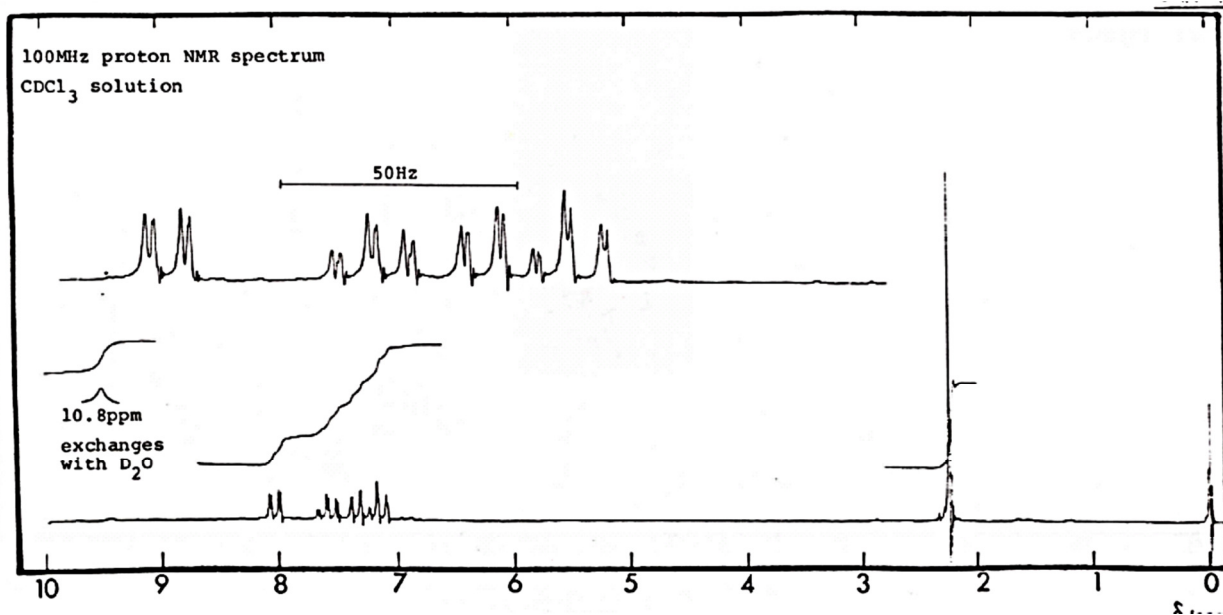


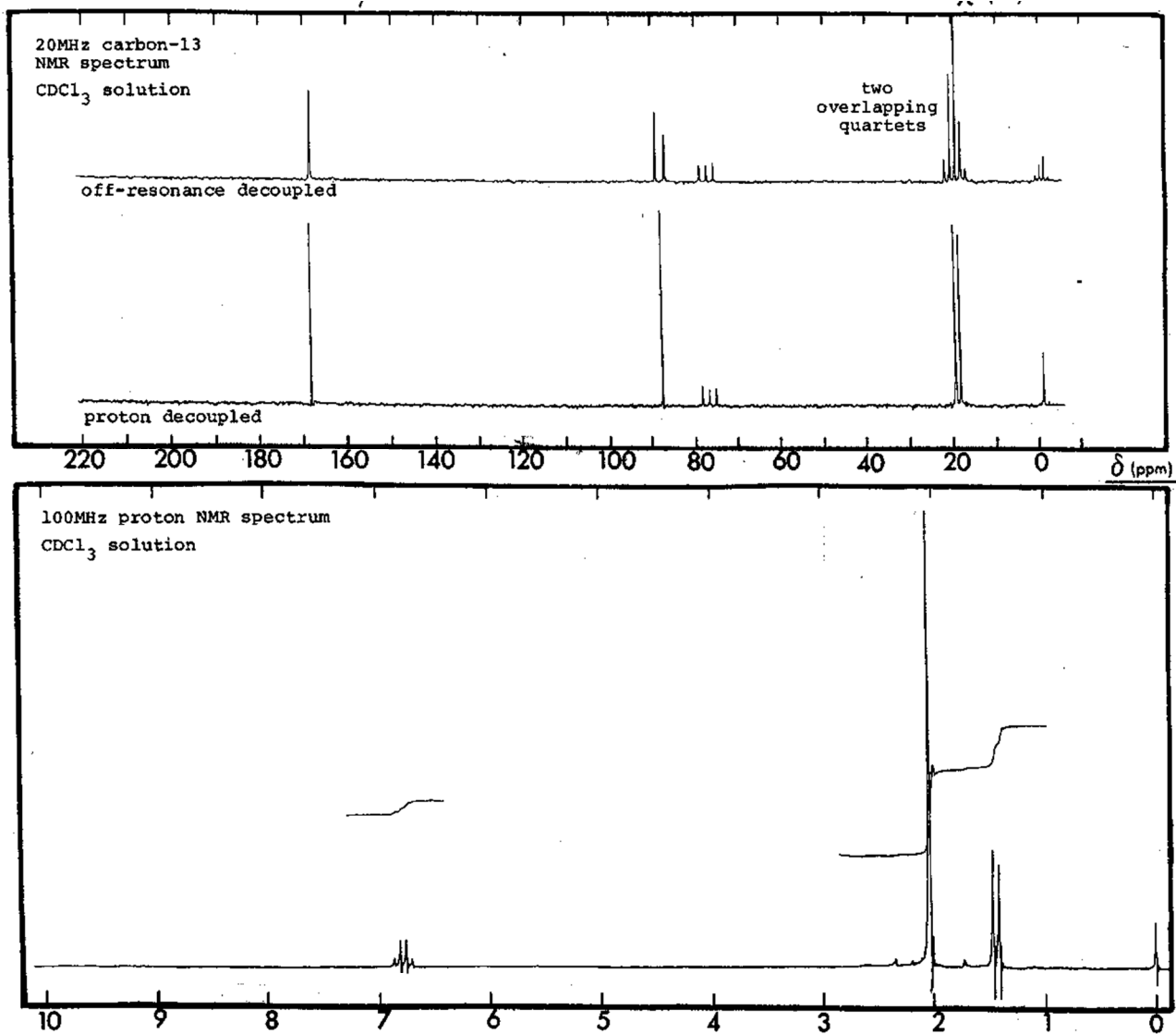
Assignment 2

- ^1H NMR spectrum of **aspirin** is shown below. Assume simple first order splitting in the multiplets signals. Calculate all the chemical shift and coupling constant values from the spectrum. Assign the spectrum to the structure.

