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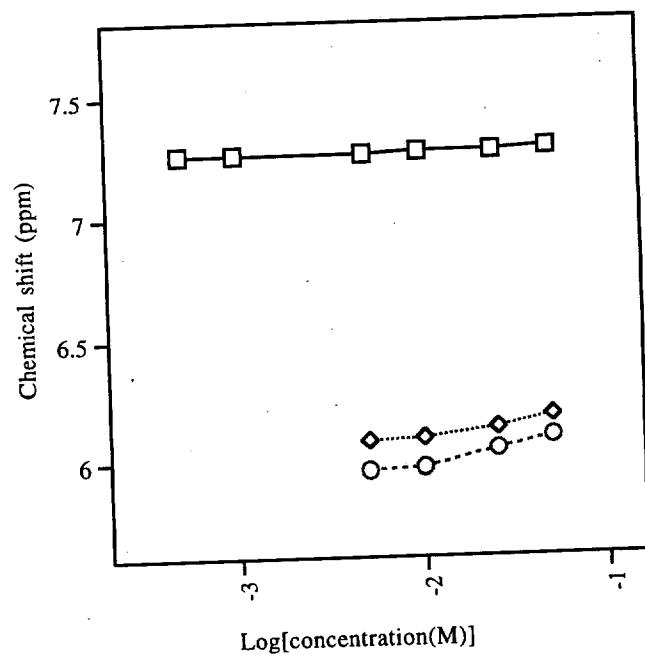
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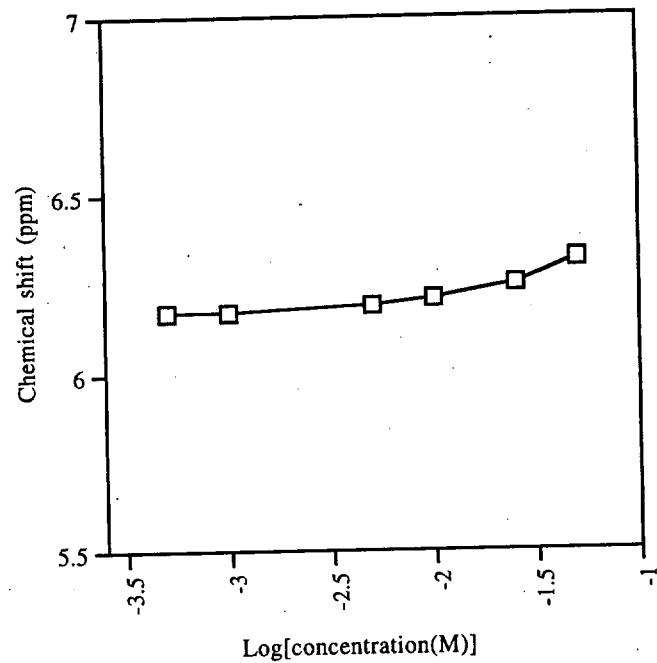
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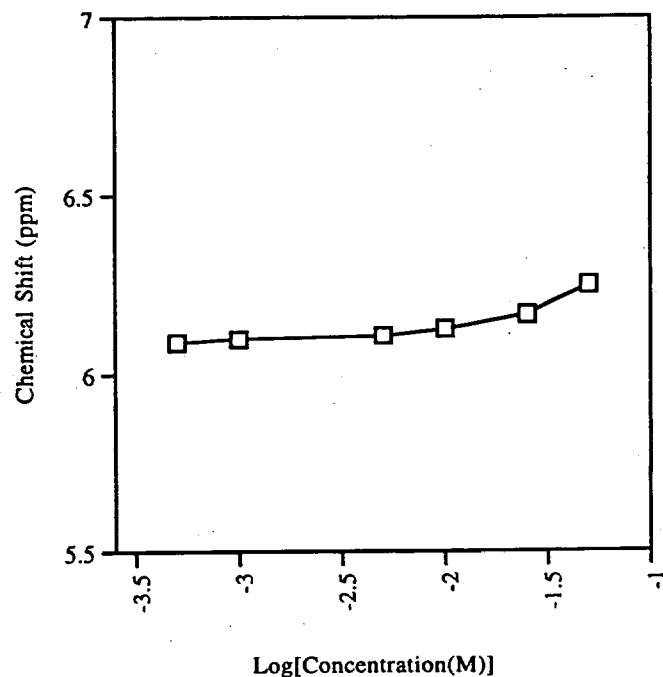
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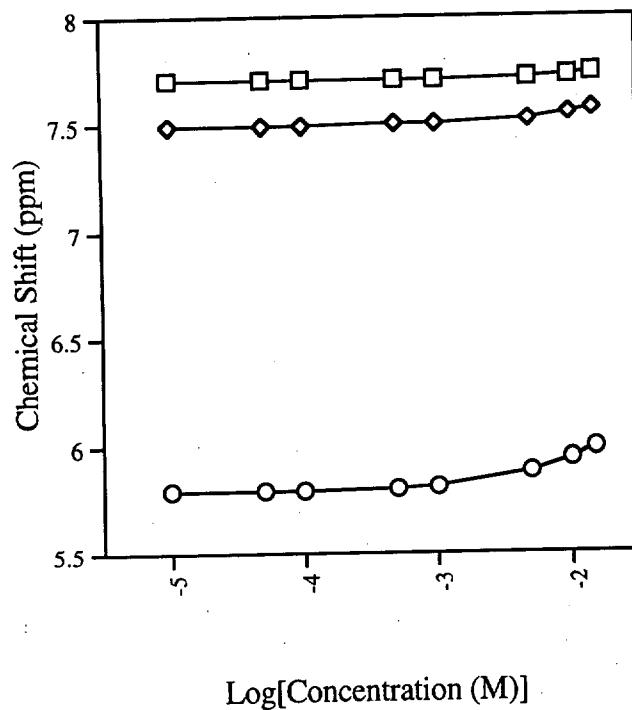
Supplementary Figure 1. Amide proton NMR chemical shifts in for **1** CD_2Cl_2 at rm temp, as a function of the logarithm of concentration. Squares: major conformer; diamonds and circles: minor conformers (detected only at higher concentrations). The lines are arbitrary.



Supplementary Figure 2. Amide proton NMR chemical shifts in for the major rotamer of 2 CD₂Cl₂ at rm temp, as a function of the logarithm of concentration. The line is arbitrary.



Supplementary Figure 3. Amide proton NMR chemical shifts in for the major rotamer of 3 CD₂Cl₂ at rm temp, as a function of the logarithm of concentration. The line is arbitrary.



Supplementary Figure 4. Amide proton NMR chemical shifts for the major rotamer of **7** in CD_2Cl_2 at rm temp, as a function of the logarithm of concentration. Circles: NH1; squares: NH2; diamonds: NH3 (numbering from N-terminus to C-terminus). The lines are arbitrary.

