

Supplementary Materials

New 2,4-bis[(substituted-aminomethyl)phenyl]phenylquinazoline and 2,4-bis[(substituted-aminomethyl)phenyl]phenylquinoline Derivatives: Synthesis and Biological Evaluation as Novel Anticancer Agents by Targeting G-Quadruplex

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Table S1. Physical properties of amines **12a-n** and **13a-e**.

Compound	Crystal color	Salt ^a	mp (°C) ^b	Yield (%) ^c
2a	Yellow	4 (COOH) ₂	147-149	67
2b	Yellow	4 (COOH) ₂	234-236	71
2c	Yellow	4 (COOH) ₂	152-155	63
2d	Pale-yellow	6 (COOH) ₂	226-228	67
2e	White	6 (COOH) ₂	165-167	50
2f	White	4 (COOH) ₂	223-225	74
2g	Pale-yellow	4 (COOH) ₂	145-147	66
2h	Pale-yellow	4 (COOH) ₂	144-146	65
2i	Pale-yellow	6 (COOH) ₂	221-223	60
2j	Pale-yellow	6 (COOH) ₂	187-189	55
2k	White	4 (COOH) ₂	211-213	81
2l	Pale-yellow	4 (COOH) ₂	186-188	73
2m	White	6 (COOH) ₂	224-226	52
2n	White	6 (COOH) ₂	177-179	58
3a	Yellow	4 (COOH) ₂	192-194	63
3b	Yellow	4 (COOH) ₂	140-142	62
3c	Pale-yellow	6 (COOH) ₂	219-221	84
3d	Yellow	6 (COOH) ₂	165-167	51
3e	Pale-yellow	4 (COOH) ₂	174-176	57

^aThe stoichiometry and composition of the salts were determined by elemental analyses and obtained values were within $\pm 0.4\%$ of the theoretical values. ^bCrystallization solvent: 2-PrOH-H₂O. ^cThe yields only included the conversions into the ammonium oxalates.

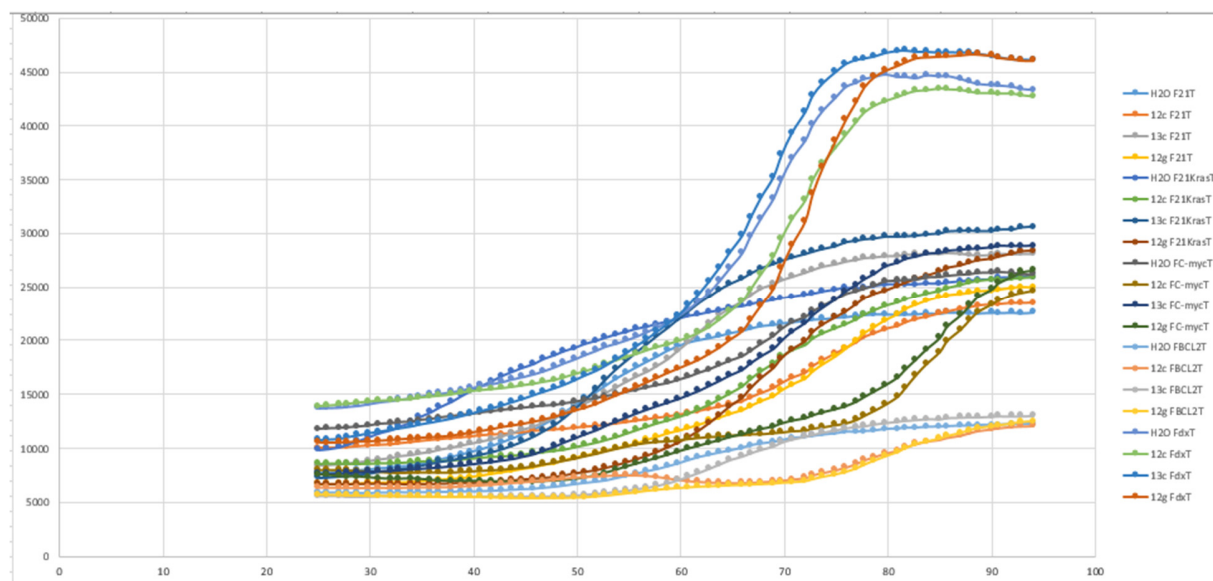


Figure S1. FRET-melting curves of compounds **12c**, **12g** and **13c**.

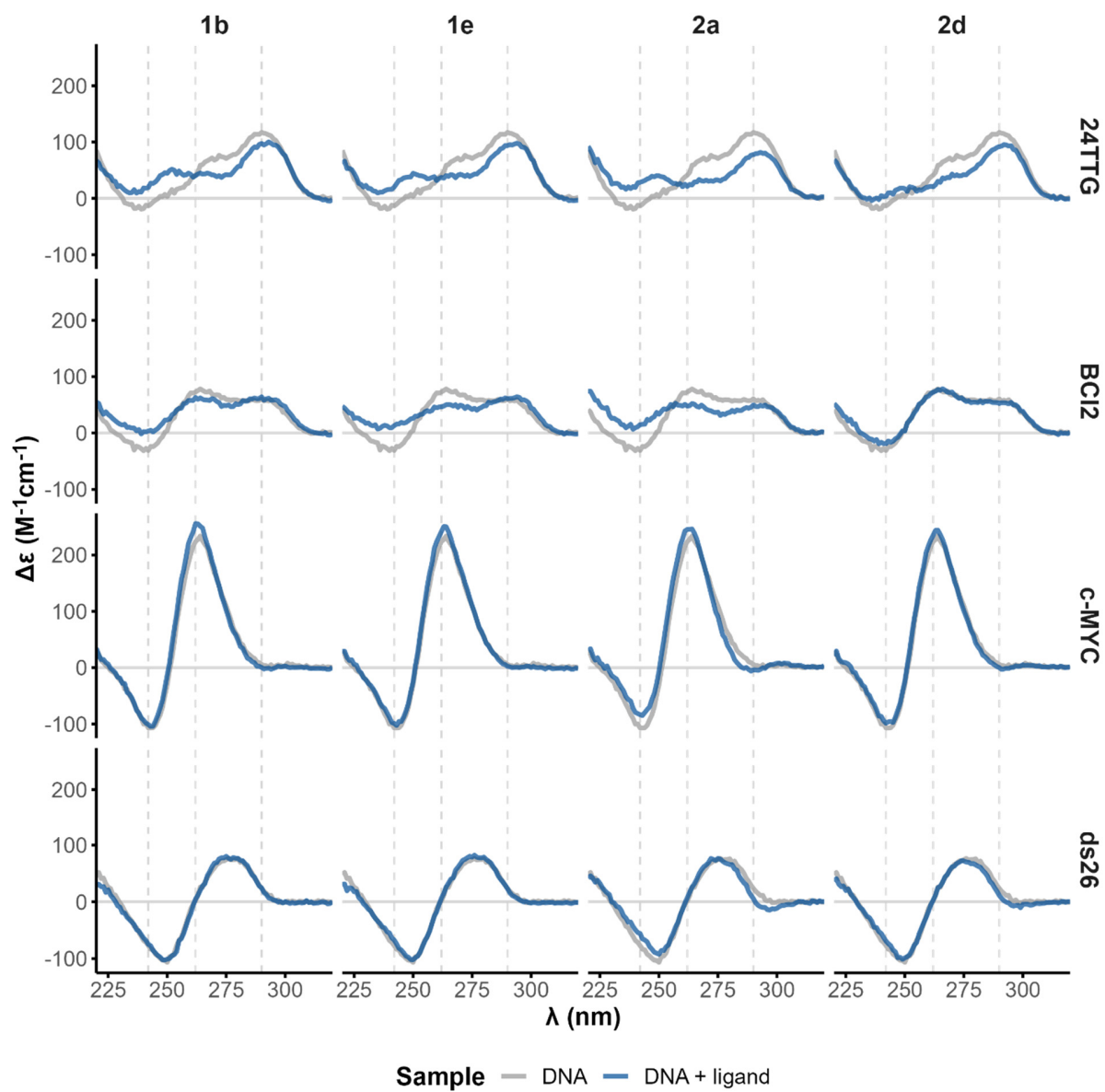


Figure S2. Circular dichroism spectra of solutions containing **12b**, **12e**, **13a** or **13d** (20 μM) with 24TTG, BCL-2 or c-MYC (10 μM) in 100 mM ammonium acetate (pH = 6.8) (DNA + ligand; blue) compared to a reference with DNA alone (grey). The positions of characteristic bands at around 240, 260, and 290 nm are shown with dashed grey lines.

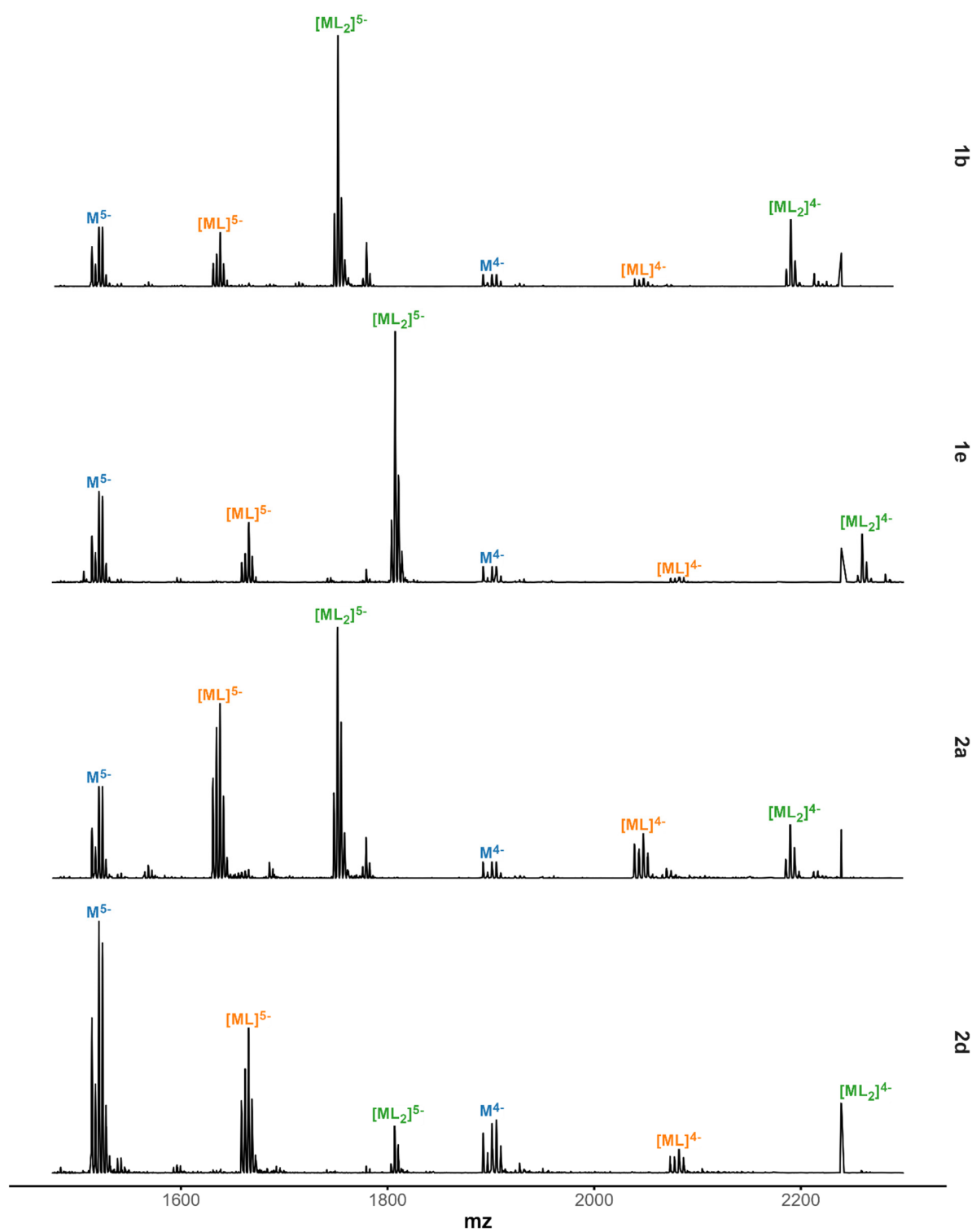


Figure S3. Native electrospray mass spectra of solutions containing **12b**, **12e**, **13a** or **13d** (20 μ M) with 24TTG (10 μ M) in 100 mM ammonium acetate (pH = 6.8), zoomed on the 4- and 5- charge states: M = oligonucleotide monomer, L = ligand.

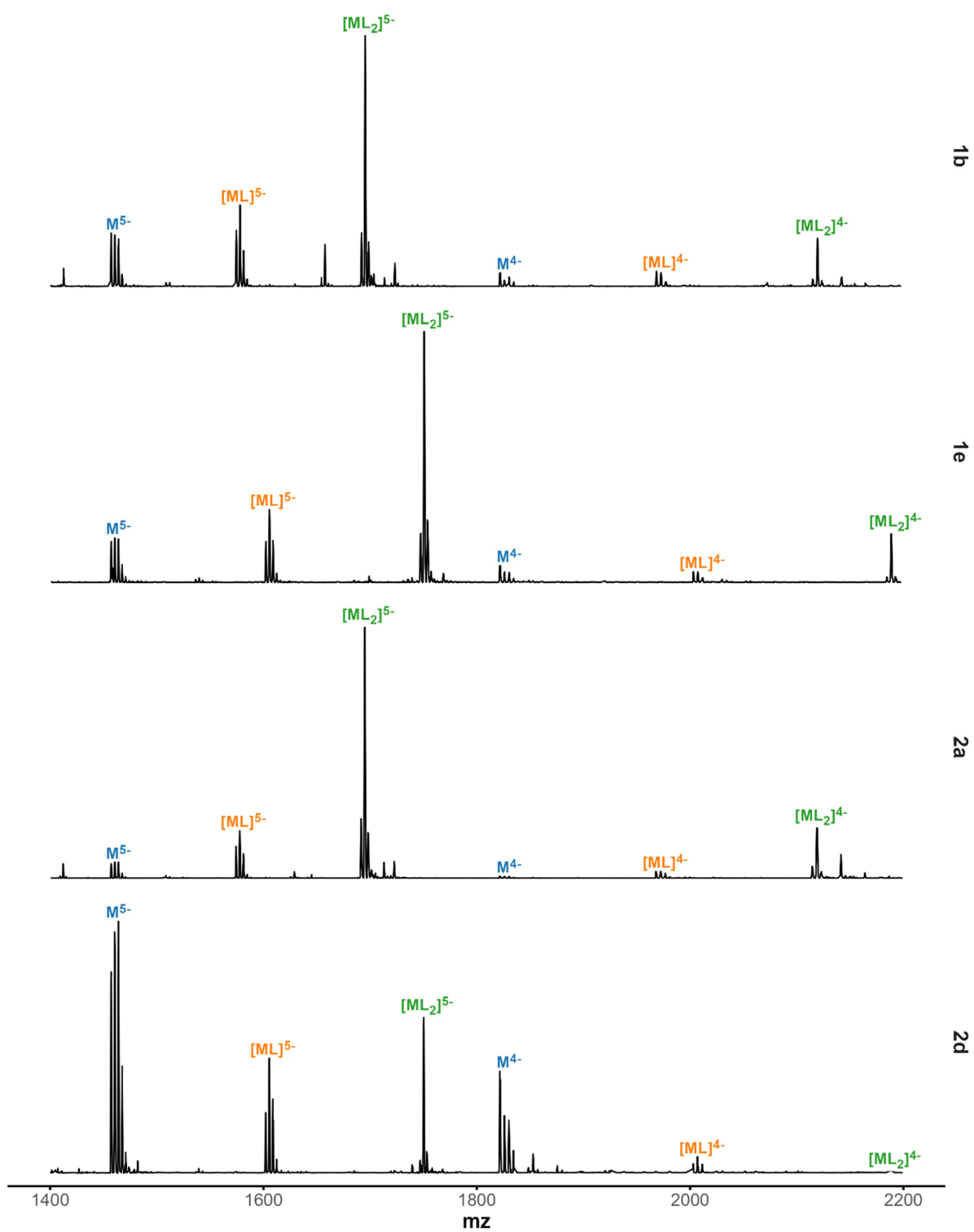


Figure S4. Native electrospray mass spectra of solutions containing **12b**, **12e**, **13a** or **13d** (20 μ M) with BCL-2 (10 μ M) in 100 mM ammonium acetate (pH = 6.8), zoomed on the 4- and 5- charge states: M = oligonucleotide monomer, L = ligand.

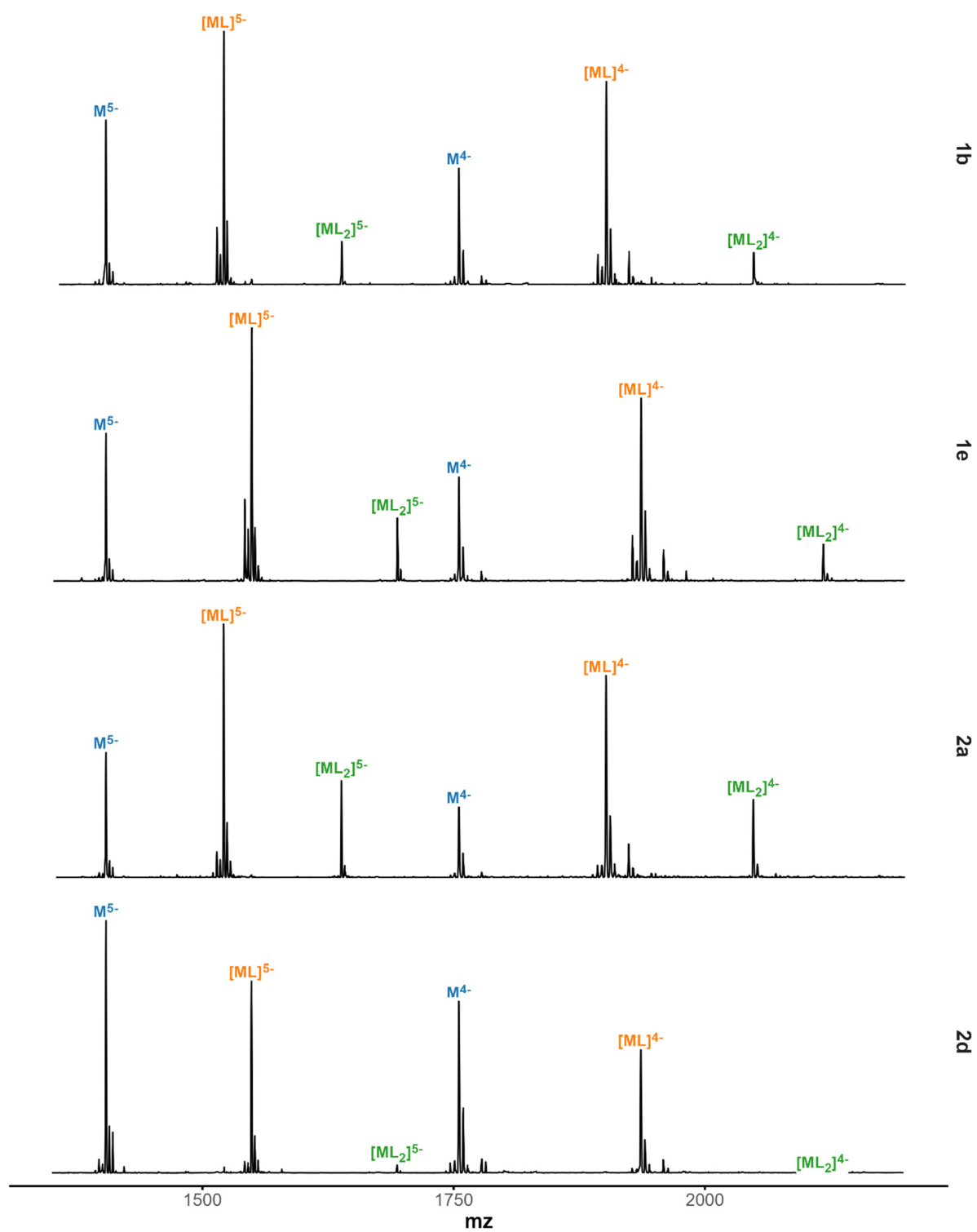


Figure S5. Native electrospray mass spectra of solutions containing **12b**, **12e**, **13a** or **13d** (20 μ M) with c-MYC (10 μ M) in 100 mM ammonium acetate (pH = 6.8), zoomed on the 4- and 5- charge states: M = oligonucleotide monomer, L = ligand.

