

Electronic Supplementary Information (ESI)

Tris(triazole) tripodal receptors as selective probes for citrate anion recognition and multichannel transition and heavy metal cations sensing

María del Carmen González, Francisco Otón, Arturo Espinosa, Alberto Tárraga and Pedro Molina.**

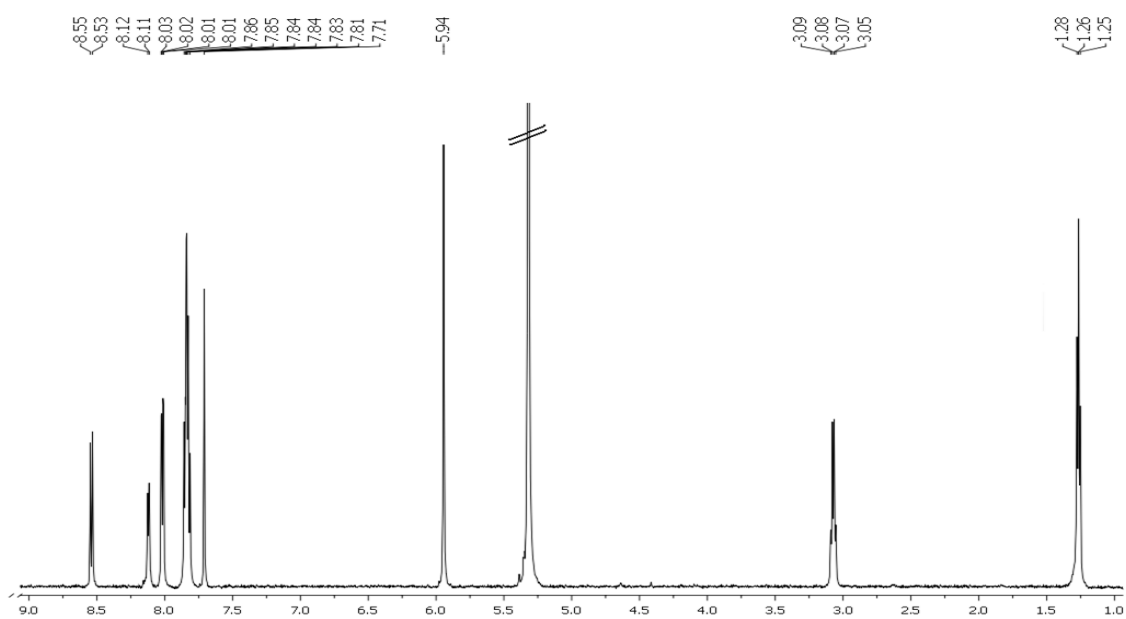
Departamento de Química Orgánica, Facultad de Química Campus de Espinardo, Universidad de Murcia, E-30100 Murcia, Spain. Fax: +34 868 884 149; Tel: +34 868 887 496;

Table of contents

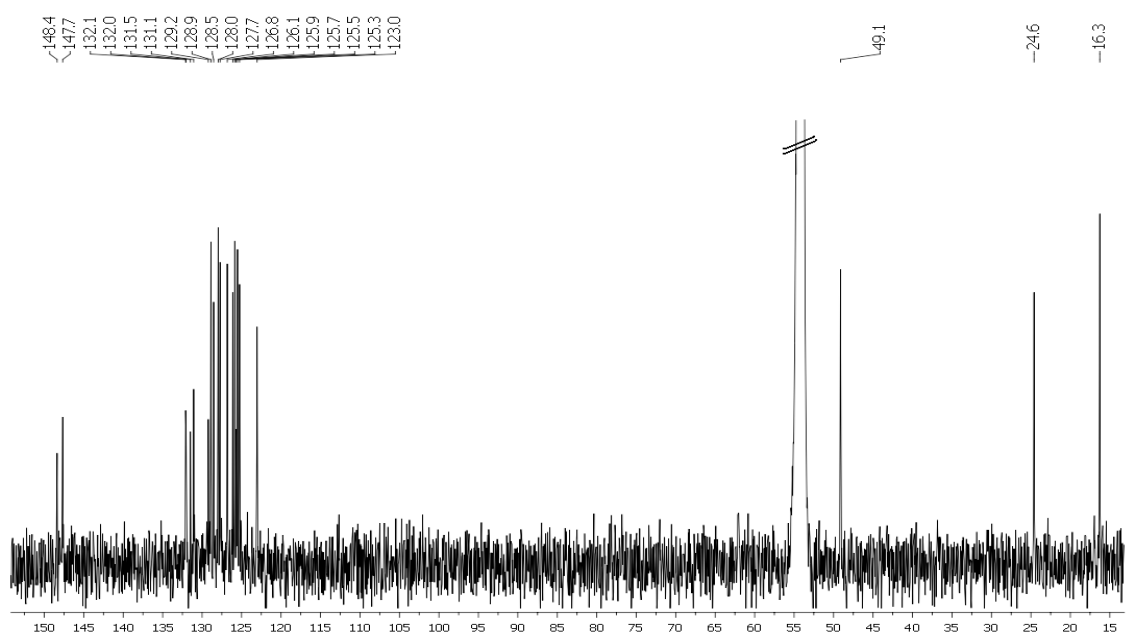
Figure S1. NMR spectra of 1 .	S3
Figure S2. NMR spectra of 2 .	S6
Figure S3. ¹ H-NMR spectra of 1 measured at -20 °C.	S8
Figure S4. UV-vis spectrum of 1 ($c = 1.5 \cdot 10^{-5}$ M) in CH ₃ CN.	S8
Figure S5. Fluorescence titration of compound 1 in CH ₃ CN ($c = 1.5 \cdot 10^{-5}$ M) upon addition of increasing amounts of citrate.	S9
Figure S6. Semilogarithmic plot for determining the detection limit of 1 towards anion citrate.	S9
Figure S7. OSWV of compound 2 in CH ₃ CN/CH ₂ Cl ₂ (4:1, $c = 5 \cdot 10^{-4}$ M) upon addition of a) H ₂ PO ₄ ⁻ ; b) F ⁻ ; c) AcO ⁻ , and d) BzO ⁻ with 0.1 M of TBAHP as supporting electrolyte.	S10
Table S1. Electrochemical data of compound 2 and of selected anion complexes.	S10
Figure S8. Evolution of the ¹ H-NMR spectra of 2 upon addition of increasing amounts of citrate.	S11
Figure S9. Titration isotherm obtained from the ¹ H NMR data	S11
Figure S10. UV-vis titration of compound 1 in CH ₃ CN ($c = 1.5 \cdot 10^{-5}$ M) upon addition of Hg ²⁺ and Job's plot showing a 1:1 stoichiometry.	S12
Figure S11. UV-vis titration of compound 1 in CH ₃ CN ($c = 1.5 \cdot 10^{-5}$ M) upon addition of Cu ²⁺ and binding profile measured at $\lambda = 382$ nm.	S12
Figure S12. Fluorescence titration of compound 1 in CH ₃ CN ($c = 1.5 \cdot 10^{-5}$ M) upon addition of Hg ²⁺ and binding profile measured at 486 nm.	S13
Figure S13. Evolution of the ¹ H-NMR spectra of 1 upon addition of increasing amounts of Hg ²⁺ .	S13
Figure S14. ESI-MS of the complex formed between receptor 1 and Hg ²⁺ .	S14
Figure S15. CV and OSWV of compound 2 in CH ₃ CN / CH ₂ Cl ₂ (1:1, $c = 5 \cdot 10^{-4}$ M) with 0.1 M of TBAHP as supporting electrolyte.	S14
Figure S16. Evolution of the LSV of 2 ($c = 5 \cdot 10^{-4}$ M) in CH ₃ CN/CH ₂ Cl ₂ (1:1, $c = 5 \cdot 10^{-4}$ M) upon addition of increasing amounts of: a) Cu ²⁺ , b) Hg ²⁺ and c) Pb ²⁺ with 0.1 M of TBAHP as supporting electrolyte.	S15
Figure S17. CV (left) and OSWV (right) of compound 2 in CH ₃ CN / CH ₂ Cl ₂ (1:1, $c = 5 \cdot 10^{-4}$ M) upon addition of Pb ²⁺ with 0.1 M of TBAHP as supporting electrolyte.	S15
Figure S18. ESI-MS of the complex formed between receptor 2 and Pb ²⁺ .	S16
Figure S19. Bond critical points and bond paths for complex [1' ·citrate] ³⁻ .	S16
Cartesian coordinates and energies for all computed species.	S17

Figure S1. NMR spectra of **1**.

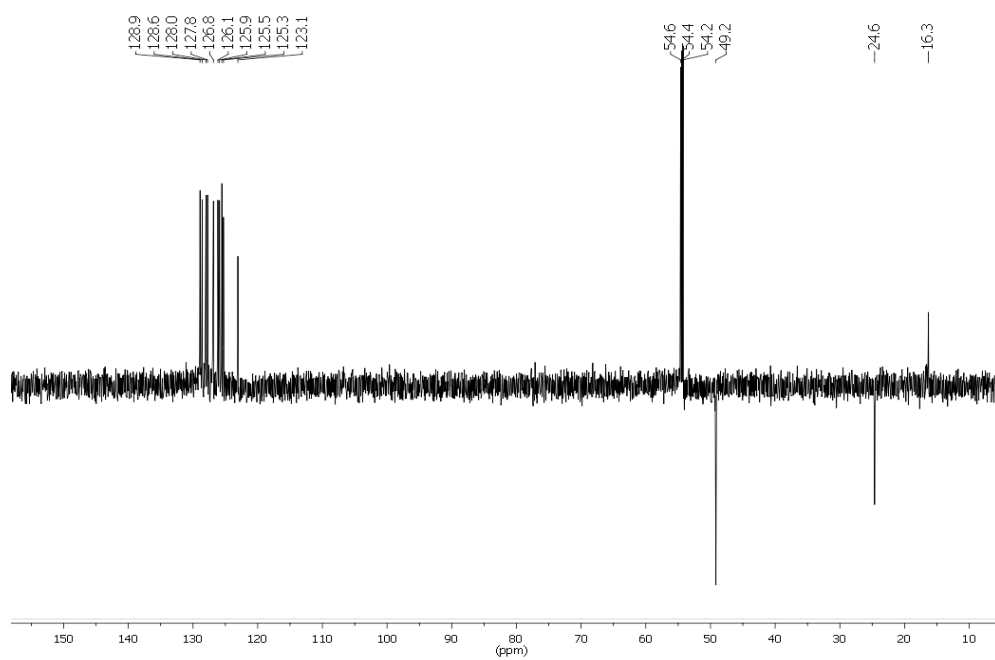
^1H NMR (CDCl_3 , 600MHz).



