Electronic Supplementary Material (ESI) for Dalton Transactions.

Zn^{II} coordination sphere and chemical structure influence over the reactivity of metallo-β-lactamase model compounds.

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Table S1: Structural data from the single-crystal XRD of the $[Zn(C_{18}H_{18}N_4)Cl](PF_6)]$ complex.

Molecular formula	$[Zn(C_{18}H_{18}N_4)Cl](PF_6)]$
Formula weight (g mol^{-1})	536.17
λ (Mo Kα, Å)	0.71073
Space group	I_{ba2}
Crystal System	Orthorhombic
a (Å)	16.794(3)
b (Å)	17.209(3)
c (Å)	14.623(3)
V (Å^3)	4226.1(15)
Z	8
T (K)	150
ρ_{calc} (g cm^{-3})	1.685
F(000)	2160
Reflections measured/independent	20046/4650 [$R_{int} = 0.052$]
Data/restraints/parameters	4650/25/301
R_1,wR_2 [$I > 2\sigma$ (I)]	0.035, 0.077
Diff. peak and hole (e/Å^3)	0.68, −0.27
Goodness of fit in F^2	1.02

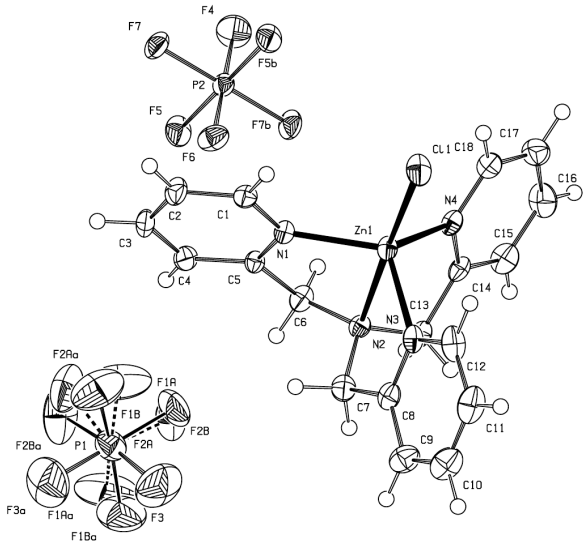

Figure S1: ORTEP image of the complex $[Zn(C_{18}H_{18}N_4)Cl](PF_6)$ with ellipsoids corresponds to 50 % probability.

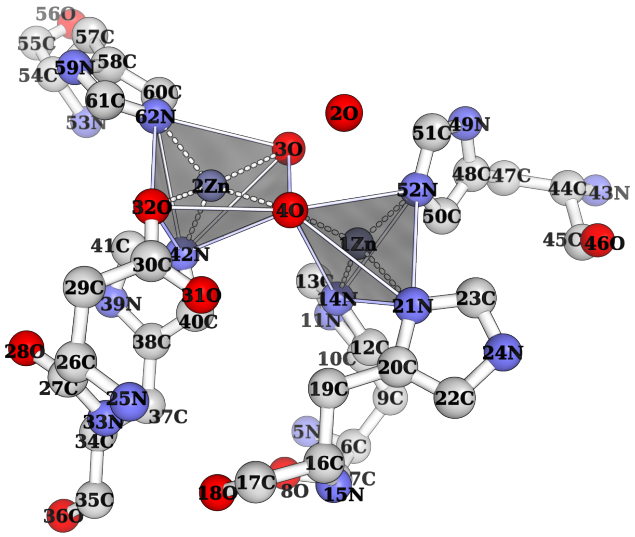

Figure S2: 1SML B3 MβL active sites numbered structure with the zinc site coordination sphere highlighted. Nitrogen atoms are colored in blue, oxygen atoms in red, zinc in grey and carbon in light grey. Hydrogens were removed for clarity.

Table S2: Bond lengths and bond angles of [Zn(N-NNN)], [Zn(N-NNO)] optimized by PBE0 functional, [ZnZn] crystals, and the retrieved 1SML pocket. See numbered structures in Figure S2 and Figure 4 main text

1SML pocket [1]		[Zn(N-NNN)]		[Zn(N-NNO)]		[ZnZn] [2]	
Measured	Length (Å)	Measured	Length (Å)	Measured	Length (Å)	Measured	Length (Å)
D(Zn2,N62)	2.0719	-	-	D(Zn1,N3)	2.1293	D(Zn1,N1)	2.1259
D(Zn2,N42)	2.0163	-	-	D(Zn1,N2)	2.1146	D(Zn1,N2)	2.1581
D(Zn2,O32)	2.0718	-	-	D(Zn1,O4)	1.9736	D (Zn1,O3)	1.9943
D(Zn2,O4)	2.2057	-	-	-	-	D(Zn1,O41)	2.0935
D(Zn2,O3)	2.4039	-	-	D(Zn1,1O)	2.2428	D(Zn1,O1)	2.0331
D(Zn2,Zn1)	3.4589	-	-	-	-	D(Zn1,Zn2)	3.1330
D(Zn1,N14)	2.0272	D(Zn1,N3)	2.0850	-	-	D(Zn2,N4)	2.1581
D(Zn1,N21)	2.1095	D(Zn1,N4)	2.0860	-	-	D(Zn2,O5)	1.9944
D(Zn1,N52)	2.0455	D(Zn1,N1)	2.0863	-	-	D(Zn2,N3)	2.1259
D(Zn1,O11)	2.0750	-	-	-	-	D(Zn2,O1)	2.0935
	Angle (°)		Angle (°)		Angle (°)		Angle (°)
A(N42,Zn2,N62)	102.0837	-	-	A(N2,Zn1,N3)	155.7314	A(N2,Zn1,N1)	81.2852
A(N42,Zn2,O32)	93.7430	-	-	A(N1,Zn1,O4)	98.6513	A(N2,Zn1,O2)	90.1501
A(O32,Zn2,N62)	92.2096	-	-	A(O4,Zn1,N3)	93.2717	A(N1,Zn1,O1)	81.5796
A(N42,Zn2,O3)	101.238	-	-	A(N2,Zn1,O1)	86.1456	A(N2,Zn1,O4)	91.6223
A(N42,Zn2,O4)	111.047	-	-	A(N1,Zn1,O2)	95.9252	A(N2,Zn2,O1)	111.049
A(N14,Zn1,N52)	99.7098	A(N4,Zn1,N3)	113.8002	-	-	A(O5,Zn2,N4)	141.5231
A(N21,Zn1,N52)	105.818	A(N1,Zn1,N3)	113.8652	-	-	A(O5,Zn2,N3)	92.8427
A(N14,Zn1,N21)	99.2391	A(N4,Zn1,N1)	114.1139	-	-	A(N3,Zn2,N4)	81.2855

Table S3: Fukui index values of $[Zn(N-NNN)Cl]^+$ atoms for Hirshfeld Population Analysis (HPA) and Natural Population Analysis (NPA) by employing PBE and PBE0 functionals.

