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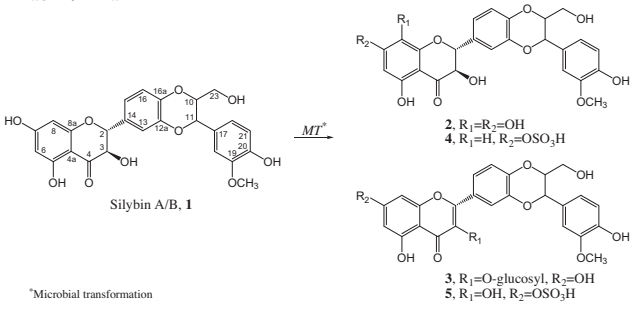
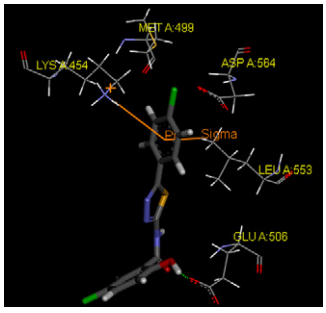
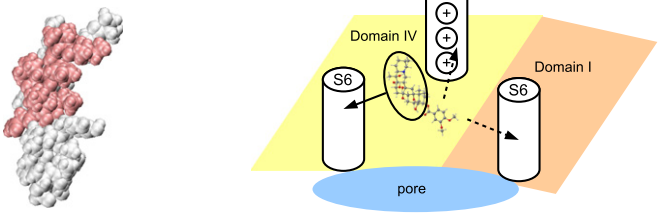
Contents

ARTICLES

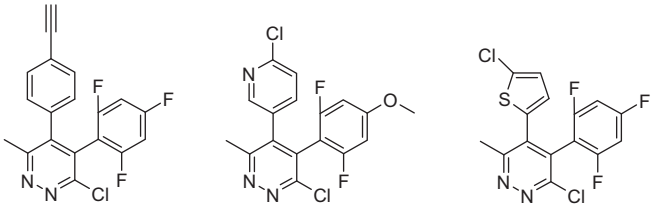




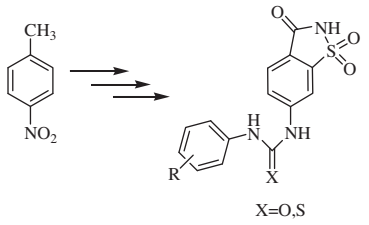
A series of 1,3,4-thiadiazol-2-amide derivatives have been designed and synthesized, and their biological activities were also evaluated as potential antiproliferation and FAK inhibitors. Compound **5h** possessed the most potent FAK inhibitory activity (IC_{50} = 5.32 μM) and anticancer activities (IC_{50} = 0.45 μM for MCF-7 and IC_{50} = 0.31 μM for B16-F10). Docking simulation was performed to insert compound **5h** into the crystal structure of FAK to determine the probable binding model.



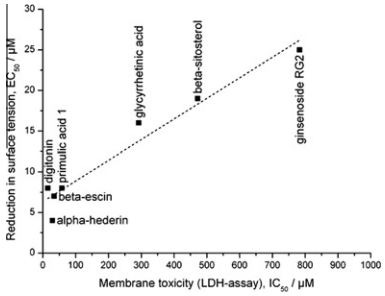
Interaction site mapping Suggested interaction manner of veratridine



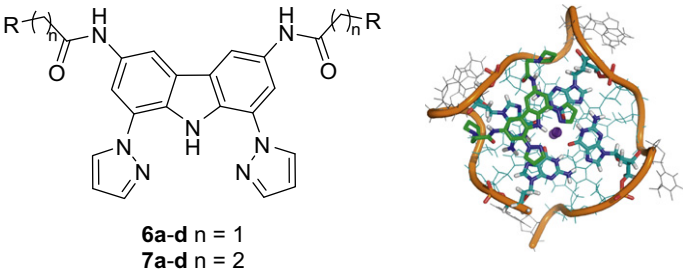
Highly active against *Botrytis cinerea* (grey mould), *Mycosphaerella graminicola* (wheat leaf blotch) and *Alternaria solani* (potato and tomato early blight).



