Supporting Information

Antiproliferative effects, Mechanism of Action and Tumor Reduction Studies in a Lung Cancer Xenograft Mouse Model of an Organometallic Gold(I) Alkynyl Complex

Uttara Basu ^{*a,b}, Anna Wilsmann^a, Sebastian Türck^a, Henrik Hoffmeister^a, Matthias Schiedel^a, Gilles Gasser ^c, Ingo Ott ^{*, a}

^a Institute of Medicinal and Pharmaceutical Chemistry, Technische Universität Braunschweig, Beethovenstr. 55, 38106 Braunschweig, Germany.

^b Department of Chemistry, BITS Pilani K K Birla Goa Campus.

^c Chimie ParisTech, PSL University, CNRS, Institute of Chemistry for Life and Health Sciences, *F*-75005 Paris, France.

Table of contents

- 1) Figures S1 to S3; additional figures from the docking studies
 - 2) Figures S4 to S6: NMR data



Figure S1: Docking of **1** into TrxR1 (PDB: 2J3N, Sec \rightarrow Cys); receptor surface: H-bonding (red), mild polar (blue), hydrophobic (grey).



Figure S2: Docking of (phosphane)Au⁺ (green) and alkynyl-Au⁺ (brown) into TrxR1 (PDB: 2J3N, Sec→Cys); receptor surface: H-bonding (red), mild polar (blue), hydrophobic (grey)



Figure S3: Docking of 1 and alkynyl-Au⁺ (brown, orange, yellow) into TrxR1 (PDB: 2J3N, Sec→Cys);



Figure S4: ¹H NMR of complex 1 recorded in CDCl₃

Kunde Basu Substanz-Code UB1_2 Exp. 13C-CPD c13cpd.ibk_32 CDCl3 {D:\u} nmr 14



20190718 12.54 AVIIIHD500 Z125869_0056 (

zgp 262

4 59523.809 Hz 0.454131 Hz 2.2020097 sec 186.82 8.400 usec 18.00 usec 298.0 K

2900 K 2,4000010 sec 0,0300000 sec 1202.5636030 Hiz 3.67 usec 51.9600022 W waltzie 18.0000000 W 0.28125000 W 0.11447000 W

 Pinis
 0.14147000 W

 F2
 - Processing parameters

 SI
 131072

 SF
 202.5331360 MHz

 NDW
 EM

 SSB
 0

 LB
 1.00 Hz

 GB
 0

 PC
 1.40

 SR
 -07.01 Hz

 HZpPT
 0.454131 Hz

PCPD2 PLW2 PLW12 PLW13

Figure S5: ¹³C NMR of complex 1 recorded in CDCl₃ **Figure S6**: ³¹P NMR of complex 1 recorded in CDCl₃