

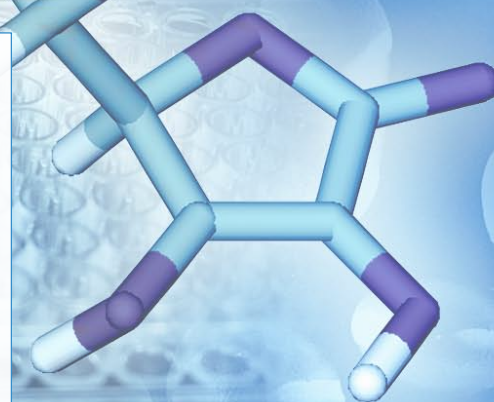
● **Molecular Profile™**

Sample: Bruker\_STR\_3427

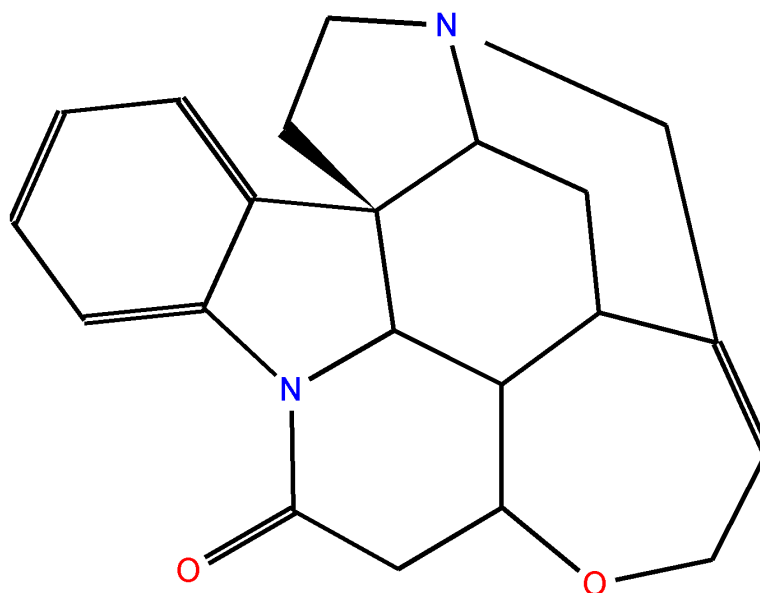
Measured on 14-Jan-2008 16:09:59

**Results Summary**

Type of Analysis	Result	Status
<b>NMR Spectroscopy</b>		
1D-Proton-verification	97%	●
2D-HSQC-verification	77%	●
Concentration [mg/ml]	1.8	
Purity	>80%	●
<b>Overall Status</b>		●



Structure to be verified:



Sum Formula:	C <sub>21</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Average Mass:	334.420913 u
Monoisotopic Neutral Mass:	334.175424 u

SMILES:

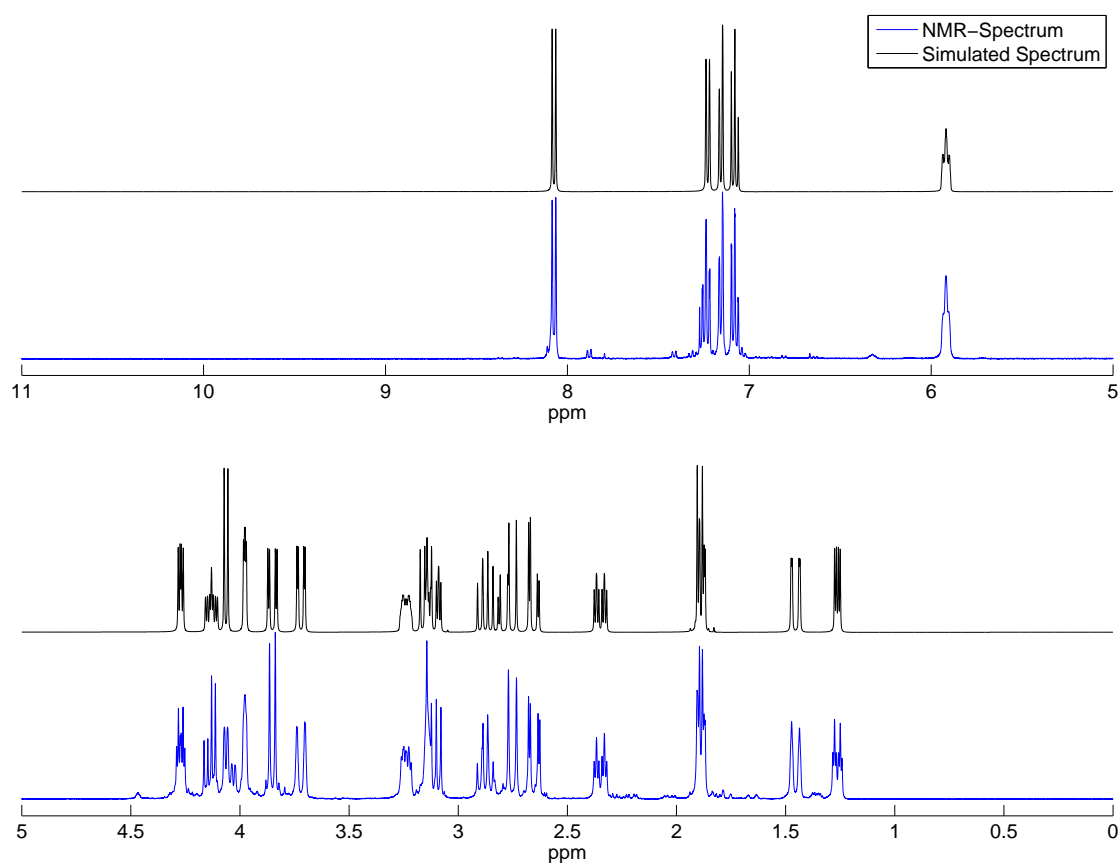
C1[C@@H]2[N@@]3CC[C@@]42[C@H]2N(c5c4cccc5)C(C[C@H]4[C@H]2[C@@H]1C(=CCO4)C3)=O

