Supporting Information

PAMAM-guanylthiourea conjugates mask furin's substrate binding site: Mechanistic insights from molecular docking and molecular dynamics studies assist the design of potential furin inhibitors

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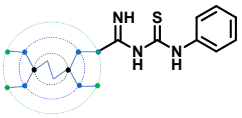
Contents of Supporting Information



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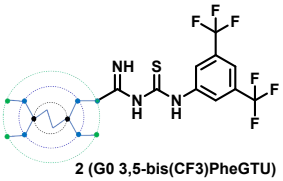

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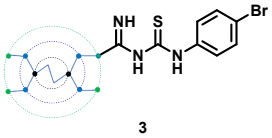

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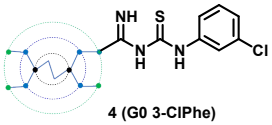

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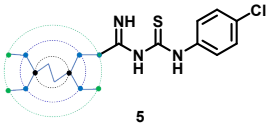

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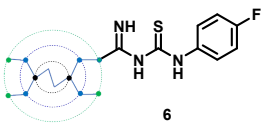

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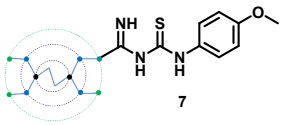

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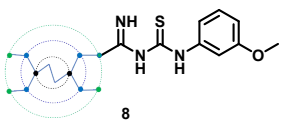

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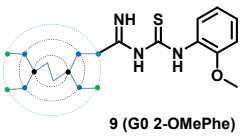

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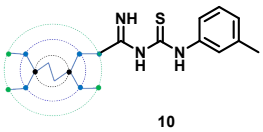

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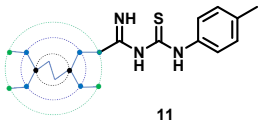

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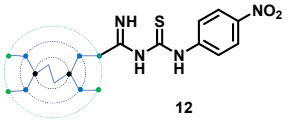

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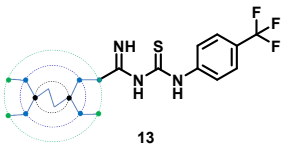

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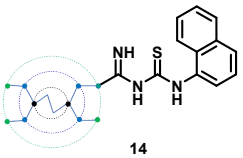

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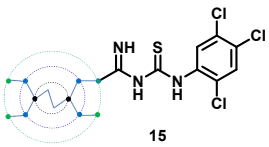

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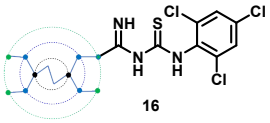

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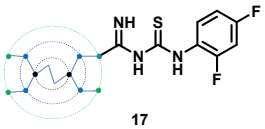

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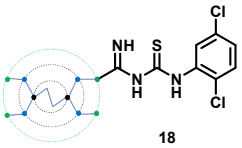

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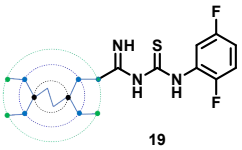

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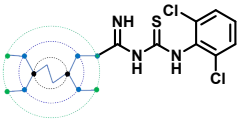

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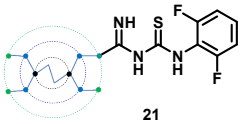

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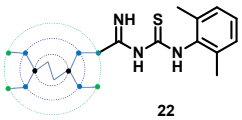

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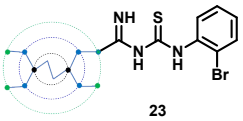

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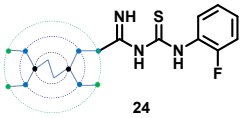

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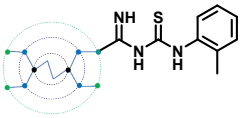

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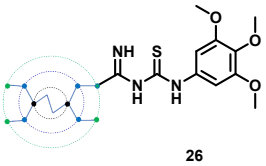

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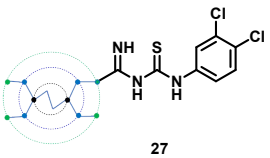

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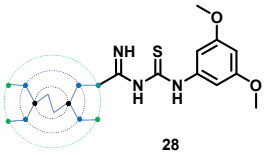

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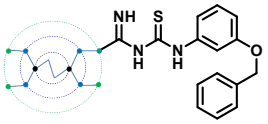

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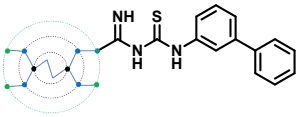

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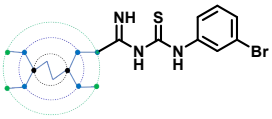

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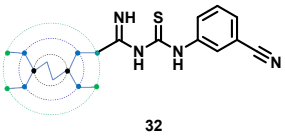

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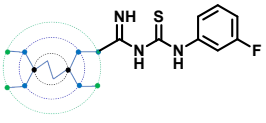

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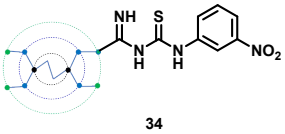

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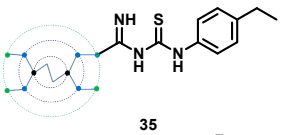

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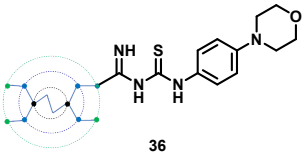

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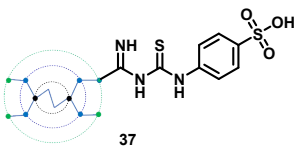

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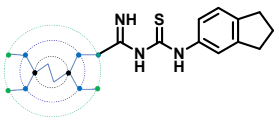

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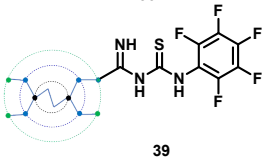

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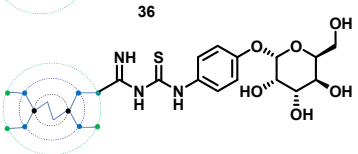

