

Supporting Information For

Design and Green Synthesis of Binuclear Organoselenium Compounds for Anticancer Evaluation against Human Lung and Breast Cancer

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**Main Title: Design and Green Synthesis of Organoselenium Compounds for Anticancer
Evaluation against Human Lung and Breast Cancer**

Table S1: Physical appearance of binuclear salts and Selenium adducts.

Sr. No.	Compound	Color	Appearance
1	ML ₁	yellow	Sticky liquid
2	ML ₂	Yellow	Sticky liquid
3	ML ₃	yellow	Sticky liquid
4	MC ₁	Brownish	Sticky liquid
5	MC ₂	Brownish	Sticky liquid
6	MMC ₃	Brownish	Sticky liquid

Table S2: Solubilities of the synthesized compounds in different solvents.

Sr. No.	Compound	Water	Methanol	DMSO	Chloroform	Dichloro- Methane
1	ML ₁	SOH	S	S	IS	IS
2	ML ₂	SOH	S	S	IS	IS
3	ML ₃	SOH	S	S	IS	IS
4	MC ₁	IS	IS	S	S	S
5	MC ₂	IS	IS	S	S	S
6	MC ₃	IS	IS	S	S	S

Where: **S**= soluble, **IS**= insoluble, **SOH**=soluble on heating

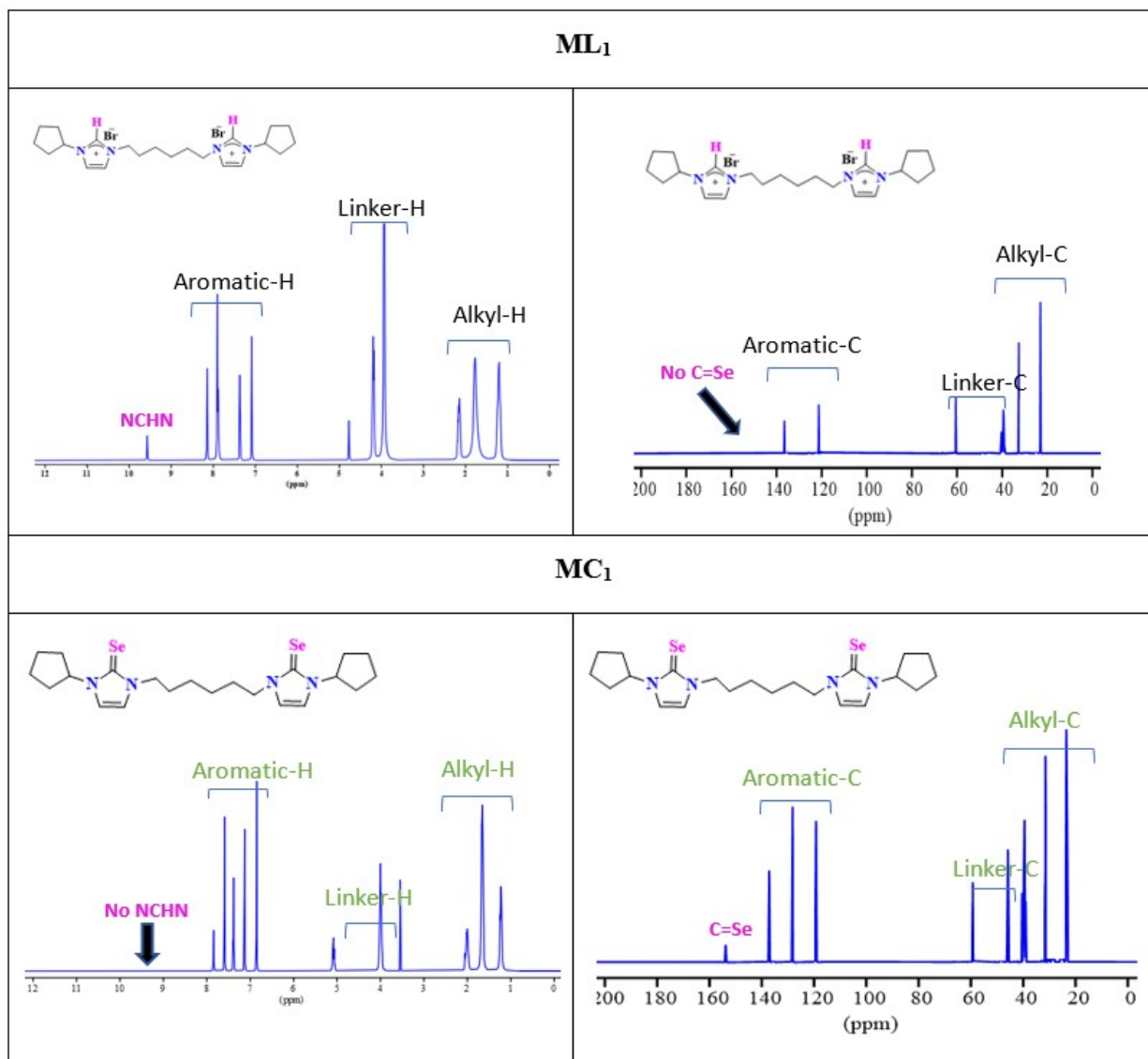


Figure S1: ¹H NMR and ¹³C NMR spectra of ML₁ and MC₁.

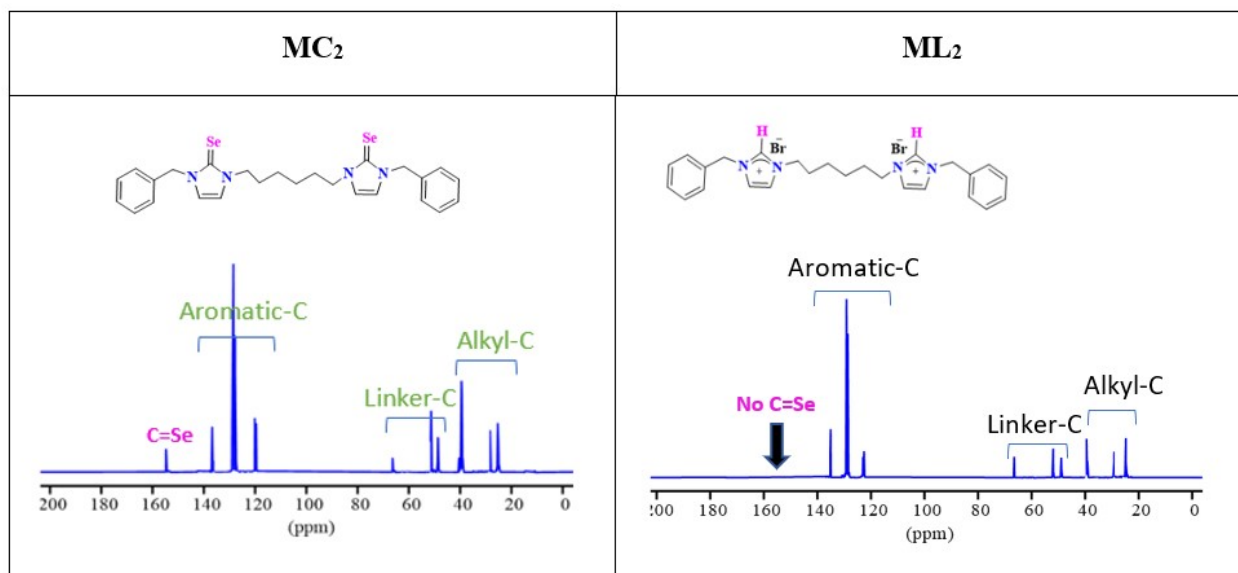


Figure S2: ¹³C NMR spectra of ML₂ and MC₂.

