



Drug likeness, *in silico* ADMET, and antioxidant study of oxindole derivatives

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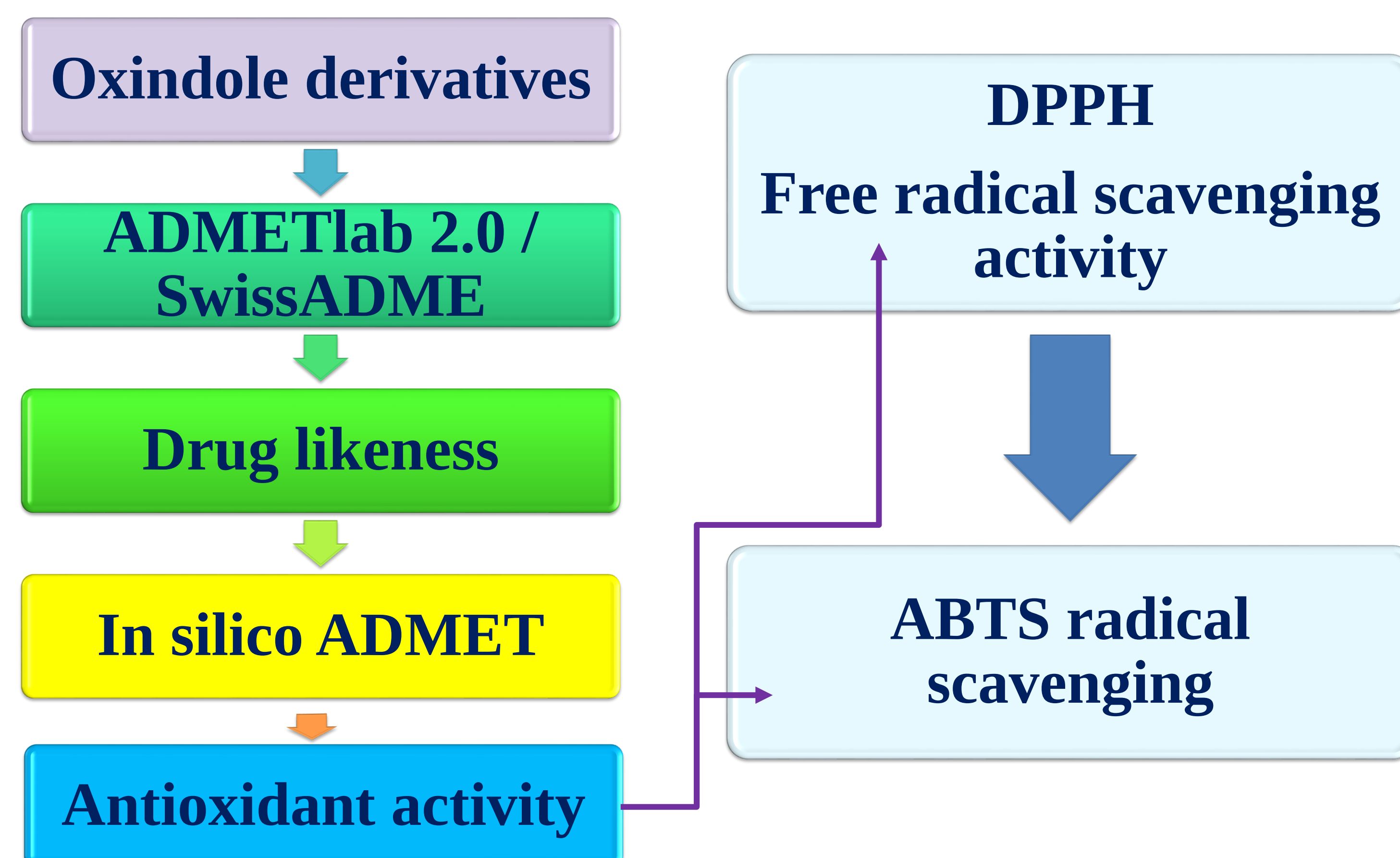


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INTRODUCTION

- ✓ Oxindoles are natural, hetero-aromatic, organic compounds found in body fluids, mammalian tissues, and various plant species.
- ✓ Oxindole derivatives have been identified with numerous pharmacological actions depending upon their structural moiety.
- ✓ Drug discovery is an interplay among physicochemical, pharmacokinetic, toxicity, and biological activities.

