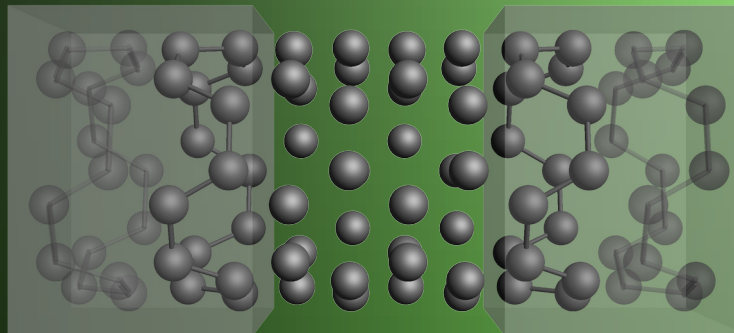


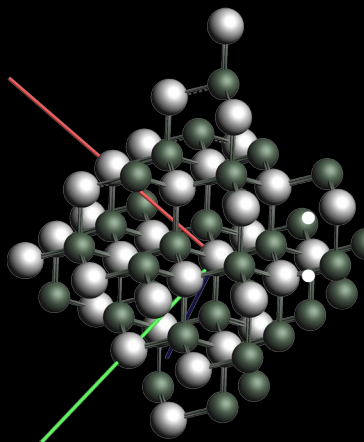


Xyngal Morph



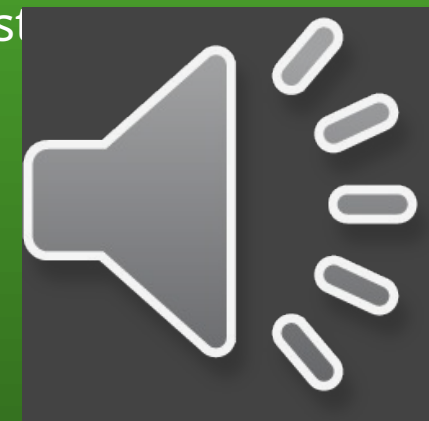
34th Conference on Intelligent Systems for Molecular Biology 2026

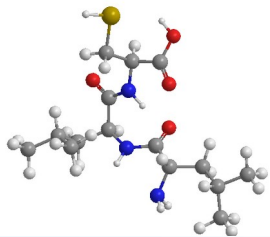
Machine Learning in Computational and Systems Biology



- Harry Shaw, D.Sc., Deborah Preston, Ph.D. co-founders, Xyngal Morph LLC
- Kimberly M. Jackson, Ph.D. Chair, Chemistry and Biochemistry, Professor of Biochemistry, Director, Food Studies Spelman College
- Renee N Shaw, JM, MPH, Spelman College

An ongoing study of novel techniques for predicting inhibitory ligand binding to prevent Androgen Receptor activation

