

## Supplemental Information

*Article*

# Development and Preclinical Evaluation of [<sup>68</sup>Ga]BMSH as a New Potent Positron Emission Tomography Tracer for Imaging Programmed Death-Ligand 1 Expression

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## 1. Characterization.

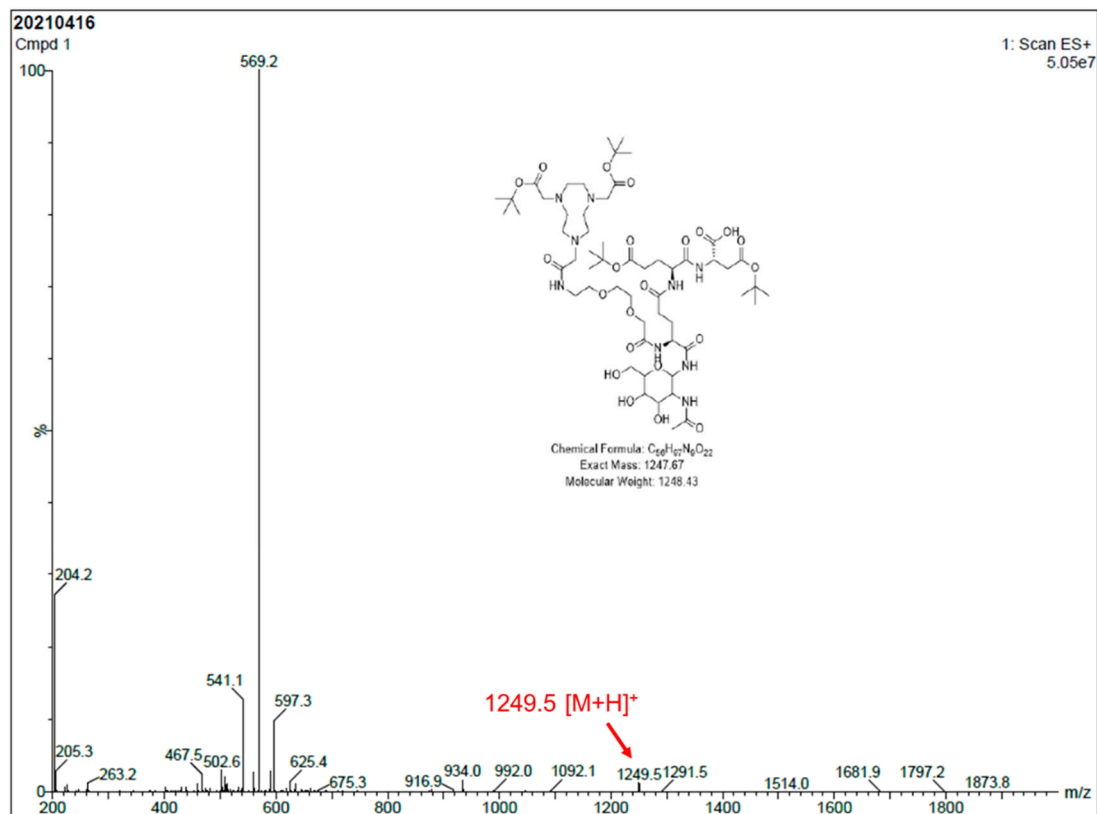


Figure S1. ESI-MS spectrum of compound 1.