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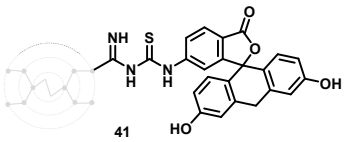
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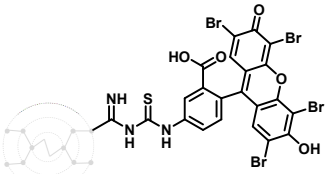
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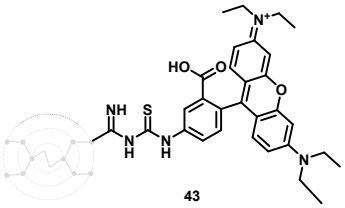
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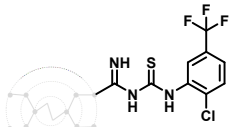
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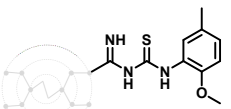
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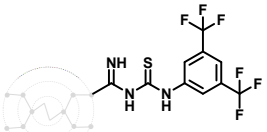
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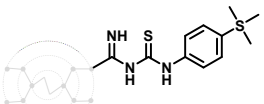
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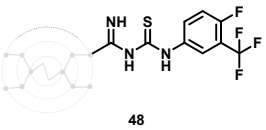
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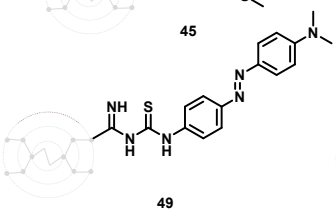
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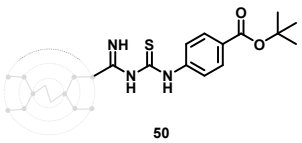
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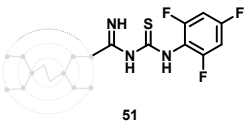
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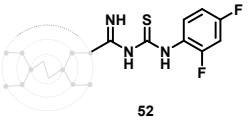
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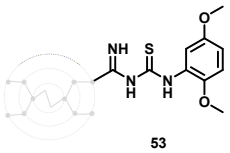
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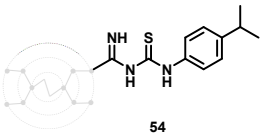
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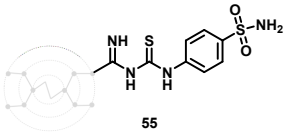
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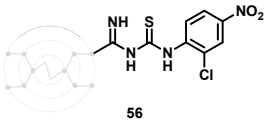
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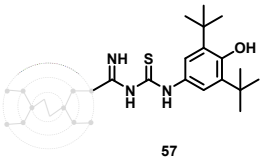
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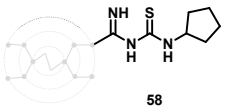
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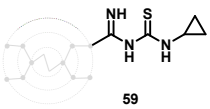
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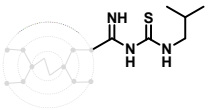
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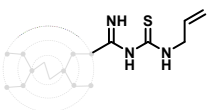
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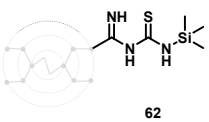
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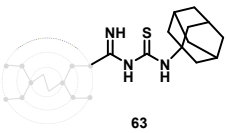
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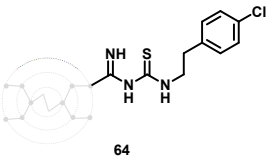
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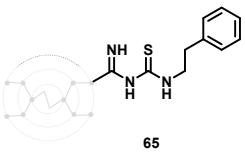
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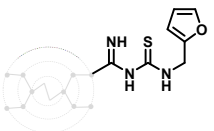
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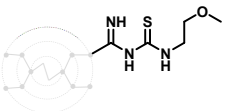
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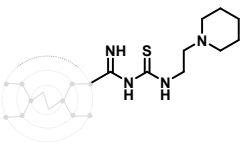
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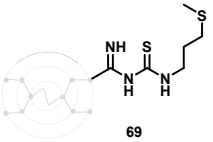
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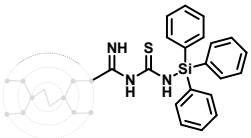
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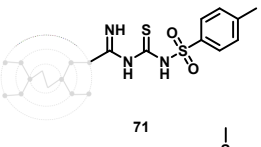
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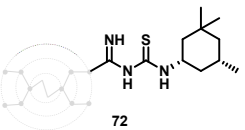
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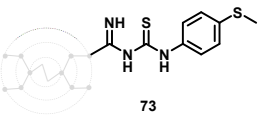
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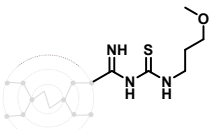
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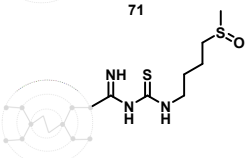
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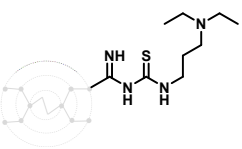
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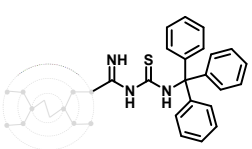
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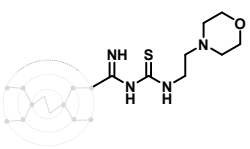
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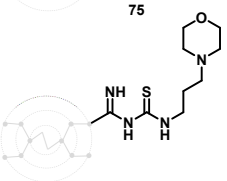
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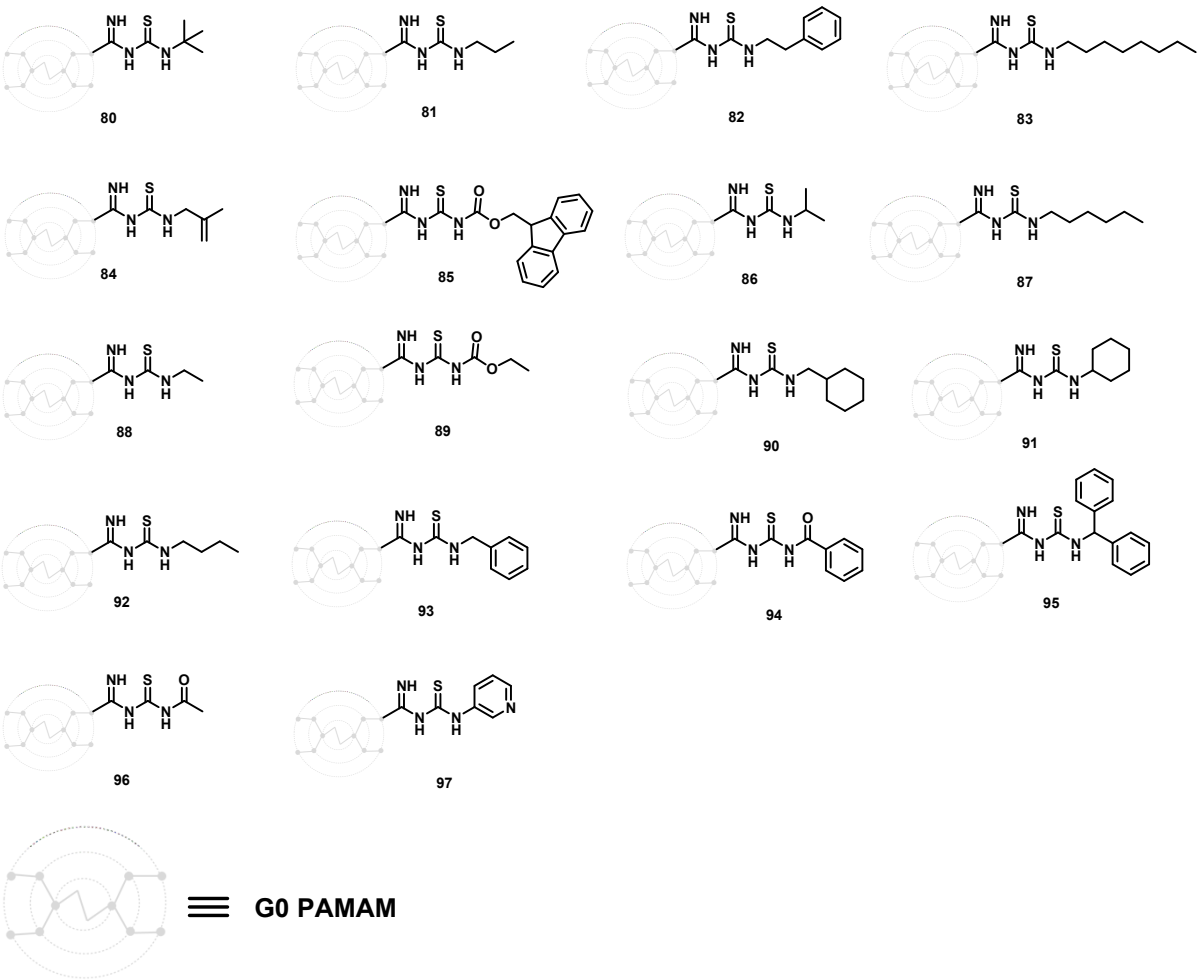