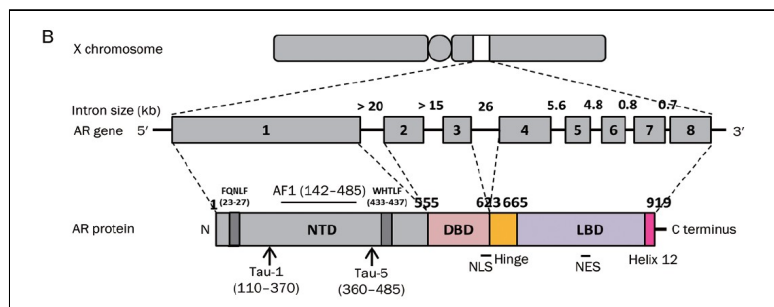




Xyngal Morph

The Importance of Androgen Receptor (AR) activity in prostate cancer

1



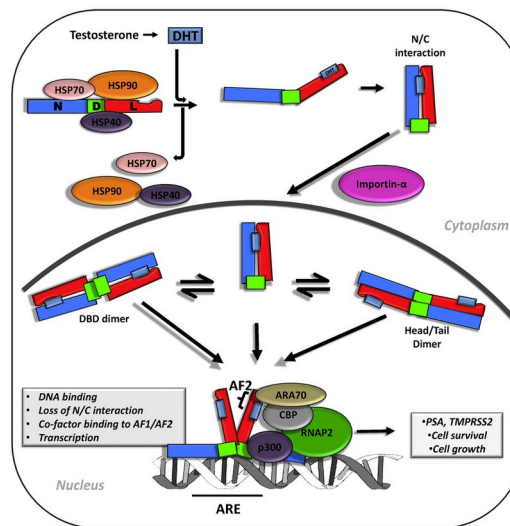
Acta Pharmacologica Sinica (2015) 36: 3–23; doi: 10.1038/aps.2014.18; published online 9 Jun 2014

Jackson, Kimberly M., Monica C. Frazier, and Wayne B. Harris.

"Suppression of androgen receptor expression by dibenzoylmethane as a therapeutic objective in advanced prostate cancer." Anticancer research 27.3B (2007): 1483-1488.

Audio contents include summarized text from the references

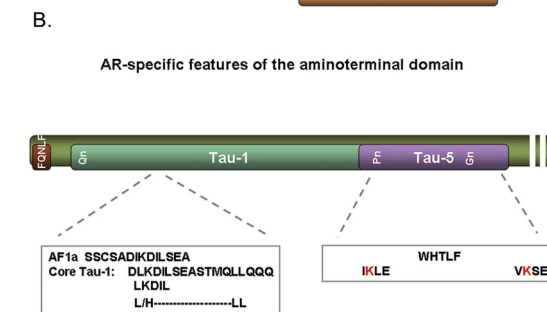
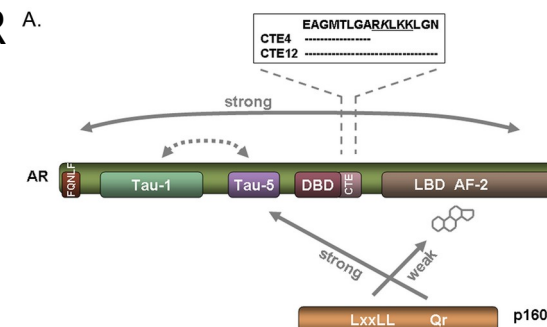
2



Int. J. Mol. Sci. 2013, 14, 12496-12519; doi:10.3390/ijms140612496

3

Known or suspected binding motifs on AR^A.

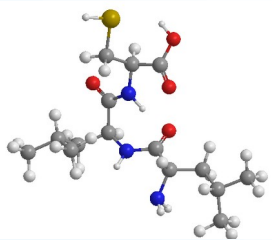


Also, FXXLF and WXXLF Sequences Mediate the NH₂-terminal Interaction with the Ligand Binding Domain of AR

Claessens, Frank, et al. "Diverse roles of androgen receptor (AR) domains in AR-mediated signaling." Nuclear receptor signaling 6.1 (2006): nrs-06008.

He B, Kempainen J, Wilson E FXXLF and WXXLF Sequences Mediate the NH₂-terminal Interaction with the Ligand Binding Domain of the Androgen Receptor, Journal of Biological Chemistry, 2000; 275: 22986-22994

