Electronic Supplementary Information for New Journal of Chemistry

Synthesis and Preliminary Evaluation of a ^{99m}Tc Labelled deoxyglucose Complex {[^{99m}Tc]DTPA-bis(DG)} as a Potential SPECT Based Probe for Tumor Imaging

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1. **Figure S1.** ^{1}H-NMR spectrum of 1-Azido-1-deoxy-β-D-glucopyranoside tetraacetate, **2**.
2. **Figure S2.** ^{13}C-NMR spectrum of 1-Azido-1-deoxy-β-D-glucopyranoside tetraacetate, **2**.
3. **Figure S3.** ESI-MS spectrum of 1-Azido-1-deoxy-β-D-glucopyranoside tetraacetate, **2.**
4. **Figure S4.** ^{1}H-NMR spectrum of (2R,3R,4S,5R,6R)-2-(acetoxymethyl)-6-(4-(aminomethyl)-1H-1,2,3-triazol-1-yl)tetrahydro-2H-pyran-3,4,5-triyl triacetate, **3**.
5. **Figure S5.** ^{13}C-NMR spectrum of (2R,3R,4S,5R,6R)-2-(acetoxymethyl)-6-(4-(aminomethyl)-1H-1,2,3-triazol-1-yl)tetrahydro-2H-pyran-3,4,5-triyl triacetate, **3**.
6. **Figure S6.** ESI-MS spectrum of (2R,3R,4S,5R,6R)-2-(acetoxymethyl)-6-(4-(aminomethyl)-1H-1,2,3-triazol-1-yl)tetrahydro-2H-pyran-3,4,5-triyl triacetate, **3**.
7. **Figure S7.** ^{1}H-NMR spectrum of (2R,3R,4S,5S,6R)-2-(4-(aminomethyl)-1H-1,2,3-triazol-1-yl)-6-(hydroxymethyl)tetrahydro-2H-pyran-3,4,5-triol, **4**.
8. **Figure S8.** ^{13}C-NMR spectrum of (2R,3R,4S,5S,6R)-2-(4-(aminomethyl)-1H-1,2,3-triazol-1-yl)-6-(hydroxymethyl)tetrahydro-2H-pyran-3,4,5-triol, **4**.
9. **Figure S9.** ESI-MS spectrum of (2R,3R,4S,5S,6R)-2-(4-(aminomethyl)-1H-1,2,3-triazol-1-yl)-6-(hydroxymethyl)tetrahydro-2H-pyran-3,4,5-triol, **4**.
10. **Figure S10.** ^{1}H-NMR spectrum of 5,8-bis(carboxymethyl)-3-oxo-11-(2-oxo-2-(((1-((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazol-4-yl)methyl)amino)ethyl)-1-(1-((2S,3S,4R,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazol-4-yl)-2,5,8,11-tetraazatridecan-13-oic acid, **5**.
11. **Figure S11.** ^{13}C-NMR spectrum of 5,8-bis(carboxymethyl)-3-oxo-11-(2-oxo-2-(((1-((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazol-4-yl)methyl)amino)ethyl)-1-(1-((2S,3S,4R,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazol-4-yl)-2,5,8,11-tetraazatridecan-13-oic acid, **5**.

12. **Figure S12.** ESI-MS spectrum of 5,8-bis(carboxymethyl)-3-oxo-11-(2-oxo-2-(((1-((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazol-4-yl)methyl)amino)ethyl)-1-(1-((2S,3S,4R,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazol-4-yl)-2,5,8,11-tetraazatridecan-13-oic acid, **5**.
13. **Figure S13.** HR-MS spectrum of 5,8-bis(carboxymethyl)-3-oxo-11-(2-oxo-2-(((1-((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazol-4-yl)methyl)amino)ethyl)-1-(1-((2S,3S,4R,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazol-4-yl)-2,5,8,11-tetraazatridecan-13-oic acid, **5**.
14. **Figure S14**. Radiolabelling efficiency of DTPA-bis-(DG) with Tc-99m as a function of time.
15. **Figure S15**. Human Serum Stability study of ^{99m}Tc-DTPA-bis-(DG).

