NTNU
Institutt for bioteknologi

Dato Referanse

Møtereferat

Til stede:	Kjetil Rasmussen, Turid Rustad, Berit L. Strand, Eivind Almaas, Catherine Nordgård, Martin Hohmann-Marriott, Ingrid Bakke, Trygve Brautaset, Finn Aachmann, Per Bruheim, Gaston Courtade, Gudmund Skjåk-Bræk, Olav Vadstein, Madeleine Gundersen (student), Oskar Speilberg (student), Kjell Morten Vårum, Marit Sletmoen.
Forfall:	Bjørn Christensen, Ann-Sissel Teialeret Ulset, Kurt I. Draget, Rahmi Lale, Trond Ellingsen
Kopi til:	
Gjelder:	Faglærermøte IBT
Møtetid:	9.5.16 kl 08:30 – 10:30 Møtested: E1-118
Signatur:	

O-saker:

- BioCat – Finn informerer om forskerskolen. Ny forskerskole også på trappene: Digital Life
- Instituttstruktur fra januar 2017 – status
- Ny budsjettmal – ta kontakt med Wenche før søknad sendes inn
- Onsager fellowship
- Status investering infrastruktur
- Vårfest 2. juni
- Opptaket vår 2016
- Sensoroppnevning for perioden t.o.m. 31.08.2018
- Gjennomgang av høstens emner

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Saksliste:

1. Evaluering av høst-emner (Jo + aktuelle faglærere)

Ikke referert

2. Gjennomgang av rutiner ifm eksamen og sensur (Jo)

- Bruk av sensorveiledning/løsningsforslag
- Oversettelse av eksamensoppgaver
- Sensur av masteroppgaver
  - Ordning for bruk av intern sensor som ikke er veileder
  - Revidert skjema til bruk ved sensur

- O-saker
  - Opptaket vår 2016
  - Sensoroppnevning for perioden t.o.m. 31.08.2018

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  - Revidert skjema til bruk ved sensur
  - Ordning for bruk av intern sensor som ikke er veileder

Eksamen V-16

Eksamensdatoer og romplassering

Eksamen våren 2016 avholdes i perioden 23.mai - 11. juni. Eksamensdatoene er publisert på emnesidene: http://www.ntnu.no/studier/emner#semester

Tre – 3 – arbeidsdager før eksamensdatoen plasseres det enkelte emnet på rom, og plasseringen publiseres på nettsiden http://www.ntnu.no/eksamen/sted/ . Legg merke til at et emne kan ha kandidater på flere rom – dette må faglærer sjekke.

Obligatorisk aktivitet

Godkjente obligatoriske aktiviteter i det enkelte emne må være registrert innen syv – 7 – arbeidsdager før eksamensdato, se frist i tabell under. Undertegnede sender ut godkjenningslister, som returneres innen fristen for registrering.

Eksamen – planlegging og gjennomføring

Se ressursside på web, her finner dere blant annet eksamensforsider, hjelpemiddelkoder mm. https://innsida.ntnu.no/eksamensforberedelse

Språkhjelp til eksamensoppgaver

Eksamenskandidatene har krav på å få eksamensoppgaven på sin målform. Sjekk derfor at eksamensoppgaven finnes i riktig målform for det enkelte emne, se under. Eksamenskontoret har navn på språkkonsulenter som kan bistå hvis faglærer mangler kompetanse på nynorsk. Undertegnede kan også bidra her. **MERK:** undertegnede har dessverre ikke kapasitet til å bidra med oversetting av eksamensoppgaver fra engelsk til norsk. De av faglærerne som har behov for dette bes finne andre løsninger.

Innlevering av eksamensoppgaver

Eksamensoppgaver sendes per e-post i word-format til undertegnede **SENEST** syv – 7 – arbeidsdager før eksamen, se frister under. Eksamensoppgaven skal ved innlevering være oversatt til valgte målformer / språk og ha korrekt utfylt forside (sjekk maler her https://innsida.ntnu.no/eksamensforberedelse).

Sensor og klagekomité

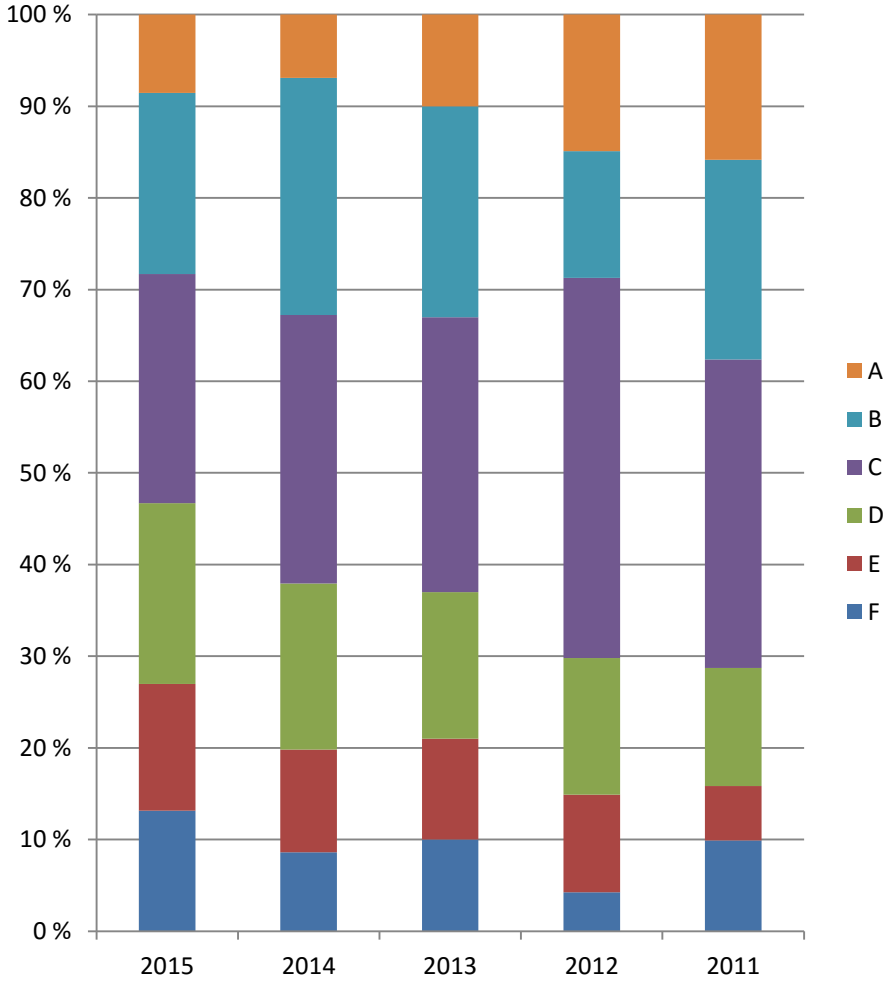
Det er vedtatt at IBT skal ha ekstern sensor i ordinære emner, ber derfor om at faglærer avklarer og melder tilbake hvem som skal være ekstern sensor. Faglærer må også ha klar ny klagekomité. Meldes til undertegnede. **Merk**: det skal lages løsningsforslag og sensorveiledning i alle emner.

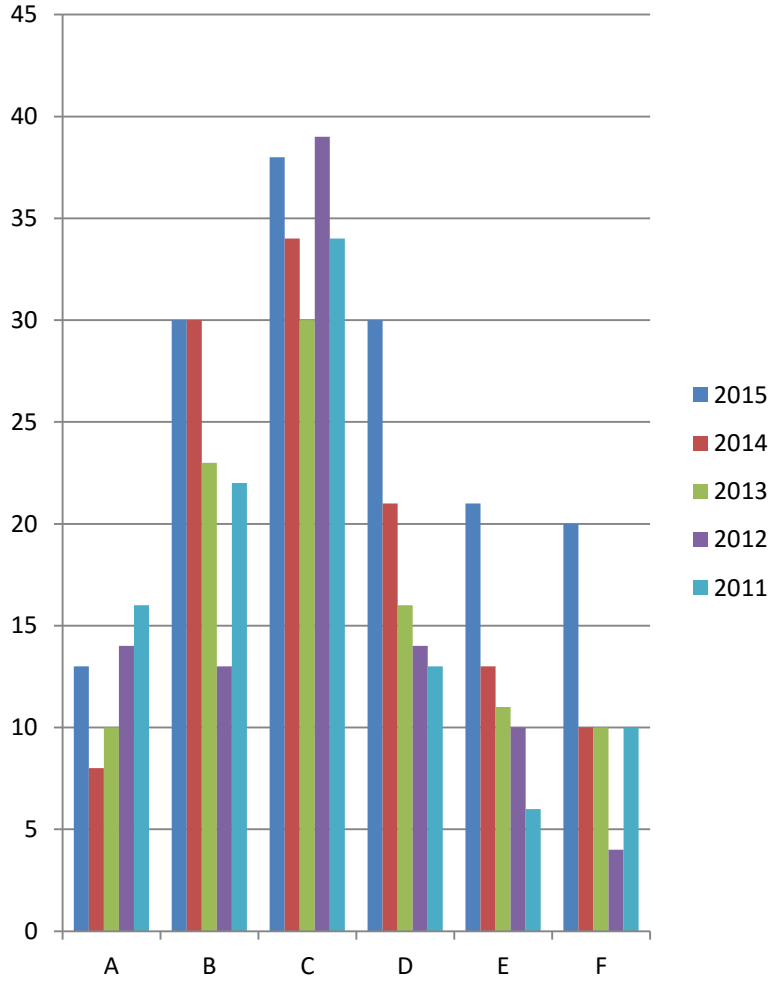
Evaluering emner H-15

- Hva er studentenes tilbakemeldinger via referansegrupper og emneevaluering?
- Hva går bra i emnet?
- Er det områder for forbedring?
- Settes det i verk tiltak i emnet på grunnlag av evalueringen?

TBT4102 Biokjemi 1

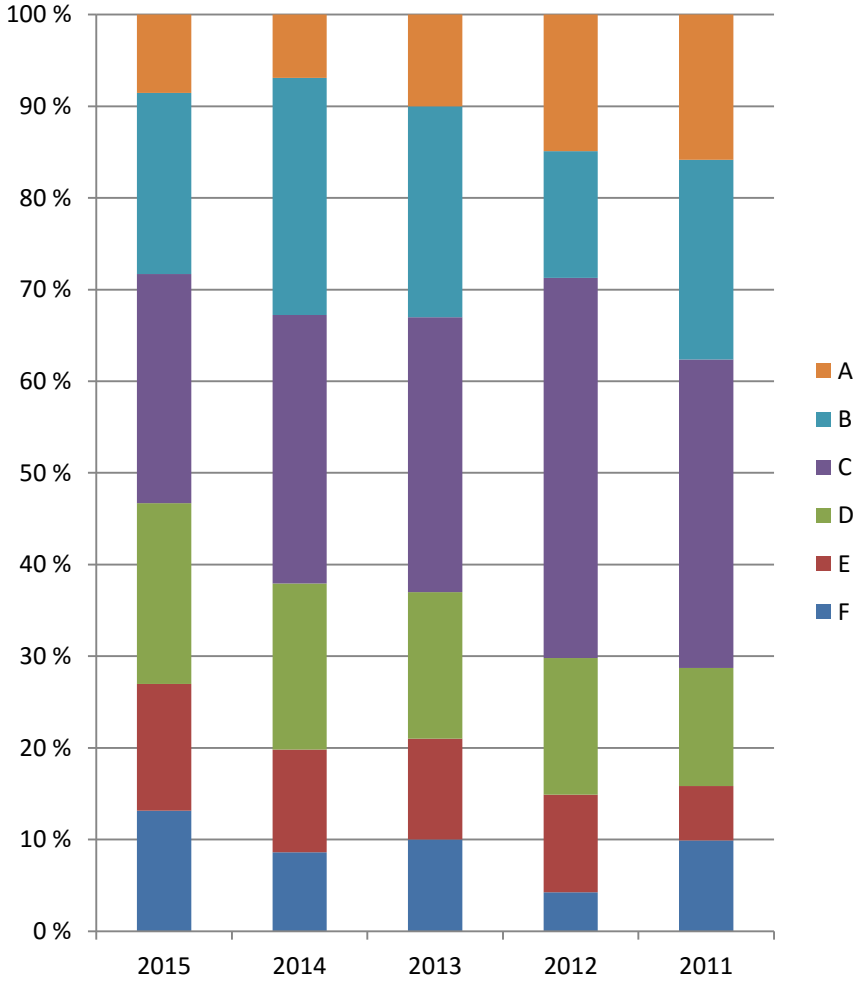
	2015	2014	2013	2012	2011
MELDT	152	136	109	110	125
MØTT	142	125	103	101	107
STRYK	20	13	10	4	10
TRUKKET/avbrutt	6	6	3	7	6
SNITT	C	C	C	C	C

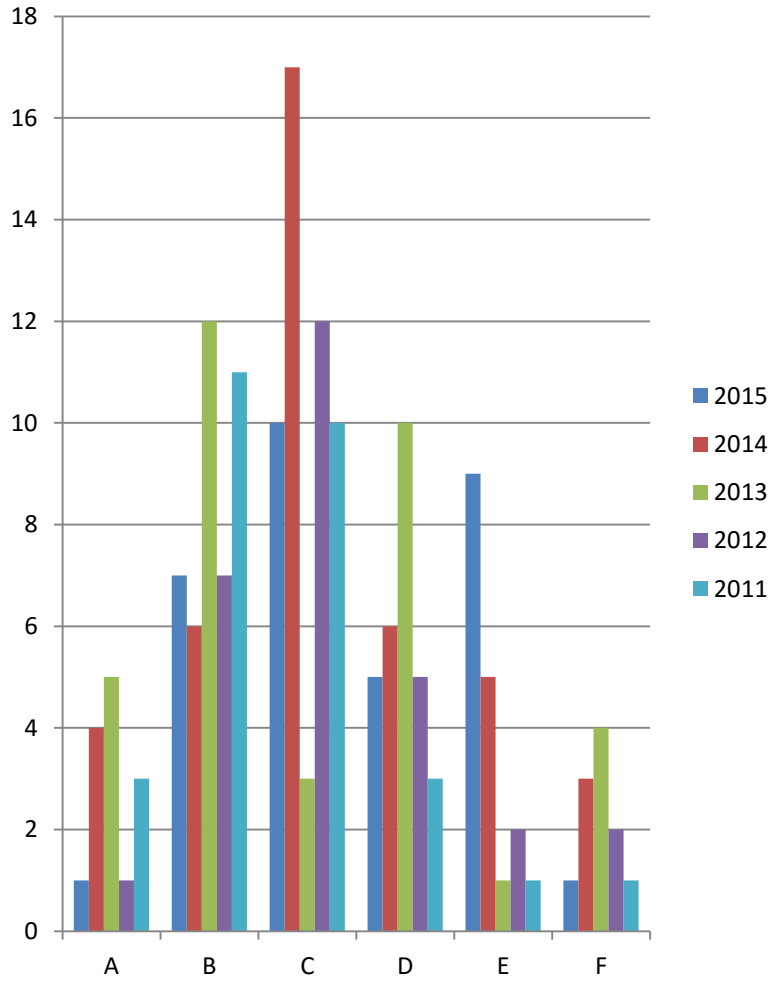




TBT4135 Biopolymer-kjemi

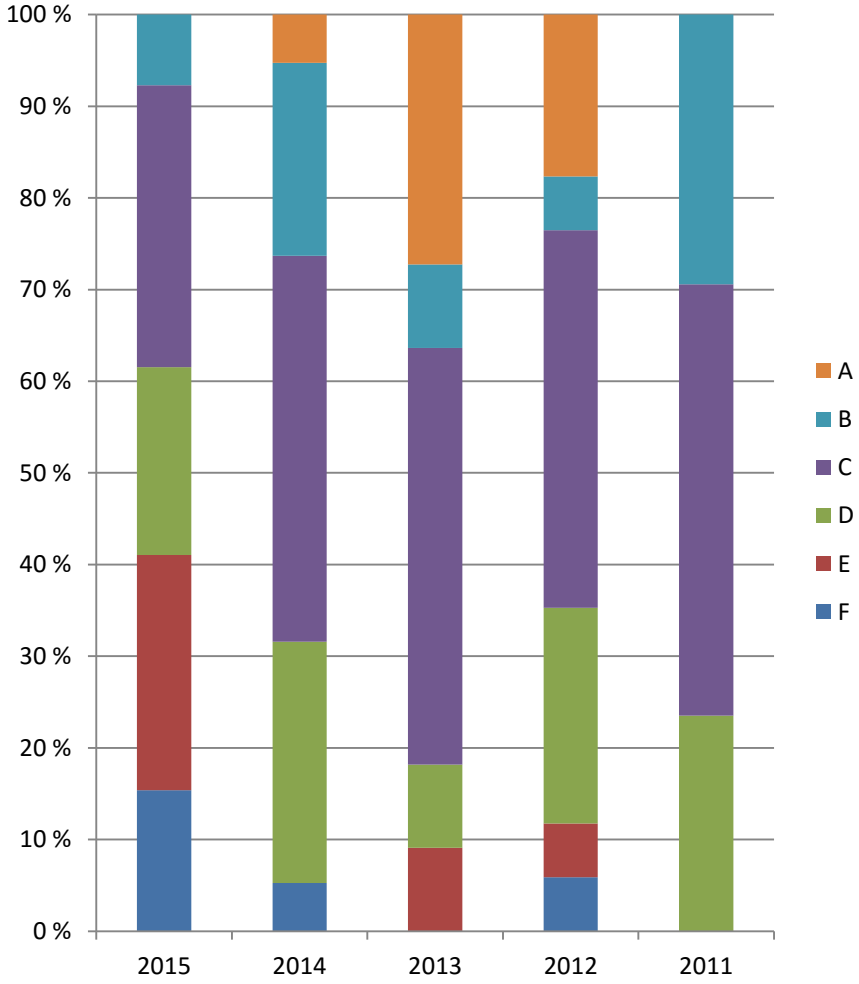
	2015	2014	2013	2012	2011
MELDT	36	43	39	31	31
MØTT	34	42	37	30	29
STRYK	1	4	4	2	1
TRUKKET	1	1	2	1	0
SNITT	C	C	C	C	C

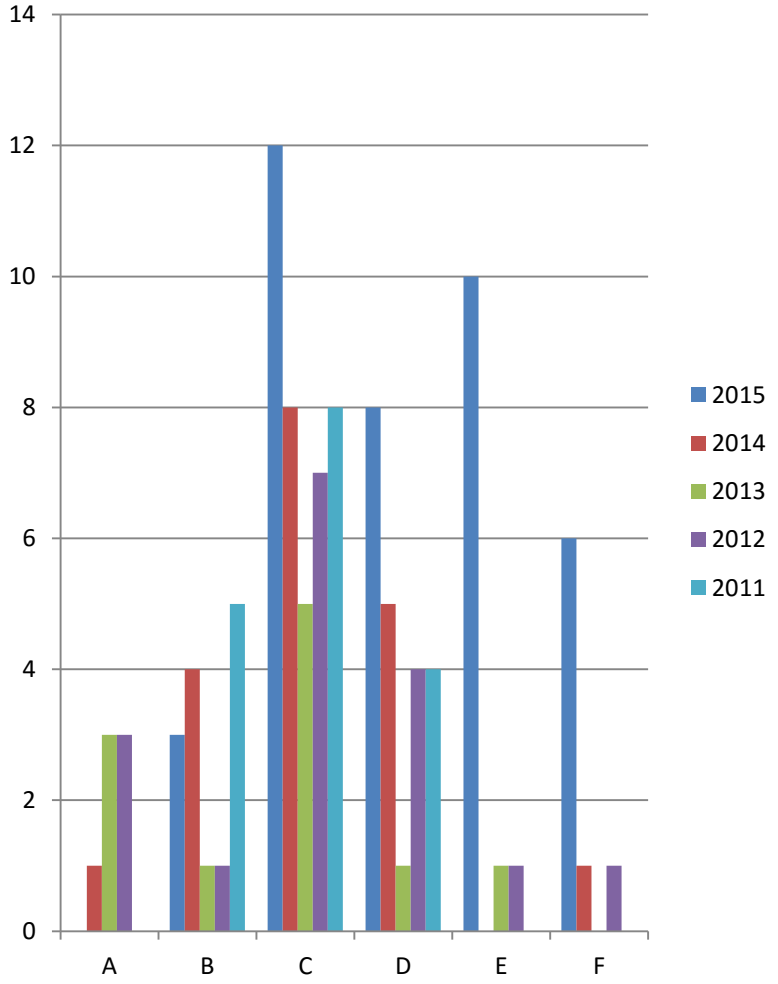




TBT4140 Biokjemi-teknikk

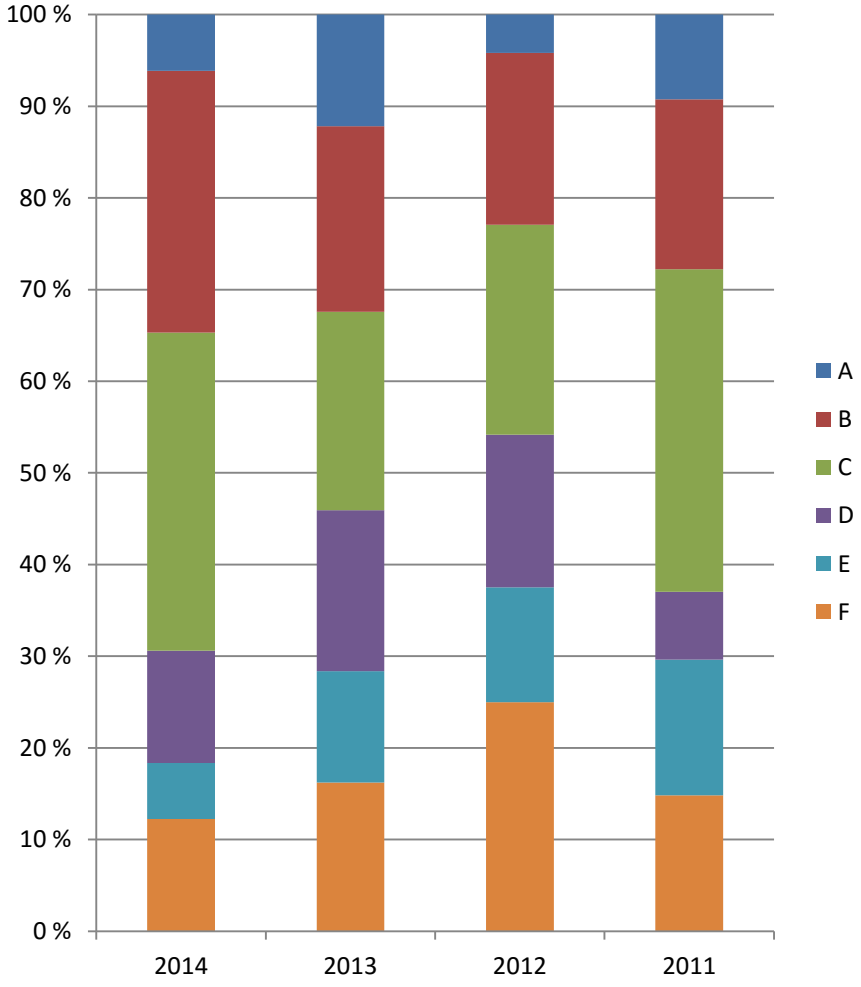
	2015	2014	2013	2012	2011
MELDT	40	21	15	22	19
MØTT	39	20	14	21	18
STRYK	6	1	0	1	0
TRUKKET	0	1	3	4	1
SNITT	D	C	C	C	C