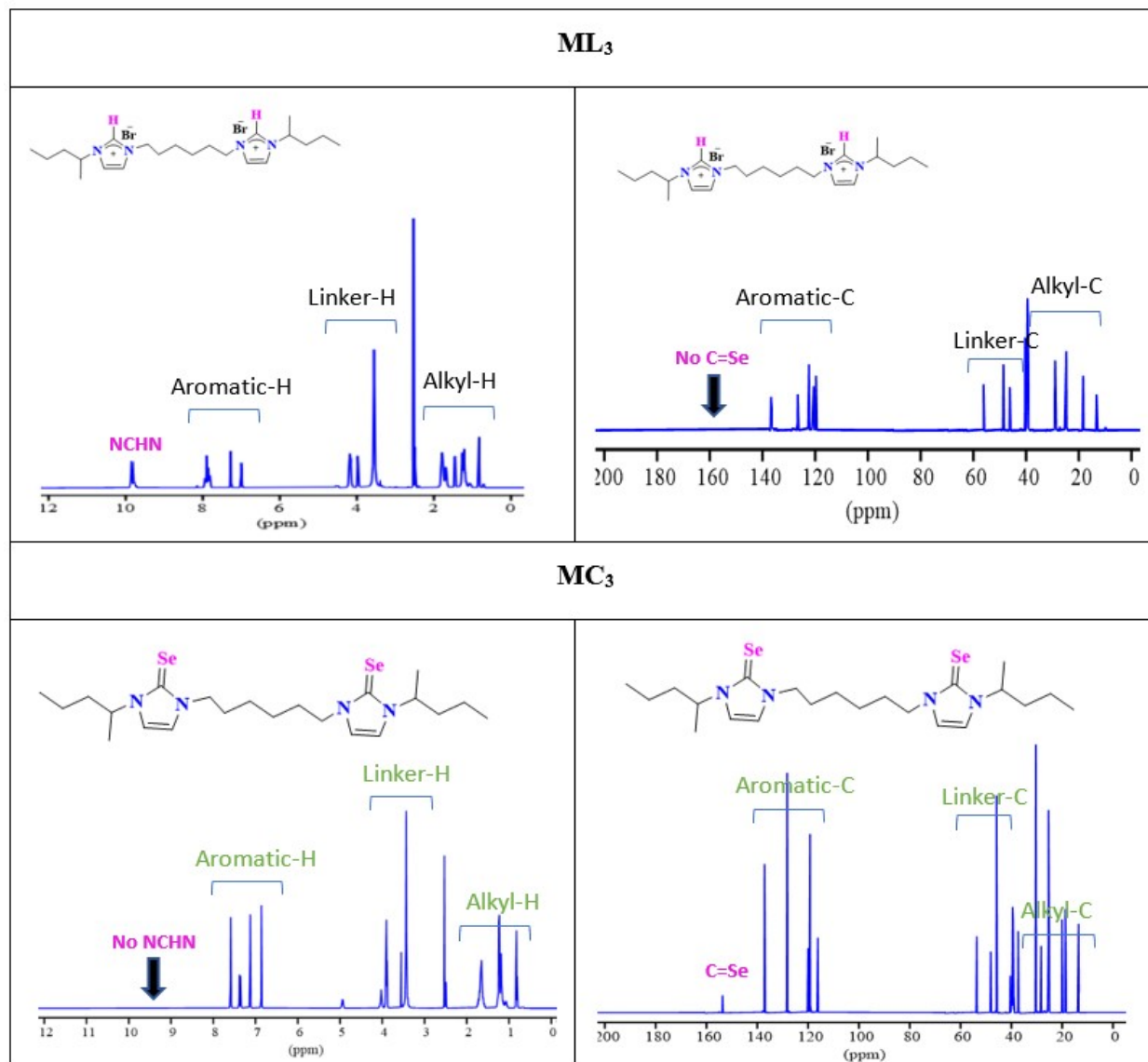


Figure S3: ¹H NMR and ¹³C NMR spectra of **ML₃** and **MC₃**.

