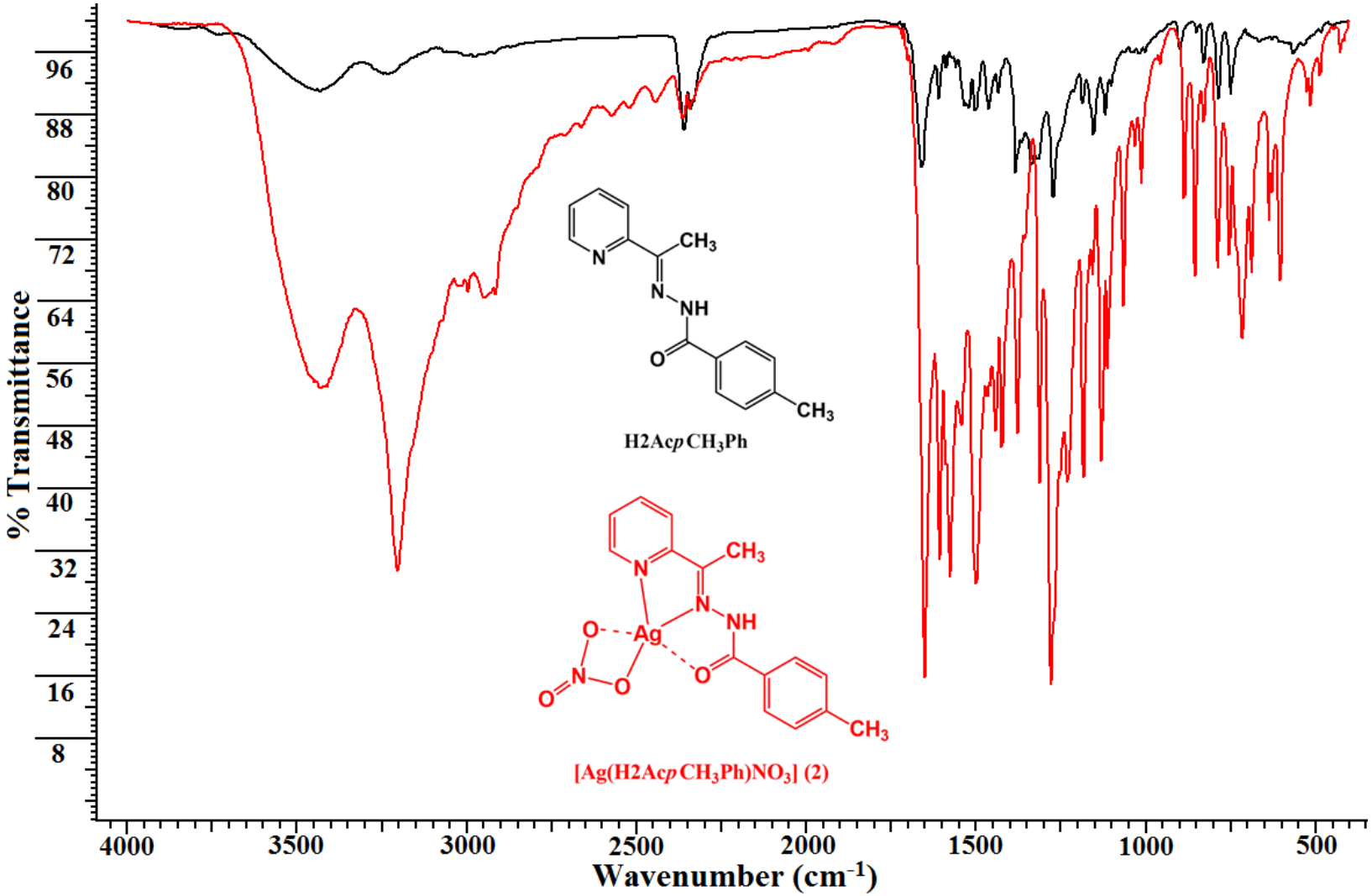

Fig. S3 IR spectrum of H2Ac*p*CH_3Ph (black) and [Ag(H2Ac*p*CH_3Ph)NO_3] (**2**) (red) obtained in KBr pellets (4000-400 cm^{-1}).

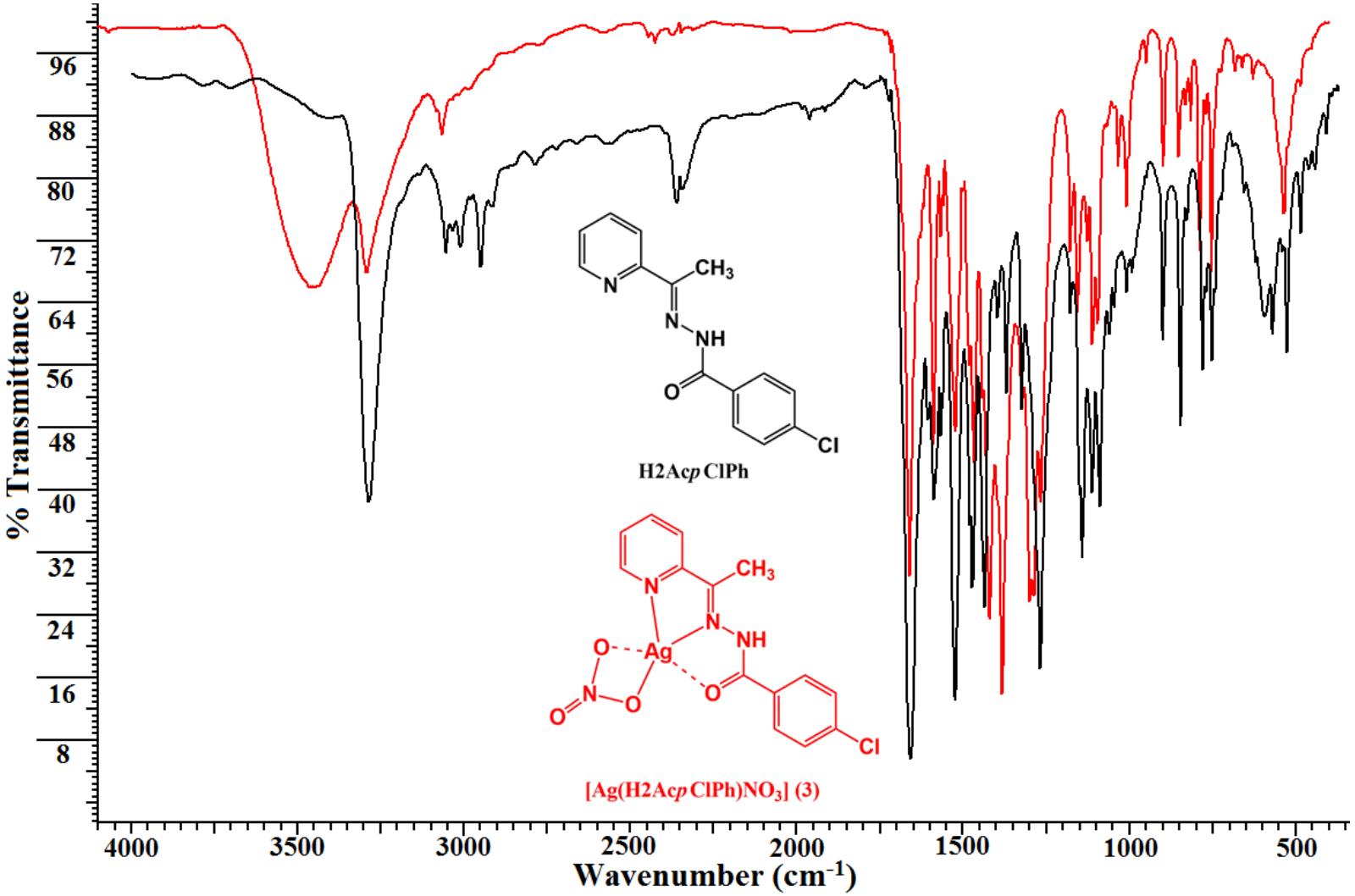

Fig. S4 IR spectrum of H2Ac*p*ClPh (black) and [Ag(H2Ac*p*ClPh)NO_3] (**3**) (red) obtained in KBr pellets (4000-400 cm^{-1}).

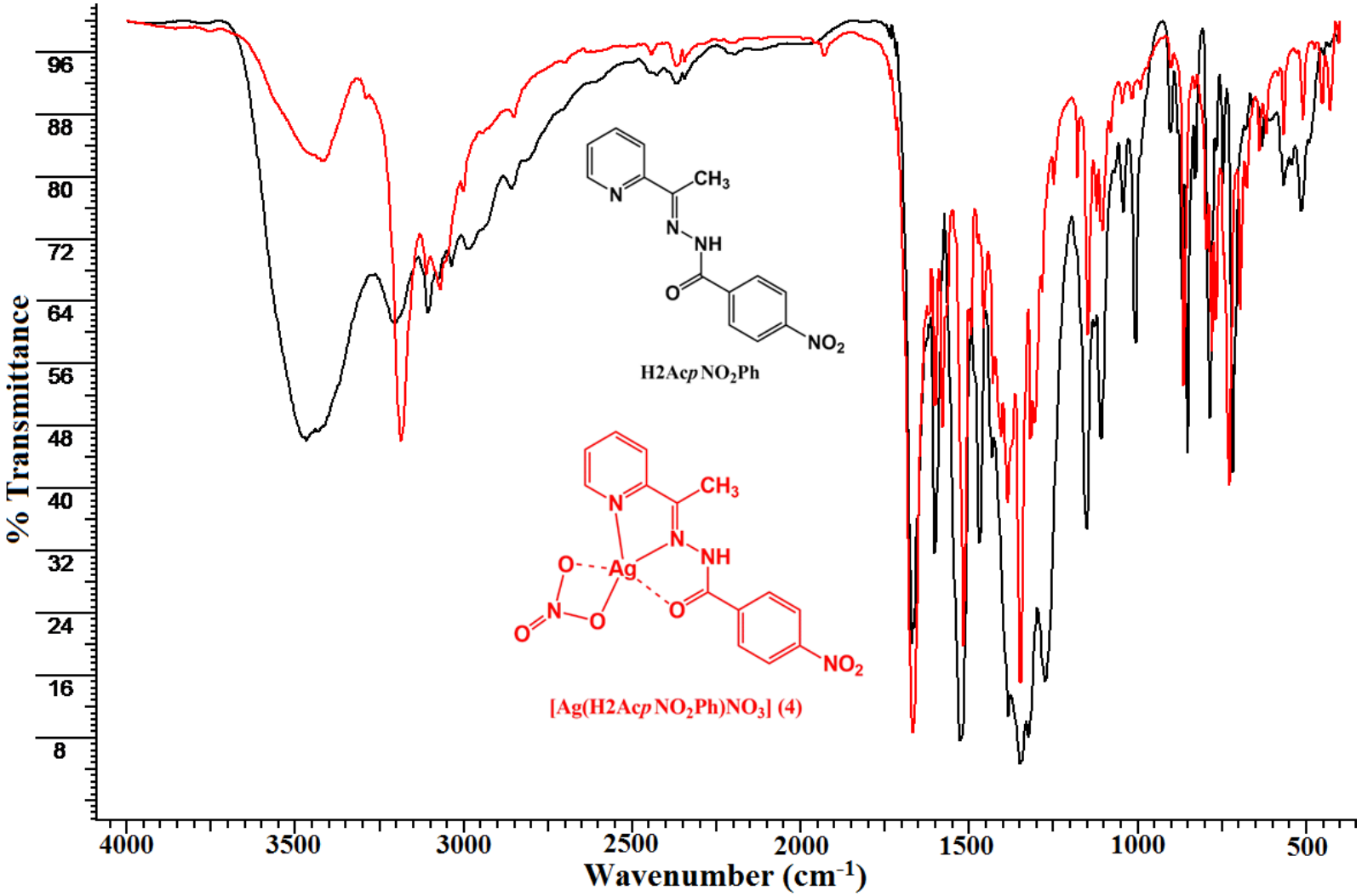

Fig. S5 IR spectrum of H2Ac*p*NO_2Ph (black) and [Ag(H2Ac*p*NO_2Ph)NO_3] (**4**) (red) obtained in KBr pellets (4000-400 cm^{-1}).

*^{1}H, COSY, $^{13}C\{^{1}H\}$ and HMQC NMR spectra of silver(I) complexes (**1-4**)*

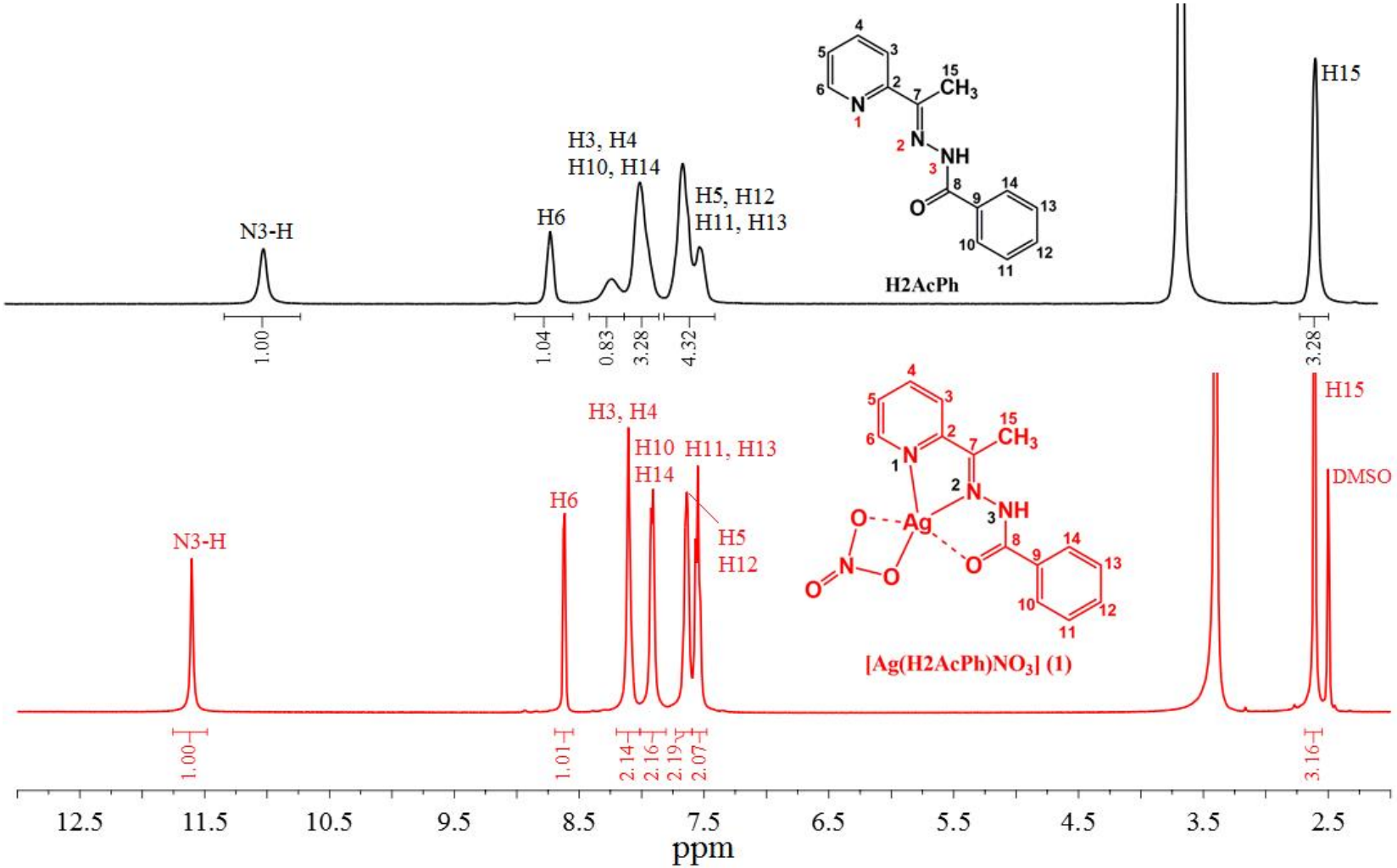

Fig. S6 ^{1}H NMR spectrum of H2AcPh (black) and [Ag(H2AcPh)NO_3] (**1**) (red) registered in DMSO-d_6 at 25ºC.