	PBE				PBE0			
Complex	HPA		NPA		HPA		NPA	
	f^+	f^-	f^+	f^-	f^+	f^-	f^+	f^-
0Zn	0.006505	0.049264	-0.004375	0.028358	0.006815	0.040195	-0.004031	0.023057
1Cl	0.033915	0.198709	0.022741	0.266628	0.031500	0.175356	0.020149	0.231773
2N	0.025521	0.001413	0.040440	-0.004529	0.026917	0.005110	0.043459	-0.000096
3N	0.000705	0.079243	0.004023	0.165915	0.000813	0.108820	0.004745	0.224198
4N	0.025461	0.006828	0.040345	0.003251	0.026841	0.004727	0.043341	-0.000681
5N	0.025421	0.005843	0.040242	0.002270	0.026730	0.005122	0.043103	-0.000157
6C	0.025565	0.011295	0.016463	0.004795	0.024972	0.012123	0.013705	0.004277
7H	0.014654	0.009339	0.014575	0.002592	0.014494	0.009824	0.014765	0.005294
8C	0.040397	0.027324	0.042393	0.029959	0.040556	0.027870	0.042537	0.029858
9H	0.024908	0.019012	0.022109	0.019480	0.024741	0.019609	0.021976	0.020471
10C	0.051995	0.026757	0.073851	0.024269	0.052957	0.027227	0.077306	0.024743
11H	0.028742	0.019709	0.023426	0.020735	0.028690	0.019667	0.023044	0.020838
12C	0.024098	0.019457	0.004748	0.019088	0.022200	0.019229	-0.001290	0.019409
13H	0.018796	0.016125	0.018954	0.016228	0.018065	0.015778	0.018860	0.016069
14C	0.024137	0.002009	0.040805	-0.008632	0.025045	-0.000270	0.043910	-0.014820
15C	0.010482	0.014615	-0.004421	-0.018620	0.010960	0.016459	-0.004477	-0.025568
16H	0.015644	0.033691	0.017383	0.048820	0.015560	0.037058	0.017243	0.054702
17H	0.015018	0.014354	0.015522	0.016114	0.015669	0.016182	0.015968	0.019241
18C	0.010470	0.014627	-0.004403	-0.018558	0.010949	0.016427	-0.004434	-0.025510
19H	0.015640	0.033069	0.017384	0.047810	0.015559	0.037009	0.017250	0.054617
20H	0.014994	0.014891	0.015472	0.017162	0.015639	0.016133	0.015891	0.019158
21C	0.024090	0.002814	0.040768	-0.009311	0.024964	-0.000405	0.043799	-0.014943
22C	0.024065	0.020449	0.004728	0.020049	0.022167	0.019080	-0.001279	0.019230
23H	0.018783	0.016971	0.018942	0.017206	0.018051	0.015693	0.018841	0.015985
24C	0.051921	0.027577	0.073710	0.025455	0.052866	0.027129	0.077130	0.024672
25H	0.028715	0.020123	0.023414	0.021064	0.028658	0.019610	0.023031	0.020781
26C	0.040395	0.027610	0.042451	0.029292	0.040546	0.027753	0.042588	0.029761
27H	0.024902	0.020041	0.022101	0.020881	0.024734	0.019524	0.021963	0.020378
28C	0.025506	0.011415	0.016361	0.004131	0.024909	0.011974	0.013610	0.004197
29H	0.014635	0.010232	0.014566	0.001986	0.014473	0.009726	0.014747	0.005176
30C	0.010462	0.014726	-0.004416	-0.018614	0.010935	0.016413	-0.004436	-0.025537
31H	0.015641	0.033543	0.017389	0.048519	0.015553	0.036962	0.017246	0.054534
32H	0.014990	0.014645	0.015473	0.016724	0.015627	0.016149	0.015887	0.019195
33C	0.024063	0.003562	0.040695	-0.007652	0.024885	-0.000299	0.043622	-0.014855
34C	0.024049	0.021552	0.004739	0.022057	0.022125	0.019166	-0.001252	0.019282
35H	0.018767	0.017257	0.018930	0.017274	0.018017	0.015762	0.018810	0.016067
36C	0.051891	0.027696	0.073663	0.024629	0.052759	0.027219	0.076947	0.024791
37H	0.028700	0.020338	0.023402	0.021382	0.028610	0.019651	0.022999	0.020816
38C	0.040362	0.028704	0.042401	0.031132	0.040470	0.027808	0.042503	0.029753
39H	0.024889	0.020112	0.022091	0.020655	0.024695	0.019595	0.021937	0.020467
40C	0.025492	0.012957	0.016366	0.005783	0.024853	0.012022	0.013580	0.004189
41H	0.014620	0.010096	0.014548	0.004224	0.014438	0.009806	0.014708	0.005192

Table S4: Fukui index values of [Zn(N−NNS)Cl] atoms for Hirshfeld Population Analysis (HPA) and Natural Population Analysis (NPA) by employing PBE and PBE0 functionals.

	PBE				PBE0			
Complex	HPA		NPA		HPA		NPA	
	f^+	f^-	f^+	f^-	f^+	f^-	f^+	f^-
0Zn	0.003865	0.053902	-0.016700	0.006828	0.003795	0.051891	-0.017274	0.001564
1S	0.043234	0.356885	0.037507	0.525846	0.038571	0.495461	0.031115	0.732709
2N	0.044379	-0.011493	0.077743	-0.029676	0.049640	-0.012535	0.088293	-0.032118
3N	-0.000824	0.019811	0.001592	0.039843	-0.000706	-0.000593	0.002218	-0.005608
4N	0.040300	-0.006323	0.072311	-0.020965	0.040975	-0.011422	0.074237	-0.032500
5C	0.011082	0.004792	-0.009496	-0.002250	0.011365	0.001377	-0.010774	0.002788
6H	0.016975	0.021351	0.016979	0.029437	0.016802	0.016699	0.016715	0.023577
7H	0.017004	0.000593	0.025991	-0.012288	0.017262	-0.005157	0.026682	-0.022659
8C	0.004734	0.011193	-0.001330	-0.010579	0.004456	0.010413	-0.001955	-0.008306
9H	0.014839	0.033044	0.018231	0.043360	0.013959	0.031669	0.017403	0.041406
10H	0.004143	0.012699	-0.001833	0.012084	0.004109	0.012764	-0.001720	0.012094
11C	0.035510	-0.004251	0.055851	-0.014740	0.038633	-0.007079	0.062035	-0.017813
12C	0.010175	0.007932	-0.004124	-0.010940	0.010157	0.005657	-0.004527	-0.008248
13H	0.017534	0.020434	0.020130	0.026812	0.017313	0.014905	0.020343	0.018566
14H	0.014819	0.011807	0.012643	0.013940	0.014778	0.011378	0.011395	0.014041
15C	0.034575	-0.001785	0.055766	-0.010769	0.035175	-0.004536	0.058869	-0.013328
16C	0.006053	0.030029	-0.006771	-0.046828	0.005363	0.035827	-0.007184	-0.068273
17H	0.009206	0.040267	0.007259	0.056423	0.008345	0.049493	0.006401	0.071917
18H	0.015896	0.036237	0.018350	0.045040	0.015278	0.038929	0.018084	0.048246
19C	0.032169	0.015200	0.007230	0.013757	0.028659	0.012986	-0.001941	0.011876
20H	0.024217	0.014327	0.023325	0.014544	0.022759	0.012405	0.022925	0.012995
21C	0.035785	0.002506	0.024207	-0.004962	0.034084	-0.000536	0.019454	-0.006392
22H	0.019365	0.005003	0.020183	-0.001236	0.018818	0.002359	0.019967	0.000294
23C	0.040021	0.004925	0.034387	0.001954	0.042314	0.004393	0.035427	0.001464
24H	0.019375	0.005773	0.020003	-0.002499	0.020425	0.005369	0.021427	0.000957
25C	0.035183	0.015258	0.011480	0.015669	0.033961	0.012963	0.003440	0.013121
26H	0.025995	0.013287	0.024436	0.013051	0.025905	0.011582	0.025204	0.011825
27C	0.050008	0.020945	0.044391	0.022006	0.050786	0.019146	0.042032	0.019550
28H	0.031488	0.016242	0.026949	0.016853	0.031860	0.015069	0.027560	0.015935
29C	0.075879	0.022904	0.118058	0.021803	0.081251	0.021067	0.130565	0.020318
30H	0.040382	0.017573	0.029170	0.018092	0.041964	0.016040	0.029560	0.016738
31C	0.070837	0.023231	0.107848	0.023344	0.070887	0.020838	0.110410	0.020949
32H	0.038371	0.017976	0.028090	0.018514	0.037685	0.016147	0.027266	0.016887
33C	0.051323	0.019394	0.052256	0.019188	0.050686	0.016713	0.051696	0.016280
34H	0.031613	0.016176	0.026566	0.017354	0.030878	0.014443	0.026068	0.015814
35Cl	0.034479	0.132148	0.021323	0.151992	0.031797	0.063865	0.018584	0.053338

Table S5: Fukui index values of $[Zn(N{-}NNO)(H_2O)_2]^+$ atoms for Hirshfeld Population Analysis (HPA) and Natural Population Analysis (NPA) by employing PBE and PBE0 functionals.

