

Journal of Medicinal Chemistry

jm- 2020-019249

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Title
Development of Novel Tetrahydroquinoline Inhibitors of NLRP3 Inflammasome for Potential Treatment of DSS-induced Mouse Colitis

RECOMMENDED COMPOUND CHARACTERIZATION CHECKLIST

NOTE: CHECKLIST IS RECOMMENDED BUT NOT REQUIRED

TO DISPLAY INSTRUCTIONS: Double-click HERE (Formula Bar must be visible: Select View>Formula Bar) TO CLOSE: Enter/Return																				
COMPOUND		IDENTITY										PURITY				BIOMEDICAL TEST				
Compound, structure, or table-entry number		New	Known	Melting point range	IR	UV-Vis	¹ H NMR	¹³ C NMR	MS	HRMS	Optical rotation/ORD/CD	Enantiomeric/Diastereomeric ratio	X-ray [ORTEP and CIF in SI*]	Copy of ¹ H/ ¹³ C NMR spectrum in SI*	Elemental analysis	Quant. GC, HPLC, or electrophoresis	Other purity method	In vitro	In vivo	Other test
I-1			✓	✓			✓	✓		✓			✓		✓					
I-2			✓	✓			✓	✓		✓			✓		✓					
1		✓		✓	✓		✓	✓		✓			✓		✓			✓		
2		✓		✓	✓		✓	✓		✓			✓		✓			✓		
3		✓		✓	✓		✓	✓		✓			✓		✓			✓		
4		✓		✓	✓		✓	✓		✓			✓		✓			✓		
5		✓		✓	✓		✓	✓		✓			✓		✓			✓		
6		✓		✓	✓		✓	✓		✓			✓		✓			✓	✓	
7		✓		✓	✓		✓	✓		✓			✓		✓			✓		
8		✓		✓	✓		✓	✓		✓			✓		✓			✓		
9		✓		✓	✓		✓	✓		✓			✓		✓			✓		

COMPOUND		IDENTITY										PURITY				BIOMEDICAL TEST				
Compound, structure, or table-entry number	New	Known	Melting point range	IR	UV-Vis	1H NMR	13C NMR	NMR	MS	HRMS	Optical rotation/ORD/CD	Enantiomeric/Diastereomeric ratio	X-ray [ORTEP and CIF in SI*]	Copy of 1H/13C NMR spectrum in SI*	Elemental analysis	Quant. GC, HPLC, or electrophoresis	Other purity method	In vitro	In vivo	Other test
10	✓		✓	✓		✓	✓			✓				✓				✓		
11	✓		✓	✓		✓	✓			✓				✓				✓		

COMPOUND	IDENTITY												PURITY			BIOMEDICAL TEST									
Compound, structure, or table-entry number	New	Known	Melting point range	IR	UV-Vis	1H NMR	13C NMR	NMR	MS	HRMS	Optical rotation/ORD/CD	Enantiomeric/Diastereomeric ratio	X-ray [ORTEP and CIF in SI*]	Copy of 1H/13C NMR spectrum in SI*	Elemental analysis	Quant. GC, HPLC, or electrophoresis	Other purity method	In vitro	In vivo	Other test					

* SI =
Supporting
Information

