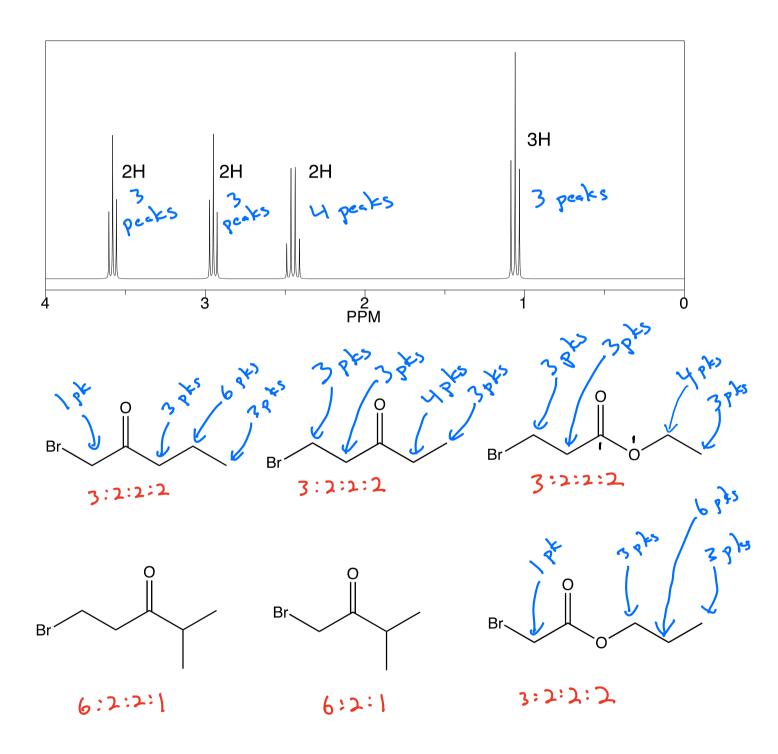
### V. When solving NMR spectra problems:

- 1) Determine number and relative integrations of signals predicted for a given structure
- 2) Make sure the splitting pattern matches with the spectrum for each signal and
- 3) If the number and relative integrations as well as splitting patterns match with the spectra, compare expected chemical shifts with those of the signals in the spectra.



MRI – Nuclear Magnetic Resonance Imaging – Produces a 3-d image inside the body.

MRI is similar in approach, but complementary to, a CAT scan, which uses X-rays for imaging.

**MRI** is therefore safer than a CAT scan (no X-rays or other damaging radiation is used). Radiofrequency electromagnetic radiation does not cause DNA damage or any other kind of damage.

**MRI** primarily visualizes soft-tissue and especially cancer tumors while a CAT scan primarily visualizes bones or Calcium based dyes drunk to visualize the digestive tract.

MRI uses the same principles and NMR.

- 1) The patient is placed in a very strong magnetic field. Creating this very strong magnetic field is technically very demanding, explaining MRI machines are so expensive ( $\sim 0.5 1.5$  \$ million)
- 2) The patient is irradiated with radiofrequency electromagnetic radiation.
- 3) The flipping (resonance) of 1H nuclear spins is monitored Actually emitted photons are measured using the FT method.
- 4) Magnetic field gradients are used to gain imaging information. The magnetic field gradients are rotated around a central point and measurements are taken at each angle around 360° to gain 2-dimensional information. This technique is called tomography.

The same three spots seen from different angles-By analyzing all angles the locations and intensities can be calculated

