## Product Data Sheet

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## Regorafénib N-oxyde (M2)-<sup>13</sup>C,d<sub>3</sub>

Cat. No.:	HY-I0678S1	
CAS No.:	2140317-01-5	
Molecular Formula:	C <sub>20</sub> <sup>13</sup> CH <sub>12</sub> D <sub>3</sub> ClF <sub>4</sub> N <sub>4</sub> O <sub>4</sub>	
Molecular Weight:	502.83	
Target:	Drug Metabolite	
Pathway:	Metabolic Enzyme/Protease	
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.	

BIOLOGICAL ACTIVITY			
BIOLOGICALACITATI			
Description	Regorafénib N-oxyde (M2)- <sup>13</sup> C,d <sub>3</sub> is the <sup>13</sup> C- and deuterium labeled Regorafénib N-oxyde (M2). Regorafénib N-oxyde M2 is an active metabolite of Regorafenib. Regorafenib is a multi-target inhibitor for VEGFR1/2/3, PDGFRβ, Kit, RET and Raf-1 with IC50s of 13/4.2/46, 22, 7, 1.5 and 2.5 nM, respectively.		
In Vitro	Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs <sup>[90]</sup> . MCE has not independently confirmed the accuracy of these methods. They are for reference only.		

## REFERENCES

[1]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019;53(2):211-223.

[2]. Allard M, et al. Simultaneous analysis of regorafenib and sorafenib and three of their metabolites in human plasma using LC-MS/MS. J Pharm Biomed Anal. 2017 Aug 5;142:42-48.

Caution: Product has not been fully validated for medical applications. For research use only.

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