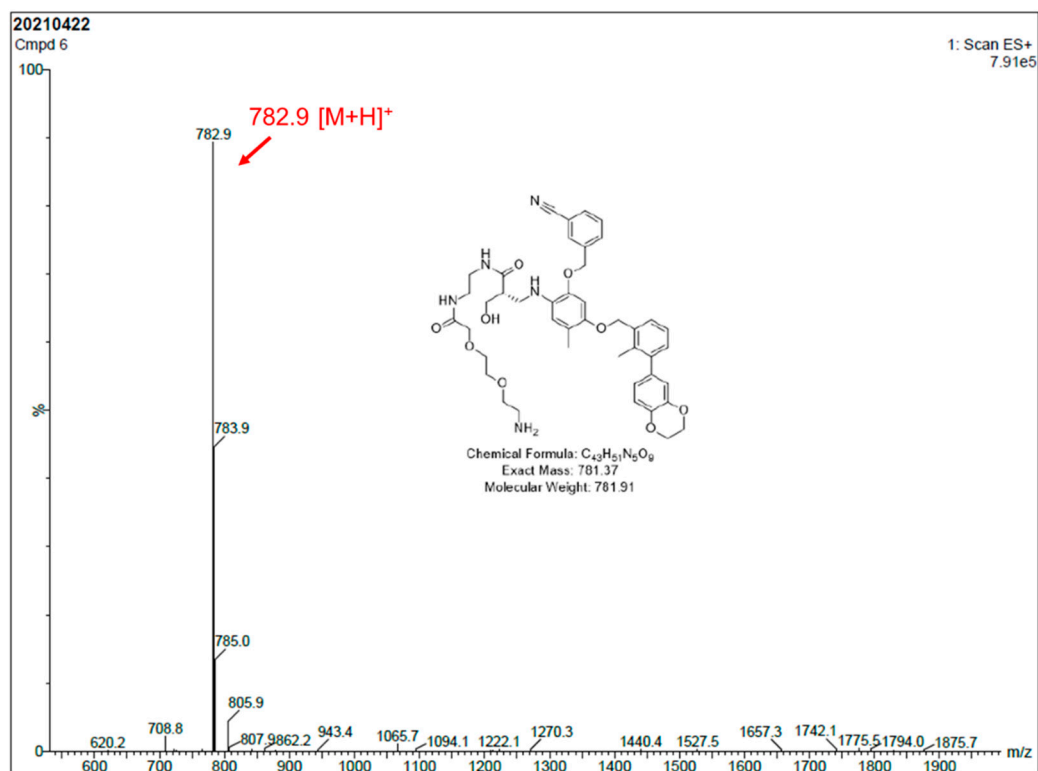
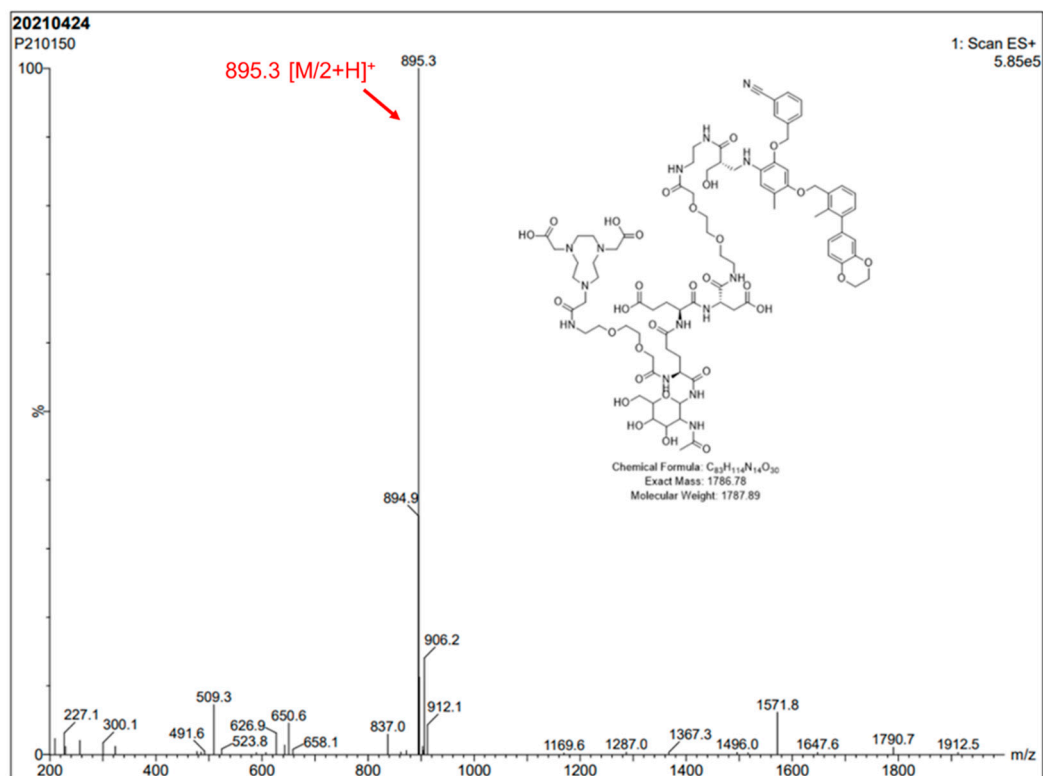
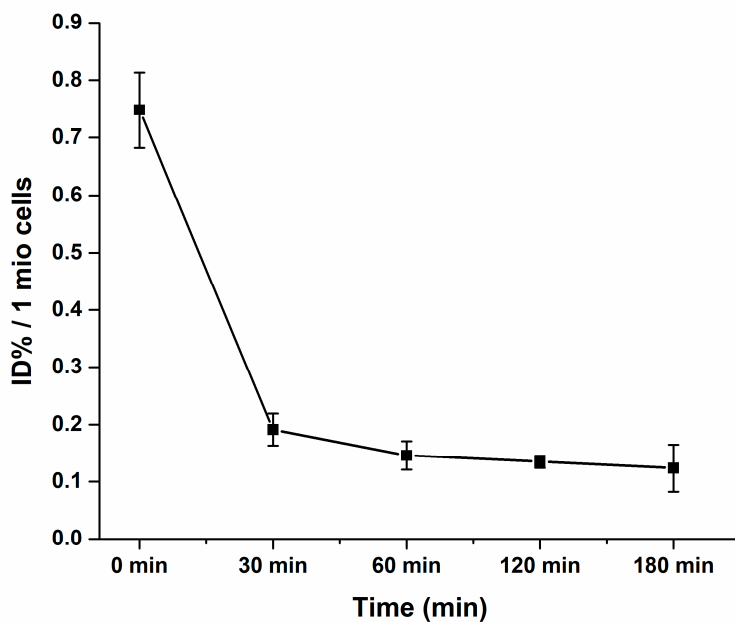


