Electronic supplementary data

for

^{68}Ga based Probe for Alzheimer's Disease: Synthesis and Preclinical Evaluation of Homodimeric Chalcone in β-Amyloid Imaging

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16. **Figure S16.** ^{1}H NMR spectrum of 5,8-bis(carboxymethyl)-13-(4-((*E*)-3-(4-(dimethylamino)phenyl)acryloyl)phenoxy)-2-(2-(2-(4-((*E*)-3-(4-(dimethylamino)phenyl)acryloyl)phenoxy)ethylamino)-2-oxoethyl)-10-oxo-2,5,8,11-tetraazatridecane-1-carboxylic acid Gallium-(III), **[$^{69/71}$Ga-]** Ch_2DT.

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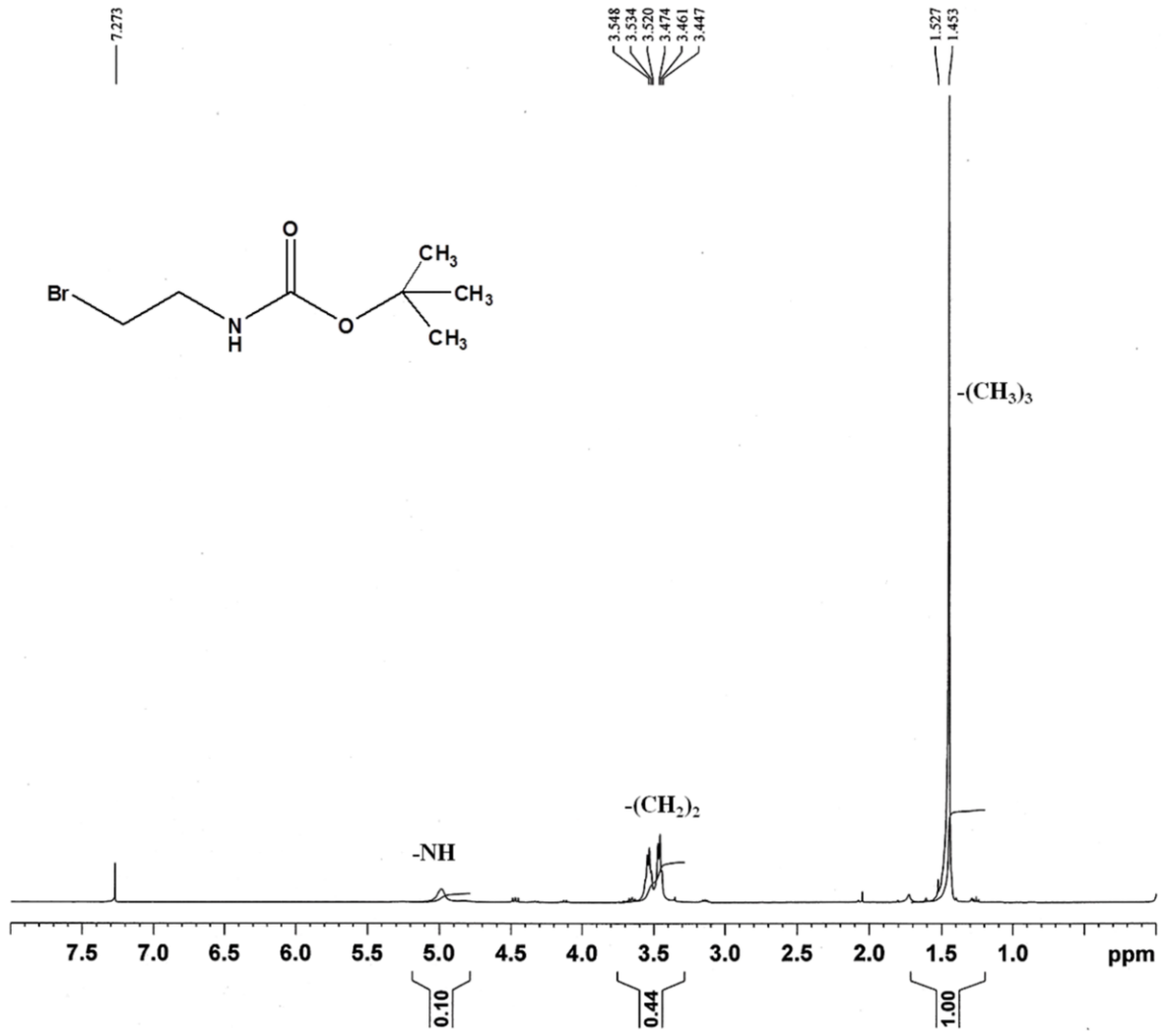


Figure S1. 1H- NMR of *tert*-Butyl 2-bromoethylcarbamate, **1**.

