Electronic Supplementary Material (ESI) for Dalton Transactions

Access to Functionalised Silver (I) and Gold(I) *N*-Heterocyclic Carbenes by [2+3] Dipolar Cycloadditions.

by

Audrey Hospital,[a] Clémentine Gibard,[a] Christelle Gaulier,[a] Lionel Nauton,[a,b] Vincent Théry,[a] Malika El–Ghozzi,[a] Daniel Avignant,[a] Federico Cisnetti*[a] and Arnaud Gautier* [a,b]

[a] *Institut de Chimie de Clermont–Ferrand, Clermont Université, Université Blaise Pascal, F–63000 Clermont–Ferrand, France Fax:+33 473 407 717; Tel: +33 473 407 110, E–mail: federico.cisnetti@univ–bpclermont.fr*
[b] *CNRS, UMR 6296, F–63177 Aubière, CEDEX, France. Fax: +33 473 407 717; Tel: +33 473 407 646; E-mail: arnaud.gautier@univ-bpclermont.fr*

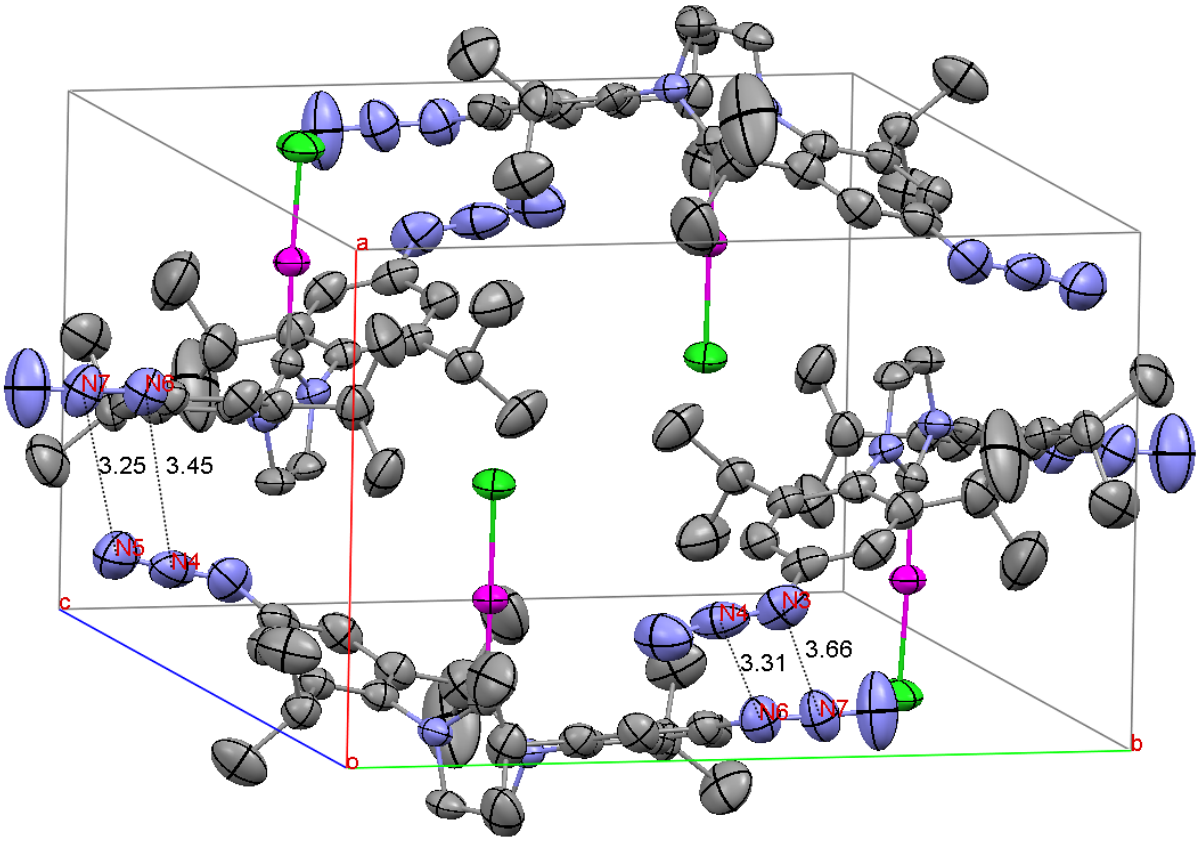
Supporting information

Contents:

Electronic Supplementary Material (ESI) for Dalton Transactions

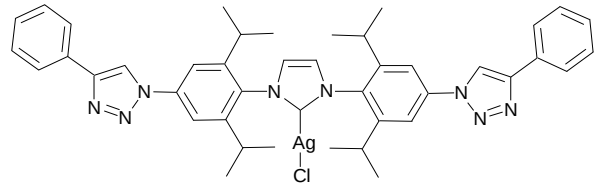
S1: Crystal packing of 22

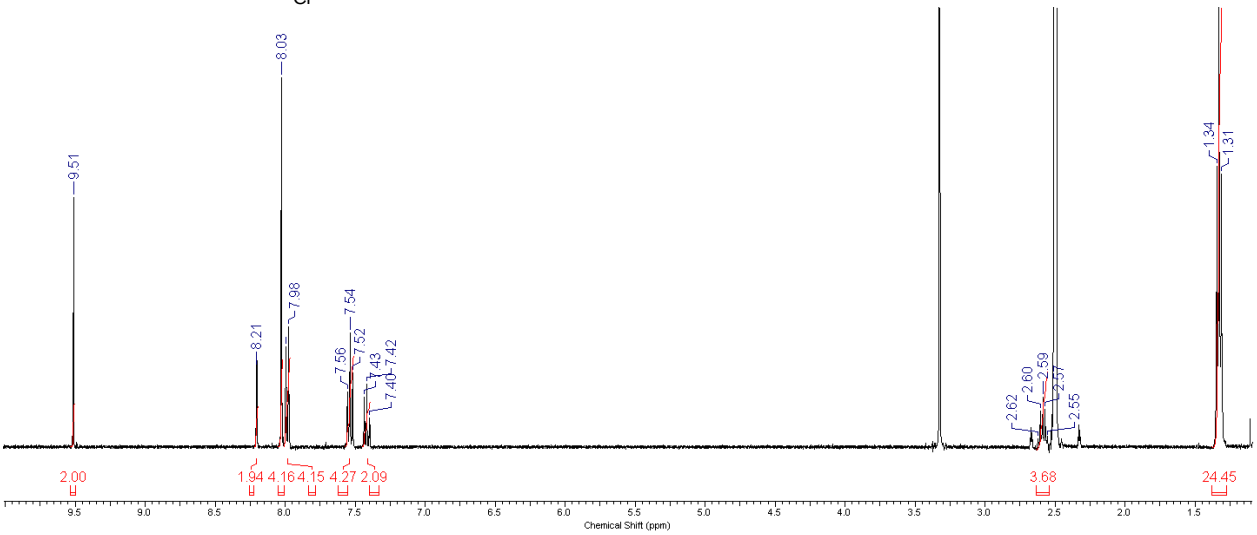
Packing of gold complex **22** showing azide–azide distances. Ellipsoids were drawn at 50% probability level and H atoms omitted for clarity

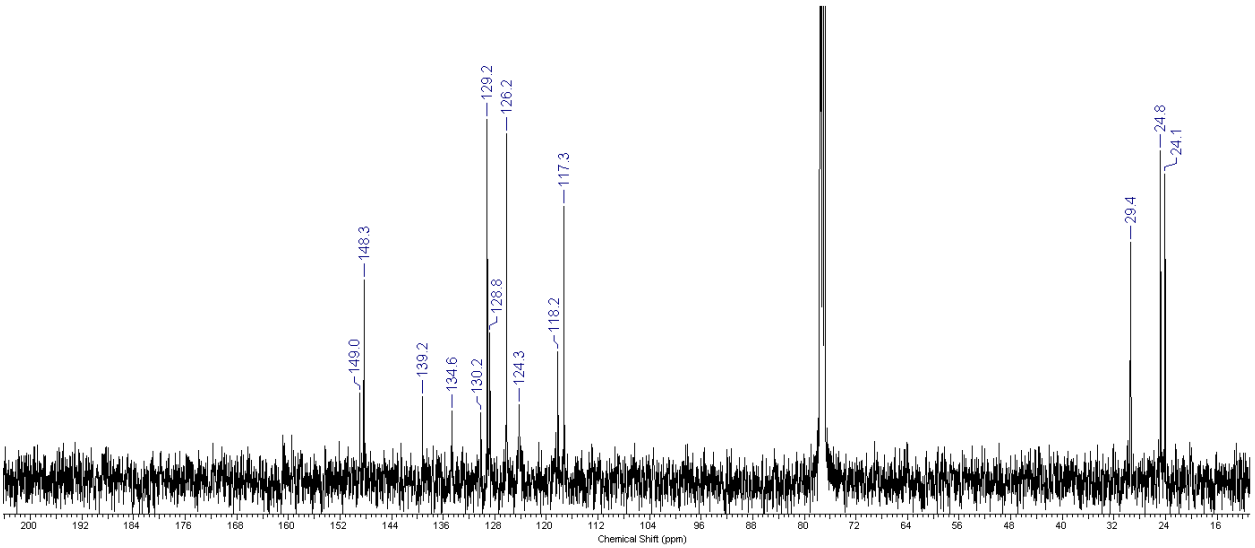


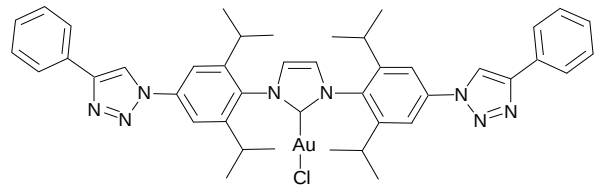
S2. Selected NMR spectra.

