2D NMR

A correlation map between two NMR parameters

$\delta_I - \delta_I$

COSY
TOCSY
NOESY
ROESY, etc.

$\delta_I - \delta_S$

HSQC
HMBC, etc.

$\delta_I - J_{I,I}$

homonuclear 2D-J

(and more… – only talking about the canned experiments here; more in Chm539 !)

COSY and TOCSY – based on resolved $J_{I,I}$-coupling

COSY (COrrelated SpectroscopY):

Single-step magnetization transfer

Connectivities through 2 or 3 chemical bonds (rarely 4), depends on torsional angle

Antiphase cross-peak structure

TOCSY (Total Correlated SpectroscopY):

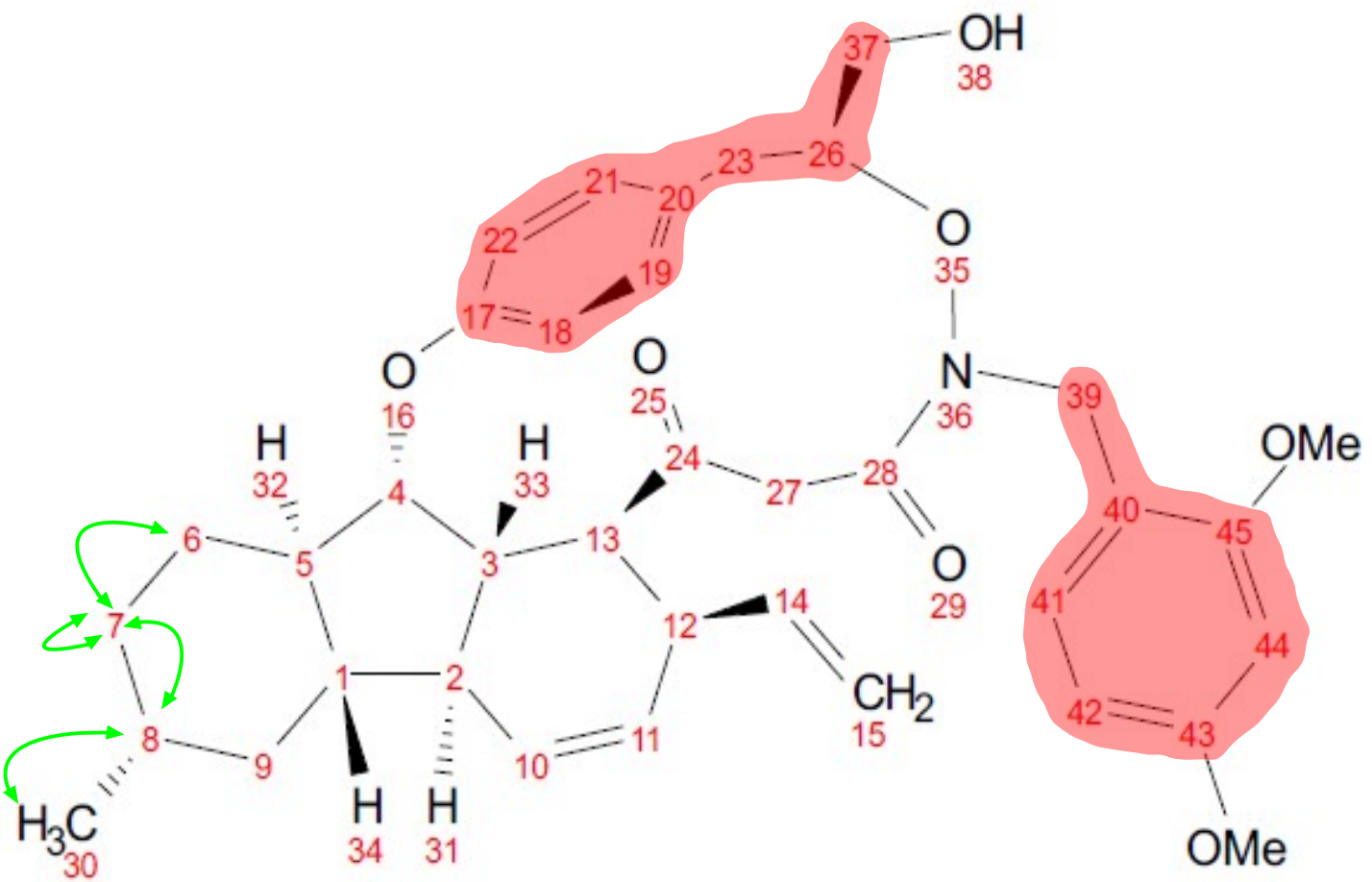
Multiple-step magnetization transfer

Connectivities throughout the whole connected spin-topology (in ideal case)