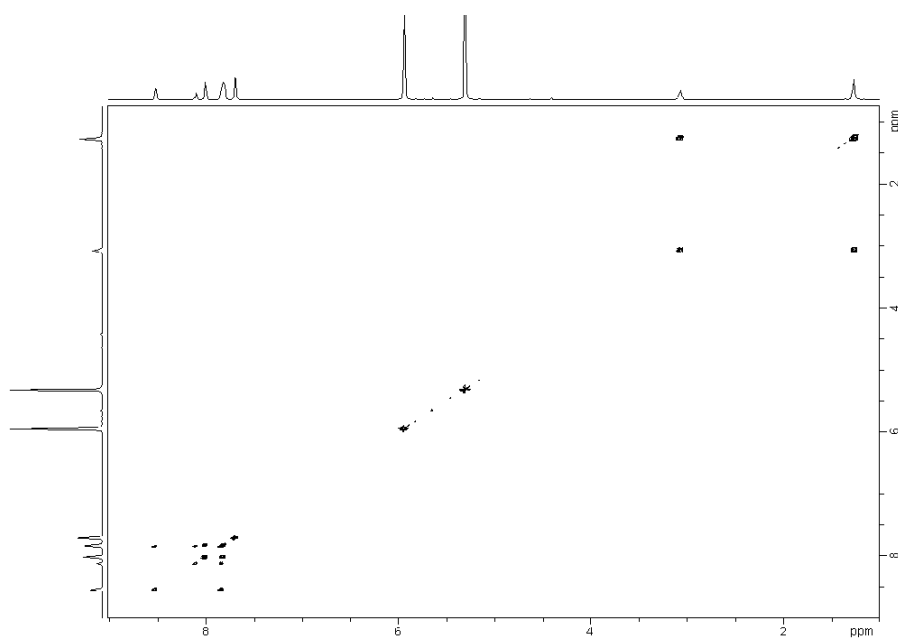
^{13}C NMR (CDCl_3 , 200MHz).



^{13}C -DEPT



^1H - ^1H COSY NMR (CDCl_3 , 600MHz).



^1H - ^{13}C HMQC NMR (CDCl_3 , 600MHz).

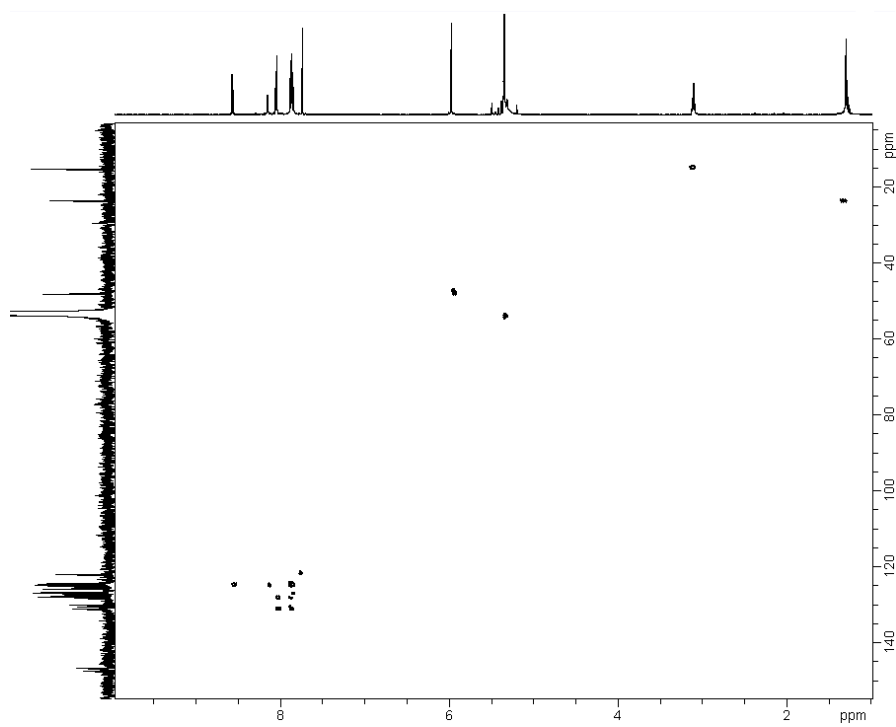
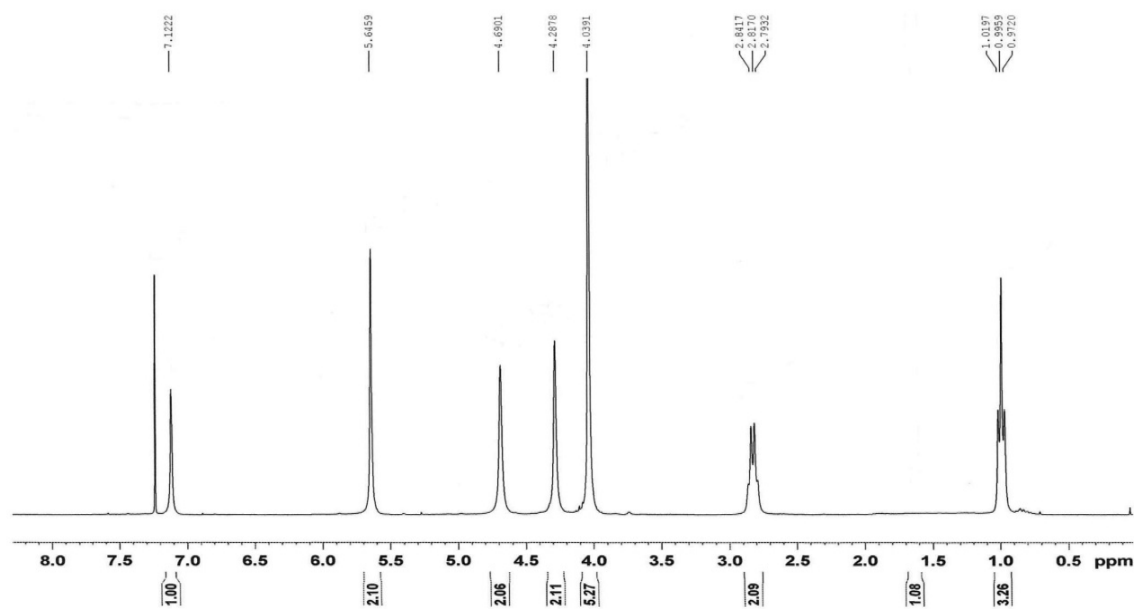
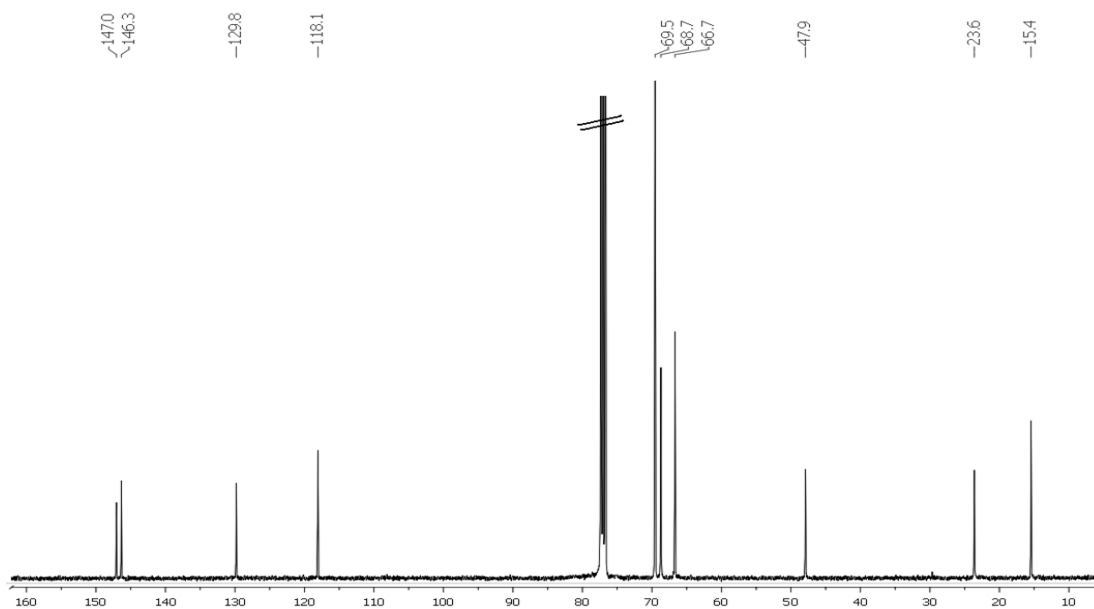


Figure S2. NMR spectra of **2**.

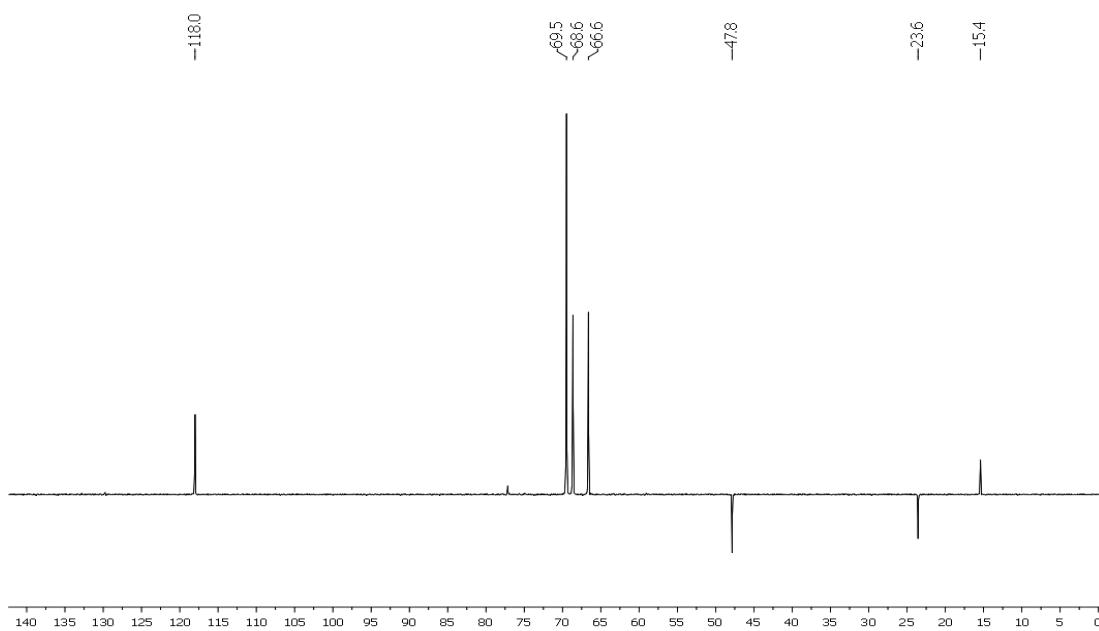
^1H NMR (CDCl_3 , 300MHz).