Figure S1: Designed PAMAM GTU library

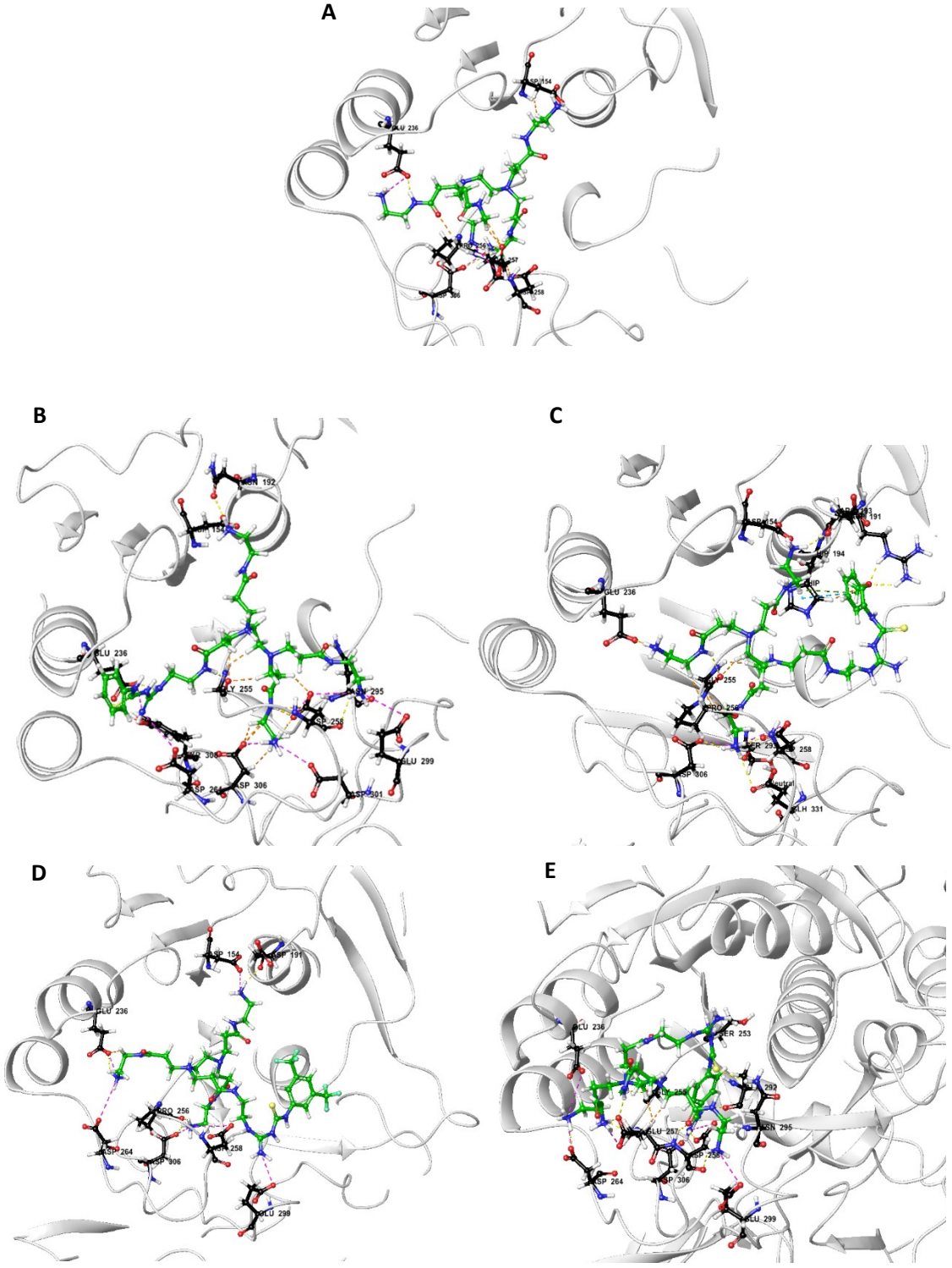

Figure S2. 3D depiction of interaction of **(A)** G0 PAMAM with Asp154, Glu236, Pro256, Glu257, Asp258, Asp306 **(B)** 2 with Asp154, Asn192, Glu236, Gly255, Asp258, Asp264, Glu299, Asp301, Asp306, Tyr308 **(C)** 3 with Asp154, Asp191, Arg193, His194, Val231, Glu236, Gly255, Pro256, Asp258, Ser293, Asp306, Glu331 **(D)** 4 with Asp154, Asp191, Glu236, Pro256, Asp258, Asp264, Glu299, Asp306 **(E)** 5 with Glu236, Asp264, Asp258, Gly255, Glu257, Ala292, Asn295, Glu299, Asp306 residues of furin