X=O,S

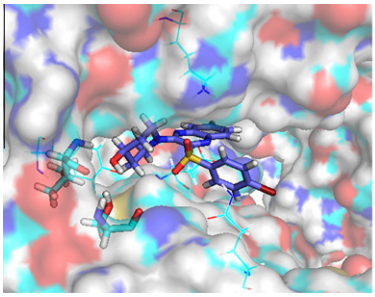


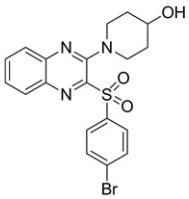
The attempt is undertaken to find a correlation between the cytotoxic effects and the physico-chemical properties of saponins.



6a-d n = 1
7a-d n = 2

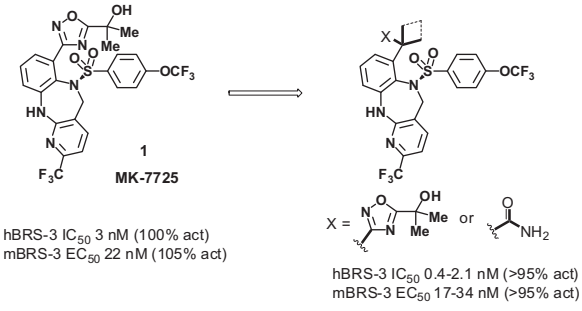
A series of 1,8-dipyrazolcarbazole derivatives were synthesized, and found to be a new type of selective binding ligands for *c-myc* G-quadruplex over duplex DNA.

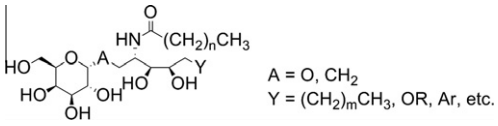


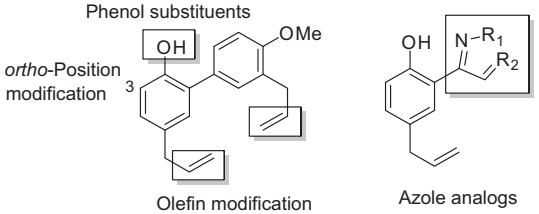


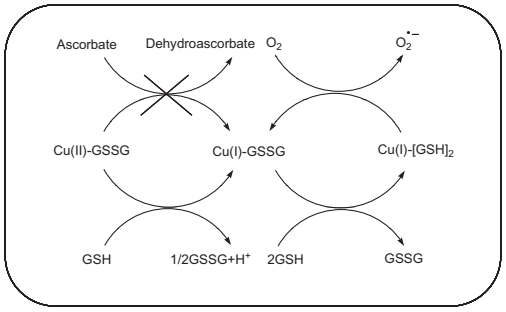
10d WR23

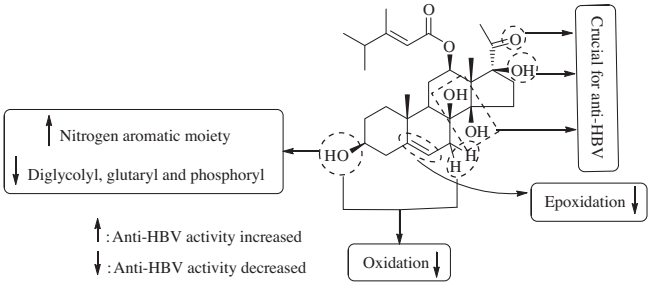
A series of novel 2-piperidinol-3-(arylsulfonyl)quinoxalines, as exemplified by compound WR23, was synthesized and evaluated as PI3Kα inhibitors.



