

Supplementary Figure S1

***In silico* and *in vitro* drug screening of curcumin and derivatives as EGFR and NF- κ B inhibitors**

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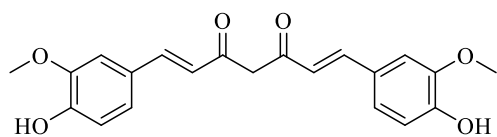
⁴ home address: Chemistry of Medicinal Plants Department, National Research Centre, 33 El-Bohouth St., Dokki, Giza 12622, Egypt.

⁵ Department of Chemistry, University of Copenhagen, Universitetsparken 5, Copenhagen 2100, Denmark

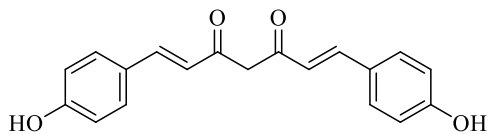
⁶ Department of Chemistry, University of the Western Cape, P/B X17, Bellville, 7535 Cape Town, South Africa.

⁷ Institute of Pharmaceutical Biology, Goethe University, Frankfurt/Main, Germany

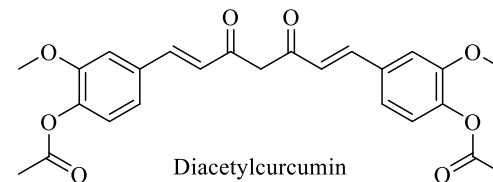
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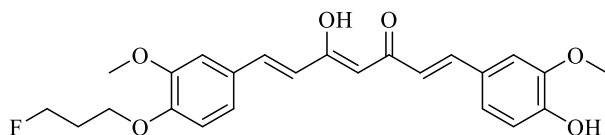
curcumin



