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# $^{13}$C-n.m.r. studies of the binding of 1,3-diazinane-2-selenone and 1,3-diazipine-2-selenone to gold(I) drugs

Anvarhusein A. Isab*, Saeed Ahmad and Waqar Ashraf
*Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia*

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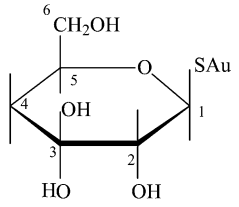
## Abstract

The interaction of gold(I) thiomalate, Myocrisin [(Autm)$_n$] with 1,3-diazinane-2-selenone (DiazSe) and 1,3-diazipine-2-selenone (DiapSe) has been studied in aqueous solution using $^{13}$C-n.m.r. spectroscopy. It is observed that ternary complexes, (DiazSe–Au–tm and DiapSe–Au–tm, respectively) are formed on coordination of these ligands to (Autm)$_n$. The $^{13}$C-n.m.r. data suggest that DiapSe binds more strongly to (Autm)$_n$ than does DiazSe, which binds more strongly compared to its analogous thione, 1,3-diazinane-2-thione (Diaz). A similar observation was made for the gold(I) thioglucose (Autg) reaction with DiazSe.

## Introduction

The exchange reactions of gold(I) drugs with thiols, $CN^-$ and selenols have been reported [1–8]. These ligands, when added to e.g. (Autm)$_n$, usually eject thiomalate (Htm) as a free ligand, forming $Au(SR)_2^-$ [3–5], $Au(CN)_2^-$ [6, 7] or $Au(SeR)_2^-$ [8, 9] type complexes respectively. Thiones, on the other hand, do not eject Htm as a free ligand. Instead, they form asymmetric complexes of the type >C═S–Au–tm [10–12]. Selenium-containing ligands e.g. selenols or selenones, are expected to form more stable complexes with class B metal ions such as gold(I) because selenium is considered to be a softer Lewis base than sulfur [13].

The complexation of gold(I) thiomalate with selenium-containing ligands is important, since selenocysteine is present at the active binding site of the enzyme, Se–glutathione peroxidase, and gold(I) is known to be a strong inhibitor of the catalytic activity of Se–glutathione peroxidase [14–16]. In the present study, we report the interaction of DiazSe and DiapSe with (Autm)$_n$ and Autg, followed by $^{13}$C-n.m.r. We hope that this work will enhance our understanding of the reaction between gold(I) drugs and selenium containing proteins and enzymes [14, 16]. The structures of (Autm)$_n$, DiazSe, DiapSe and Autg are given in Scheme 1.




Gold(I)thioglucose (Autg)

*Scheme 1.* Structures of (Autm)$_n$, Diazinane-2-selenone, Diazipine-2-selenone and Autg

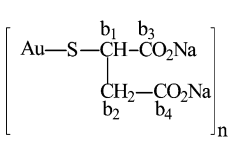
## Experimental

### *Chemicals*

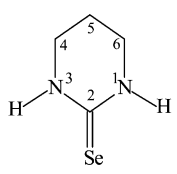
Autm and Autg were obtained from ICN K & K Labs Plainview, New York. $D_2O$ was purchased from Fluka chemical Co. Diazinane-2-selenone and Diazipine-2-selenone were synthesized as described in the literature [17, 18].

### *Spectroscopic measurements*

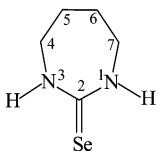
The $^{13}$C-n.m.r. spectra were obtained at 125.65 MHz with $^1$H broadband decoupling at 298 K. The spectral




Gold(I) thiomalate [(Autm)n]




Diazinane-2-selenone (DiazSe)




Diazipine-2-selenone (DiapSe)

* Author for correspondence