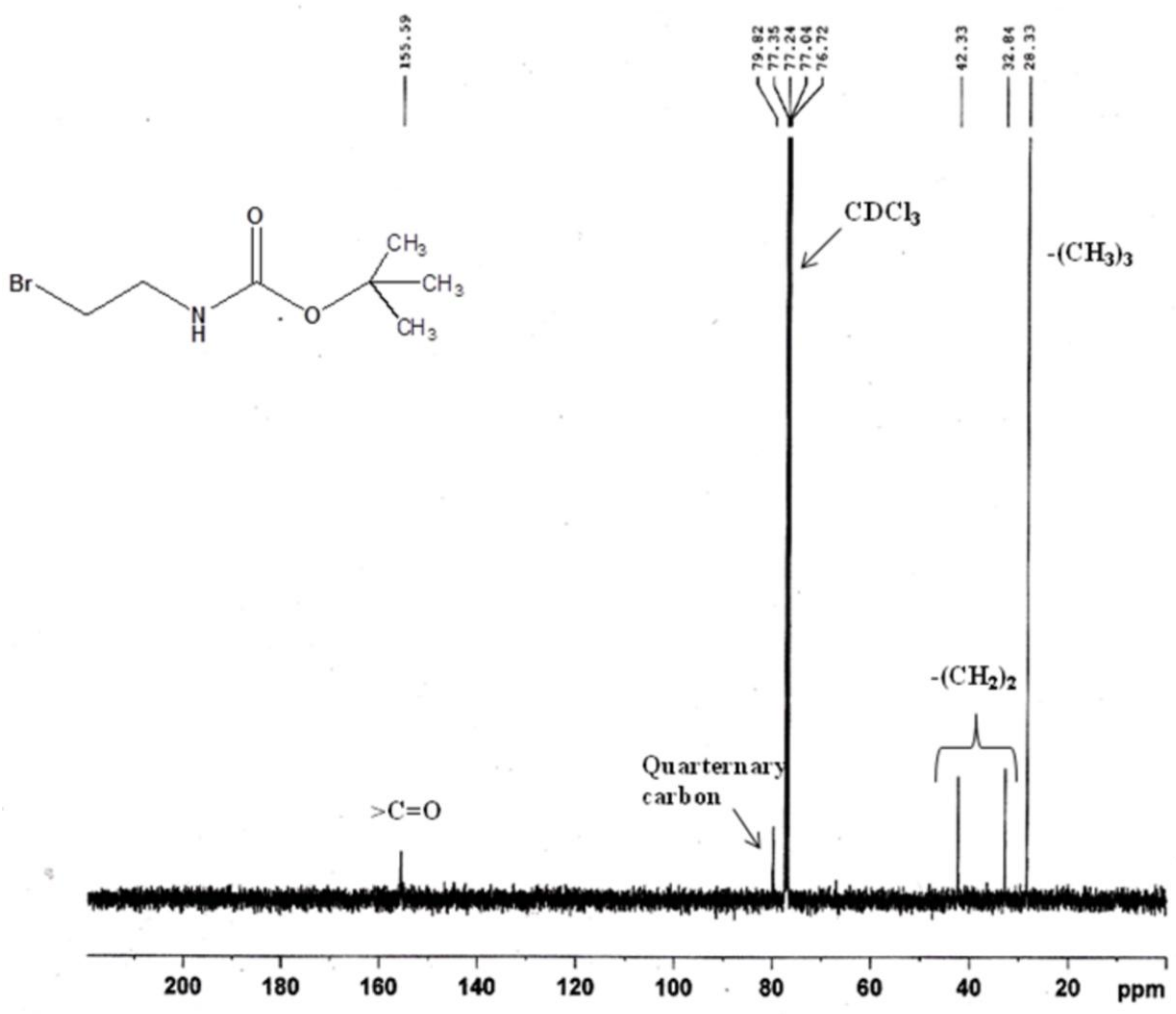


Figure S2. ^{13}C NMR spectrum of *tert*-Butyl 2-bromoethylcarbamate, **1**

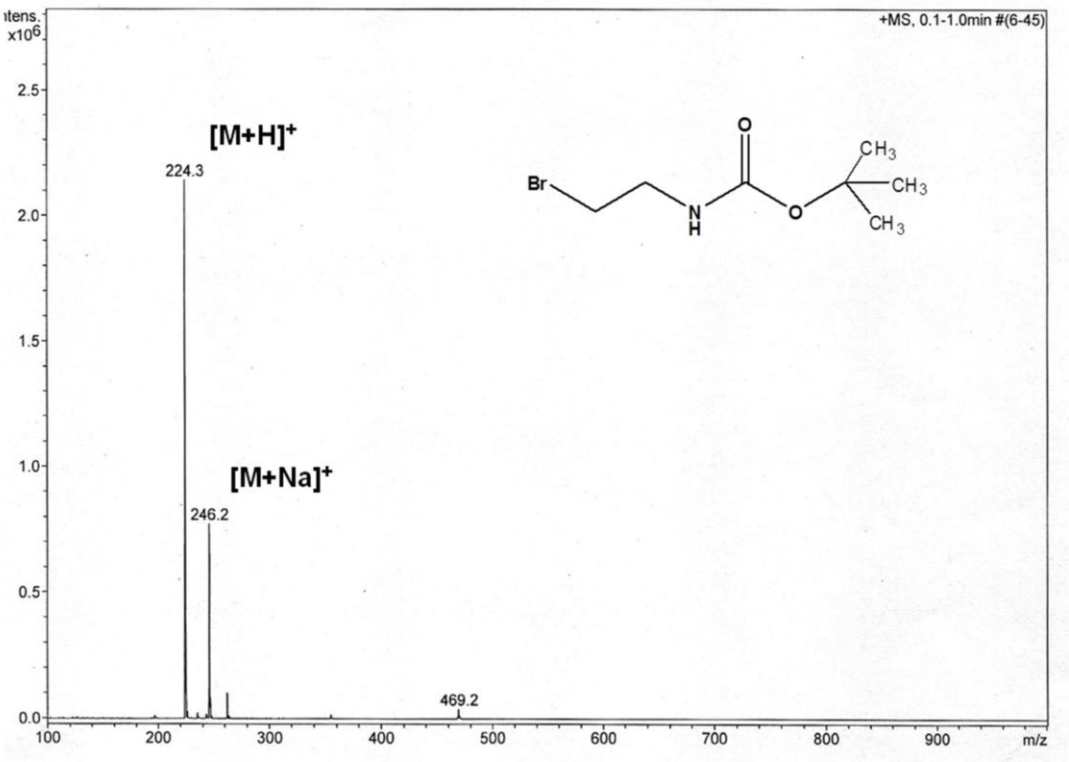


Figure S3. ESI-MS spectrum of *tert*-Butyl 2-bromoethylcarbamate, **1**.

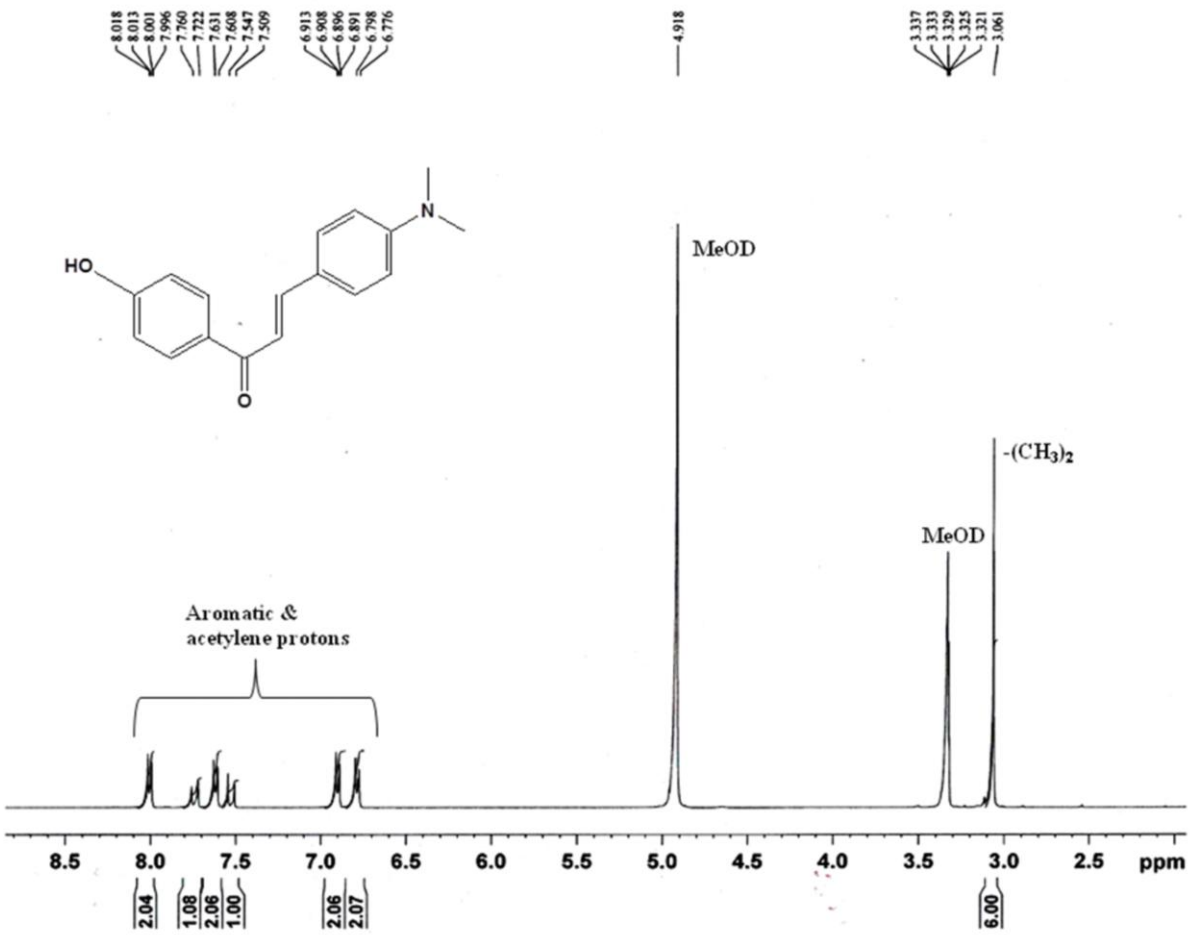


Figure S4. ^{1}H NMR spectrum of (*E*)-1-(4-hydroxyphenyl)-3-(4-isopropylphenyl)prop-2-en-1-one, **2**.

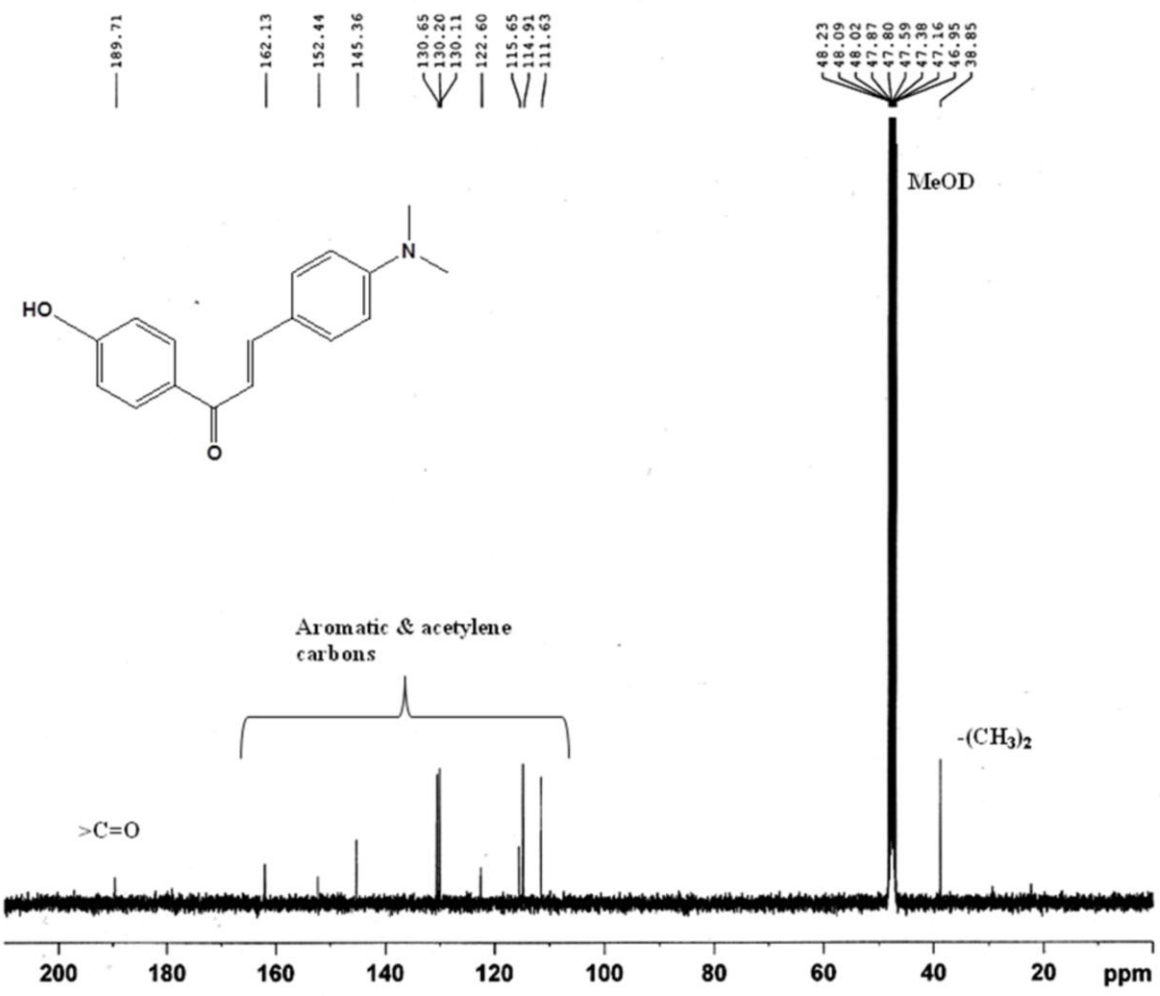


Figure S5. ^{13}C NMR spectrum of (*E*)-1-(4-hydroxyphenyl)-3-(4-isopropylphenyl)prop-2-en-1-one, **2**.