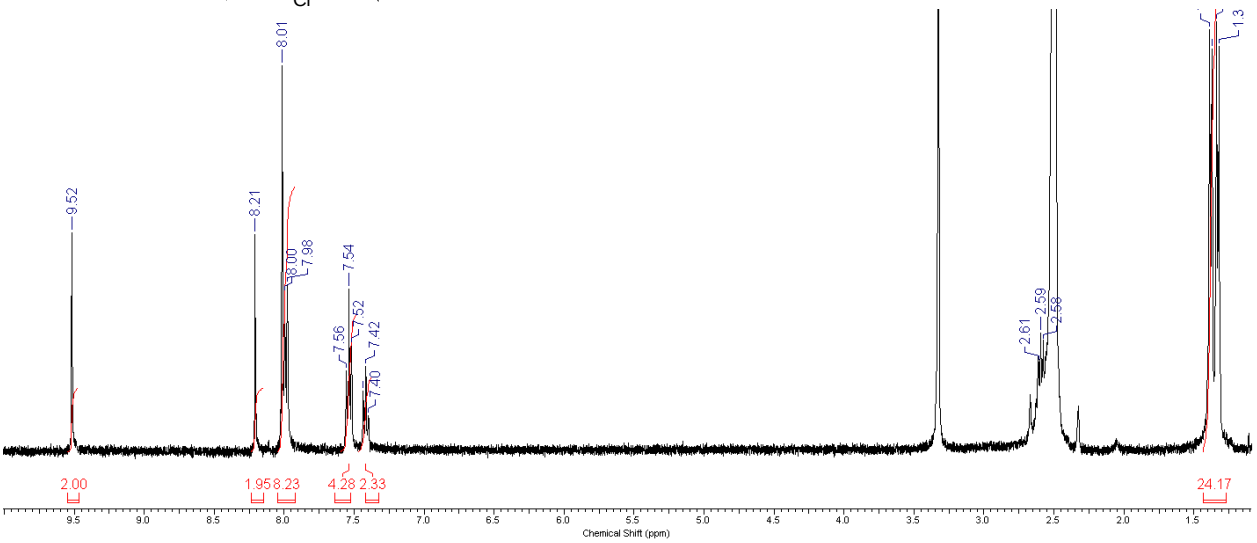
S2a: ^{1}H and ^{13}C NMR spectra of metallocarbenes

