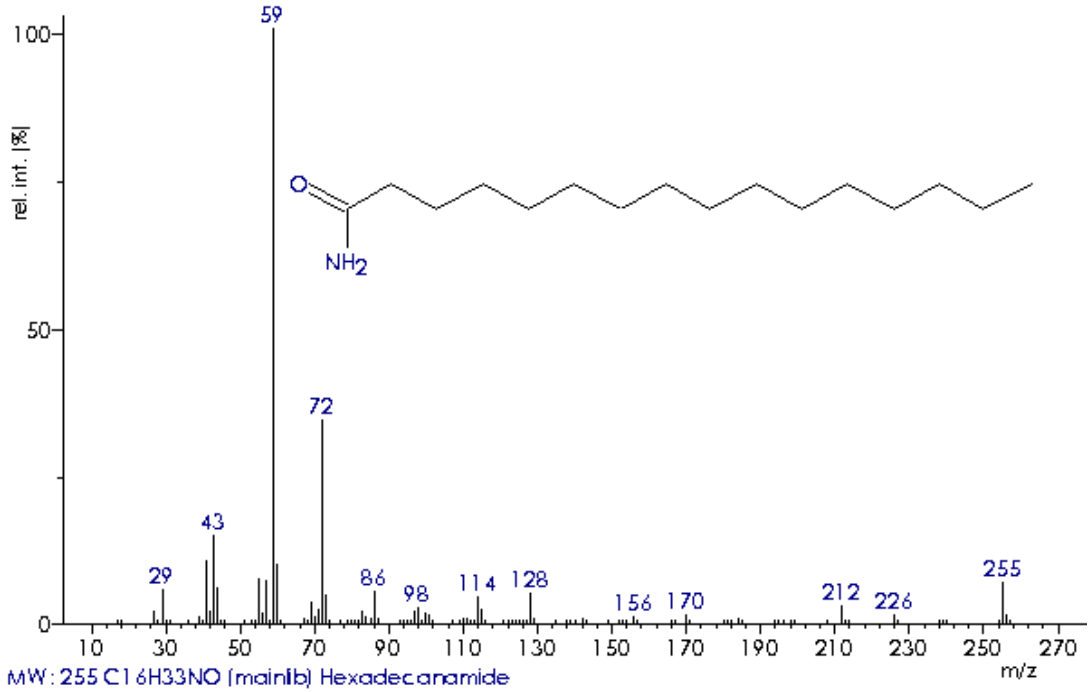
Answer 6.11

Identify the unknown from its 70 eV EI mass spectrum. The ^{1}H-NMR spectrum reveals an aliphatic chain and one signal indicating two exchangeable hydrogens.



The (presumed) monoisotopic molecular ion peak is of low intensity, located at *m/z* 255, and exhibits an isotopic pattern that seems to result from carbon alone. An odd mass indicates that the molecule contains 1, 3, 5 ... nitrogen atoms.

The general appearance of the EI mass spectrum coincides well with the findings from NMR spectroscopy, i.e., an alkyl chain with one functional group.

m/z 226	[M–29], [M–C_2H_5]$^+$
m/z 212	[M–43], [M–C_3H_7]$^+$
m/z 170	[M–43–42]
m/z 128	[M–43–42–42]
m/z 86	[M–43–42–42–42] series with stronger fragment every three carbons is common with long alkyl chains
m/z 72	γ-cleavage product of primary amides
m/z 59 (base peak)	McL product of primary amides
m/z 29, 43	alkyl ions

The compound should be a long chain primary aliphatic amide. Subtracting 44 u ($CONH_2$) from 255 u yields a rest of 211 u which fits to 15 × 14 u + 1u.

Therefore, the empirical formula is $C_{16}H_{33}NO$; r+d = 16 – 16.5 + + 0.5 + 1 = 1

The fragmentation scheme assures the structure: