

SUPPORTING INFORMATION

Triple-Helical Transition State Analogs: A New Class of Selective Matrix Metalloproteinase Inhibitors

Janelle Lauer-Fields,^{1,2} Keith Brew,² John K. Whitehead,³ Shunzi Li,³ Robert P. Hammer,³ and Gregg B. Fields^{1,*}

¹Department of Chemistry & Biochemistry and ²College of Biomedical Sciences, Florida Atlantic University, Boca Raton, FL, 33431 and ³Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803

*Corresponding author: Department of Chemistry & Biochemistry, Florida Atlantic University, 777 Glades Road, 301A Physical Sciences Building, Boca Raton, FL 33431. Phone 561-297-2093, Fax 561-297-2759, e-mail fieldsg@fau.edu

SUPPORTING INFORMATION FIGURE LEGENDS

Figure S1. ^1H NMR spectrum (250 Hz, CD_3SOCD_3) of (*R,S*)-2-isopropyl-3-((1-(*N*-(9-fluorenylmethoxycarbonyl)amino)-methyl)-adamantyloxyphosphinyl) propanoic acid (**1**).

Figure S2. ^{13}C NMR spectrum (75 Hz, CD_3SOCD_3) of (*R,S*)-2-isopropyl-3-((1-(*N*-(9-fluorenylmethoxycarbonyl)amino)-methyl)-adamantyloxyphosphinyl) propanoic acid (**1**).

Figure S3. ^{31}P NMR spectrum (101 Hz, CD_3SOCD_3) of (*R,S*)-2-isopropyl-3-((1-(*N*-(9-fluorenylmethoxycarbonyl)amino)-methyl)-adamantyloxyphosphinyl) propanoic acid (**1**).

Figure S4. ^1H NMR spectrum (250 Hz, CDCl_3) of 2-isopropyl-3-oxobutyric acid allyl ester (**2**).

Figure S5. ^{13}C NMR spectrum (63 Hz, CDCl_3) of 2-isopropyl-3-oxobutyric acid allyl ester (**2**).

Figure S6. ^1H NMR spectrum (250 Hz, CDCl_3) of 2-isopropylacrylic acid allyl ester (**6**).

Figure S7. ^{13}C NMR spectrum (75 Hz, CDCl_3) of 2-isopropylacrylic acid allyl ester (**6**).

Figure S8. ^1H NMR spectrum (300 Hz, CD_3SOCD_3) of (*R,S*)-2-isopropyl-3-((1-(*N*-(9-fluorenylmethoxycarbonyl)amino)-methyl)-phosphinic acid) propanoic acid allyl ester (**7**).

Figure S9. ^{13}C NMR spectrum (75 Hz, CD_3SOCD_3) of (*R,S*)-2-isopropyl-3-((1-(*N*-(9-fluorenylmethoxycarbonyl)amino)-methyl)-phosphinic acid) propanoic acid allyl ester (**7**).

Figure S10. ^{31}P NMR spectrum (101 Hz, CD_3SOCD_3) of (*R,S*)-2-isopropyl-3-((1-(*N*-(9-fluorenylmethoxycarbonyl)amino)-methyl)-phosphinic acid) propanoic acid allyl ester (**7**).

Figure S11. ^1H NMR spectrum (250 Hz, CDCl_3) of (*R,S*)-2-isopropyl-3-((1-(*N*-(9-fluorenylmethoxycarbonyl)amino)-methyl)-adamantyloxyphosphinyl) propanoic acid, allyl ester (**8**).

Figure S12. ^{13}C NMR spectrum (63 Hz, CDCl_3) of (*R,S*)-2-isopropyl-3-((1-(*N*-(9-fluorenylmethoxycarbonyl)amino)-methyl)-adamantylxyphosphinyl) propanoic acid, allyl ester (**8**).

Figure S13. ^{31}P NMR spectrum (101 Hz, CDCl_3) of (*R,S*)-2-isopropyl-3-((1-(*N*-(9-fluorenylmethoxycarbonyl)amino)-methyl)-adamantylxyphosphinyl) propanoic acid, allyl ester (**8**).

Complete reference 26: Reiter, L. A.; Rizzi, J. P.; Pandit, J.; Lasut, M. J.; McGahee, S. M.; Parikh, V. D.; Blake, J. F.; Danley, D. E.; Laird, E. R.; Lopez-Anaya, A.; Lopresti-Morrow, L. L.; Mansour, M. N.; Martinelli, G. J.; Mitchell, P. G.; Owens, B. S.; Pauly, T. A.; Reeves, L. M.; Schulte, G. K.; Yocum, S. A. *Bioorg. Med. Chem. Lett.* **1999**, *9*, 127-132.

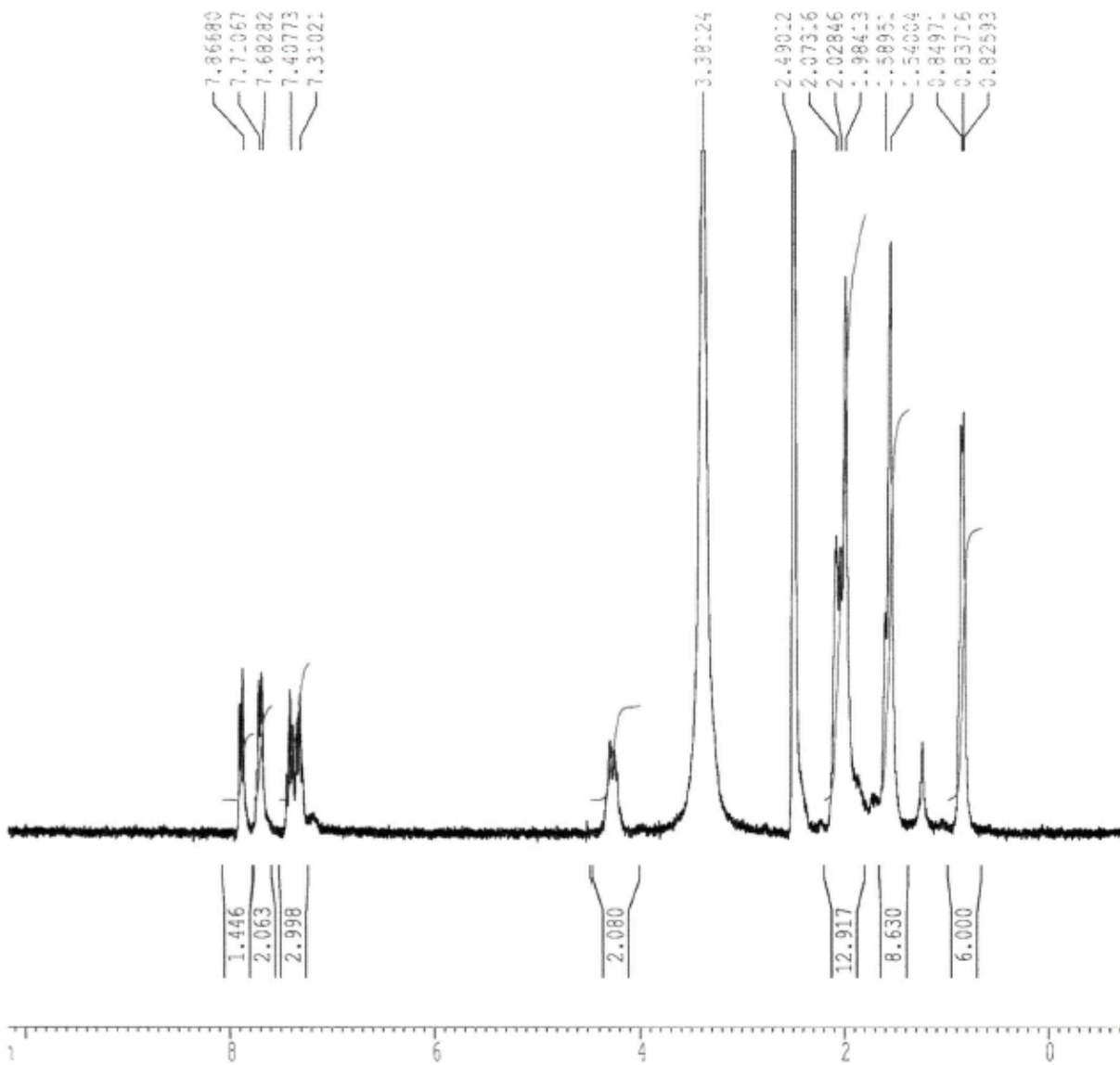
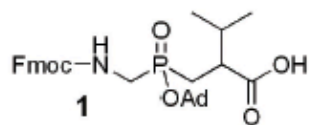


