Supplementary Information Available

Exploring the potential of gold(III) cyclometallated compounds as cytotoxic agents: variations on the C,N theme

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Compound 2-PF_6

X-ray diffraction

Figure S1 - The asymmetric unit of complex 2-PF_6.

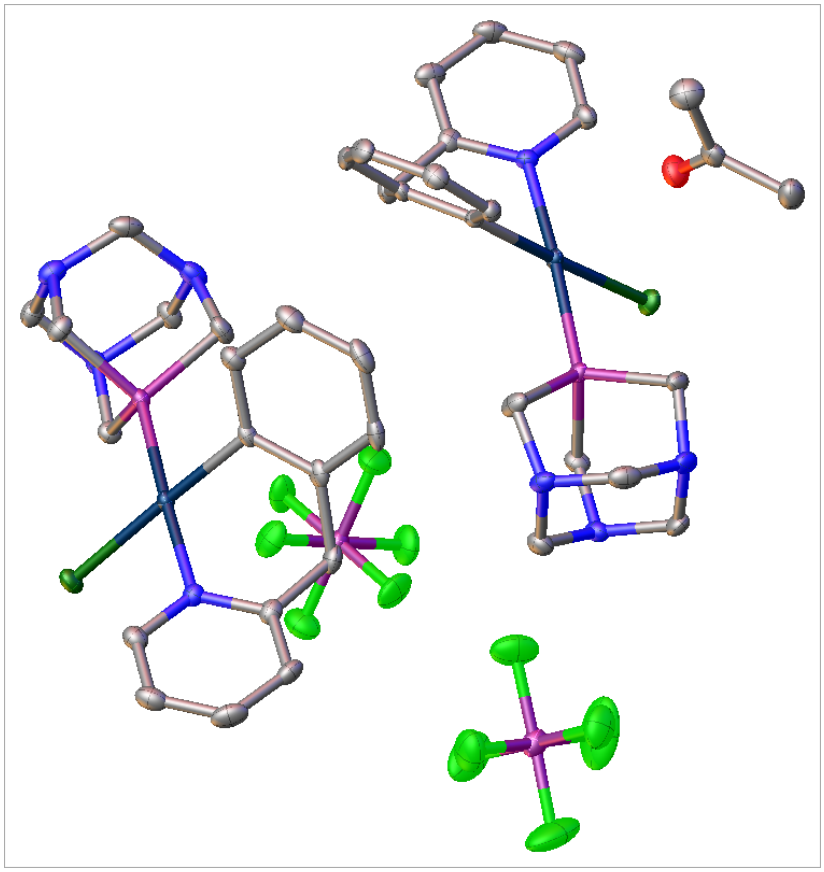
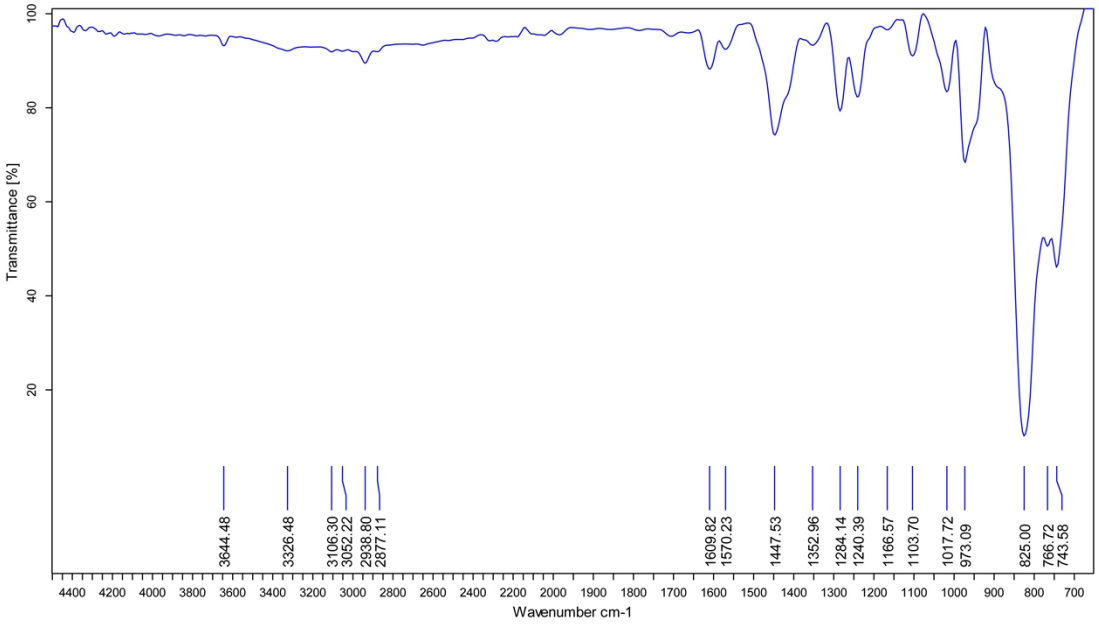
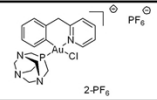


Table S1 - Crystal data and structure refinement for $[Au(py^b\text{-}H)(pta)Cl]PF_6$.

Identification code	**2**
Empirical formula	$C_{39}H_{50}Au_2Cl_2F_{12}N_8OP_4$
Formula weight	1463.58
Temperature/K	115
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.3224(9)
b/Å	17.2070(13)
c/Å	20.8871(17)
α/°	90
β/°	101.168(3)
γ/°	90
Volume/Å^3	4697.5(6)
Z	4
ρ_{calc}g/cm^3	2.069
μ/mm^{-1}	6.581
F(000)	2832.0
Crystal size/mm^3	0.5 × 0.2 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.668 to 55.038
Index ranges	$-17 \leq h \leq 14$, $-22 \leq k \leq 22$, $-26 \leq l \leq 27$
Reflections collected	105261
Independent reflections	10774 [R_{int} = 0.0327, R_{sigma} = 0.0162]
Data/restraints/parameters	10774/0/615
Goodness-of-fit on F^2	1.052
Final R indexes [I>=2σ (I)]	R_1 = 0.0155, wR_2 = 0.0351
Final R indexes [all data]	R_1 = 0.0181, wR_2 = 0.0358
Largest diff. peak/hole / e Å^{-3}	0.93/-0.62

Medium Infrared

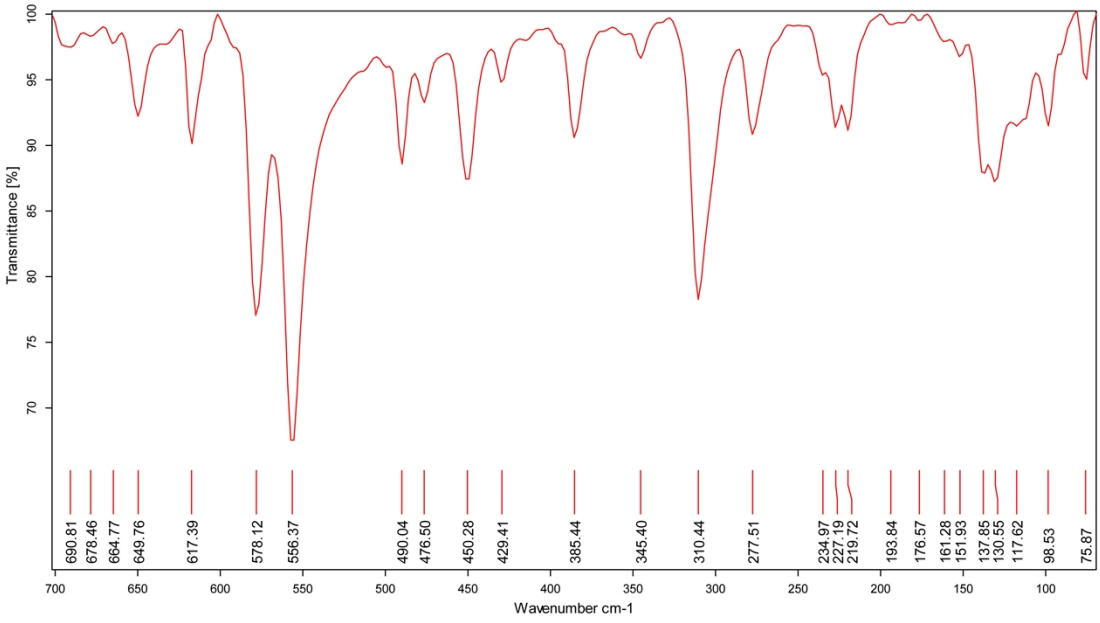


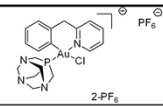
Echantillon : 