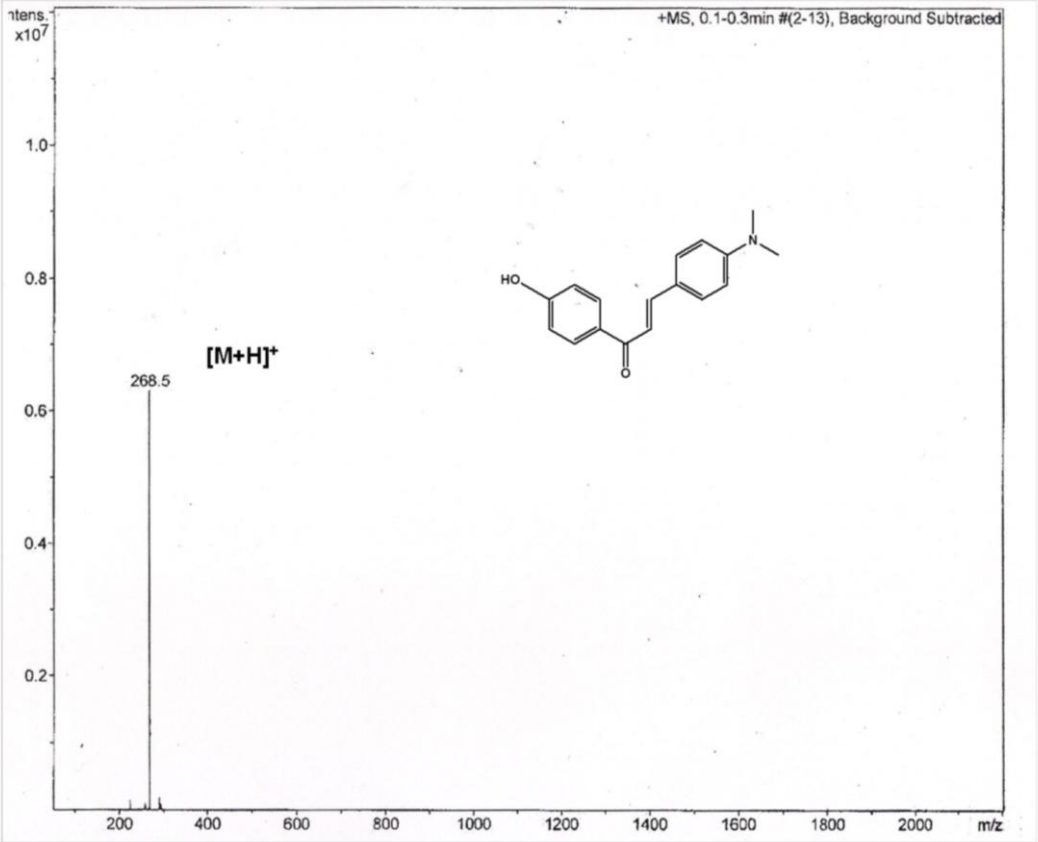


Figure S6. ESI-MS spectrum of (*E*)-1-(4-hydroxyphenyl)-3-(4-isopropylphenyl)prop-2-en-1-one, **2**.

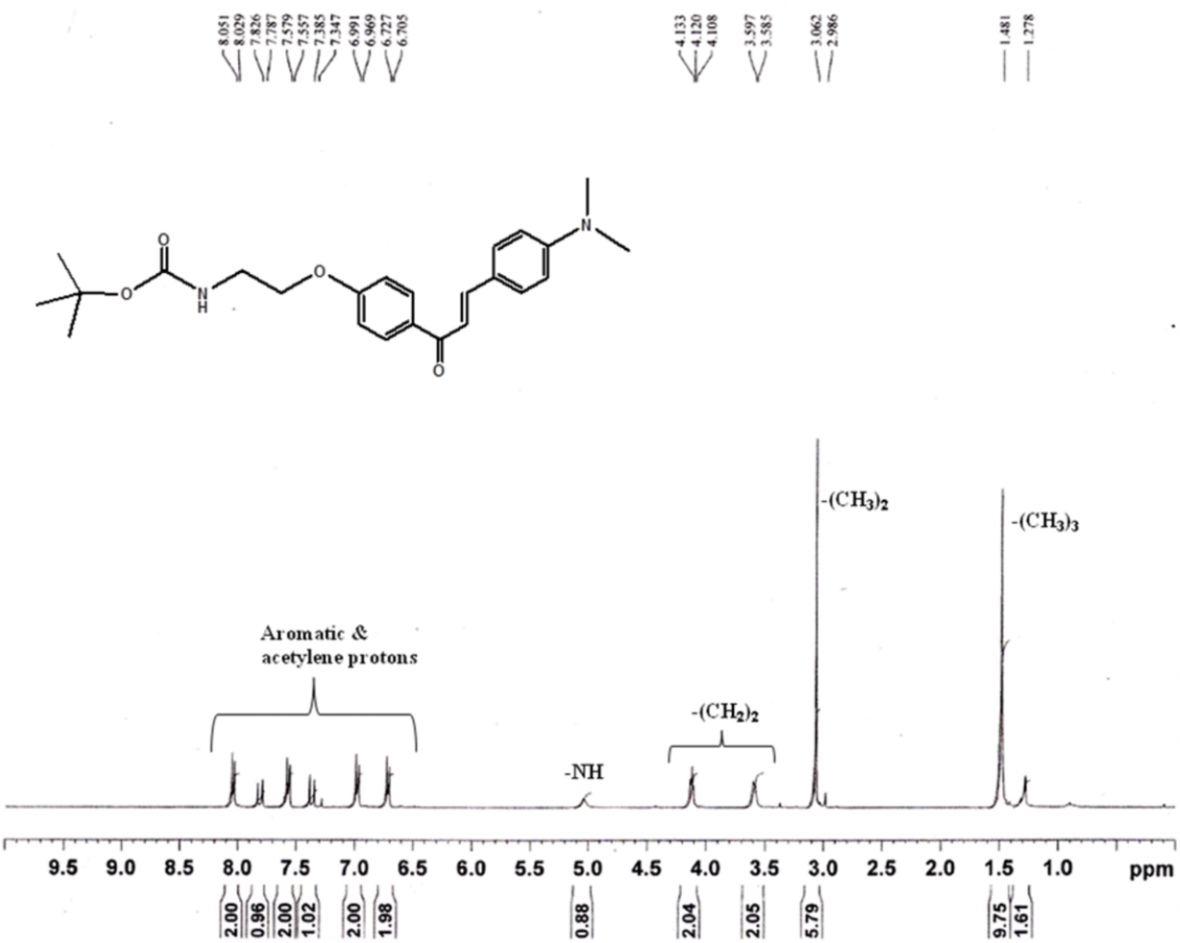


Figure S7. ^{1}H NMR spectrum of (*E*)-tert-butyl 2-(4-(3-(4-(dimethylamino)phenyl)acryloyl)phenoxy)ethylcarbamate, **3**.

