

A Calix[8]arene-Based Catalyst for Suzuki–Miyaura Couplings with Reduced Pd_Leaching

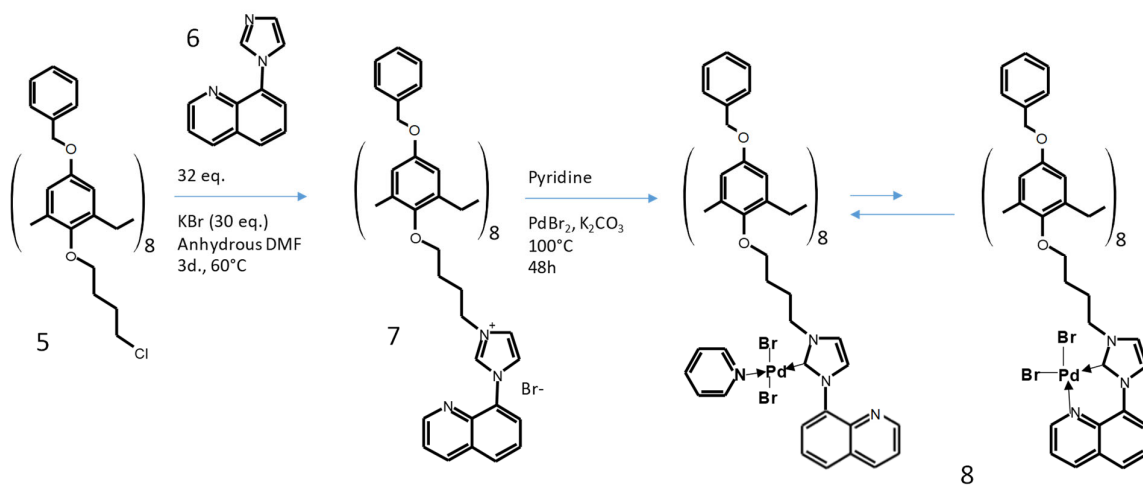
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Supplementary Materials

General:

All the solvents were purchased from TCI and Aldrich as anhydrous, and used as received. Compound **5** was purchased from NOVECAL (Orsay, France: <https://www.novecal.com/>, accessed on 22 July 2022). Compound **6** was purchased from CHEMIELIVA (JiangBei, Chongqing, China) and used as received.

Figure S1. Synthetic scheme of compound 8.