2-PF_6

Technique : Golden Gate Diamant

Far Infrared

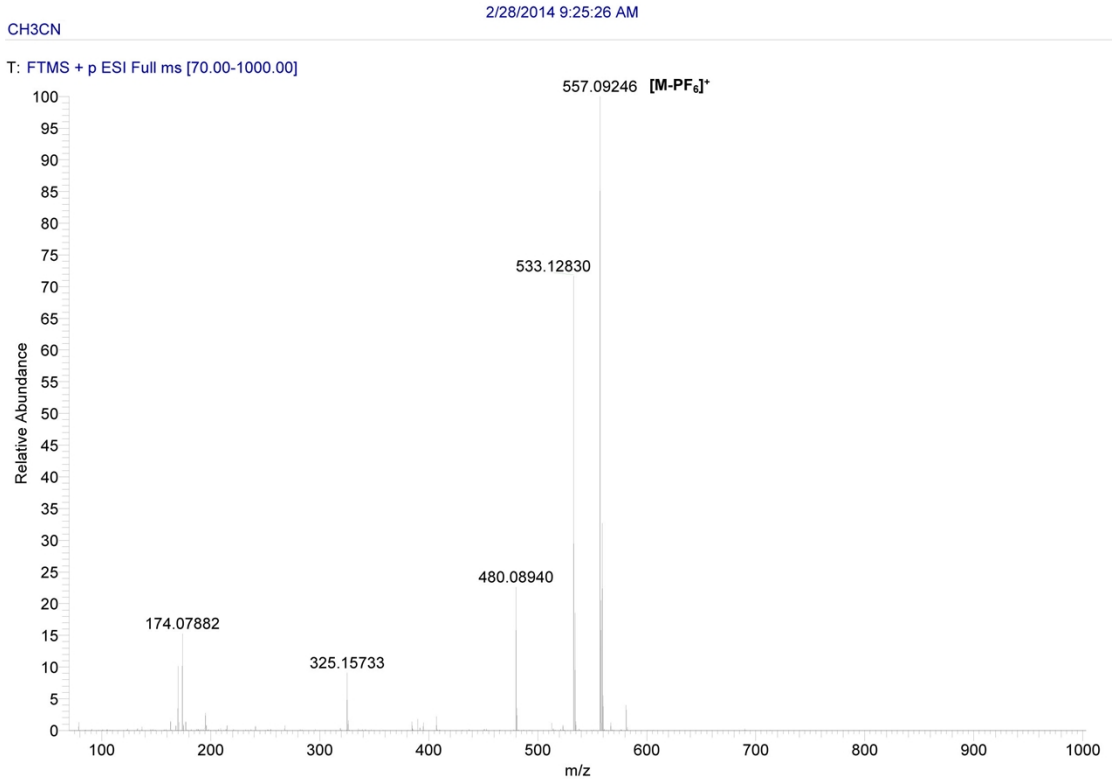


Echantillon : 