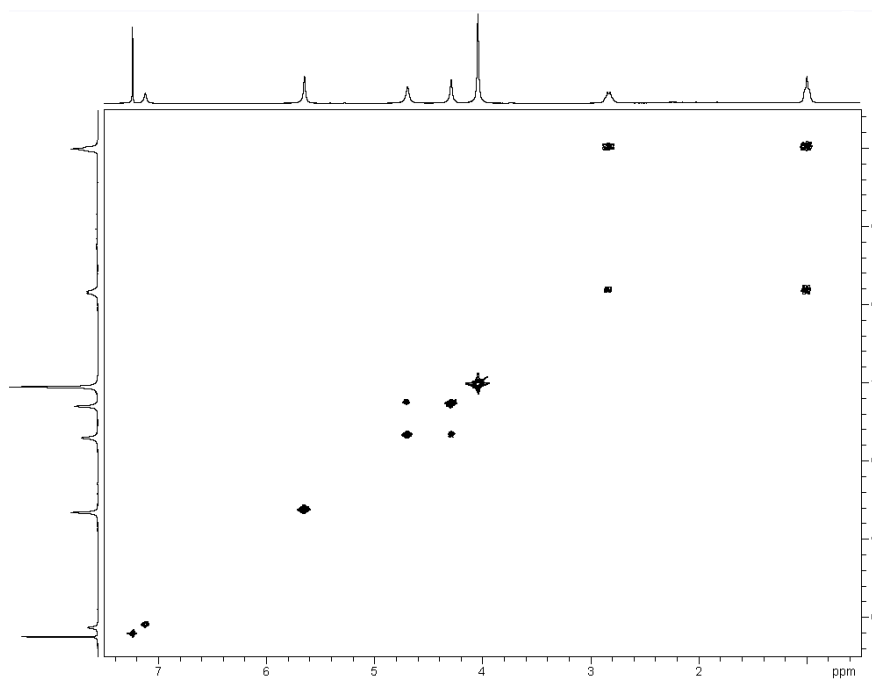
^{13}C NMR (CDCl_3 , 75 MHz).



^{13}C -DEPT (CDCl_3 , 75 MHz).



^1H - ^1H COSY NMR (CDCl_3 , 300MHz).



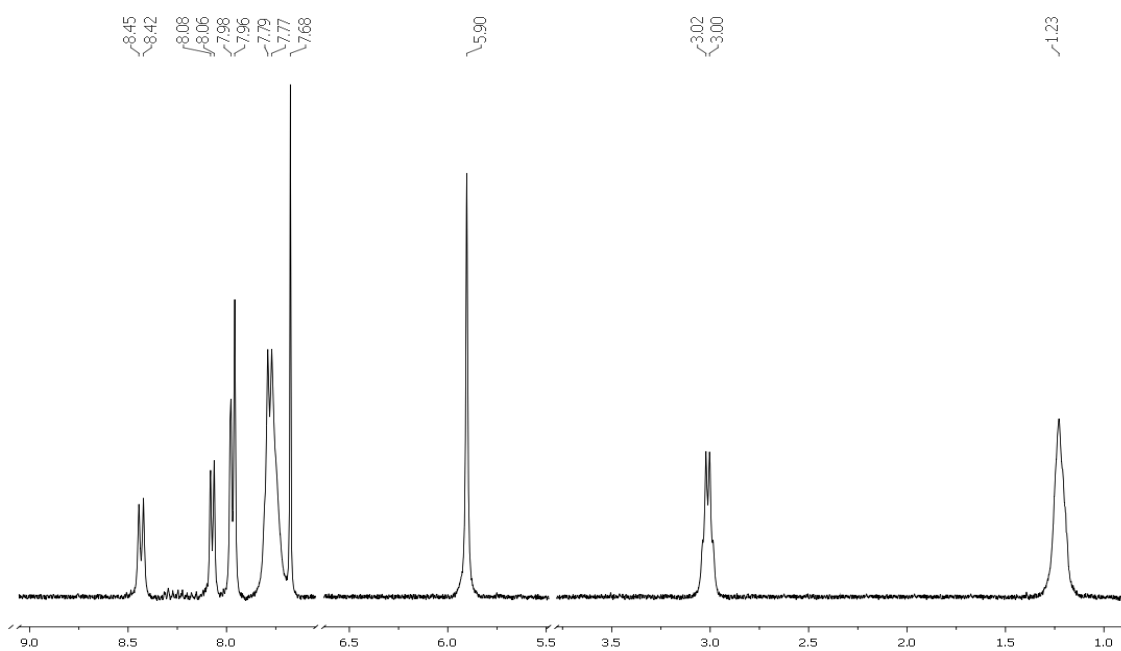


Figure S3. $^1\text{H-NMR}$ spectra of **1** measured at $-20\text{ }^\circ\text{C}$ ($c = 2 \cdot 10^{-3}\text{ M}$) in CDCl_3 .

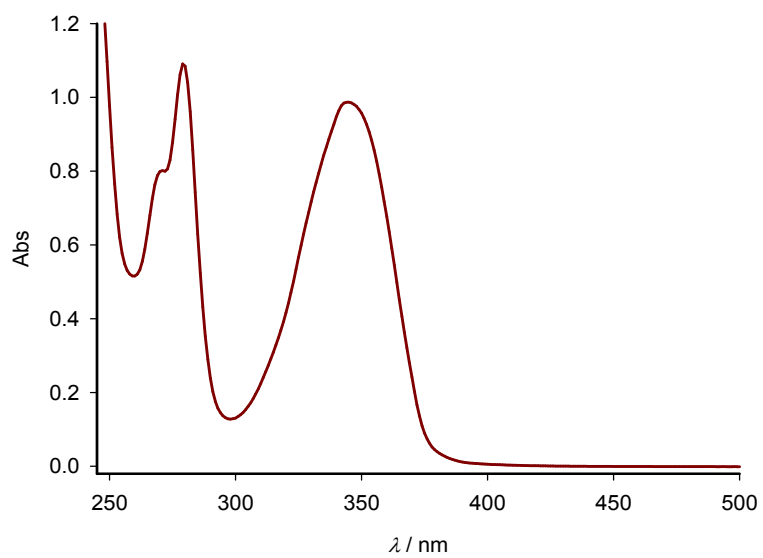


Figure S4. UV-vis spectrum of **1** ($c = 1.5 \cdot 10^{-5}\text{ M}$) in CH_3CN .

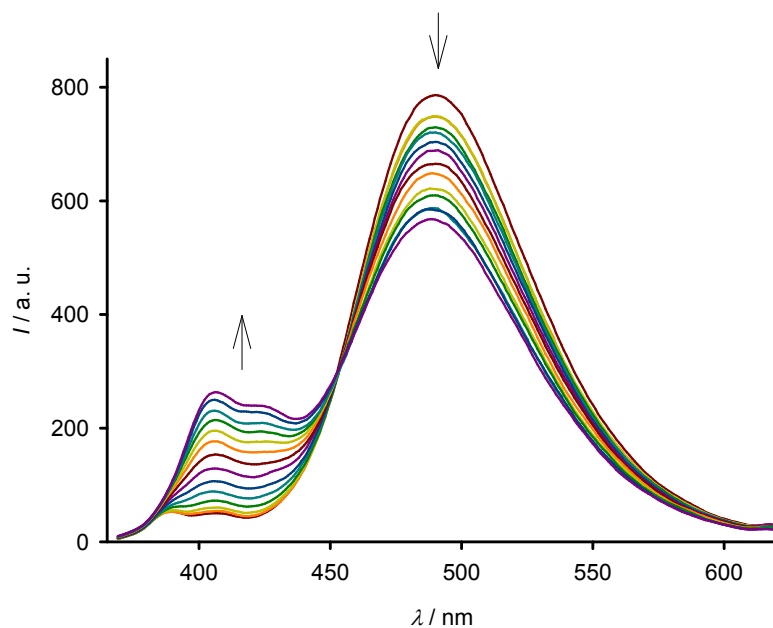


Figure S5. Fluorescence titration of compound **1** in CH_3CN ($c = 1.5 \cdot 10^{-5}$ M) upon addition of increasing amounts of citrate from 0 to 100 equiv.

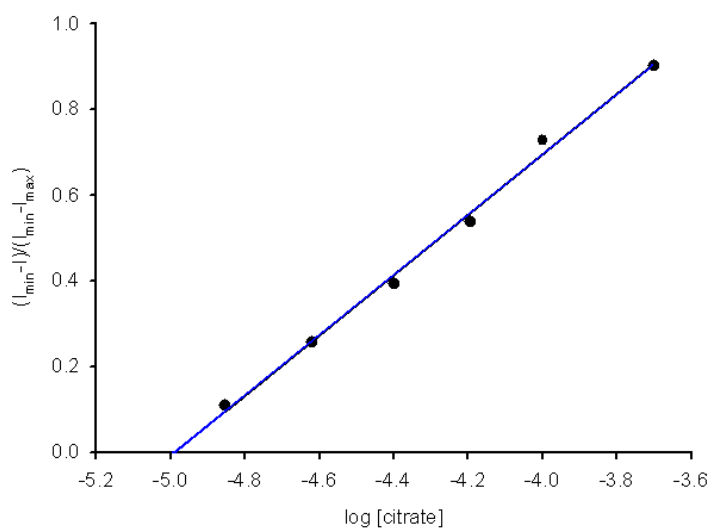


Figure S6. Fluorescence intensity of **1** ($c = 2 \cdot 10^{-6}$ M in $\text{CH}_3\text{CN}/\text{H}_2\text{O}$, 1:1) at each concentration of anión citrate added, normalized between the mínimo intensity, found at zero equiv of anion; and the maximum intensity, found at $[\text{citrate}] = 1.6 \cdot 10^{-4}$ M.

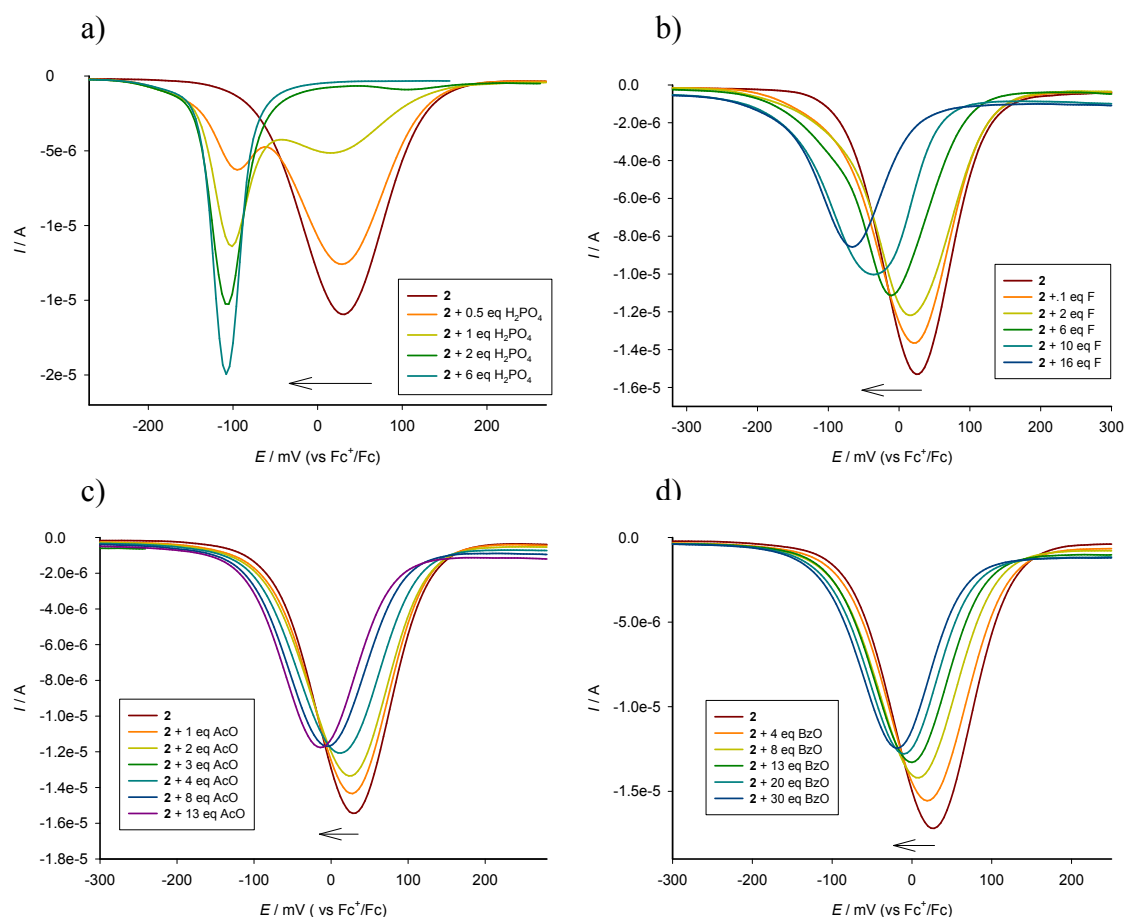


Figure S7. OSWV of compound **2** in CH₃CN / CH₂Cl₂ (4:1, $c = 5 \cdot 10^{-4}$ M) upon addition of a) H₂PO₄⁻; b) F⁻; c) AcO⁻, and d) BzO⁻ (supporting electrolyte, $c = 0.1$ M of TBAHP).

