

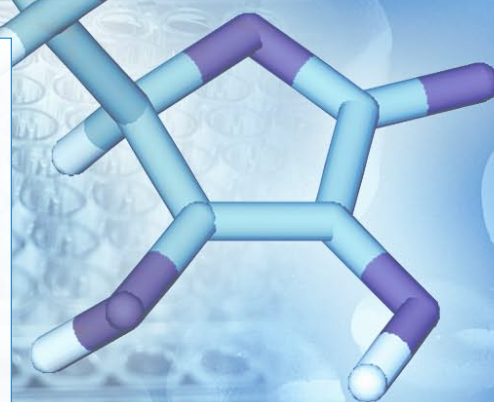
● **Molecular Profile**[™]

Sample: **Strychnine**

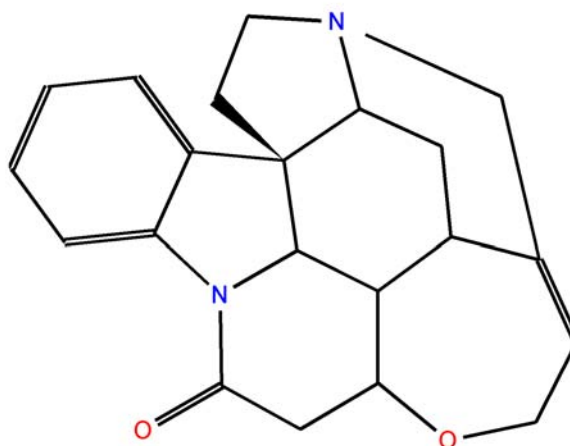
Measured on 13-Oct-2008 16:18:32

Results Summary

Type of Analysis	Result	Status
Mass Spectroscopy		
LC-MS pos. Ionisation	87%	●
LC-MS neg. Ionisation	–	○
Purity (BPC)	96%	●
NMR Spectroscopy		
1D-Proton-verification	98%	●
2D-HSQC-verification	96%	●
Concentration [mg/ml]	1.8	
Purity	91%	
Overall Status	87%	●



Structure to be verified:



Sum Formula:	C ₂₁ H ₂₂ O ₂ N ₂
Average Mass:	334.420913 u
Monoisotopic Neutral Mass:	334.168128 u

SMILES:

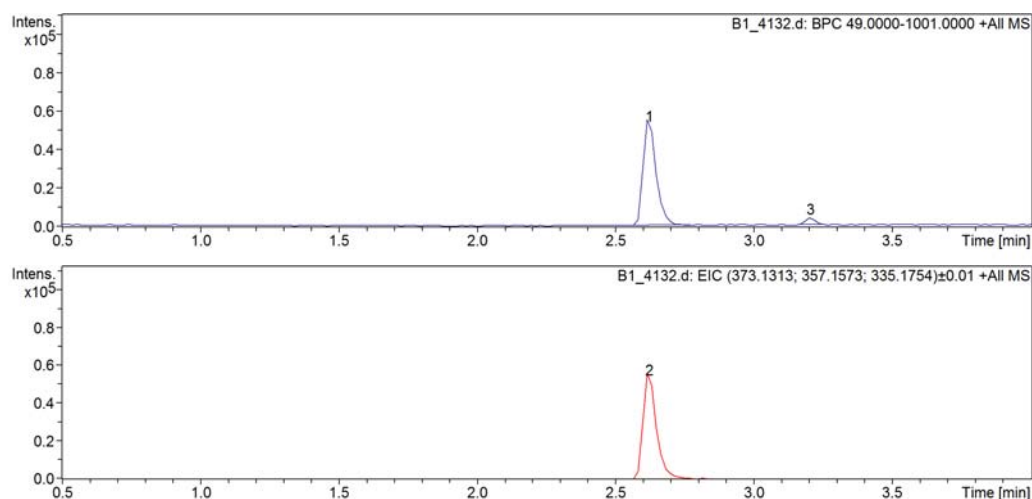
C1[C@@H]2[N@@]3CC[C@@]42[C@H]2N(c5c4cccc5)C(C[C@H]4[C@H]2[C@@H]1C(=CCO4)C3)=O

InChI:

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

LC-MS Results:

Following figure shows the chromatograms BPC, EIC and UV of your sample.



Confirm Formula Results

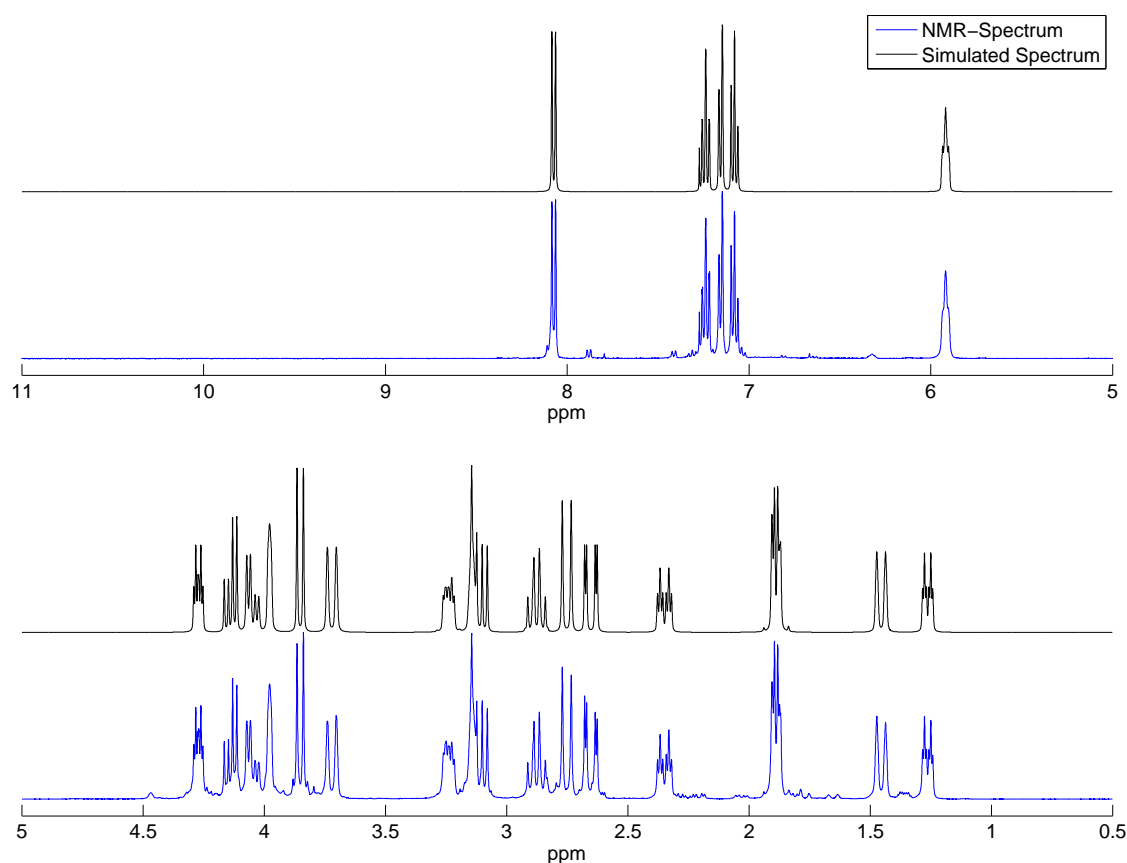
#	meas. m/z	theo. m/z	err [ppm]	Sigma	Formula	Adduct	Purity(BPC)
2	335.1752	335.1754	0.6	0.010	C ₂₁ H ₂₃ N ₂ O ₂	M+H	95.8%

Impurity Formula Results

#	meas. m/z	theo. m/z	err [ppm]	Sigma	Formula
3	229.1408	229.1410	1.2	0.008	C ₁₀ H ₂₂ NaO ₄
3	229.1408	229.1408	0	0.011	C ₈ H ₁₇ N ₆ O ₂