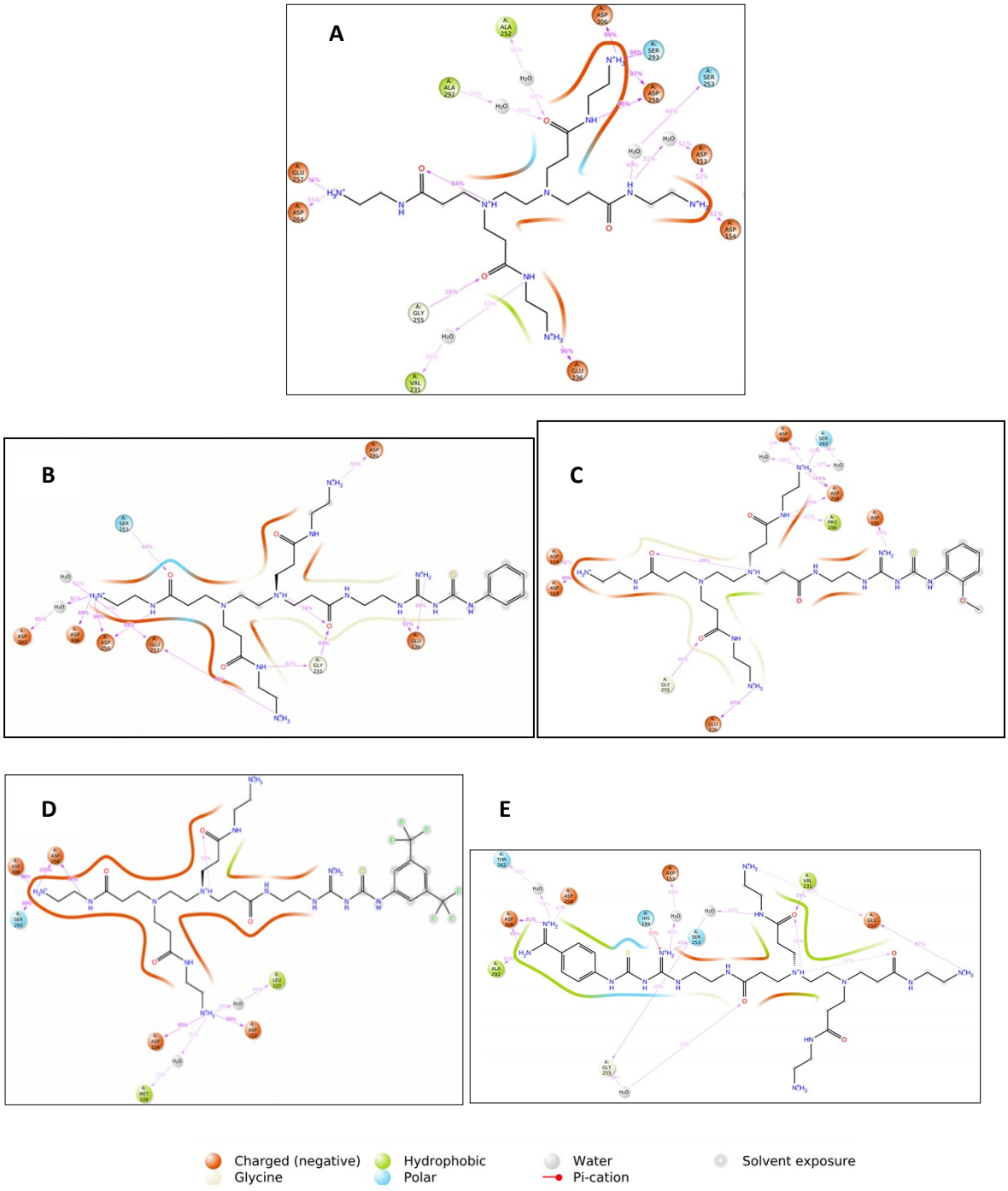

Figure S3. 2D summary of interaction analysis results of **(A)** G0 PAMAM **(B)** 2 **(C)** 3 **(D)** 4 **(E)** 5 with furin

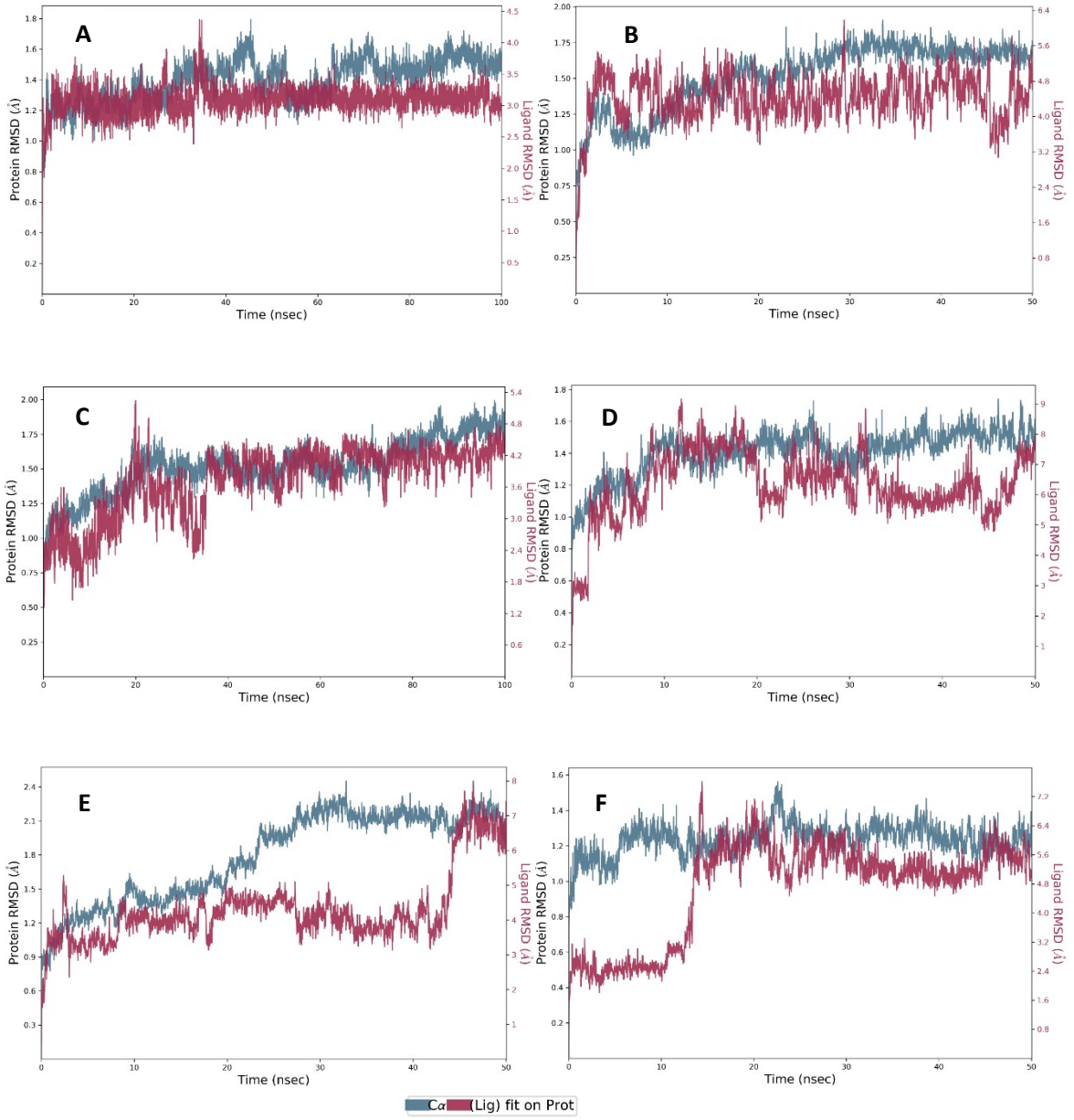

Figure S4: Protein-ligand RMSD plot of furin (A) G0 PAMAM **(B)** 1 **(C)** 2 **(D)** 3 **(E)** 4 **(F)** 5 in complex with furin.

