

Supporting Information

Syntheses of 2-nitroimidazole derivatives conjugated with 1,4,7-triazacyclononane-N,N'-diacetic acid labeled with F-18 using an aluminum complex method for hypoxia imaging

Lathika Hoigebazar,^{†,‡} Jae Min Jeong,^{*,†,‡} Ji-Youn Lee,^{†,‡} Dinesh Shetty,^{†,‡} Bo Yeun Yang,^{†,‡}
Yun-Sang Lee,^{†,‡} Dong Soo Lee,^{†,‡} June-Key Chung,^{†,‡} and Myung Chul Lee,^{†,‡}

[†]*Radiation Applied Life Sciences, Department of Nuclear Medicine, Institute of Radiation Medicine, Seoul National University College of Medicine, Seoul 110-744, Korea,*

[‡]*Cancer Research Institute, Seoul National University College of Medicine, Seoul 110-744, Korea.*

Contents

Nitroimidazole-ethylbromide (2)	
MS (ESI ⁺)	----- Figure 1S
H-3-NMR	----- Figure 2S
C-13-NMR	----- Figure 3S
NODAtBu-ethylnitroimidazole	
MS (ESI ⁺)	----- Figure 4S
H-3-NMR	----- Figure 5S
C-13-NMR	----- Figure 6S
NODA-ethylnitroimidazole (4)	
MS (ESI ⁺)	----- Figure 7S
HRMS	----- Figure 8S
H-3-NMR	----- Figure 9S
C-13-NMR	----- Figure 10S
HPLC	----- Figure 11S
Nitroimidazole-propylbromide (3)	
MS (ESI ⁺)	----- Figure 12S
H-3-NMR	----- Figure 13S
C-13-NMR	----- Figure 14S
NODAtBu-propylnitroimidazole	
MS (ESI ⁺)	----- Figure 15S
H-3-NMR	----- Figure 16S
C-13-NMR	----- Figure 17S
NODA-propylnitroimidazole (5)	
MS (ESI ⁺)	----- Figure 18S
HRMS	----- Figure 19S
H-3-NMR	----- Figure 20S
C-13-NMR	----- Figure 21S
HPLC	----- Figure 22S
HPLC of AIF-18-NODA-ethylnitroimidazole	----- Figure 23S
HPLC of AIF-18-NODA-propylnitroimidazole	----- Figure 24S
AIF-NODA-ethylnitroimidazole HRMS	----- Figure 25S
AIF-NODA-propylnitroimidazole HRMS	----- Figure 26S

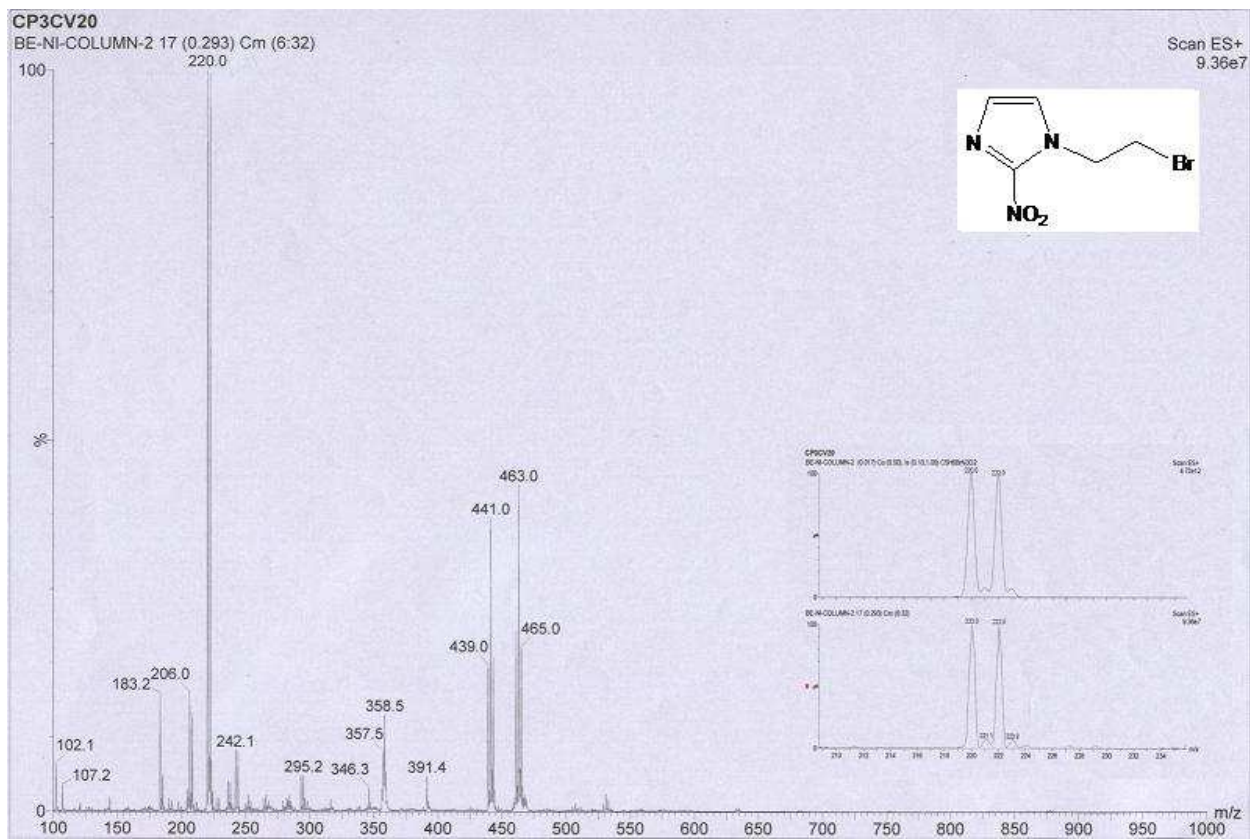


Figure 1S.

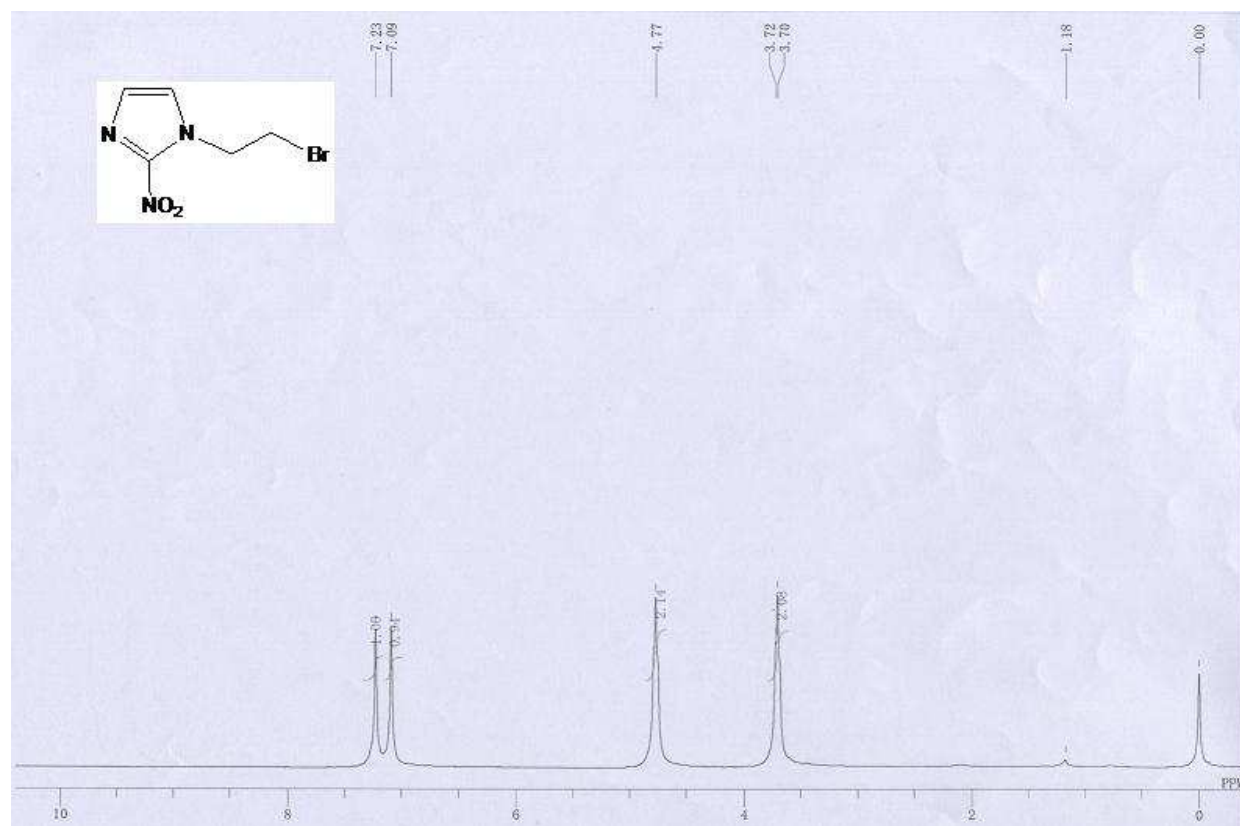


Figure 2S.