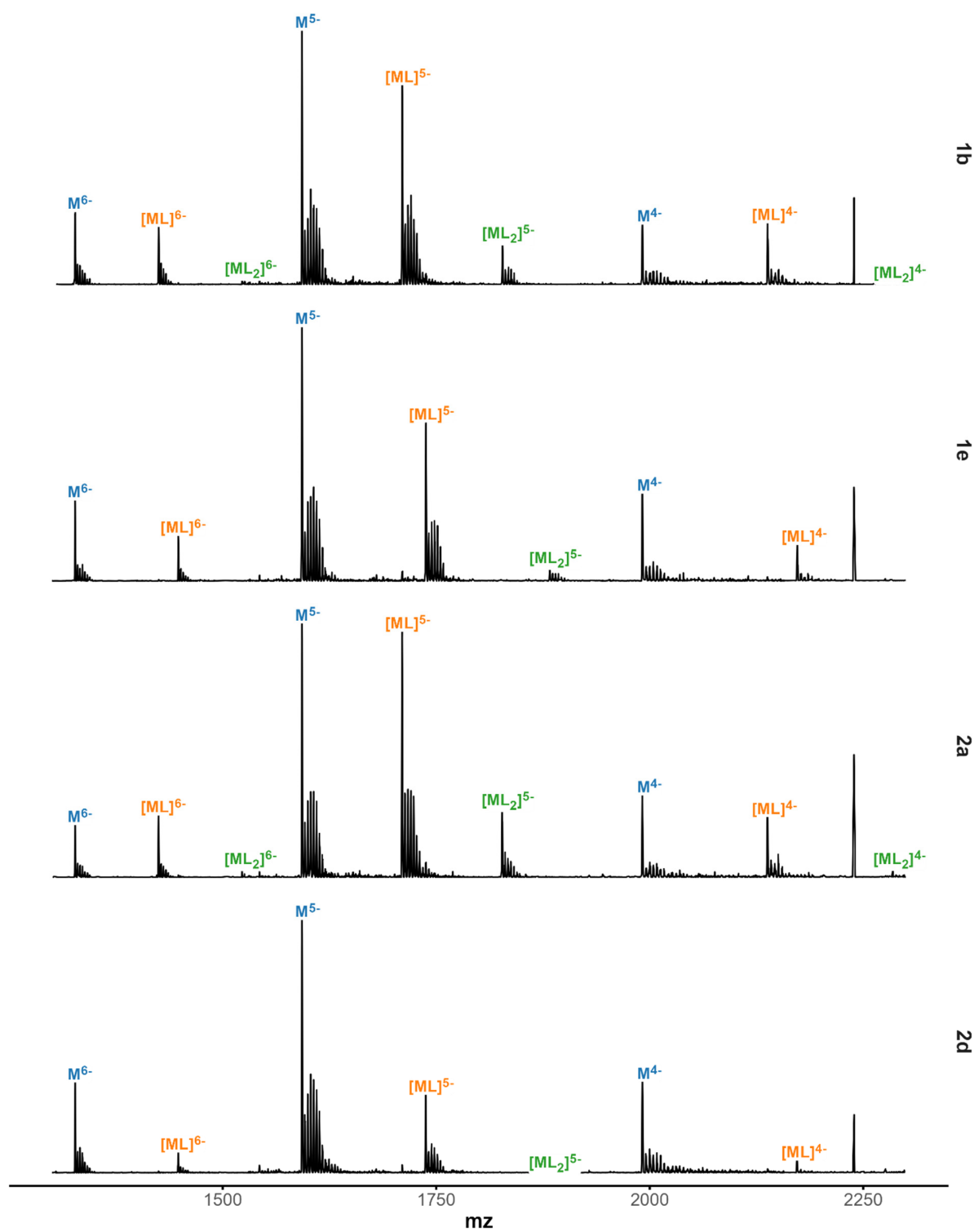
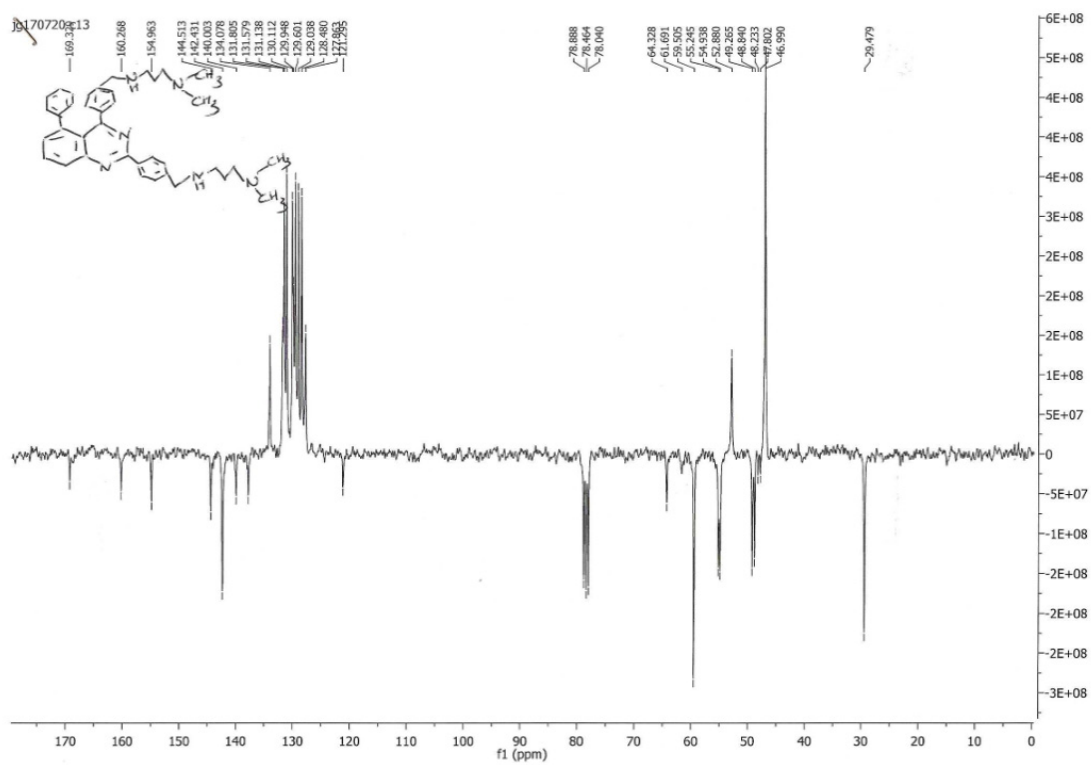
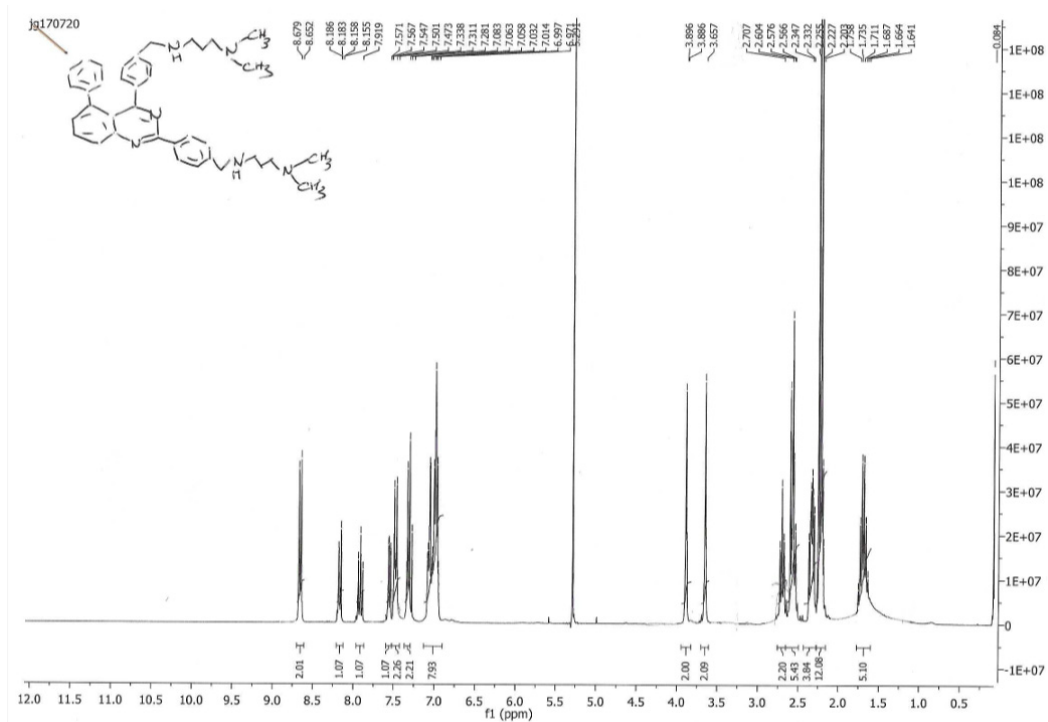


Figure S6. Native electrospray mass spectra of solutions containing **12b**, **12e**, **13a** or **13d** (20 μ M) with ds26 (10 μ M) in 100 mM ammonium acetate (pH = 6.8), zoomed on the 4-, 5- and 6- charge states: M = oligonucleotide monomer, L = ligand.



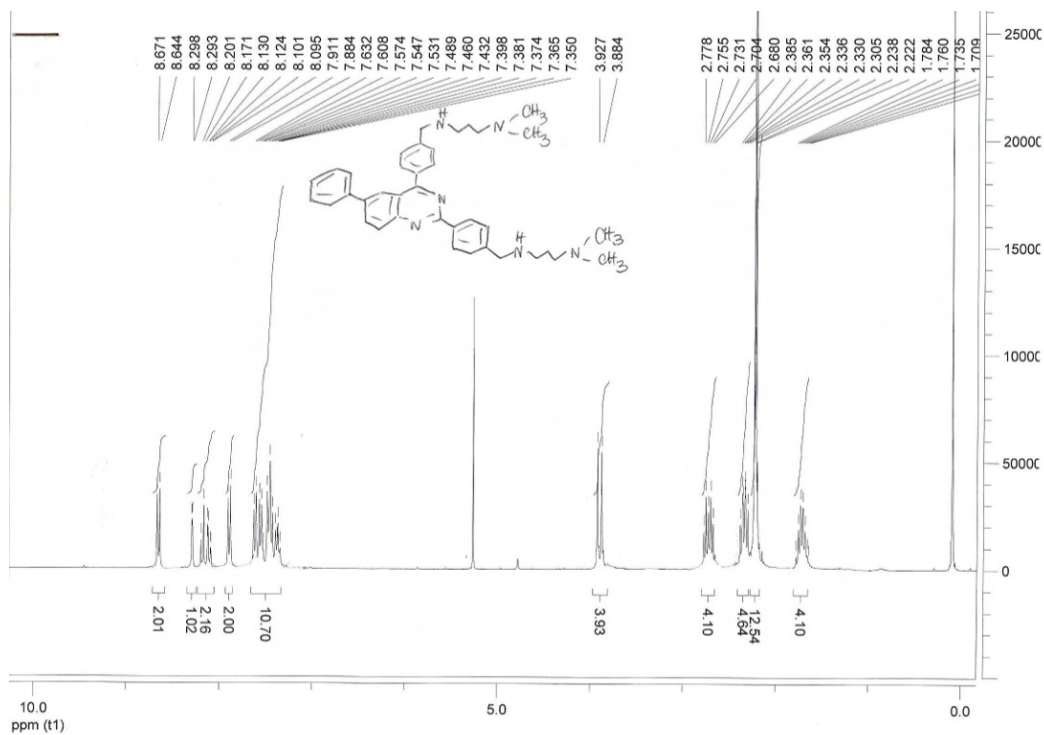


Figure S9. ¹H NMR spectrum of 12b.

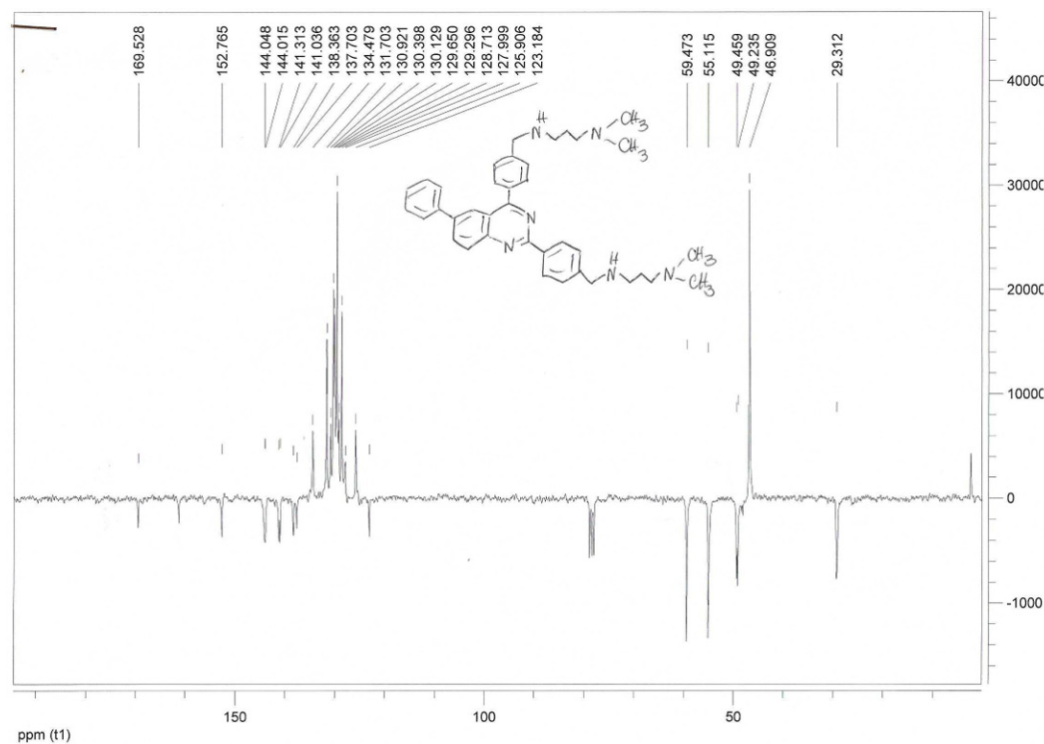


Figure S10. ¹³C NMR spectrum of 12b.

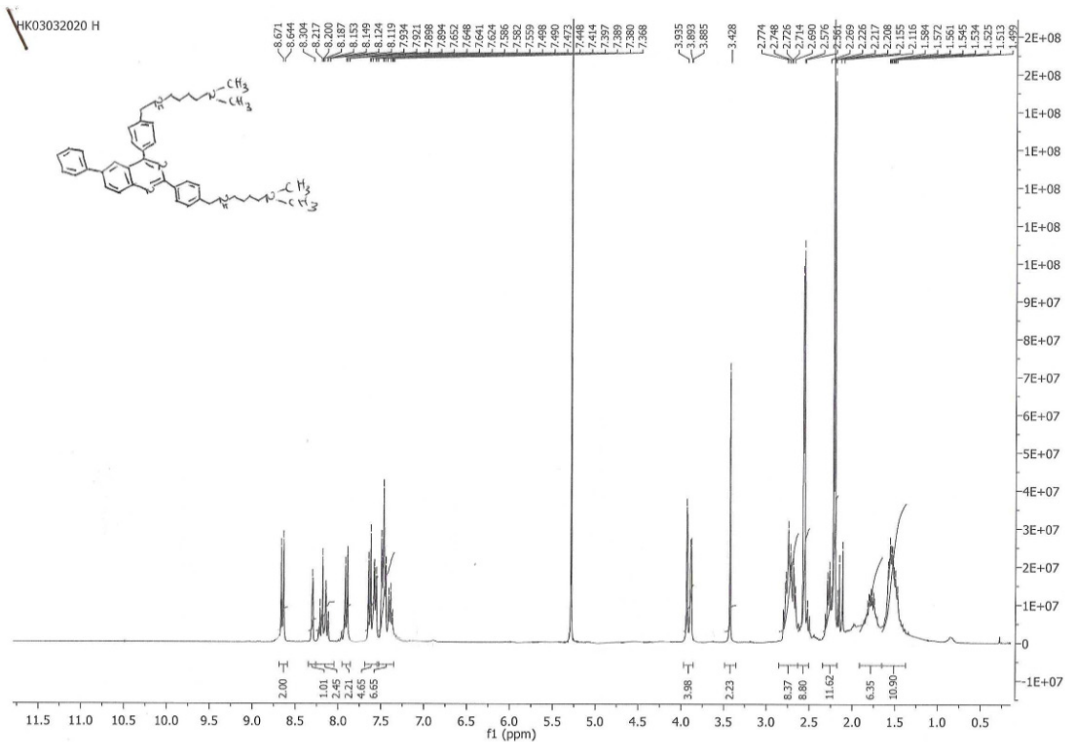


Figure S11. ^1H NMR spectrum of 12c.

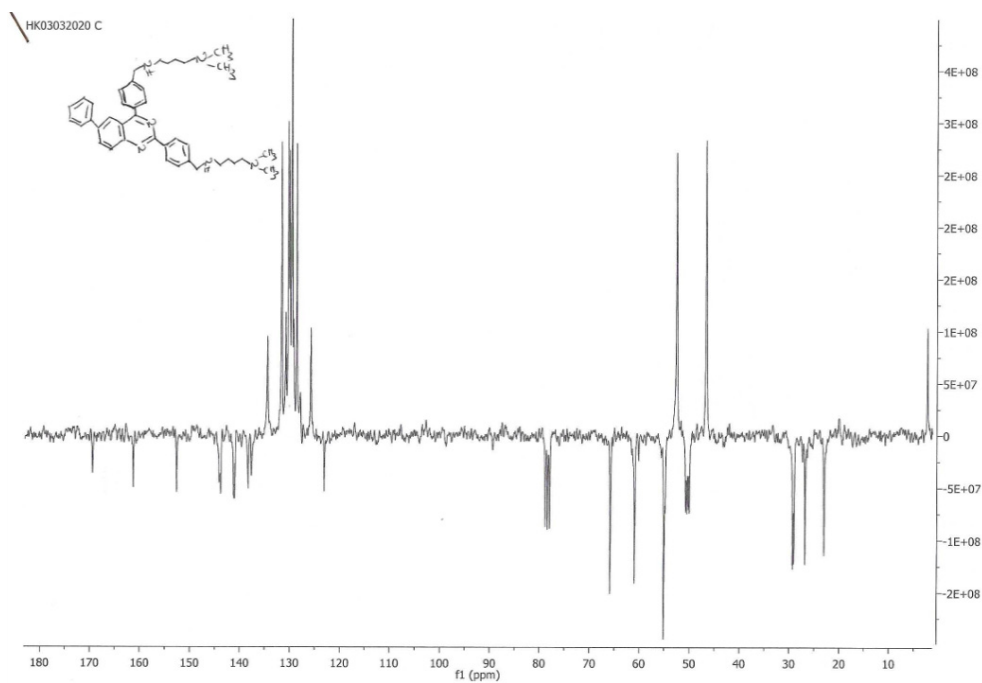


Figure S12. ^{13}C NMR spectrum of 12c.

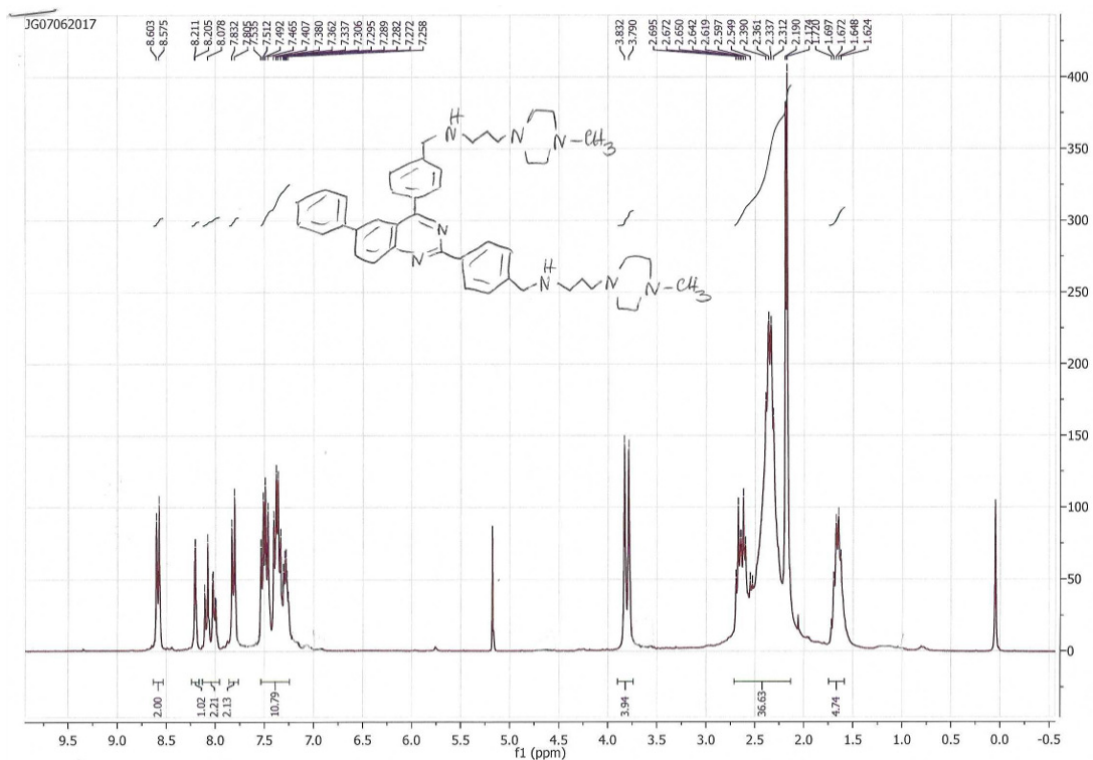


Figure S13. ^1H NMR spectrum of 12d.