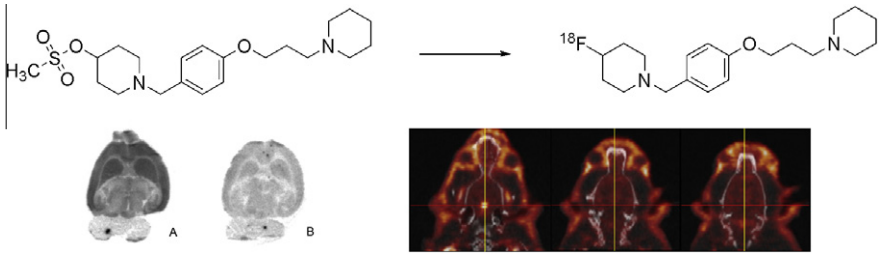


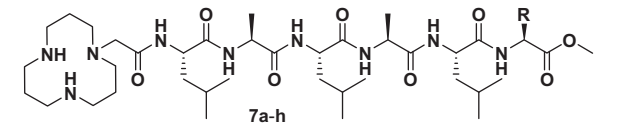




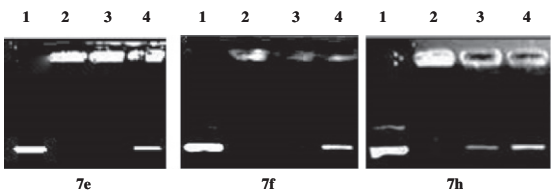


A series of caudatin derivatives were synthesized, and their anti-hepatitis B virus (HBV) activity was evaluated in HepG 2.2.15 cells. Most of the 3-O-substituted caudatin derivatives showed effective anti-HBV activity. Two compounds (**2e**, **2f**) had potent activity inhibiting not only the secretion of HBsAg, HBeAg, but also HBV DNA replication. The structure–activity relationships (SARs) of caudatin derivatives had been discussed.





a, R=H; b, R=CH_3; c, R=CH_2OH; d, R=$CH(CH_3)_2$
e, R=$CH_2CH(CH_3)_2$; f, R=$C_6H_5CH_2$; g, R=$CH_2C_6H_5OH$; h, R=$CH_2C_8H_5NH$

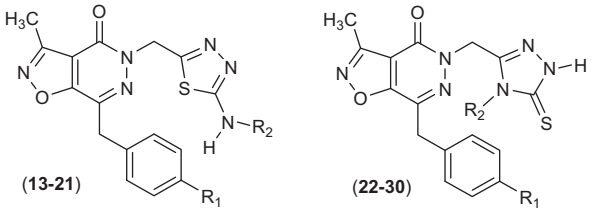


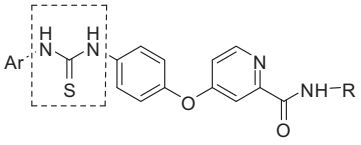
A series of oligopeptide derived macrocyclic polyamine [12]aneN$_3$ conjugates **7a–h**·3HCl have been synthesized and showed reversible DNA condensation ability.

Experimental design	Treatments	Mw (kDa) α	Mw (kDa) β
A	High Mw	300 a	280 a
	Med Mw	79 b	61 b
	Low Mw	30 c	22 c
	Oligosaccharides	5 e	4 e
B	Higher DDA (97%)	-	14 d
	Lower DDA (86-88%)	12 d	15 d

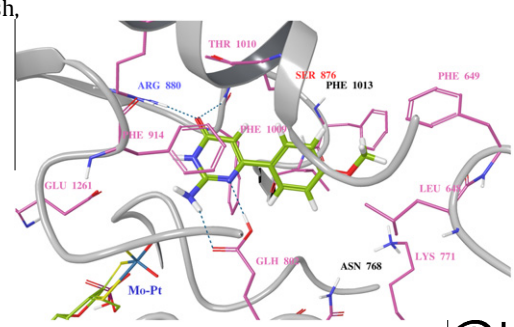
Total antioxidant activity

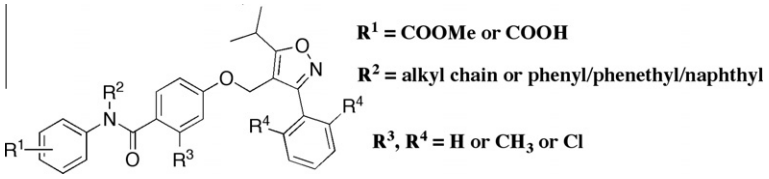
	P value			
	DPPH	Reducing	Chelating	Hydroxyl
FC	0.2915	<.0.0001	0.0171	<.0.0001
Mw	<.0.0001	<.0.0001	<.0.0001	<.0.0001
CS	<.0.0001	<.0.0001	<.0.0001	<.0.0001
FC x Mw	<.0.0001	<.0.0001	0.0016	<.0.0001
Mw x CS	<.0.0001	0.0434	<.0.0001	0.1635
FC x CS	0.5103	0.6509	0.1788	0..0093