A) imidazolium salt 7

Figure S2. ^1H NMR spectrum of compound 7

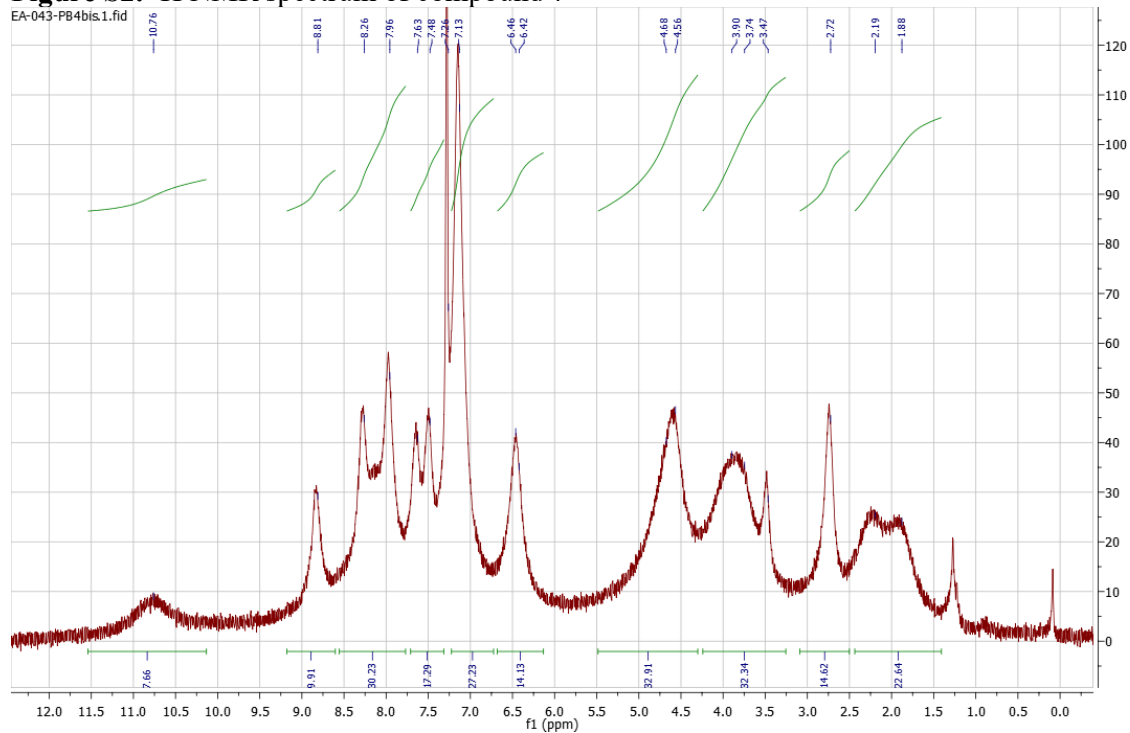