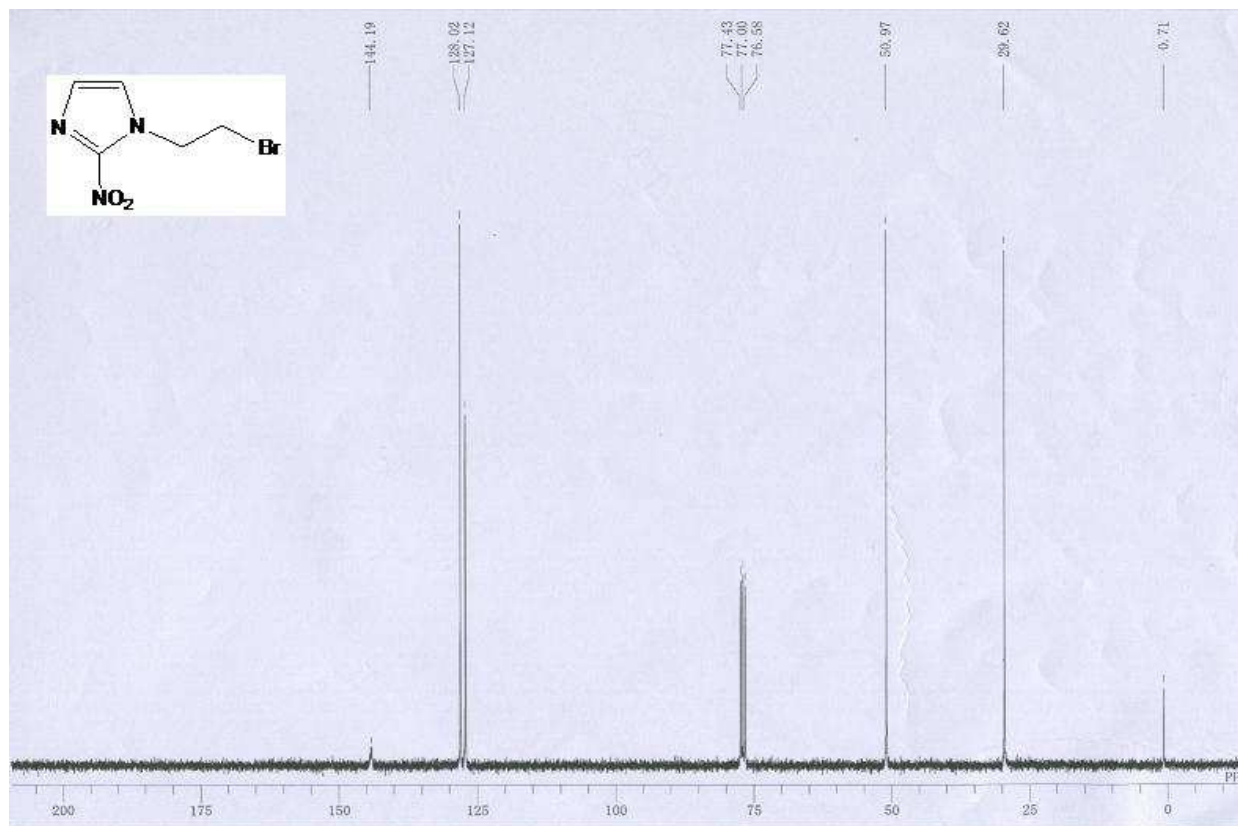


Figure 3S.

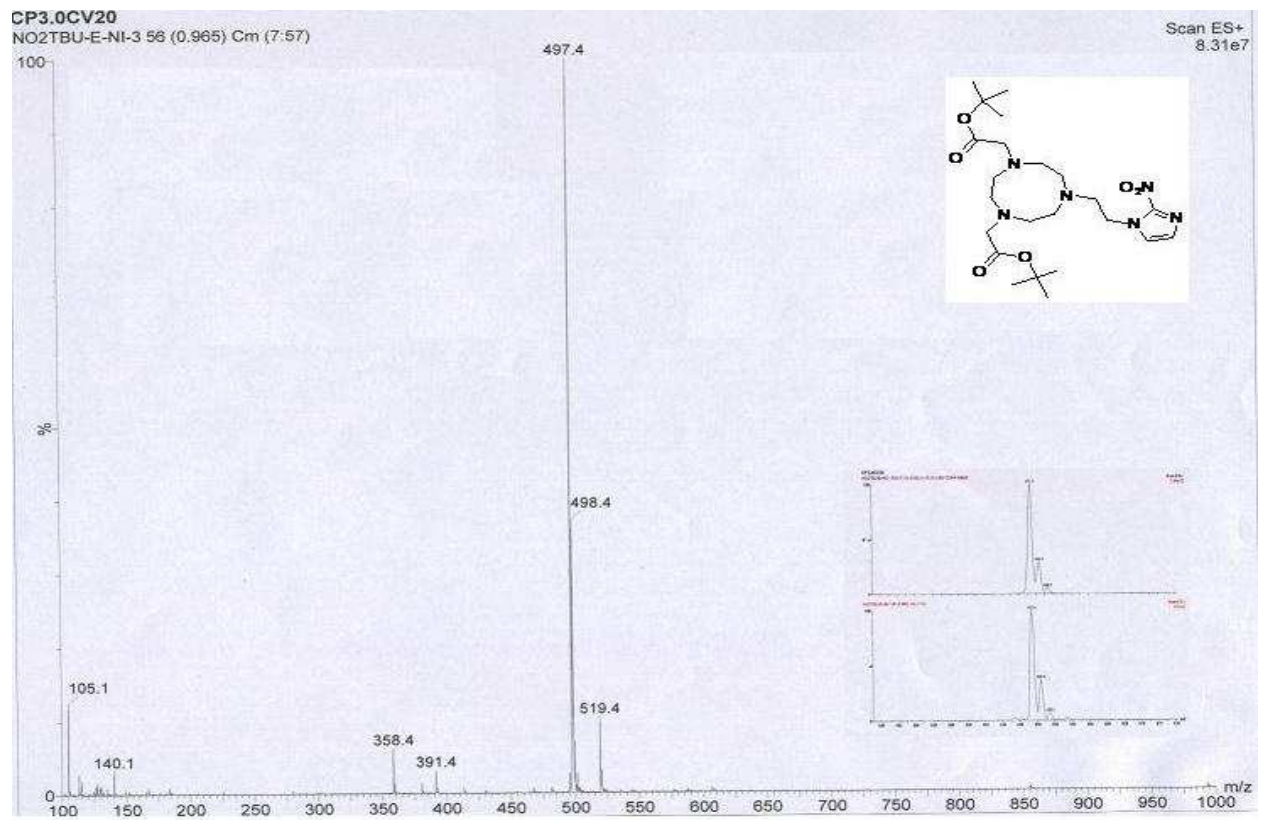


Figure 4S.

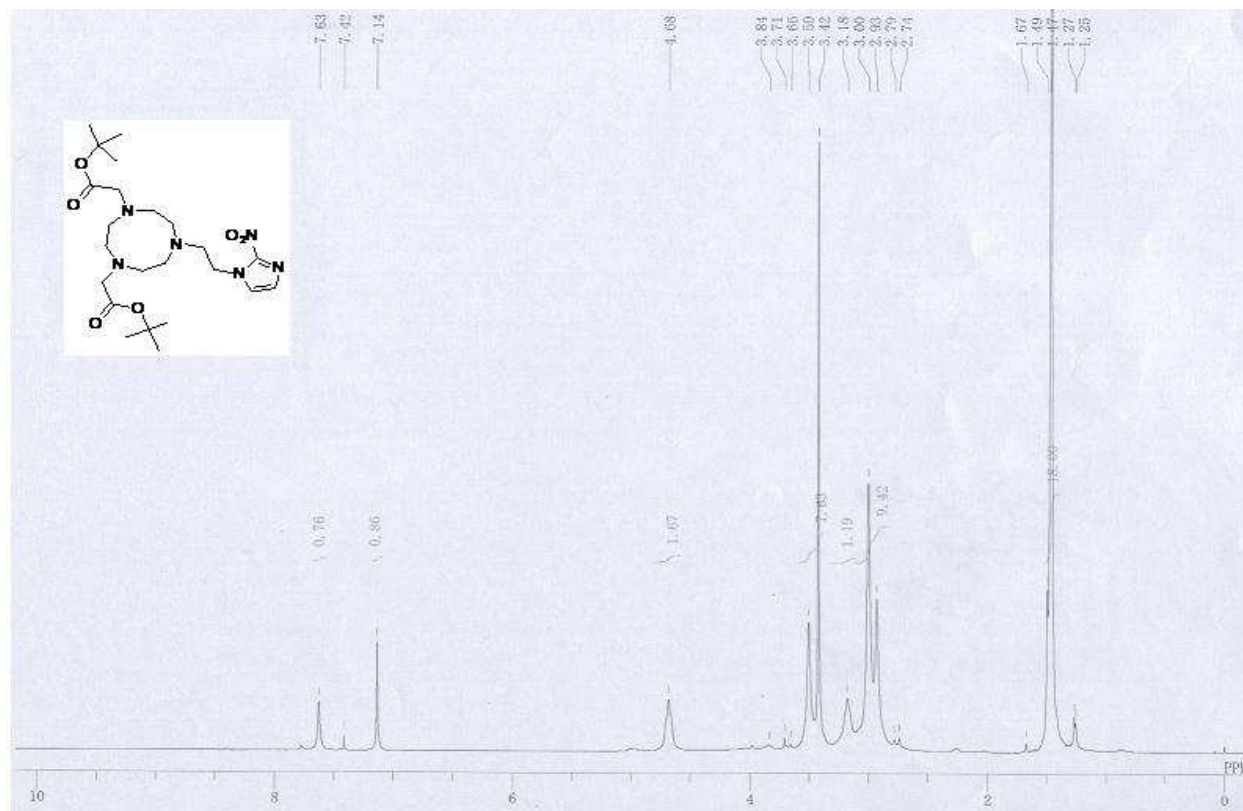


Figure 5S.

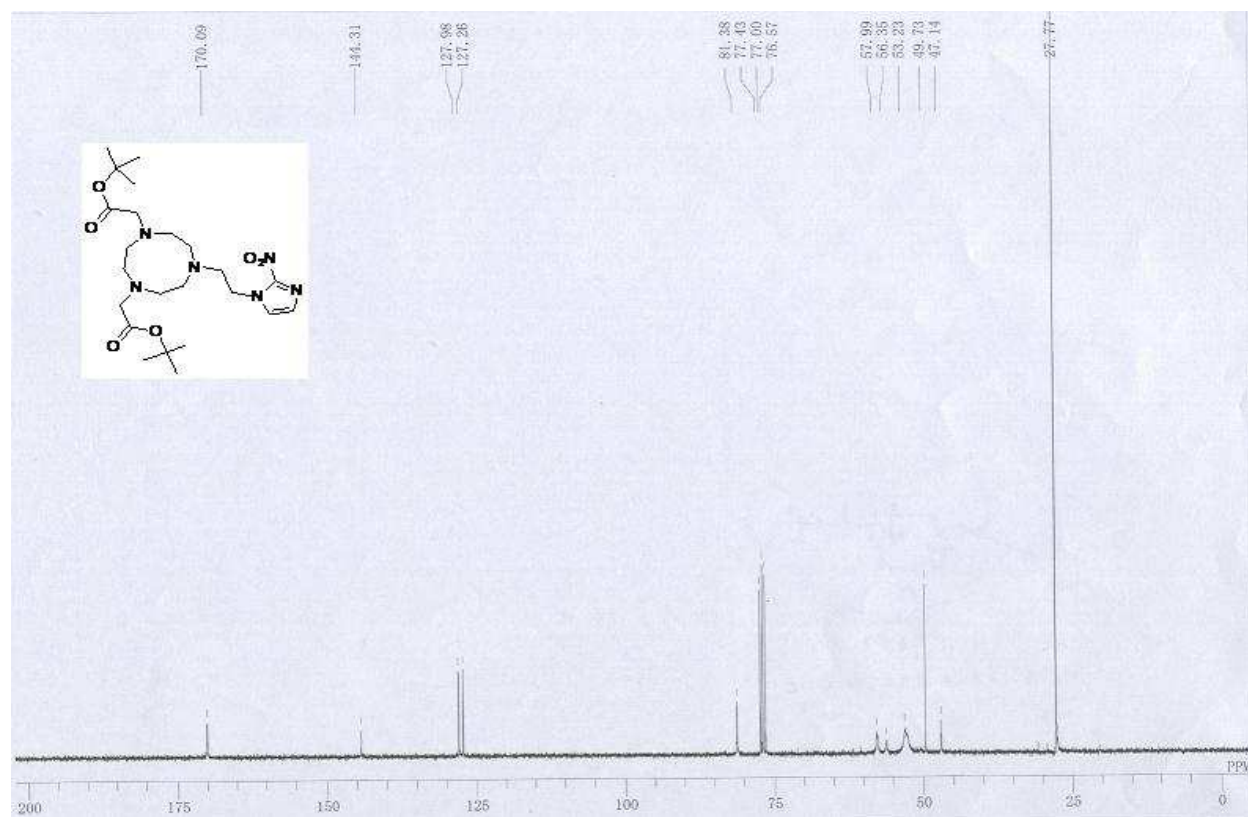


Figure 6S.