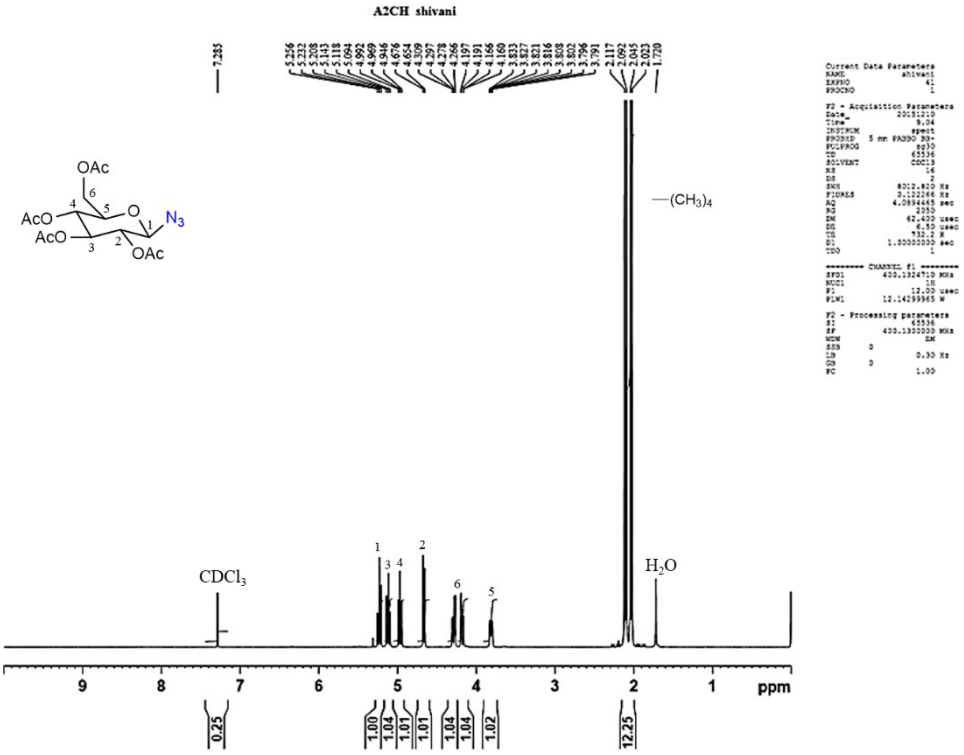


Figure S1. [1]H-NMR spectrum of 1-Azido-1-deoxy-β-D-glucopyranoside tetraacetate, **2**.

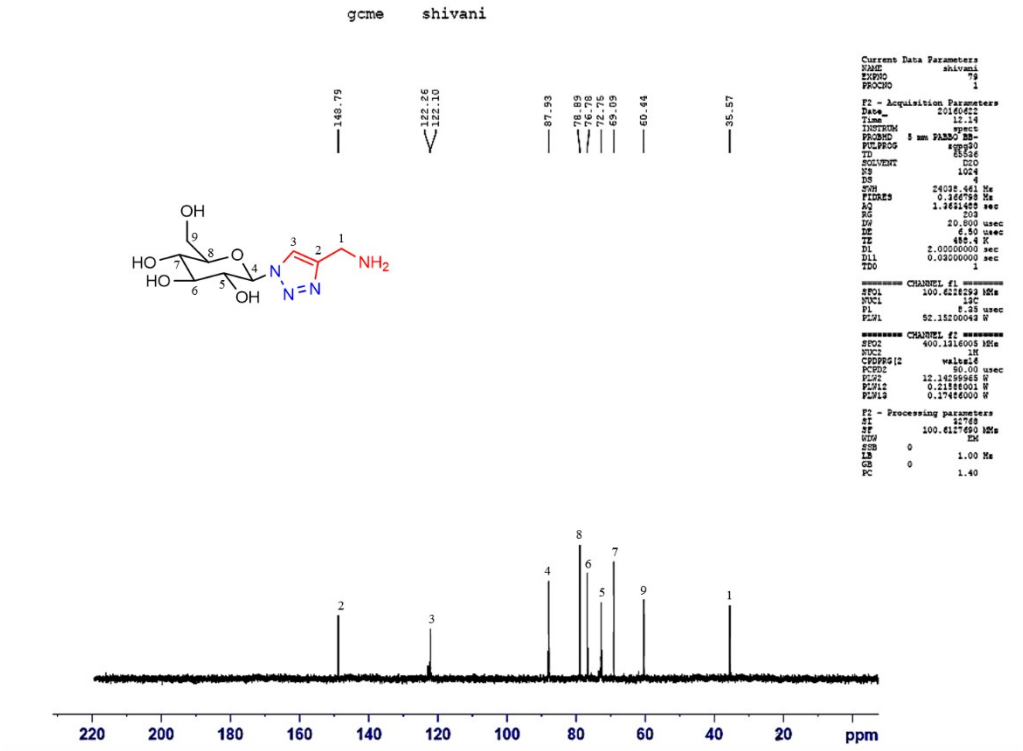


Figure S2. ^{13}C-NMR spectrum of 1-Azido-1-deoxy-β-D-glucopyranoside tetraacetate, **2**.