Figure S3. ^{13}C NMR spectrum of compound 7

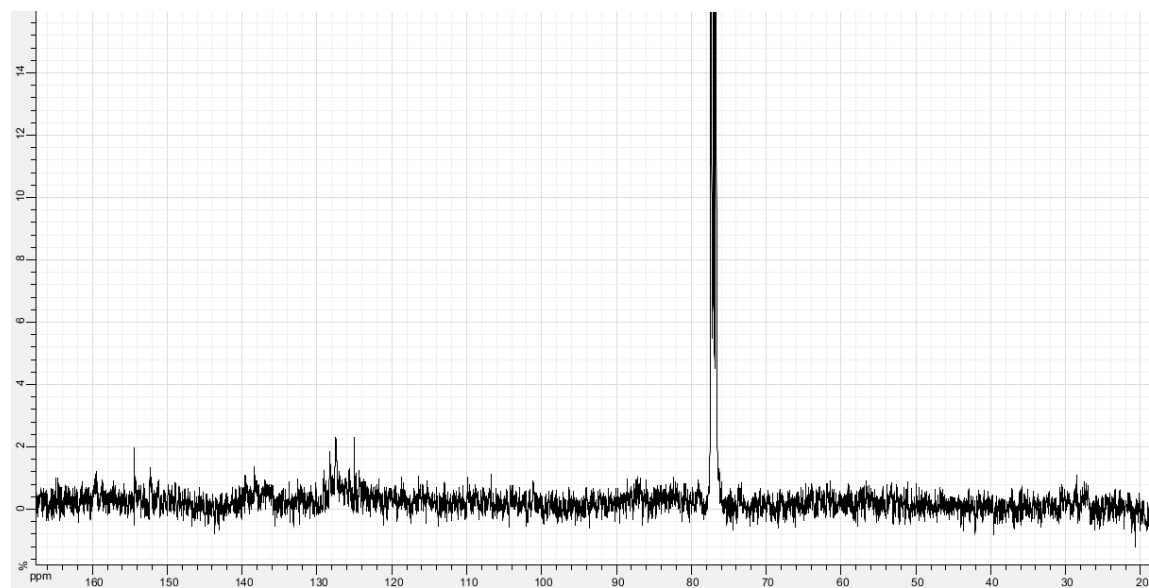
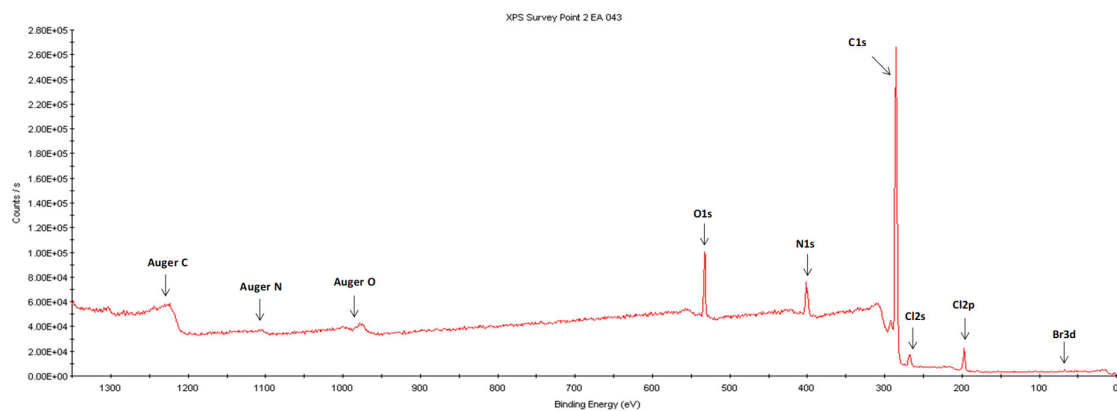