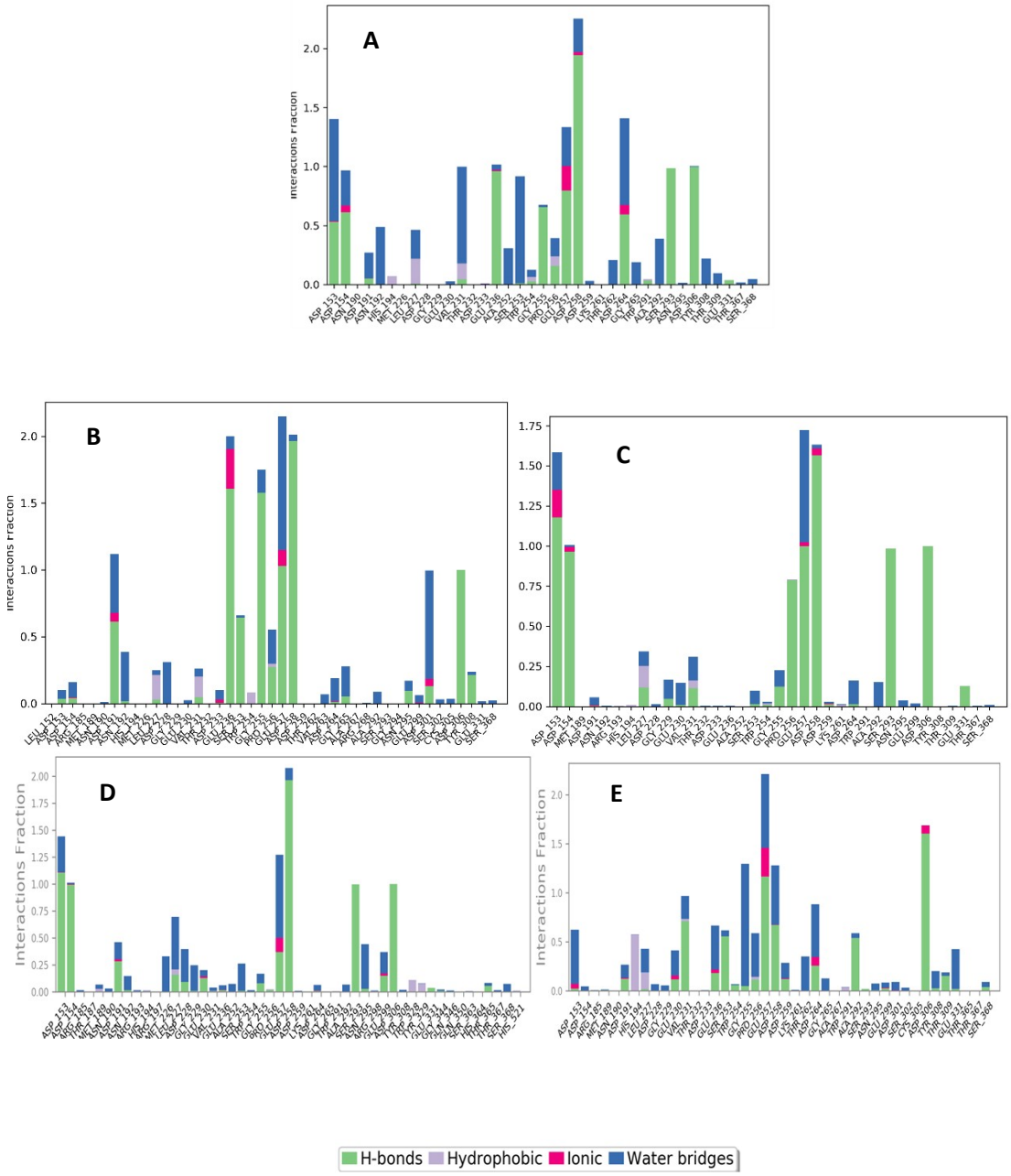

Figure S5. Interaction fraction summary of (A) G0 PAMAM (**B)** 2 **(C)** 3 **(D)** 4 **(E)** 5 in contact with furin

