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Mechanism-based inhibitors and probes for neuraminidases

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Mechanism-Based Inhibitors and Probes for Neuraminidases

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List of abbreviations

4-MU: 4-methylumbelliferyl	dt: double triplet
Å: Ångström, 1.0×10^{-10} meters	DIPEA: diisopropylethylamine
ABP: activity-based probe	DMAP: 4-dimethylaminopyridine
ABPP: activity-based protein profiling	DMBA: dimethylbarbituric acid
Ac: acetyl	DMF: <i>N,N</i> -dimethylformamide
All: allyl	Em: emission
Alloc: allyloxycarbonyl	ESI: electrospray ionisation
aq.: aqueous	eq: molar equivalents
B: boat	Et: ethyl
BF ₃ •OEt ₂ : boron trifluoride diethyl etherate	Ex: excitation
Bn: benzyl	FEL: free energy landscape
Bu: butyl	Fmoc: fluorenylmethyloxycarbonyl
C: chair	fs: femtosecond(s)
calc.: calculated	GH: glycosidase hydrolase
CAZy: Carbohydrate Active Enzyme	h: hour(s)
CBB: Coomassie Brilliant Blue	<i>K_i</i> : inhibition constant of competitive inhibitors
Cbz: carboxybenzyl	<i>K_i</i> : inactivation constant of covalent inhibitors
CEL: conformational energy landscape	<i>K_M</i> : Michaelis-Menten constant
CDCl ₃ : chloroform- <i>d</i> , deuterated chloroform	<i>k_{inact}</i> : inactivation constant
COSY: correlation spectroscopy	HA: heamagglutinin
CV: collective variable	HBTU: (2-(1H-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate
δ: chemical shift	HMBC: heteronuclear multiple-bond correlation
DBU: 1,8-diazabicyclo[5.4.0]undec-7-ene	HSQC: single quantum coherence
DCM: dichloromethane, methylene chloride	MD: molecular dynamics
dd: double doublet	NA: neuraminidase
ddd: doublet of double doublets	<i>p</i> : para
ddt: doublet of double triplets	PAGE: polyacrylamide gel electrophoresis
DFT: density functional theory	Pd/C: palladium on activated charcoal
DIBAL-H: di-isobutylaluminiumhydride	PG: protecting group
DMP: Dess-Martin periodinane	Ph: phenyl
DMDO: dimethyldioxirane	
DMSO: dimethyl sulfoxide	
DTT: dithiothreitol	
dq: double quartet	

PMB: *para*-methoxybenzyl
PPM: parts per million
ps: picosecond(s)
Quant.: quantitative yield
ROS: radical oxygen species
t: triplet
TBAF: tetrabutylammonium fluoride
TBAI tetrabutylammonium iodide
TBS, TBDMS: *tert*-butyldimethylsilyl
tBu: *tert*-butyl
TES: triethylsilyl
Tf: trifluoromethanesulfonyl
TFA trifluoroacetic acid
TFAA: Trifluoroacetic acid anhydride
THF: tetrahydrofuran
TLC: thin layer chromatography
TMEDA: tetramethylethylenediamine
TMS: tetramethylsilane
TOF: Time-of-Flight (mass spectrometry)
q: quartet
QM/MM: quantum mechanics/molecular
mechanics
UV: ultraviolet
v/v: volume/volume
WT: wild type