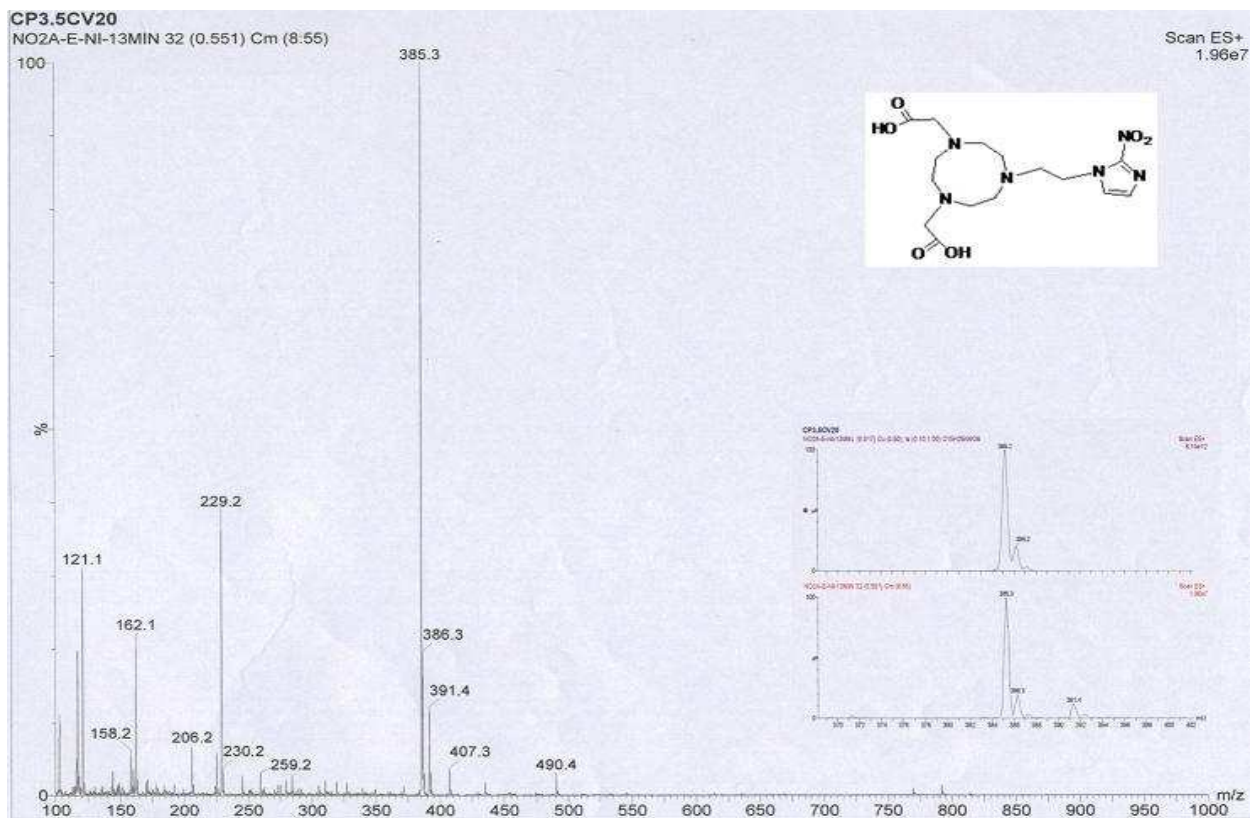


Figure 7S.

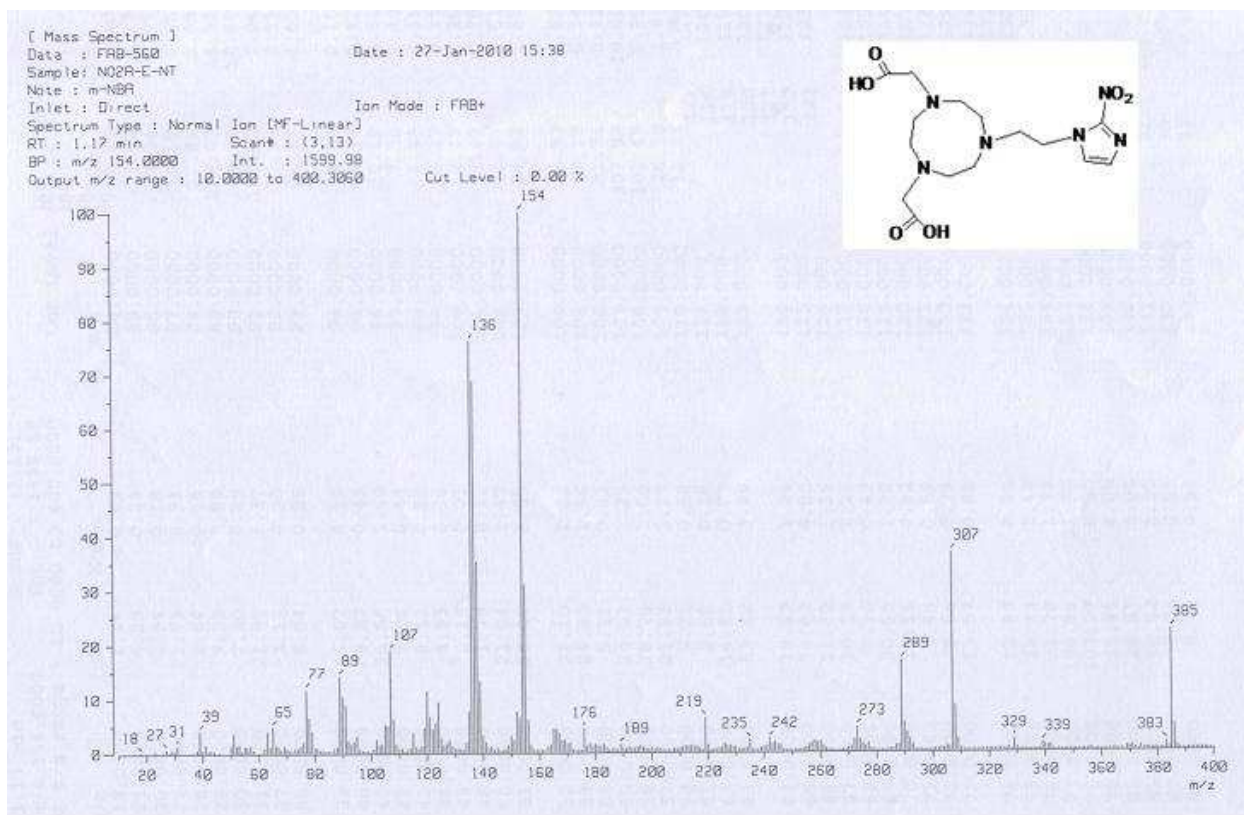


Figure 8S.

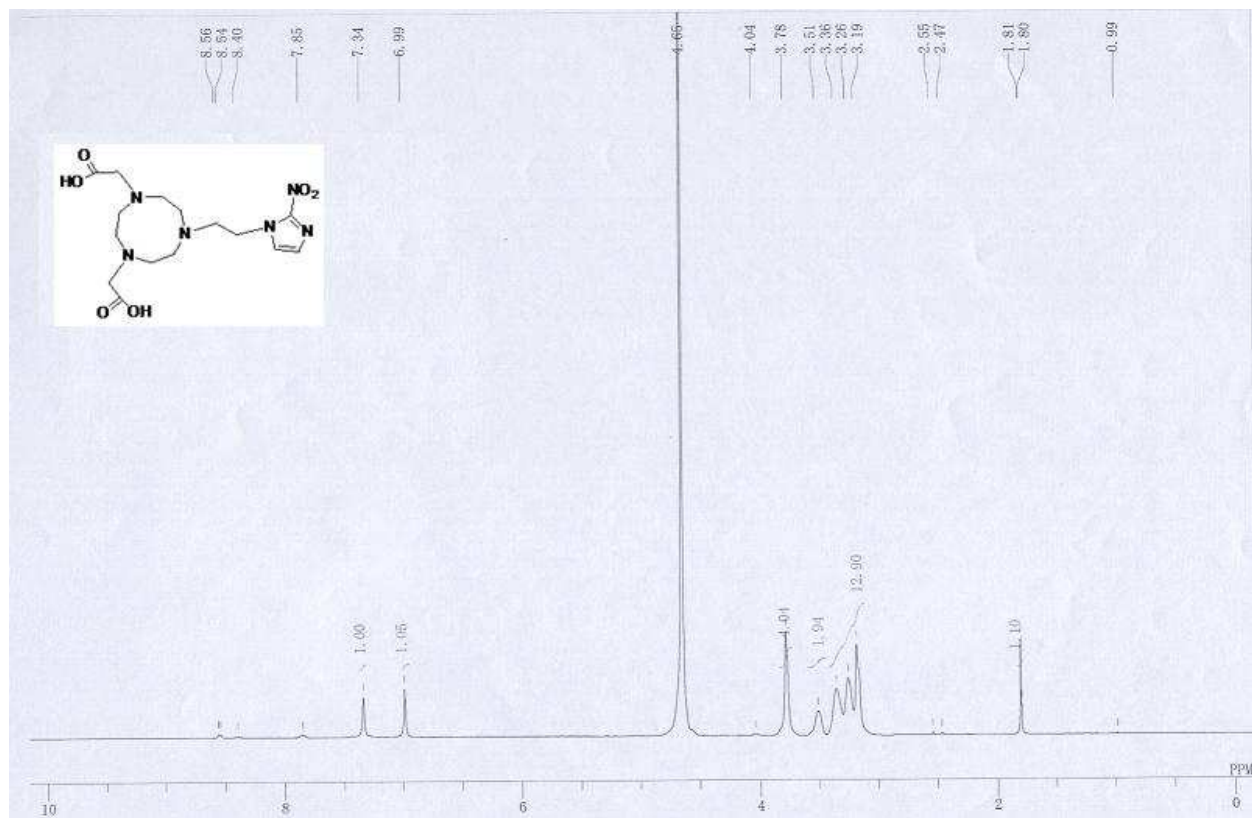


Figure 9S.

