

## Supporting Information:

# **Application of machine learning in predicting potentiometric selectivity ( $\text{Mg}^{2+}/\text{Ca}^{2+}$ ) of some amide ligands**

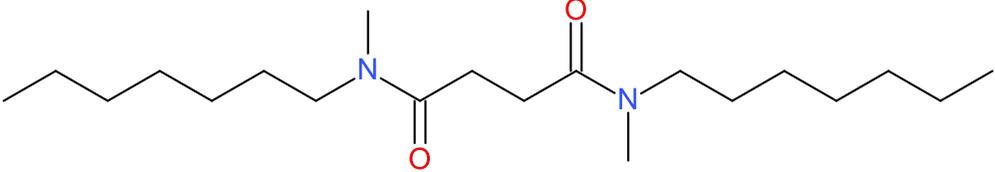
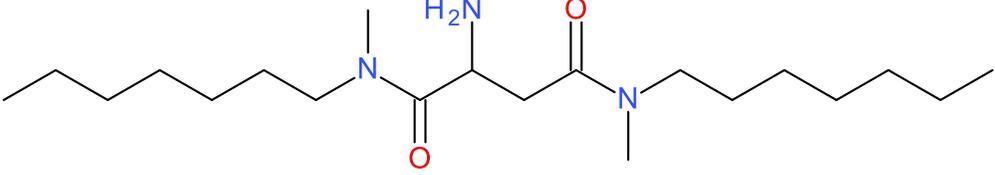
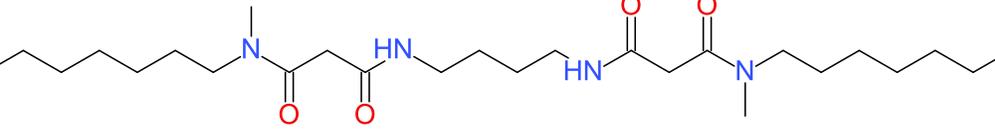
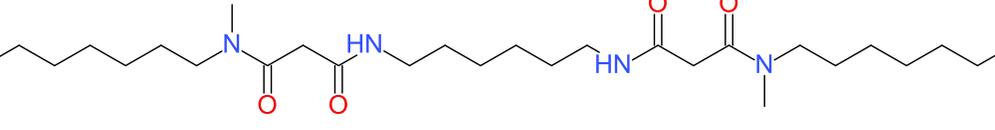
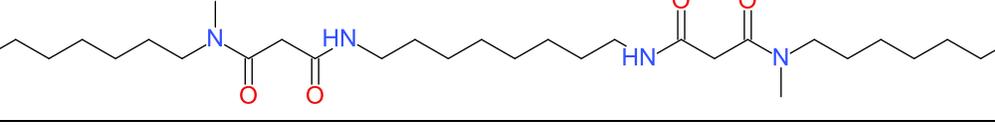
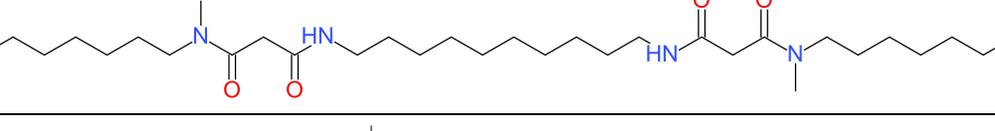
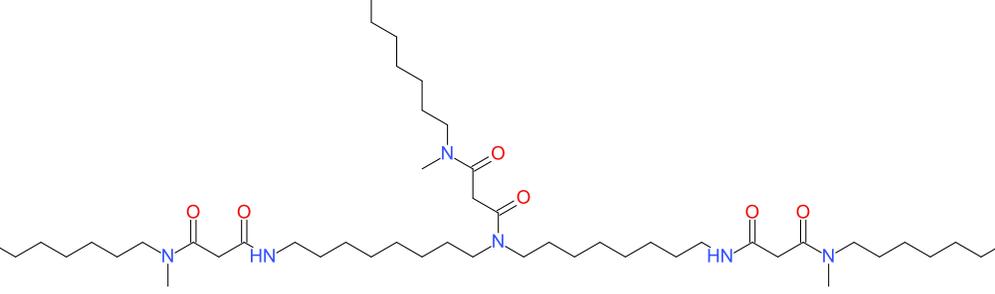
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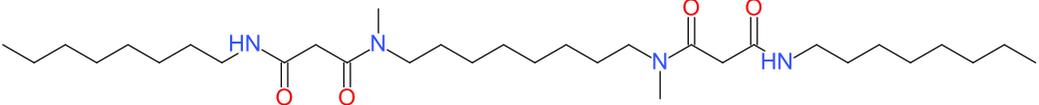
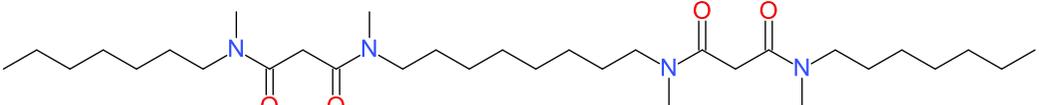
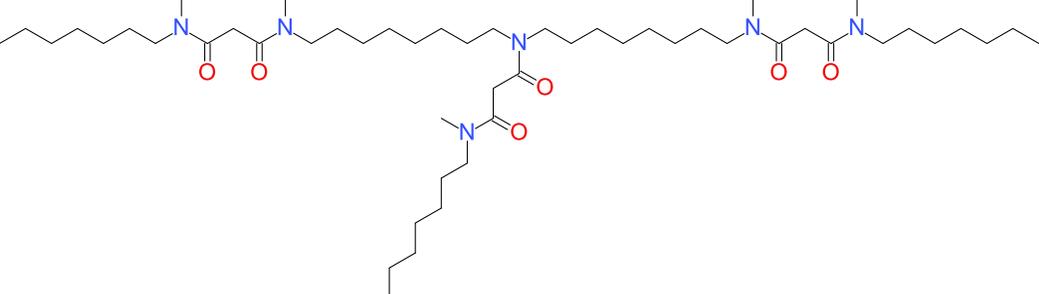
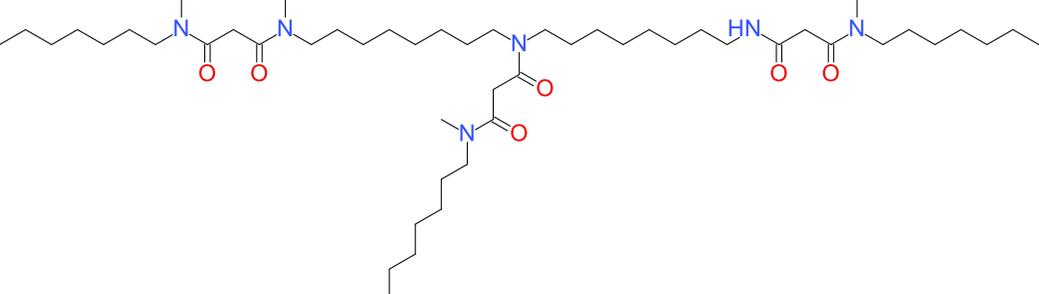
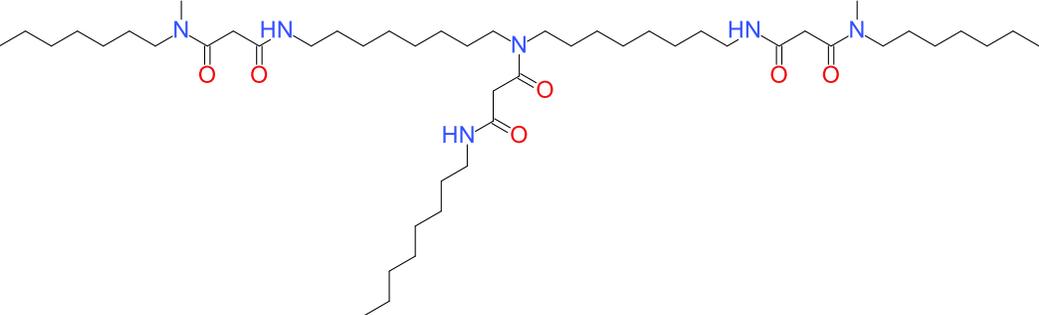
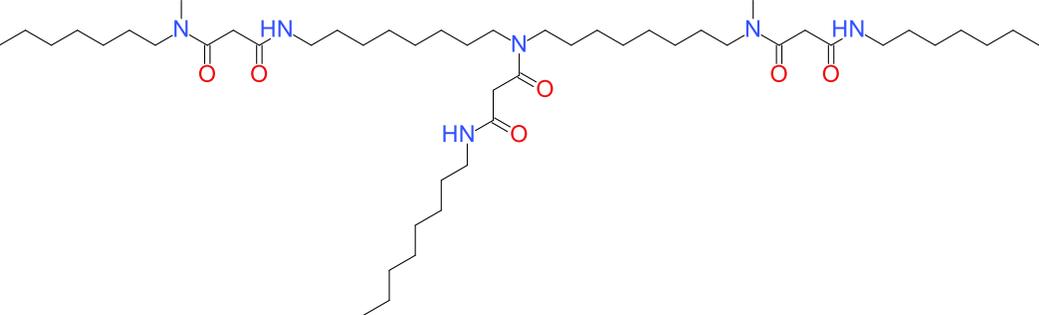
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**Table S1.** Chemical structures of the studied amide ligands

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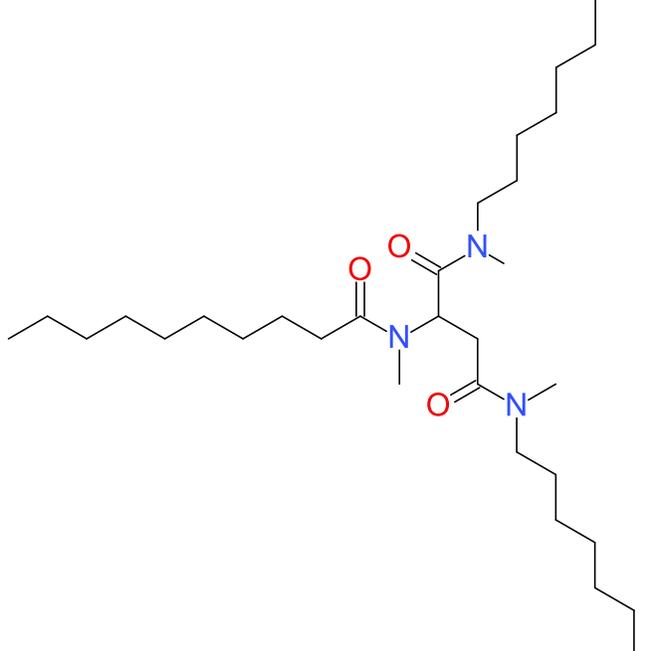
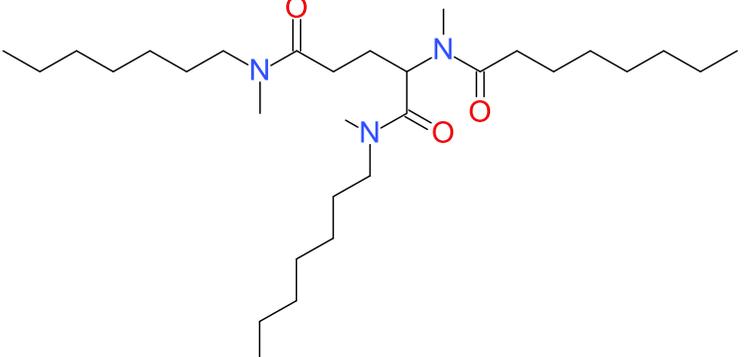
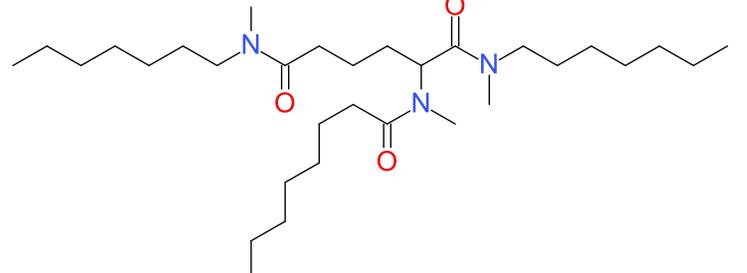
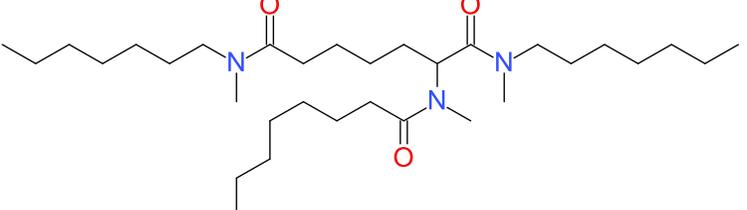