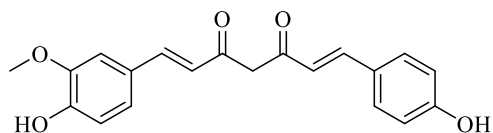
Bisdemethoxycurcumin



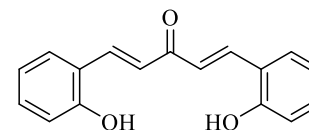
Diacetylcurcumin



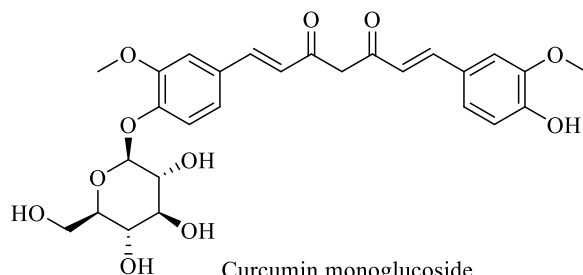
[18F]-curcumin



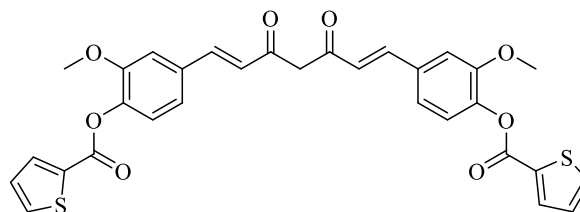
Monodemethoxycurcumin



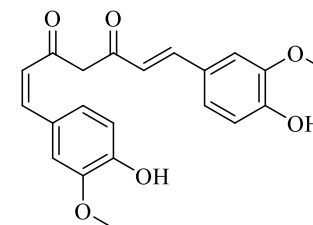
(E,E)-Bis(2-hydroxybenzylidene)acetone



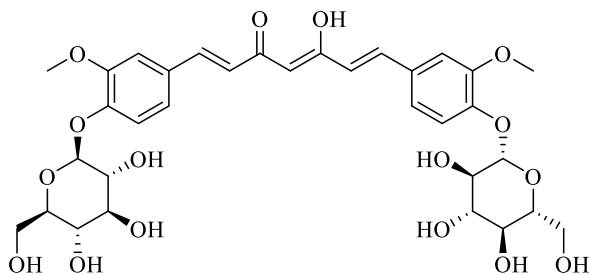
Curcumin monoglucoside



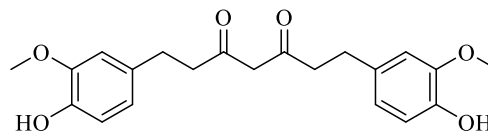
Di-O-(2-Thienoyl) curcumin



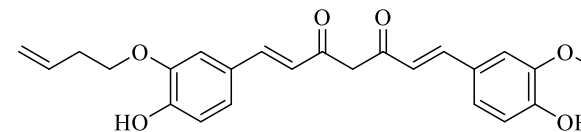
Cis-curcumin



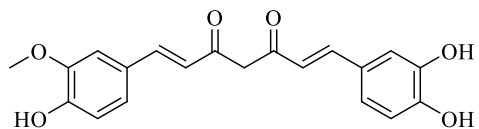
Curcumin diglucoside



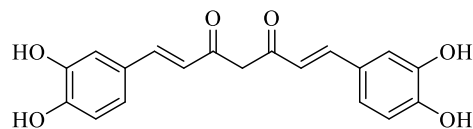
Tetrahydrocurcumin



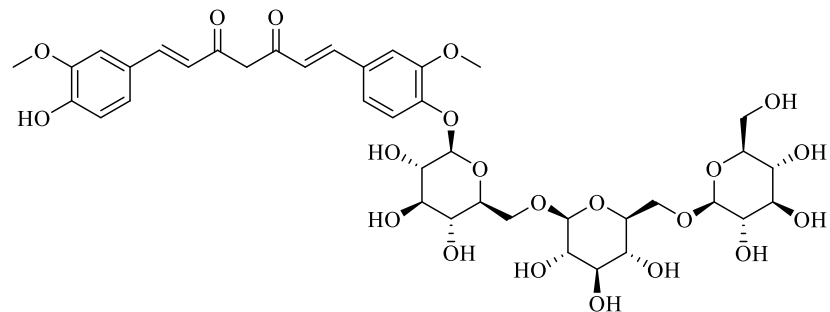
Allyl curcumin



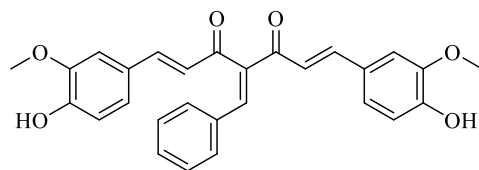
Monodemethylcurcumin



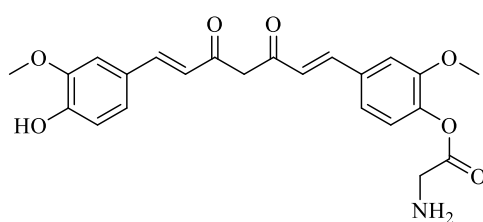
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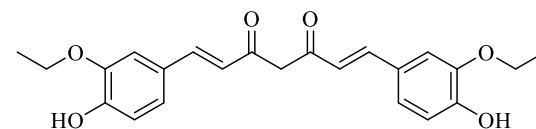
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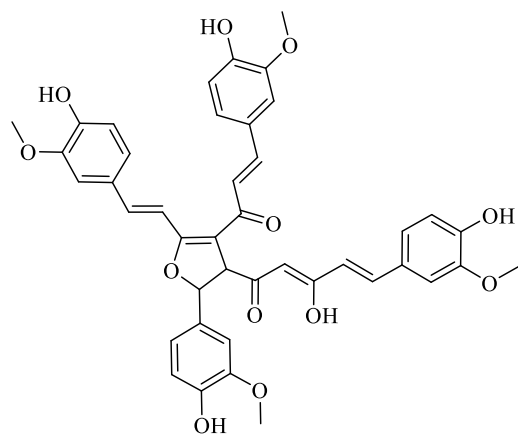
4-Benzylidene curcumin



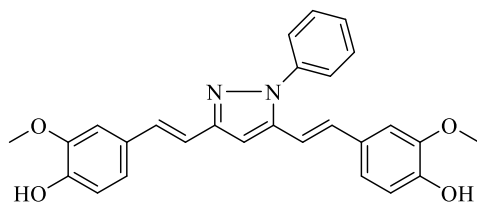
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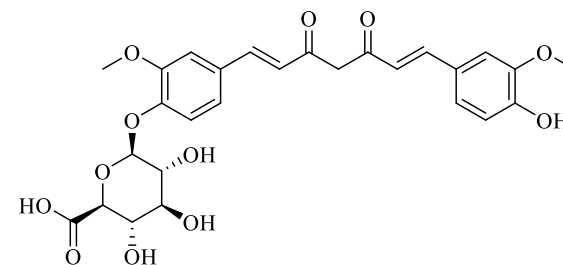
Ethylcurcumin



