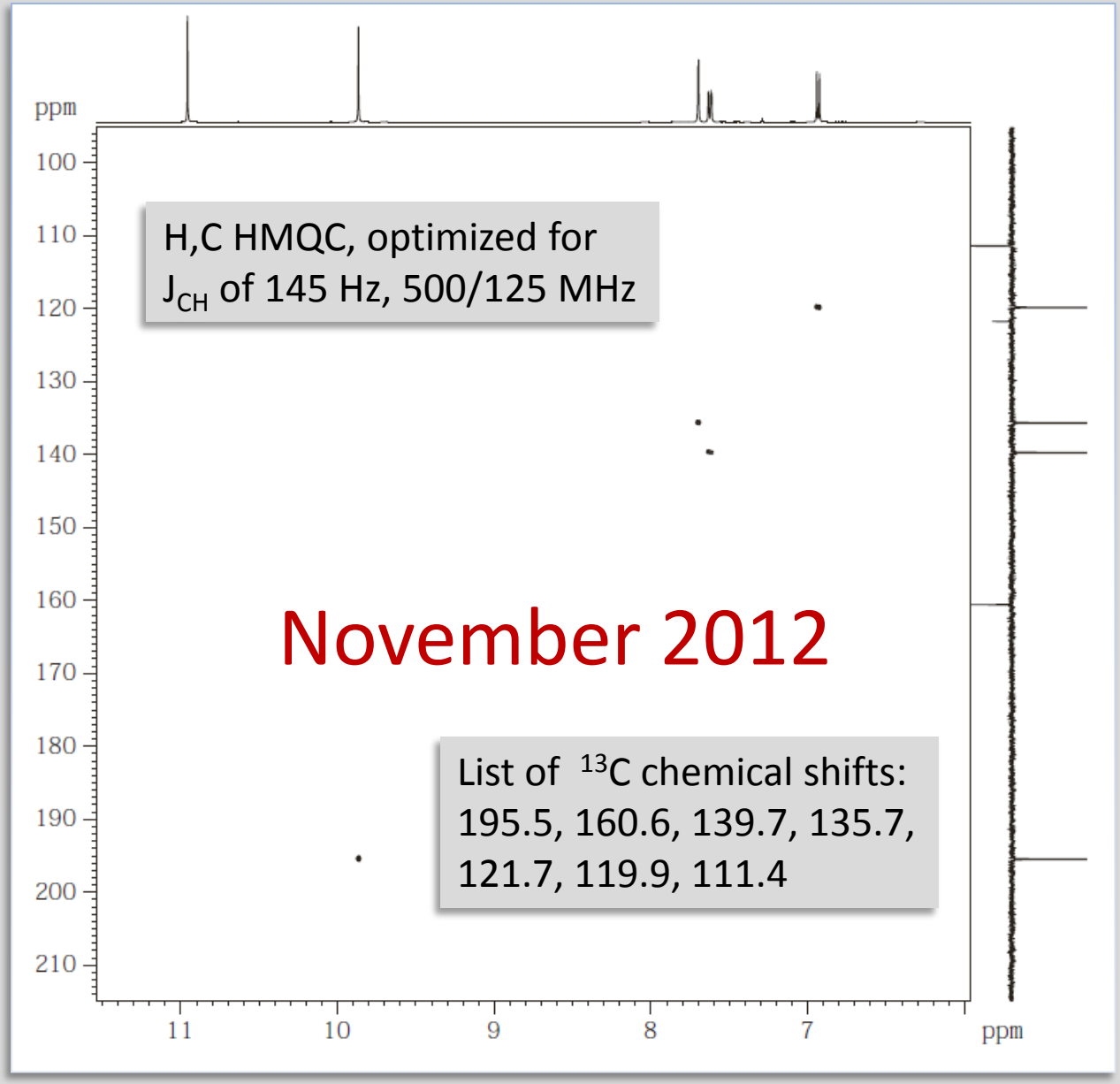
Problem of the Month:



Problem of the Month:

Strategy

(1) The molecular formula of this month's molecule is $C_7H_5BrO_2$: As a first step, determine the number of DBE.

