Homochiral imidazolium-based dicarboxylate silver(I) compounds: synthesis, characterisation and antimicrobial properties.

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ELECTRONIC SUPPLEMENTARY INFORMATION

Figure S17. ^{1}H-DOSY spectrum (500 MHz, 25 °C, H_2O) of compounds **1a** (a), **2a** (b) and $\{Na[L^H]\}_n$ (c).

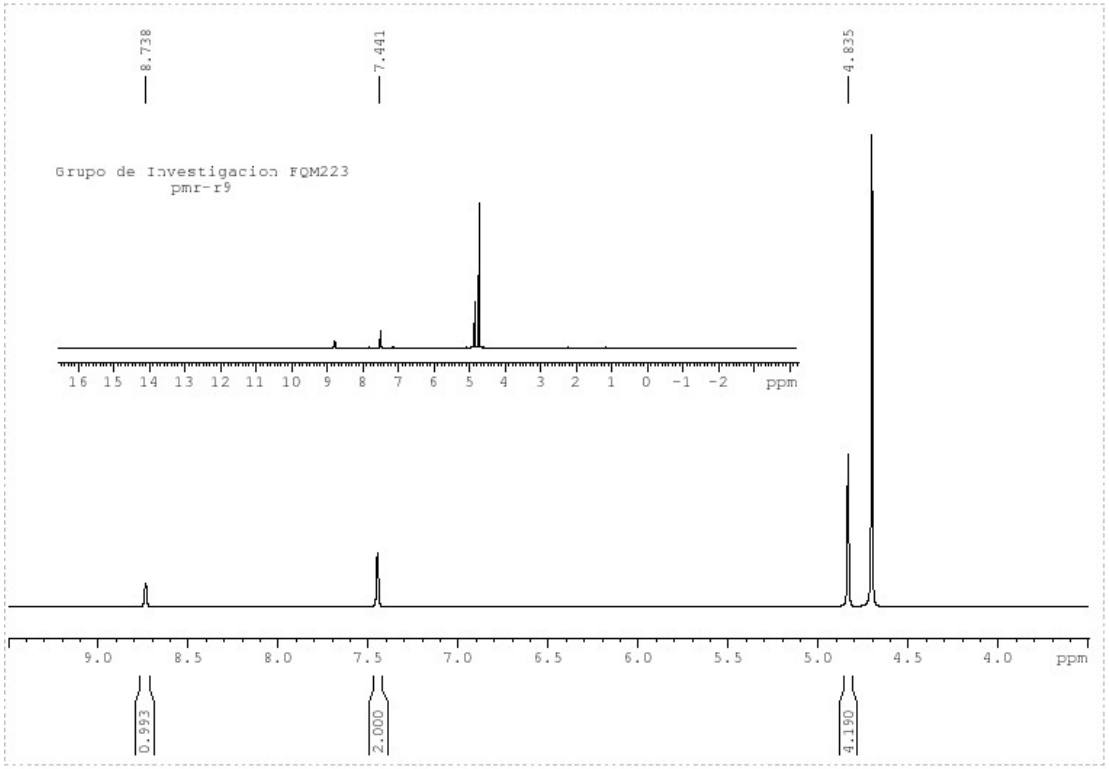
Table S1. Conductivity measurements (μs/cm) of compounds **1** and **2** at 25ºC (10^{-3}M) in mili-Q water.

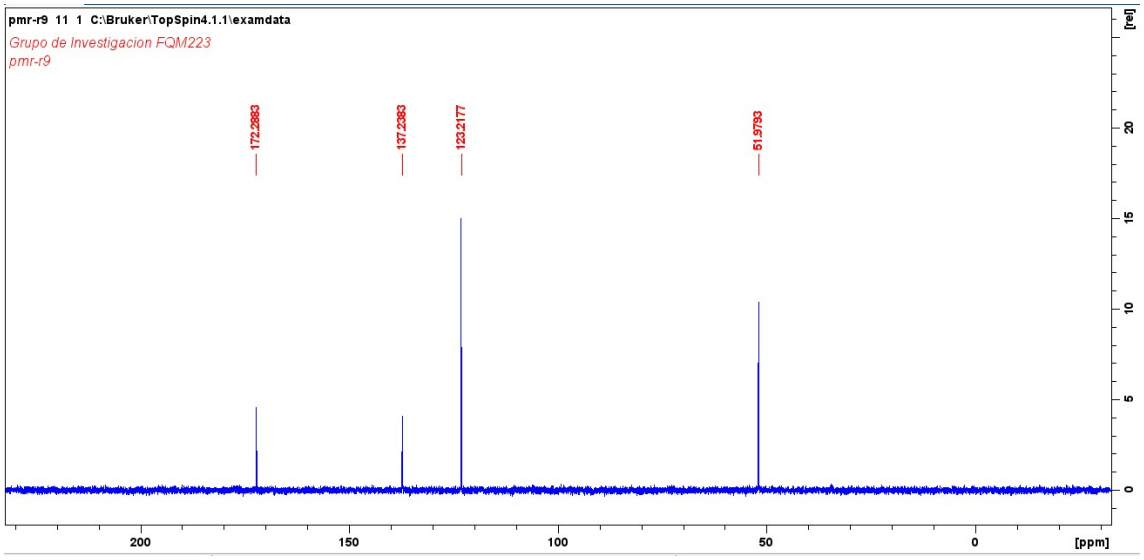
Table S2. Crystal data and structure refinement for compounds **2c**, **2c'** and **2e** from single-crystal X-ray crystallography.

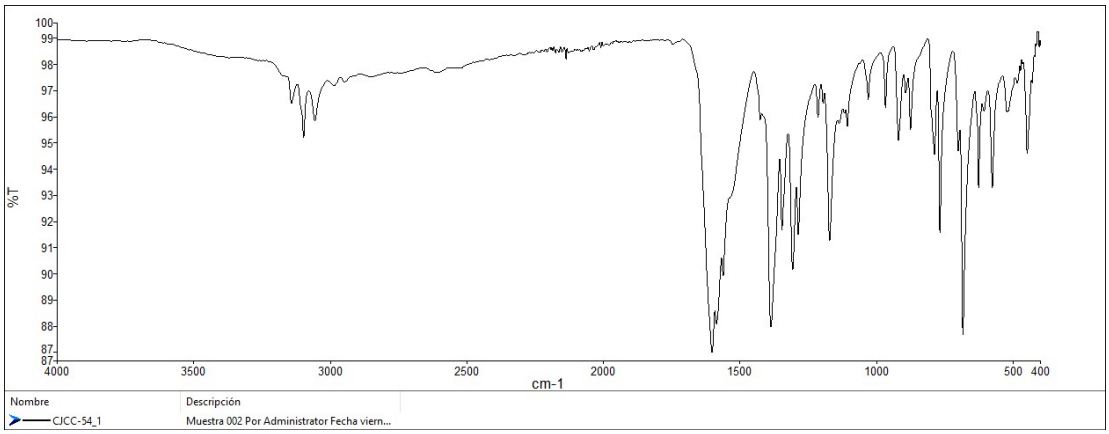
Table S3. Selected bond lengths (Å) and angles (°) for complexes **2c**, **2c'** and **2e**.[a]

Table S4. Coordinates of the optimised compounds of the H-D exchange mechanism.

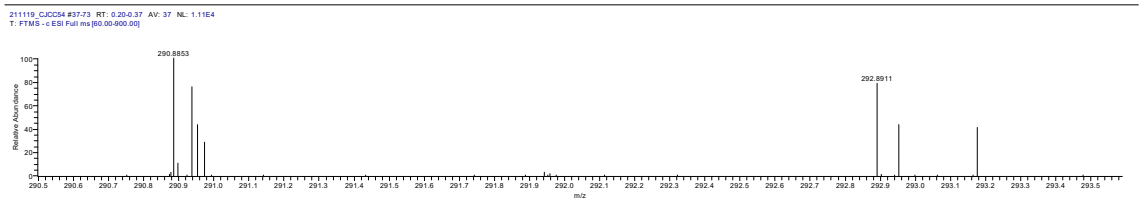
Figure S1. ^{1}H and $^{13}C\{^{1}H\}$ NMR, IR and HR-ESI-MS spectra of complex **2a**.

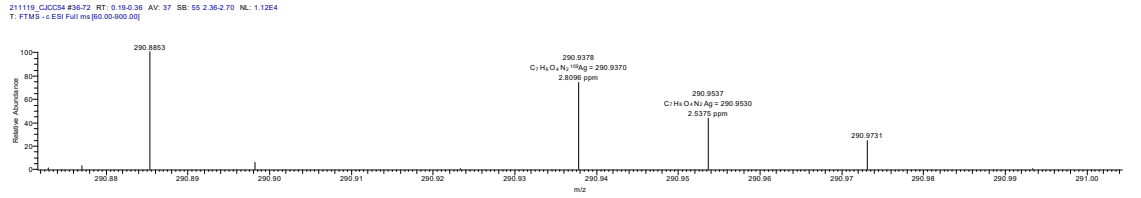






211119_CJCC54 11/19/21 12:20:20 CJCC-54 PM=290 C7H8AgN2O4+





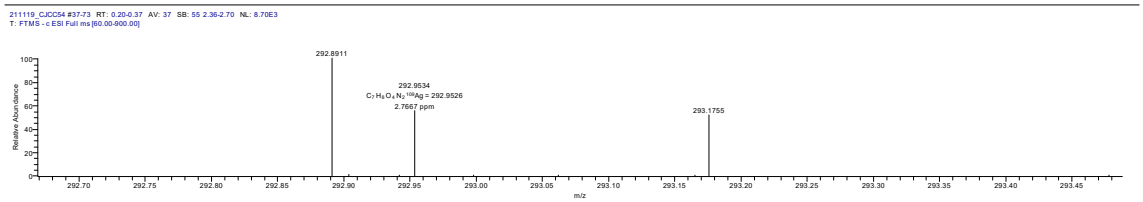
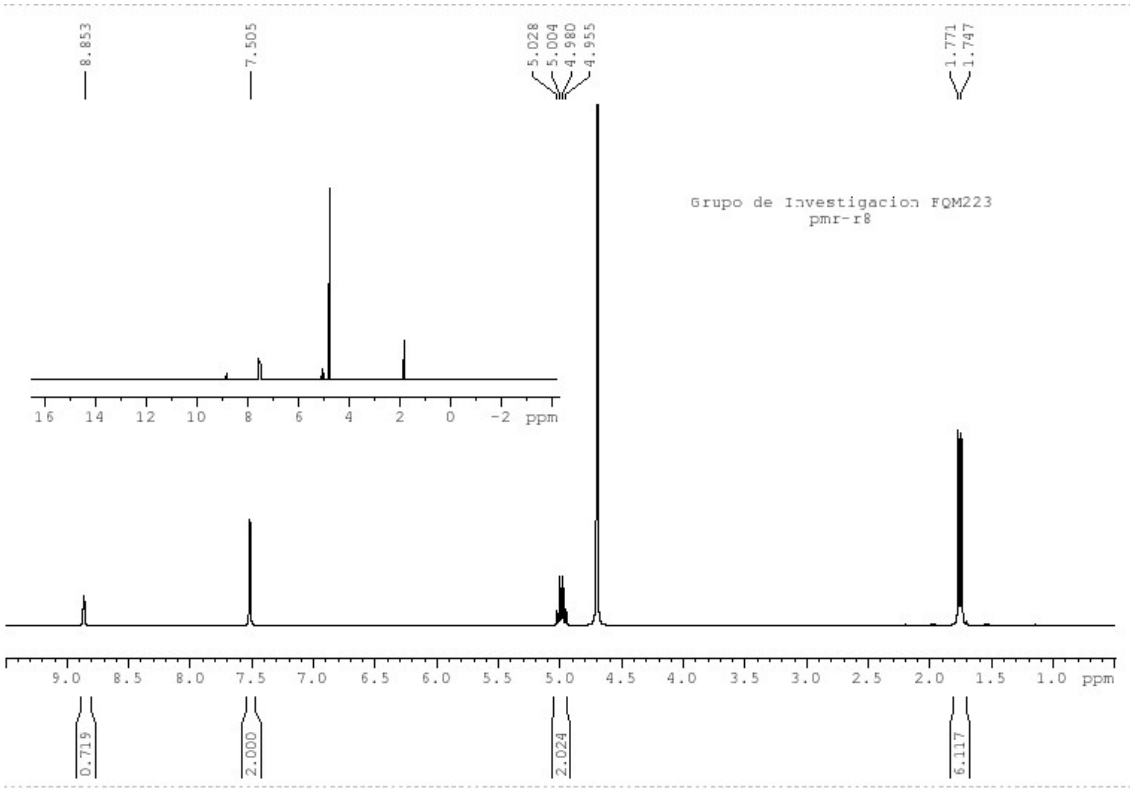
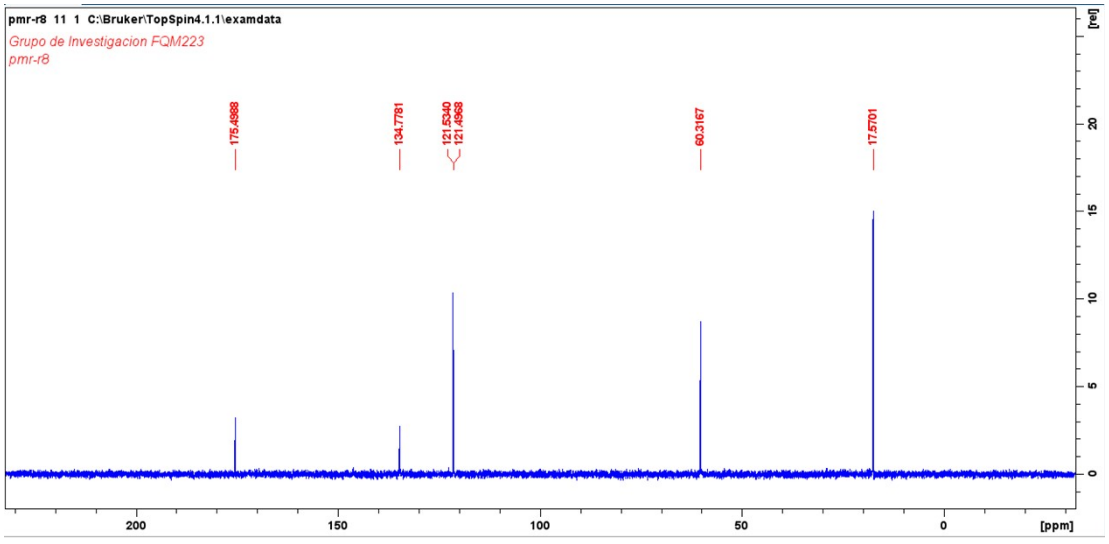
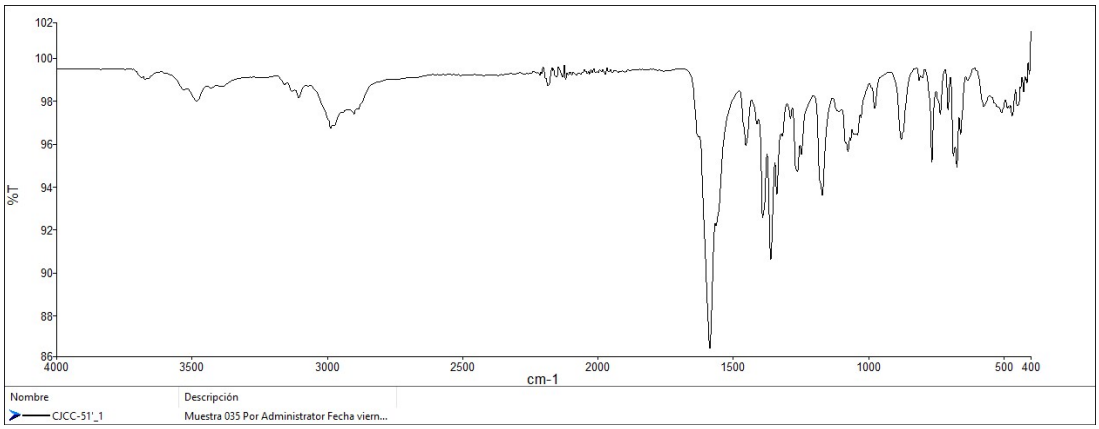


Figure S2. ^{1}H and $^{13}C\{^{1}H\}$ NMR, IR and HR-ESI-MS spectra of complexes **2b** and **2b'**.