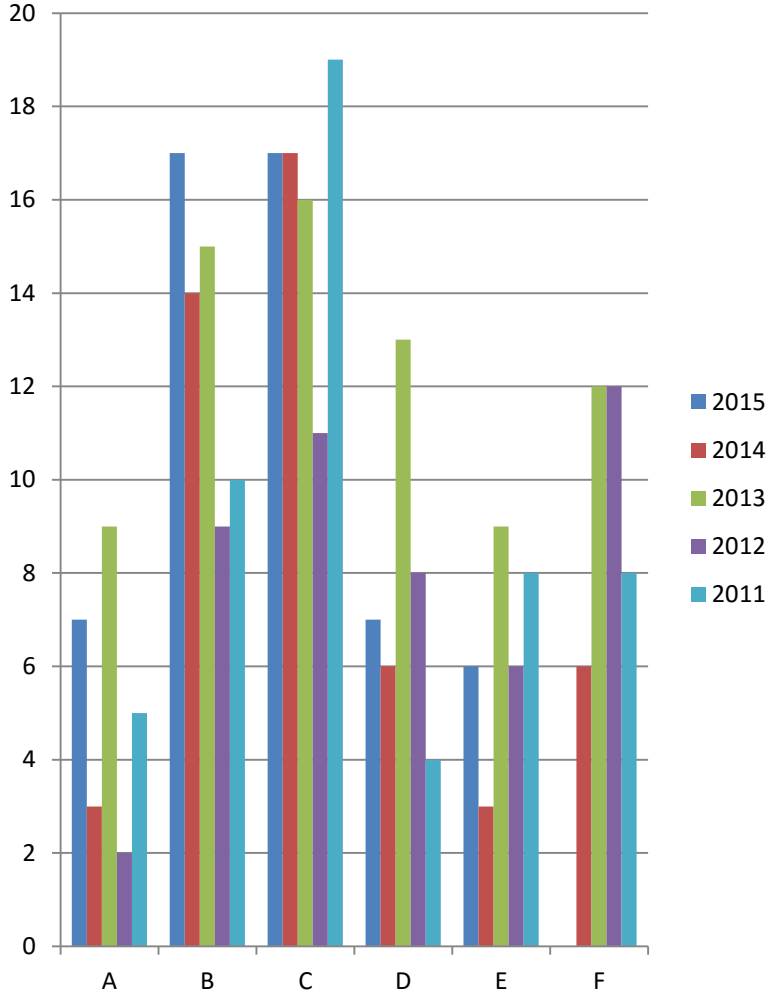




TBT4145 Molekylær-genetikk

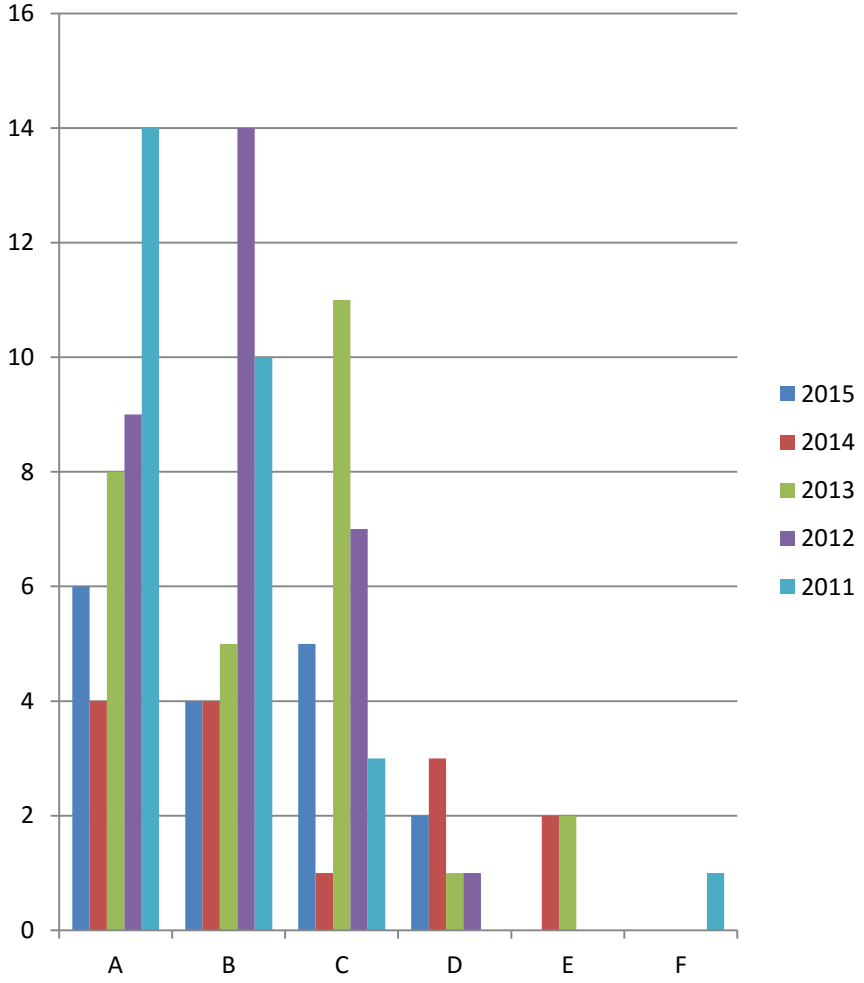
	2015	2014	2013	2012	2011
MELDT	60	55	79	59	66
MØTT	54	51	76	53	60
STRYK	0	6	12	12	8
TRUKKET	3	2	2	5	6
SNITT	C	C	B	C	C

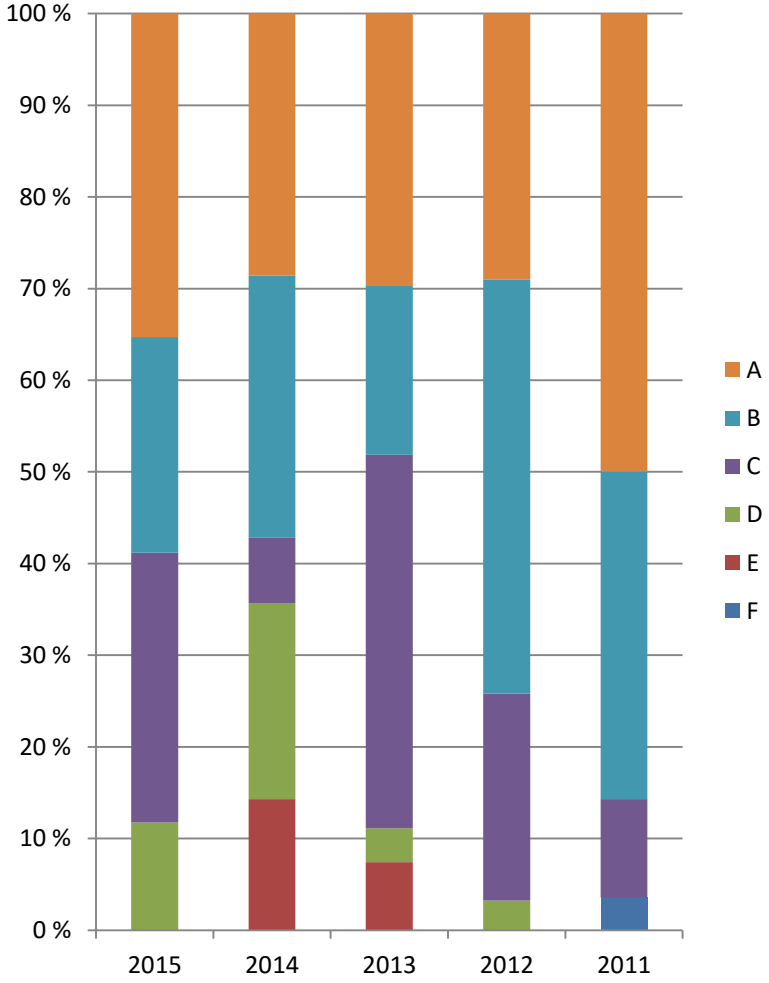




TBT4505 Bioteknologi fordypn.emne

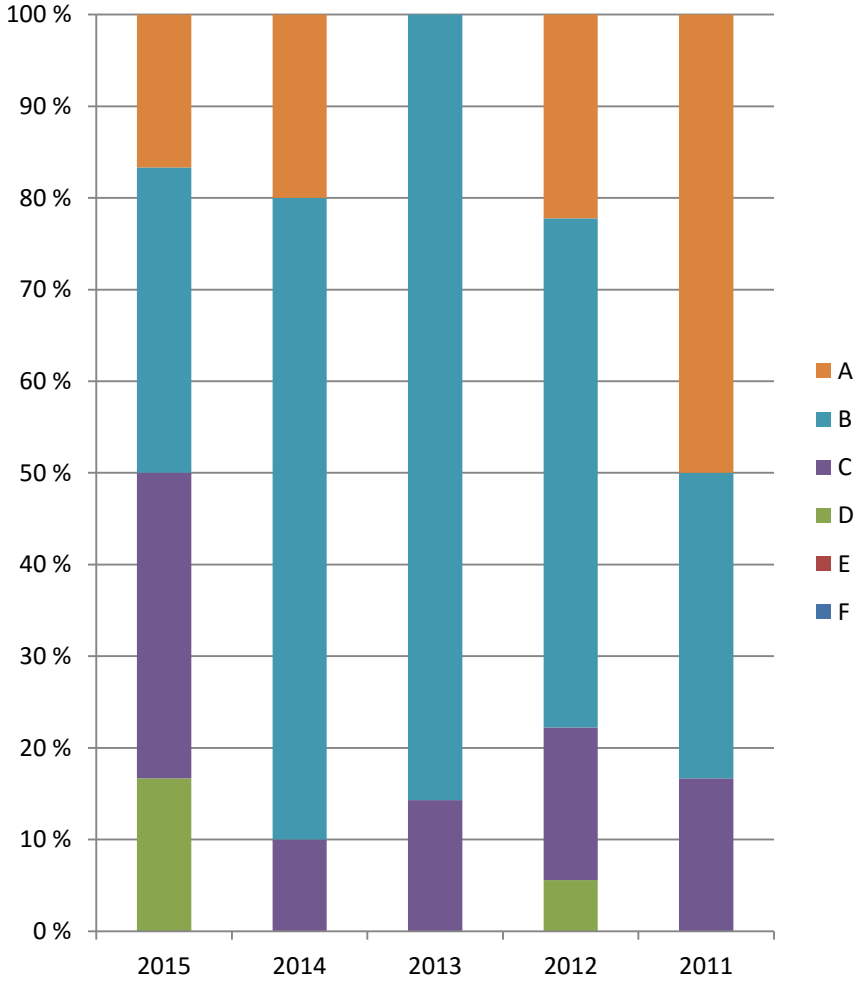
	2015	2014	2013	2012	2011
MELDT	17	16	33	34	30
MØTT	17	14	27	31	28
STRYK	0	0	0	0	1
TRUKKET	0	0	0	0	0
SNITT	B	B	B	B	B

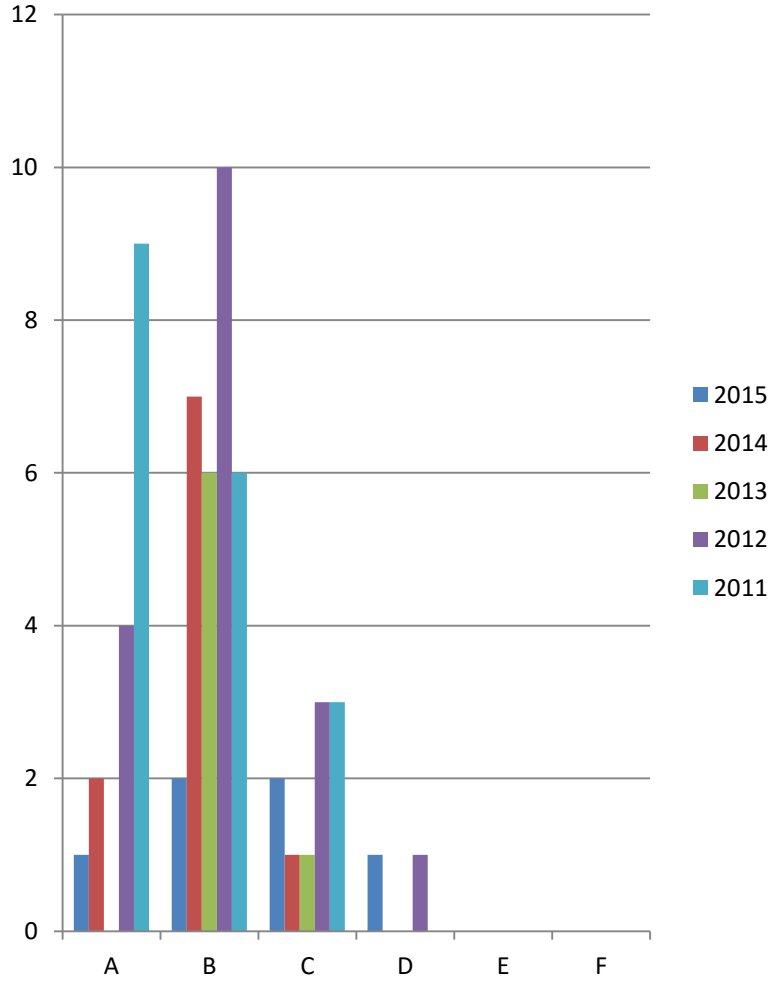




TBT4500 Bioteknologi fordypn.prosjekt

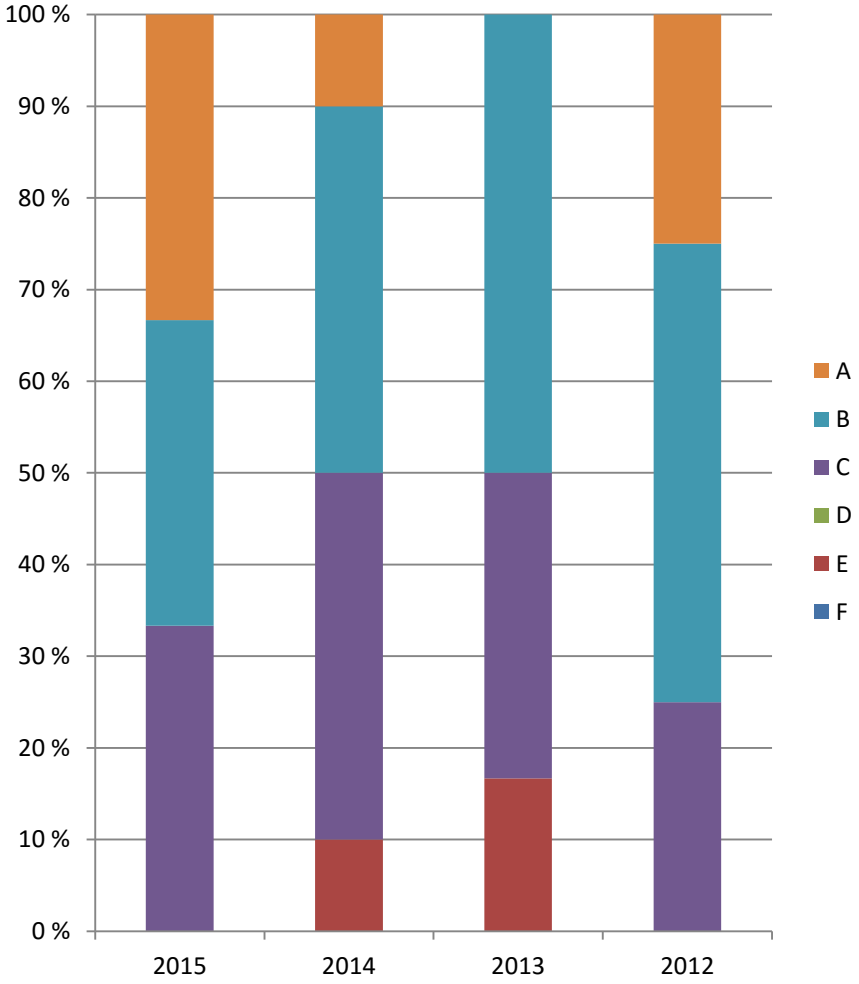
	2015	2014	2013	2012	2011
MELDT	7	10	7	19	18
MØTT	6	10	7	18	18
STRYK	0	0	0	0	0
TRUKKET	0	0	0	0	0
SNITT	B	B	B	B	B

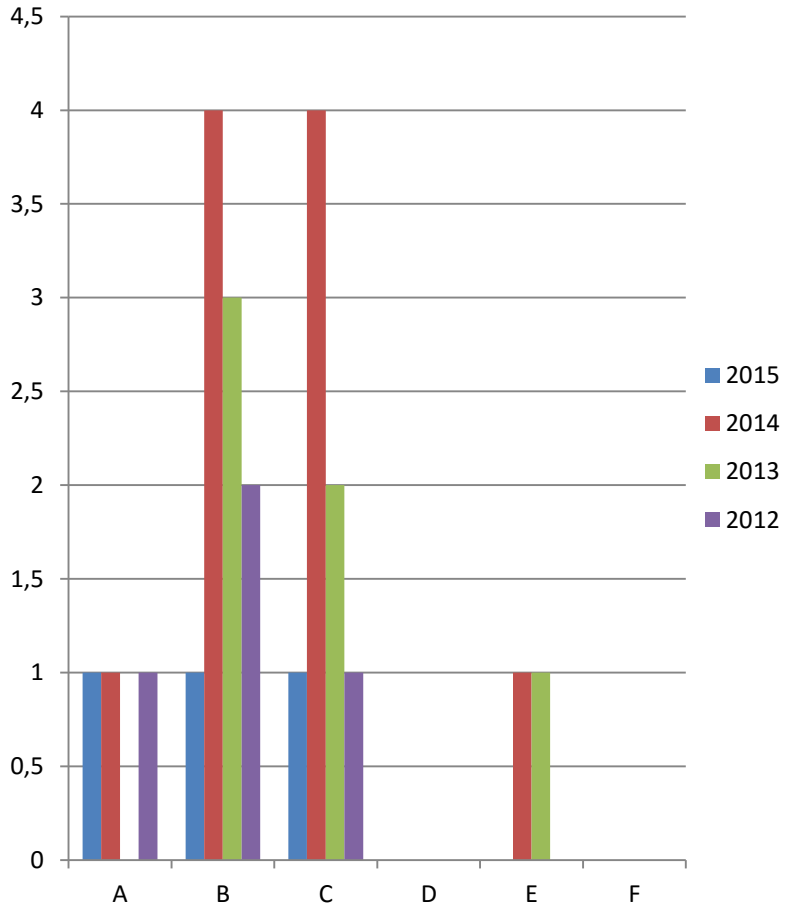




BT3110 Marine Næringsmiddelressurser

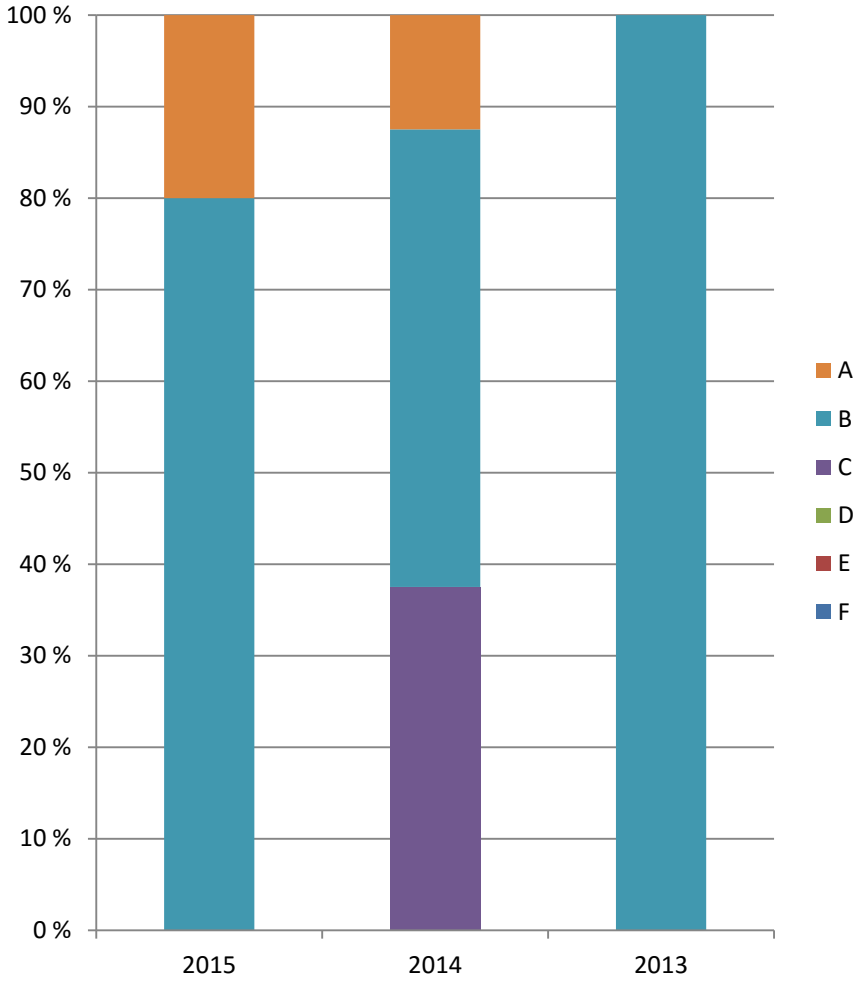
	2015	2014	2013	2012
MELDT	5	11	8	4
MØTT	3	10	7	4
STRYK	0	0	1	0
TRUKKET	0	0	0	0
SNITT	B	C	C	B

