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1D

2D

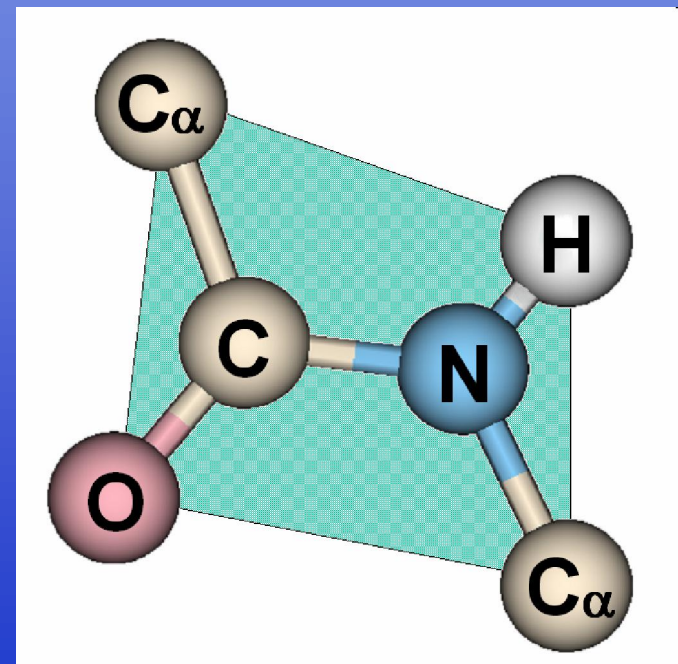
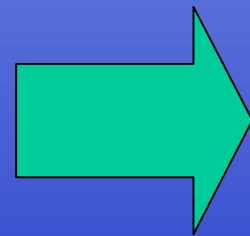
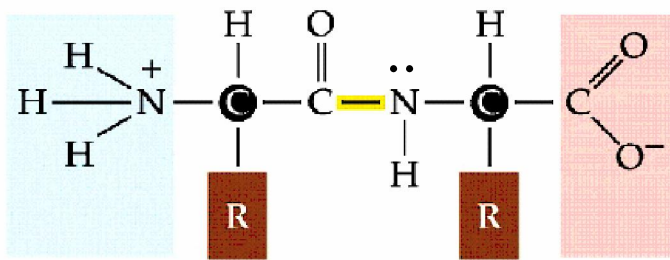
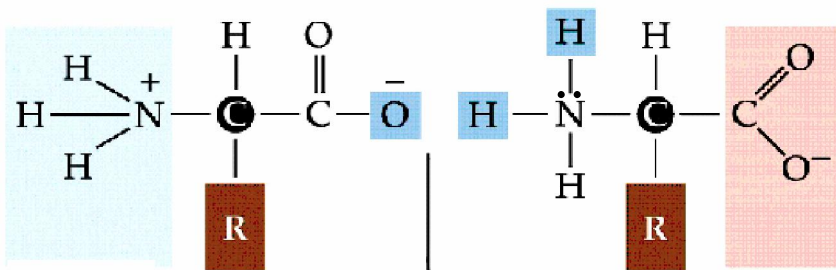
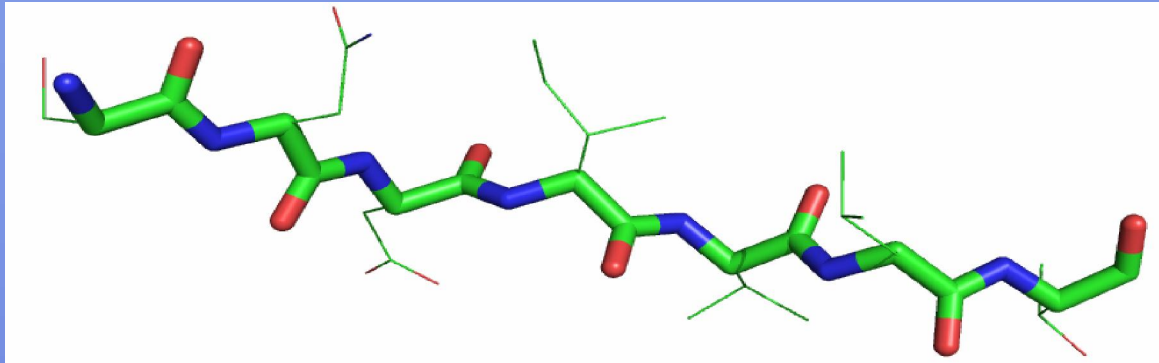
3D

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M, q, pI, hp
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2D
3D

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%H, %S, %L
3D .
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N . ./
sc-mc-MC
(2D, 3D)
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1D, 3D

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3D
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(3D)
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1D, 2D

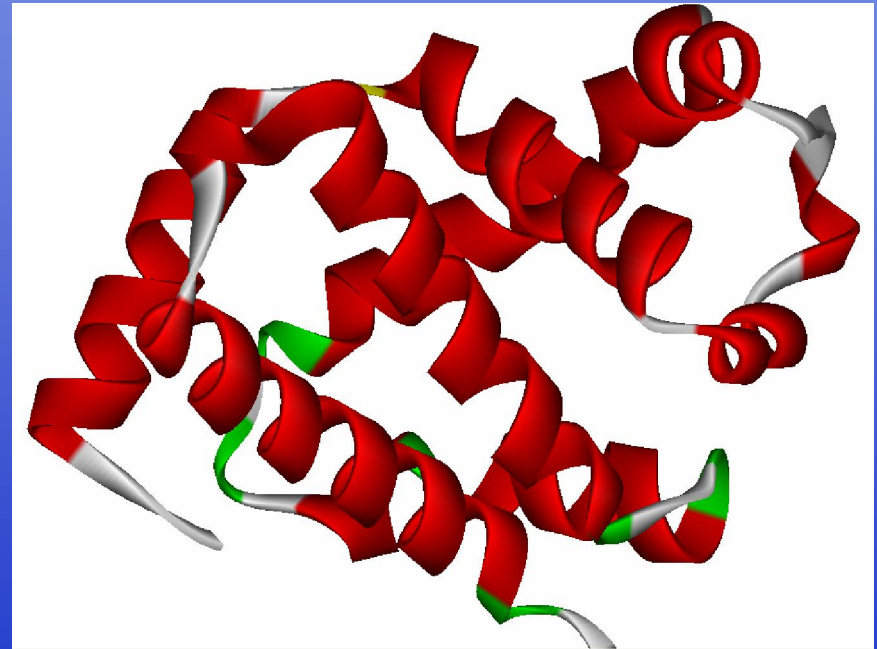
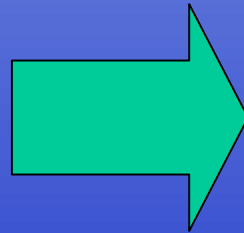
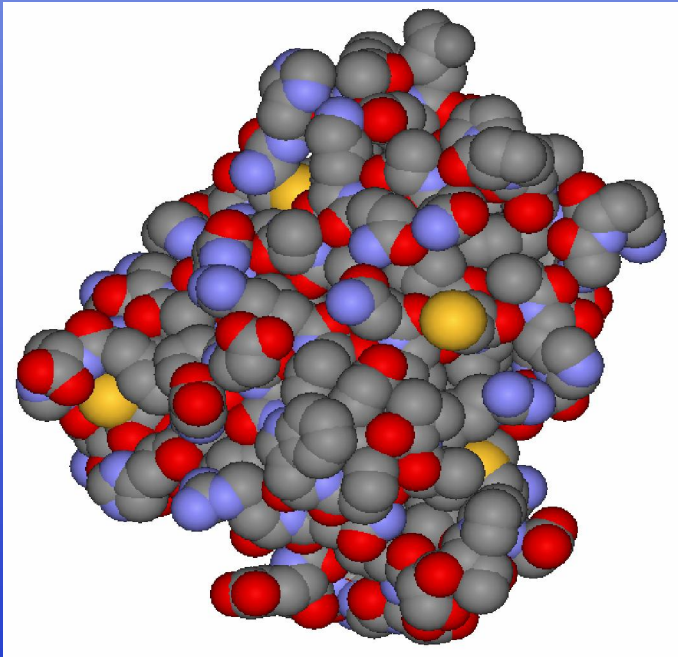


