Derivatization of dihydrotetrabenazine for technetium-99m labelling towards a radiotracer targeting vesicular monoamine transporter 2

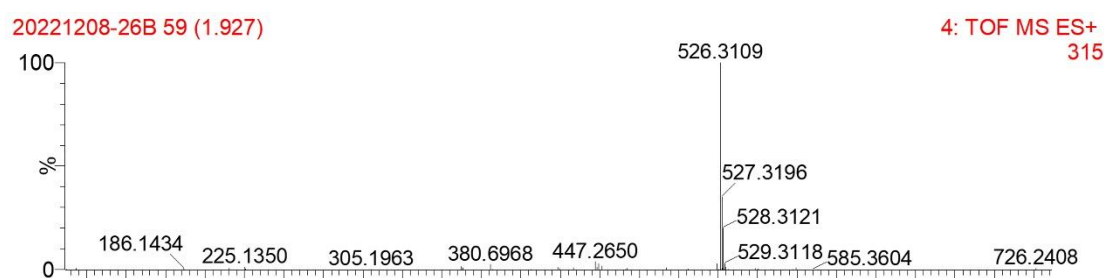Chunyi Liu, Yi Fang, Jie Tang, Zhengping Chen*

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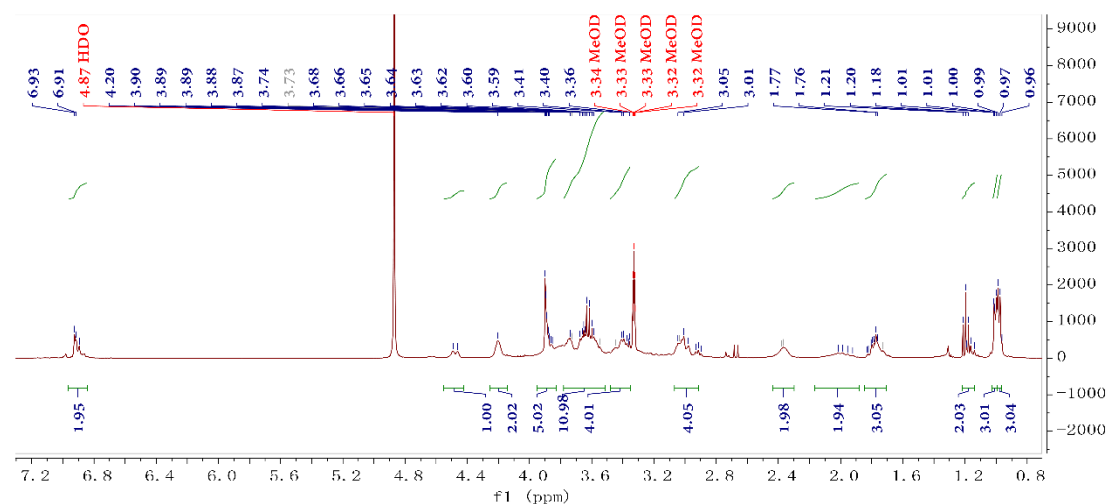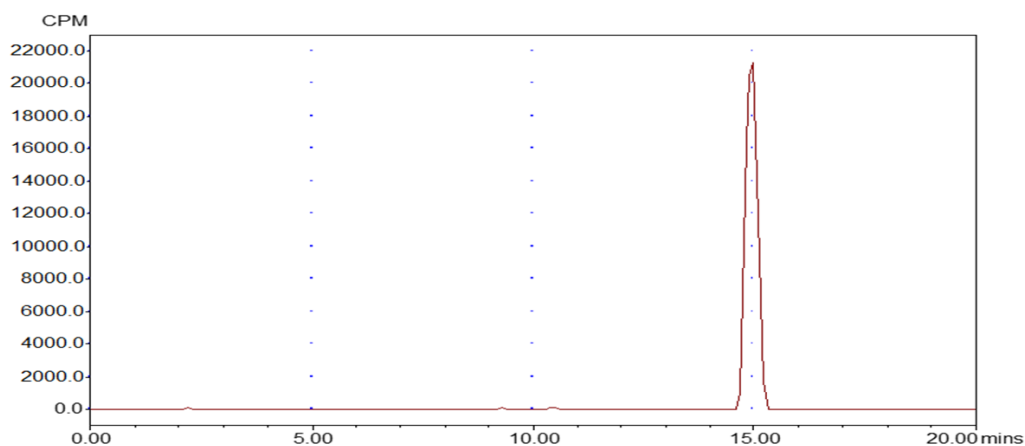Tel: 86 510 85514482 Ext. 3529
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Fig. S1 The high resolution mass spectrum of bisaminodithiol-propyl-dihydrotetrabenazine (**8**). HRMS (ESI-TOF): m/z [M + H]$^+$ calcd for $C_{27}H_{48}N_3O_3S_2^+$ 526.3137; found 526.3109.

Fig. S2 The hydrogen NMR spectrum of bisaminodithiol-propyl-dihydrotetrabenazine (**8**). ^{1}H NMR(CD$_3$OD, 400 MHz), δ: 6.98 ~ 6.84 (m, 2H), 4.49 ~ 4.46 (br. d, 1H), 4.20 (br. s, 2H), 3.90 ~ 3.85 (m, 5H), 3.83 ~ 3.55 (m, 11H), 3.45 ~ 3.36 (m, 4H), 3.05 ~ 2.89 (m, 4H), 2.46 ~ 2.27 (m, 2H), 2.14 ~ 1.89 (m, 2H), 1.83 ~ 1.69 (m, 3H), 1.21 ~ 1.14 (m, 2H), 1.01 (d, J = 5.95 Hz, 3H), 0.98 (d, J = 5.93 Hz, 3H).

Fig. S3 The chromatogram of ^{99m}Tc-BAT-P-DTBZ.

Table S1 The reaction parameters of technetium-99m radiolabelling.

Test	Reaction temperature (°C)	Reaction time (min)	EDTA-2Na (mg)	GH (mg)	pH	Labelling precursor (µg)	SnCl$_2$·2H$_2$O (µg)
1	70	5 ~ 30	1	10	7.2	100	50
2	85	5 ~ 30	1	10	7.2	100	50
3	100	5 ~ 30	1	10	7.2	100	50
4	100	30	0.2 ~ 2	10	7.2	100	50
5	100	30	1	1 ~ 25	7.2	100	50
6	100	30	1	10	2 ~ 9	100	50
7	100	30	1	10	7.2	10 ~ 200	50
8	100	30	1	10	7.2	50	10 ~ 100

Table S2 The organic liquid-water partition coefficient of ^{99m}Tc-BAT-P-DTBZ.

Organic phase (CPM)	Water Phase (CPM)	Distribution ratio	Log$P_{7.0}$	Organic phase (CPM)	Water Phase (CPM)	Distribution ratio	Log$P_{7.4}$
4791730	187080	25.61	1.41	5576742	242781	22.97	1.36
1630165	33745	48.31	1.68	1885773	39461	47.79	1.68
549780	10219	53.80	1.73	644192	13510	47.68	1.68
181379	3946	45.97	1.66	215670	4325	49.87	1.70