Experimental

A colorless prism-shaped crystal of dimensions $0.42 \times 0.18 \times 0.08$ mm was selected for structural analysis. Intensity data for this compound were collected using a Siemens SMART ccd area detector(1) mounted on a Siemens P4 diffractometer equipped with graphite-monochromated Mo K α radiation ($\lambda = 0.71073$ Å). The sample was cooled to 153(2) K. The intensity data, which nominally covered one and a half hemispheres of reciprocal space, were measured as a series of ϕ oscillation frames each of 0.4 ° for 60 sec / frame. The detector was operated in 512×512 mode and was positioned 5.26 cm from the sample. Coverage of unique data was 99.1 % complete to 25.00 degrees in θ . Cell parameters were determined from a non-linear least squares fit of 8192 peaks in the range $3.0 < \theta < 25.0$ °. The first 50 frames were repeated at the end of data collection and yielded a total of 419 peaks showing a variation of -0.01 % during the data collection. A total of 19922 data were measured in the range $2.31 < \theta < 29.14$ °. The data were corrected for absorption by the empirical method (2) giving minimum and maximum transmission factors of 0.675 and 0.956. The data were merged to form a set of 9702 independent data with $R(\text{int}) = 0.0432$.

The orthorhombic space group P2(1)2(1)2(1) was determined by systematic absences and statistical tests and verified by subsequent refinement. The structure was solved by direct methods and refined by full-matrix least-squares methods on F^2 (3). Hydrogen atom positions were initially determined by geometry and refined by a riding model. Non-hydrogen atoms were refined with anisotropic displacement parameters. A total of 478 parameters were refined against 0 restraints and 9702 data to give $wR(F^2) = 0.1078$ and $S = 0.979$ for weights of $w = 1/[\sigma^2(F^2) + (0.0438 P)^2]$, where $P = [F_0^2 + 2F_c^2] / 3$. The final $R(F)$ was 0.0526 for the 6763 observed, [$F > 4\sigma(F)$], data. The largest shift/s.u. was 0.009 in the final refinement cycle. The final difference map had maxima and minima of 0.355 and -0.272 e/Å³, respectively. The absolute structure was determined by refinement of the Flack parameter(4).

Comment

The displacement ellipsoids were drawn at the 50% probability level.

Acknowledgment

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CRYSTALLOGRAPHIC RESULTS FOR COMPOUND 8

Table 1. Crystal data and structure refinement

| | |
|-----------------------------------|--|
| Identification code | 98102 |
| Empirical formula | C41 H59 N5 O6 S |
| Formula weight | 749.99 |
| Crystal system | Orthorhombic |
| Space group | P2(1)2(1)2(1) |
| Unit cell dimensions | a = 9.9579(2) Å α = 90°. b = 18.7977(4) Å β = 90°. c = 21.8917(4) Å γ = 90°. |
| Volume | 4097.81(14) Å ³ |
| Z | 4 |
| Density (calculated) | 1.216 Mg/m ³ |
| Wavelength | 0.71073 Å |
| Temperature | 153(2) K |
| F(000) | 1616 |
| Absorption coefficient | 0.130 mm ⁻¹ |
| Absorption correction | Empirical |
| Max. and min. transmission | 0.956 and 0.675 |
| Theta range for data collection | 2.31 to 29.14°. |
| Reflections collected | 19922 |
| Independent reflections | 9702 [R(int) = 0.0432] |
| Data / restraints / parameters | 9702 / 0 / 478 |
| wR(F ² all data) | wR2 = 0.1078 |
| R(F obsd data) | R1 = 0.0526 |
| Goodness-of-fit on F ² | 0.979 |
| Observed data [I > 2σ(I)] | 6763 |
| Absolute structure parameter | -0.02(8) |
| Largest and mean shift / s.u. | 0.009 and 0.001 |
| Largest diff. peak and hole | 0.355 and -0.272 e/Å ³ |

Table 2. Atomic coordinates and equivalent isotropic displacement parameters
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij}
 tensor.

| | x | y | z | $U(\text{eq})$ |
|-------|-------------|-------------|-------------|----------------|
| S(1) | 0.01292(7) | 0.37048(4) | 0.22018(3) | 0.03403(17) |
| O(1) | 0.18738(18) | 0.21045(8) | 0.37588(7) | 0.0288(4) |
| O(2) | 0.13525(17) | 0.31918(8) | 0.41658(7) | 0.0284(4) |
| O(3) | 0.29478(17) | 0.51904(8) | 0.35530(7) | 0.0287(4) |
| O(4) | 0.57497(19) | 0.75853(8) | 0.25951(8) | 0.0356(5) |
| O(5) | 0.2379(2) | 0.70208(8) | 0.52701(8) | 0.0369(5) |
| O(6) | 0.1584(2) | 0.45639(9) | 0.62175(8) | 0.0404(5) |
| N(1) | 0.2153(2) | 0.30567(9) | 0.31947(8) | 0.0232(5) |
| N(2) | 0.44085(19) | 0.52811(9) | 0.27601(9) | 0.0221(4) |
| N(3) | 0.4946(2) | 0.74368(9) | 0.35503(9) | 0.0259(5) |
| N(4) | 0.2649(2) | 0.59914(9) | 0.47399(9) | 0.0261(5) |
| N(5) | 0.1421(2) | 0.37133(10) | 0.54974(9) | 0.0314(5) |
| C(1) | 0.2732(3) | 0.19268(14) | 0.47919(12) | 0.0388(7) |
| C(2) | 0.1678(3) | 0.17007(12) | 0.43287(11) | 0.0274(6) |
| C(3) | 0.1927(3) | 0.09400(12) | 0.41286(12) | 0.0395(7) |
| C(4) | 0.0251(3) | 0.17897(15) | 0.45568(13) | 0.0405(7) |
| C(5) | 0.1760(2) | 0.28204(11) | 0.37502(10) | 0.0225(5) |
| C(6) | 0.2260(2) | 0.38106(11) | 0.30513(10) | 0.0231(5) |
| C(7) | 0.1851(3) | 0.39394(13) | 0.23837(11) | 0.0312(6) |
| C(8) | 0.0226(3) | 0.27842(14) | 0.20053(12) | 0.0341(6) |
| C(9) | -0.0522(3) | 0.22913(16) | 0.23373(15) | 0.0473(8) |
| C(10) | -0.0566(3) | 0.15892(17) | 0.21506(18) | 0.0592(10) |
| C(11) | 0.0137(4) | 0.13710(17) | 0.16433(18) | 0.0640(11) |
| C(12) | 0.0889(4) | 0.18490(18) | 0.13164(15) | 0.0586(10) |
| C(13) | 0.0940(3) | 0.25599(15) | 0.14903(14) | 0.0445(8) |
| C(14) | 0.3711(2) | 0.40866(11) | 0.31491(10) | 0.0216(5) |
| C(15) | 0.4360(2) | 0.38275(12) | 0.37494(11) | 0.0268(6) |
| C(16) | 0.5819(3) | 0.40540(12) | 0.37958(11) | 0.0252(5) |
| C(17) | 0.6831(3) | 0.36410(13) | 0.35474(11) | 0.0313(6) |