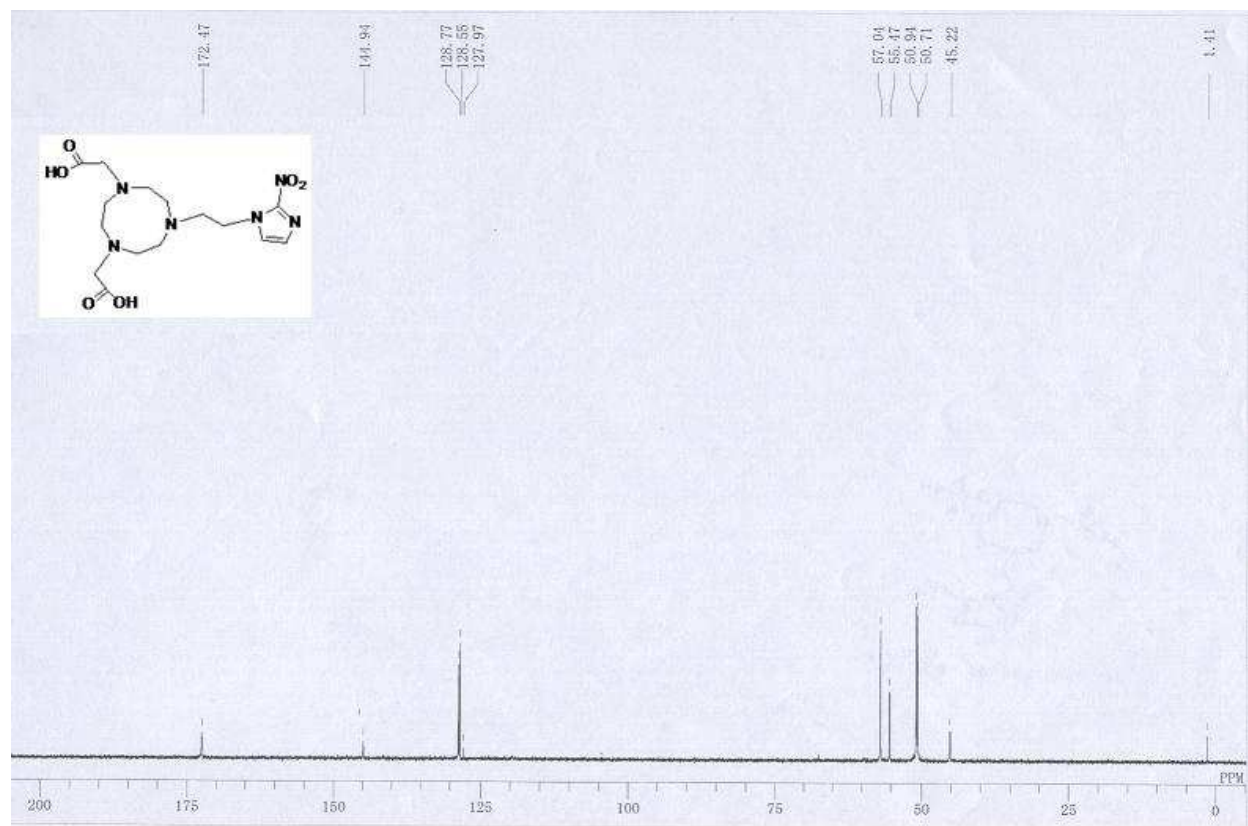


Figure 10S.

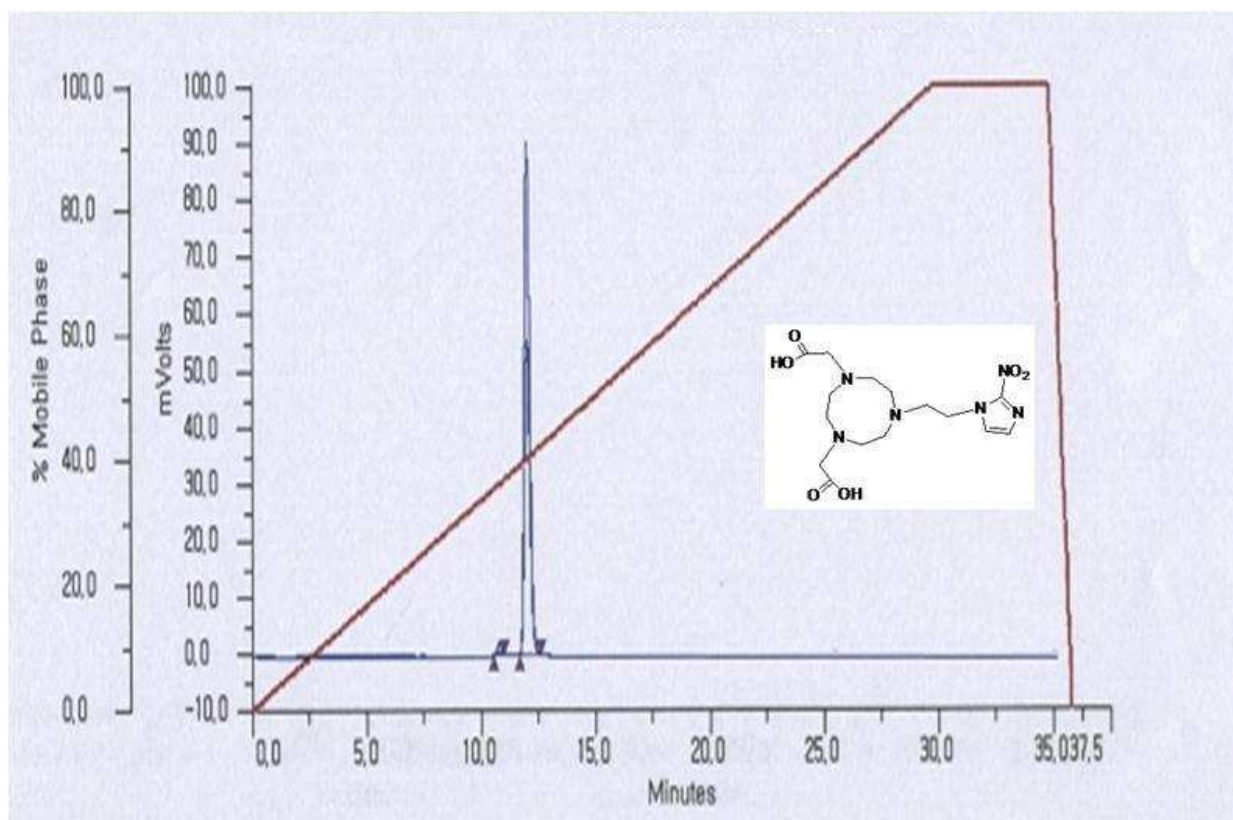


Figure 11S.

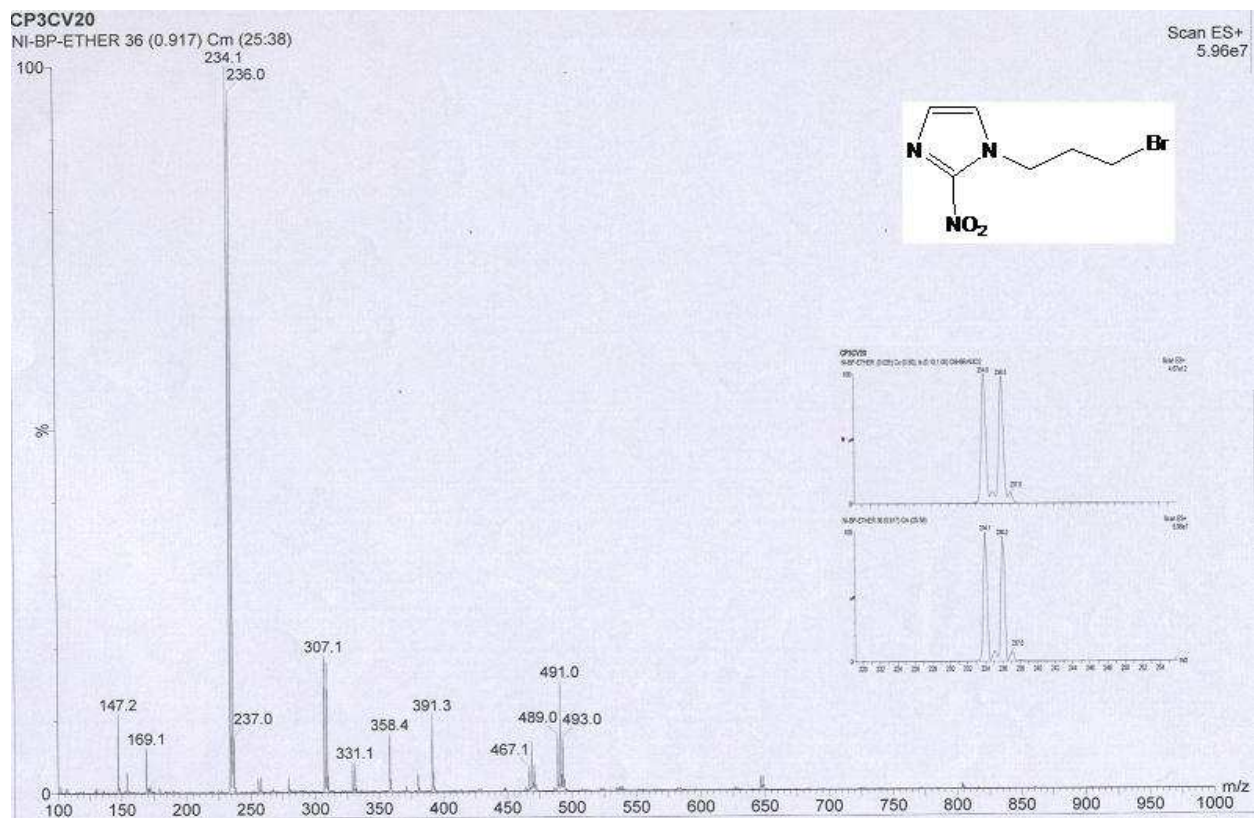


Figure 12S.