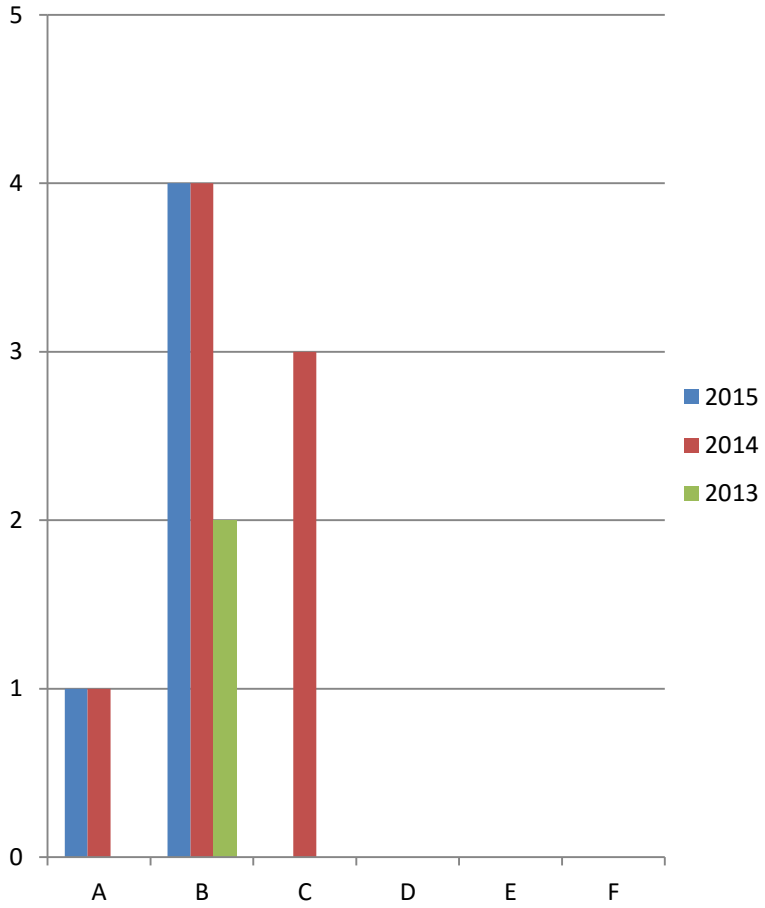




BT3115 Primærproduksjon - akvakultur og fiskeri

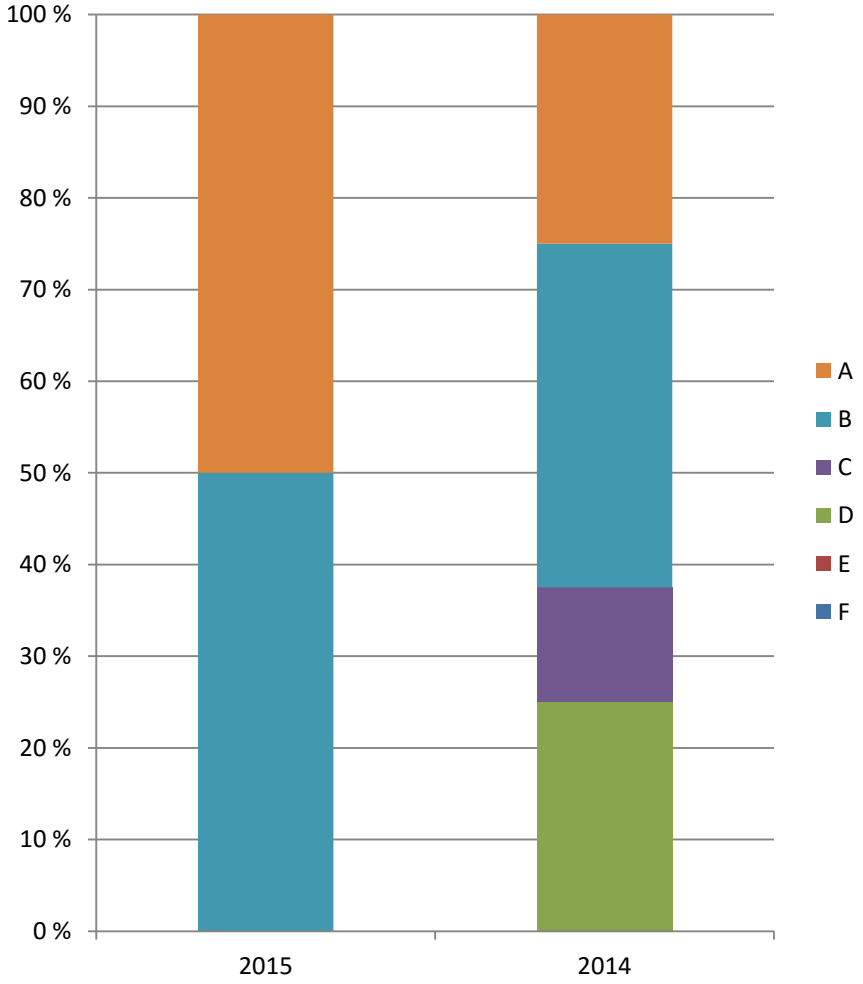
	2015	2014	2013
MELDT	5	9	4
MØTT	5	8	2
STRYK	0	0	0
TRUKKET	0	0	0
SNITT	B	B	C

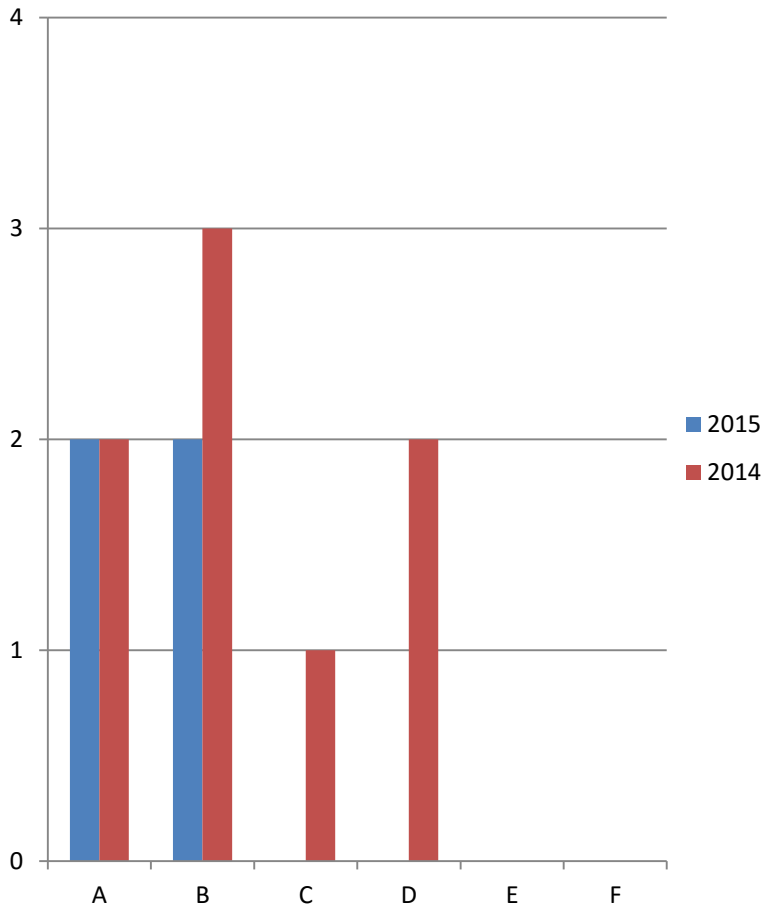




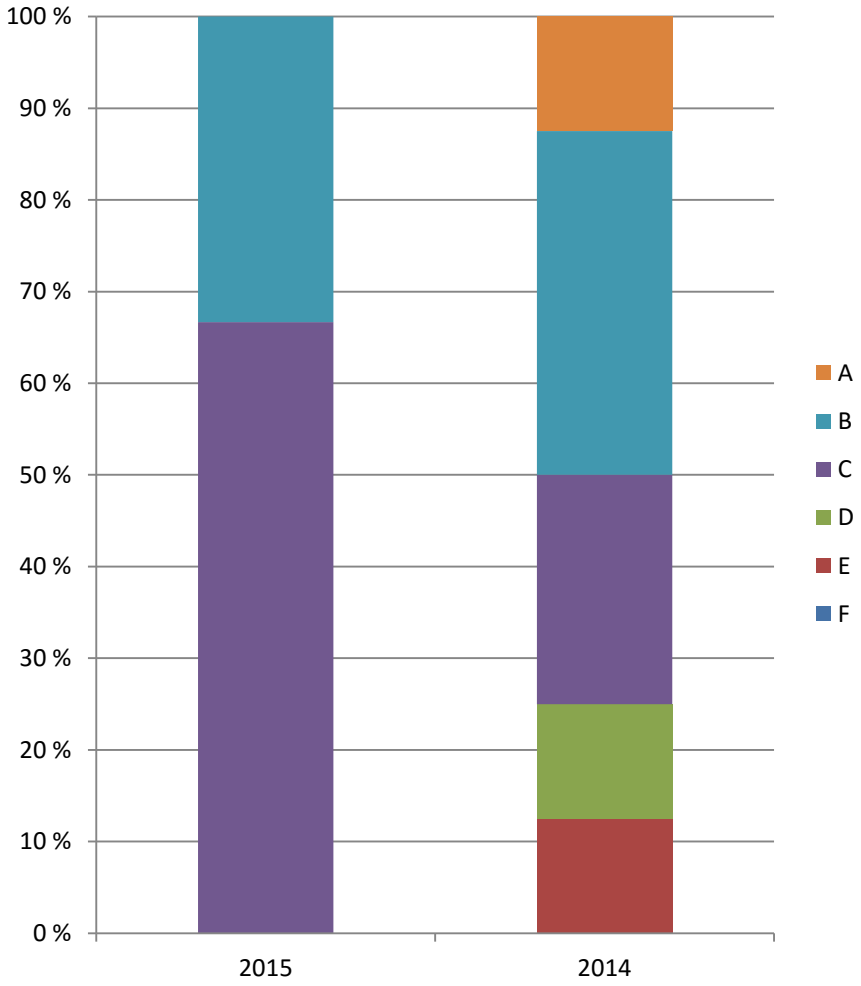
BT3120 Sjømat, styring av forsyningskjede, miljø og ressurser

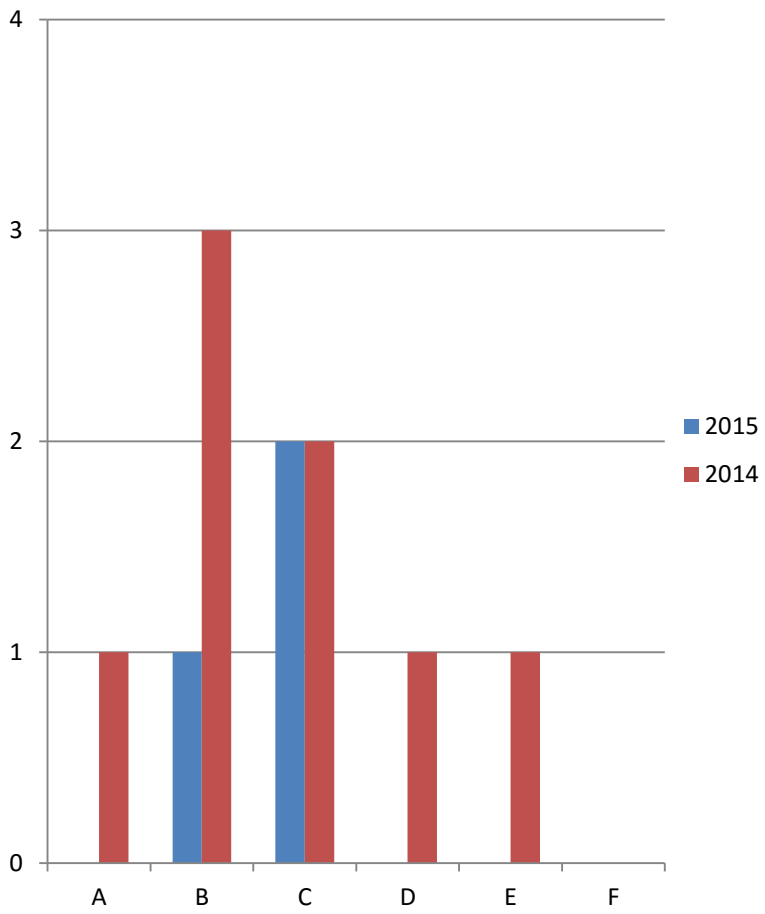
	2015	2014
MELDT	4	9
MØTT	4	8
STRYK	0	0
TRUKKET	0	0
SNITT	A	B





BT3125 Sjømat, trygghet og helseeffekter





UiT

NORGES
ARKTISKE
UNIVERSITET

ASSESSMENT GUIDELINE

For exam in: Nuclear Magnetic Resonance KJE-3303 and KJE-8303

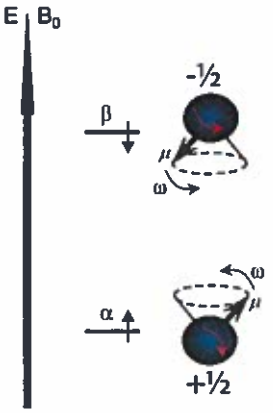
Date: Torsdag 28. May 2015

The assessment guideline contains X pages included this cover page

Contact person: Johan Isaksson

Phone: 41354726

Question 1. Theory (35 p)



$\mu = \gamma\, I\, h/2\pi$

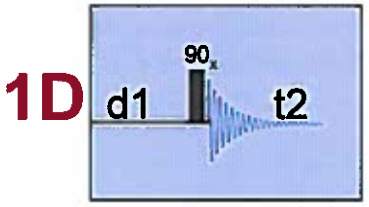
$\omega_0 = -\gamma\, B_o \qquad \nu_0 = -\gamma\, B_o/2\pi$

ω_0 = larmor frequency (rad^{-1})
γ = gyromagnetic ratio
μ = magnetic moment

$\gamma_H = +2.67 \times 10^8$ rad s^{-1} T^{-1}

1a. Above is a schematic representation of what happens when a spin ½ nuclei is put in a strong magnetic field (B_0). *Briefly* describe equilibrium, and what characterizes the energy levels. (4 p)

In a magnetic field, the spin ½ nuclei can have 2 orientations relative to the magnetic field, α and β, with slightly different energies. The difference in energy between the two levels is very small, making spontaneous emission negligible. The difference in energy corresponds to radiofrequencies. The polarization = the population difference across the transition, this is what eventually gives rise to the detectable signal.



1b. In a standard (FT) NMR experiment, we perturb the equilibrium with a short (90°) RF pulse. *Briefly* explain what happens using the vector model (at the macroscopic level), and explain what creates the NMR signal and how it is detected. (4 p)

Turning on a RF pulse of the matching frequency (on resonance) will create a moment that acts as a torque on the net magnetization of the sample. This will rotate the magnetization as long as the RF pulse is on (higher power, faster rotation). If turned off after a delay that corresponds to a 90° pulse, the net magnetization has been rotated out into the X-Y plane. After a perfect 90° pulse there is no longer any Z-magnetization (polarization or population difference), but there is a coherence between spins so that the net signal remains in the X-Y plane. The macroscopic magnetic vector rotates with the larmor frequency and creates an induction current in the receiver coil.

1c. Generally speaking, the higher the magnetic field on you spectrometer, the better spectra you get. What is improved, and why is that (give at least two)? (3 p)

1. Higher magnetic field gives bigger difference between the energy levels, which gives stronger polarization which gives more signal-to-noise

2. Higher field also leads to greater separation between peaks in Hz (because the shielding effect of the electrons have the same dependence on the field as the proton spins themselves = PPM shift is decoupled from the field)
3. For the same reason as in 2, the risk of multiplet overlap is smaller, a splitting in Hz will resonate closer to the chemical shift in PPM

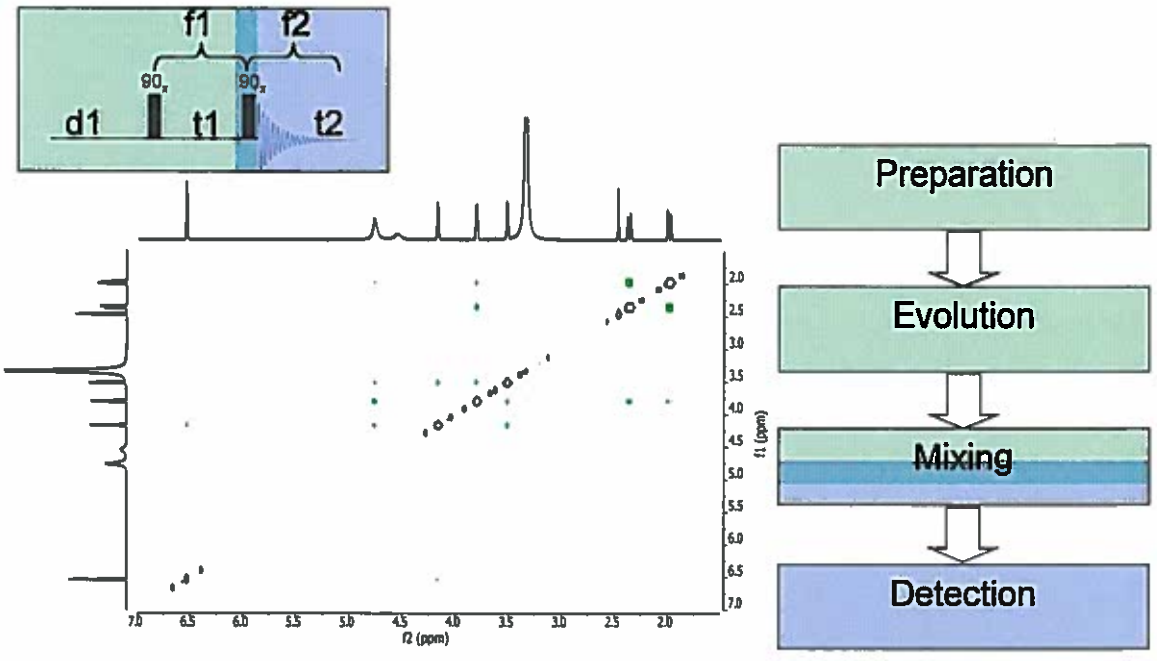
1d. Return to equilibrium is described by two relaxation processes, T_1 and T_2. *Very briefly* explain the difference between them. (4 p)

1. T1 relaxation (spin-lattice) is the enthalpic return to equilibrium (the Boltzmann distribution over the transition is restored), *i.e.* return of net magnetization on the Z-axis. Energy is emitted as tiny amounts of heat.
2. T2 relaxation (spin-spin) is the entropic loss of coherence between the X-Y components of the spins. This process is always faster than T1 (under normal circumstances). Both relaxation processes follow exponential decay with the time constant T1/T2.

1e. Why do different Hydrogen atoms in a molecule resonate at different chemical shifts? *Briefly* describe three contributing factors. (4 p)

The main factor is that protons are surrounded by moving and charged electrons who create a magnetic field opposite to the static field B0.

1. Electron density near the nucleus (e-donating/withdrawing groups, hybridization)
2. Through space shielding/deshielding from neighboring motifs (aromatic rings etc)
3. Hydrogen bonding

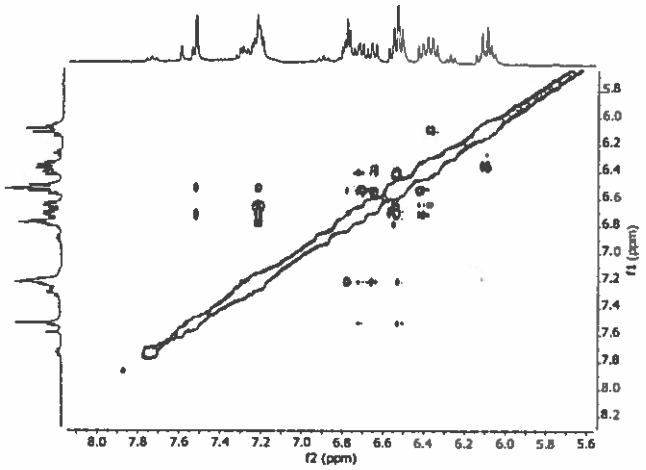


1e. Explain *briefly* how the 2D dimensions in the spectra above is constructed using the functional elements to the right. Explain *very briefly* the origin of crosspeaks (in a general form) (8 p)

2p: There is the direct dimension (f2), which is the directly detected FID, meaning: time domain t2 is fourier transformed into f2 (frequency domain). The indirect dimension (f1) is calculated from the time domain t1, which is a delay in the pulse sequence that is varied every iteration of the sequence.