	PBE				PBE0			
Complex	HPA		NPA		HPA		NPA	
	f^+	f^-	f^+	f^-	f^+	f^-	f^+	f^-
0Zn	0.015136	0.036499	0.012923	0.022996	0.015665	0.024586	0.012267	0.006114
1O	0.005841	0.000511	-0.007704	-0.012519	0.004447	-0.000899	-0.009350	-0.013271
2O	0.002736	0.023937	-0.006391	0.024334	0.001295	0.014688	-0.008402	0.011027
3O	0.032118	0.228217	0.037952	0.310964	0.030274	0.343409	0.036149	0.468870
4O	0.005059	0.061507	-0.000760	0.104621	0.003159	0.089887	-0.003849	0.155577
5N	0.001212	0.057494	0.005337	0.129770	0.001119	0.037466	0.005583	0.079465
6N	0.039079	-0.000815	0.076220	-0.006995	0.043486	-0.008945	0.085414	-0.022591
7N	0.039185	0.001661	0.075234	-0.001346	0.041704	-0.009060	0.081305	-0.022633
8C	0.036091	-0.007906	0.054078	-0.022775	0.038305	-0.012401	0.058054	-0.026793
9C	0.031970	0.011050	0.006367	0.008955	0.030640	0.007503	-0.001226	0.006573
10C	0.070308	0.022464	0.107432	0.021634	0.074904	0.018353	0.119386	0.016877
11C	0.046498	0.022660	0.039109	0.022903	0.046784	0.018533	0.036077	0.018988
12C	0.039115	0.009625	0.031762	-0.000337	0.041139	0.005228	0.032901	-0.001907
13C	0.035765	-0.004099	0.054044	-0.018987	0.036532	-0.010718	0.056164	-0.026449
14C	0.032517	0.014770	0.007208	0.013065	0.029928	0.009367	-0.001086	0.008898
15C	0.071001	0.024621	0.108332	0.023054	0.073134	0.019346	0.115970	0.017943
16C	0.047163	0.025663	0.039840	0.027098	0.046651	0.019096	0.037331	0.019775
17C	0.039890	0.011844	0.033097	0.001848	0.040059	0.005336	0.031736	-0.001014
18C	0.013217	0.011337	-0.006930	-0.016639	0.013607	0.008251	-0.007547	-0.013943
19C	0.013171	0.015170	-0.006046	-0.013131	0.013401	0.011620	-0.006309	-0.011402
20C	0.003817	0.039802	-0.004968	0.043632	0.003468	0.045453	-0.005563	0.053865
21C	0.002307	0.065988	-0.009726	-0.006050	0.000809	0.089882	-0.010927	-0.012605
22H	0.023328	0.012144	0.023179	0.013170	0.022985	0.009372	0.023468	0.010629
23H	0.036284	0.017600	0.027676	0.018951	0.037471	0.015166	0.027520	0.016805
24H	0.029115	0.018028	0.026280	0.019324	0.029122	0.015341	0.026400	0.016783
25H	0.023012	0.010870	0.021696	0.013592	0.023782	0.007567	0.022262	0.009799
26H	0.023713	0.013823	0.023435	0.014470	0.022660	0.009891	0.023076	0.010722
27H	0.036661	0.018641	0.027897	0.019865	0.036783	0.015268	0.027122	0.016642
28H	0.029383	0.018915	0.026411	0.019748	0.028853	0.015149	0.025993	0.016347
29H	0.022180	0.011372	0.021148	0.012780	0.022229	0.006869	0.021172	0.007460
30H	0.016836	0.023967	0.018599	0.032858	0.016686	0.016277	0.018443	0.020258
31H	0.021612	0.017945	0.027123	0.020715	0.021882	0.018162	0.027545	0.022773
32H	0.020925	0.018844	0.025893	0.021501	0.020792	0.018968	0.025434	0.023658
33H	0.017318	0.026094	0.018948	0.034607	0.016850	0.017551	0.018582	0.021468
34H	0.009394	0.030270	0.006118	0.035133	0.009601	0.033054	0.006566	0.040849
35H	0.011952	0.033997	0.012528	0.033330	0.011264	0.031535	0.011169	0.031043
36H	0.018238	0.011337	0.015874	0.010730	0.016182	0.009429	0.013774	0.009423
37H	0.019466	0.011022	0.016960	0.010275	0.016536	0.008957	0.013758	0.008786
38H	0.011811	0.022702	0.010793	0.019025	0.010951	0.020009	0.010774	0.018952
39H	0.005574	0.010420	0.003033	-0.006172	0.004861	0.005451	0.002866	-0.013759

Table S6: Zn^{II} fukui index values (f^+ & f^-) for Hirshfeld Population Analysis (HPA) and Natural Population Analysis (NPA) by employing PBE and PBE0 functionals.

	PBE				PBE0			
Complex	HPA		NPA		HPA		NPA	
	f^+	f^-	f^+	f^-	f^+	f^-	f^+	f^-
[Zn(N-NNO)]	0.015136	0.036499	0.012923	0.022996	0.015665	0.024586	0.012267	0.006114
[Zn(N-NNN)]	0.006505	0.049264	-0.004375	0.028358	0.006815	0.040195	-0.004031	0.023057
[Zn(N-NNS)]	0.003865	0.053902	-0.016700	0.006828	0.003795	0.051891	-0.017274	0.001564

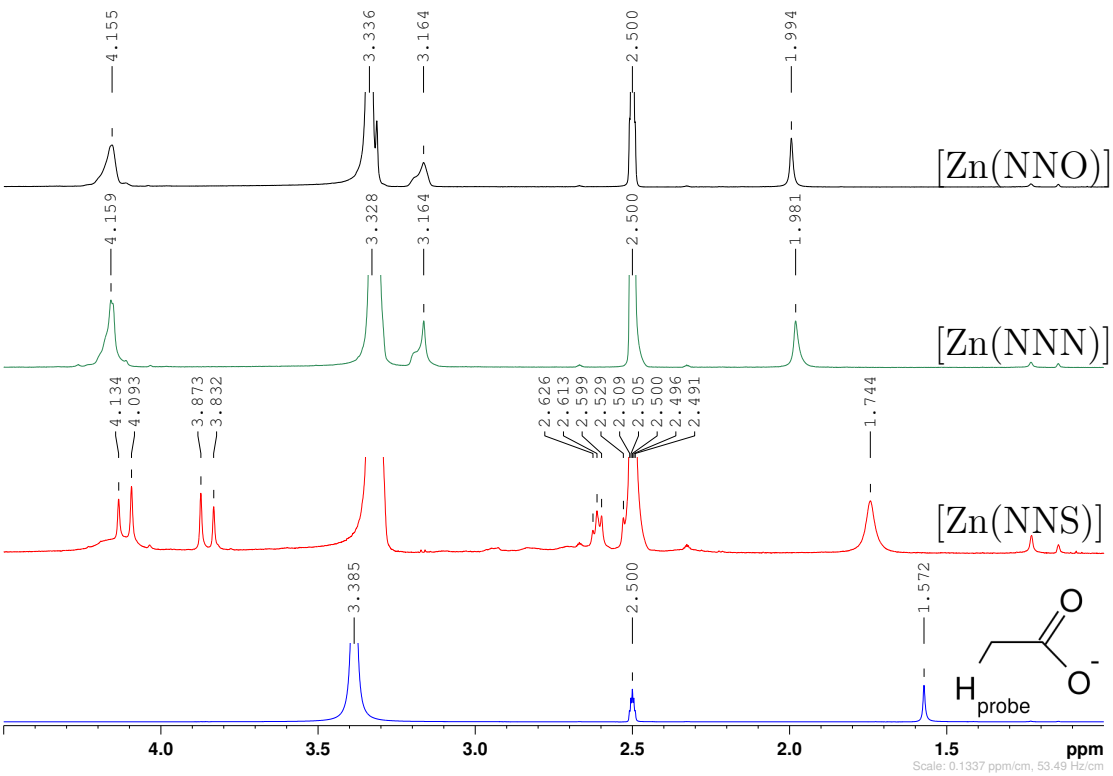

Figure S3: ^{1}H NMR spectra evaluation of the Zn^{II} Lewis acidity in the model complexes using acetate ion as probe in DMSO-d_6. KOAc (blue), [Zn(N-NNS)] + KOAc (red), [Zn(N-NNN)] + KOAc (green) and [Zn(N-NNO)] + KOAc (black). The residual solvent signals are: DMSO at 2.5 ppm and water ∼3.4-3.3 ppm. The remaining signals are in agreement with the reported in literature for each complex.[3,4]