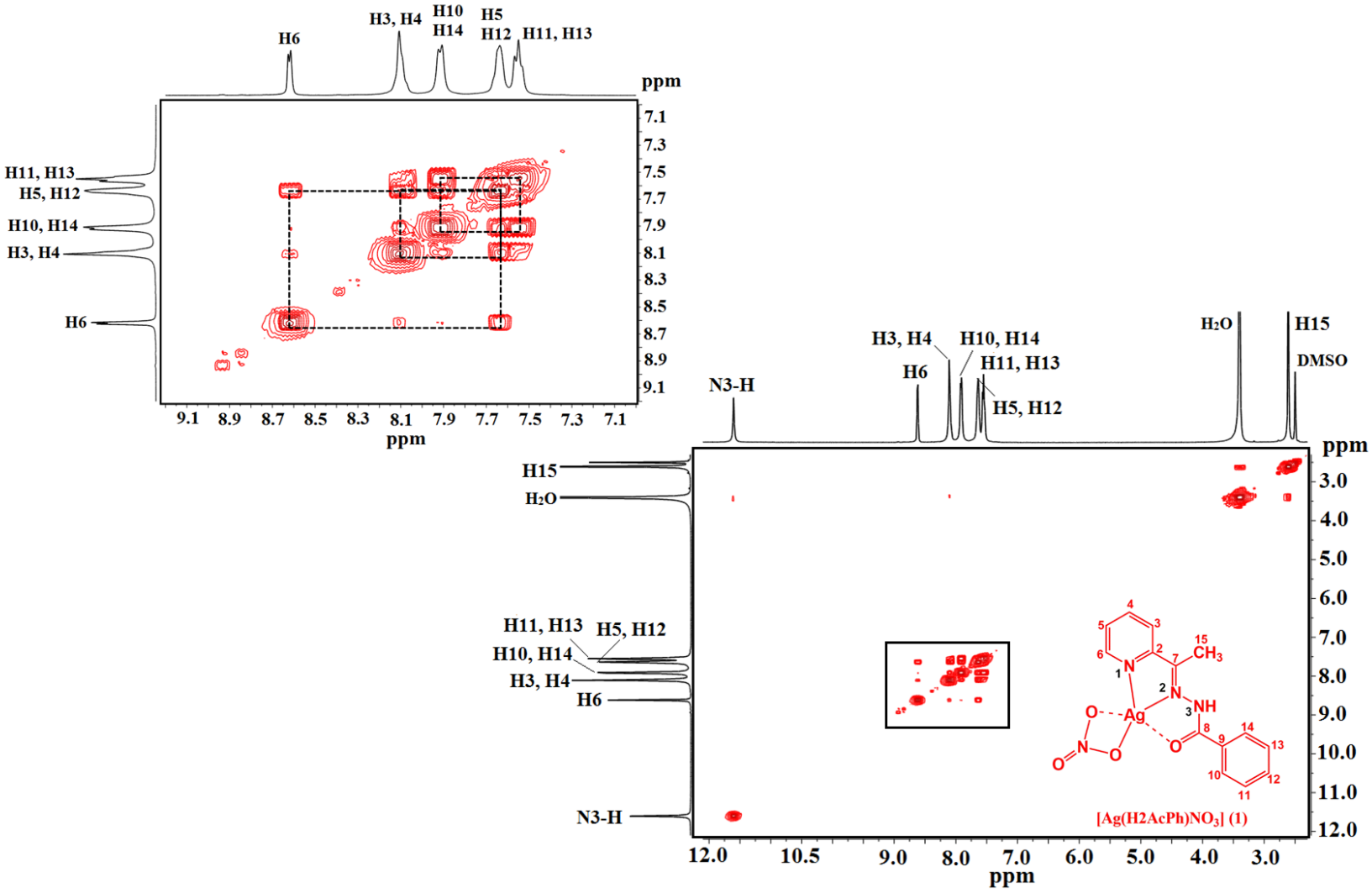

Fig. S7 COSY (^{1}H-^{1}H) contour map of [Ag(H2AcPh)NO_3] (**1**) registered in DMSO-*d*$_6$ at 25ºC.

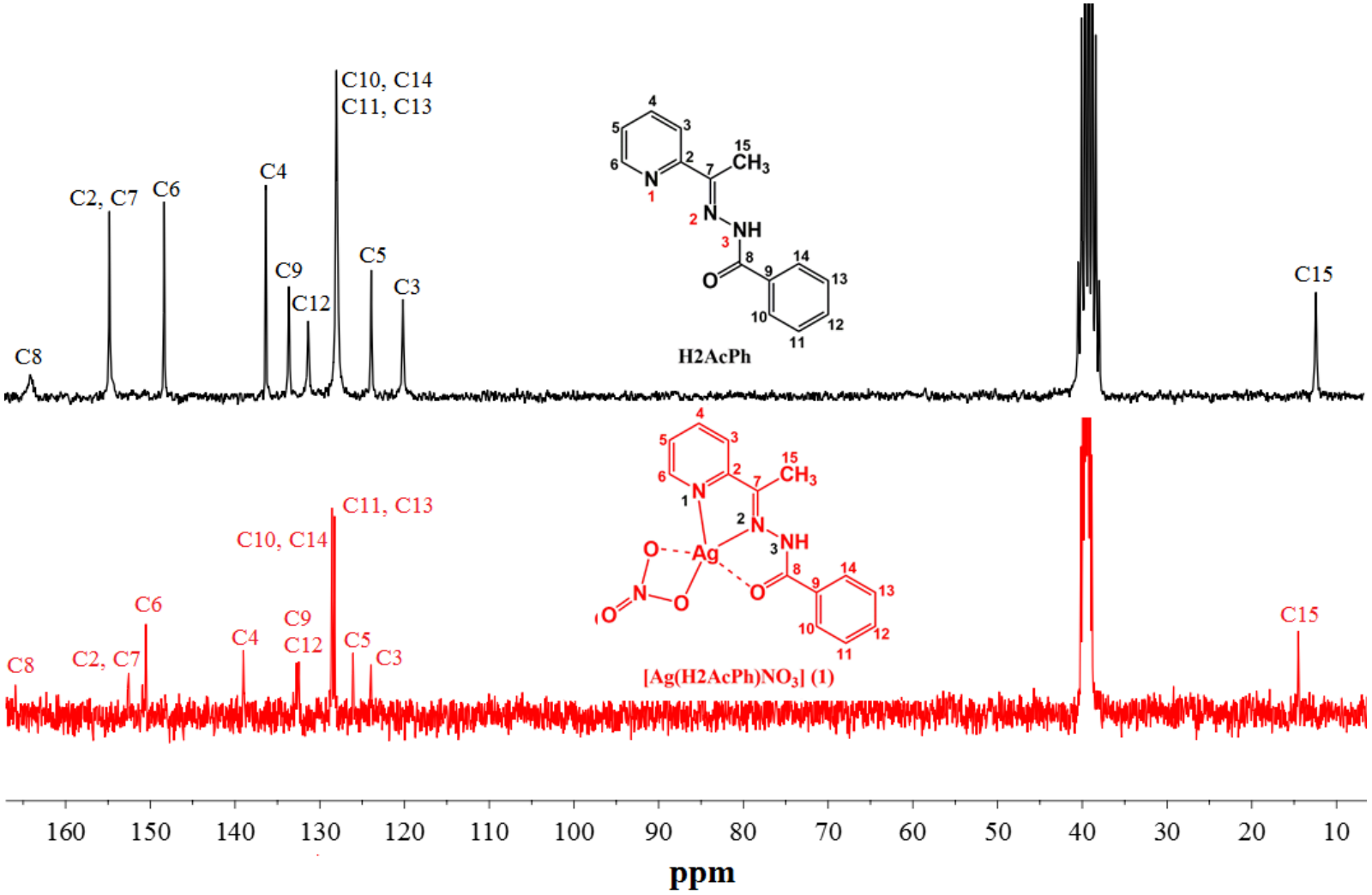

Fig. S8 $^{13}C\{^{1}H\}$ NMR spectrum of H2AcPh (black) and [Ag(H2AcPh)NO_3] (**1**) (red) registered in DMSO-d_6 at 25ºC.

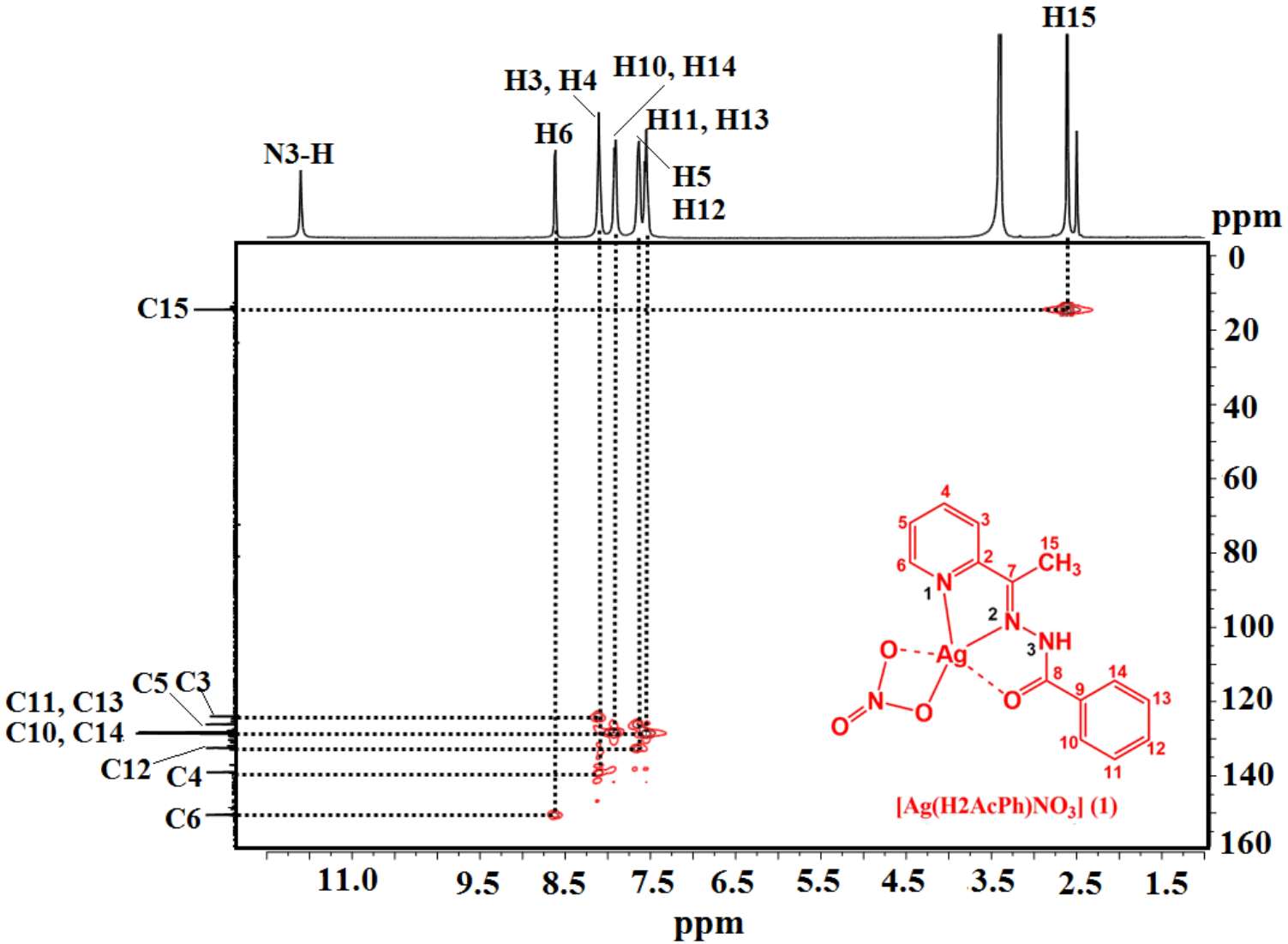

Fig. S9 HMQC (^{1}H-^{13}C{^{1}H}) contour map of [Ag(H2AcPh)NO_3] (**1**) registered in DMSO-d_6 at 25ºC.

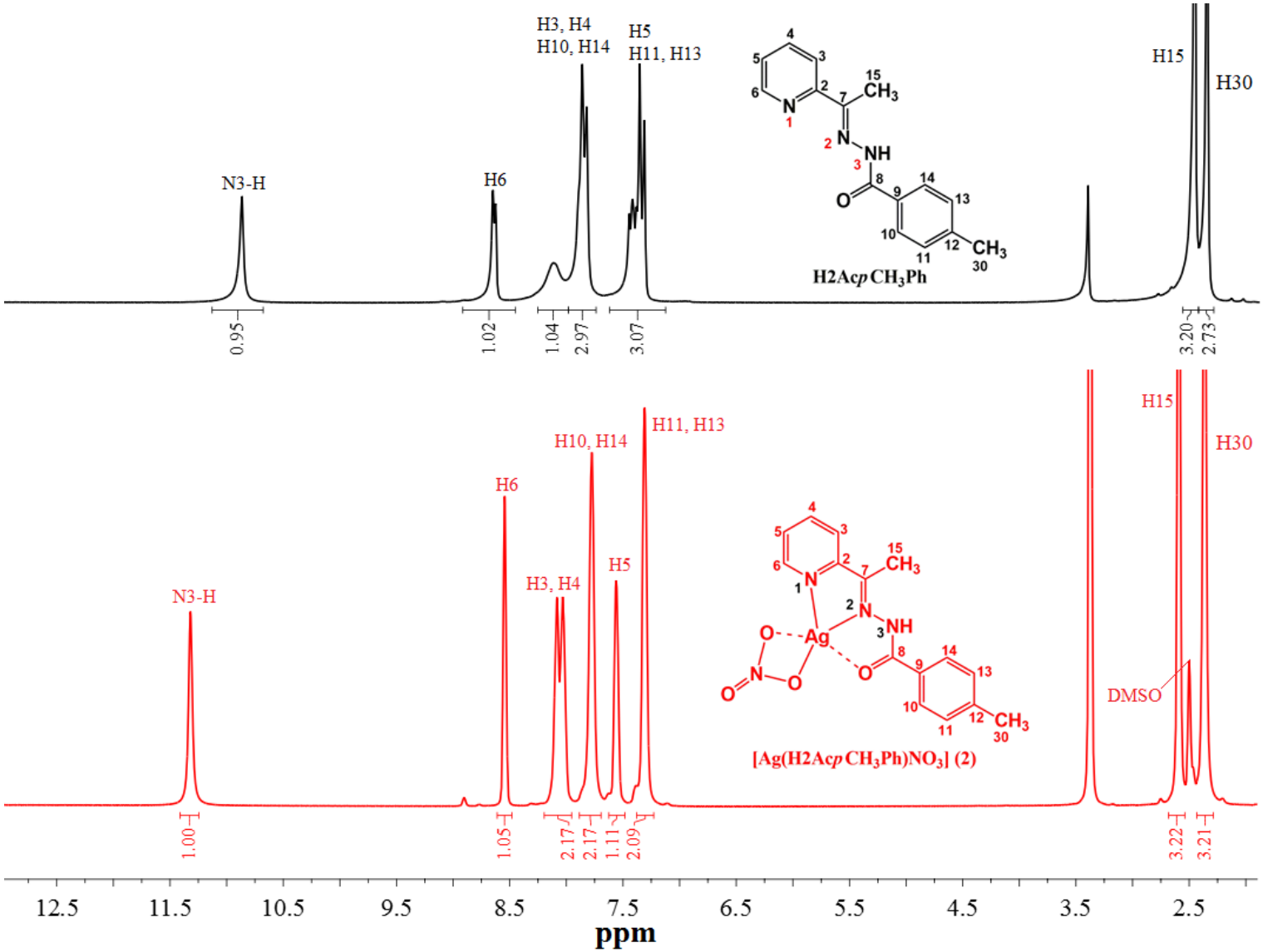

Fig. S10 ^{1}H NMR spectrum of H2Ac*p*CH_3Ph (black) and [Ag(H2Ac*p*CH_3Ph)NO_3] (**2**) (red) registered in DMSO-d_6 at 25ºC.