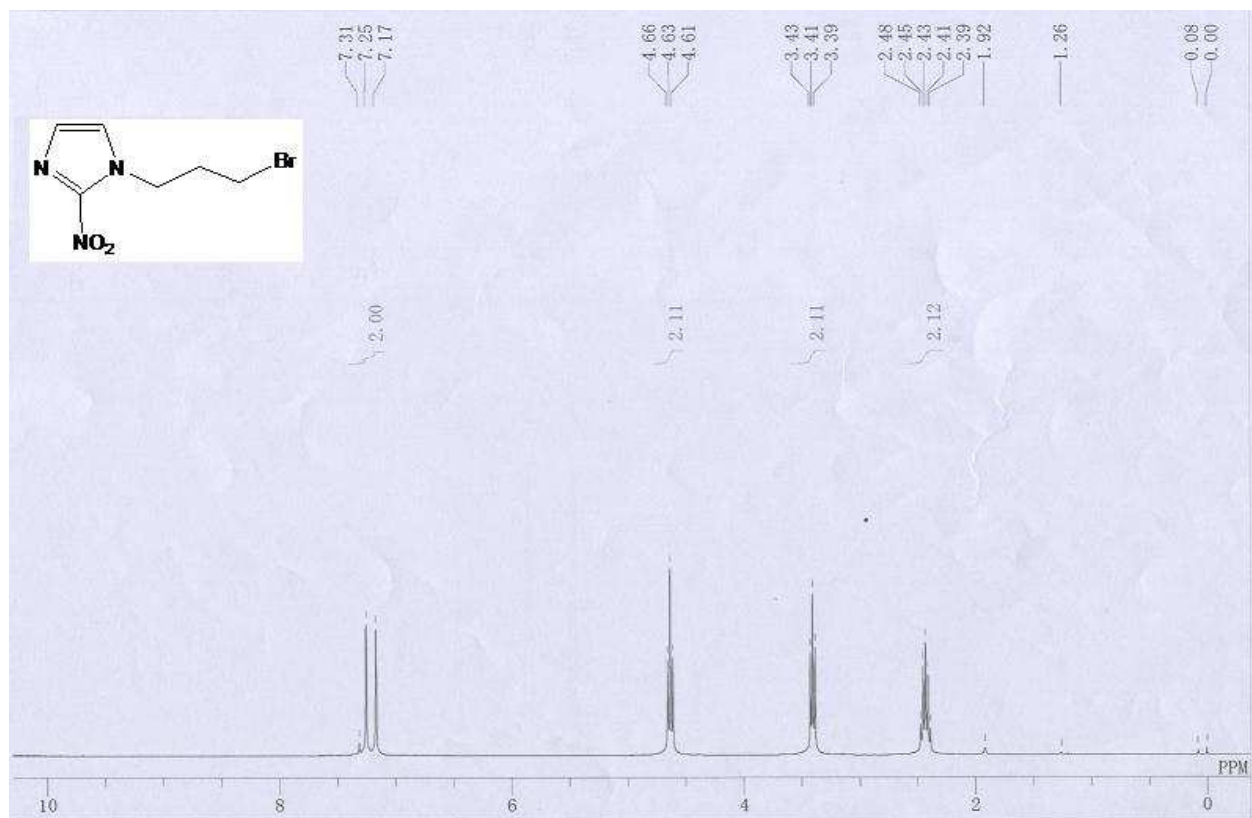


Figure 13S.

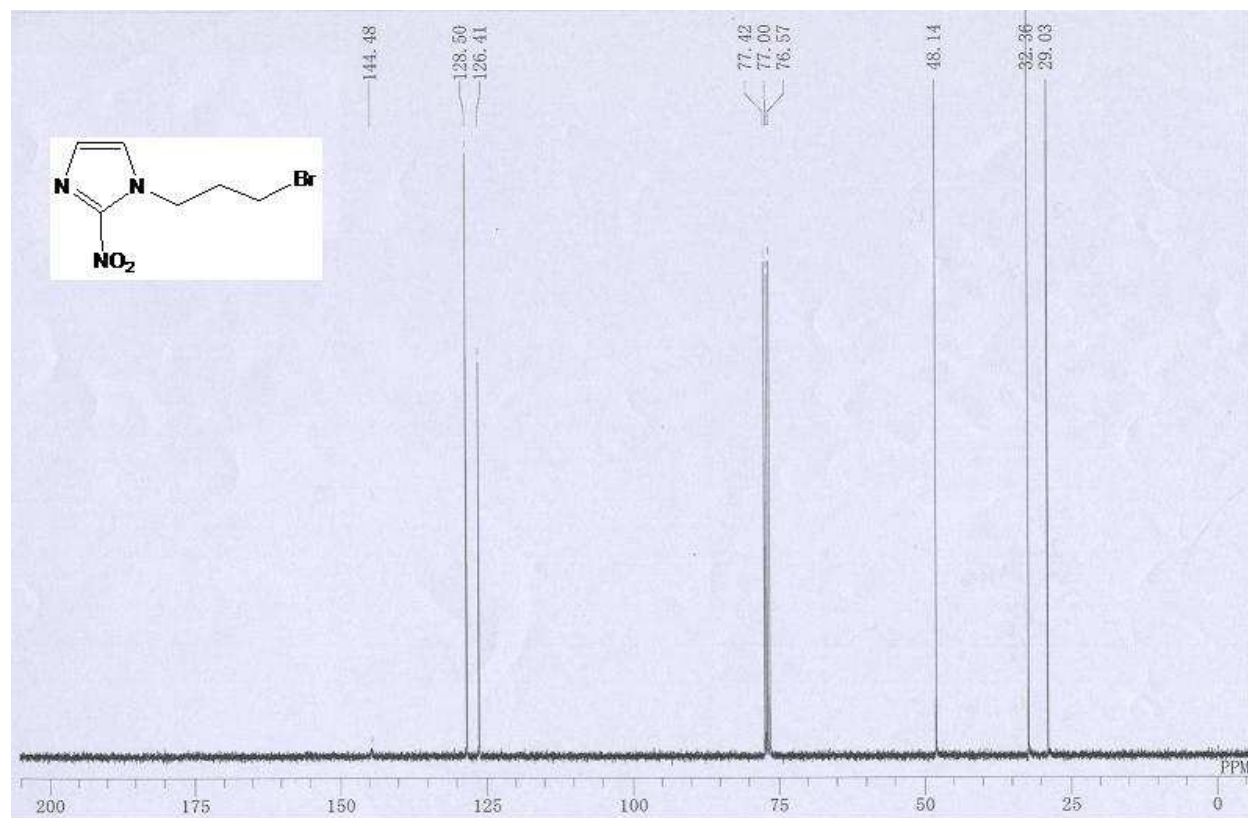


Figure 14S.

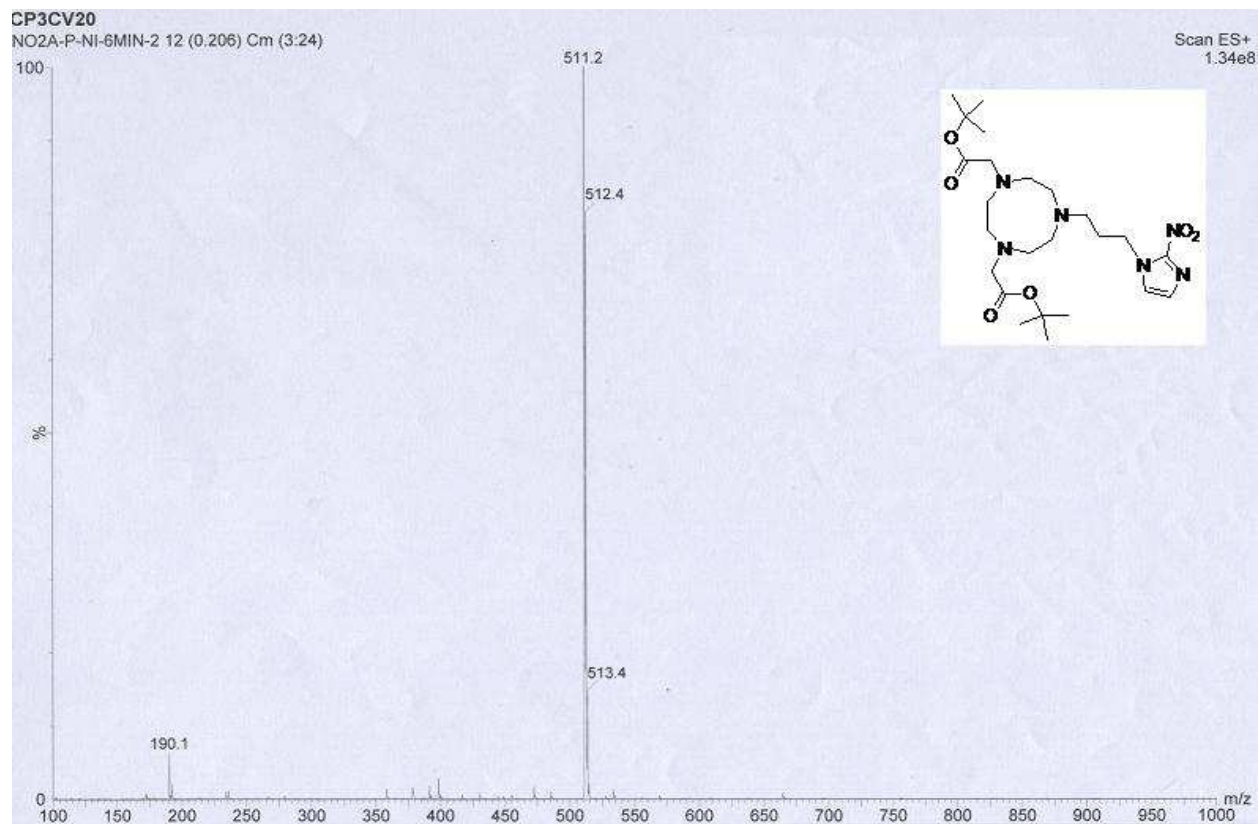


Figure 15S.