In-phase cross-peak structure (enhances sensitivity)

COSY examples

TOCSY examples



NOESY and ROESY – based on spatial closeness (r^{-6})

NOESY (Nuclear Overhauser Enhancement SpectroscopY):

Connectivities through distances up to 5-7 Å

+ or -, may be vanishing at certain mobility

ROESY (Rotating frame Overhauser Enhancement SpectroscopY):

Same as NOESY, faster buildup, faster relaxation losses

Always positive, may help to identify exchange

HSQC and HMBC – based on resolved $J_{I,S}$ -coupling

HSQC (Heteronuclear Single Quantum Coherence):

Connectivities through one chemical bond

HMBC (Heteronuclear Multiple Bond Coherence):

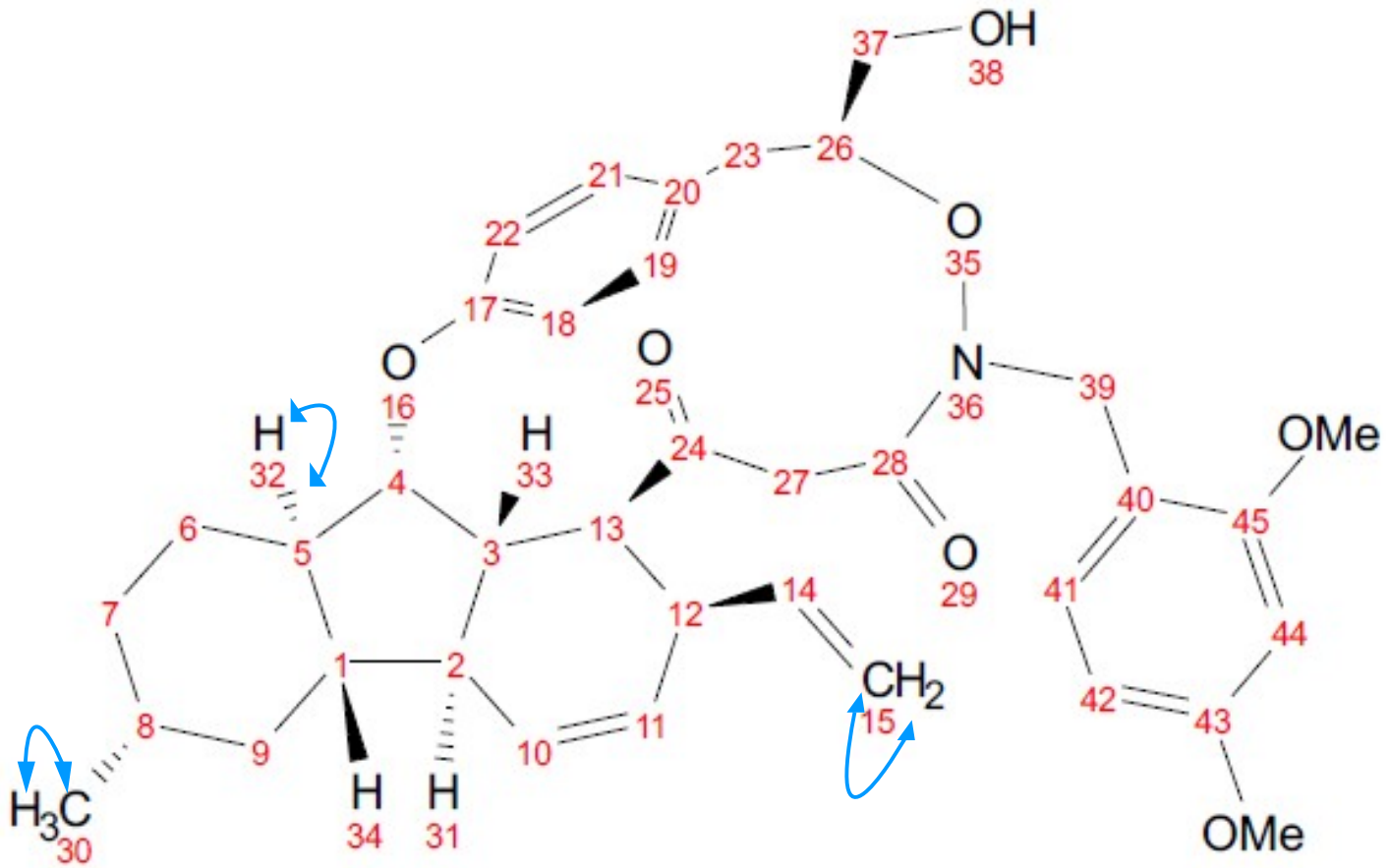
Connectivities through 2-4(5) chemical bonds

^{1}H-detected ; overall sensitivity depends on ^{1}H sensitivity – A1 is best !