Figure S4. XPS spectrum of compound **7**



Cl ₂ p	196,46	1,45	8739,12	52,02	2,8
C ₁ s	284,67	2,26	110116,29	1562,81	83,2
N ₁ s	401,39	1,4	16044,5	134,5	7,2
O ₁ s	532,48	1,54	22796,95	126,83	6,8
Br ₃ d	67,19	1,91	463,74	2,1	0,1

B) compound 8.

Figure S5. ^1H NMR spectrum of compound **8** ($\text{DMSO}-d_6$)

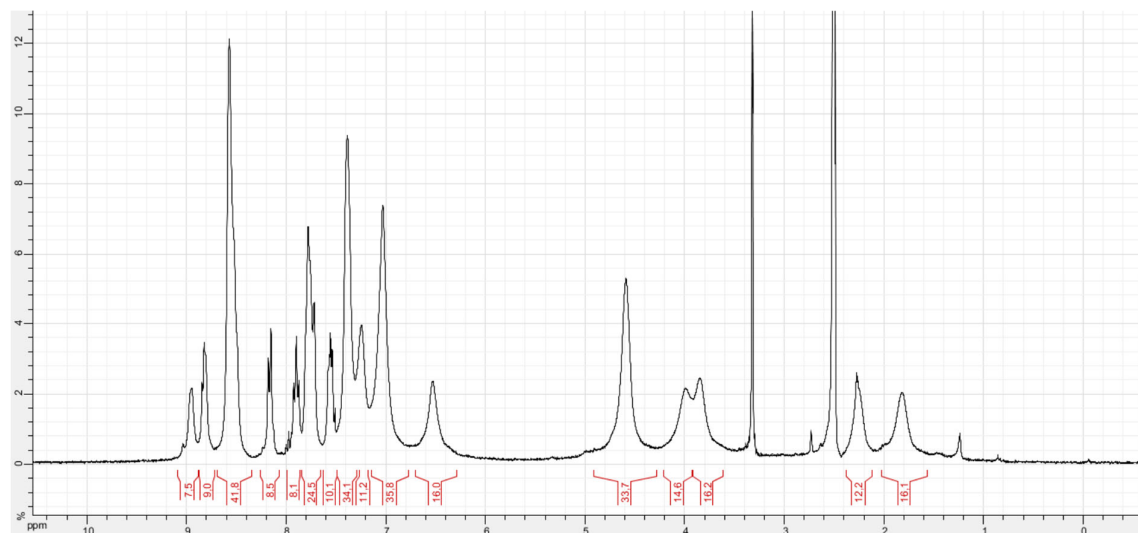
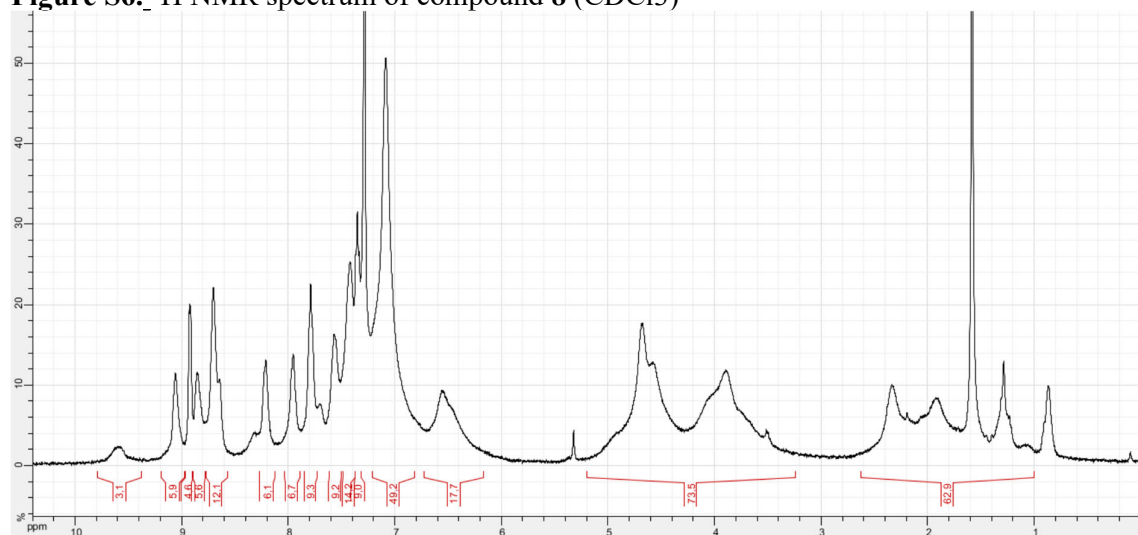


