



## How do I deposit a single structure and its associated reference to ChemSpider?

### STEP 1

You will need to be a registered user of [ChemSpider](#) and be logged in. Select the menu for **Depositions** and choose the link to **Deposit Structures**.

### STEP 2

Select the structure picture to access the structure editor. If you have the structure already in a chemical drawing format (mol, sdf, cdx, skc) use the **Browse** button to load the file into the editor.

No existing structure and no desktop drawing package? Select **Draw** or **Edit** to draw the structure in one of the two online applets in [ChemSpider](#).

### STEP 3

Accept the structure and **Add** any of the following pieces of information:

1. Description and tags – general information about the chemical entity
2. Identifiers – chemical names, synonyms, CAS RNs
3. Links to Websites – associated URLs and publication DOIs

The screenshot shows the submission process flowchart at the top: 1. Data Entry → 2. Pre-Processing → 3. Confirmation → 4. Approval by Curator → 5. Publication. Below the flowchart are buttons for 'Cancel Submission' and 'Finish Submission'. The main area displays 'Record 1 of 1' with 'New' and 'Delete' links. A chemical structure of 2-[1-(4-isopropylphenyl)triazol-4-yl]pyridine is shown in a large box. At the bottom, there are input fields for 'External ID' and 'External URL', and a 'Save' button.

When all the steps are completed click **Finish Submission** followed by **Finish and Submit**. Following review by a curator your structure will be accepted for deposition and you will receive an e-mail confirming the deposition.

The published record in [ChemSpider](#) should look like this.

The screenshot shows the published record for 2-[1-(4-isopropylphenyl)triazol-4-yl]pyridine in ChemSpider. The record includes the chemical structure, the name '2-[1-(4-isopropylphenyl)triazol-4-yl]pyridine', the ChemSpider ID '24593844', the molecular formula  $C_{16}H_{16}N_4$ , and various links for 'Similar', 'Wikibox', 'Mass', and 'Machine readable identifiers'. The 'Systematic name' is '2-[1-(4-isopropylphenyl)triazol-4-yl]pyridine', the 'SMILES' string is CC(C)c1ccc(cc1)n2cc(nn2)c3ccccc3, and the 'InChI' string is InChI=1/C16H16N4/c1-12(2)13-6-8-14(9-7-13)20-11-16(18-19-20)15-5-3-4-10-17-15/h3-12H,1-2H3. A sidebar on the right offers additional actions like 'Comments', 'Image', 'Spectrum', 'CIF', 'Identifier', 'Description', 'Data source', 'Publication', 'DOI', 'PubMed ID', and 'URL'.

**▼ Identifiers**

Names and Synonyms

Validated by Experts, Validated by Users, Non-Validated, Removed by Users, Redirected by Users, Redirect Approved by Experts Edit

1-(4-isopropyl phenyl)-4-(2-pyridyl)-1,2,3-triazole

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**▼ Associated Data Sources and Commercial Suppliers** Filter

Publishers | All Data Sources

Data Source	External ID(s)
Royal Society of Chemistry	10:1039/B910660J

The record is linked to the original publication by the DOI



## Dalton Transactions Issue 42, 2009

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**New 1,2,3-triazole ligands through click reactions and their palladium and platinum complexes**

David Schweinfurth, Roberto Pattacini, Sabine Strobel and Biprajit Sarkar

*Dalton Trans.*, 2009, 9291-9297

DOI: 10.1039/B910660J , Paper

Journal Article

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Abstract
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**Abstract**

The new ligands, 1-(4-isopropyl phenyl)-4-(2-pyridyl)-1,2,3-triazole, **1** and 1-(mesityl)-4-(2-pyridyl)-1,2,3-triazole, **2** were prepared by the reactions of the respective azides with 2-ethynylpyridine following the "click method". These ligands together with the reported ligands 1-(phenyl)-4-(2-pyridyl)-1,2,3-triazole, **3** and 1-(benzyl)-4-(2-pyridyl)-1,2,3-triazole, **4** were reacted with palladium and platinum precursors to give mononuclear *cis*-dichloropalladium and platinum complexes containing the triazole ligands. Structural characterisation of the free ligand **3** shows that the central N–N bond in the triazole ring has double bond character and hence is best described as an "azo-like" N–N double bond. The pyridine ring in **3** has an almost "anti" conformation with respect to the central triazole ring. The metal centers bind to the ligands through the pyridine N and a triazole N atom. The metal–N(triazole) distances are shorter than the metal–N(pyridine) distances. Cyclic voltammograms of the ligands show reduction processes that appear at extreme negative potentials. Coordination of metal centers induces huge anodic shifts of the reduction potentials due to  $\sigma$ -polarisation by the metal centers. UV/vis spectra of the ligands and complexes are also discussed. The properties of such chelating triazole ligands towards palladium and platinum centers is being compared and contrasted to the widely used 2,2'-bipyridine ligand.