2-PF_6

Technique : FIR BMS Si [710 - 80 cm-1] - Energie = 2

HRMS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CH3CN
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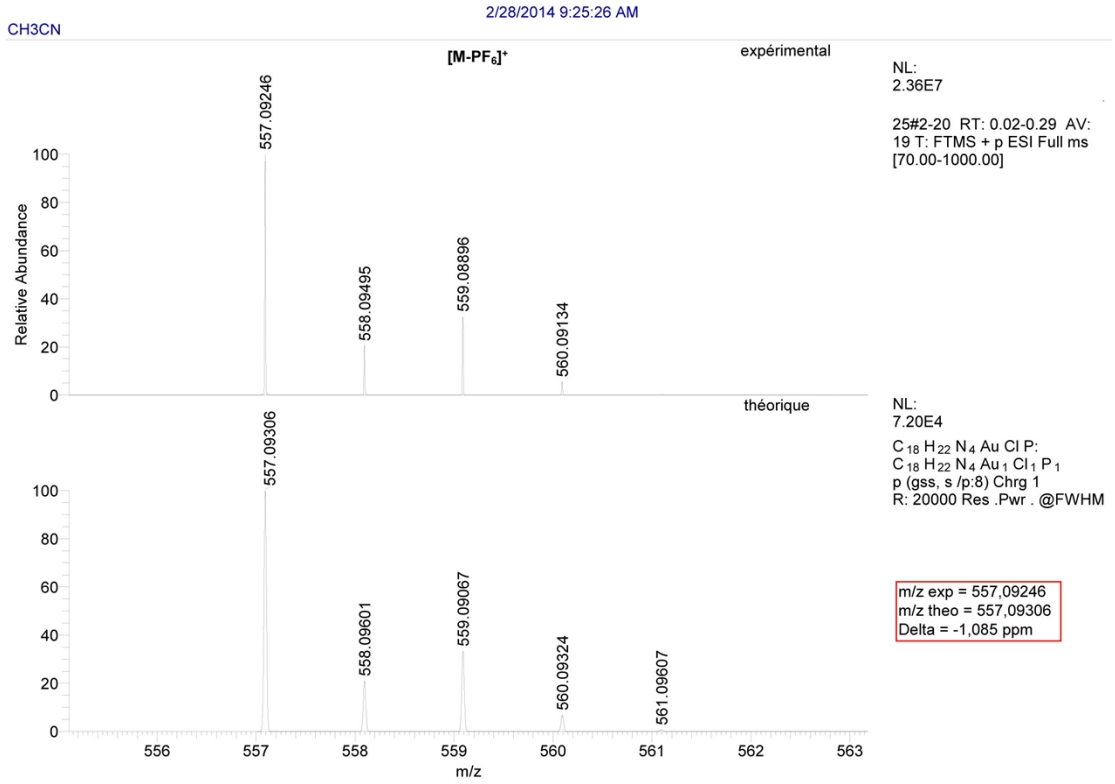
557.09246 [M-PF6]+
533.12830
480.08940
174.07882
325.15733
Relative Abundance
m/z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CH3CN
[M-PF6]+
expérimental
NL:
2.36E7
25#2-20 RT: 0.02-0.29 AV: 19 T: FTMS + p ESI Full ms [70.00-1000.00]
557.09246
558.09495
559.08896
560.09134
théorique
NL:
7.20E4
C18 H22 N4 Au Cl P:
C18 H22 N4 Au1 Cl1 P1
p (gss, s /p:8) Chrg 1
R: 20000 Res .Pwr . @FWHM
557.09306
558.09601
559.09067
560.09324
561.09607
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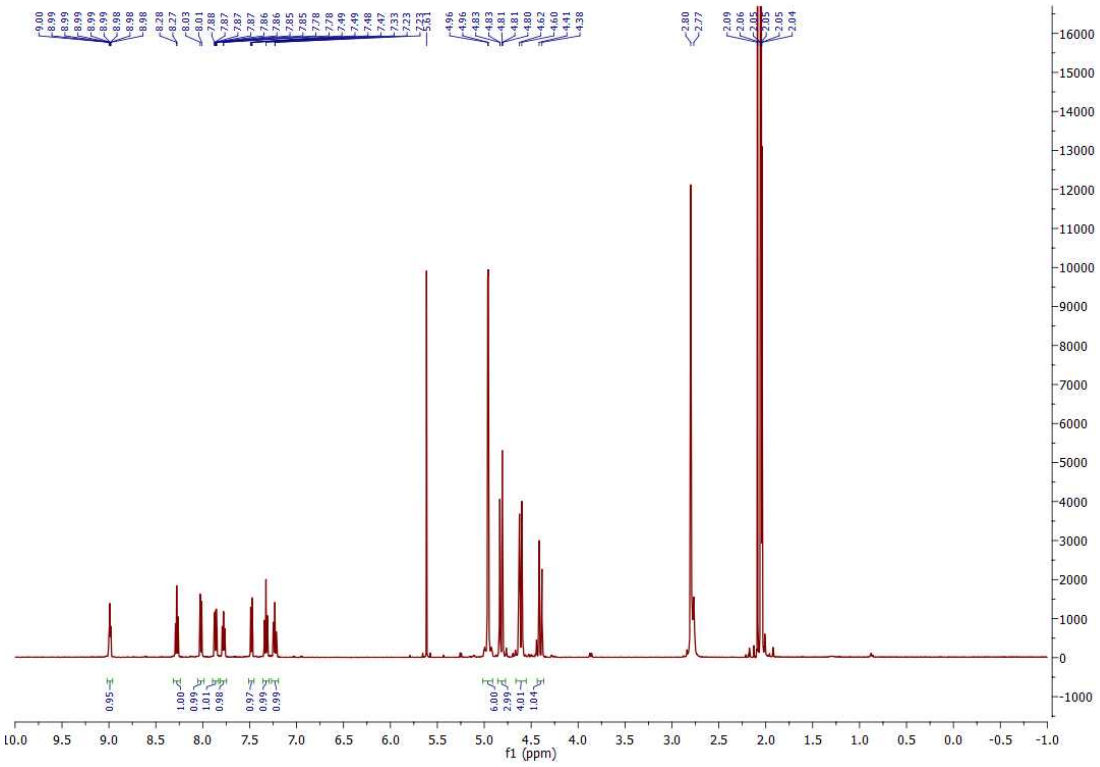
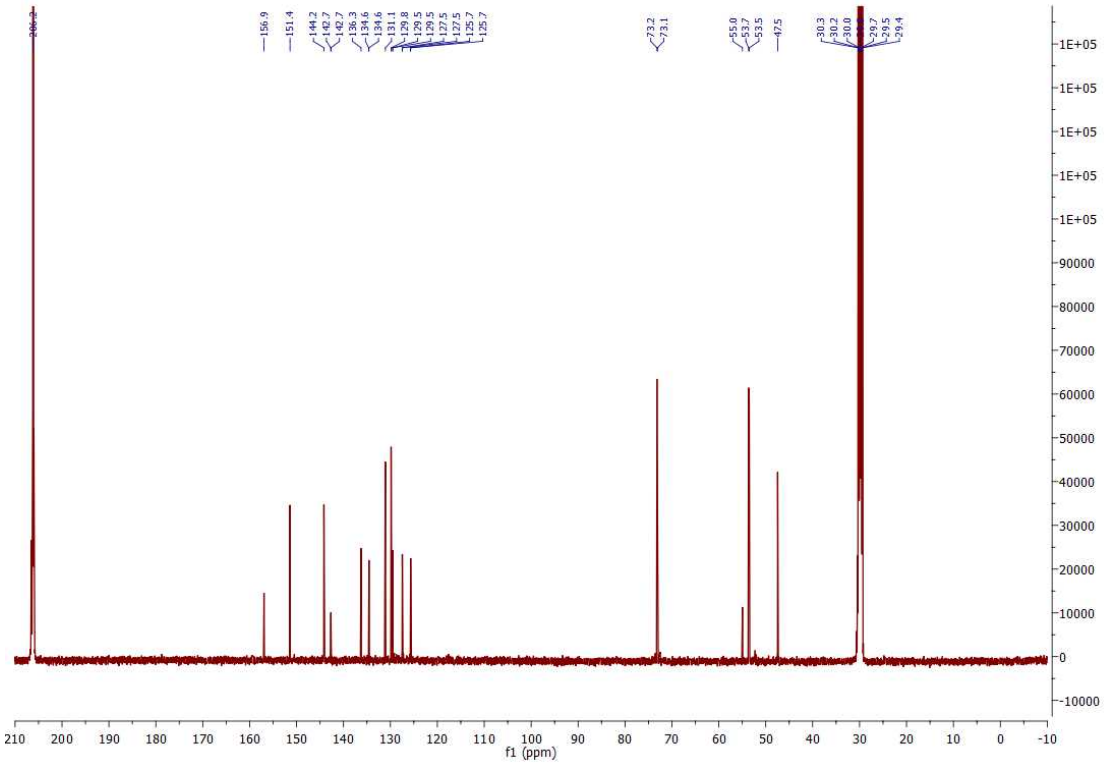
m/z theo = 557,09306
Delta = -1,085 ppm
Relative Abundance
m/z

