Supporting information

Molecular Complexes and Main-Chain Organometallic Polymers Based on Janus Bis(carbenes) Fused to Metalloprophyrins

J.-F. Longevial*, Mamadou Lo, Aurélien Lebrun, D. Laurencin, S. Clément and S. Richeter*

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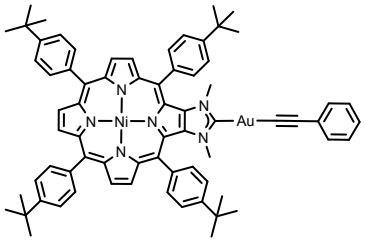


Chemical Formula: $C_{71}H_{69}AuN_6Ni$
Exact Mass: 1260,4603

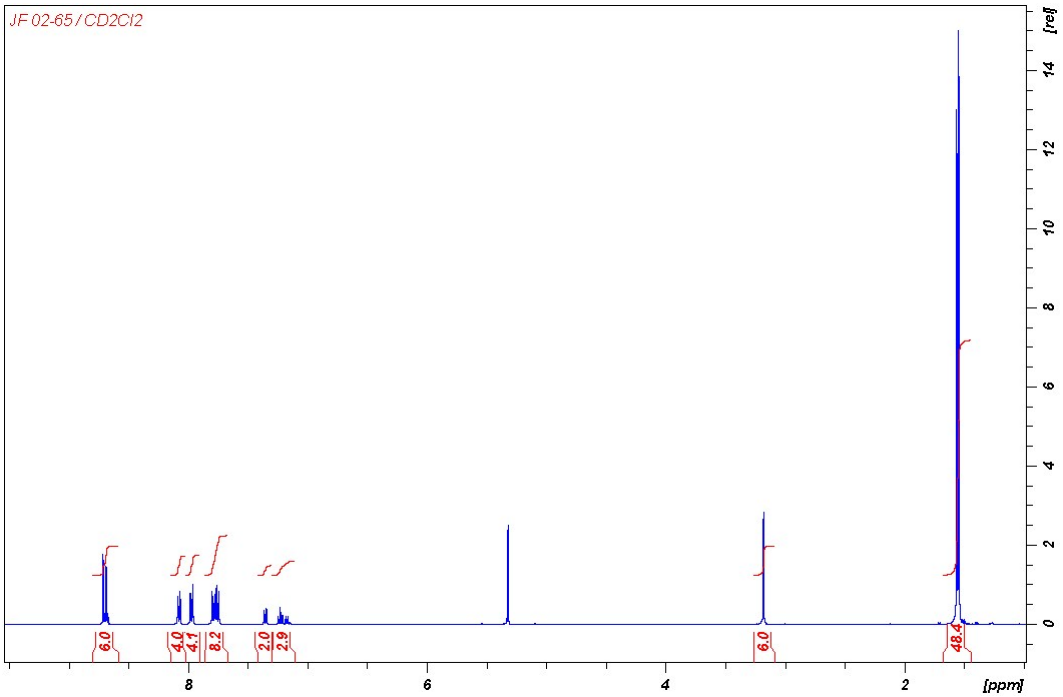


Figure S 1. ^{1}H NMR spectrum of **[NiAuPh]** in CD_2Cl_2, 400 MHz, 298K

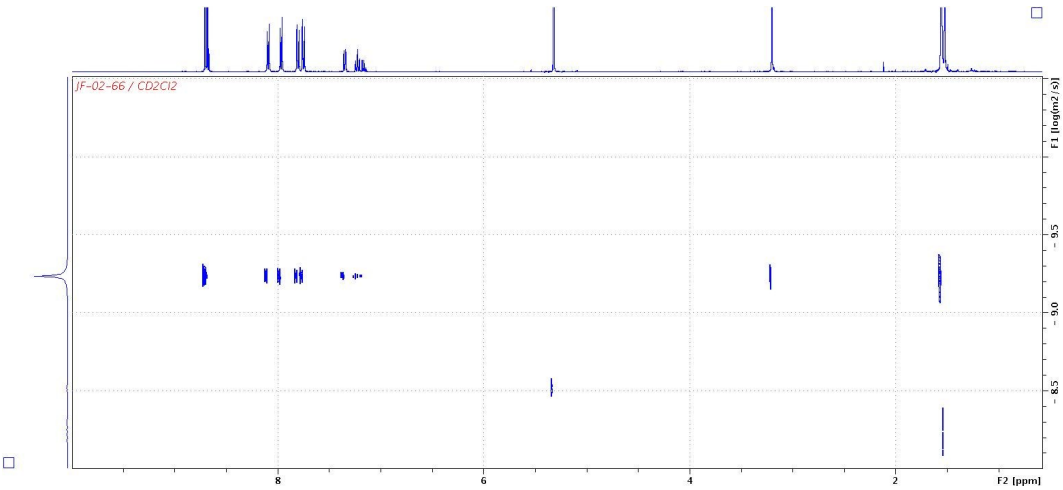


Figure S 2. ^{1}H 2D DOSY NMR spectrum of **[NiAuPh]** in CD_2Cl_2, 400 MHz, 298K

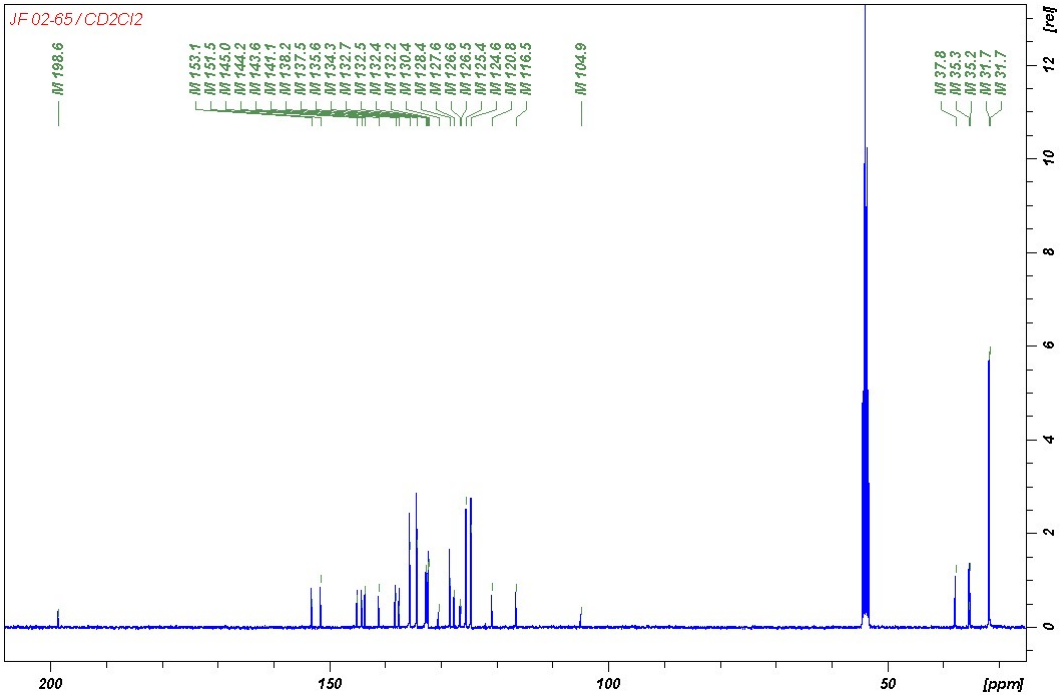


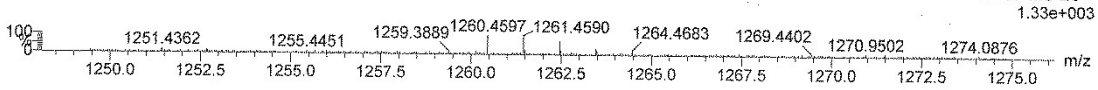
Figure S 3. $^{13}C\{^{1}H\}$ NMR spectrum of **[NiAuPh]** in CD_2Cl_2, 126 MHz, 298K

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -50.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
188 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 Ni: 1-1 Au: 0-1

SYNAPT G2-S#UEB205 JF.02.65 26-Nov-2015
Y-YG151126-02 4 (0.175) 1: TOF MS ES+
1.33e+003



Minimum:				-50.0				
Maximum:		10.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
1260.4597	1260.4603	-0.6	-0.5	41.5	326.7	n/a	n/a	C71 H69 N6 Ni Au

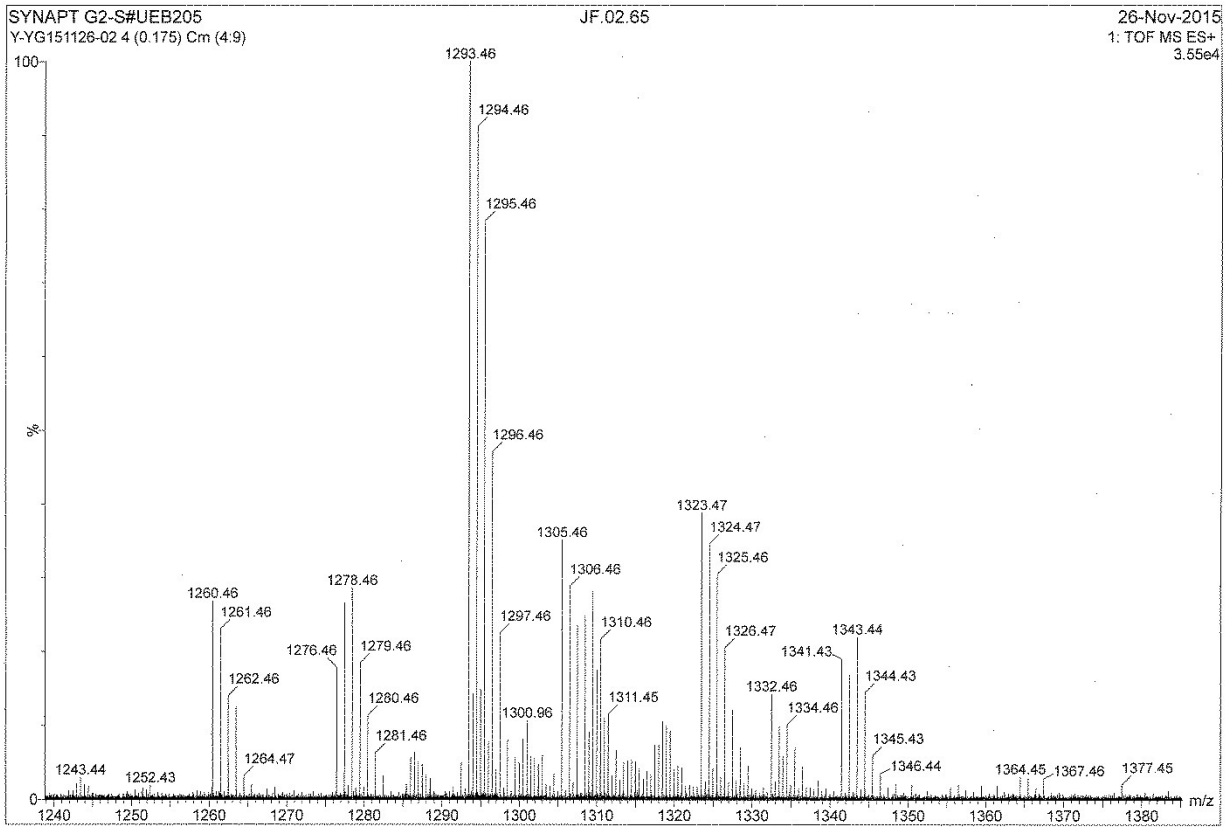
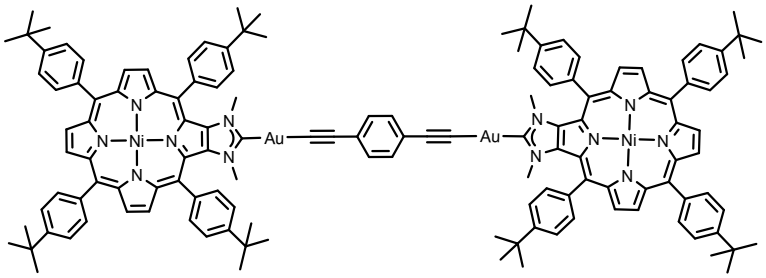


Figure S 4. HRMS ESI⁺ report for **[NiAuPh]**



Chemical Formula: $C_{136}H_{132}Au_2N_{12}Ni_2$
Exact Mass: 2442,8736

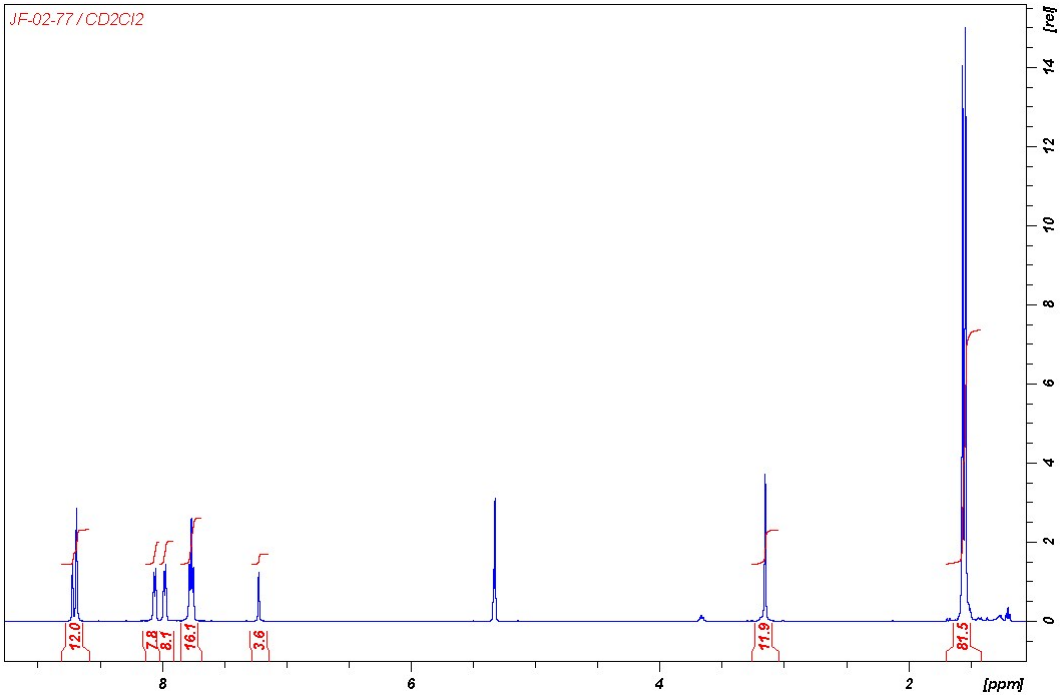


Figure S 5. ^{1}H NMR spectrum of **Ni_2** in CD_2Cl_2, 400 MHz, 298K

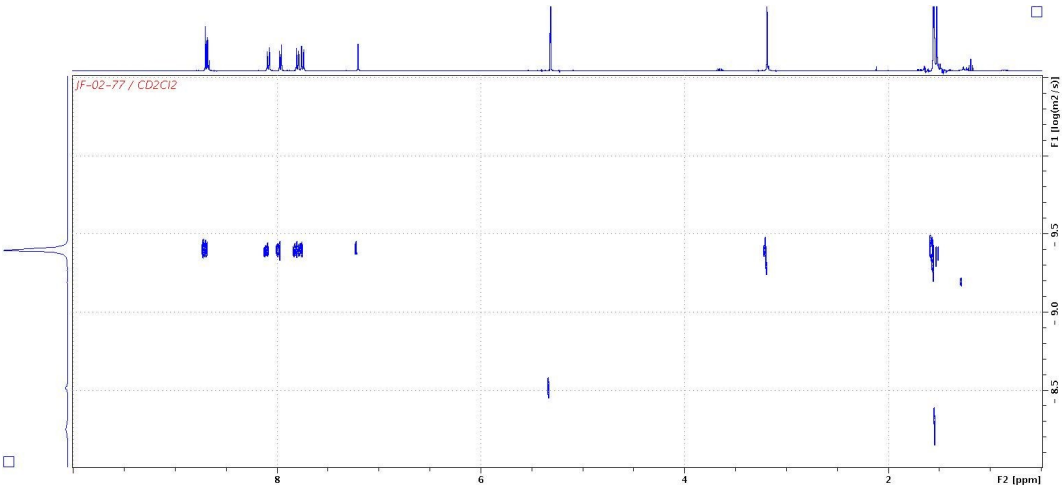


Figure S 6. ^{1}H 2D DOSY NMR spectrum of **Ni_2** in CD_2Cl_2, 400 MHz, 298K

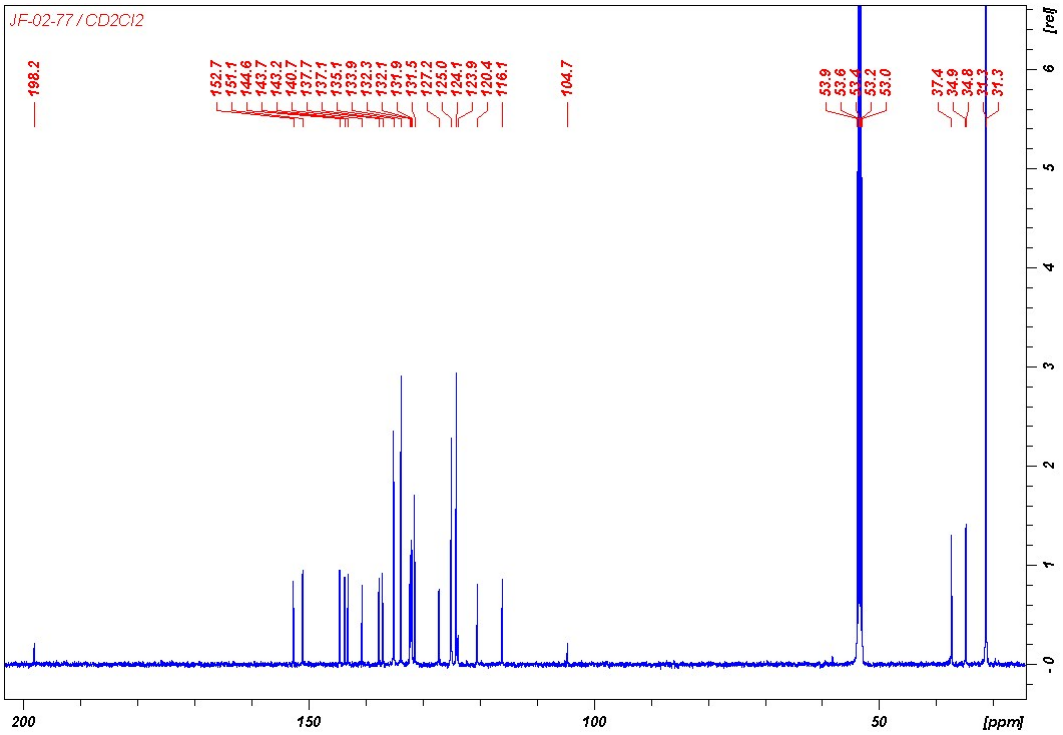


Figure S 7. $^{13}C\{^{1}H\}$ NMR spectrum of **Ni_2** in CD_2Cl_2, 126 MHz, 298K

