

SUPPORTING INFORMATION

Development of new antimicrobial oleanonic acid polyamine conjugates

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Cp d	SMILES
2a	<chem>CC1(C)CC[C@]2(C(NCCN)=O)CC[C@@]3(C)[C@]4(C)CC[C@]5([H])C(C)(C)C(CC[C@]5(C)[C@@]4([H])CC=C3[C@]2([H])C1)=O</chem>
2b	<chem>CC1(C)CC[C@]2(C(NCCCN)=O)CC[C@@]3(C)[C@]4(C)CC[C@]5([H])C(C)(C)C(CC[C@]5(C)[C@@]4([H])CC=C3[C@]2([H])C1)=O</chem>
2c	<chem>CC1(C)CC[C@]2(C(NCCCCCN)=O)CC[C@@]3(C)[C@]4(C)CC[C@]5([H])C(C)(C)C(CC[C@]5(C)[C@@]4([H])CC=C3[C@]2([H])C1)=O</chem>
2d	<chem>CC1(C)CC[C@]2(C(NCCCN3CCCC3=O)=O)CC[C@@]4(C)[C@]5(C)CC[C@]6([H])C(C)(C)C(CC[C@]6(C)[C@@]5([H])CC=C4[C@]2([H])C1)=O</chem>
2e	<chem>CC1(C)CC[C@]2(C(NCCCN3CCOCC3=O)CC[C@@]4(C)[C@]5(C)CC[C@]6([H])C(C)(C)C(CC[C@]6(C)[C@@]5([H])CC=C4[C@]2([H])C1)=O</chem>
2f	<chem>CC1(C)CC[C@]2(C(NCCCN3CCN(CCCN)CC3=O)CC[C@@]4(C)[C@]5(C)CC[C@]6([H])C(C)(C)C(CC[C@]6(C)[C@@]5([H])CC=C4[C@]2([H])C1)=O</chem>
2g	<chem>CC1(C)CC[C@]2(C(NCCNCCN)=O)CC[C@@]3(C)[C@]4(C)CC[C@]5([H])C(C)(C)C(CC[C@]5(C)[C@@]4([H])CC=C3[C@]2([H])C1)=O</chem>
2h	<chem>CC1(C)CC[C@]2(C(NCCCNCCCN)=O)CC[C@@]3(C)[C@]4(C)CC[C@]5([H])C(C)(C)C(CC[C@]5(C)[C@@]4([H])CC=C3[C@]2([H])C1)=O</chem>
2i	<chem>CC1(C)CC[C@]2(C(NCCCN(C)CCN)=O)CC[C@@]3(C)[C@]4(C)CC[C@]5([H])C(C)(C)C(CC[C@]5(C)[C@@]4([H])CC=C3[C@]2([H])C1)=O</chem>
2j	<chem>CC1(C)CC[C@]2(C(NCCNCCNCCNCCN)=O)CC[C@@]3(C)[C@]4(C)CC[C@]5([H])C(C)(C)C(CC[C@]5(C)[C@@]4([H])CC=C3[C@]2([H])C1)=O</chem>
2k	<chem>CC1(C)CC[C@]2(C(NCCNCCNCCNCCNCCN)=O)CC[C@@]3(C)[C@]4(C)CC[C@]5([H])C(C)(C)C(CC[C@]5(C)[C@@]4([H])CC=C3[C@]2([H])C1)=O</chem>
2l	<chem>CC1(C)CC[C@]2(C(NCCCNCCCCNCCCN)=O)CC[C@@]3(C)[C@]4(C)CC[C@]5([H])C(C)(C)C(CC[C@]5(C)[C@@]4([H])CC=C3[C@]2([H])C1)=O</chem>

2m	<chem>CC1(C)CC[C@@]2(C(NCCCCCCCCOCCCN)=O)CC[C@@]3(C)[C@@]4(C)CC[C@@]5([H])C(C)(C)C(CC[C@@]5(C)[C@@]4([H])CC=C3[C@@]2([H])C1)=O</chem>
2n	<chem>CC1(C)CC[C@@]2(C(NCCCN(CCCN)CCCN)=O)CC[C@@]3(C)[C@@]4(C)CC[C@@]5([H])C(C)(C)C(CC[C@@]5(C)[C@@]4([H])CC=C3[C@@]2([H])C1)=O</chem>
3	<chem>CC1(C)C(NCCCNCCCCNCCCN)CC[C@@]2(C)[C@@]1([H])CC[C@@]3(C)[C@@]2([H])CC=C4[C@@]3(C)CC[C@@]5(C(OC)=O)[C@@]4([H])CC(C)(C)CC5</chem>
4	<chem>CC1(C)C(NCCCN(CC2)CCN2CCCN)CC[C@@]3(C)[C@@]1([H])CC[C@@]4(C)[C@@]3([H])CC=C5[C@@]4(C)CC[C@@]6(C(OC)=O)[C@@]5([H])CC(C)(C)CC6</chem>
5	<chem>CC1(C)C(CC[C@@]2(C)[C@@]1([H])CC[C@@]3(C)[C@@]2([H])CC=C4[C@@]3(C)CC[C@@]5(C(NCC#C)=O)[C@@]4([H])CC(C)(C)CC5)=O</chem>
6	<chem>CC1(C)C(CC[C@@]2(C)[C@@]1([H])CC[C@@]3(C)[C@@]2([H])CC=C4[C@@]3(C)CC[C@@]5(C(NCC#CCN(CCCN)CCCN)CCCN)=O)[C@@]4([H])CC(C)(C)CC5)=O</chem>
7a	<chem>CC1(C)[C@@H](O)CC[C@@]2(C)[C@@]1([H])CC[C@@]3(C)[C@@]2([H])CC=C4[C@@]3(C)CC[C@@]5(C(NCCCNCCCN)=O)[C@@]4([H])CC(C)(C)CC5</chem>
7b	<chem>CC1(C)[C@@H](O)CC[C@@]2(C)[C@@]1([H])CC[C@@]3(C)[C@@]2([H])CC=C4[C@@]3(C)CC[C@@]5(C(NCCCN(C)CCCN)=O)[C@@]4([H])CC(C)(C)CC5</chem>
7c	<chem>CC1(C)[C@@H](O)CC[C@@]2(C)[C@@]1([H])CC[C@@]3(C)[C@@]2([H])CC=C4[C@@]3(C)CC[C@@]5(C(NCCNCCNCCNCCN)=O)[C@@]4([H])CC(C)(C)CC5</chem>