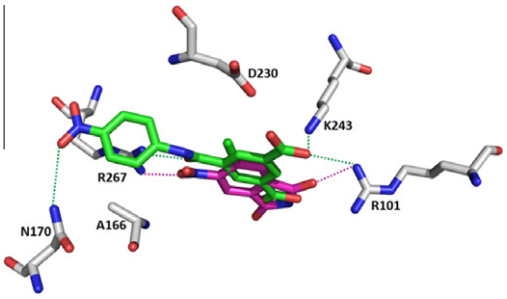


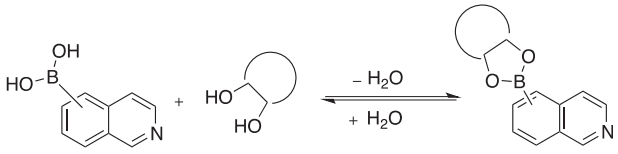
Twenty new diaryl thiourea containing sorafenib derivatives **9a**–**t** have been prepared and evaluated for their anticancer activity.





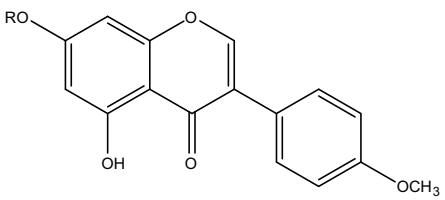
Highly E297G BSEP function enhancers, including 3-{2-Chloro-{4-[3-(2,6-dichlorophenyl)-5-isopropylisoxazol-4-yl]methoxy}-*N*-benzylbenzamido}benzoic acid, were discovered.

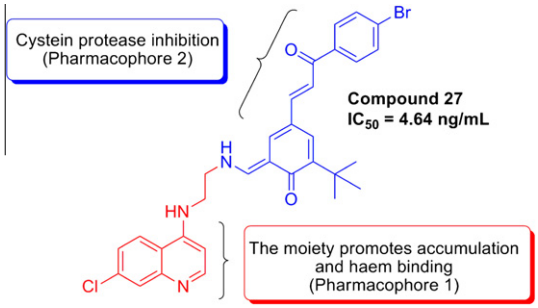




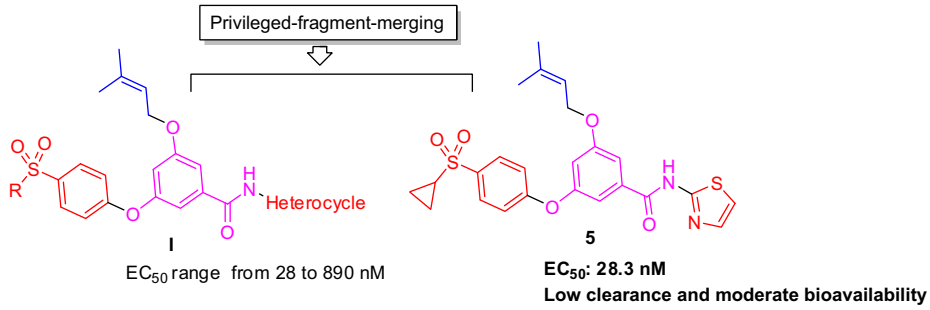
A stopped-flow method was used for the first time to study kinetic properties of binding between boronic acids and various sugars. For all the boronic acid–diol pairs examined, reactions were complete within minutes. The k_{on} values with various sugars follow the order of D-fructose > D-tagatose > D-mannose > D-glucose. The 'on' rate is the key determining factor of the binding constant.

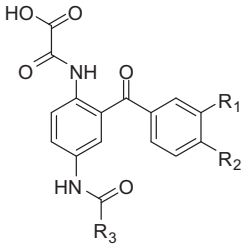
1 R = $ClCH_2CO$
2 R = $ClCH_2CH_2NCO$
3 R = $BrCH_2CO$
4 R = $BrCH_2CH_2NCO$
5 R = $CH_3(CH_2)_{10}NCO$



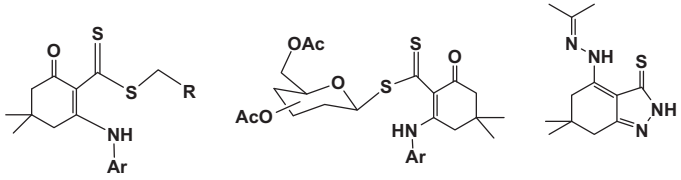


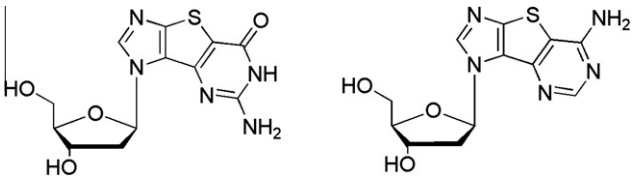
Synthesis and antimalarial evaluation of novel chalcone-chloroquine hybrids is reported.