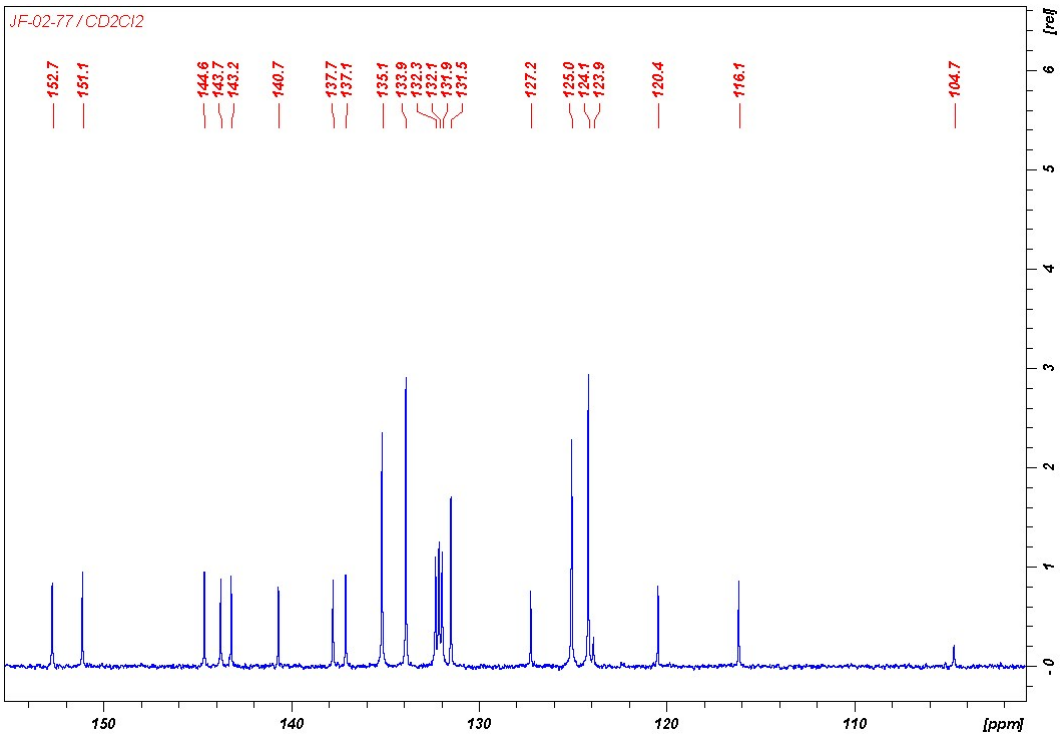


Figure S 8. $^{13}C\{^{1}H\}$ NMR spectrum of **Ni_2** (zoom) in CD_2Cl_2, 126 MHz, 298K

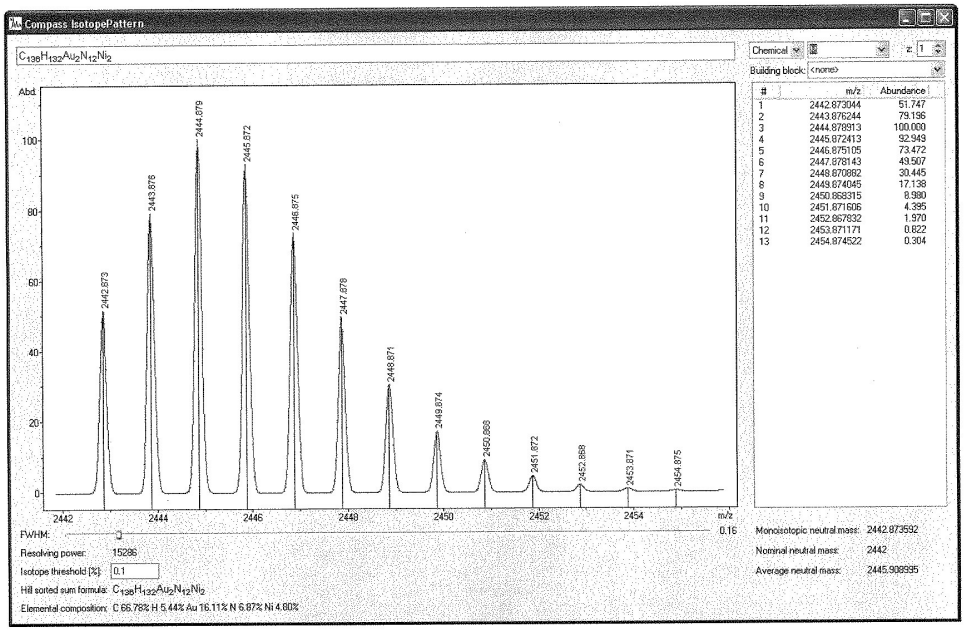


Figure S 9. Simulated mass spectrum of **Ni_2**

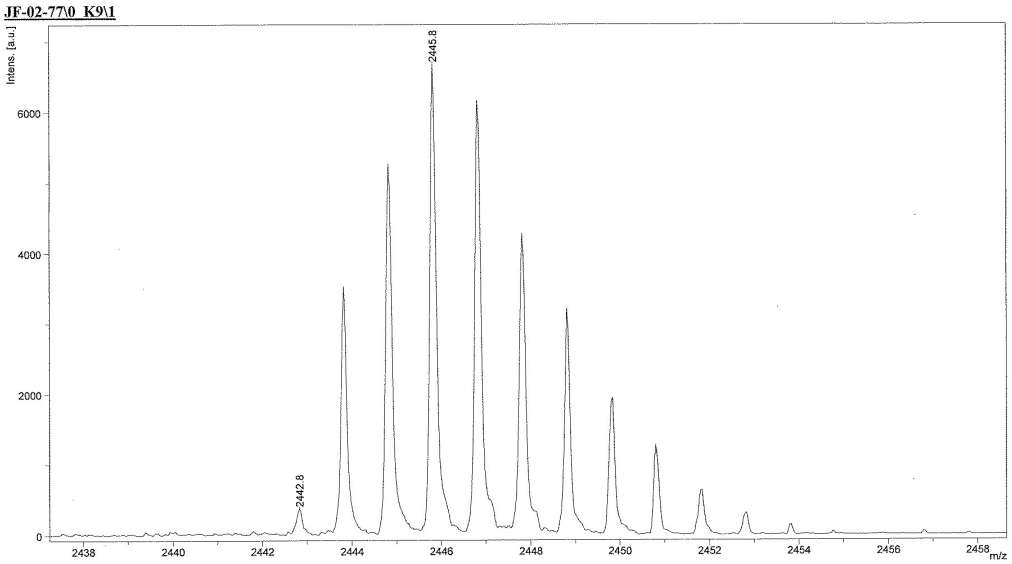
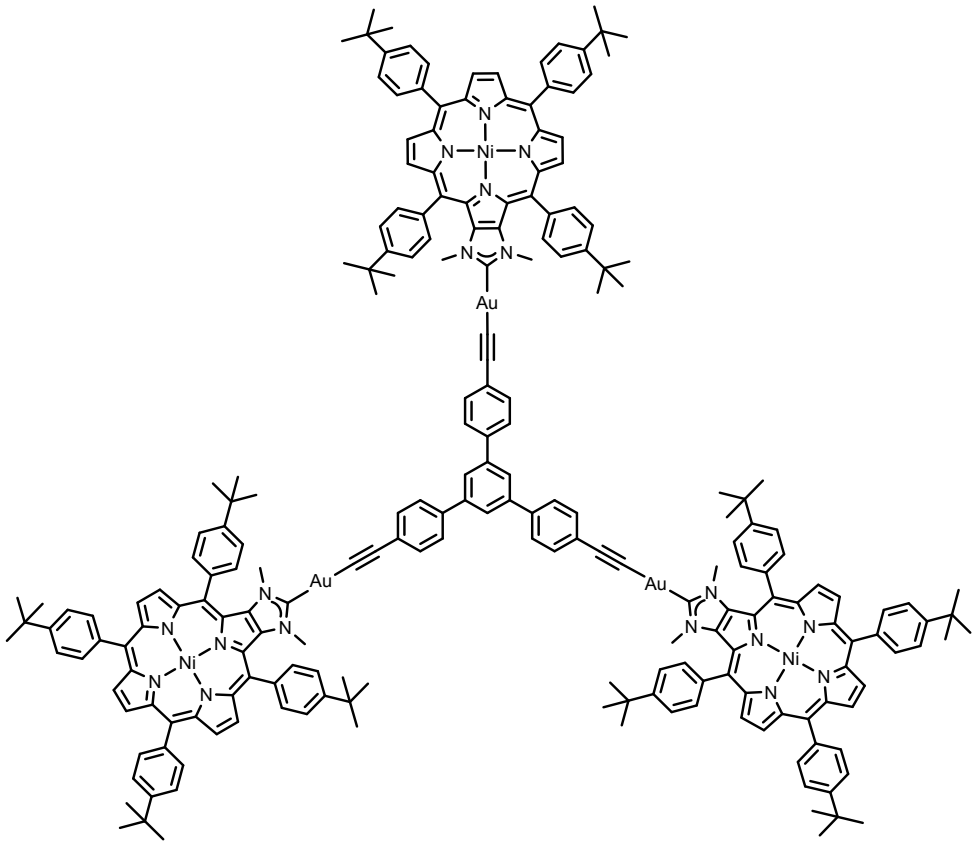


Figure S 10. Experimental mass spectrum of **Ni_2** (MALDI-TOF+)



Chemical Formula: $C_{219}H_{207}Au_3N_{18}Ni_3$
Molecular Weight: 3858,1709

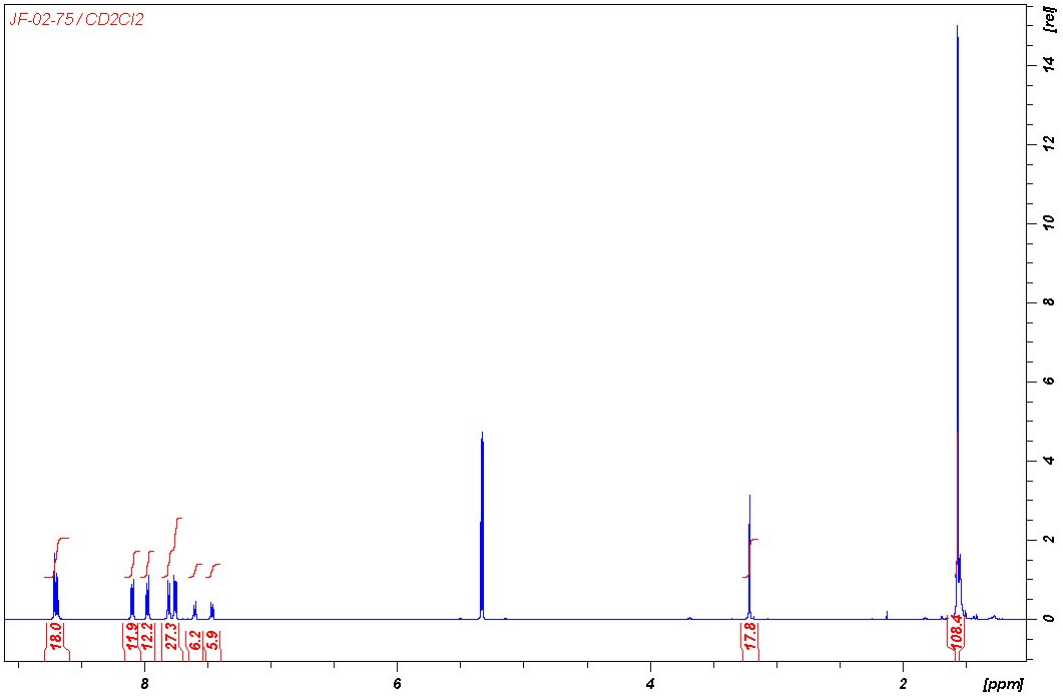


Figure S 11. ^{1}H NMR spectrum of **Ni_3** in CD_2Cl_2, 400 MHz, 298K

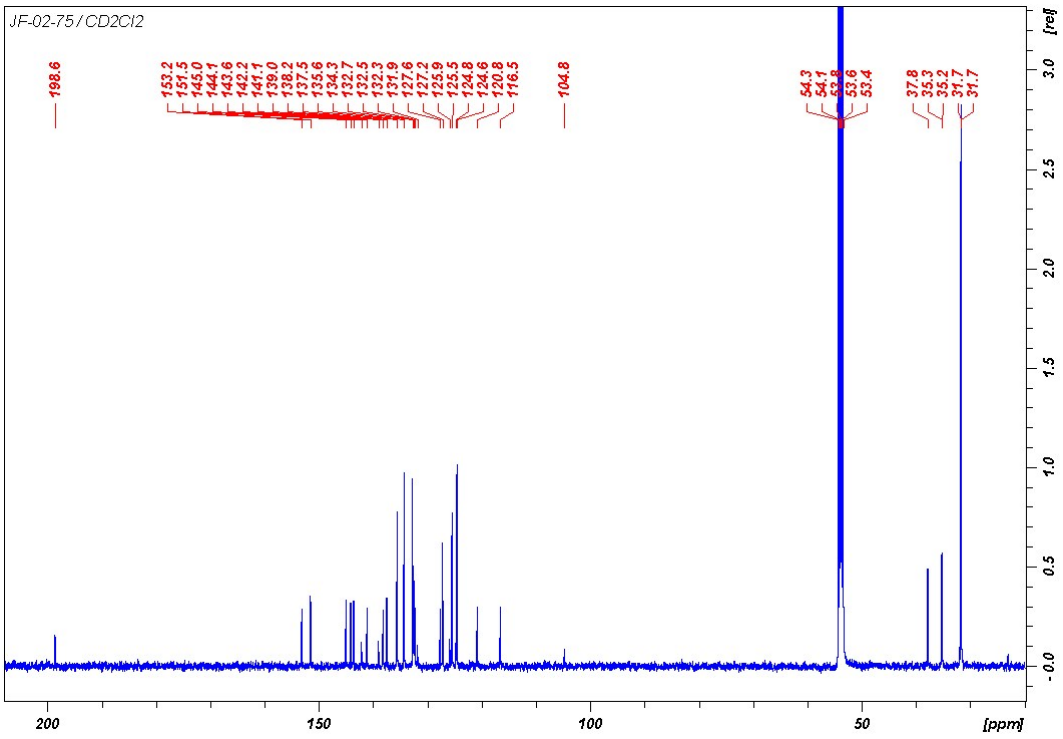


Figure S 12. $^{13}C\{^{1}H\}$ NMR spectrum of **Ni_3** in CD_2Cl_2, 126 MHz, 298K