Figure S1

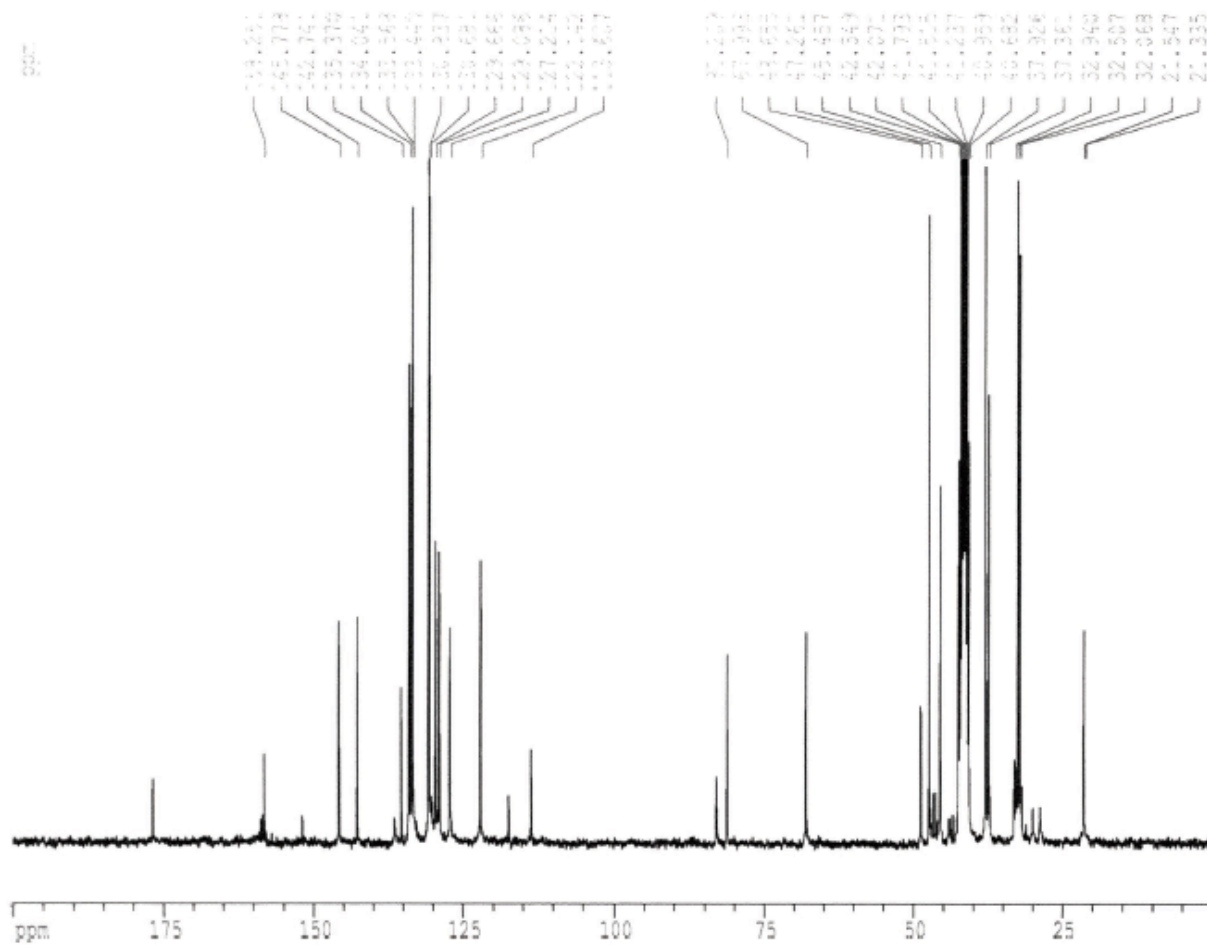
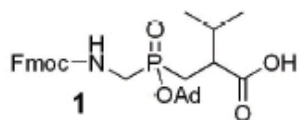