| | | | | |
|-------|-----------|-------------|-------------|-----------|
| C(18) | 0.8168(3) | 0.38379(14) | 0.35994(12) | 0.0382(7) |
| C(19) | 0.8505(3) | 0.44629(15) | 0.38907(12) | 0.0391(7) |
| C(20) | 0.7510(3) | 0.48989(14) | 0.41220(11) | 0.0337(6) |
| C(21) | 0.6173(3) | 0.46914(13) | 0.40748(11) | 0.0286(6) |
| C(22) | 0.3670(2) | 0.48984(11) | 0.31607(10) | 0.0217(5) |
| C(23) | 0.5427(3) | 0.50238(12) | 0.23223(11) | 0.0273(6) |
| C(24) | 0.6783(2) | 0.53659(12) | 0.24507(11) | 0.0267(6) |
| C(25) | 0.6691(2) | 0.61802(12) | 0.24755(11) | 0.0270(6) |
| C(26) | 0.5656(2) | 0.63822(11) | 0.29595(10) | 0.0221(5) |
| C(27) | 0.4300(2) | 0.60571(11) | 0.27749(12) | 0.0255(5) |
| C(28) | 0.5468(2) | 0.71850(12) | 0.30235(11) | 0.0244(5) |
| C(29) | 0.4686(3) | 0.82029(12) | 0.36241(12) | 0.0314(6) |
| C(30) | 0.3189(3) | 0.83268(12) | 0.37102(12) | 0.0341(6) |
| C(31) | 0.2655(3) | 0.79067(12) | 0.42574(12) | 0.0333(6) |
| C(32) | 0.3007(3) | 0.71123(12) | 0.42050(11) | 0.0248(5) |
| C(33) | 0.4520(2) | 0.70233(12) | 0.40864(11) | 0.0256(6) |
| C(34) | 0.2629(2) | 0.67109(12) | 0.47868(11) | 0.0243(5) |
| C(35) | 0.2596(2) | 0.55181(11) | 0.52689(11) | 0.0242(5) |
| C(36) | 0.3978(3) | 0.51906(13) | 0.53980(12) | 0.0308(6) |
| C(37) | 0.5098(3) | 0.57445(13) | 0.54600(12) | 0.0328(6) |
| C(38) | 0.1503(3) | 0.49501(12) | 0.51694(11) | 0.0266(6) |
| C(39) | 0.0105(3) | 0.52899(14) | 0.51712(13) | 0.0385(7) |
| C(40) | 0.1526(3) | 0.43939(13) | 0.56713(12) | 0.0291(6) |
| C(41) | 0.1320(3) | 0.31462(14) | 0.59490(12) | 0.0416(7) |

Table 3. Bond lengths [\AA] and angles [$^\circ$]

| | | | |
|------------------|----------|------------------|------------|
| S(1)-C(8) | 1.786(3) | C(9)-C(10) | 1.382(4) |
| S(1)-C(7) | 1.815(3) | C(10)-C(11) | 1.375(5) |
| O(1)-C(5) | 1.351(3) | C(11)-C(12) | 1.371(5) |
| O(1)-C(2) | 1.473(3) | C(12)-C(13) | 1.390(4) |
| O(2)-C(5) | 1.217(3) | C(14)-C(22) | 1.527(3) |
| O(3)-C(22) | 1.248(3) | C(14)-C(15) | 1.544(3) |
| O(4)-C(28) | 1.235(3) | C(15)-C(16) | 1.517(3) |
| O(5)-C(34) | 1.233(3) | C(16)-C(17) | 1.383(3) |
| O(6)-C(40) | 1.239(3) | C(16)-C(21) | 1.390(3) |
| N(1)-C(5) | 1.352(3) | C(17)-C(18) | 1.386(4) |
| N(1)-C(6) | 1.455(3) | C(18)-C(19) | 1.378(4) |
| N(2)-C(22) | 1.352(3) | C(19)-C(20) | 1.382(4) |
| N(2)-C(27) | 1.463(3) | C(20)-C(21) | 1.391(4) |
| N(2)-C(23) | 1.477(3) | C(23)-C(24) | 1.522(3) |
| N(3)-C(28) | 1.351(3) | C(24)-C(25) | 1.534(3) |
| N(3)-C(29) | 1.472(3) | C(25)-C(26) | 1.526(3) |
| N(3)-C(33) | 1.470(3) | C(26)-C(28) | 1.527(3) |
| N(4)-C(34) | 1.356(3) | C(26)-C(27) | 1.536(3) |
| N(4)-C(35) | 1.461(3) | C(29)-C(30) | 1.521(4) |
| N(5)-C(40) | 1.339(3) | C(30)-C(31) | 1.530(3) |
| N(5)-C(41) | 1.457(3) | C(31)-C(32) | 1.538(3) |
| C(1)-C(2) | 1.520(4) | C(32)-C(34) | 1.528(3) |
| C(2)-C(3) | 1.516(3) | C(32)-C(33) | 1.538(3) |
| C(2)-C(4) | 1.516(4) | C(35)-C(36) | 1.534(3) |
| C(6)-C(7) | 1.536(3) | C(35)-C(38) | 1.540(3) |
| C(6)-C(14) | 1.550(3) | C(36)-C(37) | 1.532(3) |
| C(8)-C(9) | 1.393(4) | C(38)-C(40) | 1.517(3) |
| C(8)-C(13) | 1.398(4) | C(38)-C(39) | 1.531(4) |
| C(8)-S(1)-C(7) | | C(22)-N(2)-C(23) | 128.33(18) |
| C(5)-O(1)-C(2) | | C(27)-N(2)-C(23) | 113.07(18) |
| C(5)-N(1)-C(6) | | C(28)-N(3)-C(29) | 120.28(19) |
| C(22)-N(2)-C(27) | | C(28)-N(3)-C(33) | 127.40(18) |