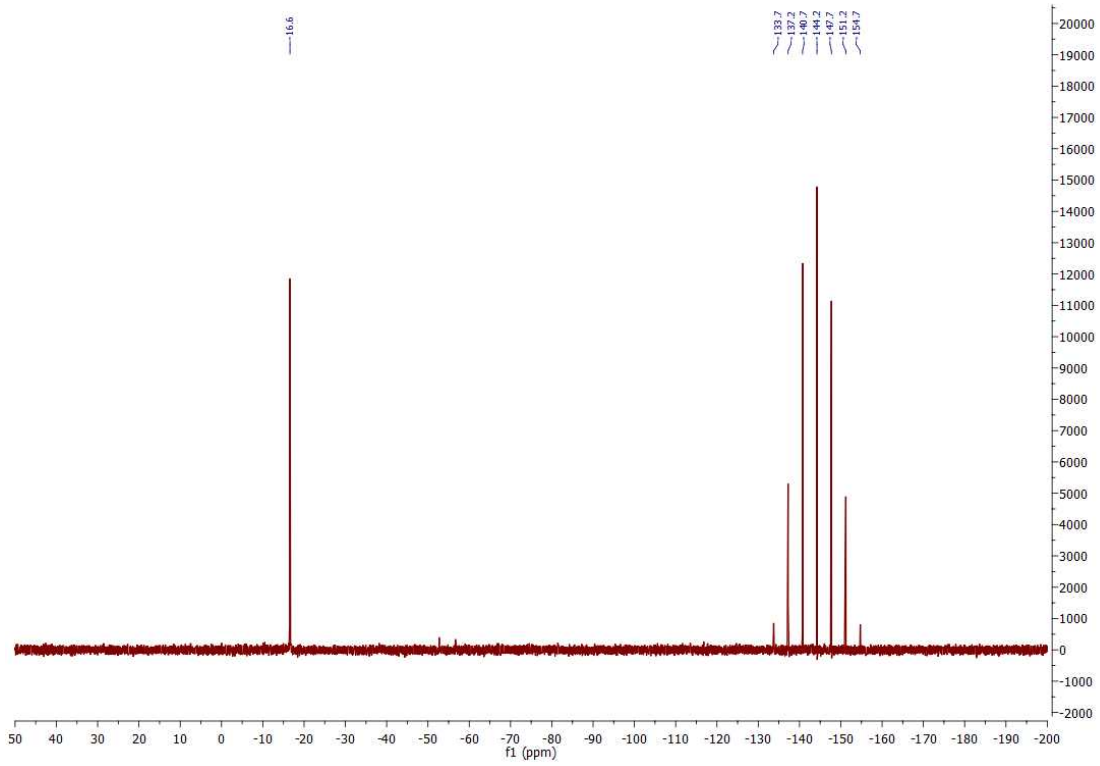
^{1}H NMR



^{13}C NMR

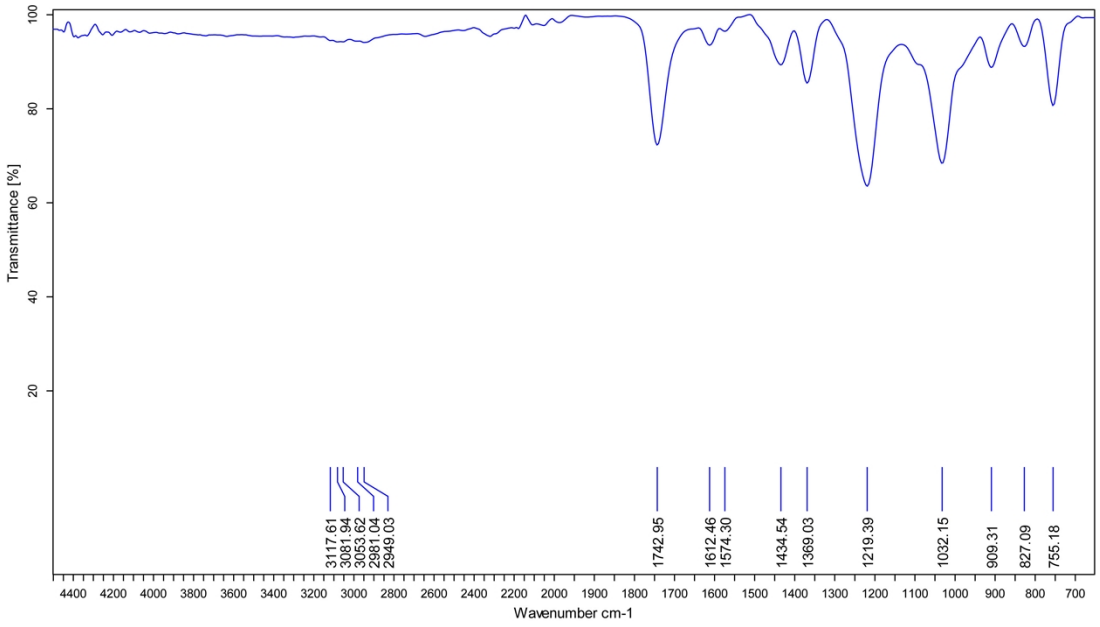


^{31}P NMR



Compound 3

Medium Infrared



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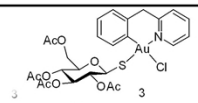
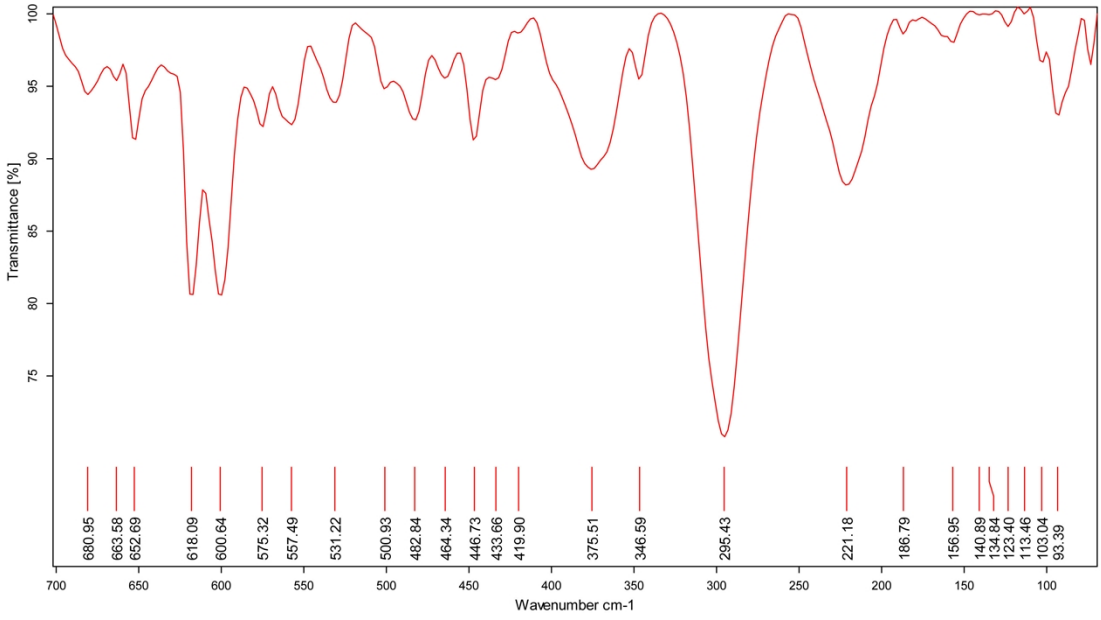


Technique : Golden Gate Diamant

Far Infrared



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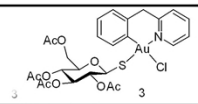
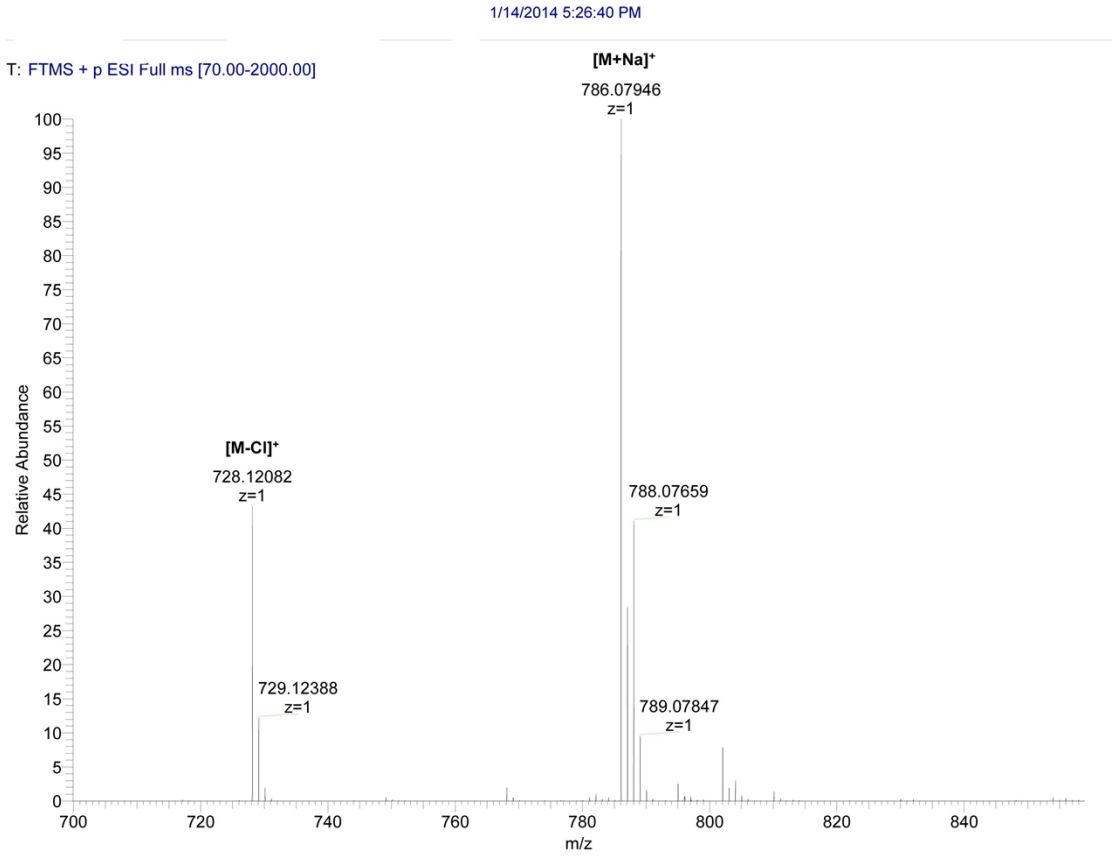