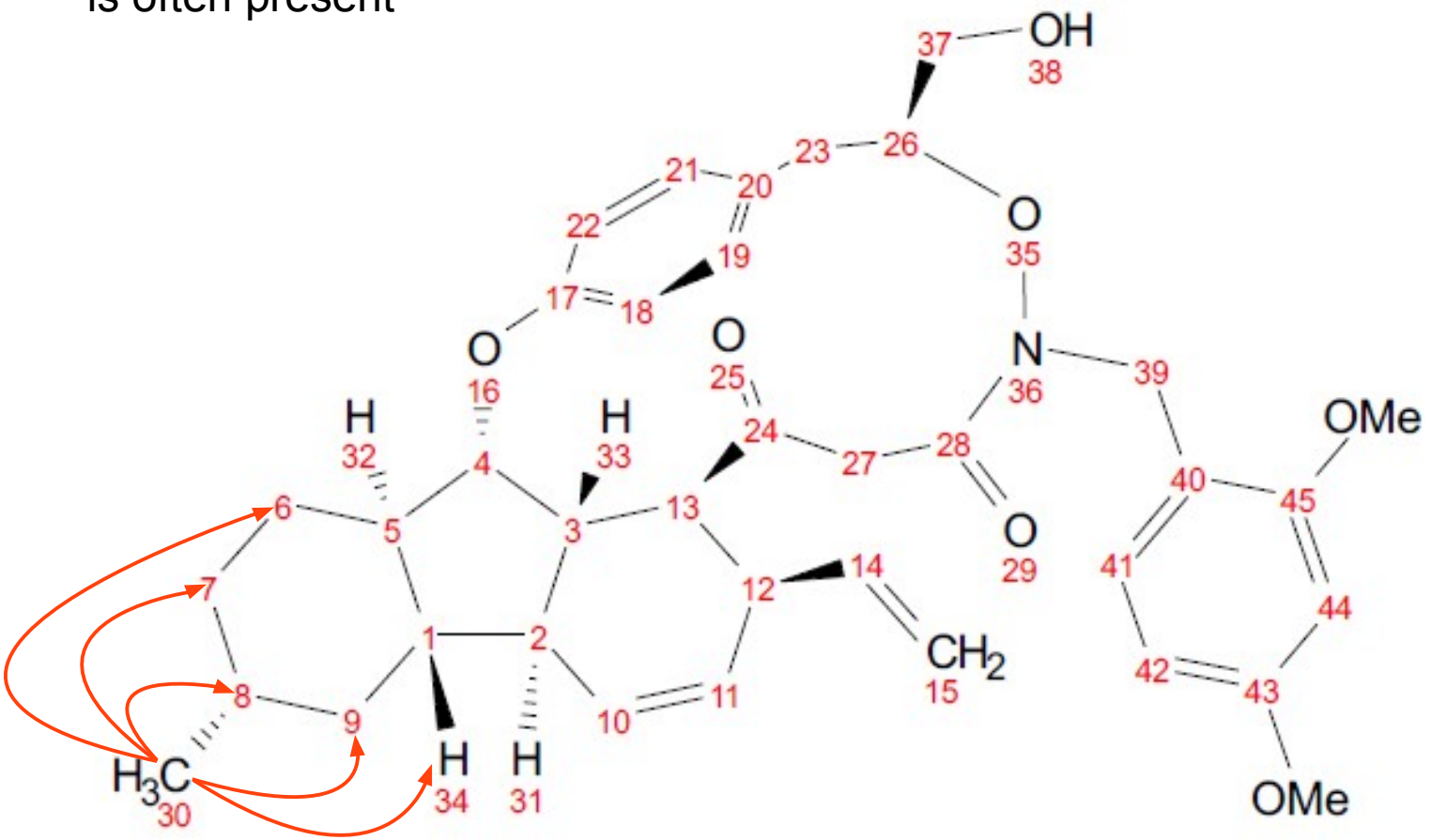
HSQC

DEPT-edited – CH_2 cross peaks

Are on the “opposite” side



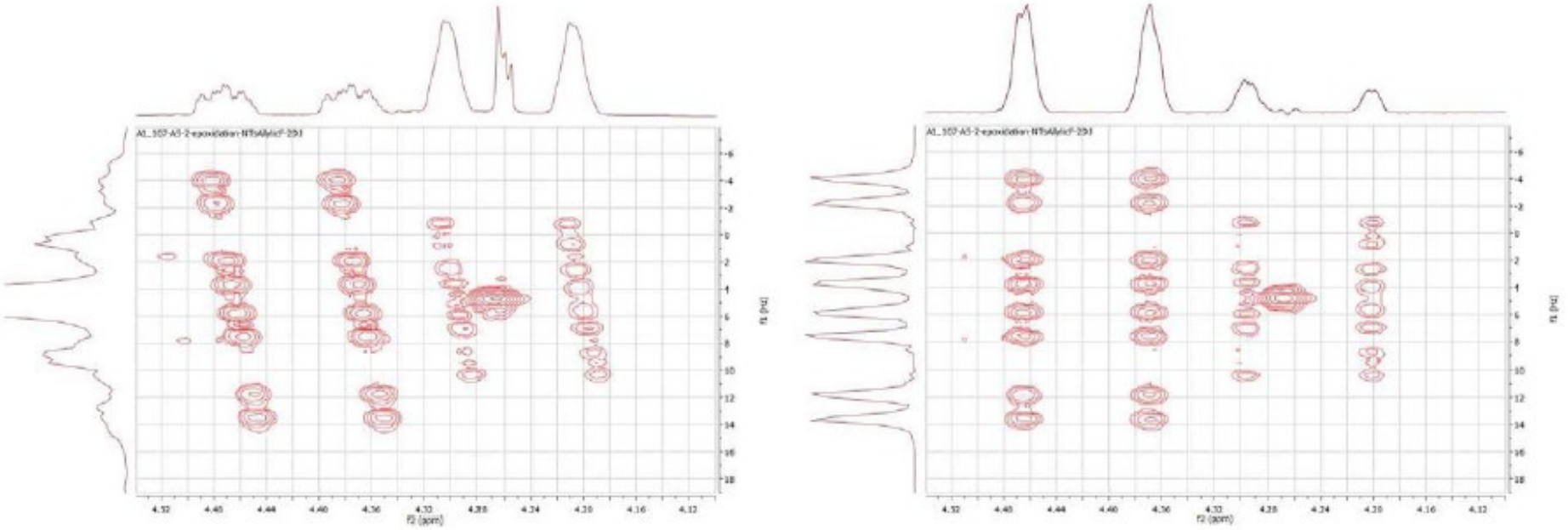
HMBC
Through 2-3-(4-(5)) bonds
Dihedral angle dependent
Residual one-bond doublet
is often present



Homonuclear 2D-J-spectroscopy

Separates – after data processing – chemical shift and $J_{I,I}$ homonuclear coupling

Heterouclear coupling ($J_{I,S}$) remains in the f2 dimension



Default data structure, processing

	phase sensitive	magnitude
COSY		+
TOCSY	+	
NOESY	+	
ROESY	+	
HSQC	+	
HMBC		+
homonuclear 2D-J		+

(Gradient selected/assisted experiments.)

Default apodization parameters, first point correction

	f2	f1
COSY	Sin2, G5-15Hz	Sin, G15-25Hz
TOCSY*	Sin2/90, G5-15Hz	Sin/90, G15-25Hz
NOESY**	Sin2/90, G5-15Hz	Sin/90, G15-25Hz
ROESY**	Sin2/90, G5-15Hz	Sin/90, G15-25Hz
HSQC*	Sin2/90, G5-15Hz	Sin/90, G15-25Hz
HMBC	Sin2/90, G5-15Hz	Sin/90, G15-25Hz
homonuclear 2D-J	Sin2(/30), G1-3Hz	Sin, G1-1.5Hz

* First point correction IS necessary in f1.

** NO first point correction in f1.

TOCSY, NOESY, ROESY – mixing/spin-lock time can be varied!

Phase correction

Automatic phase correction may work just fine…

In general:

move the Pivot point to the leftmost position
adjust PH0 (left mouse button) watching peaks on the left only
adjust PH1 (right mouse button) watching peaks on the right only
do it in few iterations…

Typical (approx.):	PH0	PH1
TOCSY :	90	0
NOESY :	90	180
ROESY :	0	180

Baseline correction

Polynomial, in both dimension

For phase sensitive spectra at the first place

Appearance, visualization options

In “Properties”

Contours, colors (red-blue)

Reference 1D-s, projections, slices