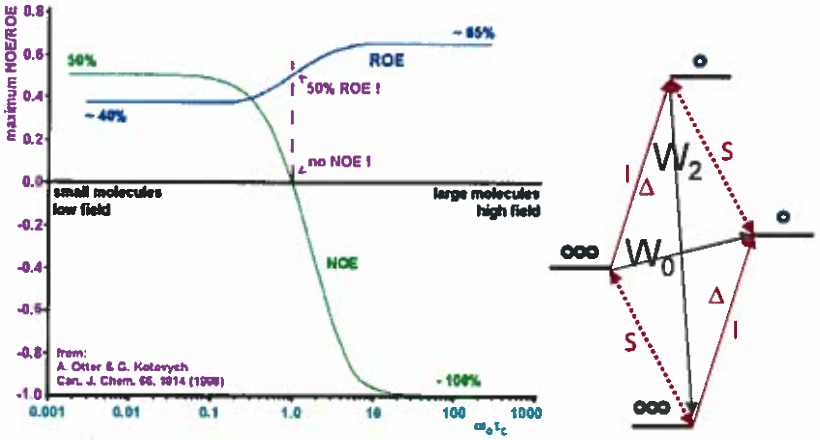
4p: The signal of every iteration is fourier transformed into a 1D spectra. The amplitude of each signal in the spectra fluctuate as a function of the t1 delay, when this is plotted versus time you get the interferogram, which resembles a FID where the signal depends on t1 instead of t2. One say that the signal has been frequency labeled during t1. The interferogram is then fourier transformed just like a normal FID into the frequency domain f1.

2p: Spins that have the same frequency during t1 and t2 give rise to diagonal peaks, spins that have changed frequency during the mixing step of the pulse sequence and thus have different frequencies during t1 and t2 give rise to crosspeaks.



1f. Above is a 2D-NOESY of an unknown molecule. Is it a small or large molecule? (2 p)

Large



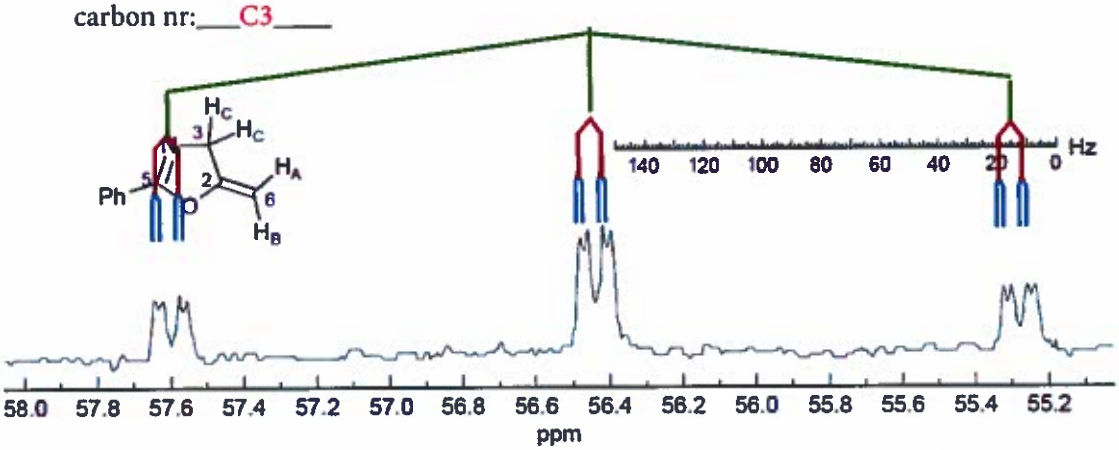
1g. Briefly motivate the answer of 1f using the figures above. (6p)

The NOE effect goes through 0 depending on which of the cross-relaxation rates dominates. W0 and W2 are "of opposite sign" because the restore population on opposite signs of the observed transition, and for large molecules W0 dominates. This leads to a negative NOE, which in turn gives a crosspeak in a NOESY spectra that is of the same sign as the diagonal peak. In the figure above, the molecule must have a correlation time so that $\omega_0\tau_c$ is on the right side of the point where the NOE goes through 0, and in this respect we call that a large molecule.

Question 2. 1D NMR (15 p)

2a. This is a non-decoupled ^{13}C spectra of an oxazoline, which carbon are we looking at? (2p)

carbon nr:___C3____



2b. Report the carbon multiplet (example: dd, J= x, y Hz) as well as the three coupling constants you can measure in the spectrum above in the standard format ($^{n}J_{CiHj}$ where n is the number of bonds, i and j are the atom id numbers in the structure above). Draw the coupling trees in the figure above. (5p)

Multiplet.__tdd, J = 146, 8, 3 Hz___

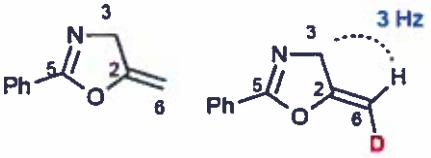
1.__$^{1}J_{C3HC}$ = 146 Hz_____ (or $^{1}J_{CH}$ = 146 Hz)

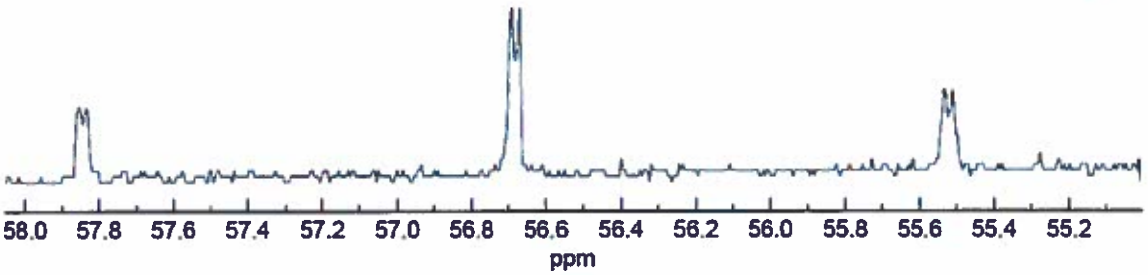
2.__$^{3}J_{C3HB}$ = 8 Hz _____ (or $^{3}J_{CH\ (trans)}$= 8 Hz)

3.__$^{3}J_{C3HA}$ = 3 Hz _____ (or $^{3}J_{CH\ (cis)}$= 3 Hz)

2c. This is the same compound where one H has been replaced by a D (deuterium, ^{2}H). Which one? Draw it on the structure below. (Hint: Couplings to deuterium is much weaker than couplings to protons) (2p)

The large *trans* coupling has disappeared and been replaced by a weak ~1 Hz coupling to deuterium, not resolved in this spectra

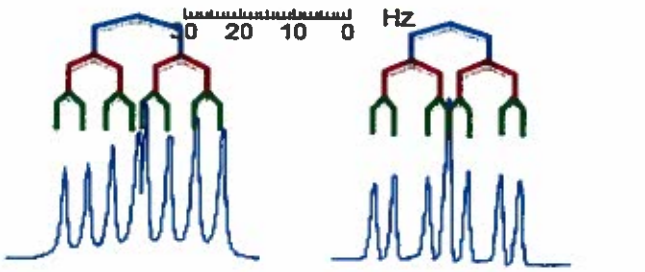




2d. You have the Hz and PPM scales in the figure (a) above, what is the approximate frequency of the spectrometer for ^{13}C and ^{1}H used in the example above? Remember that you are observing a carbon spectrum. (2p) 1 PPM = 125 Hz

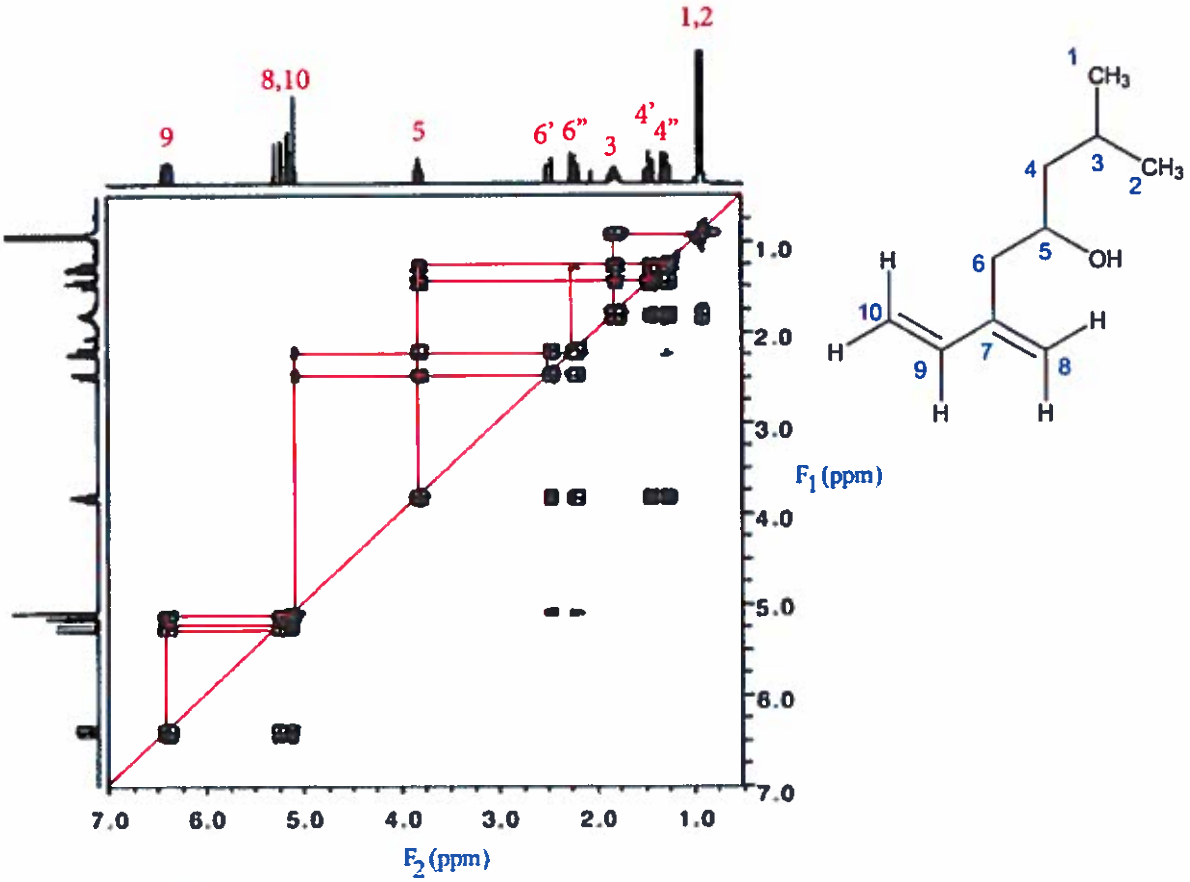
^{13}C frequency ~__125__ MHz
^{1}H frequency ~__500__ MHz

2e. Analyze the coupling patterns in the following multiplets and report them using the attached Hz scale (4p)

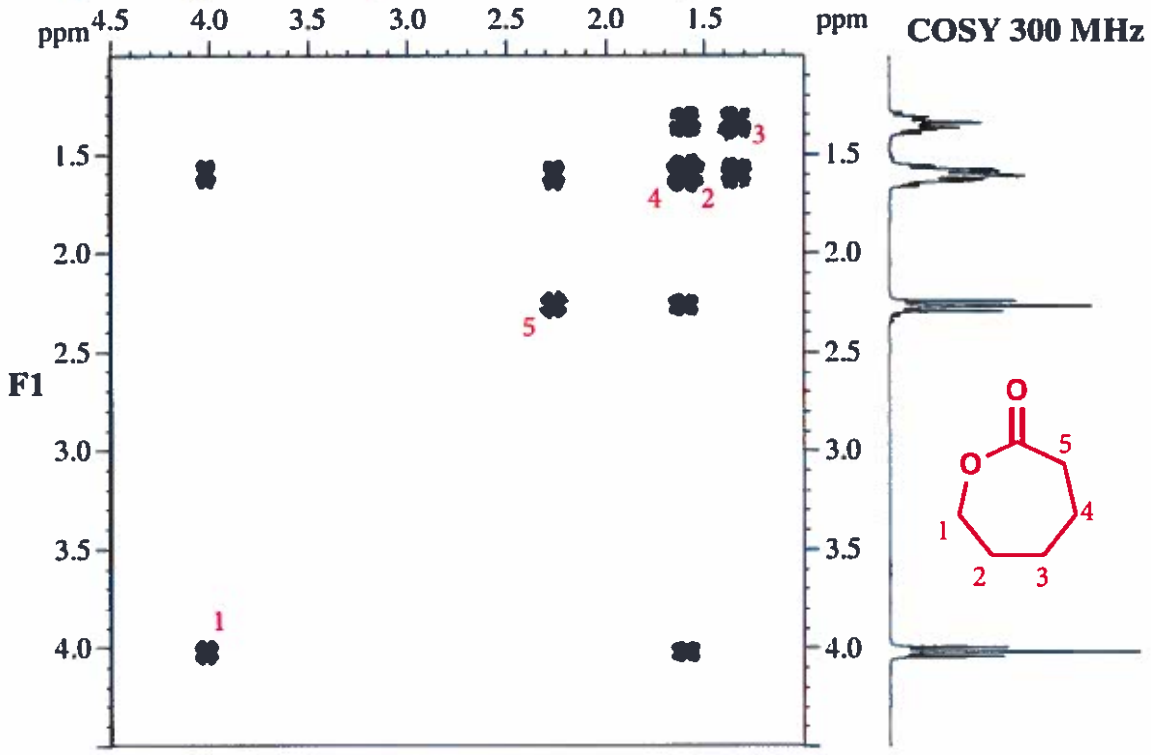


1H, ddd, *J*=16, 9, 4.5 Hz 1H, ddd, *J*=13.5, 10, 4 Hz

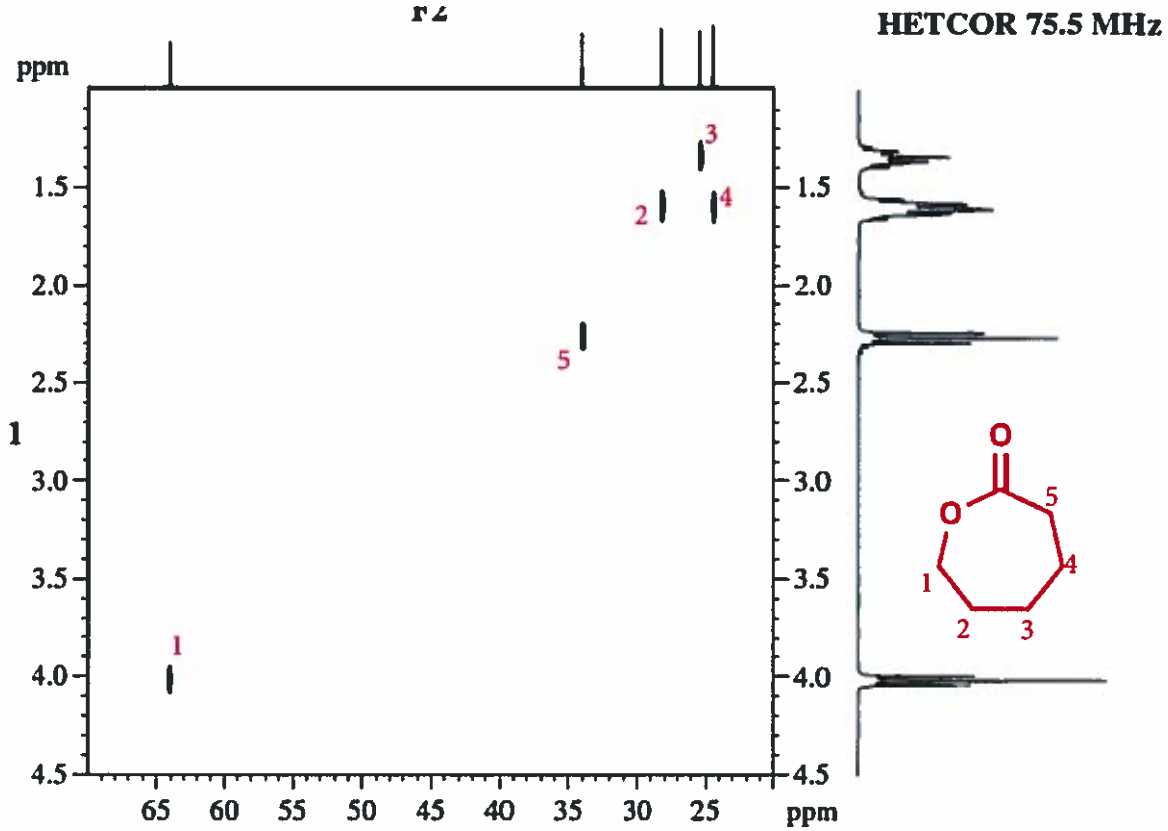
Question 3 – KJE-3303. 2D NMR (25 p)



3a. Assign all denoted protons (the overlapping protons at 0.8 and 5.1 ppm don't need to be individually assigned but note which ones are there). (15 p)



3b. Assign the CH_2 protons (5 p)

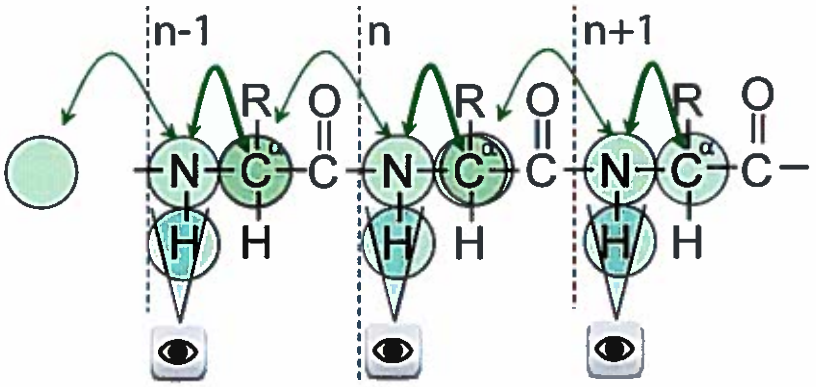


3c. Assign the CH_2 carbons (note that this is a HETCOR, pay attention to the axis', f1=^{1}H, f2=^{13}C) (5p)

Question 3 – KJE-8303. Protein NMR (25 p)

3a. Triple resonance spectra (3D ^{1}H, ^{15}N, ^{13}C correlated spectra) are central in protein backbone assignment by NMR. Describe in a general fashion what these experiments do and how this type of information is used to find the sequential backbone assignment. Draw a schematic Figure of the used correlations. (Some key words: HNCA, HN(CO)CA, HNCO, HN(CA)CO, HNCACB, slices, inter/intra-residue correlations, traces.) (15 p)

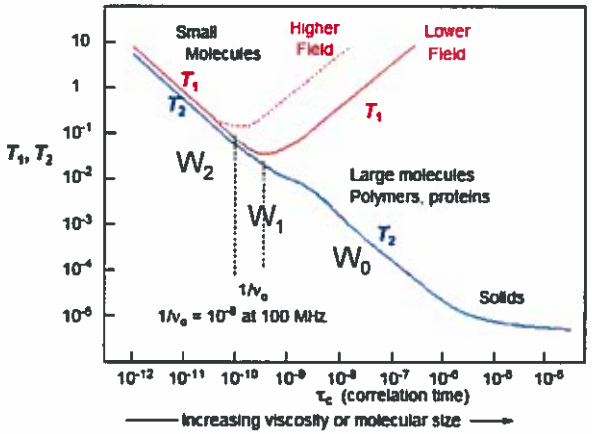
1. Triple resonance spectra are 3D experiments that specifically correlates the $^{15}N,^{1}H$-HSQC of the protein backbone with one or several near carbons atoms, either intra-residue or inter-residue, or both.
2. From carbon slices in the given experiments, for each HN, CA, CA(n-1), CO, CO(n-1), CB(n), CB(n-1) can be assigned
3. These shifts (slices) can then be matched pairwise to find sequence patches of neighboring residues
4. Sequences are fit to the protein sequence using database shifts (not required, was not emphasized in lectures)

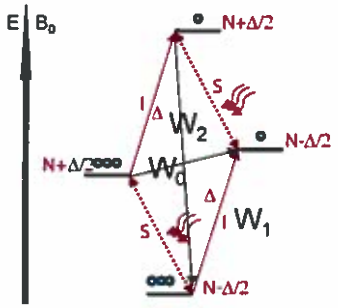


3b. Describe what Chemical Shift Perturbation (CSP) is and how that can be used in protein detected screening. What is the benefit compared to other conventional screening methods? What is the drawback? (5p)

CSP is when you monitor how much the different chemical shifts (H, N, C, CA, CB or other atoms) of each protein residue shifts when an inhibitor/fragment/co-factor/metal/pH is added to the original protein. This gives a rough picture of which residues are most affected by binding and indirectly where the interaction takes place.