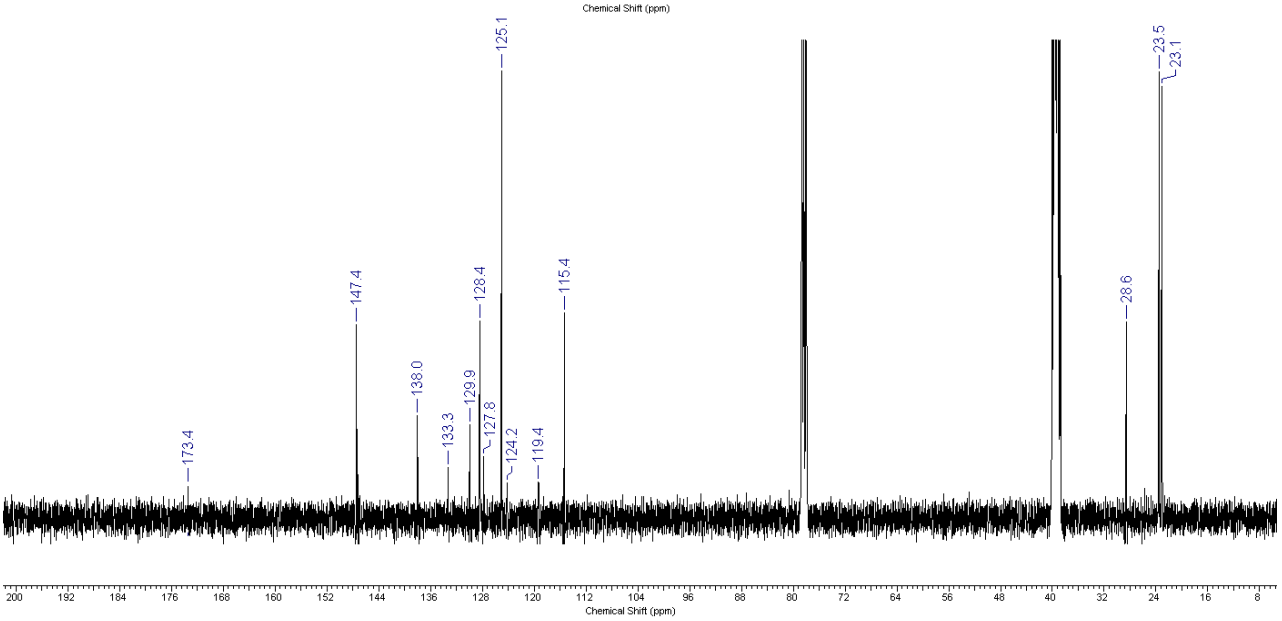


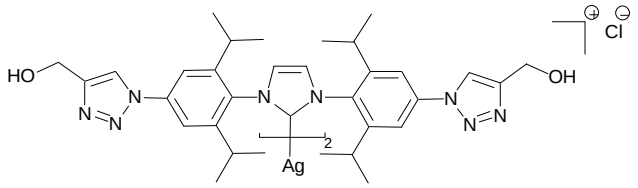


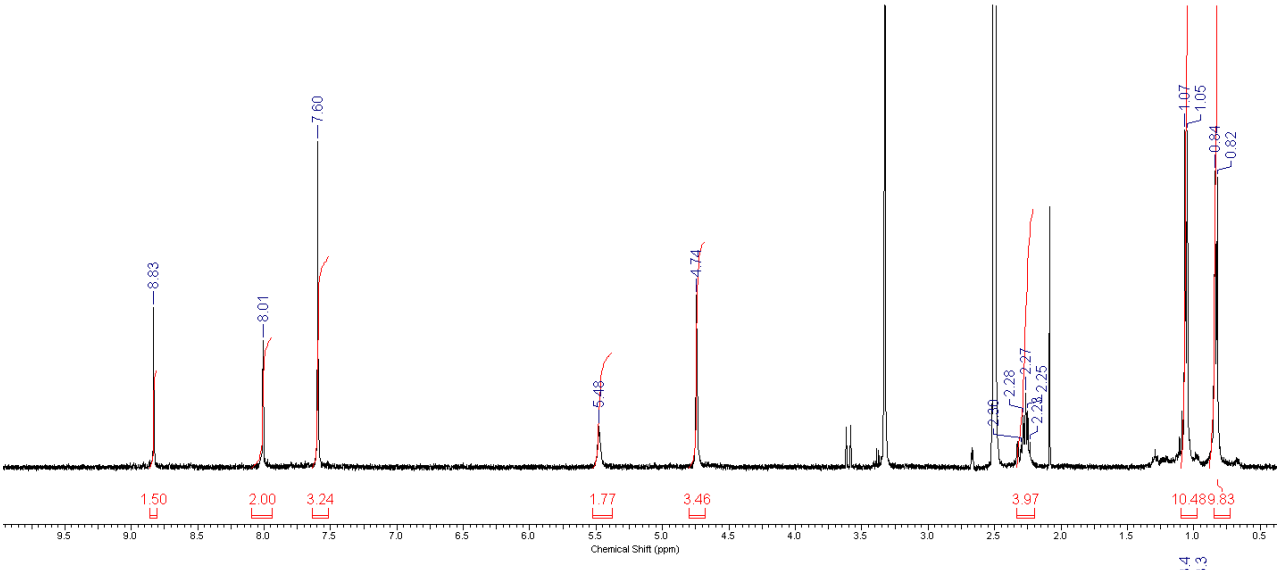


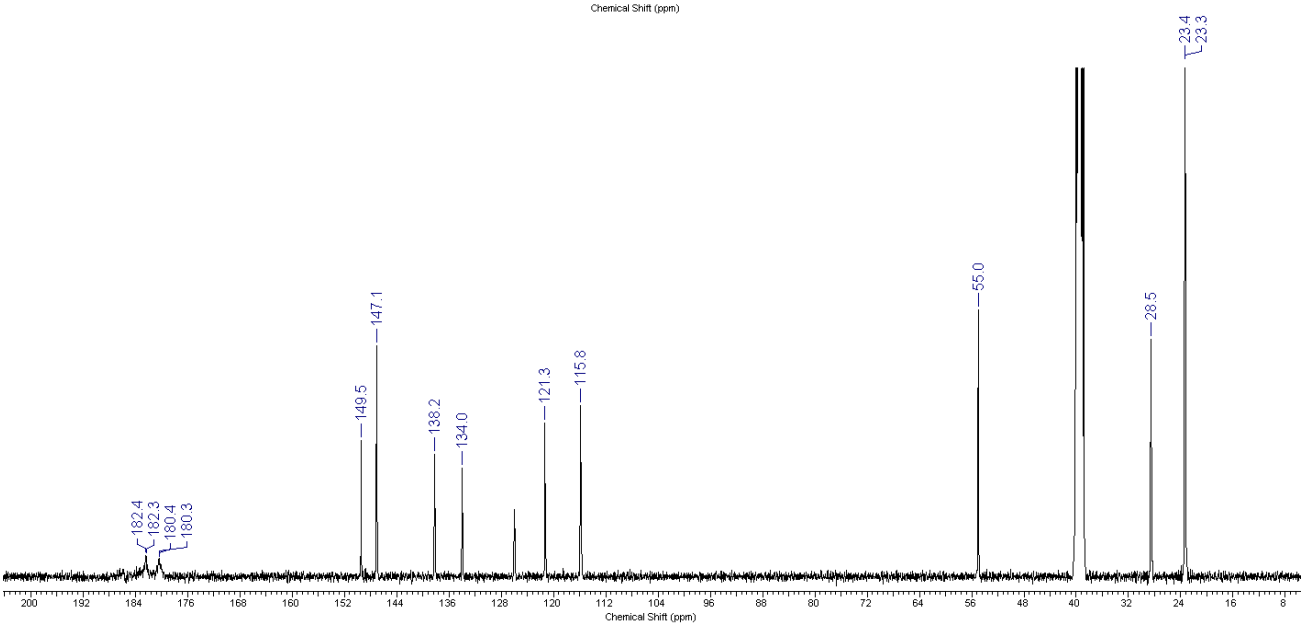


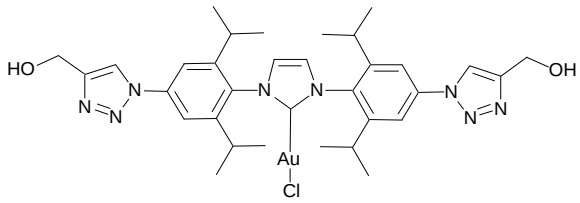


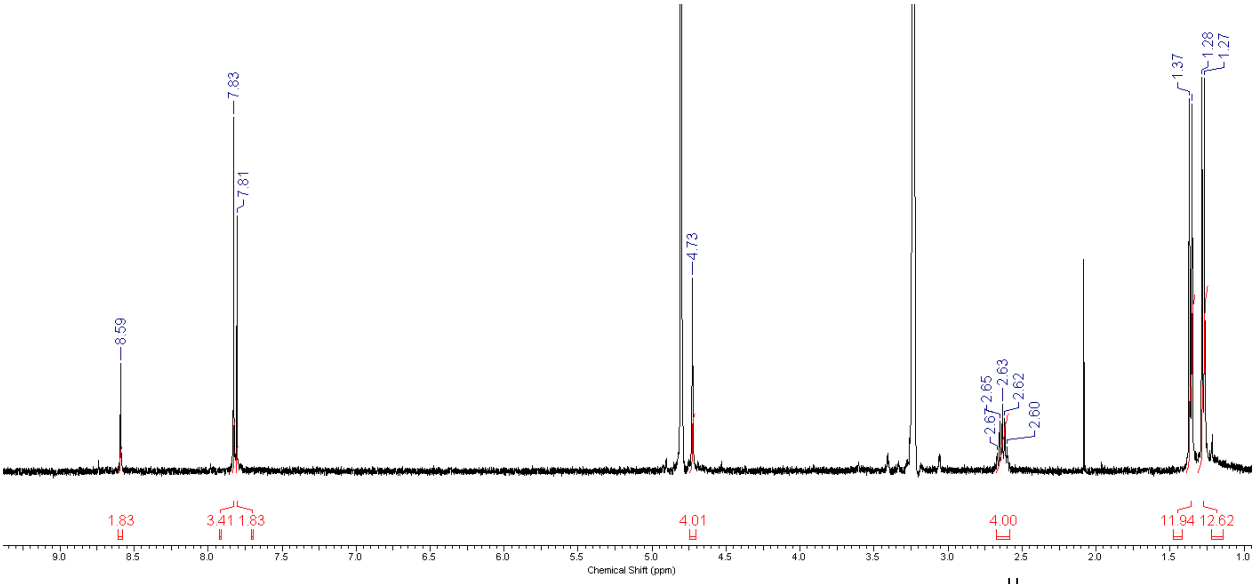


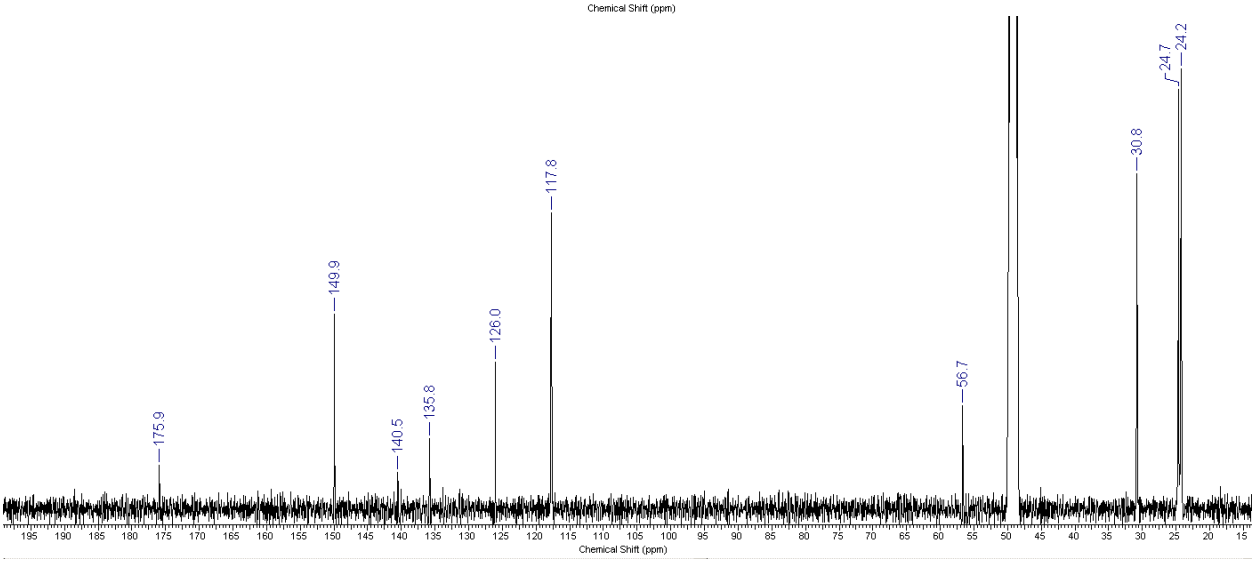


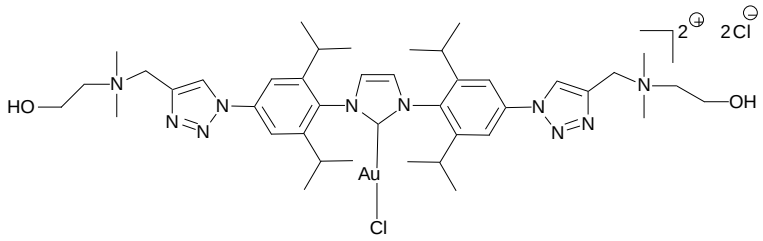