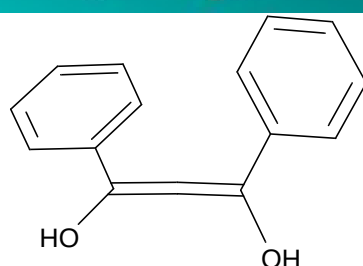
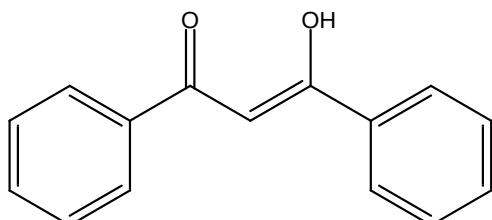
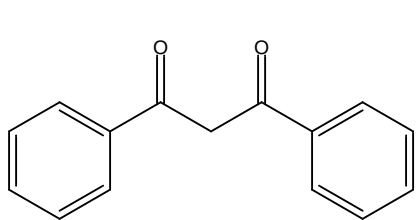
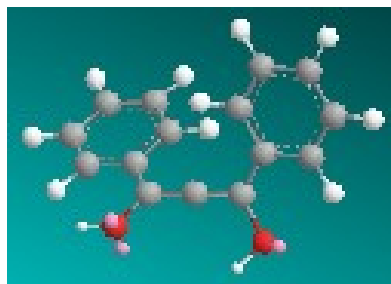
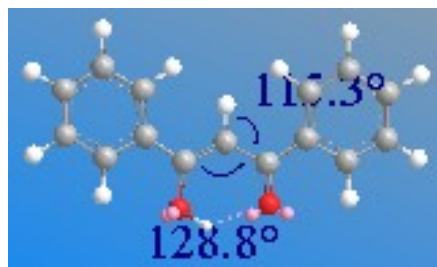
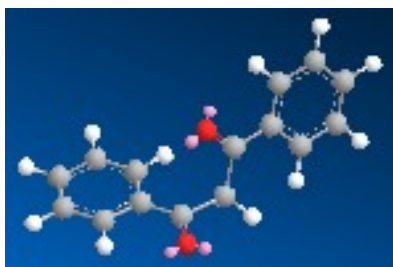




Xyngal Morph

Our research focus is on AR: Dibenzoylmethane (DBM) binding via modeling of Structure Activity Relationships (SAR)

DBM has 3 tautomeric forms: keto, enol, allene. Examining the binding prospects for each form. We are examining the Structure-Activity Relationships (SAR) for each form and thermodynamics of conversion



Stretch: 1.4331
Bend: 4.1248
Stretch-Bend: 0.2140
Torsion: -8.5186
Non-1,4 VDW: 1.6938
1,4 VDW: 17.2327
Dipole/Dipole: 0.6795
Total Energy: 16.8593 kcal/mol

keto

tretch: 2.4864
Bend: 7.7338
Stretch-Bend: 0.2013
Torsion: -11.5493
Non-1,4 VDW: 4.4907
1,4 VDW: 16.7778
Dipole/Dipole: -2.7600
Total Energy: 17.3809 kcal/mol

enol

Stretch: 0.7202
Bend: 2.3599
Stretch-Bend: 0.0056
Torsion: -15.9143
Non-1,4 VDW: -3.1485
1,4 VDW: 13.8462
Dipole/Dipole: -0.3672
Total Energy: -2.4980 kcal/mol

allene

Research indicates that DBM downregulates AR expression. But which tautomer?

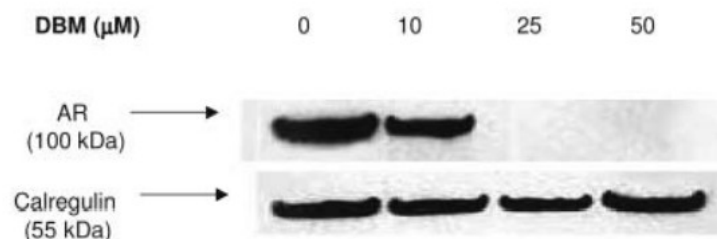
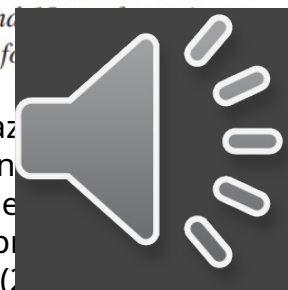
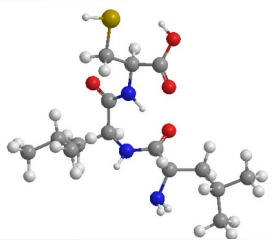