Figure S2

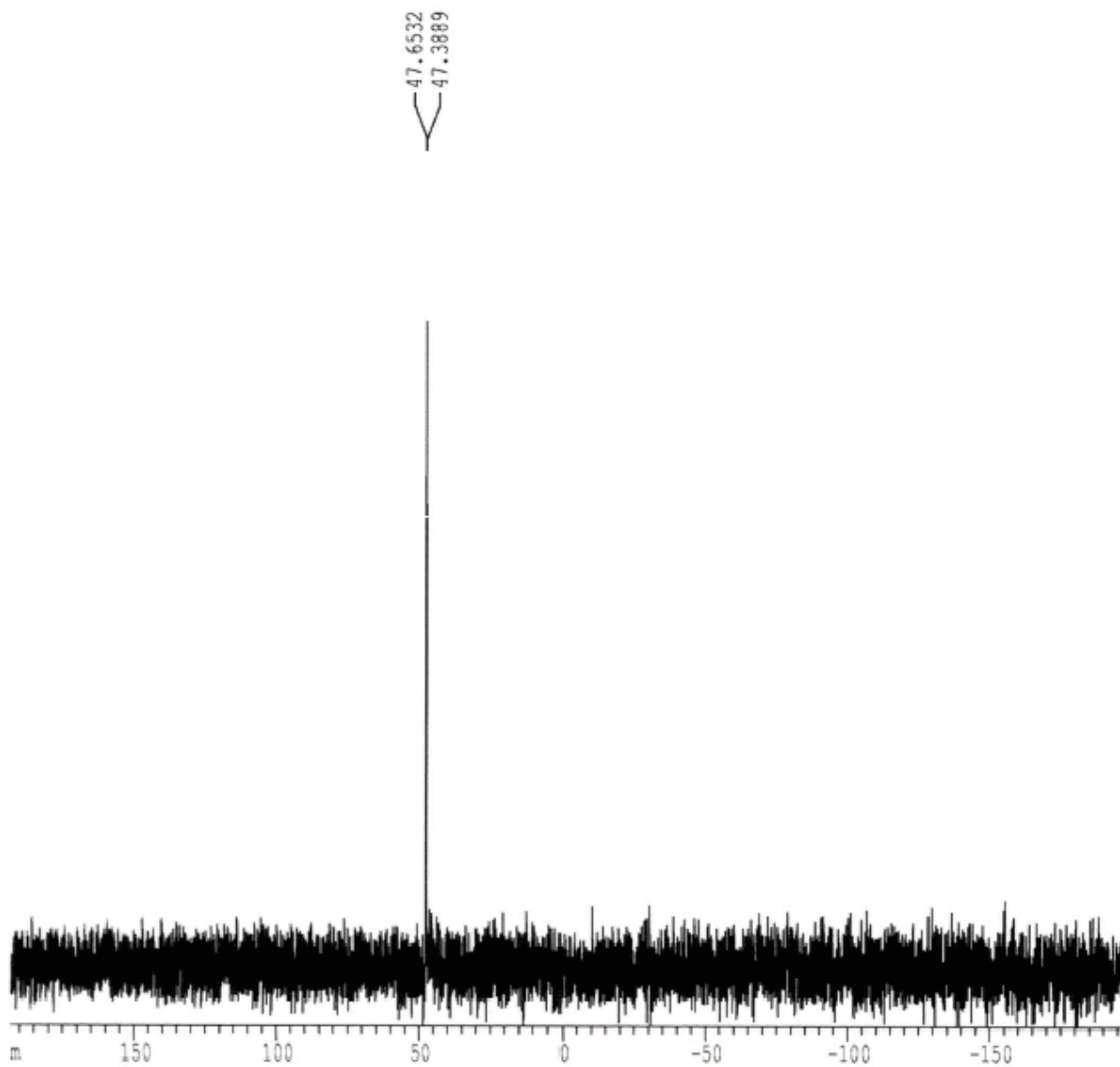
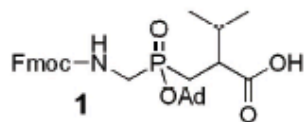


Figure S3

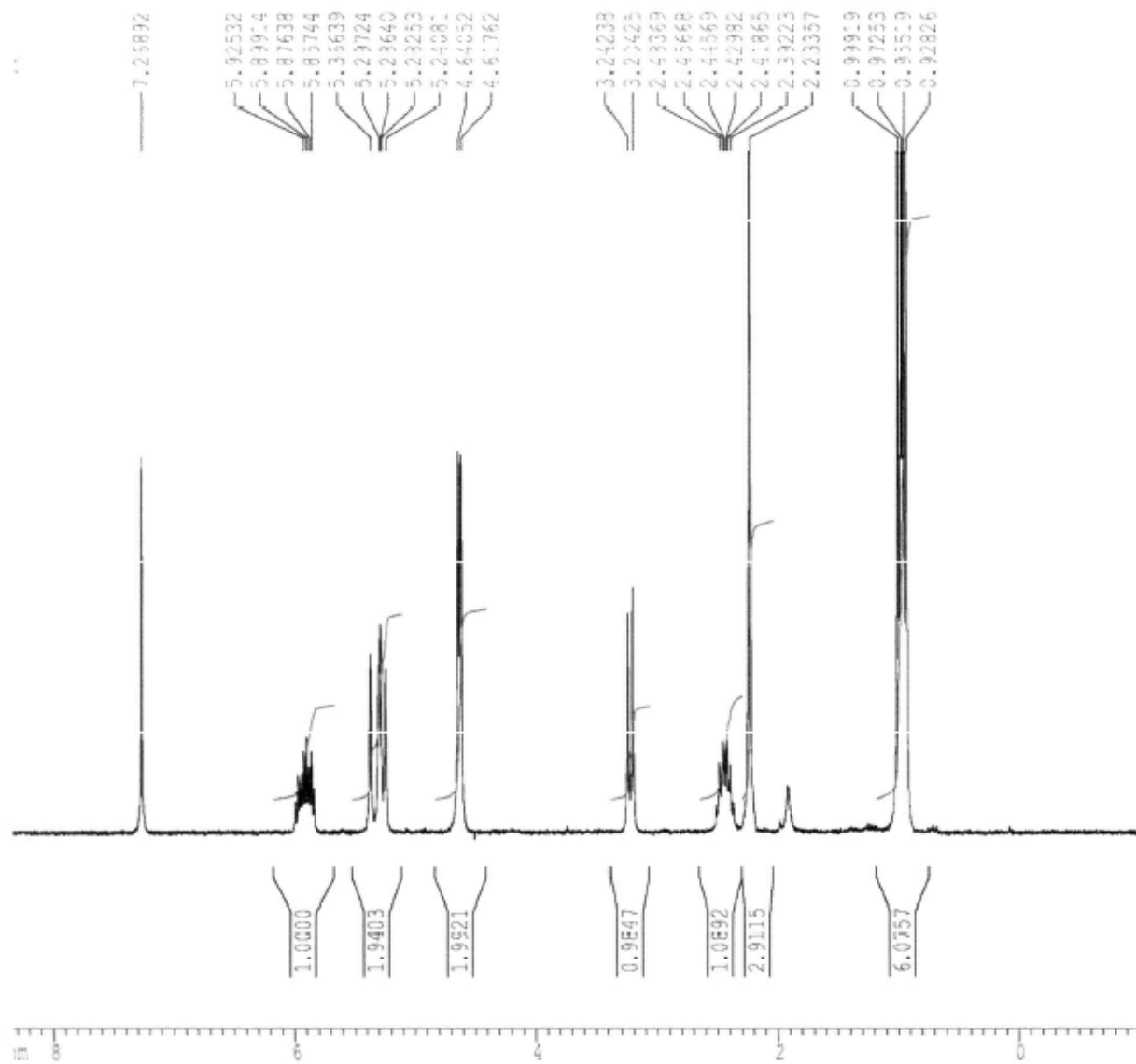
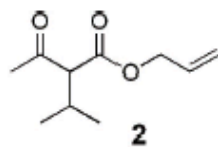