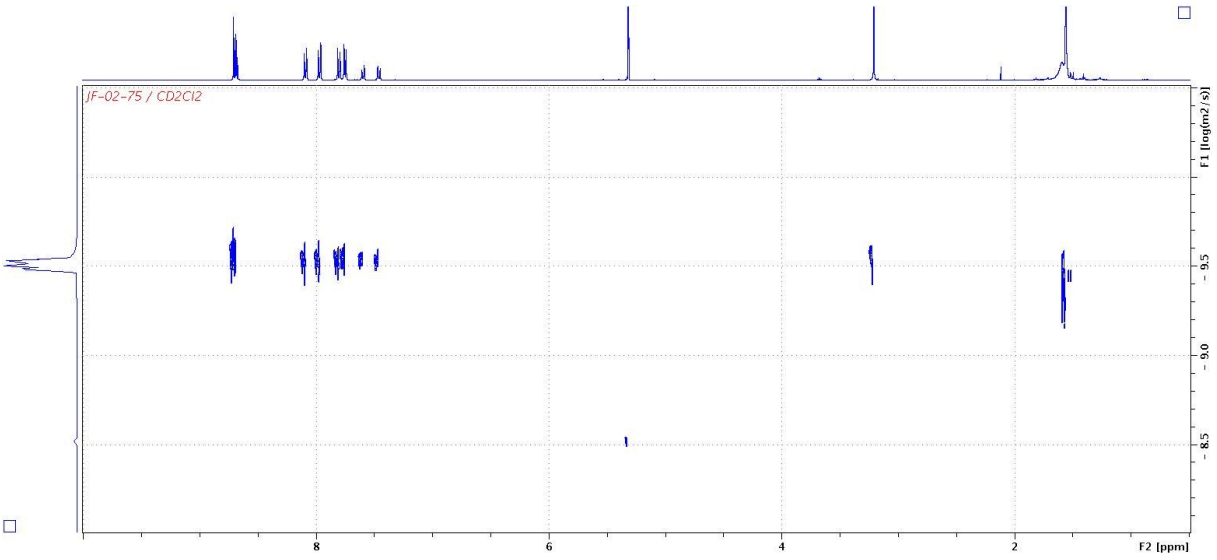


Figure S 13. ^{1}H 2D DOSY NMR spectrum of **Ni_3** in CD_2Cl_2, 400 MHz, 298K

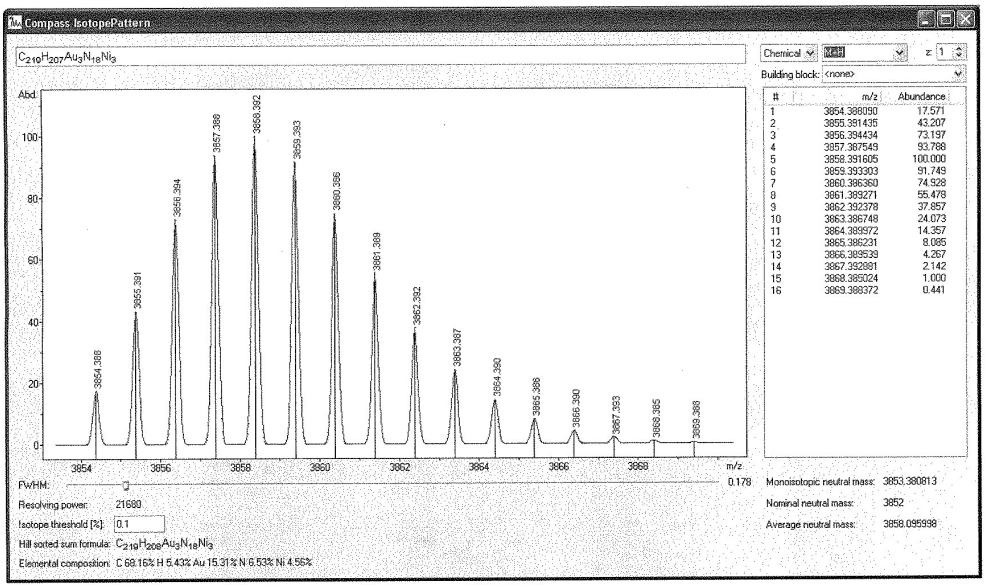


Figure S 14. Simulated mass spectrum of **Ni_3**

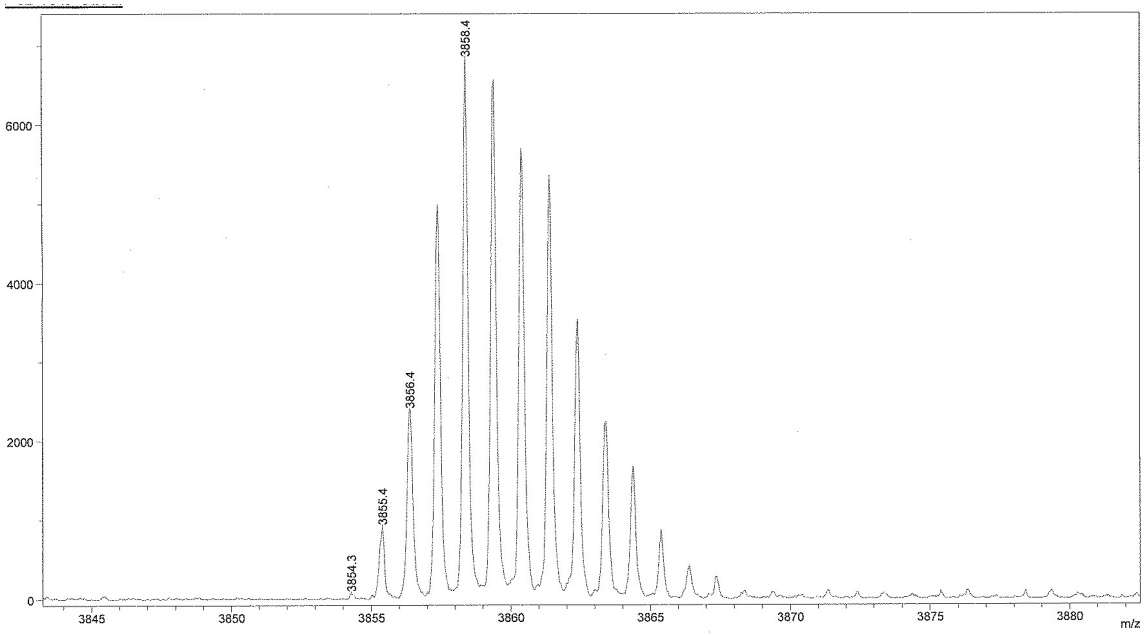
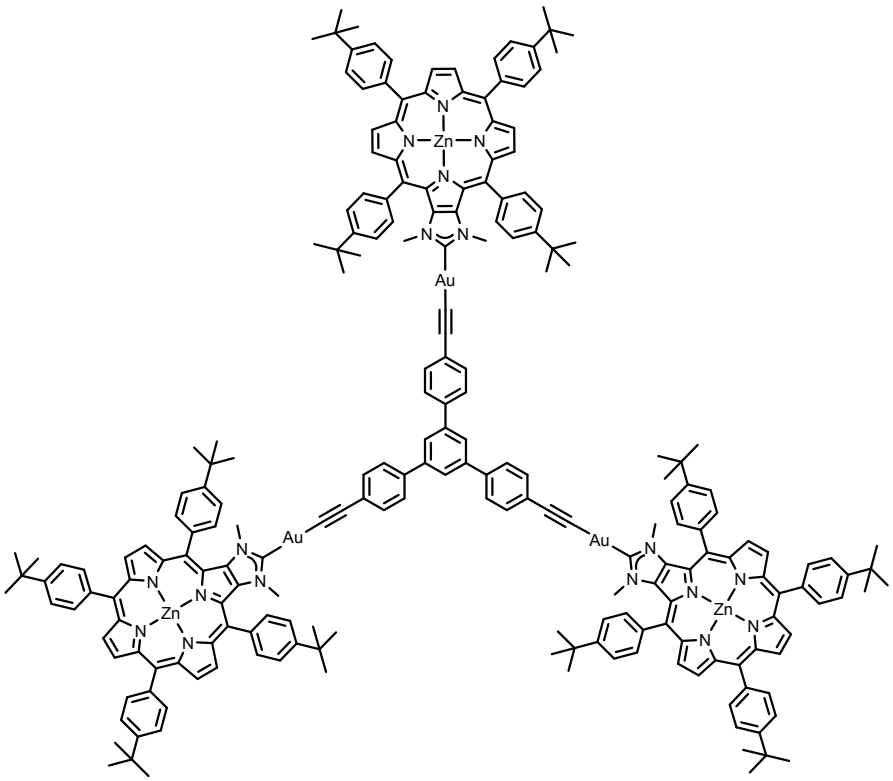


Figure S 15. Experimental mass spectrum of **Ni_3**
(MALDI-TOF+)



Chemical Formula: $C_{219}H_{207}Au_3N_{18}Zn_3$
Molecular Weight: 3871,3622

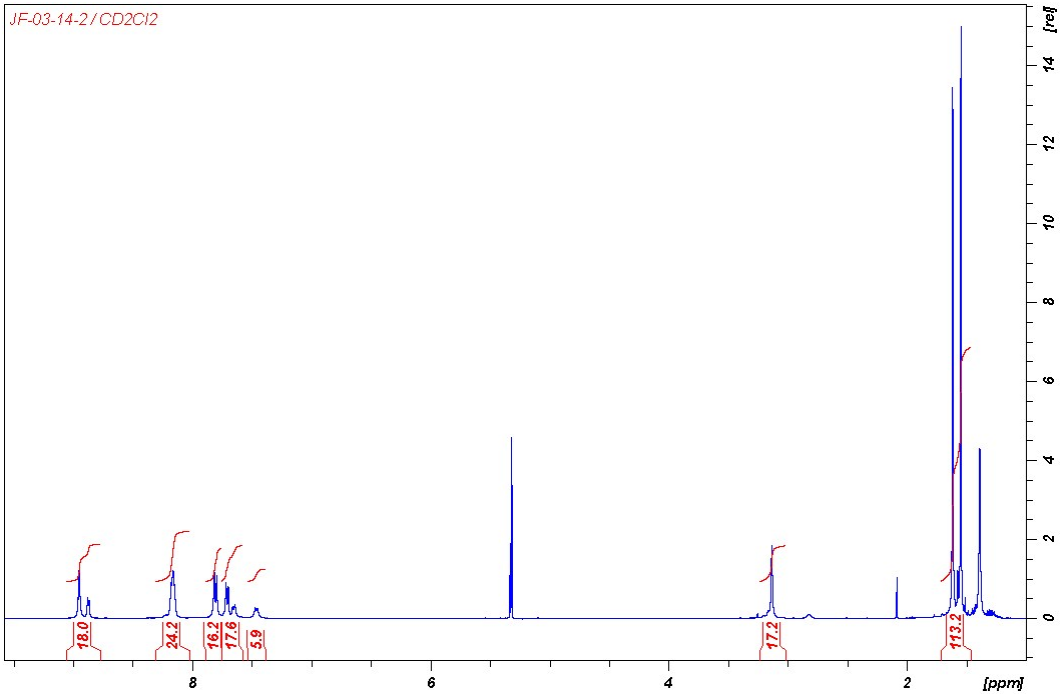


Figure S 16. ^{1}H NMR spectrum of **Zn_3** in CD_2Cl_2, 400 MHz, 298K

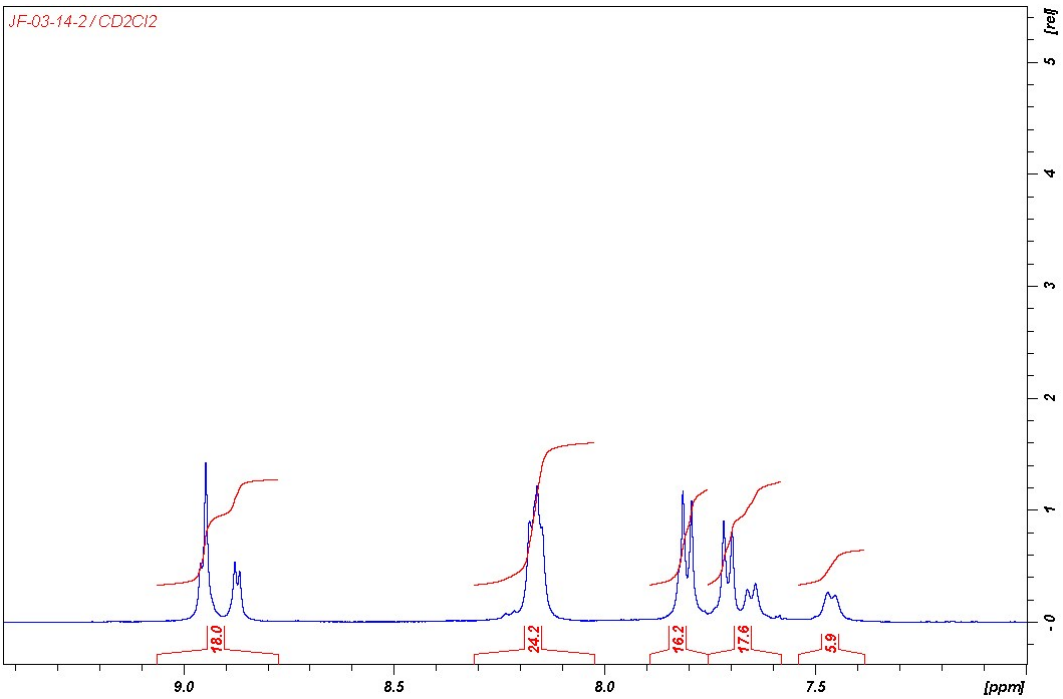


Figure S 17. ^{1}H NMR spectrum (zoom) of **Zn_3** in CD_2Cl_2, 400 MHz, 298K

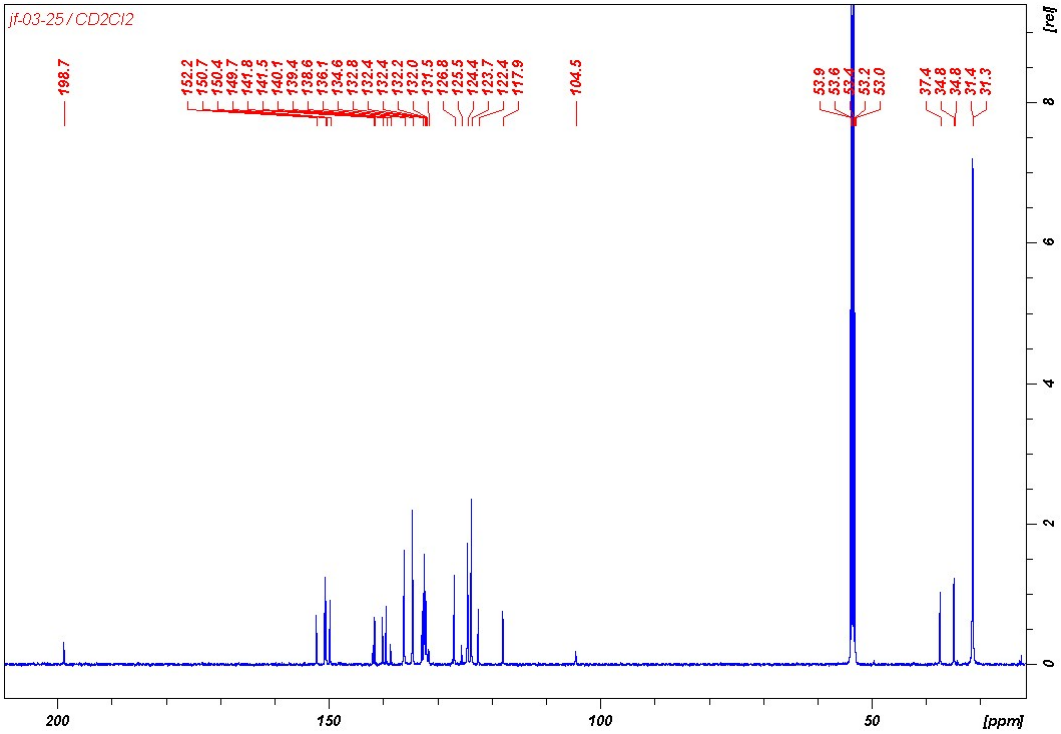


Figure S 18. $^{13}C\{^{1}H\}$ NMR spectrum of **Zn_3** in CD_2Cl_2, 126 MHz, 298K