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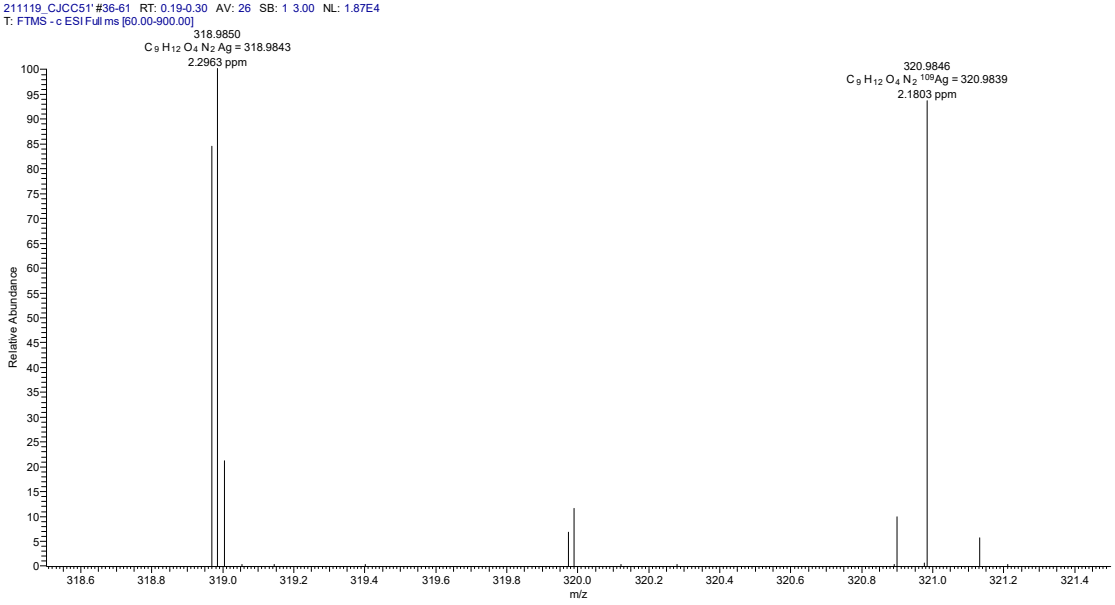
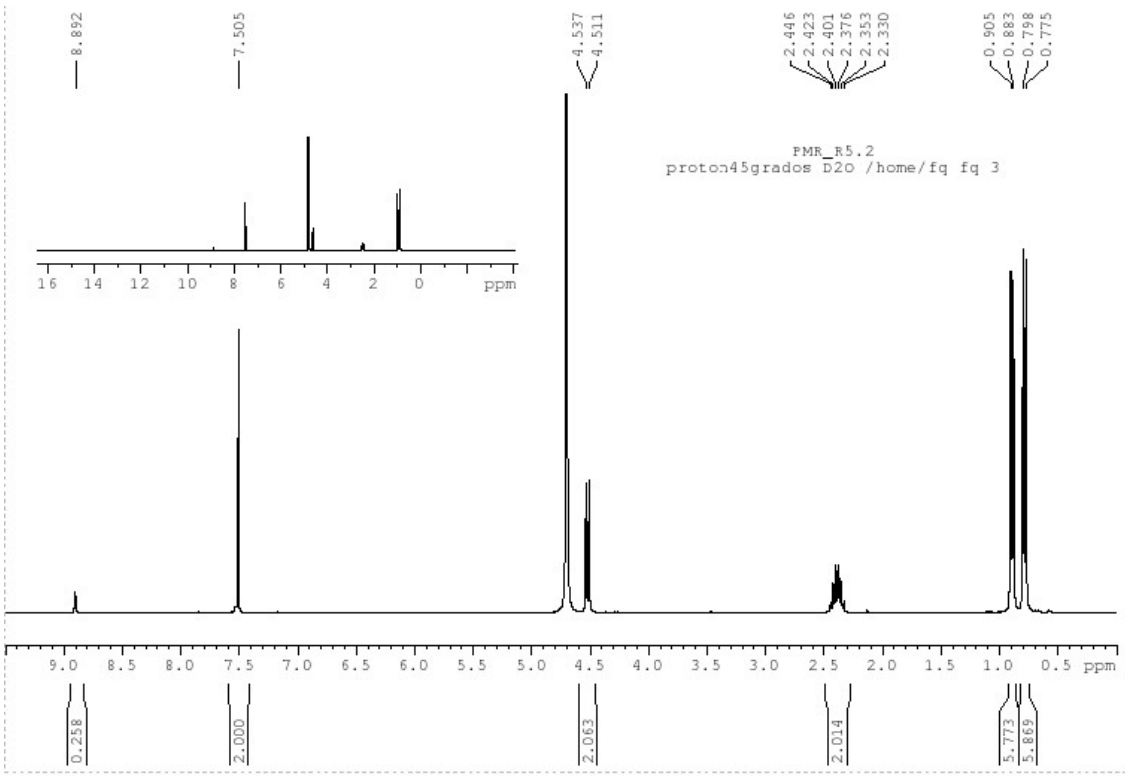
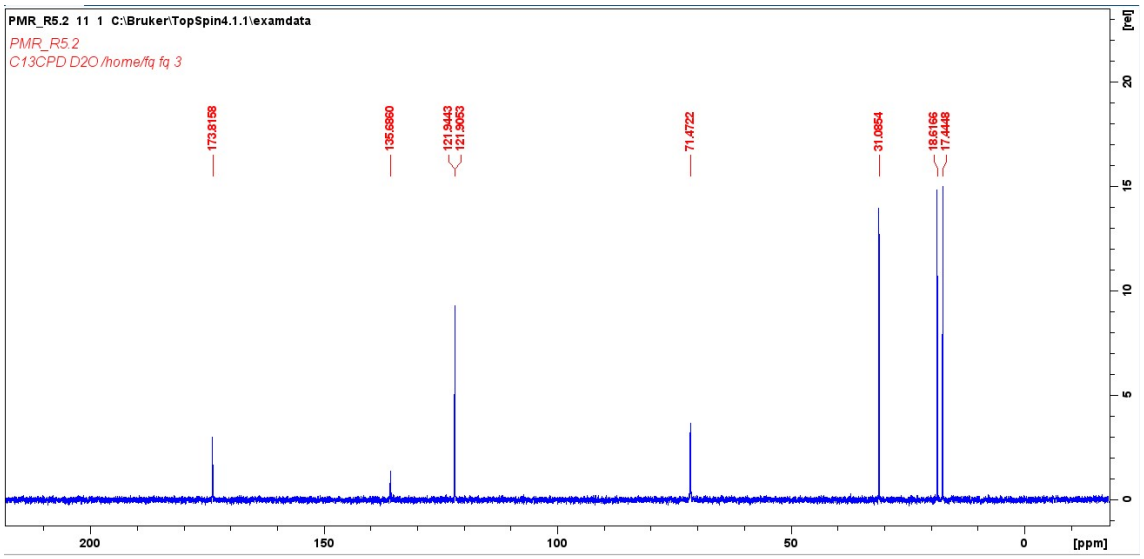
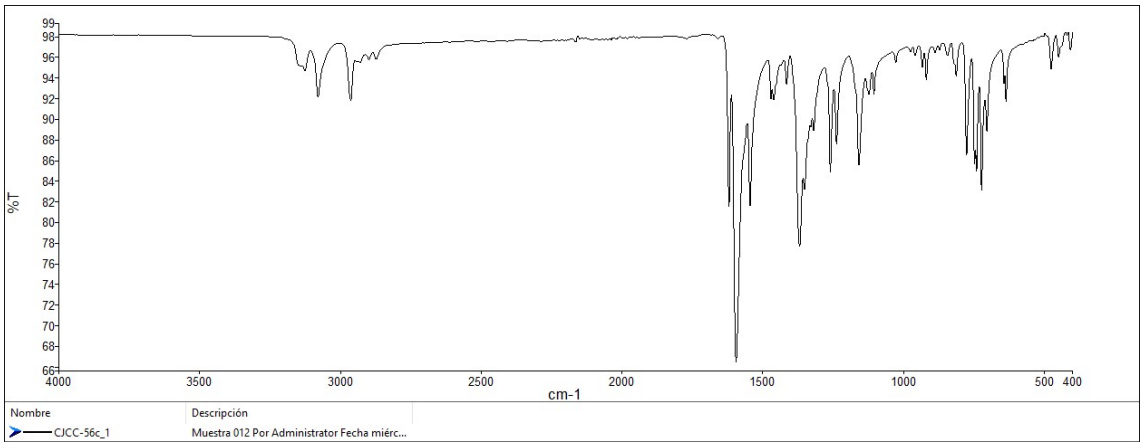


Figure S3. ^{1}H and $^{13}C\{^{1}H\}$ NMR, IR and HR-ESI-MS spectra of complexes **2c** and **2c'**.







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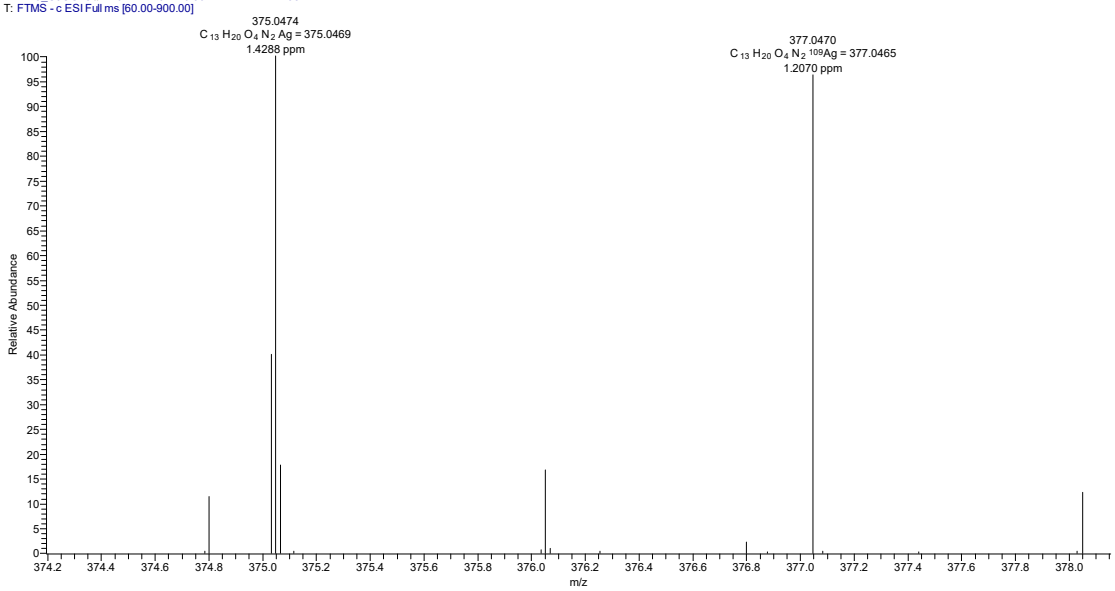
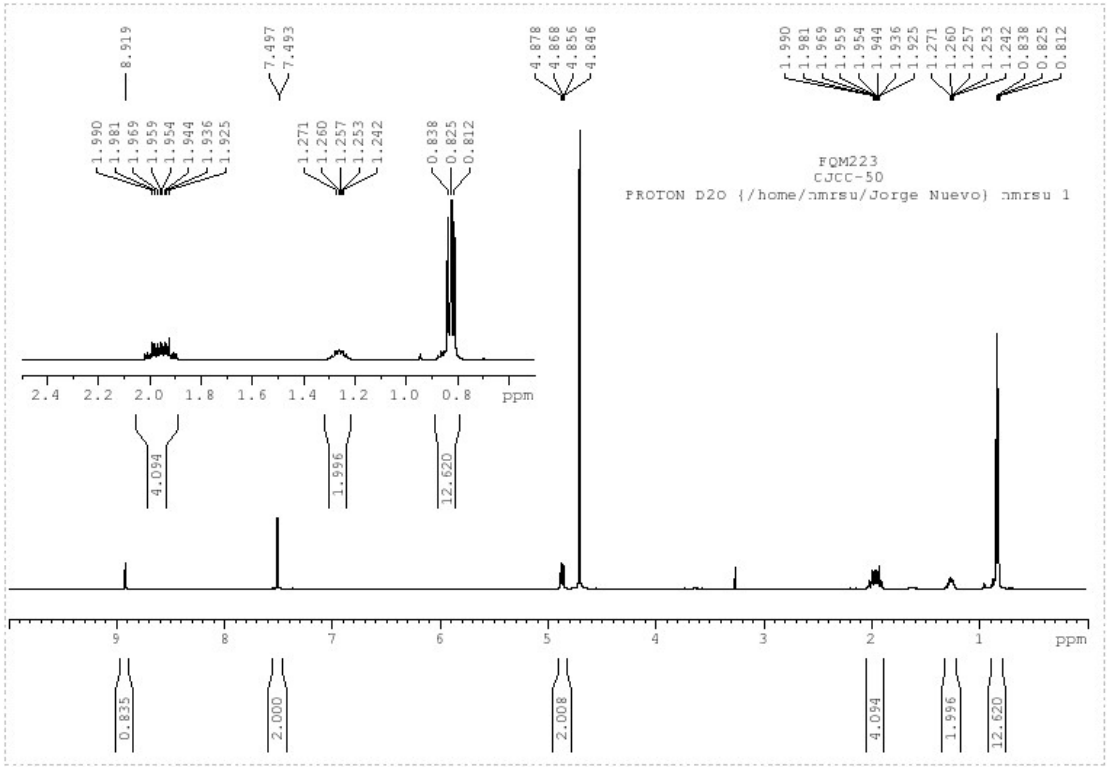
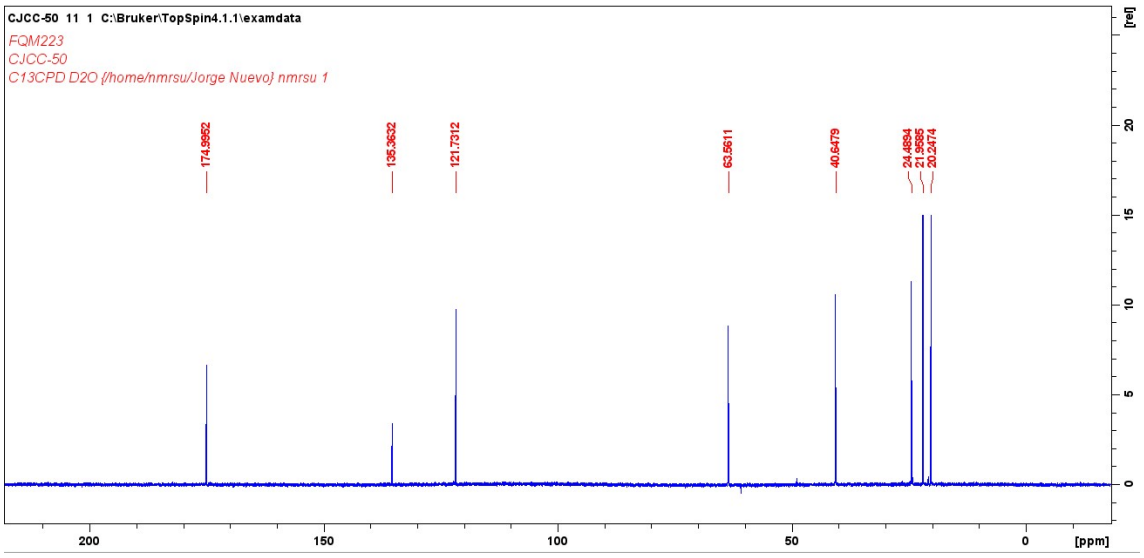
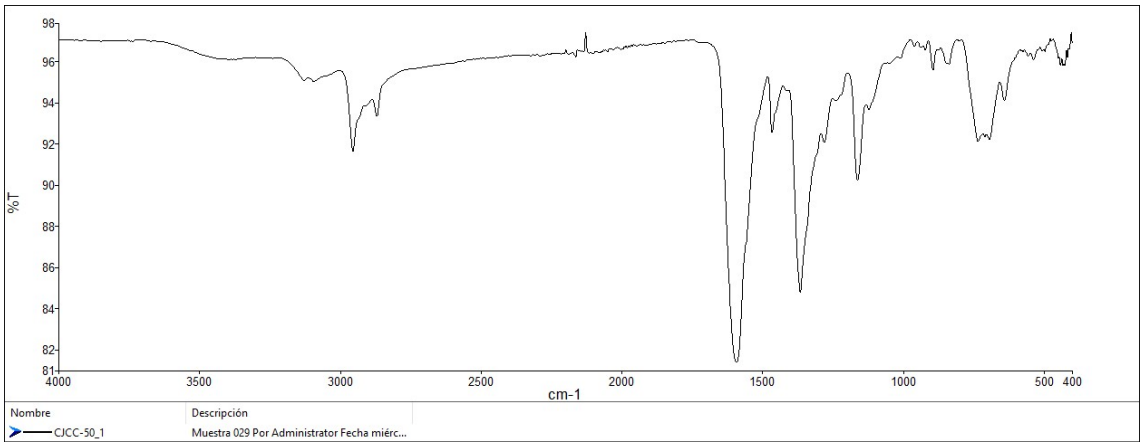