Figure 1. DBM inhibits androgen receptor (AR) protein levels in LNCaP cells. LNCaP cells were treated with different amounts of DBM for 72 h. Whole-cell lysates were extracted from these cells and analyzed by Western blotting. Calregulin was used for

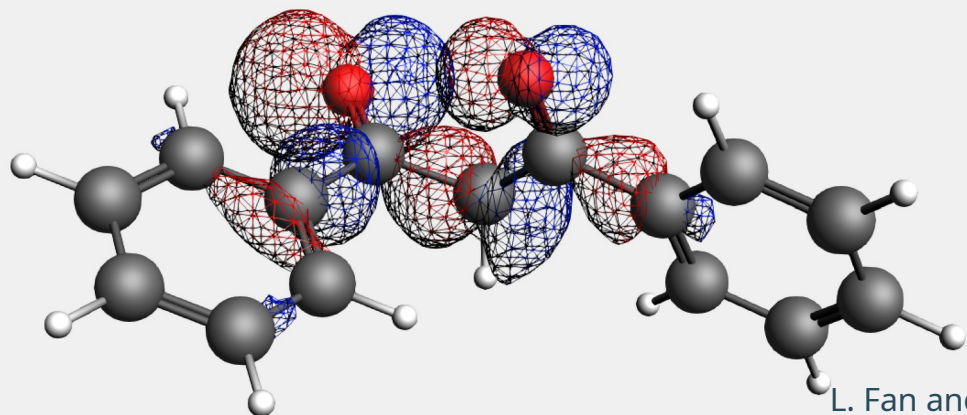
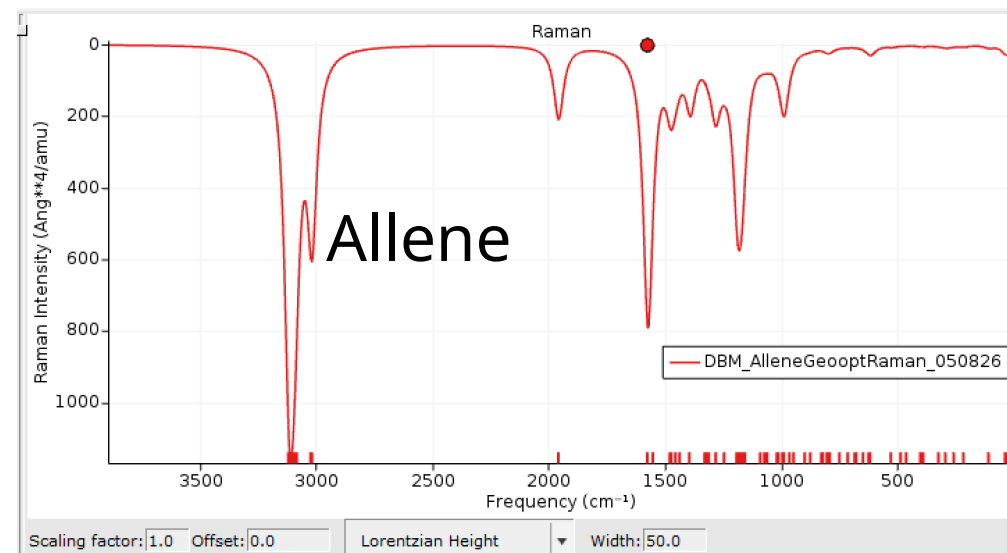
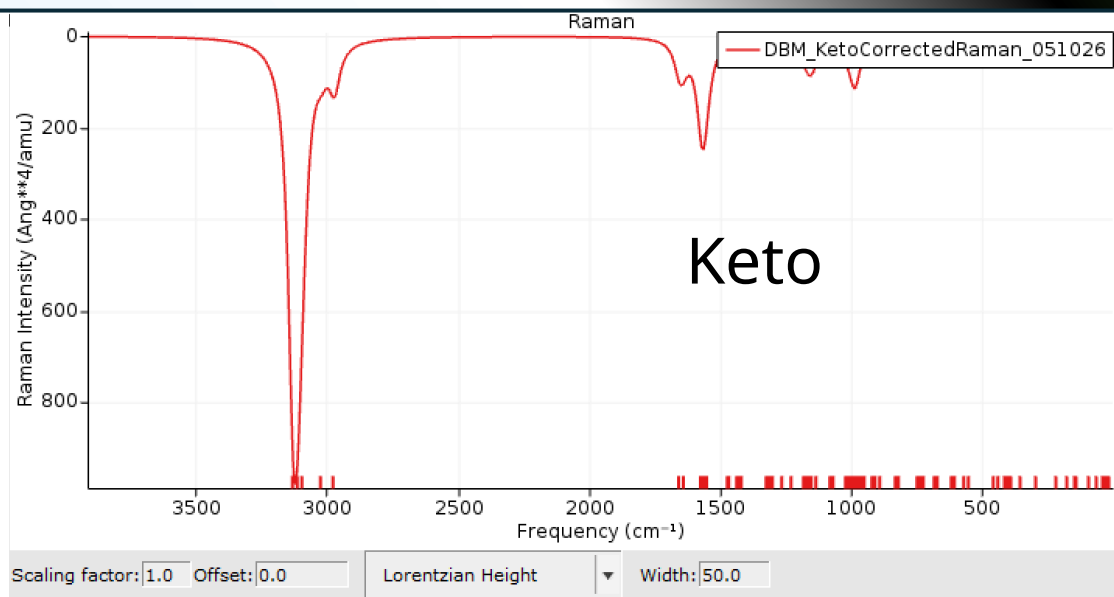
Jackson, Kimberly M., Monica C. Frazee, and Wayne B. Harris. "Suppression of androgen receptor expression by dibenzoylmethane: a novel therapeutic objective in advanced prostate cancer." *Anticancer research* 27.3B (2007): 1488.