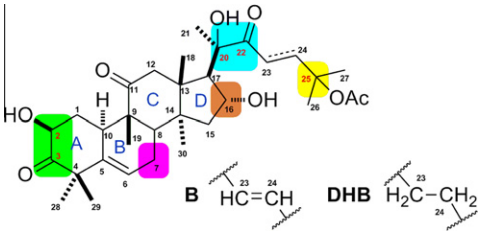


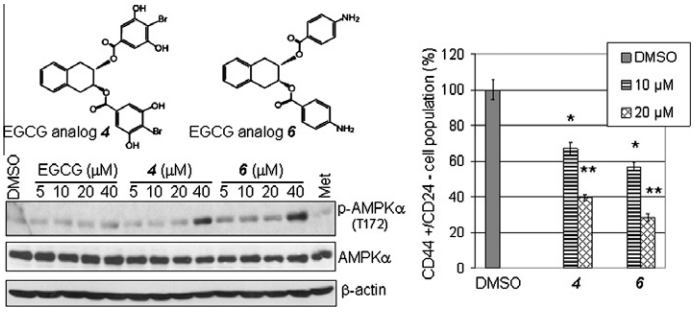


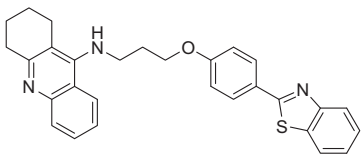
A series of novel benzophenone derivatives were prepared and their inhibitory activities were evaluated on hPin1. Of all the synthesized compounds, the most active compound displayed inhibitory activities with IC_{50} value of 5.99 μmol/L. Preliminary structure–activity relationships were analyzed in details and the binding mode of the titled compounds was predicted using FlexX algorithm.





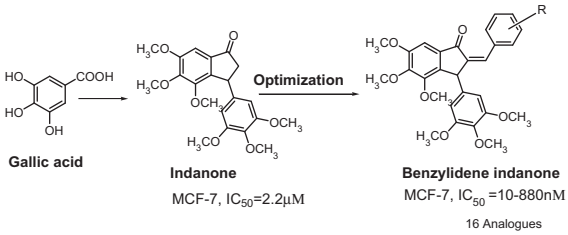




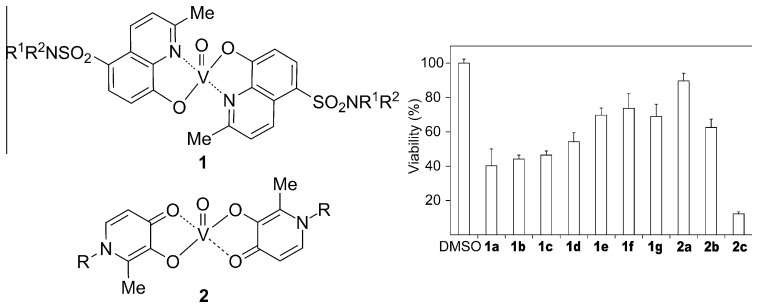


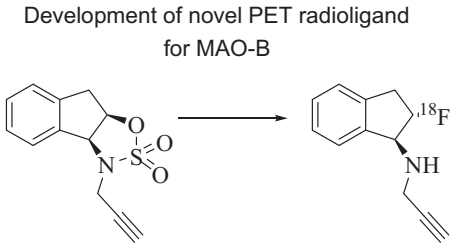
44b: IC_{50} of 0.017 μM for AChE; 51.8% for $A\beta_{1-42}$ at 20μM

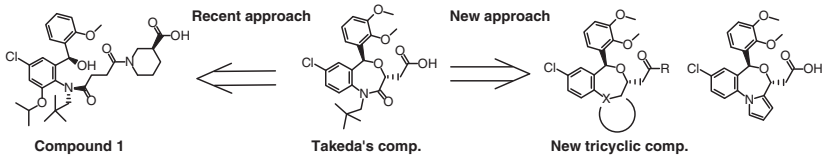
A series of berberine-phenyl-benzoheterocyclic and tacrine-phenyl-benzoheterocyclic hybrids were synthesised and evaluated as multifunctional anti-Alzheimer's disease agents. Compound **44b**, was the most potent AChE inhibitor with an IC_{50} value of 0.017 μM. This compound demonstrated similar Aβ aggregation inhibitory activity with cucurmin (51.8% vs 52.1% at 20 μM, respectively).

