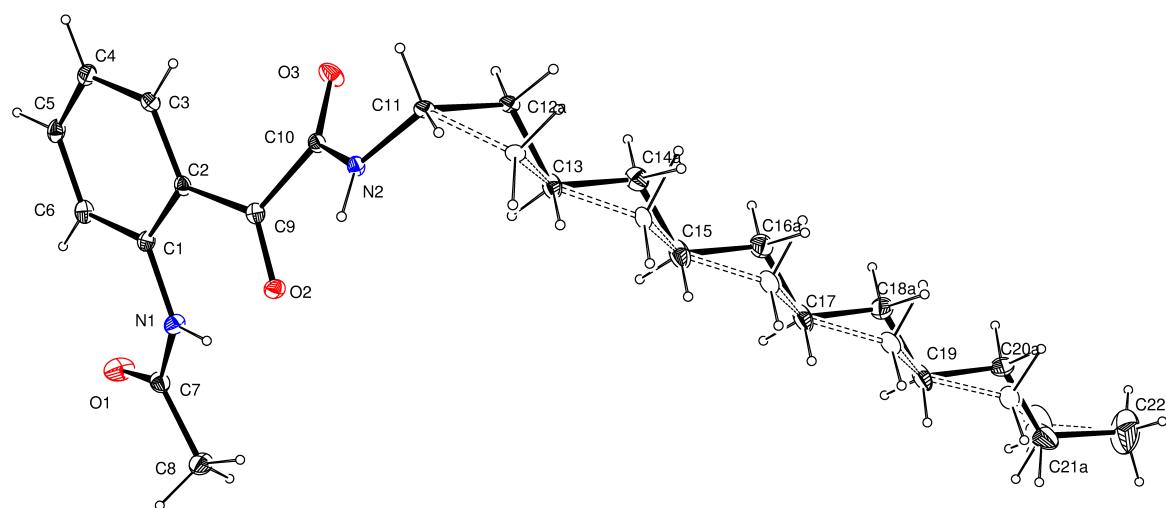
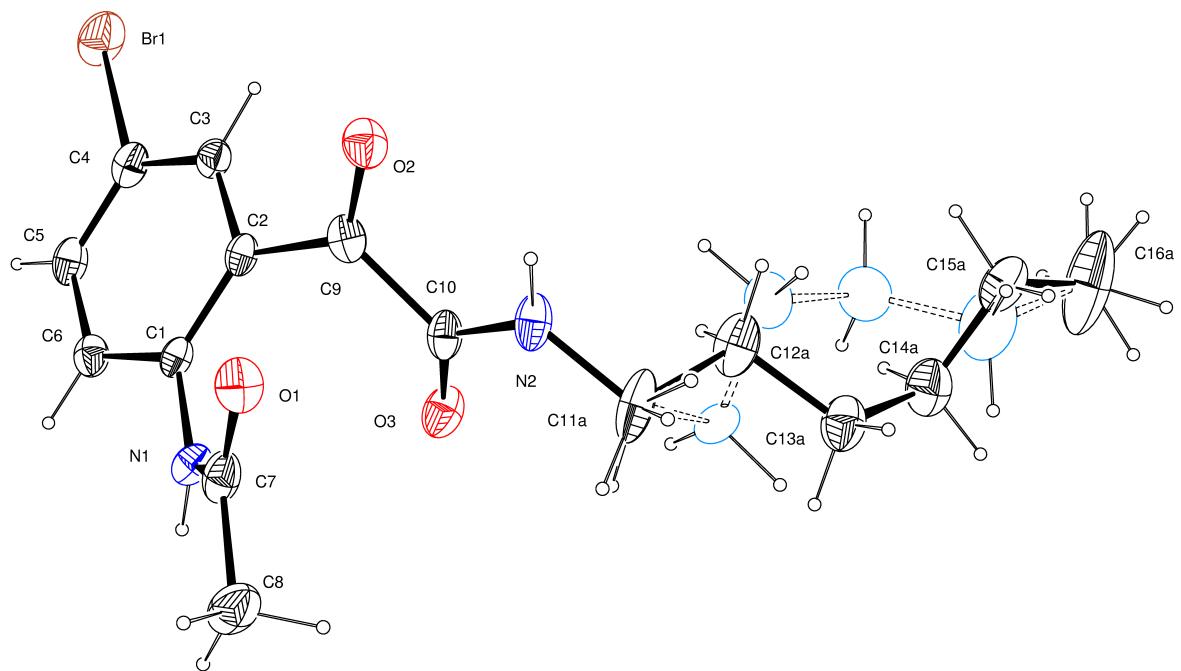