| | | | |
|-------------------|------------|-------------------|------------|
| C(29)-N(3)-C(33) | 112.27(18) | C(16)-C(21)-C(20) | 121.1(2) |
| C(34)-N(4)-C(35) | 123.1(2) | O(3)-C(22)-N(2) | 121.74(19) |
| C(40)-N(5)-C(41) | 120.8(2) | O(3)-C(22)-C(14) | 117.8(2) |
| O(1)-C(2)-C(3) | 102.69(18) | N(2)-C(22)-C(14) | 120.4(2) |
| O(1)-C(2)-C(1) | 109.25(19) | N(2)-C(23)-C(24) | 110.55(18) |
| C(3)-C(2)-C(1) | 110.1(2) | C(23)-C(24)-C(25) | 112.0(2) |
| O(1)-C(2)-C(4) | 110.2(2) | C(26)-C(25)-C(24) | 108.24(19) |
| C(3)-C(2)-C(4) | 110.6(2) | C(25)-C(26)-C(28) | 113.10(19) |
| C(1)-C(2)-C(4) | 113.4(2) | C(25)-C(26)-C(27) | 108.20(18) |
| O(2)-C(5)-N(1) | 125.5(2) | C(28)-C(26)-C(27) | 108.03(19) |
| O(2)-C(5)-O(1) | 126.1(2) | N(2)-C(27)-C(26) | 109.71(19) |
| N(1)-C(5)-O(1) | 108.39(19) | O(4)-C(28)-N(3) | 121.5(2) |
| N(1)-C(6)-C(7) | 109.83(18) | O(4)-C(28)-C(26) | 120.3(2) |
| N(1)-C(6)-C(14) | 111.37(19) | N(3)-C(28)-C(26) | 118.16(19) |
| C(7)-C(6)-C(14) | 108.99(19) | N(3)-C(29)-C(30) | 109.6(2) |
| C(6)-C(7)-S(1) | 114.87(18) | C(29)-C(30)-C(31) | 111.0(2) |
| C(9)-C(8)-C(13) | 119.5(3) | C(30)-C(31)-C(32) | 111.3(2) |
| C(9)-C(8)-S(1) | 119.4(2) | C(34)-C(32)-C(31) | 111.2(2) |
| C(13)-C(8)-S(1) | 120.9(2) | C(34)-C(32)-C(33) | 109.18(19) |
| C(10)-C(9)-C(8) | 119.9(3) | C(31)-C(32)-C(33) | 110.0(2) |
| C(11)-C(10)-C(9) | 120.5(3) | N(3)-C(33)-C(32) | 111.10(19) |
| C(12)-C(11)-C(10) | 120.3(3) | O(5)-C(34)-N(4) | 122.6(2) |
| C(11)-C(12)-C(13) | 120.5(3) | O(5)-C(34)-C(32) | 122.1(2) |
| C(12)-C(13)-C(8) | 119.4(3) | N(4)-C(34)-C(32) | 115.2(2) |
| C(22)-C(14)-C(15) | 108.19(19) | N(4)-C(35)-C(36) | 111.0(2) |
| C(22)-C(14)-C(6) | 108.20(19) | N(4)-C(35)-C(38) | 109.60(19) |
| C(15)-C(14)-C(6) | 113.74(19) | C(36)-C(35)-C(38) | 112.46(18) |
| C(16)-C(15)-C(14) | 111.69(19) | C(37)-C(36)-C(35) | 113.40(19) |
| C(17)-C(16)-C(21) | 118.1(2) | C(40)-C(38)-C(39) | 107.4(2) |
| C(17)-C(16)-C(15) | 120.9(2) | C(40)-C(38)-C(35) | 111.4(2) |
| C(21)-C(16)-C(15) | 120.9(2) | C(39)-C(38)-C(35) | 110.66(19) |
| C(16)-C(17)-C(18) | 121.1(2) | O(6)-C(40)-N(5) | 121.6(2) |
| C(19)-C(18)-C(17) | 120.0(3) | O(6)-C(40)-C(38) | 121.5(2) |
| C(18)-C(19)-C(20) | 120.0(3) | N(5)-C(40)-C(38) | 116.8(2) |
| C(19)-C(20)-C(21) | 119.5(2) | | |

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$)
 The
 anisotropic displacement factor exponent takes the form:
 $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^{*} b^{*} U_{12}]$

| | U_{11} | U_{22} | U_{33} | U_{23} | U_{13} | U_{12} |
|-------|----------|----------|----------|----------|----------|----------|
| S(1) | 32(1) | 37(1) | 33(1) | -2(1) | -5(1) | 2(1) |
| O(1) | 45(1) | 21(1) | 21(1) | 2(1) | 8(1) | -3(1) |
| O(2) | 34(1) | 29(1) | 22(1) | -3(1) | 8(1) | 1(1) |
| O(3) | 37(1) | 21(1) | 28(1) | -4(1) | 7(1) | 1(1) |
| O(4) | 49(1) | 26(1) | 32(1) | 8(1) | 12(1) | -1(1) |
| O(5) | 56(1) | 25(1) | 29(1) | -6(1) | 9(1) | 2(1) |
| O(6) | 62(1) | 37(1) | 22(1) | -5(1) | 11(1) | -12(1) |
| N(1) | 33(1) | 19(1) | 18(1) | -3(1) | 2(1) | -3(1) |
| N(2) | 25(1) | 17(1) | 24(1) | 0(1) | 2(1) | 1(1) |
| N(3) | 35(1) | 18(1) | 25(1) | 1(1) | 4(1) | 0(1) |
| N(4) | 35(1) | 23(1) | 21(1) | -2(1) | 1(1) | -2(1) |
| N(5) | 45(1) | 25(1) | 24(1) | 0(1) | 7(1) | -3(1) |
| C(1) | 39(2) | 44(2) | 34(2) | 3(1) | -2(1) | 3(1) |
| C(2) | 35(2) | 27(1) | 20(1) | 6(1) | 7(1) | -2(1) |
| C(3) | 55(2) | 28(1) | 36(2) | 10(1) | 9(2) | 0(1) |
| C(4) | 38(2) | 39(2) | 44(2) | 7(1) | 10(1) | -4(1) |
| C(5) | 22(1) | 23(1) | 22(1) | 1(1) | -1(1) | -4(1) |
| C(6) | 27(1) | 20(1) | 22(1) | 0(1) | -1(1) | -2(1) |
| C(7) | 35(2) | 30(1) | 29(2) | 3(1) | -4(1) | -5(1) |
| C(8) | 33(2) | 37(1) | 32(2) | -4(1) | -12(1) | 1(1) |
| C(9) | 37(2) | 49(2) | 56(2) | 4(2) | -8(2) | -5(1) |
| C(10) | 41(2) | 46(2) | 90(3) | 6(2) | -20(2) | -13(2) |
| C(11) | 64(2) | 42(2) | 86(3) | -20(2) | -40(2) | 12(2) |
| C(12) | 69(2) | 58(2) | 48(2) | -17(2) | -18(2) | 21(2) |
| C(13) | 53(2) | 47(2) | 33(2) | -3(1) | -11(2) | 11(2) |
| C(14) | 26(1) | 20(1) | 19(1) | 1(1) | 1(1) | 2(1) |
| C(15) | 30(1) | 23(1) | 27(1) | 5(1) | -1(1) | -2(1) |
| C(16) | 28(1) | 27(1) | 21(1) | 7(1) | -2(1) | 0(1) |
| C(17) | 38(2) | 31(1) | 25(1) | 2(1) | -1(1) | 2(1) |

| | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|
| C(18) | 37(2) | 48(2) | 29(2) | 4(1) | 10(1) | 9(1) |
| C(19) | 28(2) | 56(2) | 33(2) | 6(1) | 0(1) | -3(1) |
| C(20) | 35(2) | 38(2) | 29(2) | 1(1) | -5(1) | -6(1) |
| C(21) | 31(2) | 33(1) | 23(1) | 2(1) | 0(1) | 2(1) |
| C(22) | 26(1) | 21(1) | 18(1) | 0(1) | -5(1) | 0(1) |
| C(23) | 36(2) | 24(1) | 22(1) | -2(1) | 8(1) | -1(1) |
| C(24) | 29(2) | 29(1) | 22(1) | 2(1) | 7(1) | 5(1) |
| C(25) | 29(2) | 27(1) | 26(1) | 4(1) | 3(1) | 1(1) |
| C(26) | 27(1) | 22(1) | 17(1) | 3(1) | 2(1) | 1(1) |
| C(27) | 26(1) | 23(1) | 27(1) | 3(1) | -1(1) | -1(1) |
| C(28) | 24(1) | 23(1) | 27(1) | 4(1) | 0(1) | -1(1) |
| C(29) | 44(2) | 17(1) | 33(2) | 0(1) | 4(1) | -1(1) |
| C(30) | 37(2) | 23(1) | 42(2) | 7(1) | -1(1) | 5(1) |
| C(31) | 33(2) | 26(1) | 41(2) | 2(1) | 5(1) | 6(1) |
| C(32) | 28(1) | 25(1) | 22(1) | 2(1) | 1(1) | 1(1) |
| C(33) | 33(2) | 20(1) | 25(1) | 2(1) | 3(1) | 2(1) |
| C(34) | 24(1) | 23(1) | 26(1) | -2(1) | 0(1) | 1(1) |
| C(35) | 31(2) | 21(1) | 20(1) | -2(1) | 3(1) | 0(1) |
| C(36) | 29(2) | 28(1) | 36(2) | 3(1) | 3(1) | 2(1) |
| C(37) | 30(2) | 30(1) | 39(2) | 1(1) | -1(1) | 0(1) |
| C(38) | 33(2) | 25(1) | 22(1) | -5(1) | 3(1) | -2(1) |
| C(39) | 30(2) | 37(1) | 49(2) | -2(1) | -4(1) | -5(1) |
| C(40) | 30(2) | 31(1) | 26(1) | -3(1) | 7(1) | -4(1) |
| C(41) | 57(2) | 30(1) | 38(2) | 5(1) | 4(2) | -2(1) |

Table 5. Hydrogen coordinates and isotropic displacement parameters

| | x | y | z | U(eq) |
|--------|---------|--------|--------|-------|
| H(1) | 0.2351 | 0.2743 | 0.2910 | 0.028 |
| H(4) | 0.2696 | 0.5801 | 0.4373 | 0.031 |
| H(5) | 0.1413 | 0.3607 | 0.5106 | 0.038 |
| H(1A) | 0.2628 | 0.2434 | 0.4882 | 0.058 |
| H(1B) | 0.3630 | 0.1840 | 0.4624 | 0.058 |
| H(1C) | 0.2618 | 0.1651 | 0.5168 | 0.058 |
| H(3A) | 0.1254 | 0.0803 | 0.3824 | 0.059 |
| H(3B) | 0.1861 | 0.0624 | 0.4483 | 0.059 |
| H(3C) | 0.2826 | 0.0902 | 0.3950 | 0.059 |
| H(4A) | -0.0379 | 0.1653 | 0.4233 | 0.061 |
| H(4B) | 0.0098 | 0.2288 | 0.4670 | 0.061 |
| H(4C) | 0.0111 | 0.1485 | 0.4915 | 0.061 |
| H(6) | 0.1638 | 0.4082 | 0.3324 | 0.028 |
| H(7A) | 0.2457 | 0.3662 | 0.2116 | 0.037 |
| H(7B) | 0.1988 | 0.4449 | 0.2288 | 0.037 |
| H(9) | -0.1000 | 0.2437 | 0.2691 | 0.057 |
| H(10) | -0.1086 | 0.1255 | 0.2374 | 0.071 |
| H(11) | 0.0102 | 0.0887 | 0.1519 | 0.077 |
| H(12) | 0.1377 | 0.1693 | 0.0969 | 0.070 |
| H(13) | 0.1457 | 0.2890 | 0.1261 | 0.053 |
| H(14) | 0.4280 | 0.3929 | 0.2798 | 0.026 |
| H(15A) | 0.3855 | 0.4024 | 0.4100 | 0.032 |
| H(15B) | 0.4305 | 0.3302 | 0.3770 | 0.032 |
| H(17) | 0.6606 | 0.3215 | 0.3337 | 0.038 |
| H(18) | 0.8851 | 0.3542 | 0.3434 | 0.046 |
| H(19) | 0.9422 | 0.4594 | 0.3932 | 0.047 |
| H(20) | 0.7738 | 0.5337 | 0.4312 | 0.040 |
| H(21) | 0.5491 | 0.4990 | 0.4236 | 0.034 |
| H(23A) | 0.5140 | 0.5140 | 0.1901 | 0.033 |
| H(23B) | 0.5508 | 0.4500 | 0.2355 | 0.033 |

| | | | | |
|--------|---------|--------|--------|-------|
| H(24A) | 0.7425 | 0.5226 | 0.2127 | 0.032 |
| H(24B) | 0.7132 | 0.5187 | 0.2845 | 0.032 |
| H(25A) | 0.7577 | 0.6385 | 0.2581 | 0.032 |
| H(25B) | 0.6417 | 0.6369 | 0.2072 | 0.032 |
| H(26) | 0.5938 | 0.6181 | 0.3362 | 0.027 |
| H(27A) | 0.3600 | 0.6200 | 0.3072 | 0.031 |
| H(27B) | 0.4034 | 0.6235 | 0.2367 | 0.031 |
| H(29A) | 0.5004 | 0.8463 | 0.3258 | 0.038 |
| H(29B) | 0.5182 | 0.8385 | 0.3983 | 0.038 |
| H(30A) | 0.2704 | 0.8179 | 0.3336 | 0.041 |
| H(30B) | 0.3021 | 0.8840 | 0.3775 | 0.041 |
| H(31A) | 0.1667 | 0.7962 | 0.4281 | 0.040 |
| H(31B) | 0.3046 | 0.8101 | 0.4638 | 0.040 |
| H(32) | 0.2500 | 0.6904 | 0.3854 | 0.030 |
| H(33A) | 0.5028 | 0.7184 | 0.4450 | 0.031 |
| H(33B) | 0.4725 | 0.6514 | 0.4019 | 0.031 |
| H(35) | 0.2334 | 0.5809 | 0.5632 | 0.029 |
| H(36A) | 0.3927 | 0.4910 | 0.5780 | 0.037 |
| H(36B) | 0.4209 | 0.4860 | 0.5062 | 0.037 |
| H(37A) | 0.5945 | 0.5504 | 0.5558 | 0.049 |
| H(37B) | 0.4873 | 0.6079 | 0.5788 | 0.049 |
| H(37C) | 0.5195 | 0.6004 | 0.5074 | 0.049 |
| H(38) | 0.1655 | 0.4712 | 0.4767 | 0.032 |
| H(39A) | -0.0572 | 0.4927 | 0.5080 | 0.058 |
| H(39B) | 0.0067 | 0.5665 | 0.4861 | 0.058 |
| H(39C) | -0.0075 | 0.5495 | 0.5574 | 0.058 |
| H(41A) | 0.1165 | 0.2692 | 0.5741 | 0.062 |
| H(41B) | 0.0571 | 0.3245 | 0.6227 | 0.062 |
| H(41C) | 0.2158 | 0.3120 | 0.6183 | 0.062 |