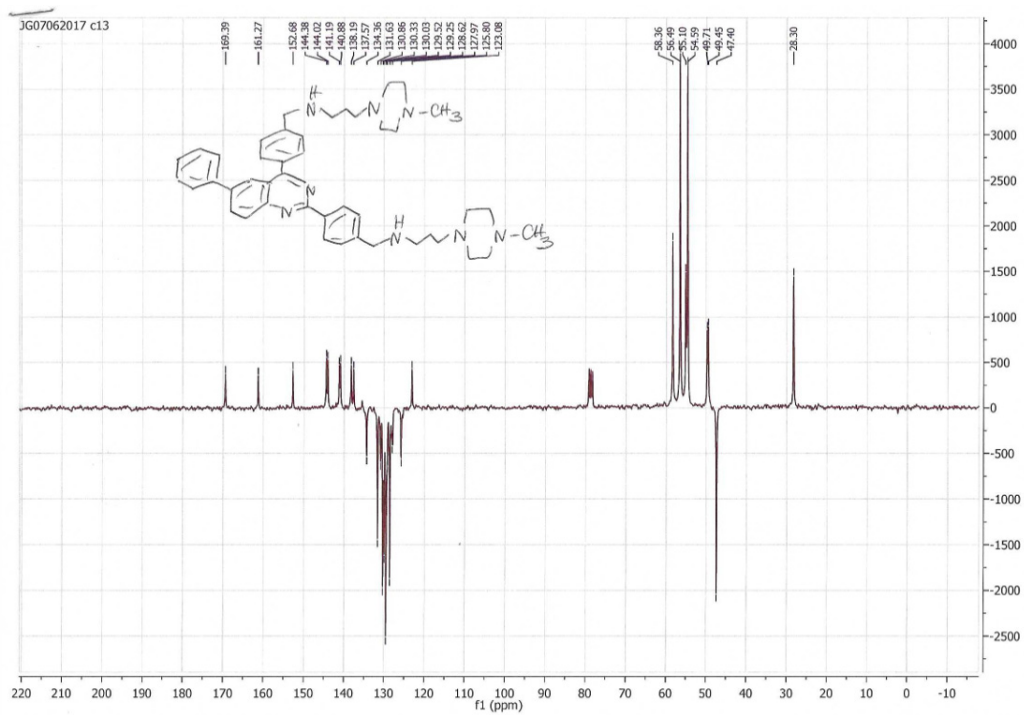


Figure S14. ^{13}C NMR spectrum of 12d.

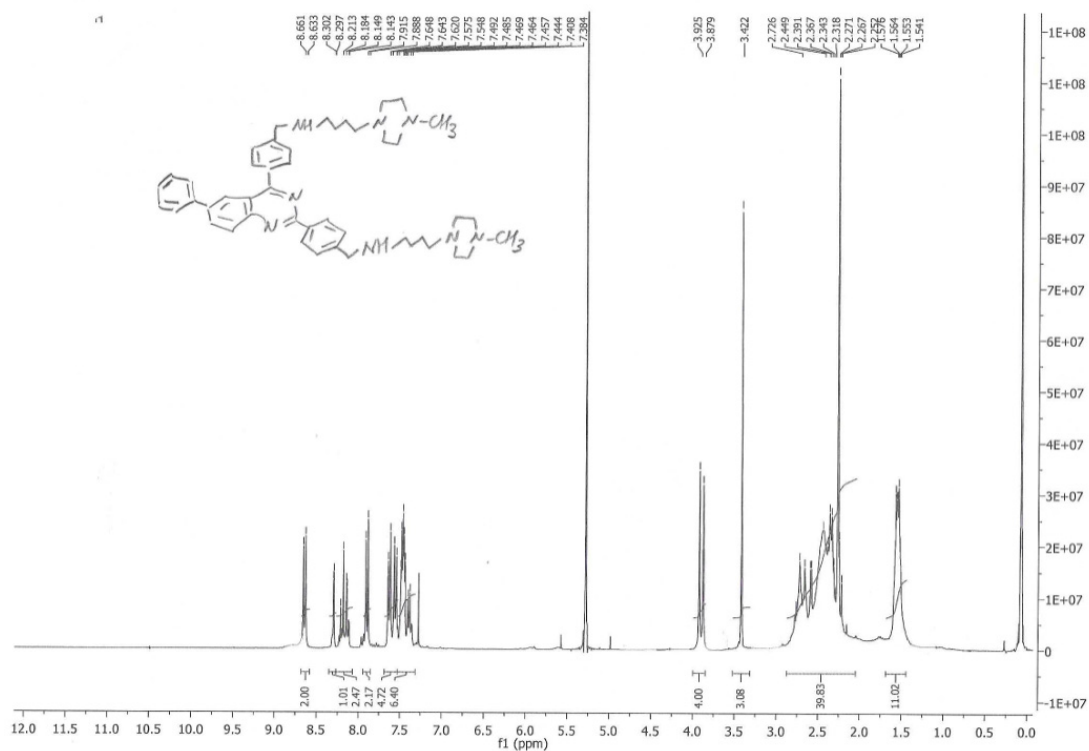


Figure S15. ¹H NMR spectrum of 12e.

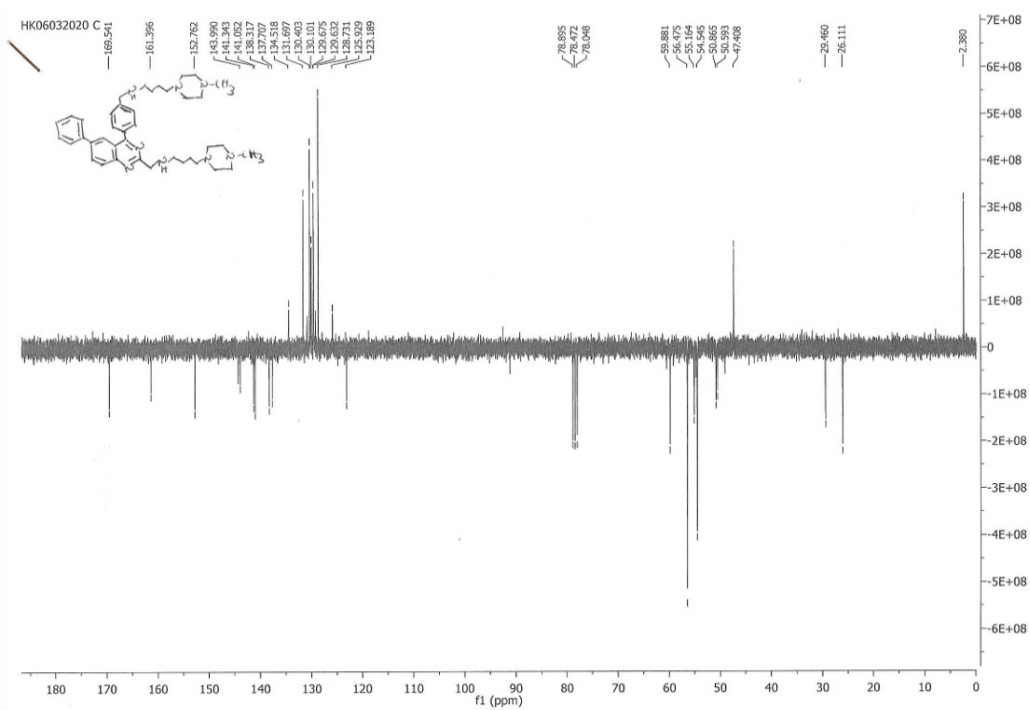


Figure S16. ¹³C NMR spectrum of 12e.

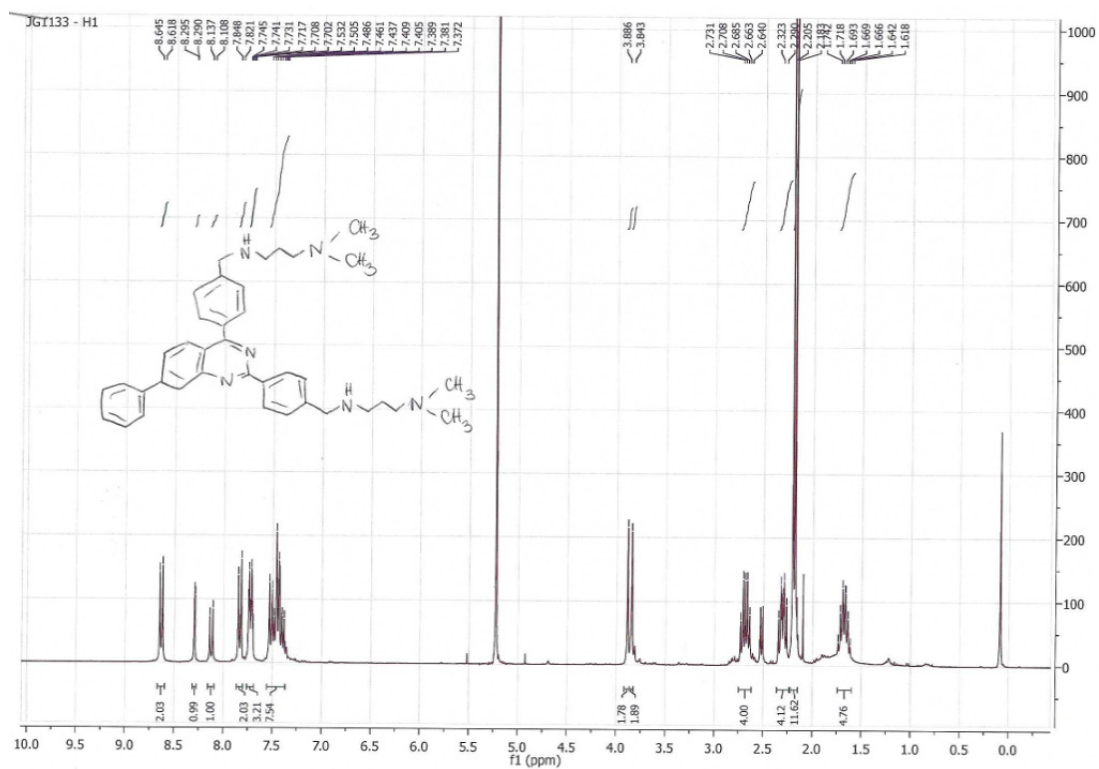


Figure S17. ^1H NMR spectrum of 12f.

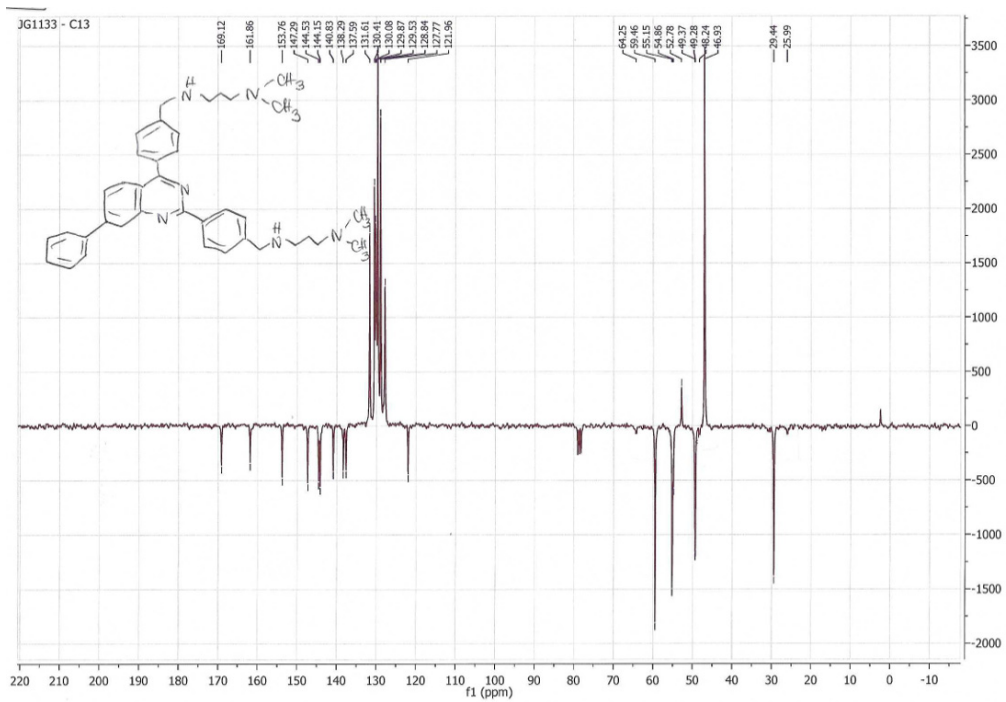


Figure S18. ^{13}C NMR spectrum of 12f.

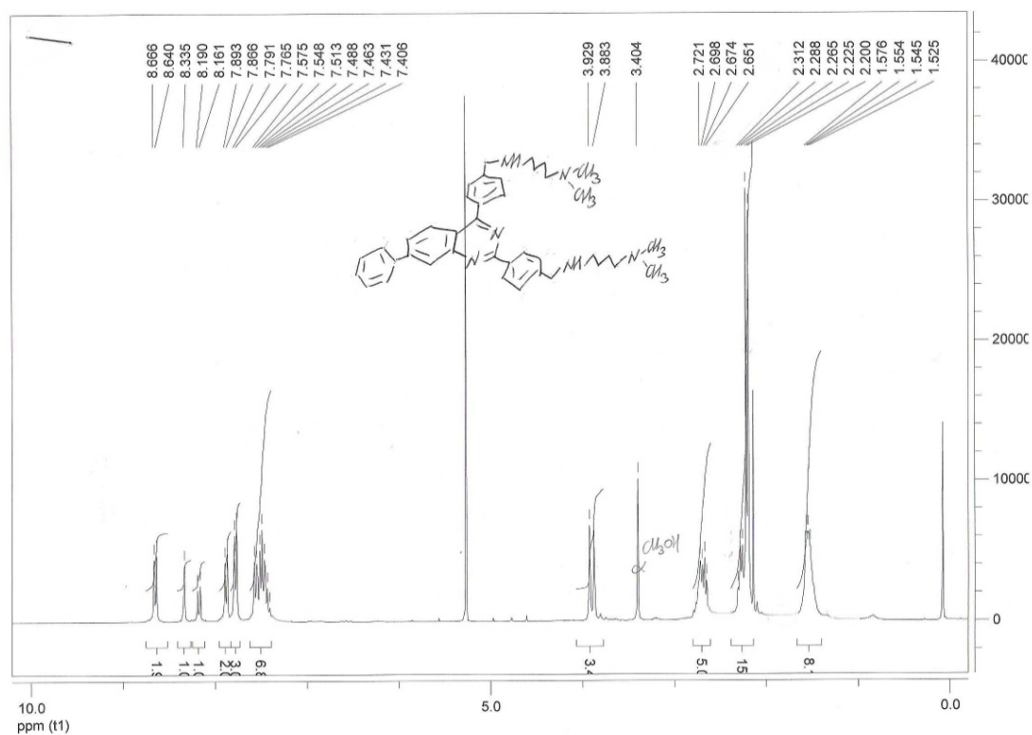


Figure S19. ¹H NMR spectrum of **12g**.

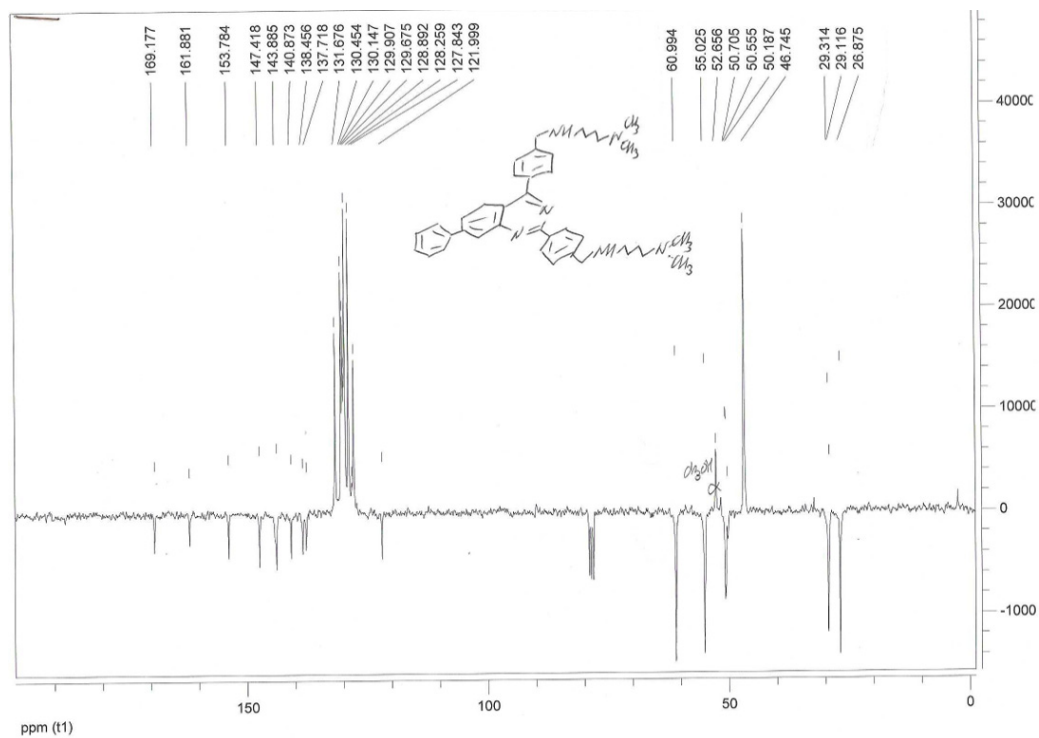


Figure S20. ¹³C NMR spectrum of **12g**.

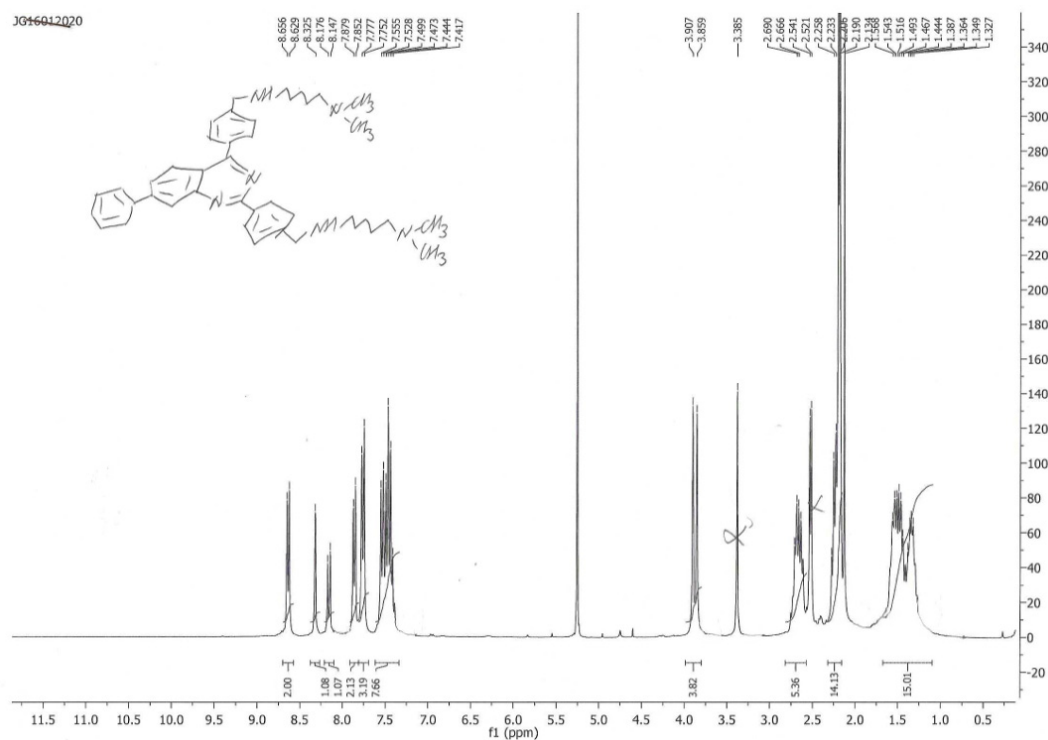


Figure S21. ¹H NMR spectrum of 12h.