Benefit: Simultaneous information about binding and location
Drawback: Requires known assignment, at least 15N labelled sample, not really a high throughput technique (though cocktails can be screened)





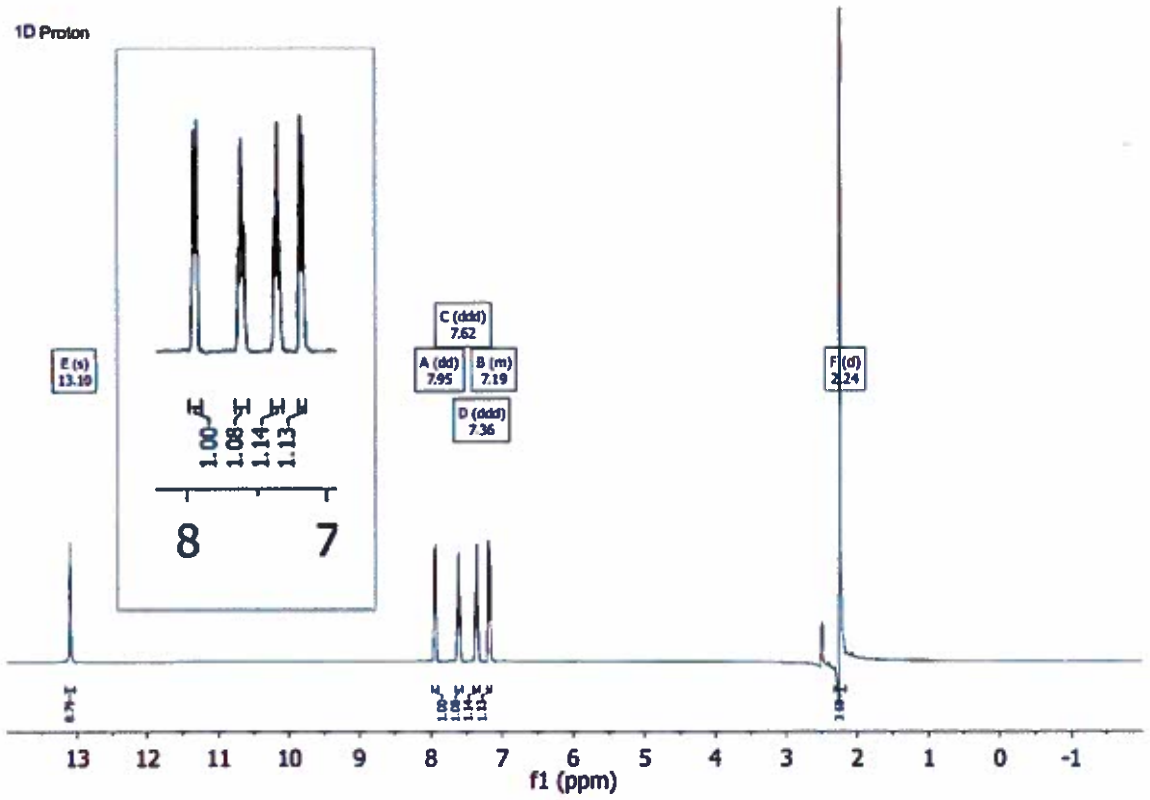
3c. Use the figure above to *very briefly* explain why Protein size is important for the quality of the NMR data you can acquire. You can also state other reasons. (3p)

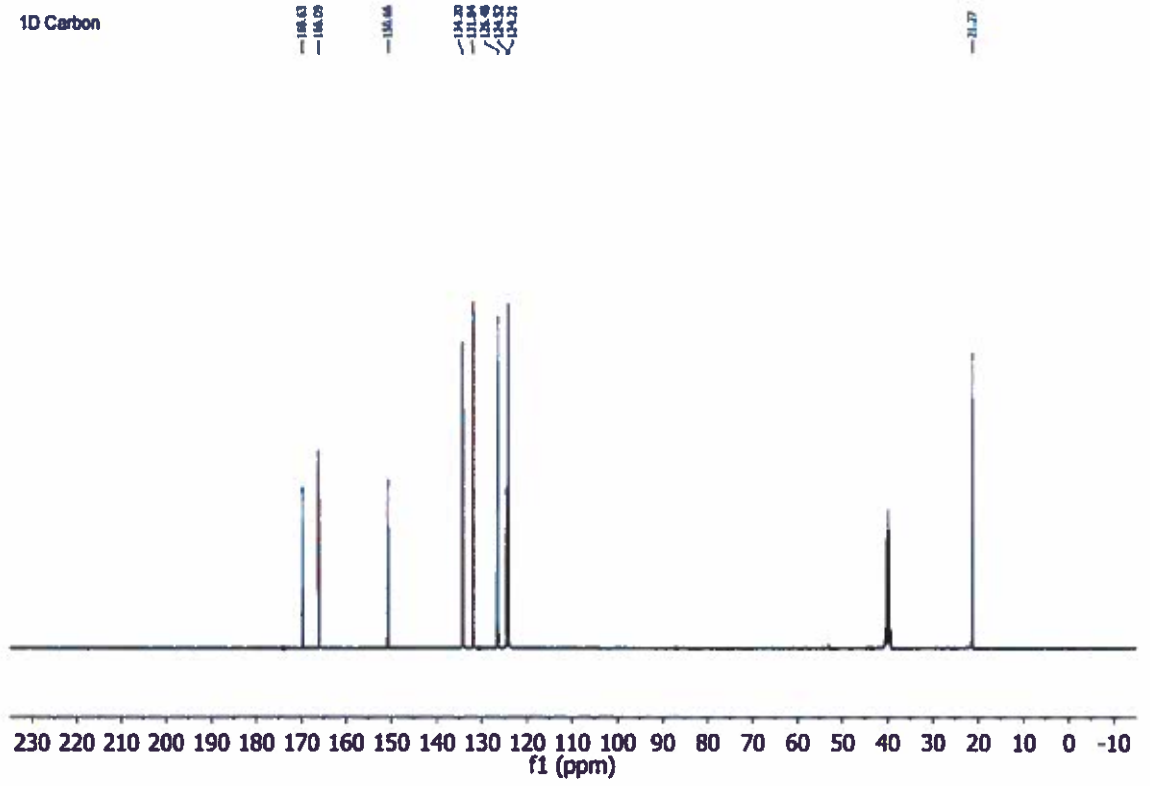
1. Spectral overlap increases with protein size (not required)
2. The larger the protein, the faster the R_2 relaxation rate because the W_0 rate becomes more and more effective the slower the protein tumbles (long τ_c). This gives severe line broadening and loss of signal during the pulse sequence.
3. Longer T_1 also affects how quickly you can pulse because it takes longer to recover magnetization (not required)

3d. Name at least two techniques/tricks used to improve the spectral quality. (2p)

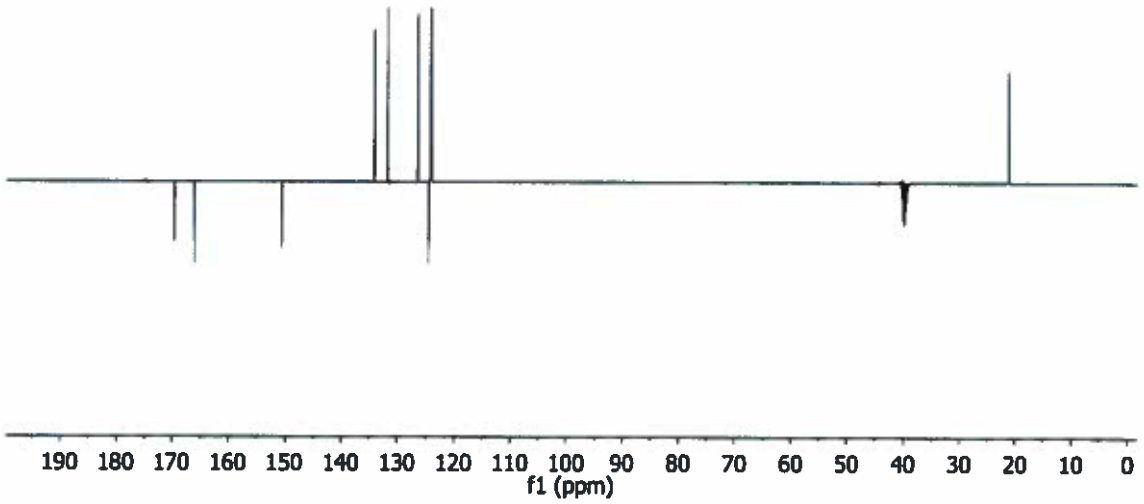
1. Partial or full deuteration reduces cross-relaxation (because of the much lower gyromagnetic ratio of ^2H, not required)
2. Use of TROSY experiments (selection of component where dipole-dipole- and CSA relaxation rates cancels out and result in slower effective relaxation rates, not required)
3. Higher field gives better resolution (could be accepted)

Question 4. 2D NMR (25 p)

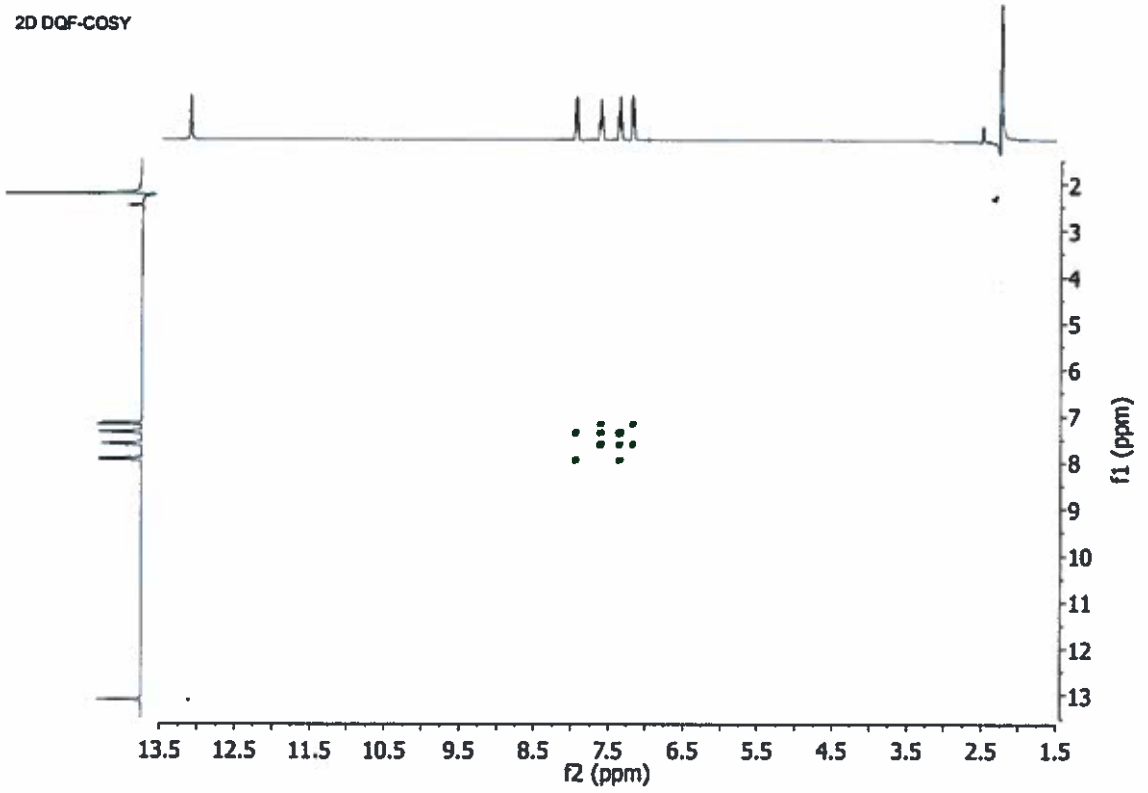


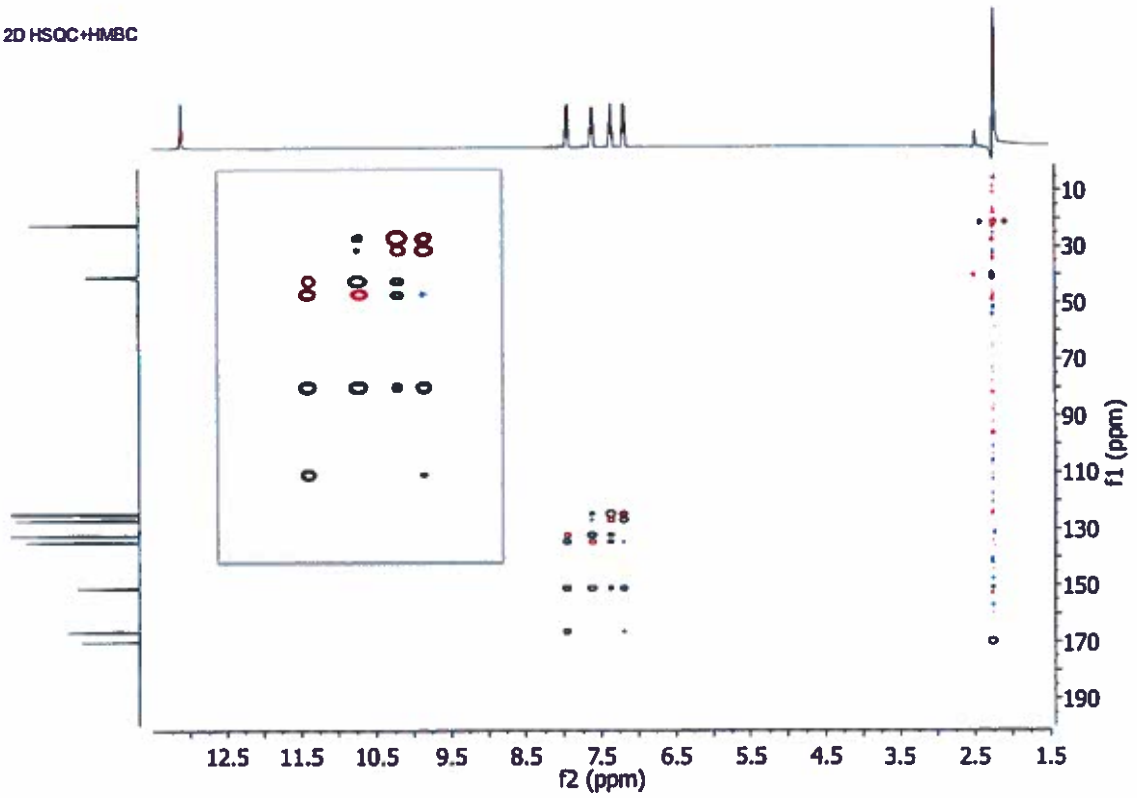


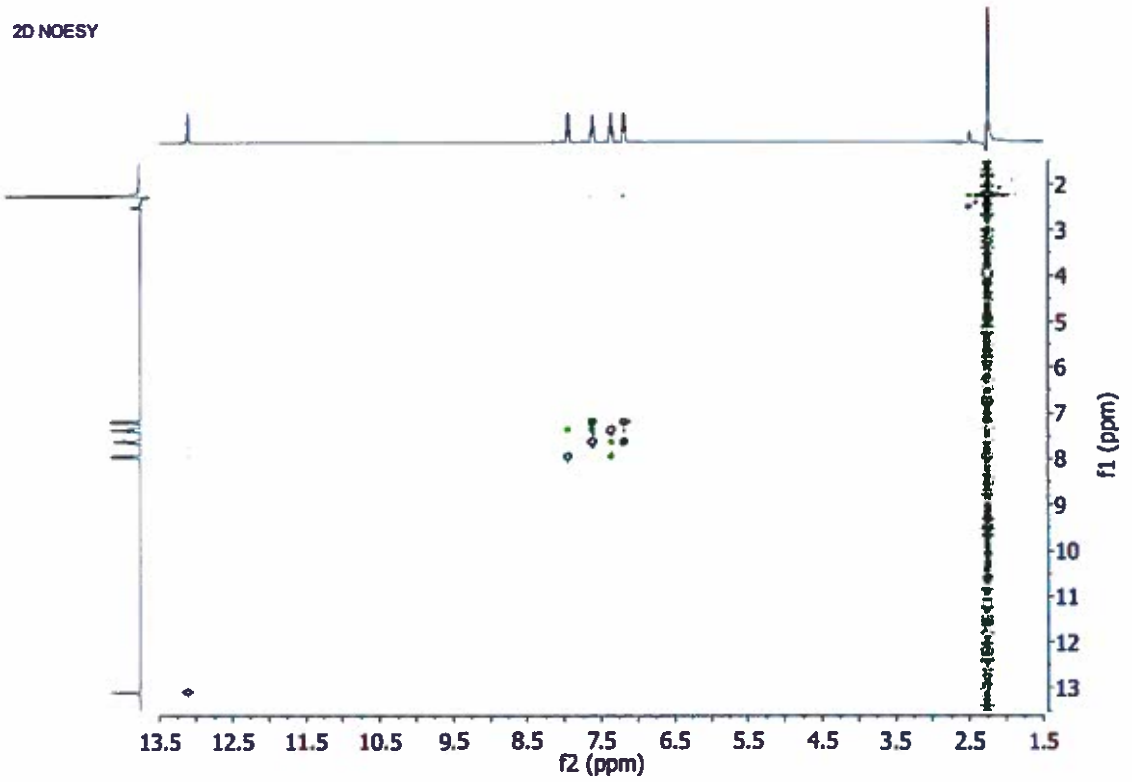
1D Apt



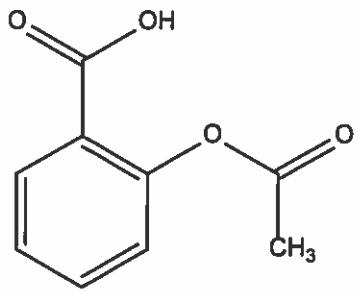
2D DQF-COSY



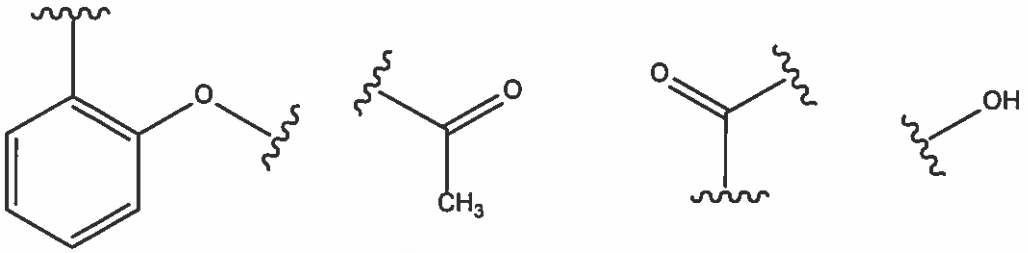




4a. The spectra above are for an unknown molecule with the molecular formula: $C_9H_8O_4$. Elucidate the structure and report the ^1H and ^{13}C assignments in the HSQC+HMBC. (21p)



Chemical Formula: $C_9H_8O_4$
Exact Mass: 180,04



Fragments you can identify. The di-substituted ring spotted from splitting pattern and couplings, the COCH3 from chemical shifts and absence of long range couplings, one carbonyl attached to the ring. The –O attached to the ring can be spotted in the HMBC from the carbon shift and the –OH needs to be attached after excluding all other options.

4b. One of the aromatic-aromatic crosspeaks in the NOESY spectra looks a bit strange, why is that? (2p) Zero quantum coherence, anti-phase character, when strongly coupled and little separated

4c. The HSQC peak at 2.3/20 PPM has one dot on each side of it in the HMBC spectra. What is that and where does it come from? It's a $^1J_{CH}$ (HMQC) artifact doublet that was not filtered away by the HMBC sequence

Good luck!

Johan

UiT

NORGES
ARKTISKE
UNIVERSITET

ASSESSMENT GUIDELINE

For exam in: Nuclear Magnetic Resonance KJE-3303 and KJE-8303

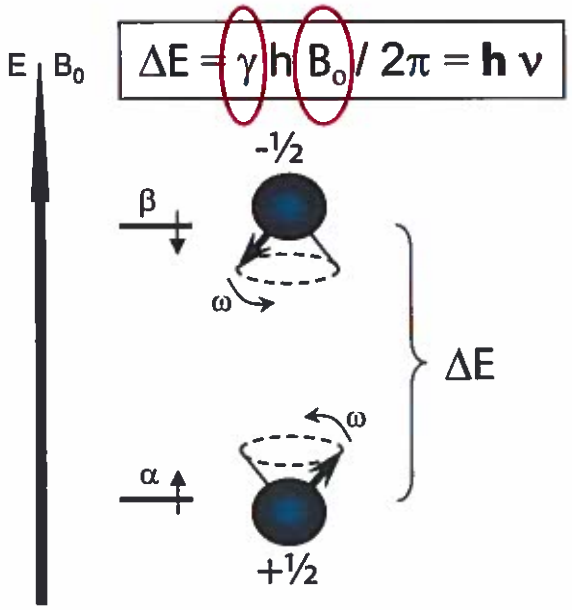
Date: Torsdag 21. September 2015

The assessment guideline contains X pages included this cover page

Contact person: Johan Isaksson

Phone: 41354726

Question 1. Theory (30 p)



$$\frac{N_2}{N_1} = \exp\left(\frac{-\Delta E}{kT}\right)$$

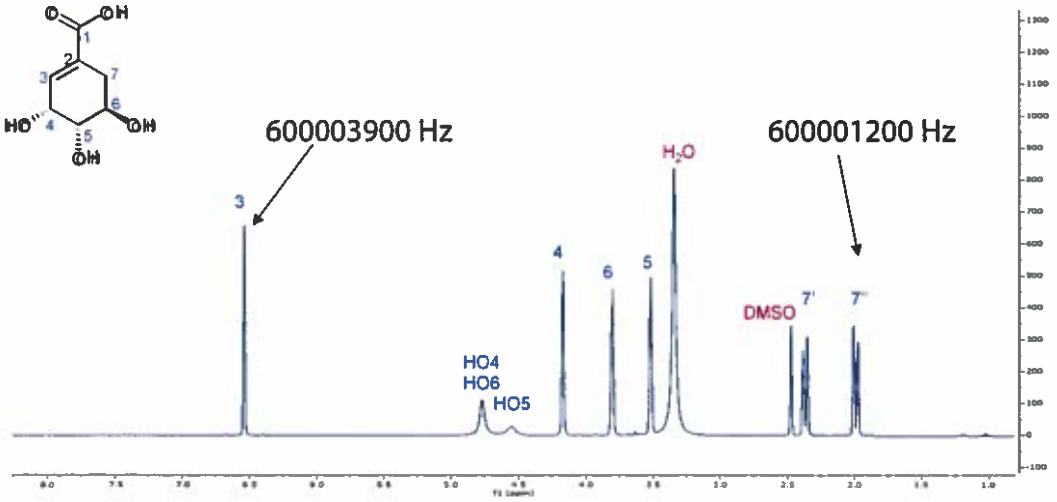
1a. Above is a schematic representation of what happens when a spin ½ nuclei is put in a strong magnetic field (B_0). *Briefly* describe what sample polarization means and how that relates to sensitivity. (4 p)

The difference in energy between the two levels is very small, corresponding to radiofrequencies. The polarization = the population difference across the transition due to the Boltzman distribution, this is what eventually gives rise to the detectable signal. The larger the energy difference between α and β, the larger the population differences and the larger the detectable signal.