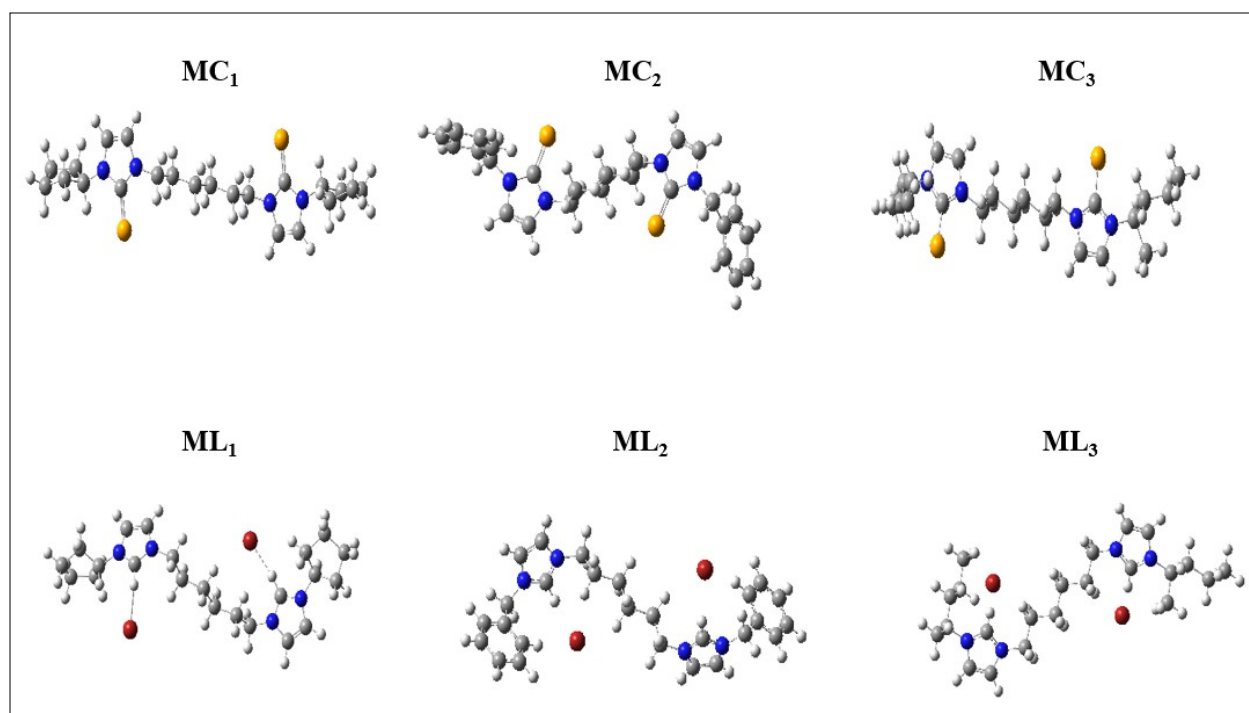


Figure S4. Optimized structures of ligands (ML_1 - ML_3) and their respective Se-adducts (MC_1 - MC_3).

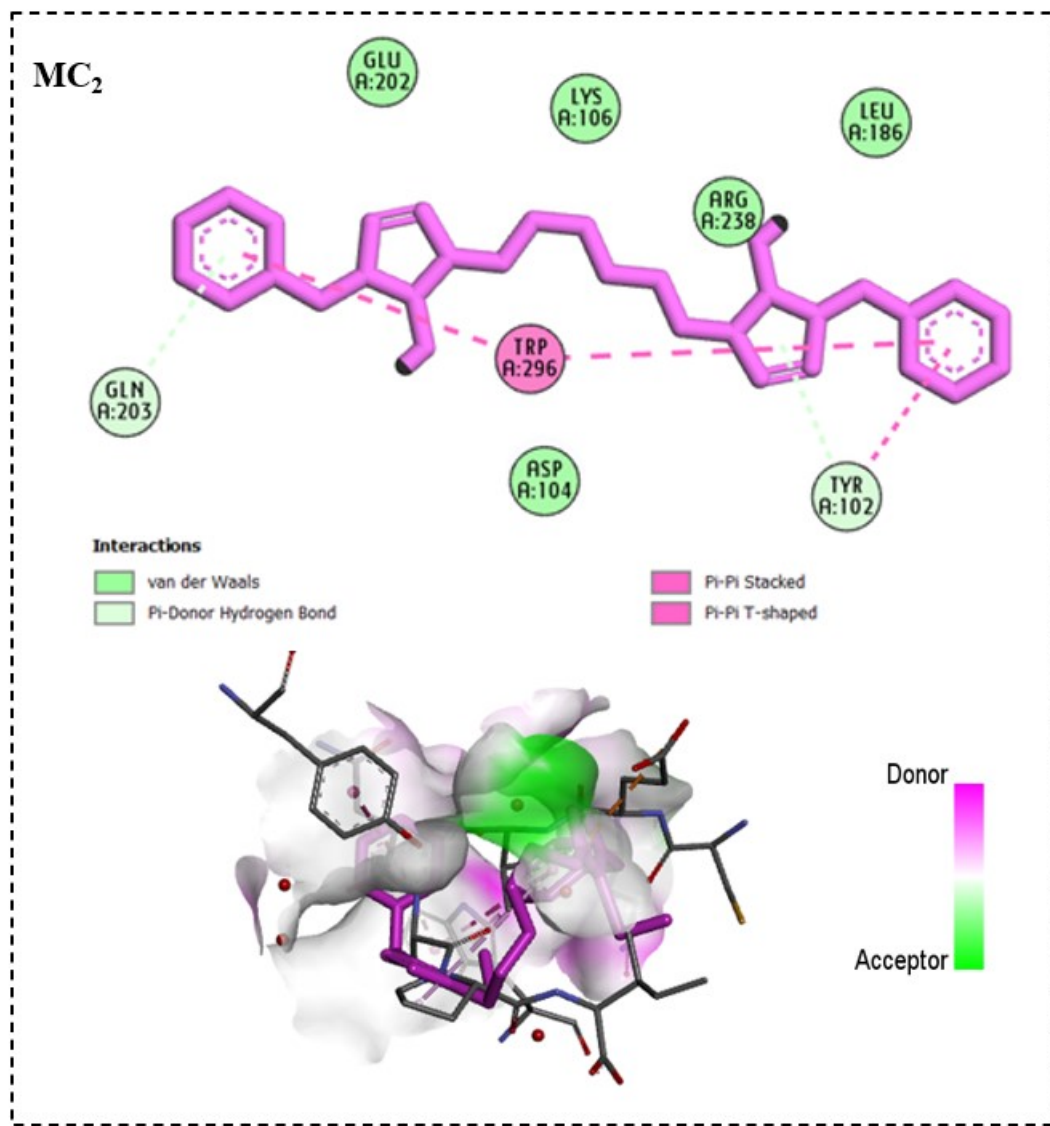


Figure S5. 2D and 3D view of the binding conformations of the selenium compound (**MC₂**) at the active site of AKR1C2.