Figure S4. ^{1}H and $^{13}C\{^{1}H\}$ NMR, IR and HR-ESI-MS spectra of complex **2d**.







210928_CJCC50 09/28/21 10:58:30 CJCC-50 PM=403 C15H24AgN2O4

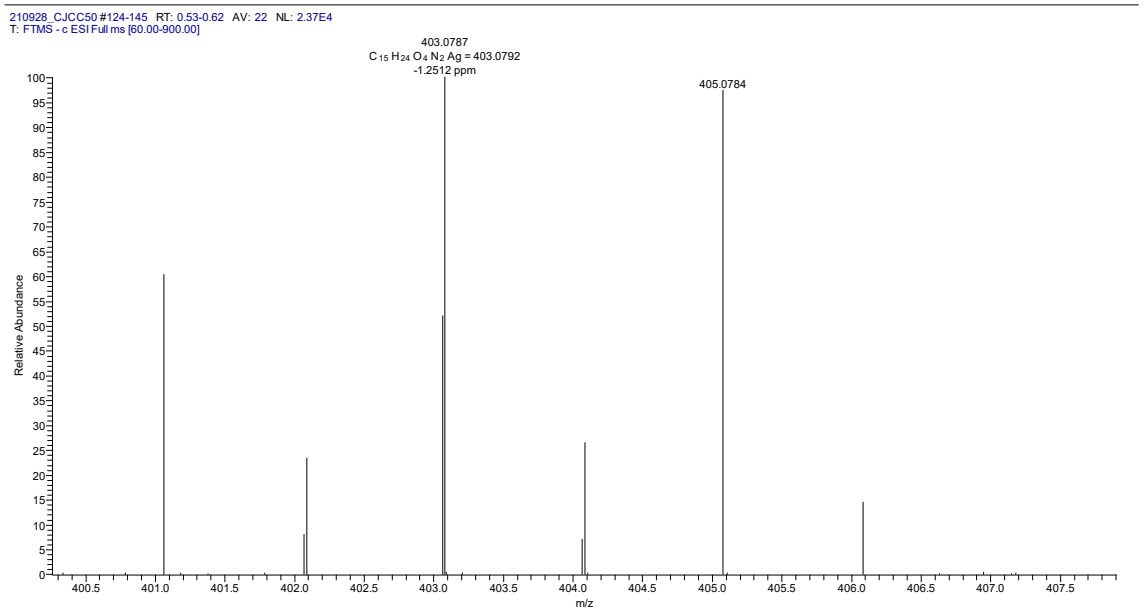
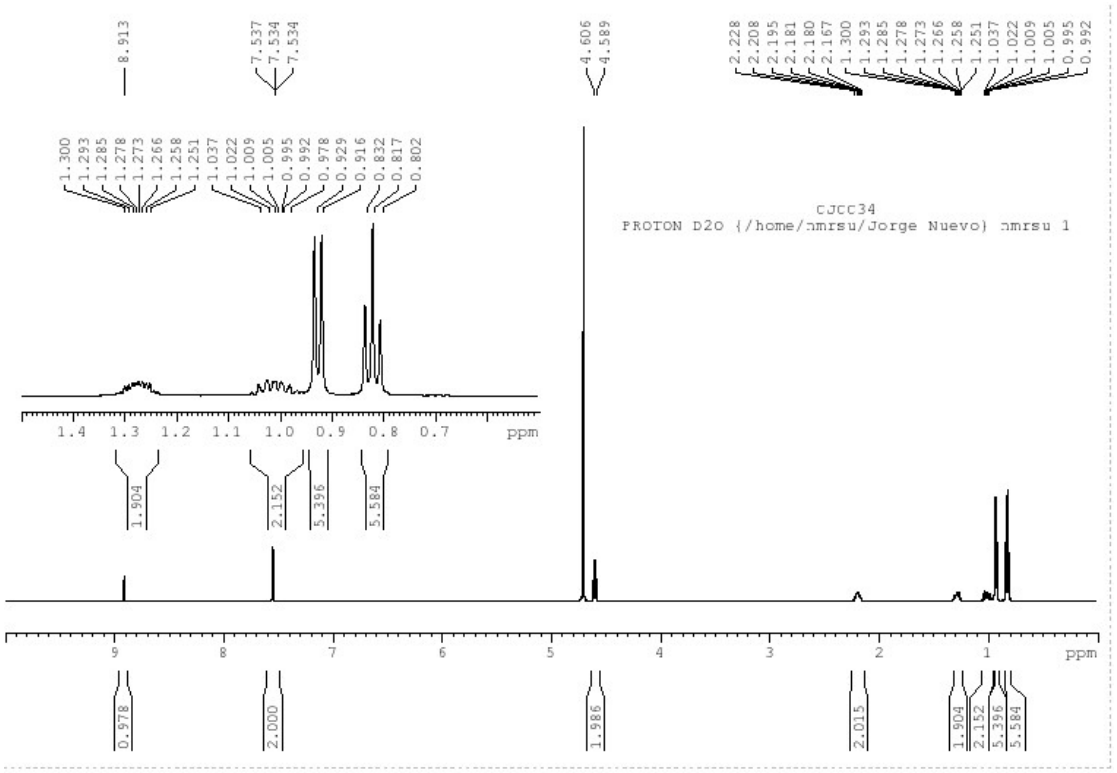
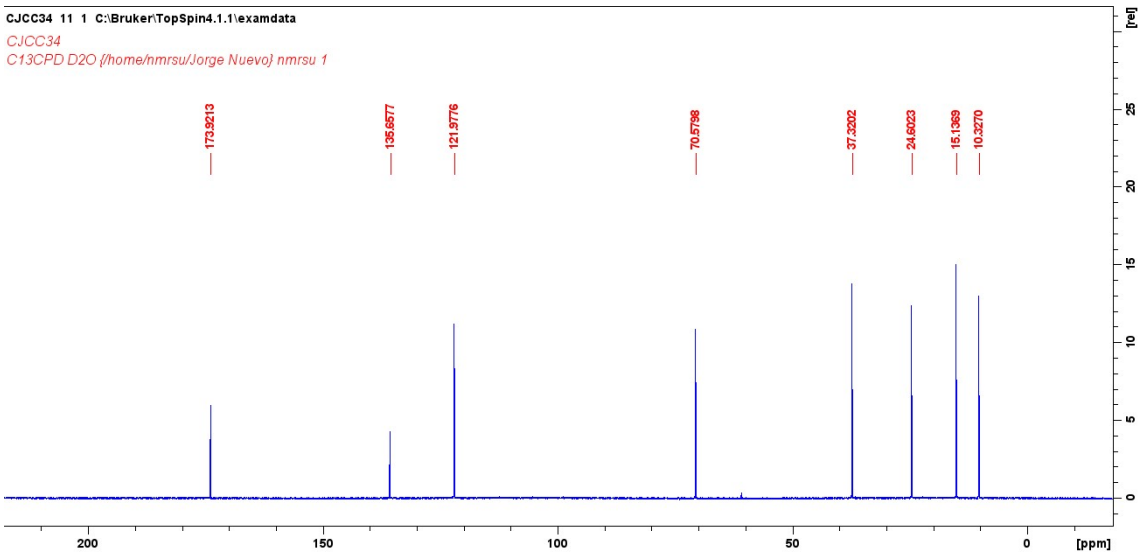
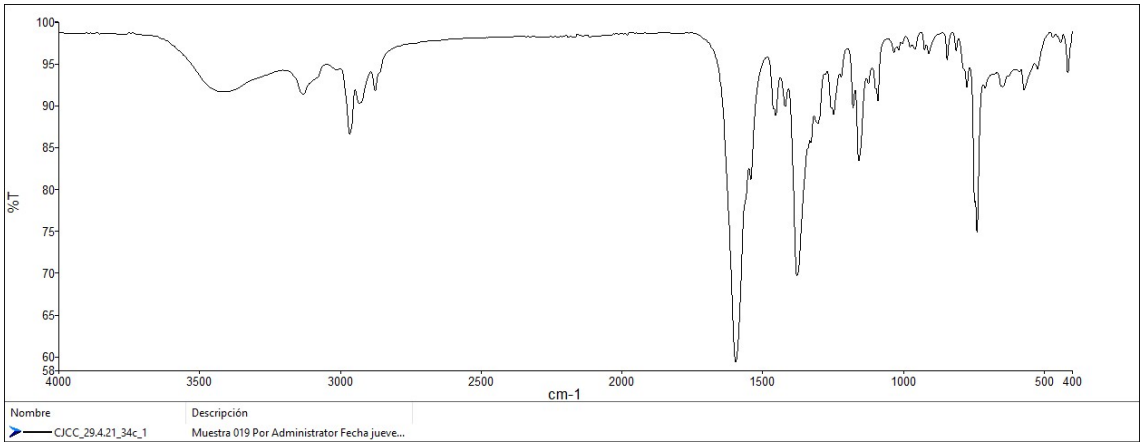


Figure S5. ^{1}H and $^{13}C\{^{1}H\}$ NMR, IR and HR-ESI-MS spectra of complex **2e**.