33	<p>Chemical structure 33: A decyl chain is attached to a carbonyl group (C=O, red oxygen). This carbonyl is part of a secondary amide (NH, blue). The nitrogen is bonded to a chiral center (wedge bond). This chiral center is also bonded to a carbonyl group (C=O, red oxygen) which is part of a tertiary amide (N, blue). The nitrogen is bonded to a methyl group and a decyl chain. The chiral center is also bonded to a nitrogen atom (blue) which is part of a quaternary ammonium salt. This nitrogen is bonded to a methyl group and a decyl chain. The nitrogen atom is also bonded to a decyl chain.</p>
34	<p>Chemical structure 34: A decyl chain is attached to a nitrogen atom (blue) which is part of a tertiary amide (C=O, red oxygen). The nitrogen is bonded to a methyl group and a chiral center (wedge bond). This chiral center is also bonded to a carbonyl group (C=O, red oxygen) which is part of a secondary amide (NH, blue). The nitrogen is bonded to a decyl chain. The chiral center is also bonded to a nitrogen atom (blue) which is part of a quaternary ammonium salt. This nitrogen is bonded to a methyl group and a decyl chain. The nitrogen atom is also bonded to a decyl chain.</p>
35	<p>Chemical structure 35: A decyl chain is attached to a nitrogen atom (blue) which is part of a tertiary amide (C=O, red oxygen). The nitrogen is bonded to a methyl group and a chiral center (wedge bond). This chiral center is also bonded to a carbonyl group (C=O, red oxygen) which is part of a secondary amide (NH, blue). The nitrogen is bonded to a decyl chain.</p>