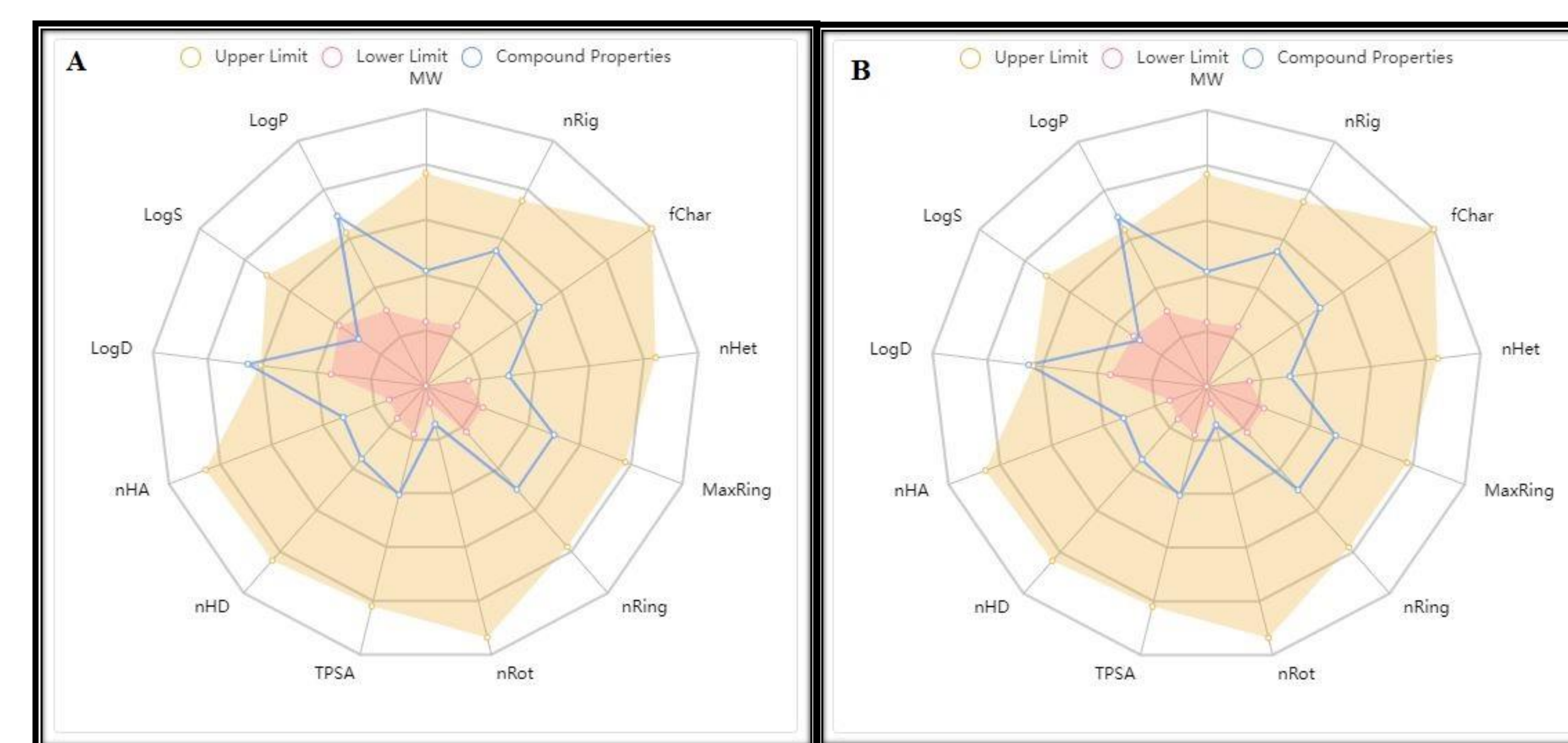
METHODOLOGY



RESULTS

Drug likeness and Medicinal chemistry parameters of oxindole derivatives

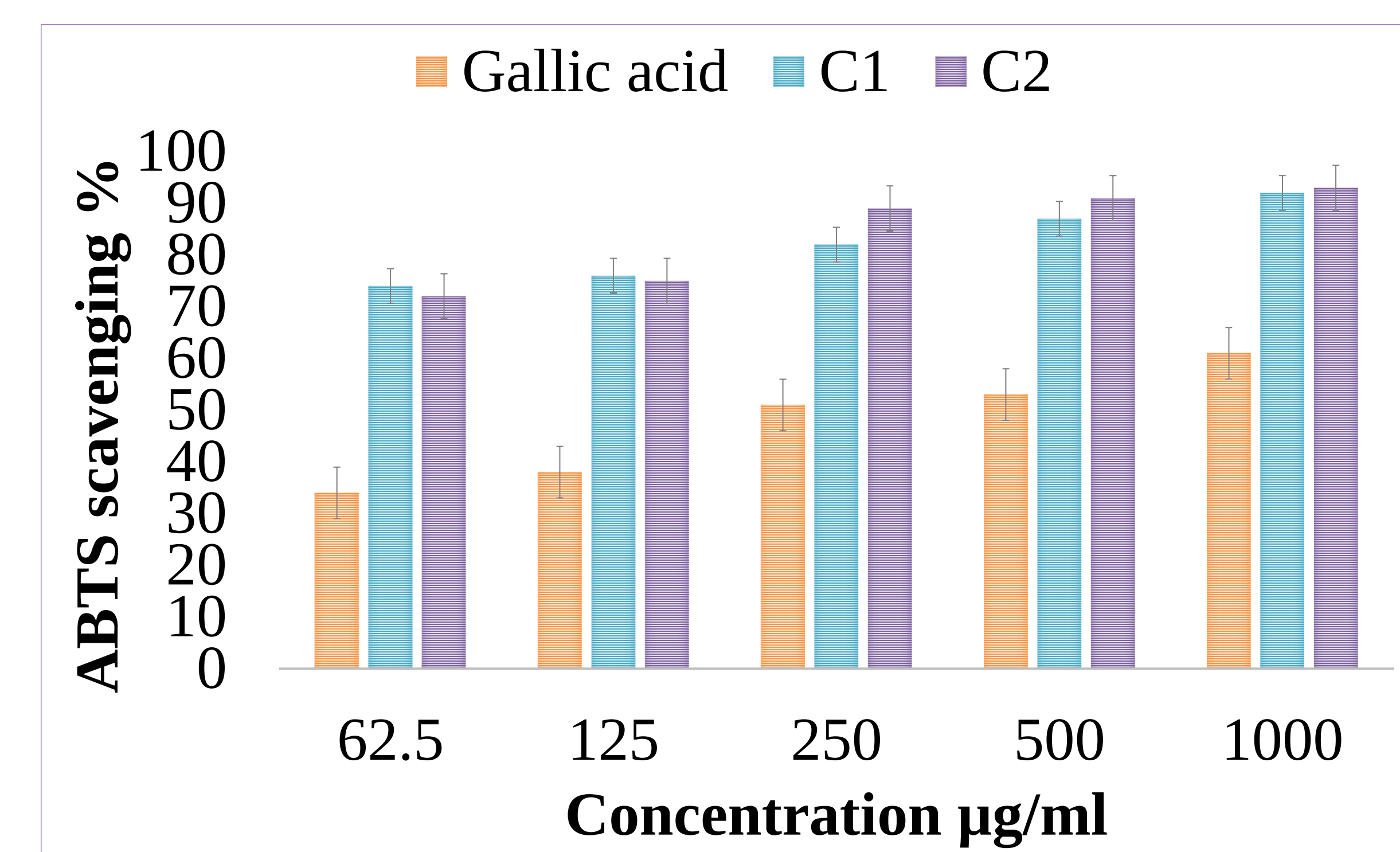
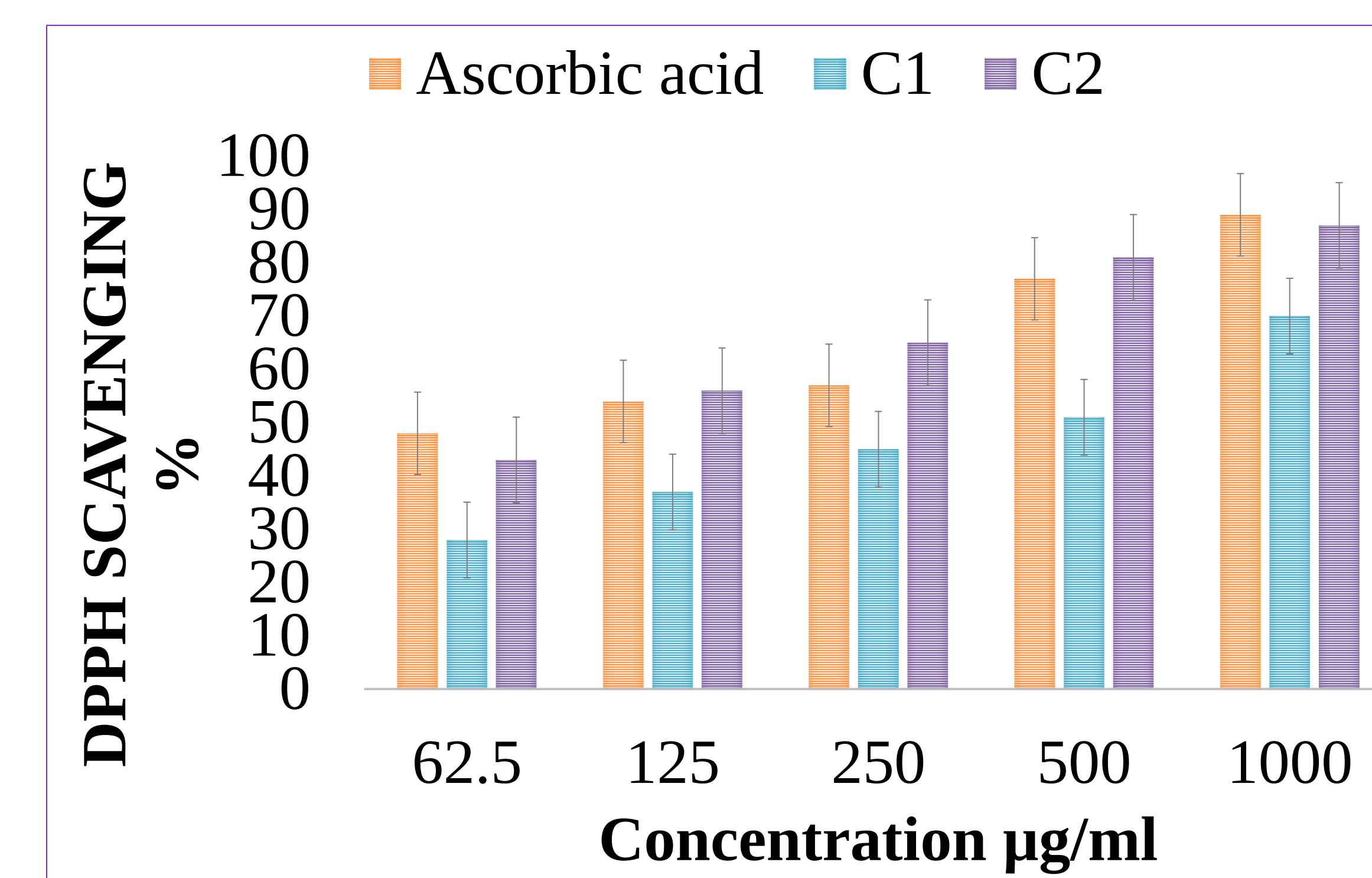
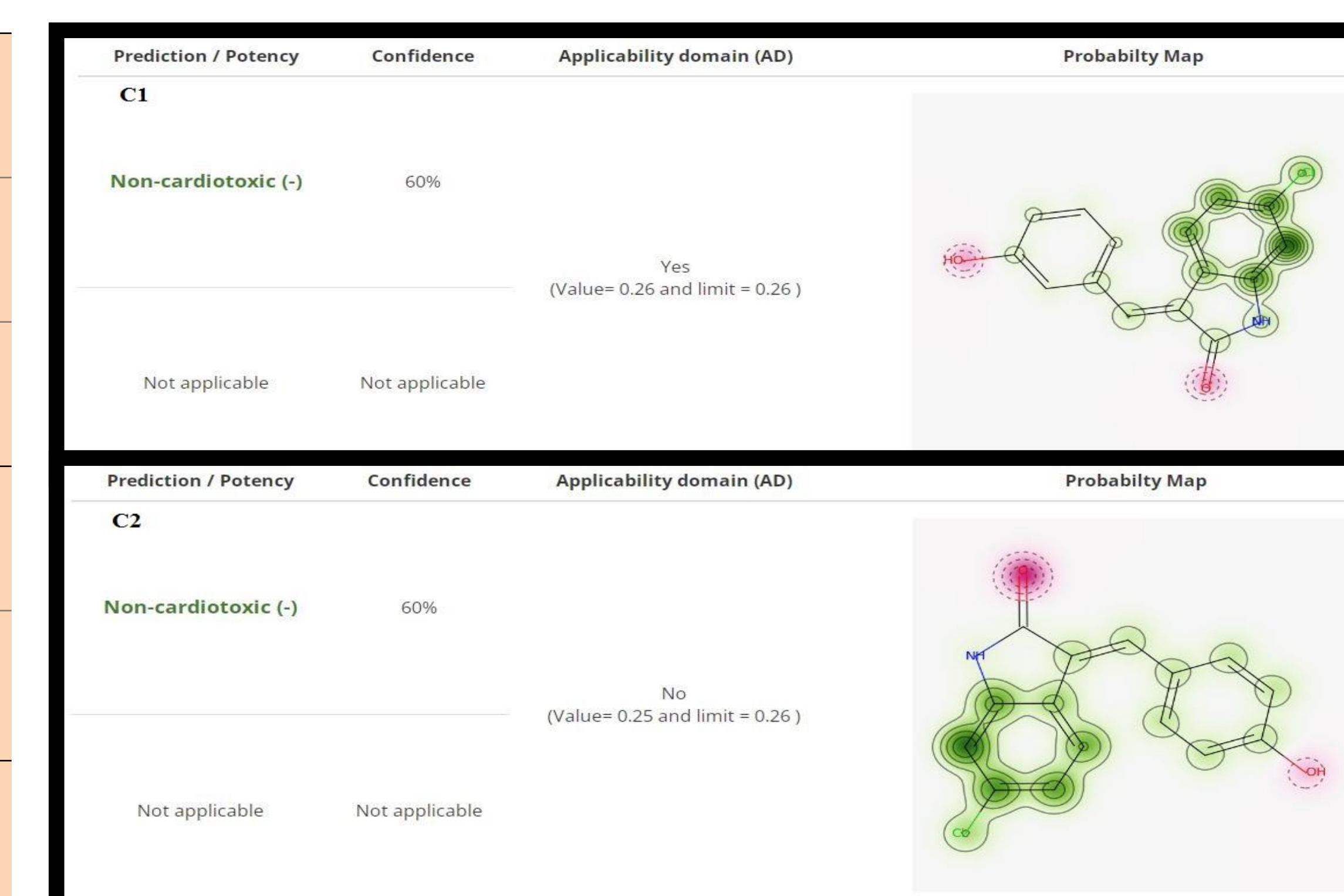
Oxindole	QED	Fsp ³	MCE-18	Lipinski Rule	Pfizer Rule	GSK Rule	Golden Triangle	PAINS	ALARM NMR	Chelator Rule
C1	0.78	0.0	32	accept	reject	accept	accept	0 alerts	2 alerts	0 alerts
C2	0.78	0.0	32	accept	reject	accept	accept	0 alerts	2 alerts	0 alerts



Physicochemical properties radar chart of C1 (A) and C2 (B)

IC₅₀ values of oxindole derivatives in µg/ml

Sample	DPPH	ABTS
C1	334.3	292.7
C2	225.7	184.171
Ascorbic acid	365.4	N/A
Gallic acid	N/A	346.7



CONCLUSION

- ✓ Oxindole derivatives possess superior drug-like properties, gastrointestinal absorption, high plasma protein binding, efficient distribution, and inhibit CYP 450 major isoforms with moderate clearance rates.
- ✓ Oxindole derivatives exhibited a concentration dependant DPPH and ABTS radical scavenging activity.
- ✓ Chemical structure-activity-pharmacokinetic relationship identified the meta position (C1) as the favorite for the electron-withdrawing groups to maintain antioxidant activity.