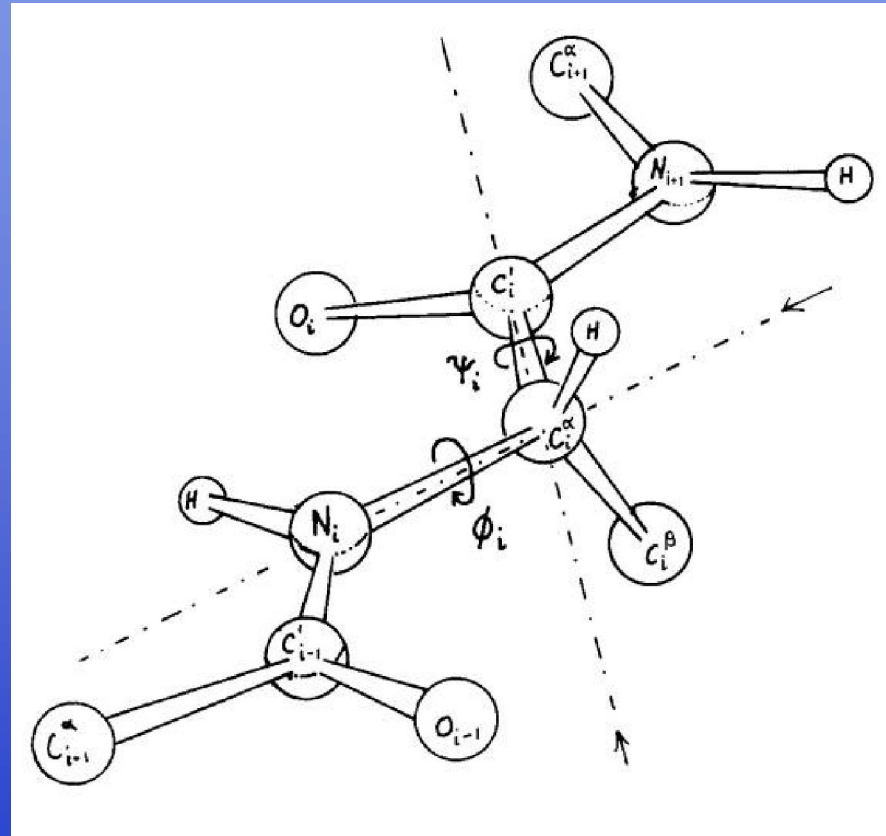
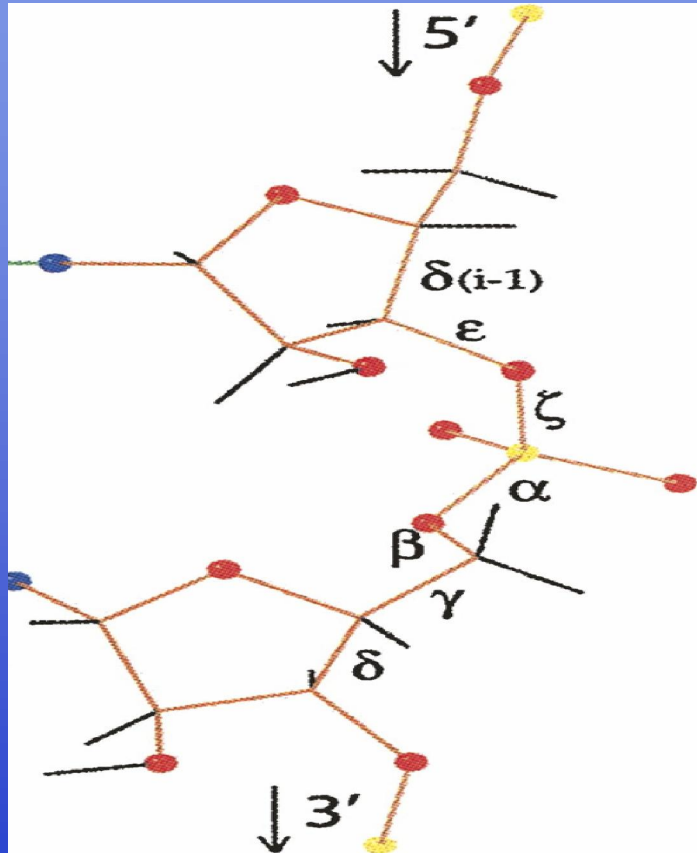