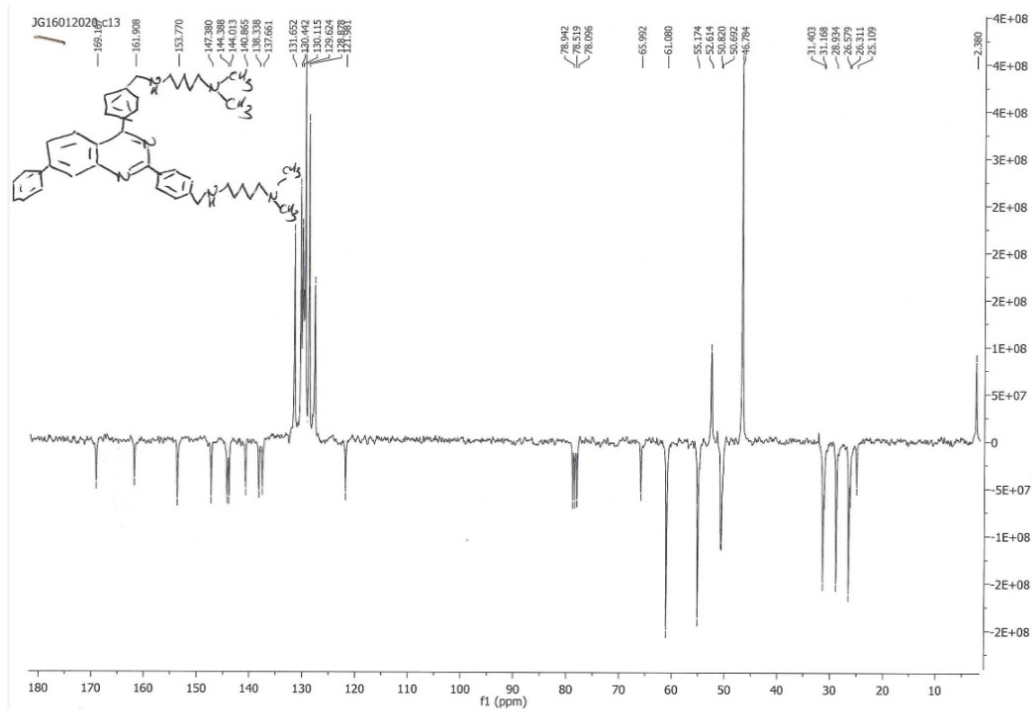


Figure S22. ¹³C NMR spectrum of 12h.

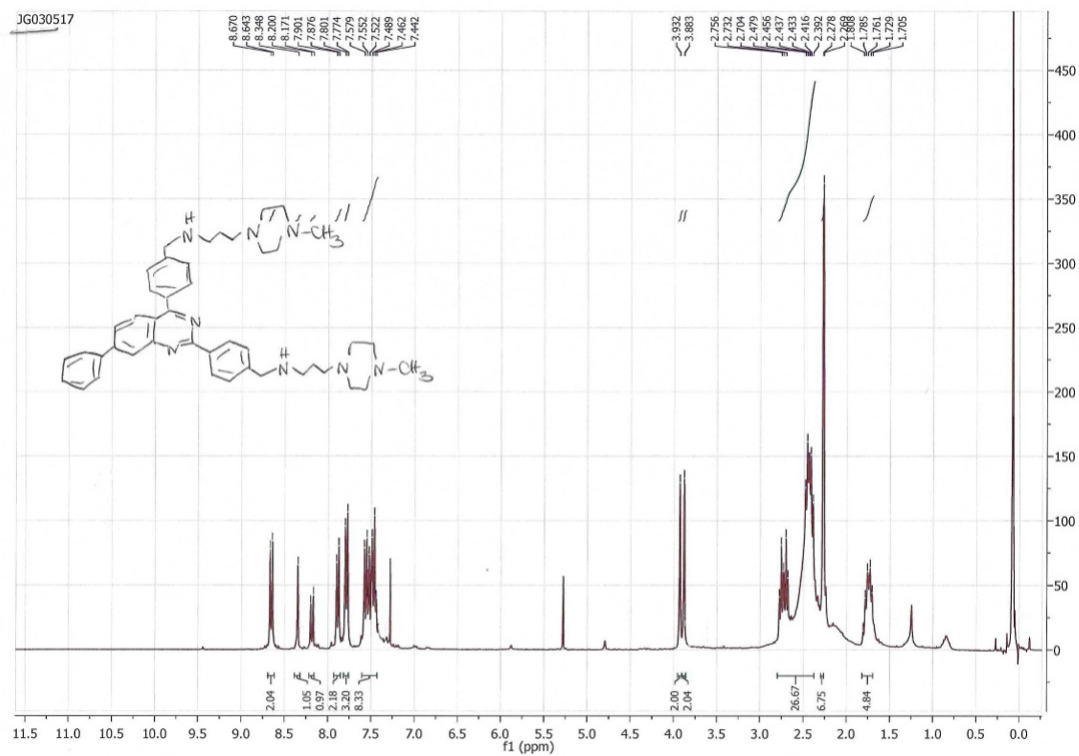


Figure S23. ^1H NMR spectrum of 12i.

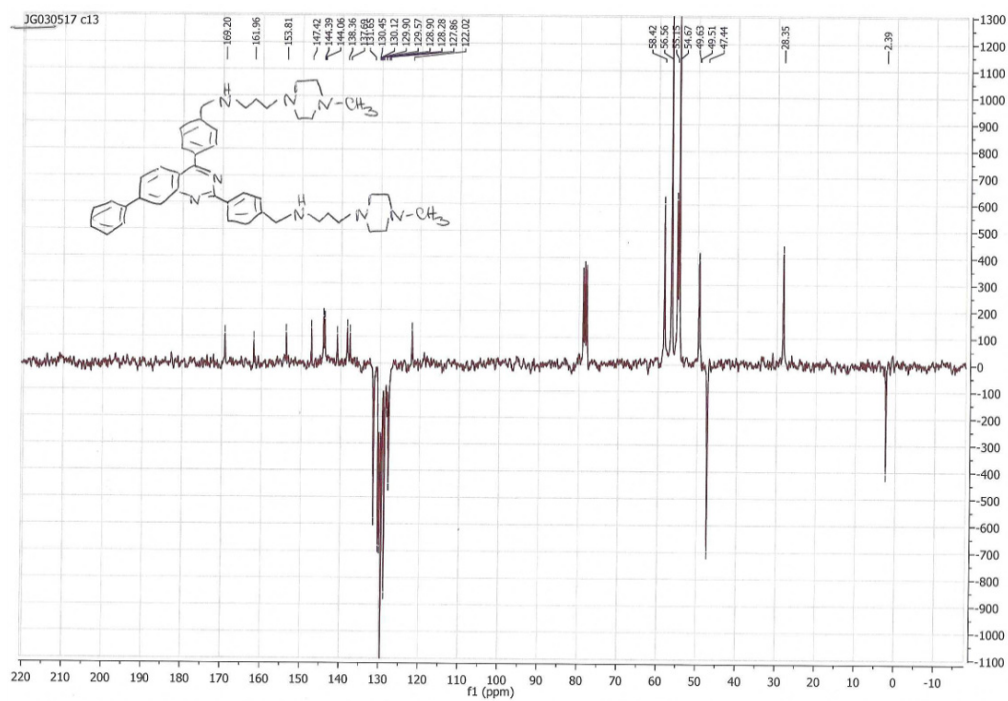
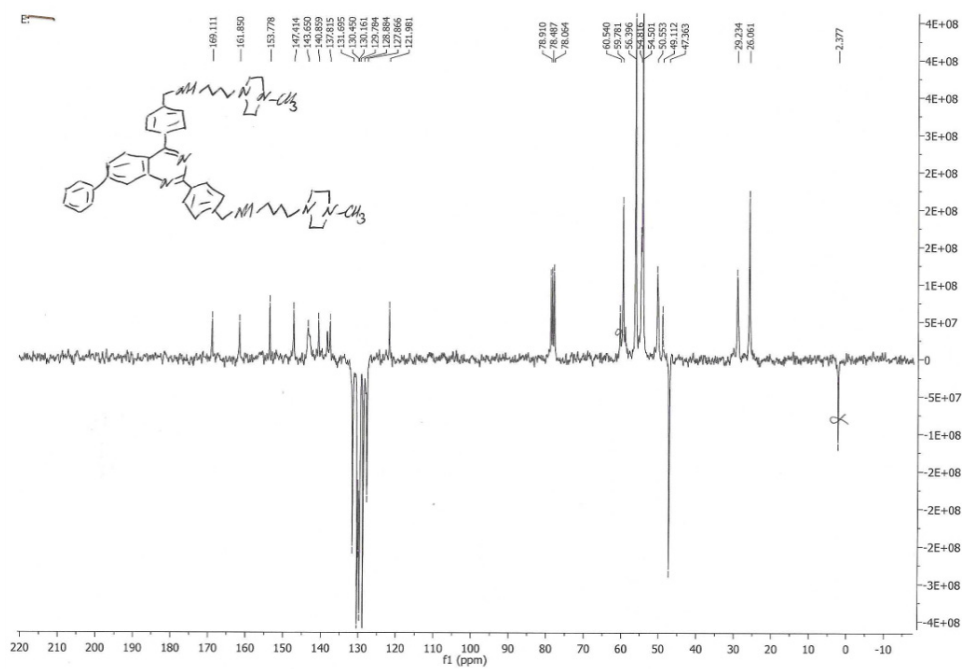
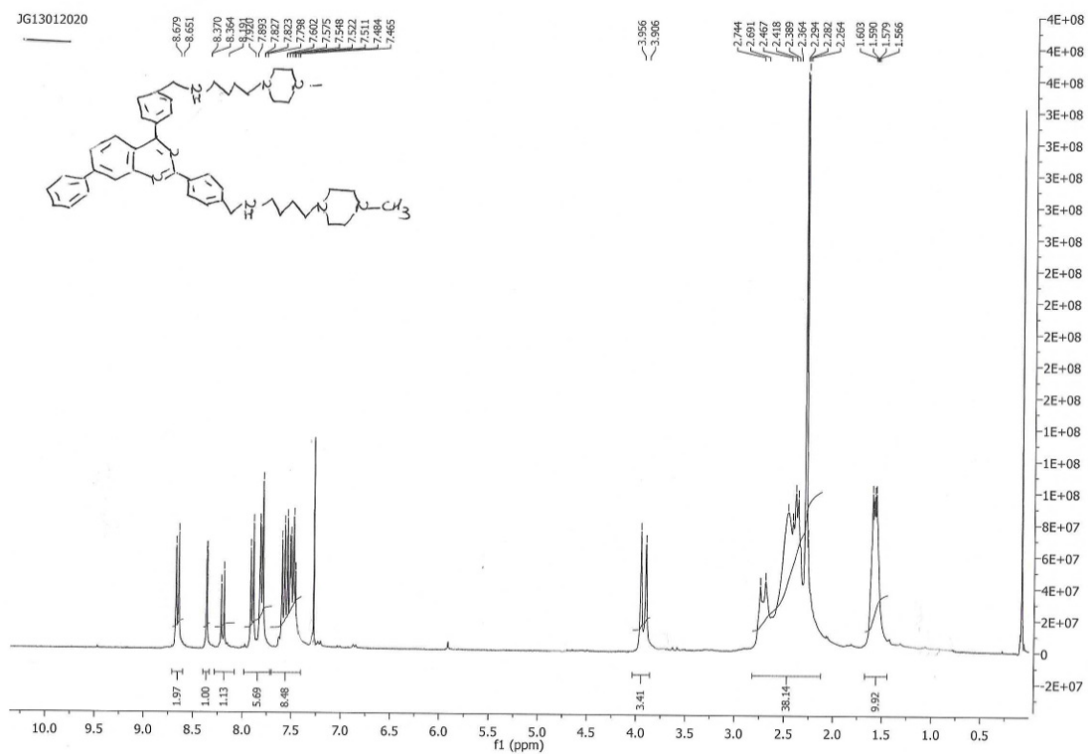


Figure S24. ^{13}C NMR spectrum of 12i.



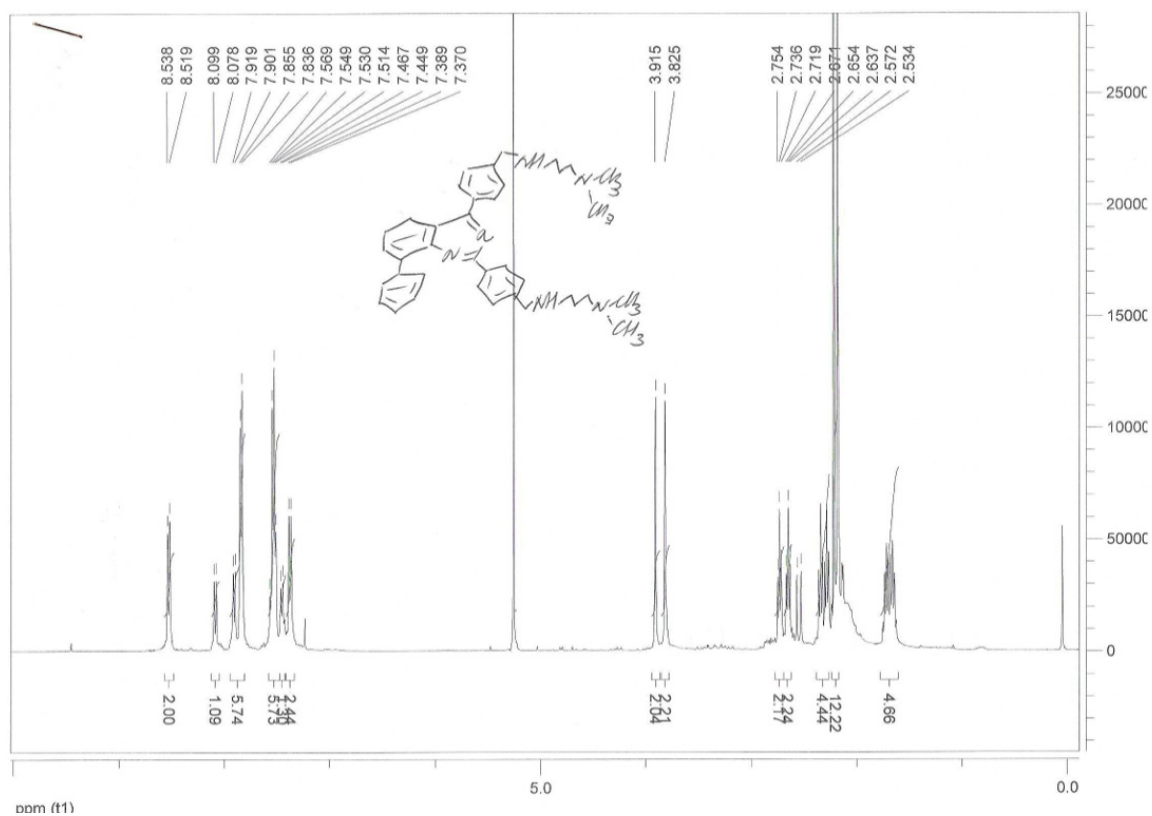


Figure S27. ¹H NMR spectrum of 12k.

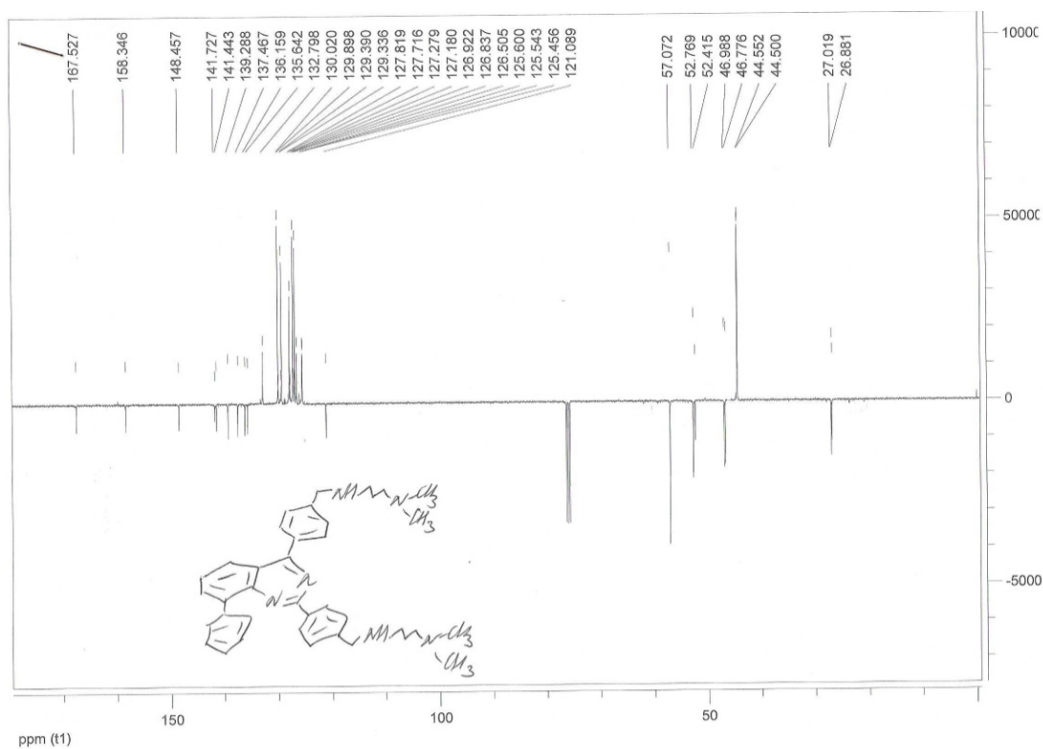


Figure S28. ¹³C NMR spectrum of 12k.

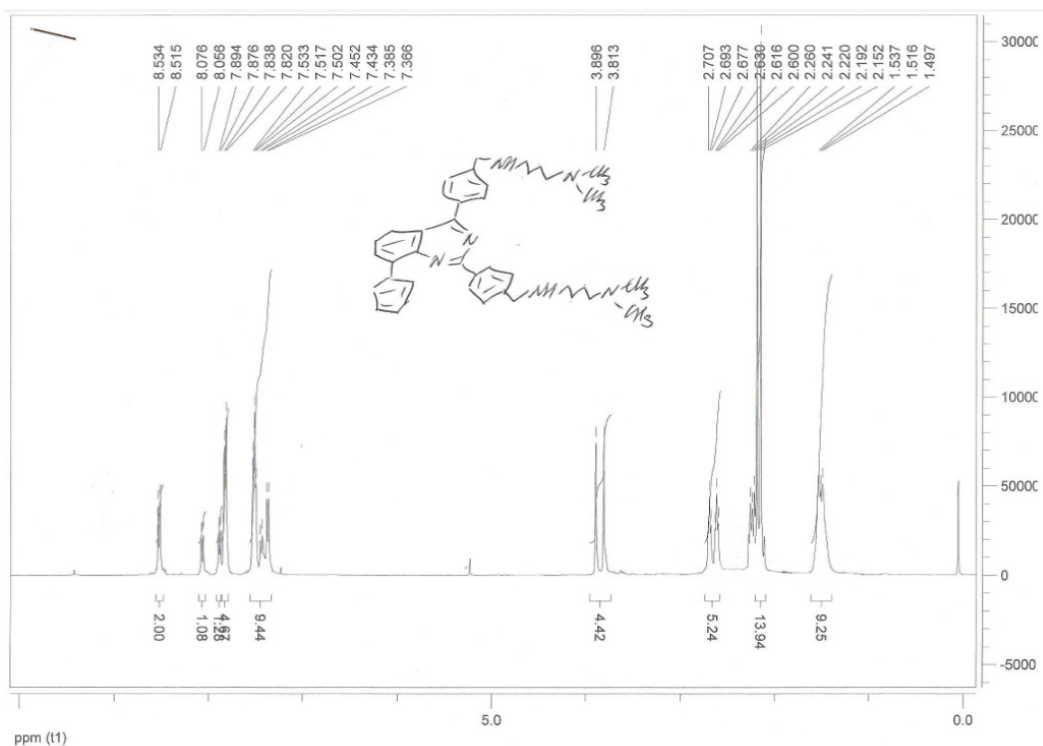


Figure S29. ¹H NMR spectrum of 12l.