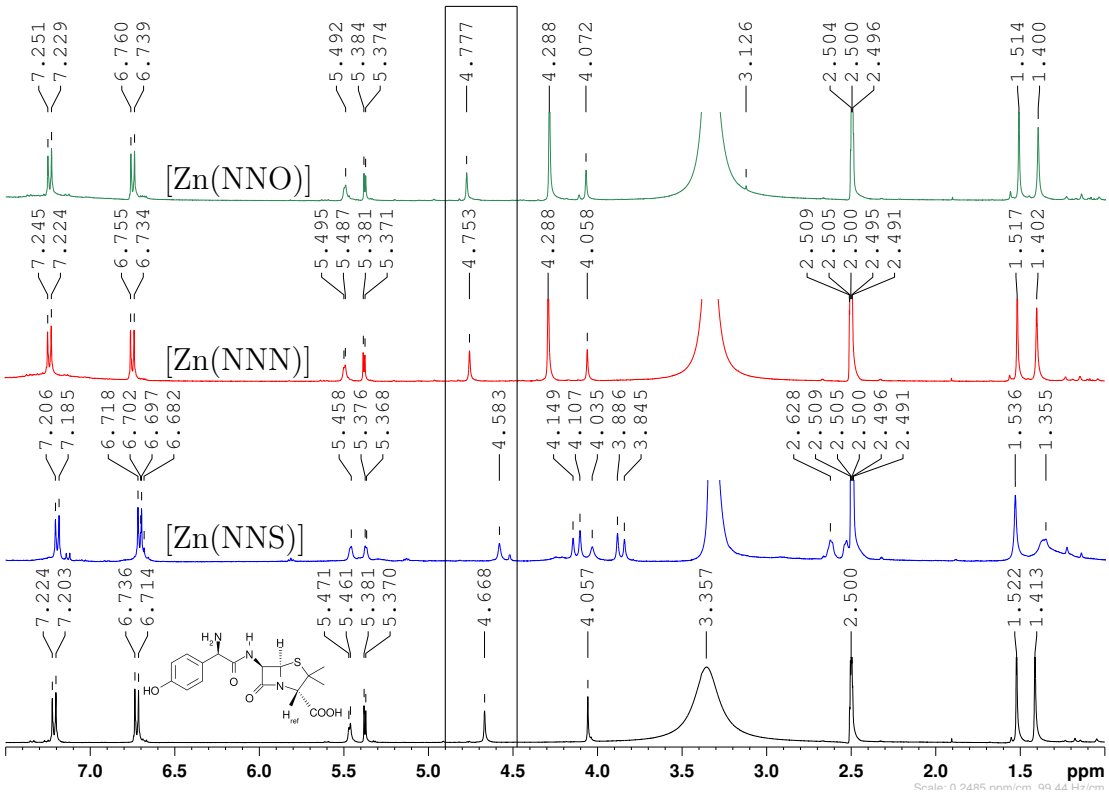

Figure S4: ^{1}H NMR spectra of the amoxicillin interaction with our mimetics in d_6-DMSO, highlighting the geminal hydrogen used as probe. [Zn(N-NNO)] + Am (green), [Zn(N-NNN)] + Am (red), [Zn(N-NNS) + Am (blue) and Amoxicillin (Am) (black).

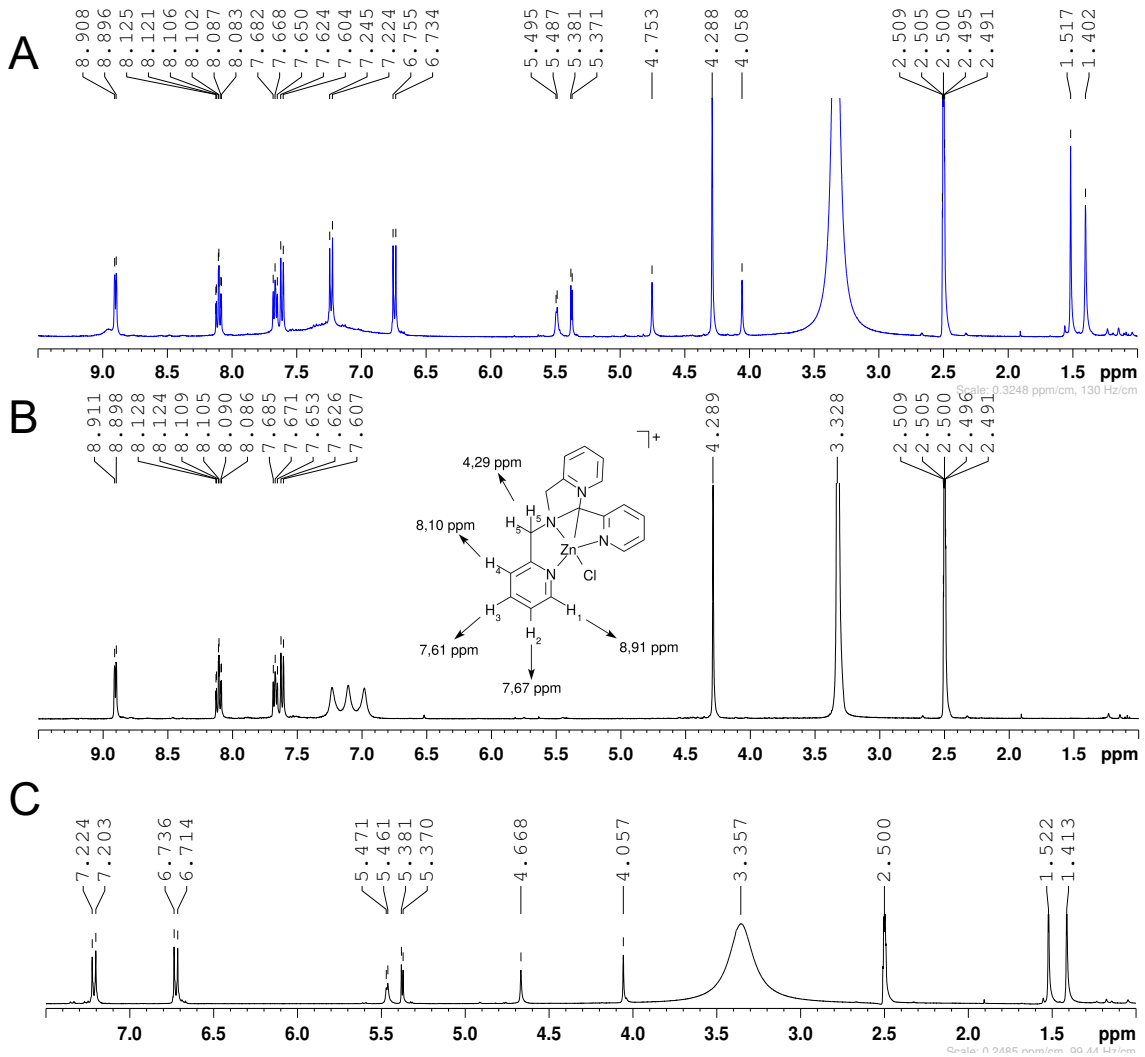

Figure S5: ^{1}H NMR spectra of the complex [Zn(N−NNN)Cl](PF$_6$) (A) and amoxicillin with [Zn(N−NNN)Cl](PF$_6$) (B) in d$_6$-DMSO. The signal centered in 7.1 ppm is due to NH_4^+ from NH_4PF_6 used in excess for precipitation. Amoxicillin spectrum in d$_6$-DMSO is shown for reference (C)