NMR Results (1D-Proton-Verification):

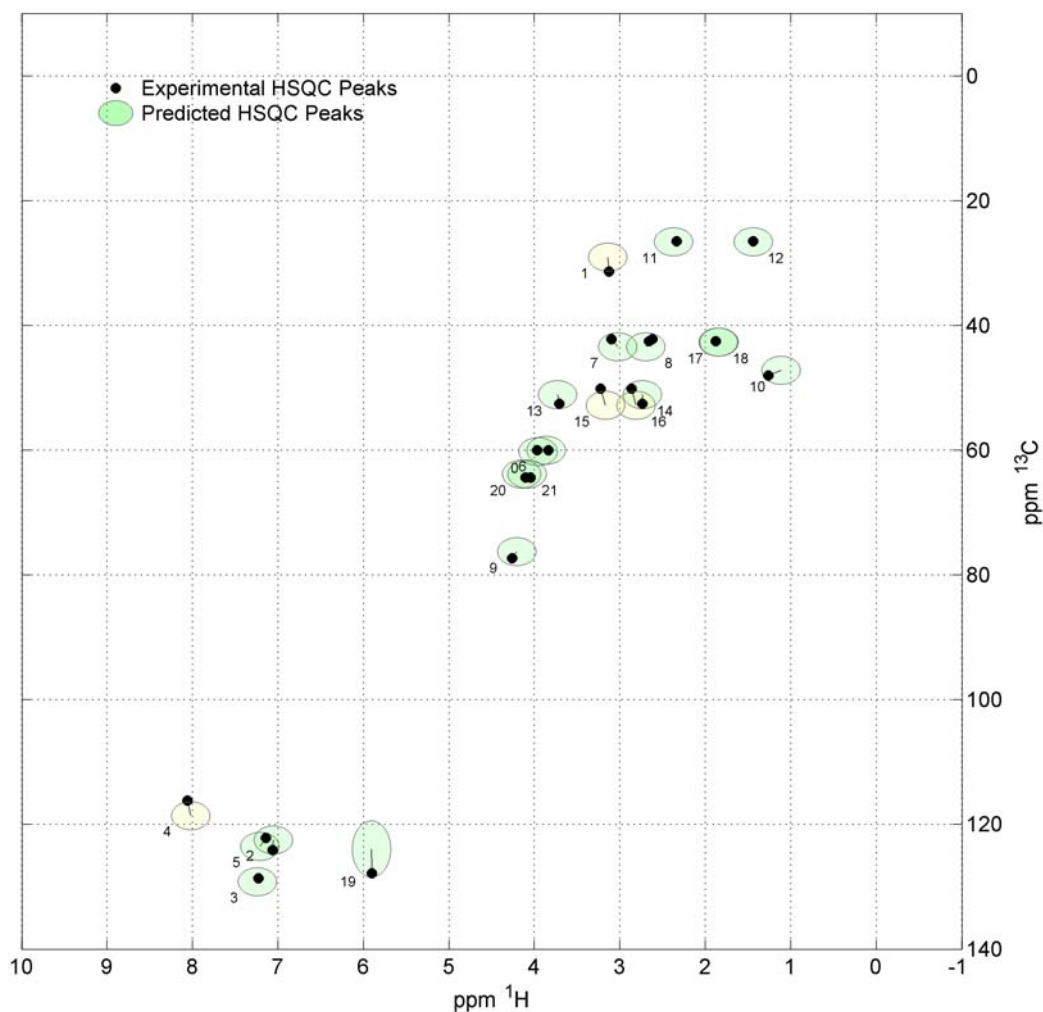
Following figure shows the comparison of the measured ¹H-NMR spectrum with the predicted and iterated spectrum of the given molecule.



Overall Rating	98%
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NMR Results (2D-HSQC-Verification):

Following figure shows the HSQC-Spectrum of your sample.



Overall Rating	96%
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