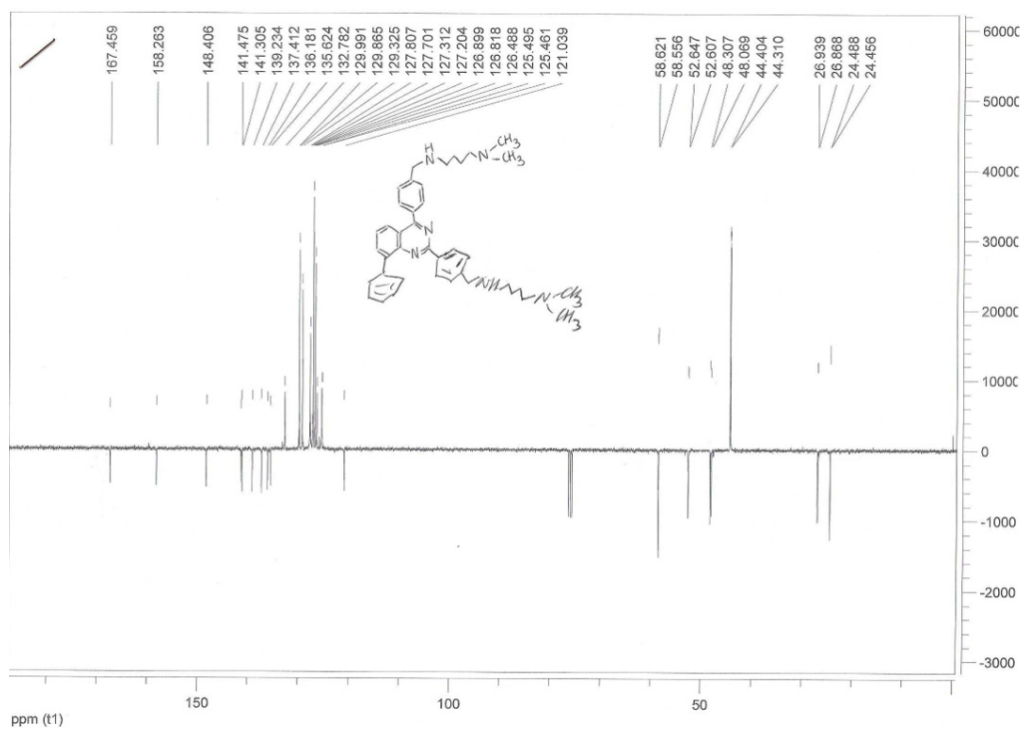


Figure S30. ¹³C NMR spectrum of 12l.

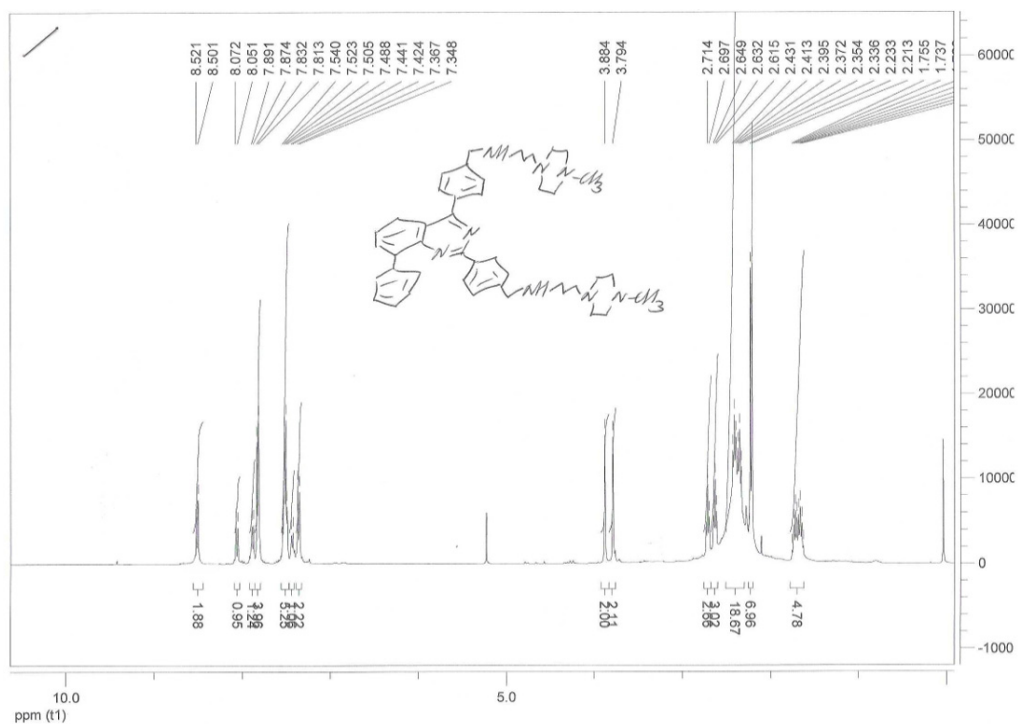


Figure S31. ¹H NMR spectrum of 12m.

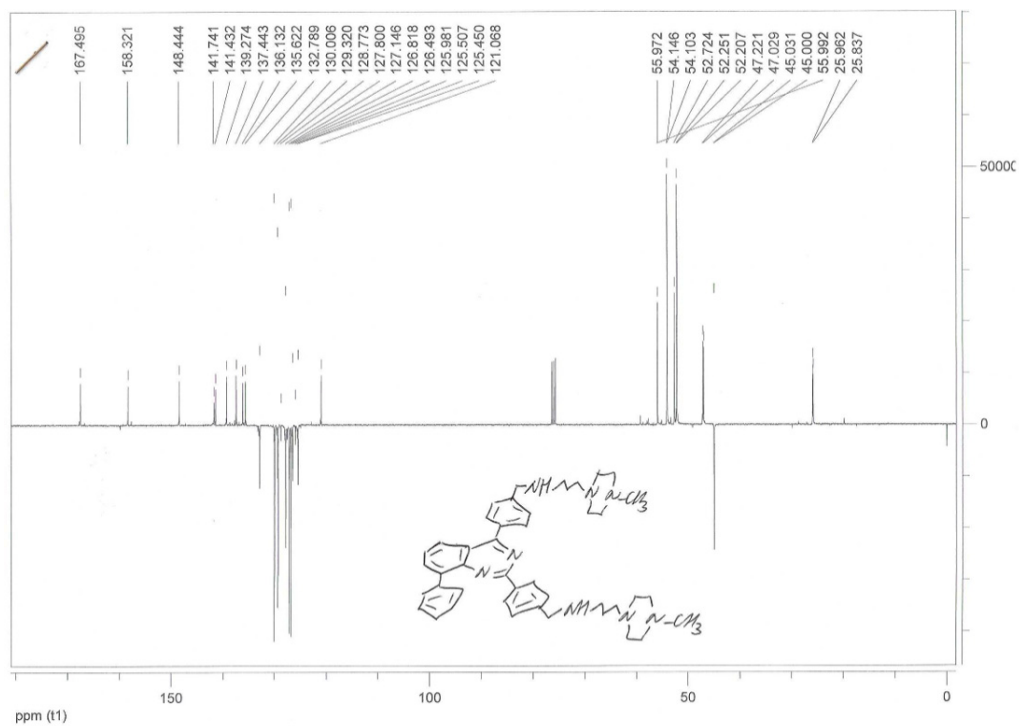


Figure S32. ¹³C NMR spectrum of 12m.

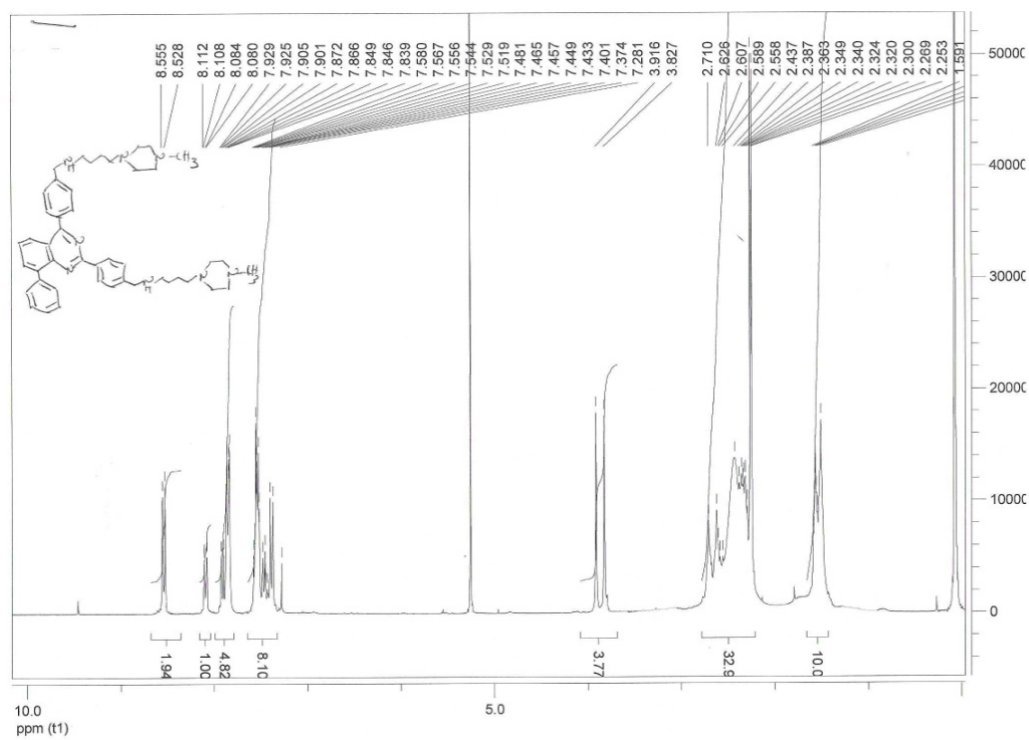


Figure S33. ¹H NMR spectrum of 12n.

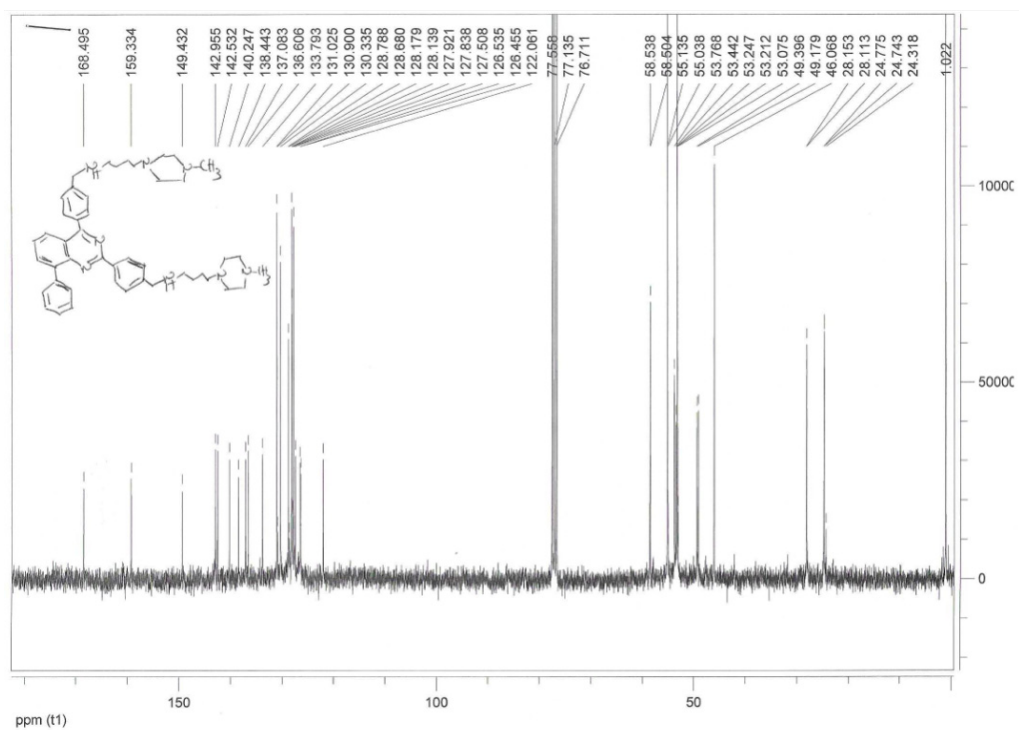


Figure S34. ¹³C NMR spectrum of 12n.

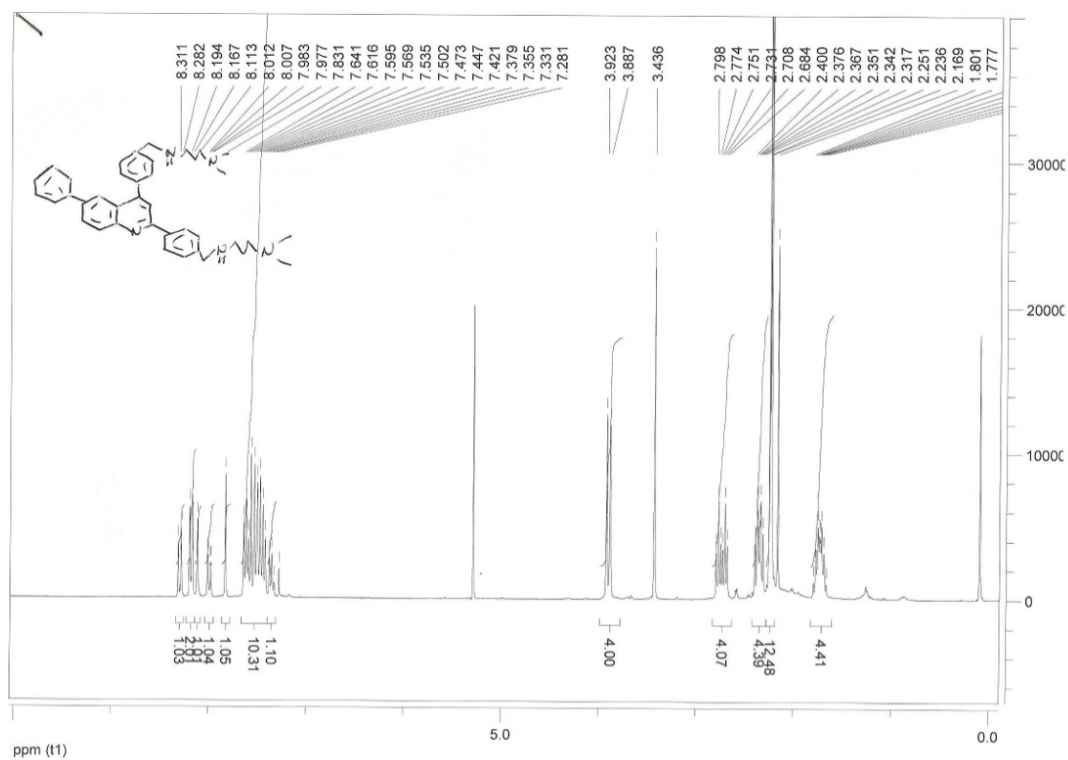


Figure S35. ^1H NMR spectrum of 13a.

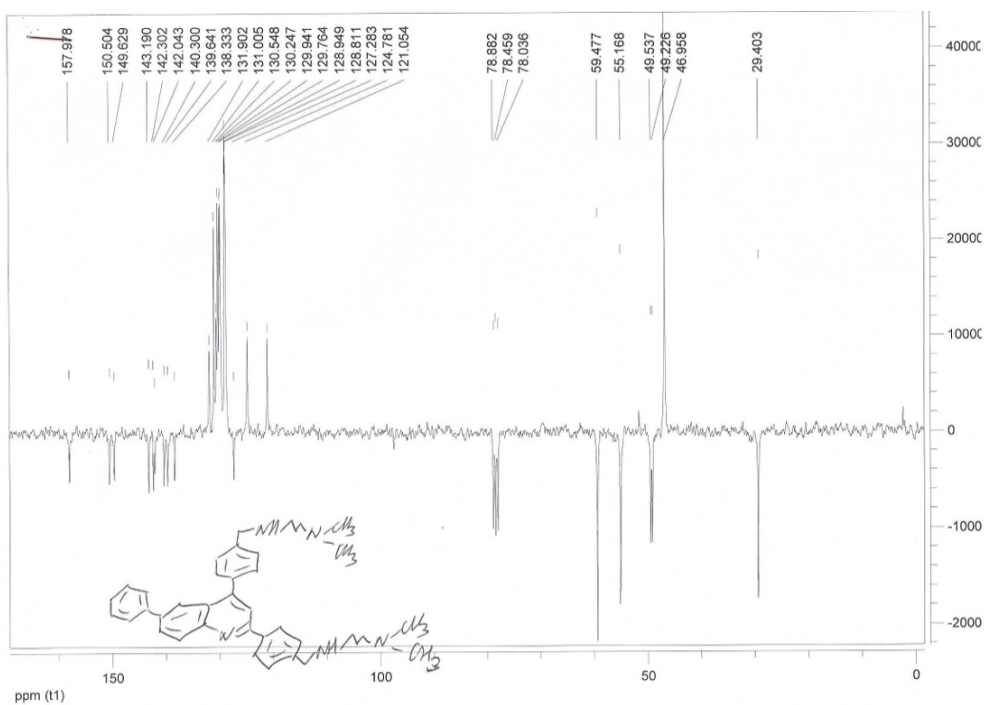


Figure S36. ^{13}C NMR spectrum of 13a.

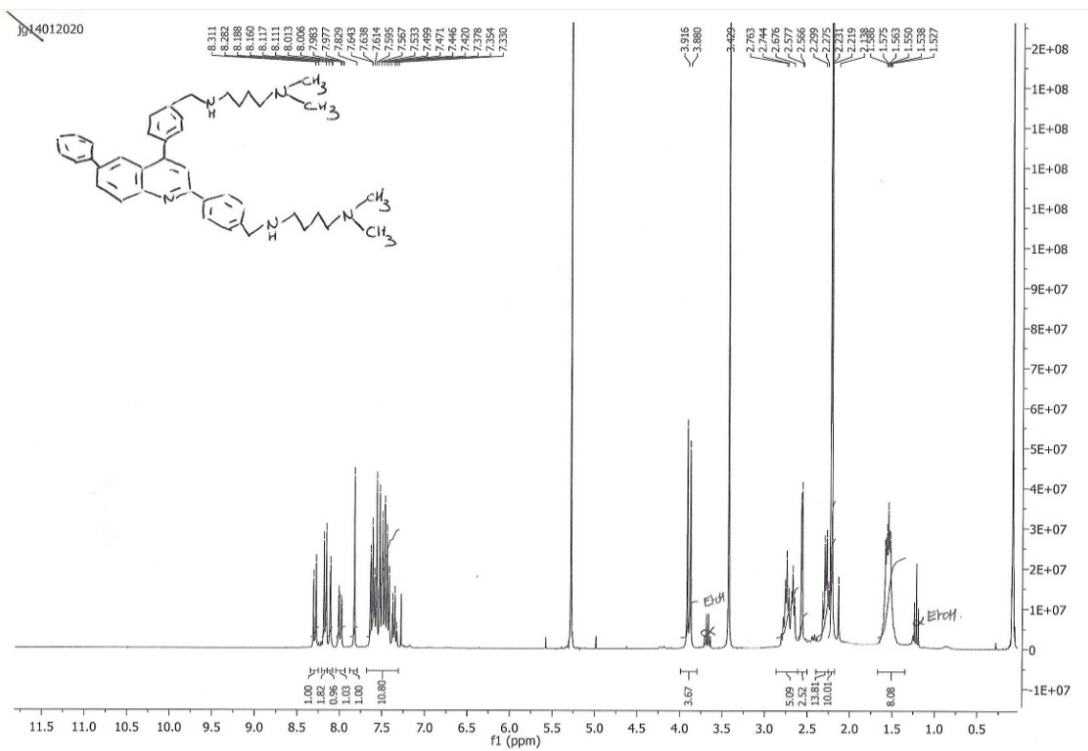


Figure S37. ¹H NMR spectrum of 13b.

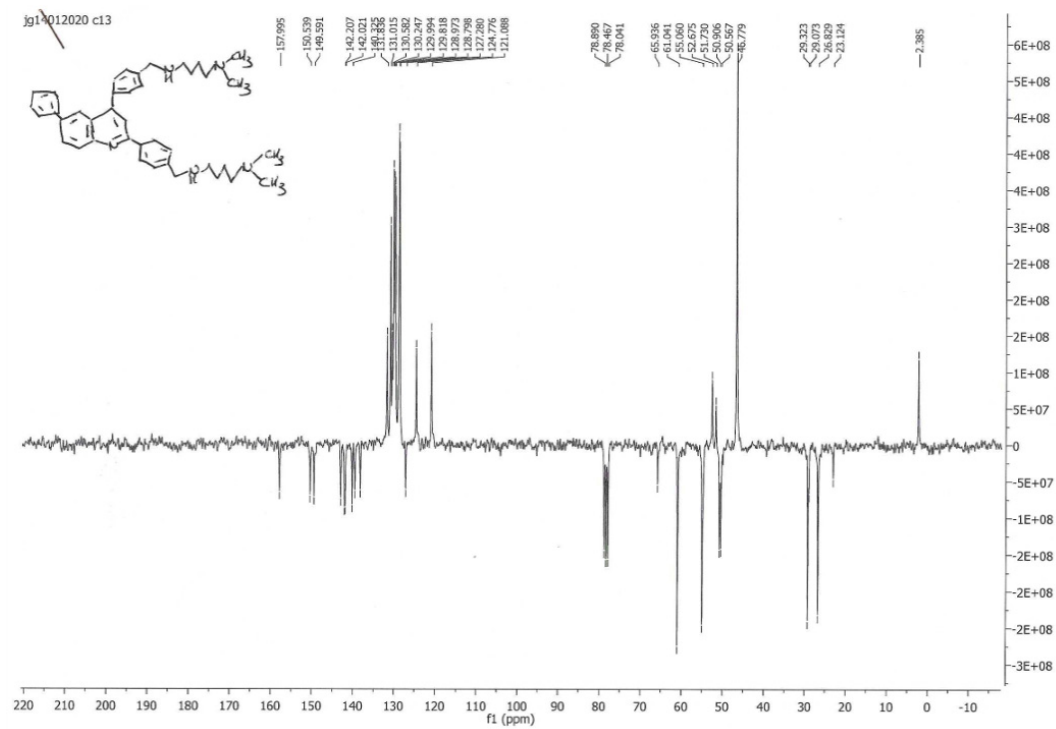


Figure S38. ¹³C NMR spectrum of 13b.