Figure S6. ^1H NMR spectrum of compound **8** (CDCl_3)



(300 MHz, CDCl_3): δ (ppm)= 8.82 (d, *o*-pyridine); 7.69 (t, *p*-pyridine); 7.26 (t, *m*-pyridine) – 8.95 (m, *o*-quinoline), 7.87 (m, *p*-quinoline); 7.70 (m, *m*-quinoline); 8.8-8.6 (Ar quinoline); 7.2-6.80 (Ar benzyl), 6.8-6.2 (Ar-hydroquinone); 5-4.25 (Ar- CH_2 -O-); 4.2-3.2 (Ar- CH_2 -Ar / CH_2 -O / CH_2 -N+); 2.6-1.6 ($-\text{CH}_2-\text{CH}_2-$)

Figure S7. ^{13}C NMR spectrum of compound **8**

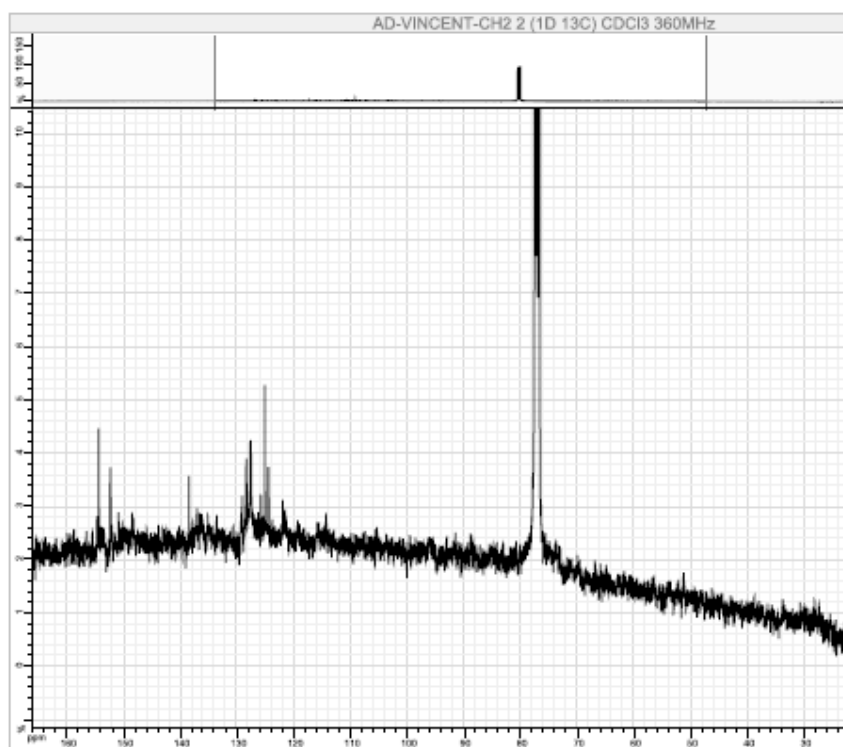


Figure S8. 2D COSY NMR spectrum of compound **8**

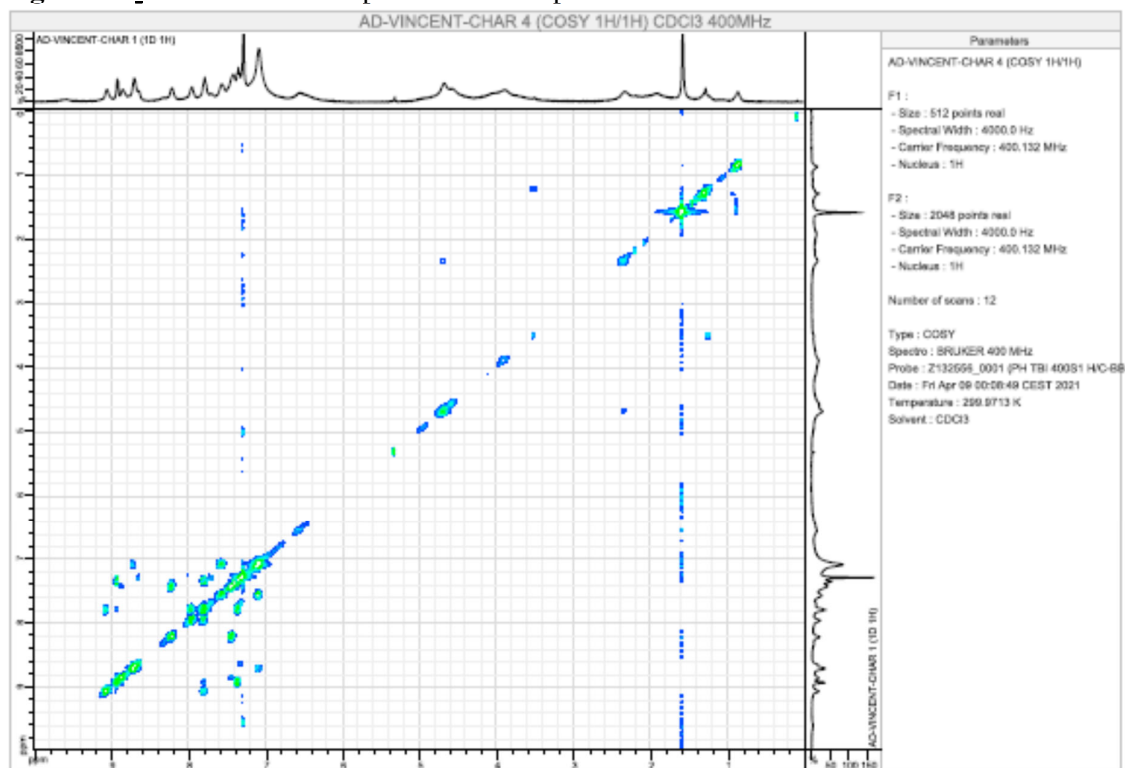


Figure S9. 2D HSQC NMR spectrum of **8**

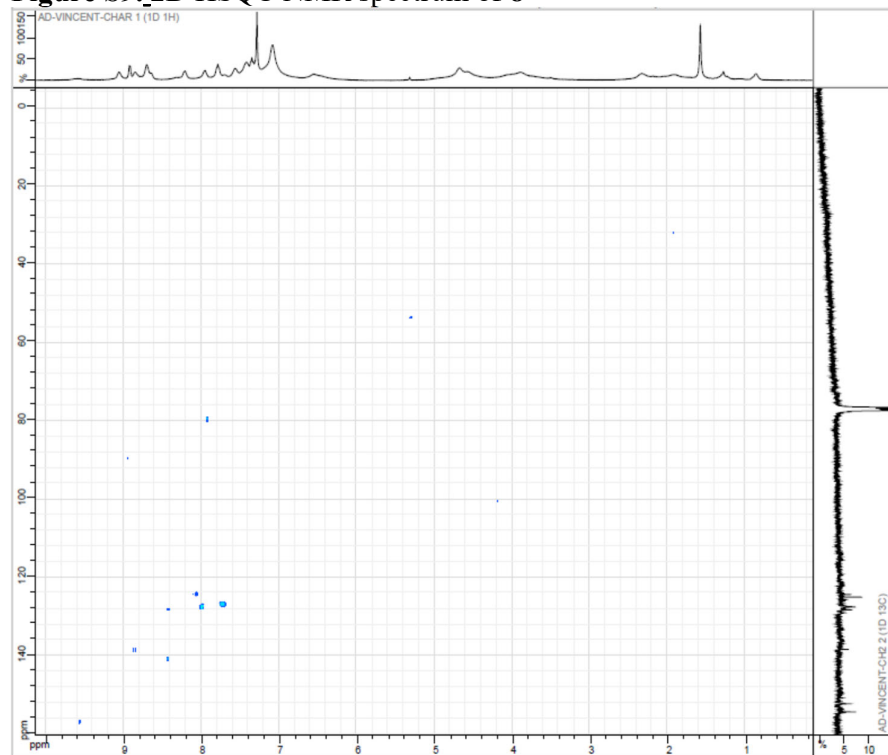


Figure S10. 2D HMBC NMR spectrum of **8**

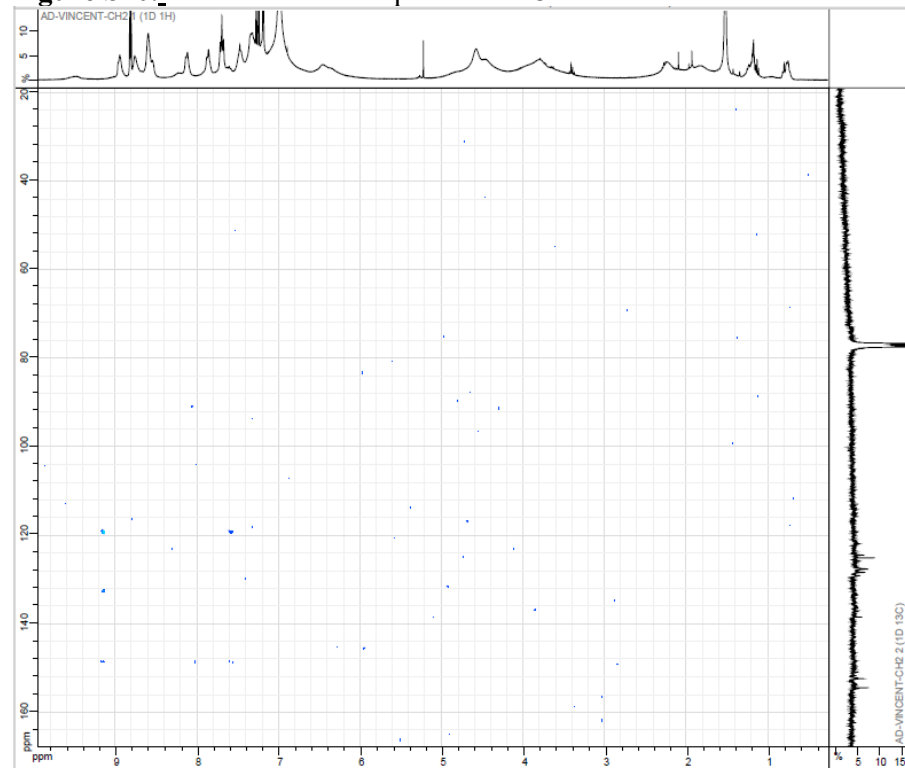
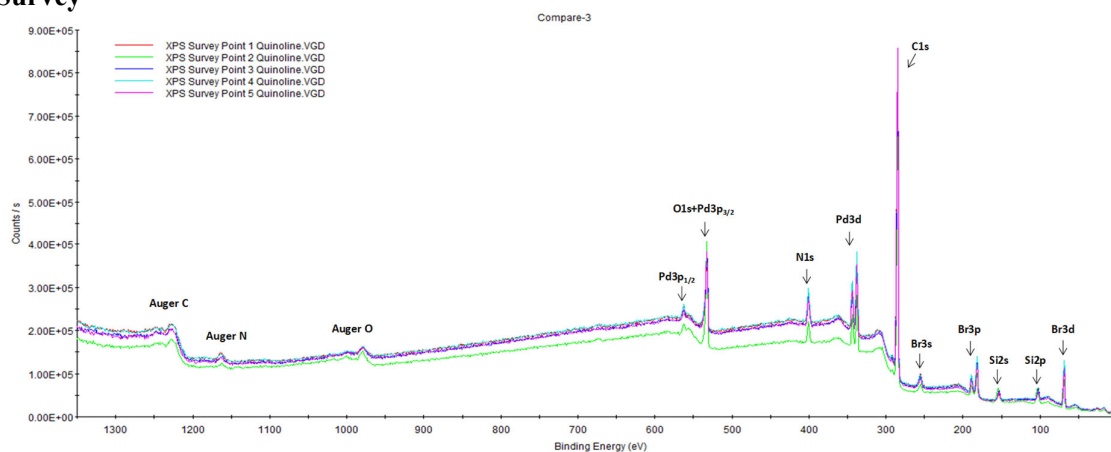


Figure S11. XPS spectra of compound **8**
Survey



Note: the XPS analysis was performed on different areas of the same sample, to check the homogeneity of the composition. The compositions were found constant.

Name	Peak BE	FWHM eV	Area (N)	Atomic %
Br3d 2	68,28	2,04	159,9	3,9
Pd3d 2	337,7	1,3	86,05	2,1
C1s	284,62	1,83	3641,99	88,4
N1s	400,53	1,9	231,54	5,6

Figure S12. XPS spectra of compound **8** Pd 3d
Pd 3d

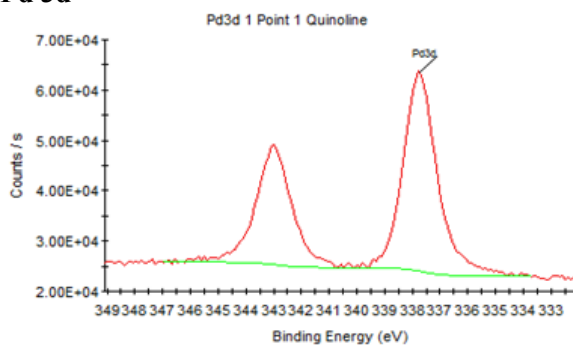


Figure S13. XPS spectra of compound **8** Br 3d
Br 3d