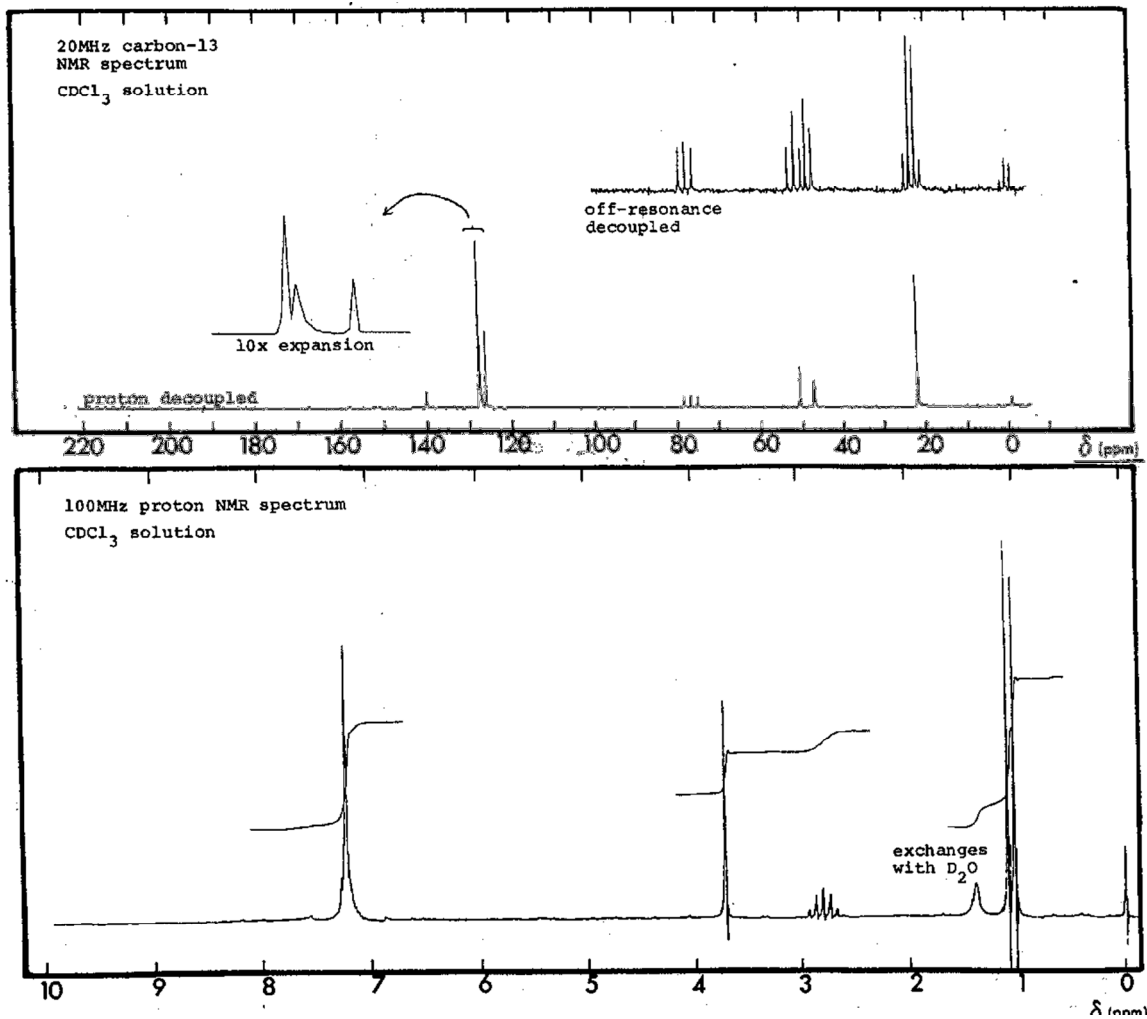


2. Identify the structure of the organic compound from the given NMR data.

Molecular formula: $C_6H_{10}O_4$



3. Identify the structure of the organic compound from the given NMR data.
Molecular formula: $C_{10}H_{15}N$



4. $C_6H_{12}O_2$ 1H NMR: 3.9 (s, br, 1H, D_2O exch), 2.6 (s, 2H), 2.2 (s, 3H), 1.2 (s, 6H); ^{13}C NMR: 211 (s), 69 (s), 44 (t), 30.5 (q), 29 (q).
5. $C_6H_{12}O_3$ 1H NMR: 4.8 (t, $J = 7.0$, 1H), 3.3 (s, 6H), 2.8 (d, $J = 7.0$, 2H), 2.05 (s, 3H); ^{13}C NMR: 205 (s), 101 (d), 53 (q), 48 (t), 30 (q).
6. $C_{14}H_{22}O$ 1H NMR: 6.95 (t, $J = 1.9$, 1H), 6.8 (d, $J = 1.9$, 2H), 5.0 (br, s, 1H, D_2O exch), 1.3 (s, 18H); ^{13}C NMR: 156 (s), 153 (s), 115 (d), 110 (d), 35 (s), 31 (q).
7. $C_6H_5NBr_2$ 1H NMR: 7.3 (d, 2H, $J = 7.9$), 6.5 (t, 1H, $J = 7.9$), 4.5 (br, s, 2H, D_2O exch); ^{13}C NMR: 141 (s), 131 (d), 119 (d), 108 (s).