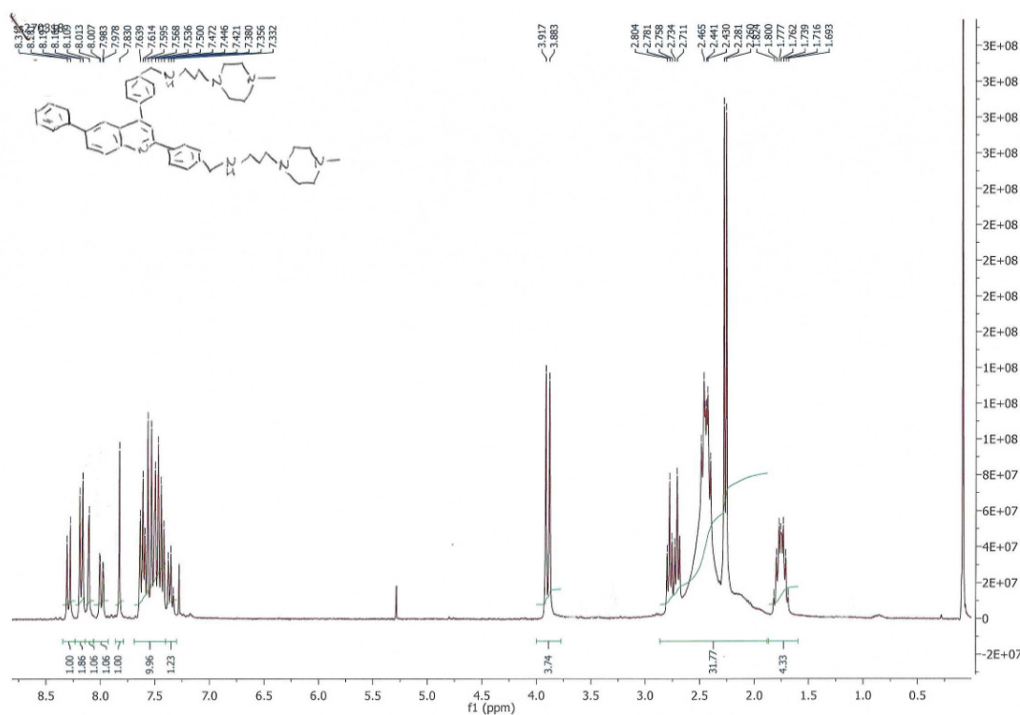


Figure S39. ¹H NMR spectrum of 13c.

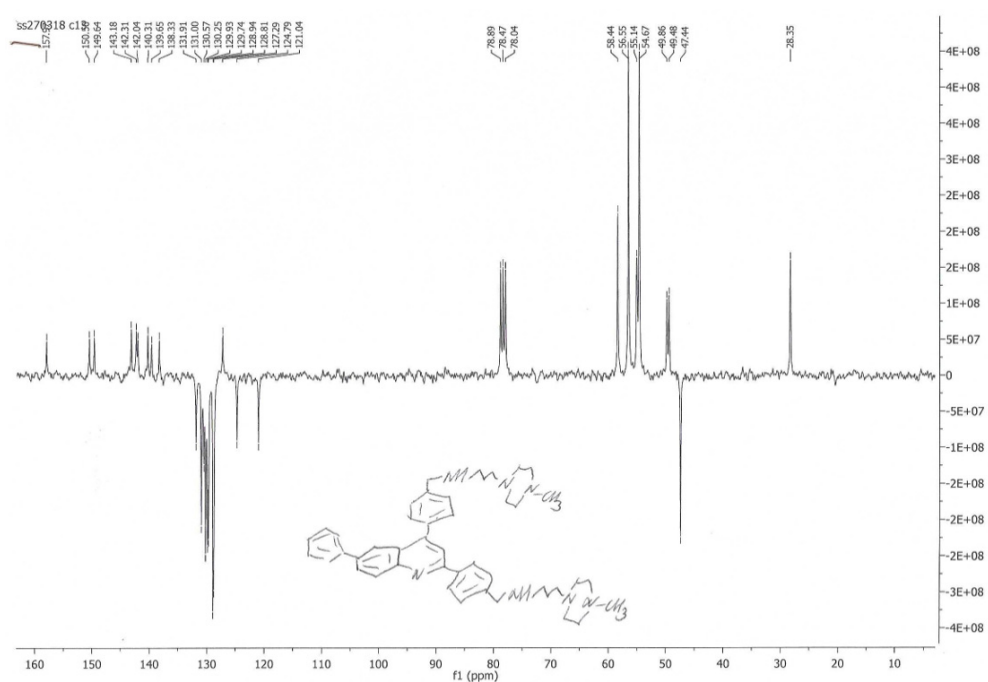


Figure S40. ¹³C NMR spectrum of 13c.

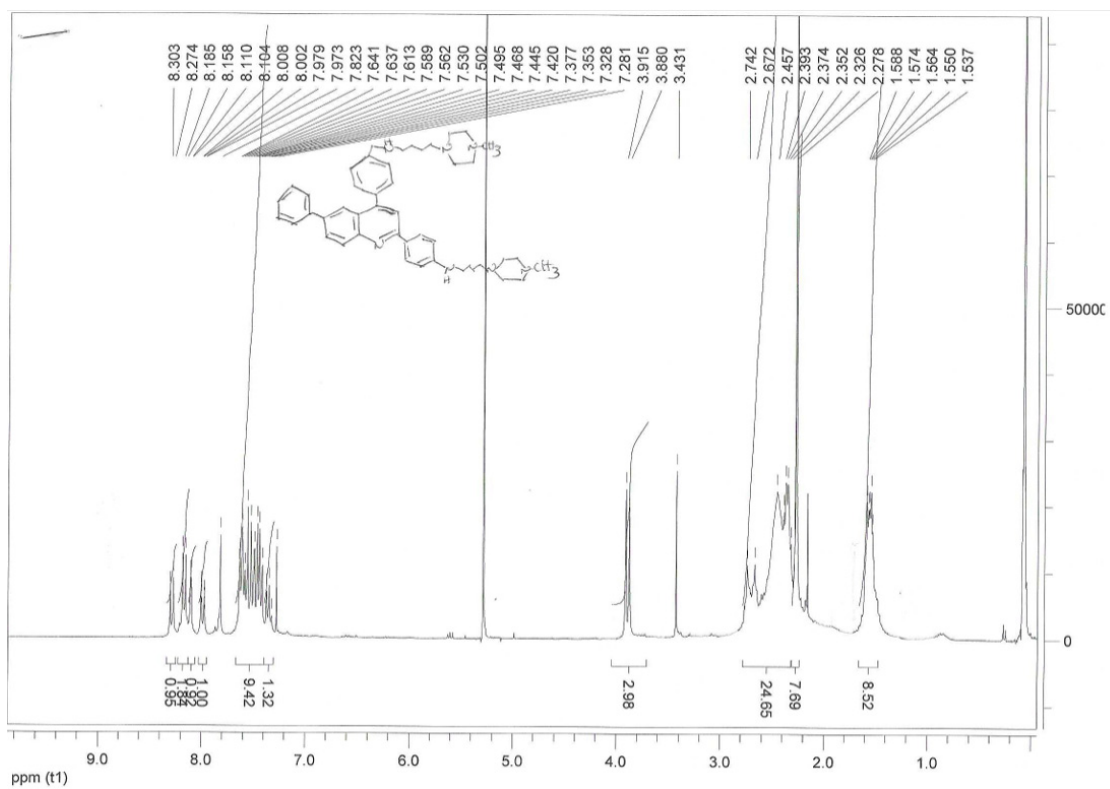


Figure S41. ¹H NMR spectrum of 13d.

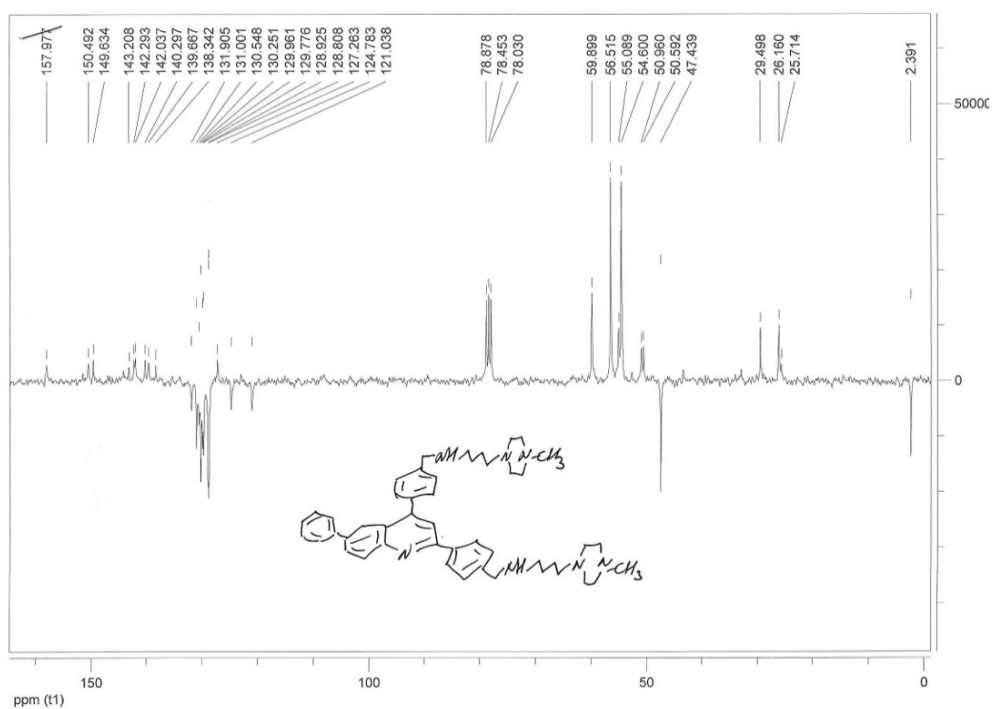


Figure S42. ¹³C NMR spectrum of 13d.

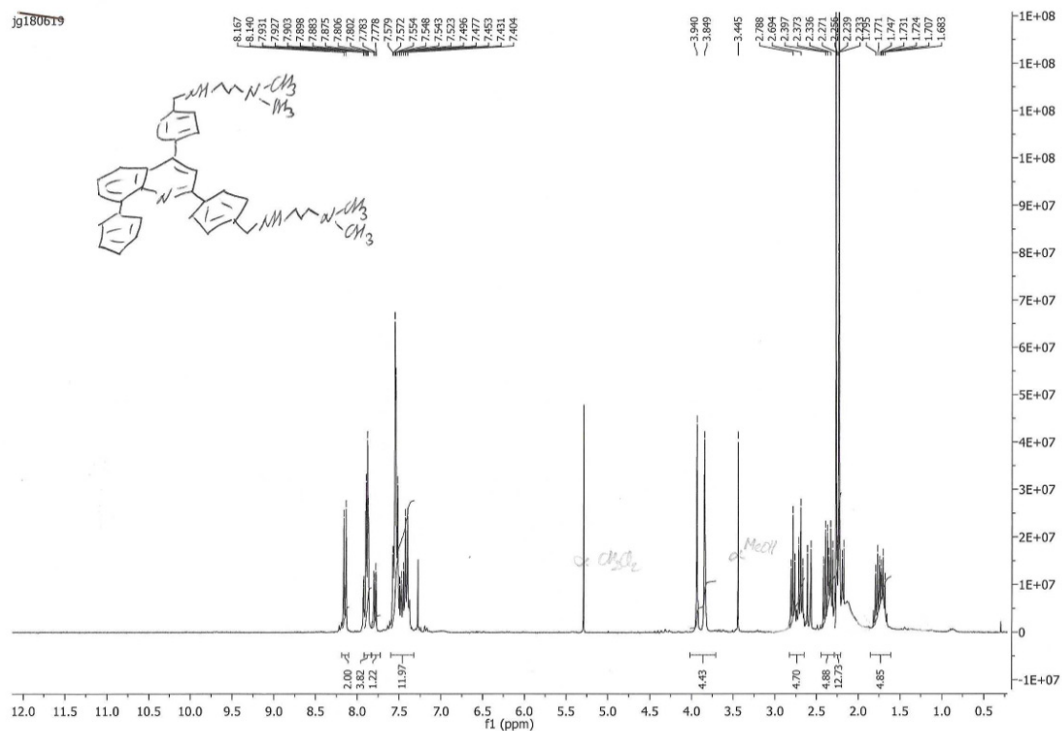


Figure S43. ¹H NMR spectrum of 13e.

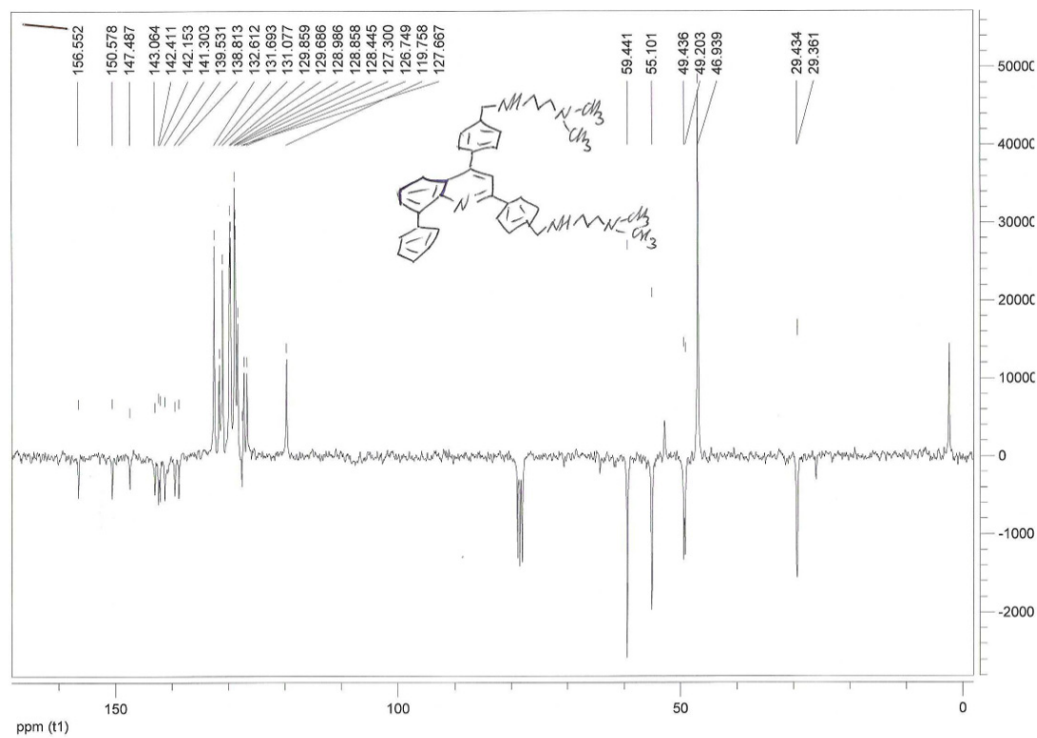


Figure S44. ¹³C NMR spectrum of 13e.

JG1468_200617091047 #1 RT: 0.01 AV: 1 NL: 4.97E7
T: FTMS Lp-ESI-Lens [150.00-2000.00]

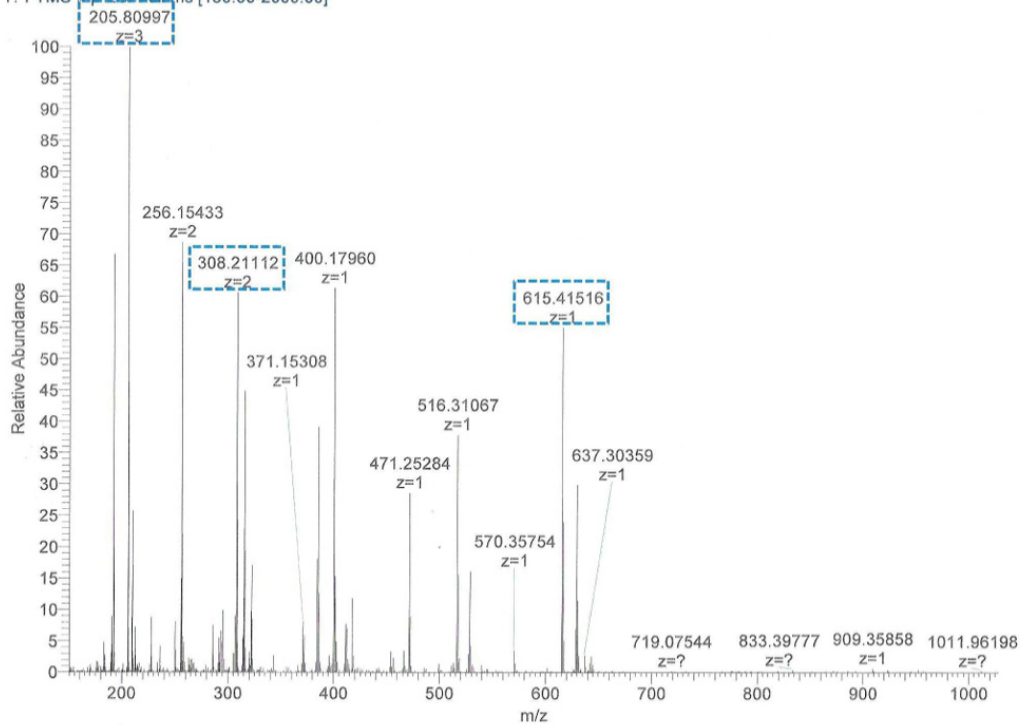


Figure S45. ESI-MS data for compound 12a.

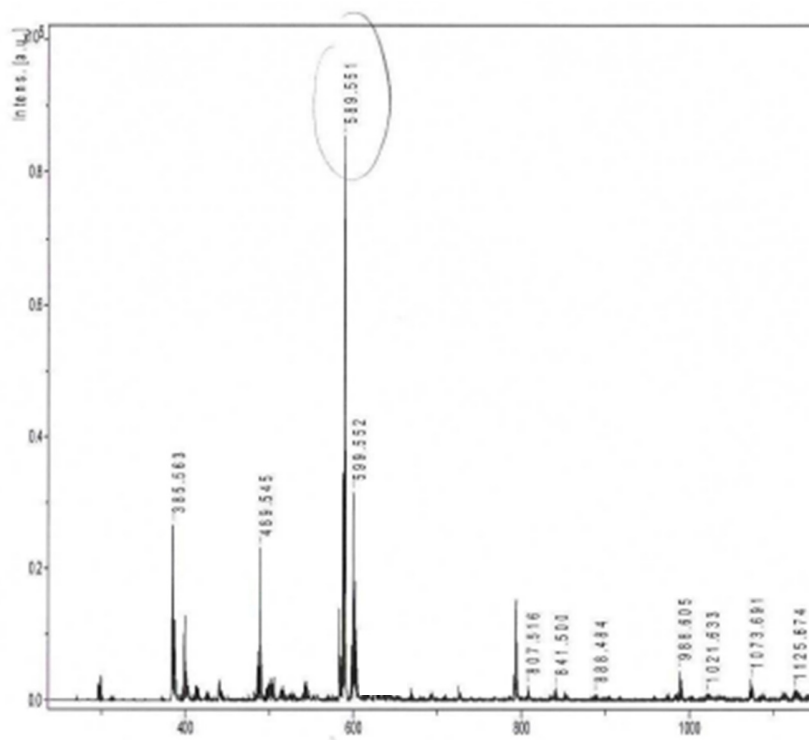


Figure S46. ESI-MS data for compound 12b.