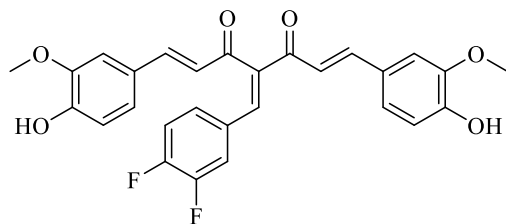
Curcumin dimer 1



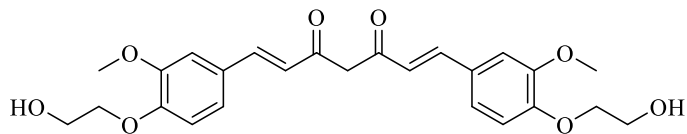
N-phenylpyrazole curcumin



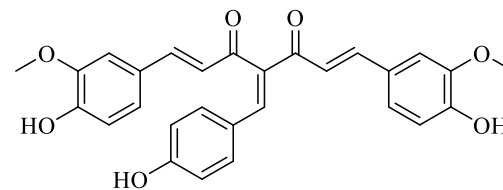
Curcumin β -*D*-glucuronide



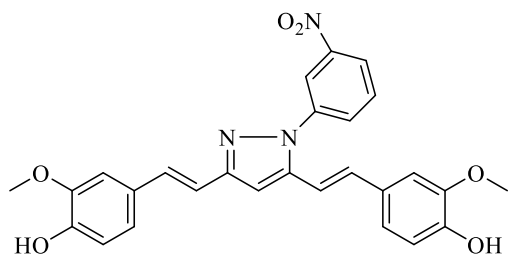
3,4-Difluorobenzylidene curcumin



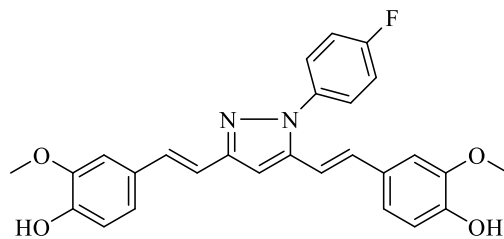
Di-*O*-(2-hydroxyethyl) curcumin



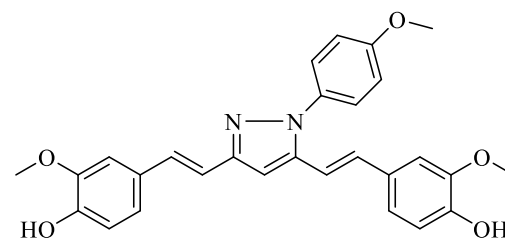
4-(4-hydroxybenzylidene) curcumin



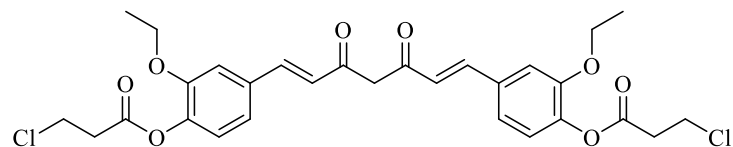
N-(3-nitrophenylpyrazole) curcumin



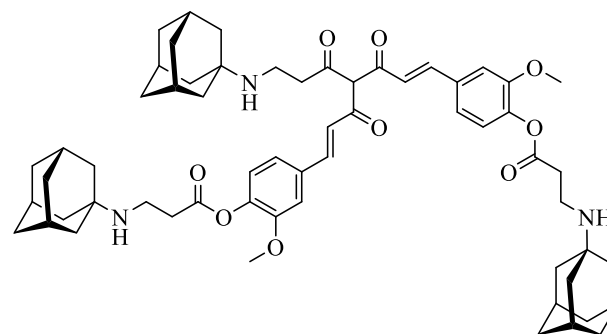
N-(4-fluorophenylpyrazole) curcumin



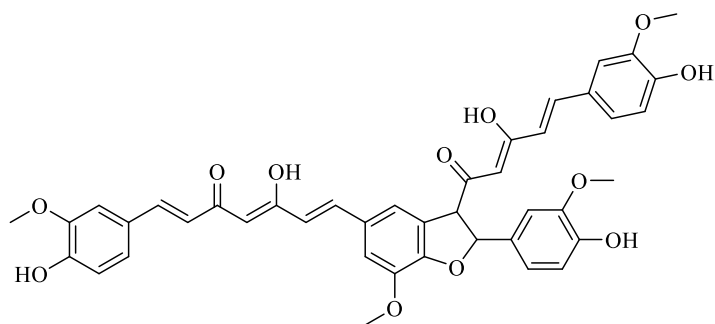