Table S1. Electrochemical data of compound **2** and of selected anion complexes.

Anion	$\Delta E_{1/2}$ (mV)	N ^o of quiv of anions added
HP ₂ O ₇ ⁻³	-145	12
F ⁻	-95	16
H ₂ PO ₄ ⁻	-145	6
AcO ⁻	-50	13
BzO ⁻	-50	30
Citrate	-60	10
Malate	-55	15
Tartrate	-60	12
Oxalate	-65	10
Trimesate	-65	8

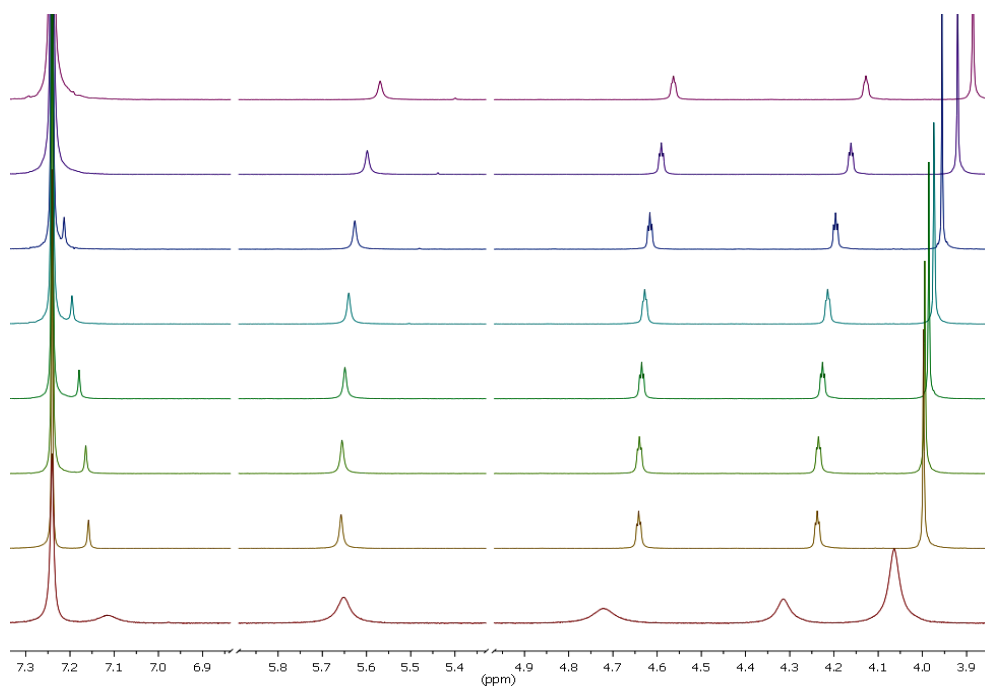


Figure S8. Evolution of the ^1H -NMR spectra of **2** upon addition of 0 (bottom), 0.5, 1, 3, 6, 10, 20 and 30 (top) equivalents of citrate anion.

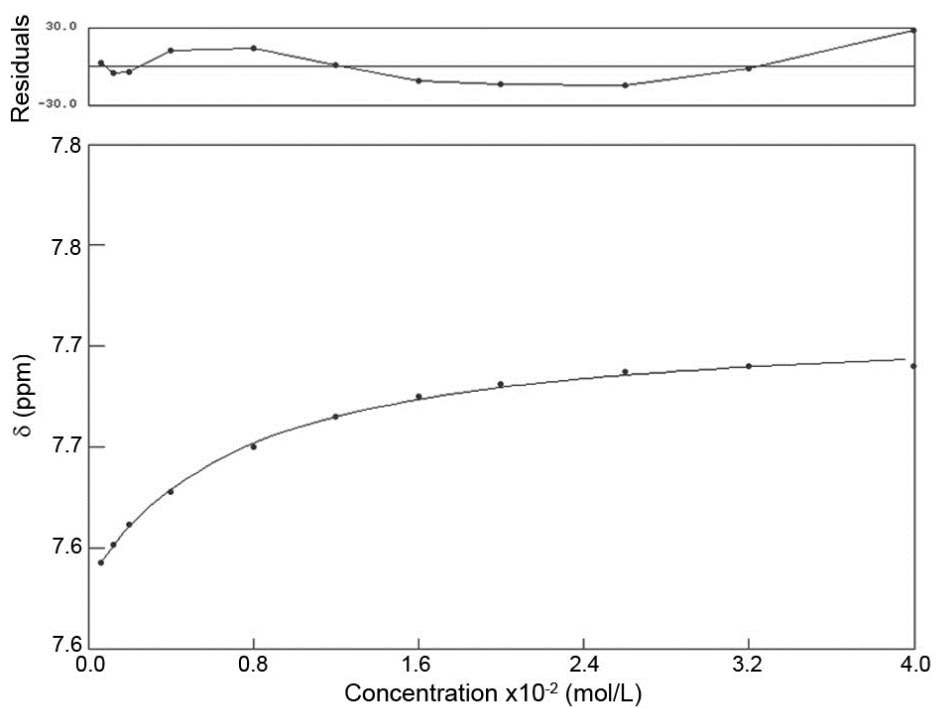


Figure S9. Titration isotherm obtained from the variation of the ^1H NMR chemical shift of the triazole CH-proton upon addition of increasing amounts of citrate anion.

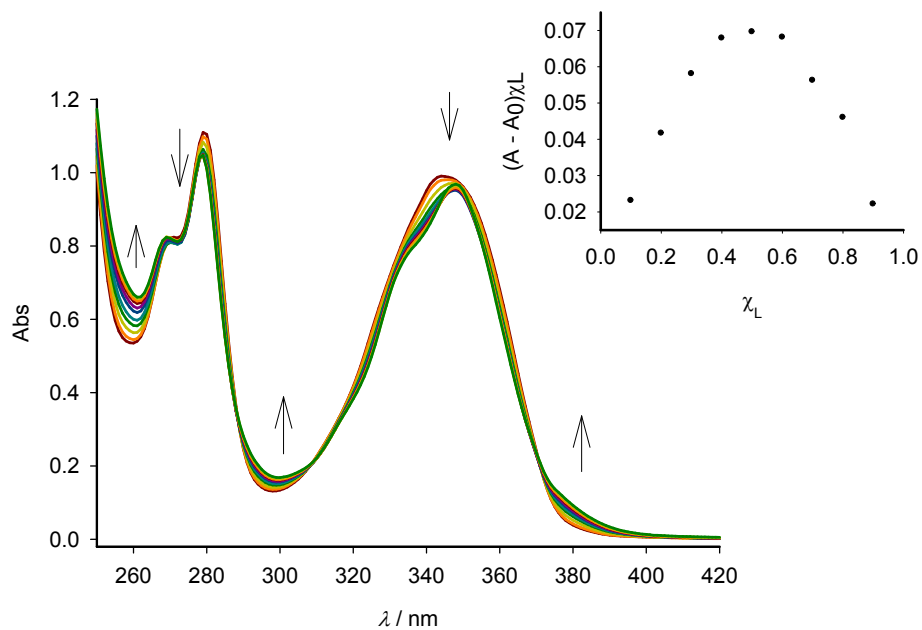


Figure S10. UV-vis titration of compound **1** in CH_3CN ($c = 1.5 \cdot 10^{-5} \text{ M}$) upon addition of Hg^{2+} from 0 to 10 equiv. Inset: Job's plot showing a 1:1 stoichiometry. The total $[\mathbf{1}] + [\text{Hg}^{2+}] = 1.5 \cdot 10^{-5} \text{ M}$.

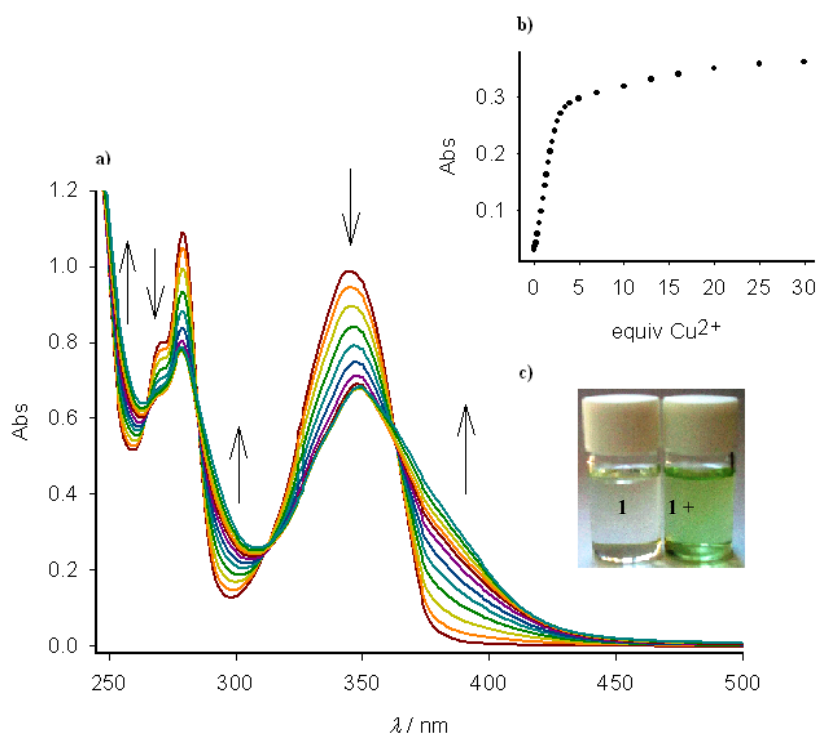


Figure S11. a) UV-vis titration of compound **1** in CH₃CN ($c = 1.5 \cdot 10^{-5}$ M) upon addition of Cu²⁺ from 0 to 30 equiv; b) Binding profile measured at $\lambda = 382$ nm; c) Colour changes observed.