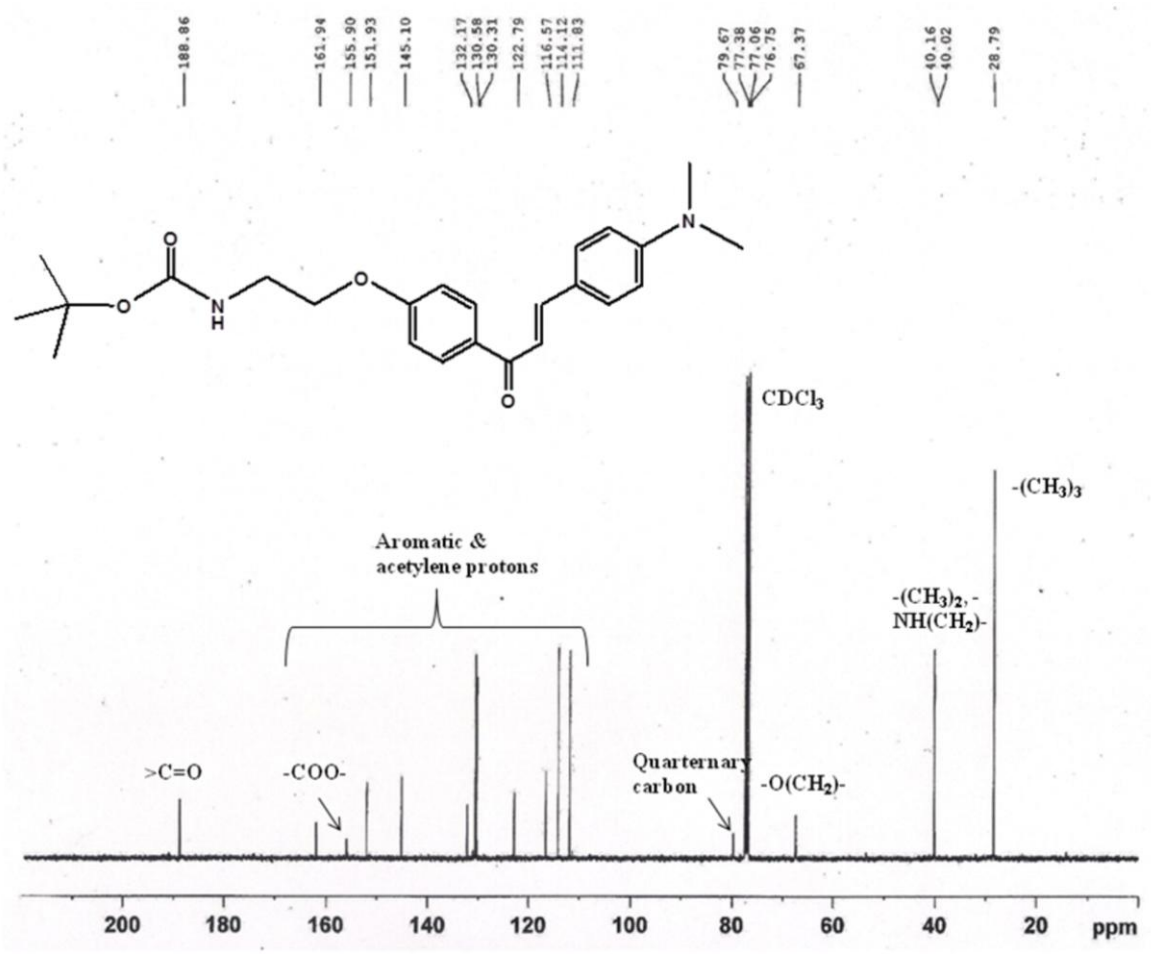


Figure S8. ^{13}C NMR spectrum of (*E*)-tert-butyl 2-(4-(3-(4-(dimethylamino)phenyl)acryloyl)phenoxy)ethylcarbamate, **3**.

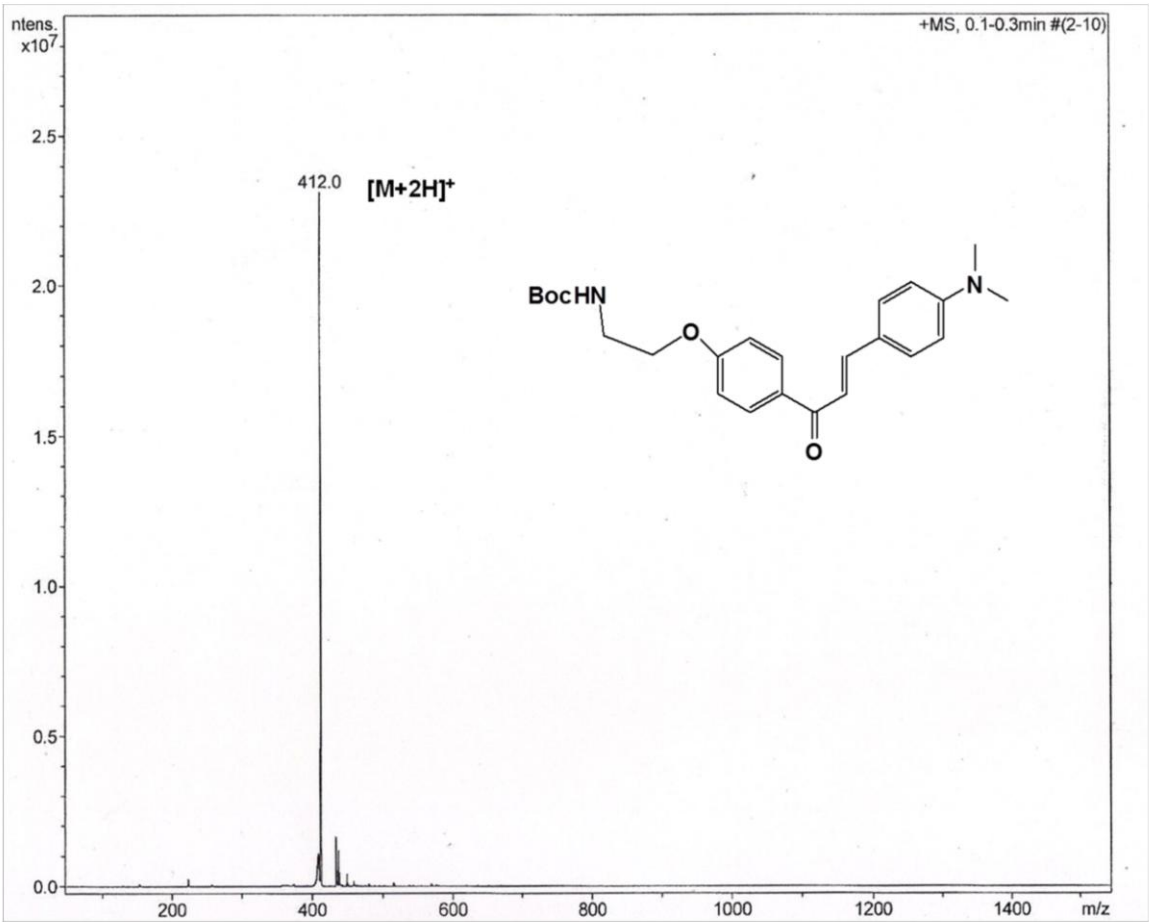


Figure S9. ESI-MS spectrum of (*E*)-tert-butyl 2-(4-(3-(4-(dimethylamino)phenyl)acryloyl)phenoxy)ethylcarbamate, **3**.

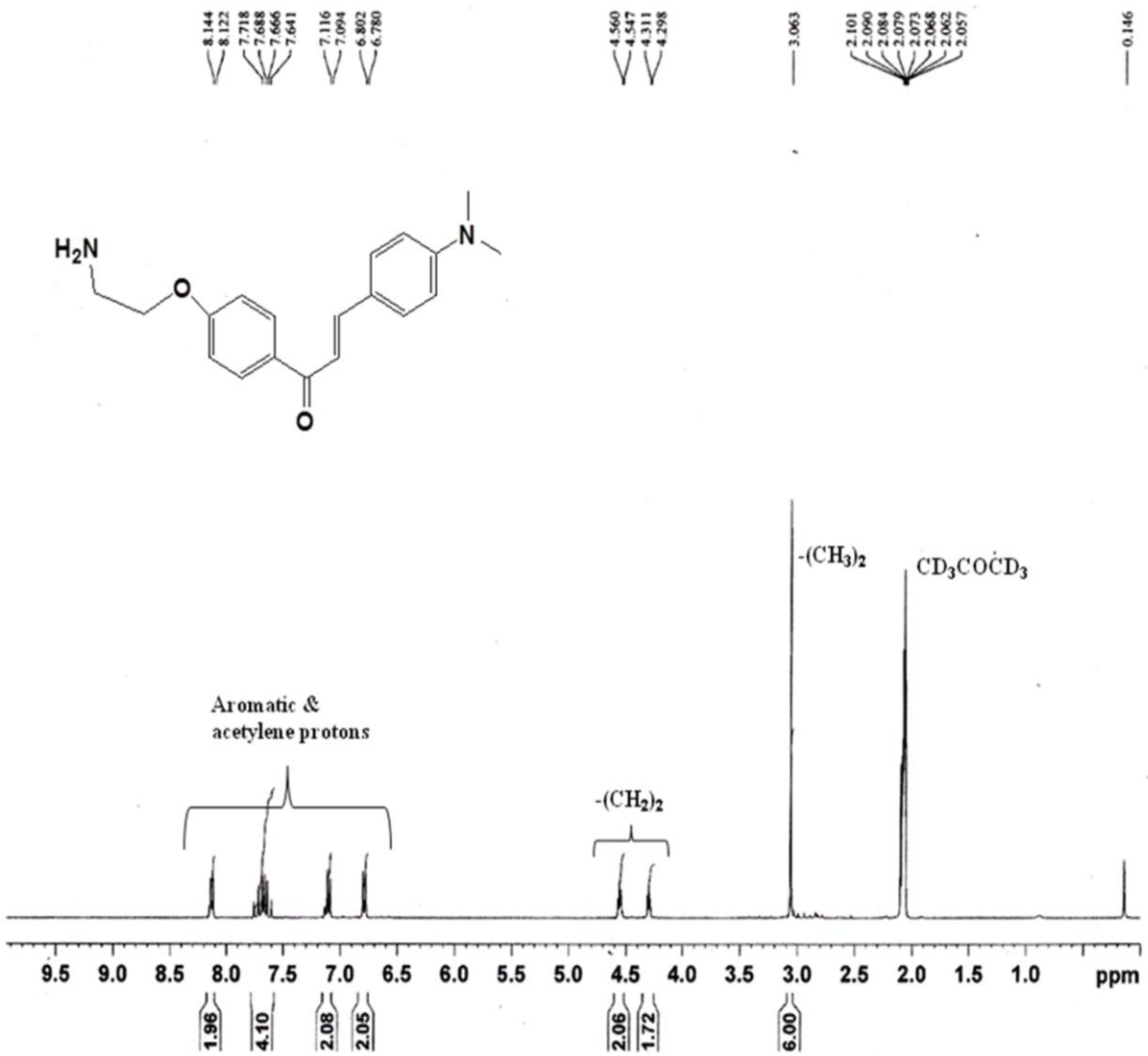


Figure S10. ^{1}H NMR spectrum of (*E*)-1-(4-(2-aminoethoxy)phenyl)-3-(4-(dimethylamino)phenyl)prop-2-en-1-one, **4**.