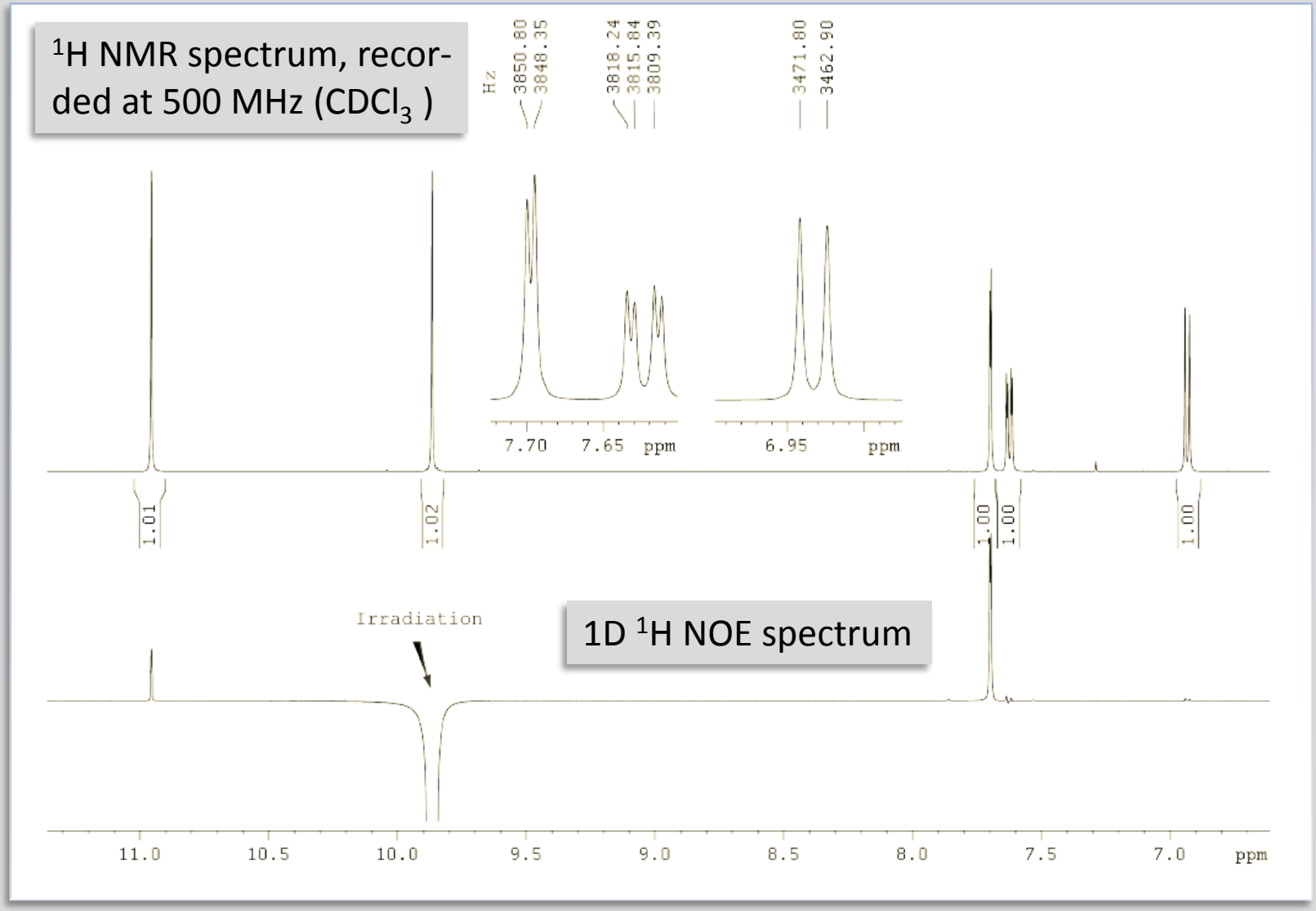
(2) Assign H,C connectivities from the HMQC (cover page). There is one ^{1}H signal without cross peak. Identify the different types of protons in the target compound by comparison with the ^{1}H NMR spectrum on the next page (upper trace). Note: The 1D projection of the ^{13}C NMR spectrum is multiplicity-edited!

(3) Do a „search by spectrum" in nmrshiftdb2 (select option „subspectrum"), and enter the carbon shift corresponding to the ^{1}H signal at 9.9 ppm (enter „195.5 D" for a shift at 195.5 ppm having one proton attached to it). This provides you with a valuable hint.

(4) Finally, evaluate the through-space information yielded from the 1D NOE spectrum (next page, lower trace).