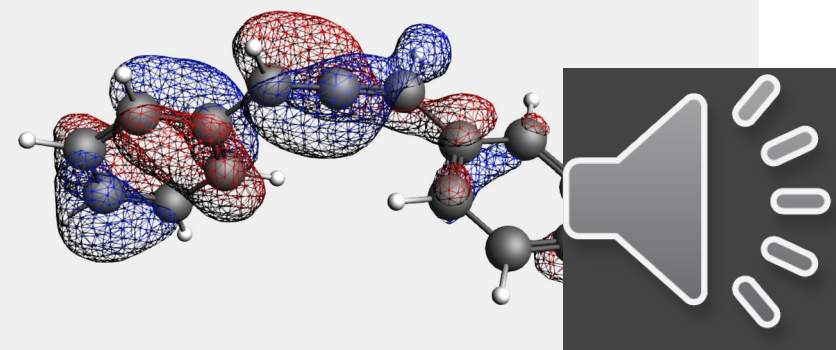


Xyngal Morph

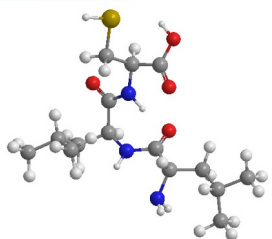
Sample data of the SAR investigations using Raman spectra



HOMO (red is negative, blue is positive)



L. Fan and T. Ziegler, *Application of density functional theory to infrared absorption intensity calculations on main group molecules*, [Journal of Chemical Physics 96, 9005 \(1992\)](#)



Xyngal Morph

Finding binding ligands to AR using AI

Raw: CC(O)