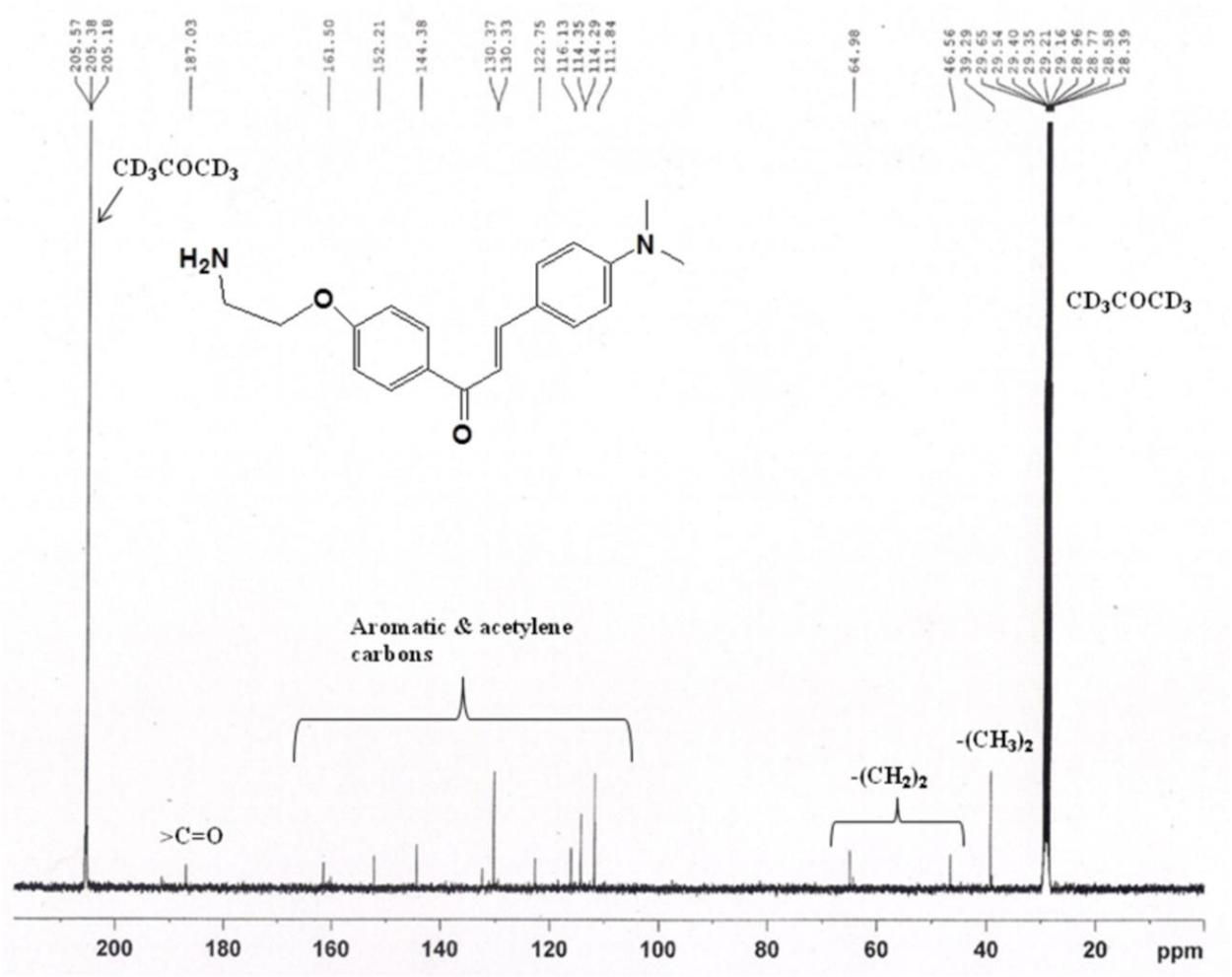


Figure S11. ^{13}C NMR spectrum of (*E*)-1-(4-(2-aminoethoxy)phenyl)-3-(4-(dimethylamino)phenyl)prop-2-en-1-one, **4**.

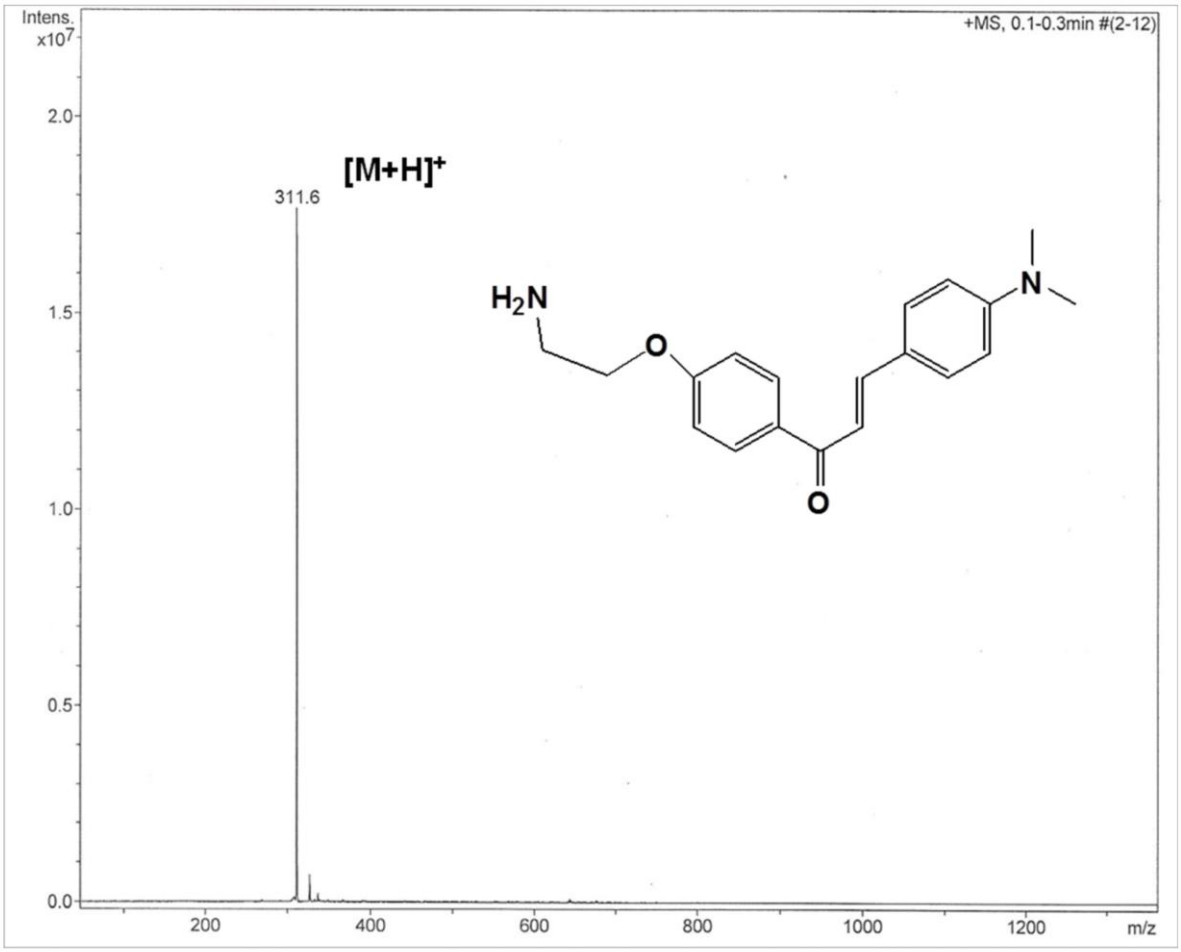


Figure S12. ESI-MS spectrum of (*E*)-1-(4-(2-aminoethoxy)phenyl)-3-(4-(dimethylamino)phenyl)prop-2-en-1-one, **4**.