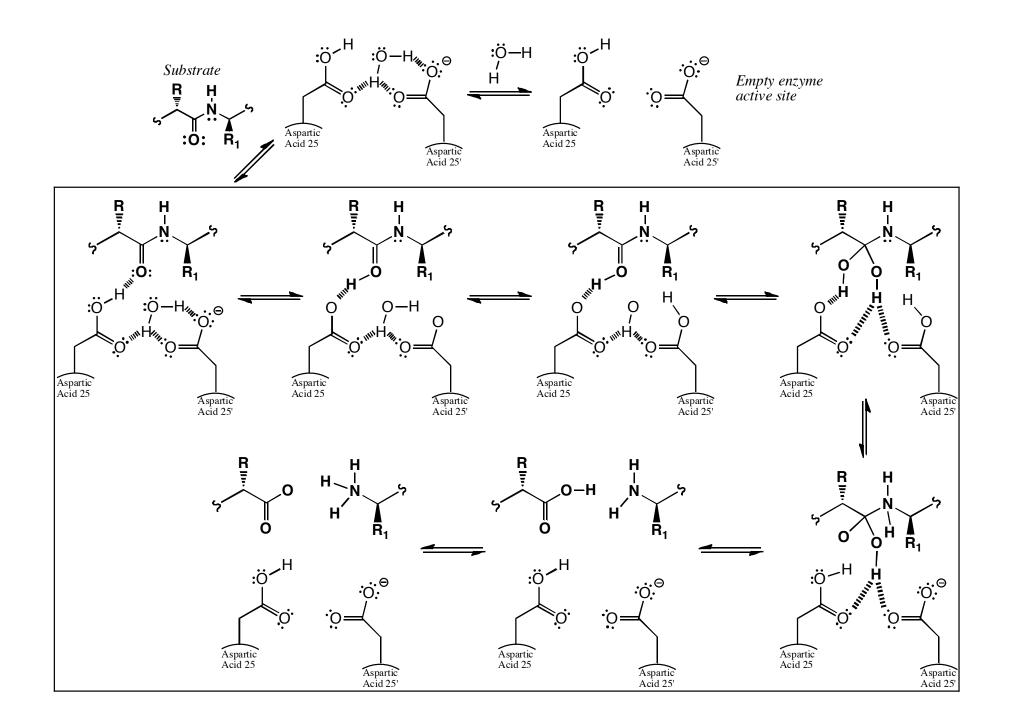
The overall MRI imaging approach involves looking at each 2-dimensional slice.

Each slice is added to give a 3-dimensional stack (analogous to stacking DVD's or CD's).

Each slice is shaded to indicate differences in the amount of <sup>1</sup>H atoms in different areas/tissues.

Water and fat have the highest density of <sup>1</sup>H atoms, so these are primarily being monitored in an MRI image.

The popular medical diagnostic technique of magnetic resonance imaging (MRI) is based on the same principles as NMR, namely the flipping (i.e. resonance) of nuclear spins of H atoms by radio frequency irradiation when a patient is placed in a strong magnetic field. Magnetic field gradients are used to gain imaging information, and rotation of the gradient around the center of the object gives imaging in an entire plane (i.e. slice inside patient). In an MRI image, you are looking at individual slices that when stacked make up the threedimensional image of relative amounts of H atoms, especially the H atoms from water and fat, in the different tissues [Memorize the preceding passage, as it will be worth 14 points on the final. No I am not kidding, 14 points right there.]



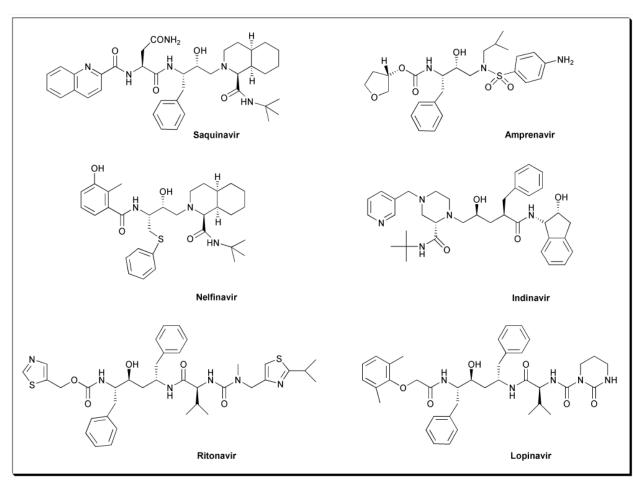


Fig. 10 FDA approved HIV-1 protease inhibitors.