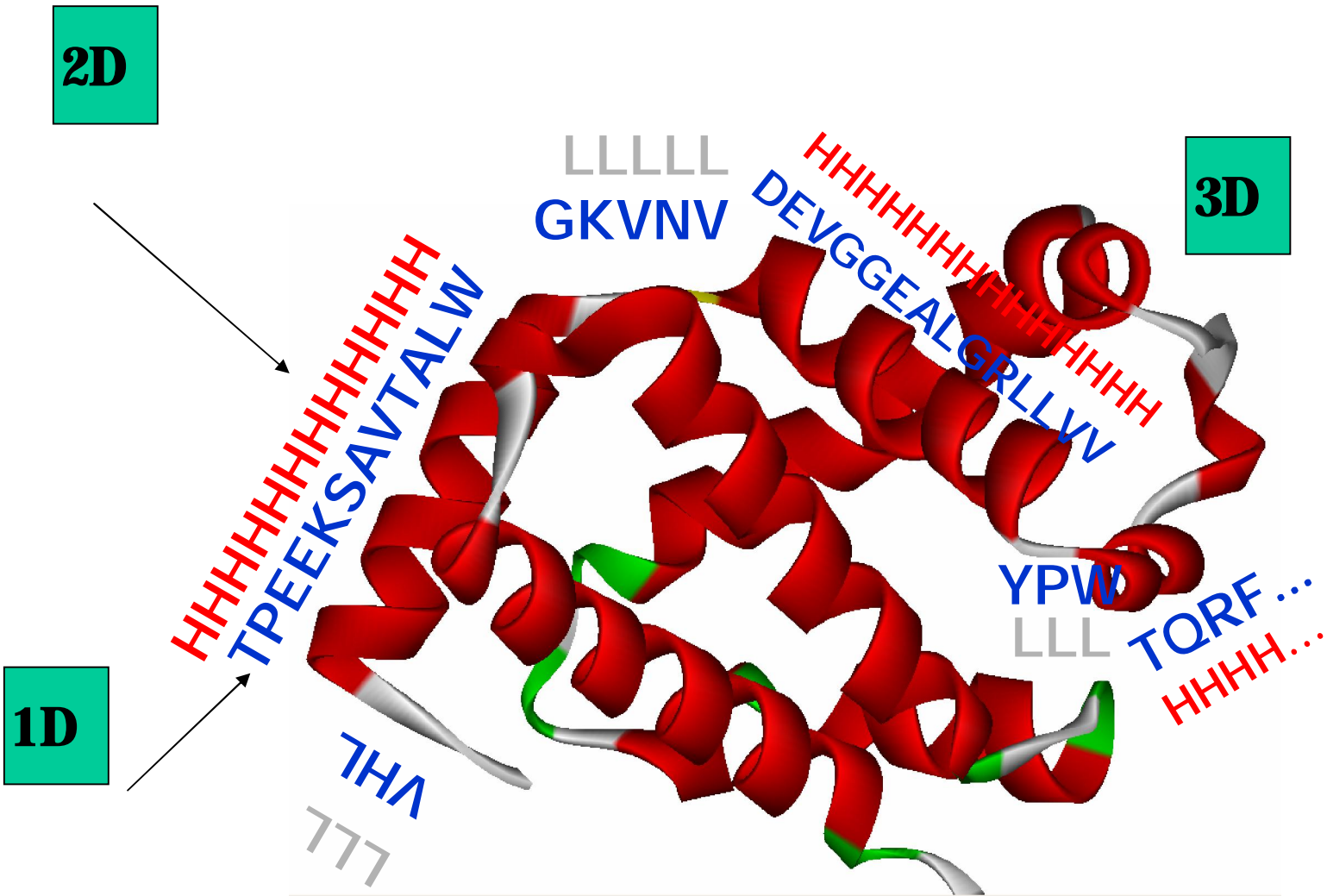
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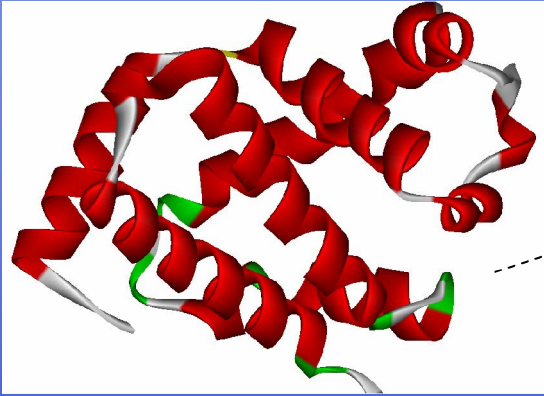
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~ 3D

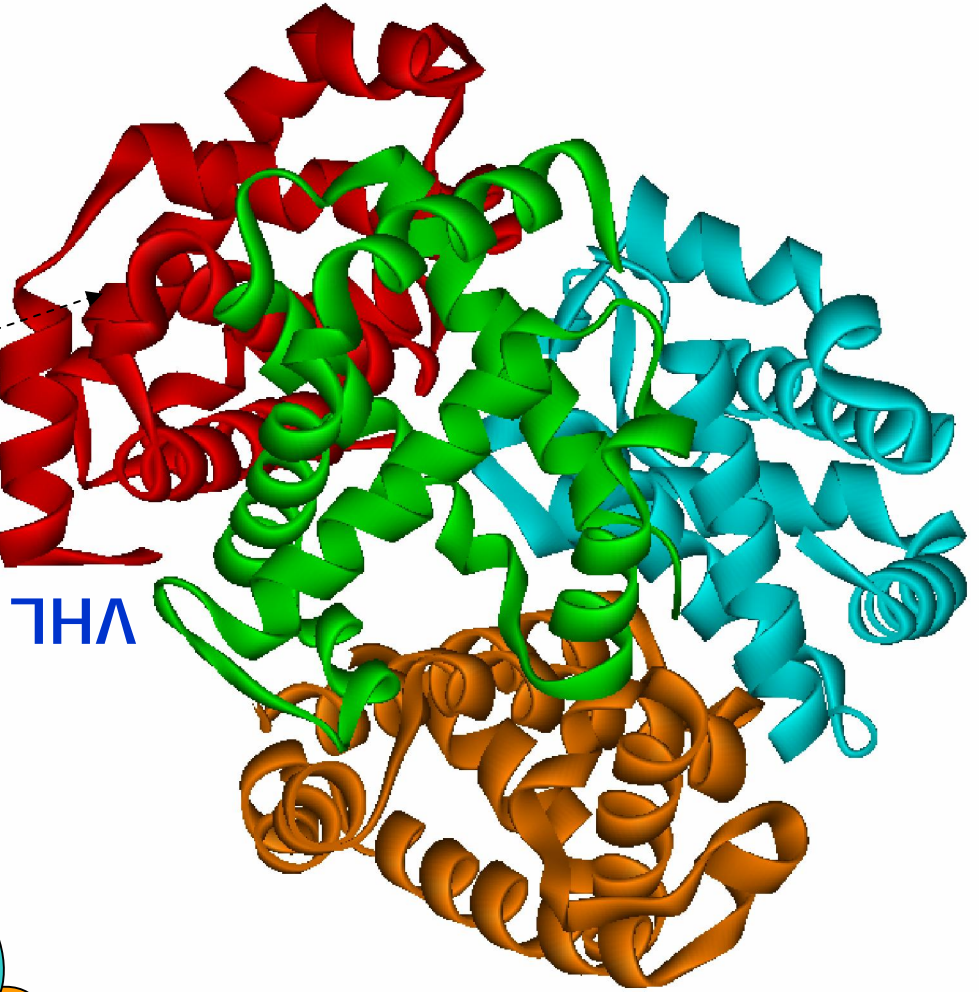




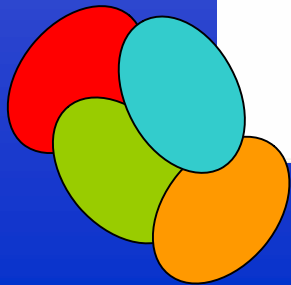


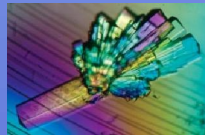


TPEEKSAVTALW...

