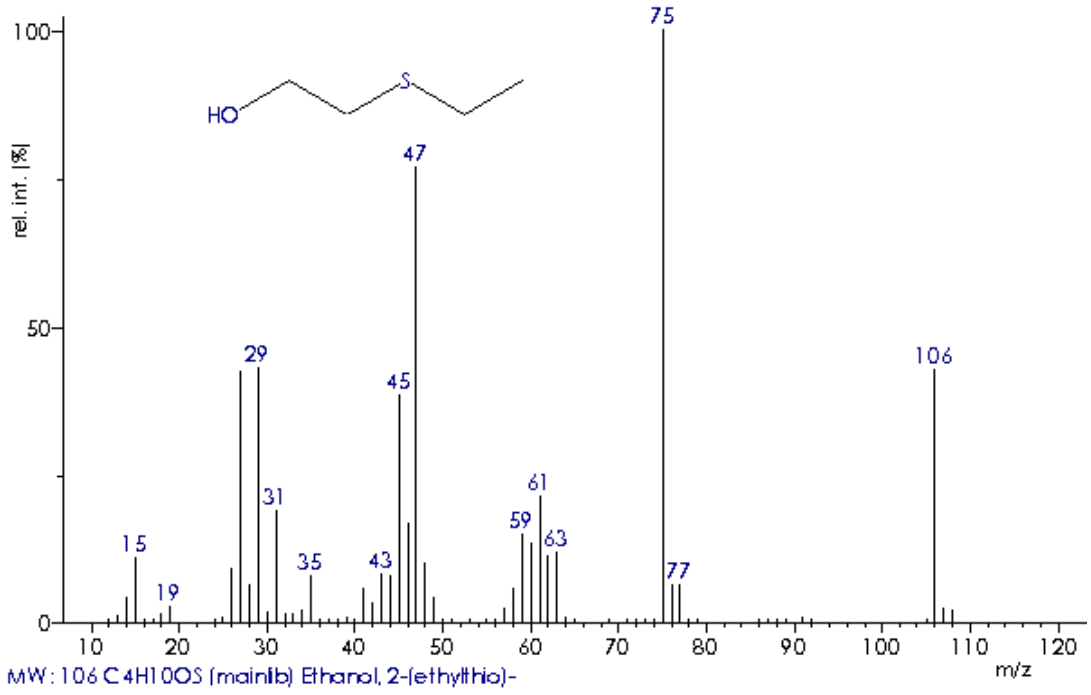
Answer 6.10

Identify the unknown from its 70 eV EI mass spectrum.



The (presumed) monoisotopic molecular ion peak is of medium intensity, located at *m/z* 106, and exhibits an isotopic pattern that cannot result from carbon alone, but Cl and Br can be excluded. In case of Si, the pattern wouldn't allow for additional carbons. Thus, S is reasonable.
Again, even mass indicates that the molecule contains 0, 2, 4, ... nitrogen atoms.
The [M+1] peak has slightly larger intensity than the ^{34}S isotopic peak, *m/z* 108, which corresponds to just above 5 % or 4–5 carbon atoms.

m/z 75 (base peak)	[M–31], S pattern → $[M–OCH_3]^+$
m/z 61	[M–45] → $[M–C_2H_4OH]^+$ or $[M–COOH]^+$?
m/z 47	[M–31–28], $[M– OCH_3–CO]^+$ or $[M– OCH_3–C_2H_4]^+$?
m/z 45	$[COOH]^+$ or $[C_2H_5O]^+$ (oxonium ion)?
m/z 31	oxonium ion
m/z 29	$C_2H_5^+$
	m/z 47, 61, 75 are sulfonium ions → thioether, thiol

The compound contains S and O. Assuming one each, 106 u – 16 u – 32 u = 58 u has to be C and H, i.e., the formula is $C_4H_{10}OS$; r+d = 4 – 5 + 1 = 0

The unknown possesses thioether and alcohol or thioether and ether functionality.

Here, the fragmentation scheme clearly serves to assure the structure: