Subject: Name to structure - Triple bonds are not parsed Posted by MaxPeters on Thu, 18 Feb 2016 11:38:53 GMT

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Entering the SMILES for HCN: C#N

in the web form results in

CH4.

The same is true for organic nitriles, they either result in terminal groups or parsing errors.

Subject: Re: Name to structure - Triple bonds are not parsed Posted by thomas on Sun, 21 Feb 2016 12:24:35 GMT View Forum Message <> Reply to Message

Thank you for reporting this. I found and fixed the bug. The # sign was not properly encoded in the URL sent to the server causing the smiles to to be truncated at the #-position.