Technique : FIR BMS Si [710 - 80 cm-1] - Energie = 2

HRMS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T: FTMS + p ESI Full ms [70.00-2000.00]
[M+Na]+
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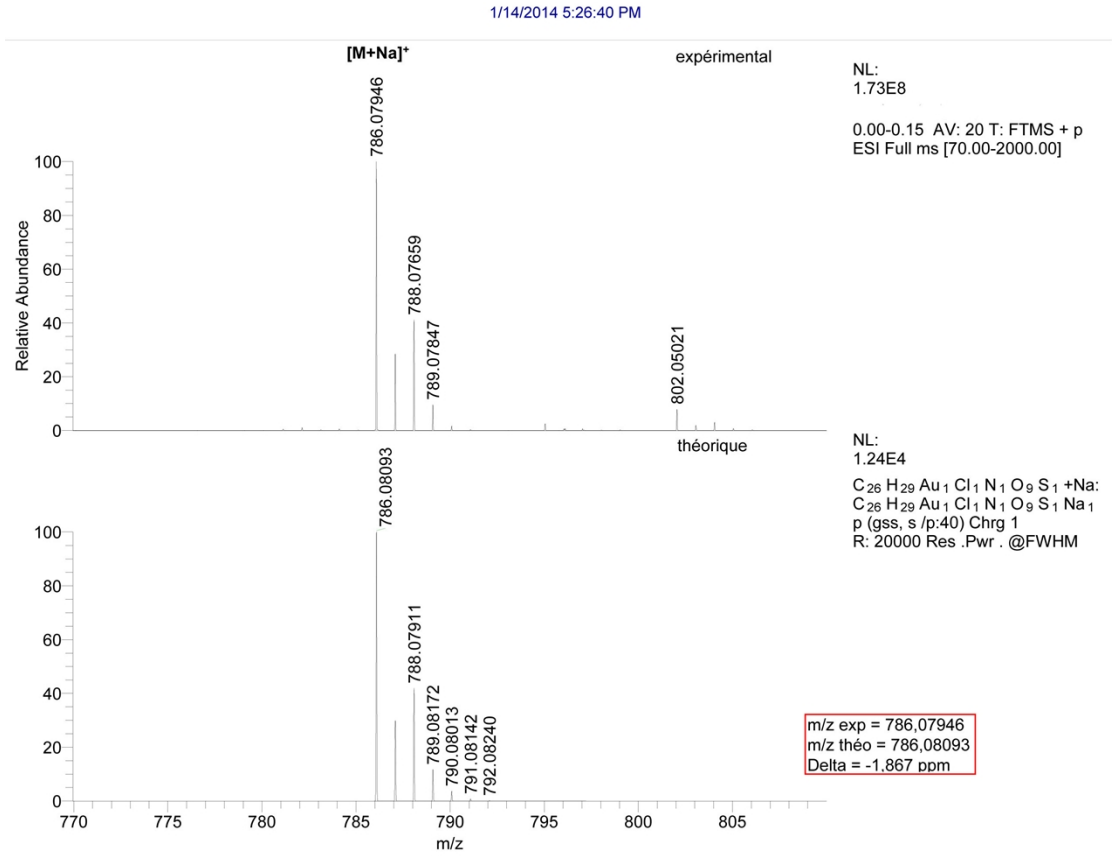
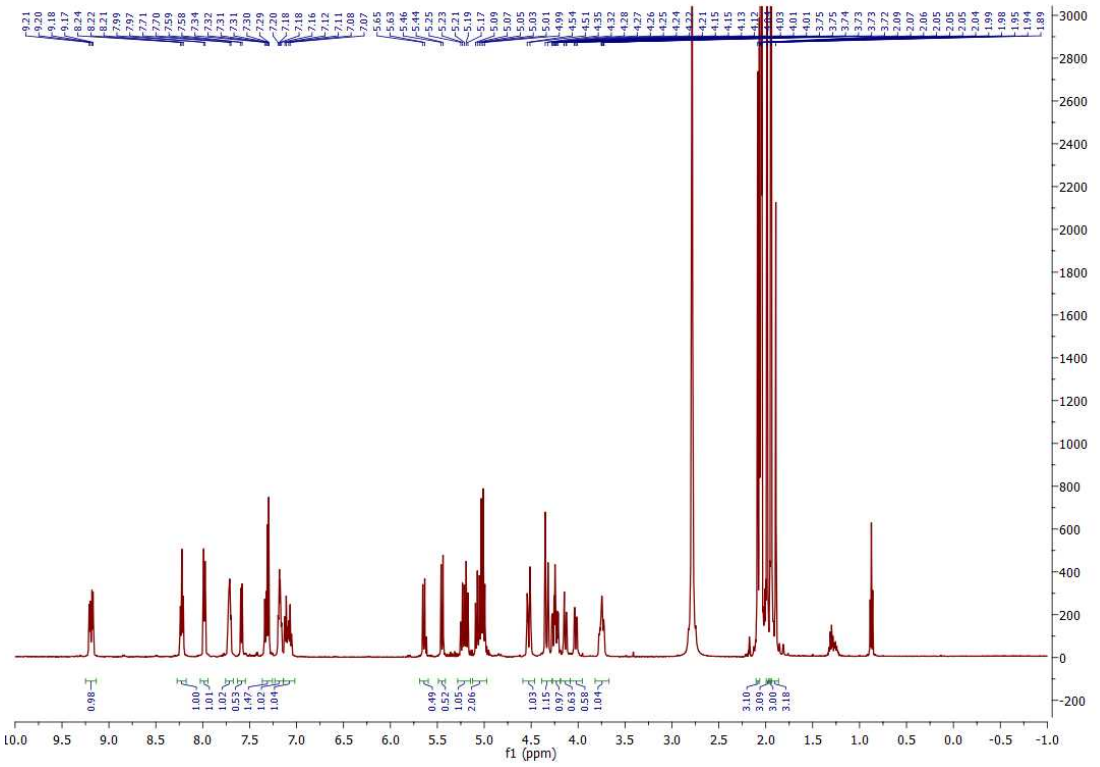
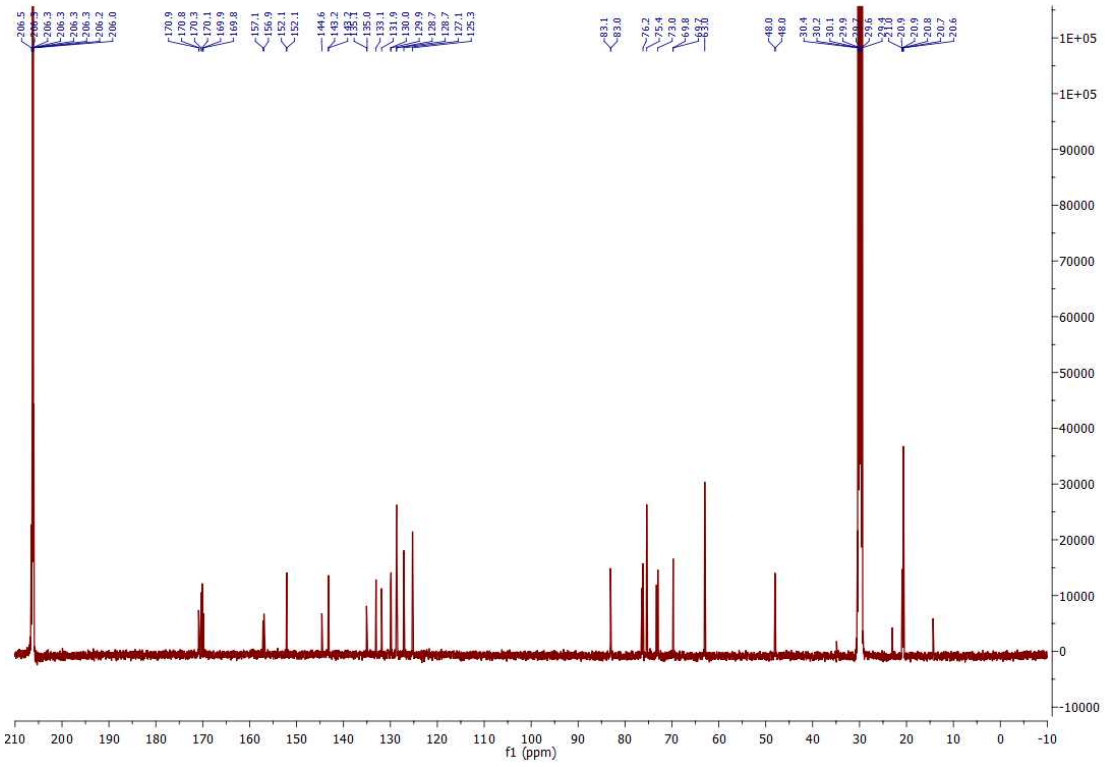
z=1
[M-Cl]+
728.12082
z=1
788.07659
z=1
729.12388
z=1
789.07847
z=1
Relative Abundance
m/z