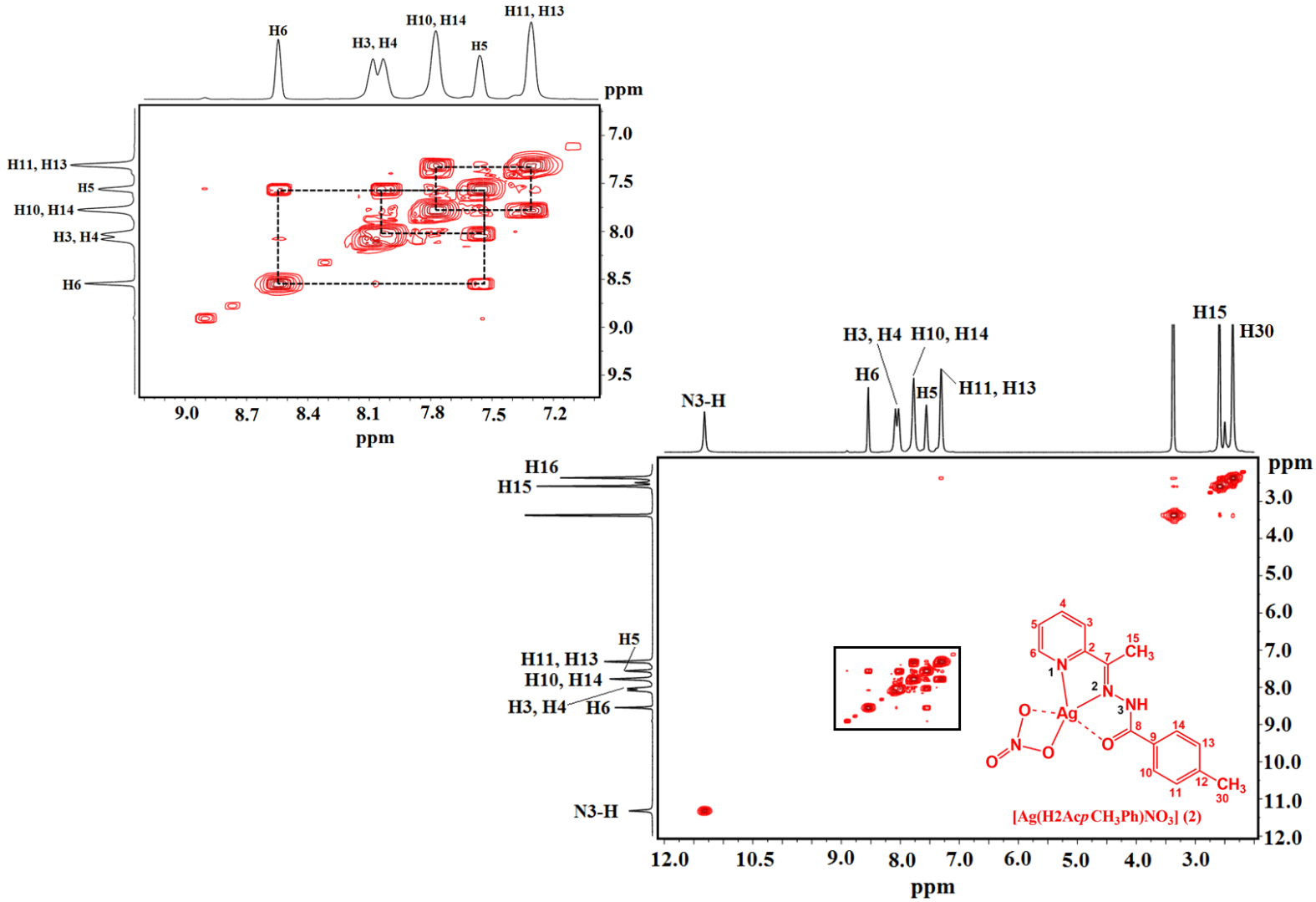

Fig. S11 COSY (^{1}H-^{1}H) contour map of [Ag(H2Ac*p*CH_3Ph)NO_3] (**2**) registered in DMSO-d_6 at 25ºC.

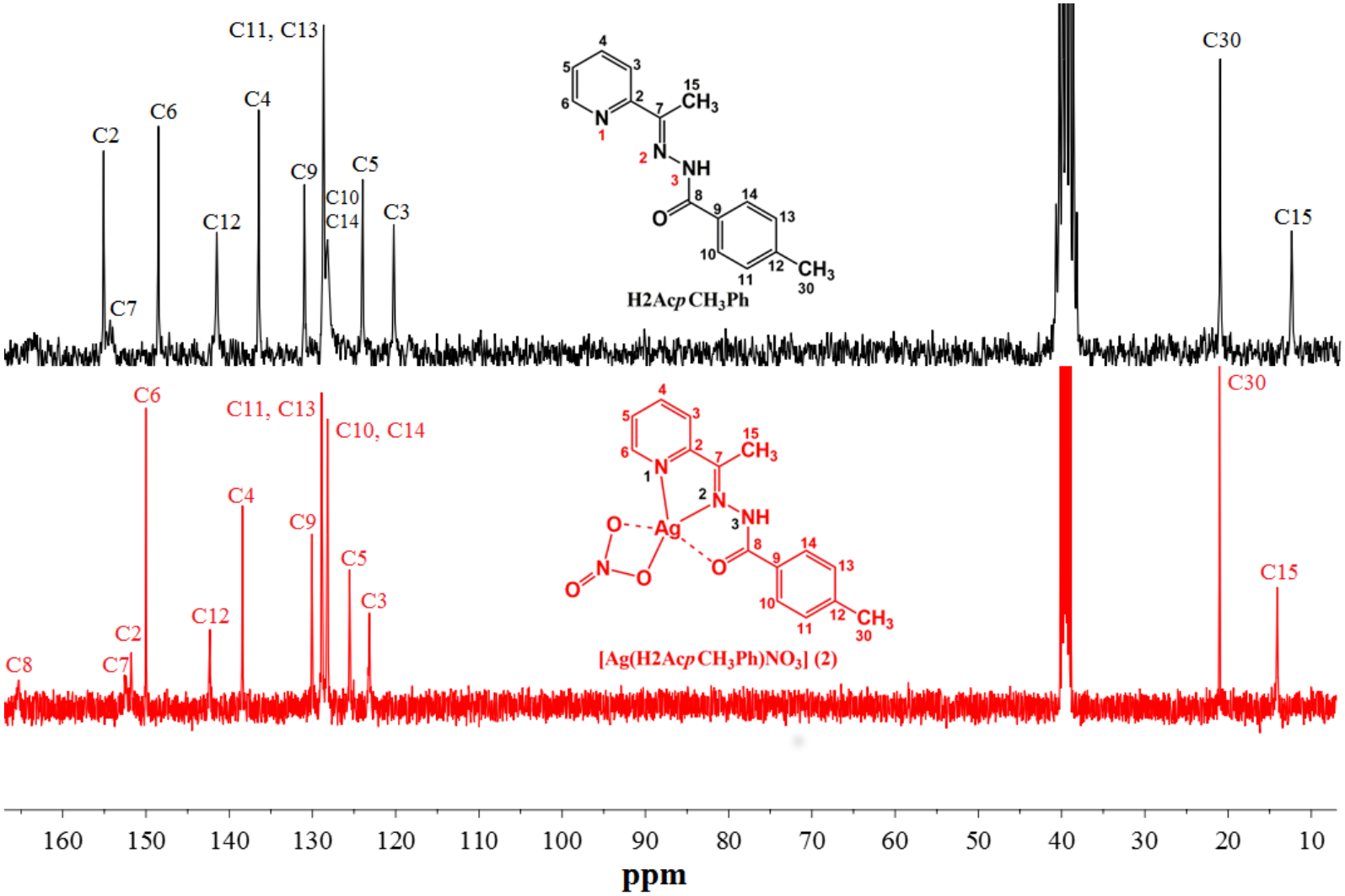

Fig. S12 $^{13}C\{^{1}H\}$ NMR spectrum of H2Ac*p*CH_3Ph (black) and [Ag(H2Ac*p*CH_3Ph)NO_3] (**2**) (red) registered in DMSO-d_6 at 25ºC.

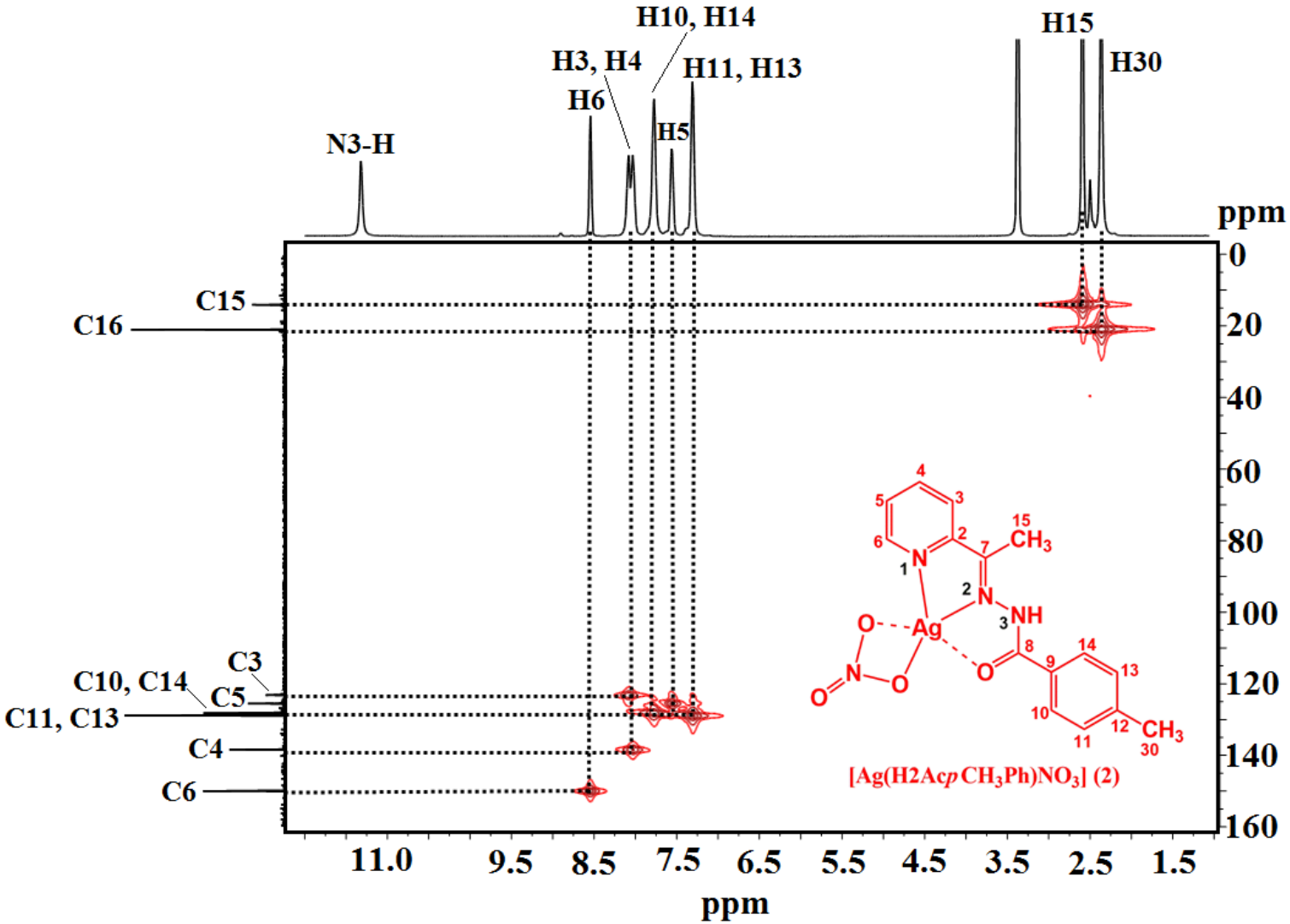

Fig. S13 HMQC (^{1}H-^{13}C{^{1}H}) contour map of [Ag(H2Ac*p*CH$_3$Ph)NO$_3$] (**2**) registered in DMSO-d_6 at 25ºC.