# **Opiates** (heroin, morphine, etc.)

The human body naturally produces its own opiate-like substances and uses them as neurotransmitters. These substances include endorphins, enkephalins, and dynorphin, often collectively known as endogenous opioids. Endogenous opioids modulate our reactions to painful stimuli. They also regulate vital functions such as hunger and thirst and are involved in mood control, immune response, and other processes.

The reason that opiates such as heroin and morphine affect us so powerfully is that these exogenous substances bind to the same receptors as our endogenous opioids. There are three kinds of receptors widely distributed throughout the brain: mu, delta, and kappa receptors.

These receptors, through second messengers, influence the likelihood that ion channels will open, which in certain cases reduces the excitability of neurons. This reduced excitability is the likely source of the euphoric effect of opiates and appears to be mediated by the mu and delta receptors.

This euphoric effect also appears to involve another mechanism in which the GABA-inhibitory interneurons of the ventral tegmental area come into play. By attaching to their mu receptors, exogenous opioids reduce the amount of GABA released (see animation). Normally, GABA reduces the amount of dopamine released in the nucleus accumbens. By inhibiting this inhibitor, the opiates ultimately increase the amount of dopamine produced and the amount of pleasure felt.

Chronic consumption of opiates inhibits the production of cAMP, but this inhibition is offset in the long run by other cAMP production mechanisms. When no opiates are available, this increased cAMP production capacity comes to the fore and results in neural hyperactivity and the sensation of craving the drug.

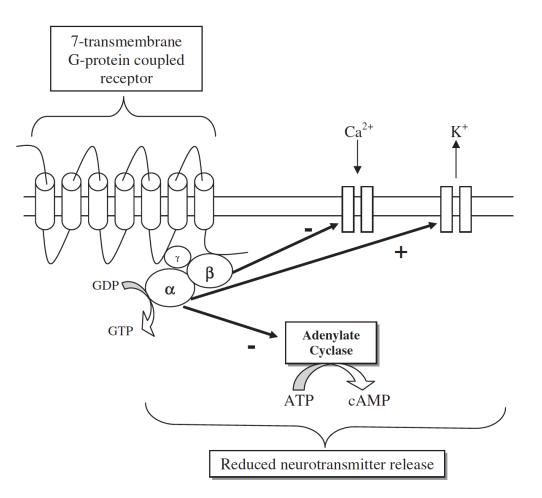
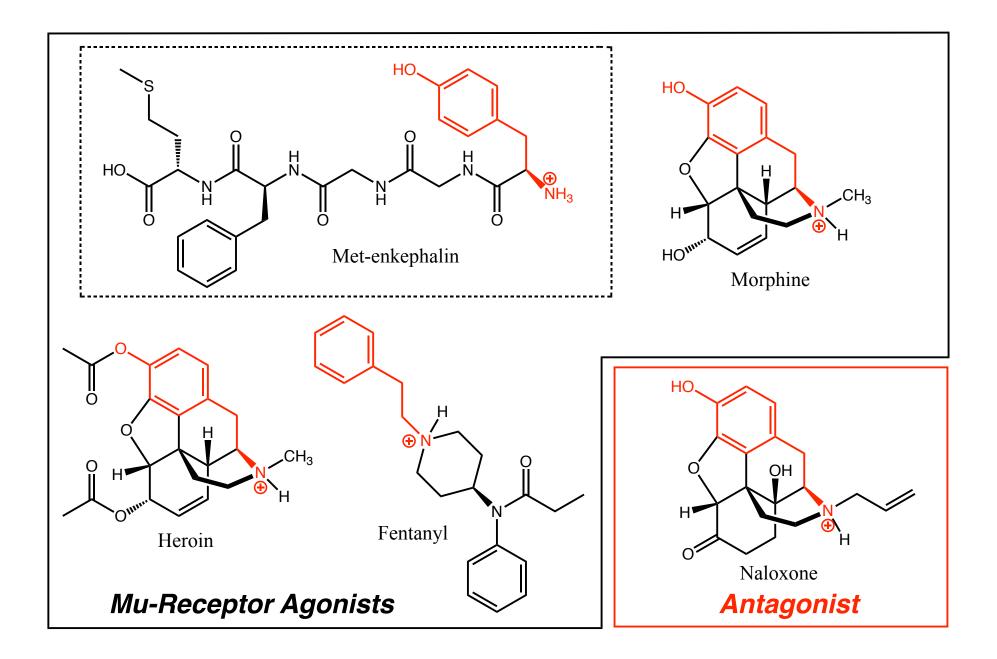