Figure S4

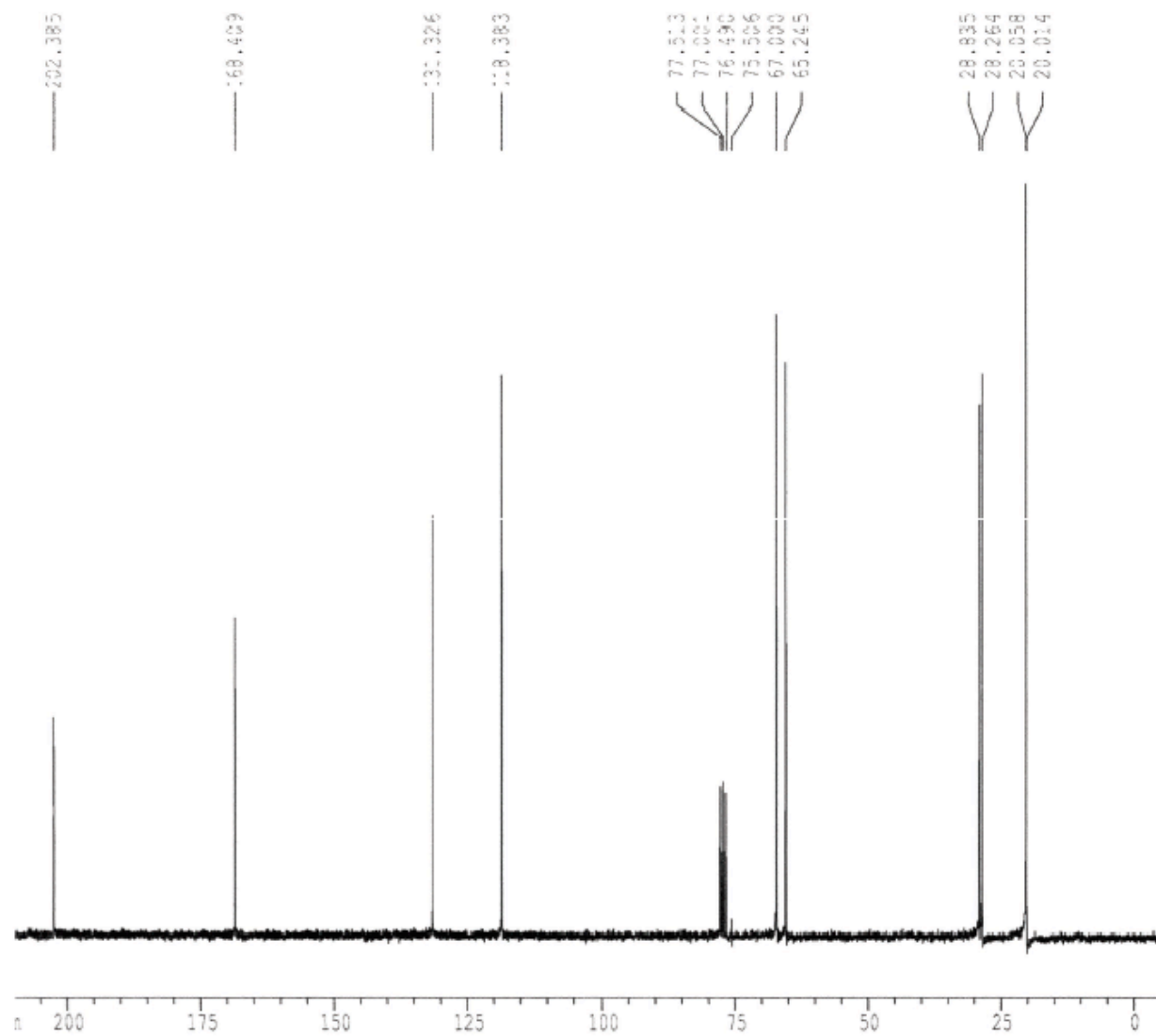
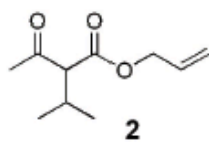


Figure S5

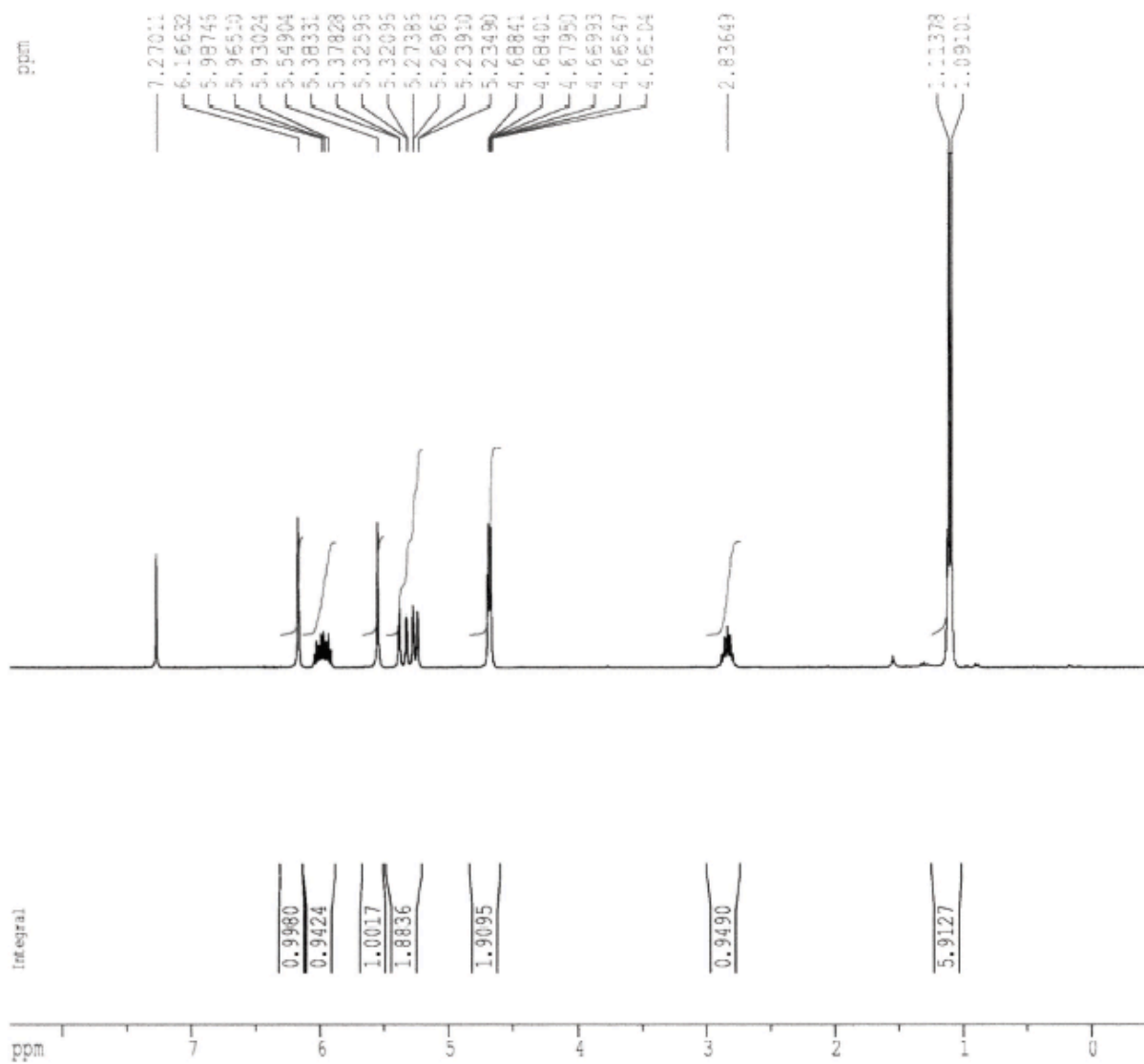
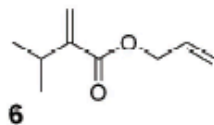