210517_CJCC-34 05/17/21 12:32:23 CJCC-34 PM=403 C15H23AgN4O8

210517_CJCC-34 #55-79 RT: 0.24-0.34 AV: 25 SB: 48 1.08-1.31 NL: 1.58E5
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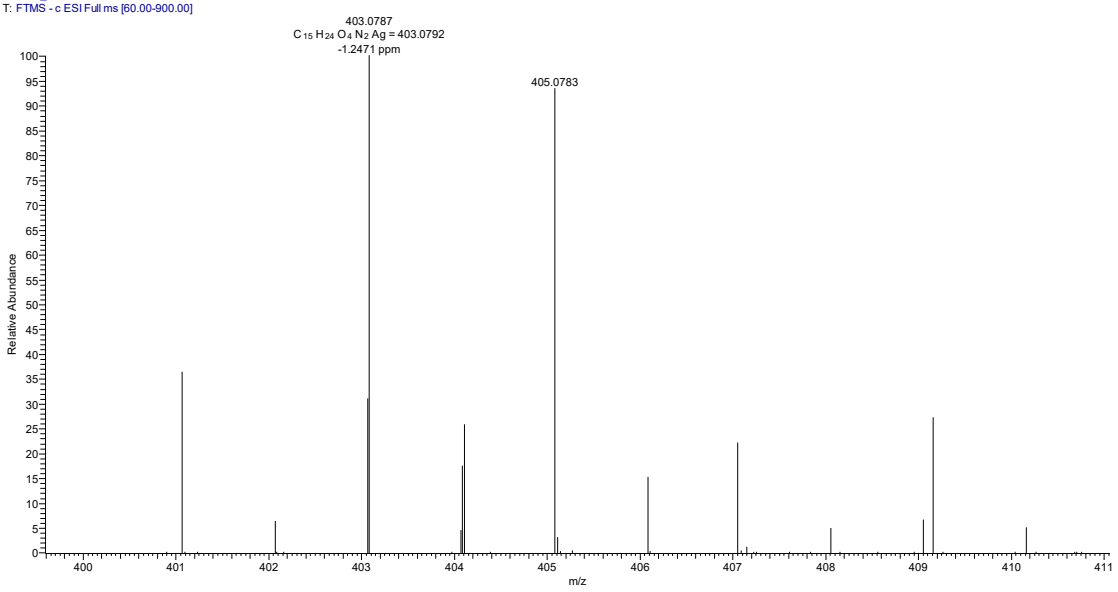
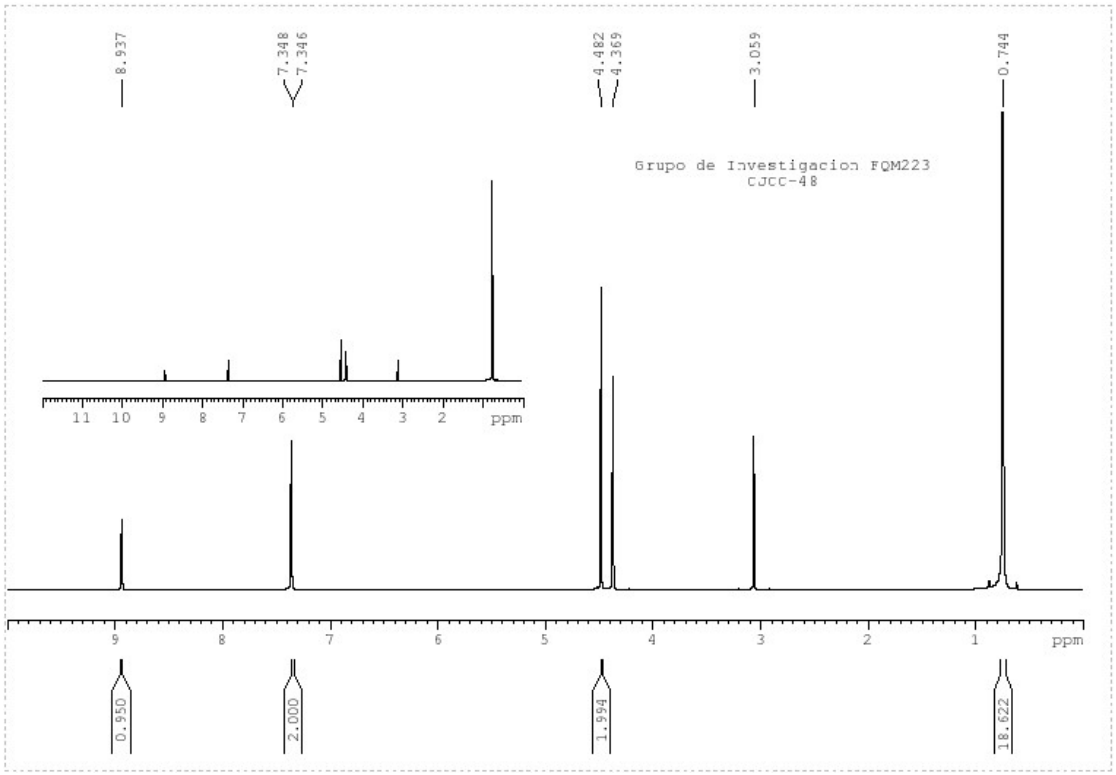
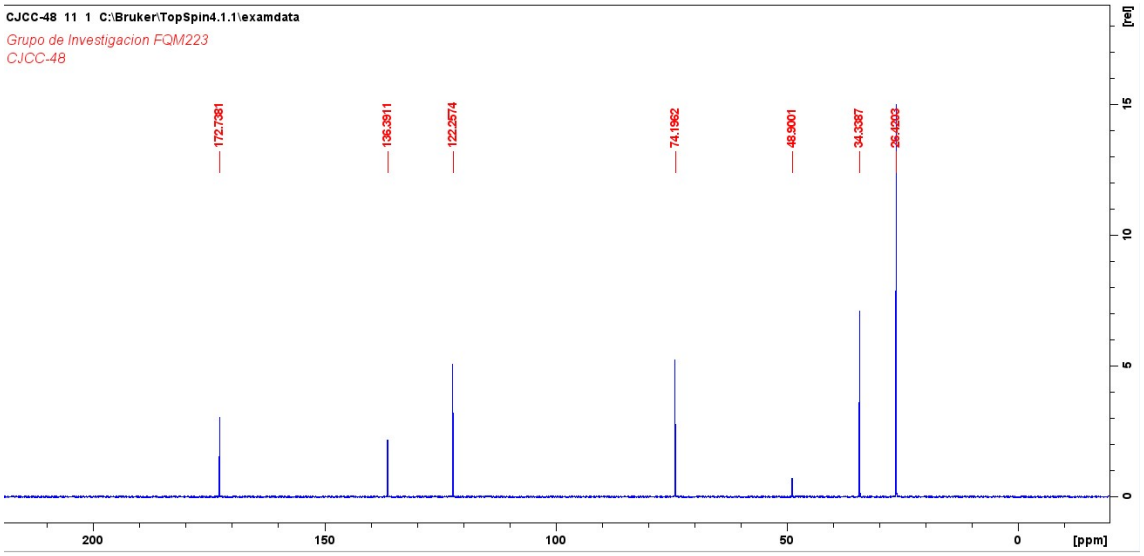
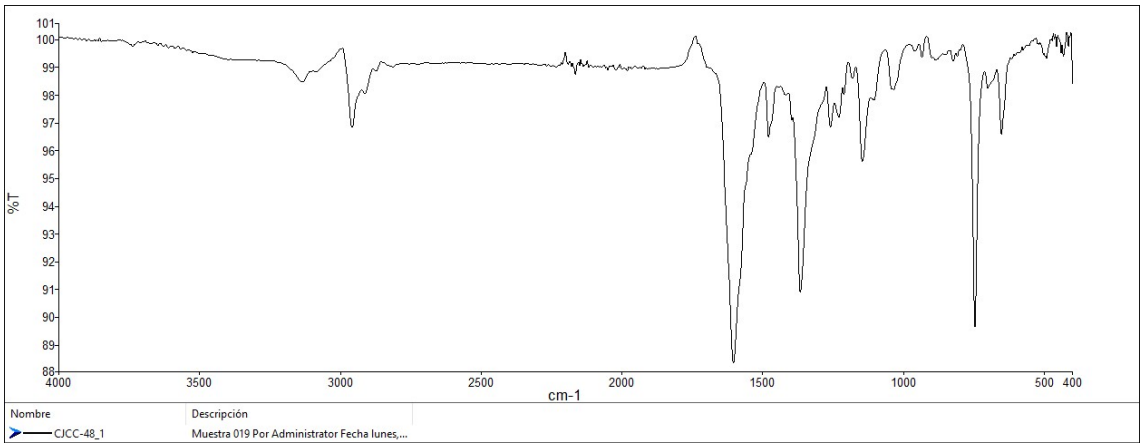


Figure S6. ^{1}H and $^{13}C\{^{1}H\}$ NMR, IR and HR-ESI-MS spectra of complex **2f**.







210527_CJCC48 05/27/21 14:10:18 CJCC-48 PM=403 C15H24AgN2O4

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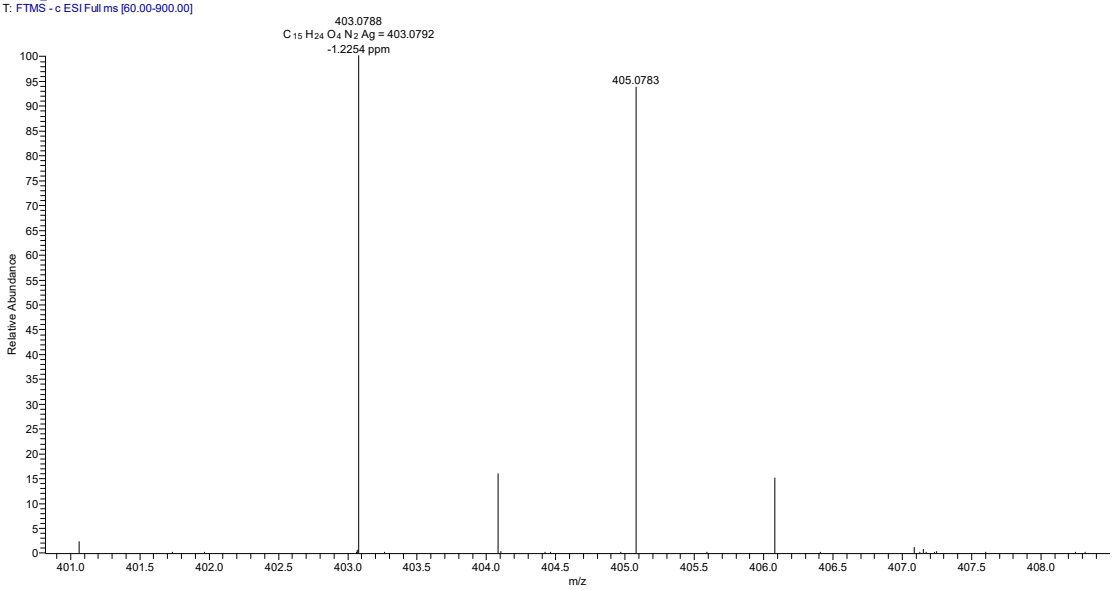
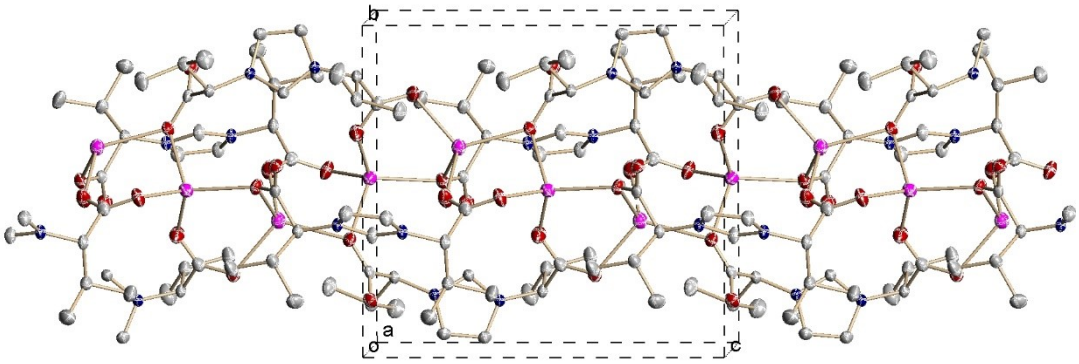
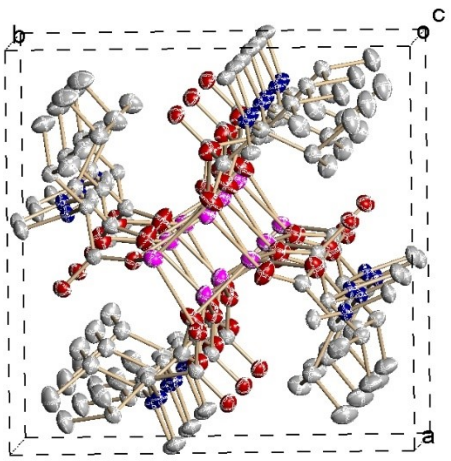


Figure S7. Views of the coordination polymer of $\{Ag[(S,S)\text{-}L^{iPr}]\}_n$ (**2c**): (a), along *a* axis (b) along *c* axis.

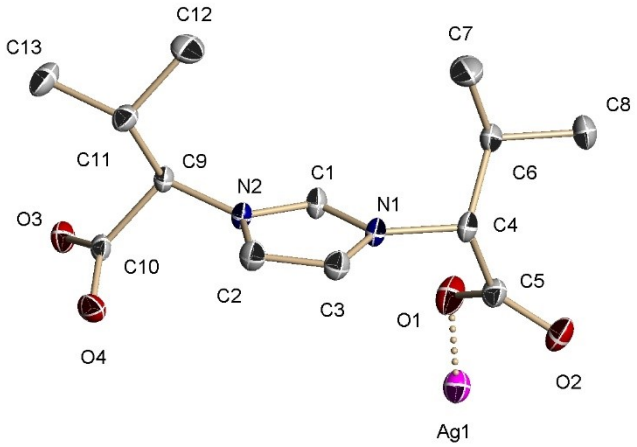


(a)

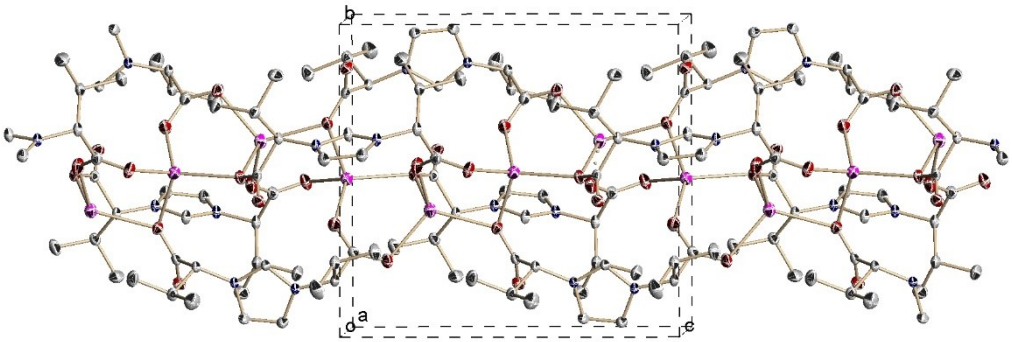


(b)

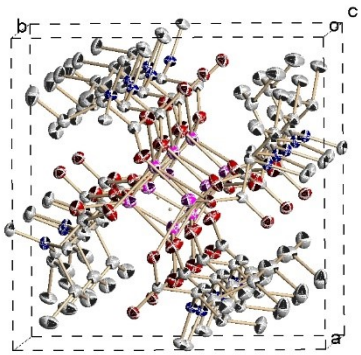
Figure S8. (a) Asymmetric unit of {Ag[(*R*,*R*)-L^{iPr}]}$_n$ (**2c'**) and views of the coordination polymer: (b), along *a* axis (c) along *c* axis.



(a)



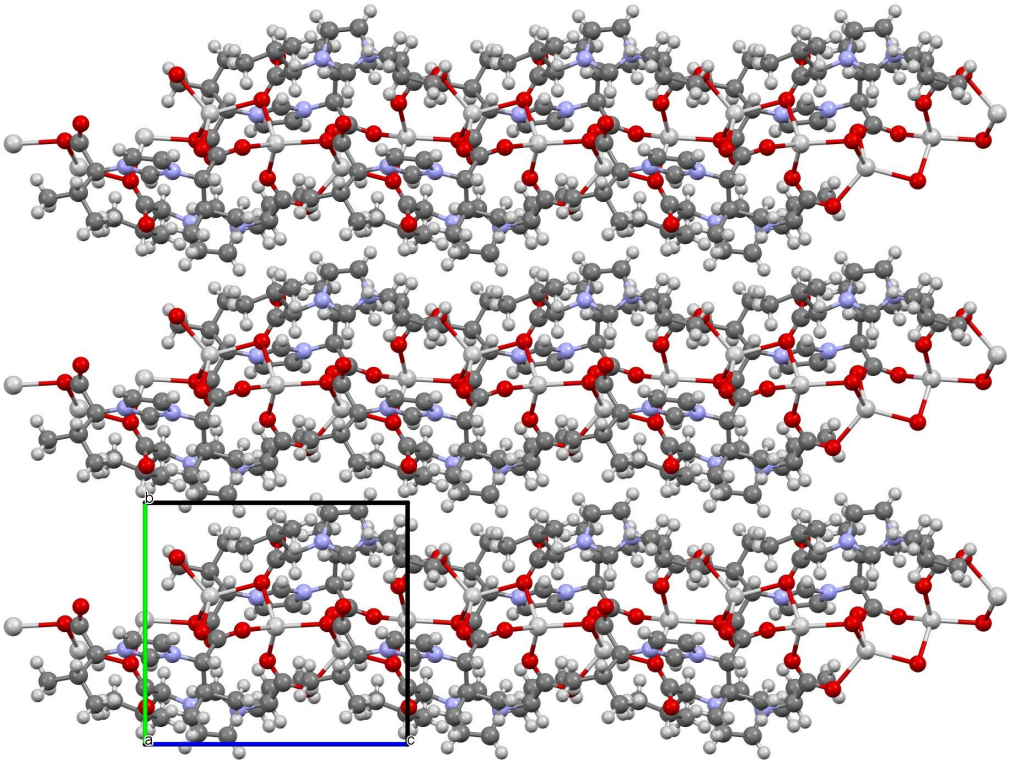
(b)



(c)

Figure S9. View of the 3D architecture of compounds **2c** and **2c'**, with three 1D coordination polymers along *a* axis (three unit cells).