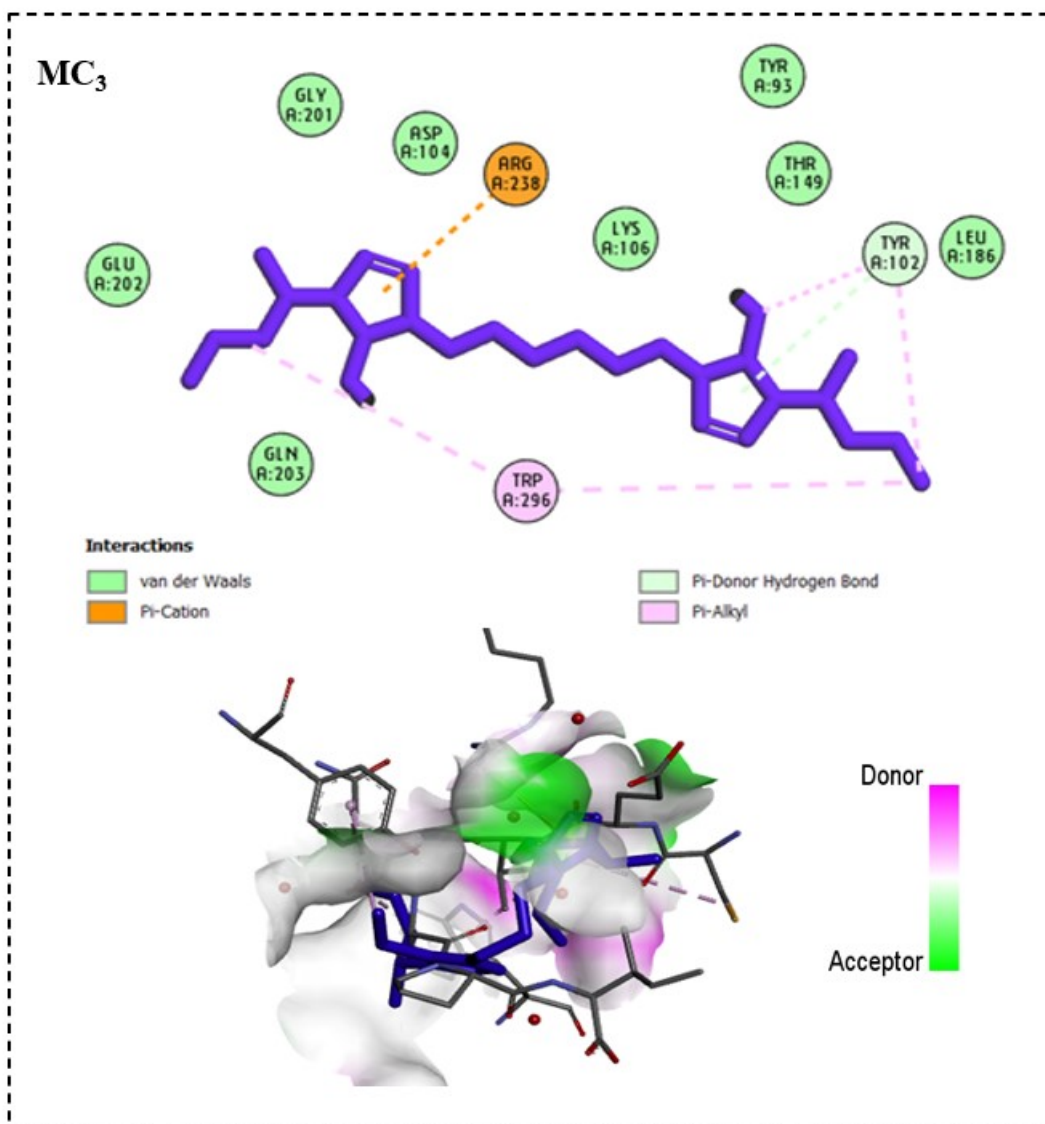


Figure S6. 2D and 3D view of the binding conformations of the selenium compound (**MC₃**) at the active site of AKR1C2.