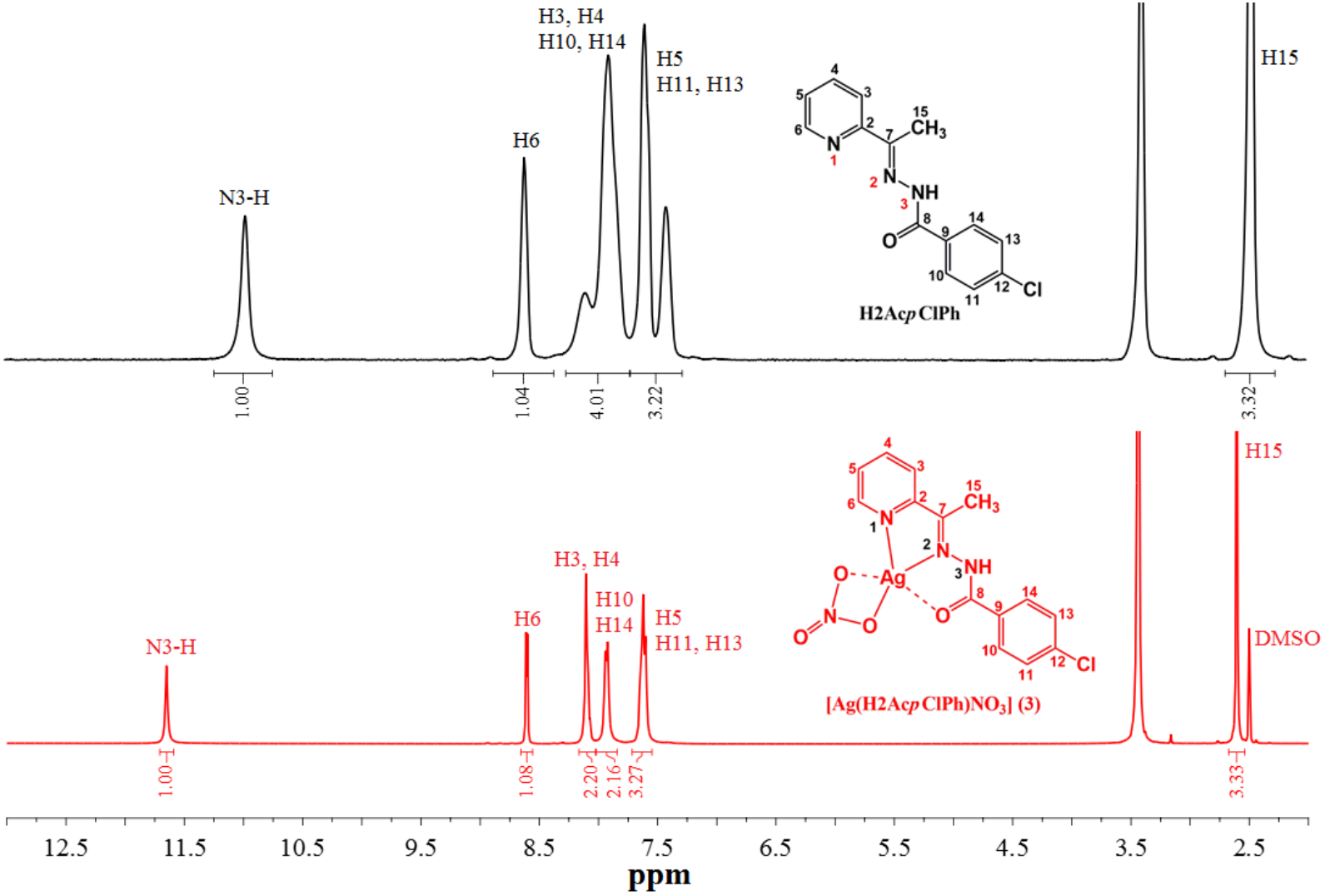

Fig. S14 ^{1}H NMR spectrum of H2Ac*p*ClPh (black) and [Ag(H2Ac*p*ClPh)NO_3] (**3**) (red) registered in DMSO-d_6 at 25ºC.

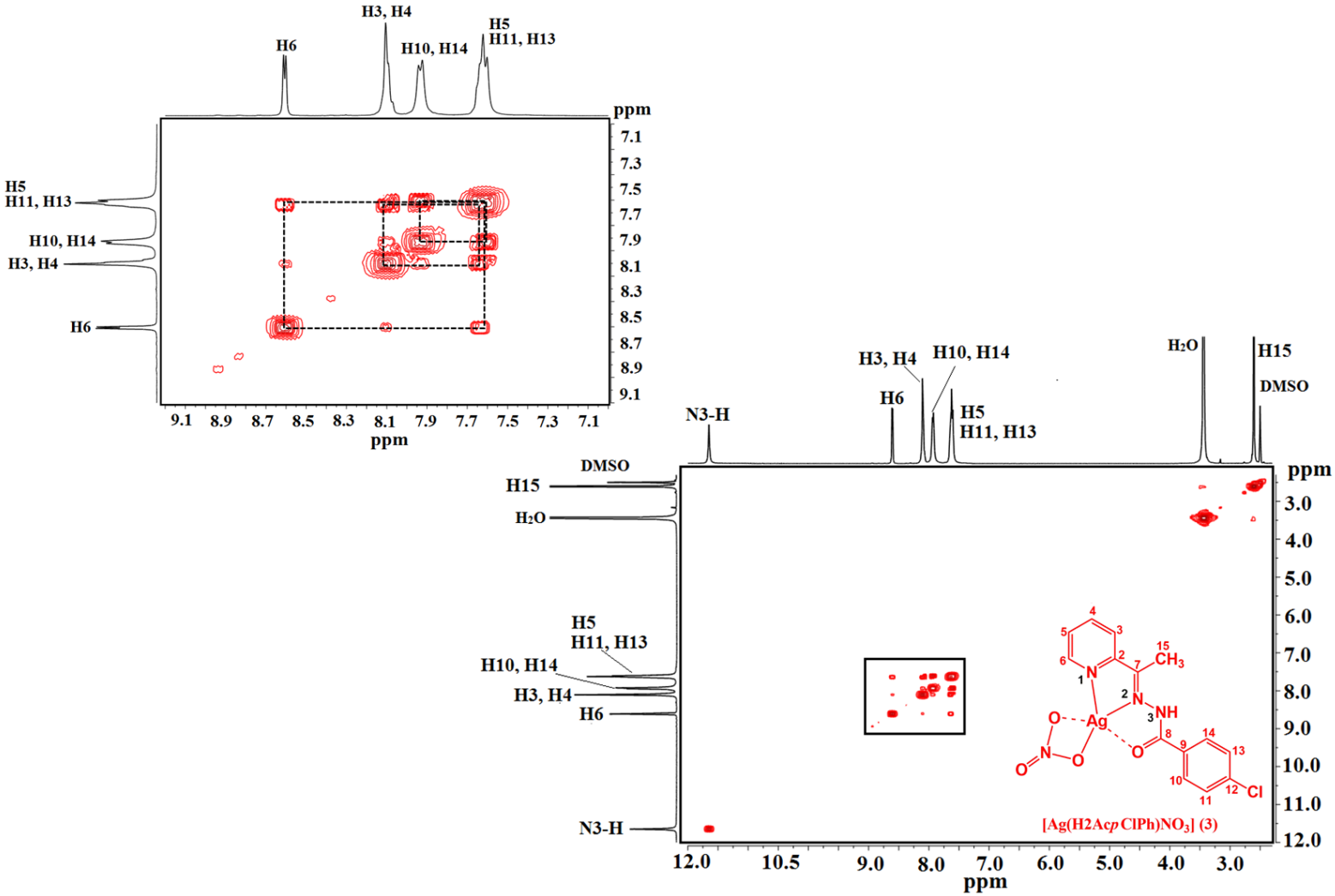

Fig. S15 COSY (^{1}H-^{1}H) contour map of [Ag(H2A*cp*ClPh)NO_3] (**3**) registered in DMSO-d_6 at 25ºC.

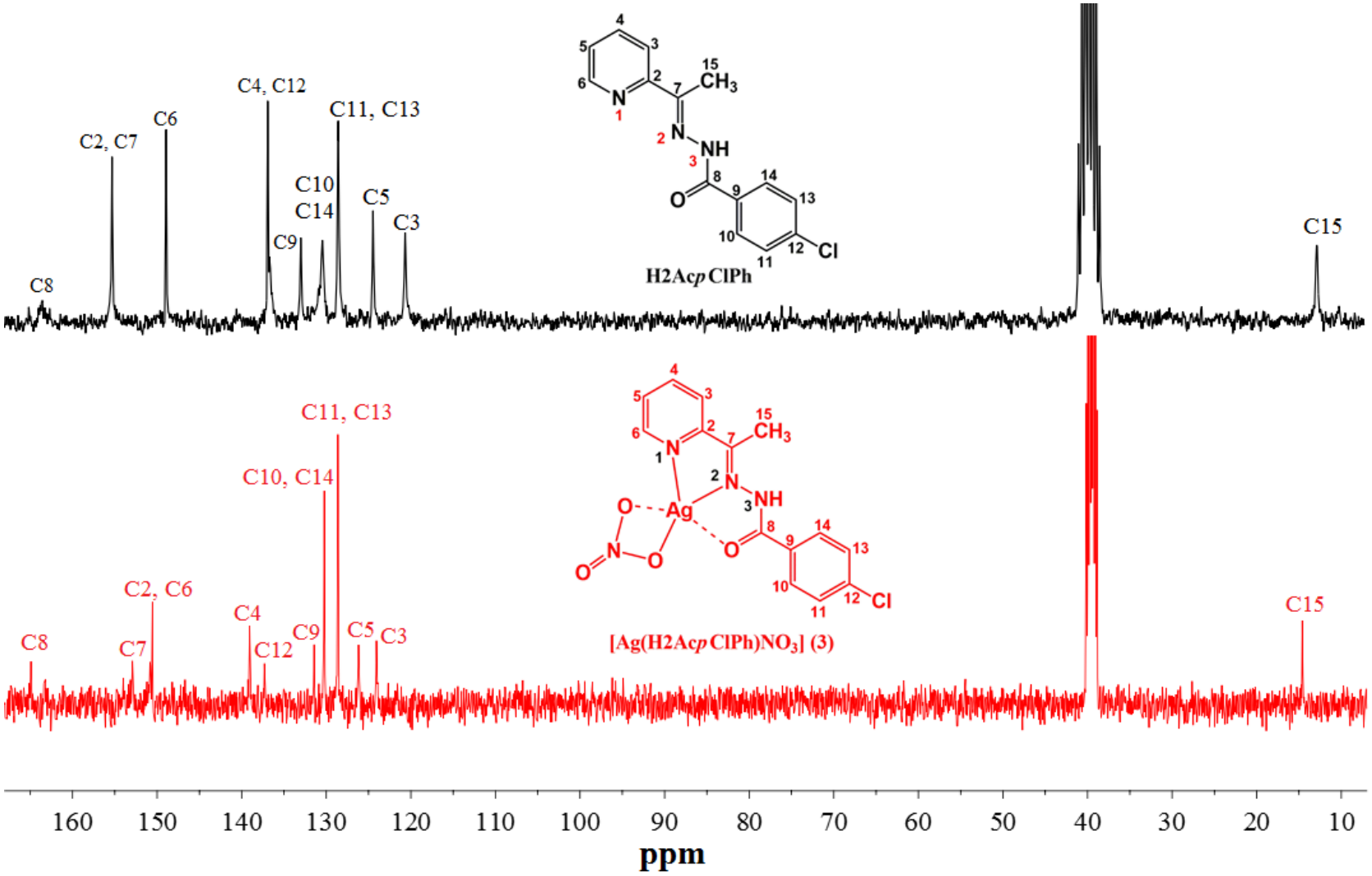

Fig. S16 $^{13}C\{^{1}H\}$ NMR spectrum of H2A*cp*ClPh (black) and [Ag(H2A*cp*ClPh)NO_3] (**3**) (red) registered in DMSO-d_6 at 25ºC.

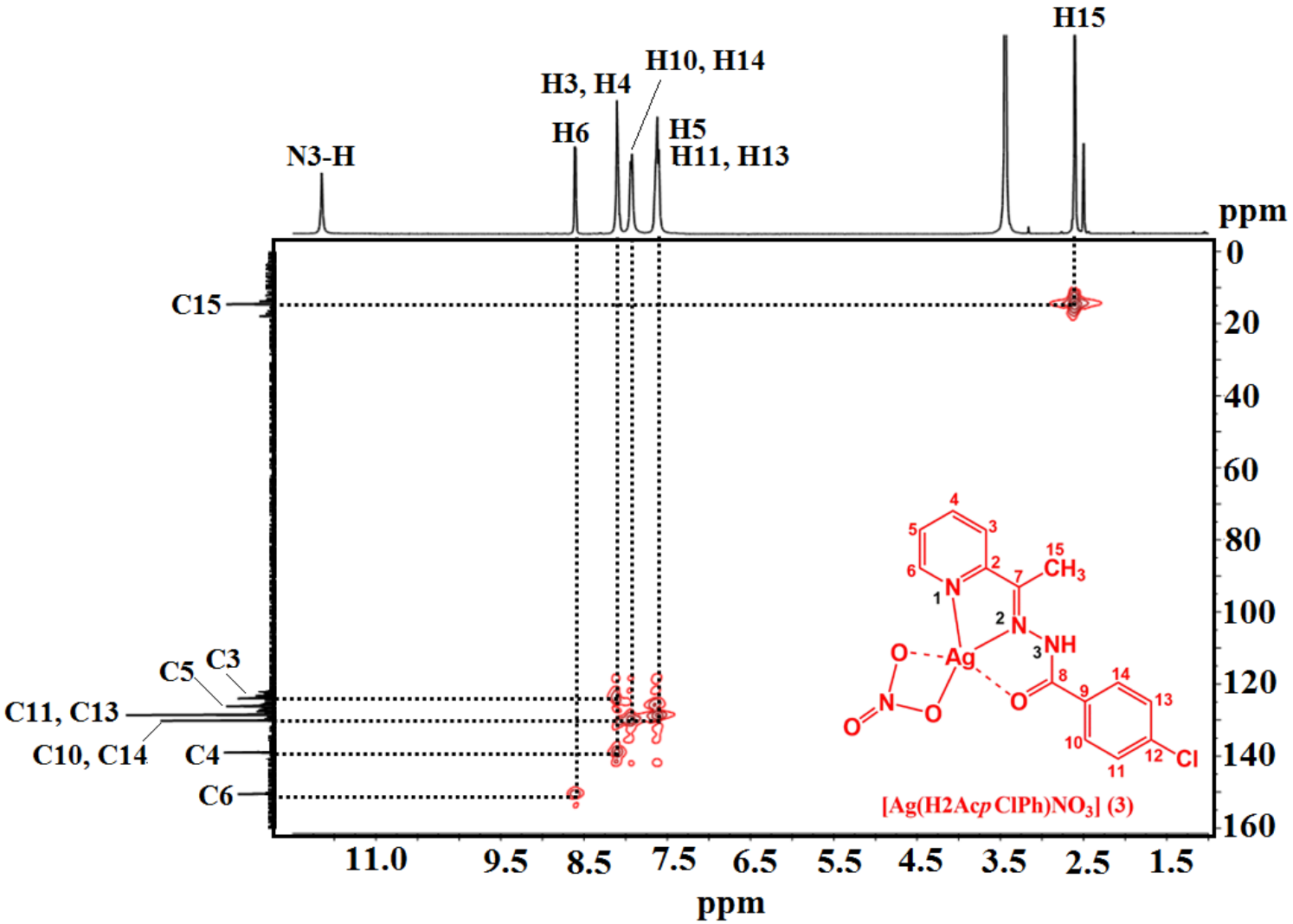

Fig. S17 HMQC (^{1}H-^{13}C{^{1}H}) contour map of [Ag(H2A*cp*ClPh)NO_3] (**3**) registered in DMSO-d_6 at 25ºC.