(CSc1ccccc1Cl)c1cc2cc(Cl)c(cc2[nH]1)C

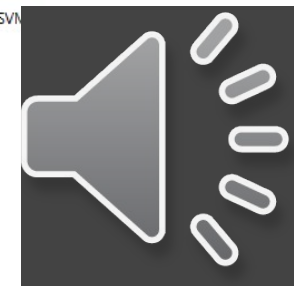
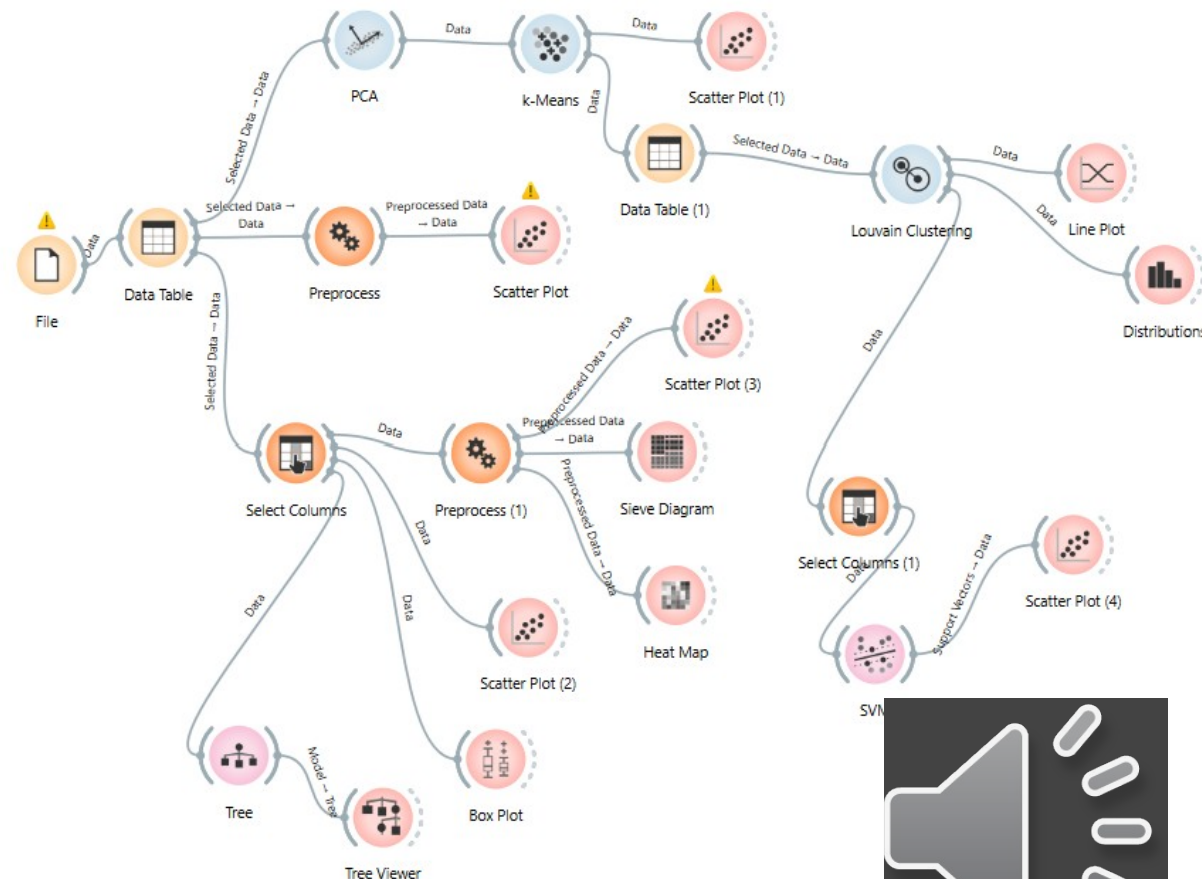
(F)(F)F