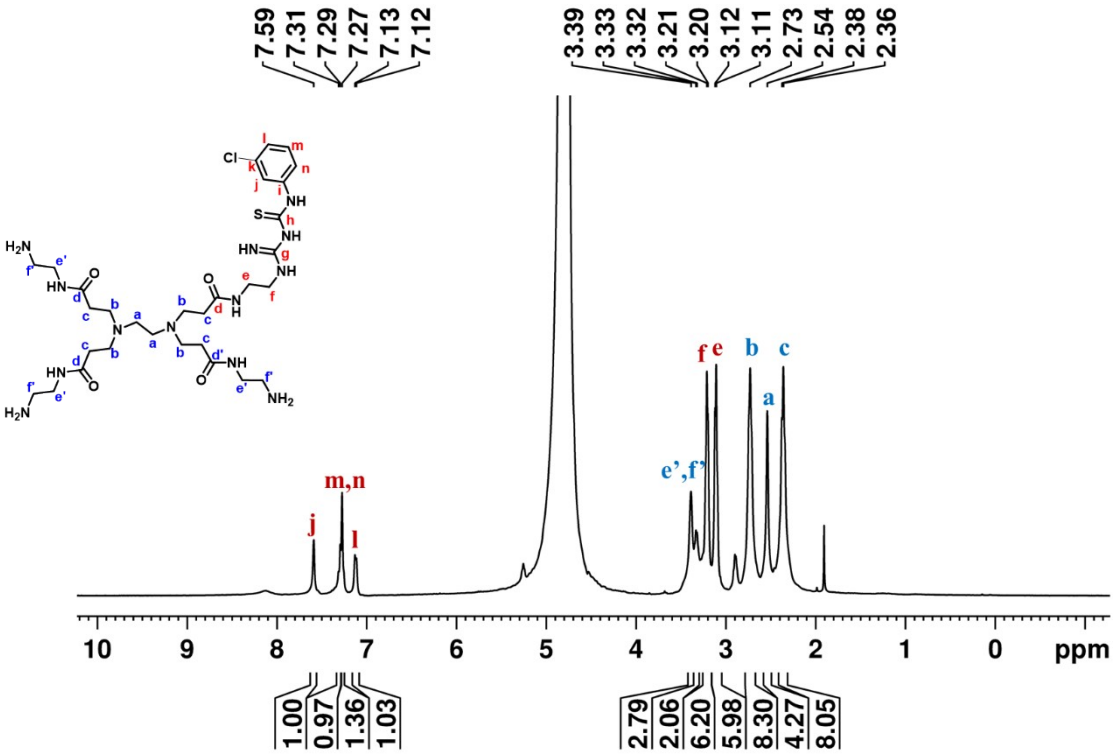

Figure S6: ^{1}H NMR (400 MHz, Deuterium Oxide) of 1

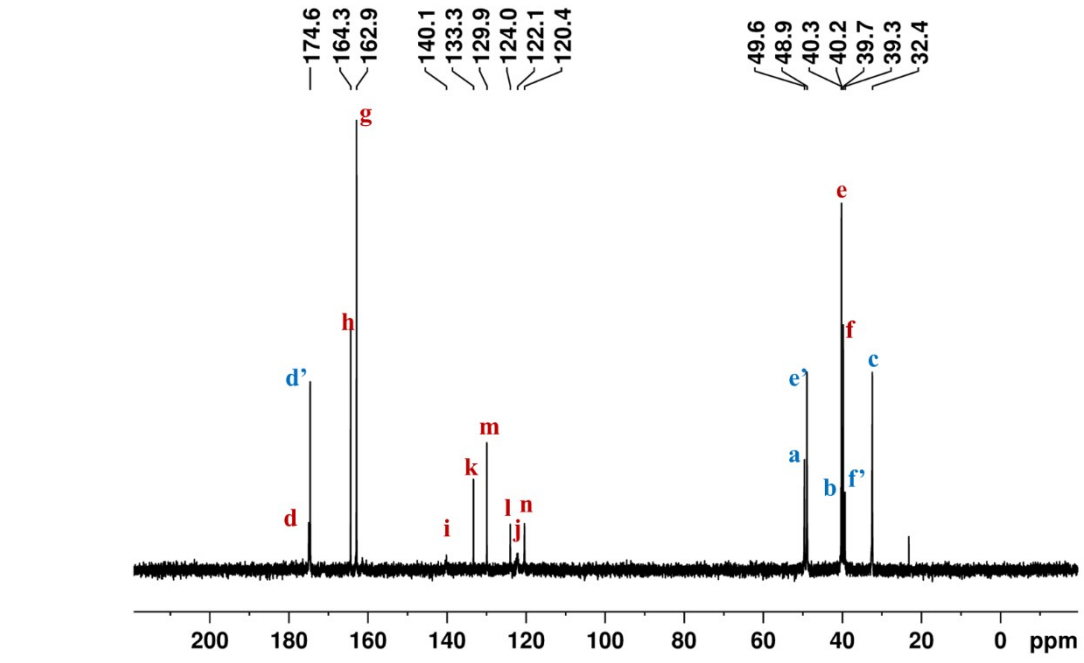

Figure S7: ^{13}C NMR (100 MHz, Deuterium Oxide) of 1

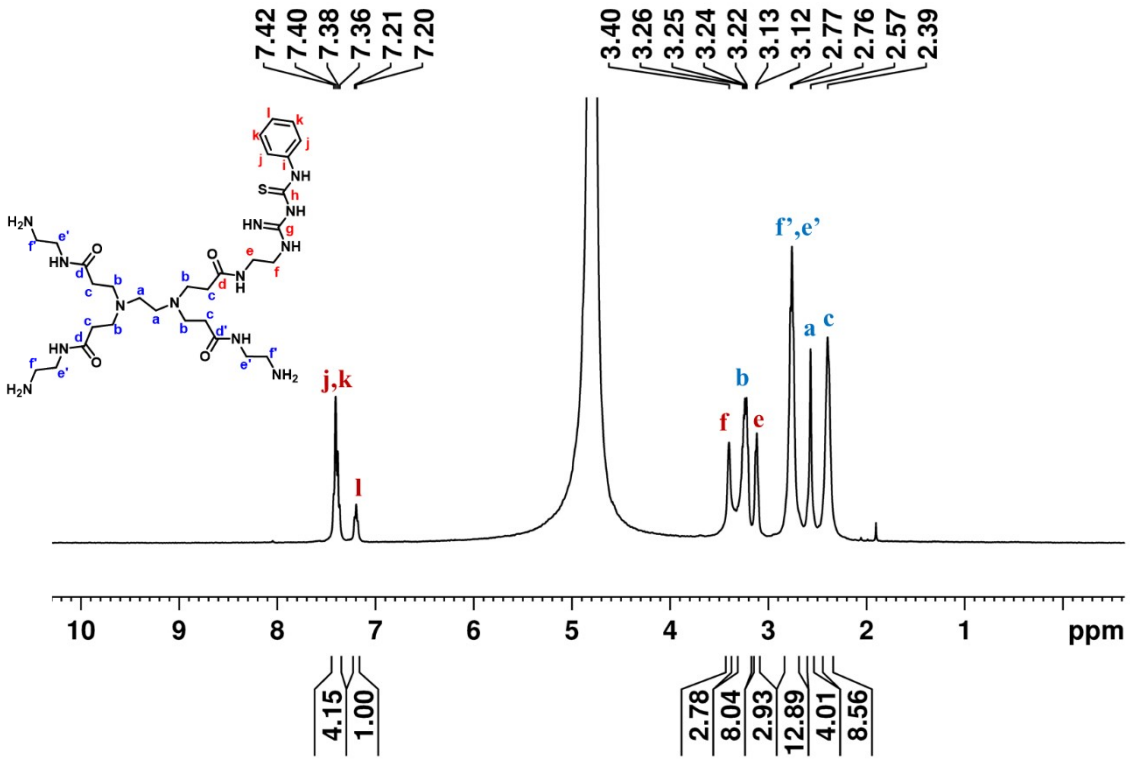