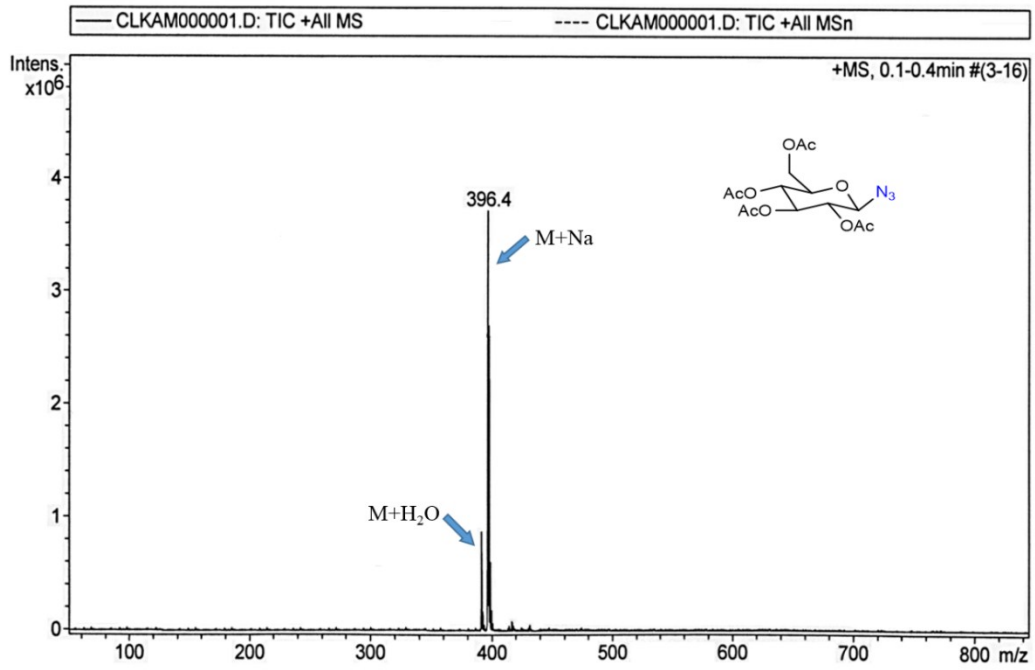


Figure S3. ESI-MS spectrum of 1-Azido-1-deoxy-β-D-glucopyranoside tetraacetate, **2**.

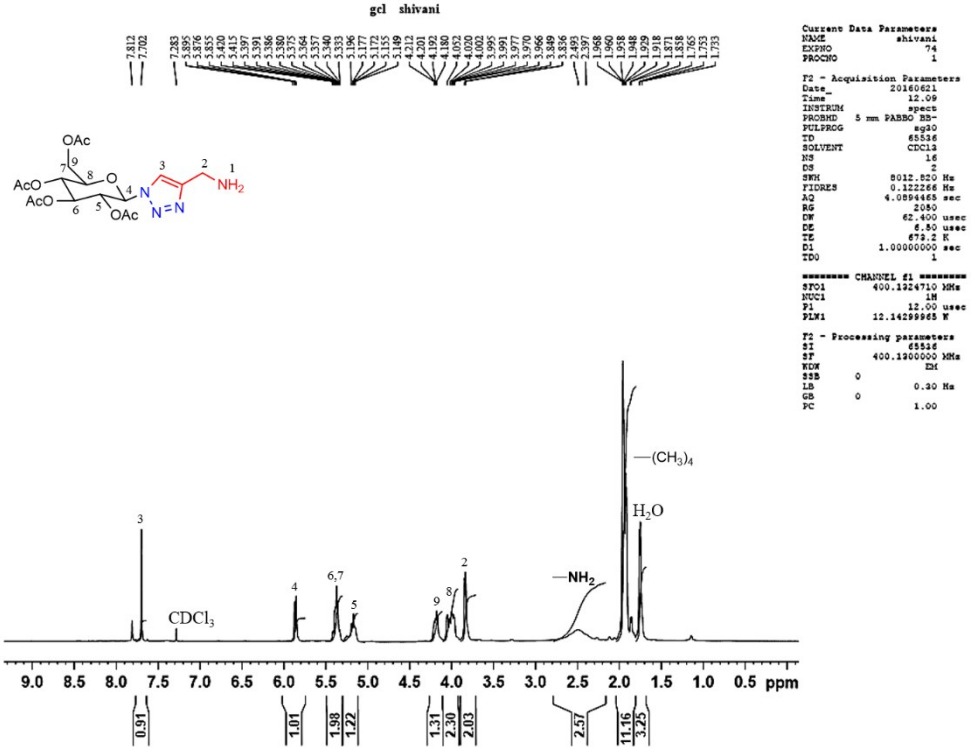


Figure S4. ^{1}H-NMR spectrum of (2R,3R,4S,5R,6R)-2-(acetoxymethyl)-6-(4-(aminomethyl)-1H-1,2,3-triazol-1-yl)tetrahydro-2H-pyran-3,4,5-triyl triacetate, **3**.

