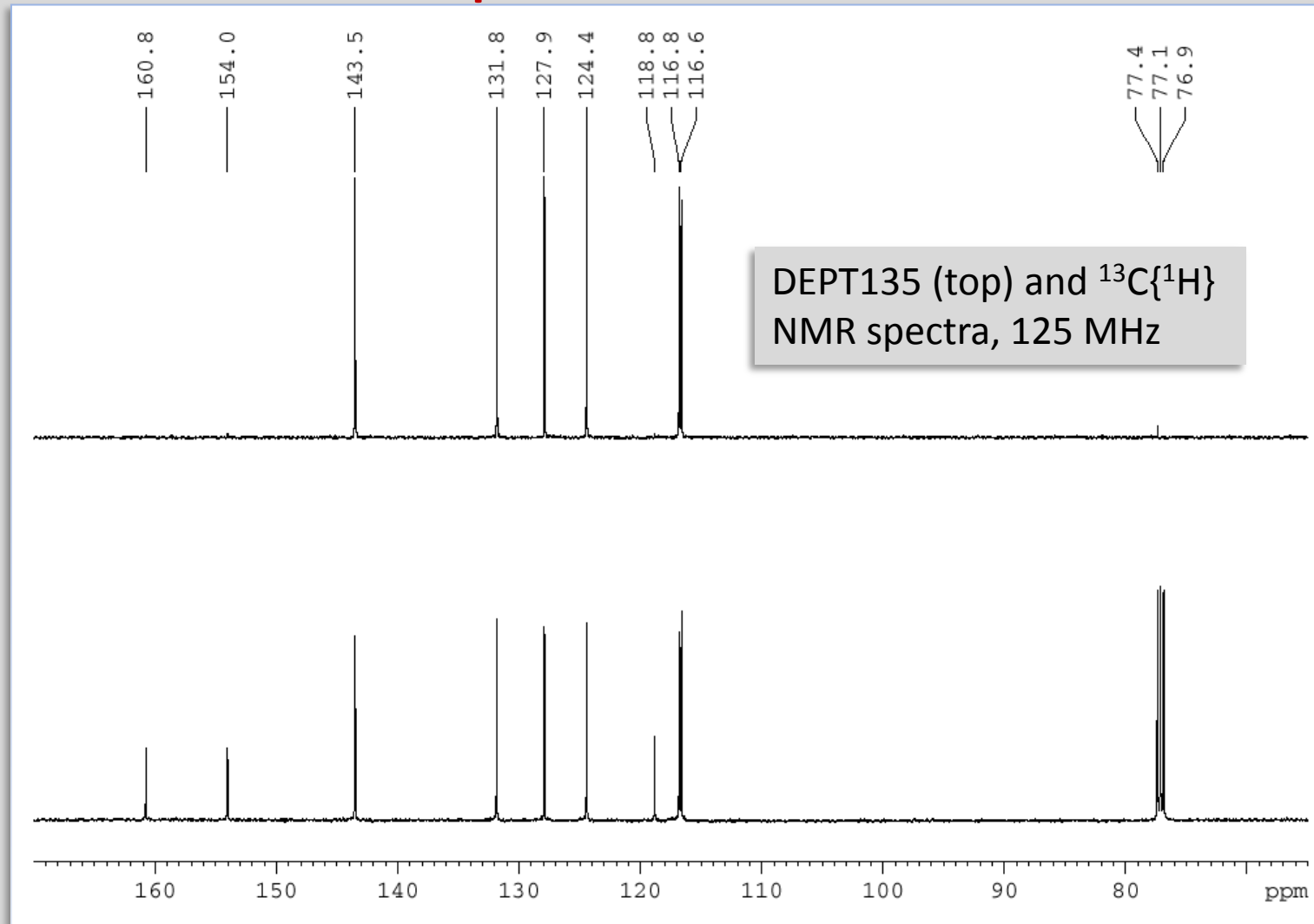


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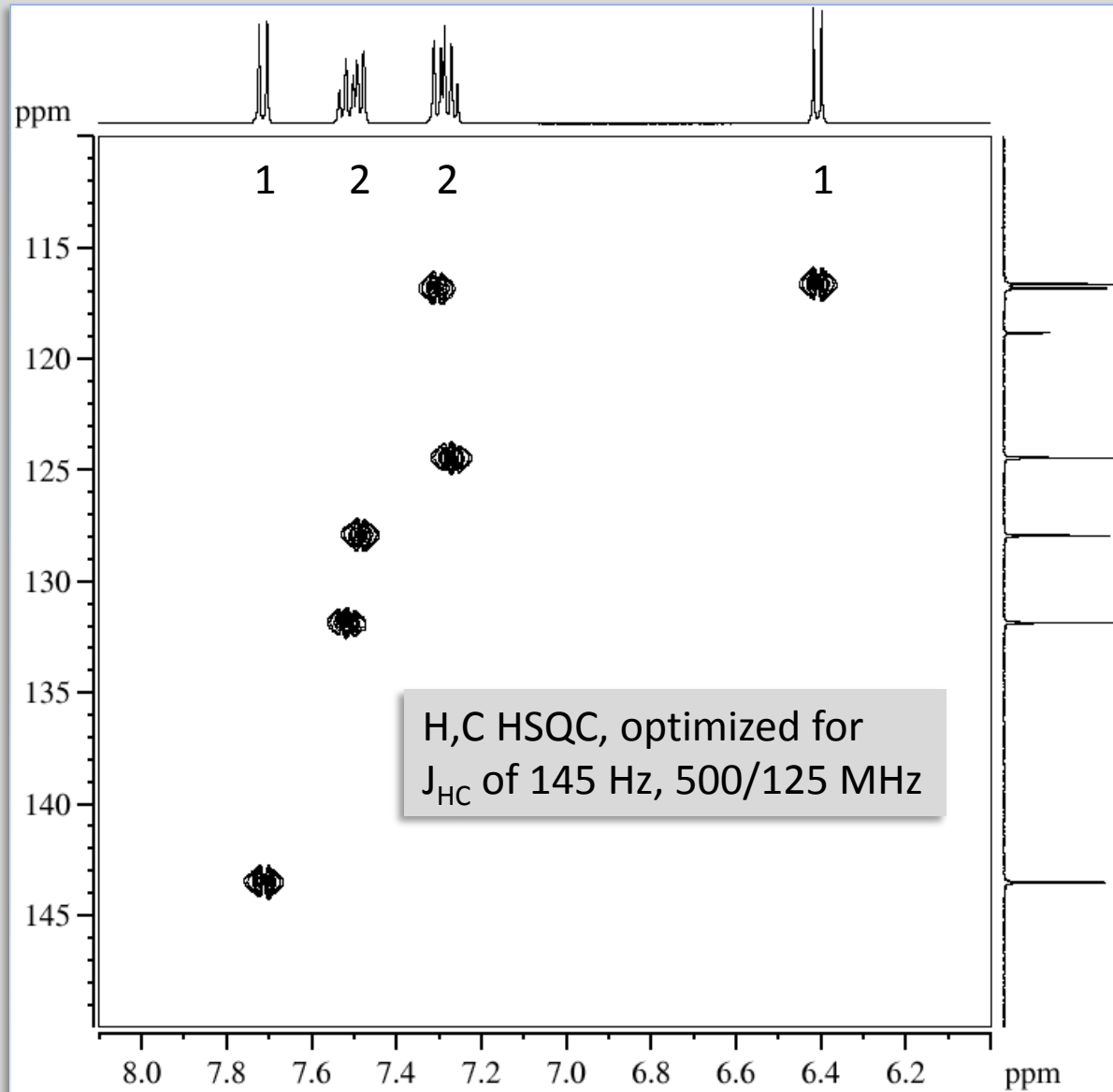
Strategy

(1) This month's molecule has the formula $C_9H_6O_2$. Check first the number of DBE.

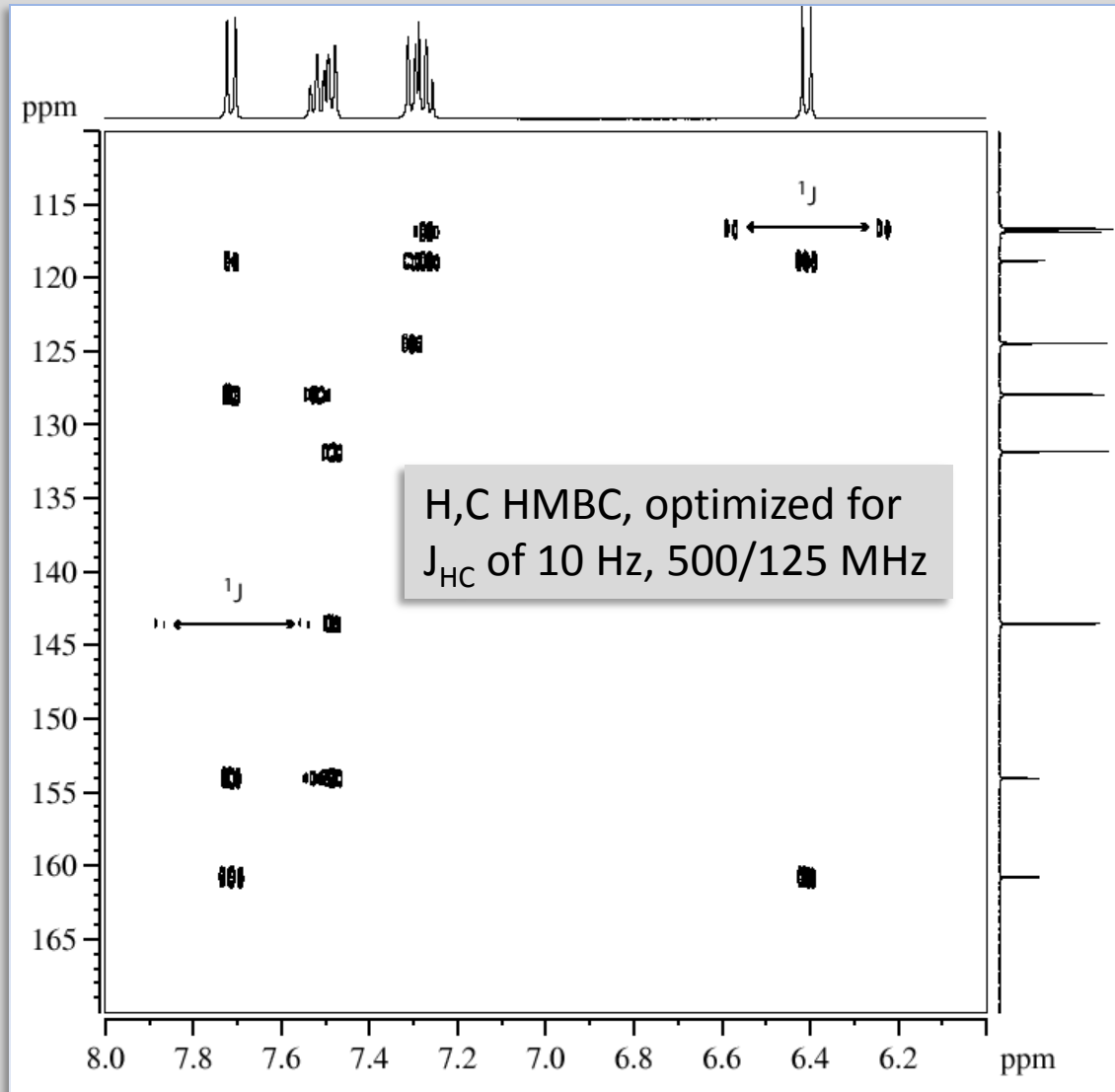
(2) After assigning H,C connectivities (next page), try to identify existing spin systems from the 1H projection of the HSQC. Relative intensities are indicated below the 1H trace.

(3) Do a „search by spectrum“ in nmrshiftdb2 (select option „subspectrum“), and enter the two leftmost carbon shifts with their corresponding multiplicity (e.g. enter „123.4 T“ for a shift at 123.4 ppm with a triplet splitting).