Table S1: SMILES Code of the synthesized compounds

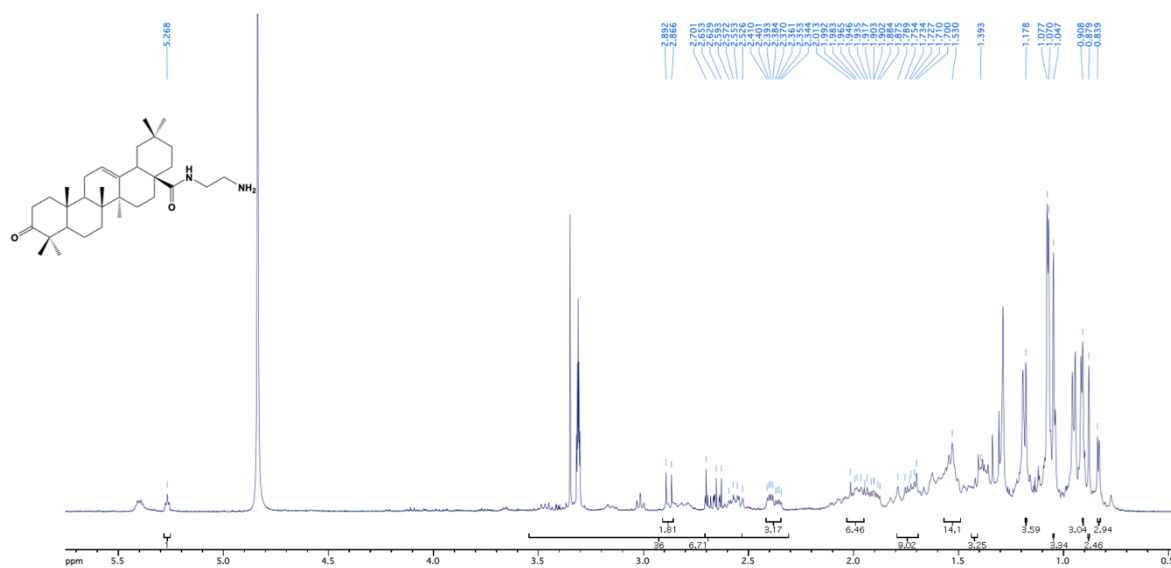


Figure S1. ^1H NMR spectrum of compound **2a**

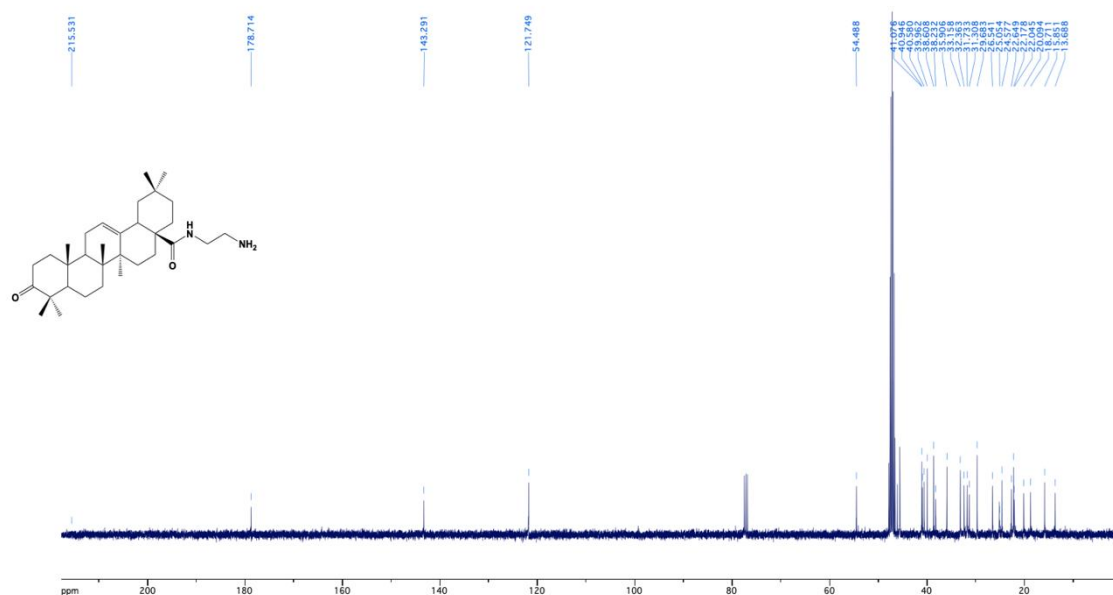


Figure S2. ^{13}C NMR spectrum of compound **2a**

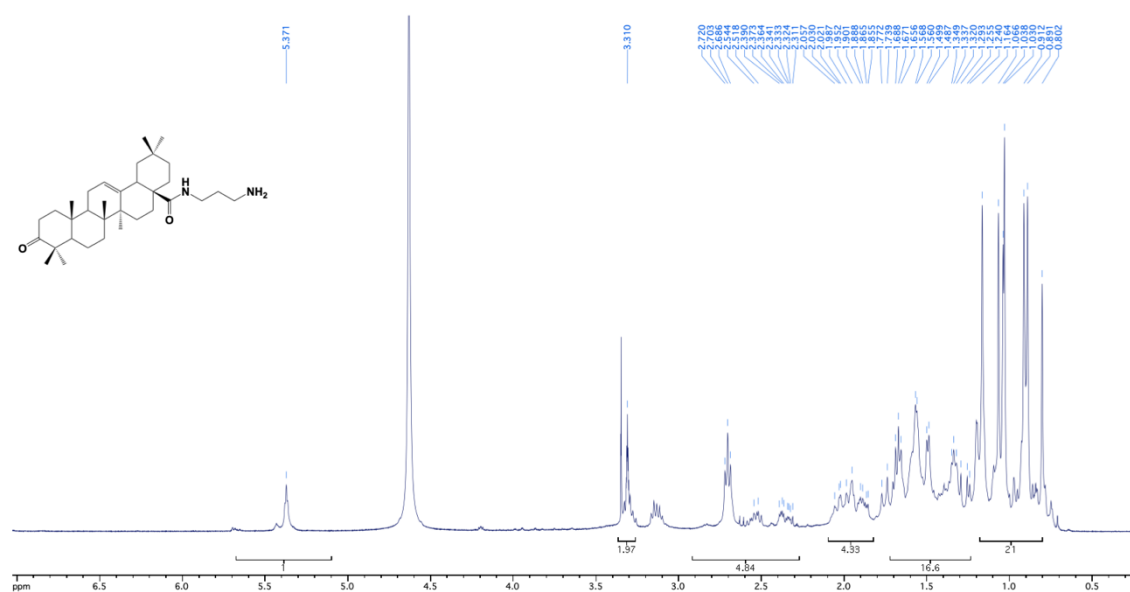


Figure S3. ^1H NMR spectrum of compound **2b**

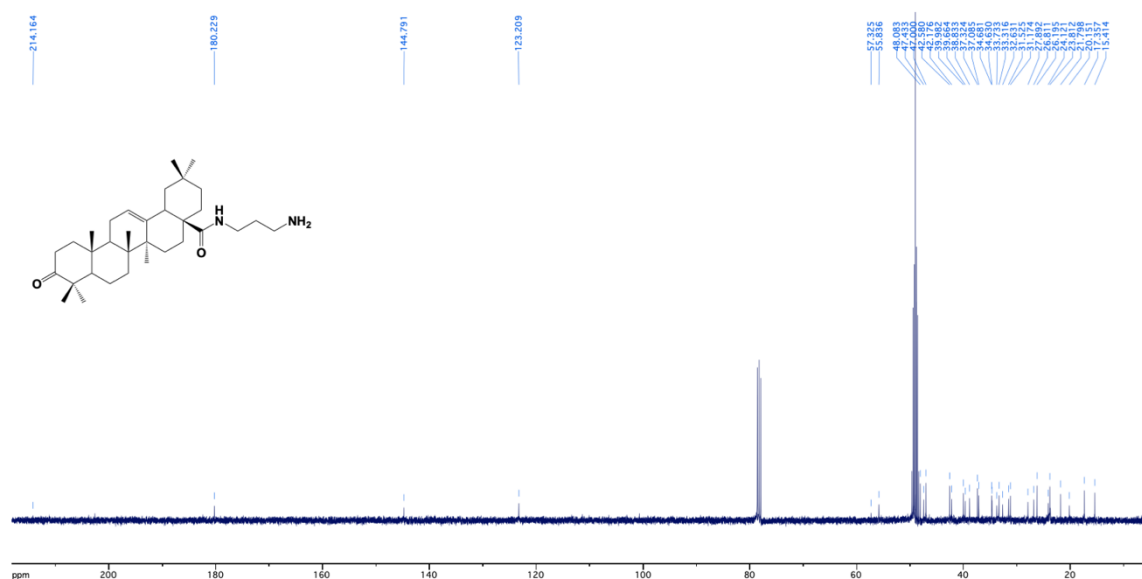


Figure S4. ^{13}C NMR spectrum of compound **2b**