1b. How is the sensitivity affected by the encircled factors in the equations above? (6 p)

i. Gyromagnetic ratio, compare for example ^{13}C with ^{1}H
ii. Static magnetic field strength, compare for example a 400 MHz and a 600 MHz NMR
iii. Temperature, compare for example room temperature to a hypothetical super-cooled sample

i. Higher gyromagnetic ratio (^{1}H) gives higher polarization and better sensitivity
ii. Higher field strength gives higher polarization and better sensitivity
iii. Lower temperature gives higher polarization and better sensitivity

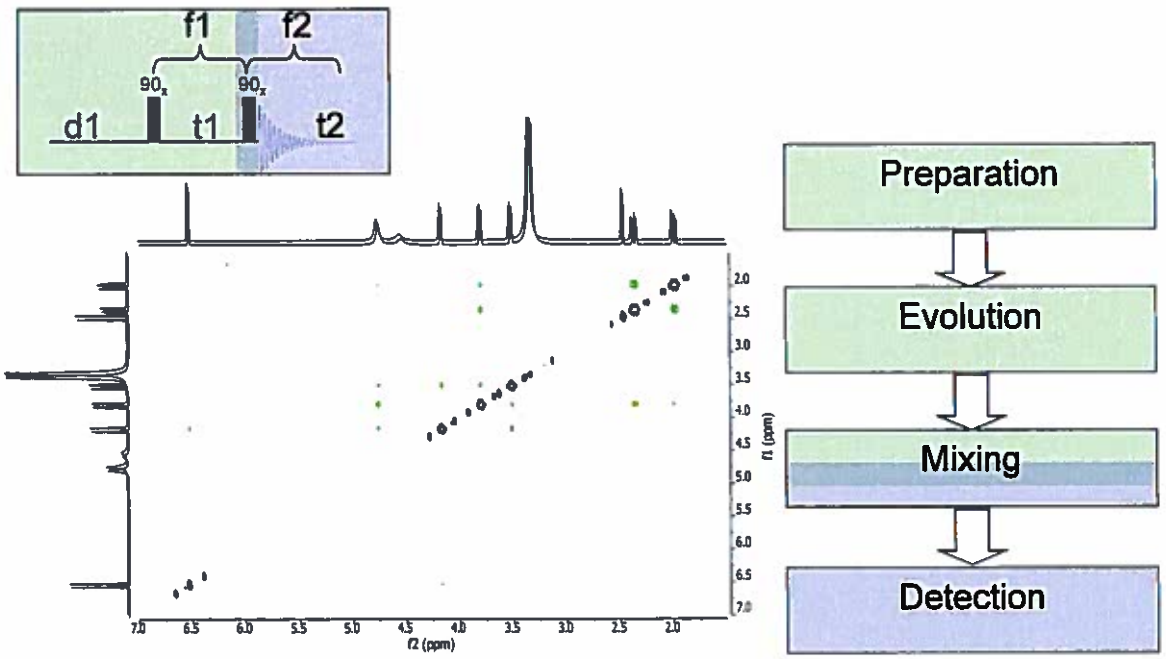


1c. What is chemical shift of protons? Briefly explain why different protons in a molecule have different chemical shifts and three factors that greatly affect the observed chemical shift. (6 p)

Protons are surrounded by moving charges (electrons) which create a magnetic field opposed to the static field. The effective magnetic field strength at the nucleus is, $B = B_0 - B_e$. and the larmor frequency is $\omega_0 = \gamma B/2\pi$ (equations not required). The chemical shift is mainly affected by i) electron density at the nucleus, ii) through space shielding/deshielding effects and iii) hydrogen bonding.

1d. Draw in the figure above, what is upfield and downfield, which part of the spectra is shielded, which is deshielded and which part resonates at higher larmor frequency and which resonates at lower larmor frequency. (6 p)

← downfield, deshielded, higher larmor frequency
→ upfield, shielded, lower larmor frequency



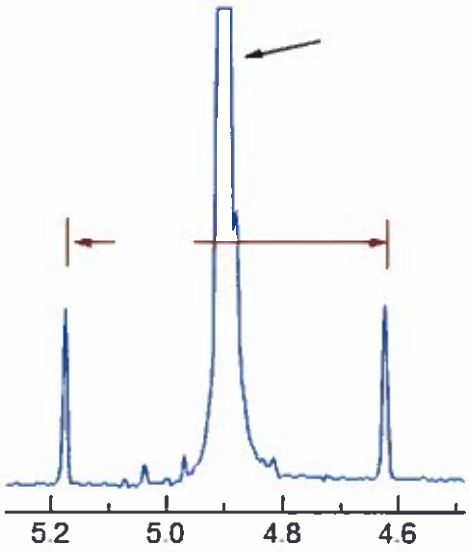
1e. Explain *briefly* how the 2D dimensions in the spectra above is constructed using the functional elements to the right. Explain *very briefly* the origin of crosspeaks (in a general form) (8 p)

2p: There is the direct dimension (f2), which is the directly detected FID, meaning: time domain t2 is fourier transformed into f2 (frequency domain). The indirect dimension (f1) is calculated from the time domain t1, which is a delay in the pulse sequence that is varied every iteration of the sequence.

4p: The signal of every iteration is fourier transformed into a 1D spectra. The amplitude of each signal in the spectra fluctuate as a function of the t1 delay, when this is plotted versus time you get the interferogram, which resembles a FID where the signal depends on t1 instead of t2. One say that the signal has been frequency labeled during t1. The interferogram is then fourier transformed just like a normal FID into the frequency domain f1.

2p: Spins that have the same frequency during t1 and t2 give rise to diagonal peaks, spins that have changed frequency during the mixing step of the pulse sequence and thus have different frequencies during t1 and t2 give rise to crosspeaks.

Question 2. 1D NMR (20 p)

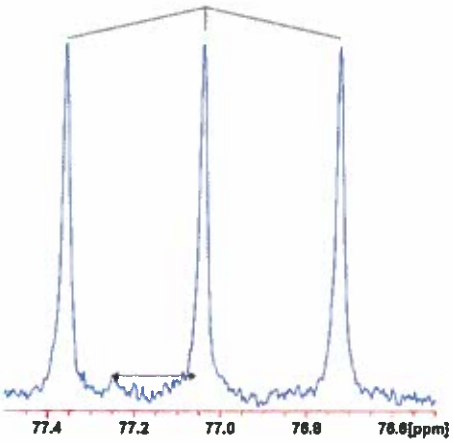


2a. This is a singlet -CH peak in a ^{1}H spectra of a non-labelled compound (natural abundance).

i. There are two small peaks around the main peak, where do they come from and what are they called? (3p)

ii. Denote the coupling in the figure (1p)

Carbon satellites, arise from the protons being coupled to ^{13}C (~1%) and not ^{12}C (~99%), producing a small ^{13}C-coupled doublet around the ^{12}C-bonded singlet. The coupling is the $^{1}J_{CH}$ coupling.



2b. The spectra above is a proton-decoupled Carbon spectra of the solvent peak of a sample acquired in $CDCl_3$.

i. Why do we see a 1-1-1 triplet? Denote the coupling it in the figure (4p)

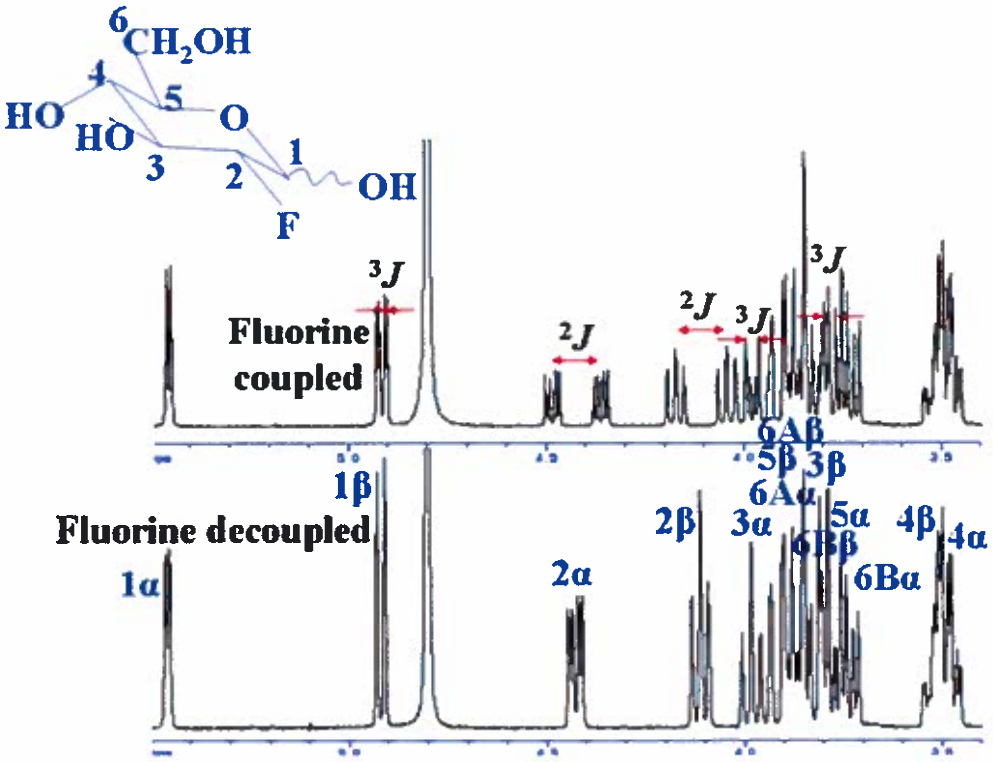
ii. What is the small singlet at 77.25 ppm? (1p)

iii. Any idea why the small singlet does not overlap with the triplet? (1p)

The coupling is denoted $^1J_{CD}$, and the triplet arise from the one bond coupling to deuterium. Deuterium is a spin=1 nuclei, and can have 3 orientations in a magnetic field instead of the 2 orientations for a spin=1/2 nuclei (with nearly the same energy), therefore resulting in a 1-1-1 triplet instead of a 1-1 doublet.

The small peak comes from the ~0.2% non-deuterated $CHCl_3$ in the deuterated solvent.

(difficult) The offset is the isotope shift, coming from if the carbon is connected to a H or a D.

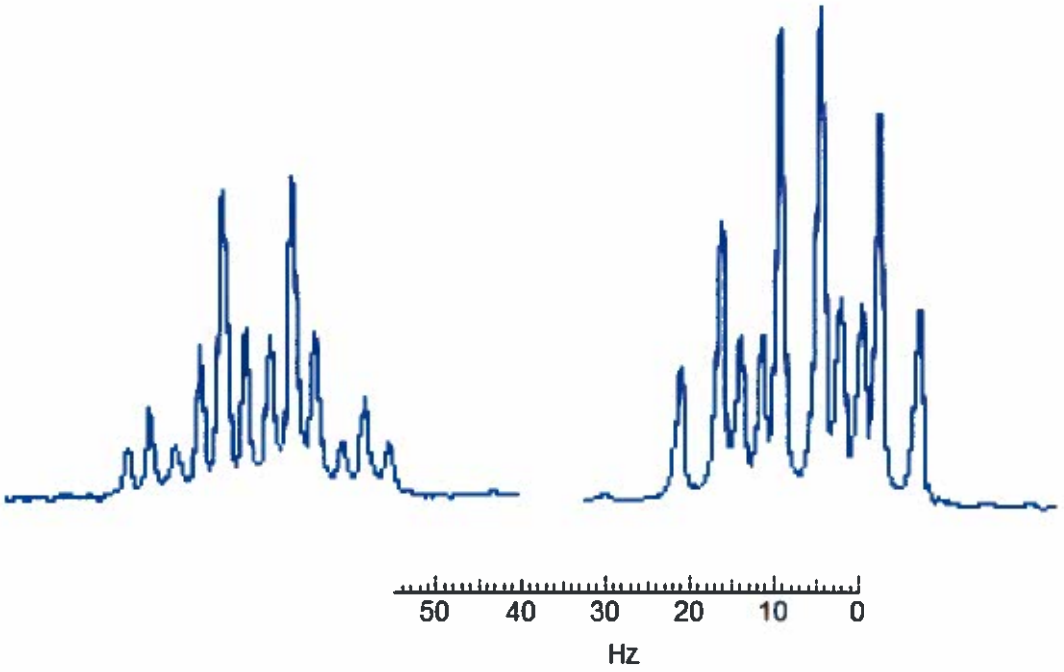


2c. The figure above shows two proton spectra of a 50:50 mixture of two OH-isomers (1-OH *R* and 1-OH *S*) of 2-fluoro-2-deoxy-glucose. The top spectra is a normal proton, and the bottom spectra is a Fluorine decoupled Proton spectra.

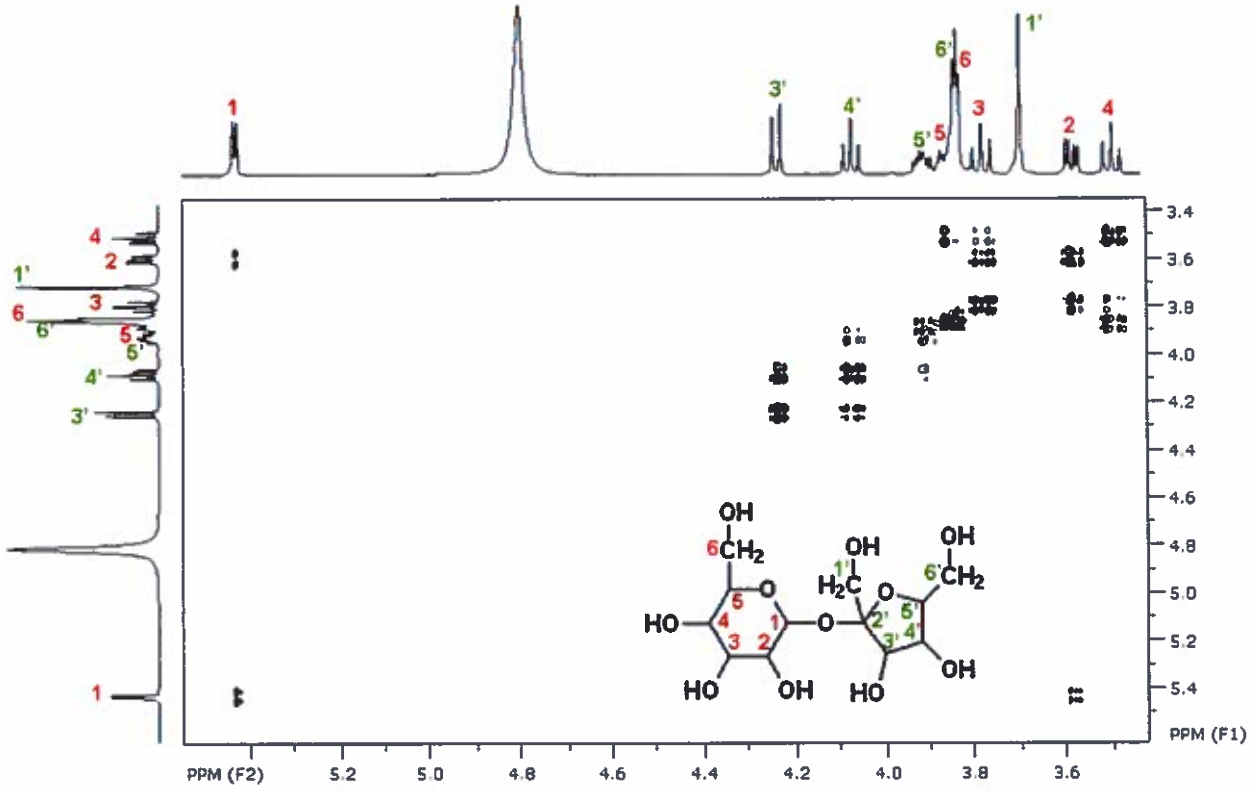
i. What is the meaning of a "fluorine decoupled proton" spectra? (2p)
ii. In the lower spectra, assign proton 2-H based on its coupling to the fluorine 2-F. Remember that since this is a mixture of two isomers, there will be two resonances belonging to 2-H, you can denote them 2α-H and 2β-H (we cannot know which one is which). (2p)
iii. In the top spectra, draw the $^2J_{FH}$ (2p)

Fluorine decoupled: fluorine frequency is saturated during acquisition, thereby collapsing the proton to fluorine coupling.

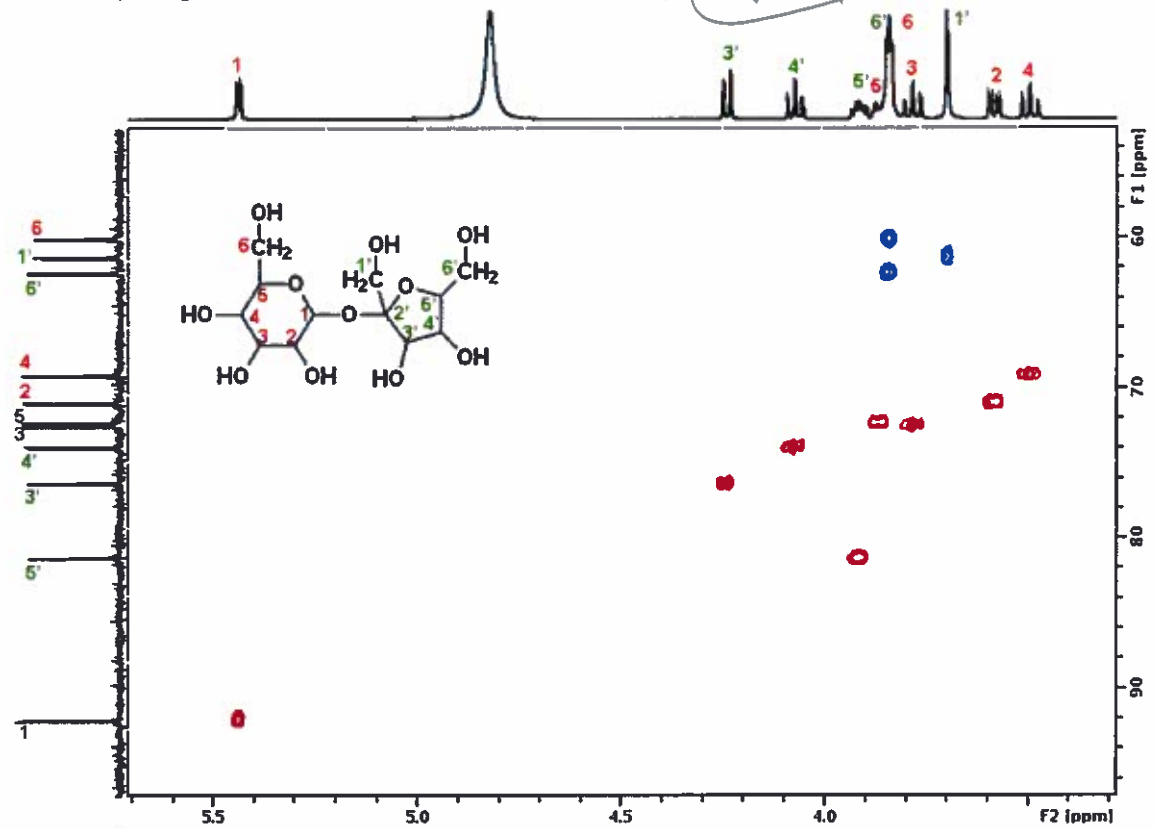
2d. Analyze the coupling patterns in the following multiplets and report them using the attached Hz scale (4p)



Question 3 – KJE-3303. 2D NMR (25 p)

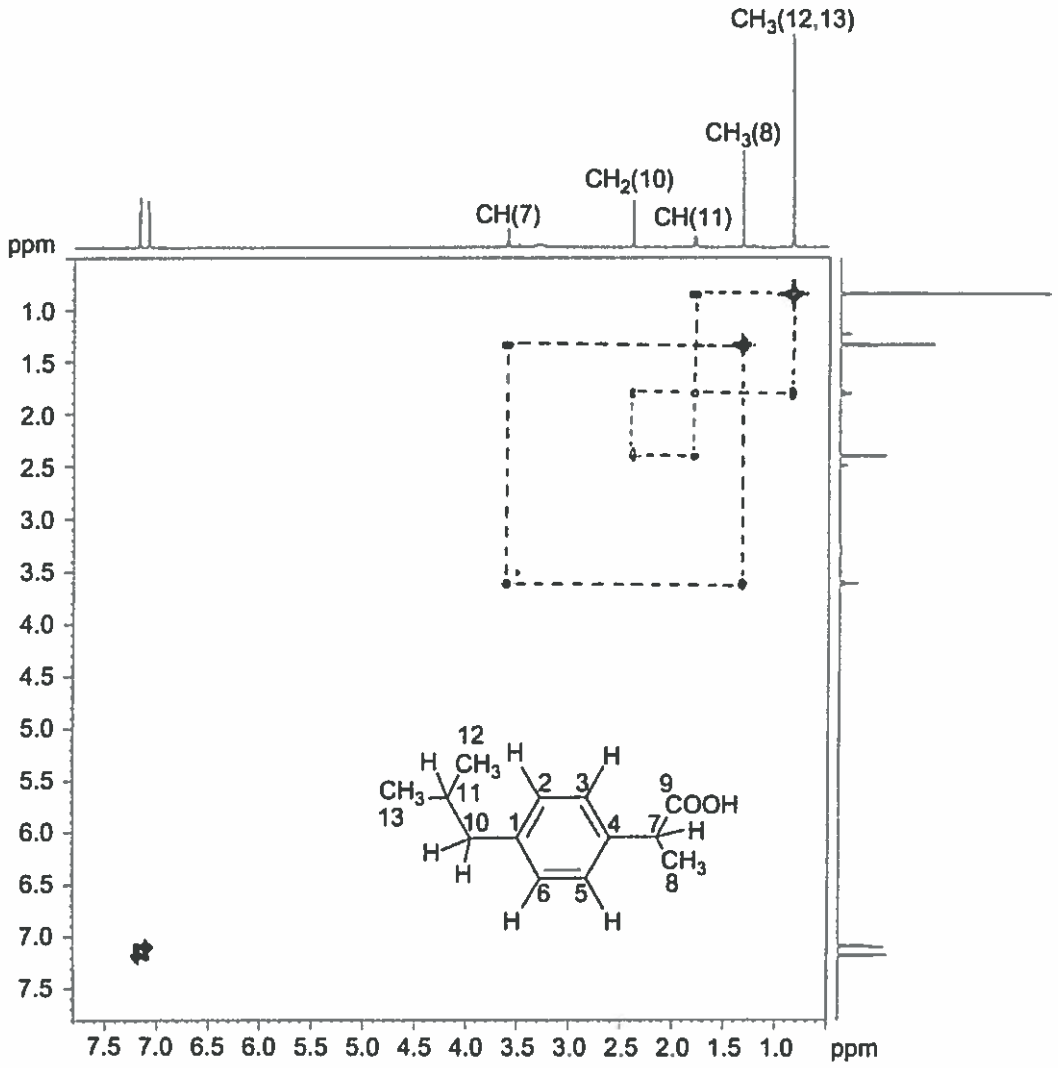


3a. Assign all denoted protons (the overlapping protons at 3.9 ppm don't need to be individually assigned but note which ones are there). (15 p) 4-5p