InChi:

1/C21H22N2O2/c24-18-10-16-19-13-9-17-21(6-7-22(17)11-12(13)5-8-25-16)14-3-1-2-4-15(14)23(18)20(19)21/h1-5,13,16-17,19-20H,6-11H2/t13-,16-,17-,19-,20-,21+/m0/s1

### NMR Results (1D-Proton-Verification):

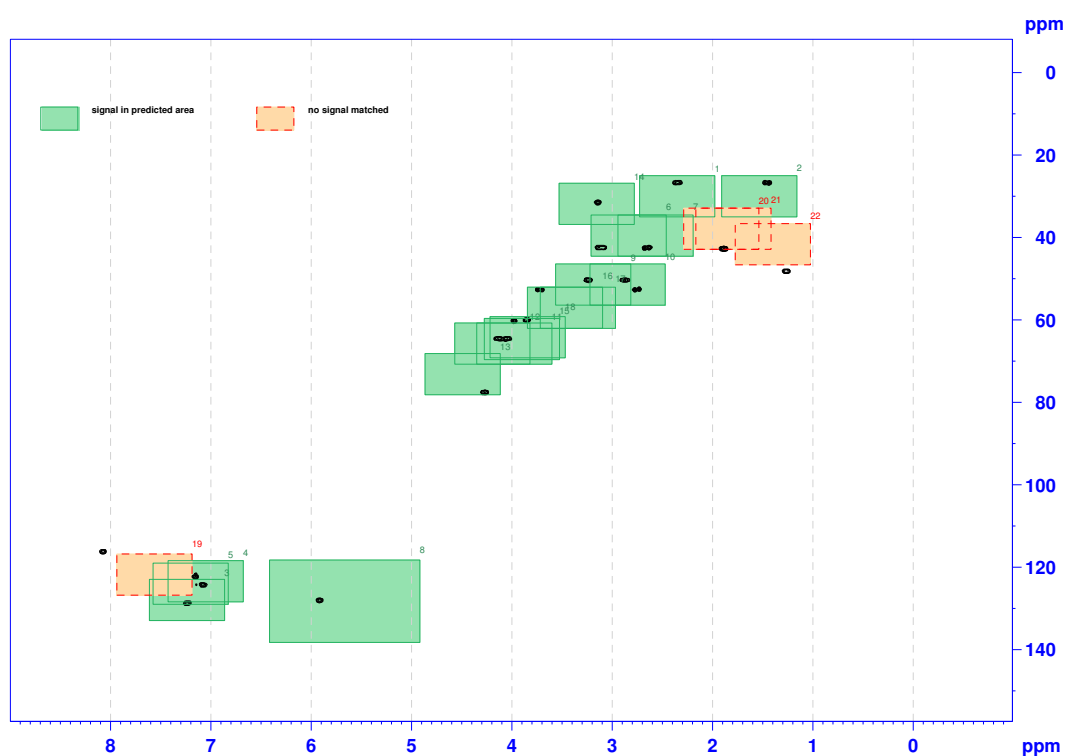
Following figure shows the comparison of the measured <sup>1</sup>H-NMR spectrum with the predicted and iterated spectrum of the given molecule.



Overall Rating	97 %
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### NMR Results (2D-HSQC-Verification):

Following figure shows the HSQC-Spectrum of your sample. The boxes drawn inside represent the NMR-prediction of your molecule (with error bar). If the peaks of the spectrum can be mapped bijective to the predicted boxes, the verification result is 100%.



### HSQC Prediction Results:

Type of Analysis	Result
Patterns hit	18 of 22
Peaks covered	44 of 47
<b>Overall Rating</b>	<b>77 %</b>