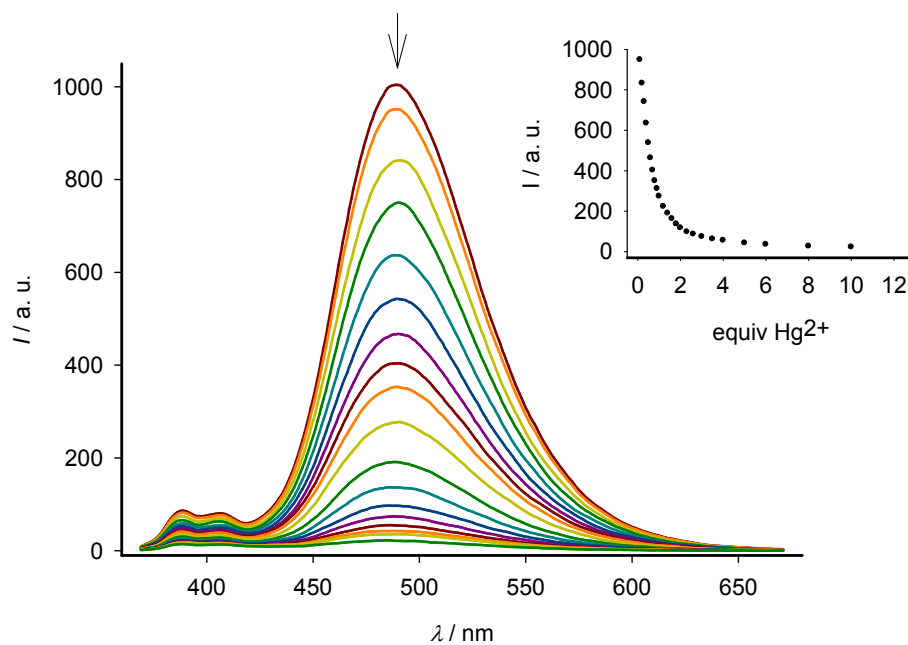


Figure S12. Fluorescence titration of compound **1** in CH₃CN ($c = 1.5 \cdot 10^{-5}$ M) upon addition of Hg²⁺ from 0 to 30 equiv. Inset: Binding profile measured at 486 nm.

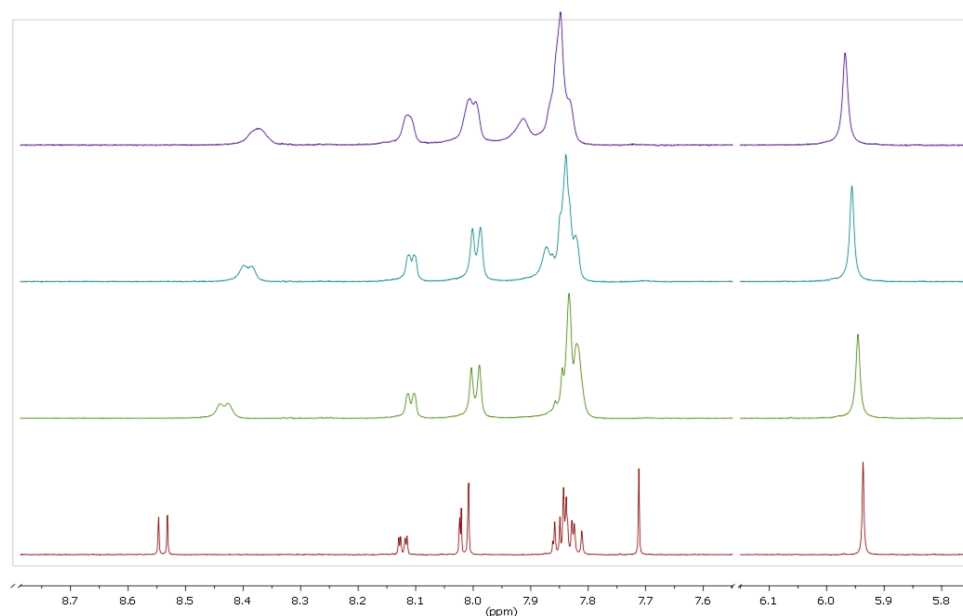


Figure S13. Evolution of the ¹H-NMR spectra of **1** upon addition of 0 (bottom), 0.3, 0.6 and 1.0 (top) equivalents of Hg²⁺.

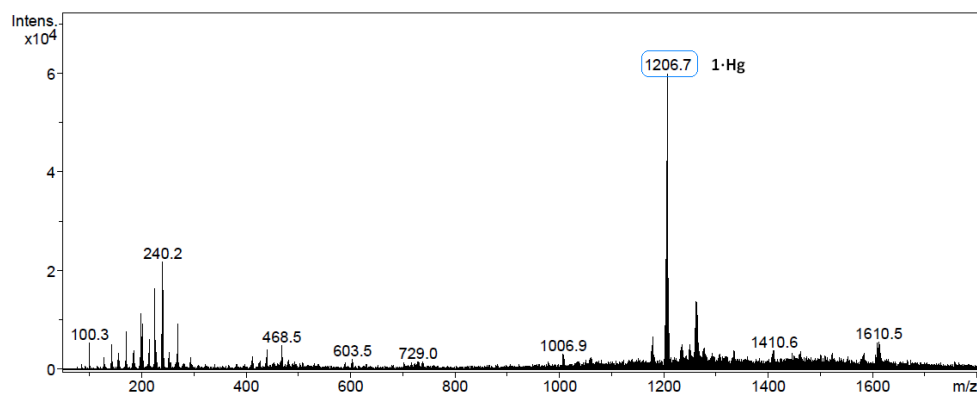


Figure S14. ESI-MS of the complex formed between receptor **1** and Hg^{2+} .

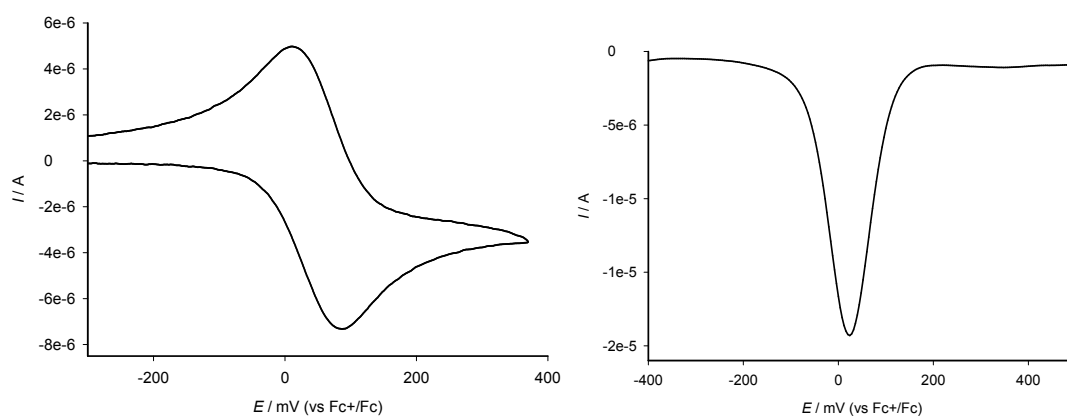


Figure S15. CV (left) and OSWV (right) of compound **2** in $\text{CH}_3\text{CN} / \text{CH}_2\text{Cl}_2$ (1:1, $c = 5 \cdot 10^{-4}$ M) with 0.1 M of TBAHP as supporting electrolyte.

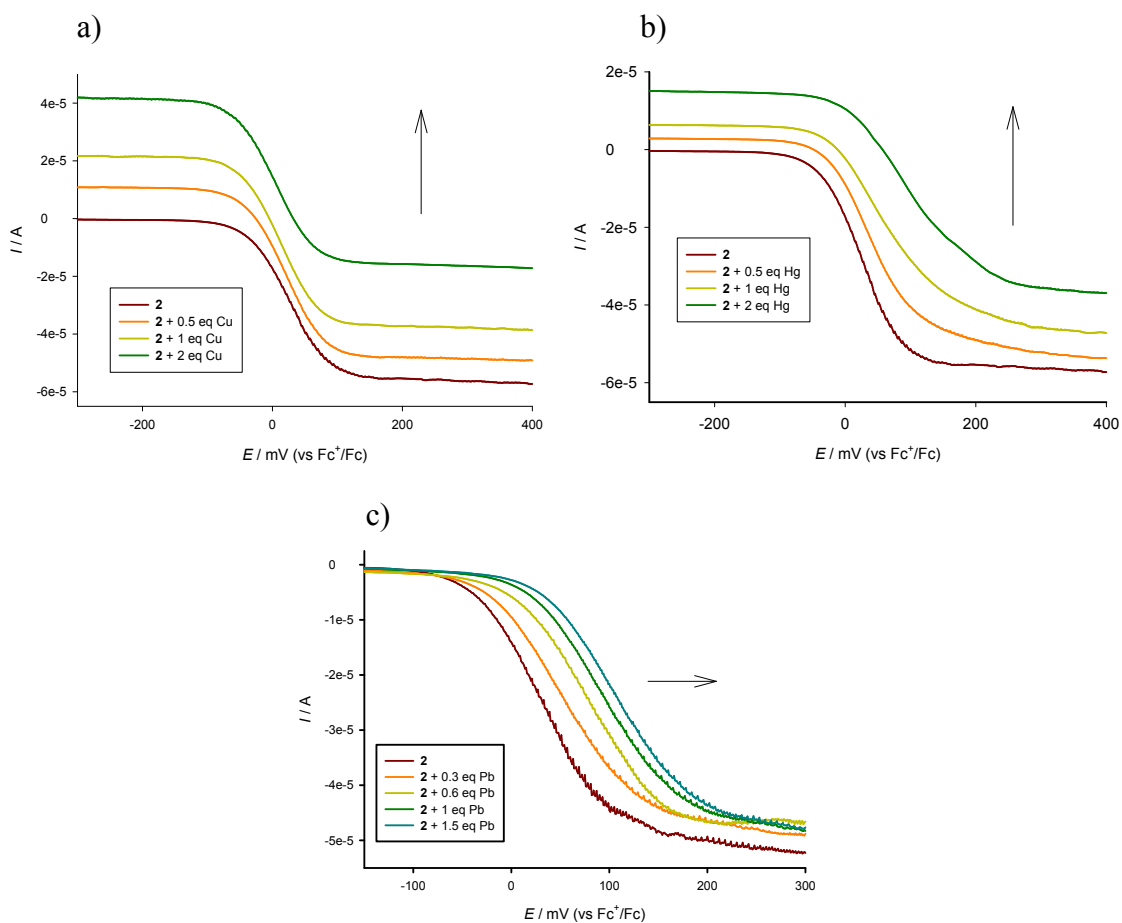


Figure S16. Evolution of the LSV of **2** ($c = 5 \cdot 10^{-4}$ M) in CH_3CN/CH_2Cl_2 (1:1, $c = 5 \cdot 10^{-4}$ M) upon addition of increasing amounts of: a) Cu^{2+} , b) Hg^{2+} and c) Pb^{2+} (supporting electrolyte, $c = 0.1$ M of TBAHP).