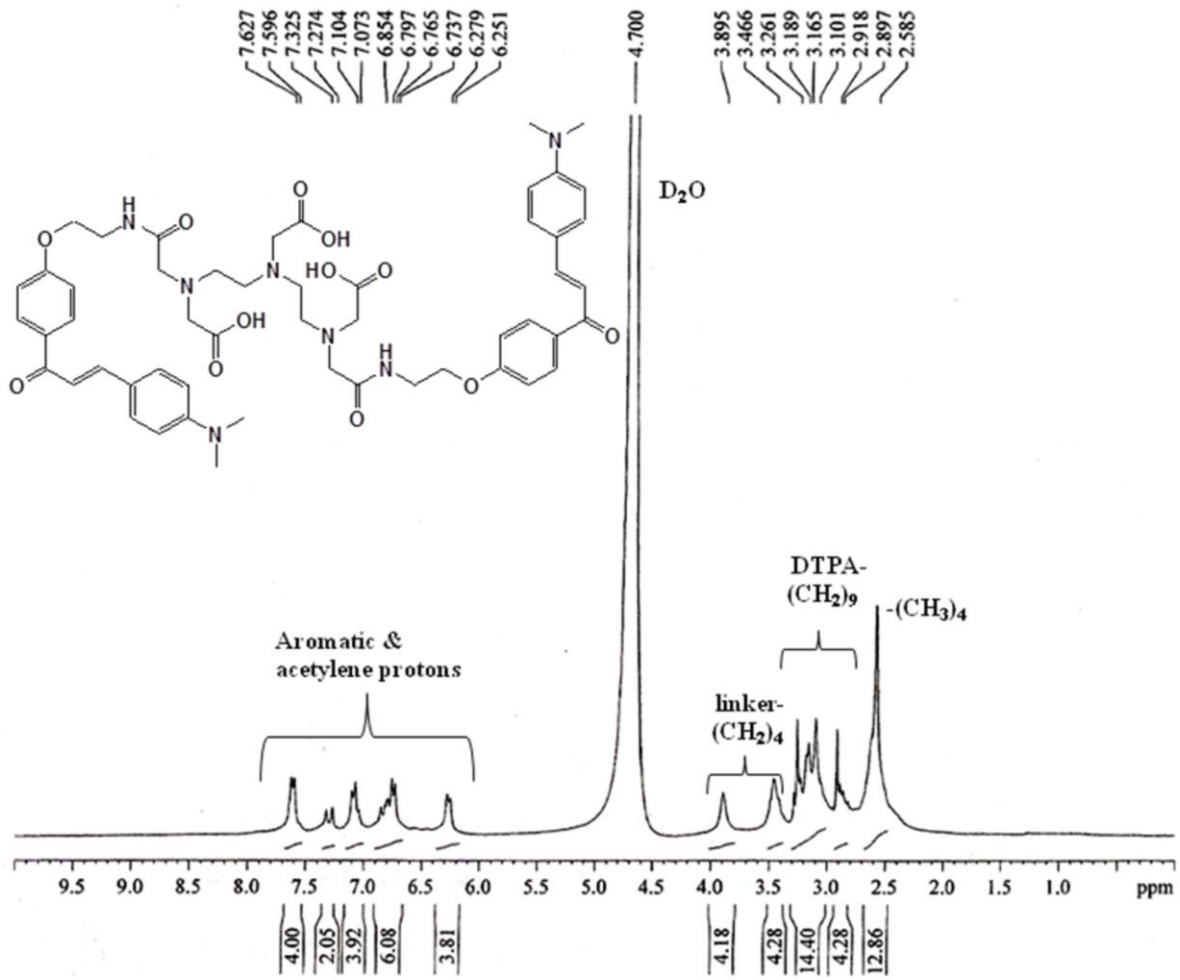


Figure S13. ^{1}H NMR spectrum of 5,8-bis(carboxymethyl)-13-(4-((*E*)-3-(4-(dimethylamino)phenyl)acryloyl)phenoxy)-2-(2-(2-(4-((*E*)-3-(4-(dimethylamino)phenyl)acryloyl)phenoxy)ethylamino)-2-oxoethyl)-10-oxo-2,5,8,11-tetraazatridecane-1-carboxylic acid **5**.

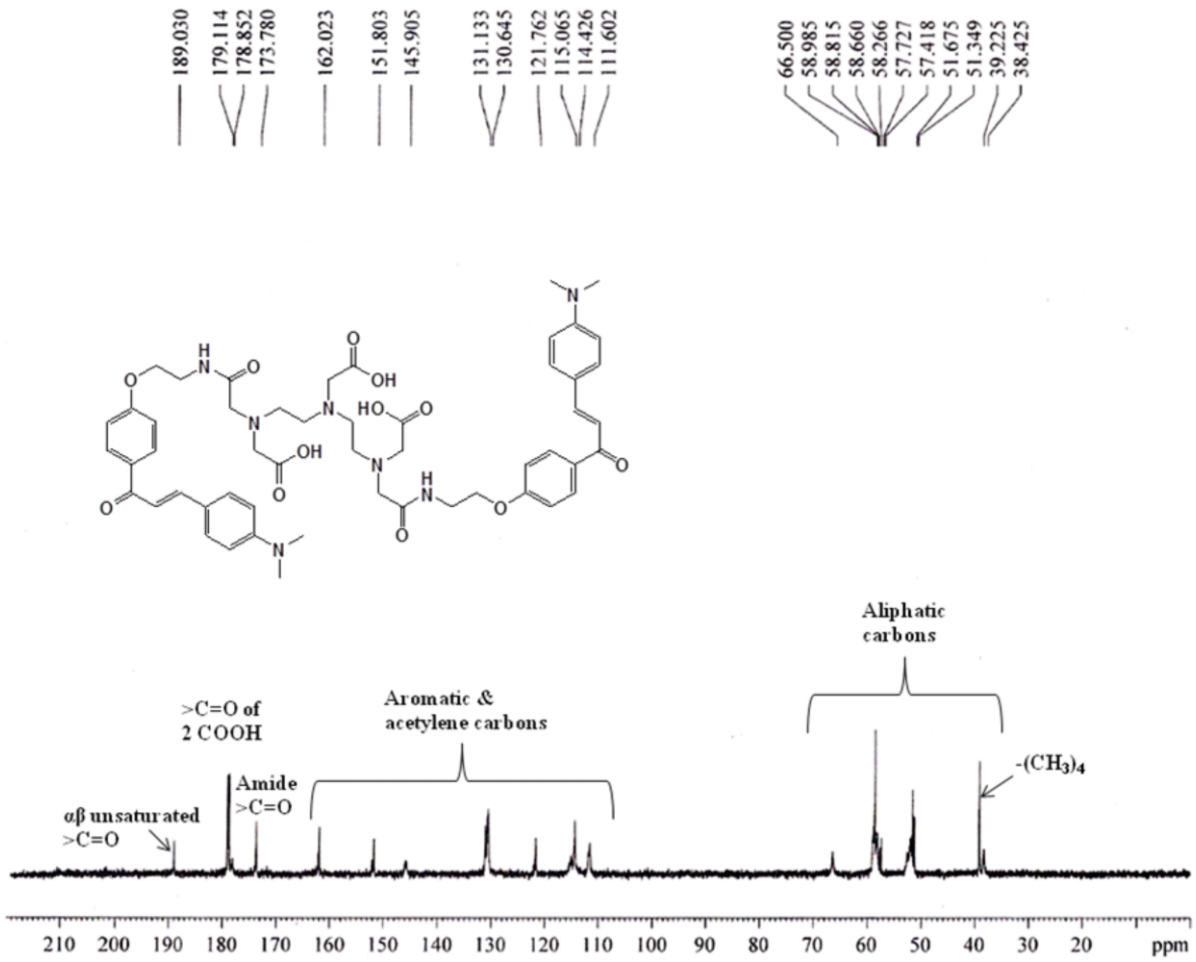


Figure S14. ^{13}C NMR spectrum of 5,8-bis(carboxymethyl)-13-(4-((*E*)-3-(4-(dimethylamino)phenyl)acryloyl)phenoxy)-2-(2-(2-(4-((*E*)-3-(4-(dimethylamino)phenyl)acryloyl)phenoxy)ethylamino)-2-oxoethyl)-10-oxo-2,5,8,11-tetraazatridecane-1-carboxylic acid **5**.