Figure S8: ^{1}H NMR (400 MHz, Deuterium Oxide) of 2

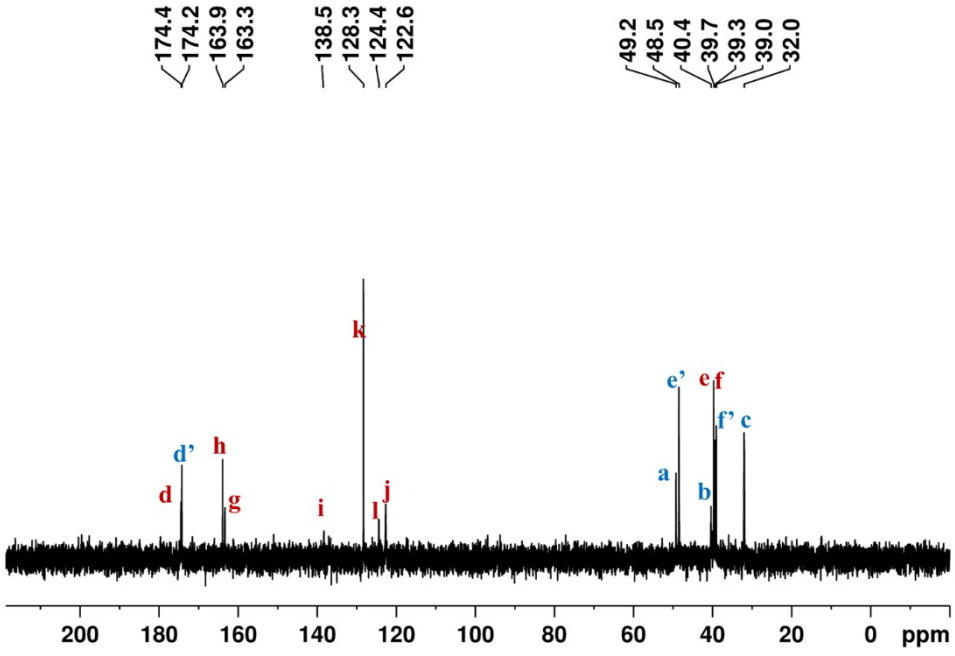

Figure S9: ^{13}C NMR (100 MHz, Deuterium Oxide) of 2

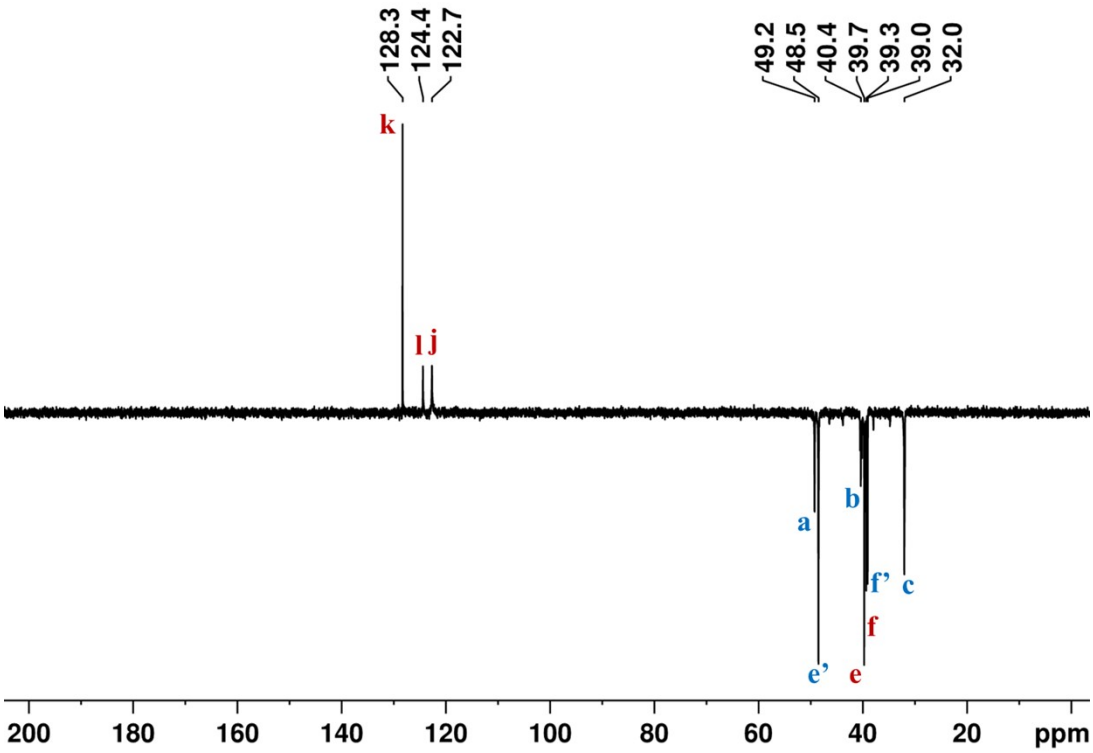

Figure S10: DEPT-135 NMR of 2 (in D_2O)