2c



2c'

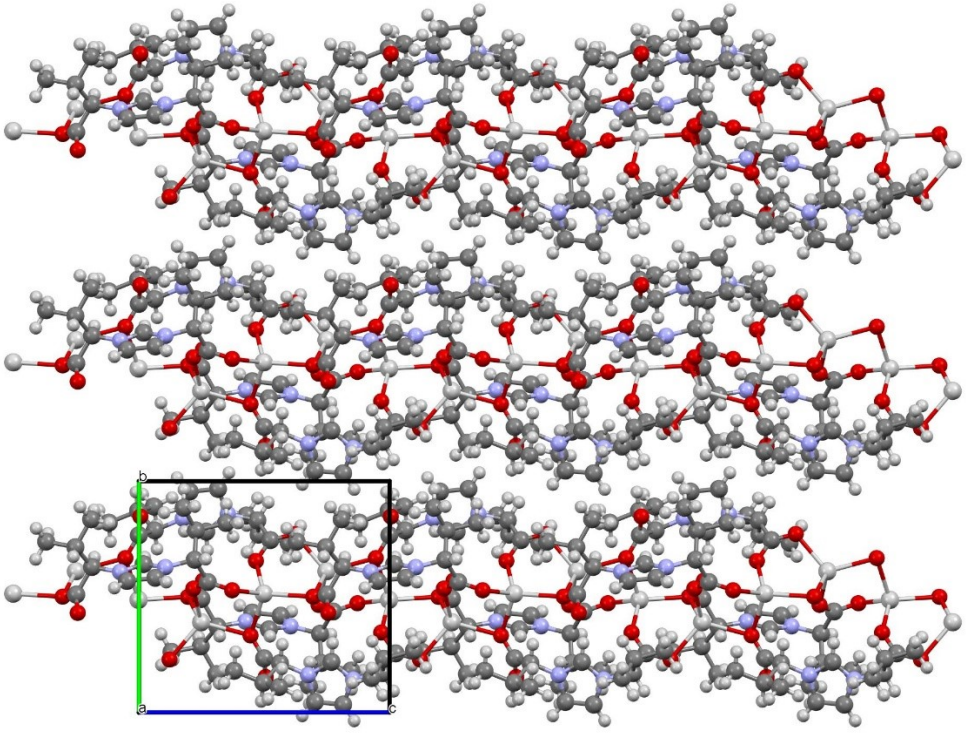


Figure S10. DFT profile of the mechanism for the carbene intermediate formation.

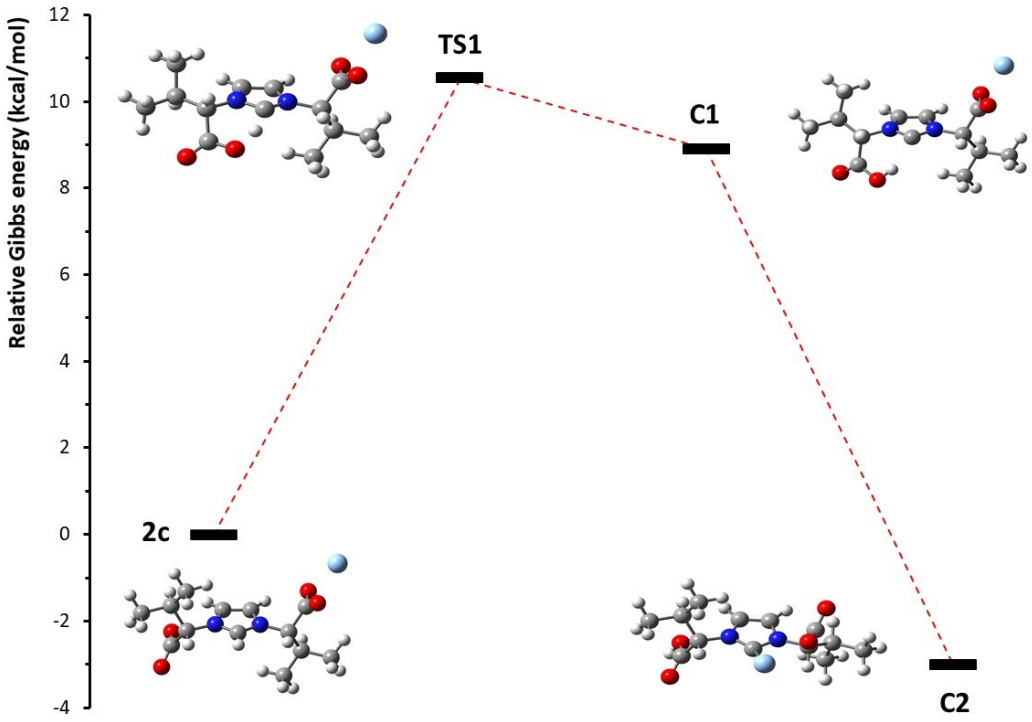


Figure S11. DFT profile of the mechanism for the H-D exchange with D2O mediated by silver(I).

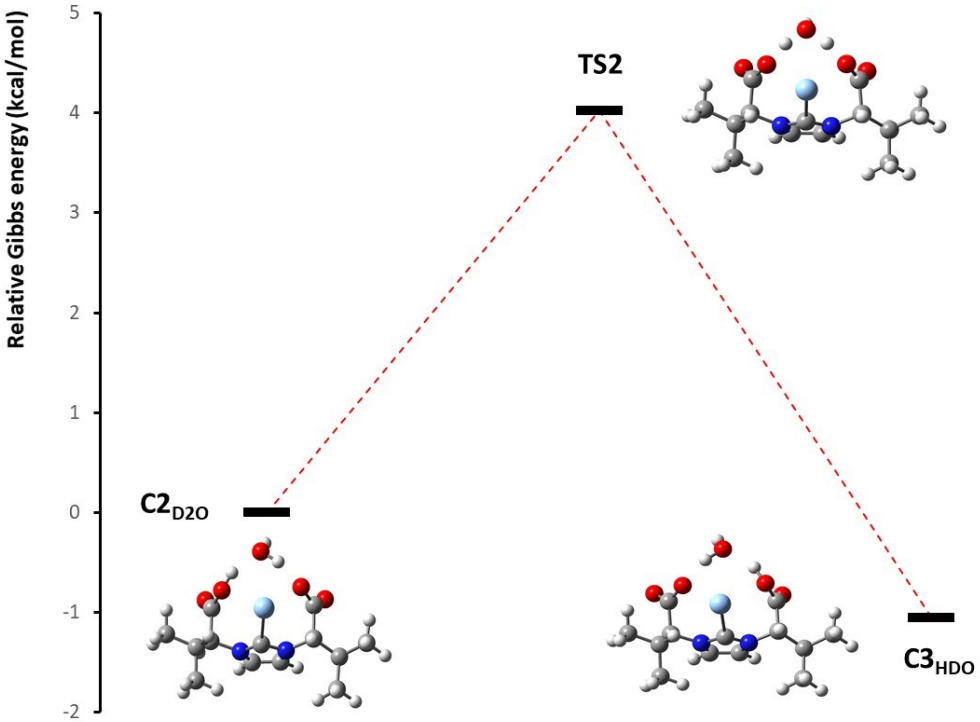


Figure S12. DFT profile of the deuteration mechanism of the C^2-H position.

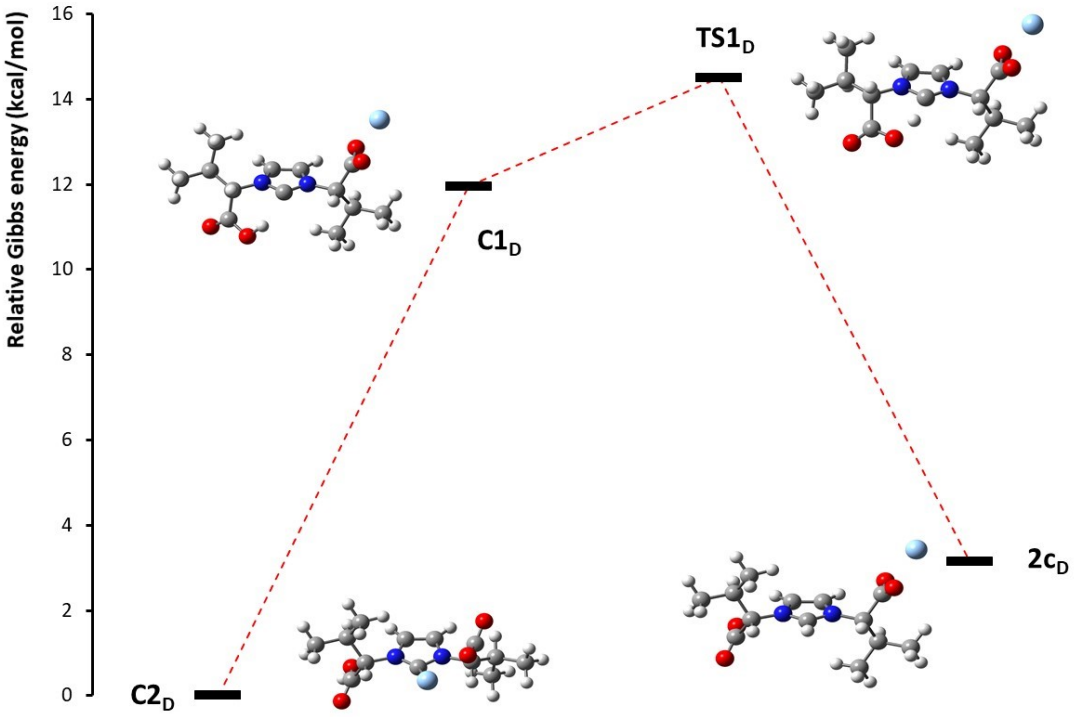


Figure S13. Relative MDA quantification for complex **2c** (control is considered as 100%) for *E. coli* (in blue) and *P. aeruginosa* (in red) assays. Control ranges are 0-0.2 nMol/mg for *E.coli* and 0.1-0.27 nMol/mg for *P. aeruginosa*.

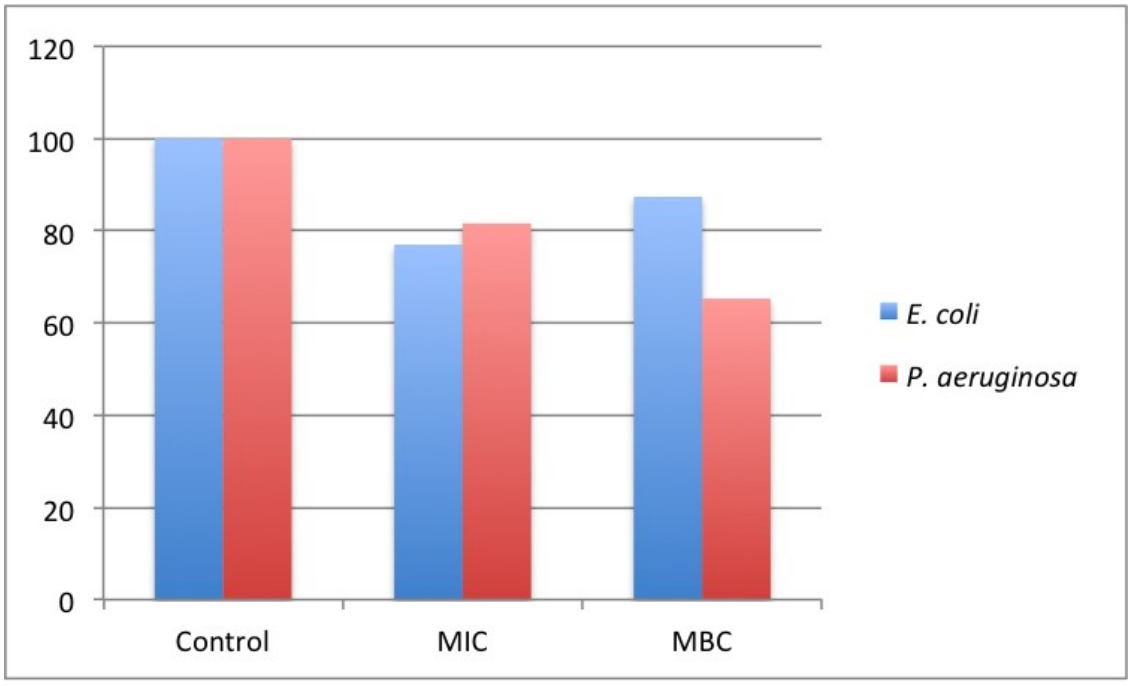


Figure S14. Relative MDA quantification for complex **2c'** (control is considered as 100%) for *E. coli* (in blue) and *P. aeruginosa* (in red) assays. Control ranges are 0-0.2 nMol/mg for *E.coli* and 0.1-0.27 nMol/mg for *P. aeruginosa*.

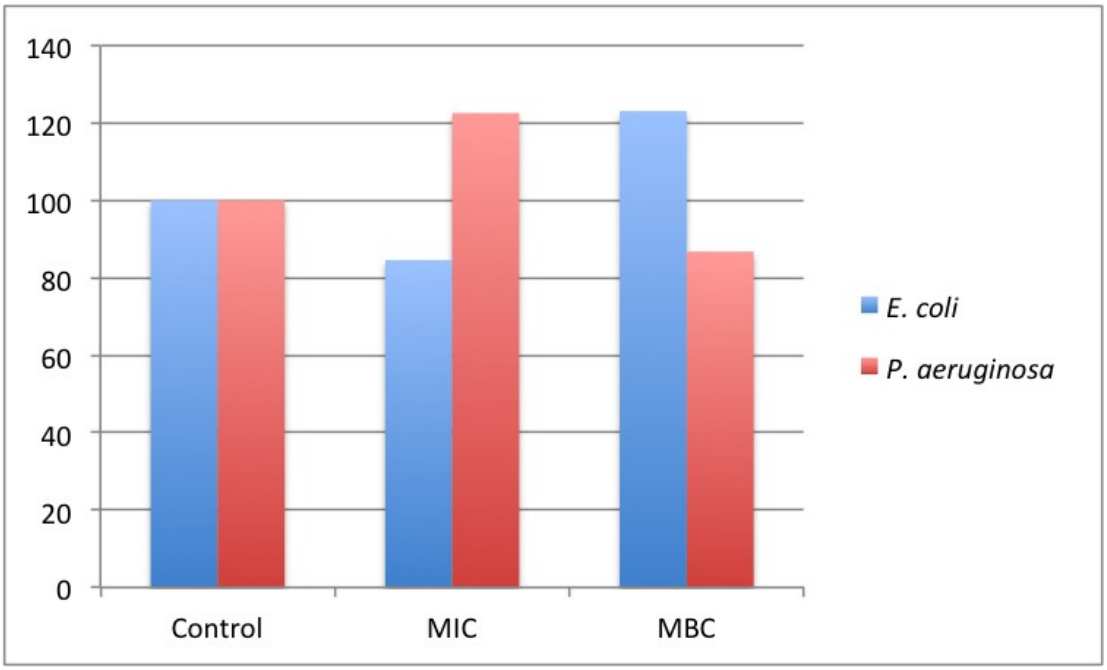


Figure S15. Evaluation of biofilm formation of *E. coli* (top) and *P. aeruginosa* (bottom) exposed to complex **2c** (A: control, B: MIC, C: MBC).