Table 6. Torsion angles [°]

| | | | |
|-------------------------|-------------|-------------------------|-------------|
| C(5)-O(1)-C(2)-C(3) | -178.8(2) | C(17)-C(18)-C(19)-C(20) | -1.1(4) |
| C(5)-O(1)-C(2)-C(1) | -62.0(3) | C(18)-C(19)-C(20)-C(21) | 1.9(4) |
| C(5)-O(1)-C(2)-C(4) | 63.3(3) | C(17)-C(16)-C(21)-C(20) | -2.1(3) |
| C(6)-N(1)-C(5)-O(2) | 6.5(4) | C(15)-C(16)-C(21)-C(20) | 179.6(2) |
| C(6)-N(1)-C(5)-O(1) | -174.7(2) | C(19)-C(20)-C(21)-C(16) | -0.3(4) |
| C(2)-O(1)-C(5)-O(2) | -8.8(4) | C(27)-N(2)-C(22)-O(3) | -2.8(3) |
| C(2)-O(1)-C(5)-N(1) | 172.32(19) | C(23)-N(2)-C(22)-O(3) | 172.0(2) |
| C(5)-N(1)-C(6)-C(7) | -144.7(2) | C(27)-N(2)-C(22)-C(14) | 177.9(2) |
| C(5)-N(1)-C(6)-C(14) | 94.4(3) | C(23)-N(2)-C(22)-C(14) | -7.4(4) |
| N(1)-C(6)-C(7)-S(1) | 62.0(2) | C(15)-C(14)-C(22)-O(3) | -65.3(3) |
| C(14)-C(6)-C(7)-S(1) | -175.77(15) | C(6)-C(14)-C(22)-O(3) | 58.4(3) |
| C(8)-S(1)-C(7)-C(6) | -87.54(19) | C(15)-C(14)-C(22)-N(2) | 114.1(2) |
| C(7)-S(1)-C(8)-C(9) | 121.0(2) | C(6)-C(14)-C(22)-N(2) | -122.3(2) |
| C(7)-S(1)-C(8)-C(13) | -65.0(2) | C(22)-N(2)-C(23)-C(24) | -120.2(2) |
| C(13)-C(8)-C(9)-C(10) | -0.9(4) | C(27)-N(2)-C(23)-C(24) | 54.8(3) |
| S(1)-C(8)-C(9)-C(10) | 173.3(2) | N(2)-C(23)-C(24)-C(25) | -53.0(3) |
| C(8)-C(9)-C(10)-C(11) | 0.8(5) | C(23)-C(24)-C(25)-C(26) | 56.7(3) |
| C(9)-C(10)-C(11)-C(12) | -0.1(5) | C(24)-C(25)-C(26)-C(28) | -179.6(2) |
| C(10)-C(11)-C(12)-C(13) | -0.5(5) | C(24)-C(25)-C(26)-C(27) | -60.0(2) |
| C(11)-C(12)-C(13)-C(8) | 0.4(5) | C(22)-N(2)-C(27)-C(26) | 115.7(2) |
| C(9)-C(8)-C(13)-C(12) | 0.3(4) | C(23)-N(2)-C(27)-C(26) | -59.9(3) |
| S(1)-C(8)-C(13)-C(12) | -173.8(2) | C(25)-C(26)-C(27)-N(2) | 62.1(2) |
| N(1)-C(6)-C(14)-C(22) | -164.86(18) | C(28)-C(26)-C(27)-N(2) | -175.15(19) |
| C(7)-C(6)-C(14)-C(22) | 73.8(2) | C(29)-N(3)-C(28)-O(4) | 0.6(4) |
| N(1)-C(6)-C(14)-C(15) | -44.6(3) | C(33)-N(3)-C(28)-O(4) | 177.6(2) |
| C(7)-C(6)-C(14)-C(15) | -165.94(18) | C(29)-N(3)-C(28)-C(26) | -177.2(2) |
| C(22)-C(14)-C(15)-C(16) | -65.1(3) | C(33)-N(3)-C(28)-C(26) | -0.1(4) |
| C(6)-C(14)-C(15)-C(16) | 174.66(19) | C(25)-C(26)-C(28)-O(4) | 23.7(3) |
| C(14)-C(15)-C(16)-C(17) | -87.0(3) | C(27)-C(26)-C(28)-O(4) | -96.0(3) |
| C(14)-C(15)-C(16)-C(21) | 91.3(3) | C(25)-C(26)-C(28)-N(3) | -158.5(2) |
| C(21)-C(16)-C(17)-C(18) | 3.0(4) | C(27)-C(26)-C(28)-N(3) | 81.7(3) |
| C(15)-C(16)-C(17)-C(18) | -178.6(2) | C(28)-N(3)-C(29)-C(30) | 116.9(2) |
| C(16)-C(17)-C(18)-C(19) | -1.5(4) | C(33)-N(3)-C(29)-C(30) | -60.6(3) |

| | | | |
|-------------------------|-------------|-------------------------|------------|
| N(3)-C(29)-C(30)-C(31) | 57.0(3) | C(34)-N(4)-C(35)-C(36) | -105.1(3) |
| C(29)-C(30)-C(31)-C(32) | -53.9(3) | C(34)-N(4)-C(35)-C(38) | 130.1(2) |
| C(30)-C(31)-C(32)-C(34) | 172.9(2) | N(4)-C(35)-C(36)-C(37) | 53.3(3) |
| C(30)-C(31)-C(32)-C(33) | 51.9(3) | C(38)-C(35)-C(36)-C(37) | 176.5(2) |
| C(28)-N(3)-C(33)-C(32) | -117.4(3) | N(4)-C(35)-C(38)-C(40) | 173.06(19) |
| C(29)-N(3)-C(33)-C(32) | 59.9(3) | C(36)-C(35)-C(38)-C(40) | 49.1(3) |
| C(34)-C(32)-C(33)-N(3) | -176.59(18) | N(4)-C(35)-C(38)-C(39) | -67.5(2) |
| C(31)-C(32)-C(33)-N(3) | -54.4(3) | C(36)-C(35)-C(38)-C(39) | 168.6(2) |
| C(35)-N(4)-C(34)-O(5) | -10.3(4) | C(41)-N(5)-C(40)-O(6) | 2.3(4) |
| C(35)-N(4)-C(34)-C(32) | 166.8(2) | C(41)-N(5)-C(40)-C(38) | -174.8(2) |
| C(31)-C(32)-C(34)-O(5) | -15.6(3) | C(39)-C(38)-C(40)-O(6) | -74.0(3) |
| C(33)-C(32)-C(34)-O(5) | 105.9(3) | C(35)-C(38)-C(40)-O(6) | 47.3(3) |
| C(31)-C(32)-C(34)-N(4) | 167.3(2) | C(39)-C(38)-C(40)-N(5) | 103.1(3) |
| C(33)-C(32)-C(34)-N(4) | -71.2(3) | C(35)-C(38)-C(40)-N(5) | -135.6(2) |