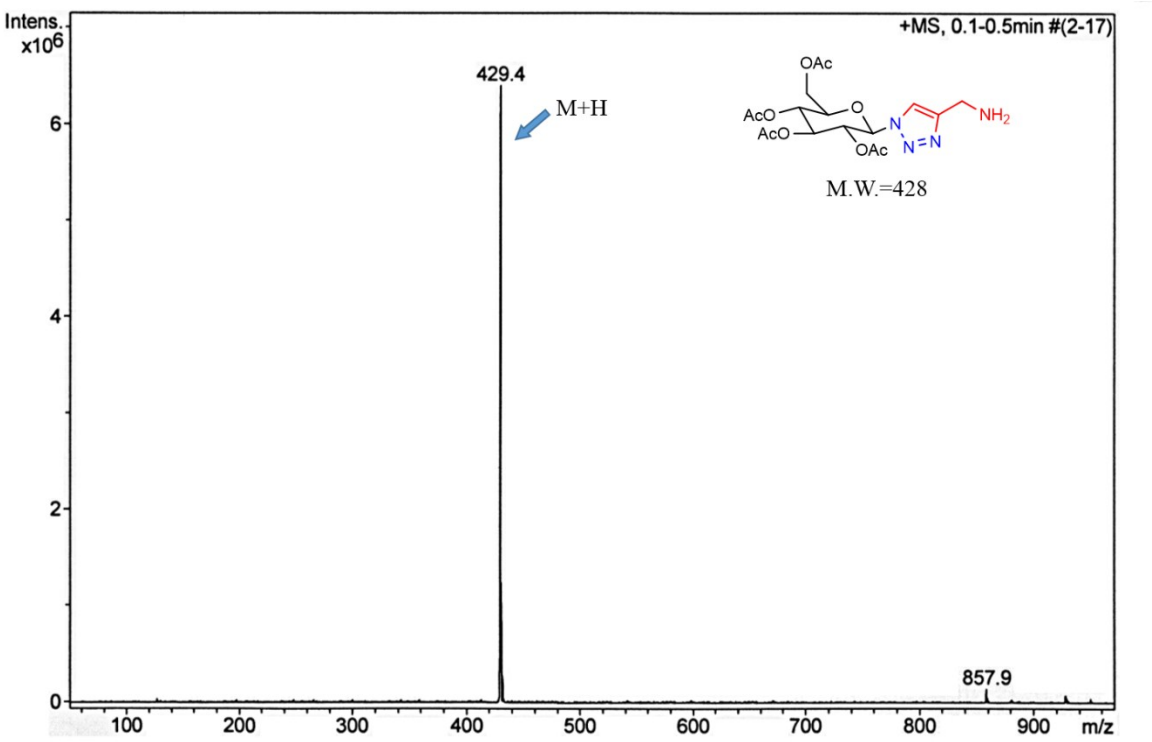


Figure S6. ESI-MS spectrum of (2R,3R,4S,5R,6R)-2-(acetoxymethyl)-6-(4-(aminomethyl)-1H-1,2,3-triazol-1-yl)tetrahydro-2H-pyran-3,4,5-triyl triacetate, **3**.