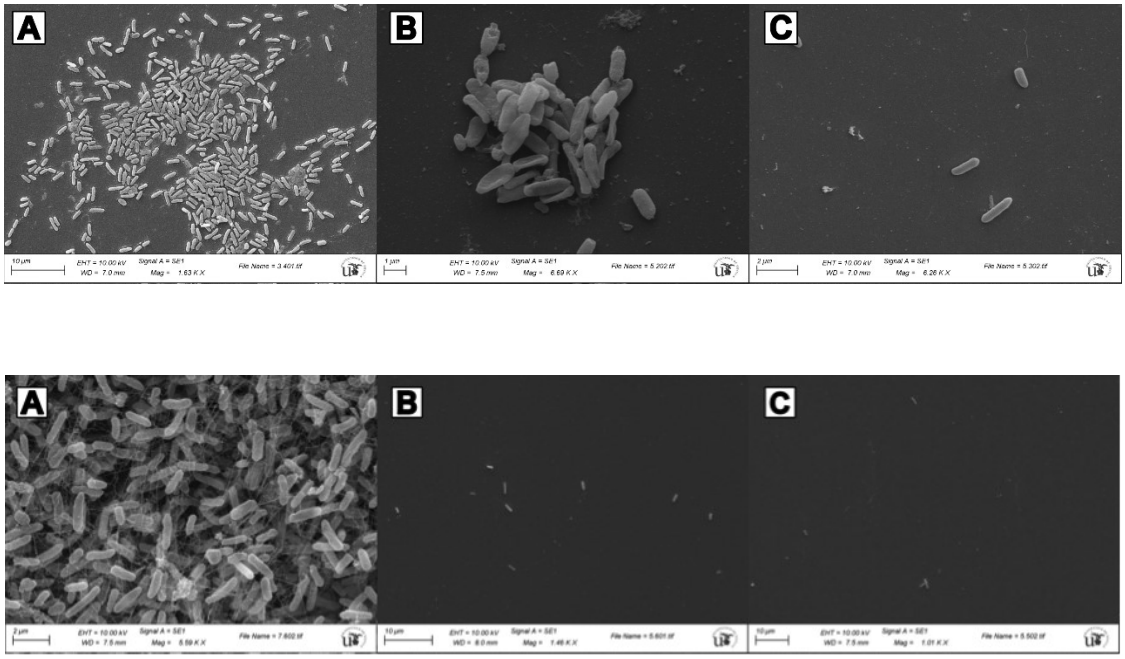
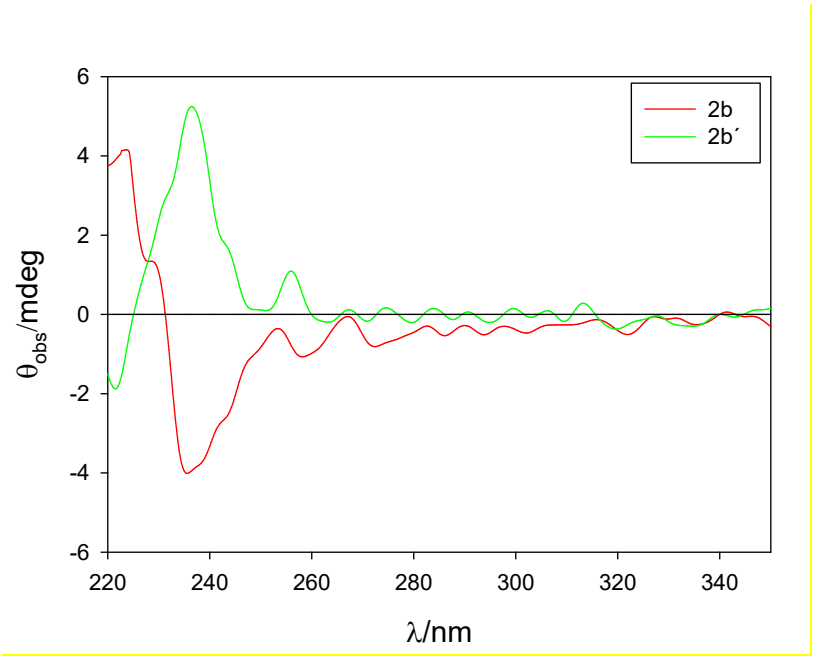


Fig. S16. CD spectra of the enantiomeric pairs **2b-2b'** (a) and **2c-2c'** (b). Electronic circular dichroism (CD) spectra were recorded in a Biologic Mos-450 spectropolarimeter. Spectra were collected under air at a concentration value of 10^{-3} M. Sweeps were taken from 220 to 350 nm. Each spectrum was obtained from an average of 5 runs, using a standard quartz cell of 10 mm path length. The spectra obtained were expressed in terms of ellipticity, Θ_{obs}.

(a)



(b)

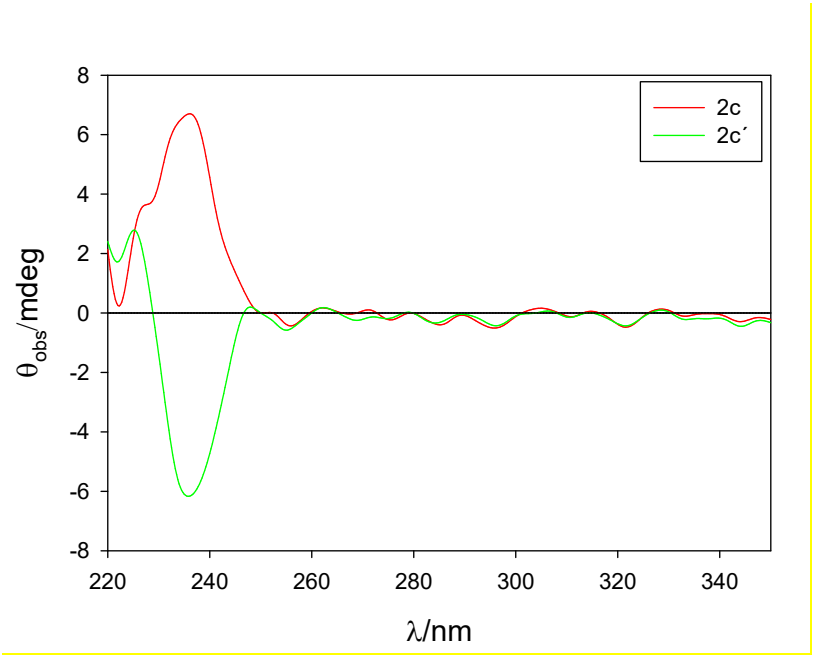
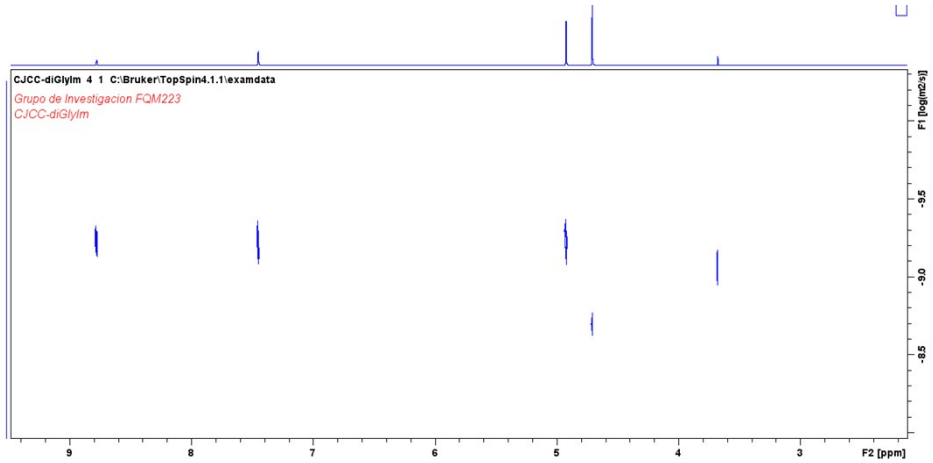
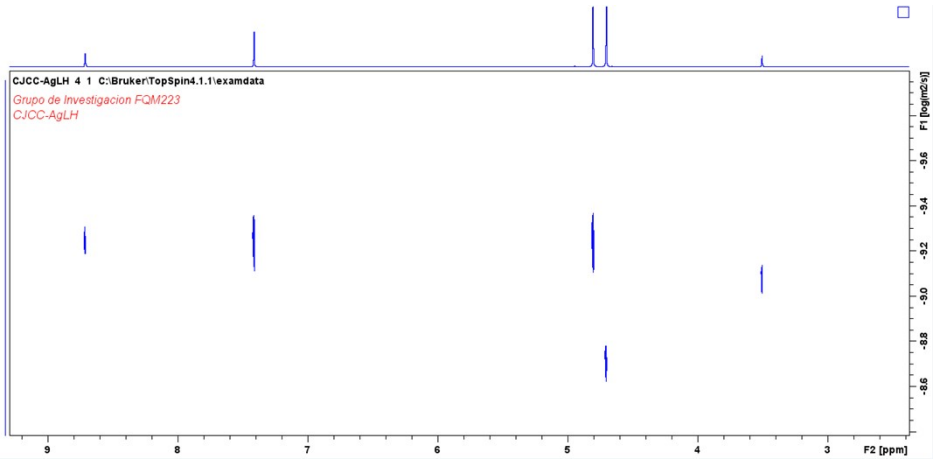


Figure S17. ^{1}H-DOSY spectrum (500 MHz, 25 °C, H_2O) of compounds **1a** (a), **2a** (b) and $\{Na[L^{H}]\}_n$ (c). Pulse program: ledbpgp2s, δ = 0.9 ms, Δ = 120 ms, LED = 5 ms, recycle delay: 5 s, 16 scans, time domain: 38k x 24 points, measurement time: 55 min, apodization: exponential broadening (0.3 Hz), spectrum: 32 k x 64 points.

(a)



(b)



(c)

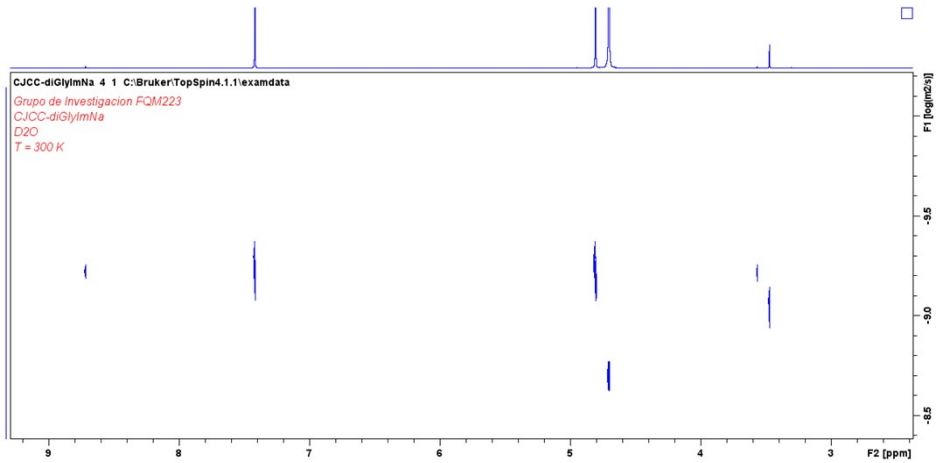


Table S1. Conductivity measurements (μS/cm) of compounds **1** and **2** at 25ºC (10^{-3}M) in mili-Q water.

R Group	HL^R, **1**	$\{Ag[(S,S)\text{-}L^R]\}_n$, **2**
H (**a**)	255	87.1
Me (**b**)	270	72.4
^{i}Pr (**c**)	279	84.0
^{i}Bu (**d**)	257	75.5
^{s}Bu (**e**)	269	60.3
^{t}Bu (**f**)	242	85.6

H_2O mili-Q	0.1
$\{Na[(S,S)\text{-}L^{iPr}]\}_n$	78.9
$AgNO_3$	153.5
NaCl	128.4

Table S2. Crystal data and structure refinement for compounds **2c**, **2c'** and **2e** from single-crystal X-ray crystallography.

Compound	**2c**	**2c'**	**2e**
Formula	$C_{13}H_{19}AgN_2O_4$	$C_{13}H_{19}AgN_2O_4$	$C_{15}H_{27}AgN_2O_6$
M	375.17	375.17	439.25
T [K]	193(2)	193(2)	193(2)
Wavelength [Å]	0.71073	0.71073	0.71073
Crystal system	Tetragonal	Tetragonal	Monoclinic
Space group	$P4_1$	$P4_3$	C_2
a [Å]	10.9520(4)	10.9697(5)	27.9770(19)
b [Å]	10.9520(4)	10.9697(5)	8.3951(6)
c [Å]	11.9218(5)	11.8981(7)	7.9560(5)
α = γ [°]	90	90	90
β [°]	90	90	92.298(2)
V [Å^3]	1429.98(12)	1431.75(16)	1867.1(2)
Z	4	4	4
$D_{calcd.}$ [Mg·m^{-3}]	1.743	1.740	1.434
μ [mm^{-1}]	1.424	1.422	1.110
F(000)	760	760	904
Crystal size [mm^3]	0.400 x 0.400 x 0.200	0.500 x 0.450 x 0.400	0.400 x 0.200 x 0.100
θ range for data collection [º]	2.525 to 30.512	2.525 to 30.527	2.562 to 30.528°
Index ranges	-15≤h≤15, -15≤k≤15, -16≤l≤17	-15≤h≤15, -15≤k≤15, -16≤l≤17	-39≤h≤39, -11≤k≤12, -11≤l≤11
Reflections collected	79993	23660	20315
Independent reflections	4288 [R(int) = 0.0267]	3329 [R(int) = 0.0288]	5555 [R(int) = 0.0364]
Completeness to theta	= 25.242° 99.9 %	= 25.242° 90.7 %	= 25.242° 96.6 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.6494	0.7461 and 0.6489	0.7461 and 0.5425
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	4288 / 1 / 186	3329 / 1 / 185	5555 / 25 / 233
Goodness-of-fit on F^2	1.090	1.039	1.157
Final R indices [I>2σ(I)]	R1 = 0.0140, wR2 = 0.0339	R1 = 0.0183, wR2 = 0.0509	R1 = 0.0334, wR2 = 0.0772
R indices (all data)	R1 = 0.0147, wR2 = 0.0347	R1 = 0.0185, wR2 = 0.0510	R1 = 0.0337, wR2 = 0.0774
Absolute structure parameter	-0.022(4)	-0.005(8)	0.018(7)
Extinction coefficient	0.0367(11)	n/a	n/a
Largest diff. peak and hole [e·Å^{-3}]	0.351 and -0.41	0.655 and -0.616	1.421 and -1.167

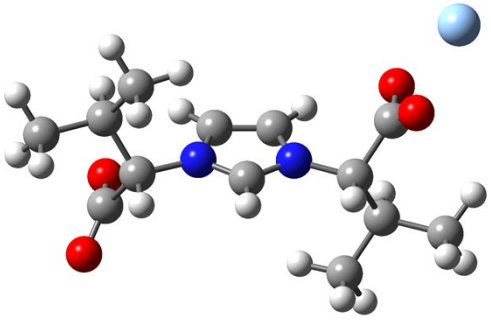
Table S3. Selected bond lengths (Å) and angles (°) for complexes **2c**, **2c'** and **2e**.[a]