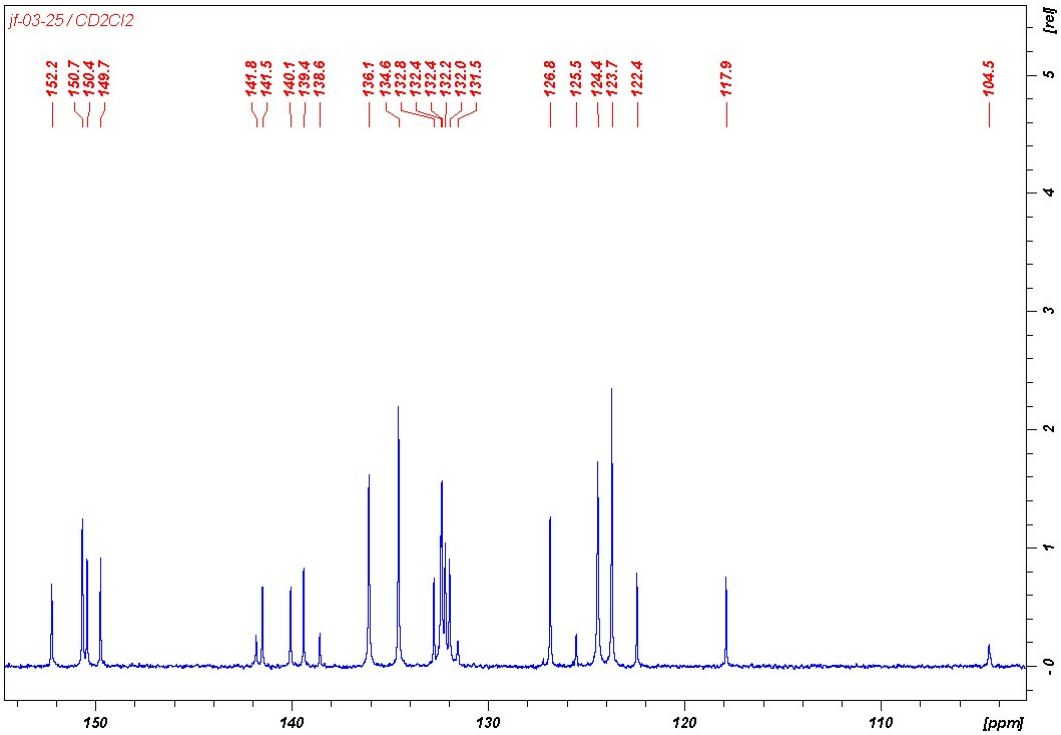


Figure S 19. $^{13}C\{^{1}H\}$ NMR spectrum (zoom) of **Zn_3** in CD_2Cl_2, 126 MHz, 298K

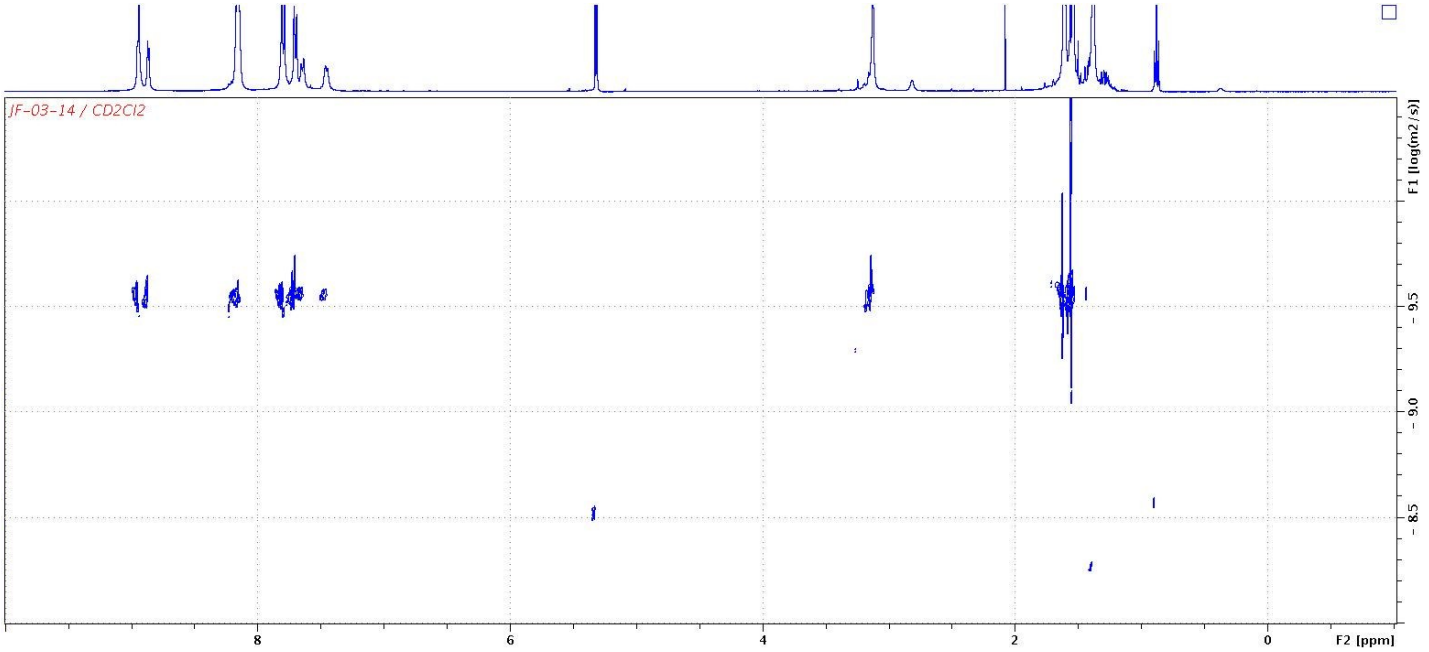


Figure S 20. ^{1}H 2D DOSY NMR spectrum of **Zn_3** in CD_2Cl_2, 400 MHz, 298K

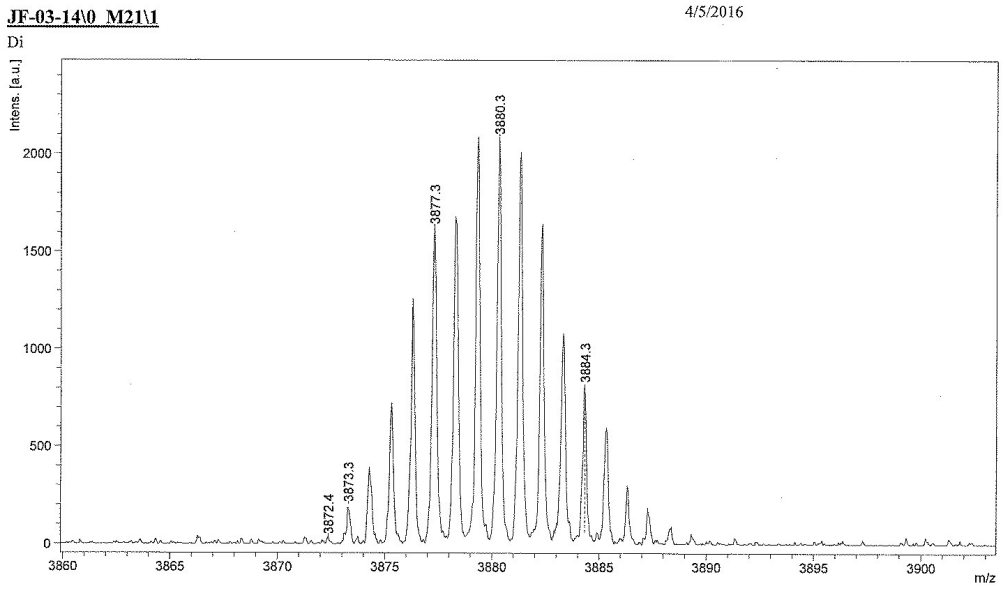


Figure S 21. Experimental mass spectrum of **Zn_3** (MALDI-TOF$^+$)

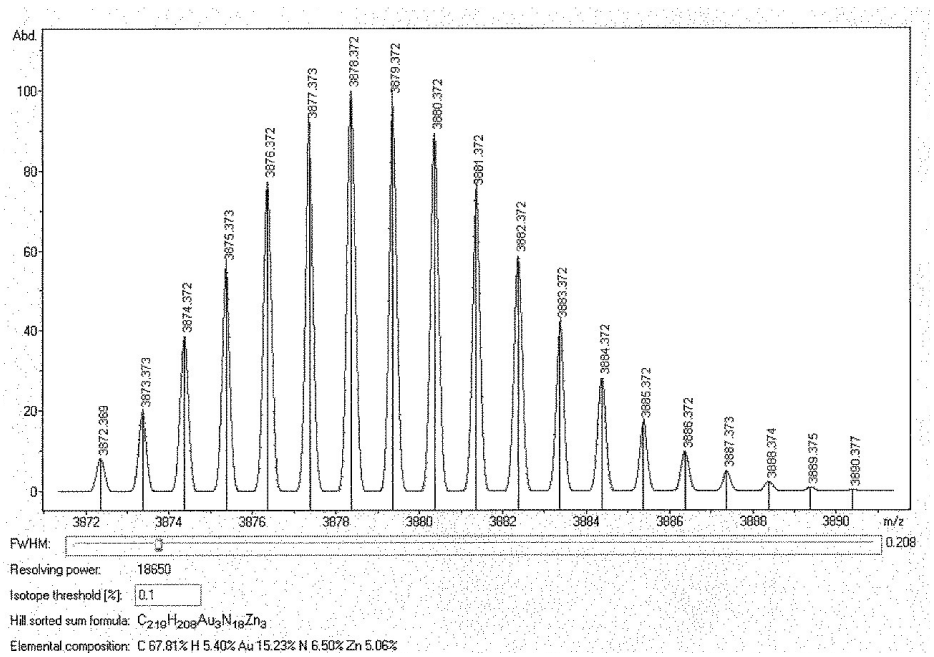
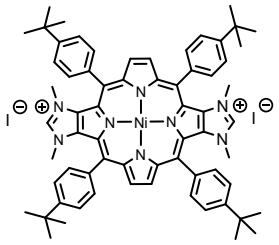


Figure S 22. Simulated mass spectrum of **Zn_3**



Chemical Formula: $C_{66}H_{70}I_2N_8Ni$
Molecular Weight: 1287,84

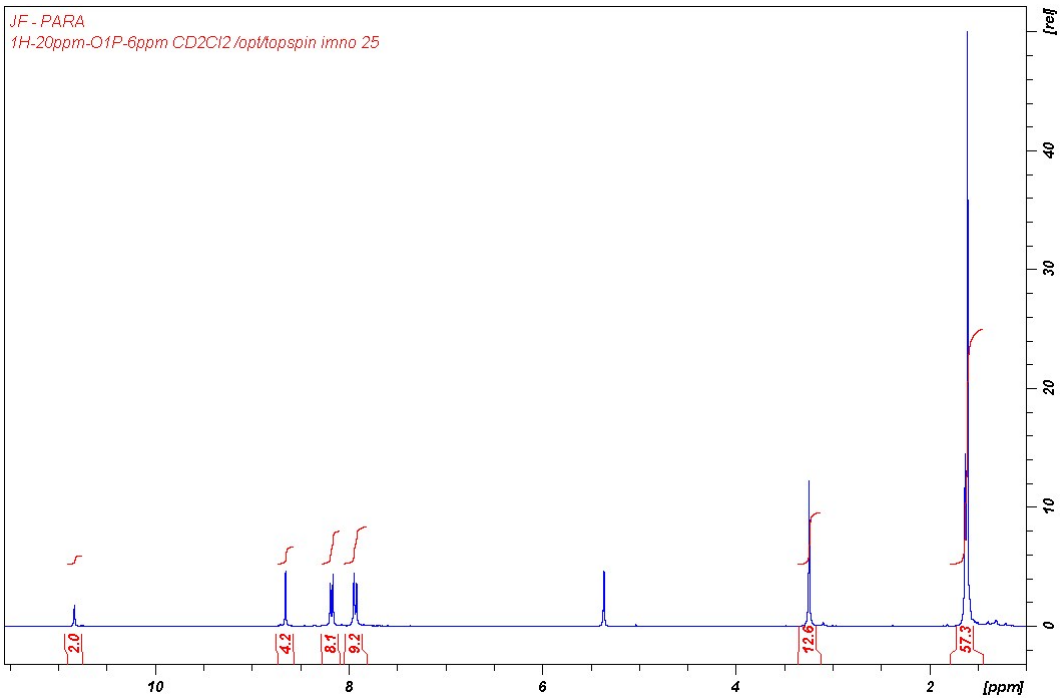


Figure S 23. ^{1}H NMR spectrum of **Ni-I_2** in CD_2Cl_2, 400 MHz, 298K

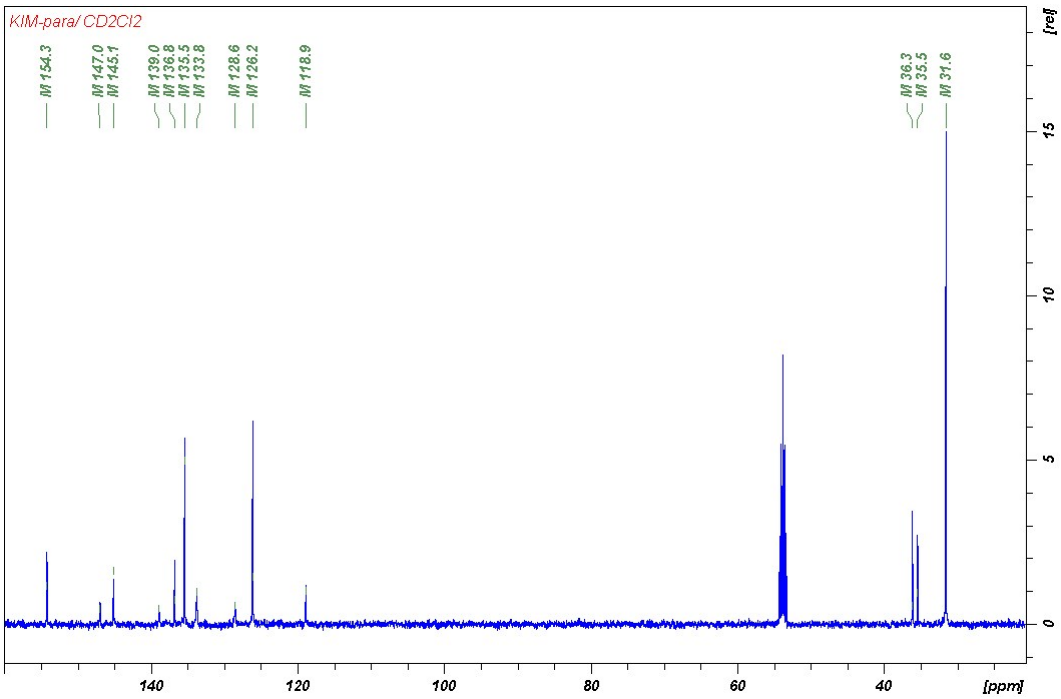


Figure S 24. $^{13}C\{^{1}H\}$ NMR spectrum of **Ni-I_2** in CD_2Cl_2, 126 MHz, 298K

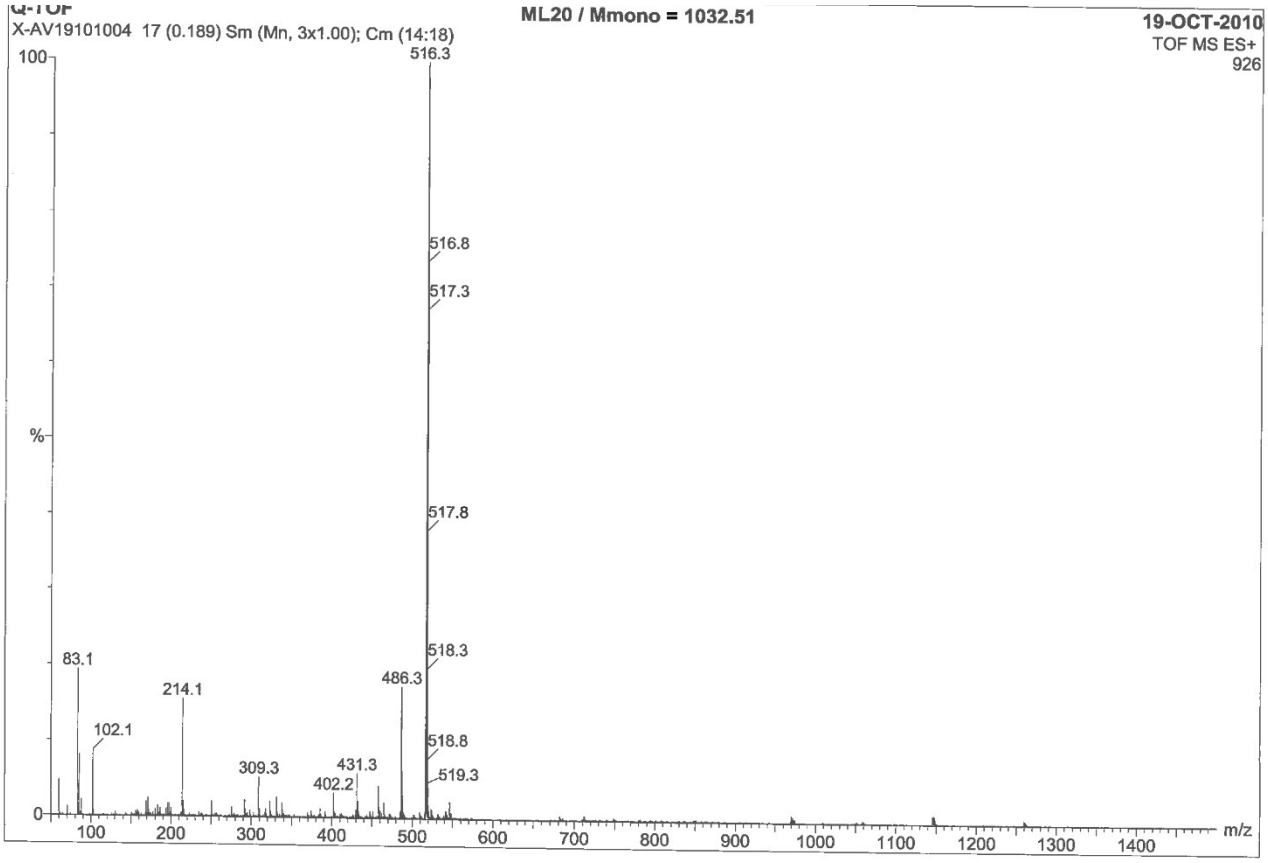
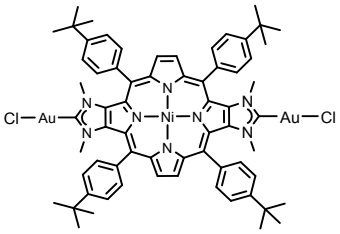