Supplementary Information: On Side Chain Disorder



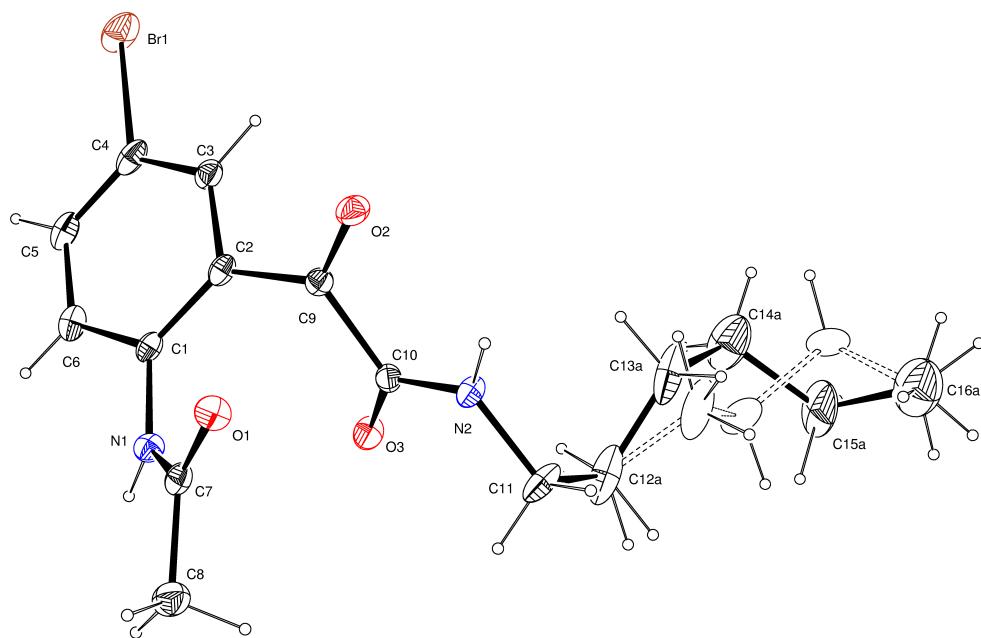
Structure 5d

The alkyl side chain exhibits orientational disorder over two almost equally populated sites. The end atoms C11 and C22 are not affected by this disorder, but atoms C12 - C21 are influenced in a gradually decreasing manner. The two orientations were separated using PART 1 and PART 2 instructions, the C-C lengths were restrained to be the same using SADI (0.01) instruction, the anisotropic displacement parameters were kept within reasonable limits using DELU (0.01) and SIMU (0.01) instructions (for C12a and C12b the s.u.s were 0.001) in the SHELXL full-matrix least-squares refinement.



Structure 5b-1

Atoms in the flexible side chain exhibit disorder, which is modeled over two positions of slightly unequal (56:44) occupancies. The starting and the end atoms are not affected by this disorder, but positions of four atoms C12, C13, C14 and C15 are influenced by this to a varying degree. In the disorder model, atoms C11a and C11b and C16a and C16b were kept in the same position using EXYZ and EADP commands, the PART 1 and PART 2 instructions were used to separate the two positions of atoms C12, C13, C14 and C15. The bond lengths C-C were restrained to be the same using SADI (0.01) instructions and the atomic displacement parameters were restrained using DELU and SIMU (0.02) instructions in SHELXL full-matrix least-squares refinement.



Structure of 5b-2

Atoms in the flexible side chains exhibit disorder, which is modelled over two positions of almost equal occupancies (51:49). The start and the end atoms are not affected by this disorder, but the atoms along the chain, C13, C14 and C15 are influenced to a varying degree. Atoms C12a, C12b and C16a, C16b were restrained to occupy the same positions using EXYZ instruction, the rest three were refined in two parts using PART 1 and PART 2 instructions. The C-C bond lengths were restrained using SADI (0.01), whereas atomic displacement parameters were restrained using DELU (0.002) and SIMU (0.002) instructions in the SHELXL program of full-matrix least-squares refinement.