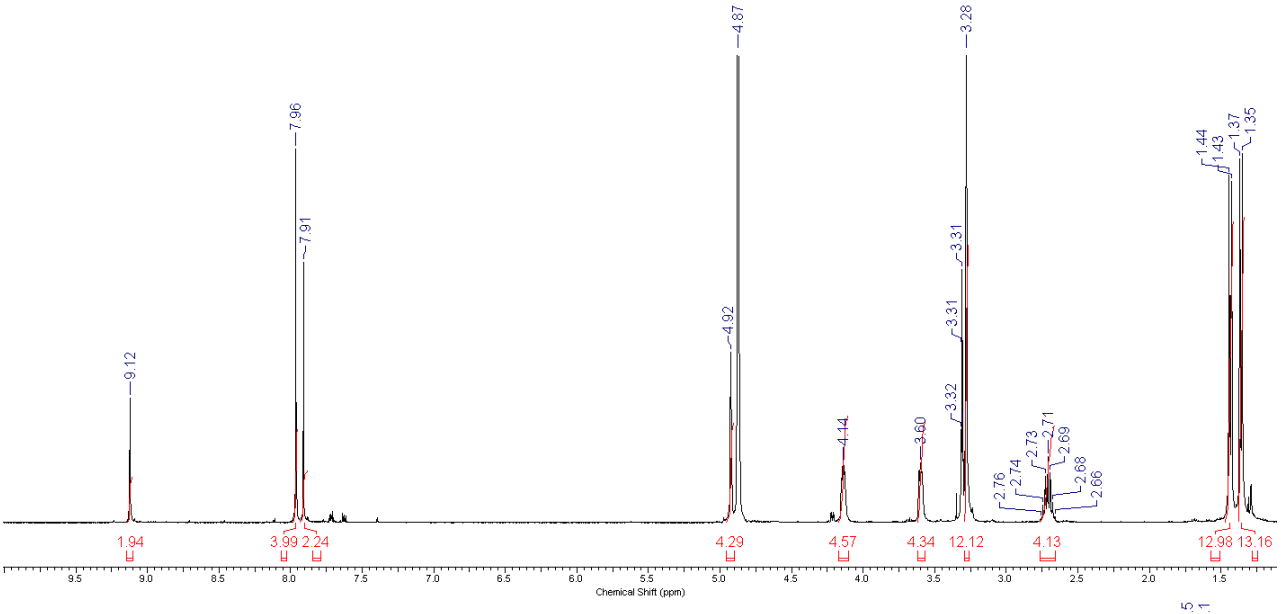


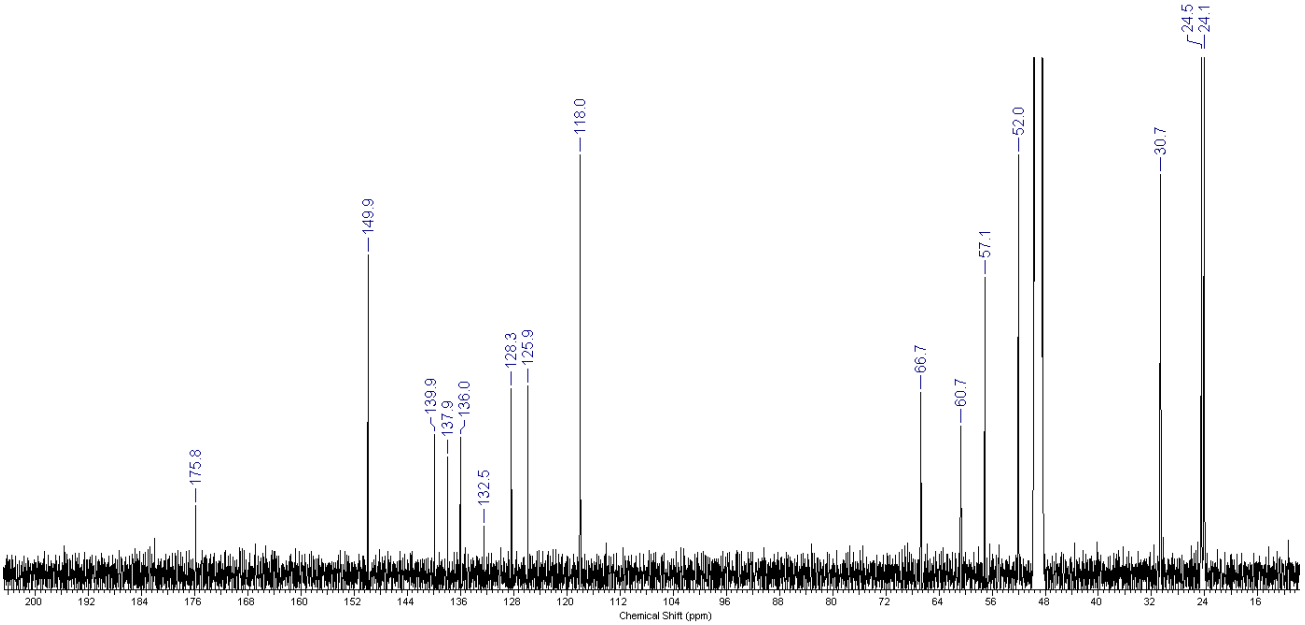


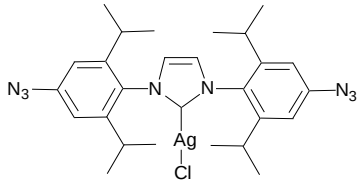


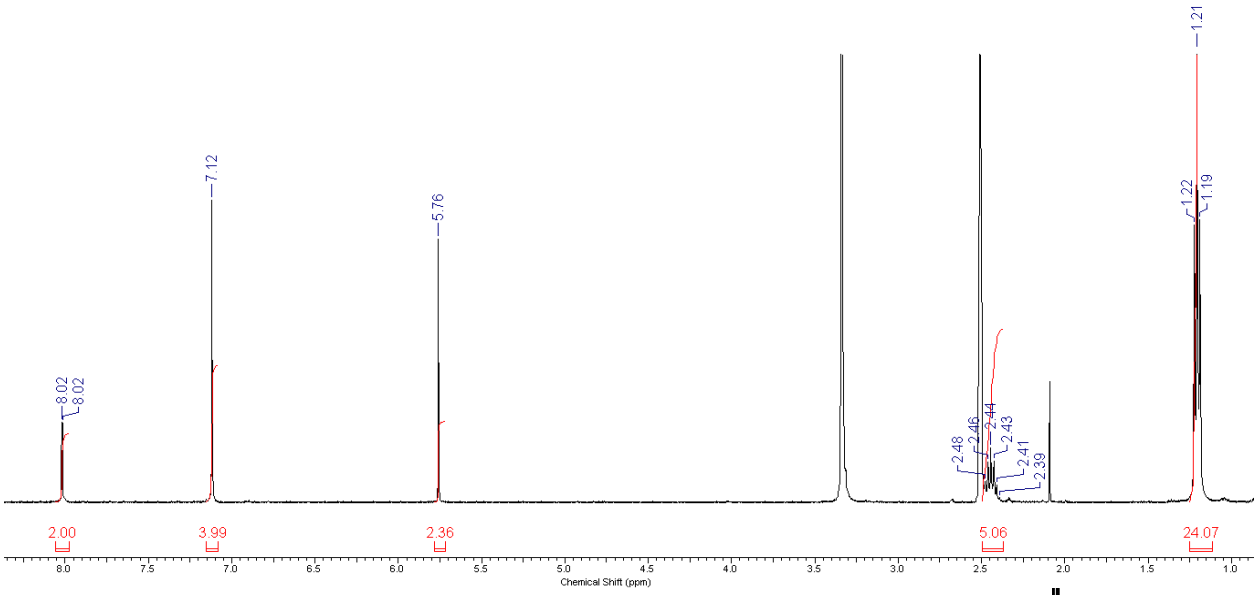


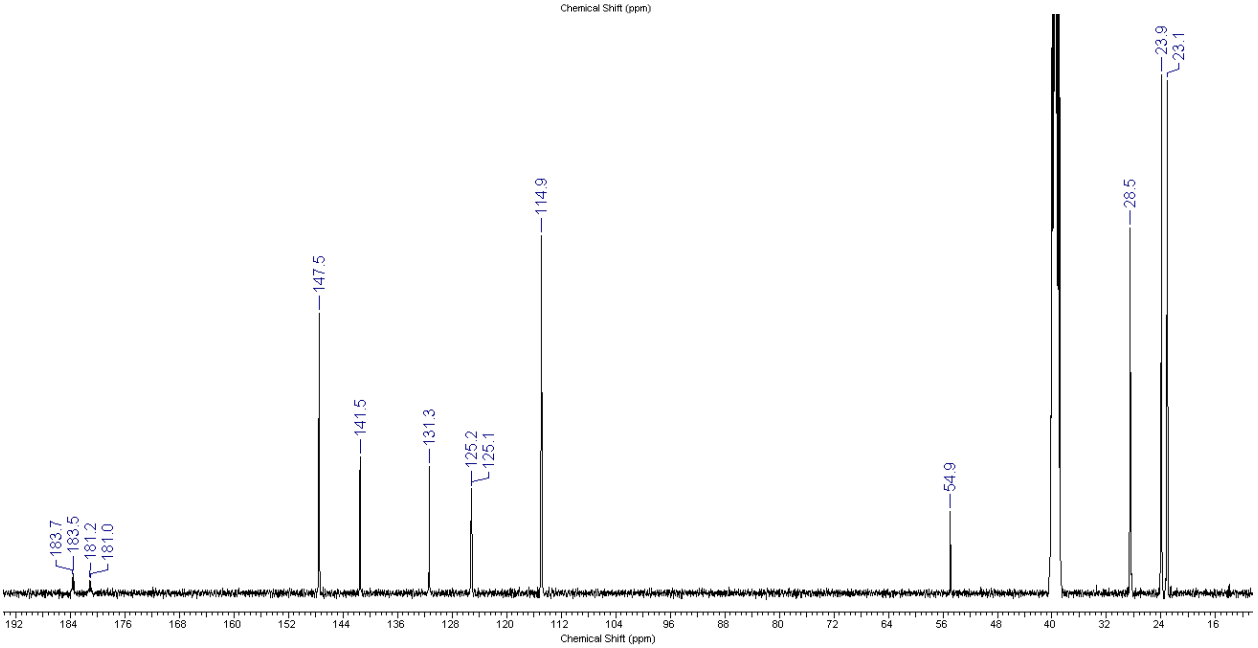

HO
N
N
N
N
N
N
N
N
N
N
OH
2⊕
2Cl⊖
Au
Cl

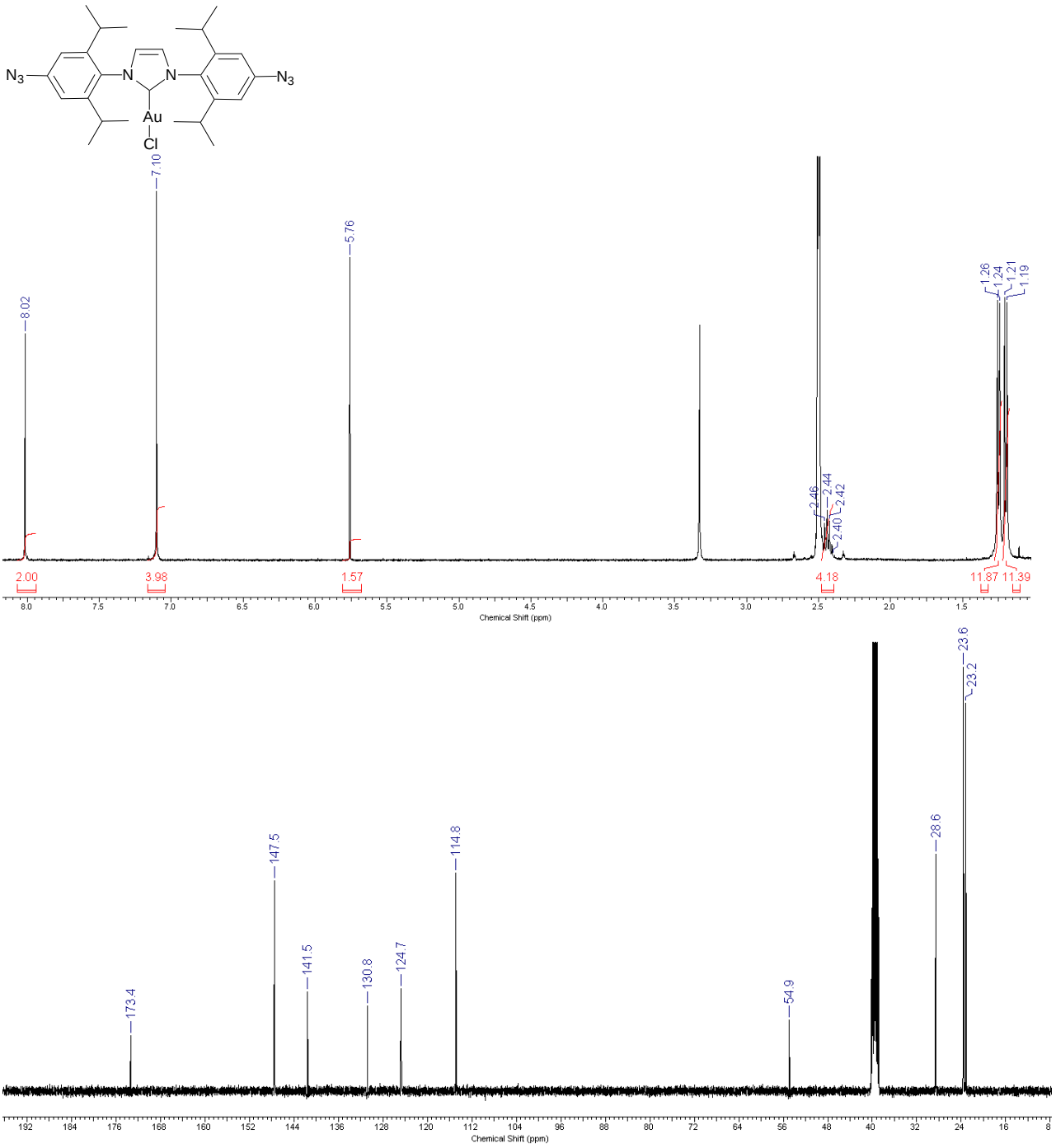

9.12
7.96
7.91
4.92
4.87
4.14
3.60
3.32
3.31
3.31
3.28
2.76
2.74
2.73
2.71
2.69
2.68
2.66
1.44
1.43
1.37
1.35
1.94
3.99
2.24
4.29
4.57
4.34
12.12
4.13
12.98
13.16
Chemical Shift (ppm)

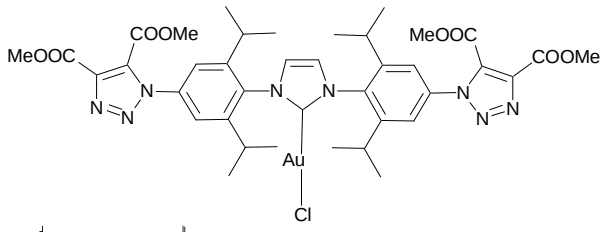

175.8
149.9
139.9
137.9
136.0
132.5
128.3
125.9
118.0
66.7
60.7
57.1
52.0
30.7
24.5
24.1
Chemical Shift (ppm)

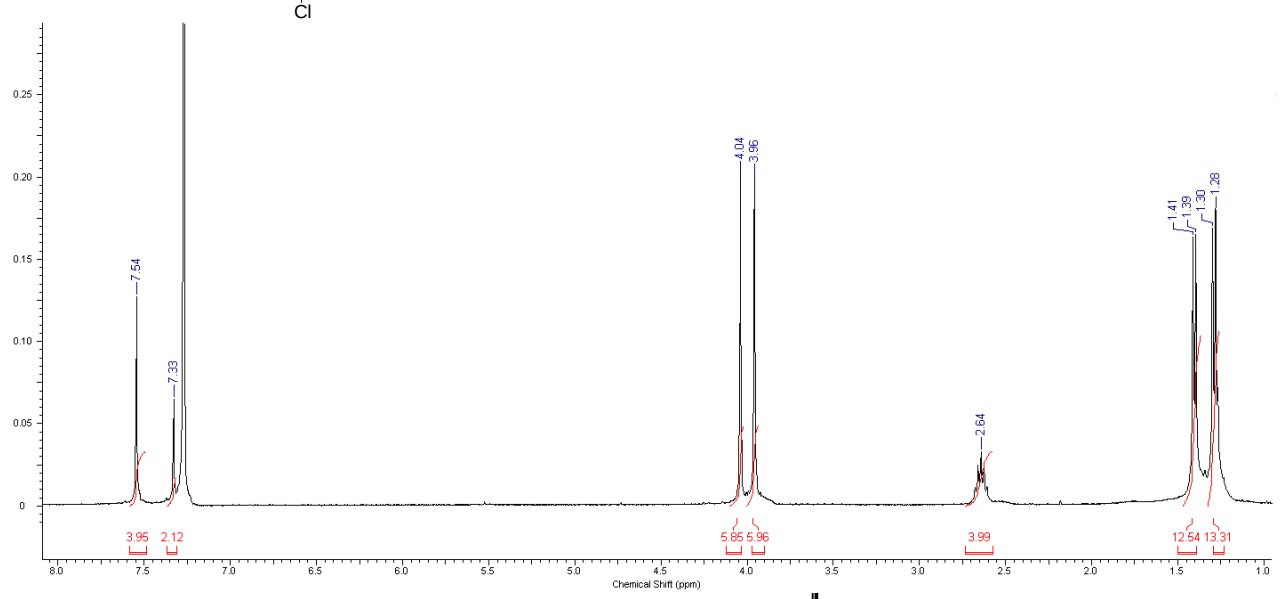


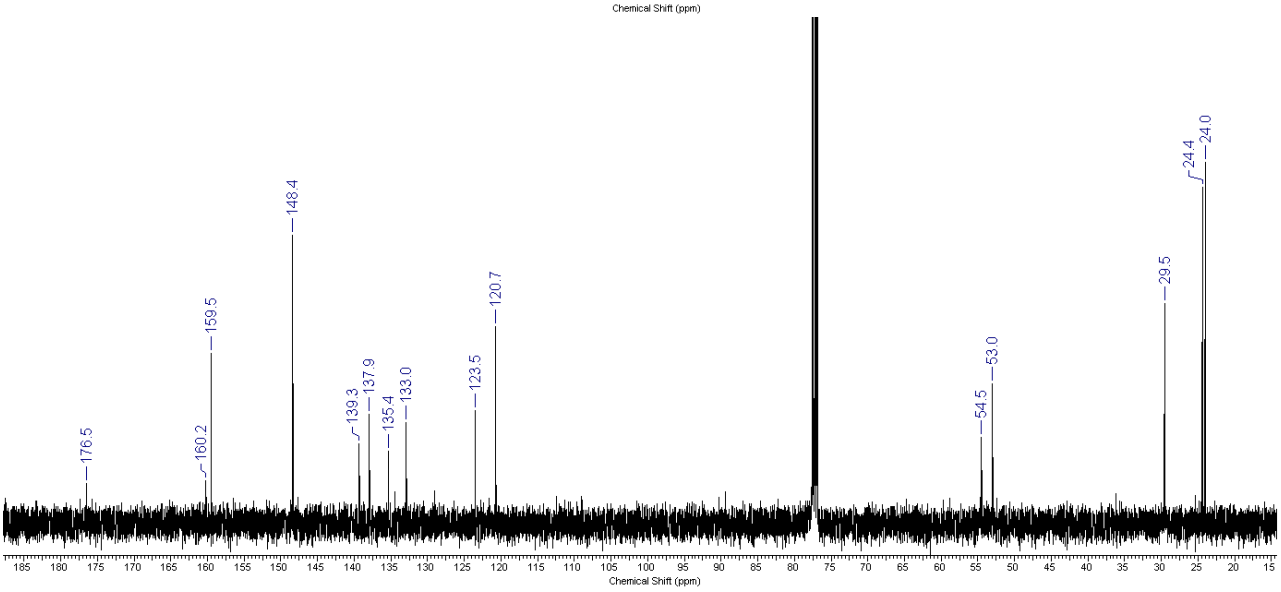




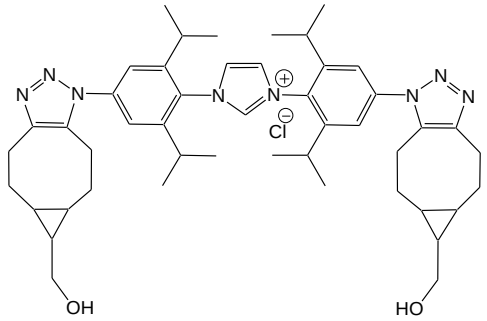


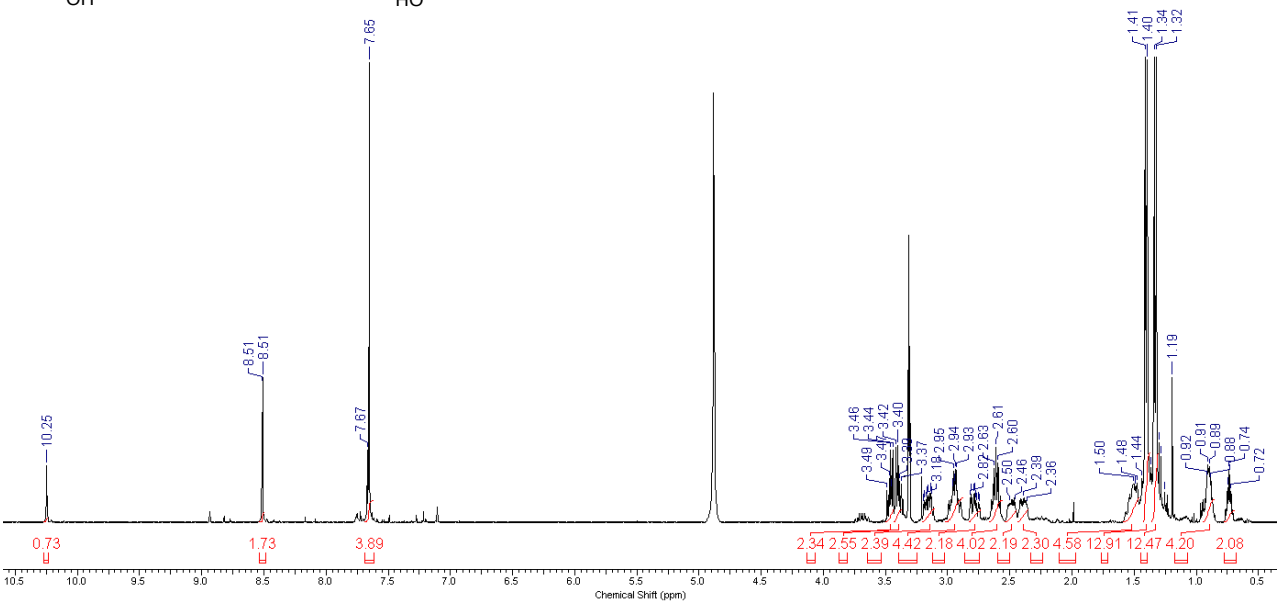


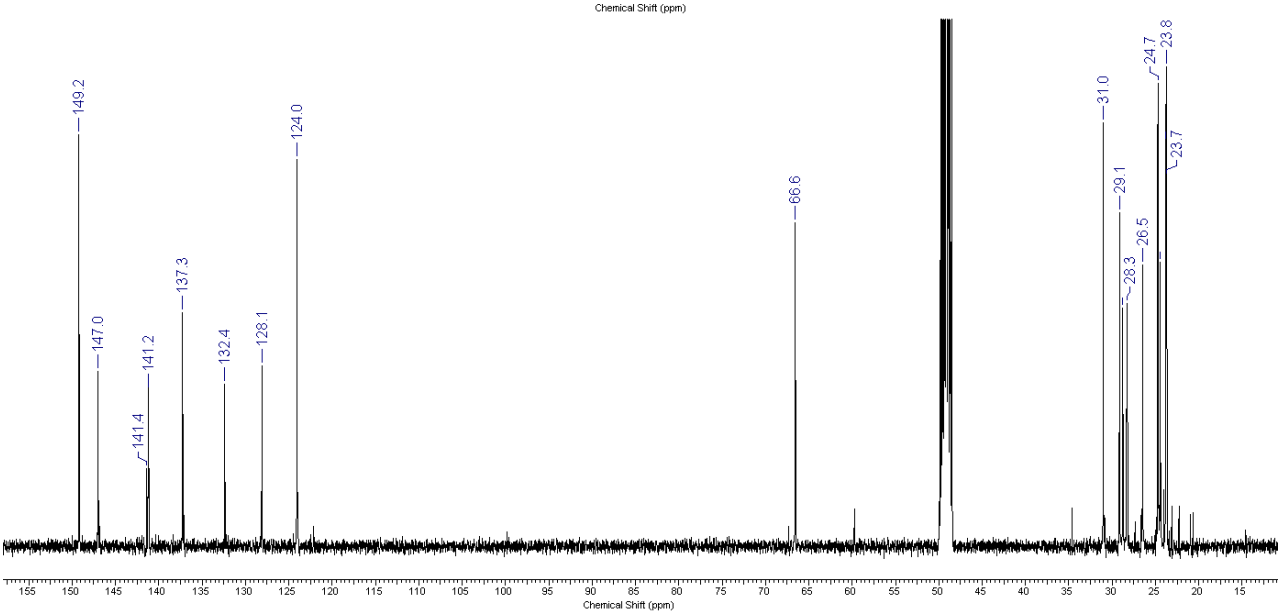




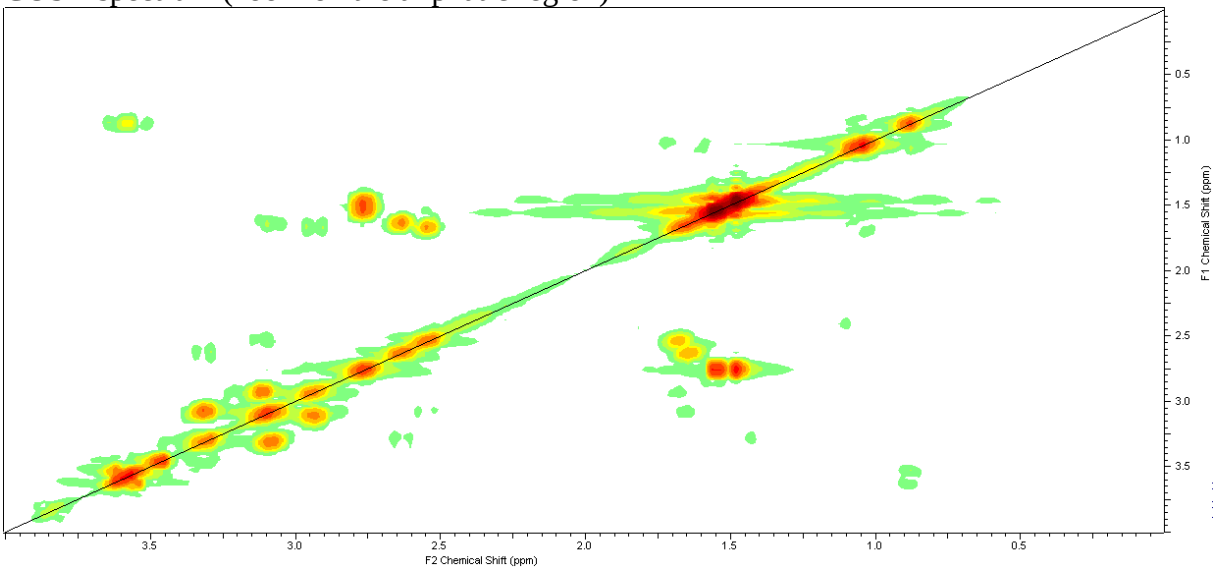
S2b: ^{1}H, ^{13}C, COSY and HSQC spectra of cyclooctyne adducts.







COSY spectrum (zoom on the aliphatic region)



^{1}H-^{13}C HSQC spectrum

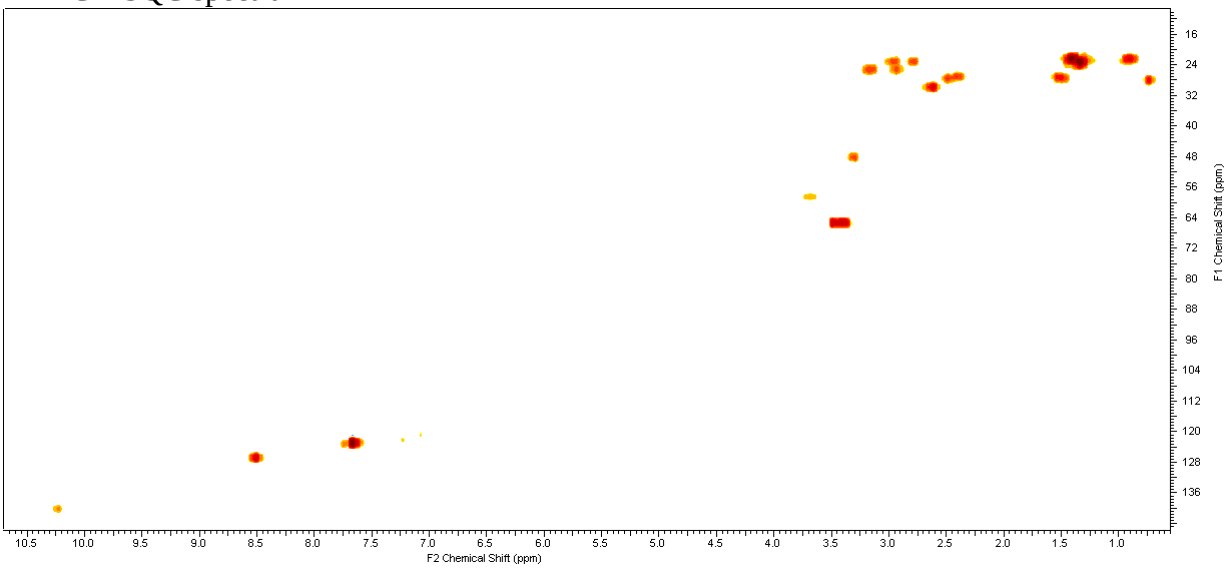
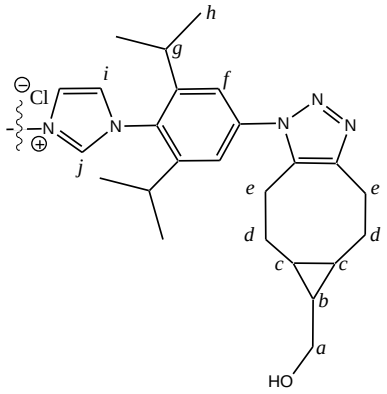
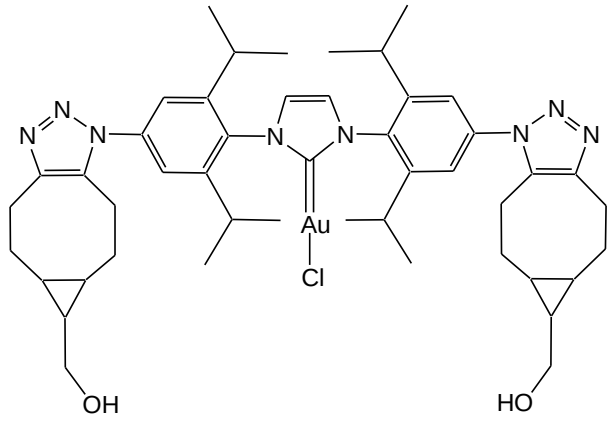


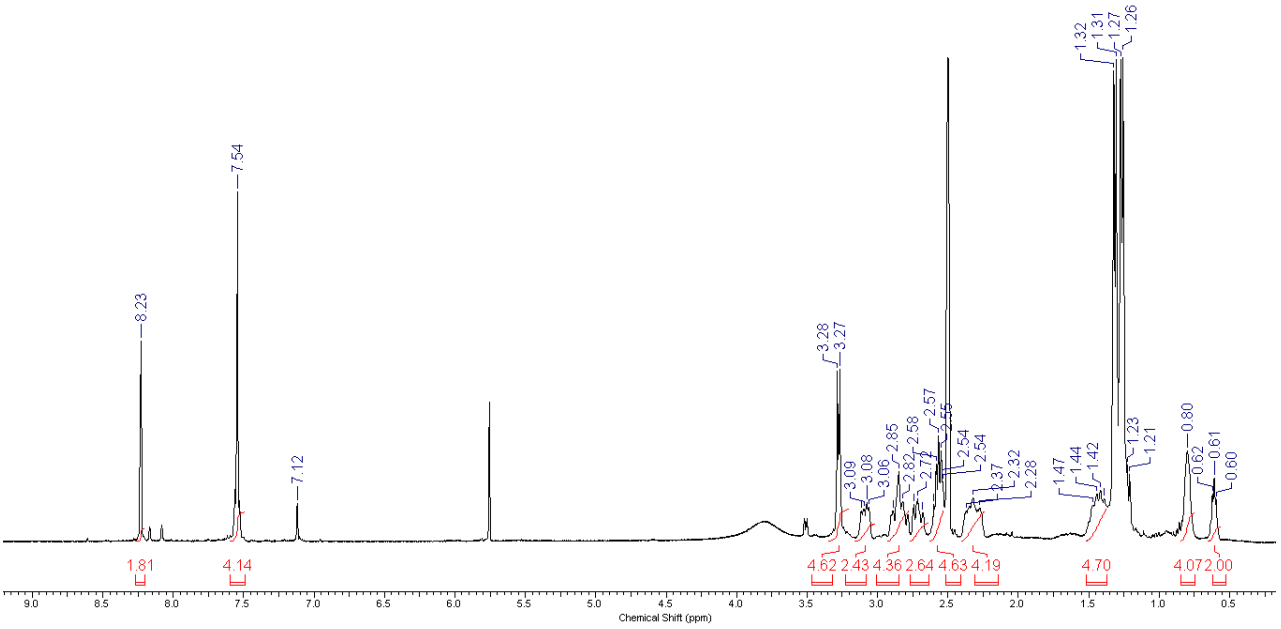
Table S1 – Partial NMR attribution (COSY, HSQC, JMOD) of **9**

