

# Correction to “Development of $^{11}\text{C}$ -Labeled ASEM Analogues for Detection of Neuronal Nicotinic Acetylcholine Receptors ( $\alpha 7$ -nAChR)”

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Article Recommendations

Unfortunately, a column in Table 2 in this article was duplicated. Correct entries in the column with heading KI-n83 are now included in the corrected version of this table.

The text “, and KI-n85” at page 354, left column, line 9 from below, should be removed. The corrected sentence reads “For the compounds substituted at positions R1 and R2, we can see that when  $\Delta\Delta G$  relative to ASEM is greater than 1 kcal/mol (e.g., KI-n74, KI-n75, and KI-n77), the compounds show low inhibition (inhibition <15%).”

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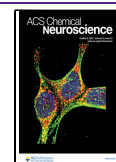









Table 2. PET Tracer Data for  $\alpha 7$ -nAChR Using Rational Tracer Design and Machine Learning Methods<sup>a</sup>

Compound ID	ASEM	KI-n83	KI-n84	KI-n85
Substituent				
$\Delta\Delta G$ (kcal/mol) <sup>b</sup>	0	0.10	-0.18	-0.28
K <sub>i</sub> (nM) <sup>c</sup>	0.35	0.41	0.26	0.22
Inhibition	94.2%	98.8%	97.8%	97.4%
Residence time (ns) <sup>d</sup>	53.38	40.81	40.37	75.63
AlogP <sup>e</sup>	2.92	2.79	2.83	2.85
Plasma protein binding	1.19	0.81	0.89	1.06
BBB	(+)	(+)	(+)	(+)
P-gp substrate	0.65 (+)	0.74(+)	0.74(+)	0.74 (+)
Autoradiography	<b>Y</b>	<b>Y</b>	<b>Y</b>	<b>Y</b>
Compound ID	KI-n74	KI-n75	KI-n77	
Substituent				
$\Delta\Delta G$ (kcal/mol)	1.10	1.70	1.51	
K <sub>i</sub> (nM) <sup>c</sup>	2.23	6.06	4.47	
Inhibition	ND	14.8%	11.9%	
Residence time (ns) <sup>d</sup>	28.68	30.01	ND	
AlogP <sup>e</sup>	2.79	2.83	2.85	
Plasma protein binding	1.12	1.00	1.04	
BBB	(+)	(+)	(+)	
P-gp substrate	0.59 (+)	0.68(+)	0.66 (+)	
Autoradiography	<b>Y</b>	<b>Y</b>	<b>N</b>	

<sup>a</sup>Data for ASEM and Kin85 are excerpts from tabulation given in ref 22. <sup>b</sup>(1) The binding free energy is calculated using FEP+ of Schrodinger.<sup>23</sup> (2) The relative free energy is calculated with ASEM as the reference. Lower is better.<sup>24</sup> <sup>c</sup>The K<sub>i</sub> value is calculated using  $\Delta G = -RT \ln(K/K_0)$ . The K<sub>i</sub> value of ASEM was reported previously.<sup>20</sup> <sup>d</sup>The residence time is calculated with potential scaled MD simulations using Gromacs. <sup>e</sup>The physicochemical properties are predicted by machine learning methods based on cheminformatics using Python, sklearn and rdkit.