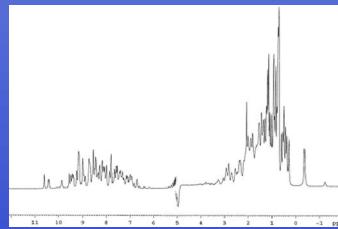
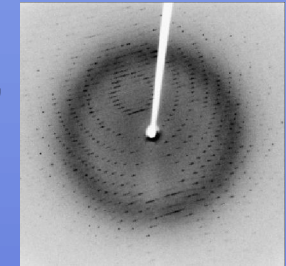


THA





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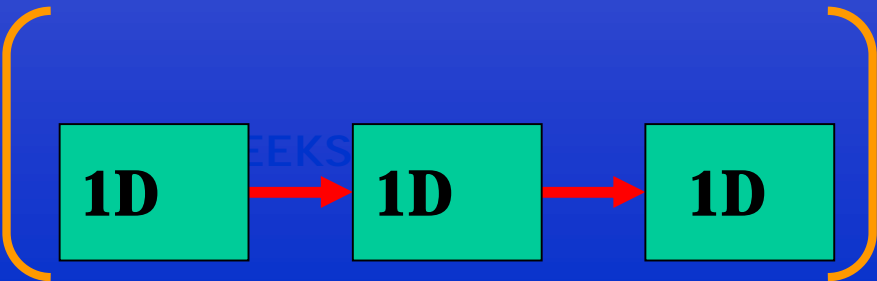
1D



1D



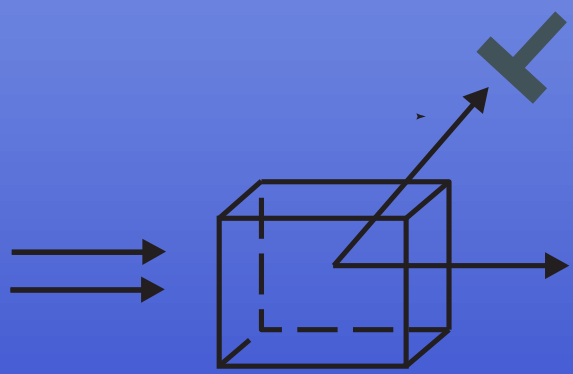
1D



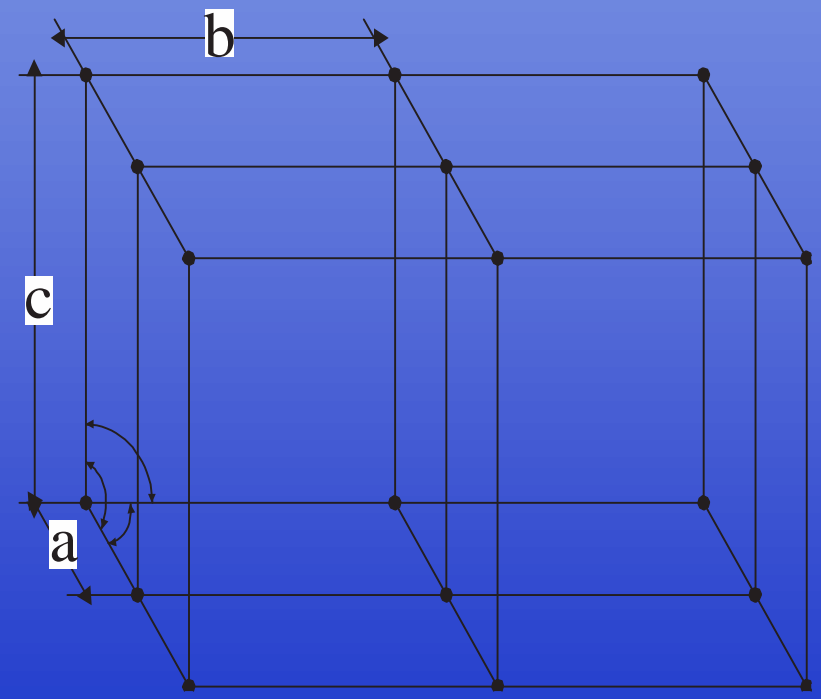
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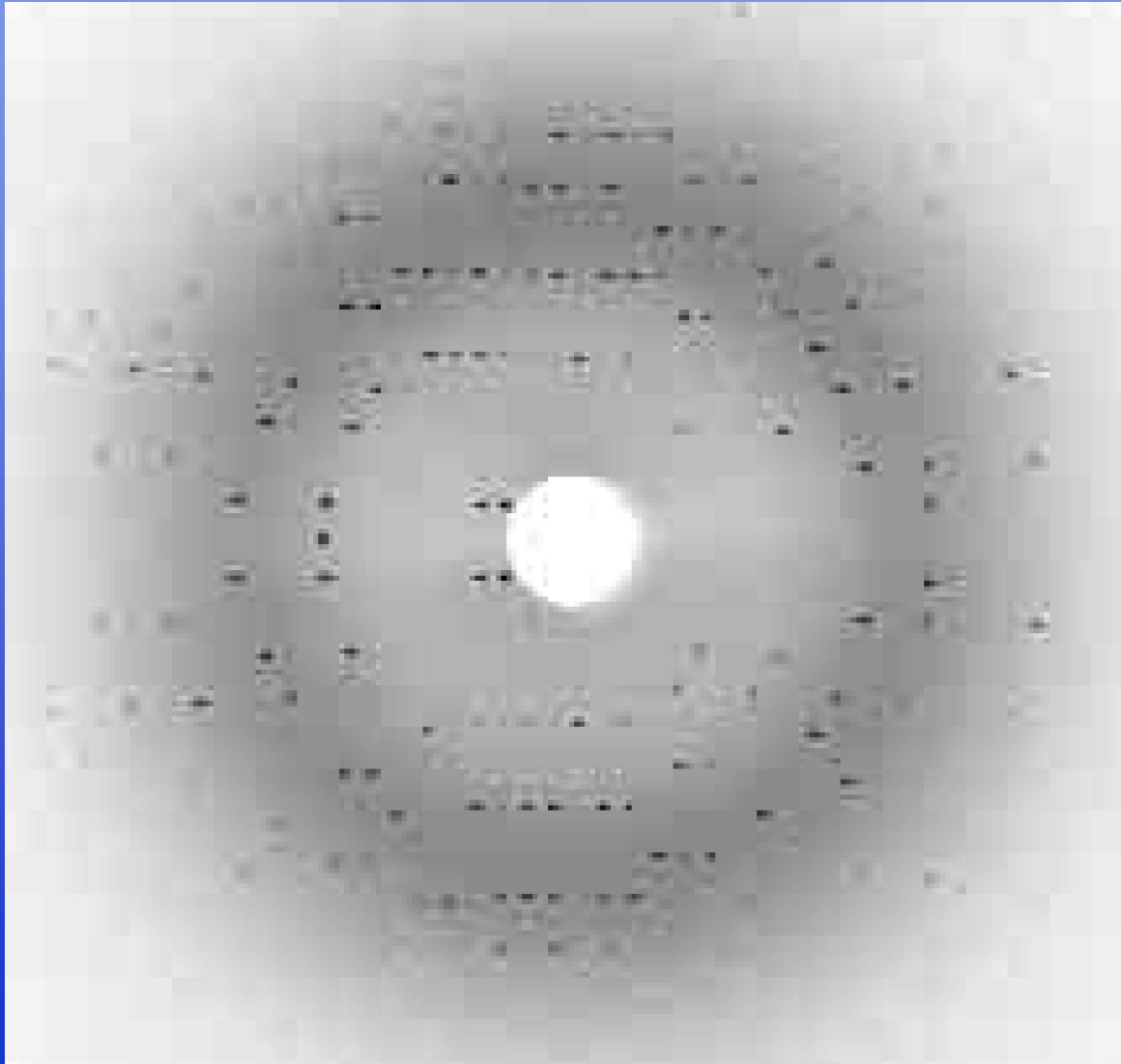
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$h_1, k_1, l_1, I_1;$

