Supplementary information

Table 1. Band gap energy (E_g) of ZnC and 6Cnt@ZnC samples.

	Bandgap (eV)	E_{cb} (eV)	E_{vb} (eV)
ZnC	3.1	-0.26	2.84
	2.2	-0.66	1.54
6Cnst@ZnC	2.9	-0.16	2.74
	1.78	-0.45	1.33

Table 2. Physicochemical properties of compound (**6**)

Property	Value	Comment
Molecular Weight	273.13	Contain hydrogen atoms. Optimal:100-600
Volume	268.436	Van der Waals volume
nHA	4	Number of hydrogen bond acceptors. Optimal:0-12
nHD	0	Number of hydrogen bond donors. Optimal:0-7
nRot	1	Number of rotatable bonds. Optimal:0-11
MaxRing	11	Number of atoms in the biggest ring. Optimal:0-18
nHet	5	Number of heteroatoms. Optimal:1-15
fChar	0	Formal charge. Optimal: -4-~4
nRig	20	Number of rigid bonds. Optimal:0-30
Flexibility	0.05	Flexibility =nRot /nRig
Stereo Centers	0	Optimal: ≤ 2

TPSA	20.64	Topological Polar Surface Area. Optimail: 0-140
logS	-3.669	Log of the aqueous solubility. Optimal: -4-0.5 log mol/L
LogP	2.704	Log of the octanol/water partition coefficient. Optimal: 0-3
logD	2.361	logP at physiological pH 7.4. Optimal: 1-3

Table 3. Medicinal Chemistry of compound (**6**)

Property	**Value**	**Comment**
QED	0.786	A measure of drug-likeness based on the concept of desirability; Attractive: > 0.67; unattractive: 0.49~0.67; too complex: < 0.34
SAscore	3.746	Synthetic accessibility score is designed to estimate ease of synthesis of drug-like molecules. SAscore ≥ 6, difficult to synthesize; Sashcord <6, easy to synthesize.
Fsp^3	0.467	The number of sp3 hybridized carbons / total carbon count, correlating with melting point and solubility. $Fsp^3 \geq 0.42$ is considered a suitable value
MCE-18	50.909	MCE-18 stands for medicinal chemistry evolution. MCE-18 ≥ 45 is considered a suitable value.
NPscore	-0.547	Natural product-likeness score. This score is typically in the range from -5 to 5. The higher the score is, the higher the probability is that the molecule is a NP
Lipinski Rule	Accepted	MW ≤ 500; logP ≤ 5; Hacc ≤ 10; Hdon ≤ 5; If two properties are out of range, a poor absorption or permeability is possible, one is acceptable.
Pfizer Rule	Accepted	logP > 3; TPSA < 75; Compounds with a high log P (>3) and low TPSA (<75) are likely to be toxic.
GSK Rule	Accepted	MW ≤ 400; logP ≤ 4; Compounds satisfying the GSK rule

Property	Value	Comment
		may have a more favorable ADMET profile
Golden Triangle	Accepted	00 ≤ MW ≤ 50; -2 ≤ logD ≤ 5; Compounds satisfying the Golden Triangle rule may have a more favorable ADMET profile
PAINS	0 alerts	Pan Assay Interference Compounds, frequent hitters, Alpha-screen artifacts and reactive compound.
ALARM NMR	0 alerts	Thiol reactive compounds
BMS	0 alerts	Undesirable, reactive compounds
Chelator Rule	0 alerts	Chelating compounds

Table 4. The properties of the drug metabolism of compound (**6**)

Property	Value	Comment
CYP1A2 inhibitor	0.896	Category 1: Inhibitor; Category 0: Non-inhibitor; The output value is the probability of being inhibitor
CYP1A2 substrate	0.858	Category 1: Substrate; Category 0: Non-substrate. The output value is the probability of being substrate
CYP2C19 inhibitor	0.47	Category 1: Inhibitor; Category 0: Non-inhibitor. The output value is the probability of being inhibitor
CYP2C19 Substrate	0.932	Category 1: Substrate; Category 0: Non-substrate; The output value is the probability of being substrate
CYP2C9 inhibitor	0.114	Category 1: Inhibitor; Category 0: Non-inhibitor. The output value is the probability of being inhibitor.
CYP2C9 substrate	0.708	Category 1: Substrate; Category 0: Non-substrate;

Property	Value	Comment
		The output value is the probability of being substrate.
CYP2D6 inhibitor	0.492	Category 1: Inhibitor; Category 0: Non-inhibitor;The output value is the probability of being inhibitor.
CYP2D6 Substrate	0.919	Category 1: Substrate; Category 0: Non-substrate; The output value is the probability of being substrate
CYP3A4 inhibitor	0.143	Category 1: Inhibitor; Category 0: Non-inhibitor; The output value is the probability of being inhibitor
CYP3A4 Substrate	0.831	Category 1: Substrate; Category 0: Non-substrate; The output value is the probability of being substrate

Table 5. The properties of the drug excretion of compound (**6**)

Property	Value	Comment
CL	6.709	Clearance; High: >15 mL/min/kg; moderate: 5-15 mL/min/kg; low: <5 mL/min/kg
T1/2	0.07	Category 1: long half-life ; Category 0: short; half-life; long half-life: >3h; short half-life: <3h; The output value is the probability of having long half-life.

Table 6. The properties of the drug toxicity of compound (**6**)

Property	Value	Comment
Herg Blockers	0.54	Category 1: active; Category 0: inactive; The output value is the probability
H-HT	0.899	Human Hepatotoxicity; Category 1: H-HT positive

		(+); Category 0: H-HT negative (-); The output value is the probability of
DILI	0.942	Drug Induced Liver Injury. Category 1: drugs with a high risk of DILI; Category 0: drugs with no risk of DILI. The output value is the probability of being toxic.
Rat Oral Acute Toxicity	0.542	Category 0: low-toxicity; Category 1: high-toxicity; The output value is the probability of being highly toxic
FDAMDD	0.322	Maximum Recommended Daily Dose; Category 1: FDAMDD (+); Category 0: FDAMDD (-); The output value is the probability of being positive.
Skin Sensitization	0.732	Category 1: Sensitizer; Category 0: Non-sensitizer; The output value is the probability of being sensitizer.
Carcinogencity	0.906	Category 1: carcinogens; Category 0: non-carcinogens; The output value is the probability of being toxic.
Eye corrosion	0.003	Category 1: corrosives; Category 0: noncorrosives; The output value is the probability of being corrosives
Eye irritation	0.012	Category 1: irritants; Category 0: nonirritants; The output value is the probability of being irritants.
Respiratory Toxicity	0.94	Category 1: respiratory toxicants; Category 0: respiratory nontoxicants; The output value is the probability of being toxic.

Table 7. The properties of the environmental toxicity of compound (**6**)

Property	Value	Comment
Bioconcentration Factors	1.713	Bioconcentration factors are used for considering secondary poisoning potential and assessing risks to human health via the food chain. The unit is -log10[(mg/L)/(1000*MW)]
IGC_{50}	3.06	Tetrahymena pyriformis 50 percent growth inhibition concentration; The unit is -log10[(mg/L)/(1000*MW)].
$LC_{50}FM$	4.397	96-hour fathead minnow 50 percent lethal concentration; The unit is -log10[(mg/L)/(1000*MW)].
$LC_{50}DM$	6.089	48-hour daphnia magna 50 percent lethal concentration; The unit is -log10[(mg/L)/(1000*MW)].