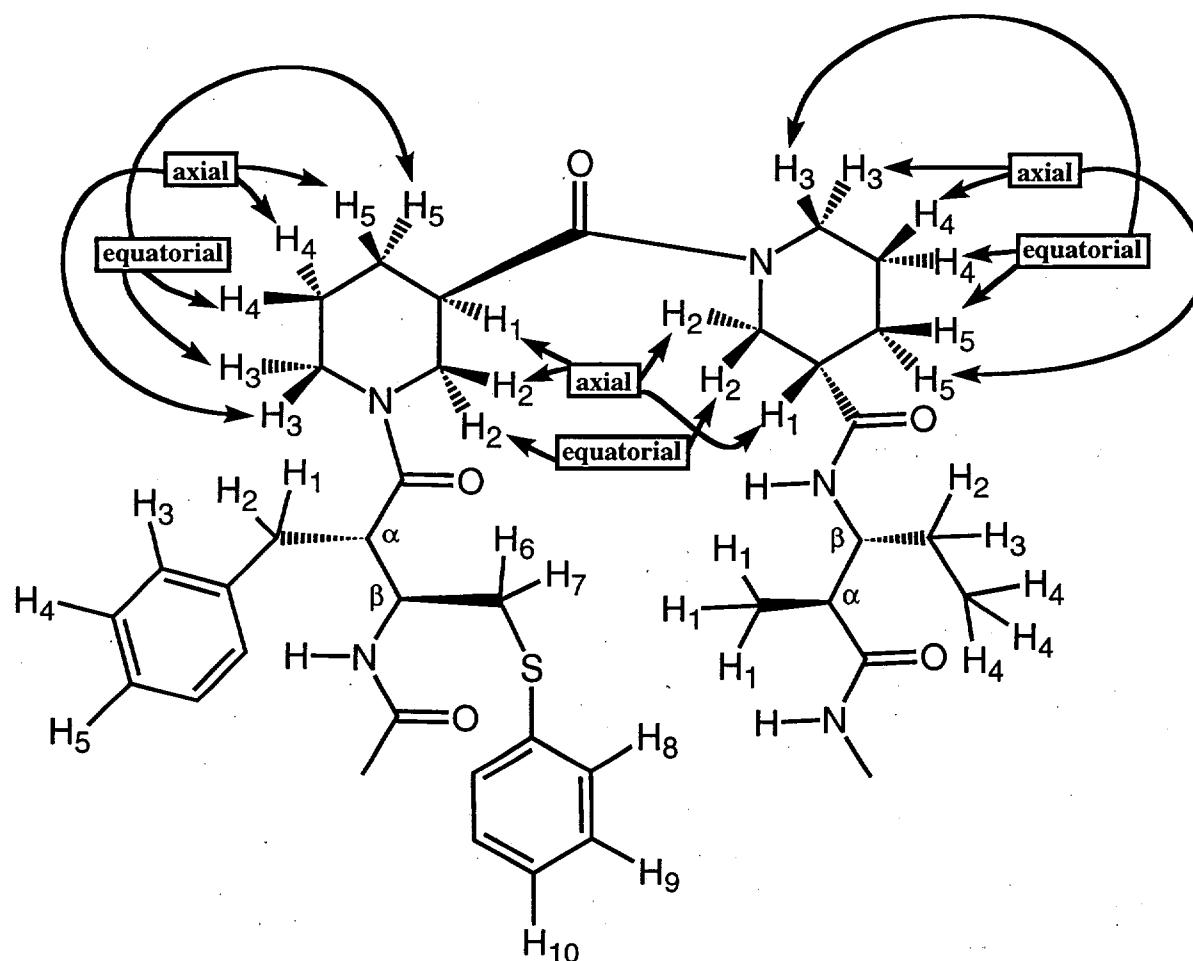
Table 7. Hydrogen bonds [Å and °].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | ∠(DHA) |
|--------------------|--------|----------|----------|--------|
| N(1)-H(1)...O(4)#1 | 0.88 | 2.21 | 2.852(3) | 129.5 |
| N(4)-H(4)...O(3) | 0.88 | 2.15 | 3.018(2) | 170.8 |
| N(5)-H(5)...O(2) | 0.88 | 2.20 | 3.076(3) | 172.3 |

Symmetry transformation used to generate equivalent atom:
#1 -x+1,y-1/2,-z+1/2

Proton Numbering Scheme for ROESY Data

19



Proton Resonances (ppm) for JC-267 (1mM in CD₂Cl₂)

| Residue | N-H | α H | β H | Others |
|-------------------|------|------------|-----------|---|
| N-terminus | ---- | ---- | ---- | -CH ₃ 1.90 |
| 1 | 5.80 | 3.27 | 4.84 | H ₁ , H ₂ 2.92 H ₃ 7.14 H ₄ 7.28 H ₅ 7.20 H ₆ , H ₇ 3.16, 2.97 H ₈ , H ₉ , H ₁₀ 7.37, 7.31 |
| 2 | ---- | ---- | ---- | 1 2.20 (tt) 2 _{ax} 2.26 (t) 2 _{eq} 4.63 (dd) 3 _{ax} 2.73 (td) 3 _{eq} 3.51 (dd) 4 _{ax} -0.56 (qt) 4 _{eq} 1.15 (buried) 5 _{ax} 1.60 (qd) 5 _{eq} 1.41 (buried) |
| 3 | ---- | ---- | ---- | 1 2.53 (buried) 2 _{ax} 3.08 (t) 2 _{eq} 4.30 (dd) 3 _{ax} 2.39 (td) 3 _{eq} 4.57 (dd) 4 _{ax} 1.35 (qt) 4 _{eq} 1.76 (broad d) 5 _{ax, eq} 1.98, 1.89 (buried) |
| 4 | 7.70 | 2.54 | 4.04 | H ₁ 1.11 H ₂ , H ₃ 1.66, 1.47 H ₄ 0.91 |
| C-terminus | 7.49 | ---- | ---- | -CH ₃ 2.74 |

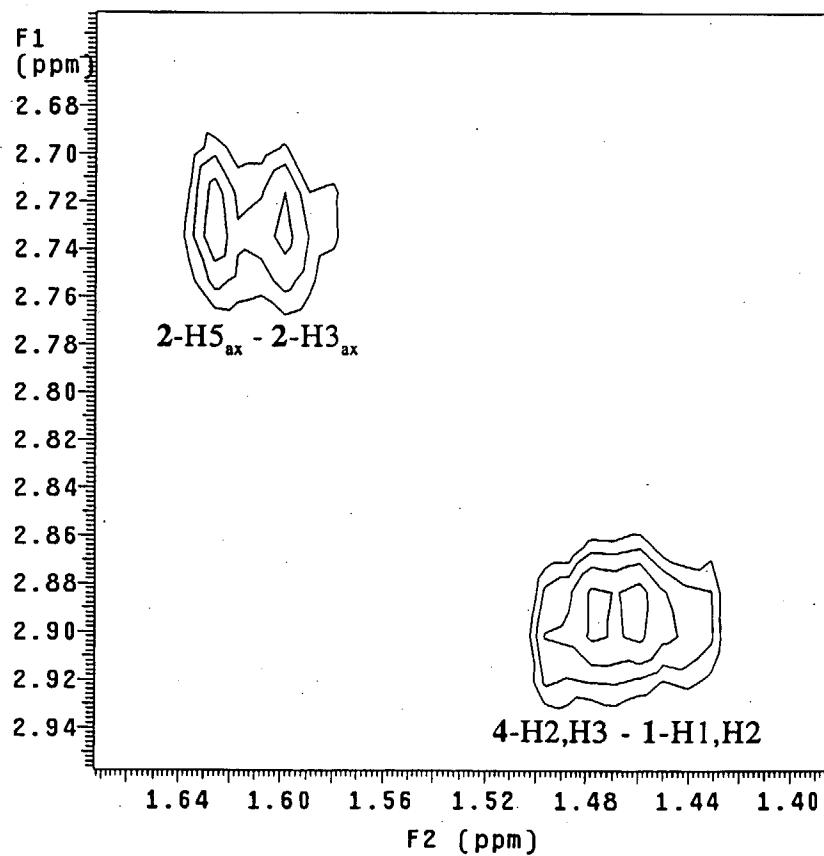
Residue numbering scheme is based on standard peptide convention, proceeding from the N-terminus to the C-terminus.