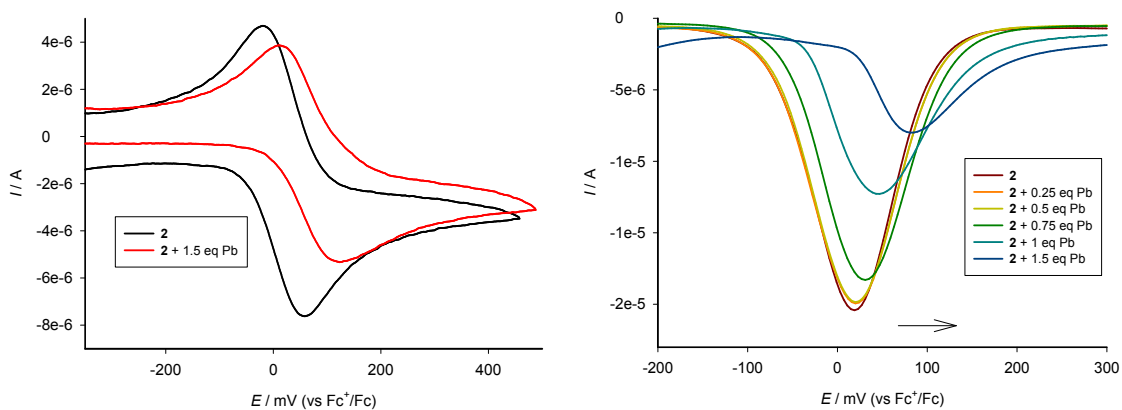


Figure S17. CV (left) and OSWV (right) of compound **2** in CH_3CN / CH_2Cl_2 (1:1, $c = 5 \cdot 10^{-4}$ M) upon addition of Pb^{2+} from 0 to 1.5 equivalents (supporting electrolyte, $c = 0.1$ M of TBAHP).

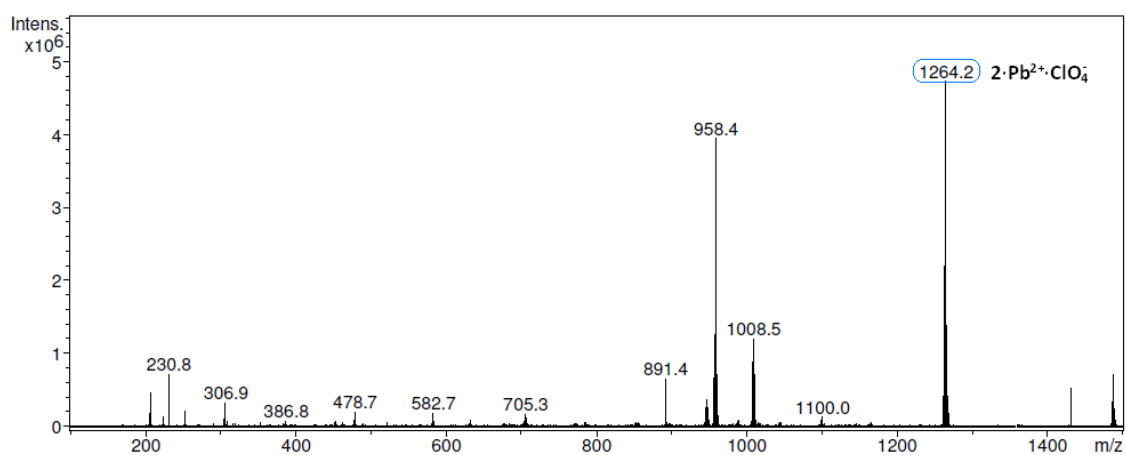


Figure S18. ESI-MS of the complex formed between receptor **2** and Pb^{2+} .

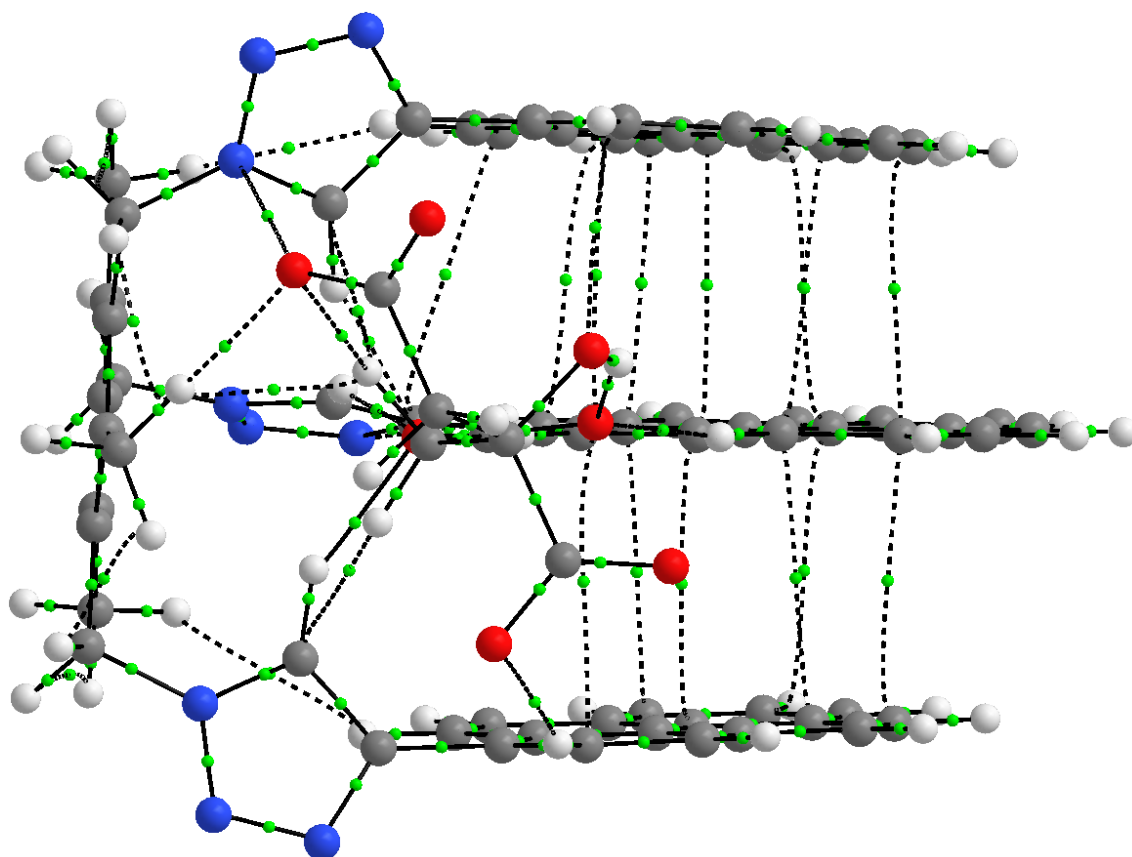


Figure S19. Bond critical points (small green spheres) and bond paths for complex $[\mathbf{1}'\cdot\text{citrate}]^{3-}$.

Cartesian coordinates (in Å) and energy (computed at the COSMOH2O/B3LYP-D3/def2-TZVPP level, in hartrees) for all computed species

1'	E= -3034.573354270911 au		
C	-0.20518472766342	0.13600042762510	-0.08854823208323
C	1.18716310978409	-0.01799392143373	-0.03540411940500
C	1.99963554739973	1.12845052864652	-0.04059210620761
C	1.43117335770018	2.41057946149949	0.01054699708260
C	0.03631359573991	2.54103149304033	-0.04141641712810
C	-0.78862093779380	1.41153494019153	-0.09318526445017
C	-1.08826306952274	-1.05204195712535	-0.38836983864068
H	-2.02187571315945	-1.04336765189780	0.16582703716248
H	-0.59823168403071	-1.99831669437848	-0.18925220798308
N	-1.45925620450618	-1.02036663622814	-1.81006788368614
N	-2.72698805156752	-1.19780414172405	-2.20456656441408
N	-2.75611811999286	-1.08855668118434	-3.50539184555396
C	-1.49506131637880	-0.83681198934352	-3.97132603217994
C	-0.65934012249088	-0.78847809102945	-2.86868551655341
H	0.39845983961067	-0.61828272006283	-2.77156881271934
C	-1.10378662304741	-0.64318159515464	-5.37204189873388
C	0.01006373966586	0.17047385258808	-5.61342645061496
C	0.50625631180581	0.37257461532647	-6.88435505066778
C	-0.08958203890196	-0.24084199920725	-7.98862415160090
C	0.41320037549528	-0.06047582462808	-9.31501389638958
C	-0.18235632316707	-0.64991939778654	-10.37995919326659
C	-1.34690678219261	-1.46408841358567	-10.21529629408127
C	-2.00056268937736	-2.05152229775248	-11.30501260226924
C	-3.14036598724233	-2.82288469034449	-11.11955377752156
C	-3.64495928639936	-3.03756003717505	-9.84343904867228
C	-3.02029354241793	-2.47425778876393	-8.72552831484369
C	-3.50583327452265	-2.67666556208513	-7.39711464343904
C	-2.90180108565320	-2.10751844094444	-6.32406740747114
C	-1.75107873752984	-1.26342527178119	-6.46599026953475
C	-1.23470504115956	-1.05850041733982	-7.78195684633969
C	-1.86374190379673	-1.66798234173380	-8.90390438159221
H	0.49912519836320	0.66403392764478	-4.78572834610485
H	1.35895238726083	1.01824744551774	-7.03016410321765
H	1.27500310359911	0.57889820658302	-9.45264678622242
H	0.20002305826495	-0.49276033453944	-11.38145093829858
H	-1.60958369913829	-1.88927360625021	-12.30234323798737
H	-3.63817278959368	-3.26124732152974	-11.97559408171052
H	-4.53344850752982	-3.64128365957618	-9.70254547169818
H	-4.38172301051039	-3.29992574949427	-7.25913922626776
H	-3.30135267881039	-2.26990223253618	-5.33618046460723
C	3.46505516281399	0.98848475599376	-0.40191902904161
H	3.85494051968163	-0.00332973388579	-0.21226065173727
H	4.11313168549786	1.69819437161593	0.09993486469625
N	3.58103641243978	1.24082273083779	-1.84769376157830
N	3.01699145803751	0.38749967283879	-2.71744366245505
N	3.01814316447663	0.95590736174509	-3.88934648841566
C	3.57513770099589	2.20169627449740	-3.79306883830466
C	3.94201476787107	2.37967849318794	-2.47074198591360
H	4.42093744544119	3.19141259680658	-1.95539491912699
C	3.61574912525783	3.18173381596291	-4.88117857569315
C	3.49580522434985	4.53296369188455	-4.53257977333496
C	3.42922539381889	5.53134351610706	-5.48461426903278
C	3.44245538556163	5.21573671142425	-6.84669350869318
C	3.27251299112895	6.21652568160972	-7.85548423890037
C	3.21555613855656	5.88744795653232	-9.17016138957608
C	3.34826472623993	4.52702248756179	-9.59709502846792
C	3.27183272218061	4.16293218949170	-10.94674817713741