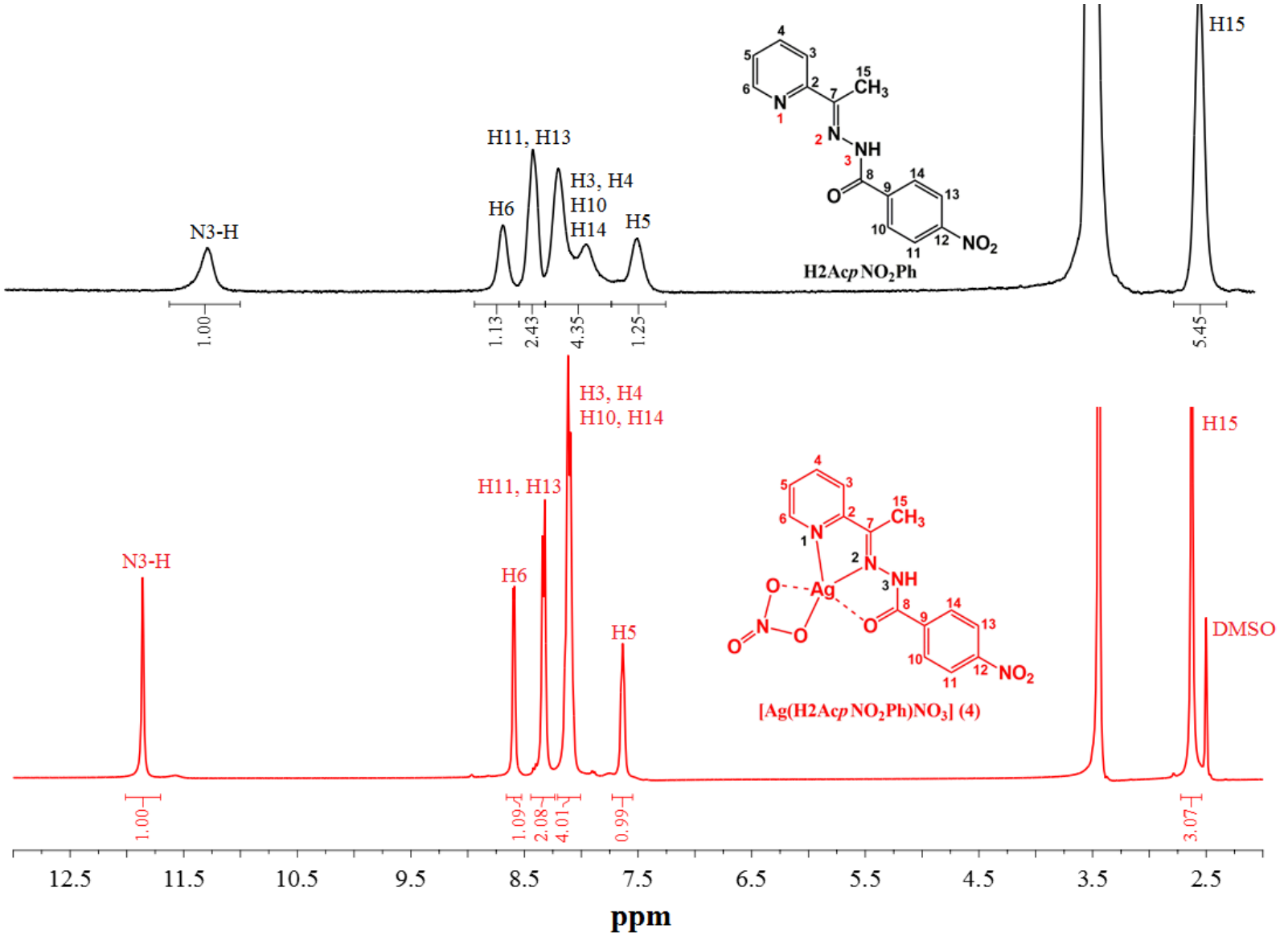

Fig. S18 ^{1}H NMR spectrum of H2Ac*p*NO_2Ph (black) and [Ag(H2Ac*p*NO_2Ph)NO_3] (**4**) (red) registered in DMSO-d_6 at 25ºC.

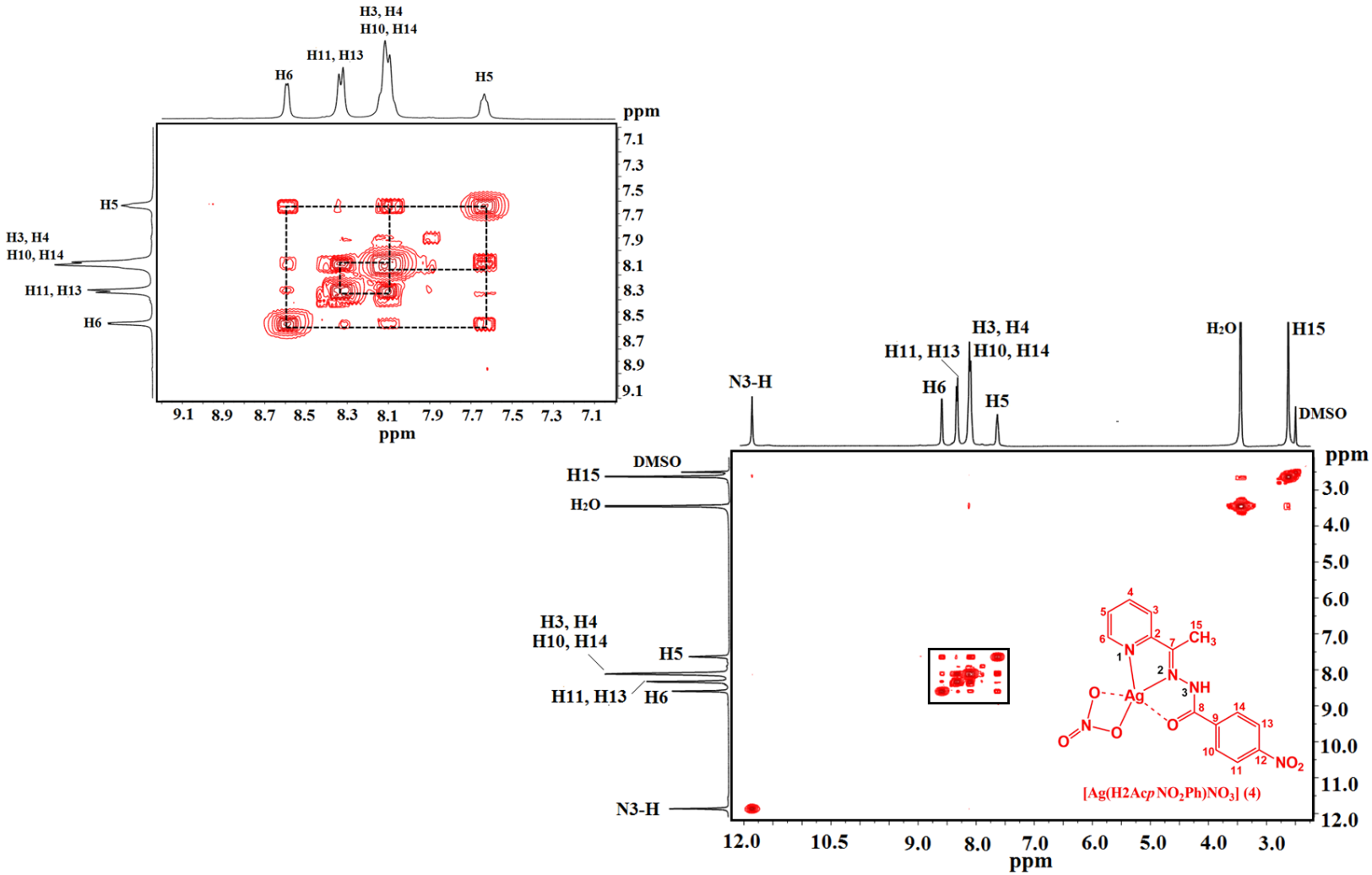

Fig. S19 COSY (^{1}H-^{1}H) contour map of [Ag(H2A*cp*NO_2Ph)NO_3] (**4**) registered in DMSO-d_6 at 25ºC.

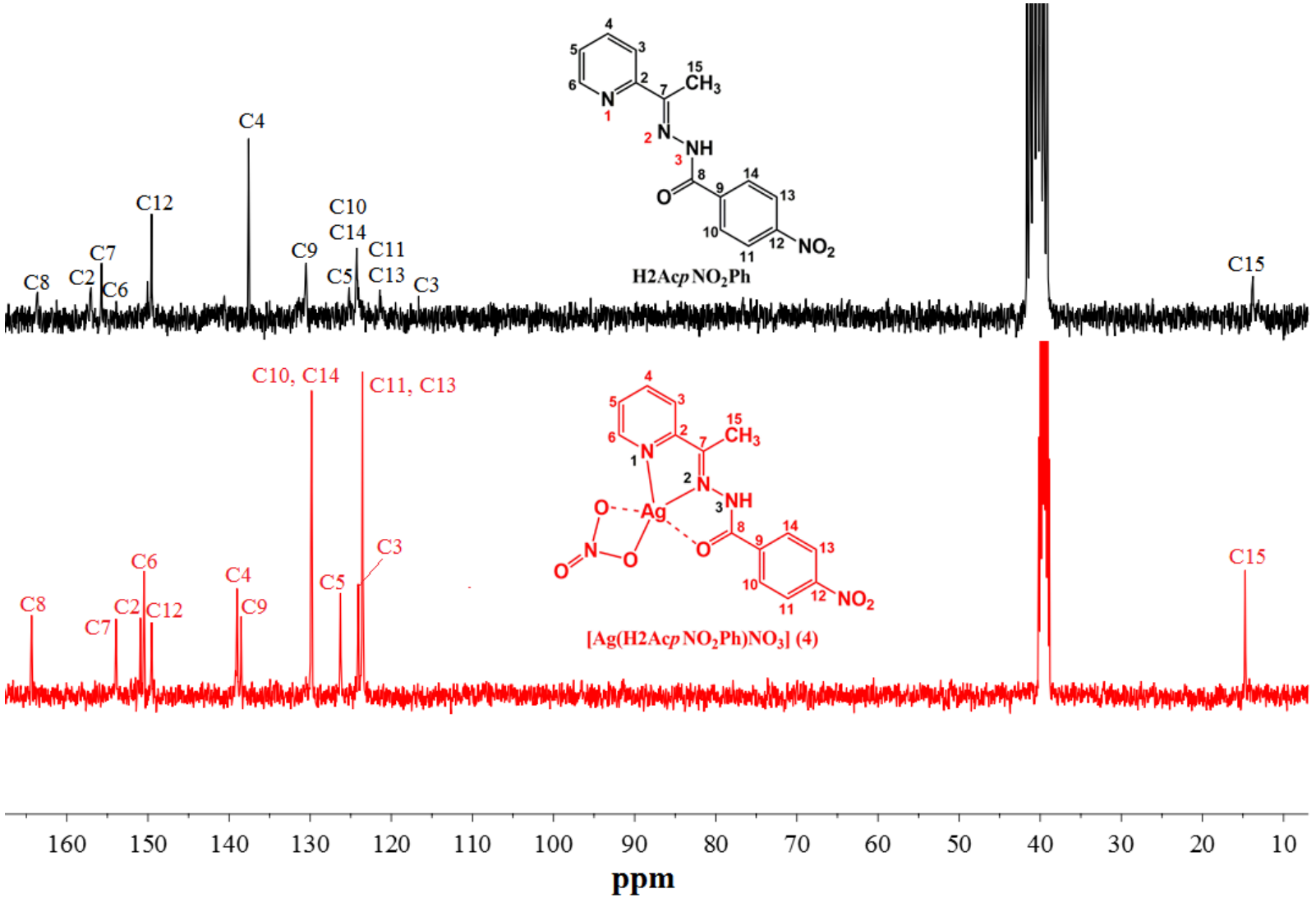

Fig. S20 $^{13}C\{^{1}H\}$ NMR spectrum of H2Ac*p*NO_2Ph (black) and [Ag(H2Ac*p*NO_2Ph)NO_3] (**4**) (red) registered in DMSO-d_6 at 25ºC.

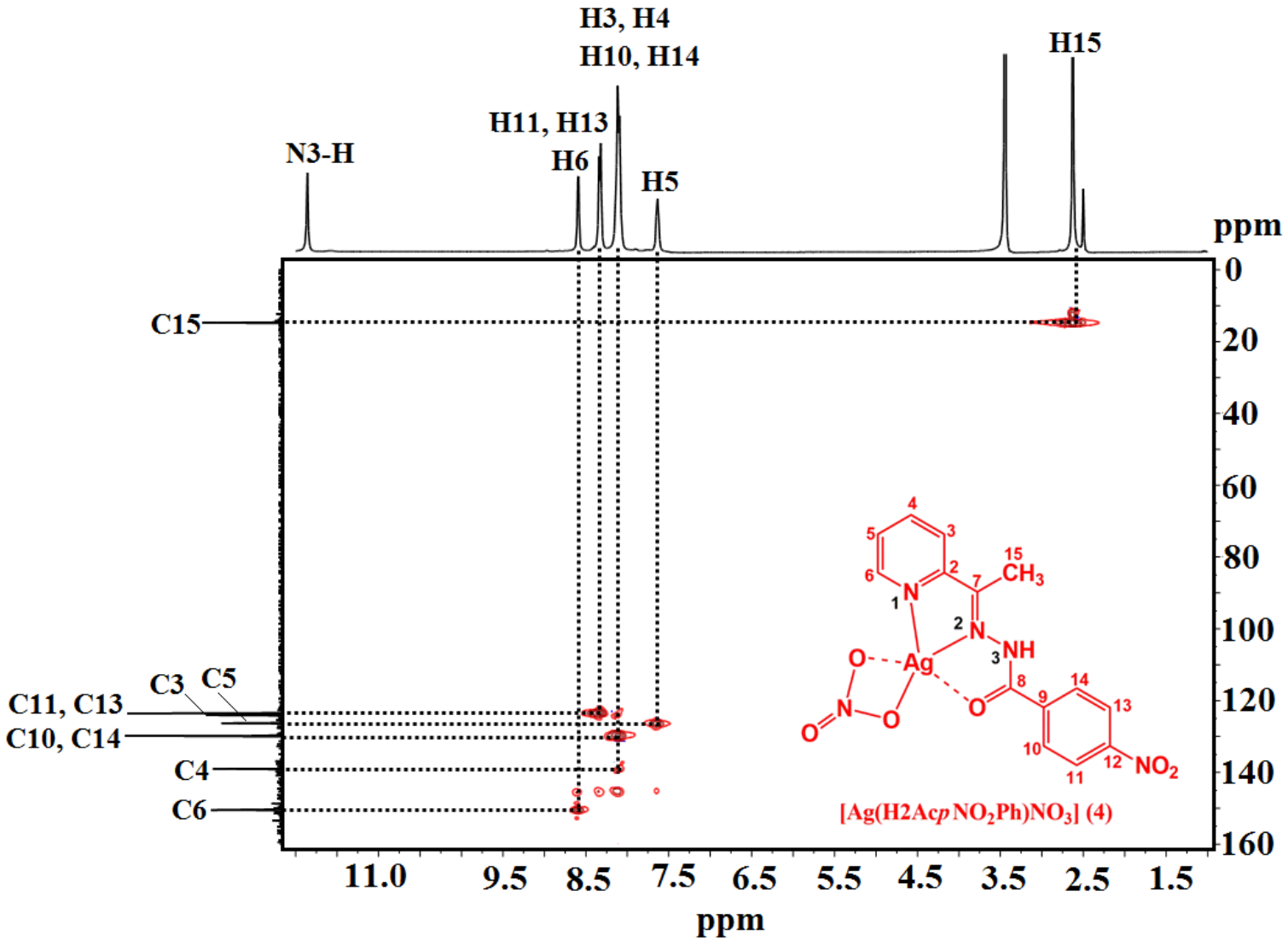

Fig. S21 HMQC (^{1}H-^{13}C{^{1}H}) contour map of [Ag(H2Ac*p*NO_2Ph)NO_3] (**4**) registered in DMSO-d_6 at 25ºC.