Figure S 25. Experimental mass spectrum of **Ni-I_2** (ESI-TOF$^+$)



Chemical Formula: $C_{66}H_{68}Au_2Cl_2N_8Ni$
Exact Mass: 1494,36

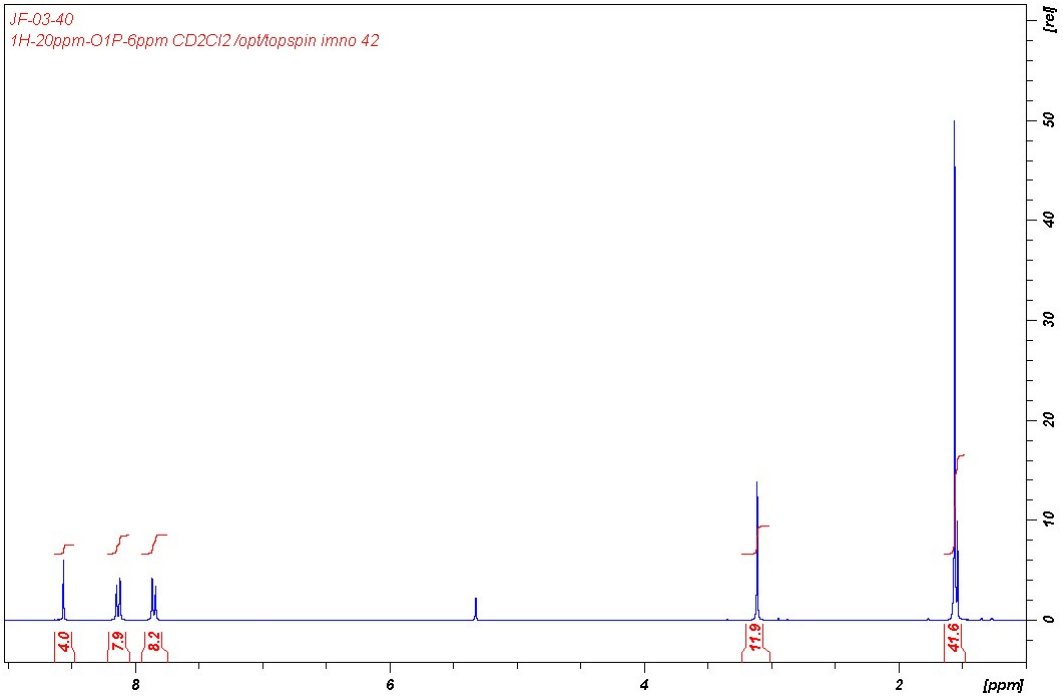


Figure S 26. ^{1}H NMR spectrum of **[Ni(AuCl)$_2$]** in CD_2Cl_2, 400 MHz, 298K

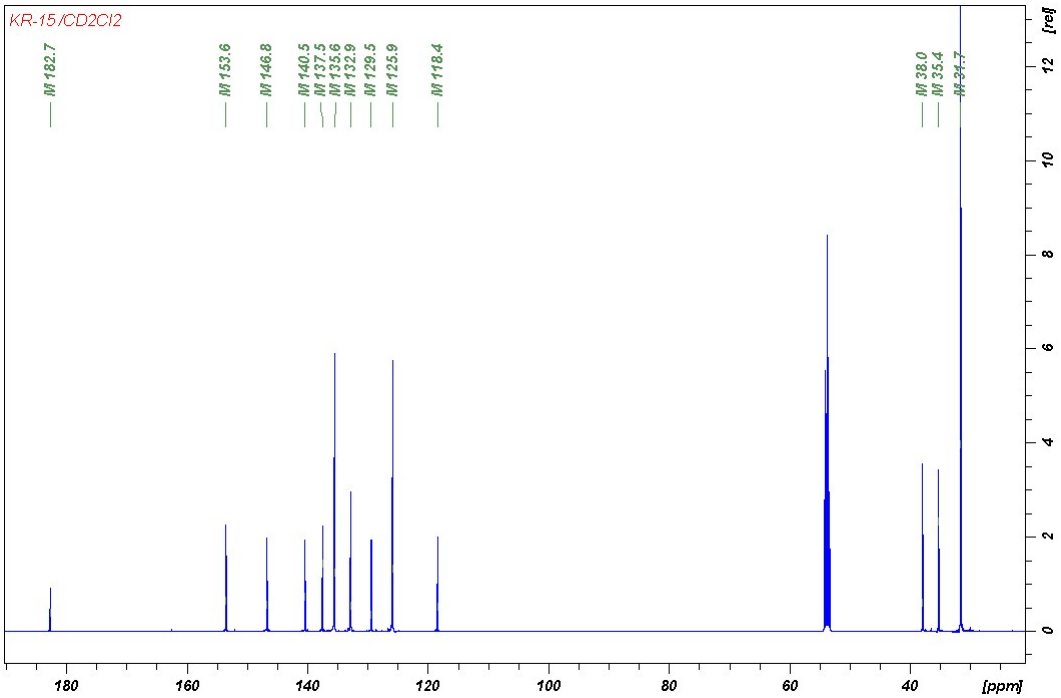


Figure S 27. $^{13}C\{^{1}H\}$ NMR spectrum of **[Ni(AuCl)$_2$]** in CD_2Cl_2, 126 MHz, 298K

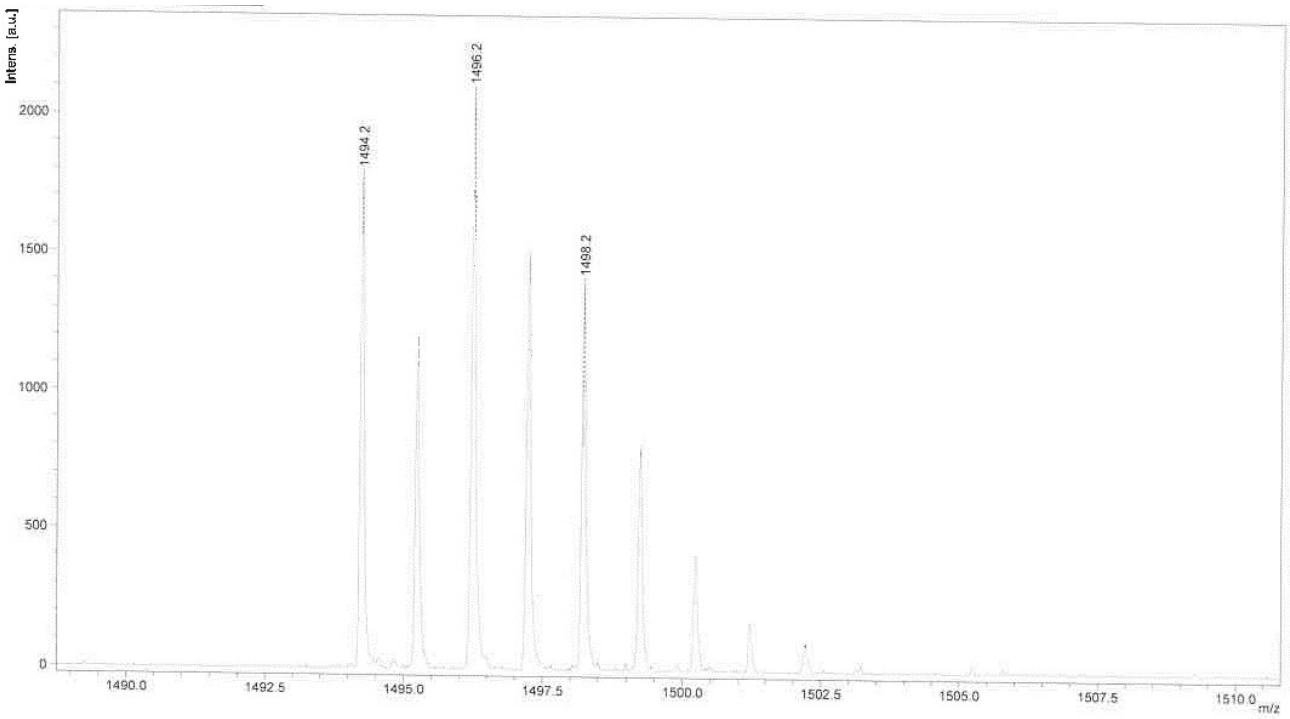
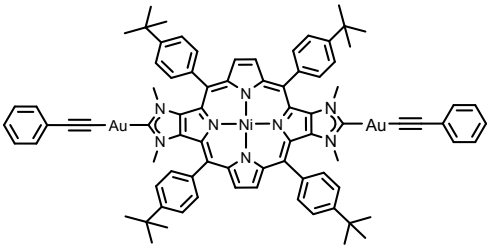


Figure S 28. Experimental mass spectrum of **[Ni(AuCl)$_2$]** (MALDI-TOF+)



Chemical Formula: $C_{82}H_{78}Au_2N_8Ni$
Molecular Weight: 1626,5

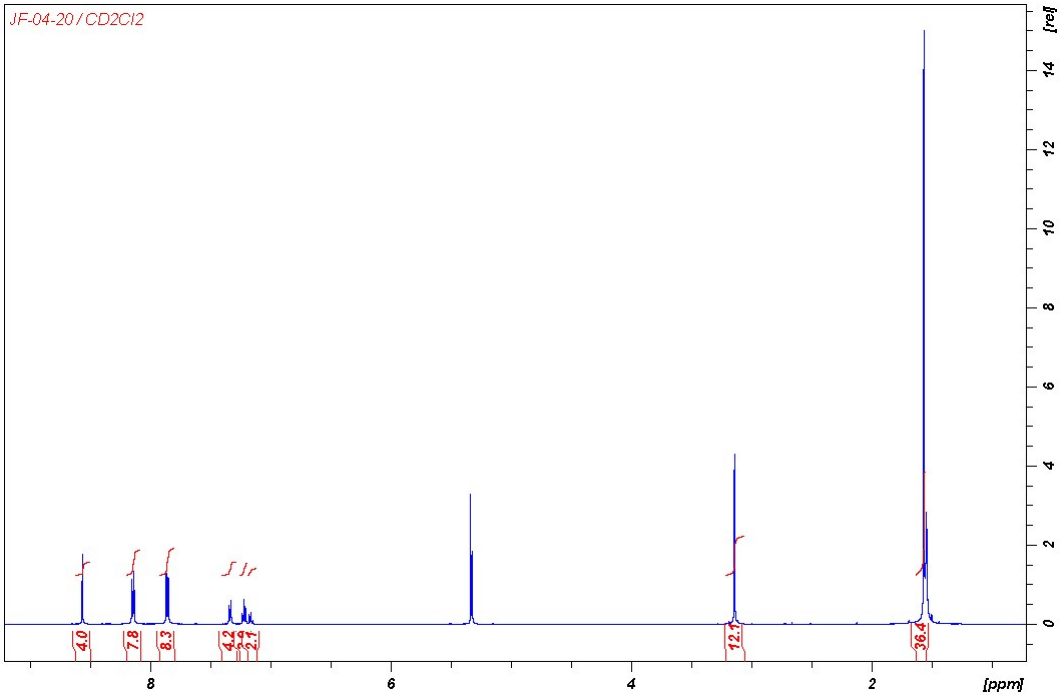


Figure S 29. ^{1}H NMR spectrum of **[Ni(AuPh)$_2$]** in CD_2Cl_2, 400 MHz, 298K

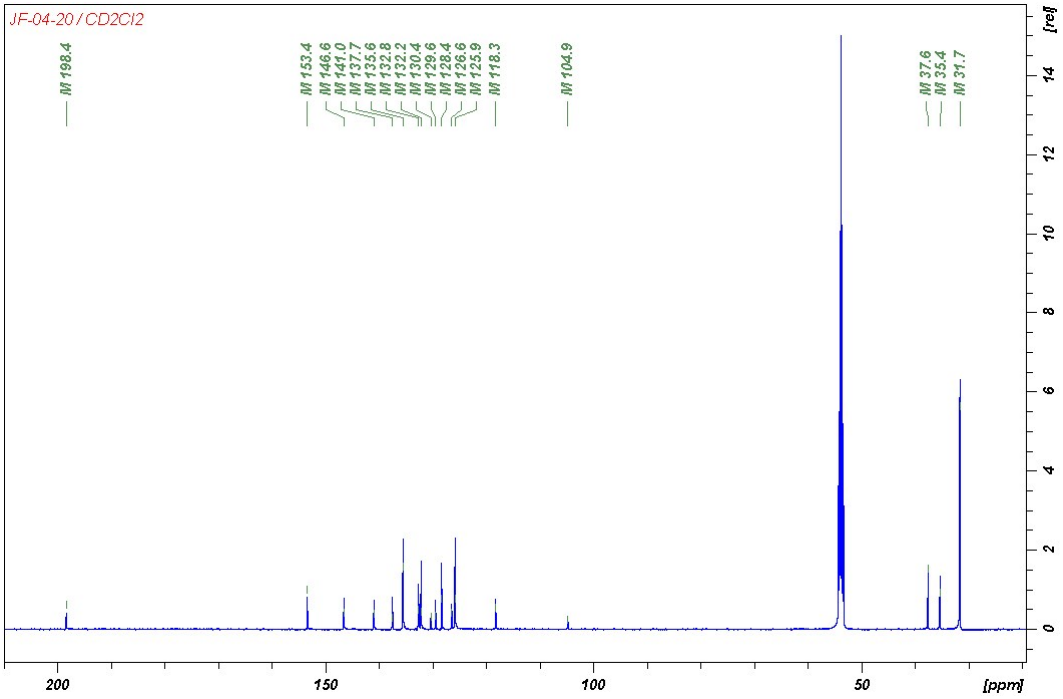


Figure S 30. $^{13}C\{^{1}H\}$ NMR spectrum of **[Ni(AuPh)$_2$]** in CD_2Cl_2, 126 MHz, 298K

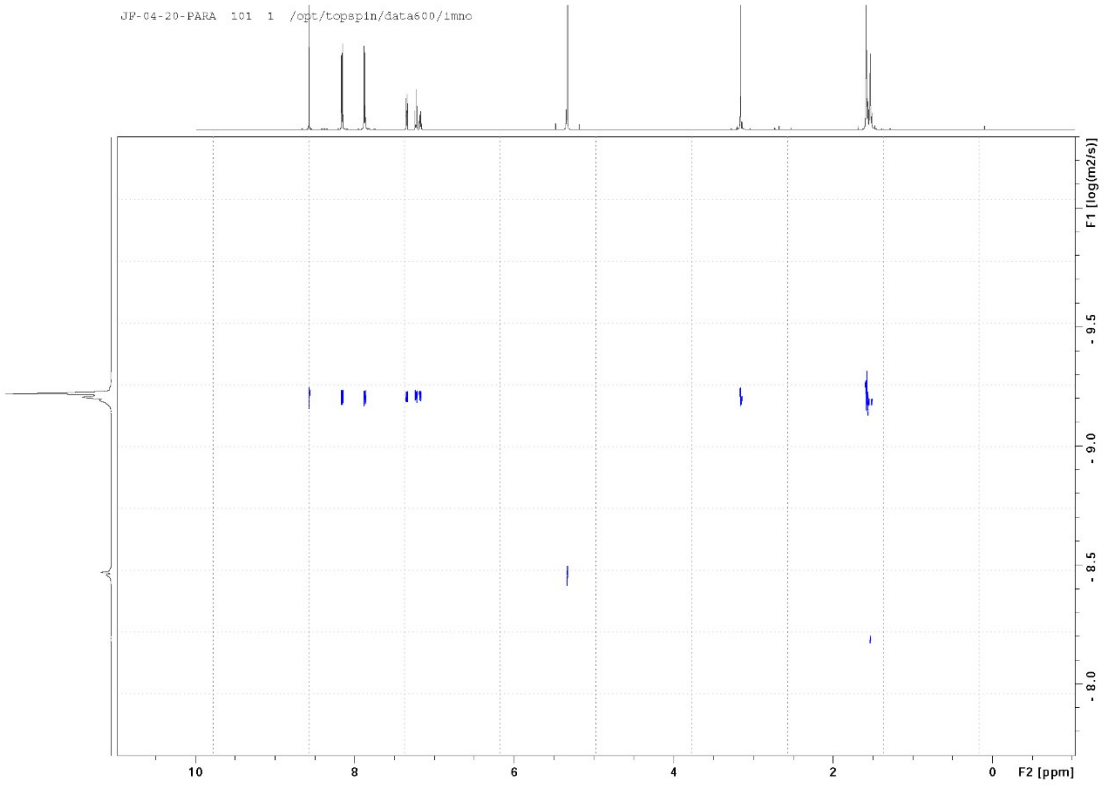


Figure S 31. ^{1}H 2D DOSY NMR spectrum of **[Ni(AuPh)$_2$]** in CD_2Cl_2, 600 MHz, 298K