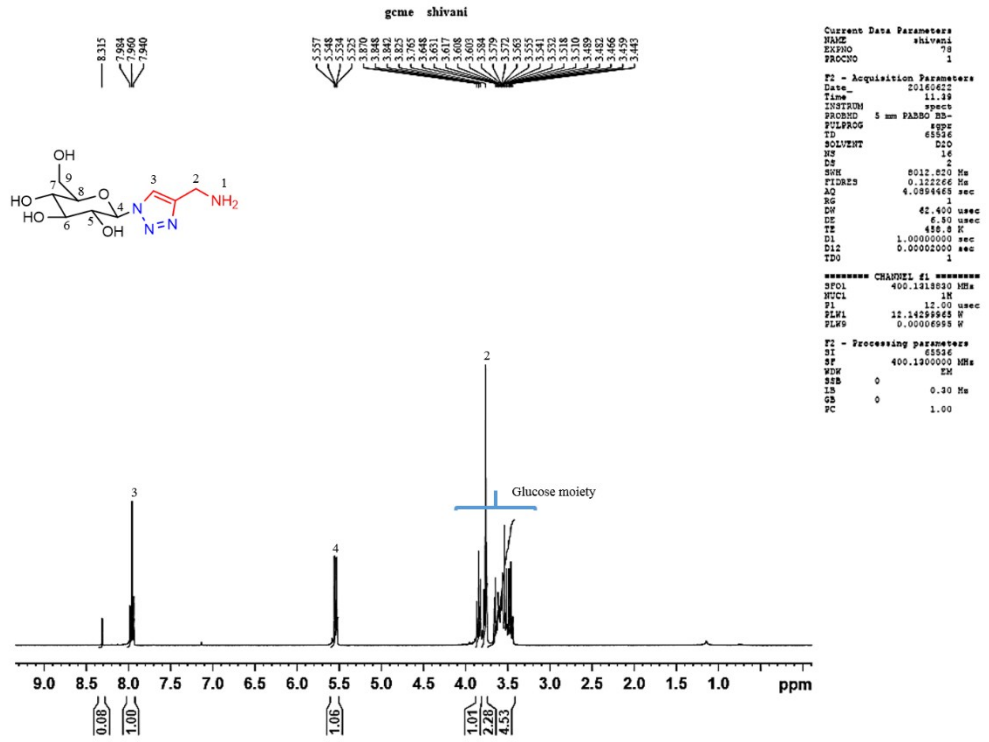


Figure S7. [1]H-NMR spectrum of (2R,3R,4S,5S,6R)-2-(4-(aminomethyl)-1H-1,2,3-triazol-1-yl)-6-(hydroxymethyl)tetrahydro-2H-pyran-3,4,5-triol, **4**.

Figure S8. [13]C-NMR spectrum of (2R,3R,4S,5S,6R)-2-(4-(aminomethyl)-1H-1,2,3-triazol-1-yl)-6-(hydroxymethyl)tetrahydro-2H-pyran-3,4,5-triol, **4**.

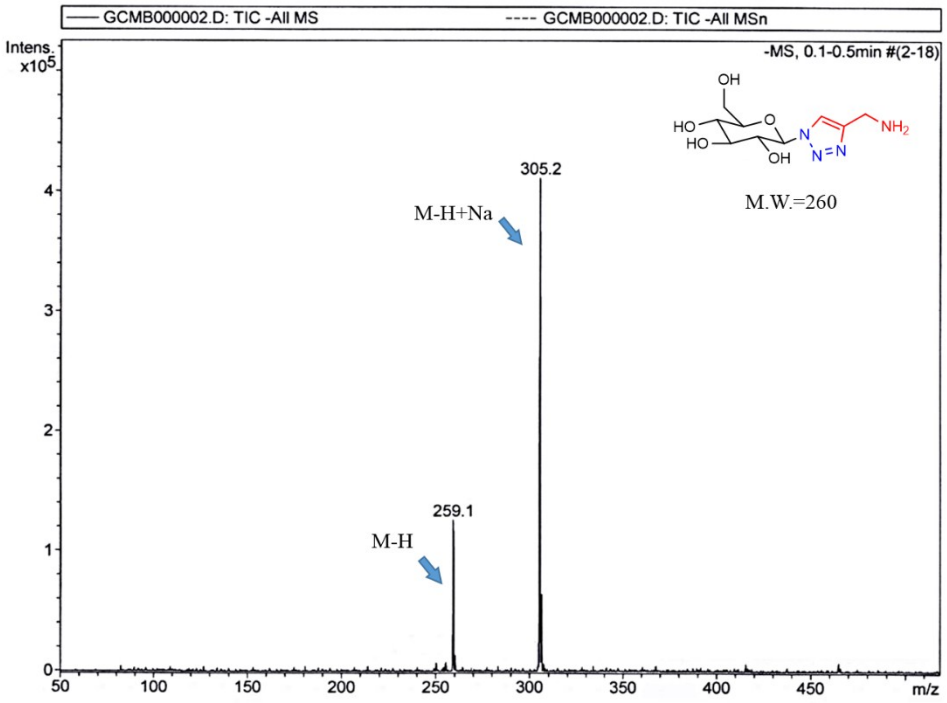


Figure S9. ESI-MS spectrum of (2R,3R,4S,5S,6R)-2-(4-(aminomethyl)-1H-1,2,3-triazol-1-yl)-6-(hydroxymethyl)tetrahydro-2H-pyran-3,4,5-triol, **4**.