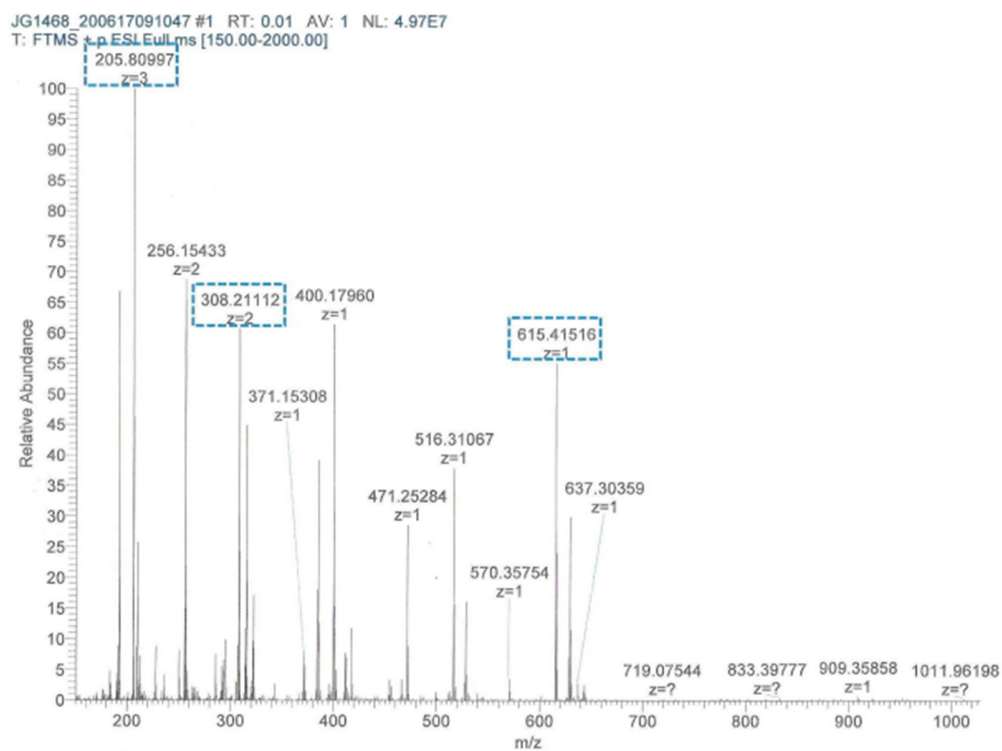


Figure S47. ESI-MS data for compound 12c.

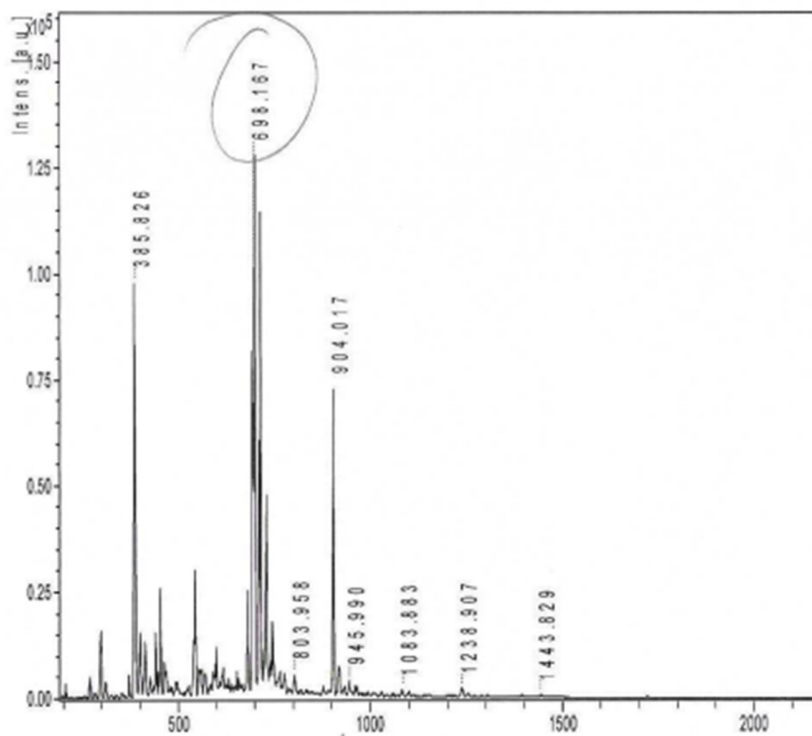


Figure S48. ESI-MS data for compound 12d.

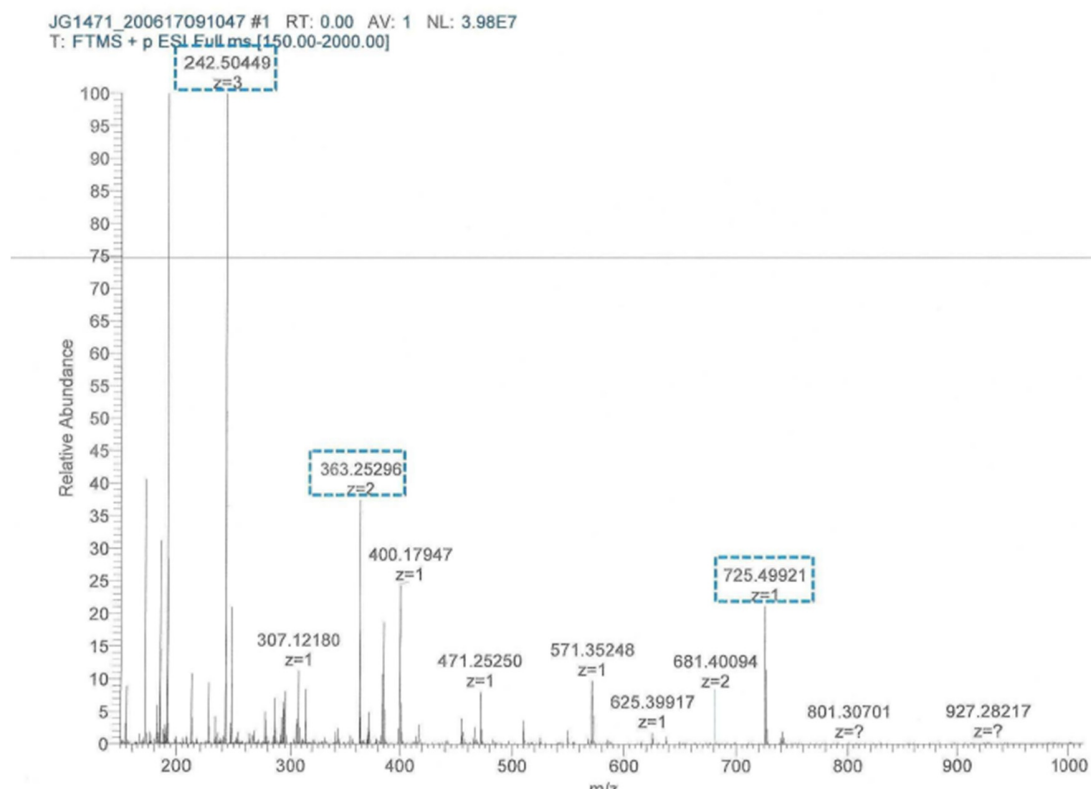


Figure S49. ESI-MS data for compound 12e.

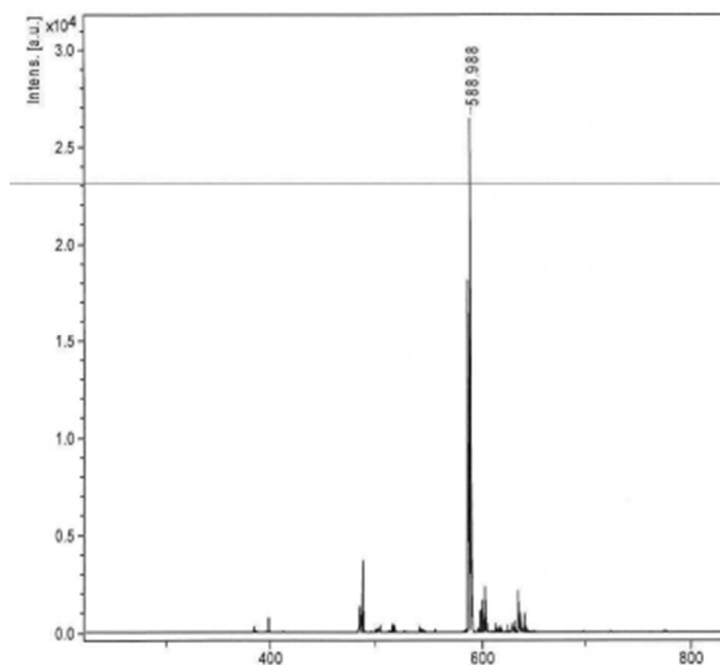


Figure S50. ESI-MS data for compound 12f.

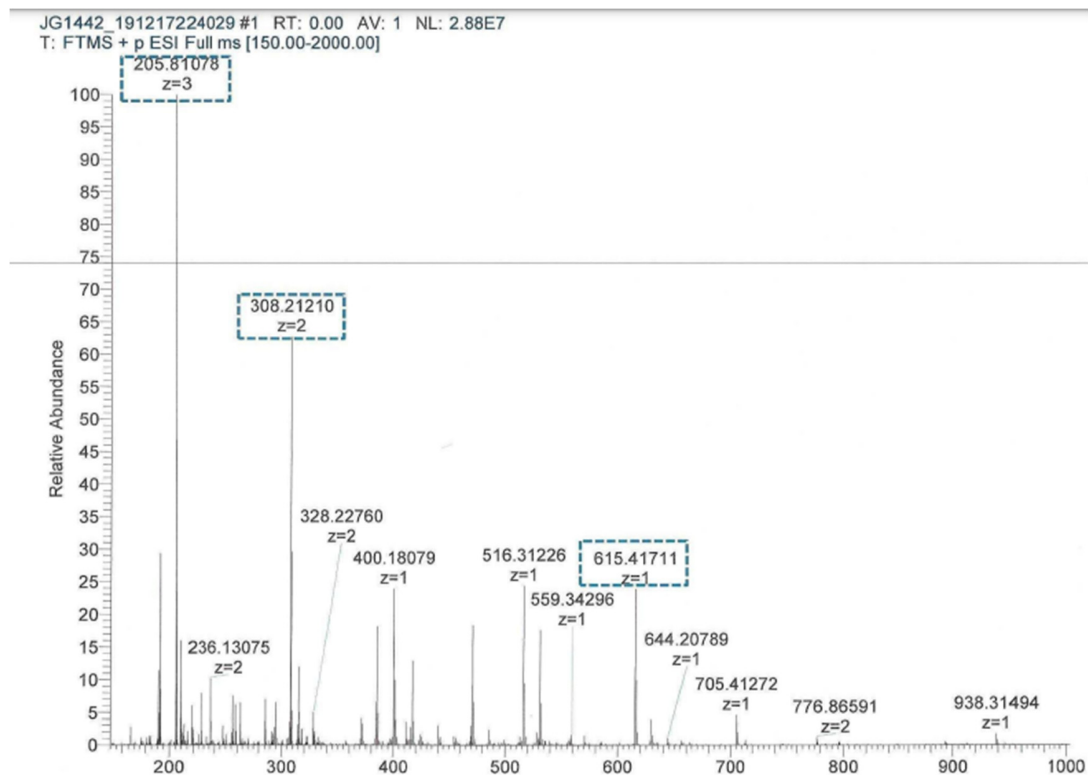


Figure S51. ESI-MS data for compound 12g.

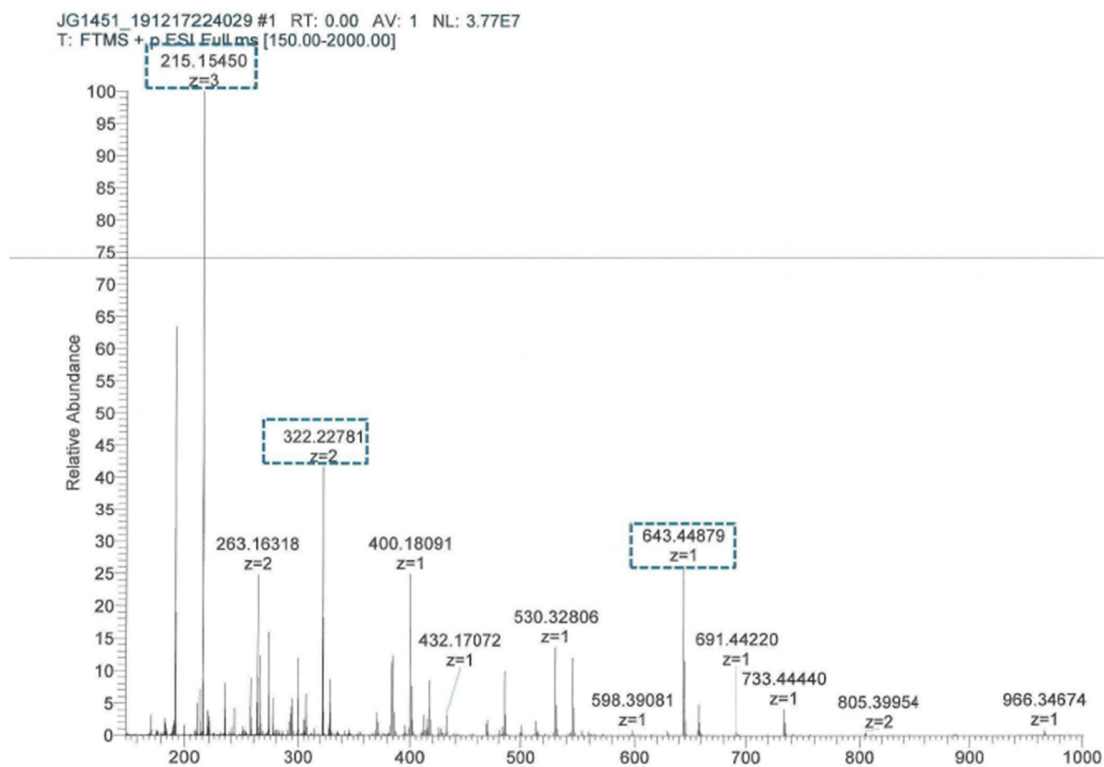


Figure S52. ESI-MS data for compound 12h.

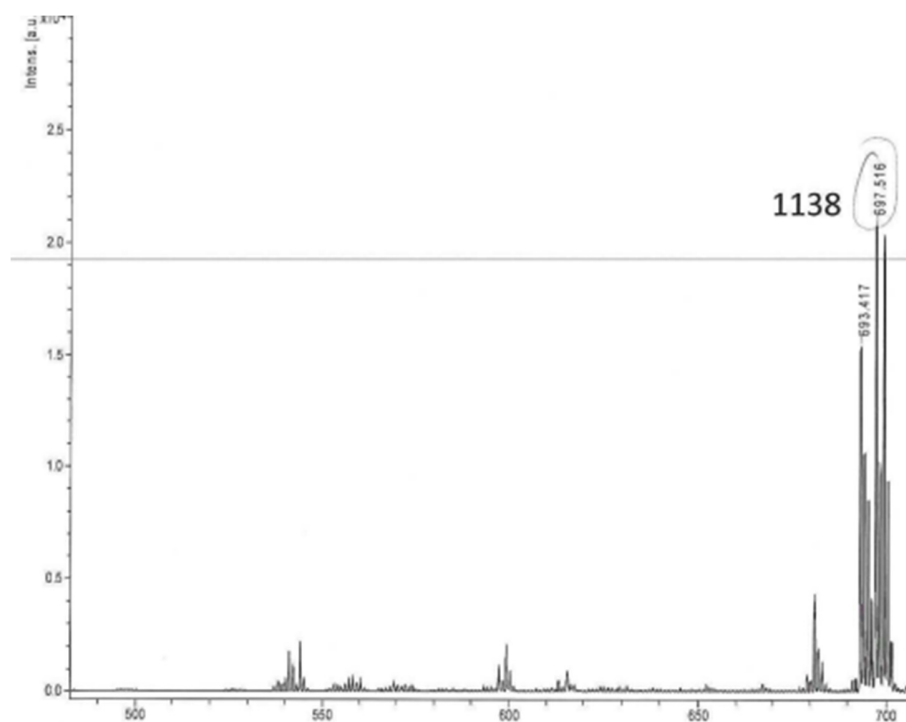


Figure S53. ESI-MS data for compound 12i.

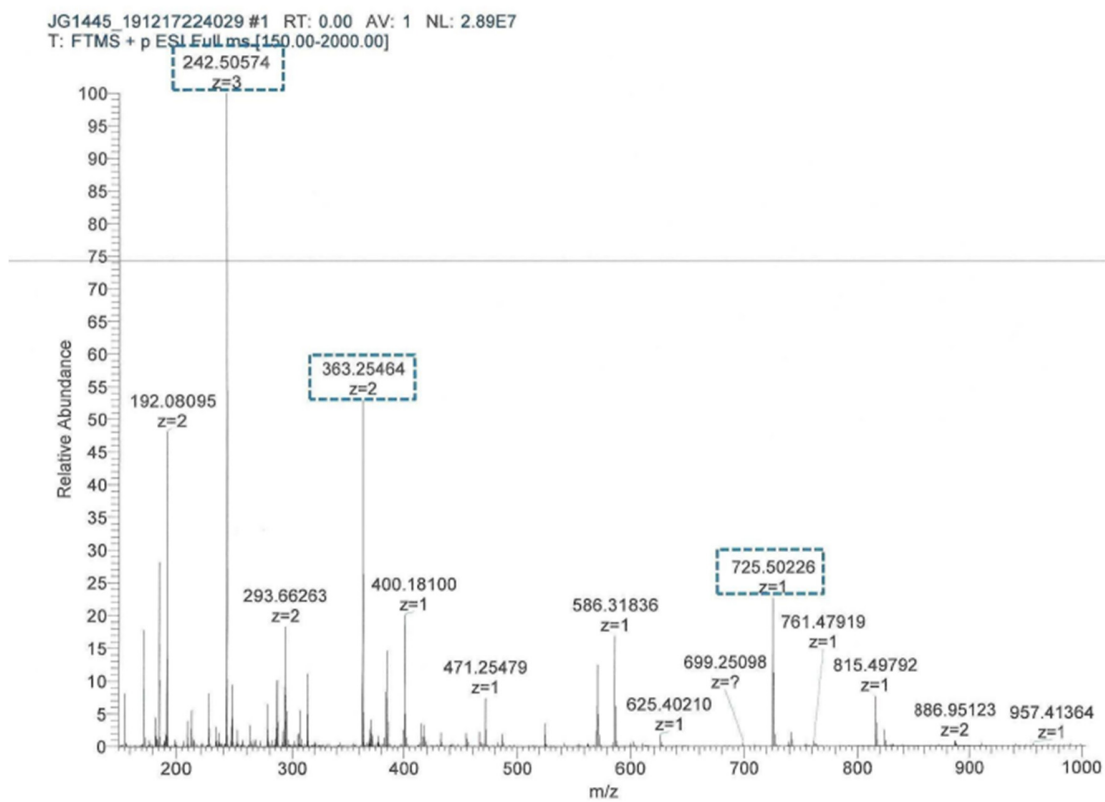


Figure S54. ESI-MS data for compound 12j.

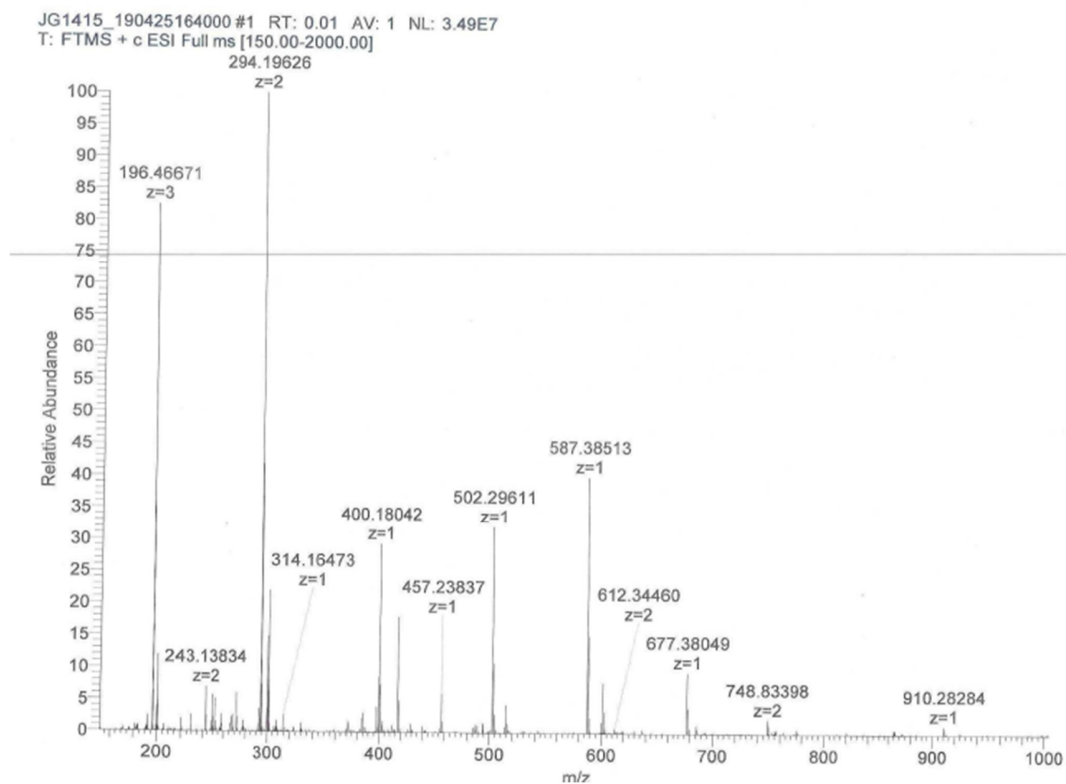


Figure S55. ESI-MS data for compound 12k.