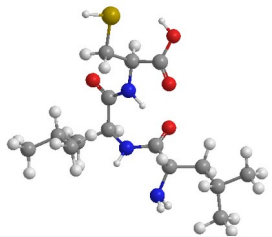
Coded:

c1cc,F,ccccc,Cl,c1cccc

c1

<https://www.bindingdb.org/rwd/bind/index.jsp>



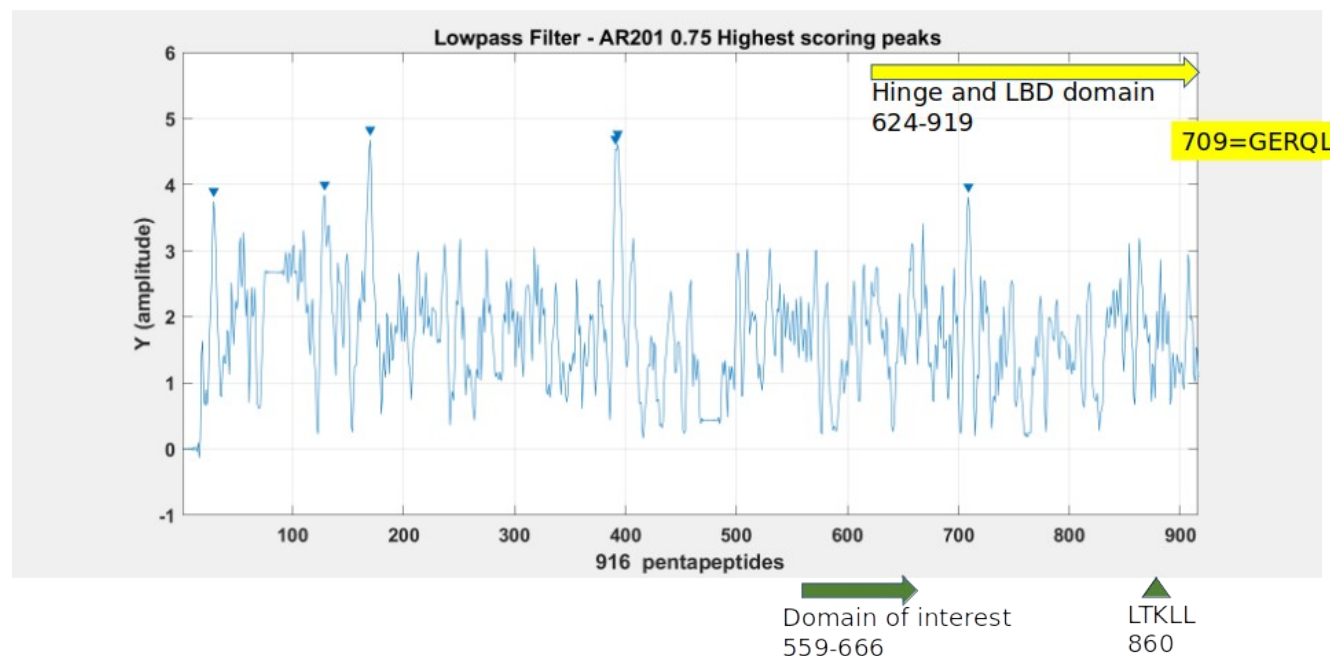


Xyngal Morph

Information theory based modeling to determine AR:DBM binding sites

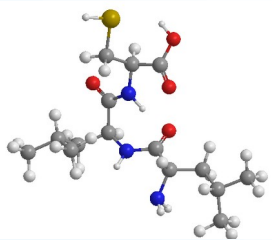
$$H_i = 10 * \left(\frac{(-p_i) * \log_{10}(p_i)}{\log_{10}(2)} \right) \quad H_{n_{\text{pentapeptide}}} = \frac{\sum_{n=1:916} H_n}{5}$$

Figure 4



Sigma Aldrich Hydrophobicity index	Amino Acid	Probability of appearing in AR
-55	D	0.040217
-46	P	0.080435
-31	E	0.059783
-28	N	0.021739
-23	K	0.043478
-14	R	0.044565
-10	Q	0.077174
-5	S	0.088043
1	G	0.10435
8	H	0.020652
13	T	0.040217
41	A	0.088043
49	C	0.029348
63	Y	0.03587
74	M	0.023913
76	V	0.043478
97	L	
97	W	
99	I	
100	F	