Complex	2c	2c'	2e
O-$C_{(carboxy.)}$	O(1)-C(5) 1.244(2)	O(1)-C(5) 1.244(2)	O(1)-C(1) 1.243(4)
	O(2)-C(5) 1.252(2)	O(2)-C(5) 1.256(2)	O(2)-C(1) 1.257(4)
	O(3)-C(10) 1.240(2)	O(3)-C(10) 1.264(3)	O(3)-C(7) 1.240(4)
	O(4)-C(10) 1.265(2)	O(4)-C(10) 1.244(3)	O(4)-C(7) 1.258(4)
Ag-O	Ag(1)-O(1) 2.262(2)	Ag(1)-O(1) 2.256(2)	Ag(1)-O(2) 2.230(3)
	Ag(1)-O(2)#1 2.330(2)	Ag(1)-O(2)#1 2.327(2)	Ag(1)-O(4)#1 2.310(2)
	Ag(1)-O(4)#2 2.402(1)	Ag(1)-O(3)#2 2.401(2)	
	Ag(1)-O(4)#3 2.434(1)	Ag(1)-O(3)#3 2.432(2)	
Ag···Ag	Ag(1)···Ag(1)# 3.447(1)	Ag(1)···Ag(1)# 3.436(1)	Ag(1)···Ag(1) 3.958 [b]
			Ag(1)···Ag(1) 4.045 [b]
O-C-O	O(1)-C(5)-O(2) 128.8(2)	O(1)-C(5)-O(2) 127.9(3)	O(1)-C(1)-O(2) 126.9(3)
	O(3)-C(10)-O(4) 126.1(2)	O(3)-C(10)-O(4) 126.1(2)	O(3)-C(7)-O(4) 125.2(3)
O-Ag-O	O(1)-Ag(1)-O(2)#1 112.59(6)	O(1)-Ag(1)-O(2)#1 112.49(8)	O(2)-Ag(1)-O(4)#1 170.04(10)
	O(1)-Ag(1)-O(4)#2 99.57(6)	O(1)-Ag(1)-O(3)#2 99.82(8)	
	O(2)#1-Ag(1)-O(4)#2 105.56(6)	O(2)#1-Ag(1)-O(3)#2 105.61(8)	
	O(1)-Ag(1)-O(4)#3 112.16(5)	O(1)-Ag(1)-O(3)#3 112.46(7)	
	O(2)#1-Ag(1)-O(4)#3 115.85(5)	O(2)#1-Ag(1)-O(3)#3 115.50(6)	
	O(4)#2-Ag(1)-O(4)#3 109.57(4)	O(3)#2-Ag(1)-O(3)#3 109.50(6)	
Ag···Ag···Ag	Ag(1)#4-Ag(1)-Ag(1)#1 138.4(1)	Ag(1)#1-Ag(1)-Ag(1)#4 138.5(1)	Ag(1)-Ag(1)-Ag(1) 167.5 [b]

[a] Symmetry transformations used to generate equivalent atoms: **2c**: #1 y,-x+1,z-1/4; #2 -x+1,-y+1,z+1/2; #3 y,-x+1,z+3/4; #4 -y+1,x,z+1/4; #5 -x+1,-y+1,z-1/2; #6 -y+1,x,z-3/4. **2c'**: #1 -y+1,x,z-1/4; #2 -x+1,-y+1,z+1/2; #3 -y+1,x,z+3/4; #4 y,-x+1,z+1/4; #5 -x+1,-y+1,z-1/2; #6 y,-x+1,z-3/4. **2e**: #1 -x+1, y+1, -z+1; #2 -x+1, y-1, -z+1. [b] measurement performed across the unit cell boundary.

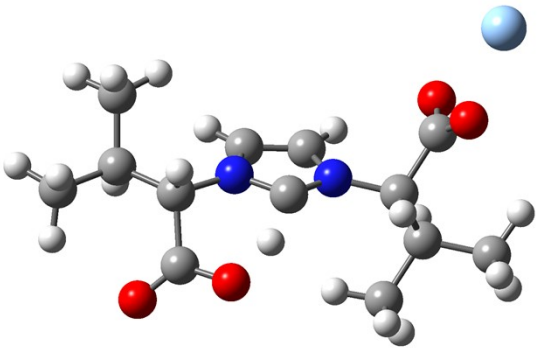
Table S4. Coordinates of the optimised compounds of the H-D exchange mechanism.

2c



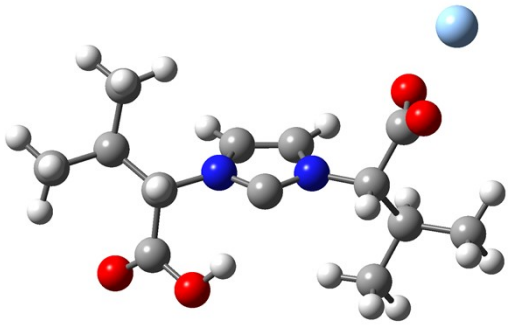
Ag	4.22317600	-1.26807800	0.20138300
O	-4.60773700	0.45993100	1.73833300
O	2.39309500	0.05504100	0.90544200
O	2.75602600	-0.14591200	-1.28692900
N	-2.38150300	-0.02204400	0.03783600
N	-0.30928200	0.65625600	-0.04437500
C	-1.42106400	0.42870200	-0.76631200
C	-0.58304100	0.33280800	1.27494900
H	0.16886000	0.41414400	2.03828100
C	-1.87770100	-0.08865000	1.32467300
H	-2.52553100	-0.35848300	2.14075200
C	-3.77990600	-0.30919900	-0.36683500
H	-3.85291500	-0.00380400	-1.41280800
C	-4.75545400	0.60701300	0.50667600
C	0.92877000	1.24391600	-0.58550800
H	0.79687300	1.28691900	-1.66729400
C	2.11792900	0.30142700	-0.30037700
O	-5.52111100	1.31019400	-0.16437200
C	1.18089100	2.67017600	-0.03603600
H	1.30660500	2.57560700	1.04772900
C	-4.10277100	-1.80907500	-0.22257800
H	-4.00346000	-2.05357000	0.84089100
C	-5.56102800	-2.06448800	-0.62965100
H	-5.80460300	-3.12383200	-0.50913900
H	-6.25410600	-1.47989500	-0.02364700
H	-5.72839000	-1.79662600	-1.67802900
C	-3.14664000	-2.69667100	-1.03267500
H	-3.22077200	-2.47865200	-2.10436200
H	-2.10228100	-2.56886600	-0.73202900
H	-3.39706400	-3.75250300	-0.89602200
C	-0.00792200	3.59651600	-0.32131500
H	-0.17370100	3.70787500	-1.39831600
H	-0.93498800	3.24006100	0.13231300
H	0.19075100	4.59150200	0.08382200
C	2.47796900	3.24300100	-0.62426500
H	3.34887800	2.63293600	-0.37456000
H	2.41897000	3.31596600	-1.71487100
H	2.65241700	4.24740300	-0.23194700
H	-1.52169300	0.59710200	-1.82425500

TS1



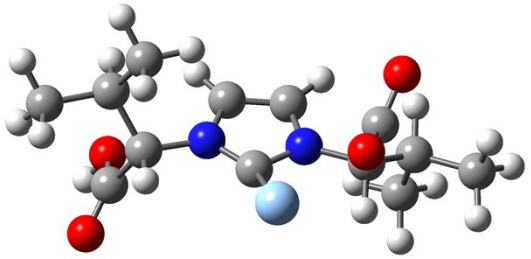
Ag	4.25603600	-1.23066400	-0.22677400
O	-5.26425100	1.27301100	-0.37641700
O	2.45205600	-0.20581700	0.89972500
O	2.73173900	0.22777600	-1.26981000
N	-2.28730400	-0.40406700	0.12542900
N	-0.31631000	0.46246300	0.21069200
C	-1.41060700	0.34999600	-0.57384800
C	-0.50808200	-0.21360200	1.40996800
H	0.26313800	-0.28616200	2.15542800
C	-1.75662900	-0.74731600	1.36053400
H	-2.28046000	-1.33391200	2.09219000
C	-3.66326200	-0.57391600	-0.43117400
H	-3.52493200	-1.06409900	-1.40114300
C	-4.18321300	0.88228300	-0.77341100
C	0.86222200	1.25802400	-0.16485700
H	0.67759300	1.58560700	-1.18720900
C	2.11183100	0.35270700	-0.18159900
O	-3.35334600	1.55009400	-1.51917300
C	1.05891800	2.48913900	0.75364900
H	1.23310300	2.11095000	1.76719600
C	-4.56146700	-1.48502300	0.42047600
H	-4.62657900	-1.06537300	1.43144400
C	-5.98880500	-1.56396400	-0.15128200
H	-6.56863900	-2.29557000	0.41865700
H	-6.49037300	-0.60107800	-0.11389800
H	-5.96745700	-1.90281500	-1.19330000
C	-3.99327500	-2.91804500	0.48631100
H	-4.02945500	-3.38021800	-0.50588000
H	-2.96059800	-2.97590600	0.83282000
H	-4.60320100	-3.53250000	1.15405800
C	-0.18970500	3.38029000	0.76051000
H	-0.40750000	3.76505000	-0.24057500
H	-1.07629800	2.84992900	1.11262500
H	-0.03201500	4.23754400	1.42025800
C	2.29710100	3.28688000	0.32059600
H	3.21151000	2.69122600	0.37312200
H	2.19071800	3.65165400	-0.70583900
H	2.42784100	4.15504400	0.97113200
H	-2.22453600	1.07784000	-1.36538600

C1



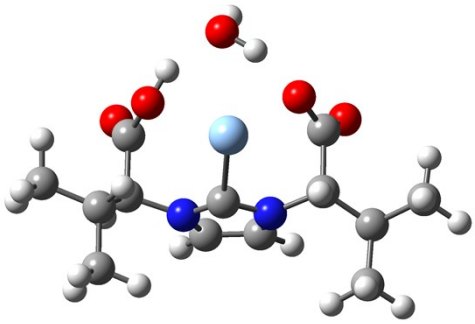
Ag	4.17878300	-1.30364000	-0.11734200
O	-5.44727300	0.98034000	0.20950800
O	2.40231500	-0.12105500	0.91369600
O	2.74667300	0.14192000	-1.27284300
N	-2.27330500	-0.27167000	0.09372300
N	-0.32367300	0.59895400	0.13244700
C	-1.38283400	0.39233300	-0.69890500
C	-0.55650300	0.10202300	1.41158700
H	0.18575400	0.13187100	2.18910900
C	-1.80162900	-0.43179600	1.39383100
H	-2.35997300	-0.91482500	2.17631500
C	-3.63516000	-0.54173600	-0.40518400
H	-3.50176300	-0.79039800	-1.46293200
C	-4.40727600	0.80572300	-0.36985600
C	0.88575200	1.30991700	-0.29914200
H	0.72172500	1.54078400	-1.35059300
C	2.10443900	0.36745900	-0.21205900
O	-3.81221700	1.78338700	-1.06819000
C	1.12104100	2.61740800	0.49672100
H	1.24900200	2.33927500	1.54893700
C	-4.34592300	-1.72314300	0.27607600
H	-4.53776000	-1.45812300	1.32190400
C	-5.70298800	-1.99756700	-0.39521400
H	-6.17820500	-2.86317000	0.07378800
H	-6.37827900	-1.14847000	-0.30856000
H	-5.56865500	-2.23324500	-1.45698600
C	-3.48432300	-2.99663500	0.21916300
H	-3.29937900	-3.28954100	-0.81963700
H	-2.51550100	-2.88337100	0.70737700
H	-4.01045600	-3.82242100	0.70512300
C	-0.08275200	3.56050100	0.37553100
H	-0.24196600	3.86182800	-0.66472900
H	-1.00489000	3.10066700	0.73484200
H	0.08961300	4.46651600	0.96276000
C	2.40696900	3.31371600	0.02845200
H	3.29072900	2.68779200	0.17284700
H	2.34953600	3.57352300	-1.03335300
H	2.55907300	4.23859000	0.59073400
H	-2.90143500	1.49687800	-1.33841700

C2



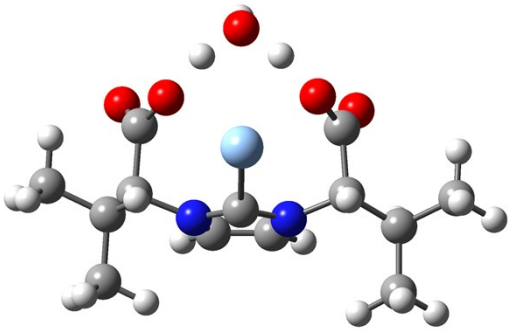
Ag	0.59994100	-1.88237400	-0.81233200
O	3.07324900	-0.35298100	2.06244200
O	-3.54247200	2.33630500	-0.47157300
O	-3.80180700	0.78596900	-2.08044000
N	0.90468800	0.89554300	0.17292300
N	-1.24363700	0.70824600	0.18078400
C	-0.11163200	0.14156400	-0.31525300
C	-0.93418400	1.80372600	0.98009600
H	-1.68415400	2.41628700	1.44650000
C	0.41762300	1.90840400	0.98137400
H	1.05627100	2.60884200	1.48821600
C	2.33585400	0.53687900	-0.04667000
H	2.37809700	0.16143900	-1.07189400
C	2.68323500	-0.65467900	0.93842500
C	-2.58581200	0.17430000	-0.07565400
H	-2.43165300	-0.74180400	-0.64563100
C	-3.36843600	1.10455100	-1.00529500
O	2.50042600	-1.82778900	0.45668900
C	-3.36010000	-0.15313300	1.22713300
H	-3.46124200	0.77834800	1.79484600
C	3.28374200	1.73894800	0.06544800
H	3.22420900	2.12025800	1.09023400
C	4.73029500	1.26905500	-0.15968000
H	5.41488400	2.11888200	-0.09332100
H	5.02888200	0.53308600	0.58675700
H	4.84807300	0.82606900	-1.15483900
C	2.93286200	2.85395300	-0.93382600
H	3.03186400	2.49449600	-1.96374900
H	1.91591300	3.23453200	-0.81406600
H	3.61741100	3.69829600	-0.81419600
C	-2.58471800	-1.16610900	2.07921200
H	-2.48498800	-2.12259600	1.55571000
H	-1.58419000	-0.81430000	2.33643900
H	-3.12098400	-1.35611300	3.01215300
C	-4.76930900	-0.67113800	0.90460900
H	-5.37127500	0.06173200	0.36174100
H	-4.72656200	-1.58270300	0.30044400
H	-5.29775700	-0.91014600	1.83024100
H	-4.02905800	2.87049800	-1.11840900

$C2_{D2O}$



Ag	-0.14628800	-0.99952800	-1.44737700
O	2.83896400	-1.20945900	1.61860000
O	-2.10145900	-1.40285900	0.45580800
O	-2.73260600	-0.62521100	2.47542100
N	1.12930500	1.09360100	0.34138700
N	-0.98858700	1.33834000	0.66228500
C	-0.08055700	0.82135300	-0.20531800
C	-0.34466900	1.92970800	1.74726900
H	-0.88359800	2.39348000	2.55560700
C	0.98466300	1.77066600	1.54635900
H	1.82046300	2.06716000	2.15390600
C	2.35915300	0.39322600	-0.11832400
H	2.24653700	0.29409600	-1.20071100
C	2.28812400	-1.04291400	0.53672400
C	-2.42300600	0.97192200	0.69036300
H	-2.89060000	1.63269300	1.42257700
C	-2.46829000	-0.44213100	1.31391500
O	1.58349500	-1.90791300	-0.10926800
C	-3.14264400	1.13056600	-0.65939500
H	-2.63595200	0.49006500	-1.38687200
C	3.65036200	1.16460900	0.17860000
H	3.76003800	1.23088100	1.26589900
C	4.85414600	0.37011200	-0.35229200
H	5.78190100	0.90987900	-0.14547100
H	4.92207100	-0.61069500	0.11915300
H	4.78659800	0.23302700	-1.43739400
C	3.62957800	2.57565400	-0.42967300
H	3.54990700	2.52747600	-1.52110200
H	2.79783600	3.18191300	-0.06365900
H	4.55605400	3.10509100	-0.19123400
C	-3.06857100	2.58119100	-1.15287900
H	-3.56856700	3.26017900	-0.45382200
H	-2.03694500	2.91677800	-1.27490800
H	-3.56833300	2.67678200	-2.12017000
C	-4.59917400	0.66059500	-0.53157000
H	-4.66742400	-0.38957100	-0.23766200
H	-5.14401500	1.25591600	0.20850400
H	-5.11477300	0.77060000	-1.48868700
H	-1.66485500	-2.17658700	0.92475900
O	-0.37533400	-3.20464000	1.24626400
H(Iso=2)	0.46317000	-2.84930500	0.85067500
H(Iso=2)	-0.15814300	-3.47229700	2.14438400