*Mass spectra (ESI) of silver(I) complexes (**1-4**)*

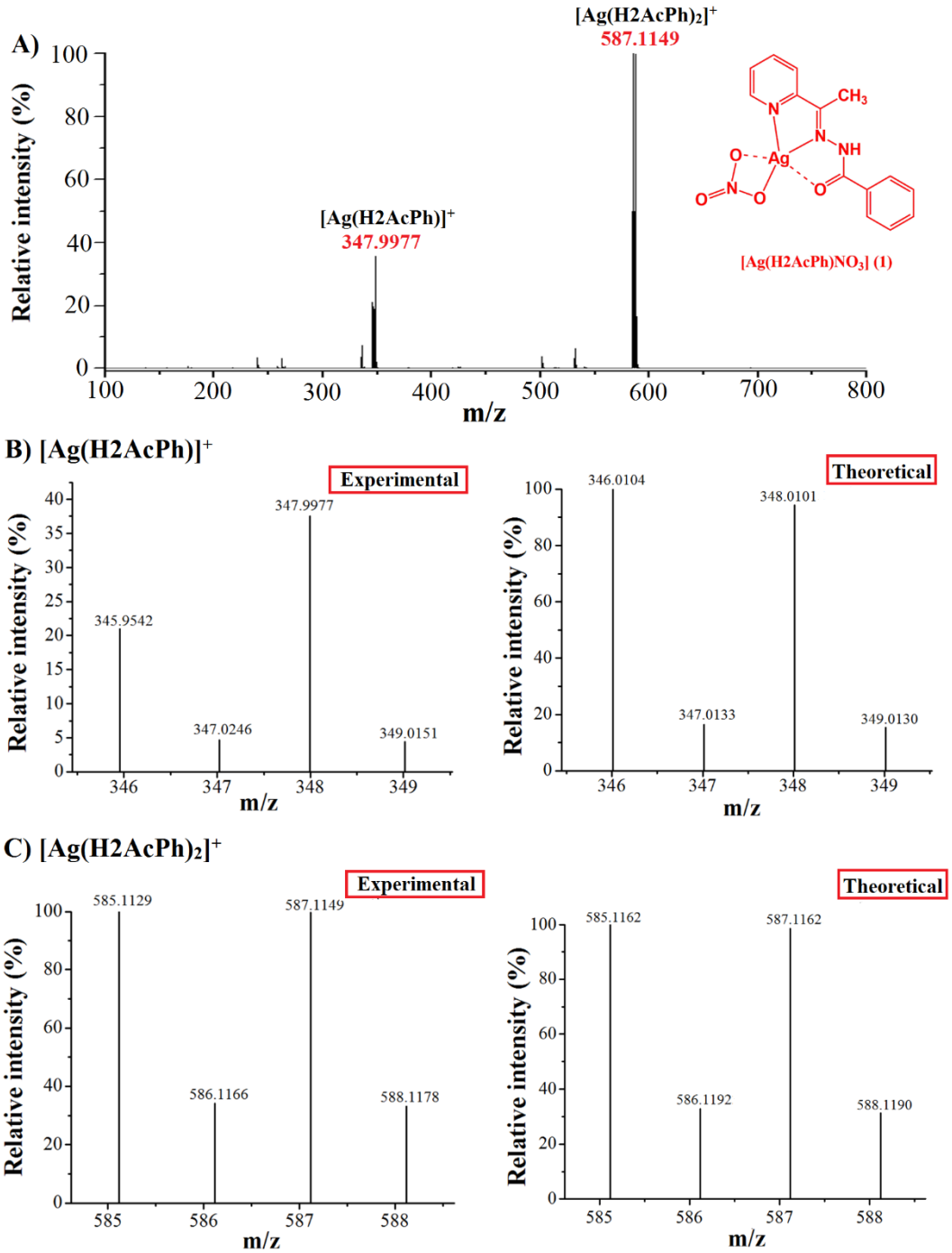

Fig. S22 A) Mass spectrum ESI-MS (+) of [Ag(H2AcPh)NO_3] (**1**). B) Comparison between the experimental (m/z 347.9977) and theoretical (m/z 348.0101) isotopic pattern of the species $[Ag(H2AcPh)]^+$. C) Comparison between the experimental (m/z 587.1149) and theoretical (m/z 587.1162) isotopic pattern of the species $[Ag(H2AcPh)_2]^+$.

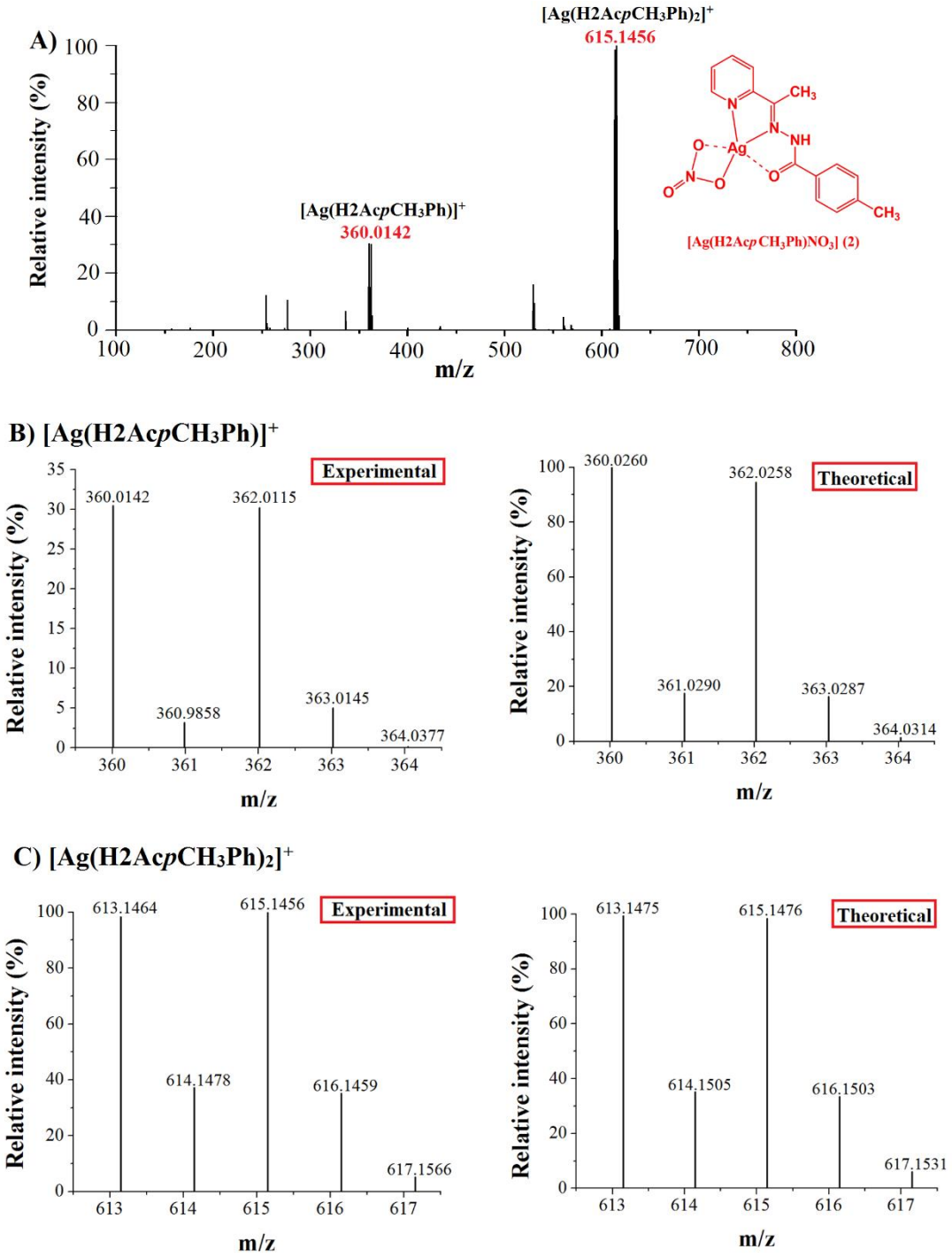

Fig. S23 A) Mass spectrum ESI-MS (+) of [Ag(H2Ac*p*CH$_3$Ph)NO$_3$] (**2**). B) Comparison between the experimental (m/z 360.0142) and theoretical (m/z 360.0260) isotopic pattern of the species [Ag(H2Ac*p*CH$_3$Ph)]$^+$. C) Comparison between the experimental (m/z 615.1456) and theoretical (m/z 615.1476) isotopic pattern of the species [Ag(H2Ac*p*CH$_3$Ph)$_2$]$^+$.

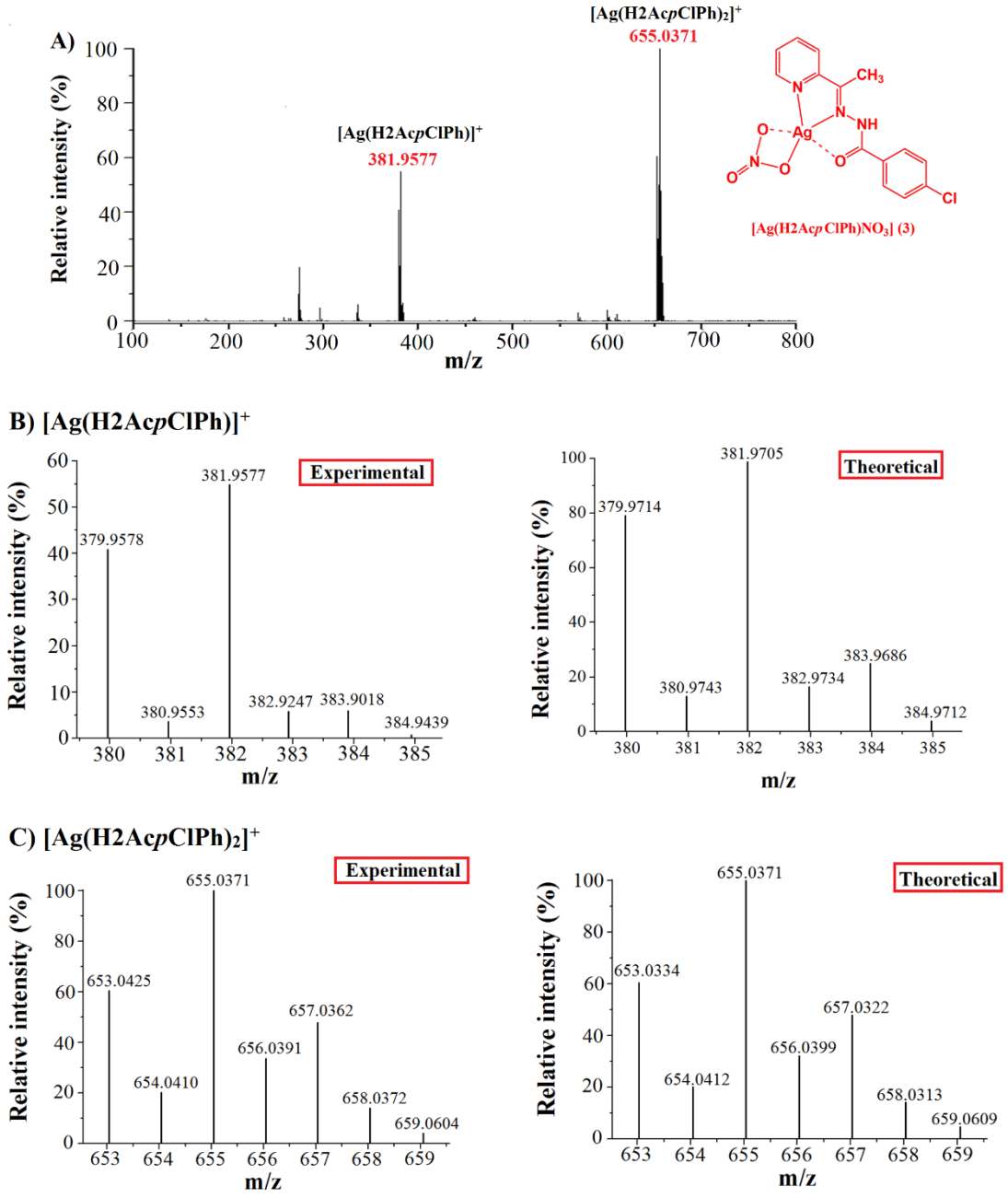

Fig. S24 A) Mass spectrum ESI-MS (+) of [Ag(H2Ac*p*ClPh)NO_3] (**3**). B) Comparison between the experimental (m/z 381.9577) and theoretical (m/z 381.9705) isotopic pattern of the species [Ag(H2Ac*p*ClPh)]$^+$. C) Comparison between the experimental (m/z 655.0371) and theoretical (m/z 655.0371) isotopic pattern of the species [Ag(H2Ac*p*ClPh)$_2$]$^+$.

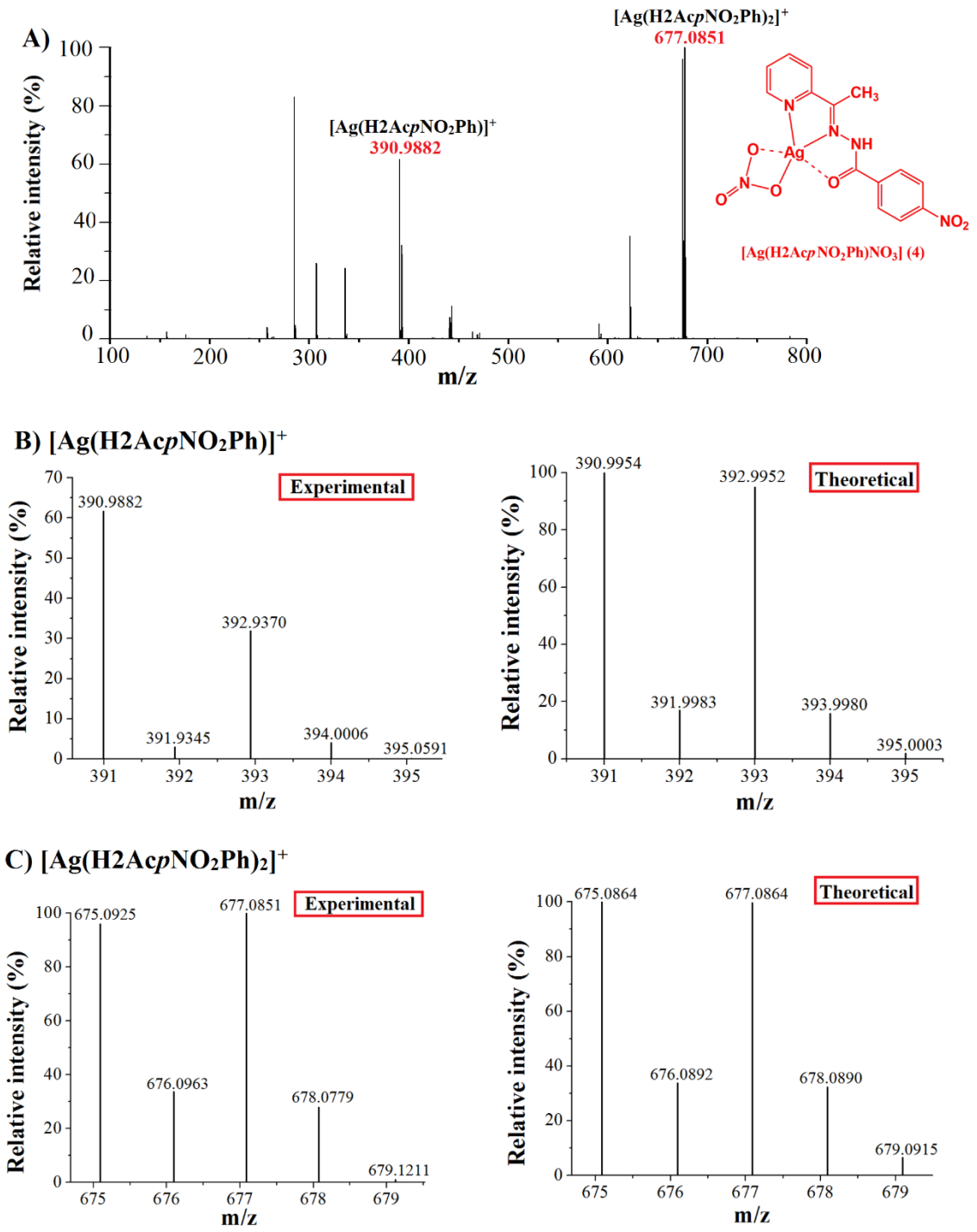

Fig. S25 A) Mass spectrum ESI-MS (+) of [Ag(H2Ac*p*NO$_2$Ph)NO$_3$] (**4**). B) Comparison between the experimental (m/z 390.9882) and theoretical (m/z 390.9954) isotopic pattern of the species [Ag(H2Ac*p*NO$_2$Ph)]$^+$. C) Comparison between the experimental (m/z 677.0851) and theoretical (m/z 677.0864) isotopic pattern of the species [Ag(H2Ac*p*NO$_2$Ph)$_2$]$^+$.