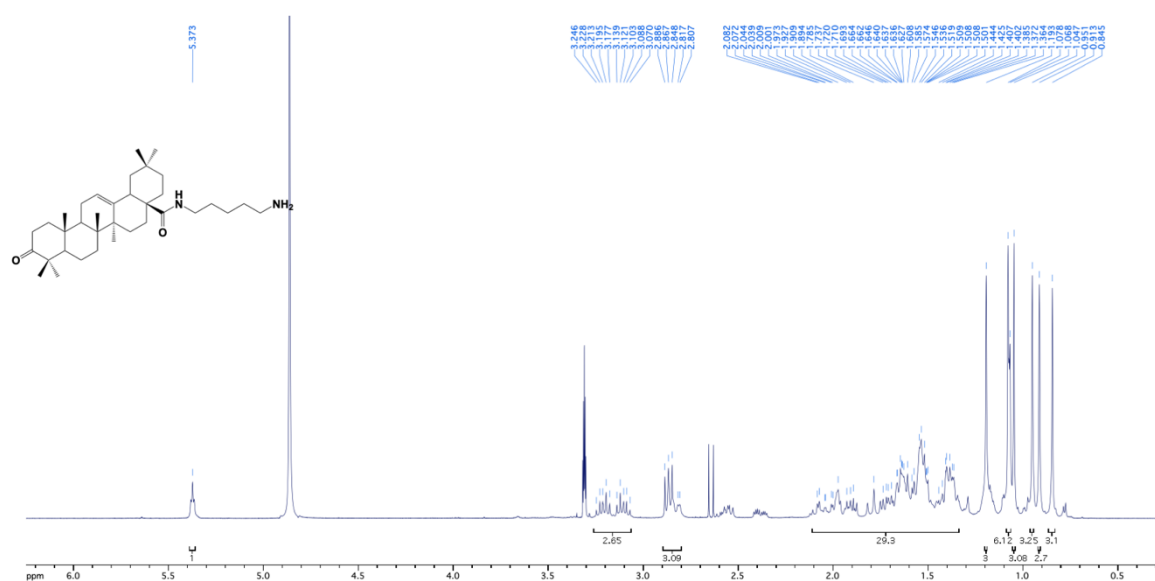


Figure S5. ^1H NMR spectrum of compound **2c**

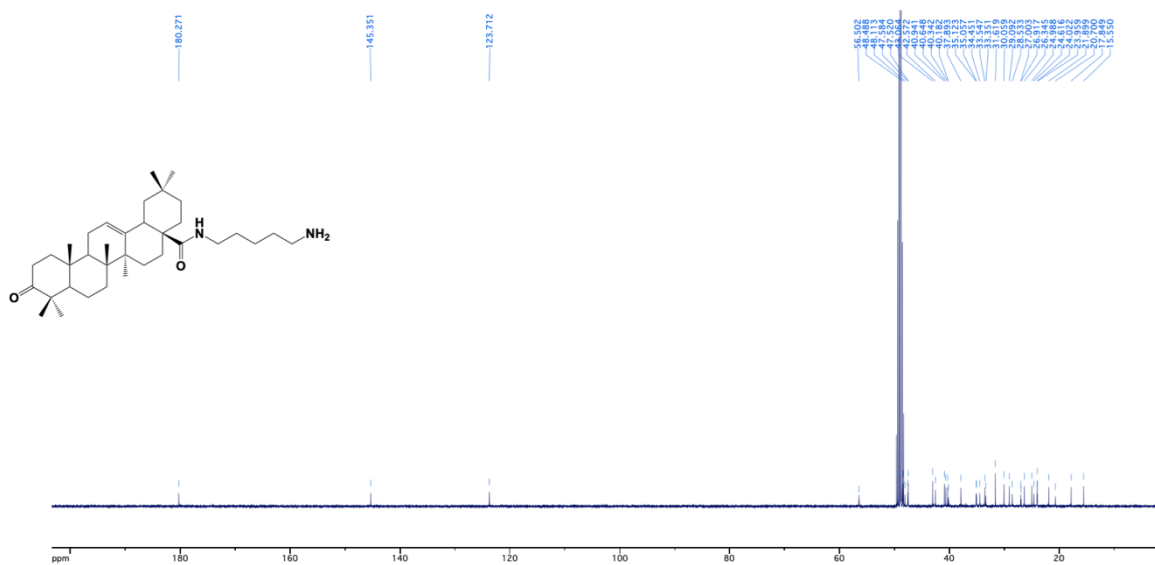


Figure S6. ^{13}C NMR spectrum of compound **2c**

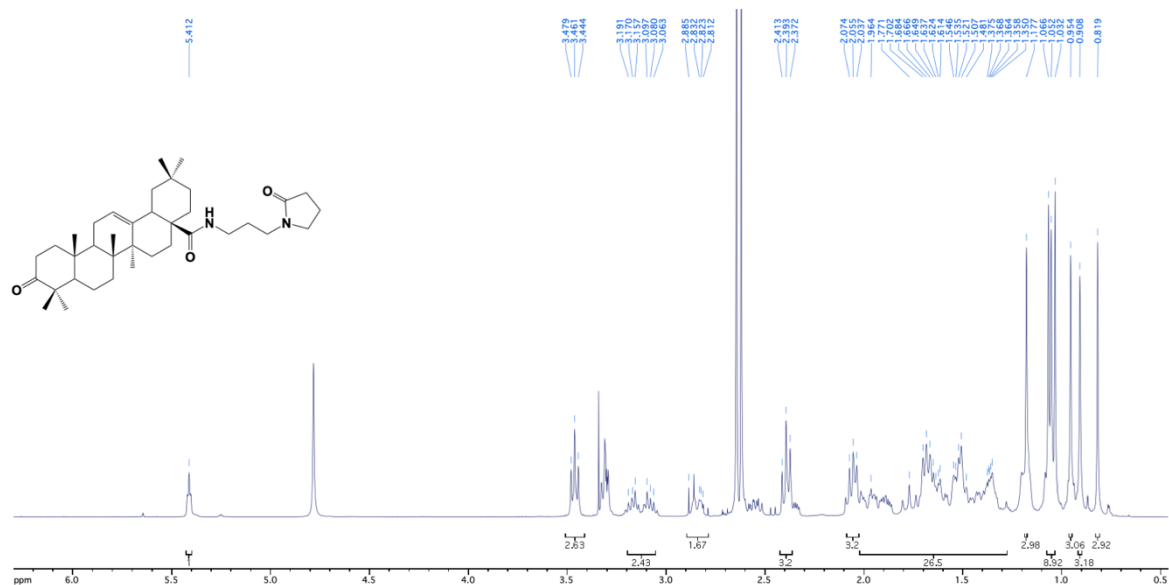


Figure S7. ^1H NMR spectrum of compound **2d**

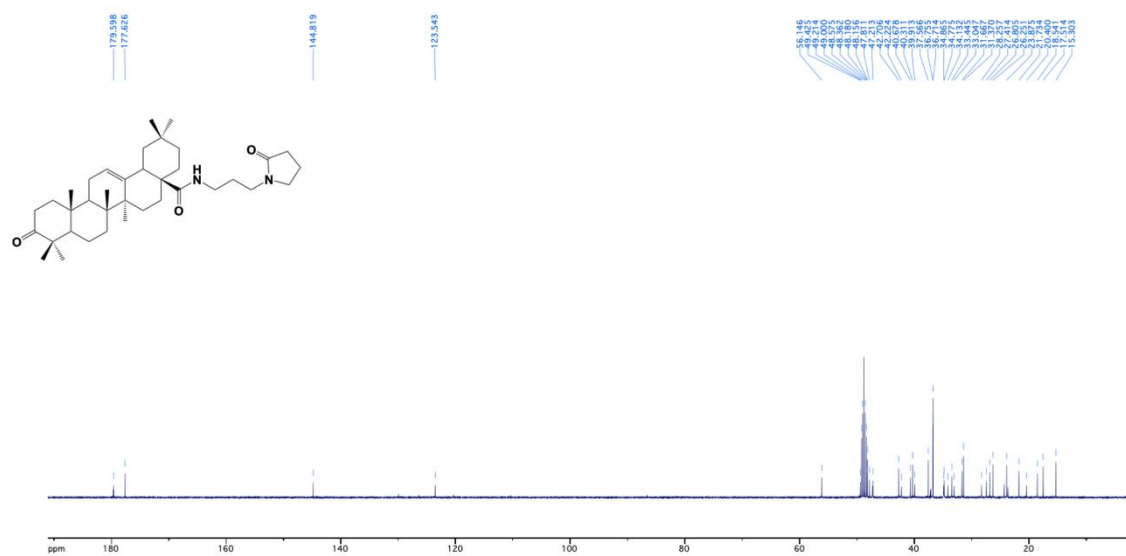


Figure S8. ^{13}C NMR spectrum of compound **2d**

