Generate PDB and CIF restrain files for ligands of the LH series

1. Prepare the 2D chemical structure using Marvin Sketch (ChemAxon)
2. Add hydrogen atoms to the structure (Structure>Add>Explicit hydrogens)
3. Convert to 3D (Structure>Clean 3D>Clean in 3D)
4. Save as Tripos mol2 file (*.mol2)
5. Go to GRADE server http://grade.globalphasing.org/cgi-bin/grade/server.cgi
6. Choose the mol2 file import option
7. Indicate a 3 letter code and the complete ligand name
8. Indicate the net charge if necessary
9. Check the resulting 2D structure displayed and save PDB and CIF files

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