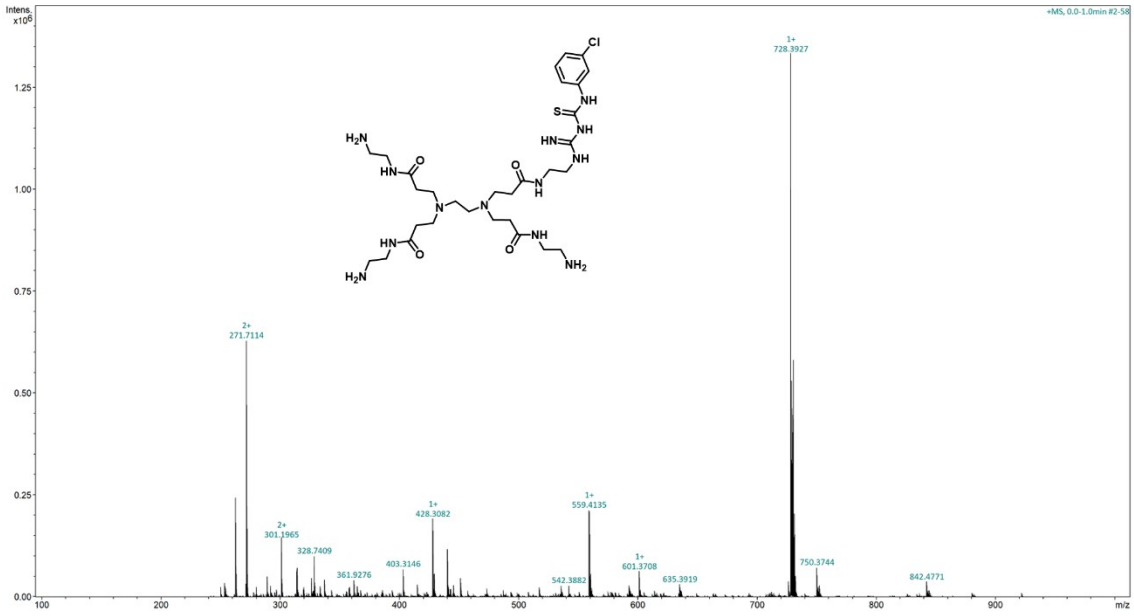

Figure S11: ESI-MS Spectrum of 1 calcd mass $(M+H)^+$, 728.3904; found, 728.3927

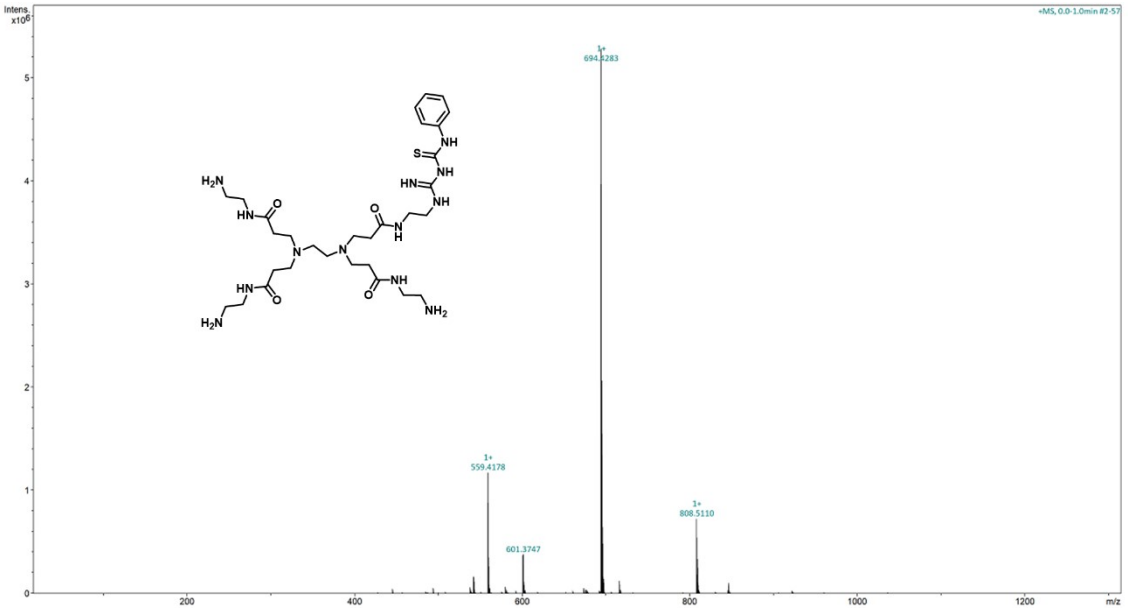

Figure S12: ESI-MS Spectrum of 2 calcd mass $(M+H)^+$, 694.4293; found, 694.4283

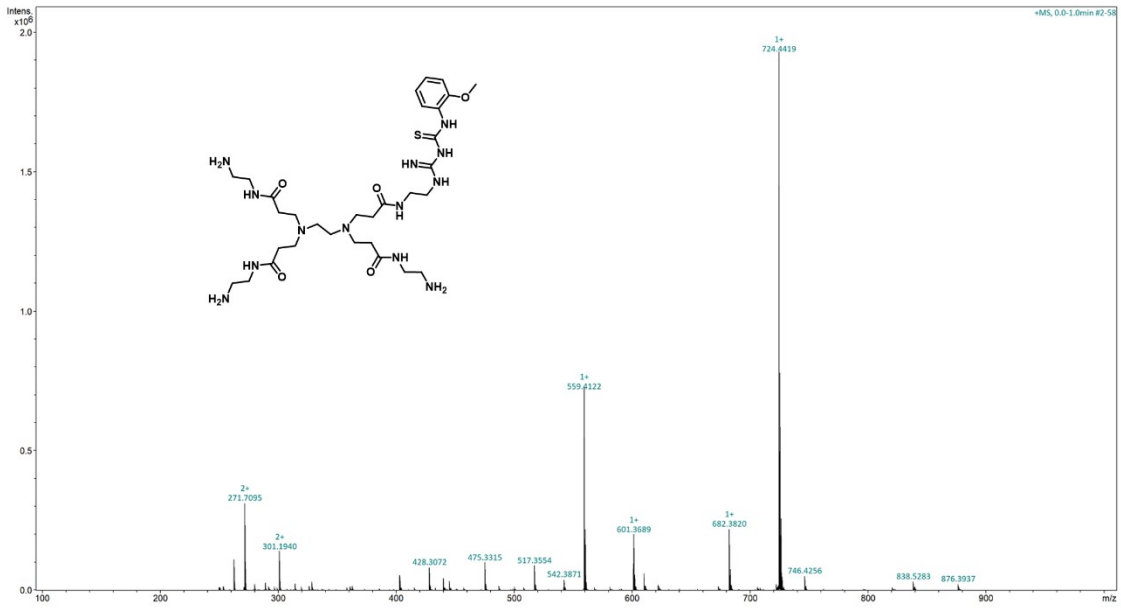

Figure S13: ESI-MS Spectrum of 3 calcd mass $(M+H)^+$, 724.4399; found, 746.4419

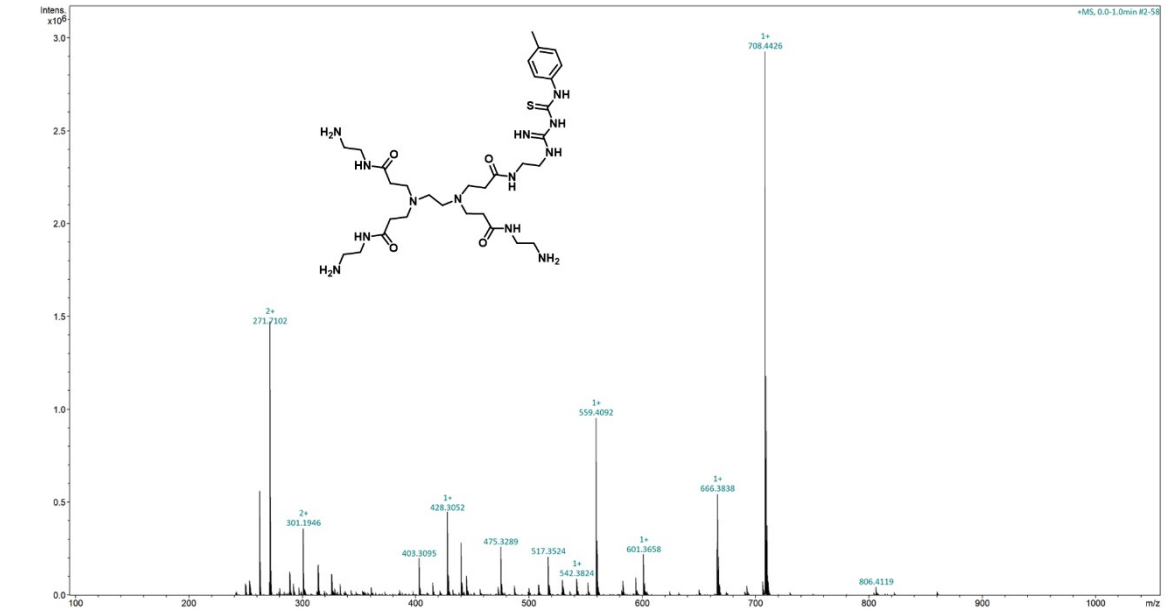

Figure S14: ESI-MS Spectrum of 6 calcd mass $(M+H)^+$, 708.4450; found, 708.4419

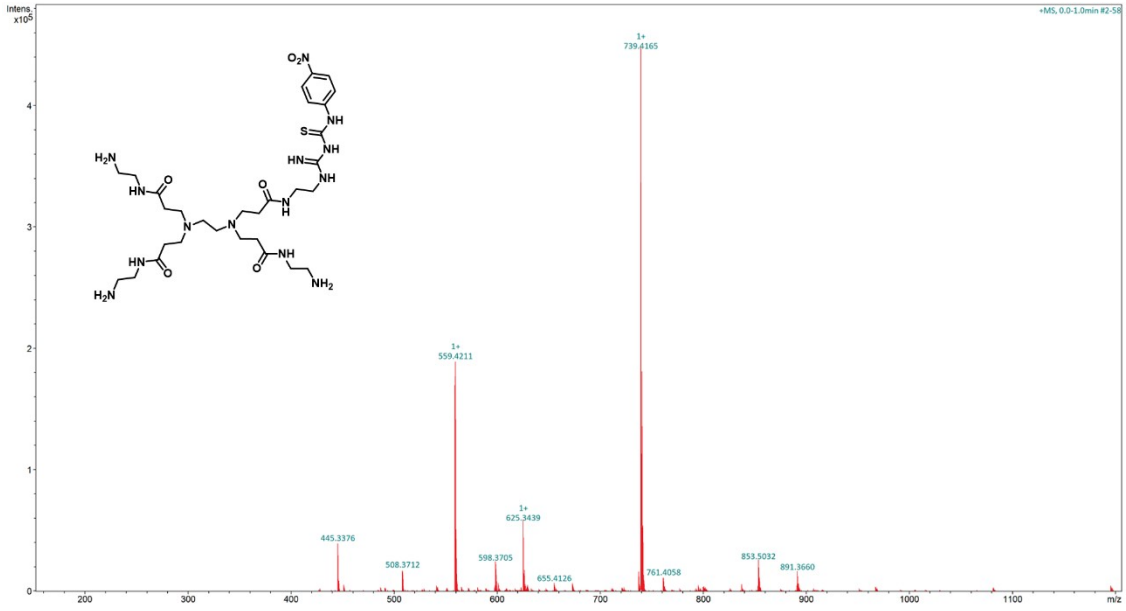

Figure S15: ESI-MS Spectrum of 7 calcd mass $(M+H)^+$, 739.4144; found, 739.4165