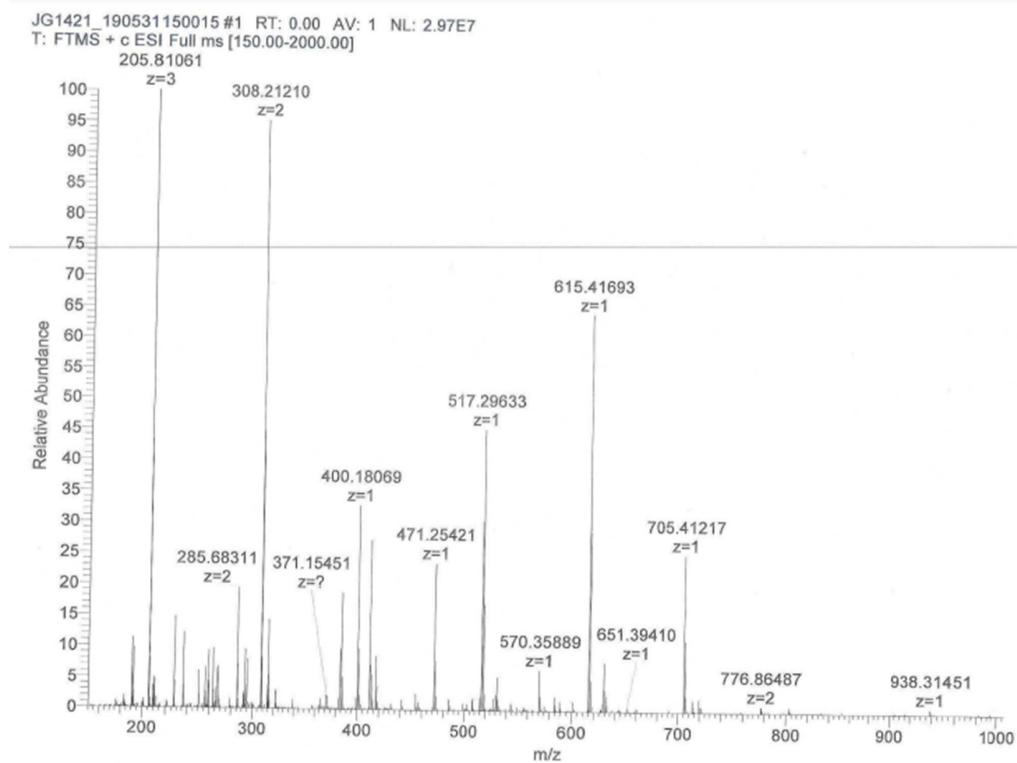


Figure S56. ESI-MS data for compound 12l.

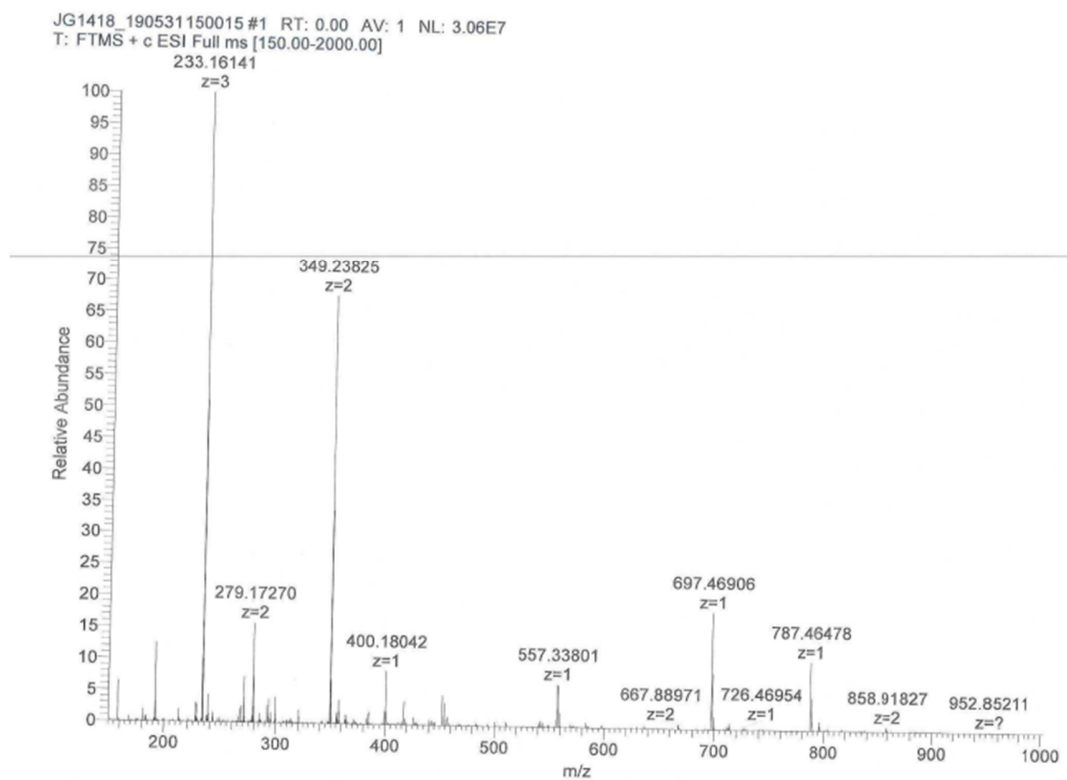


Figure S57. ESI-MS data for compound 12m.

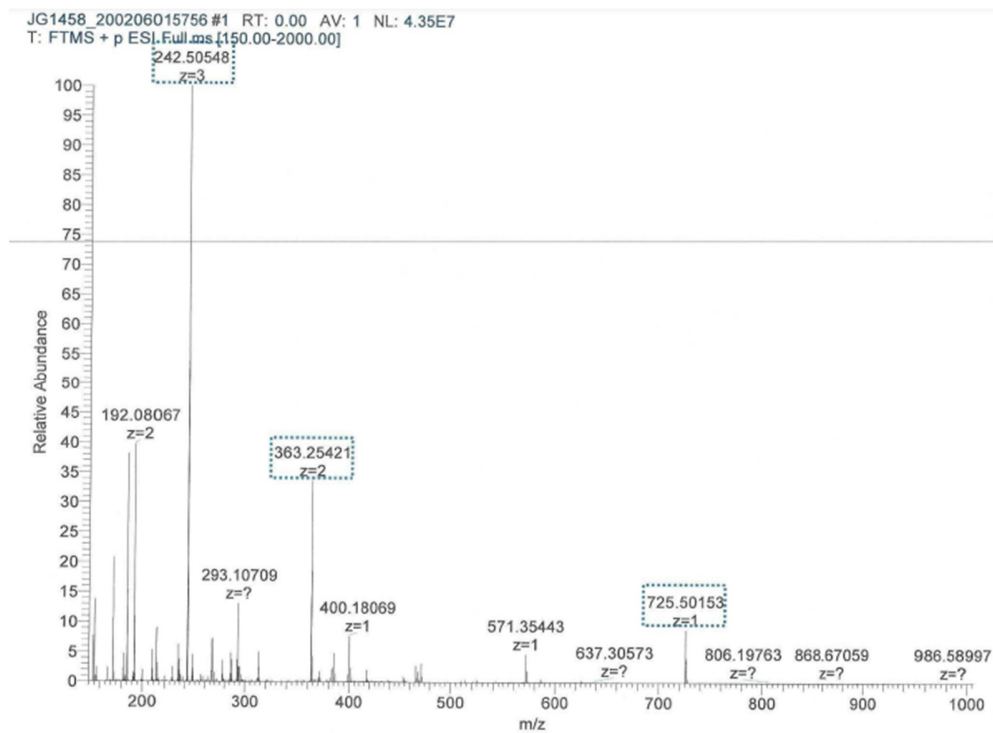


Figure S58. ESI-MS data for compound 12n.

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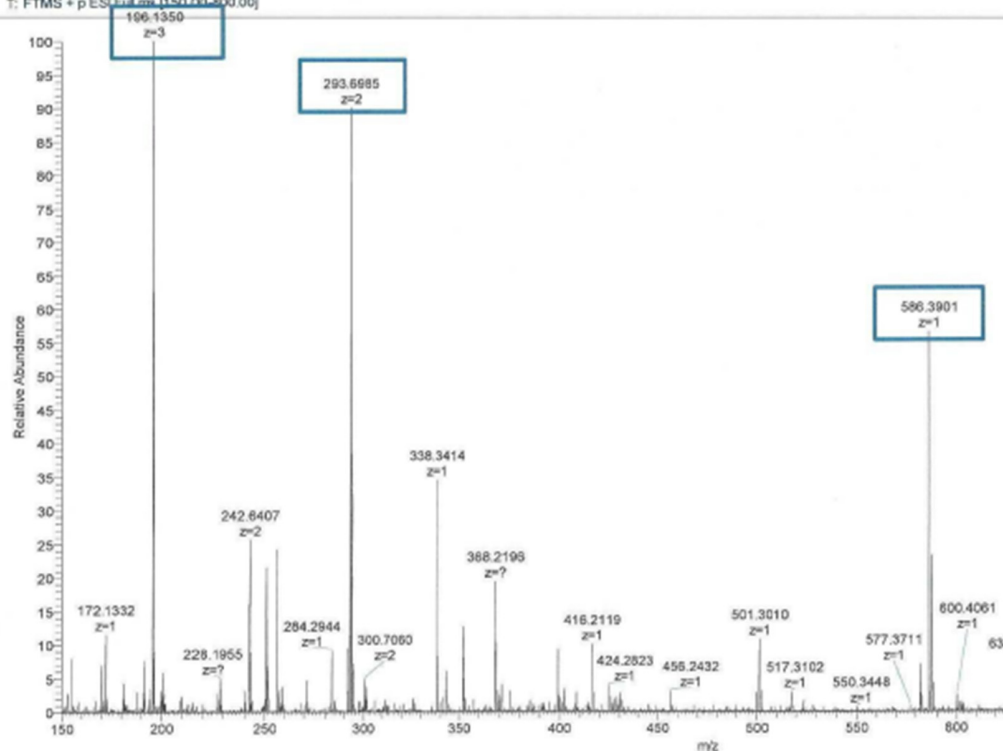


Figure S59. ESI-MS data for compound 13a.

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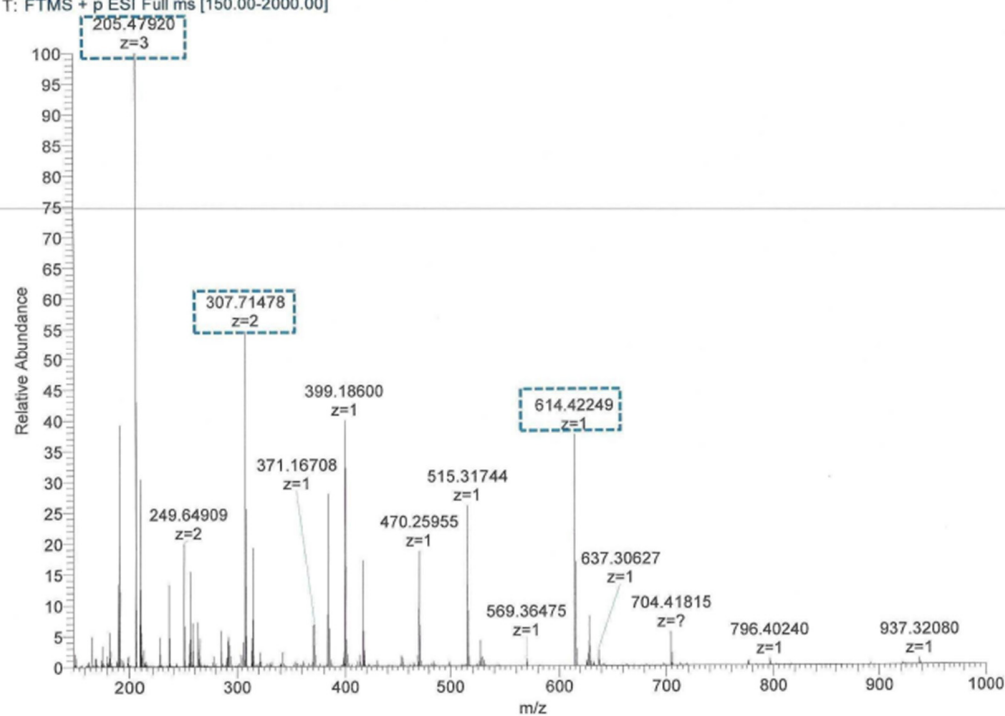


Figure S60. ESI-MS data for compound 13b.

JG1265_180702115925 #2-41 RT: 0.02-0.56 AV: 40 NL: 1.28E7
T: FTMS + p ESI Full ms [150.00-2000.00]

Ok z=

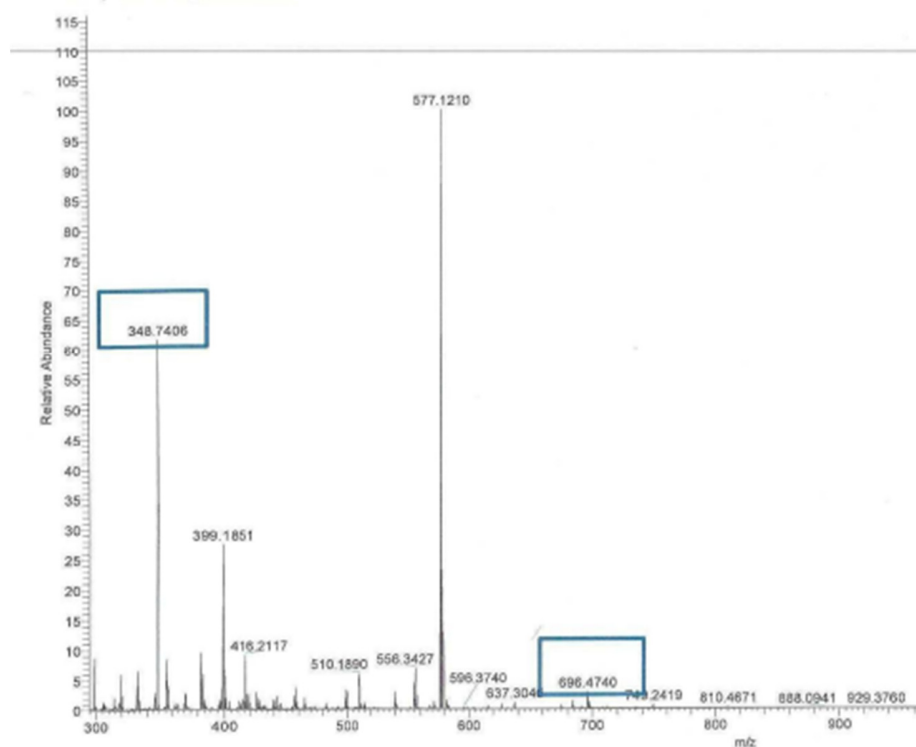


Figure S61. ESI-MS data for compound 13c.

JG1454_200206015756 #1 RT: 0.00 AV: 1 NL: 2.13E7
T: FTMS + p ESI Full ms [150.00-2000.00]

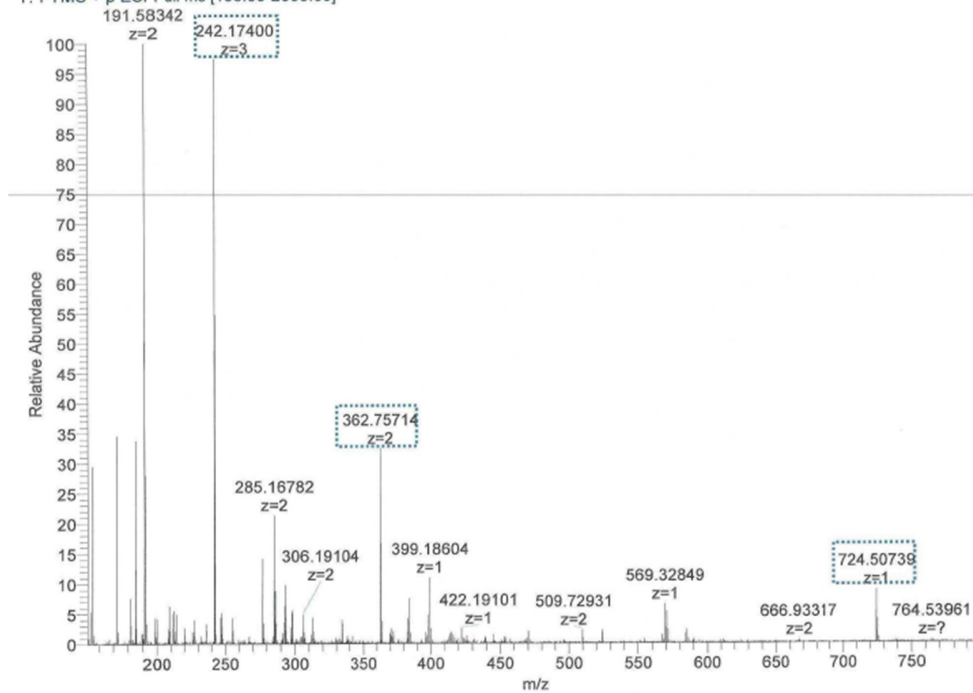


Figure S62. ESI-MS data for compound 13d.

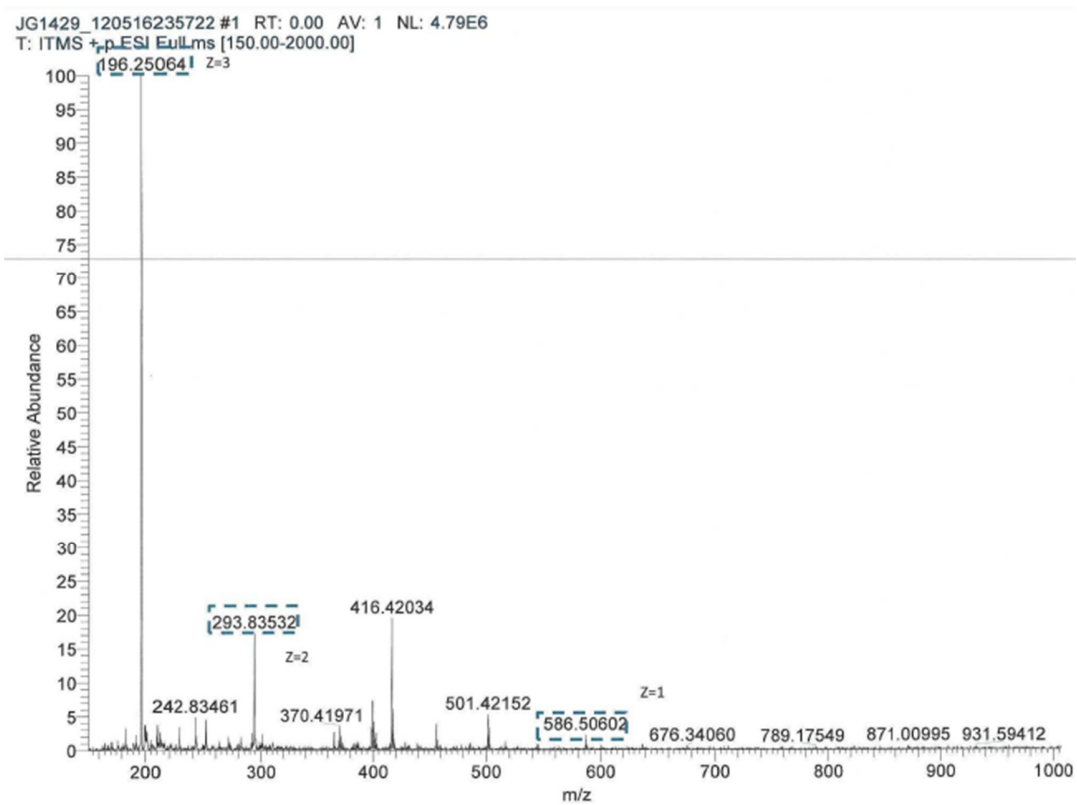


Figure S63. ESI-MS data for compound 13e.