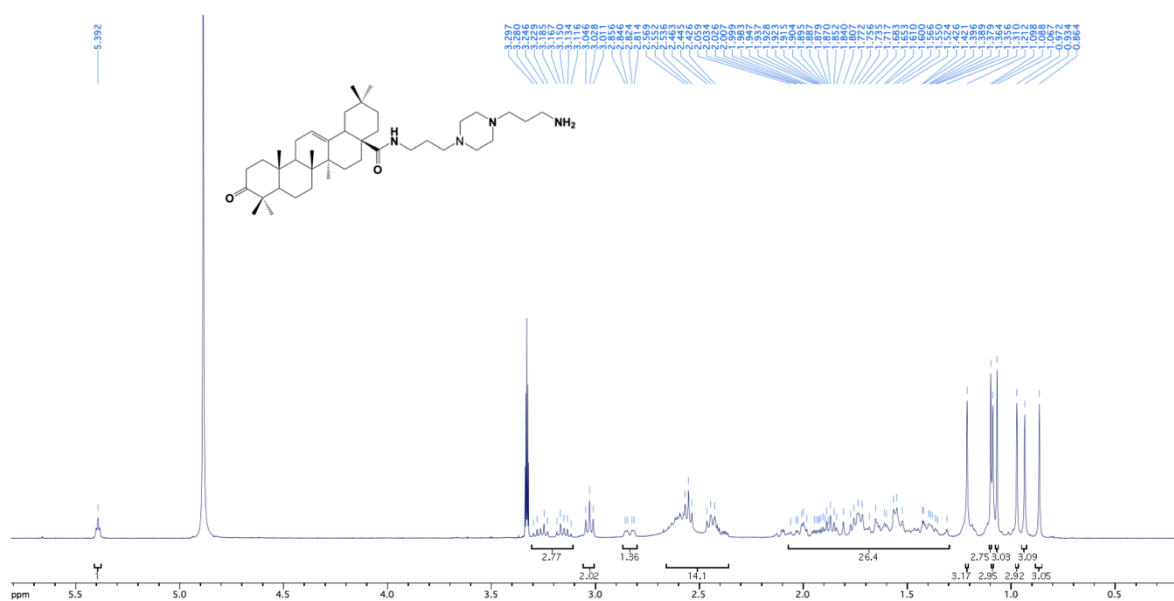


Figure S11. ^1H NMR spectrum of compound **2f**

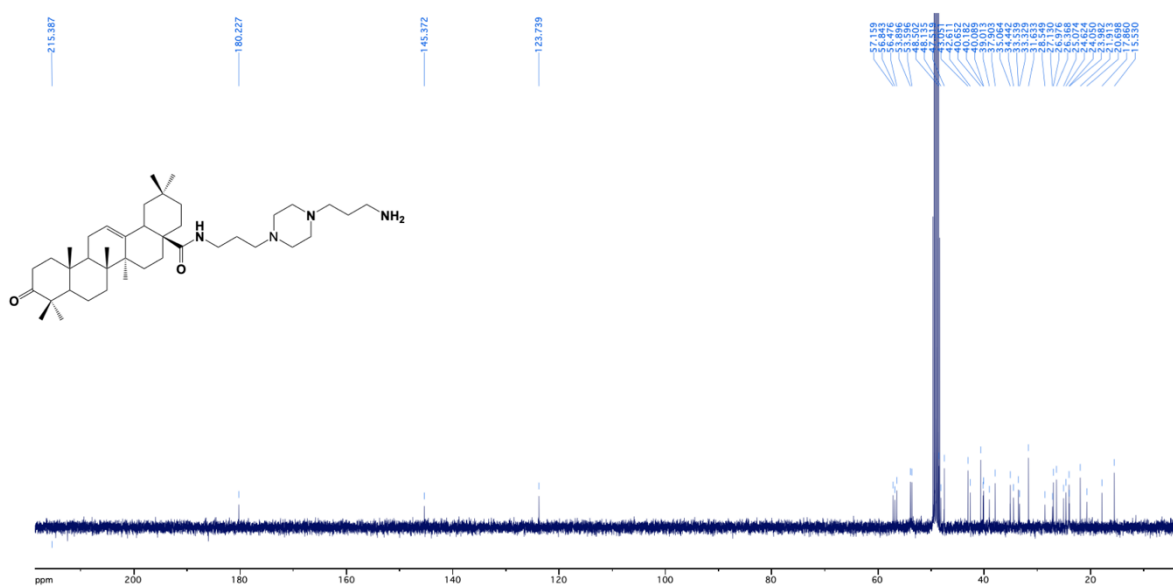


Figure S12. ^{13}C NMR spectrum of compound **2f**

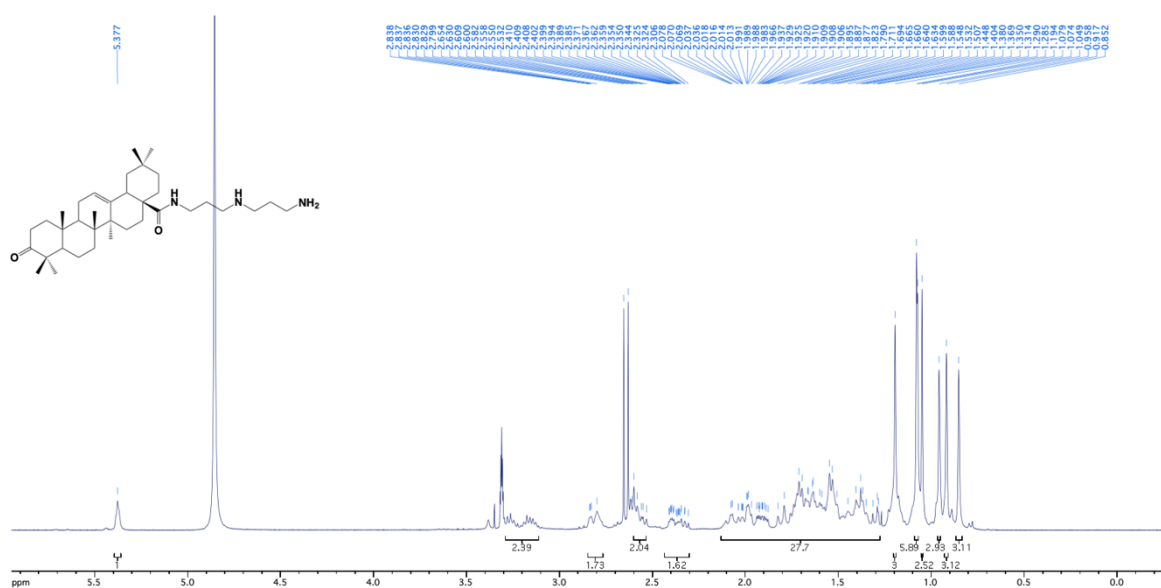


Figure S13. ^1H NMR spectrum of compound **2h**

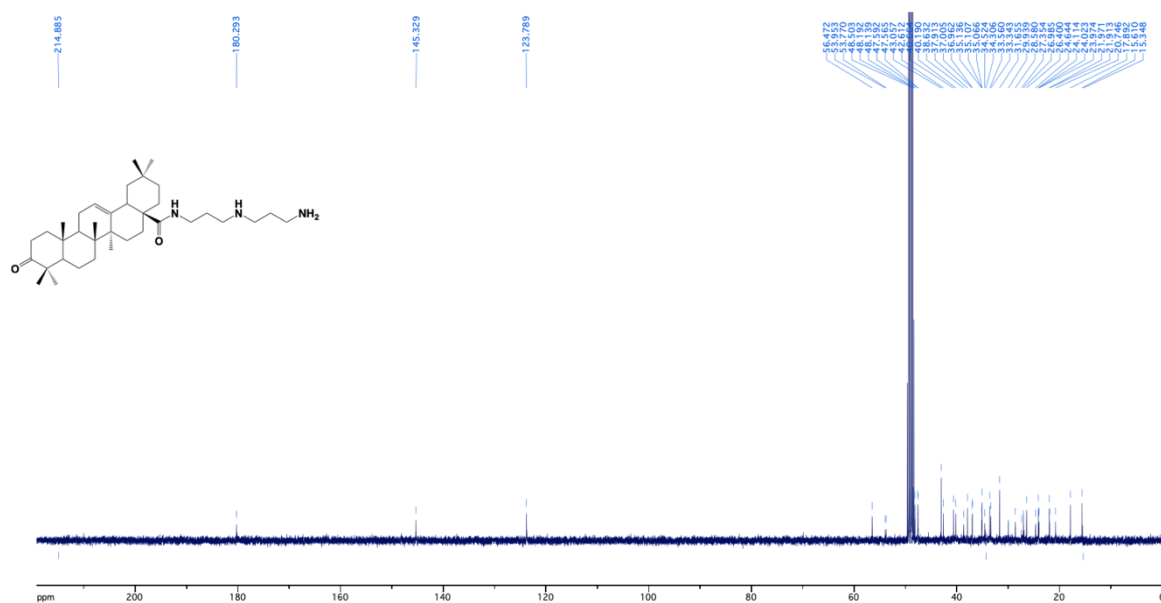


Figure S14. ^{13}C NMR spectrum of compound **2h**

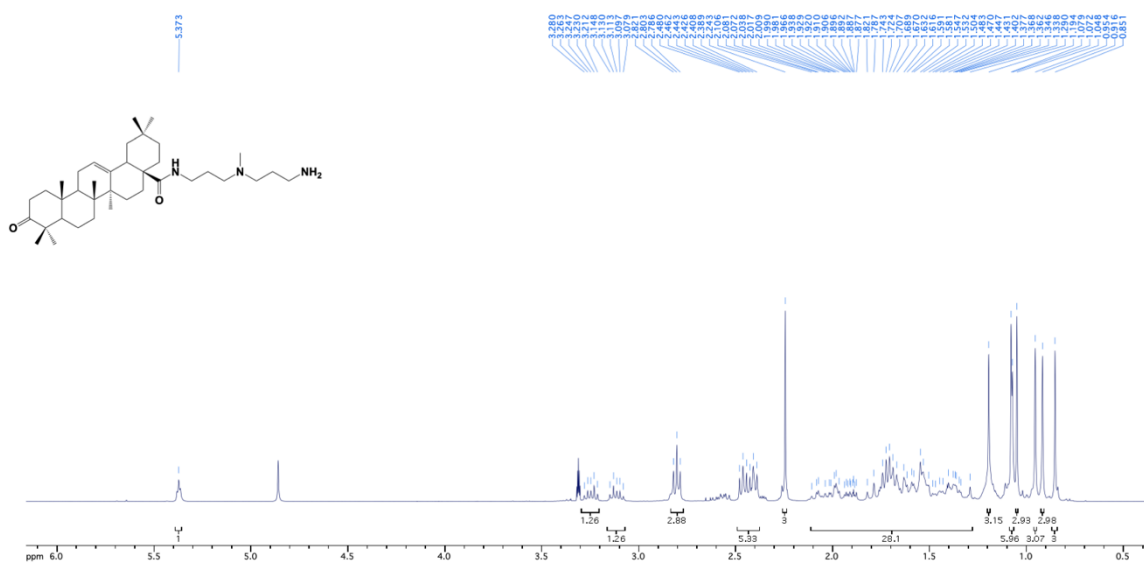