1/14/2014 5:26:40 PM
[M+Na]+
expérimental
786.07946
788.07659
789.07847
802.05021
théorique
786.08093
788.07911
789.08172
790.08013
791.08142
792.08240
NL:
1.73E8
0.00-0.15 AV: 20 T: FTMS + p
ESI Full ms [70.00-2000.00]
NL:
1.24E4
C26 H29 Au1 Cl1 N1 O9 S1 +Na:
C26 H29 Au1 Cl1 N1 O9 S1 Na1
p (gss, s /p:40) Chrg 1
R: 20000 Res .Pwr . @FWHM
m/z exp = 786,07946
m/z théo = 786,08093
Delta = -1,867 ppm
Relative Abundance
m/z

^{1}H NMR

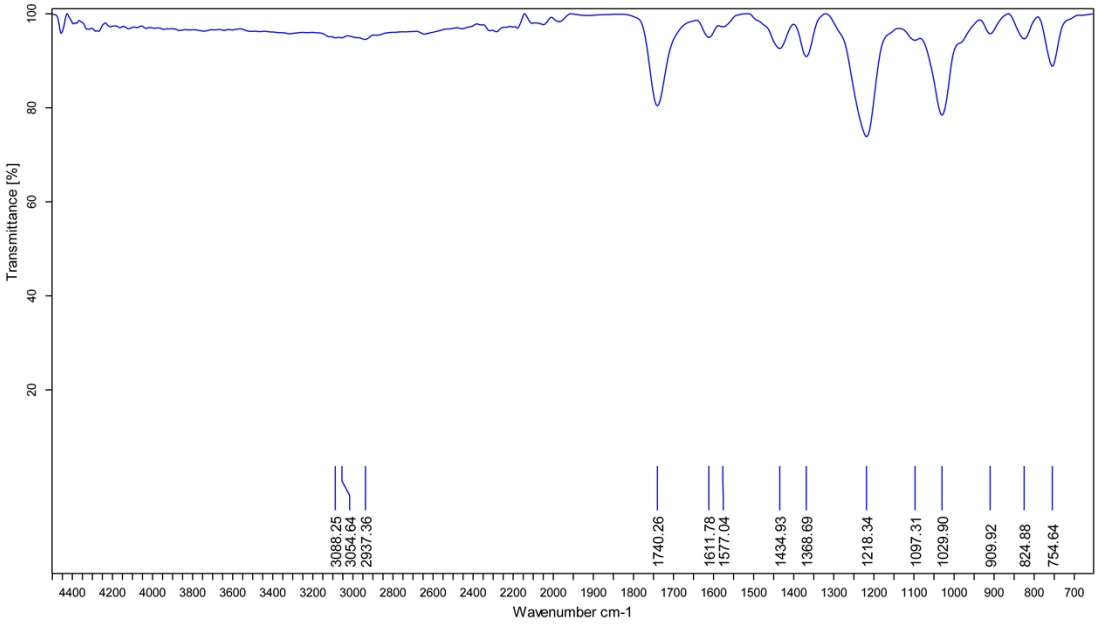


^{13}C NMR

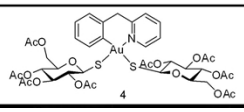


Compound 4

Medium Infrared



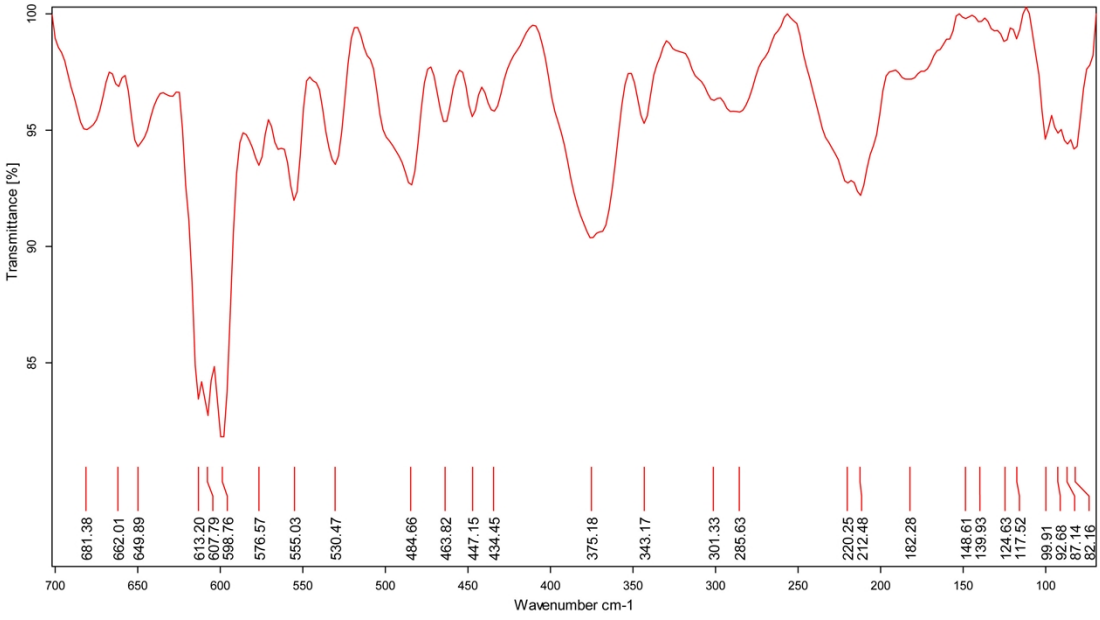
Echantillon :