Figure S6

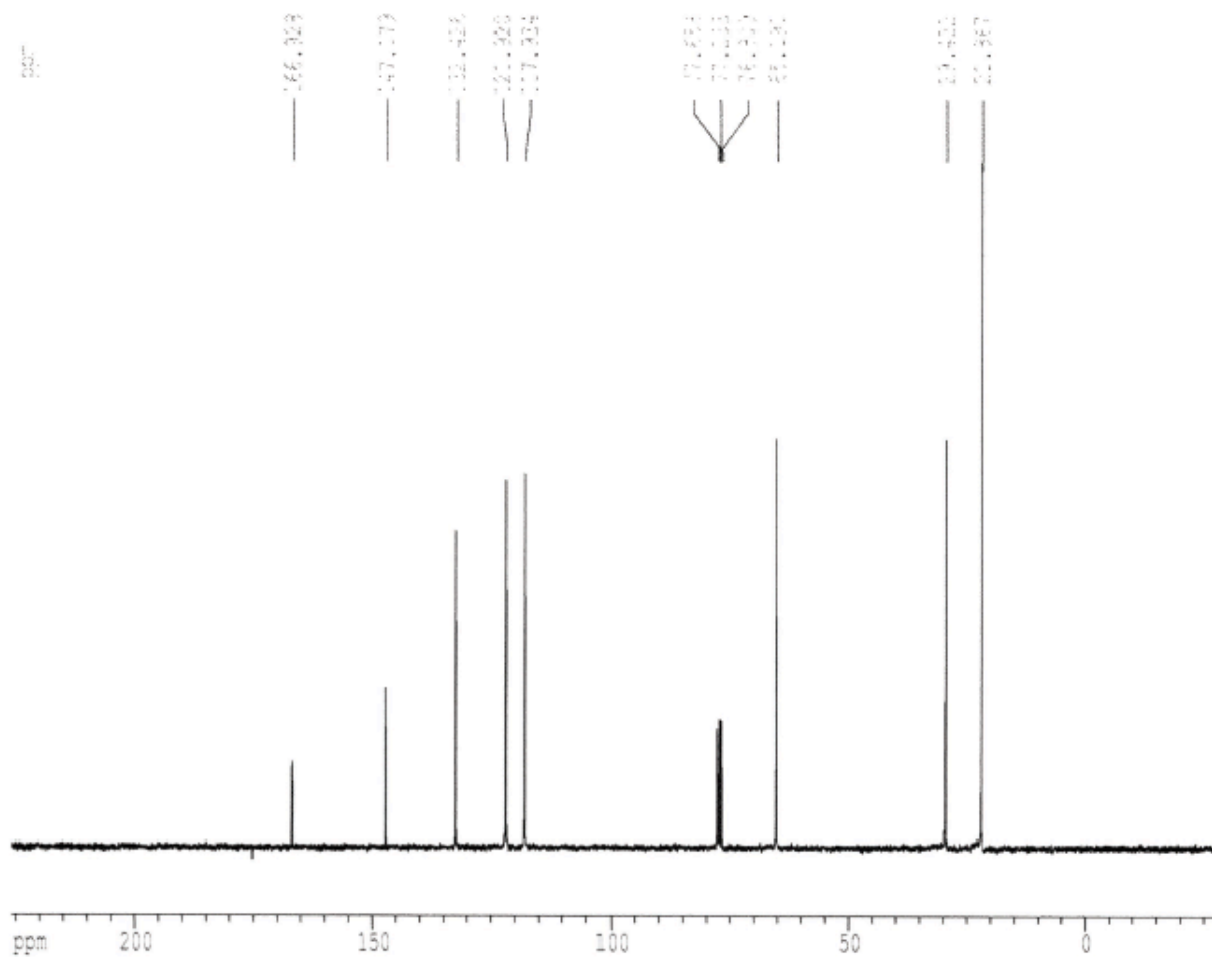
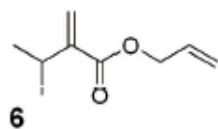


Figure S7

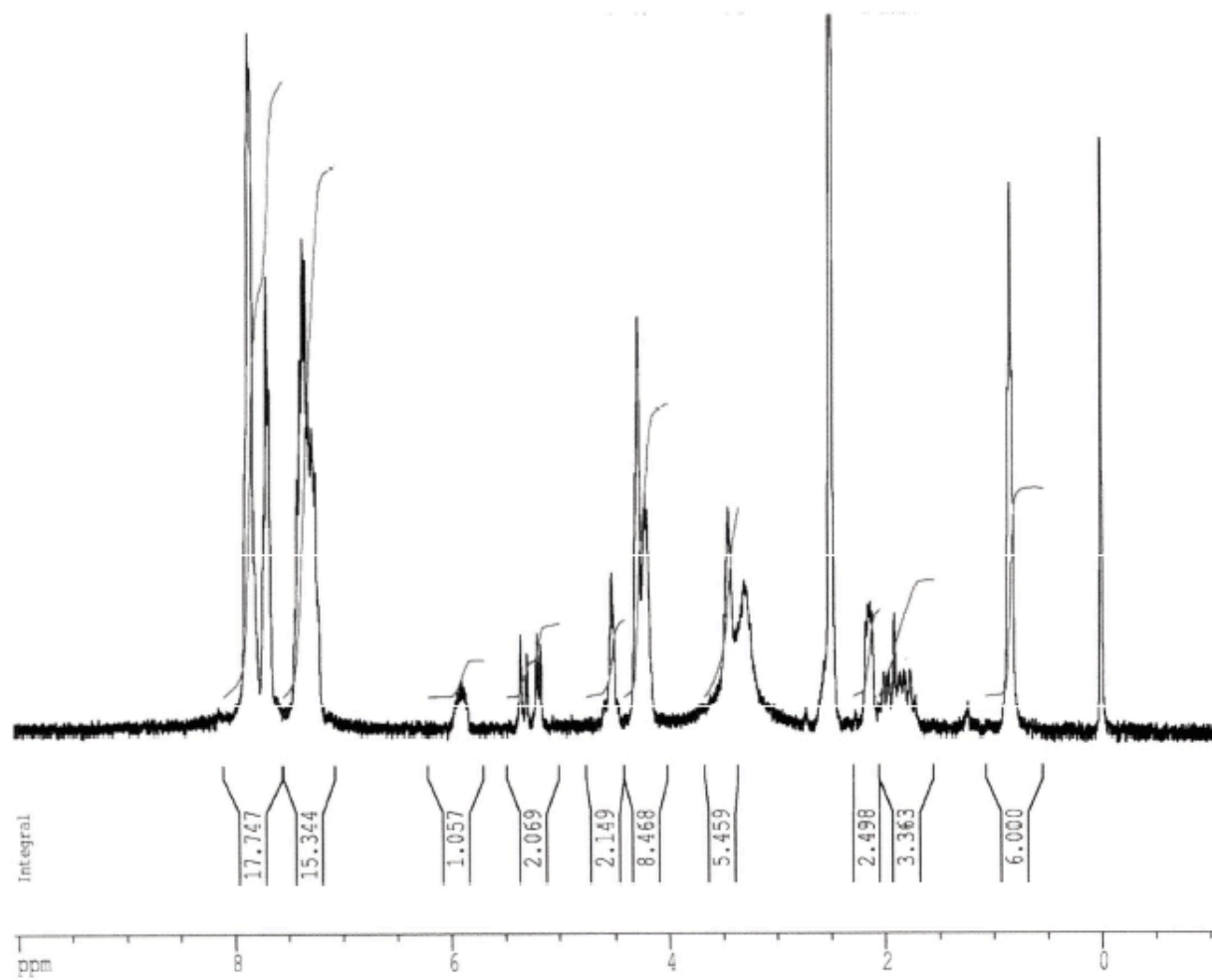
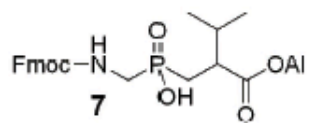