Figure S15. ^1H NMR spectrum of compound **2i**

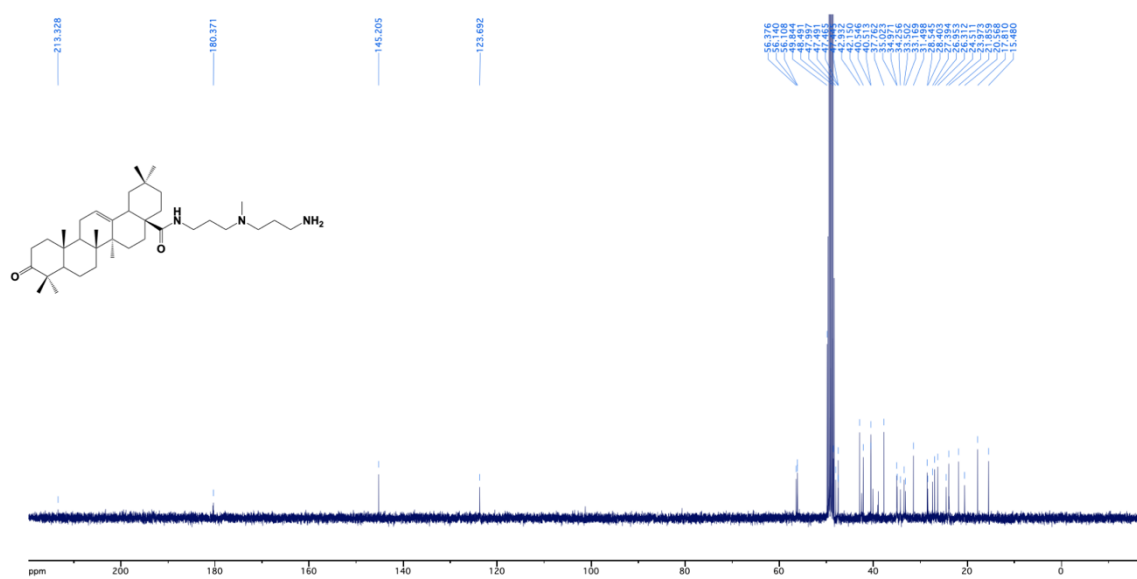


Figure S16. ^{13}C NMR spectrum of compound **2i**

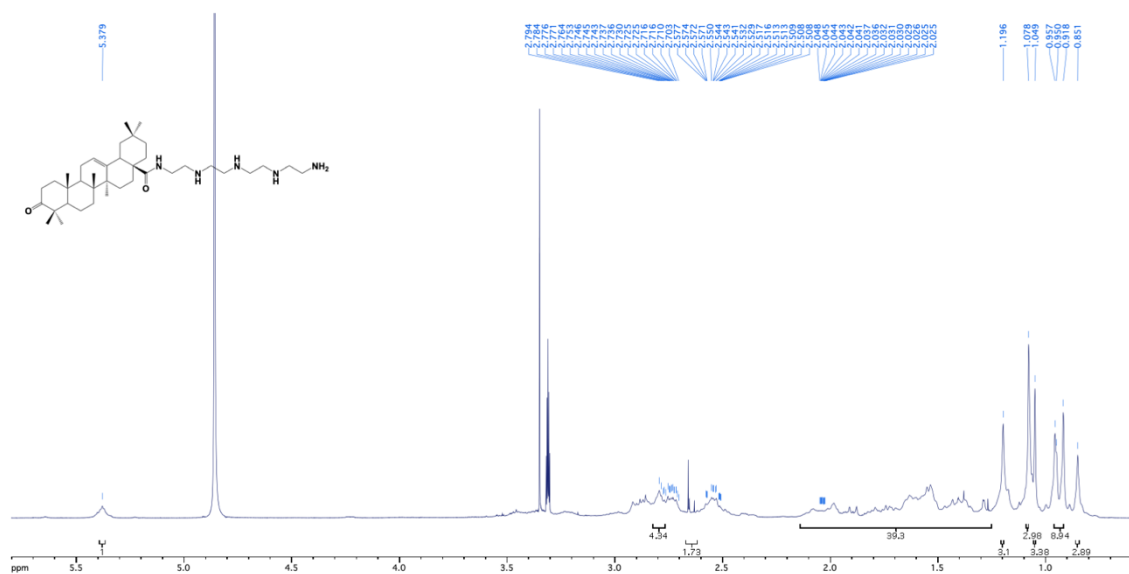


Figure S17. ^1H NMR spectrum of compound **2j**

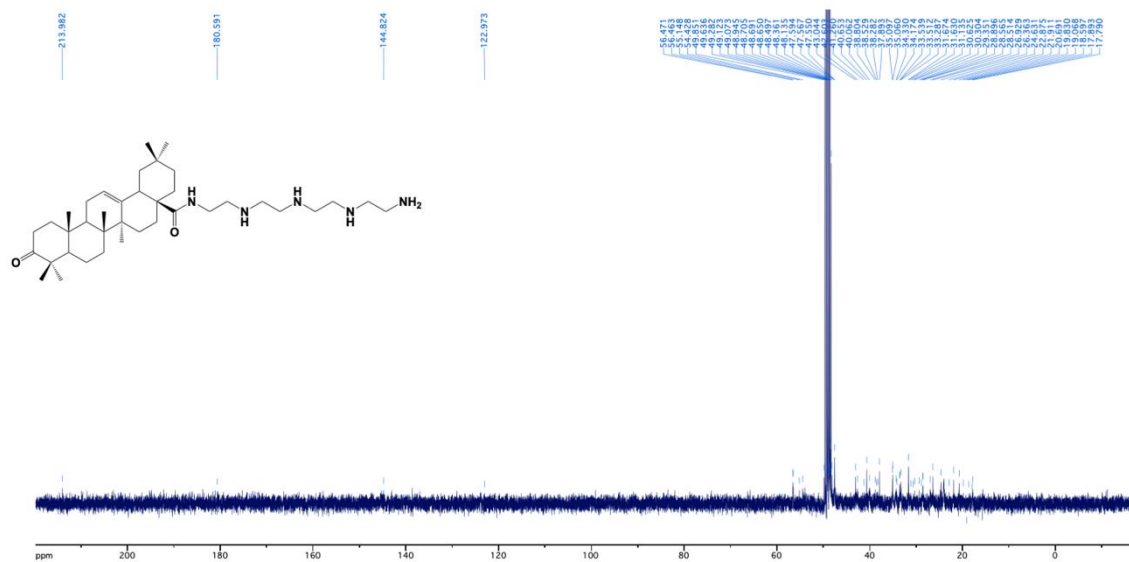


Figure S18. ^{13}C NMR spectrum of compound **2j**

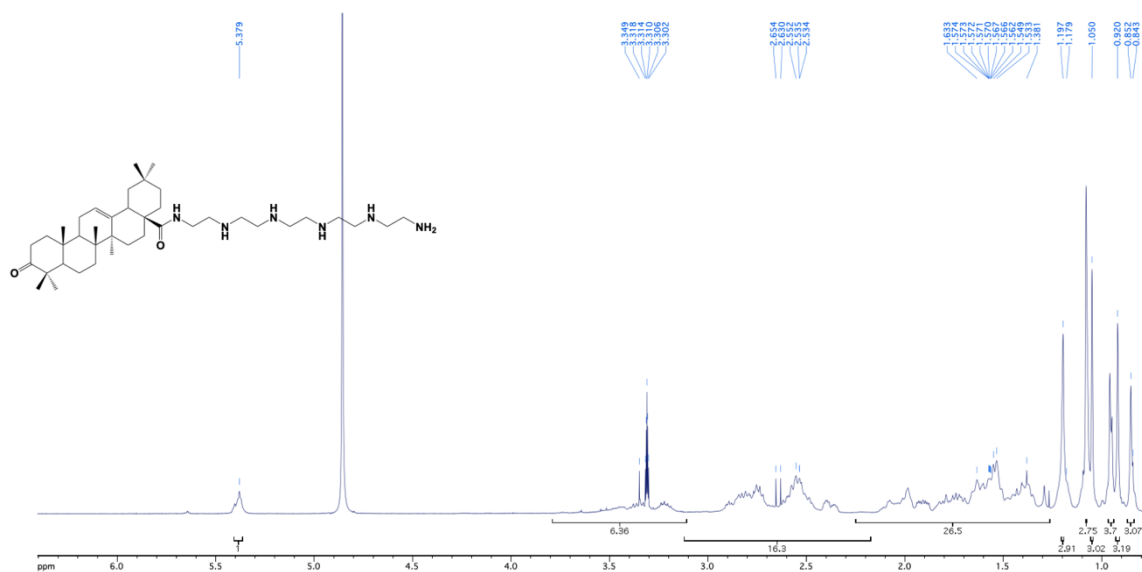
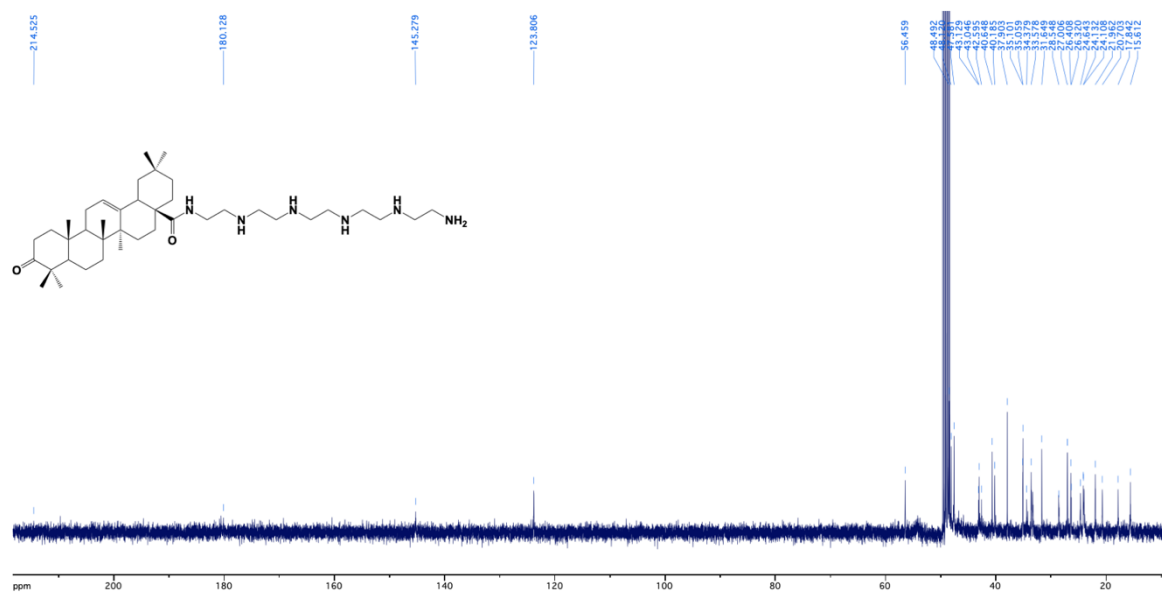