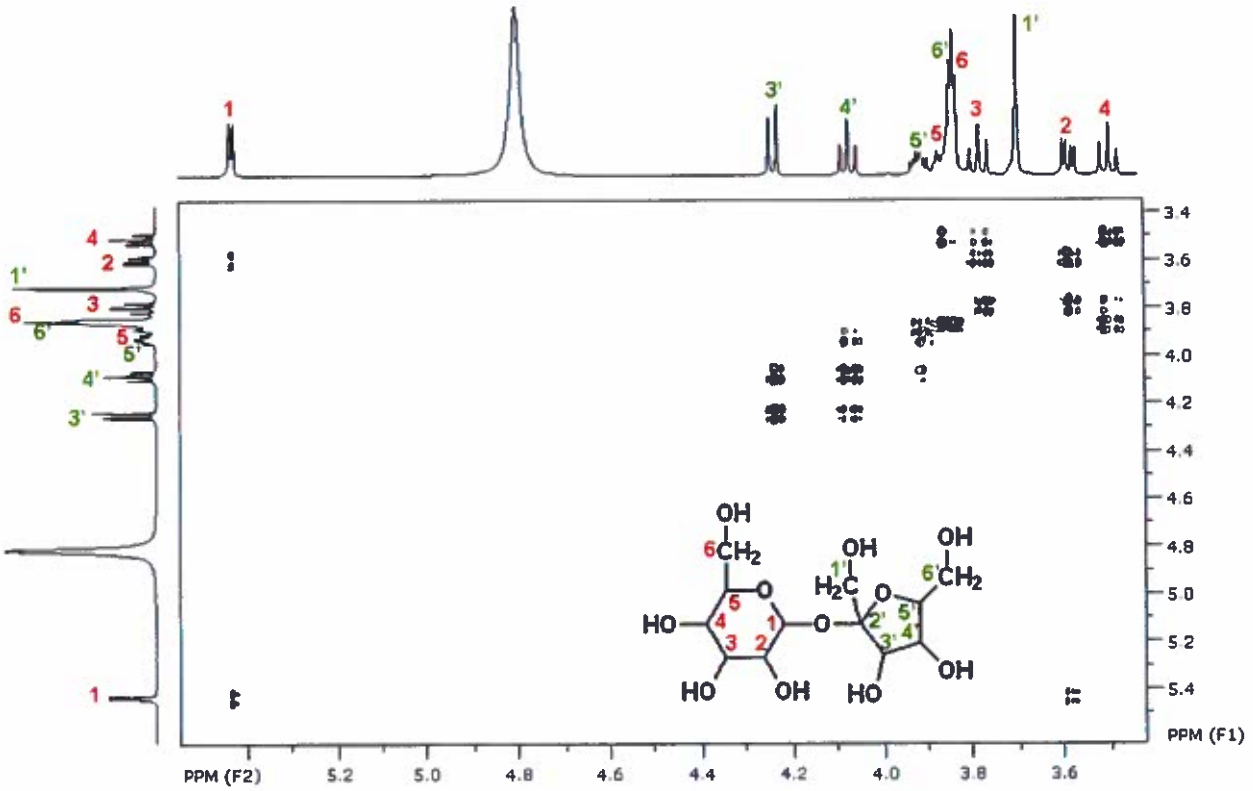
3b. Assign the carbons (5p)

1p



3c. Assign the non-aromatic protons (5 p)

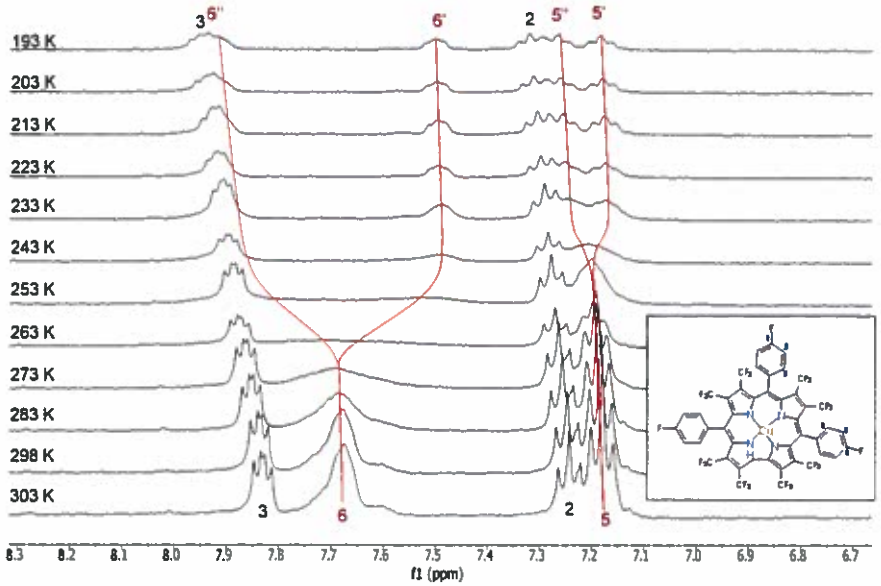
Question 3 – KJE-8303. 2D and Protein NMR (25 p)



3a. Assign all denoted protons (the overlapping protons at 3.9 ppm don't need to be individually assigned but note which ones are there). (15 p)

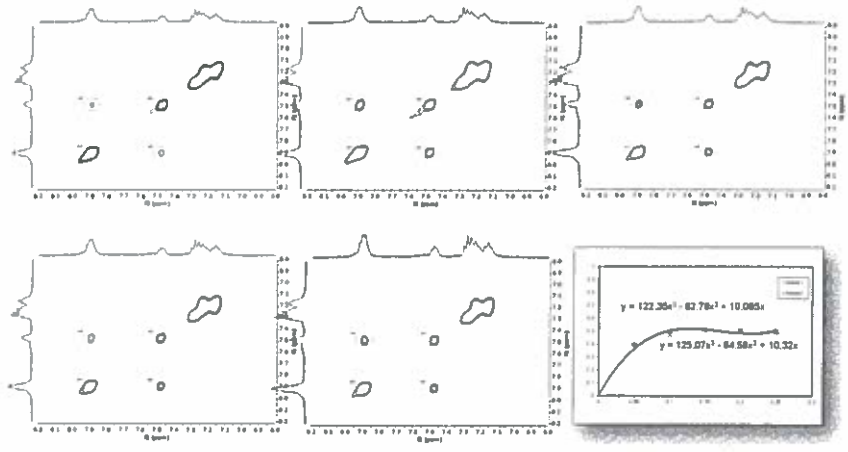
3b. List 3 types of NMR data that provide structural information, and which information you get from each experiment (very briefly)? (3p)

NOEs->distances, scalar couplings->dihedrals, RDCs->(long distance) relative angles + allowed: Chemical shifts->dihedrals, relaxation mapping->distance from label, exchange mapping->solvent exposure



3c. The figure above shows the temperature dependence of the proton spectra of the copper complex in the right corner (note about the molecule: it has a twisted conformation, and therefore not flat and symmetric – the 6' and 6" denote the two orto protons of the para-substituted fluoro-phenyls, the 5' and 5" denote the meta protons of the same ring). What can be the underlying mechanism that can make a doublet at low temperature collapse into a singlet at high temperature? (3p)

There is conformational exchange going on in the molecule (slow phenyl ring rotation). At low temperature the residence time of each conformation is long enough to be individually detected during acquisition, thus 6' and 6" give one peak each (corresponding to the proton being above or below the plane of the macrocycle). As temperature is increased, the two states interconvert quicker and finally coalesce into the average singlet in the time scale of NMR acquisition.



3d. Above you can see ROESY spectra with 5 different mixing times of the 6" and 6' protons of the same copper complex at 233 K. The graph shows crosspeak volume vs mixing time.

i. How can you tell from these spectra what kind of phenomenon we are observing? (2p)
ii. What information can you get out by integrating the crosspeaks? (1p)

iii. Can you extract themodynamics from this data? (1p)

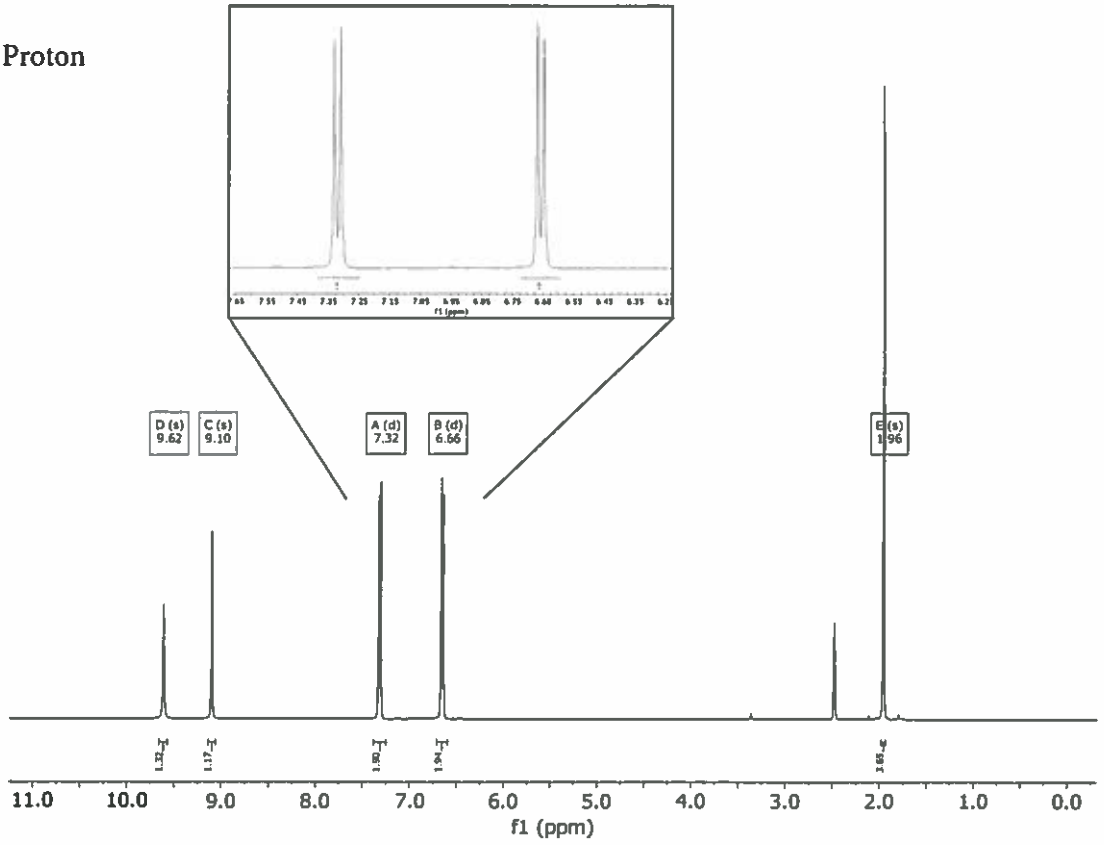
The crosspeaks being the same sign as the diagonal peaks means that we are observing a exchange process, it can be a chemical or conformational exchange. In this case we see the phenyl ring rotations. In a ROESY, cross-relaxation always produce crosspeaks with a sign opposite to the diagonal peaks (ROE is always positive), so true ROE peaks would have the opposite sign.

The initial buildup of the crosspeak is directly proportional to the rate constant of the exchange process. By plotting the curve we can determine the rate (= the slope at time 0)

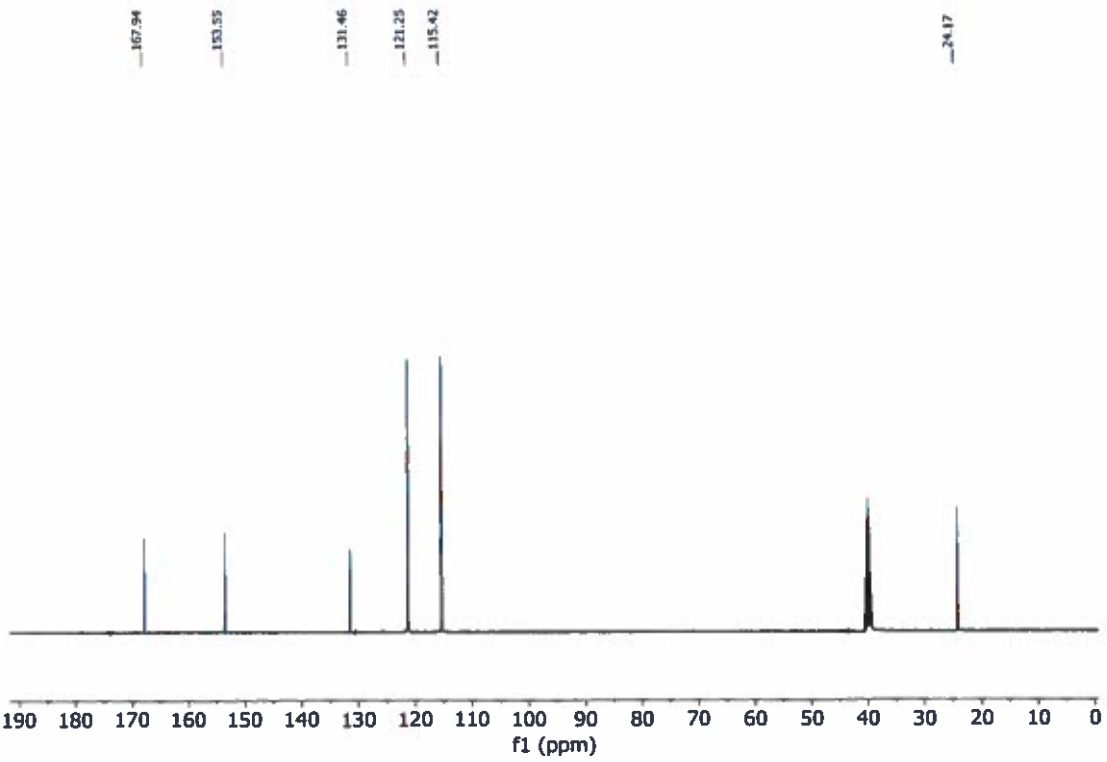
Yes, by calculating the rate at several temperatures (we can calculate energy of activation, ΔH, ΔS and ΔG of activation from Arrhenius/Eyring plots).

Question 4. 2D NMR (25 p)

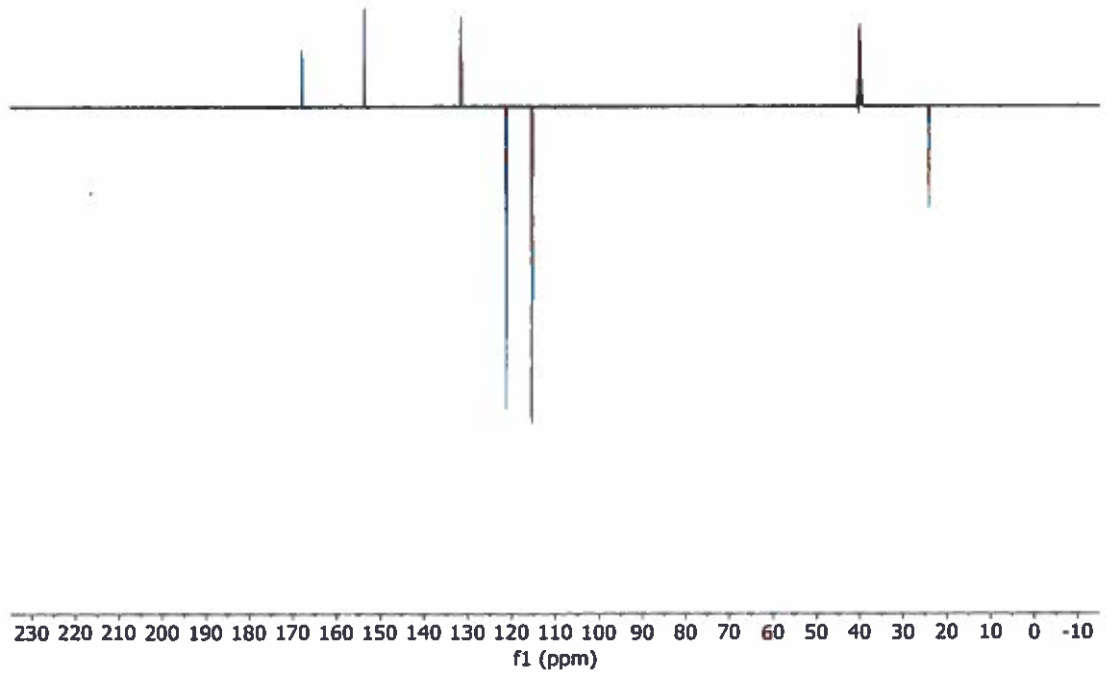
Proton



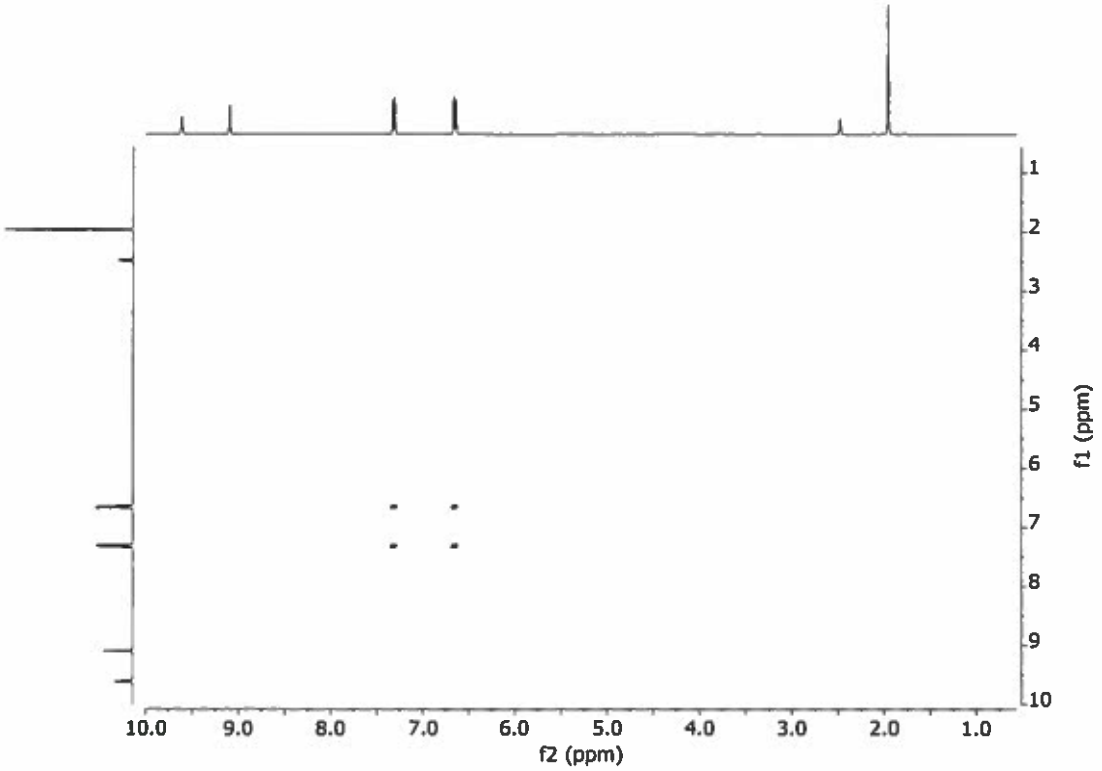
Carbon


167.94
153.55
131.46
121.25
115.42
24.17
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

