## Capture of the volatile carbonyl metabolite of flecainide on 2,4-dinitrophenylhydrazine cartridge for quantitation by stable-isotope dilution mass spectrometry coupled with chromatography

Laszlo Prokai<sup>a,\*</sup>, Szabolcs Szarka<sup>a</sup>, Xiaoli Wang<sup>1</sup>, Katalin Prokai-Tatrai<sup>a,b</sup> <sup>a</sup>Department of Molecular Biology and Immunology, University of North Texas Health Science Center, 3500 Camp Bowie Boulevard, Fort Worth, TX 76107-2699, USA <sup>b</sup>Department of Pharmacology and Neuroscience, University of North Texas Health Science Center, 3500 Camp Bowie Boulevard, Fort Worth, TX 76107-2699, USA

## **Supplementary Information**



**Fig. S7.** Full-scan LC-ESI mass spectrum (**A**) of TFAA-*d*<sub>3</sub>-DNPH and CID-MS/MS spectrum (**B**) of the *m/z* 280 [M-H]<sup>-</sup> ion.

[M-H]-► 281 100] Relative Abundance 0 100 120 140 160 180 200 220 240 260 280 300 m/z 60 80 MS/MS CID <mark>183</mark> 113 171 183 Н <u>15</u>⊖ —N 100 В 15 167 Relative Abundance F<sub>3</sub>C 153 15 NO<sub>2</sub> 121 Ο 233 202 250 263 281 0 180 200 220 240 260 280 100 140 160 80 120 m/z

**Fig. S8.** Full-scan LC-ESI mass spectrum (**A**) of TFAA-<sup>15</sup>N<sub>4</sub>-DNPH and CID-MS/MS spectrum (**B**) of the *m/z* 281 [M-H]<sup>-</sup> ion.

## **Supplementary Table 1**

Summary method validation results for of the LC-ESI-MS using narrow-range scans (*m/z* 275 to 283).

	Repeatability					
TFAA-DNPH	Area Ratio (RSD %) <sup>a</sup>			Retention Time (RSD %) <sup>b</sup>		
(ng injected)	Intra-day <sup>c</sup>	Inter	-day <sup>d</sup>	Intra-day <sup>c</sup>	Inter-day <sup>d</sup>	
5	6.1	11.8		0.19	0.49	
10	3.7	4.0		0.25	0.56	
100	2.8	2.6		0.29	0.57	
	Accuracy					
$C_Q^{e}(ng/\mu L)$	$C_M^{f} \pm SD (ng/\mu L)$	.)	Precision (	RSD %)	Accuracy (%)	
1.56	$1.45 \pm 0.05$		3.7		-7.3	
6.25	$5.95\pm0.08$		1.4		-4.9	
25	$25.4 \pm 0.7$		2.8		1.7	

<sup>a</sup> Area Ratio (RSD %) denotes precision expressed in RSD % of analyte/IS area ratios.

<sup>b</sup> Retention Time (RSD %) denotes precision expressed in RSD % of retention times.

 $n^{c} n = 5.$  $n^{d} n = 15.$ 

<sup>e</sup>  $C_Q$  denotes the nominal concentration of TFAA-DNPH in QC samples. <sup>f</sup>  $C_M$  denotes the measured concentration of TFAA-DNPH in QC samples.