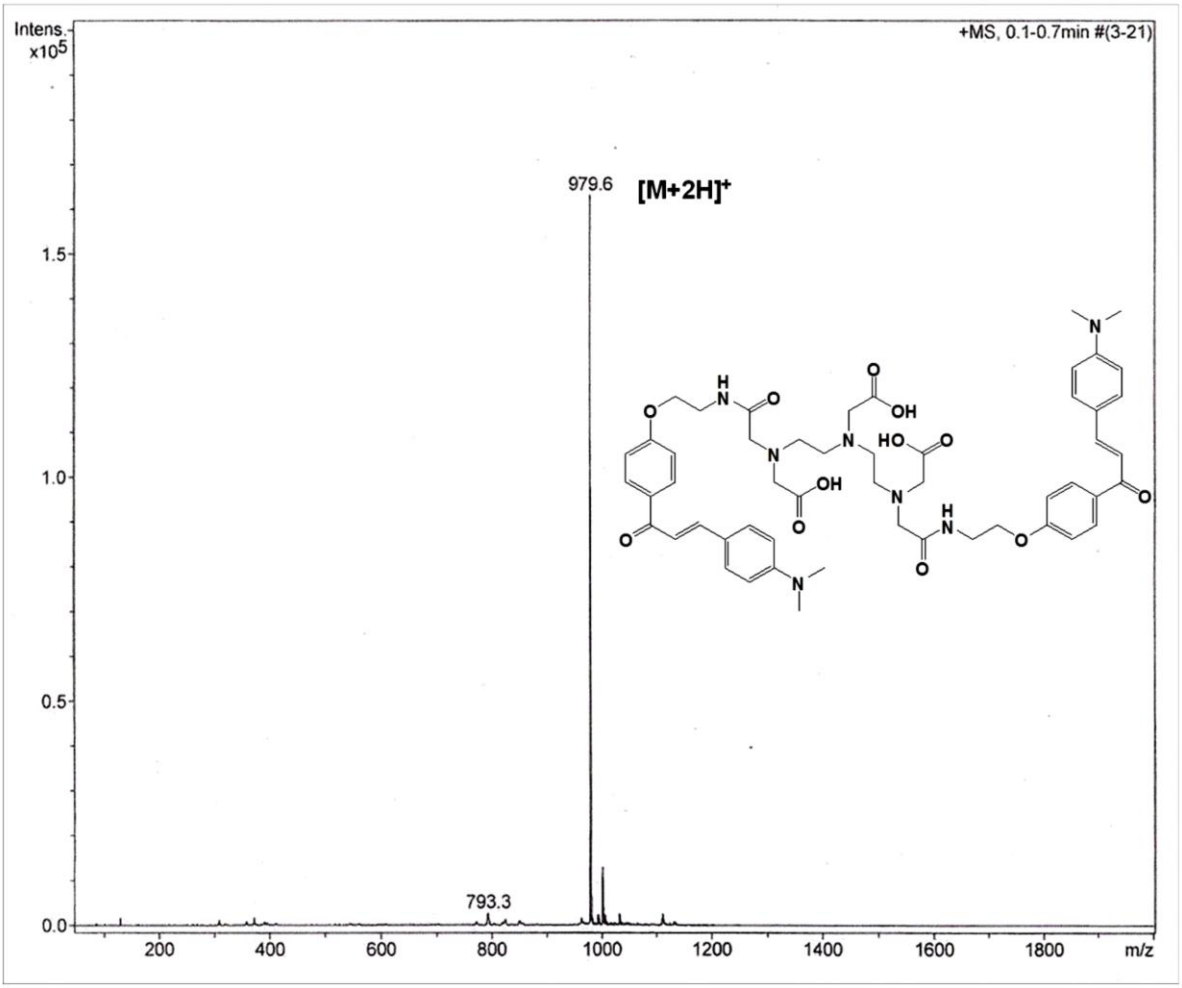


Figure S15. ESI-MS spectrum of 5,8-bis(carboxymethyl)-13-(4-((*E*)-3-(4-(dimethylamino)phenyl)acryloyl)phenoxy)-2-(2-(2-(4-((*E*)-3-(4-(dimethylamino)phenyl)acryloyl)phenoxy)ethylamino)-2-oxoethyl)-10-oxo-2,5,8,11-tetraazatridecane-1-carboxylic acid **5**.

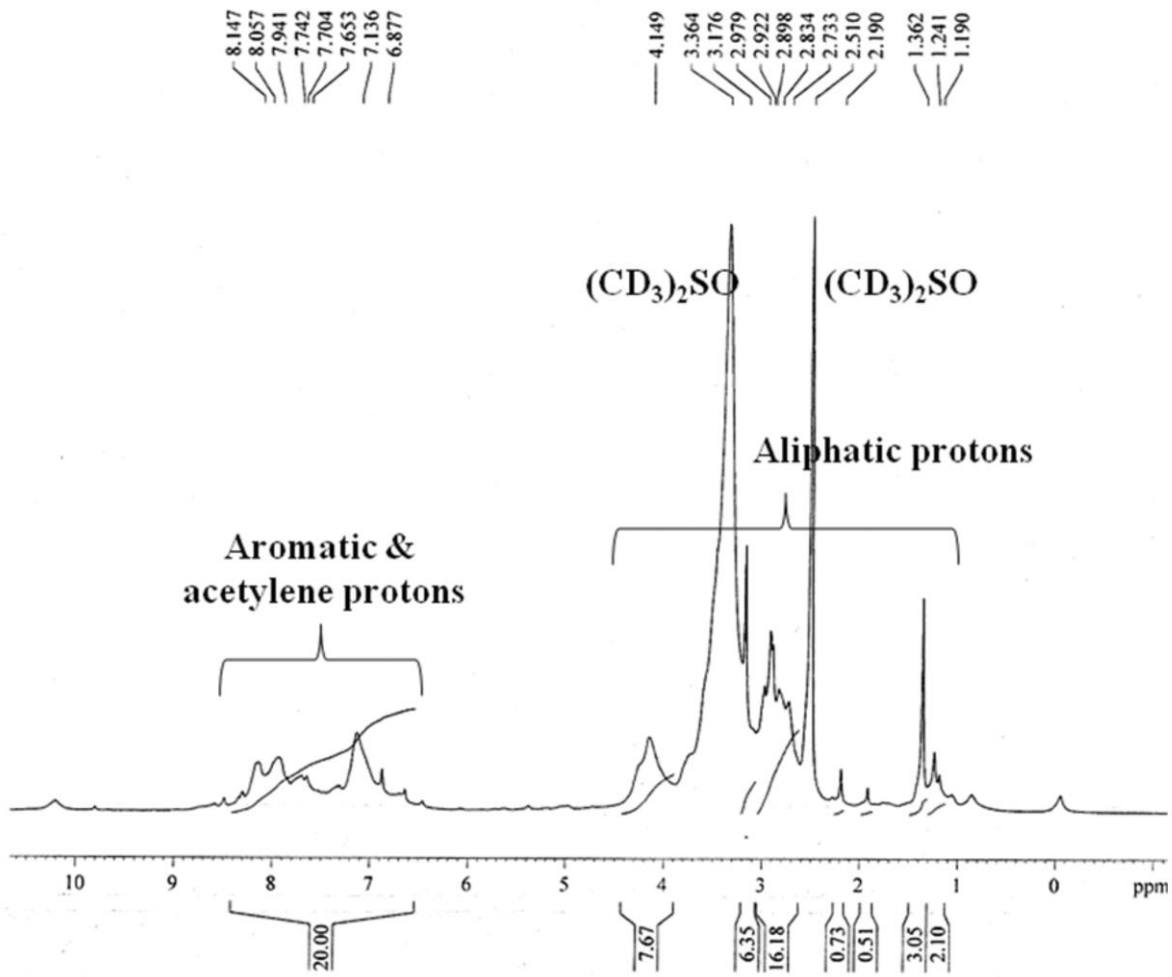
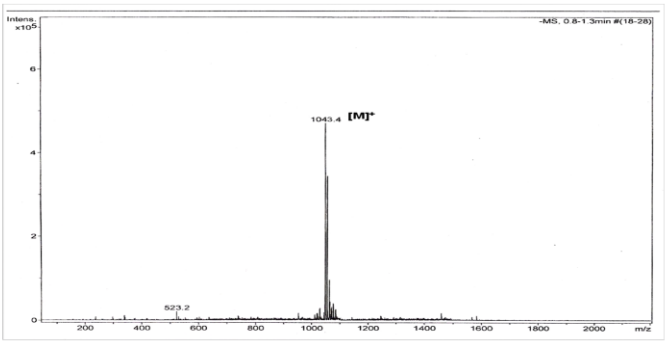
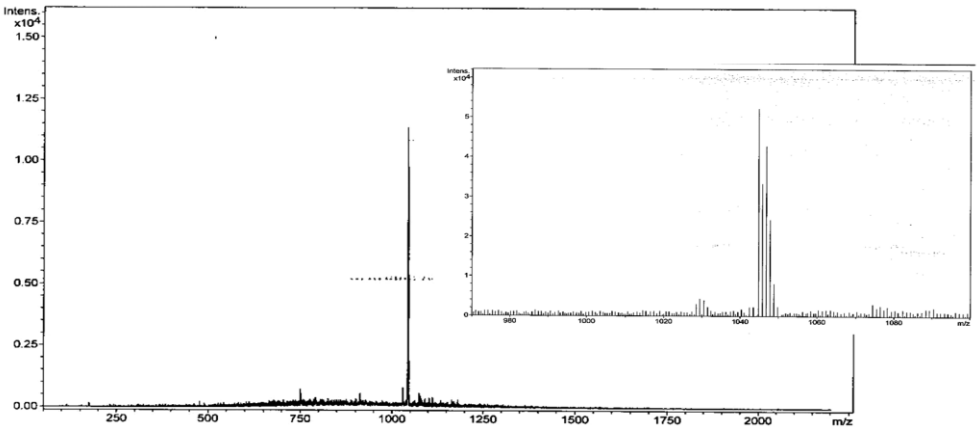


Figure S16. ^{1}H NMR spectrum of 5,8-bis(carboxymethyl)-13-(4-((*E*)-3-(4-(dimethylamino)phenyl)acryloyl)phenoxy)-2-(2-(2-(4-((*E*)-3-(4-(dimethylamino)phenyl)acryloyl)phenoxy)ethylamino)-2-oxoethyl)-10-oxo-2,5,8,11-tetraazatridecane-1-carboxylic acid Gallium-(III), **[$^{69/71}$Ga-] Ch_2DT** (at pH 4.5).





Mass Spectrum SmartFormula Report

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Sample Name	exoprot oct 27	Instrument / Ser#	micrOTOF-Q II 10262
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
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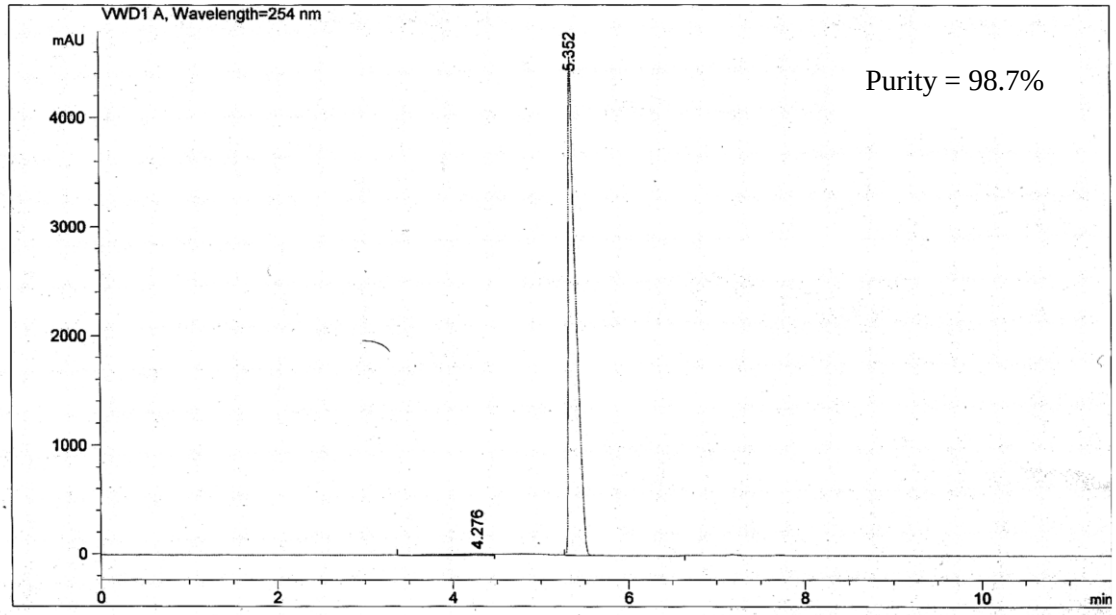
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source

Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
1044.3623	1	C 52 H 61 Ga N 7 O 12	100.00	1044.3629	0.5	3.4	252.4	26.5	even	ok

Figure S18. ESI-MS spectra and HR-ESI-MS data of 5,8-bis(carboxymethyl)-13-(4-((*E*)-3-(4-(dimethylamino)phenyl)acryloyl)phenoxy)-2-(2-(2-(4-((*E*)-3-(4-(dimethylamino)phenyl)acryloyl)phenoxy)ethylamino)-2-oxoethyl)-10-oxo-2,5,8,11-tetraazatridecane-1-carboxylic acid Gallium-(III), **[$^{69/71}$Ga-] Ch$_2$DT**.