Problem of the Month:

November 2012



Problem of the Month:
November 2012

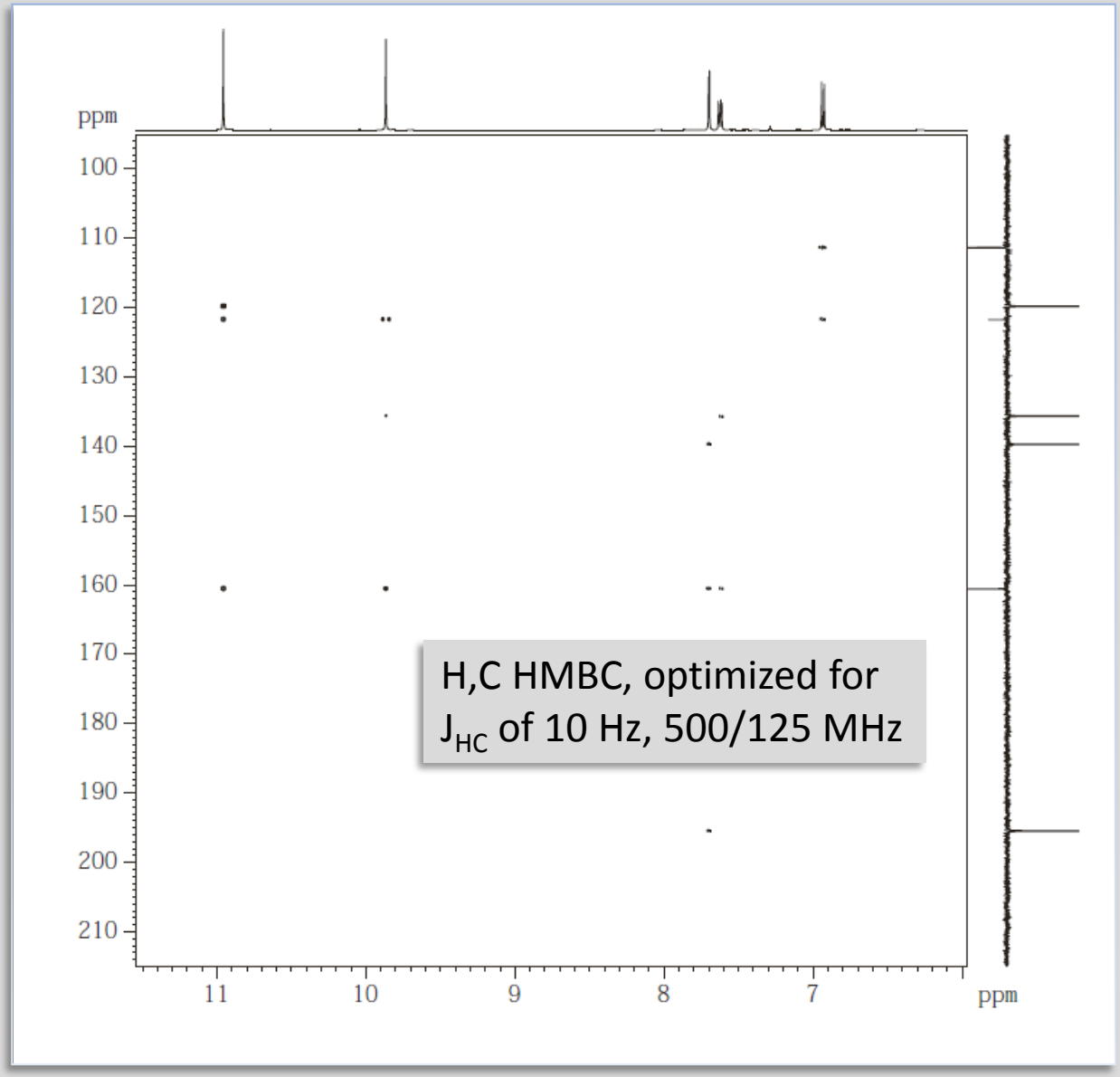
Hints

(1) There is only one coupled spin system visible in the ^{1}H NMR spectrum. Also, from the number of DBE, an aromatic compound should be considered.

(2) The information yielded from nmrshiftdb2 search derives a characteristic functional group which is present in the molecule. Its neighbour protons are visible in the 1D NOE experiment.

(3) Summing up these informations, an aromatic molecule is identified. The substitution pattern can be deduced from NOE, ^{1}H coupling pattern and HMBC (as additional information available on the next page)

Problem of the Month:



Problem of the Month:
November 2012

Solution

(1) An AMX system, made up from protons attached to sp^2 hybridized (aromatic) carbons, can be identified. There is long range coupling (1.4 Hz) and ^3J coupling (8.9 Hz) present. The total number of DBE‘s is 5.

(2) Subspectrum search for the ^{13}C signal at δ_C 195.5 indicates presence of an aldehyde. From the NOE spectrum, neighbouring OH and H protons can be identified. The third substituent on the aromatic moiety is Br. The substitution pattern can be cross-checked by evaluation of the HMBC spectrum.

(3) Hint: Enter the chemical shifts of the ^{13}C signals in nmrsshiftdb2 as a „spectrum search“ (option „complete“) or click here.