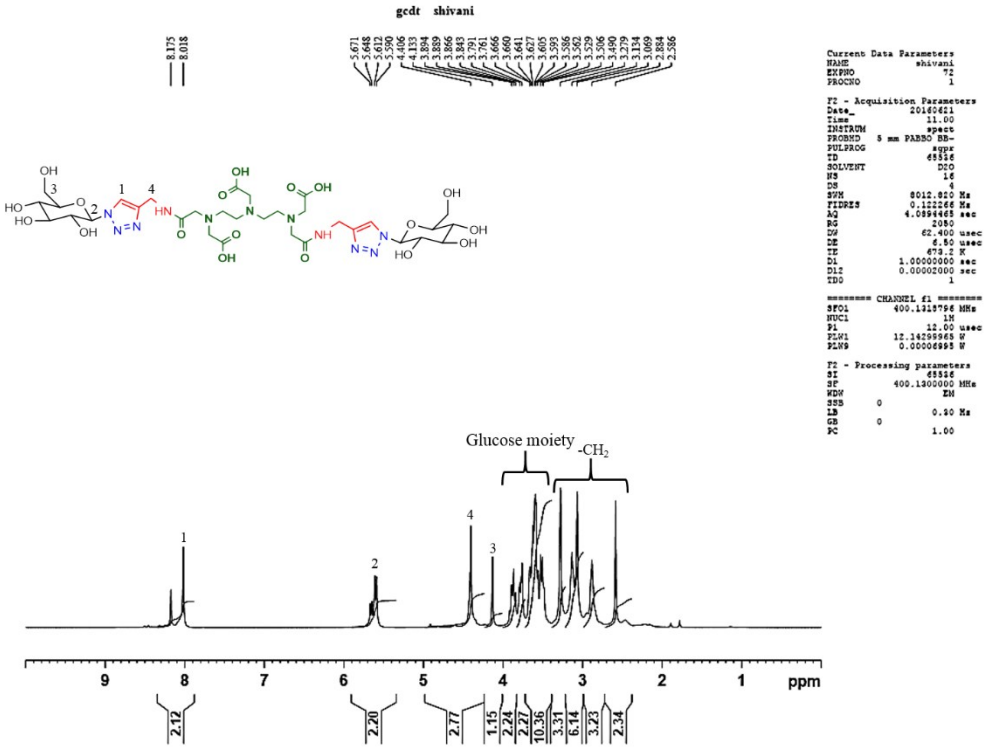


Figure S10. ^{1}H-NMR spectrum of 5,8-bis(carboxymethyl)-3-oxo-11-(2-oxo-2-(((1-((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazol-4-yl)methyl)amino)ethyl)-1-(1-((2S,3S,4R,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazol-4-yl)-2,5,8,11-tetraazatridecan-13-oic acid, **5**.

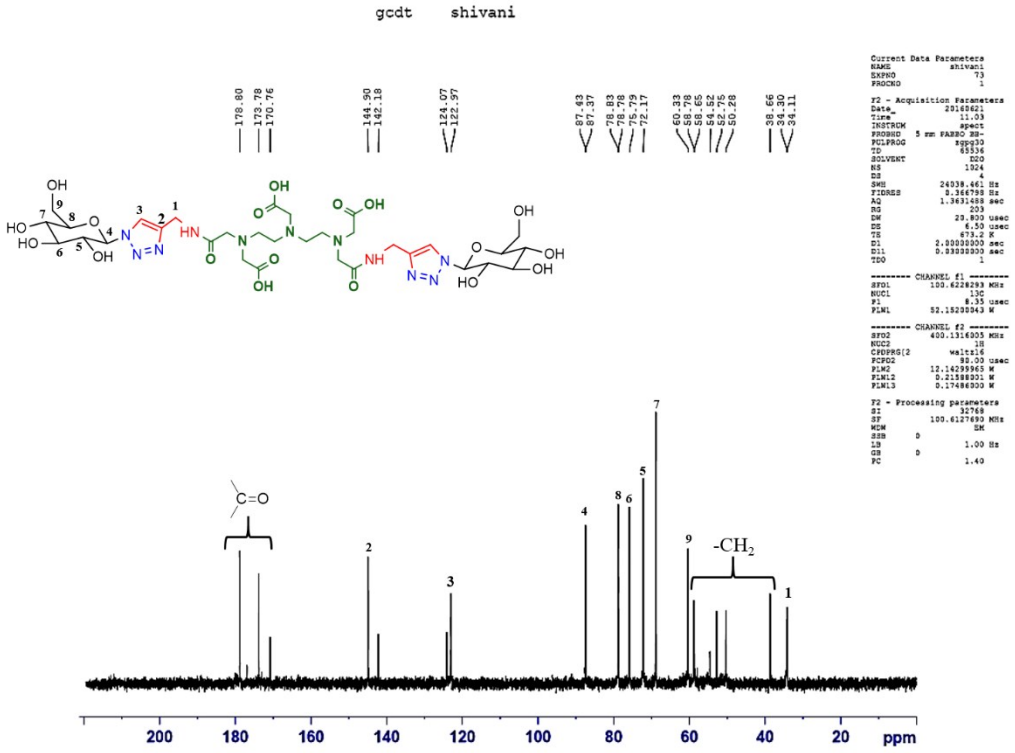


Figure S11. ^{13}C-NMR spectrum of 5,8-bis(carboxymethyl)-3-oxo-11-(2-oxo-2-(((1-((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazol-4-yl)methyl)amino)ethyl)-1-(1-((2S,3S,4R,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazol-4-yl)-2,5,8,11-tetraazatridecan-13-oic acid, **5**.