Fig. I Seven transmembrane structure of opioid G-protein-coupled receptor. Receptor activation by opioid receptor ligands leads to initiation of intracellular transduction pathways that include stimulation of potassium efflux, inhibition of VSCCs and inhibition of adenylyl cyclase. In this diagram the G-protein is denoted  $\alpha$ ,  $\beta$ ,  $\gamma$  but the  $\alpha$ -subunit interacts with K<sup>+</sup>/Ca<sup>2+</sup> channel and adenylate cyclase.

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# Shape of $S_N 2$ $\longrightarrow$ Br + ?

 $S_N 2$ 

The club ain't the best place to find nucleophiles So the lab is where I go Me and my friends in solvent Moving fast but reacting slow Come over and start up a reaction with just me And trust me I'll give it a chance now Let's react, stop, put your charge over here And then we start to react, and now I'm singing like You know I want to make a bond Your charge was handmade for a reagent like me Come on now, follow my lead I'm an electrophile, don't mind me Say now let's not talk too much Get through solvent and put your electrons on me Come on now, follow my lead, Come, come on now, follow my lead

I'm attracted to the charge of you We push and pull like charges do Although my orbitals are reacting too Come on let's get bonding Transition state is coming true Time to finish the  $S_N 2$ Creating a bond brand new Come on let's get bonding Oh-I-oh-I-oh-I Come on let's get bonding Oh-I-oh-I-oh-I-oh-I Come on let's get bonding Oh-I-oh-I-oh-I Come on let's get bonding We need to make a bond brand new Come on now let's  $S_N 2$ .

#### "<u>Don't Stop, Believin'</u>

Just a Houston girl, Living in a Longhorn world. She took the premed train Straight to OChem 1

Just a Plano boy, Born and raised in full burnt orange, He took the premed train Straight to OChem 1

They study in a smoky room, Smell of vapes and Mountain Dew For an A they study all night It goes on and on and on and on

Alkanes to alkynes Up and down the I-35 Two students studying in the night Roadmaps, reactions Living just to pass the final Will they ever get it right

Working hard to get my grade Everybody wants an "A" Trying anything to ace this class Just one more exam Some will win, some will lose I don't want to sing the blues OChem never seems to end It goes on and on and on and on

Alkanes to alkynes Up and down the I-35 Two students studying in the night Roadmaps, reactions Living just to pass the final Will they ever get it right

Don't stop believin' Hold on to that "A" feelin' Roadmaps, reactions Ohohohohoh

Don't stop believin' Hold on Roadmaps, reactions Ohohohohoh

Don't stop believin' Hold on to that "A" feelin' Roadmaps, reactions Ohohohohoh

## We All Love Organic Chemistry

In the town where I was born, Lived a man of chemistry. And he told us of his life In the organic laboratory.

Making molecules to fight disease Coming up with their syntheses. So we sit in 320M Learning organic chemistry.

Refrain: We all love organic chemistry Synthetic chemistry Molecules with "C" We all love organic chemistry Synthetic chemistry Molecules with "C"

All our friends think we're a bore Our grade point averages begin with 4. But we await graduation day To work in lab for meager pay.

But its OK, who else can say They're curing cancer or fighting AIDS. We hope that you in 320M Respect organic chemistry

Refrain: We all love organic chemistry Synthetic chemistry Molecules with "C" We all love organic chemistry Synthetic chemistry Molecules with "C