Sample preparation procedure: $^{69/71}$Ga-DT(Ch)$_2$ was dissolved in HPLC grade MeOH (1 mg/mL) at pH 4.5 and passed through 0.20 μm hydrophobic DISMIC – 13$_{JP}$ filter (disposable syringe filter unit). The filtrate was collected and used for mass analysis.



Area Percent Report

Sorted By : Retention Time
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Sig	Type	Area [mAU*s]	Height [mAU]	Area %
1	4.276	1	BV	396.85281	9.05114	1.2976
2	5.352	1	BB	3.01857e4	4583.69043	98.7024
Totals :				3.05825e4	4592.74157	

Figure S19. HPLC profile of **[$^{69/71}$Ga]-DT(Ch)$_2$** with retention time = 5.35 min.

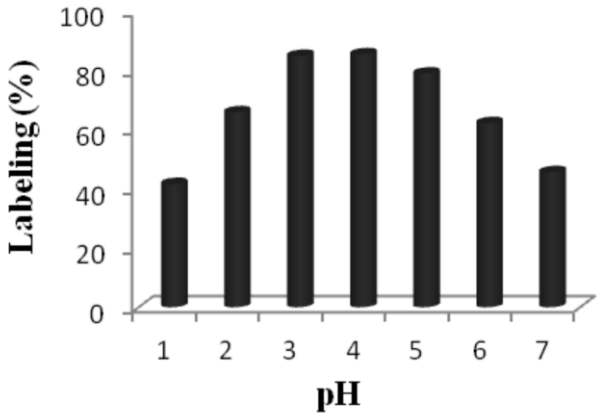


Figure S20. Radiolabeling efficiency of ^{68}Ga-DT(Ch)$_2$ at different pH.

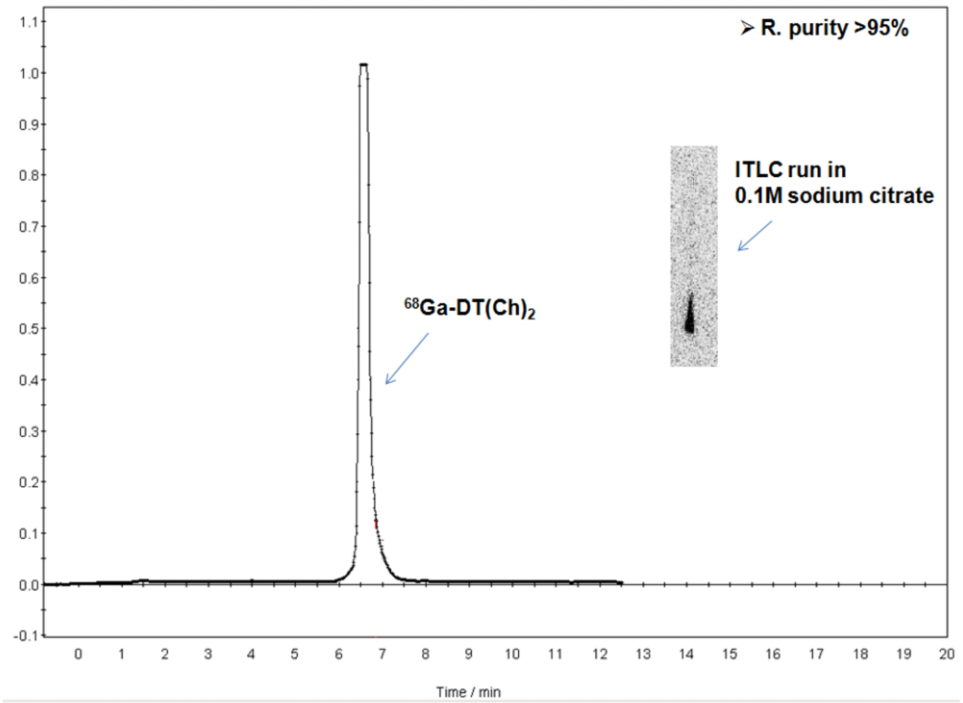


Figure S21. Radio-HPLC profile of ^{68}Ga-DT(Ch)$_2$ with retention time = 6.2 min.

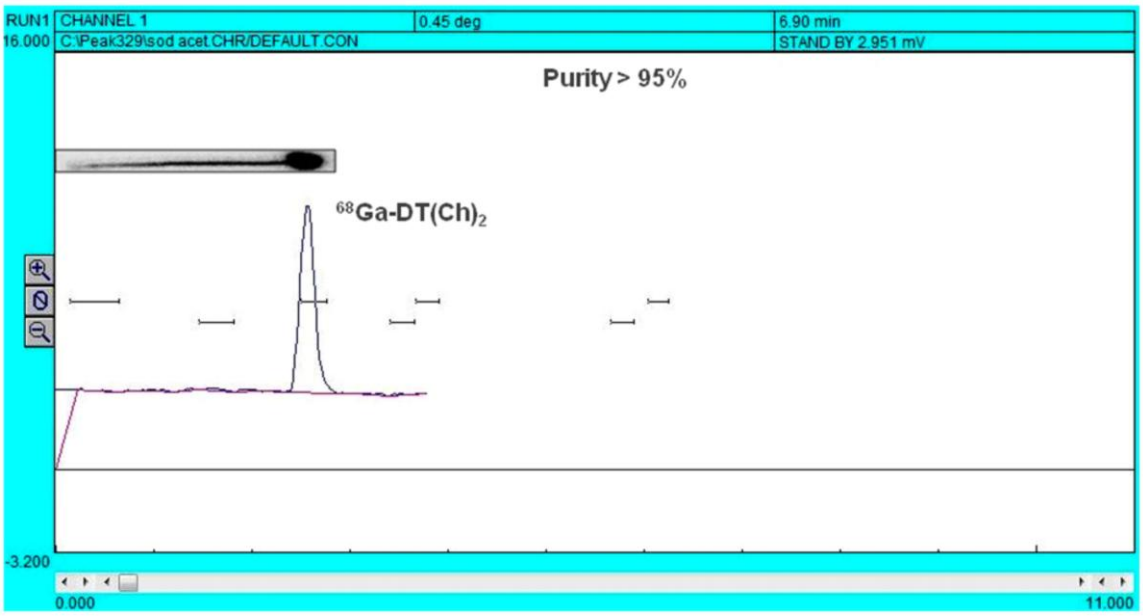


Figure S22. Radio-TLC profile of ^{68}Ga-DT(Ch)$_2$ run in 1:1 ammonium acetate and methanol.

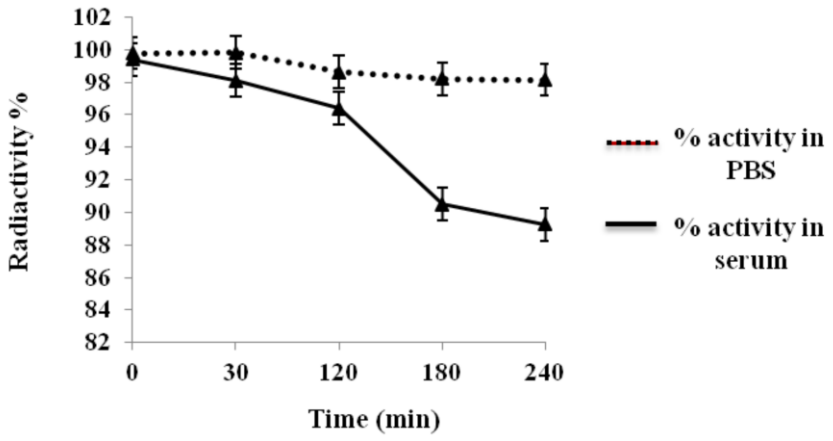


Figure S23. In-vitro serum stability of ^{68}Ga-DT(Ch)$_2$ at 37°C (n=3).

Table S1. Fluorescence profile of $DT(Ch)_2$ with Aβ42 aggregates.

	Excitation max. (nm)		Emission max. (nm)		Fold increase
	before	after	before	after	
$DT(Ch)_2$	410	410	540	520	5.55