N-(4-methoxyphenylpyrazole) curcumin



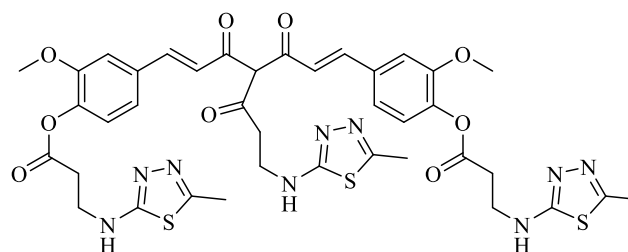
Di-*O*-chloropropionylethyl curcumin



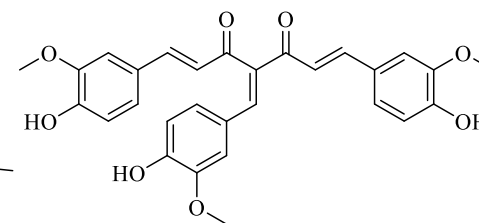
Curcumin tri adamantylaminoethylcarbonate



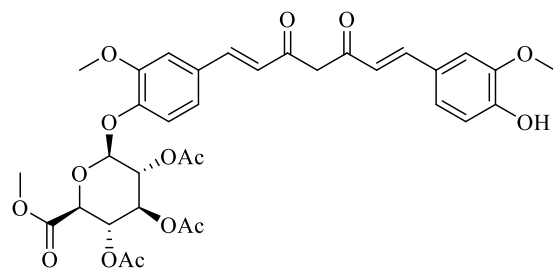
Curcumin dimer 2



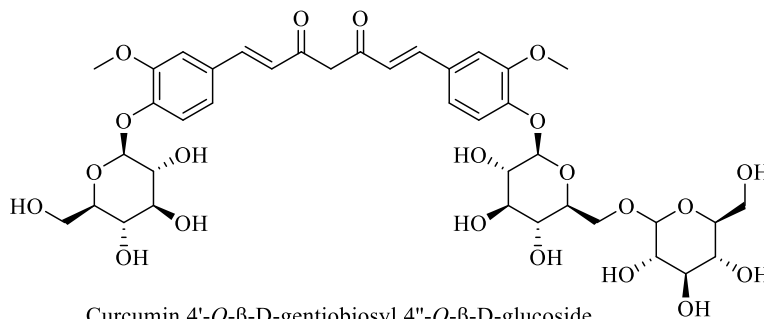
Curcumin tri-trithiadiazolaminoethylcarbonate



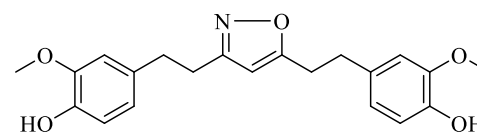
4-(4-hydroxy-3-methoxybenzylidene) curcumin



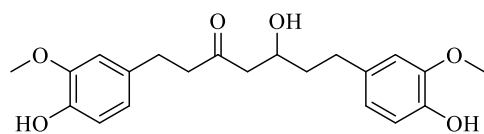
Curcumin β -D-glucuronide triacetate methyl ester



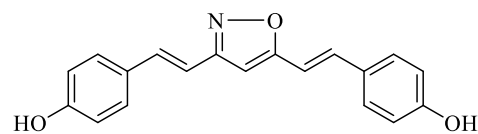
Curcumin 4'-O- β -D-gentiobiosyl 4''-O- β -D-glucoside