Figure S19. ^1H NMR spectrum of compound **2k**



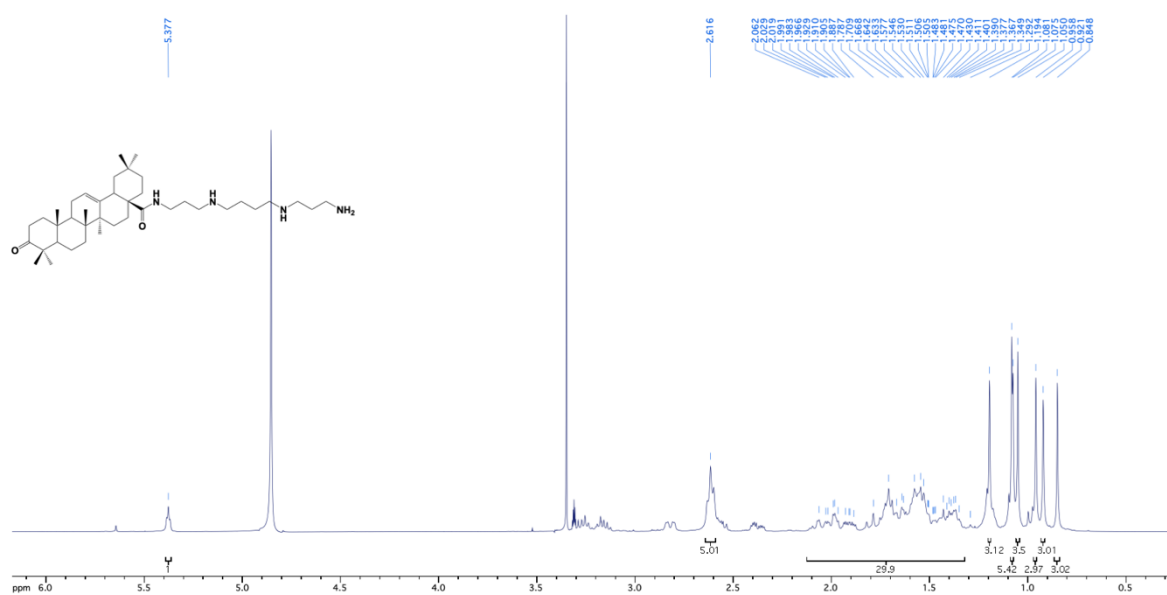


Figure S21. ^1H NMR spectrum of compound **21**

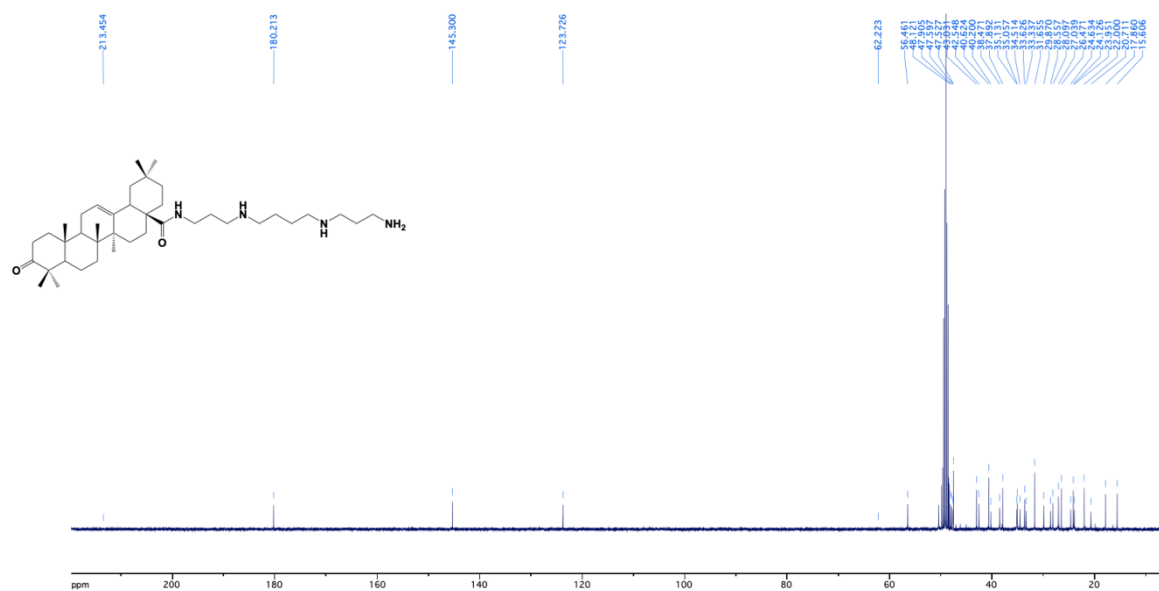


Figure S22. ^{13}C NMR spectrum of compound **21**

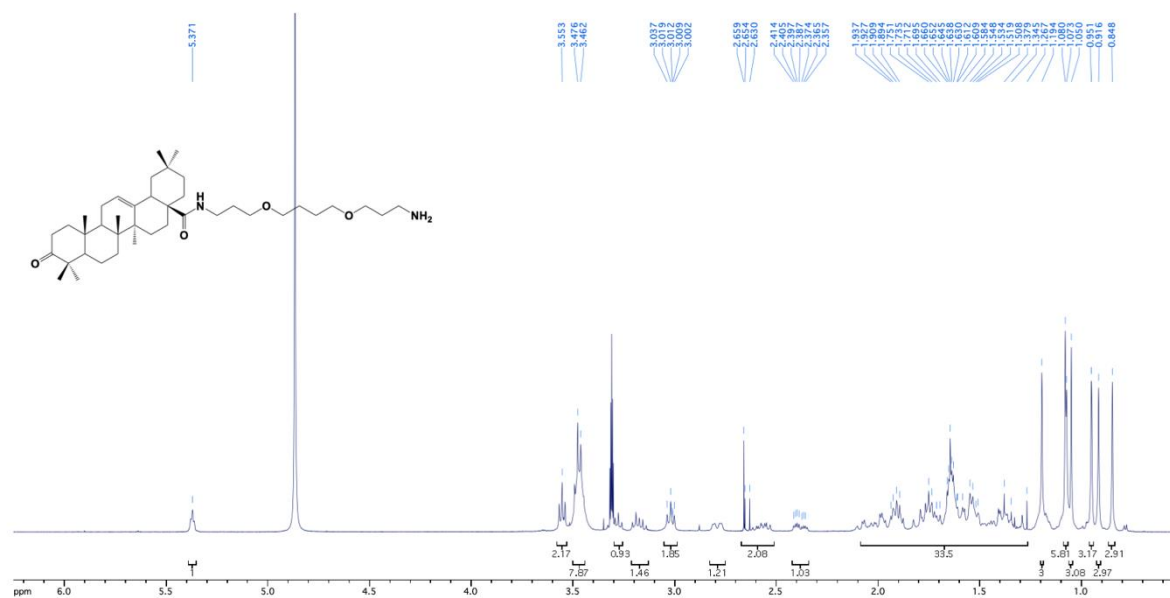


Figure S23. ^1H NMR spectrum of compound **2m**

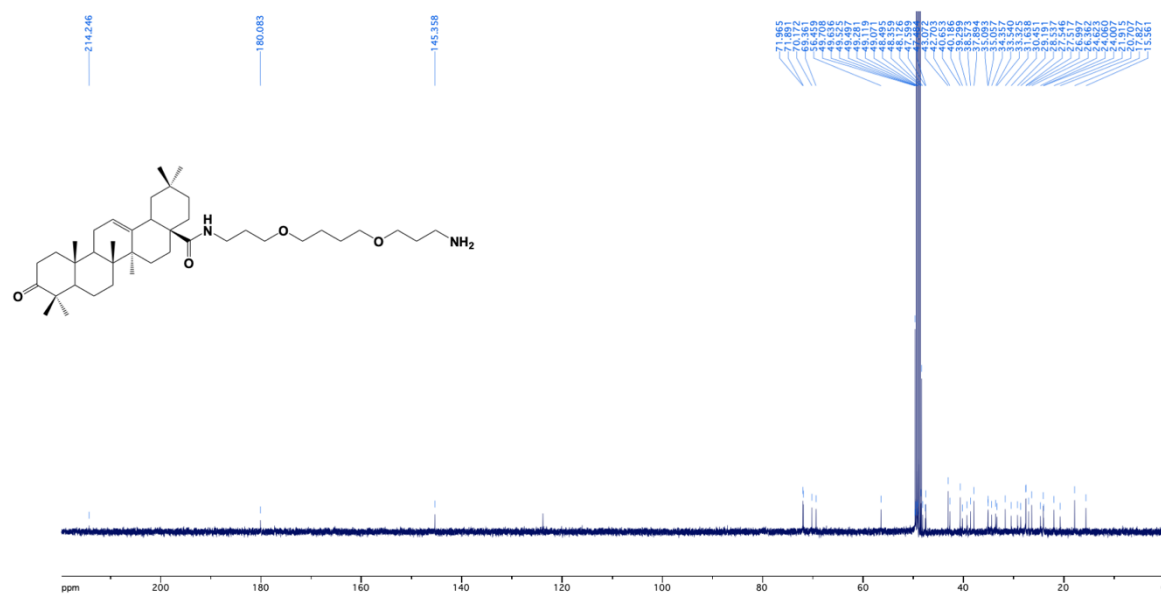


Figure S24. ^{13}C NMR spectrum of compound **2m**

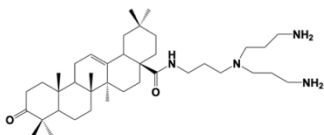


Figure S25. ^1H NMR spectrum of compound **2n**

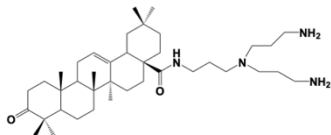
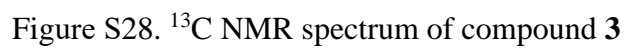
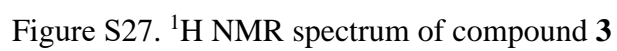