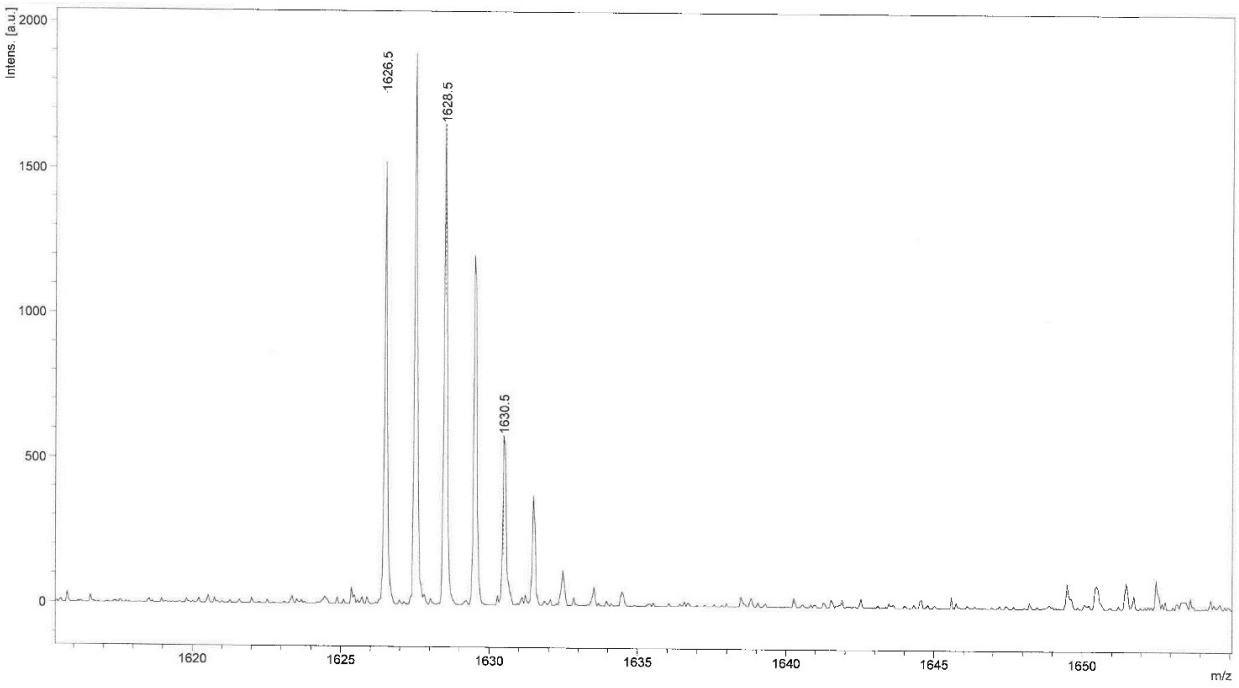
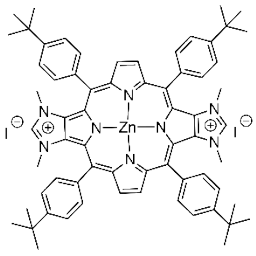


Figure S 32. Experimental Mass spectrum of **[Ni(AuPh)$_2$]** (MALDI-TOF$^+$)



Chemical Formula: $C_{66}H_{70}I_2N_8Zn$
Molecular Weight: 1294.5309

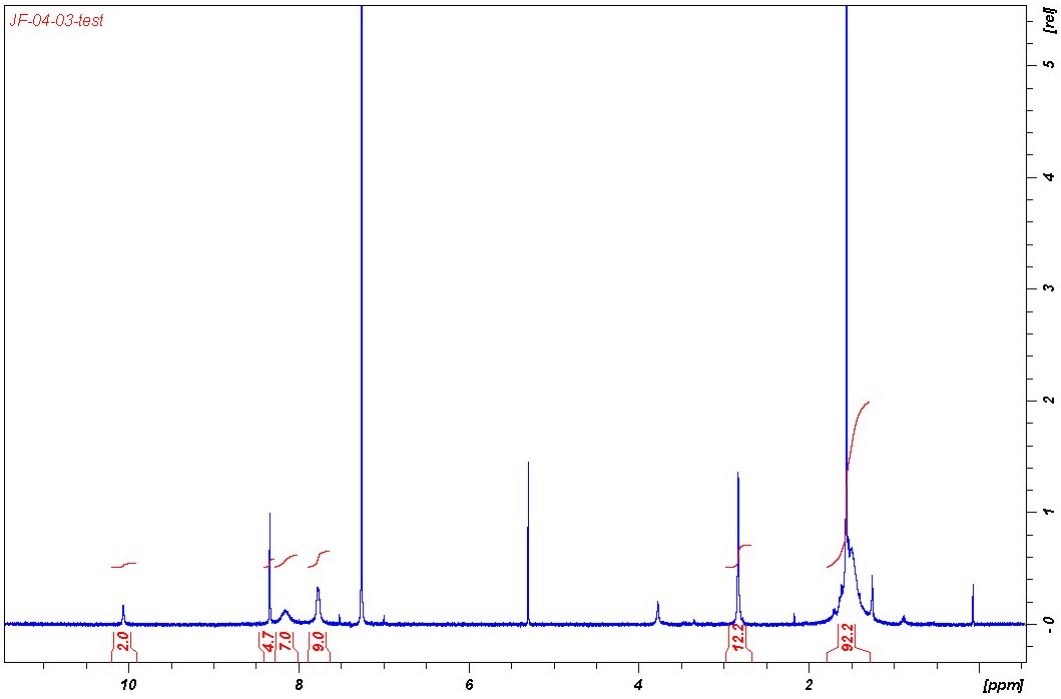


Figure S 33. ^{1}H NMR spectrum of **Zn-I_2** in $CDCl_3$, 400 MHz, 298K

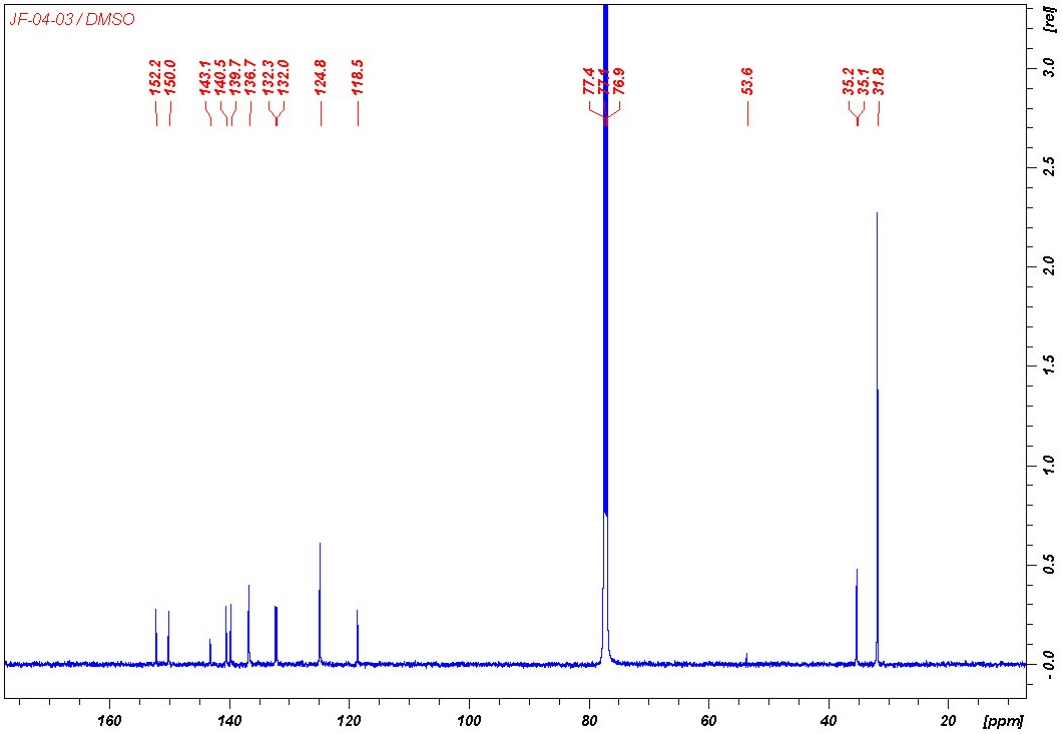


Figure S 34. $^{13}C\{^{1}H\}$ NMR spectrum of **Zn-I$_2$** in $CDCl_3$, 126 MHz, 298K

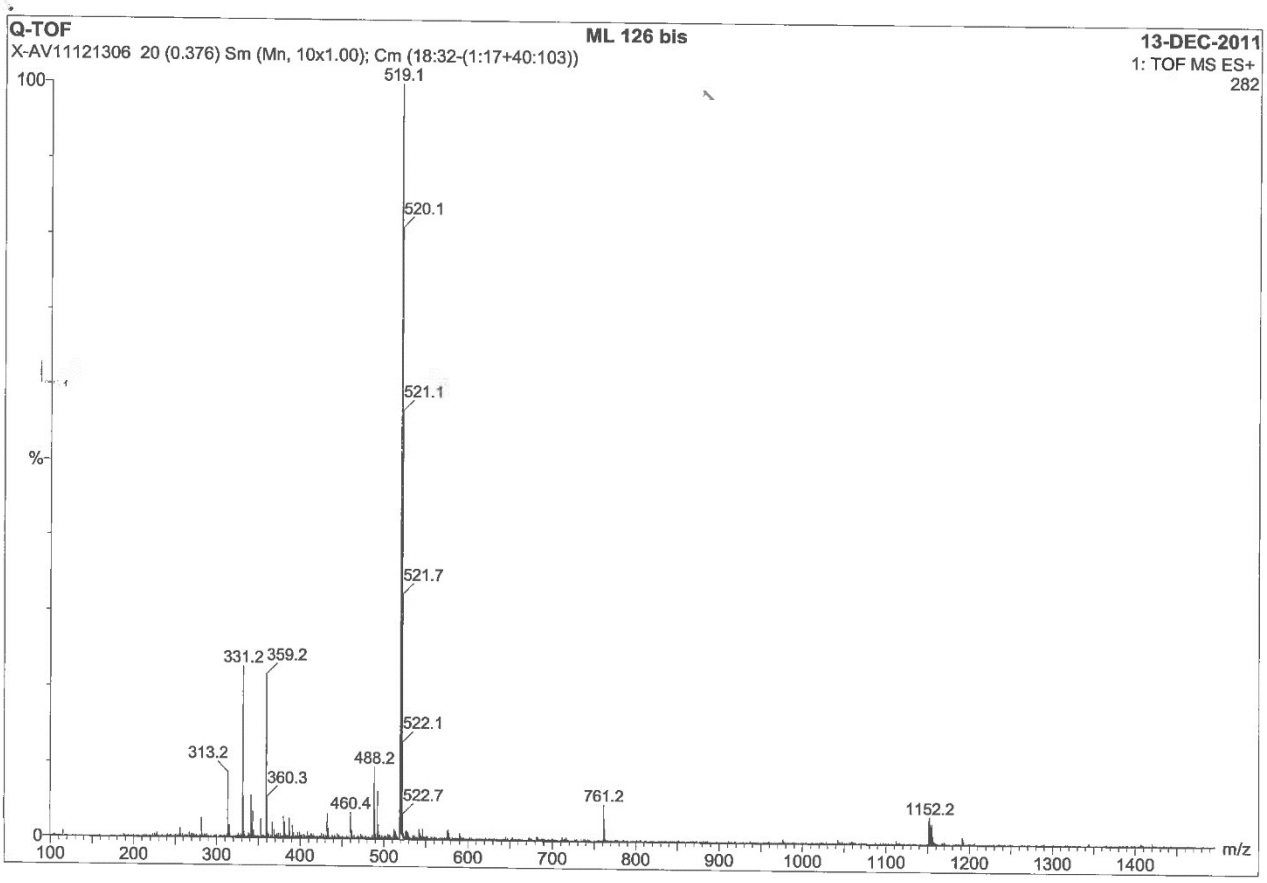
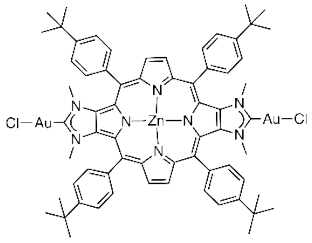


Figure S 35. Experimental Mass spectrum of **Zn-I$_2$** (ESI-TOF$^+$)



Chemical Formula: $C_{66}H_{68}Au_2Cl_2N_8Zn$
Molecular Weight: 1500,3500

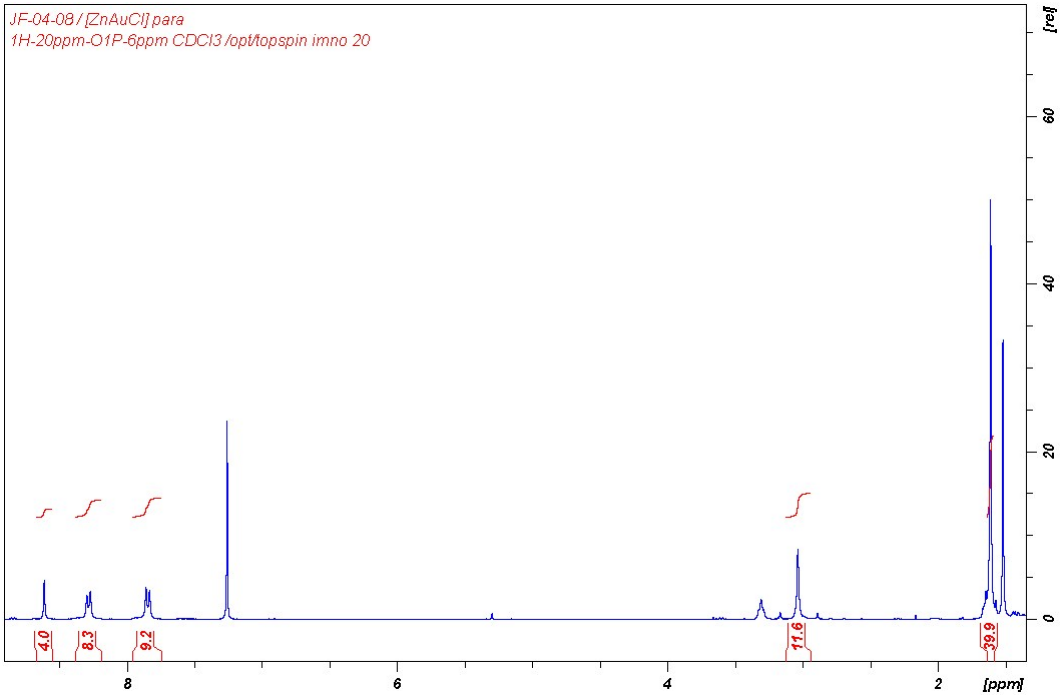


Figure S 36. ^{1}H NMR spectrum of **$[Zn(AuCl)_2]$** in $CDCl_3$, 400 MHz, 298K

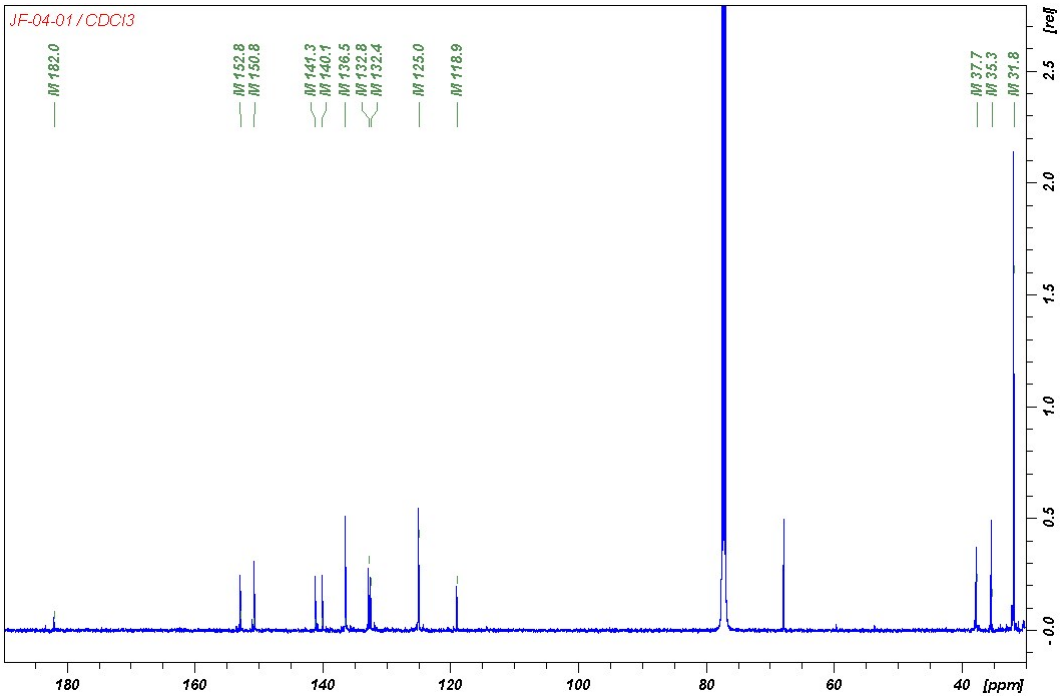


Figure S 37. $^{13}C\{^{1}H\}$ NMR spectrum of **$[Zn(AuCl)_2]$** in CD_2Cl_2, 126 MHz, 298K