36	<p>Chemical structure 36: A decyl chain is attached to a nitrogen atom (blue) which is part of a quaternary ammonium salt. This nitrogen is bonded to a methyl group and a decyl chain. The nitrogen atom is also bonded to a decyl chain. The quaternary ammonium salt is bonded to a chiral center (wedge bond). This chiral center is also bonded to a carbonyl group (C=O, red oxygen) which is part of a secondary amide (NH, blue). The nitrogen is bonded to a decyl chain. The chiral center is also bonded to a carbonyl group (C=O, red oxygen) which is part of a tertiary amide (N, blue). The nitrogen is bonded to a methyl group and a decyl chain.</p>
37	<p>Chemical structure 37: A decyl chain is attached to a nitrogen atom (blue) which is part of a tertiary amide (C=O, red oxygen). The nitrogen is bonded to a methyl group and a chiral center (wedge bond). This chiral center is also bonded to a hydroxyl group (OH, red). The chiral center is also bonded to a carbonyl group (C=O, red oxygen) which is part of a secondary amide (NH, blue). The nitrogen is bonded to a decyl chain.</p>
38	<p>Chemical structure 38: A decyl chain is attached to a nitrogen atom (blue) which is part of a tertiary amide (C=O, red oxygen). The nitrogen is bonded to a methyl group and a chiral center (wedge bond). This chiral center is also bonded to a methoxy group (O, red). The chiral center is also bonded to a carbonyl group (C=O, red oxygen) which is part of a secondary amide (NH, blue). The nitrogen is bonded to a decyl chain.</p>

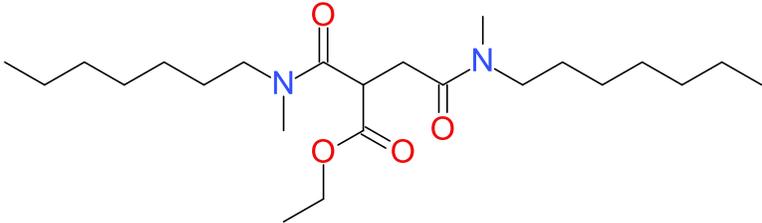
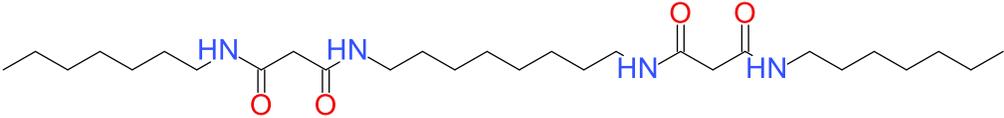
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66	 <p>The structure shows a six-membered cyclic amide ring. One nitrogen atom is substituted with a heptyl chain. The carbon atom adjacent to this nitrogen is part of a side chain that includes another heptyl chain and a carbonyl group. The carbon atom adjacent to the carbonyl group is substituted with an ethoxy group. The carbon atom adjacent to the ethoxy group is also part of a side chain that includes a carbonyl group and another heptyl chain.</p>
67	 <p>The structure shows a linear polyamide chain consisting of four heptyl chains connected by amide bonds. The amide bonds are shown with blue 'HN' labels and red oxygen atoms. The chain is symmetrical, with two heptyl chains on each side of the central amide linkage.</p>