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Autodock tutorial pdf



4 Ligand → Torsion Tree → Set Number of Torsions...

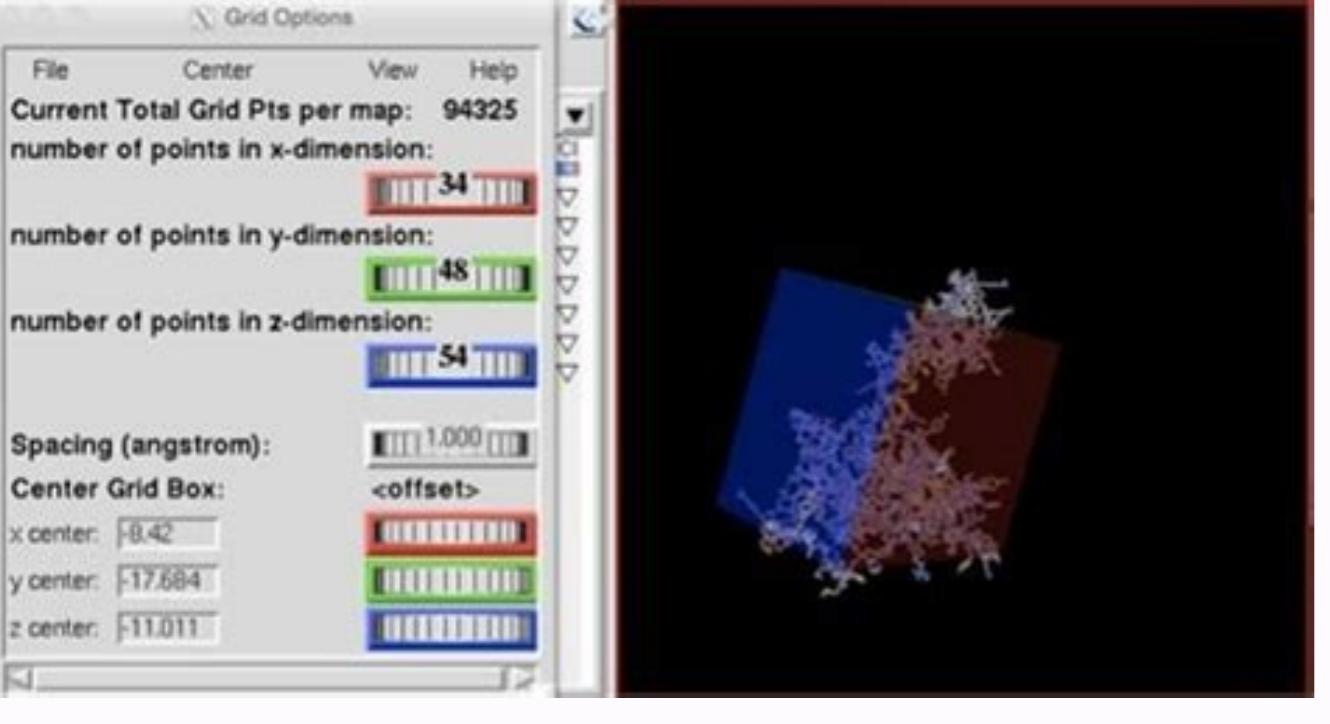
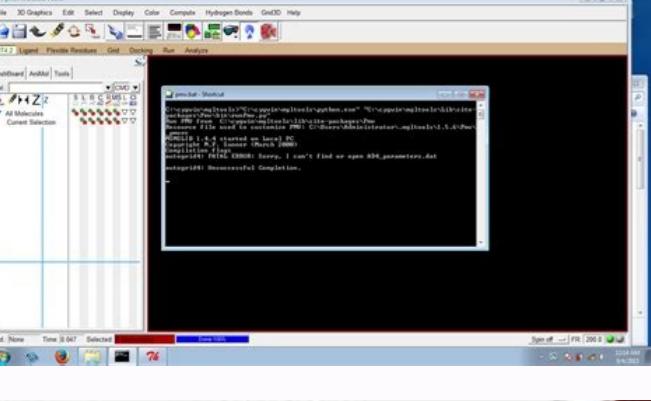
This feature allows you to set the total number of active bonds while specifying whether you want active bonds which move the fewest atoms or those which move the most. To see this distinction, set the radiobutton for **fewest atoms**, type '6' in the entry and then press <Enter> on your keyboard. ADT will turn off all but six torsions, leaving active the torsions which move the fewest atoms.

Set the radiobutton to **most atoms** and type <Enter> in the entry window. You will see a very different set of 6 rotatable bonds.

For our exercise, leave the **6 torsions** that move the **fewest** atoms **active**. Click **Dismis** to close the widget.

5 Ligand → Output → Save as PDBQ...[AD3]

Opens a file browser allowing you to enter a name. Type in 'ind.out.pdbq' and click **Save**.



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