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Hints

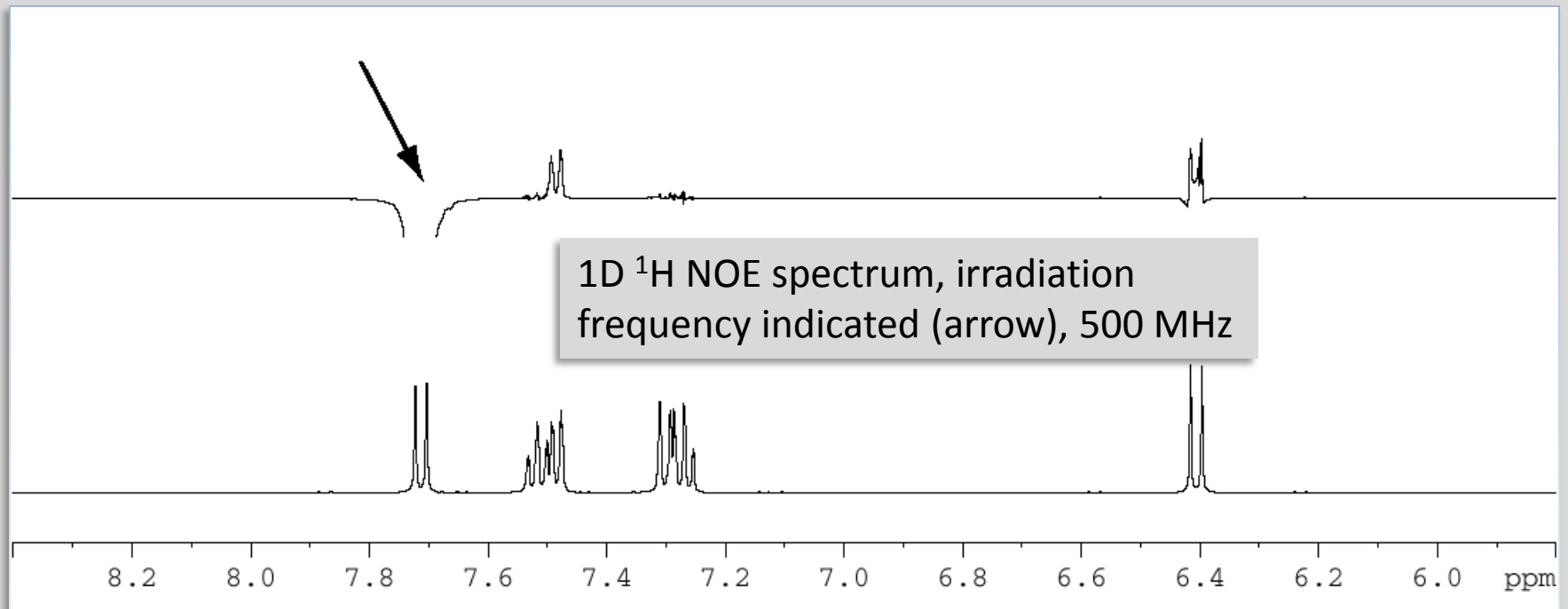
(1) There are two spin systems visible in the ^1H NMR spectrum.

(2) From your search for the two signals at δ_{C} 160.8 and 154.0, you should obtain an idea, which type of compound we are looking for.

(3) Additional information can be gained from the selective 1D NOE experiment provided on the next slide.

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Solution

(1) An AMPX and an AX system, each made up from protons attached to sp^2 hybridized carbons, can be identified. Also, vicinity between them can be derived from the NOE spectrum.

(2) A (subspectrum) search for ^{13}C signals δ_{C} 160.8 and 154.0 indicates that there is an aromatic ester in the compound. The total number of DBE's is 7. Connectivities can be derived from evaluation of the HMBC spectrum.

(3) Hint: Enter the chemical shifts of the ^{13}C signals in nmrshiftdb2 as a „spectrum search“ (option „complete“) or click [here](#).