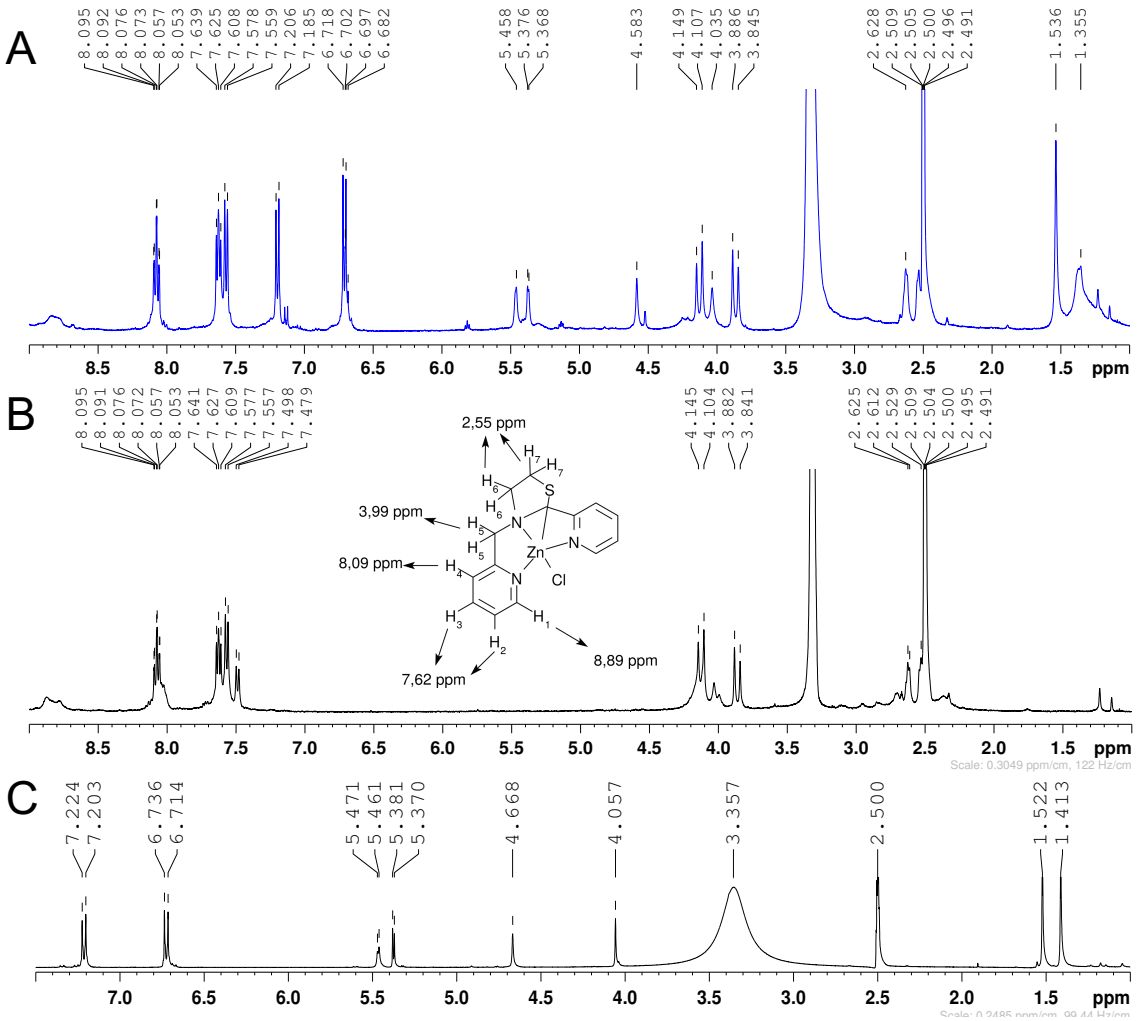

Figure S6: ^{1}H NMR spectra of the complex [Zn(N−NNS)Cl] (A) and amoxicillin with [Zn(N−NNS)Cl] (B) in d_6-DMSO. Amoxicillin spectrum in d_6-DMSO is shown for reference (C).

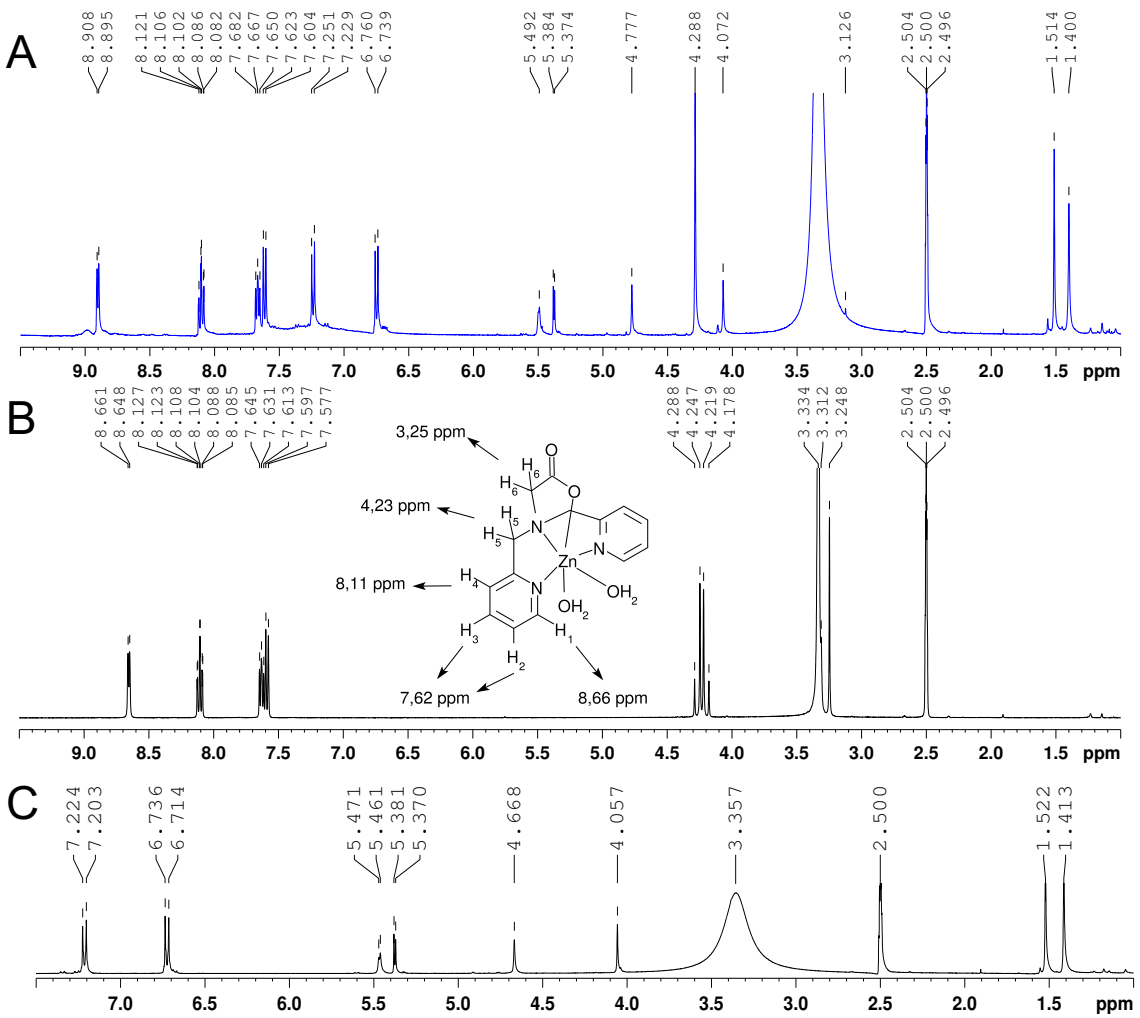

Figure S7: ^{1}H NMR spectra of the complex $[Zn(N\text{-}NNO)(H_2O)_2](NO_3)$ (A) and amoxicillin with $[Zn(N\text{-}NNO)(H_2O)_2](NO_3)$ (B) in d_6-DMSO. The spectrum of amoxicillin in d_6-DMSO is shown for reference (C)