C	3.41104855699036	2.83632571339004	-11.33333776799511
C	3.64012362435778	1.84619359465668	-10.38643113481061
C	3.71413413116709	2.16354808437666	-9.02538416393227
C	3.93975010607657	1.17303655403376	-8.01948352923325
C	3.92724249767623	1.48632283485059	-6.69987987142280
C	3.70789361528336	2.82959561021115	-6.24720494548267
C	3.58287694364687	3.85378469376472	-7.23321035295395
C	3.55639775404370	3.51606538750670	-8.61589559377038
H	3.41647804261853	4.80170742692757	-3.48737962014253
H	3.32052416241192	6.56433928213915	-5.17849464187749
H	3.16739648047239	7.24793115997668	-7.54157913019843
H	3.06475593239432	6.65208207630013	-9.92245550360325
H	3.10059508171651	4.93163138272926	-11.69036241851843
H	3.34498738866143	2.57266855814793	-12.38119987139801
H	3.75840881622950	0.81465307406137	-10.69499920236081
H	4.10011857240213	0.14816513229487	-8.33173992260075
H	4.06217067230640	0.70944355462994	-5.96458464380847
C	-0.58069357375029	3.90177084055447	-0.26434189924201
H	0.12180442286890	4.70872611680194	-0.08861363200464
H	-1.45108293412625	4.08412201669923	0.35976425613483
N	-1.05092076138393	3.99707580009561	-1.65411815408339
N	-2.26806994179901	4.47242647437558	-1.93909932580706
N	-2.43901932266657	4.37948950511371	-3.23037169012733
C	-1.32061291314560	3.83481289468556	-3.79718029577273
C	-0.42414460042502	3.58892849762582	-2.77938033402652
H	0.55624874312757	3.14856707511635	-2.77729447295585
C	-1.15984362202130	3.63157306499028	-5.24363208203864
C	-0.05710978359667	4.20928244916357	-5.87762598757196
C	0.12570850306686	4.10431137407820	-7.24486027763241
C	-0.78644220826241	3.40142943597692	-8.03513963724512
C	-0.62299014051622	3.28232857805409	-9.45207303011578
C	-1.50268881316652	2.57428988588425	-10.20132259161060
C	-2.62037632432156	1.90940550609396	-9.60207146641587
C	-3.51743471038089	1.14122995741831	-10.35204221434200
C	-4.57231078945653	0.48027756337313	-9.73787675862000
C	-4.75821718583110	0.57157722130902	-8.36498728355003
C	-3.89204235857203	1.33491504219790	-7.57574187750992
C	-4.03986803768538	1.43950703618968	-6.15674690400634
C	-3.18853390202320	2.18255953052432	-5.40781925802291
C	-2.08764310667974	2.88464682725163	-6.00016867511173
C	-1.89862514689875	2.77423851525462	-7.40844233819014
C	-2.80724467902785	2.01410261965556	-8.19497598071060
H	0.65557587373394	4.76874053826205	-5.28646408852586
H	0.97475638848317	4.57773031586278	-7.71500010258535
H	0.23767072835560	3.75419350113111	-9.91081487595412
H	-1.35911502657023	2.47511615684882	-11.27026703675342
H	-3.36676832417199	1.04926956411643	-11.42026392814793
H	-5.24202459265151	-0.12832097414946	-10.33103642845908
H	-5.57070191249005	0.03696100619395	-7.88885904073833
H	-4.84223815594750	0.88894818553515	-5.68144813861999
H	-3.31775145301510	2.22927757135712	-4.33672370491825
C	1.80375991745744	-1.39751949798323	-0.03447798037146
H	2.76619477922470	-1.40601432693898	0.47033316111151
H	1.17583427709418	-2.11514557476835	0.48715096234226
H	1.96459428949524	-1.76543412910129	-1.05087682624534
C	2.28866390479606	3.65312906271858	0.08116369105621
H	1.91113843478333	4.33567915155606	0.84186698961265
H	3.31800061352738	3.43244859599089	0.34374376295674
H	2.30017510235360	4.20064504923744	-0.86441604645085
C	-2.28125265995673	1.56374801018202	-0.23180800338671
H	-2.81682509130596	0.75561277445445	0.26029130676735
H	-2.63777975462339	2.49615749449664	0.19621935000857
H	-2.58074616129612	1.55429670025789	-1.28320735538526

[1⁻·citrate]³⁻

E= -3793.277405776694 au

C	0.51286497471390	-0.71165571300135	0.41695483420565
C	1.83194165045216	-0.25234942112167	0.26453190793532
C	2.11198991082167	1.10523717915579	0.48815282274987
C	1.07943546449768	2.00757859691825	0.78765966313484
C	-0.24183111808960	1.54655142775905	0.83074197999101
C	-0.53277854278419	0.18705960530457	0.66385465454169
C	0.19070837172033	-2.17261483367313	0.22137490843494
H	-0.55704278866471	-2.51113925628366	0.93519531246021
H	1.06326666824359	-2.80317718399900	0.35463116054915
N	-0.34613439351742	-2.40388008749266	-1.12683697316573
N	-0.79121960586485	-3.61270585383329	-1.50430064621009
N	-1.24575988157109	-3.49348277507898	-2.73040561424328
C	-1.09617766233093	-2.20153800426867	-3.13786305585785
C	-0.51684413845101	-1.49859018479957	-2.10740603981992
H	-0.18326510475846	-0.47239355532547	-2.07644201317067
C	-1.49335261064312	-1.68265670599173	-4.45813694881588
C	-0.73910303653559	-2.02020386015091	-5.57973764007961
C	-1.06158815633393	-1.52367016158546	-6.83280666340288
C	-2.15594101820481	-0.67259092464724	-7.00839243138546
C	-2.51789591268626	-0.14648717726759	-8.29217732992760
C	-3.58286810860415	0.67861950448458	-8.44226819256137
C	-4.38655663492302	1.06515180108232	-7.32129315865793
C	-5.48039723548188	1.92581179941800	-7.45148601803371
C	-6.22293911368437	2.30371291375997	-6.34014296754561
C	-5.89032717360524	1.83380143777167	-5.07808100416296
C	-4.80588265487660	0.96694672295522	-4.90055882126733
C	-4.42637153670350	0.46810209380043	-3.61473283350992
C	-3.37723571512704	-0.37784755147043	-3.46522983186119
C	-2.58896101063041	-0.80279176002523	-4.58478369241667
C	-2.93108700737660	-0.30441773502294	-5.87372650904320
C	-4.04198216009865	0.57061352164057	-6.03179596212372
H	0.14601680406566	-2.63034542911285	-5.45072261752448
H	-0.44269306403431	-1.77671499959756	-7.68510520741246
H	-1.91344118671954	-0.42373249887922	-9.14805344868963
H	-3.83706398149753	1.07656793330252	-9.41708162155340
H	-5.72662605585804	2.32075859496166	-8.42910658295247
H	-7.04820567024140	2.99400185719052	-6.45652689961162
H	-6.45530731482717	2.15433512192977	-4.21180140946462
H	-4.99279488045184	0.79217433145402	-2.75006739969134
H	-3.11252234181483	-0.73735803559198	-2.48096715951365
C	3.52525913172787	1.62149352690817	0.34018756669315
H	4.23957469059895	0.81514565303086	0.21768145486380
H	3.82787879448731	2.20311179422294	1.21012752069186
N	3.64852302896131	2.49754715597577	-0.83008310930862
N	4.73286732075439	3.26148004240084	-1.00983407443607
N	4.57398410260038	3.90494330566550	-2.14199878052100
C	3.37579022710830	3.55322463366974	-2.68940034931545
C	2.78026161217944	2.64535976312962	-1.84341171869916
H	1.86138723450859	2.09103050819340	-1.94253051968339
C	2.86383063273349	4.06531345163897	-3.96945056910897
C	3.55816343424967	3.77843755516567	-5.14335309285760
C	3.08735465396495	4.19387687550552	-6.37804321007167
C	1.90261992033533	4.92891825265525	-6.48270578165827
C	1.38675166280067	5.37210931800025	-7.74473348183486
C	0.25218163667266	6.11020272162426	-7.82318949278972
C	-0.47743583807831	6.47637558437745	-6.64654897081858
C	-1.64301522682714	7.24631522805815	-6.70385528812093
C	-2.33549522709676	7.57422922123407	-5.54554874433813

C	-1.88491766009069	7.13720132249860	-4.30856919398841
C	-0.72435875839142	6.36244886288044	-4.20360800645944
C	-0.23196255968929	5.88734377937465	-2.94804007097188
C	0.90280797105623	5.15007525664733	-2.86639668187703
C	1.66326127002566	4.80480305752903	-4.03129428798502
C	1.18671981847627	5.25135360278209	-5.29686871046921
C	-0.00263680927517	6.02864928399272	-5.38172820008187
H	4.45223273550148	3.17319774508069	-5.08172119350758
H	3.63145625240073	3.93630038110243	-7.27911329536212
H	1.92900643154831	5.10183157613509	-8.64341257039303
H	-0.12964084826968	6.43170492006818	-8.78448642182894
H	-2.01663574424138	7.56510049124022	-7.66881157624405
H	-3.24977968937312	8.14926149608986	-5.61187078389035
H	-2.44333562839058	7.37337486674496	-3.41141054036762
H	-0.79325398998704	6.12560521454916	-2.05259123875764
H	1.25406050024454	4.80908509582234	-1.90366163956506
C	-1.37577968153017	2.51945531882595	1.01670229437729
H	-1.03486437504908	3.45262887491622	1.45439991821659
H	-2.14688658041596	2.11978315853141	1.67078803311994
N	-2.04881246059589	2.84672473528263	-0.25175754249727
N	-3.28240945210365	3.37306818139962	-0.21338280991964
N	-3.63186552973745	3.64365189799683	-1.44389734828192
C	-2.62348264360802	3.29851628817805	-2.29790207929101
C	-1.59672990869706	2.77621833290435	-1.51762148571719
H	-0.64521480664184	2.35064540865397	-1.78733525456740
C	-2.61736846315875	3.44803418747749	-3.75963853565156
C	-1.58561752172719	2.79130897592699	-4.43903894349727
C	-1.43747731314873	2.87780368424019	-5.80537383124983
C	-2.32758233523217	3.62533377168150	-6.57479956999981
C	-2.19555873452209	3.72755455229997	-7.99291880244107
C	-3.06464749426470	4.45535024180328	-8.73355808545286
C	-4.15212896293988	5.14922803368510	-8.11439595291734
C	-5.06527853958502	5.90481763170863	-8.85870307365725
C	-6.11259873611335	6.57415088625087	-8.23599240615694
C	-6.26765515921037	6.50576338601627	-6.85787289427807
C	-5.37584563391382	5.76133195251183	-6.07517577357892
C	-5.49602595585475	5.67555271621859	-4.65550196908817
C	-4.62682127269826	4.94712739626060	-3.91043245544063
C	-3.54302041791417	4.22033222971572	-4.50272870713995
C	-3.39284893725083	4.30191056041600	-5.92105351664344
C	-4.30462687190686	5.06760678228218	-6.69998084066128
H	-0.86789657926729	2.18630158204458	-3.90078058788493
H	-0.60930333629644	2.35031752977881	-6.25933284292495
H	-1.37428250006525	3.20279211852148	-8.46394976789992
H	-2.95245729589802	4.52541715490896	-9.80927263080868
H	-4.94639492384350	5.96248116875939	-9.93449005020870
H	-6.80980653477833	7.15338506470105	-8.82933060537324
H	-7.08259586162577	7.03091439639678	-6.37318150079477
H	-6.30589302999447	6.21243798898716	-4.17405771523044
H	-4.74768462252318	4.89966085461793	-2.84103353820593
C	2.92728843862298	-1.19841269431743	-0.16459402437211
H	3.48618774510690	-1.57467962482594	0.69823143582968
H	2.52745308641085	-2.05800596233067	-0.69550663651249
H	3.63387247300206	-0.72560415656155	-0.84520560239272
C	1.35893532991203	3.47416257859013	1.01946342702041
H	2.41692996971603	3.71036237132973	1.00520087310616
H	0.88137898696811	4.09109754907506	0.25516595925180
H	0.96792497792384	3.79787267346810	1.98543798868842
C	-1.97437977132696	-0.25748166802487	0.69505133183082
H	-2.45179333788267	0.01563640019834	1.63812405911499
H	-2.54005181597316	0.22730018597171	-0.10335211222657
H	-2.09503302741028	-1.32734693080041	0.56701988481360
C	1.35989216397954	0.68448257876983	-4.01413237396633