$h_2, k_2, l_2, I_2;$

...

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...

$h_n, k_n, l_n, I_n;$

- $\rho(\mathbf{r})$ — плотность заряда в кристалле — периодическая функция:

$$\rho(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{h}} \mathbf{F}_{\mathbf{h}} e^{2\pi i(\mathbf{h}; \mathbf{r})},$$

- V — объём элементарной ячейки, $\mathbf{h} = (h, k, l)$ — «индекс Гюйса», $\mathbf{r} = (x, y, z)$ — радиус-вектор точки в кристалле, $\mathbf{F}_{\mathbf{h}}$ — амплитуда Фурье-ряда.

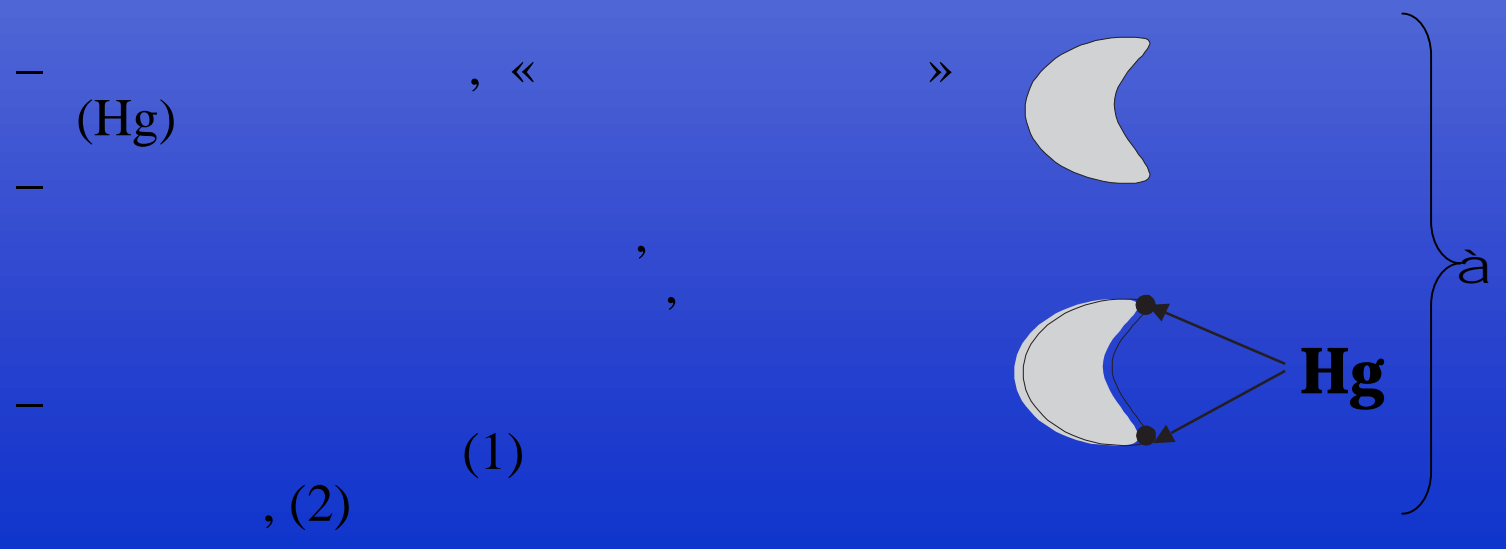
$$\mathbf{F}_{\mathbf{h}} = |\rho_{\mathbf{h}}| \cdot e^{i\varphi_{\mathbf{h}}},$$

- $|\rho_{\mathbf{h}}|$ — амплитуда Фурье-ряда (интенсивность дифракции), $\varphi_{\mathbf{h}}$ — фаза Фурье-ряда.

- \therefore () $I_{hkl} \sim |F_{hkl}|^2$

$$\mathbf{F}_h = |F_h| \cdot e^{i\phi_h},$$

- \therefore —
- —



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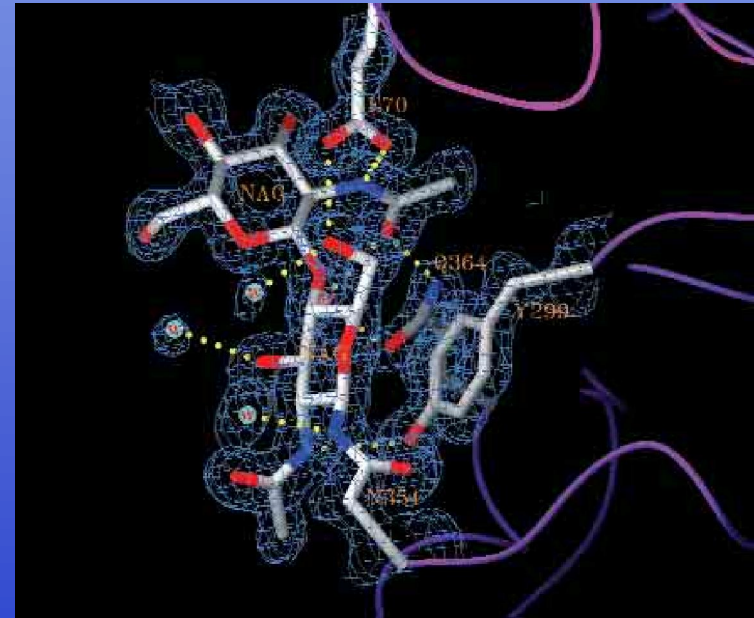
(r)