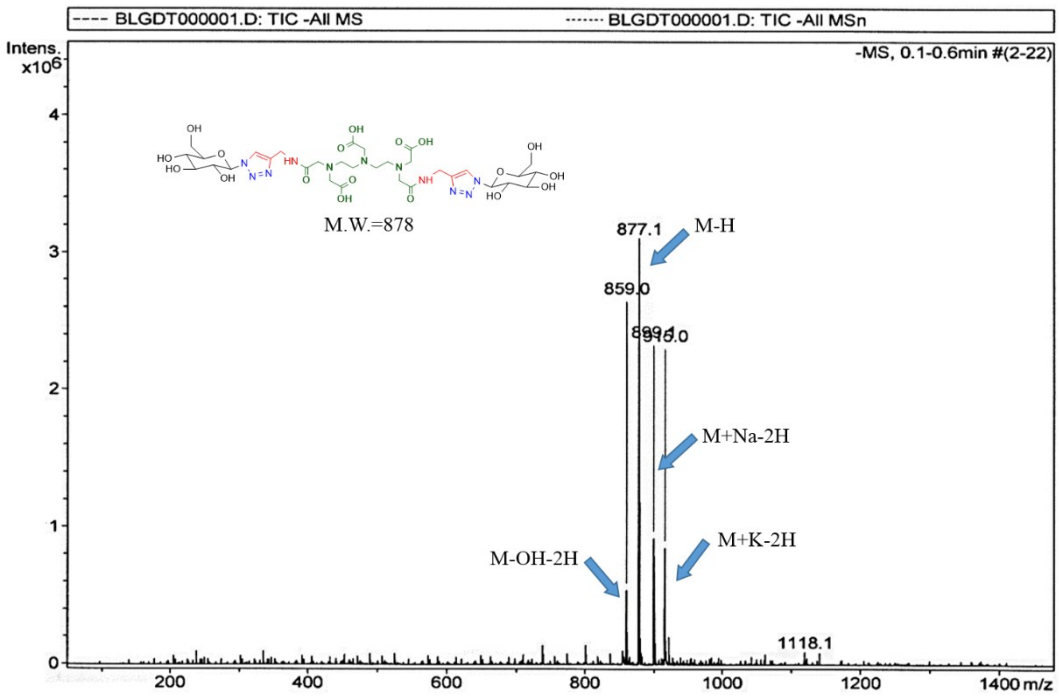


Figure S12. ESI-MS spectrum of 5,8-bis(carboxymethyl)-3-oxo-11-(2-oxo-2-(((1-((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazol-4-yl)methyl)amino)ethyl)-1-(1-((2S,3S,4R,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazol-4-yl)-2,5,8,11-tetraazatridecan-13-oic acid, **5**.

Qualitative Compound Report

Data File	GLDT.d	**Sample Name**	GLDT
Sample Type	Sample	**Position**	P1-B6
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	13-08-2018 12:04:00
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

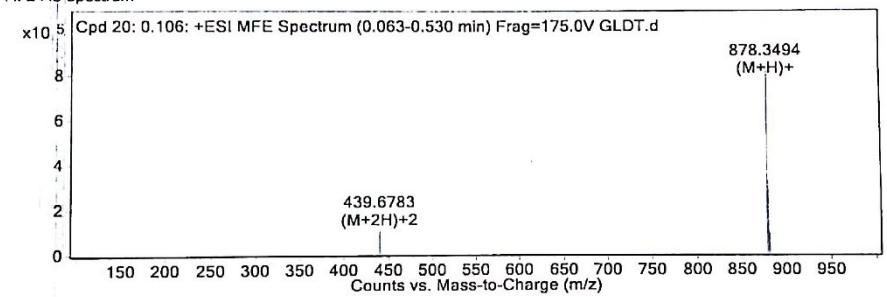
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

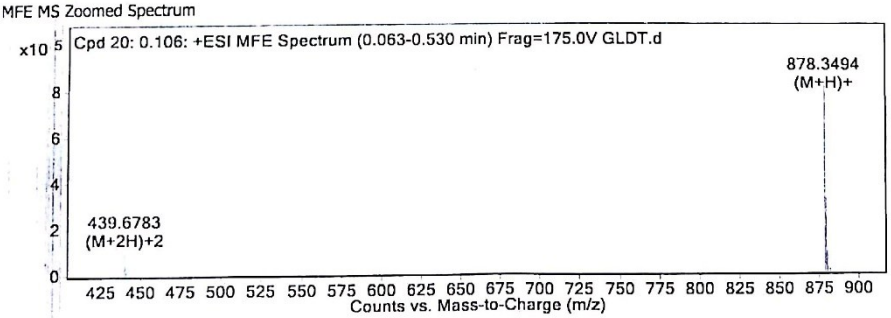
Compound Label	RT	Mass	MFG Formula
Cpd 20: 0.106	0.106	877.3421	> limit