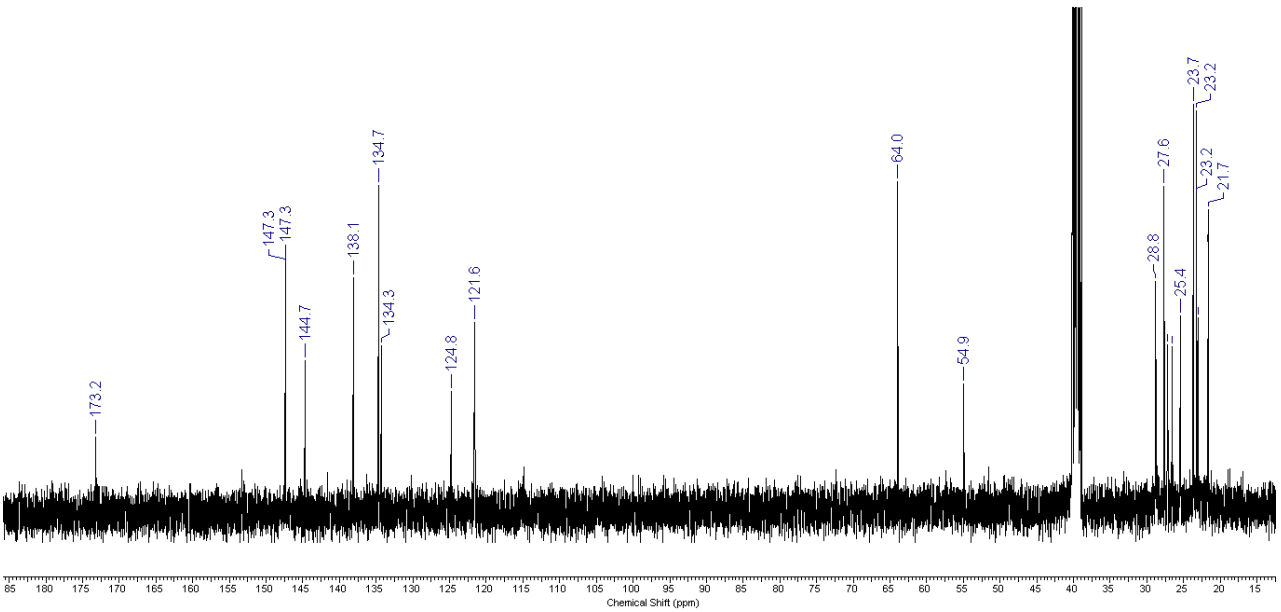


position(s)	^{1}H NMR (δ/ ppm)	^{13}C NMR (δ/ ppm)
a	3.46 (dd, 2H, ^{3}J =7.0 Hz, ^{2}J = 11 Hz) 3.40 (dd, 2H, , ^{3}J =7.0 Hz, ^{2}J = 11 Hz)	66.6
b	0.73 (m, 2H)	29.1
c	0.90 (m, 4H)	23.7-23.8 (2 signals)*
d	1.51 (m, 4H), 2.39 (m, 2H), 2.48 (m, 2H)	28.8, 28.3
e	3.08 (ddd, 2H, ^{3}J = 3.0 Hz, ^{3}J = 7.5 Hz, ^{2}J =16.0 Hz), 2.99-2.90 (m, 4H), 2.78 (ddd, 2H, ^{3}J = 3.0 Hz, ^{3}J = 9.5 Hz, ^{2}J =16.0 Hz)	26.5, 24.5
f	7.65 (s, 4H)	124.0
g	2.61 (hept, 4H, ^{3}J = 7.0 Hz)	31.0
h	1.41 (d, ^{3}J = 7.0 Hz), 1.33 (d, ^{3}J = 7.0 Hz)	24.74, 24.72, 23.7-23.8 (2 signals)*
i	8.50 (d, 2H, ^{4}J = 1.5 Hz)	128.1
j	10.24 (t, 1H, ^{4}J = 1.5 Hz)	141.2

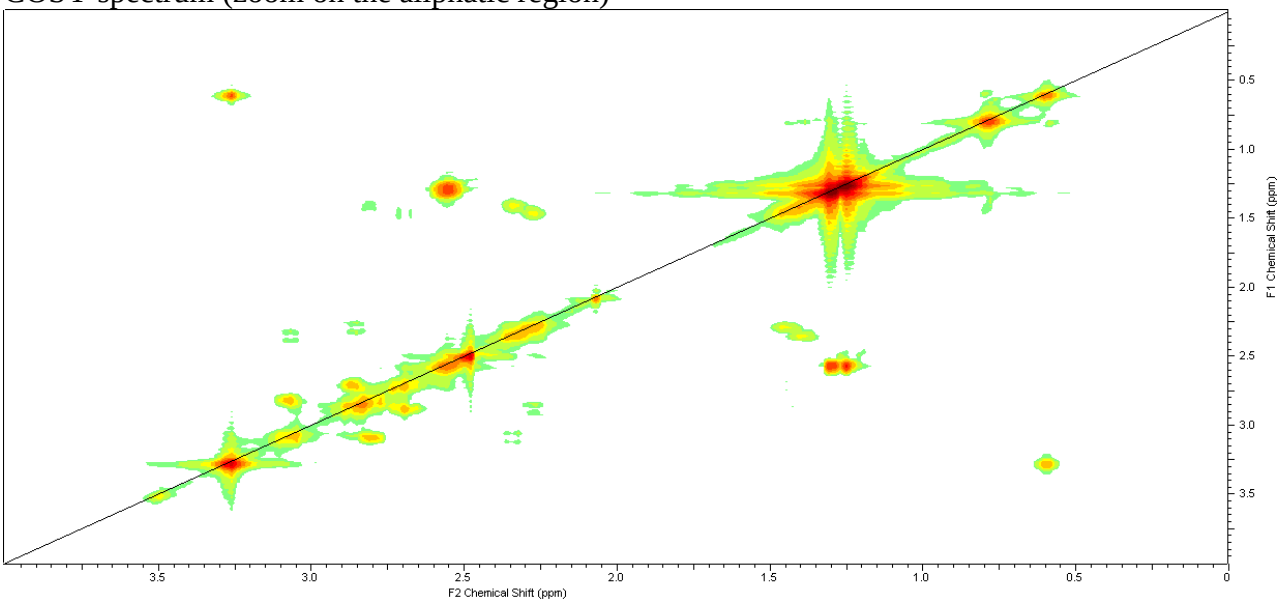
*4 signals are observed between in the spectrum 23.7 and 23.8 ppm







COSY spectrum (zoom on the aliphatic region)



^{1}H-^{13}C HSQC spectrum

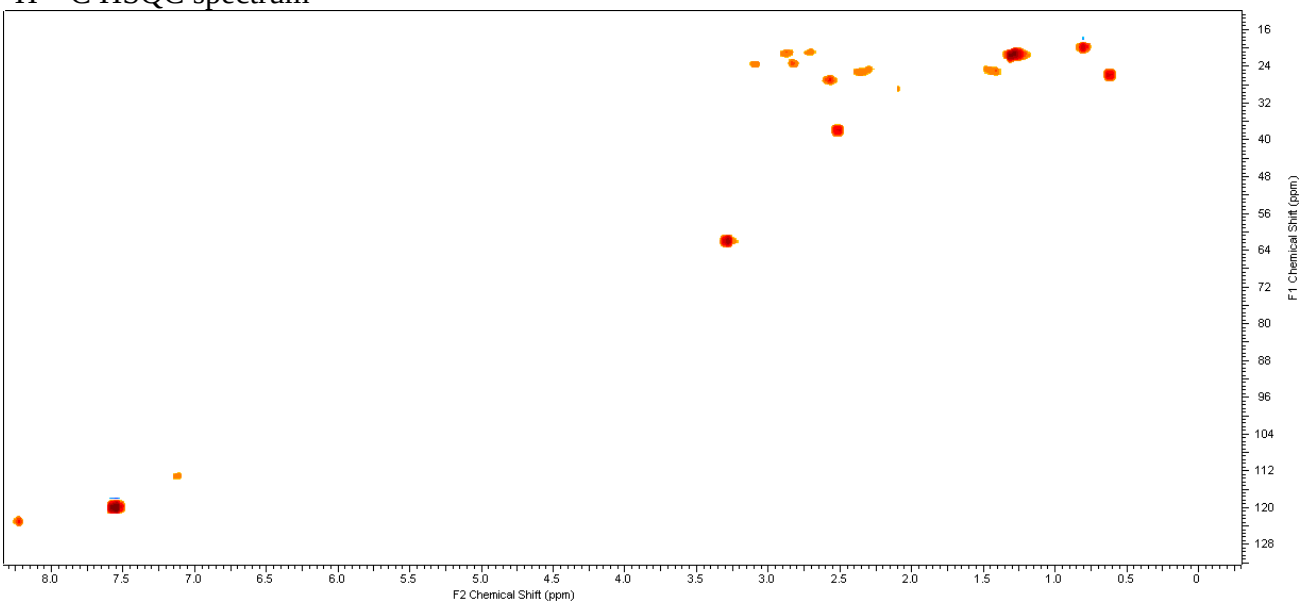
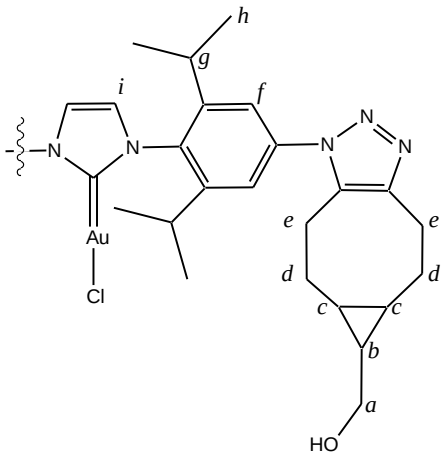


Table S2 – Partial NMR attribution (by COSY, HSQC and JMOD) of **24**



position(s)	^{1}H NMR (δ / ppm)	^{13}C NMR (δ / ppm)
a	3.28 (d, 4H, ^{3}J = 6.5 Hz)	64.0
b	0.60 (m, 2H)	27.6
c	0.76-0.83 (m, 4H)	21.72, 21.66
d	1.37-1.51 (m, 4H), 2.35 (m, 2H), 2.29 (m, 2H)	26.6, 27.2
e	3.08 (ddd, 2H, ^{3}J = 2.5 Hz, ^{3}J = 7.5 Hz, ^{2}J =15.5 Hz), 2.91-2.78 (m, 4H), 2.71 (ddd, 2H, ^{3}J = 3.0 Hz, ^{3}J = 10.0 Hz, ^{2}J =15.5 Hz)	23.1, 25.4
f	7.54 (s, 4H)	121.6
g	2.56 (hept, 4H, ^{3}J = 7.0 Hz)	28.8
h	1.32 (d, ^{3}J = 7.0 Hz), 1.27 (d, ^{3}J = 7.0 Hz)	23.69, 23.66, 23.24, 23.20
i	8.22 (s, 2H)	124.8

S3: Representation of the calculated transition states.