X-ray crystallography

Table S1 Crystal data and structure refinement results for [Ag(H2AcPh)NO_3] (**1**), [Ag(H2Ac*p*CH_3Ph)$_2$]NO_3 (**2a**), [Ag(H2Ac*p*ClPh)$_2$]NO_3 (**3a**) and [Ag(H2Ac*p*NO_2Ph)(H_2O)(NO_3)] (**4a**).

Compound	(**1**)	(**2a**)	(**3a**)	(**4a**)
Empirical formula	$C_{14}H_{13}N_4O_4Ag$	$C_{30}H_{30}N_7O_5Ag$	$C_{28}H_{24}Cl_2N_7O_5Ag$	$C_{14}H_{14}N_5O_7Ag$
Molecular weight (g mol^{-1})	409.15	676.48	717.31	472.17
T (K)	270(2)	270(2)	270(2)	270(2)
Crystal system	monoclinic	triclinic	triclinic	monoclinic
Space group	P 2_1/n	P -1	P -1	P 2_1/c
Unit cell dimensions				
a (Å)	6.7603(7)	8.4416(6)	8.2925(4)	7.2535(4)
b (Å)	13.0051(7)	12.9864(5)	13.1239(7)	13.2543(7)
c (Å)	16.5751(9)	14.7636(6)	14.7518(7)	17.9111(8)
α (º)	90	112.115(4)	112.238(5)	90
β (º)	97.889(7)	99.194(4)	98.638(4)	99.214(4)
γ (º)	90	95.337(4)	96.159(4)	90
V ($Å^3$)	1443.46(19)	1459.23(14)	1445.35(13)	1699.76(15)
Z	4	2	2	4
Density calculated (Mg m^{-3})	1.883	1.540	1.648	1.845
Absorption coefficient (mm^{-1})	1.424	0.743	0.934	1.237
F(000)	816	692	724	944
Crystal size (mm)	0.21 x 0.06 x 0.06	0.39 x 0.19 x 0.08	0.43 x 0.13 x 0.05	0.36 x 0.09 x 0.07
θ °range for data collection	2.0 to 26.4	2.5 to 26.4	2.5 to 26.4	1.9 to 29.5
Index ranges	$-8 \le h \le 8$ $-16 \le k \le 15$ $-20 \le l \le 20$	$-10 \le h \le 9$ $-16 \le k \le 16$ $-18 \le l \le 18$	$-10 \le h \le 10$ $-16 \le k \le 16$ $-18 \le l \le 18$	$-10 \le h \le 9$ $-18 \le k \le 15$ $-24 \le l \le 24$
Reflections collected	12186	12718	22505	13375
Independent reflections (R_{int})	2968 (0.0762)	5972 (0.0283)	5925 (0.0521)	4195 (0.0325)
Completeness to θ = 25.242 (%)	100	99.9	99.9	100
Data/restraints/parameters	2968/0/209	5972/12/420	5925/12/388	4195/3/ 251
Goodness-of-fit on F^2	1.079	1.032	1.037	1.023
Final R indices [I >2σ(I)]	R_1 = 0.0625, wR_2 = 0.1508	R_1 = 0.0293, wR_2 = 0.0655	R_1 = 0.0452, wR_2 = 0.1024	R_1 = 0.0623, wR_2 = 0.1419
R indices (all data)	R_1 = 0.1019 wR_2 = 0.1764	R_1 = 0.0409, wR_2 = 0.0708	R_1 = 0.0735, wR_2 = 0.1204	R_1 = 0.0932, wR_2 = 0.1617
Largest diff. peak and hole ($eÅ^{-3}$)	1.562 and -0.668	0.276 and -0.441	1.149 and -0.796	2.549 and -0.894

Table S2 Selected bond lengths (Å) for[Ag(H2AcPh)NO_3] (**1**), [Ag(H2Ac*p*CH_3Ph)$_2$]NO_3 (**2a**), [Ag(H2Ac*p*ClPh)$_2$]NO_3 (**3a**) and [Ag(H2Ac*p*NO_2Ph)(H_2O)(NO_3)] (**4a**) along with data for H2AcPh and H2Ac*p*ClPh.

Atoms	H2AcPh[40]	(**1**)	(**2a**)	H2Ac*p*ClPh[13]	(**3a**)	(**4a**)
N1-C2	1.325(3)	1.350(8)	1.344(3)	1.3345(19)	1.343(5)	1.342(6)
C2-C7	1.487(2)	1.494(8)	1.492(3)	1.4900(18)	1.496(6)	1.491(7)
C7-N2	1.264(3)	1.280(7)	1.282(3)	1.2860(18)	1.279(5)	1.278(6)
N2-N3	1.375(2)	1.369(7)	1.377(2)	1.3810(15)	1.380(4)	1.369(6)
N3-C8	1.347(3)	1.365(8)	1.367(3)	1.3590(17)	1.364(5)	1.359(6)
C8-O1	1.219(2)	1.219(7)	1.219(3)	1.2260(16)	1.219(4)	1.217(6)
Ag1-N1	–	2.338(5)	2.3709(19)	–	2.372(3)	2.378(4)
Ag1-N2	–	2.378(5)	2.3930(16)	–	2.401(3)	2.372(4)
Ag1-O1	–	2.564(4)	2.5923(16)	–	2.619(3)	2.629(4)
Ag1-O2	–	2.384(6)	–	–	–	2.488(5)
Ag1-O3	–	2.692(6)	–	–	–	2.665(4)
Ag1-N4	–	–	2.3631(17)	–	2.371(3)	–
Ag1-N5	–	–	2.3565(17)	–	2.376(3)	–
Ag1-O1W	–	–	–	–	–	2.359 (4)

Table S3 Selected angles (º) for [Ag(H2AcPh)NO_3] (**1**), [Ag(H2Ac*p*CH_3Ph)$_2$]NO_3 (**2a**), [Ag(H2Ac*p*ClPh)$_2$]NO_3 (**3a**) and [Ag(H2Ac*p*NO_2Ph)(H_2O)(NO_3)] (**4a**) along with data for H2AcPh and H2Ac*p*ClPh.

Atoms	H2AcPh[40]	(**1**)	(**2a**)	H2Ac*p*ClPh[13]	(**3a**)	(**4a**)
N1-C2-C7	116.2(1)	117.2(5)	117.14(19)	116.40(12)	117.2(3)	116.8(4)
C2-C7-N2	114.5(1)	114.2(5)	115.23(19)	115.12(12)	115.4(3)	115.8(4)
C7-N2-N3	119.0(1)	120.0(5)	118.86(18)	116.22(11)	118.6(3)	119.5(4)
N2-N3-C8	117.0(1)	118.1(5)	117.51(16)	117.89(11)	117.7(3)	118.0(4)
N3-C8-O1	123.3(2)	122.3(5)	121.82(19)	123.28(13)	122.2(4)	122.8(5)
N1-Ag1-N2	–	68.18(17)	68.26(6)	–	68.25(11)	68.52(13)
N1-Ag1-O2	–	118.35(19)	–	–	–	116.77(14)
N2-Ag1-O2	–	118.97(18)	–	–	–	120.45(13)
N1-Ag1-O1	–	133.45(16)	132.39(6)	–	132.01(10)	132.60(13)
N2-Ag1-O1	–	65.27(15)	64.15(5)	–	63.82(10)	64.23(12)
O2-Ag1-O1	–	85.17(15)	–	–	–	90.81(15)
N1-Ag1-O3	–	92.69(18)	–	–	–	93.85(14)
N2-Ag1-O3	–	150.62(18)	–	–	–	152.95(14)
O2-Ag1-O3	–	49.84(16)	–	–	–	48.33(13)
O1-Ag1-O3	–	129.51(16)	–	–	–	131.23(14)
N4-Ag1-N5	–	–	68.82(6)	–	68.71(10)	–
N5-Ag1-O1	–	–	115.74(6)	–	118.86(10)	–
N1-Ag1-N5	–	–	106.96(6)	–	106.56(11)	–

Table S4 Hydrogen-bond geometry (Å,°) for (**1-4a**).

Compound	D—H···A	D-H	H···A	D···A	D—H···A
(**1**)	N3-H3N···O2^{i}	0.86	2.23	2.996(7)	149
(**2a**)	N3-H3N···O4A^{ii}	0.86	2.22	3.051(10)	164
(**2a**)	N3-H3N···O4B^{ii}	0.86	2.52	3.374(17)	173
(**2a**)	N6-H6N···O2A	0.86	2.33	2.974(12)	132
(**2a**)	N6-H6N···O2B	0.86	2.21	2.905(13)	138
(**3a**)	N3-H3N···O4A^{ii}	0.86	2.23	3.079(7)	169
(**3a**)	N3-H3N···O4B^{ii}	0.86	2.30	3.109(8)	156
(**3a**)	N6-H6N···O2A	0.86	2.33	2.987(7)	134
(**3a**)	N6-H6N···O2B	0.86	2.34	3.071(9)	142
(**4a**)	N3-H3N···O2^{iii}	0.86	2.33	3.124(6)	154
(**4a**)	O1W-H1W···O4^{vi}	0.82(1)	2.01(4)	2.770(6)	154(8)
(**4a**)	O1W-H2W···O5^{v}	0.82(1)	2.50(7)	3.122(7)	134(8)
(**4a**)	O1W-H2W···O6^{v}	0.82(1)	2.51(3)	3.305(7)	164(8)

Symmetry codes: i = -x+1,-y+2,-z; ii = x,y+1,z; iii = -x+1,-y+1,-z; iv = x+1,y,z; v = x,y-1,z.

Table S5 Stereo-electronic parameters for 2-acetylpyridine-derived hydrazones and their silver(I) complexes (**1-4**).

Compound		E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A (Å^2)	V (Å^3)	logP
H2AcPh	(*E*)	-6.332	-1.767	4.565	4.675	343.76	222.34	1.98
H2Ac*p*CH_3Ph	(*E*)	-6.283	-1.763	4.520	9.332	375.47	239.27	2.49
H2Ac*p*ClPh	(*E*)	-6.300	-1.887	4.413	4.139	359.64	236.23	2.58
H2Ac*p*NO_2Ph	(*E*)	-6.394	-2.871	3.523	6.243	384.56	245.6	1.92
H2AcPh	(*Z*)	-6.319	-1.920	4.399	9.970	342.03	222.52	1.98
H2Ac*p*CH_3Ph	(*Z*)	-6.277	-1.899	4.378	10.108	374.83	239.38	2.49
H2Ac*p*ClPh	(*Z*)	-6.350	-1.934	4.416	10.064	359.36	236.36	2.58
H2Ac*p*NO_2Ph	(*Z*)	-6.443	-2.828	3.615	11.325	383.97	245.71	1.92
[Ag(H2AcPh)NO_3]	(**1**)	-6.894	-2.520	4.374	7.440	336.52	239.79	2.80
[Ag(H2Ac*p*CH_3Ph)NO_3]	(**2**)	-6.812	-2.471	4.341	7.567	369.91	256.68	3.27
[Ag(H2Ac*p*ClPh)NO_3]	(**3**)	-6.842	-2.540	4.302	11.170	354.07	253.73	3.32
[Ag(H2Ac*p*NO_2Ph)NO_3]	(**4**)	-7.007	-3.106	3.902	15.896	378.38	263.12	2.76

Table S6 Correlation Matrix between the IC_{50} data for *Aspergillus flavus* and the Stereo-Electronic parameters of the free-ligands H2AcPh, H2Ac*p*CH_3Ph and H2Ac*p*NO_2Ph (*Z* and *E* isomers).

		IC_{50}							
Compounds	Isomer	*Aspergillus flavus*	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A (Å^2)	V (Å^3)	LogP
H2AcPh	Z	48.6	-6.319	-1.920	4.399	9.970	342.03	222.52	1.98
H2Ac*p*CH_3Ph	Z	23.6	-6.277	-1.899	4.378	10.108	374.83	239.38	2.49
H2Ac*p*NO_2Ph	Z	42.1	-6.443	-2.828	3.615	11.325	383.97	245.71	1.92
H2AcPh	E	48.6	-6.332	-1.767	4.565	4.675	343.76	222.34	1.98
H2Ac*p*CH_3Ph	E	23.6	-6.283	-1.763	4.520	9.332	375.47	239.27	2.49
H2Ac*p*NO_2Ph	E	42.1	-6.394	-2.871	3.523	6.243	384.56	245.6	1.92

Correlation matrix

	Aspergillus flavus	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A (Å^2)	V (Å^3)	LogP
Aspergillus flavus	1							
E_{HOMO} (eV)	-0.54497	1						
E_{LUMO} (eV)	-0.27508	0.89878	1					
ΔE (eV)	-0.23329	0.87047	0.99815	1				
μ (D)	-0.38759	-0.02417	-0.09964	-0.10853	1			
S.A (Å^2)	-0.53567	-0.38345	-0.65381	-0.68091	0.31922	1		
V (Å^3)	-0.48824	-0.43295	-0.69820	-0.72389	0.33659	0.99773	1	
LogP	-0.93965	0.78600	0.58460	0.54739	0.30870	0.21464	0.16021	1

Table S7 Correlation Matrix between the IC_{50} data obtained for *Penicillium citrinum* and the Stereo-Electronic parameters of the free-ligands H2AcPh, H2Ac*p*CH_3Ph, H2Ac*p*ClPh and H2Ac*p*NO_2Ph (*Z* and *E* isomers)

		IC_{50}							
Compounds	Isomer	*Penicillium citrinum*	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A (Å^2)	V (Å^3)	LogP
H2AcPh	Z	72.5	-6.319	-1.920	4.399	9.970	342.03	222.52	1.98
H2Ac*p*CH_3Ph	Z	33.4	-6.277	-1.899	4.378	10.108	374.83	239.38	2.49
H2Ac*p*ClPh	Z	44.1	-6.350	-1.934	4.416	10.064	359.36	236.36	2.58
H2Ac*p*NO_2Ph	Z	53.9	-6.443	-2.828	3.615	11.325	383.97	245.71	1.92
H2AcPh	E	72.5	-6.332	-1.767	4.565	4.675	343.76	222.34	1.98
H2Ac*p*CH_3Ph	E	33.4	-6.283	-1.763	4.520	9.332	375.47	239.27	2.49
H2Ac*p*ClPh	E	44.1	-6.300	-1.887	4.413	4.139	359.64	236.23	2.58
H2Ac*p*NO_2Ph	E	53.9	-6.394	-2.871	3.523	6.243	384.56	245.6	1.92