O	1.28980056338480	1.08963260263320	-5.19988084382787
O	0.58509601985044	1.03371280269061	-3.07715405305365
C	2.48533002558106	-0.26850891712383	-3.60200120537641
H	2.03207462672977	-1.15072026760725	-3.15175888338666
H	3.05343131210203	0.23040308596846	-2.81889089413211
C	3.46260013016905	-0.70899235773781	-4.69940177692784
C	4.75685887304138	-1.28954879336661	-4.09535092849890
H	5.35387381342574	-1.70152809682790	-4.91247318203194
H	4.46866141829216	-2.10802154890800	-3.43473348084539
C	5.63955276298067	-0.30274170360125	-3.31080000444670
O	6.72346301686084	0.04702018459267	-3.85647185294040
O	5.26076697965935	0.05073951305752	-2.16483428056665
C	2.83301467052819	-1.85287321279640	-5.56297289434833
O	2.78920456070392	-1.71176402200012	-6.80791339501315
O	2.44484820927062	-2.87095352698812	-4.92889779695543
O	3.83168990402001	0.41481020717245	-5.49431956495938
H	2.96761950571446	0.85928314773761	-5.65465534839184

[1'-citrate]³⁻ isomer

E= -3793.245361512534 au

C	0.59054574675090	-0.21904455467457	-0.23101683449968
C	1.94019252262226	0.03845535388581	0.06913988472514
C	2.39158614261310	1.36946554323385	0.06147243511996
C	1.58559777835695	2.38895492225597	-0.47314129376474
C	0.28331545284767	2.08447525412651	-0.88460775209183
C	-0.25996883613687	0.81933284949464	-0.62433302305566
C	0.03401420814472	-1.61783959232185	-0.06449944424123
H	-0.59428569801488	-1.68624388738299	0.82506264902198
H	0.83471156672859	-2.34229345285643	0.02794196376468
N	-0.80591989896313	-2.05083323790707	-1.17627851288727
N	-2.02076630333586	-2.58250054137779	-0.94751085284145
N	-2.54058352109486	-2.87808093938806	-2.10965460711163
C	-1.65430210684420	-2.53691533956251	-3.09425907339552
C	-0.53409445186603	-2.00660920054436	-2.48958695448636
H	0.38109468487383	-1.62721506260167	-2.91836468266480
C	-1.85908704941340	-2.83260707029792	-4.51561711714158
C	-0.83922468008914	-3.50421117091077	-5.19820858891089
C	-1.01675116473691	-3.92527639029865	-6.50470937972894
C	-2.21128696488280	-3.67485018861945	-7.18819571017245
C	-2.44139982294585	-4.13899311784625	-8.52228695064626
C	-3.58047746666040	-3.82984842679441	-9.18958176986687
C	-4.59016015004948	-3.00995305951832	-8.59097017137254
C	-5.74376935531269	-2.62424724400771	-9.28225540566015
C	-6.69045917004855	-1.80530596764459	-8.68266462060367
C	-6.51392100184630	-1.36002535907094	-7.37935403231190
C	-5.38084190915174	-1.72620268017753	-6.64604474662270
C	-5.15602032319384	-1.27671710563261	-5.30629423271131
C	-4.05118456514747	-1.64505508540902	-4.61210022964848
C	-3.04153086297511	-2.47883010802049	-5.19621214770718
C	-3.22107724820401	-2.91005321265177	-6.54187022114142
C	-4.39928571039177	-2.55603719346069	-7.25544521302178
H	0.10152851246096	-3.69575689206491	-4.69183128075992
H	-0.22323653755120	-4.46333612888530	-7.01062937644191
H	-1.67006131269806	-4.73261424330712	-8.99887980443466
H	-3.73349844072874	-4.17430225129138	-10.20544164761597
H	-5.87938684974513	-2.95452793822742	-10.30475464576973
H	-7.56396392307708	-1.49624131712424	-9.24176462882301
H	-7.24777596987289	-0.70683218806503	-6.92322769111031
H	-5.88521764560254	-0.61237673774661	-4.85870937742953
H	-3.89854972374683	-1.28118903128640	-3.60672868395167
C	3.68744314990929	1.72233445006244	0.76511798112544

H	4.12227772507962	0.84832117581019	1.23795532457524
H	3.48508691482363	2.44159934308413	1.55812583951279
N	4.73070848681389	2.35510949286956	-0.04629403246186
N	5.23643823115878	3.54219466269169	0.32708618733072
N	6.13015026734697	3.88659973326940	-0.55590875221291
C	6.21670234186380	2.91865343328854	-1.51769677224159
C	5.31658977211185	1.92162932302471	-1.17501590975665
H	5.09496163820547	0.96669758444004	-1.61708914538792
C	7.13420377704616	2.94605654739621	-2.66299927694538
C	7.59213363413371	1.71396049555975	-3.14646699193764
C	8.46515629118576	1.62979827275262	-4.21431936997234
C	8.93722607173005	2.78379251068367	-4.84666657847201
C	9.86887779565721	2.72607289940561	-5.93253838984515
C	10.31782287126728	3.85398533485804	-6.53717926811865
C	9.86682283951947	5.14651049769933	-6.11562322576693
C	10.31288804170151	6.32336636491044	-6.72920780059077
C	9.85238642761324	7.56455232750584	-6.30736506348361
C	8.93490882780299	7.65973229395192	-5.26869237960764
C	8.46426085596817	6.50912354542705	-4.62424047375580
C	7.50997700080337	6.56430778473931	-3.56041297244820
C	7.07847448078352	5.44096694717133	-2.93329271031991
C	7.55373654135215	4.13780282227548	-3.30289659234103
C	8.47384210071932	4.05077012358364	-4.39255873991923
C	8.93402542809920	5.23298735208695	-5.04165474335167
H	7.26035781127087	0.79995482091403	-2.67036347161570
H	8.78893651859644	0.65608866129229	-4.55992700707554
H	10.21161496838206	1.75232537458639	-6.26196476369841
H	11.02561858929510	3.79603455671535	-7.35541401397186
H	11.02442563821756	6.25507681940080	-7.54327420045094
H	10.20894523486116	8.46343979326848	-6.79457471364707
H	8.57303074355718	8.62908404345362	-4.94759424478226
H	7.12879248623361	7.53325859122920	-3.25988963395169
H	6.36491658687243	5.51938705872123	-2.12882170672345
C	-0.56318878941156	3.13187155687221	-1.57683002927731
H	0.05417274361349	3.95067628147258	-1.93199016997982
H	-1.32492934966242	3.55550627357971	-0.92111551425889
N	-1.29396590643910	2.60925827594571	-2.73291581437519
N	-2.61235744383653	2.83799623483561	-2.84148602589569
N	-3.01882714169105	2.27744908065588	-3.94554562617183
C	-1.96117667977238	1.67687711485392	-4.57213665996575
C	-0.84033393567370	1.89098726983226	-3.77708921139333
H	0.20068921983269	1.60570552633123	-3.89861692896519
C	-1.99632637244853	0.97224787123988	-5.86146230619719
C	-0.90598985070334	0.13628410516236	-6.14421242194645
C	-0.77857553255530	-0.49888564349111	-7.36212040661274
C	-1.73912516680443	-0.34091379172730	-8.36434205171980
C	-1.61693652719161	-0.97662994006835	-9.63864198044636
C	-2.56392396909073	-0.82876467144656	-10.59692608786838
C	-3.73109459893277	-0.03697019542482	-10.36065321547959
C	-4.73232775609190	0.11360492278959	-11.32793998751961
C	-5.86035627844941	0.88130417221516	-11.07169878371636
C	-6.01147689216398	1.52145477855631	-9.84885717324557
C	-5.03491329839944	1.39930164084631	-8.85415427609817
C	-5.15218532223196	2.04253858801145	-7.58462354040125
C	-4.19586626027730	1.91748792999374	-6.63006319102534
C	-3.01708815622948	1.12501356524504	-6.83348148251213
C	-2.87891335940076	0.46544313068676	-8.09438435633248
C	-3.87868073915167	0.60965492483439	-9.09970163616720
H	-0.14022729759621	-0.04395380788266	-5.39747799787060
H	0.07092805121479	-1.14776786762821	-7.53418741971884
H	-0.74839440038708	-1.59888503063279	-9.81643050055055
H	-2.46399978538837	-1.32893012014946	-11.55282393553603
H	-4.62018202128038	-0.38713938049658	-12.28221397399705

H	-6.62804887105650	0.97907429156561	-11.82940194079993
H	-6.89420451932396	2.11751453304219	-9.64965620484701
H	-6.03492569939485	2.64132461059722	-7.39091984067462
H	-4.32118690669276	2.40728148861838	-5.67907153938613
C	2.86846539824065	-1.10687059891836	0.40088669954938
H	2.71929984602946	-1.48078465886031	1.41829416229780
H	2.69783716051537	-1.93019374629814	-0.29567922838685
H	3.91342252348537	-0.82577602566860	0.299688842601994
C	2.11031555248349	3.80144321641216	-0.56399667175581
H	2.77390872342436	4.03407770240768	0.26455052296065
H	2.68406799673894	3.95049972759418	-1.48366882755642
H	1.31386091133682	4.54057324561718	-0.54373311783768
C	-1.74986040584587	0.60480887647237	-0.71868267608908
H	-2.07912647883554	-0.12352148641923	0.01848397862740
H	-2.28676111652231	1.53059160574424	-0.52682265661230
H	-2.06295201748198	0.23976535257553	-1.69860188778698
C	2.30761497827373	-0.04629557447489	-4.08802027733161
O	1.50393589137627	-0.96372375826064	-4.33577535699241
O	2.14793424800679	1.17795098764587	-4.38792024038502
C	3.59144571135540	-0.36928372678475	-3.31318543383512
H	3.32363684311953	-0.44450208875366	-2.25927141392408
H	4.23449107582461	0.50401082481142	-3.41886951297167
C	4.39223052747830	-1.61515271799107	-3.72937568823778
C	4.04732847984895	-2.93374821897476	-3.00505120704364
H	4.34413431742361	-2.79293570524210	-1.96675477075799
H	4.70299262429698	-3.69291729949022	-3.44448338141169
C	2.62324716777417	-3.51443401670802	-2.99911950548795
O	1.96434646825368	-3.35649689712788	-1.93481768519357
O	2.25583519342944	-4.19650554572455	-3.98889181061190
C	5.88613463255181	-1.34687928106851	-3.34369654277463
O	6.72511348079905	-1.43520427649562	-4.28214527245309
O	6.14021497096083	-1.06854225291763	-2.14950355244517
O	4.34176513653905	-1.76778814885103	-5.15051655471538
H	5.29120544113330	-1.74606516723514	-5.38667981158179