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 20: 0.106	878.3494	0.106	Find by Molecular Feature	877.3421

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Ion
439.6783	2	106708.02	(M+2H)+2
440.1794	2	43974.38	(M+2H)+2
440.6807	2	12759.9	(M+2H)+2
441.1827	2	3343.35	(M+2H)+2
878.3494	1	817153.88	(M+H)+
879.3517	1	325865.91	(M+H)+

Figure S13. HR-MS spectrum of 5,8-bis(carboxymethyl)-3-oxo-11-(2-oxo-2-(((1-((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazol-4-yl)methyl)amino)ethyl)-1-(1-((2S,3S,4R,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazol-4-yl)-2,5,8,11-tetraazatridecan-13-oic acid, **5**.

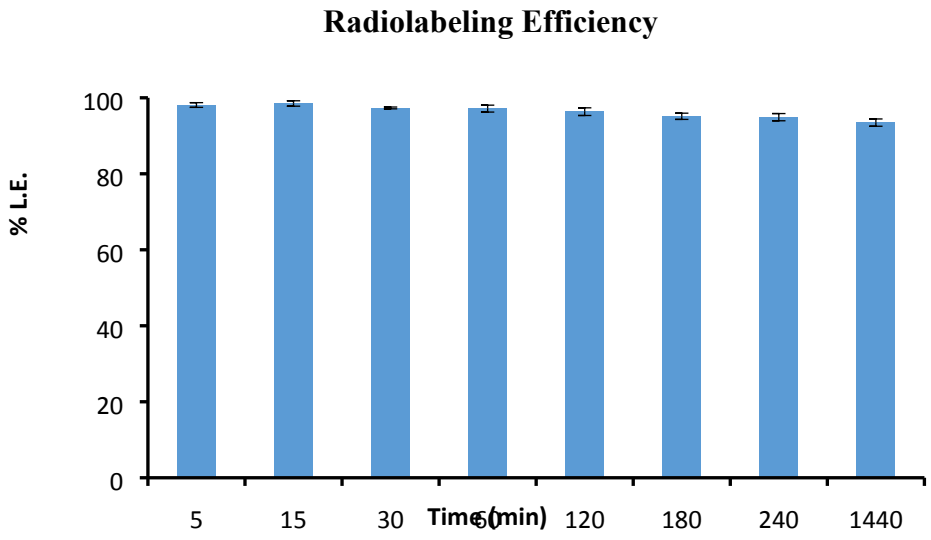


Figure S14. Radiolabelling efficiency of DTPA-bis-(DG) with Tc-99m as a function of time.

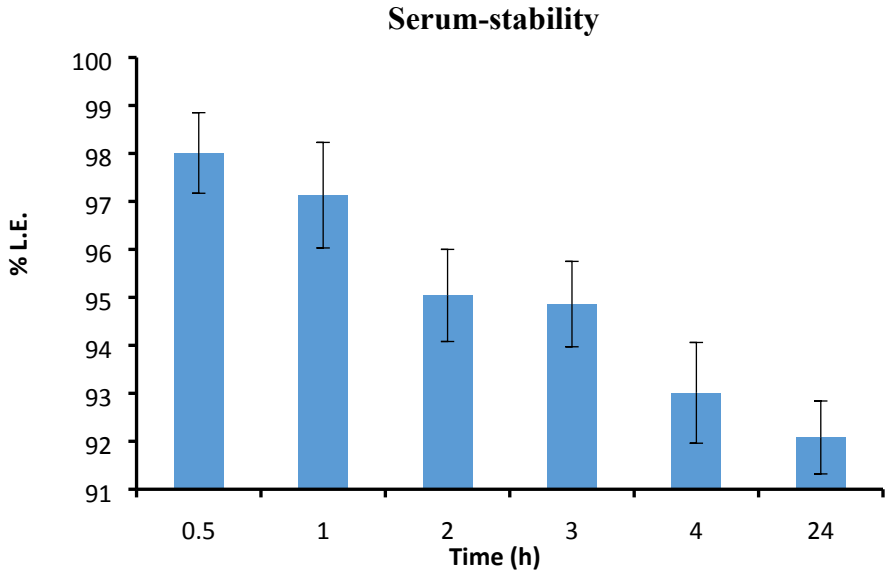


Figure S15. Human Serum Stability study of ^{99m}Tc-DTPA-bis-(DG).