Figure S2. ESI-MS spectrum of compound 6.



**Figure S3.** ESI-MS spectrum of NOTA-BMSH

## 2. Cell study



**Figure S4.** Efflux kinetics of [<sup>68</sup>Ga]BMSH after incubation of A549-hPDL1 cells with radiolabeled compounds for 60 min followed by incubation with a compound-free medium for 0–180 min.

### 3. Estimated human dosimetry of [ $^{68}\text{Ga}$ ]BMSH.

Table S1. Estimated human dosimetry data of [ $^{68}\text{Ga}$ ]BMSH in mSv/MBq(male).

Target Organ	Total	EDE Cont.	ED Cont.
Adrenals	1.36E-02	0.00E00	1.26E-04
Brain	1.48E-03	0.00E00	1.48E-05
Esophagus	3.34E-03	0.00E00	1.34E-04
Eyes	1.97E-04	0.00E00	0.00E00
Gallbladder Wall	3.65E-03	0.00E00	3.37E-05
Left colon	2.39E-03	0.00E00	1.16E-04
Small Intestine	1.93E-02	1.16E-03	1.78E-04
Stomach Wall	3.37E-03	0.00E00	4.05E-04
Right colon	1.70E-03	0.00E00	8.22E-05
Rectum	6.02E-04	0.00E00	1.39E-05
Heart Wall	2.53E-02	1.52E-03	2.33E-04
Kidneys	1.22E-01	7.31E-03	1.12E-03
Liver	1.75E-02	1.05E-03	6.99E-04
Lungs	3.52E-02	4.23E-03	4.23E-03
Pancreas	2.97E-03	0.00E00	2.74E-05
Prostate	5.35E-04	0.00E00	2.47E-06
Salivary Glands	2.74E-04	0.00E00	2.74E-06
Red Marrow	3.43E-03	4.12E-04	4.12E-04
Osteogenic Cells	3.26E-03	9.79E-05	3.26E-05
Spleen	8.45E-02	5.07E-03	7.80E-04
Testes	7.35E-05	1.84E-05	2.94E-06
Thymus	3.03E-03	0.00E00	2.79E-05
Thyroid	1.39E-03	4.17E-05	5.55E-05
Urinary Bladder Wall	2.92E-04	0.00E00	1.17E-05
Total Body	2.71E-03	0.00E00	0.00E00
Effective Dose		2.09E-02	8.74E-03