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R,



R

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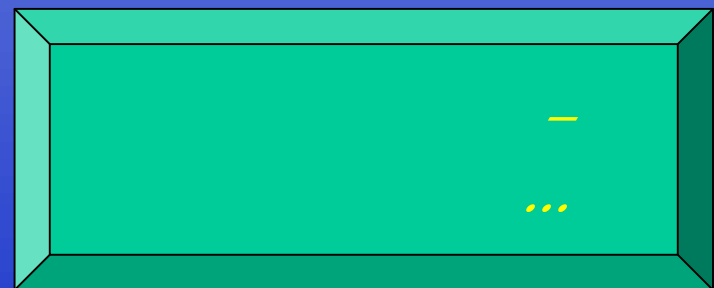
$$R\text{-factor} = \frac{\sum_{(h,k,l)} \left| |F_{obs}(h,k,l)| - |F_{calc}(h,k,l)| \right|}{\sum_{(h,k,l)} |F_{obs}(h,k,l)|}$$

: R=(0,1-0,15)

- R, $R_{free} - R$

(10%

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hkl

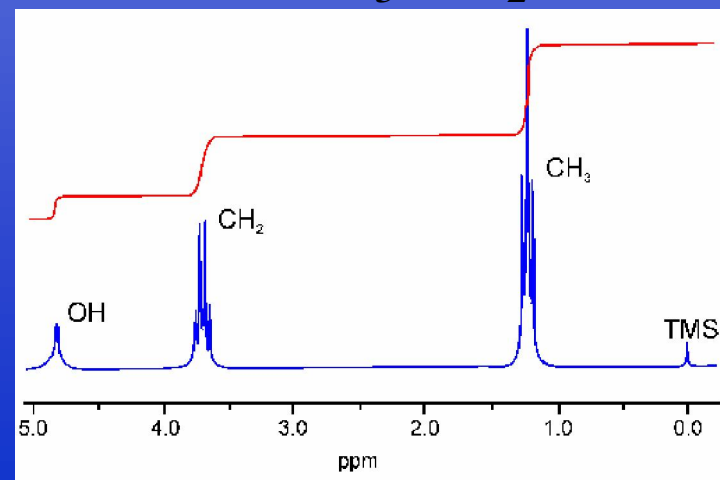
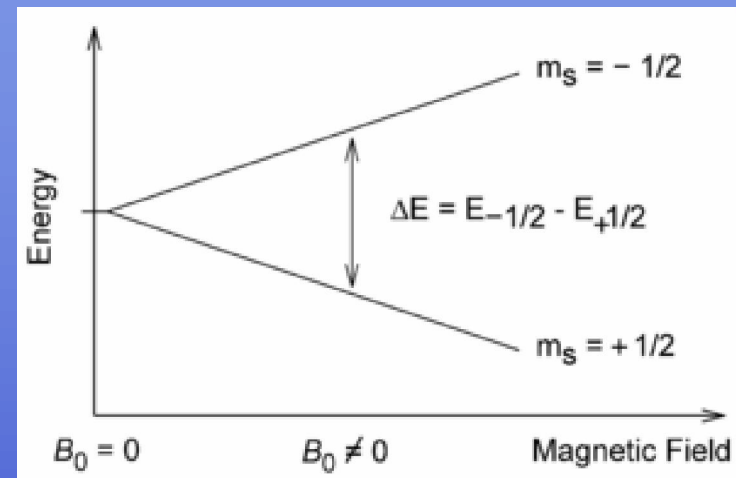


CCV...

1D, 2D ... !

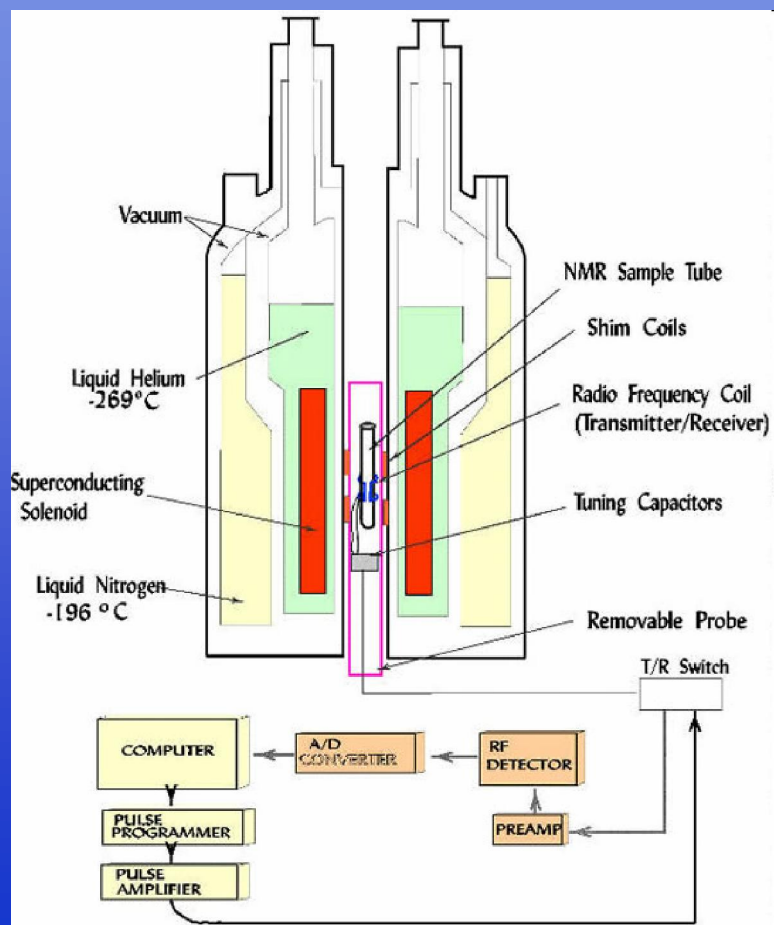
• : ^1H , ^{13}C , ^{15}N ,
 $1/2$, $m = -1/2$

$m =$



• ^{13}C , ^{15}N

• (. .)- :