Figure S26. ^{13}C NMR spectrum of compound **2n**



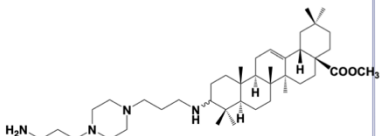


Figure S29. ^1H NMR spectrum of compound **4**

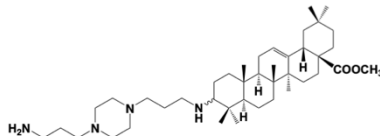


Figure S30. ^{13}C NMR spectrum of compound **4**

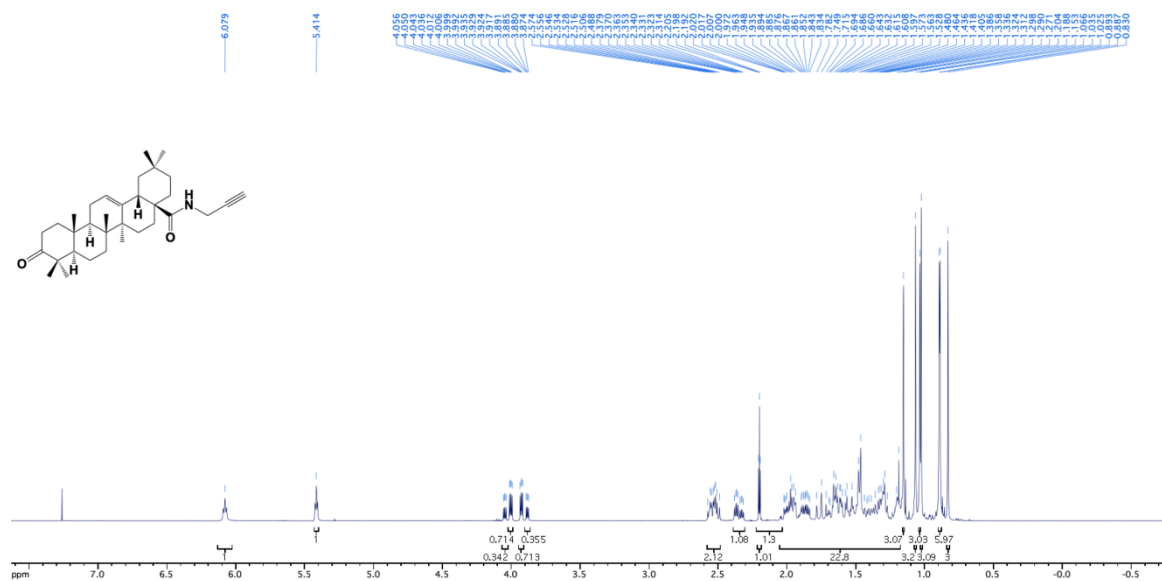


Figure S31. ^1H NMR spectrum of compound **5**

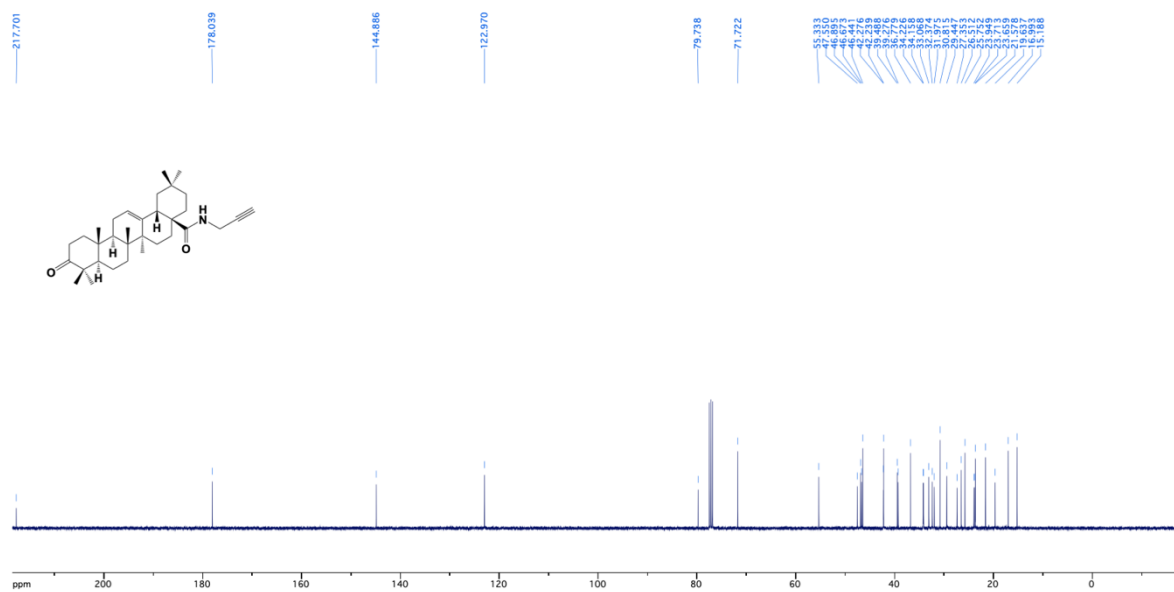


Figure S32. ^{13}C NMR spectrum of compound **5**

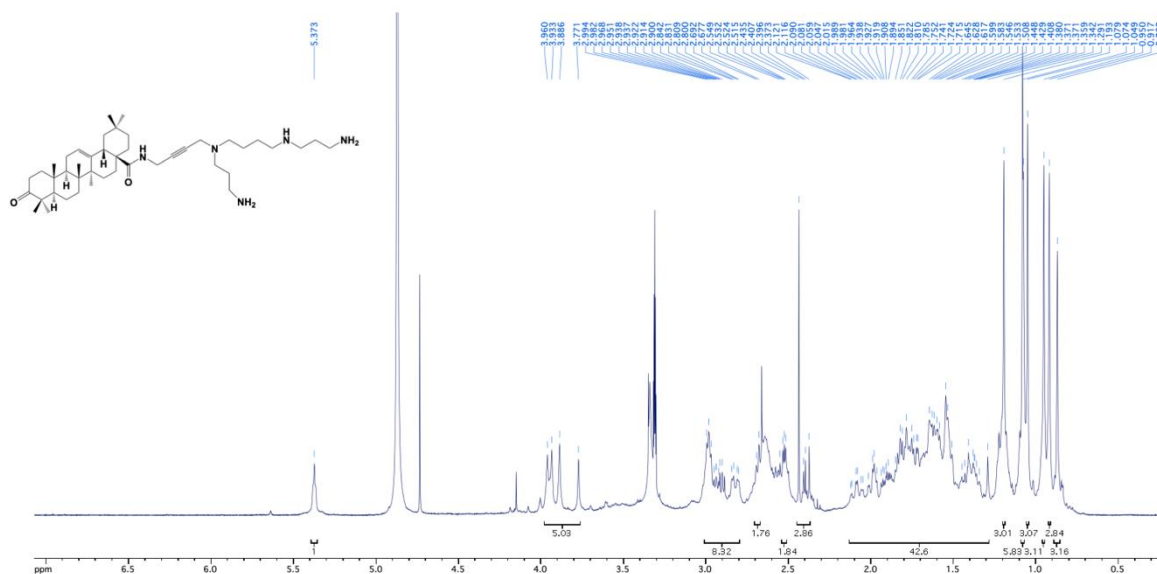