8. C_4H_7OCl 1H NMR: 6.2 (dd, 1H, $J = 15$ and 10), 4.0 (dd, 1H, $J = 15$, 2), 3.9 (dd, 1H, $J = 10$, 2) (AMX type pattern), 3.4 and 3.2 (AA'BB' pattern, 4H); ^{13}C NMR: 152 (d), 89 (t), 69 (t), 41 (t).
9. $C_{10}H_9NO_4Br_2$ 1H NMR: 8.2 and 7.5 (AA'BB' pattern, 4H, $J = 8$), 5.5 and 4.85 (AB pattern, 2H, $J = 12$), 3.95 (s, 3H); ^{13}C NMR: 168 (s), 148 (s), 144 (s), 130 (d), 123 (d), 53 (q), 48 (d), 45 (d).
10. C_9H_{10} 1H NMR: 7.1-7.5 (m, 5H), 5.3 (m, 1H), 5.1 (m, 1H), 2.15 (s, 3H); ^{13}C NMR: 144 (s), 140 (s), 129 (d), 128 (s), 126 (d), 112 (t), 21 (q).
11. C_7H_9NO 1H NMR: 8.3 (m, 1H), 7.1 (m, 1H), 6.6-6.8 (m, 2H), 4.9 (br, s, 1H, D_2O exch), 4.0 (t, 2H, $J = 8$), 2.9 (t, 2H, $J = 8$); ^{13}C NMR: 160 (s), 149 (d), 137 (d), 124 (d), 121 (d), 61 (t), 40 (t).

END