Figure S8

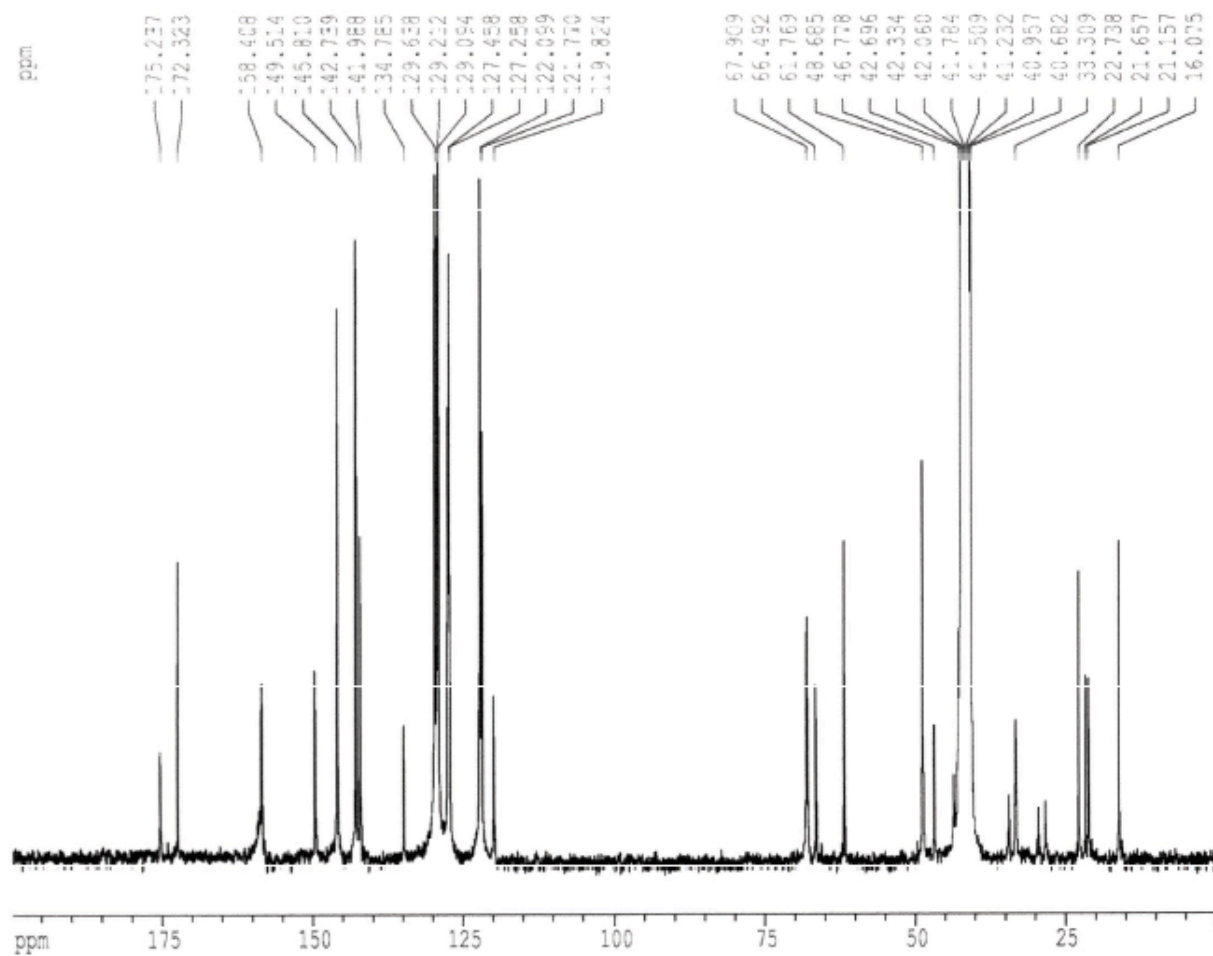
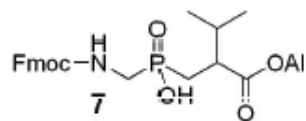