TS2



Ag	-0.39095800	-0.88269900	-1.49377000
O	2.72875800	-1.23313300	1.64235600
O	-1.91264300	-1.46631900	0.43279800
O	-2.52165100	-0.76289700	2.47443400
N	1.21818400	1.11064700	0.29842300
N	-0.89230500	1.34258400	0.69024200
C	-0.01110300	0.86238100	-0.21905100
C	-0.21553900	1.90101500	1.77204200
H	-0.73130700	2.33604200	2.61087100
C	1.10777600	1.75014300	1.53048200
H	1.96028600	2.02685600	2.12411300
C	2.40159100	0.33884400	-0.16398200
H	2.26480800	0.21067600	-1.23971400
C	2.24032700	-1.05120300	0.53948200
C	-2.31267800	0.91375300	0.77045500
H	-2.75563000	1.50587300	1.57305400
C	-2.28102900	-0.55935400	1.29583100
O	1.47629600	-1.89054300	-0.10310400
C	-3.11525100	1.14986700	-0.51831600
H	-2.64545000	0.57449500	-1.32322200
C	3.74084800	1.03321400	0.10438300
H	3.86640000	1.11517600	1.18889400
C	4.88683300	0.15598300	-0.42379600
H	5.84934300	0.63570400	-0.22916000
H	4.89769000	-0.82261500	0.05854800
H	4.80318000	0.00962000	-1.50634400
C	3.79345300	2.43193600	-0.52807100
H	3.69489800	2.37131500	-1.61719800
H	3.00220100	3.08861700	-0.15963700
H	4.75205400	2.91020700	-0.31028900
C	-3.10846100	2.63197000	-0.91528200
H	-3.57764300	3.24661000	-0.13936900
H	-2.09500900	3.00524800	-1.07714200
H	-3.67224000	2.78133600	-1.83997700
C	-4.54812000	0.62859600	-0.33623300
H	-4.56504900	-0.43933400	-0.10799900
H	-5.05913600	1.15614100	0.47582300
H	-5.12638900	0.78649600	-1.25020600
H	-1.10707100	-2.38149200	0.92477400
O	-0.23325700	-3.05201800	1.16631900
H(Iso=2)	0.66092100	-2.60083500	0.66017000
H(Iso=2)	-0.09489700	-3.08551100	2.12043900

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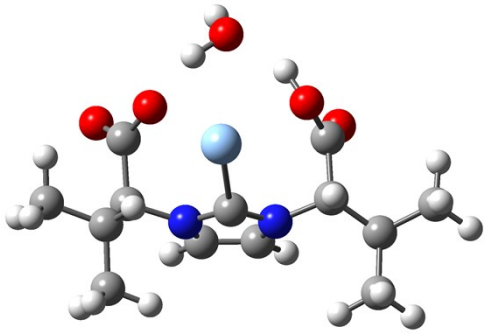

Ag	-0.60748400	-0.85896500	-1.45412300
O	2.92307300	-1.29003600	1.59970500
O	-2.03405400	-1.48539700	0.30415100
O	-2.85467900	-0.86585500	2.29753000
N	1.30602500	1.02227600	0.35156500
N	-0.79775900	1.23069300	0.77638600
C	0.06873800	0.78127000	-0.15945900
C	-0.11185300	1.75495800	1.86600100
H	-0.62006400	2.16360700	2.72254600
C	1.20985300	1.61755400	1.60748800
H	2.06786900	1.87730500	2.20100000
C	2.50170600	0.32159000	-0.16956800
H	2.32381900	0.19020600	-1.23822500
C	2.43703100	-1.06204900	0.52114700
C	-2.24823000	0.90536900	0.81358900
H	-2.64354100	1.45254800	1.67049200
C	-2.40751700	-0.62034800	1.18278800
O	1.68325200	-1.91825000	-0.17987700
C	-3.01049700	1.35669300	-0.44501500
H	-2.58202600	0.83732000	-1.31076500
C	3.82032600	1.07218000	0.05256200
H	3.98459800	1.15807500	1.13172900
C	4.98374800	0.25301200	-0.52828800
H	5.92869300	0.77808600	-0.37010400
H	5.06674900	-0.72732000	-0.05530500
H	4.86264000	0.10805700	-1.60719800
C	3.77678400	2.47484600	-0.57001100
H	3.63666800	2.41641500	-1.65446000
H	2.96965000	3.08677100	-0.16226700
H	4.71857200	2.99822100	-0.38669100
C	-2.87127200	2.86741700	-0.67608300
H	-3.30082700	3.43078800	0.15938500
H	-1.82761500	3.16980800	-0.78823800
H	-3.40425800	3.16558500	-1.58307800
C	-4.48603900	0.94656800	-0.33329500
H	-4.59889300	-0.13479000	-0.23323500
H	-4.95846200	1.41453500	0.53630400
H	-5.03513000	1.26476500	-1.22343000
H	-0.96314900	-2.75180400	0.88184500
O	-0.16676500	-3.32236100	1.03483500
H(Iso=2)	1.23011500	-2.59444300	0.40483600
H(Iso=2)	-0.24480700	-3.66233600	1.93107600

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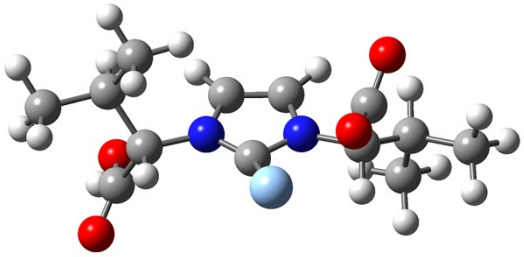

Ag	0.59994100	-1.88237400	-0.81233200
O	3.07324900	-0.35298100	2.06244200
O	-3.54247200	2.33630500	-0.47157300
O	-3.80180700	0.78596900	-2.08044000
N	0.90468800	0.89554300	0.17292300
N	-1.24363700	0.70824600	0.18078400
C	-0.11163200	0.14156400	-0.31525300
C	-0.93418400	1.80372600	0.98009600
H	-1.68415400	2.41628700	1.44650000
C	0.41762300	1.90840400	0.98137400
H	1.05627100	2.60884200	1.48821600
C	2.33585400	0.53687900	-0.04667000
H	2.37809700	0.16143900	-1.07189400
C	2.68323500	-0.65467900	0.93842500
C	-2.58581200	0.17430000	-0.07565400
H	-2.43165300	-0.74180400	-0.64563100
C	-3.36843600	1.10455100	-1.00529500
O	2.50042600	-1.82778900	0.45668900
C	-3.36010000	-0.15313300	1.22713300
H	-3.46124200	0.77834800	1.79484600
C	3.28374200	1.73894800	0.06544800
H	3.22420900	2.12025800	1.09023400
C	4.73029500	1.26905500	-0.15968000
H	5.41488400	2.11888200	-0.09332100
H	5.02888200	0.53308600	0.58675700
H	4.84807300	0.82606900	-1.15483900
C	2.93286200	2.85395300	-0.93382600
H	3.03186400	2.49449600	-1.96374900
H	1.91591300	3.23453200	-0.81406600
H	3.61741100	3.69829600	-0.81419600
C	-2.58471800	-1.16610900	2.07921200
H	-2.48498800	-2.12259600	1.55571000
H	-1.58419000	-0.81430000	2.33643900
H	-3.12098400	-1.35611300	3.01215300
C	-4.76930900	-0.67113800	0.90460900
H	-5.37127500	0.06173200	0.36174100
H	-4.72656200	-1.58270300	0.30044400
H	-5.29775700	-0.91014600	1.83024100
H(Iso=2)	-4.02905800	2.87049800	-1.11840900

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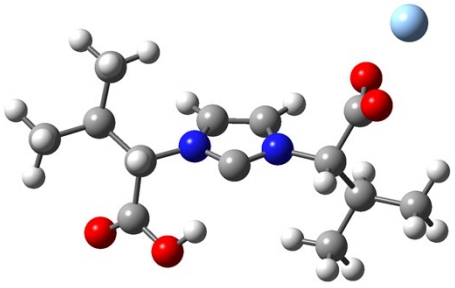

Ag	4.17890400	-1.30356100	-0.11731300
O	-5.44725200	0.98061400	0.20950400
O	2.40259500	-0.12066000	0.91391000
O	2.74623900	0.14123300	-1.27292000
N	-2.27339600	-0.27161400	0.09376700
N	-0.32373600	0.59895000	0.13251900
C	-1.38286200	0.39230000	-0.69887300
C	-0.55664500	0.10213300	1.41168800
H	0.18561100	0.13191300	2.18921000
C	-1.80167800	-0.43190300	1.39384000
H	-2.36004300	-0.91491400	2.17631000
C	-3.63526700	-0.54168900	-0.40516300
H	-3.50187400	-0.79032400	-1.46292100
C	-4.40727200	0.80586100	-0.36985500
C	0.88575200	1.30982600	-0.29909600
H	0.72173700	1.54062100	-1.35056100
C	2.10440500	0.36731600	-0.21198900
O	-3.81193200	1.78333300	-1.06806200
C	1.12111400	2.61734900	0.49665400
H	1.24924500	2.33928700	1.54886700
C	-4.34604500	-1.72314200	0.27601200
H	-4.53786100	-1.45817100	1.32185200
C	-5.70310400	-1.99757600	-0.39535600
H	-6.17851800	-2.86293900	0.07390200
H	-6.37830600	-1.14838000	-0.30907700
H	-5.56862100	-2.23365400	-1.45701200
C	-3.48451700	-2.99668000	0.21893600
H	-3.29957400	-3.28945000	-0.81990800
H	-2.51567900	-2.88361700	0.70716900
H	-4.01073500	-3.82249500	0.70475300
C	-0.08277100	3.56033900	0.37561600
H	-0.24215700	3.86163800	-0.66462700
H	-1.00482000	3.10042500	0.73506500
H	0.08959300	4.46637800	0.96280600
C	2.40693800	3.31371600	0.02815100
H	3.29075600	2.68785000	0.17244000
H	2.34932800	3.57345600	-1.03366000
H	2.55907200	4.23863100	0.59035600
H(Iso=2)	-2.90121600	1.49648600	-1.33812500

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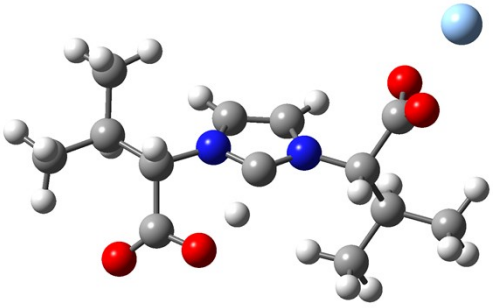

Ag	4.25603600	-1.23066400	-0.22677400
O	-5.26425100	1.27301100	-0.37641700
O	2.45205600	-0.20581700	0.89972500
O	2.73173900	0.22777600	-1.26981000
N	-2.28730400	-0.40406700	0.12542900
N	-0.31631000	0.46246300	0.21069200
C	-1.41060700	0.34999600	-0.57384800
C	-0.50808200	-0.21360200	1.40996800
H	0.26313800	-0.28616200	2.15542800
C	-1.75662900	-0.74731600	1.36053400
H	-2.28046000	-1.33391200	2.09219000
C	-3.66326200	-0.57391600	-0.43117400
H	-3.52493200	-1.06409900	-1.40114300
C	-4.18321300	0.88228300	-0.77341100
C	0.86222200	1.25802400	-0.16485700
H	0.67759300	1.58560700	-1.18720900
C	2.11183100	0.35270700	-0.18159900
O	-3.35334600	1.55009400	-1.51917300
C	1.05891800	2.48913900	0.75364900
H	1.23310300	2.11095000	1.76719600
C	-4.56146700	-1.48502300	0.42047600
H	-4.62657900	-1.06537300	1.43144400
C	-5.98880500	-1.56396400	-0.15128200
H	-6.56863900	-2.29557000	0.41865700
H	-6.49037300	-0.60107800	-0.11389800
H	-5.96745700	-1.90281500	-1.19330000
C	-3.99327500	-2.91804500	0.48631100
H	-4.02945500	-3.38021800	-0.50588000
H	-2.96059800	-2.97590600	0.83282000
H	-4.60320100	-3.53250000	1.15405800
C	-0.18970500	3.38029000	0.76051000
H	-0.40750000	3.76505000	-0.24057500
H	-1.07629800	2.84992900	1.11262500
H	-0.03201500	4.23754400	1.42025800
C	2.29710100	3.28688000	0.32059600
H	3.21151000	2.69122600	0.37312200
H	2.19071800	3.65165400	-0.70583900
H	2.42784100	4.15504400	0.97113200
H(Iso=2)	-2.22453600	1.07784000	-1.36538600

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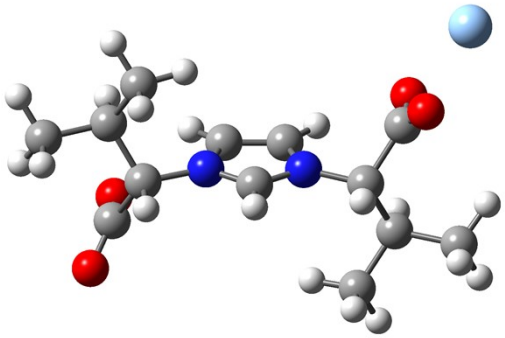

Ag	4.22317600	-1.26807800	0.20138300
O	-4.60773700	0.45993100	1.73833300
O	2.39309500	0.05504100	0.90544200
O	2.75602600	-0.14591200	-1.28692900
N	-2.38150300	-0.02204400	0.03783600
N	-0.30928200	0.65625600	-0.04437500
C	-1.42106400	0.42870200	-0.76631200
C	-0.58304100	0.33280800	1.27494900
H	0.16886000	0.41414400	2.03828100
C	-1.87770100	-0.08865000	1.32467300
H	-2.52553100	-0.35848300	2.14075200
C	-3.77990600	-0.30919900	-0.36683500
H	-3.85291500	-0.00380400	-1.41280800
C	-4.75545400	0.60701300	0.50667600
C	0.92877000	1.24391600	-0.58550800
H	0.79687300	1.28691900	-1.66729400
C	2.11792900	0.30142700	-0.30037700
O	-5.52111100	1.31019400	-0.16437200
C	1.18089100	2.67017600	-0.03603600
H	1.30660500	2.57560700	1.04772900
C	-4.10277100	-1.80907500	-0.22257800
H	-4.00346000	-2.05357000	0.84089100
C	-5.56102800	-2.06448800	-0.62965100
H	-5.80460300	-3.12383200	-0.50913900
H	-6.25410600	-1.47989500	-0.02364700
H	-5.72839000	-1.79662600	-1.67802900
C	-3.14664000	-2.69667100	-1.03267500
H	-3.22077200	-2.47865200	-2.10436200
H	-2.10228100	-2.56886600	-0.73202900
H	-3.39706400	-3.75250300	-0.89602200
C	-0.00792200	3.59651600	-0.32131500
H	-0.17370100	3.70787500	-1.39831600
H	-0.93498800	3.24006100	0.13231300
H	0.19075100	4.59150200	0.08382200
C	2.47796900	3.24300100	-0.62426500
H	3.34887800	2.63293600	-0.37456000
H	2.41897000	3.31596600	-1.71487100
H	2.65241700	4.24740300	-0.23194700
H(Iso=2)	-1.52169300	0.59710200	-1.82425500