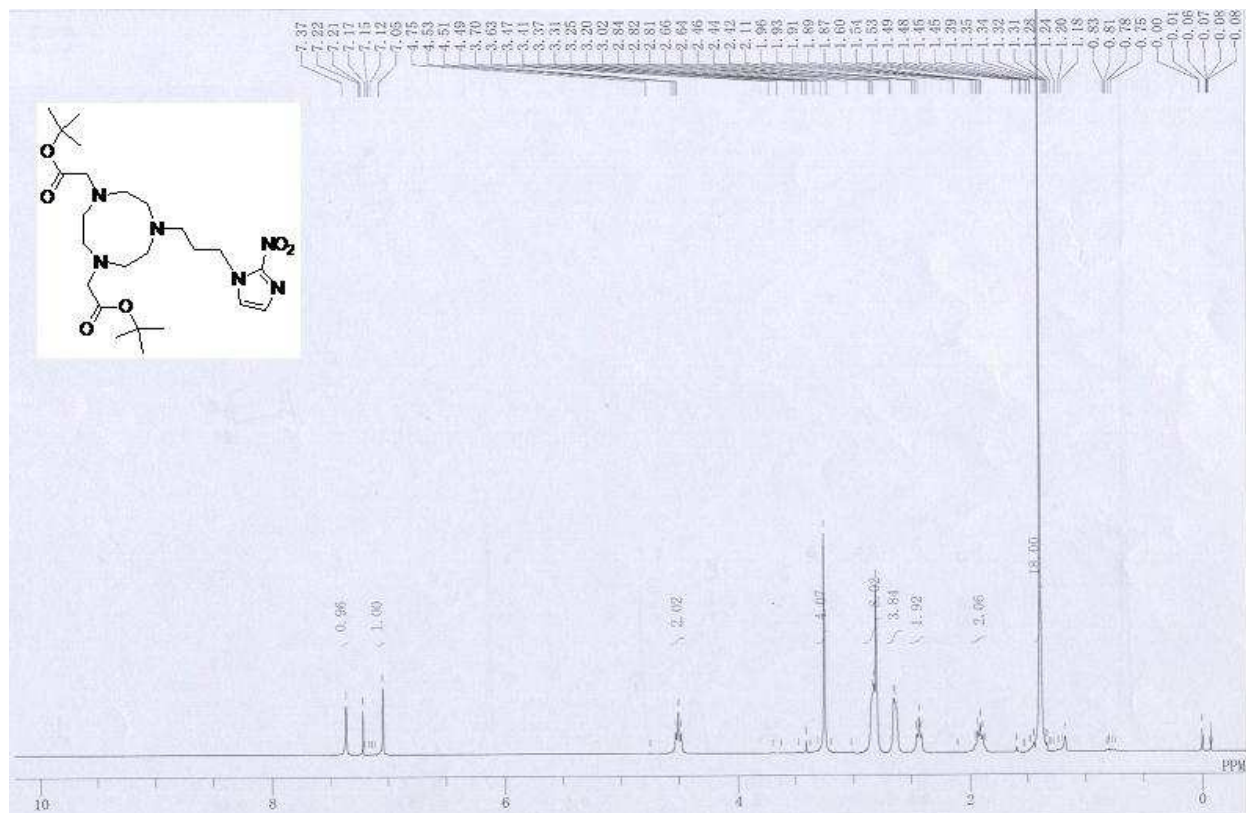


Figure 16S.

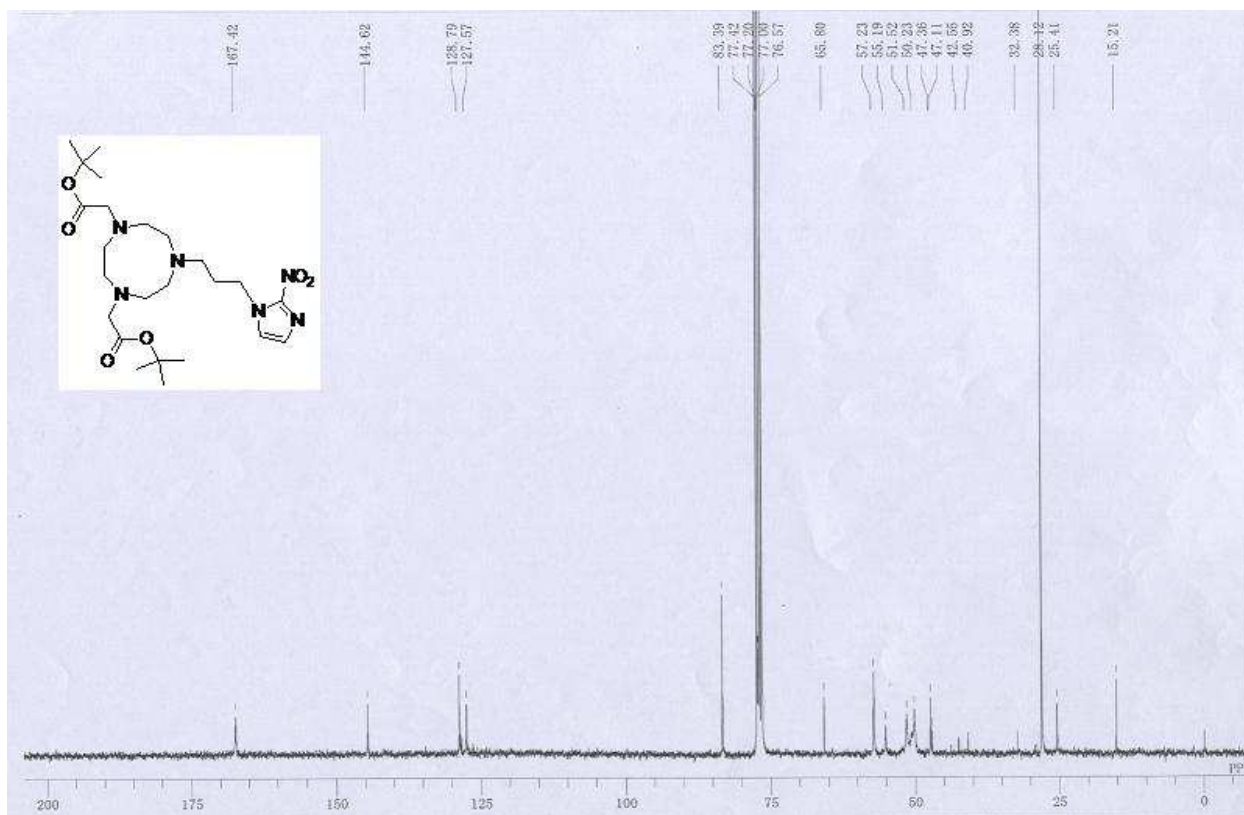


Figure 17S.

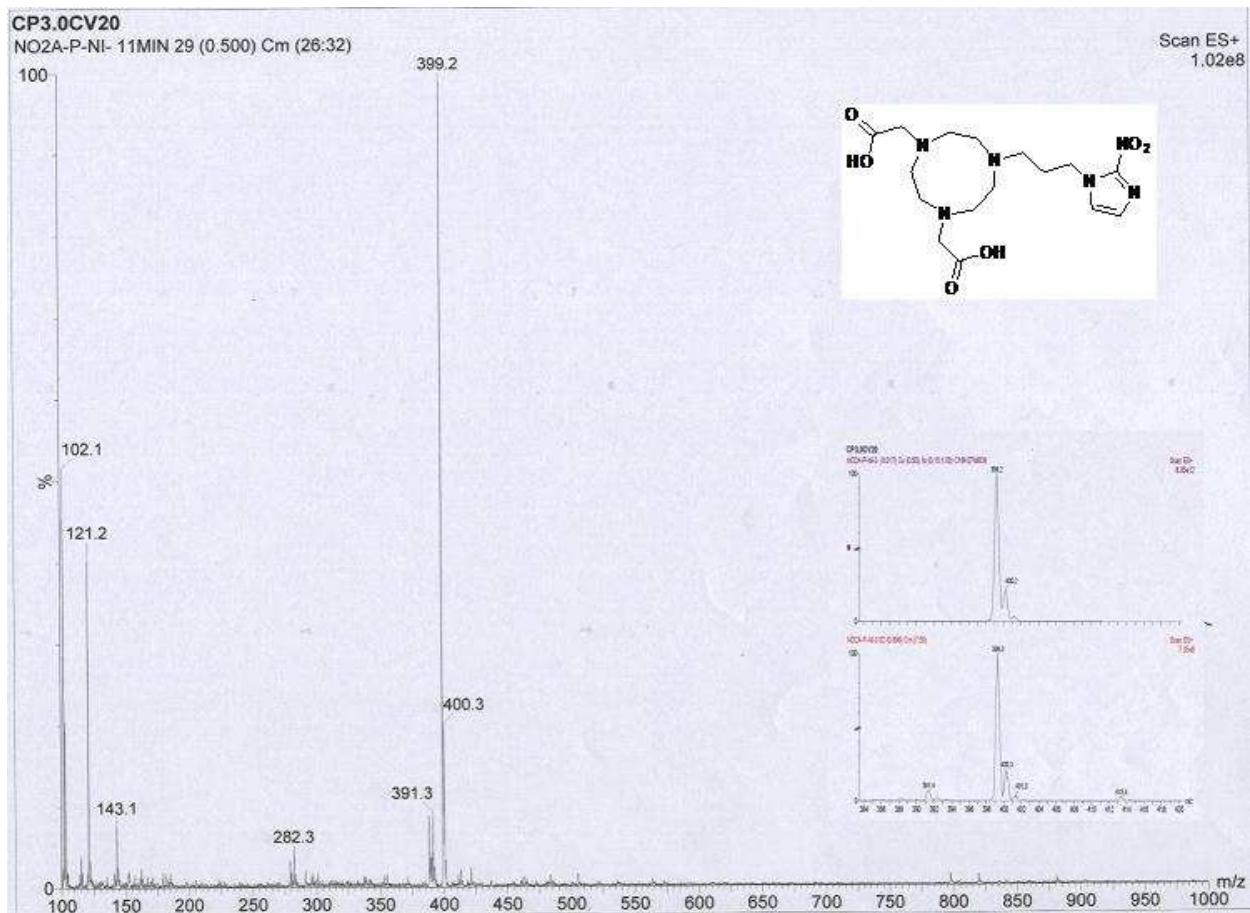


Figure 18S.

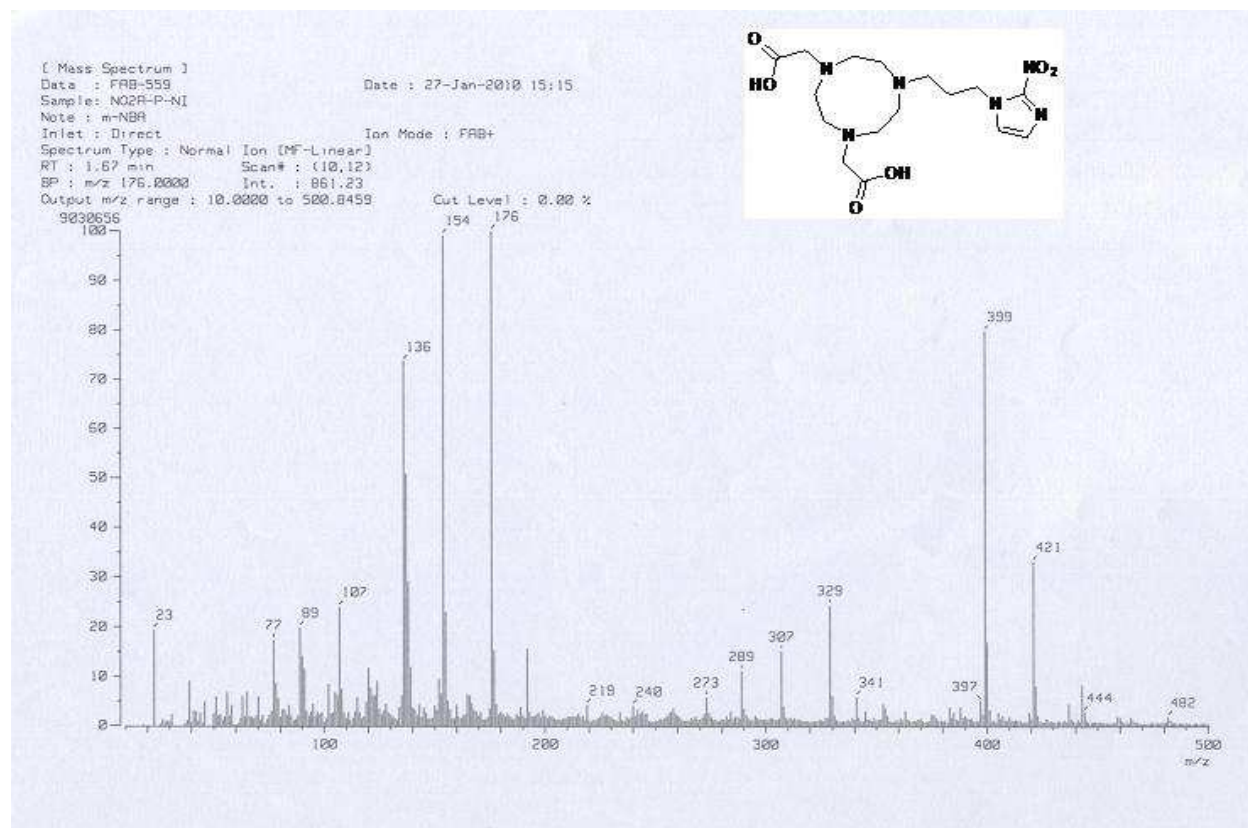


Figure 19S.

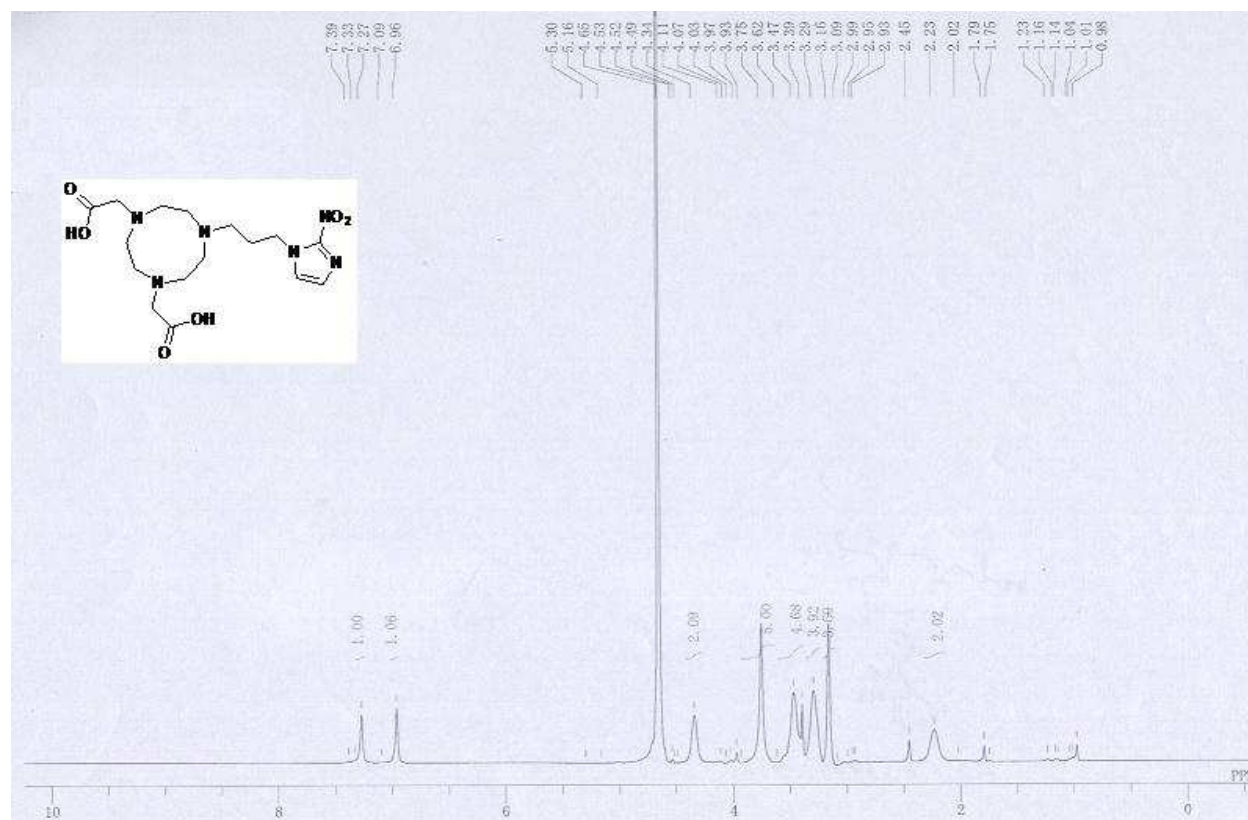


Figure 20S.

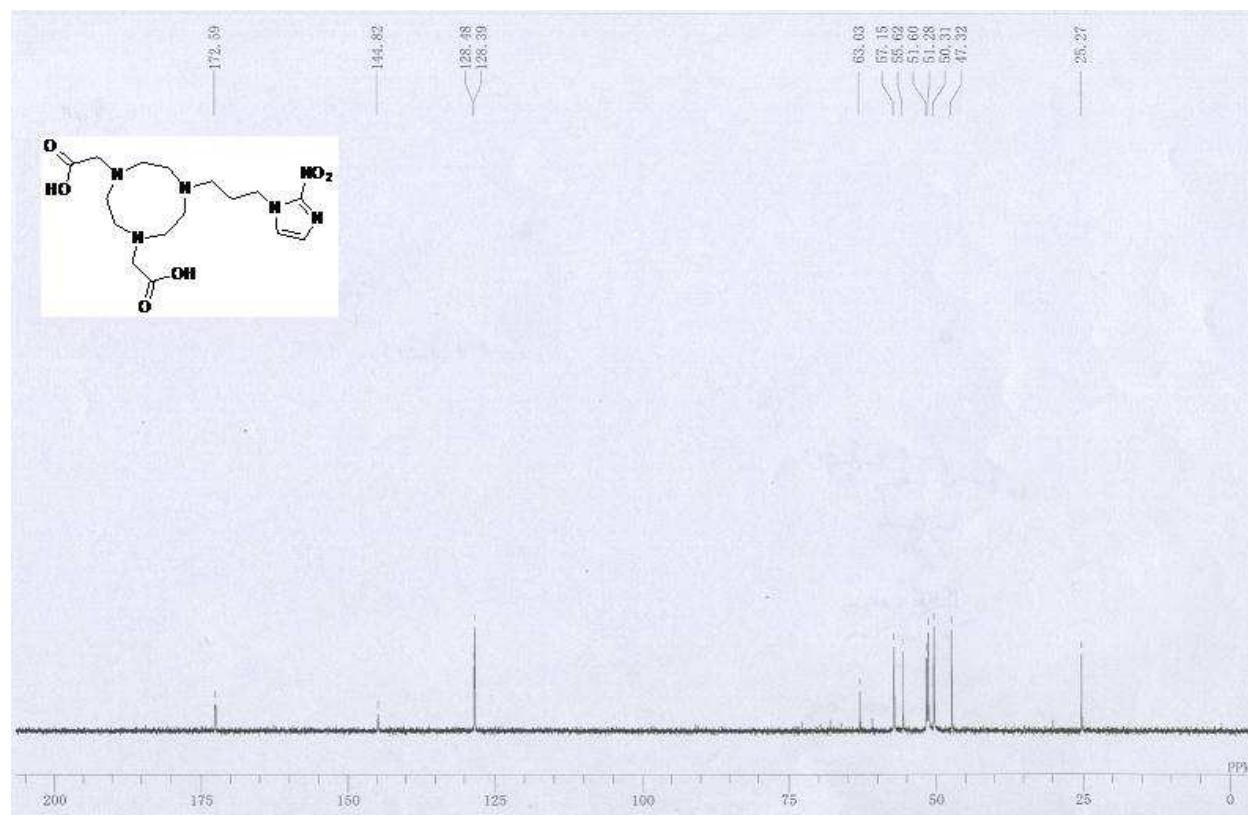


Figure 21S.

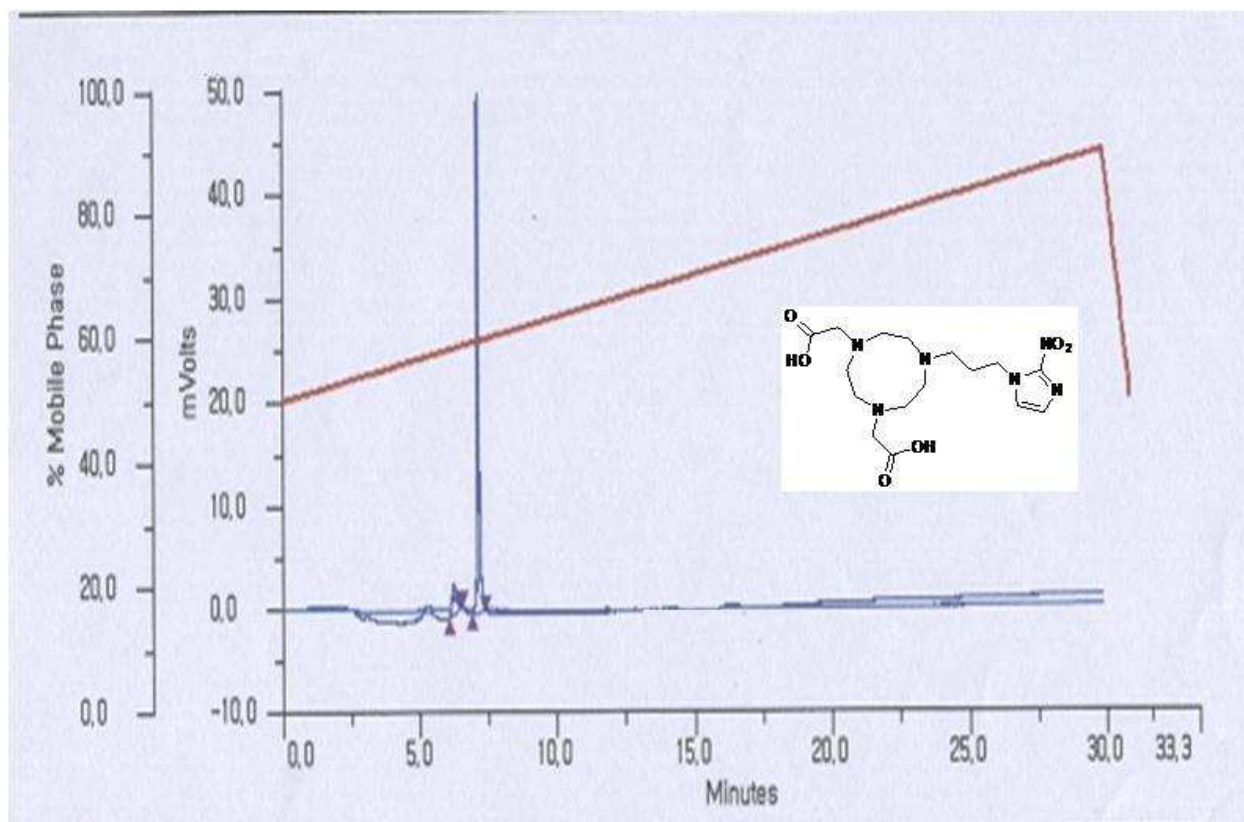


Figure 22S.

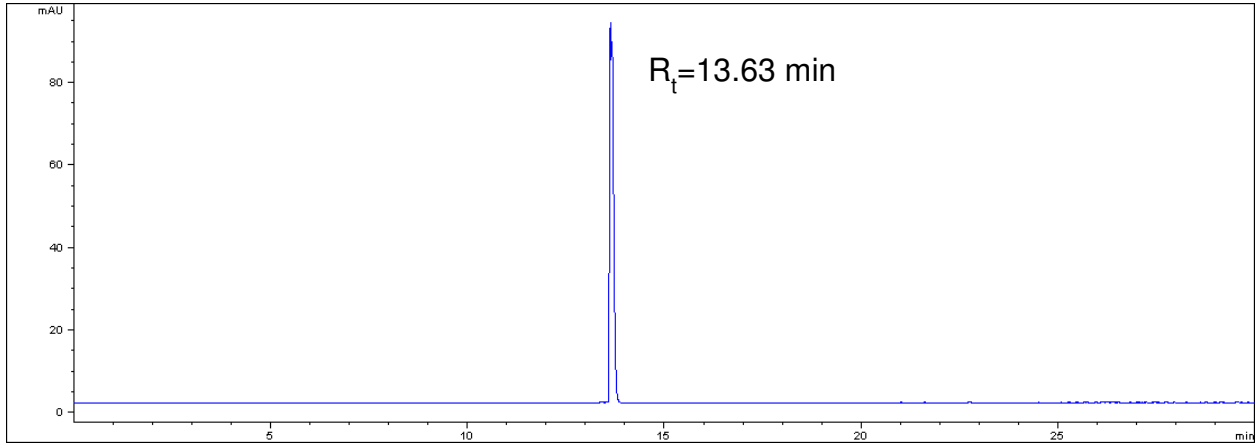


Figure 23S.

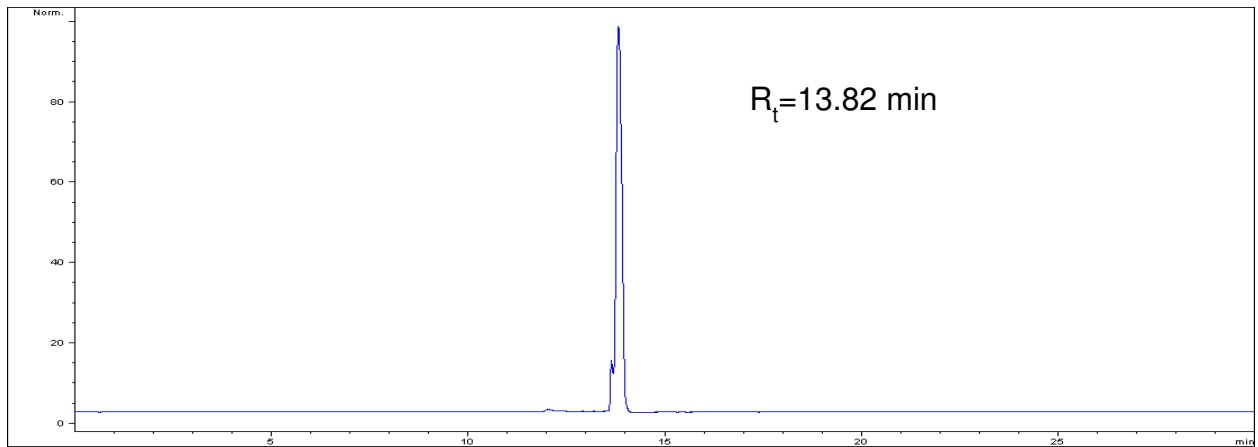
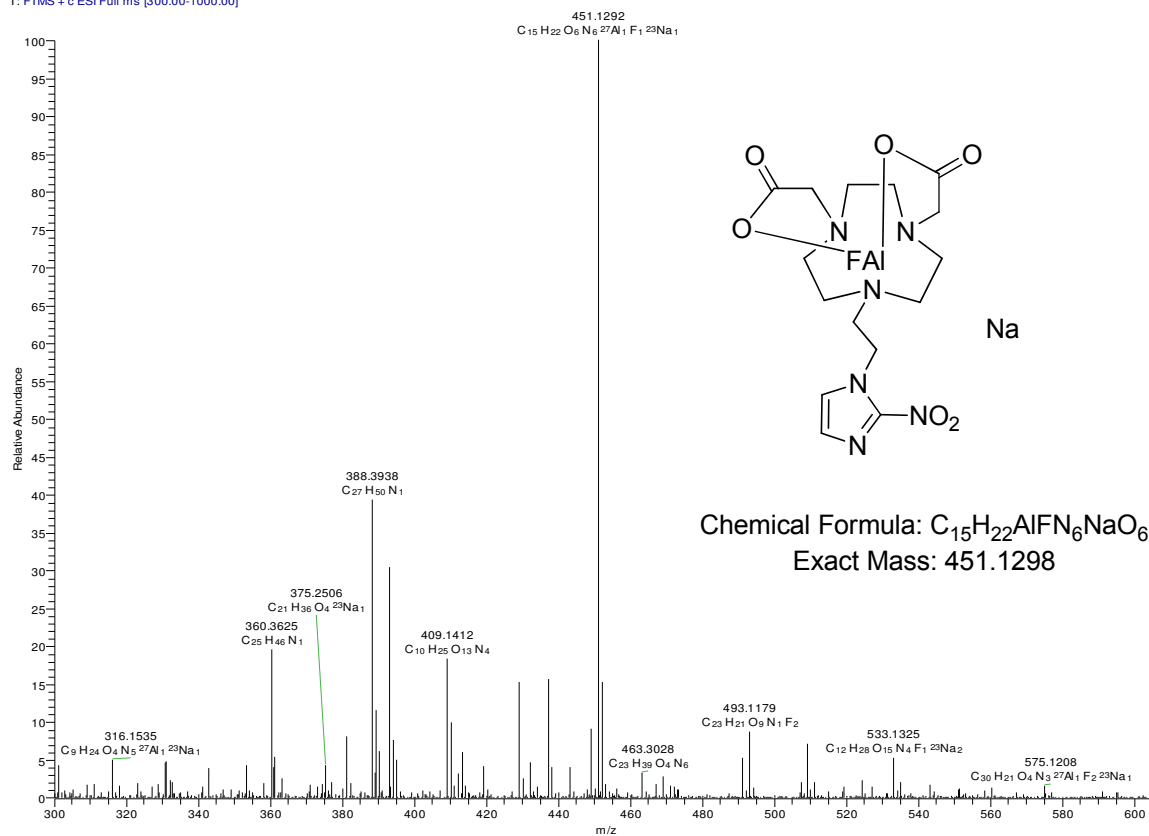


Figure 24S.

YangBH_1_#110-121 RT: 1.38-1.48 AV: 12 NL: 1.11E7
T: FTMS + c ESI Full ms [300.00-1000.00]



C16H25AlFN6O6: C16 H25 Al1 F1 N6 O6 pa Chrg 1

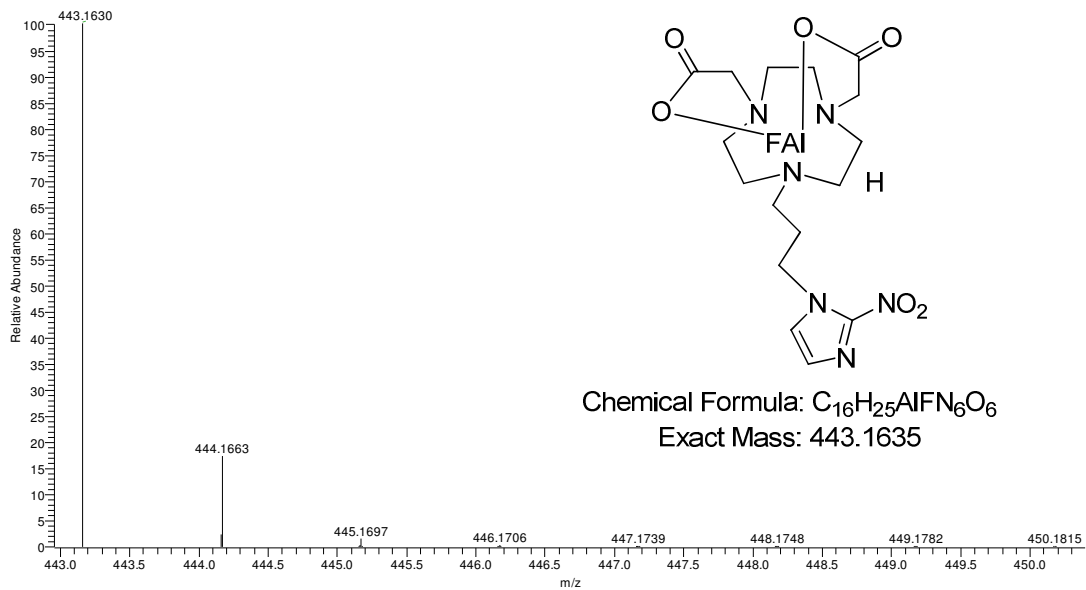


Figure 26S.