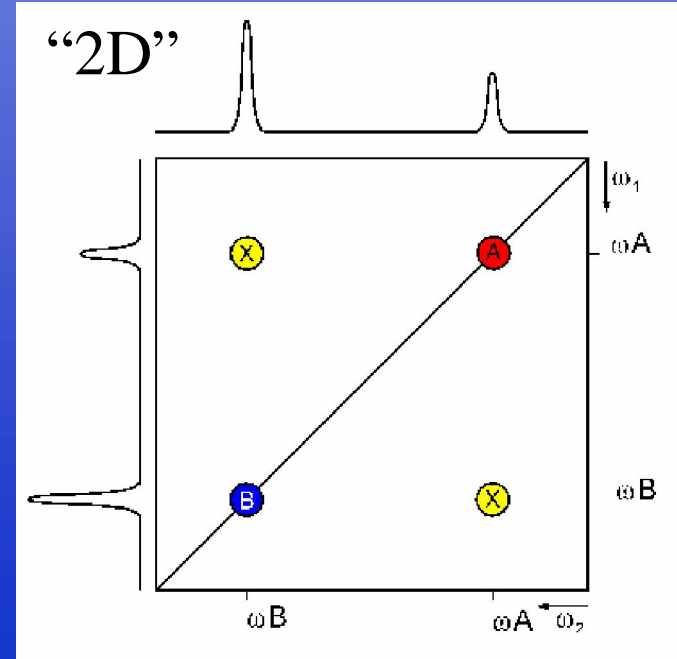
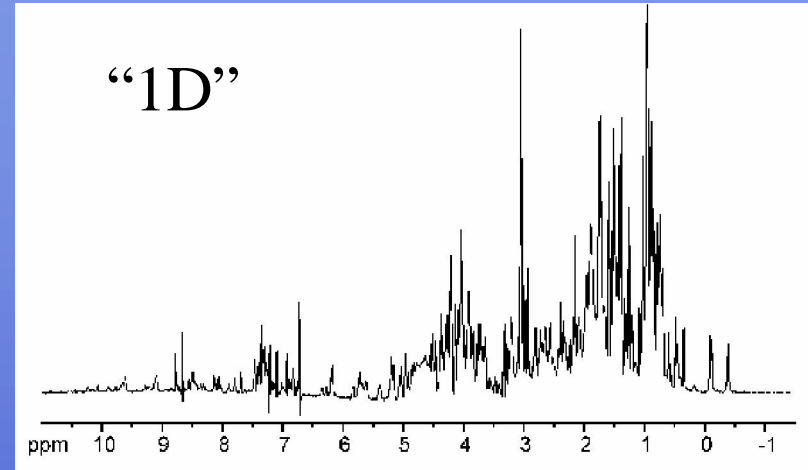


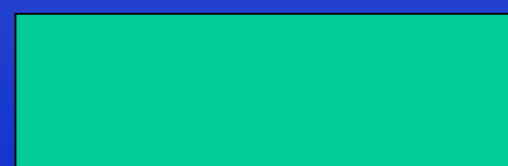
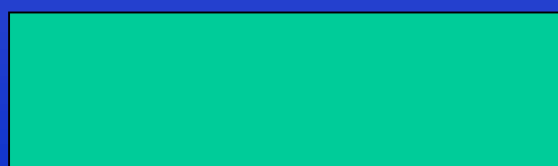
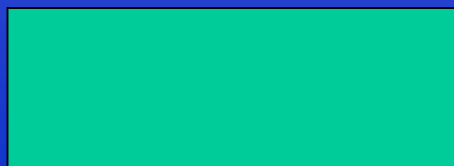
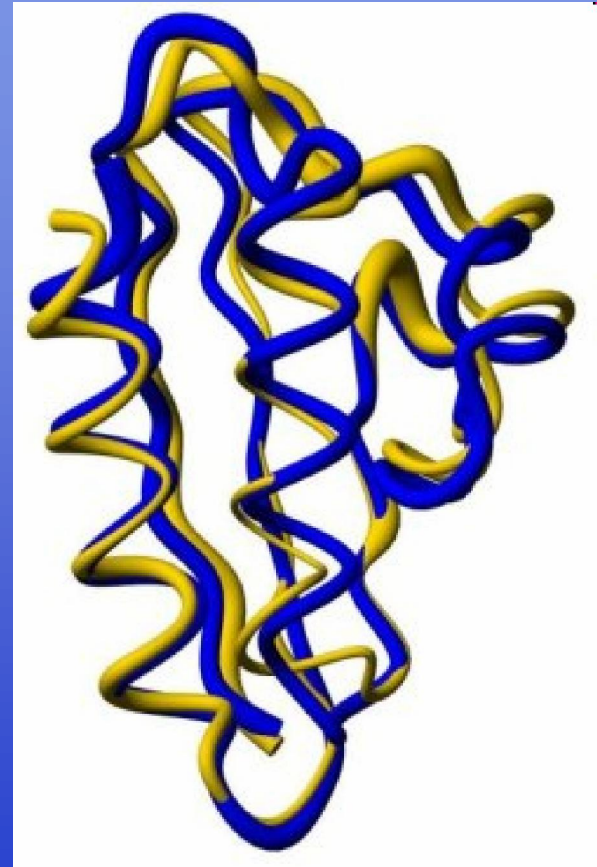
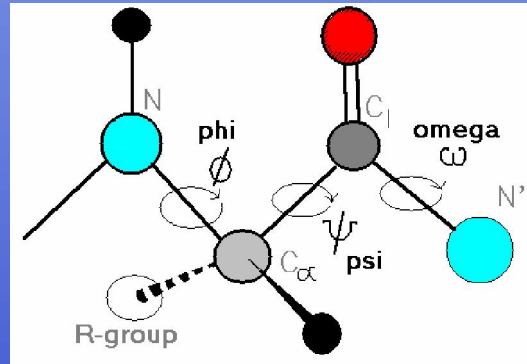
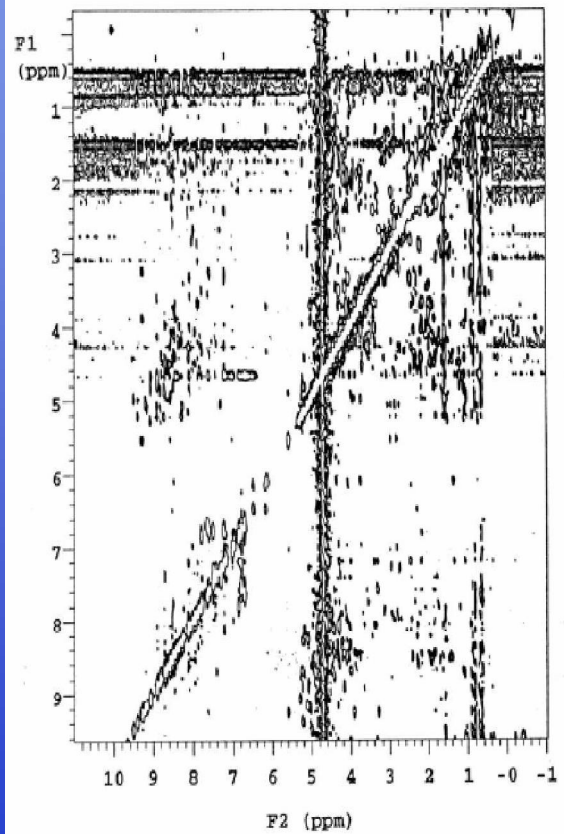
(2D)