Correlation matrix

	Penicillium citrinum	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A (Å^2)	V (Å^3)	LogP
Penicillium citrinum	1							
E_{HOMO} (eV)	-0.34849	1						
E_{LUMO} (eV)	-0.10861	0.87592	1					
ΔE (eV)	-0.07333	0.84179	0.99777	1				
μ (D)	-0.24292	-0.18460	-0.15718	-0.15034	1			
S.A (Å^2)	-0.61756	-0.38830	-0.67268	-0.69896	0.29597	1		
V (Å^3)	-0.66355	-0.41449	-0.66623	-0.68813	0.25913	0.96790	1	
LogP	-0.78128	0.65584	0.59805	0.57847	0.01541	0.01320	0.13680	1

Table S8 Correlation Matrix between the IC_{50} data for *Aspergillus flavus* and the Stereo-Electronic parameters of complexes (**1-4**)

	IC_{50}							
Compounds	*Aspergillus flavus*	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A ($Å^2$)	V ($Å^3$)	LogP
[Ag(H2AcPh)NO_3] (**1**)	12.4	-6.894	-2.520	4.374	7.440	336.52	239.79	2.80
[Ag(H2Ac*p*CH_3Ph)NO_3] (**2**)	10.5	-6.812	-2.471	4.341	7.567	369.91	256.68	3.27
[Ag(H2Ac*p*ClPh)NO_3] (**3**)	41.4	-6.842	-2.540	4.302	11.170	354.07	253.73	3.32
[Ag(H2Ac*p*NO_2Ph)NO_3] (**4**)	32.9	-7.007	-3.106	3.902	15.896	378.38	263.12	2.76

Correlation matrix								
	Aspergillus flavus	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A ($Å^2$)	V ($Å^3$)	LogP
Aspergillus flavus	1							
E_{HOMO}(eV)	-0,30915	1						
E_{LUMO} (eV)	-0.44226	0.93629	1					
ΔE (eV)	-0,47910	0.87953	0.99063	1				
μ (D)	0.73959	-0.79621	-0.92604	-0.94497	1			
S.A ($Å^2$)	0.23590	-0.32975	-0.62292	-0.71562	0.62611	1		
V ($Å^3$)	0.45714	-0.32005	-0.63168	-0.73130	0.72076	0.97010	1	
LogP	0.15092	0.84746	0.62831	0.52156	-0.35444	0.06685	0.15783	1

Table S9 Correlation Matrix between the IC_{50} data for *Penicillium citrinum* and the Stereo-Electronic parameters of complexes (**1**), (**2**) and (**4**)

	IC_{50}							
Compounds	*Penicillium citrinum*	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A ($Å^2$)	V ($Å^3$)	LogP
[Ag(H2AcPh)NO_3] (**1**)	39.8	-6.894	-2.520	4.374	7.440	336.52	239.79	2.80
[Ag(H2Ac*p*CH_3Ph)NO_3] (**2**)	17.1	-6.812	-2.471	4.341	7.567	369.91	256.68	3.27
[Ag(H2Ac*p*NO_2Ph)NO_3] (**4**)	31.6	-7.007	-3.106	3.902	15.896	378.38	263.12	2.76

Correlation matrix								
	Penicillium citrinum	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A ($Å^2$)	V ($Å^3$)	LogP
Penicillium citrinum	1							
E_{HOMO}(eV)	-0.55528	1						
E_{LUMO}(eV)	-0.22645	0.93580	1					
ΔE (eV)	-0.09691	0.88156	0.99138	1				
μ (D)	0.14531	-0.90352	-0.99659	-0.99881	1			
S.A ($Å^2$)	-0.64098	-0.28243	-0.60247	-0.70183	0.66627	1		
V ($Å^3$)	-0.57923	-0.35631	-0.66283	-0.75520	0.72235	0.99696	1	
LogP	-0.90675	0.85419	0.61605	0.50757	-0.54896	0.25754	0.18147	1

Table S10 Correlation Matrix between the IC_{50} data for *Candida dubliniensis* and the Stereo-Electronic parameters of complexes (**1-4**)

Compounds	IC_{50} *Candida dubliniensis*	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A (Å^2)	V (Å^3)	LogP
[Ag(H2AcPh)NO_3] (**1**)	40.7	-6.893	-2.519	4.373	7.440	336.52	239.79	2.80
[Ag(H2Ac*p*CH_3Ph)NO_3] (**2**)	44.3	-6.811	-2.470	4.341	7.566	369.91	256.68	3.27
[Ag(H2Ac*p*ClPh)NO_3] (**3**)	14.5	-6.842	-2.540	4.302	11.170	354.07	253.73	3.32
[Ag(H2Ac*p*NO_2Ph)NO_3] (**4**)	13.9	-7.000	-3.105	3.901	15.896	378.38	263.12	2.76

Correlation matrix

	Candida dubliniensis	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A (Å^2)	V (Å^3)	LogP
Candida dubliniensis	1							
E_{HOMO}(eV)	0.52858	1						
E_{LUMO}(eV)	0.64759	0.93715	1					
ΔE (eV)	0.67205	0.88115	0.99076	1				
μ (D)	-0.87703	-0.79832	-0.92643	-0.94503	1			
S.A (Å^2)	-0.34712	-0.33147	-0.62277	-0.71504	0.62608	1		
V (Å^3)	-0.53839	-0.32244	-0.63179	-0.73077	0.72073	0.97010	1	
LogP	0.05939	0.84565	0.62789	0.52208	-0.35447	0.06685	0.15783	1

Table S11 Correlation Matrix between the IC_{50} data for *Candida glabrata* and the Stereo-Electronic parameters of complexes (**1-4**)

Compounds	IC_x *Candida glabrata*	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A (Å^2)	V (Å^3)	LogP
[Ag(H2AcPh)NO_3] (**1**)	52.8	-6.894	-2.520	4.374	7.440	336.52	239.79	2.80
[Ag(H2Ac*p*CH_3Ph)NO_3] (**2**)	44.3	-6.812	-2.471	4.341	7.567	369.91	256.68	3.27
[Ag(H2Ac*p*ClPh)NO_3] (**3**)	42.1	-6.842	-2.540	4.302	11.170	354.07	253.73	3.32
[Ag(H2Ac*p*NO_2Ph)NO_3] (**4**)	52.6	-7.007	-3.106	3.902	15.896	378.38	263.12	2.76

Correlation matrix

	Candida glabrata	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A (Å^2)	V (Å^3)	LogP
Candida glabrata	1							
E_{HOMO}(eV)	-0.78690	1						
E_{LUMO}(eV)	-0.55795	0.93715	1					
ΔE (eV)	-0.45015	0.88115	0.99076	1				
μ (D)	0.25670	-0.79832	-0.92643	-0.94503	1			
S.A (Å^2)	-0.09711	-0.33147	-0.62277	-0.71504	0.62608	1		
V (Å^3)	-0.21152	-0.32244	-0.63179	-0.73077	0.72073	0.97010	1	
LogP	-0.99321	0.84565	0.62789	0.52208	-0.35447	0.06685	0.15783	1

Table S12 Correlation Matrix between the IC_{50} data for *Candida lusitaniae* and the Stereo-Electronic parameters of complexes (**1-4**)

IC_{50}

Compounds	*Candida lusitaniae*	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A (Å^2)	V (Å^3)	LogP
[Ag(H2AcPh)NO_3] (**1**)	29.1	-6.894	-2.520	4.374	7.440	336.52	239.79	2.80
[Ag(H2Ac*p*CH_3Ph)NO_3] (**2**)	33.7	-6.812	-2.471	4.341	7.567	369.91	256.68	3.27
[Ag(H2Ac*p*ClPh)NO_3] (**3**)	20.2	-6.842	-2.540	4.302	11.170	354.07	253.73	3.32
[Ag(H2Ac*p*NO_2Ph)NO_3] (**4**)	17.5	-7.007	-3.106	3.902	15.896	378.38	263.12	2.76

Correlation matrix

	Candida lusitaniae	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A (Å^2)	V (Å^3)	LogP
Candida lusitaniae	1							
E_{HOMO}(eV)	0.67426	1						
E_{LUMO}(eV)	0.73494	0.93715	1					
ΔE (eV)	0.73378	0.88115	0.99076	1				
μ (D)	-0.90496	-0.79832	-0.92643	-0.94503	1			
S.A (Å^2)	-0.28474	-0.33147	-0.62277	-0.71504	0.62608	1		
V (Å^3)	-0.45535	-0.32244	-0.63179	-0.73077	0.72073	0.97010	1	
LogP	0.26189	0.84565	0.62789	0.52208	-0.35447	0.06685	0.15783	1

Table S13 Correlation Matrix between the IC_{50} data for *Penicillium citrinum* and the Stereo-Electronic parameters of the ligands H2AcPh, H2Ac*p*CH_3Ph, H2Ac*p*ClPh and H2Ac*p*NO_2Ph (*Z* and *E* isomers) and complexes (**1-4**)

		IC_{50}							
Compounds	Isomer	*Penicillium citrinum*	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A ($Å^2$)	V ($Å^3$)	LogP
H2AcPh	Z	72.5	-6.319	-1.920	4.399	9.970	342.03	222.52	1.98
H2Ac*p*CH_3Ph	Z	33.4	-6.277	-1.899	4.378	10.108	374.83	239.38	2.49
H2Ac*p*ClPh	Z	44.1	-6.350	-1.934	4.416	10.064	359.36	236.36	2.58
H2Ac*p*NO_2Ph	Z	53.9	-6.443	-2.828	3.615	11.325	383.97	245.71	1.92
H2AcPh	E	72.5	-6.332	-1.767	4.565	4.675	343.76	222.34	1.98
H2Ac*p*CH_3Ph	E	33.4	-6.283	-1.763	4.520	9.332	375.47	239.27	2.49
H2Ac*p*ClPh	E	44.1	-6.300	-1.887	4.413	4.139	359.64	236.23	2.58
H2Ac*p*NO_2Ph	E	53.9	-6.394	-2.871	3.523	6.243	384.56	245.6	1.92
[Ag(H2AcPh)NO_3] (**1**)		39.8	-6.894	-2.520	4.374	7.440	336.52	239.79	2.80
[Ag(H2Ac*p*CH_3Ph)NO_3] (**2**)		17.1	-6.812	-2.471	4.341	7.567	369.91	256.68	3.27
[Ag(H2Ac*p*NO_2Ph)NO_3] (**4**)		31.6	-7.007	-3.106	3.902	15.896	378.38	263.12	2.76

Correlation matrix

	Penicillium citrinum	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A ($Å^2$)	V ($Å^3$)	LogP
Penicillium citrinum	1							
E_{HOMO}(eV)	0.49680	1						
E_{LUMO}(eV)	0.23835	0.70106	1					
ΔE (eV)	-0.04445	0.21367	0.84643	1				
μ (D)	-0.26999	-0.40002	-0.45060	-0.31859	1			
S.A ($Å^2$)	-0.42733	0.01954	-0.47457	-0.66473	0.38684	1		
V ($Å^3$)	-0.76776	-0.70576	-0.76950	-0.52715	0.50840	0.66692	1	
LogP	-0.86887	-0.61535	-0.07679	0.35431	0.11992	-0.02843	0.56163	1

Table S14 Correlation Matrix between the IC_{50} data for *Candida glabrata* and the Stereo-Electronic parameters of the ligands H2Ac*p*ClPh and H2Ac*p*NO_2Ph (*Z* and *E* isomers) and complexes (**1-4**)

		IC_{50}							
Compounds	Isomer	*Candida glabrata*	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A (Å^2)	V (Å^3)	LogP
H2Ac*p*ClPh	Z	102.8	-6.350	-1.934	4.416	10.064	359.36	236.36	2.58
H2Ac*p*NO_2Ph	Z	77.0	-6.443	-2.828	3.615	11.325	383.97	245.71	1.92
H2Ac*p*ClPh	E	102.8	-6.300	-1.887	4.413	4.139	359.64	236.23	2.58
H2Ac*p*NO_2Ph	E	77.0	-6.394	-2.871	3.523	6.243	384.56	245.6	1.92
[Ag(H2AcPh)NO_3] (**1**)		52.8	-6.894	-2.520	4.374	7.440	336.52	239.79	2.80
[Ag(H2Ac*p*CH_3Ph)NO_3] (**2**)		44.3	-6.812	-2.471	4.341	7.567	369.91	256.68	3.27
[Ag(H2Ac*p*ClPh)NO_3] (**3**)		42.1	-6.842	-2.540	4.302	11.170	354.07	253.73	3.32
[Ag(H2Ac*p*NO_2Ph)NO_3] (**4**)		52.6	-7.007	-3.106	3.902	15.896	378.38	263.12	2.76

Correlation matrix								
	Candida glabrata	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A (Å^2)	V (Å^3)	LogP
Candida glabrata	1							
E_{HOMO}(eV)	0.90610	1						
E_{LUMO}(eV)	0.59964	0.52035	1					
ΔE (eV)	0.00290	-0.16028	0.75951	1				
μ (D)	-0.38215	-0.53503	-0.57311	-0.25489	1			
S.A (Å^2)	0.12232	0.26304	-0.53300	-0.81645	0.26905	1		
V (Å^3)	-0.76774	-0.73458	-0.71121	-0.26251	0.64968	0.40027	1	
LogP	-0.59212	-0.65469	0.21859	0.75137	0.12441	-0.56143	0.4026	1

Table S15 Correlation Matrix between the IC_{50} data for *Candida tropicalis* and the Stereo-Electronic parameters of the ligands H2Ac*p*ClPh and H2Ac*p*NO_2Ph (*Z* and *E* isomers) and complexes (**1-4**)

		IC_{50}							
Compounds	Isomer	*Candida tropicalis*	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A (Å^2)	V (Å^3)	LogP
H2Ac*p*ClPh	Z	164.1	-6.350	-1.934	4.416	10.064	359.36	236.36	2.58
H2Ac*p*NO_2Ph	Z	99.0	-6.443	-2.828	3.615	11.325	383.97	245.71	1.92
H2Ac*p*ClPh	E	164.1	-6.300	-1.887	4.413	4.139	359.64	236.23	2.58
H2Ac*p*NO_2Ph	E	99.0	-6.394	-2.871	3.523	6.243	384.56	245.6	1.92
[Ag(H2AcPh)NO_3] (**1**)		45.2	-6.894	-2.520	4.374	7.440	336.52	239.79	2.80
[Ag(H2Ac*p*CH_3Ph)NO_3] (**2**)		60.7	-6.812	-2.471	4.341	7.567	369.91	256.68	3.27
[Ag(H2Ac*p*ClPh)NO_3] (**3**)		40.5	-6.842	-2.540	4.302	11.170	354.07	253.73	3.32
[Ag(H2Ac*p*NO_2Ph)NO_3] (**4**)		50.8	-7.007	-3.106	3.902	15.896	378.38	263.12	2.76

Correlation matrix								
	Candida tropicalis	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	μ (D)	S.A (Å^2)	V (Å^3)	Log P
Candida tropicalis	1							
E_{HOMO}(eV)	0.90452	1						
E_{LUMO}(eV)	0.69676	0.52035	1					
ΔE (eV)	0.11636	-0.16028	0.75951	1				
μ (D)	-0.42414	-0.53503	-0.57311	-0.25489	1			
S.A (Å^2)	0.11492	0.26304	-0.53300	-0.81645	0.26905	1		
V (Å^3)	-0.72338	-0.73458	-0.71121	-0.26251	0.64968	0.4002	1	
LogP	-0.45914	-0.65469	0.21859	0.75137	0.12441	-0.5614	0.4026	1