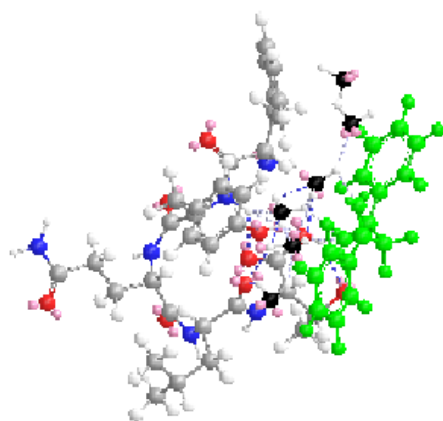
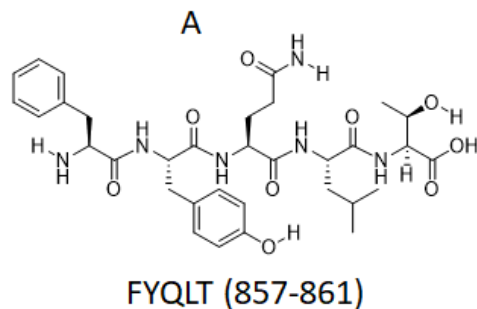
Xyngal Morph

Next steps

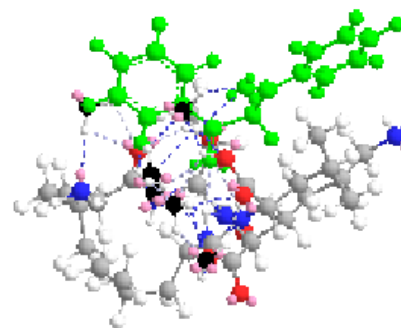
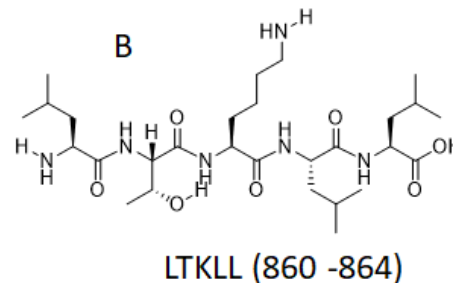
1. Continue the classical modelling of AR:DBM binding investigations with DFT
2. Convert the AR:DBM binding problem into a clique detection problem approachable by a Gaussian Bosonic Sampling processor under development. Clique graphs can be constructed from properties such as the hydrogen bonding networks of

AR peptide sequence

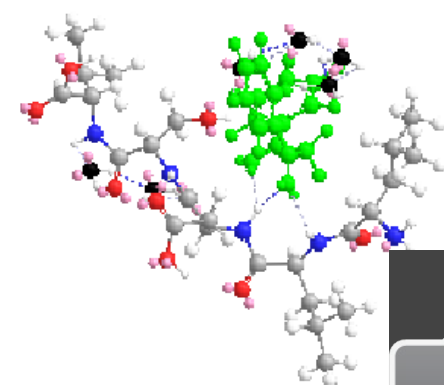
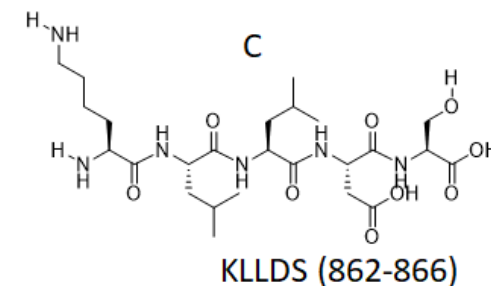
... F Y Q L T K L L D S ...



FYQLT:DBM:6H₂O



LTKLL:DBM:6H₂O



LLDSV:DBM:6H₂O