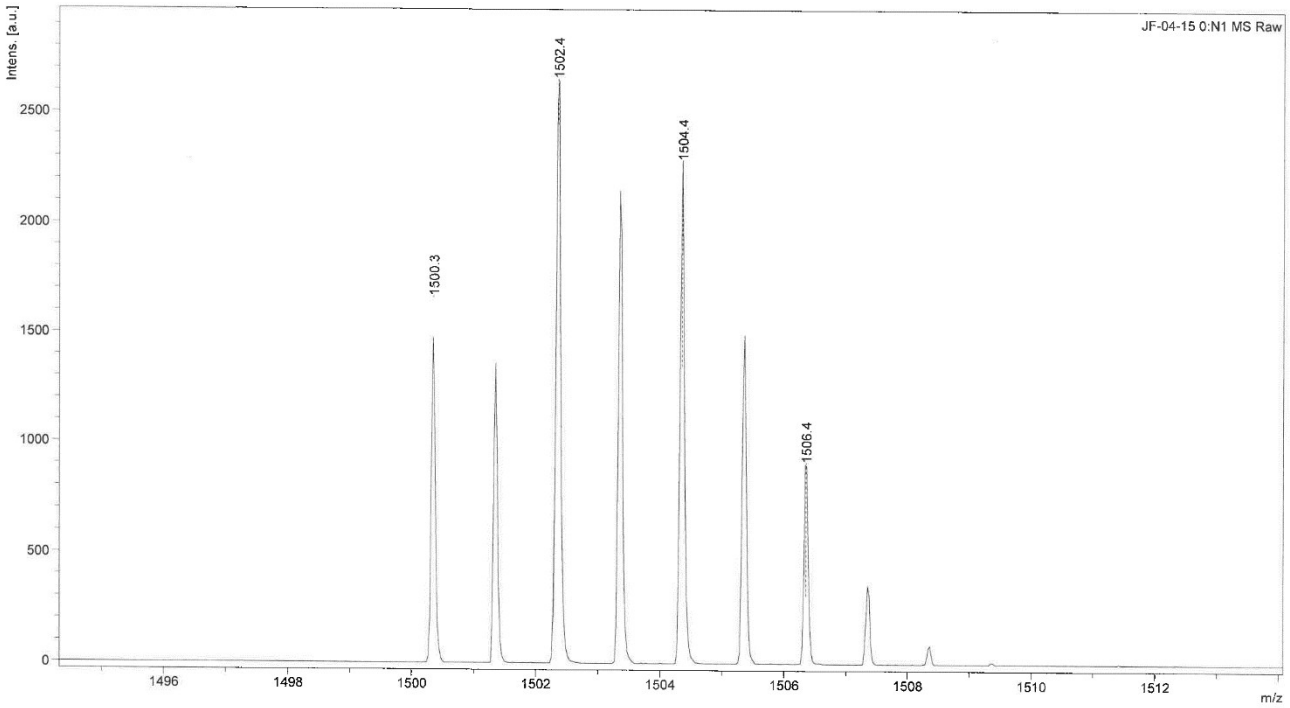


Figure S 38. Experimental mass spectrum of **[Zn(AuCl)$_2$]** (MALDI-TOF$^+$)

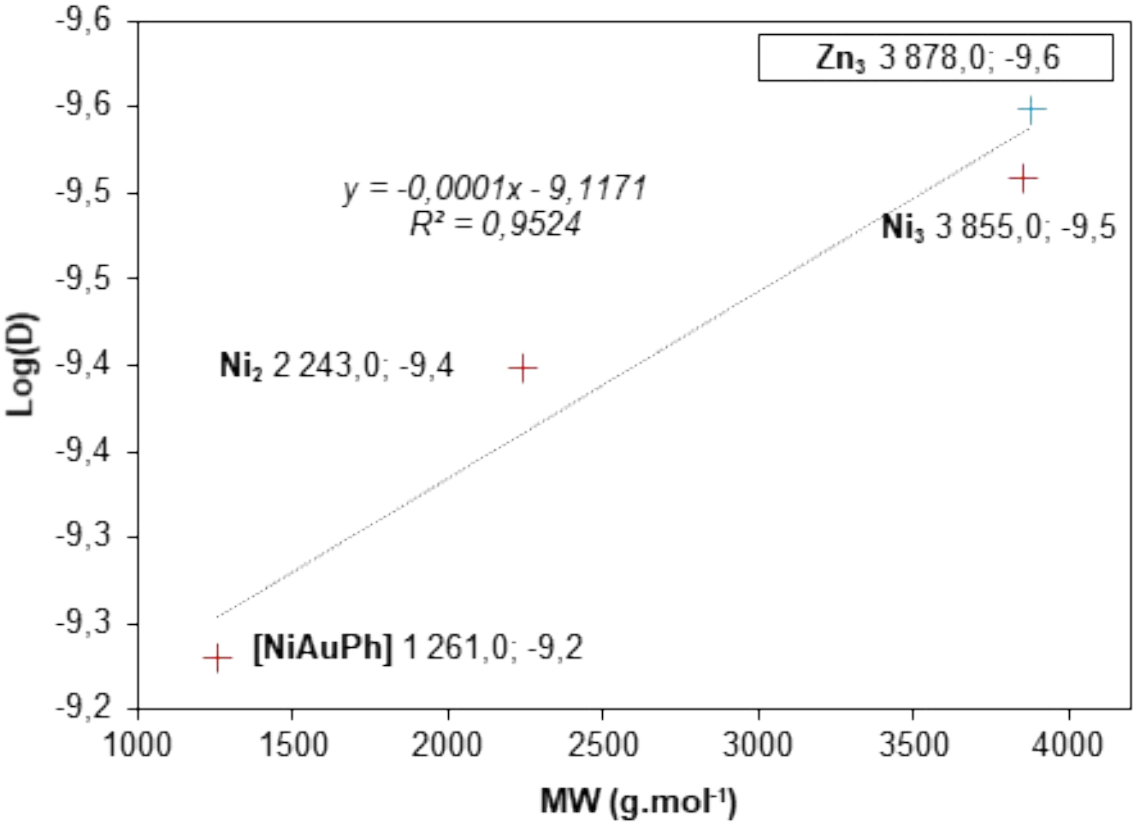
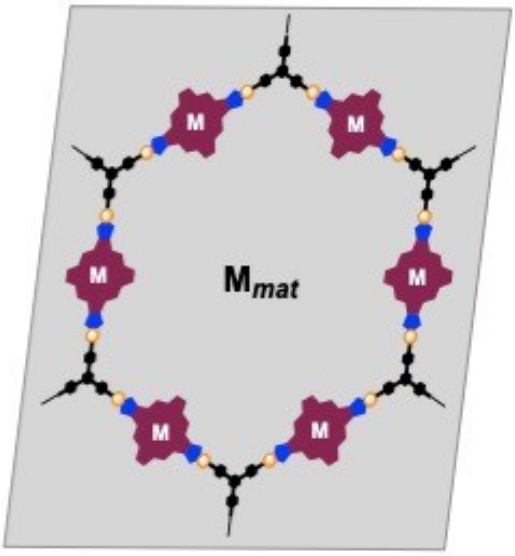


Figure S 39. Plot of log(D) = f(MW) for the studied compounds

Ni$_{mat}$



Ni$_{mat}$ **M = Ni** 74%

EDX Trials	Au	Ni	Au/Ni
1	1.60	0.96	1.66
2	1.61	0.92	1.75
3	1.73	1.02	1.79
average	1.64	0.96	1.71

Figure S 40. Relative ratio of Au/Ni present in **Ni$_{mat}$** measured by EDX. Measured were repeated 3 times.

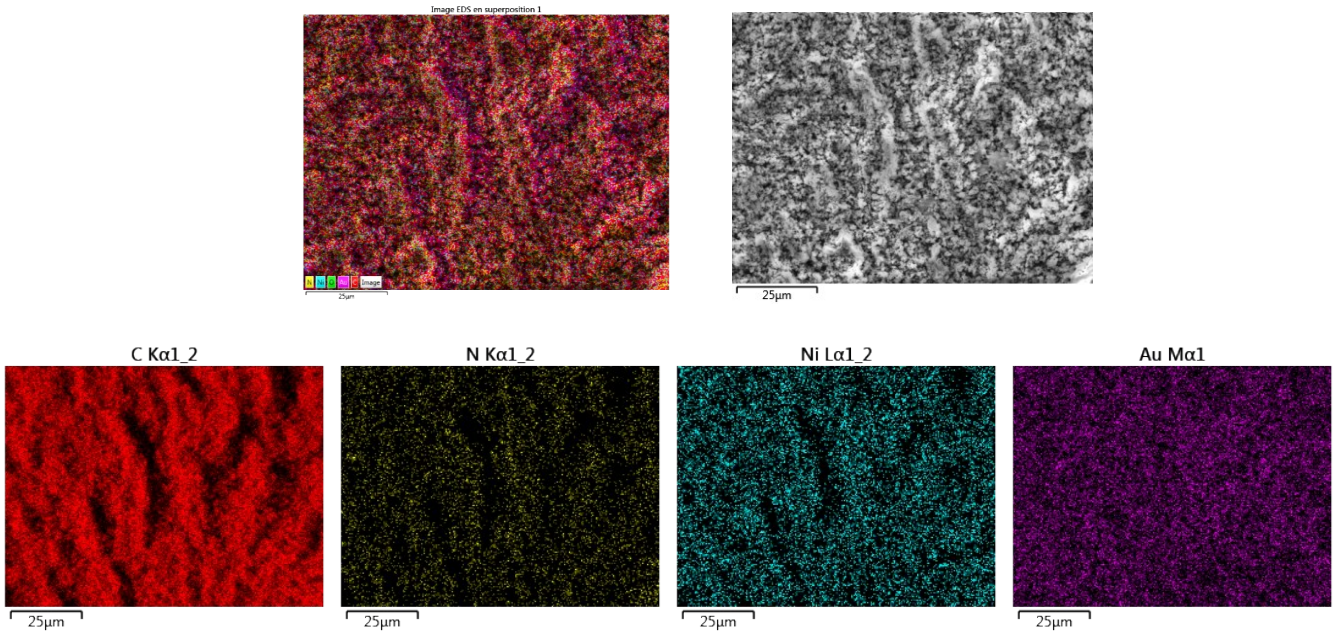


Figure S 41. Elemental mapping analysis of **Ni$_{mat}$** realized by means of EDX in zone 1

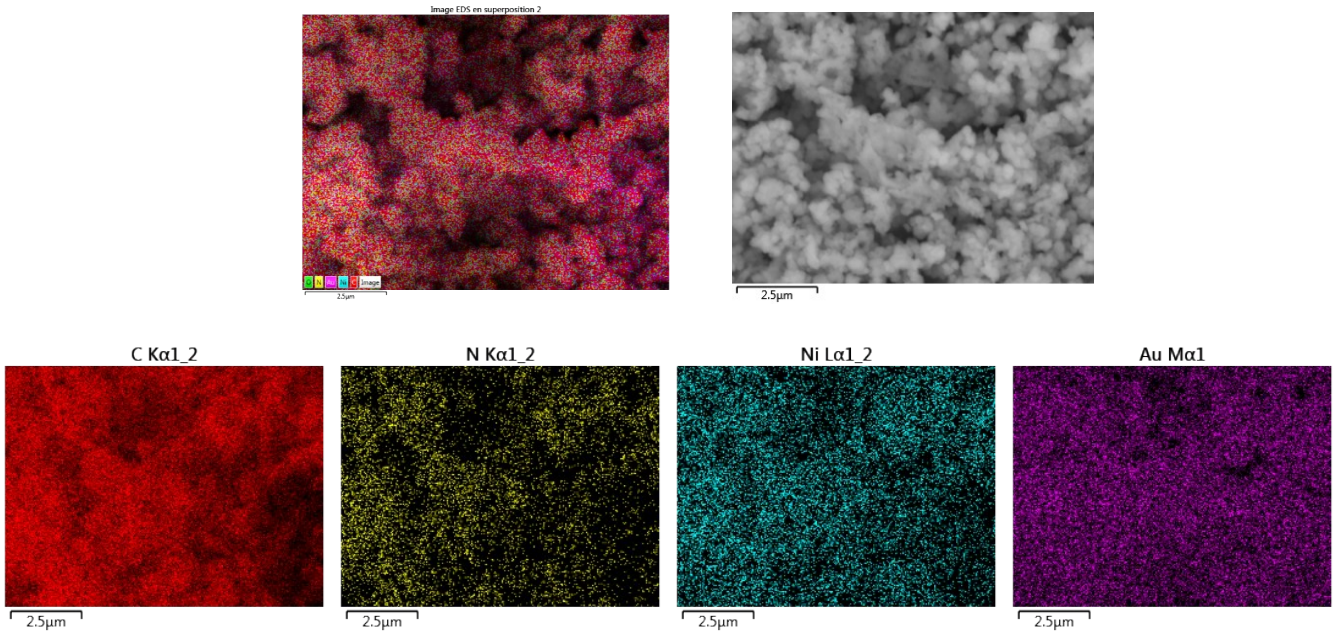


Figure S 42. Elemental mapping analysis of **Ni*mat*** realized by means of EDX in zone 2

