



Gina Luciano <gina@visallimedia.com>

Today's Meeting

Hoch, Jeffrey <hoch@uchc.edu>

Tue, Mar 7, 2017 at 3:42 PM

To: Joel Markus <joel@jmarkusdesign.com>, "Schuyler, Adam" <schuyler@uchc.edu>

Cc: Visalli Media <gina@visallimedia.com>

Thanks Joel!

Below is a first stab at categories and exemplars.

- J

1. Spectral

a. Processing

NMRPipe

RNMRTK

NMRfx

b. Visualization

NMRDraw

Sparky

NMRViewJ

2. Assignment

PINE

Abacus

3. Relaxation

ModelFree

DASHA

4. Chemical shift

a. Prediction

SHIFTS

SHIFTX

SHIFTX2

b. Analysis

TALOS+

CS23D

CS-ROSETTA

5. Molecular modeling

a. Dynamics simulation

AMBER

GROMACS

MOSART

b. Docking

HADDOCK

c. Structure determination

AMBER

XPLOR-NIH

CS-ROSETTA

6. Structure

a. Visualization

MOLMOL

VMD

PyMOL

b. Validation

ASDP

ProCheckNMR

7. Redidual dipole couplings

REDCAT

REDCRAFT

PALES

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From: Joel Markus <joel@jmarkusdesign.com>
Sent: Tuesday, March 7, 2017 3:12 PM
To: Schuyler,Adam; Hoch,Jeffrey
Cc: Visalli Media
Subject: Today's Meeting

Adam and Jeff,

Thanks for taking the time to meet this morning to go over a few fundamental flow diagrams for content flow and navigation.

Attached are the two documents that were presented this morning.