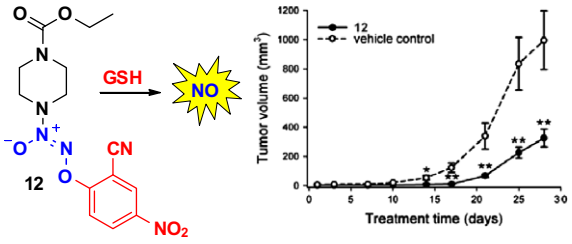


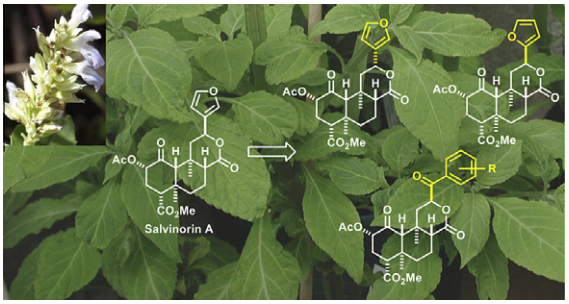
Gallic acid has been modified to 2-benzylidene indanones. Three of the analogues exhibited potent anticancer activity (IC_{50} in nM) through tubulin polymerization inhibition.

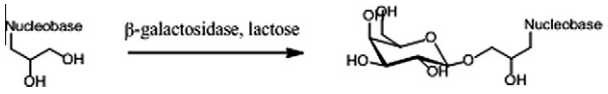


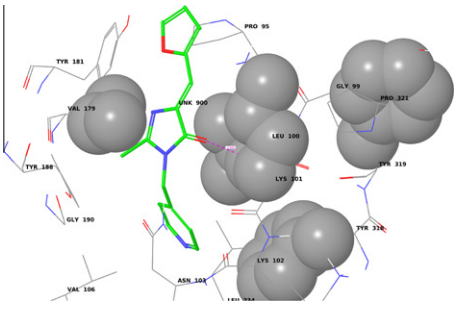




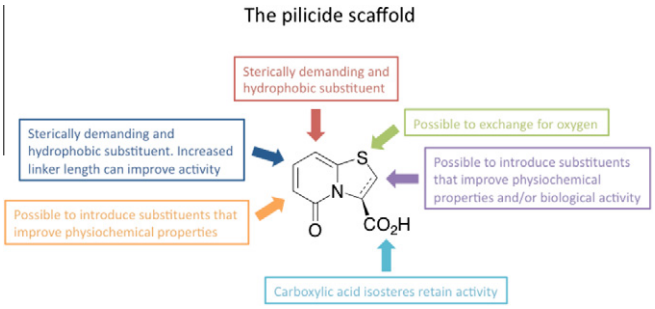








A novel series of substituted imidazol-5-ones were designed, synthesized and evaluated for reverse transcriptase inhibition activity using reverse transcriptase (RT) assay kit (Roche, Colorimetric). Docking study was performed to study the binding orientation and affinity of synthesized compounds for RT enzyme.



*Corresponding author
Supplementary data available via SciVerse ScienceDirect

COVER

Dipyrone (metamizol) is a common antipyretic drug and the most popular non-opioid analgesic in many countries. In spite of its long and widespread use, molecular details of its fate in the body are not fully known. Two unknown metabolites were now found, viz. arachidonoyl amides, and positively tested for cannabis receptor binding (CB1 and CB2) and cyclooxygenase inhibition. Two more puzzle pieces of the dipyrone story found! (Rogosch, T.; Sinning, C.; Podlewski, A.; Watzer, B.; Schlosburg, J.; Lichtman, A.H.; Cascio, M.G.; Bisogno, T.; Di Marzo, V.; Nüsing, R.; Imming, P. *Bioorg. Med. Chem.* **2012,** *20,* 103–109.]

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