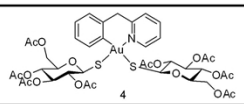
4

Technique : Golden Gate Diamant

Far Infrared



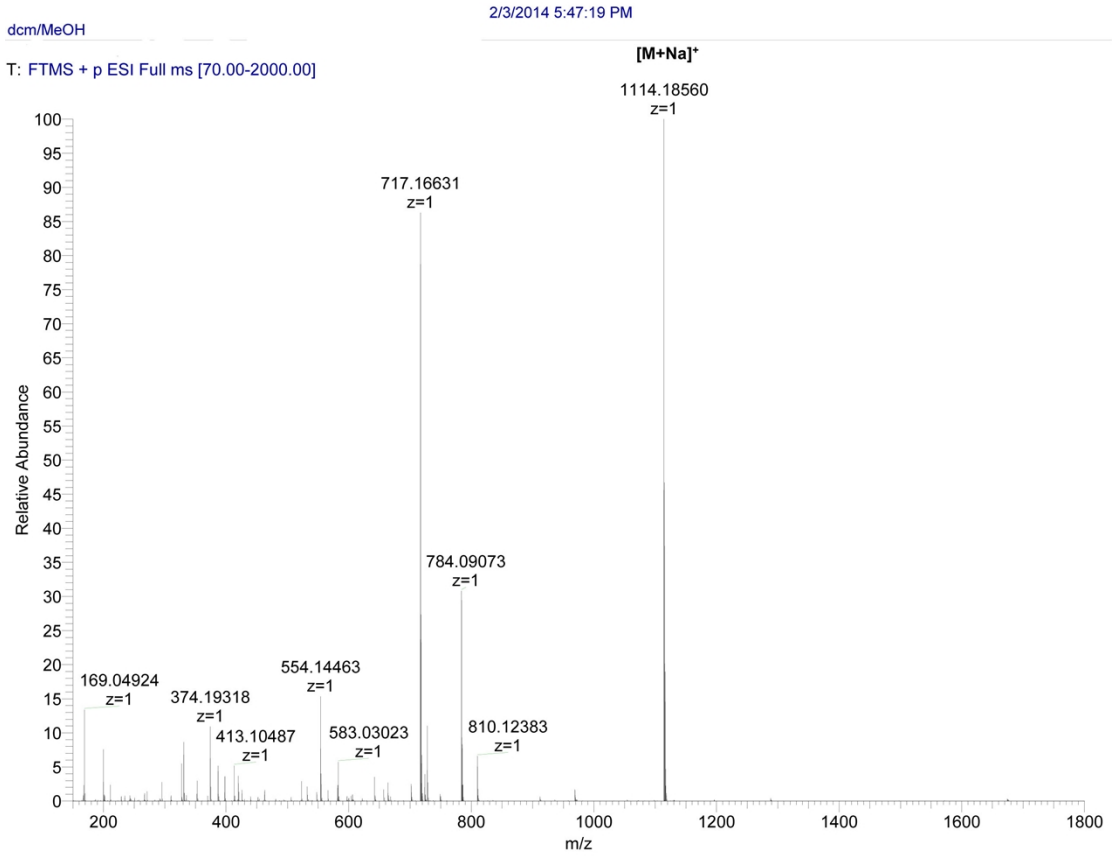
Echantillon :