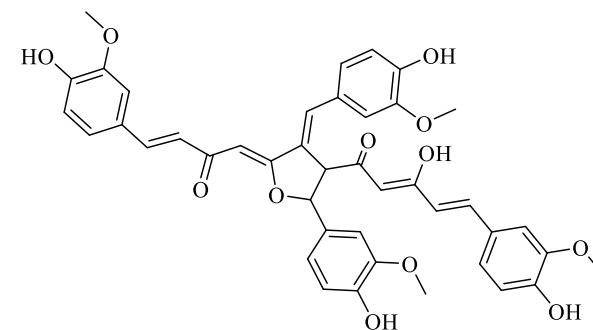
Tetrahydrocurcumin isoxazole



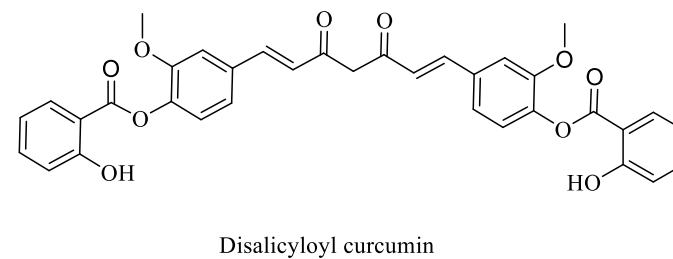
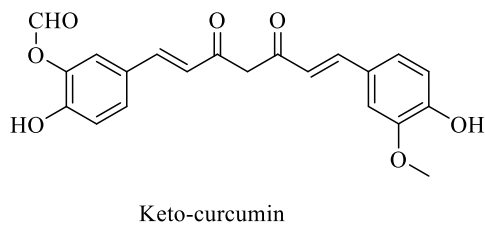
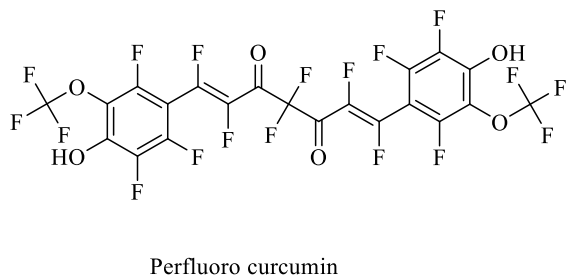
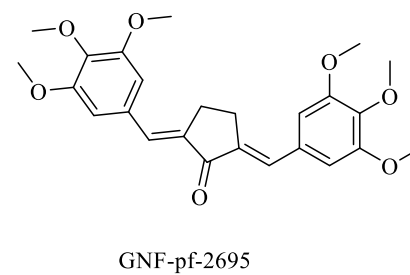
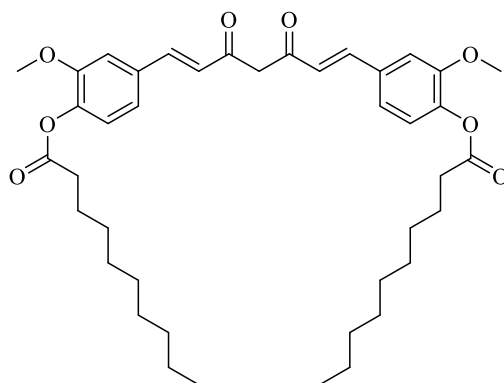
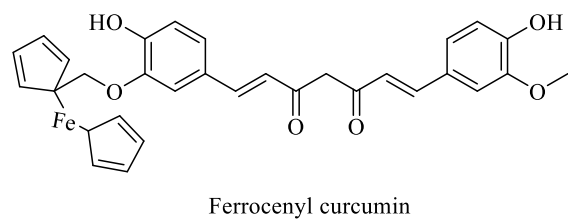
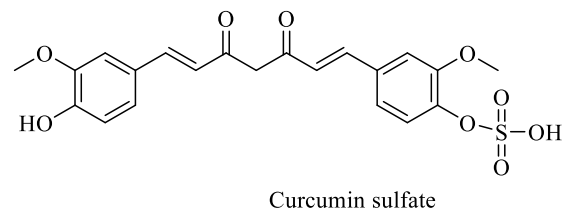
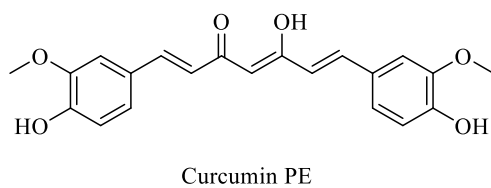
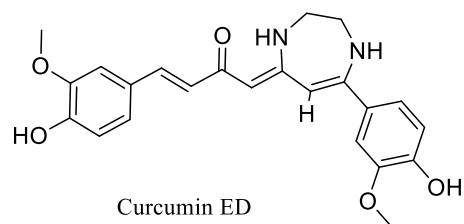
Hexahydrocurcumin

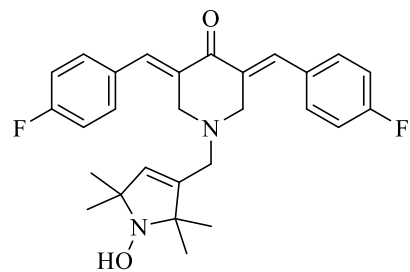


Bisdemethoxycurcumin isoxazole

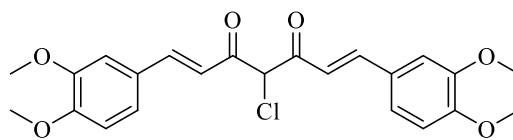


Curcumin dimer 3

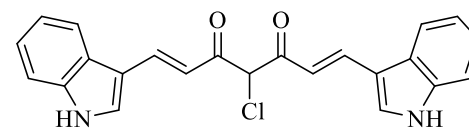




HO-3867



1A6



1A9