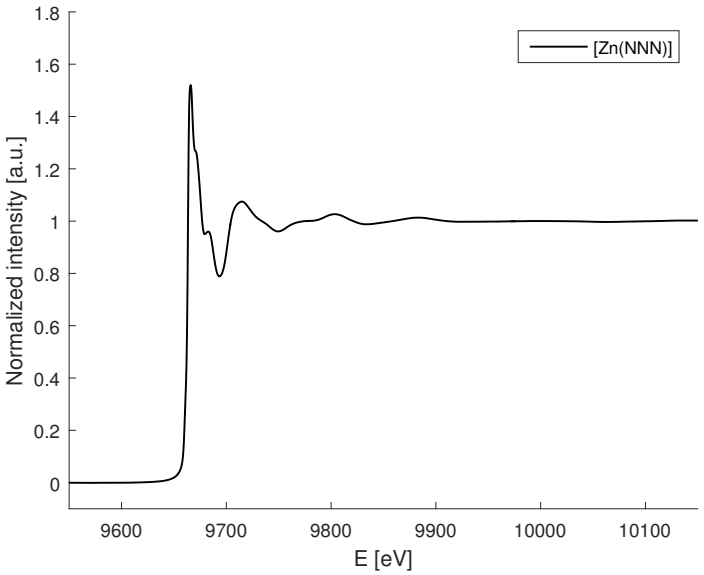

Figure S8: Zn K-edge X-ray absorption spectrum of the [Zn(N−NNN)Cl](PF_6) complex in solid state.

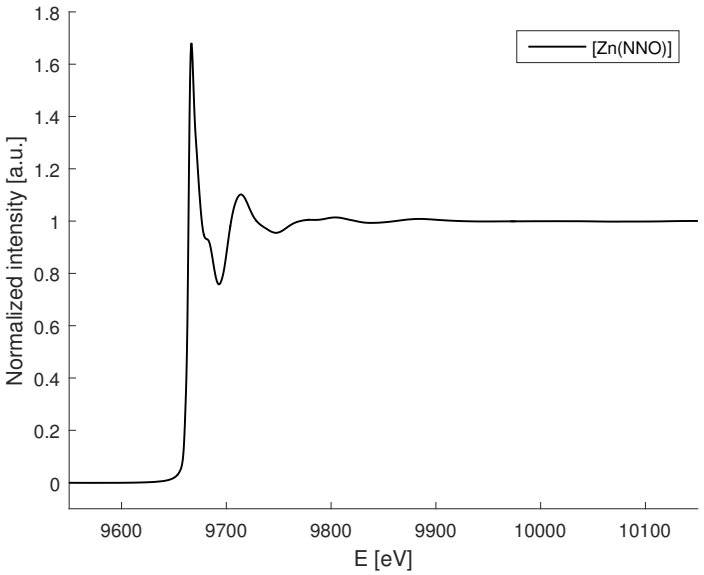

Figure S9: Zn K-edge X-ray absorption spectrum of the $[Zn(N{-}NNO)(H_2O)_2](NO_3)$ complex in solid state.

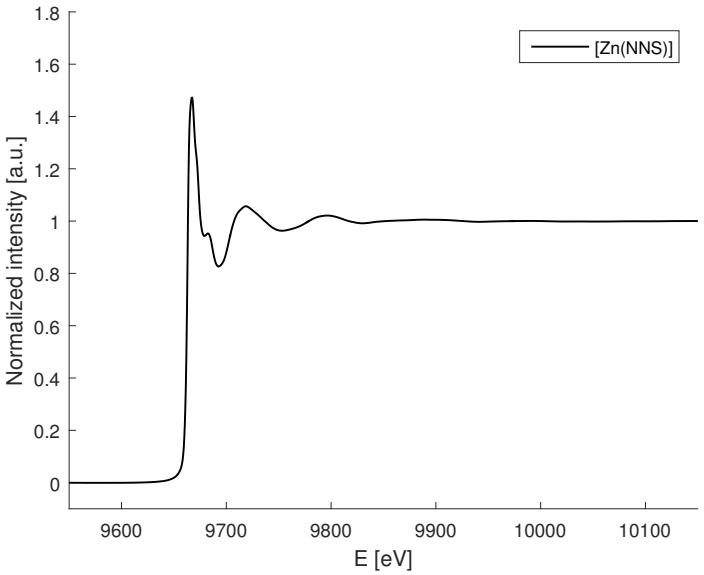

Figure S10: Zn K-edge X-ray absorption spectrum of the [Zn(N−NNS)Cl] complex in solid state.

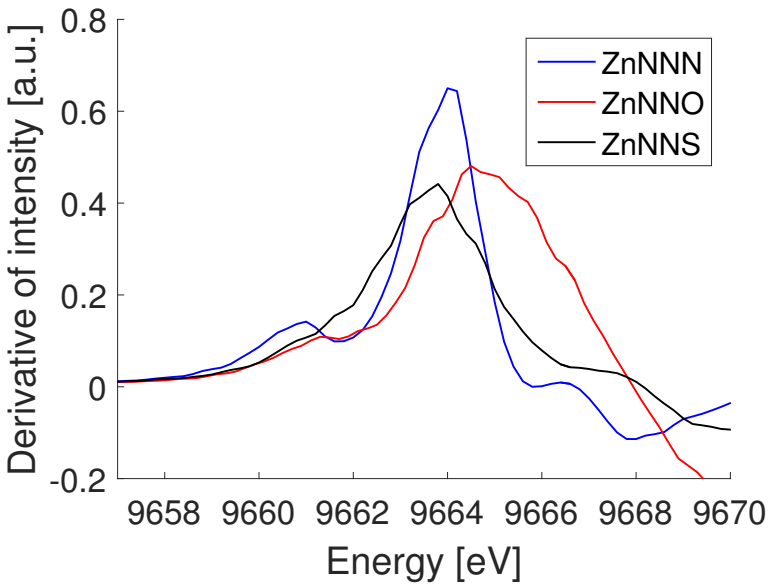

Figure S11: First derivative of Zn K-edge XAS spectra of solid model complexes [Zn(N-NNX)], with X = O, N or S, ([Zn(N-NNN) in blue, [Zn(N-NNO)] in red, and [Zn(N-NNS)] in black). The rising edge energies were taken as the maximum of the edge (9663-4 eV). It is possible to see the variation between its position for each complex and also highlighting the pre-edge absorption around 9661 eV.

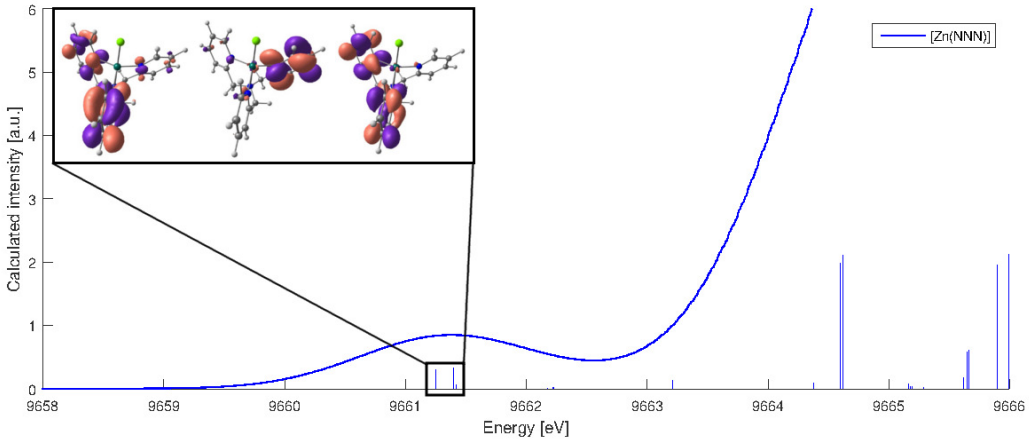

Figure S12: TDDFT spectra of [Zn(N-NNN)] focusing in the pre-edge absorption and highlighting molecular orbitais involved in these transitions. Nitrogen atoms are colored in blue, oxygen in red,chlorine atoms in green, zinc in grey and carbon in light grey.