Figure S9

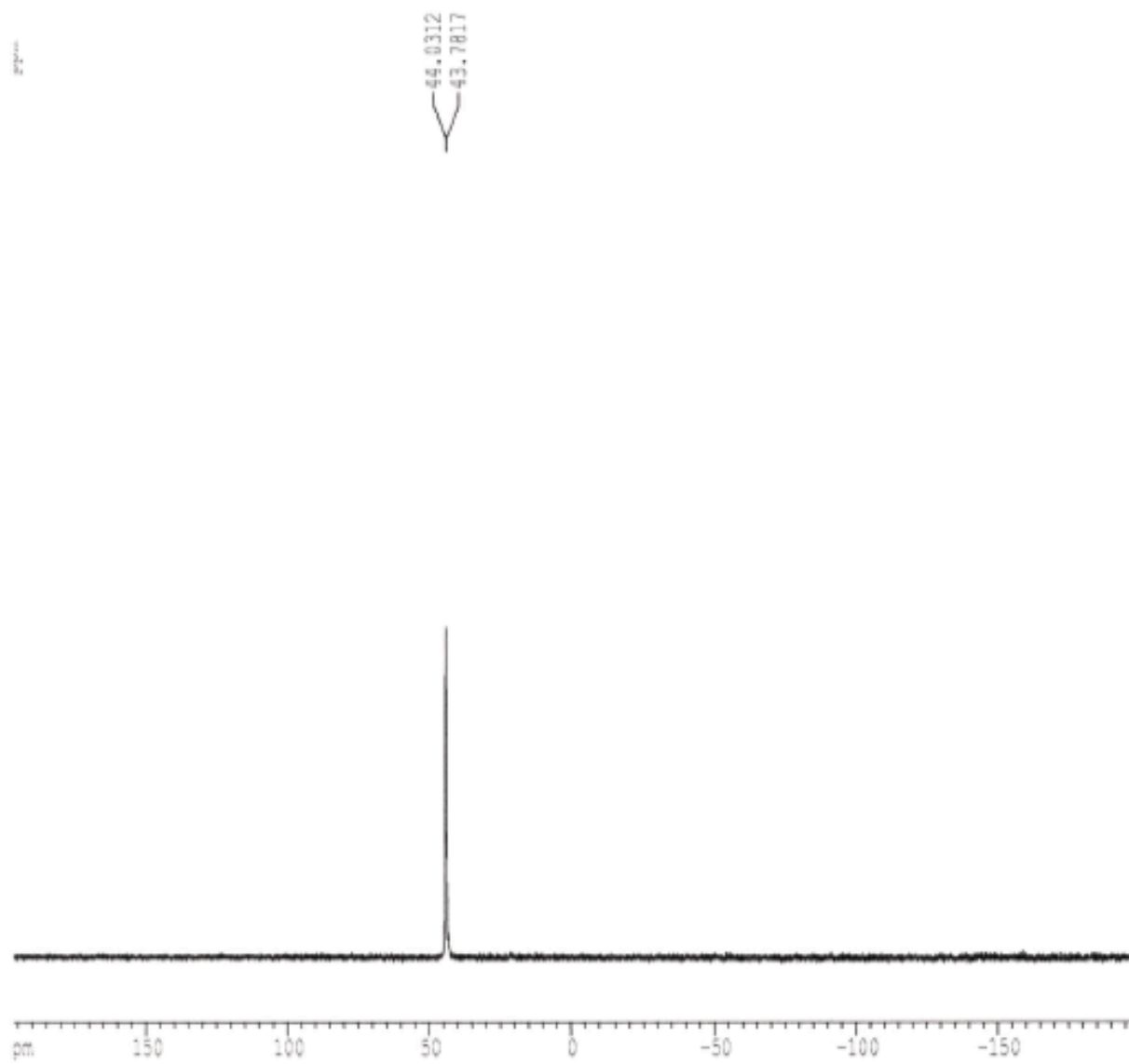
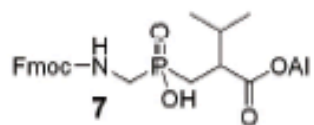


Figure S10

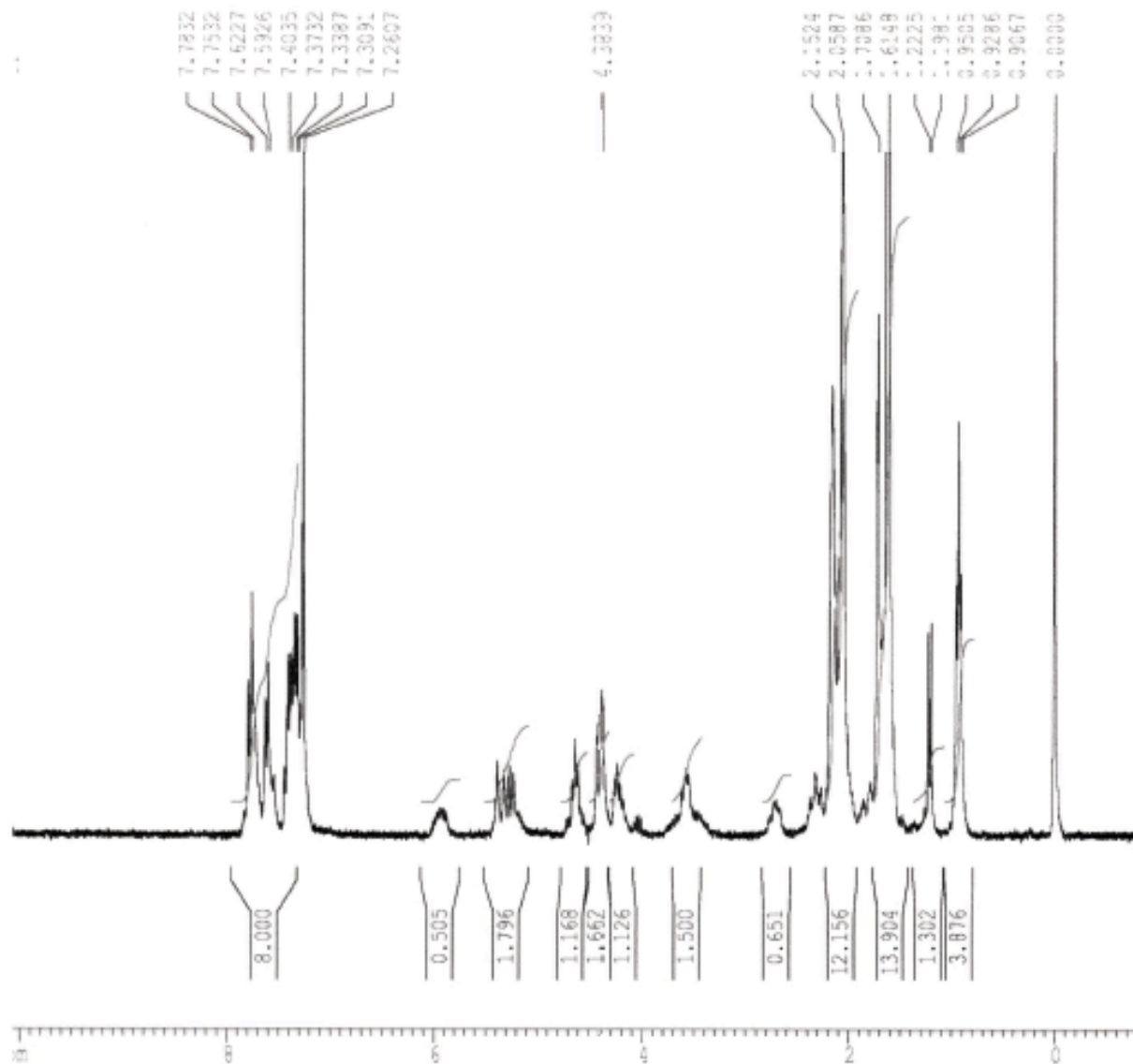
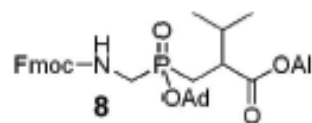