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• 2, 3, n- —

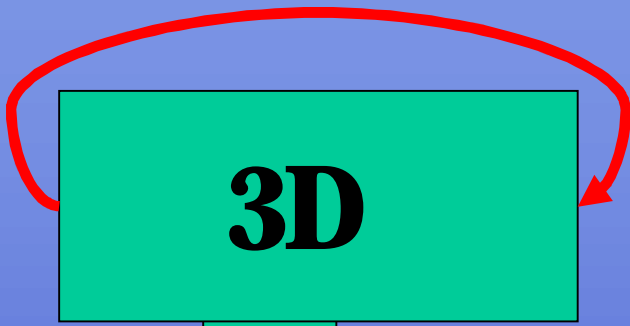
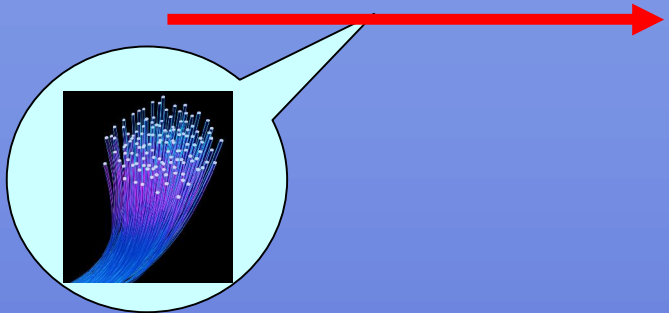
• 2- —



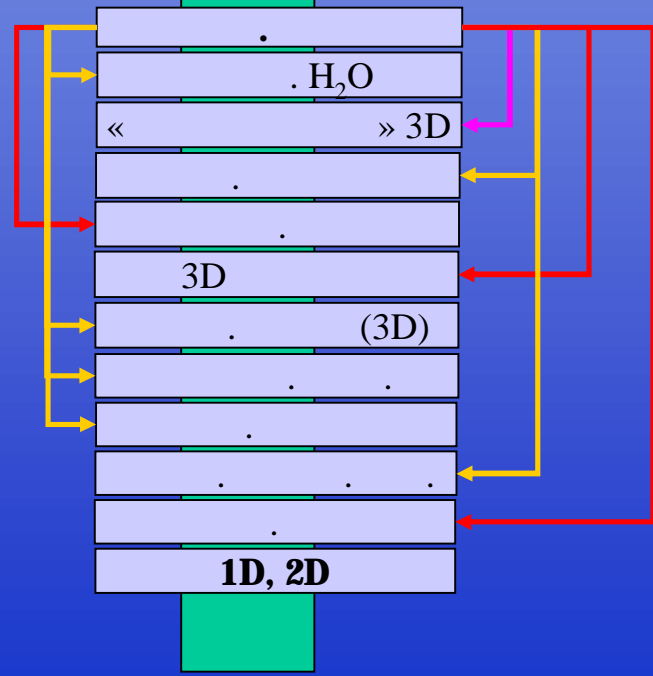


3D-3D

3D > 3D



3D



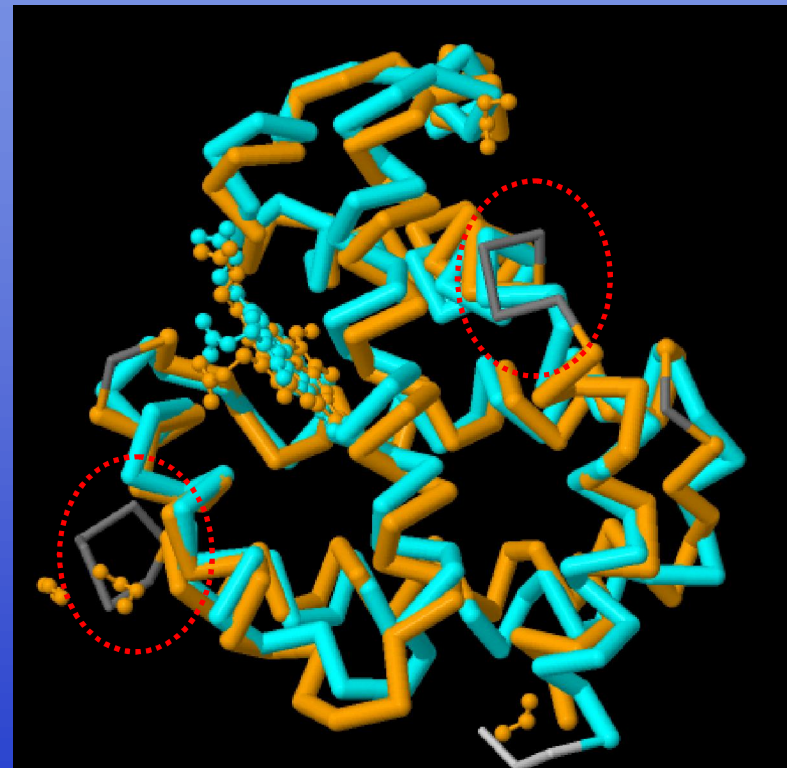
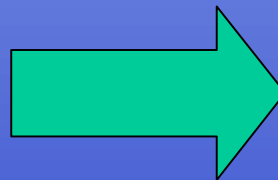
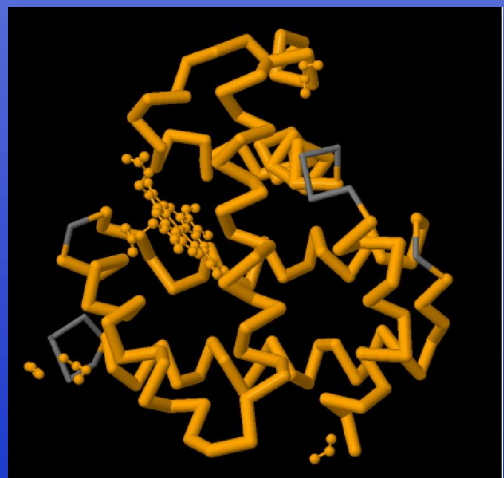
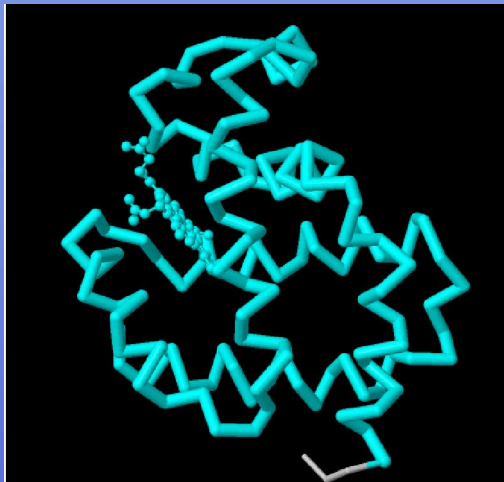
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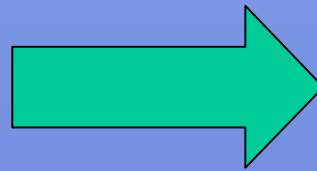
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3D

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+	376
	66
	58
« »	90
	1195

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(PDB 2009)