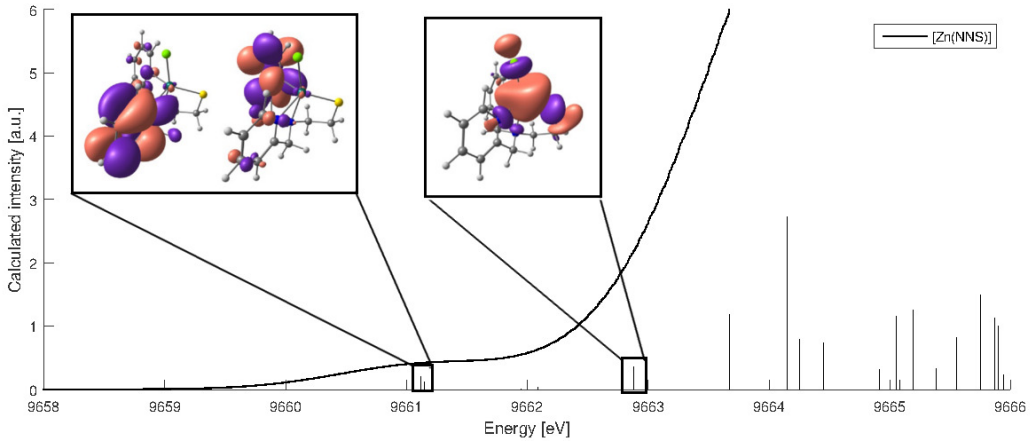

Figure S13: TDDFT spectra of [Zn(N-NNS)] focusing in the pre-edge absorption and highlighting molecular orbitais involved in these transitions. Nitrogen atoms are colored in blue, oxygen in red, sulfur in yellow, chlorine atoms in green, zinc in grey and carbon in light grey.

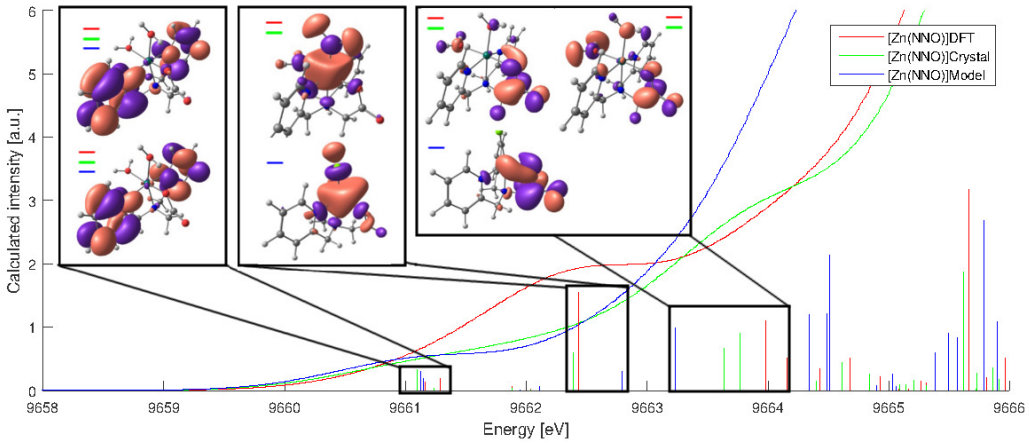

Figure S14: TDDFT spectra of [Zn(N-NNO)] models focusing in the pre-edge absorption and highlighting molecular orbitais involved in these transitions. Nitrogen atoms are colored in blue, oxygen atoms in red, zinc in grey and carbon in light grey.

Table S7: Experimental Zn K-edge XAS rising edge energies (E_{K-edge}) and pre-edge absorptions ($E_{pre-edge}$) for [Zn(NNX)], with N = O, N or S, and ΔE_{K-edge} relative to the [Zn(NNS)] E_{K-edge}. All data were acquired with 0.2 eV sampling step in the near-edge region (9644 to 9704 eV).

Compound	E_{K-edge} (eV)	ΔE_{K-edge} (eV)	$E_{pre-edge}$ (eV)
Zn foil	9659.0	-	-
[Zn(NNS)]	9663.0	0.0	-
[Zn(NNN)]	9663.5	+ 0.5	9660.0
[Zn(NNO)]	9664.3	+ 1.3	9660.2

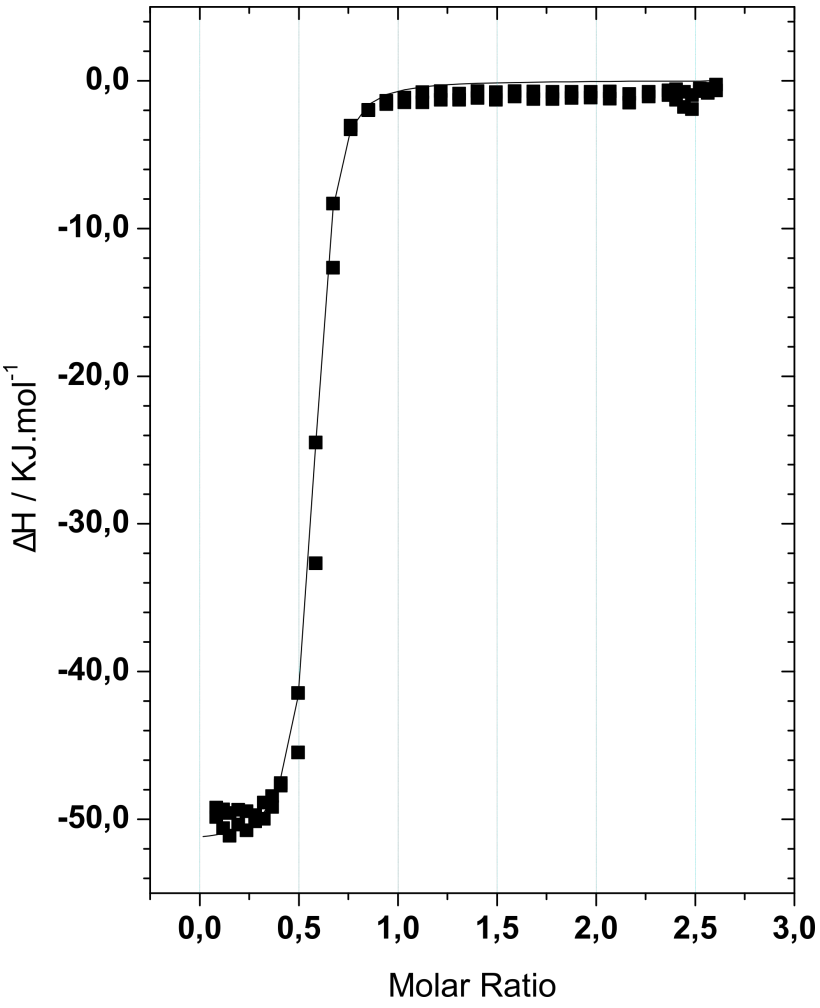

Figure S15: Enthalpy variation by molar ratio of amoxicillin titrated to a solution of [Zn(NNN)Cl](PF_6) complex and the curve resultant of the one-site fitting analysis.