4

Technique : FIR BMS Si [710 - 80 cm-1] - Energie = 2

HRMS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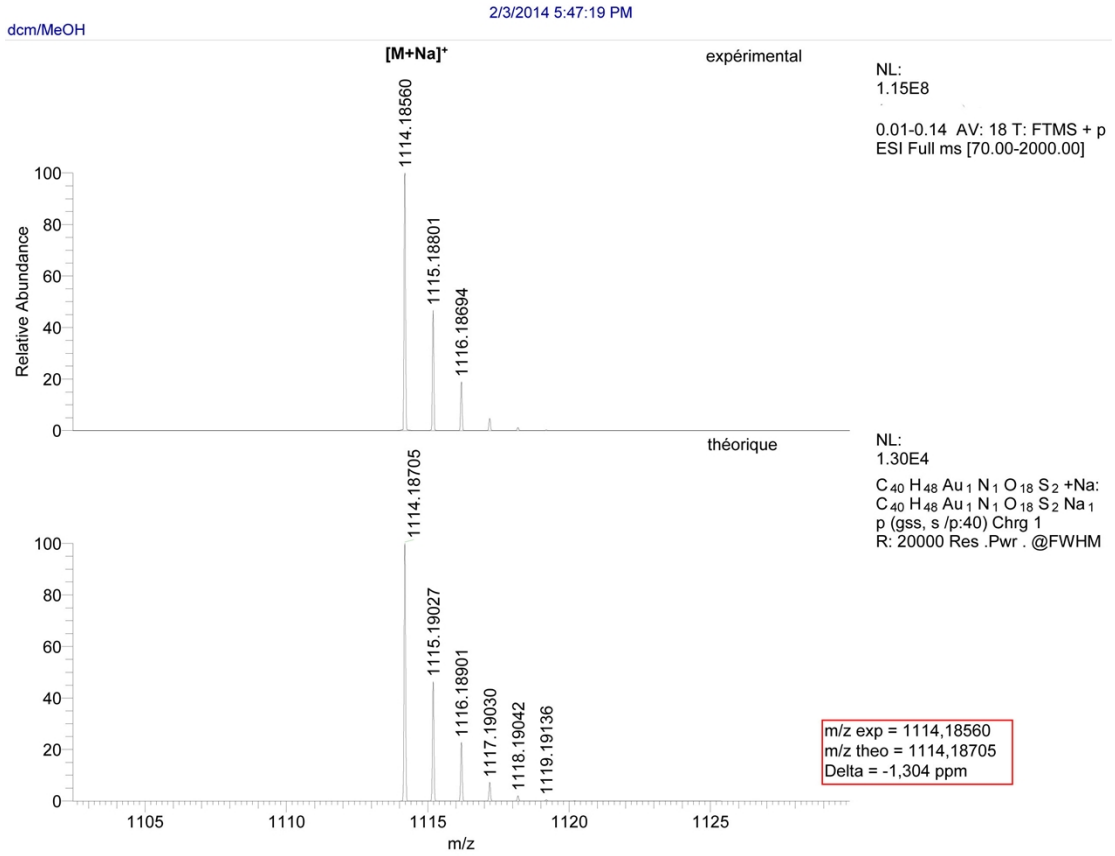
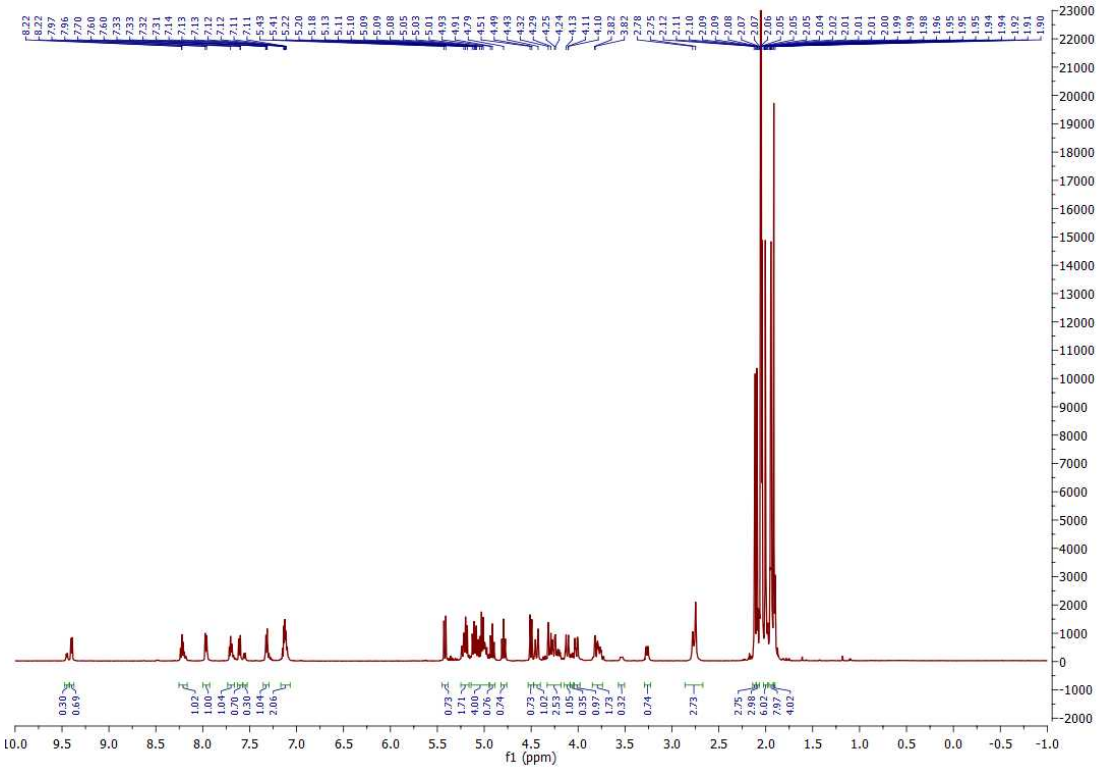
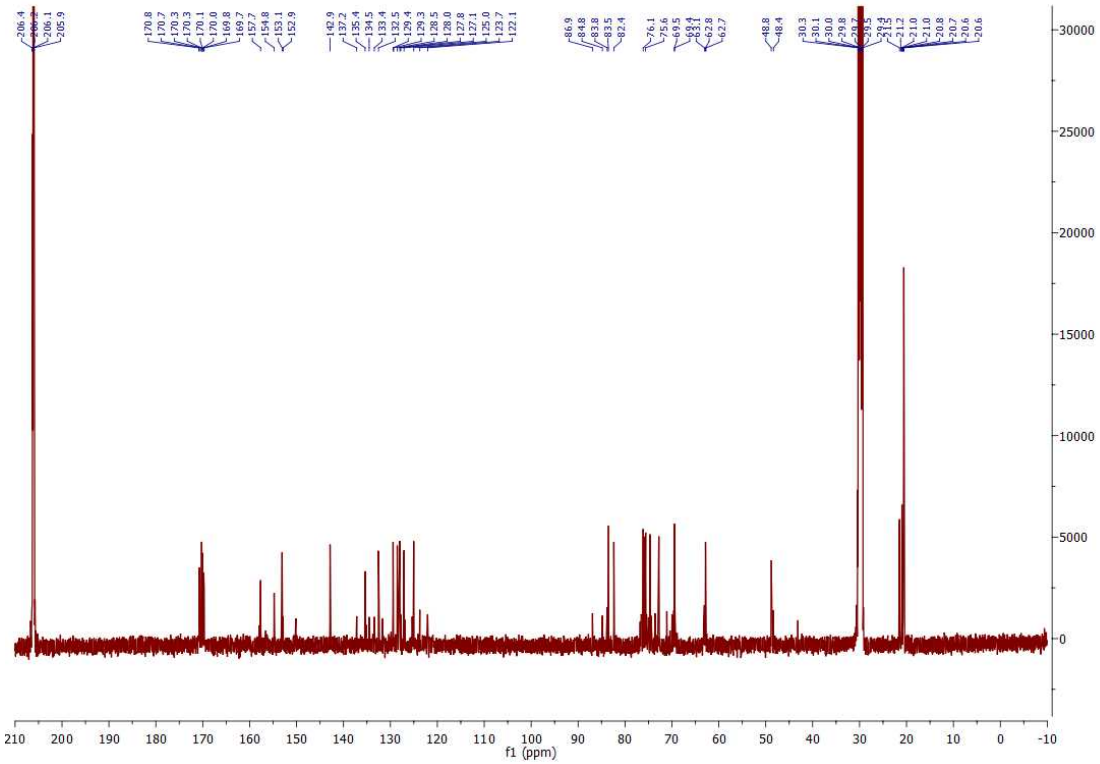
dcm/MeOH
T: FTMS + p ESI Full ms [70.00-2000.00]
[M+Na]+
1114.18560
z=1
717.16631
z=1
784.09073
z=1
554.14463
z=1
169.04924
z=1
374.19318
z=1
413.10487
z=1
583.03023
z=1
810.12383
z=1
Relative Abundance
m/z


2/3/2014 5:47:19 PM
dcm/MeOH
[M+Na]+
expérimental
1114.18560
1115.18801
1116.18694
NL:
1.15E8
0.01-0.14 AV: 18 T: FTMS + p ESI Full ms [70.00-2000.00]
théorique
1114.18705
1115.19027
1116.18901
1117.19030
1118.19042
1119.19136
NL:
1.30E4
C40 H48 Au1 N1 O18 S2 +Na:
C40 H48 Au1 N1 O18 S2 Na1
p (gss, s /p:40) Chrg 1
R: 20000 Res .Pwr . @FWHM
m/z exp = 1114,18560
m/z theo = 1114,18705
Delta = -1,304 ppm
Relative Abundance
m/z

^{1}H NMR



^{13}C NMR



Miscellaneous information

Figure S2 – Schematic representation of the two possible isomers of the monosubstituted Au(III) compounds.

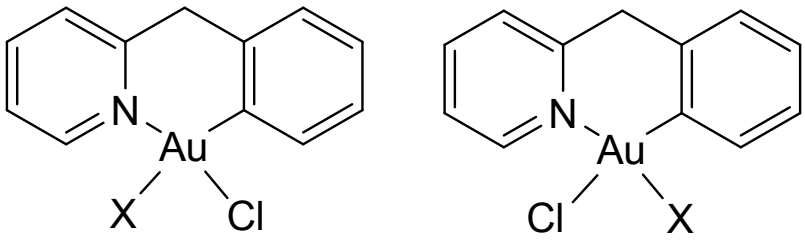


Table S2 - Far-IR absorption bands of the (2-benzylpyridine)-based cyclometallated Au(III) complexes (cm^{-1}).

Compound	$\bar{\upsilon}$(Au-Cl) *trans* to N	$\bar{\upsilon}$(Au-Cl) *trans* to C	$\bar{\upsilon}$(Au-S)
1	358	287	-
5-BF_4	-	305[a]; 310[b]	-
2-PF_6	-	310	-
3	-	295	372
4	-	-	375, 369

[a] M. Z. Cinellu, A.; Stoccoro, S.; Minghetti, G.; Manassero, M.; Sansoni, M., *J. Chem. Soc. Dalton Trans.,* 1996, 4217-4225

[b] Fuchita : Y. Fuchita, H. Ieda, Y. Tsunemune, J. Kinoshita-Nagaoka and H. Kawano, *Dalton Trans*, 1998, 791-796