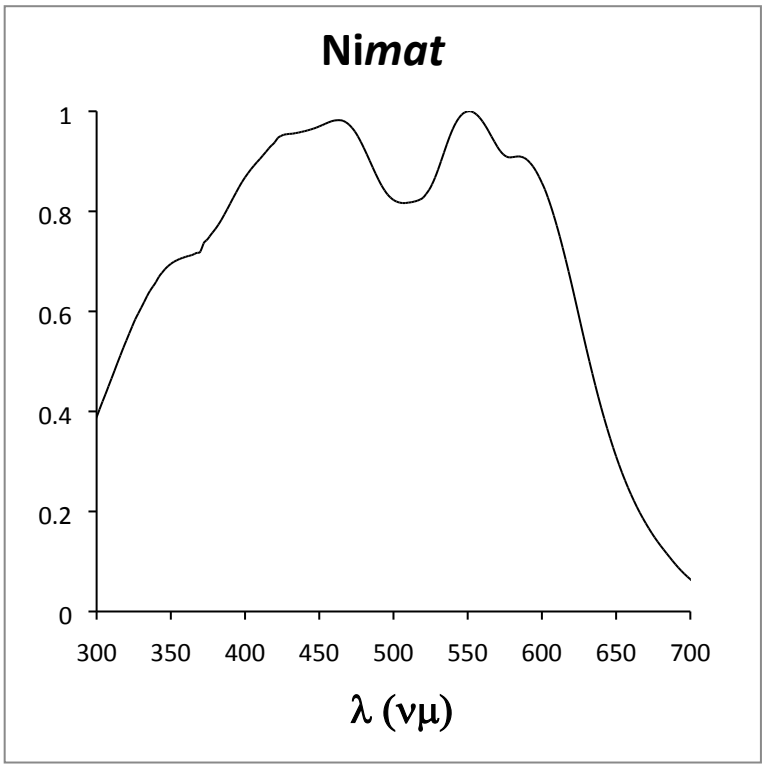


Figure S 43. Solid state UV-Vis spectrum of **Ni*mat***

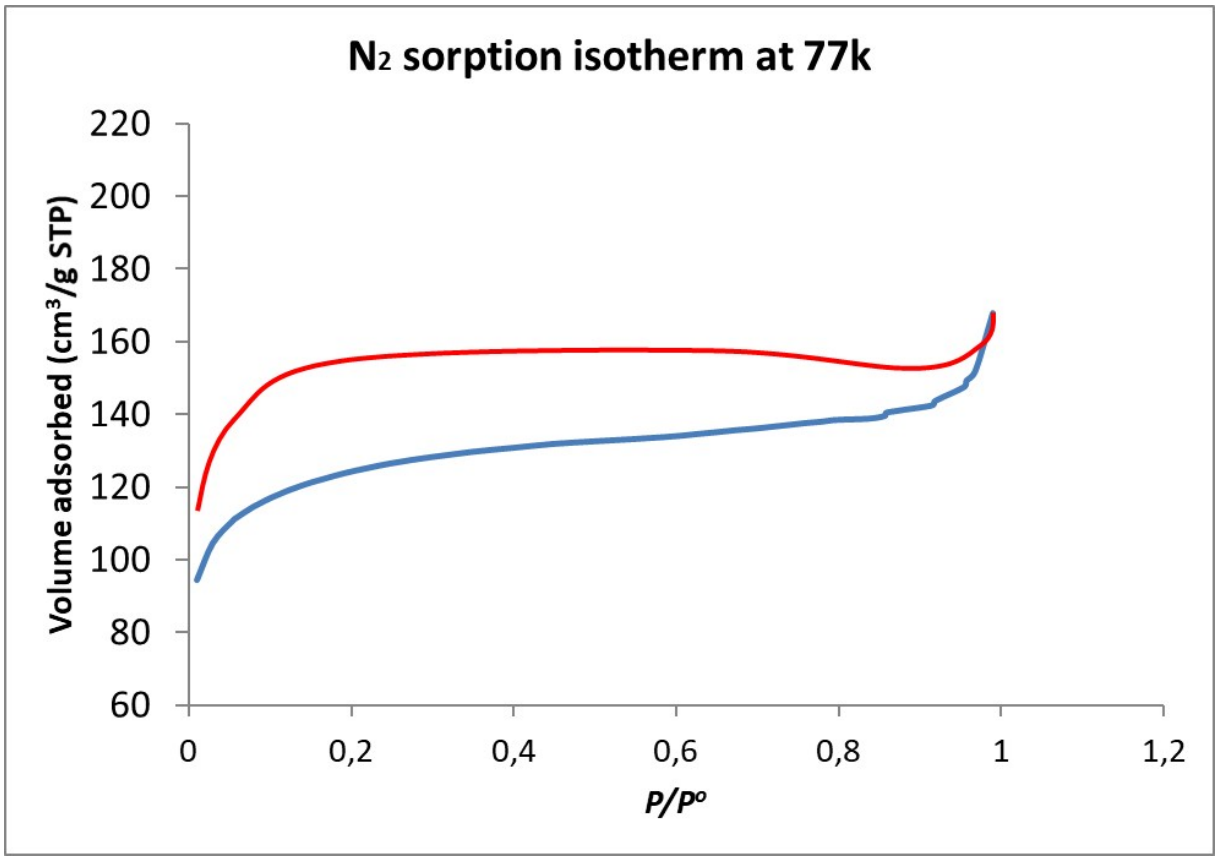


Figure S 44. N_2 adsorption/desorption isotherms of **Ni**$_{mat}$

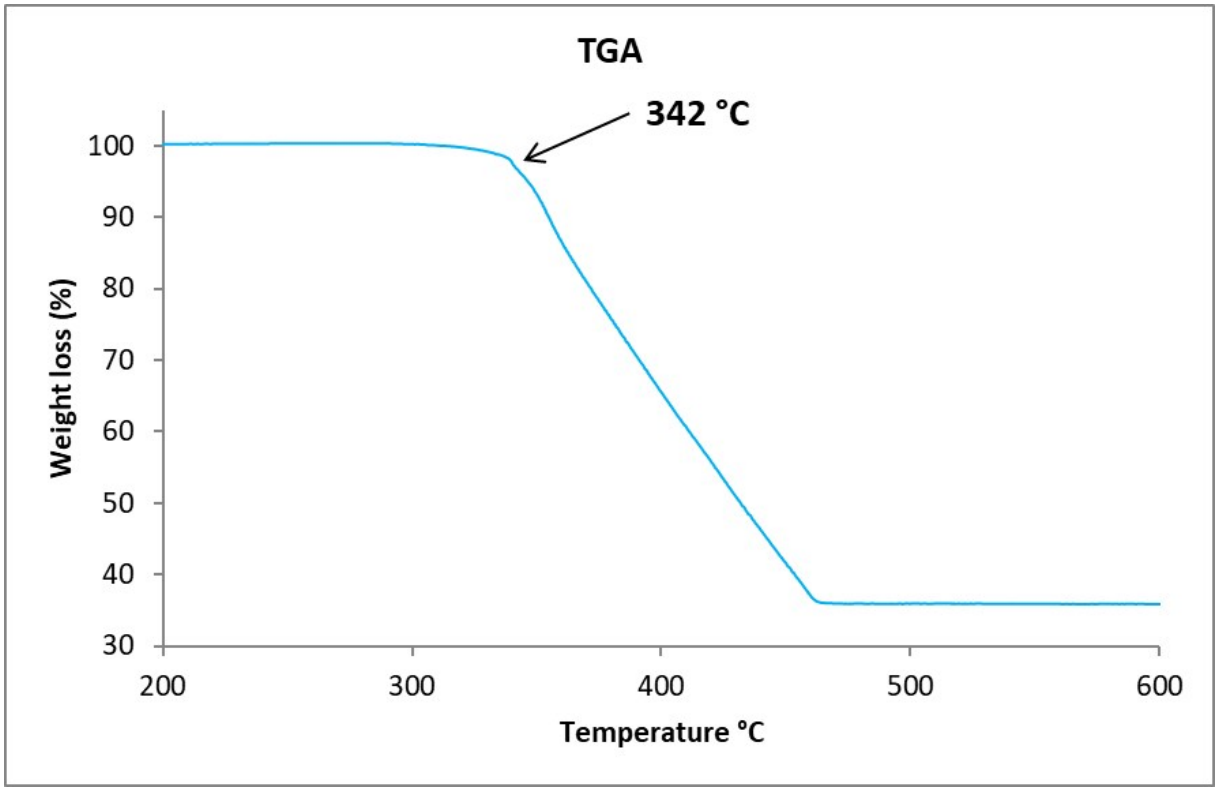


Figure S 45. Thermogravimetric analysis of **Ni**$_{mat}$

Zn$_{mat}$

EDX Trials	Au	Zn	Au/Zn
1	2.26	0.97	2.32
2	2.22	0.95	2.33
3	2.22	0.97	2.28
average	2.23	0.96	2.32

Figure S 46. Relative ratio of Au/Ni present in **Zn$_{mat}$** measured by EDX. Measured were repeated 3 times.

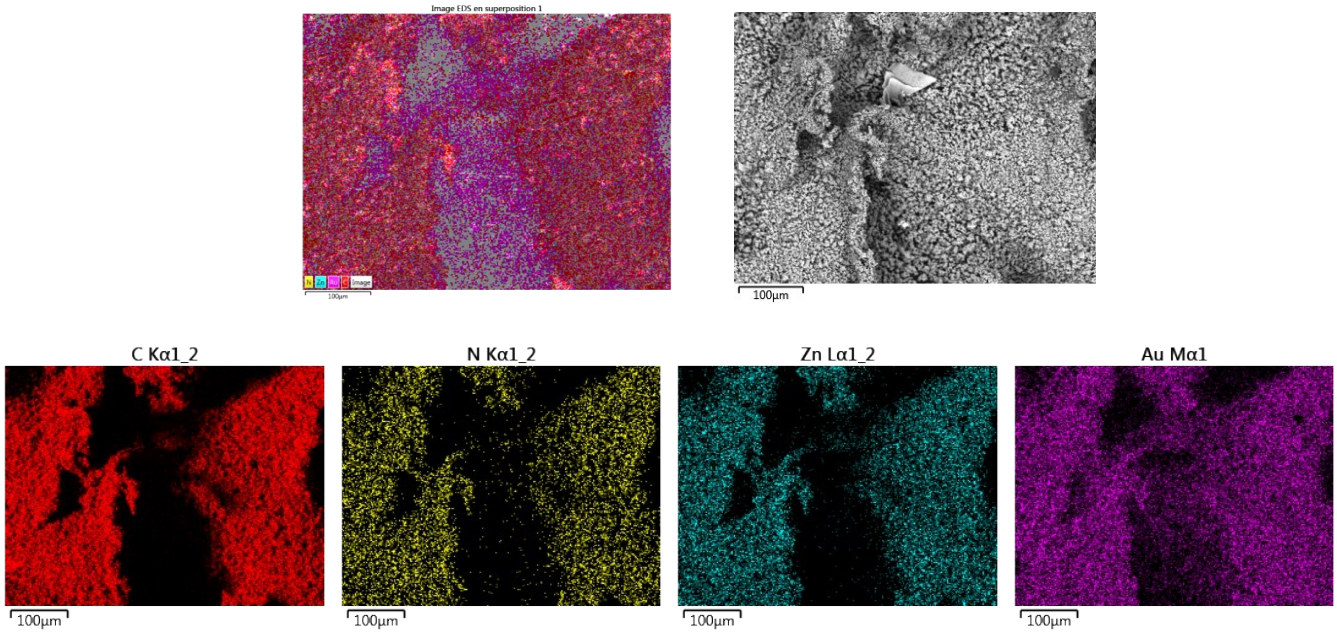


Figure S 47. Elemental mapping analysis of **Zn$_{mat}$** realized by means of EDX in zone 1.

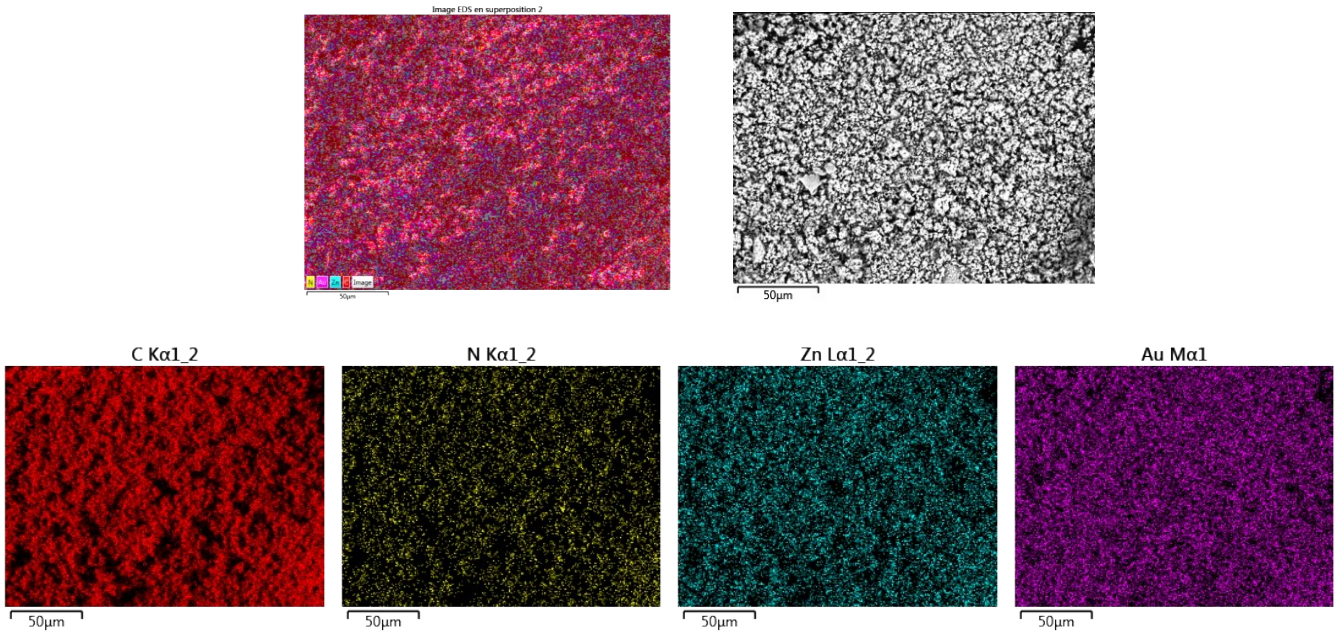


Figure S 48. Elemental mapping analysis of **Zn**$_{mat}$ realized by means of EDX in zone 2.

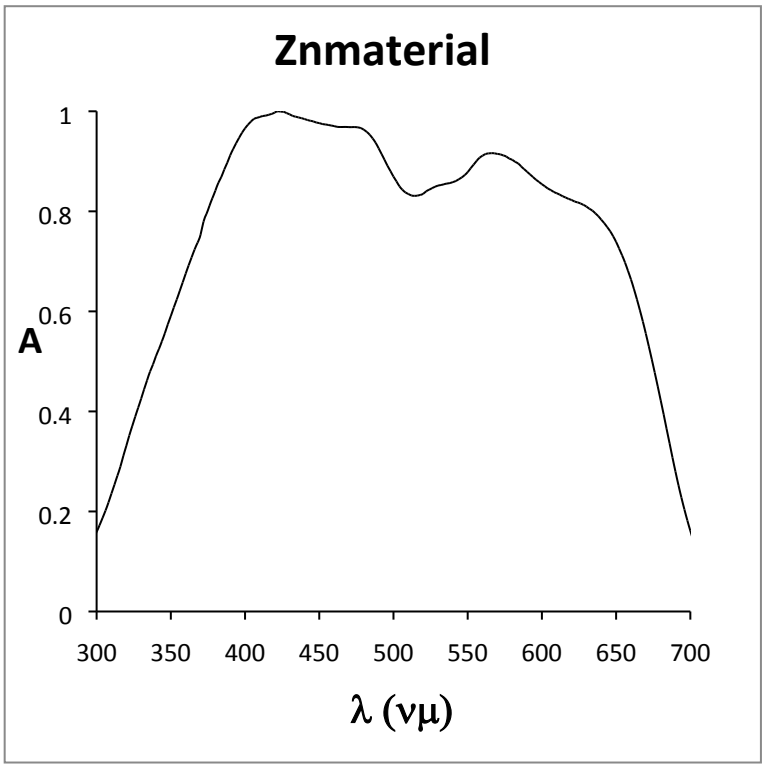


Figure S 49. Solid state UV-Vis spectrum of **Zn**$_{mat}$

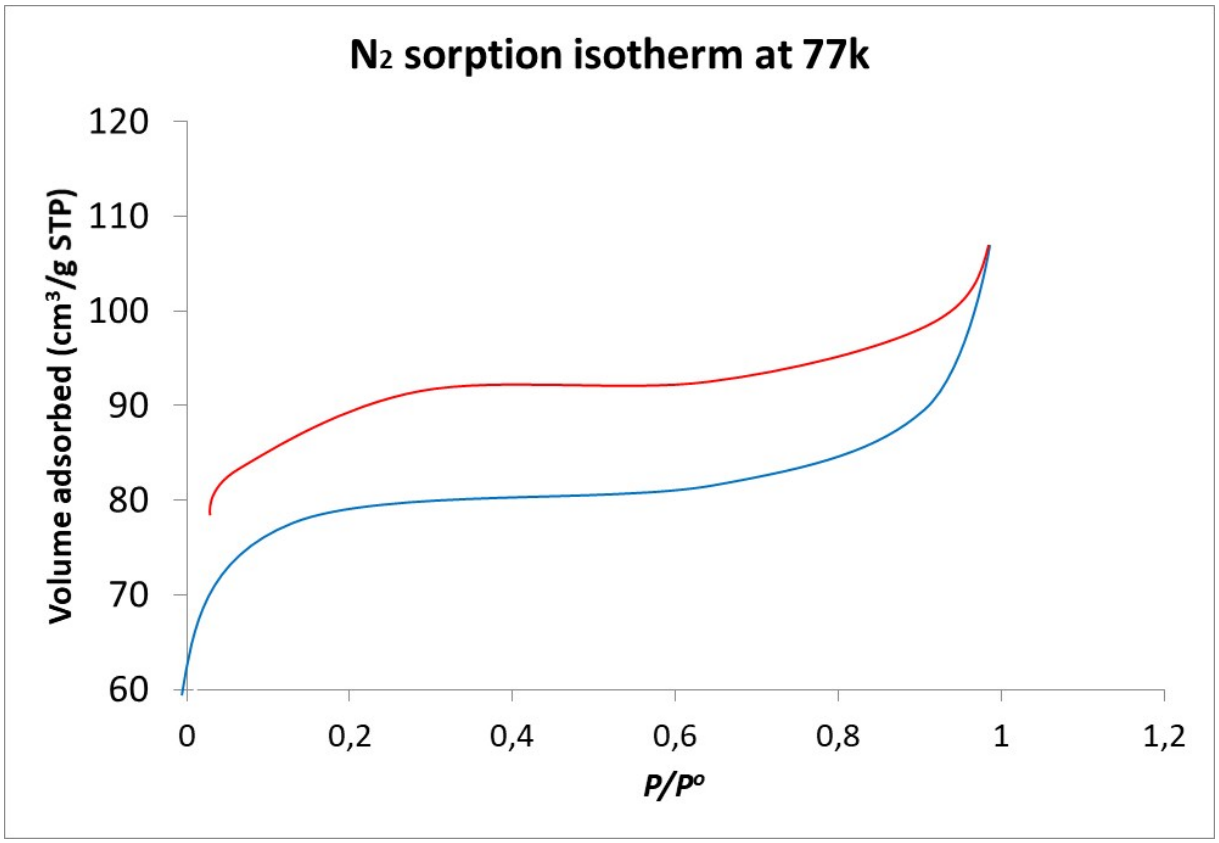


Figure S 50. N_2 adsorption/desorption isotherms of **Zn_{mat}**