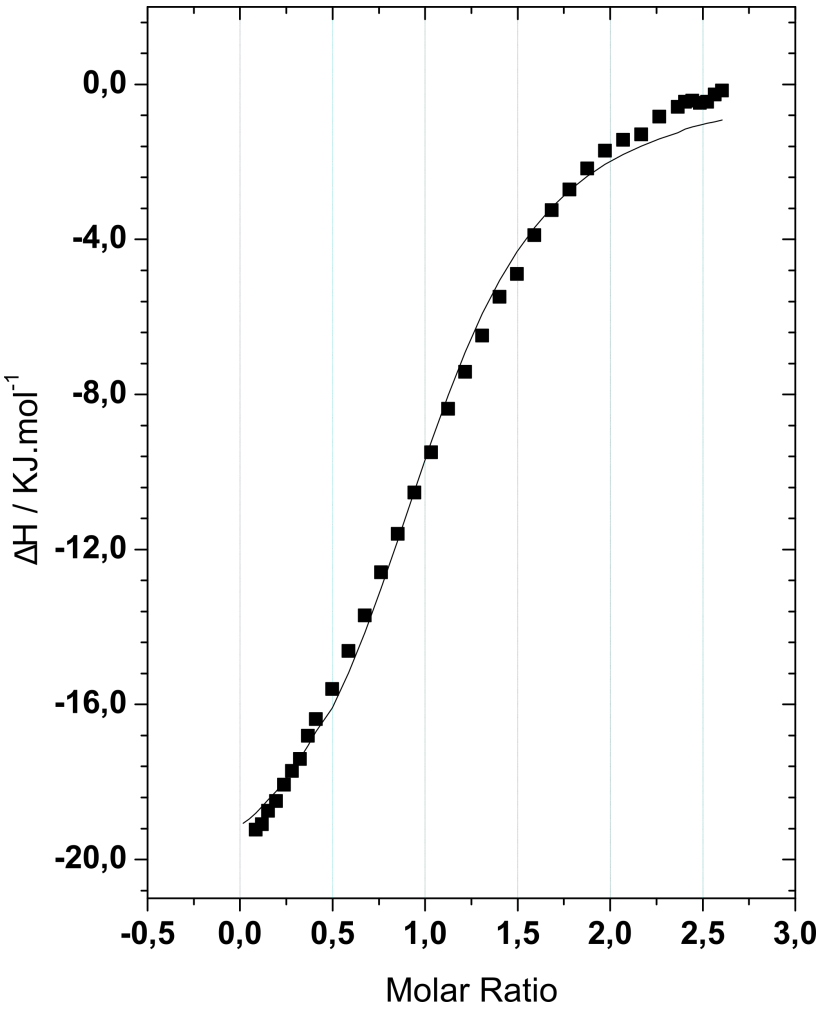

Figure S16: Enthalpy variation by molar ratio of amoxicillin titrated to a solution of $[Zn(NNO)(H_2O)_2](NO_3)$ complex and the curve resultant of the one-site fitting analysis.

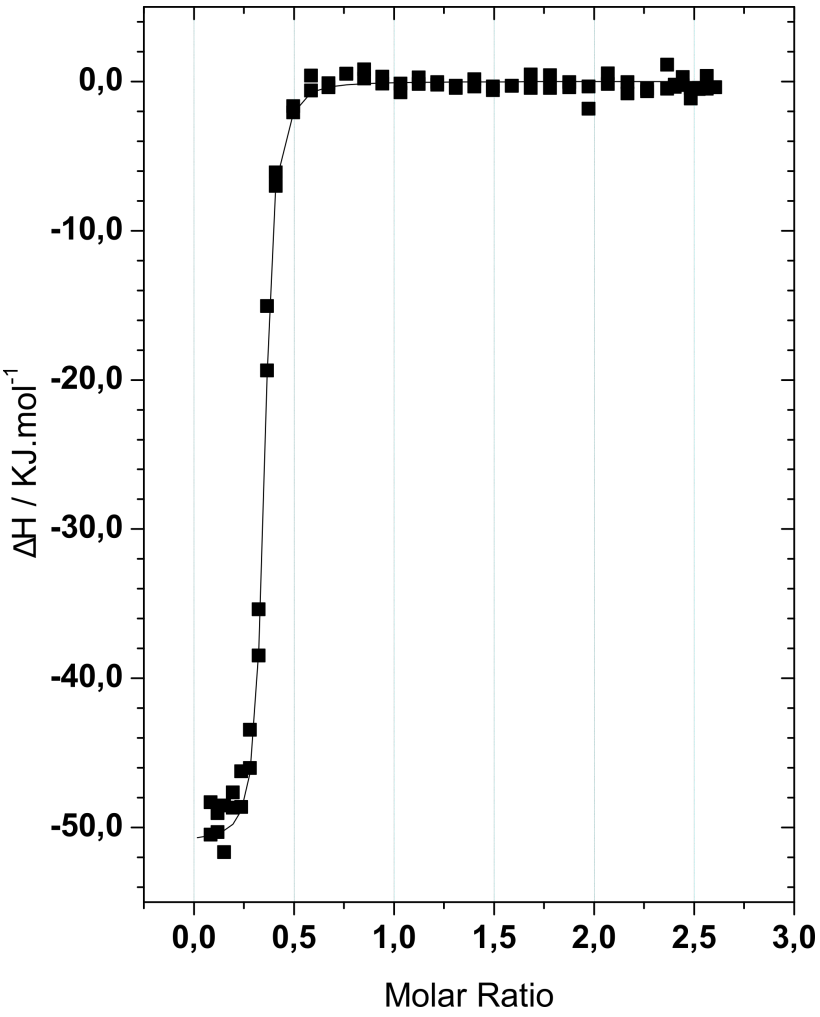

Figure S17: Enthalpy variation by molar ratio of amoxicillin titrated to a solution of [Zn(NNS)Cl] complex and the curve resultant of the one-site fitting analysis.

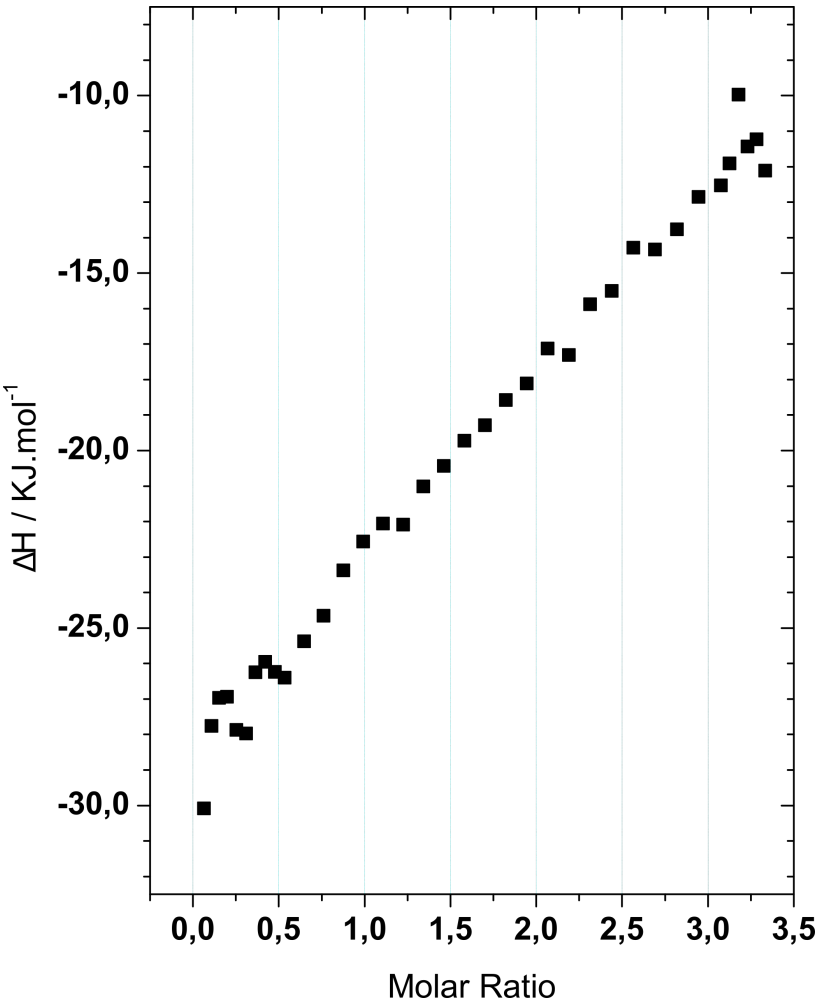

Figure S18: Enthalpy variation by molar ratio of amoxicillin titrated to a solution of the literature zinc complex $[Zn_2(C_{11}H_{17}N_2O_1)_2(C_2H_3O_2)_2]$.

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