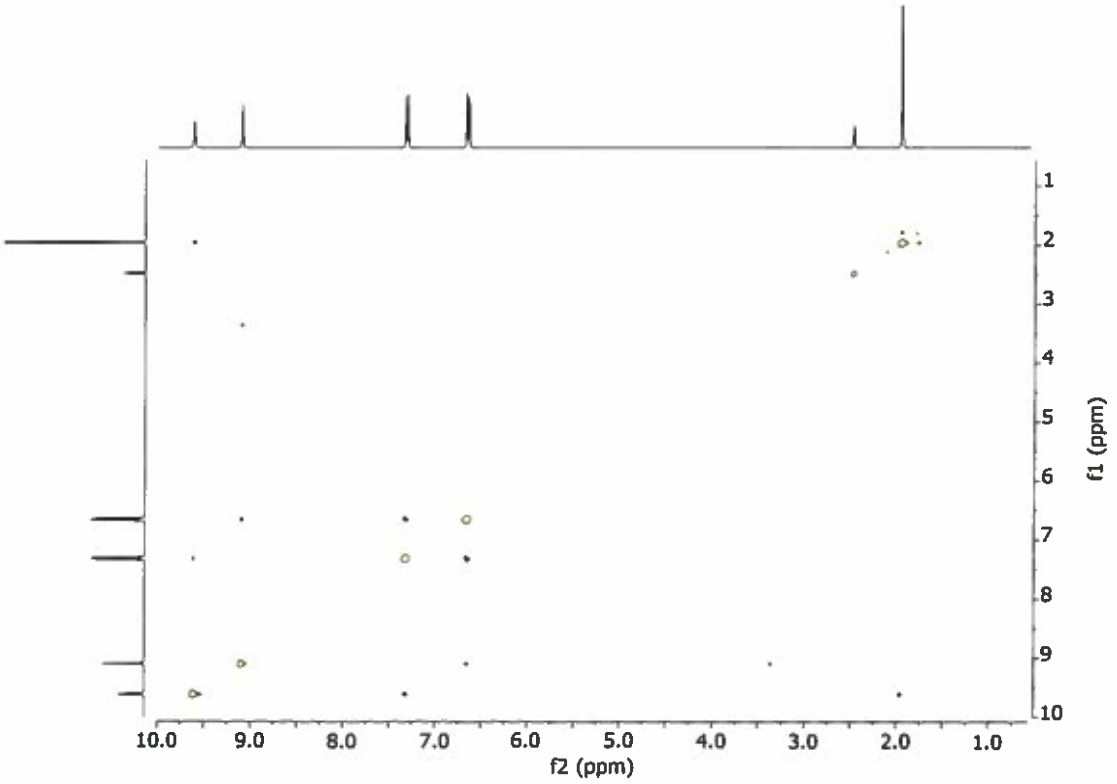
APT


230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

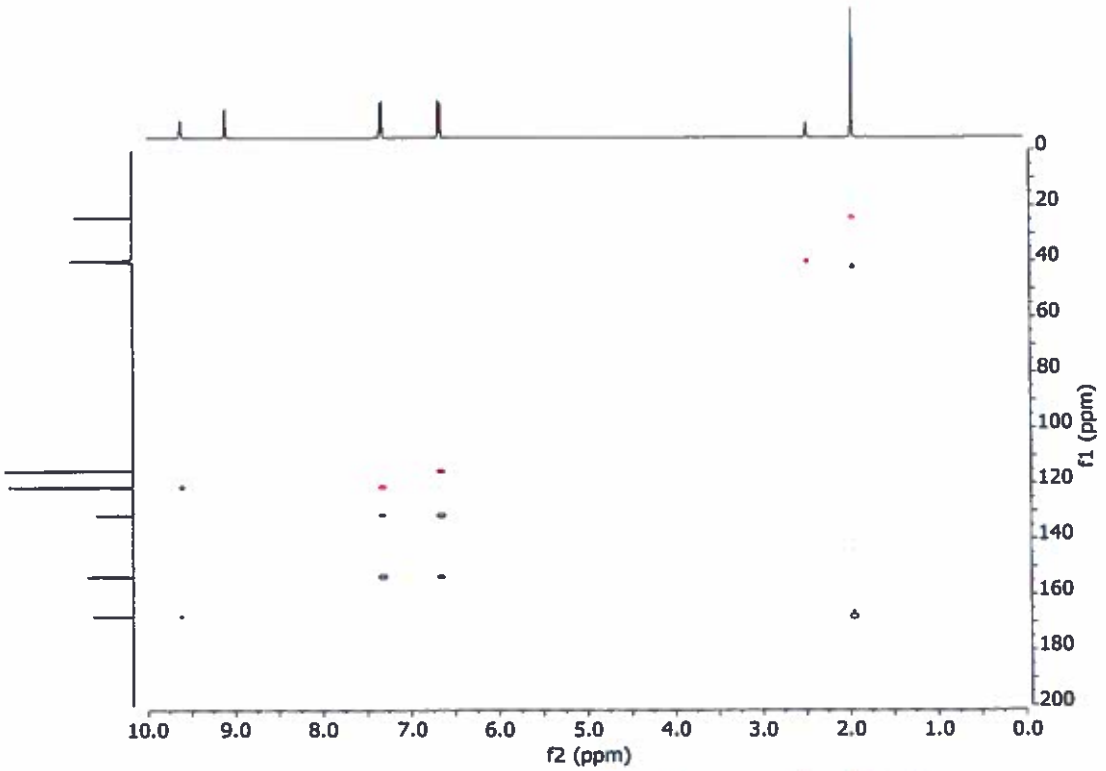
DQF-COSY



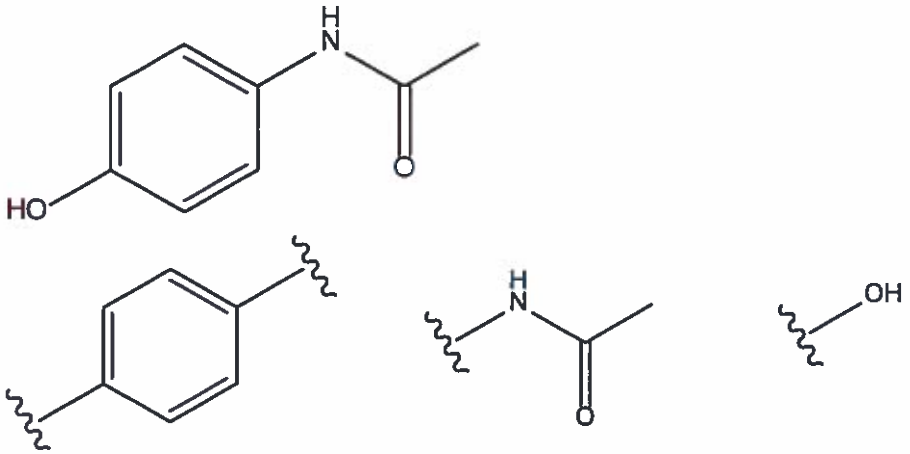
ROESY 300ms



HSQC+HMBC



4a. The spectra above are for an unknown molecule with the molecular formula: $C_8H_9NO_2$. Elucidate the structure and report the ^1H and ^{13}C assignments in the HSQC+HMBC. (20p)



Fragments you can identify. The para di-substituted ring spotted from symmetric aromatic resonances (Proton and HSQC/HMBC), the NH-CO-CH3 from long range couplings and chemical shifts, one hydroxyl attached to the ring. The –O attached to the ring can be spotted in the HMBC from the carbon shift and the –OH needs to be attached after excluding all other options.

4b. There is a crosspeak at 9.1/3.3 PPM in the ROESY, what is that? (2p) Chemical exchange with a small amount of water present in the DMSO. In a ROESY, exchange is identified with crosspeaks with the same sign as the diagonal.

4c. The aromatic HSQC $^1J_{CH}$ peaks also overlaps with HMBC $^nJ_{CH}$ peaks, how is that possible? (3p) Each of the two overlapping protons will correlate with both the directly

attached carbon (HSQC) as well as the rotationally equivalent carbon on the opposite side of the ring (3-bond HMBC). Because of the rotational symmetry, both these correlations result in a crosspeak in the same place in both experiments.

Good luck!

Johan

Veiledende hjelpemiddel: Standardisert sensurskjema

Anbefalt av NTs utdanningsutvalg 21.03.14. Endret 29.03.16 iht. dekani vedtak 2016/83 om sensorording for masteroppgaver.

Vurdering av	**Delpunkt:** ***Kommentar***	**E/I/V[1]**	**Maks. poeng**	**Forhånds-vurdering**	**Endelig poeng**	**Kommentarer**
Innledning og teori (maks. 21 p.)	Faglig forankring:	E	5			
	Teoretisk innsikt:	E+I[2)]	8			
	Målbeskrivelse:	E	3			
	Eget bidrag:	E+I[2)]	5			
Metoder og arbeidsform (maks. 26 p.)	Ferdighetsnivå:	E+I[2)]	10			
	Arbeidsform:	E+I[2)]	3			
	Arbeidsinnsats:	E+I[2)]	5			
	Selvstendighet:	E+I[2)]	8			
Resultater og diskusjon (maks. 37 p.)	Resultat (Arbeidet):	E+I[2)]	10			
	Analyse, diskusjon og konklusjon:	E	15			
	Kritisk refleksjon:	E	6			
	Eget bidrag/måloppnåelse:	E	6			

Fremstilling (maks. 16 p.)	Struktur:	E	5			
	Språk:	E	6			
	Form:	E	5			
Muntlig[3] (maks. 0 p.)	Presentasjon i forbindelse med avsluttende eksamen:	E+I	0			
		SUM	**100**			

1) Her står E for at vurderingen primært gjøres av Ekstern **S**ensor, mens der det står I betyr det at vurderingen primært gjøres av Intern Sensor (kan ikke være veileder).

2) **V**eilederes vurderinger gitt på eget skjema gir grunnlag for poenggivingen.

3) Vurdering av masteroppgaven omfatter en vurdering av det skriftlige arbeidet, og kan i tillegg inkludere en muntlig eksaminasjon og/eller muntlig presentasjon. «Muntlig presentasjon» vurderes til godkjent/ikke godkjent. Hvis presentasjonen ikke er godkjent, må studenten presentere oppgaven på nytt etter avtale. Formålet med den «muntlige eksaminasjonen» i forbindelse med avsluttende mastereksamen i realfagstudiet er å vurdere bl.a. kandidatens beherskelse av innholdet i masteroppgaven, og ut fra dette justere de andre delpunktene, opp eller ned. Det vises til utfyllende regler for realfagstudiet, og dekani vedtak om eksamensordning ved NT-fakultetet ved avsluttende mastereksamen for realfag.

Bruk av sensurskjema
Sensurskjemaet skal være et arbeidsdokument for eksamenskommisjoner og vil ikke være egnet som begrunnelse eller tilbakemelding til studentene. Det skal heller ikke fungere som sensurprotokoll. Egen sensurprotokoll sendes til eksamenskommisjonene.

Poengsummer:
Fakultet har satt en max poengsum på hvert punkt slik at summen blir 100. Hvert delpunkt har en poengsum slik at summen av delpunktene blir lik punktets max-sum. Dersom et delpunkt, slik som "Faglig forankring", gis maksimal uttelling på 5 poeng, fordeles poeng for eksempel etter følgende skala:

5 poeng - bortimot perfekt
4 poeng - meget godt, bare små mangler
3 poeng - godt, men med klare mangler
2 poeng - akkurat nok til å være en akseptabel prestasjon for mastergraden
1 poeng - noe av verdi, men ikke godt nok til å være akseptabelt
0 poeng - lite eller intet av verdi

Dette betyr at vurderingen av delpunktene gjøres i hht de relevante delene av den overordnede karakterbeskrivelsen. Der andre maksimale uttellinger enn 5 poeng benyttes, må dette naturlig nok skaleres tilsvarende.

Vurdering:
Ekstern Sensor og Intern Sensor gjør en forhåndsvurdering og setter foreløpige poengsummer for sine punkter (merket med E og I). Etter muntlig eksaminasjon og sensurmøte kan alle poengsummene bortsett fra for punktene "Fremstilling" og "Muntlig eksamen", justeres. Det er markert hvilke underpunkter som henholdsvis ekstern sensor (E) og intern sensor (I) har ansvar for å vurdere. For tre punkter har ekstern sensor og intern sensor (E + I) et delt ansvar for å sette en poengsum.

Karaktertabell:

Karakter	**Poengintervall**
A	89 - 100
B	77 - 88
C	65 - 76
D	53 - 64
E	41 - 52
F	0 - 40

VURDERINGSSKJEMA VEILEDER (ARBEIDSDOKUMENT)

Vurdering av	**Kommentar**
Arbeidet	
Teoretisk innsikt og eget bidrag	
Ferdighetsnivå	
Arbeidsform	
Arbeidsinnsats	
Selvstendighet	
Progresjon	

Hjelpespørsmål ved veileders vurdering av kandidaten

Veileder vurderer for hvert punkt i hvilken grad kandidaten har oppnådd disse målene:

Arbeidet:
Vurder kandidatens arbeid med hensyn til

- Det vises kreativitet og/eller bidrar til nytenkning/nyskapning
- Det gir inntrykk av å være spesielt omfattende

Teoretisk innsikt og eget bidrag:
Vurder kandidatens teoretiske innsikt og eget bidrag, blant annet om

- Kandidaten selv har generert viktige elementer/problemstillinger i oppgaven.
- Kandidaten bruker aktuell og oppdatert litteratur og bakgrunnskunnskap for arbeidet.

Ferdighetsnivå:
Vurder om kandidaten behersker relevante metoder og bruker dem i eget arbeid på en hensiktsmessig og integrert måte. Vurder kandidatens evne til strukturere avhandlingen hensiktsmessig. Vurder kandidatens språklige ferdigheter.

Arbeidsform:
Vurder kandidatens evne til planmessig og metodisk arbeid.

Arbeidsinnsats:
Vurder om kandidaten viser evne til høy arbeidsinnsats og solid faglig engasjement.

Selvstendighet:
Vurder kandidatens evne til å arbeide og bruke relevante metoder selvstendig og gjennomføre et selvstendig forsknings- eller utviklingsprosjekt under veiledning. Vurder dette spesielt med hensyn til om det

- Vises det personlig initiativ
- Hvilke typer hjelp og veiledning har kandidaten mottatt i ulike faser av arbeidet
- Kandidatens evne til å dra nytte av forskningsgruppens fagkompetanse i eget arbeid

Progresjon:
Gi en kort beskrivelse av kandidatens progresjon vært i løpet av tiden.

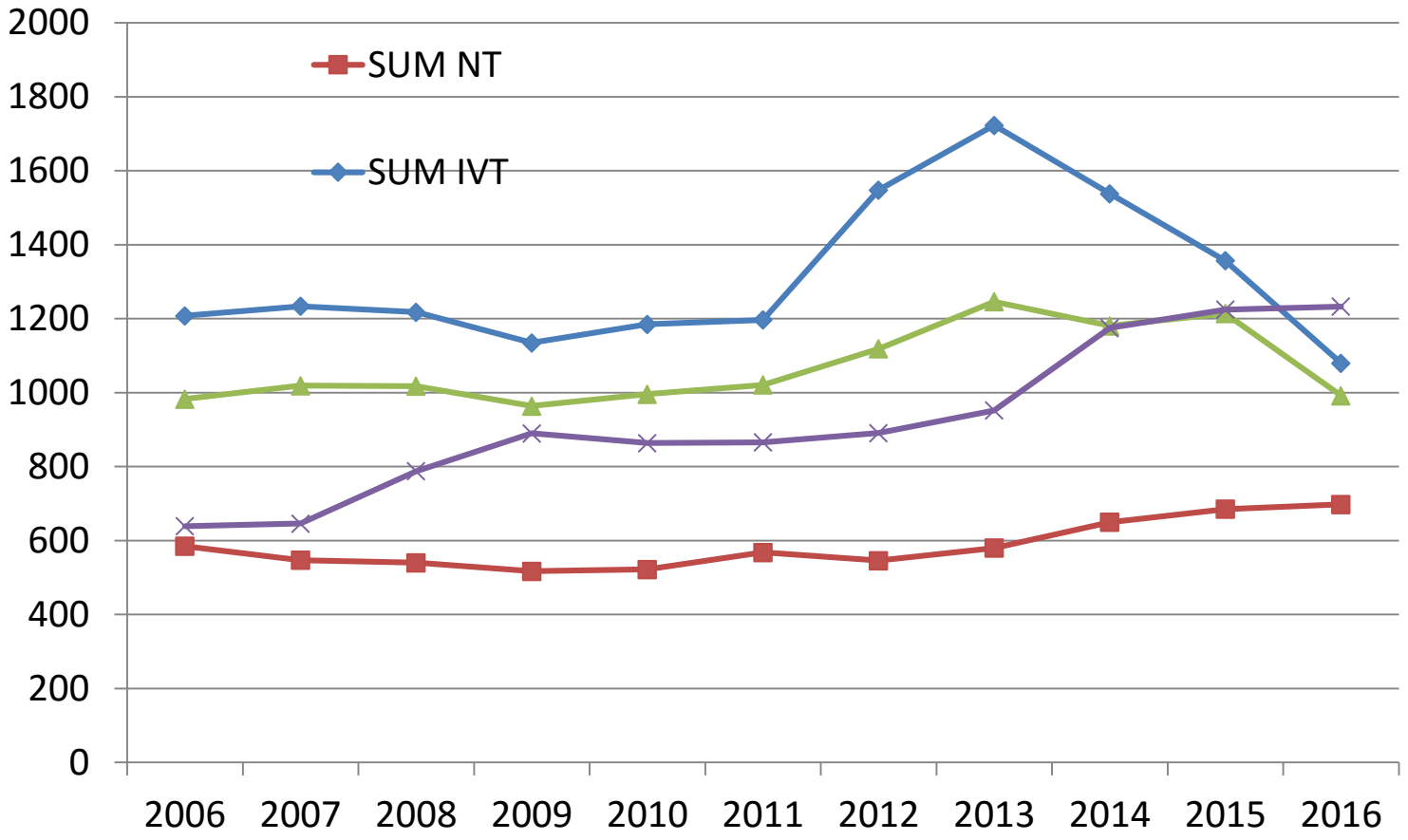
NTNU

Kunnskap for en bedre verden

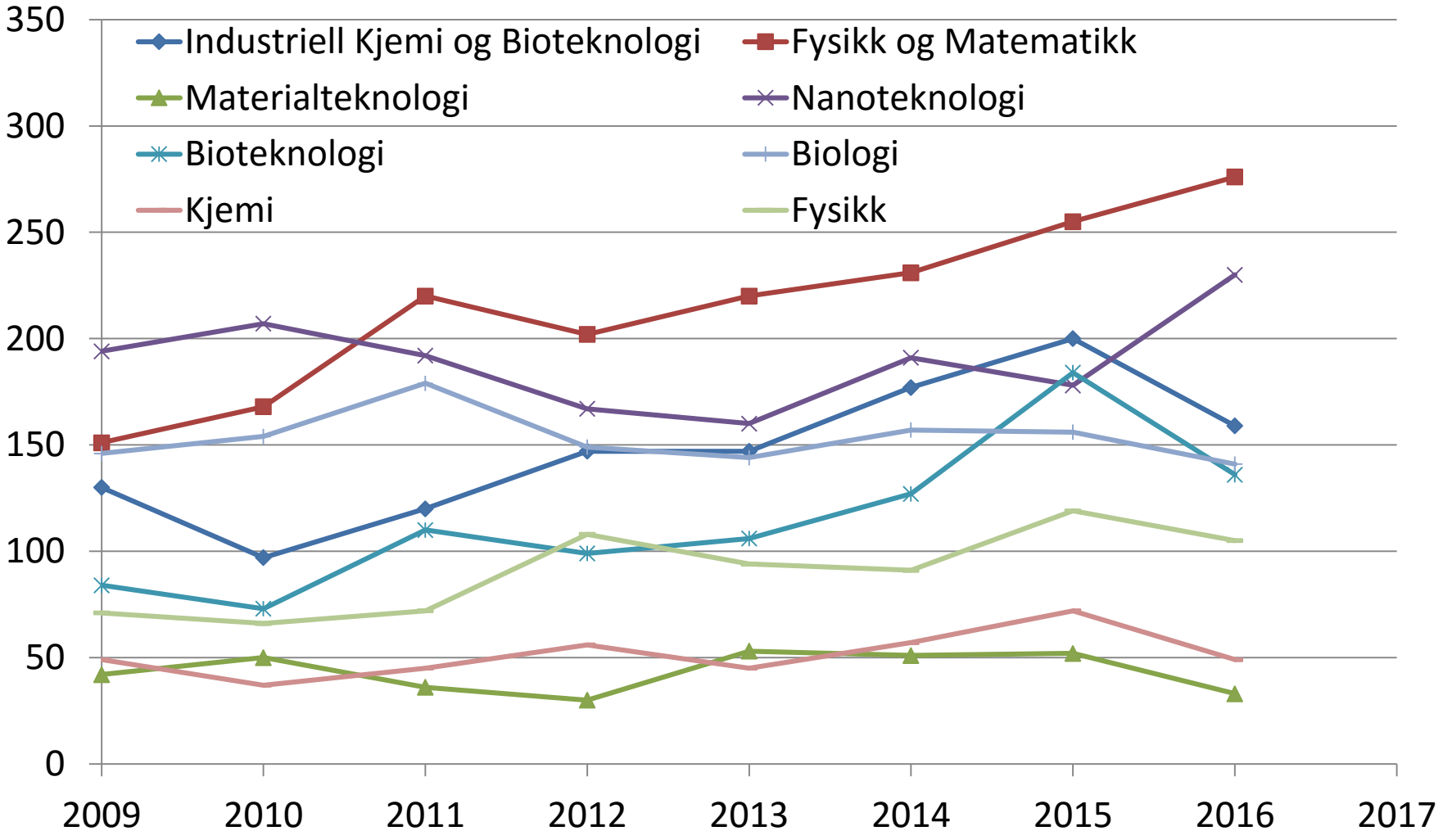
Søkertall NT-2016

Øyvind Gregersen

Pimærsøkere til teknologi 2006-2016



Primærsøkere pr program ved NT



Søker pr studieplass

	2016	2016 ramme	Søkere pr plass 2016	Søkere pr plass 2015
Industriell Kjemi og Bioteknologi	159	107	1,5	1,9
Fysikk og Matematikk	276	99	2,8	2,7
Materialteknologi	33	36	0,92	1,3
Nanoteknologi	230	32	**7,2**	**5,7**
Bioteknologi	136	35	3,9	**5,3**
Biologi	141	75	1,9	2,1
Kjemi	49	30	1,6	2,4
Fysikk	105	40	2,6	3,0
Teknologiprogrammene, snitt			2,54	2,56
Realfagsprogrammene, snitt			2,47	2,95

Søkere til 2-årige masterprogram

PROGRAM	2015	2016
Biology - (MSc)	54	122
Biotechnology (MSc)	39	162
Chemistry (Msc)	24	55
Environmental Toxicology and Chemistry (MSc)	30	94
Natural Resources Management - (MSc)	46	131
Physics (MSc)	20	90
Marine Coastal Development (MSc)	24	64
Chemical Engineering (MSc)	11	175
Materials technolgy (MSc)	1	79
Materialteknologi	28	49
Industriell kjemi og bioteknologi	19	59