Figure S33. ¹H NMR spectrum of compound 6

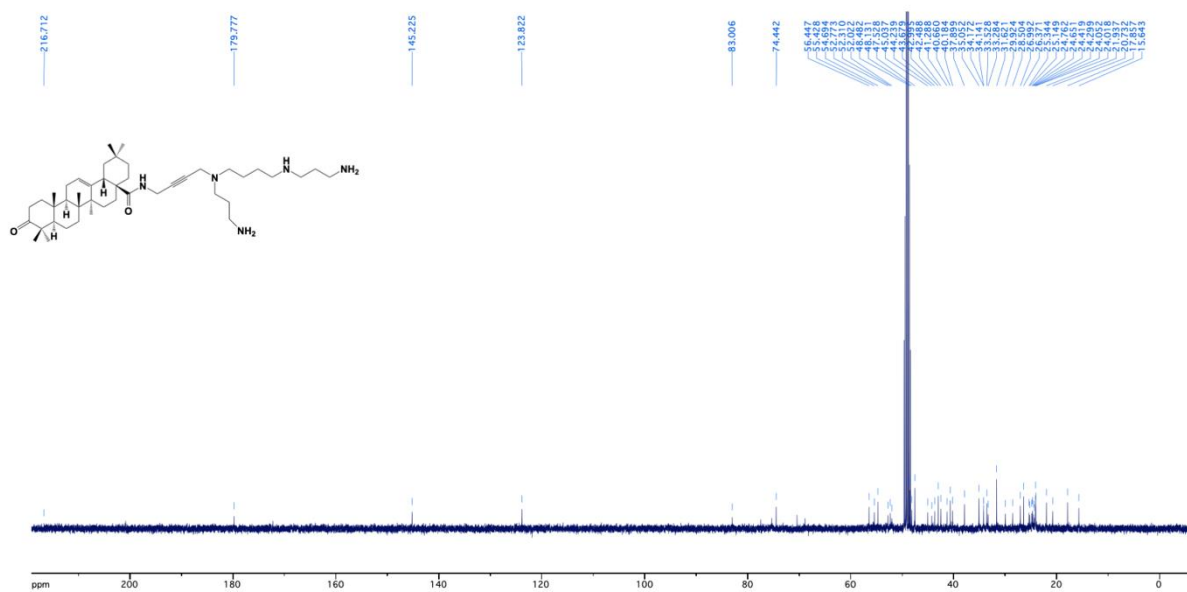


Figure S34. ¹³C NMR spectrum of compound 6

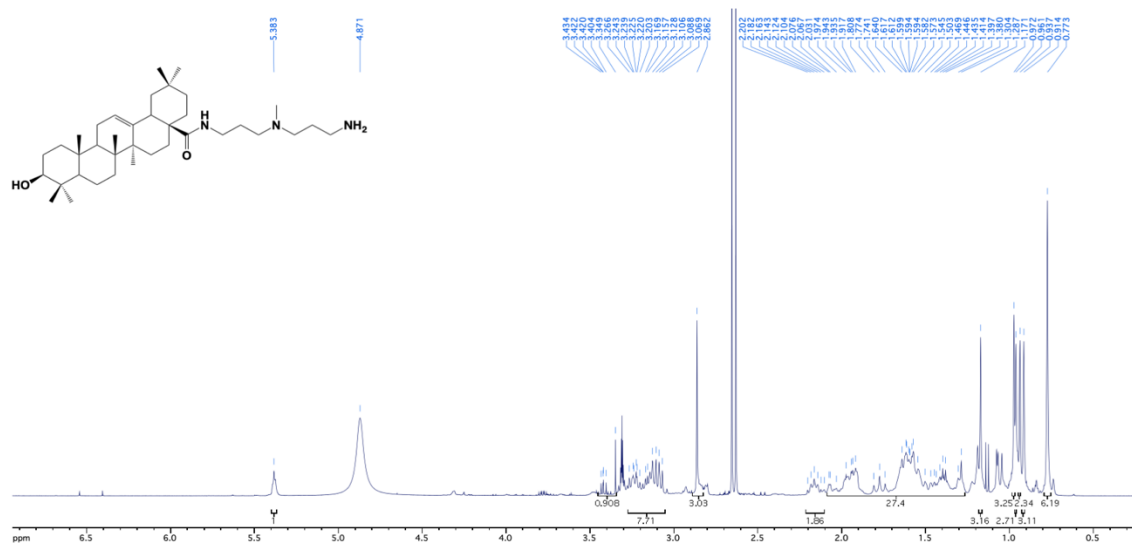


Figure S37. ^1H NMR spectrum of compound **7b**

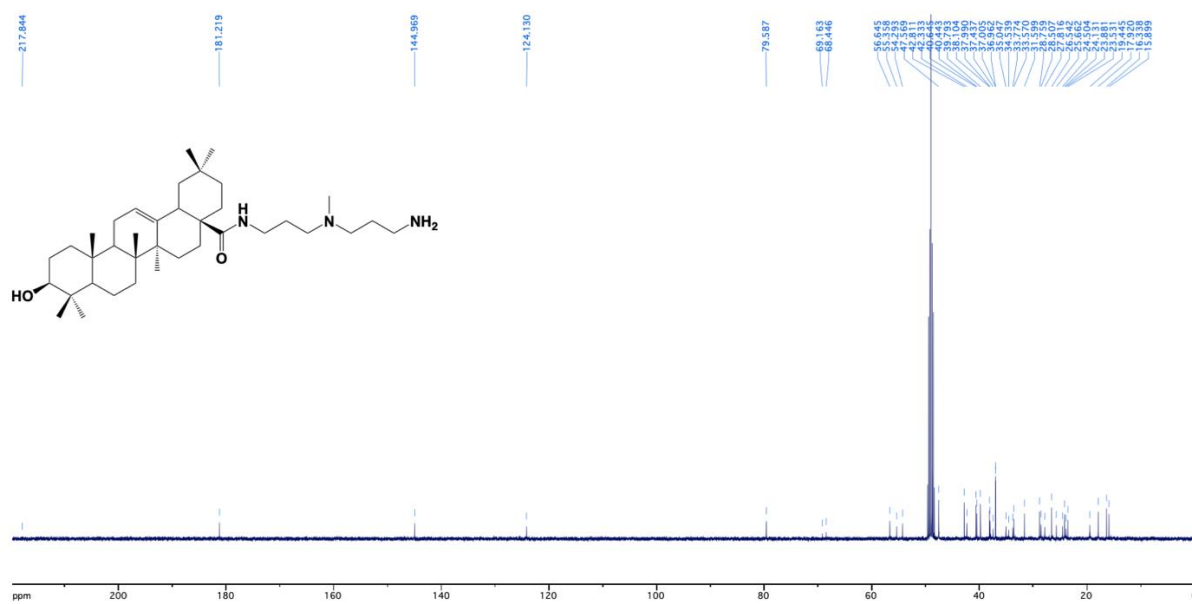


Figure S38. ^{13}C NMR spectrum of compound **7b**

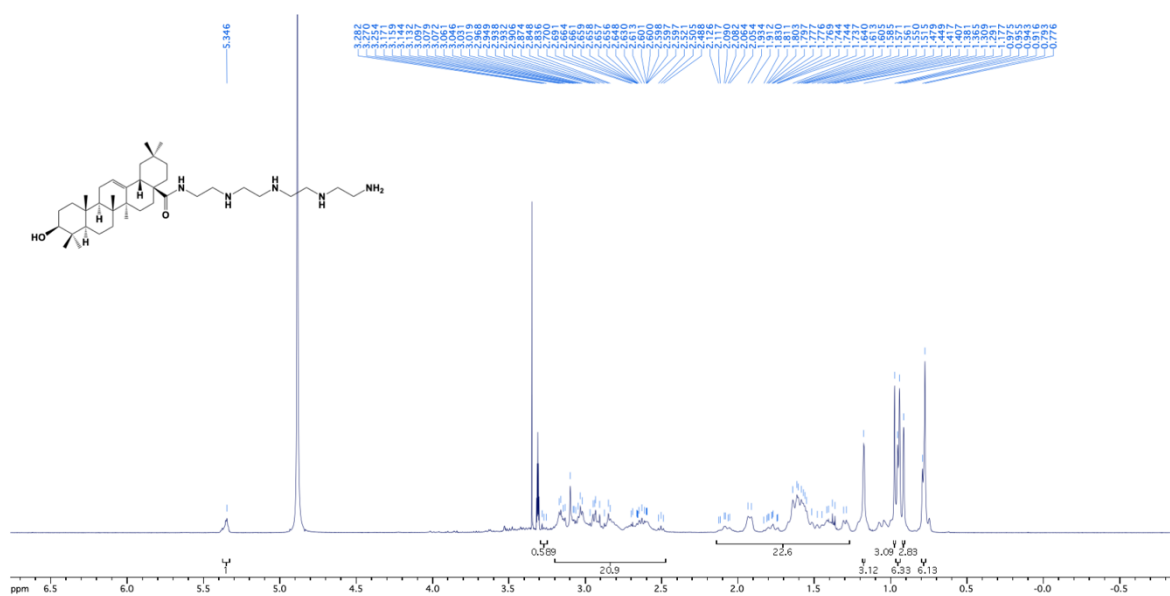


Figure S37. ^1H NMR spectrum of compound **7c**

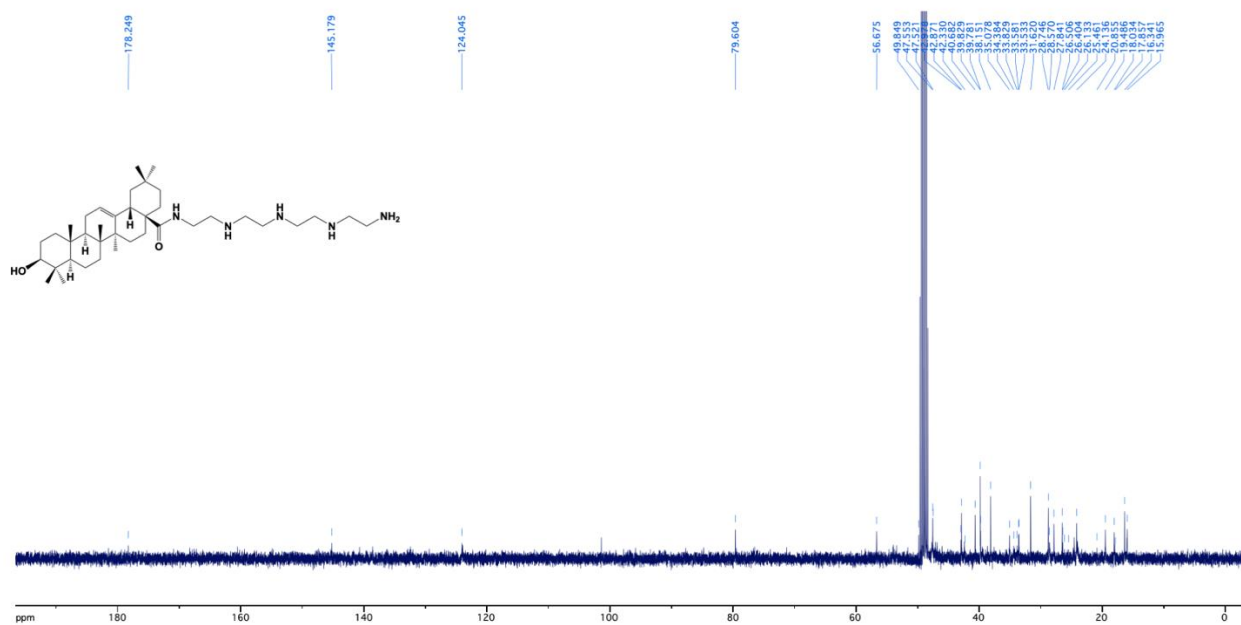


Figure S40. ^{13}C NMR spectrum of compound **7c**