Figure S11

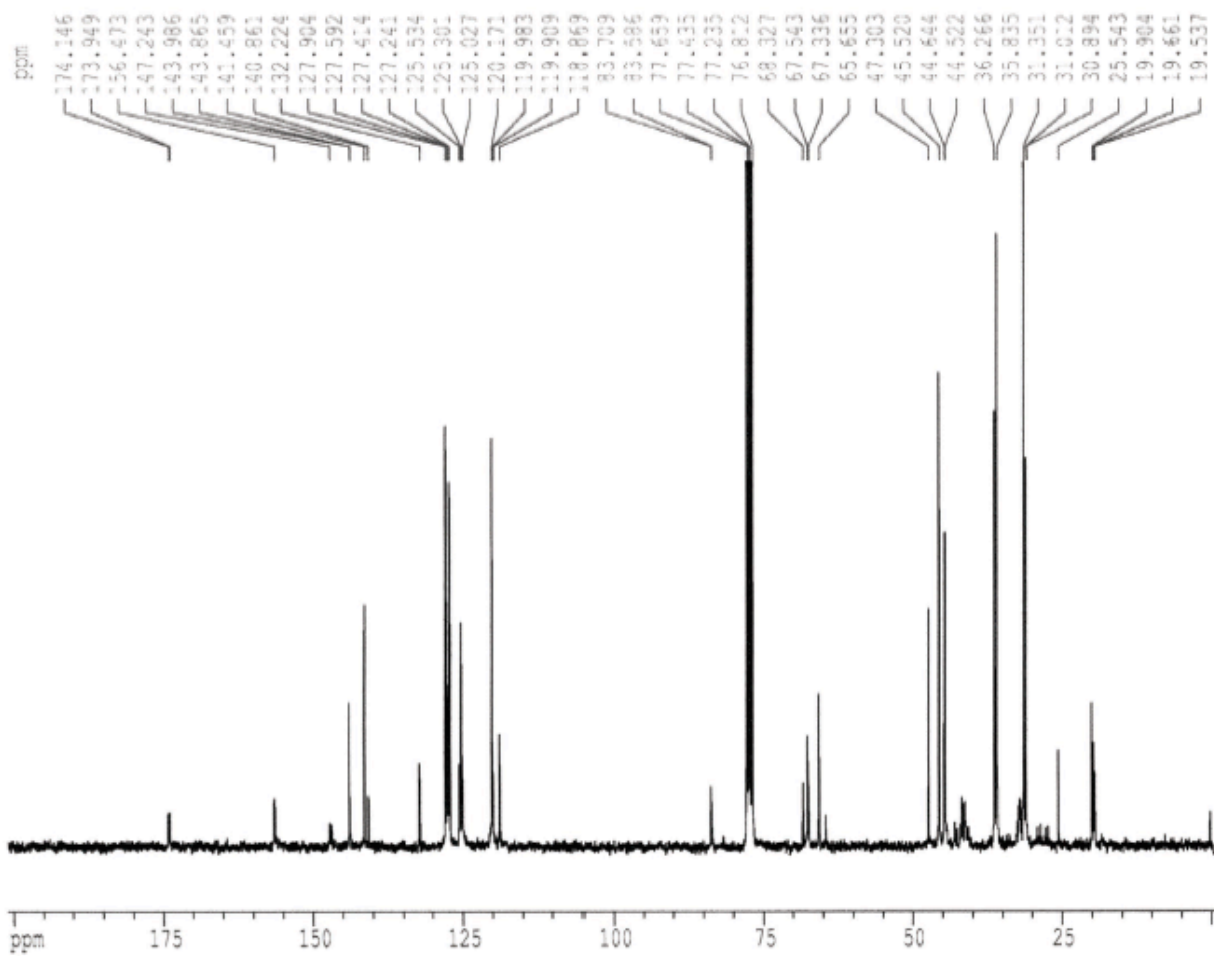
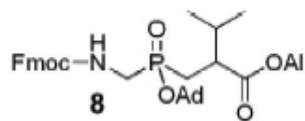


Figure S12

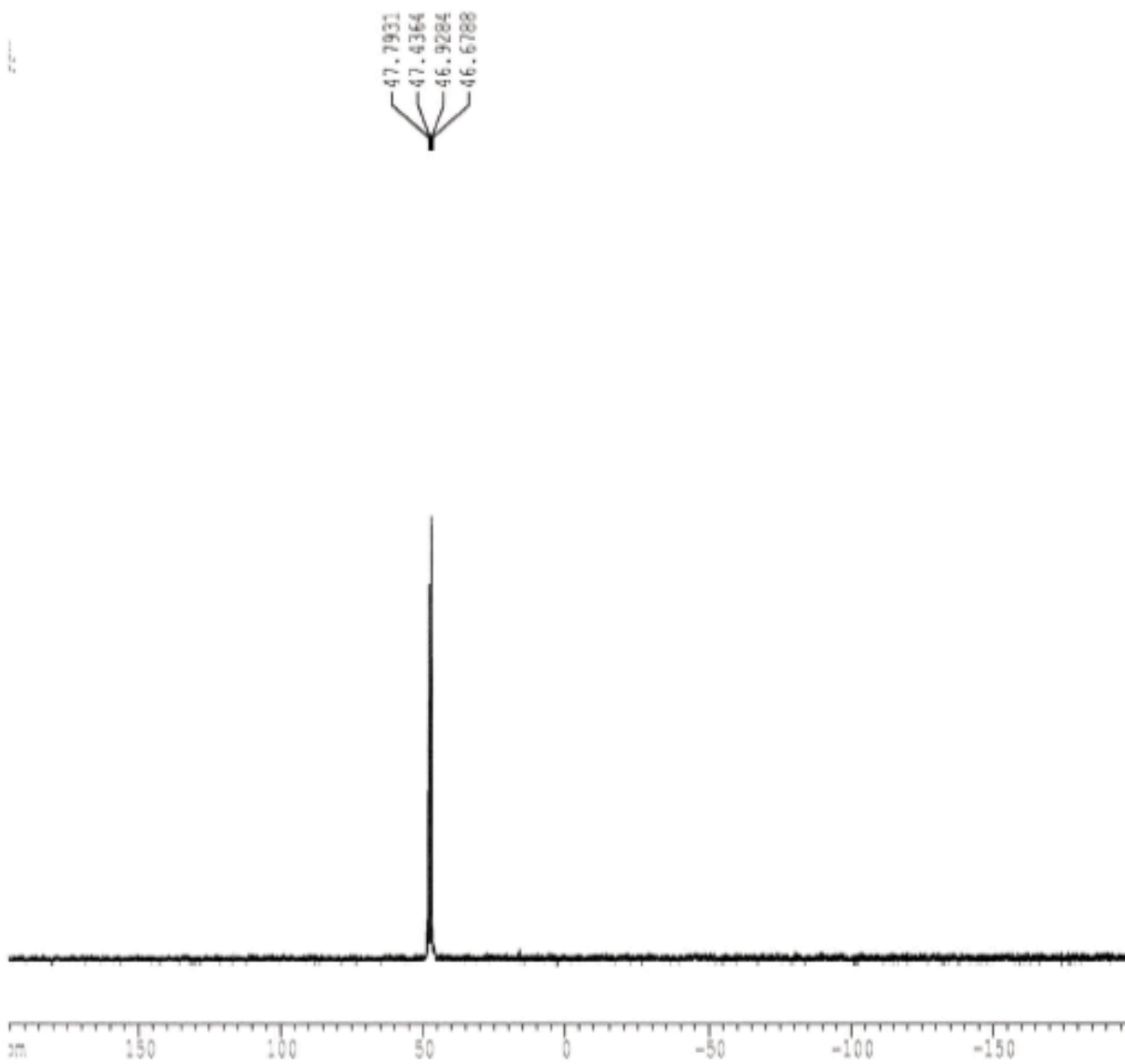
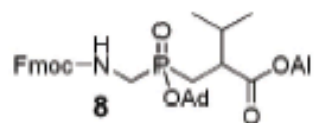


Figure S13