Each ROESY crosspeak shown in the supplementary material is labeled. The bold number corresponds to the residue number; the proton specification follows the bold number.

Chung's JC-267 ROESY, 300msec mixing time

exp5 roesy

| SAMPLE | DEC. & VT | ACQUISITION ARRAYS |
|---------------------|---------------------|--------------------|
| date May 1 1998 | dfrq 500.254 | array phase |
| solvent cd2c12 | dn H1 | arraydim 716 |
| file /europa/stang~ | dpwr 0 | |
| er/JC-267/CD2C12/j~ | dof 0 | 1 |
| c-267-1mM-roesy300~ | dm nnn | 1 |
| -050198-wkup-wftbc~ | dmm c | 2 |
| | 5 dmf 0 | |
| ACQUISITION | | |
| sfrq 500.253 | dseq | 1.0 |
| tn H1 | homo | n |
| at 0.216 | PROCESSING | |
| np 2048 | gf 0.100 | |
| sw 4750.0 | gfs not used | |
| fb 3000 | wtfile | |
| bs 4 | proc ft | |
| ss 8 | fn 2048 | |
| tpwr 54 | math f | |
| pw 3.1 | | |
| p1 9.2 | | |
| di 1.000 | werr | |
| presat 0 | wexp svf('/europa/~ | |
| tof -600.0 | stanger/lnova/chun~ | |
| ratio 8.0 | g/JC-267-1mM-roesy~ | |
| mix 0.300 | 300-050198') | |
| nt 32 | wbs | |
| ct 32 | wnt | |
| clock n | 2D PROCESSING | |
| gain 50 | gfi 0.025 | |
| FLAGS | gfs1 not used | |
| fl n | wtfile1 | |
| in n | proc1 ft | |
| dp y | fn1 1024 | |
| hs y | | |
| sspul y | | |
| rocomp y | | |
| 2D ACQUISITION | | |
| sw1 4750.0 | | |
| ni 358 | | |
| phase arrayed | | |
| DISPLAY | | |
| sp 688.1 | | |
| wp 148.6 | | |
| vs 2000 | | |
| sc 0 | | |
| wc 100 | | |
| hzmm 1.49 | | |
| is 33.57 | | |
| rfl 3152.6 | | |
| rfp 2661.4 | | |
| th 2 | | |
| ins 1.000 | | |
| ai cdc ph | | |
| 2D DISPLAY | | |
| sp1 1321.4 | | |
| wpl 158.0 | | |
| sc2 0 | | |
| wc2 100 | | |
| rfl1 3152.6 | | |
| rfp1 2661.4 | | |

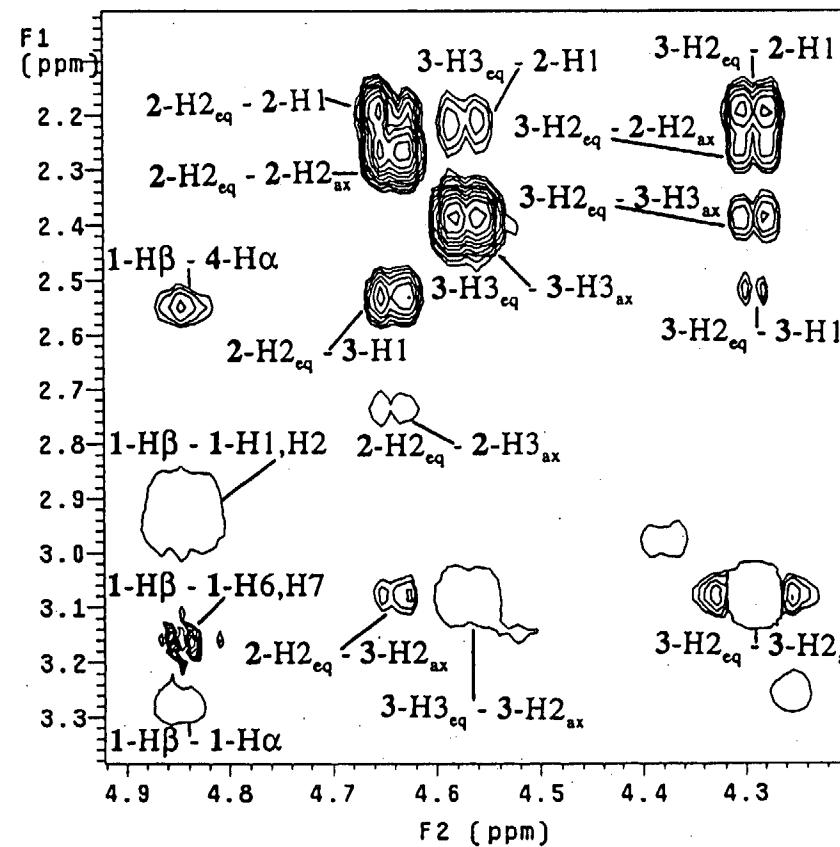


LJ

Chung's JC-267 ROESY, 300msec mixing time

exp5 roesy

| SAMPLE | DEC. & VT | ACQUISITION ARRAYS |
|---------------------|---------------------|--------------------|
| date May 1 1998 | dfreq 500.254 | array H1 |
| solvent cd2c12 | dn arraydim 716 | |
| file /europa/stang~ | dpwr 0 | |
| er/Jc-267/CD2C12/J~ | dof 0 | phase 1 |
| c-267-1mH-roesy300~ | dm nnn 1 | 1 |
| -050198-wftbc~ | dmm c 2 | 2 |
| | 5 dmf 0 | |
| ACQUISITION | | |
| sfrq 500.253 | dseq | |
| tn H1 | pres | 1.0 |
| at 0.216 | homo | n |
| np 2048 | PROCESSING | |
| sw 4750.0 | gf 0.100 | |
| fb 3000 | gfs not used | |
| bs 4 | wtfile | |
| ss 8 | proc ft | |
| tpwr 54 | fn 2048 | |
| pw 3.1 | math f | |
| p1 9.2 | werr | |
| di 1.000 | wexp svf('/europa/~ | |
| presat 0 | stanger/lnova/chun~ | |
| tof -600.0 | g/jc-267-1mH-roesy~ | |
| ratio 8.0 | 300-050198") | |
| mix 0.300 | wbs | |
| nt 32 | wnt | |
| ct 32 | 2D PROCESSING | |
| alock n | gfi 0.025 | |
| gain 50 | gfs1 not used | |
| FLAGS | wtfile1 | |
| 11 n | proc1 ft | |
| in n | fn1 1024 | |
| dp y | | |
| hs yy | | |
| sspu1 yy | | |
| rocomp yy | | |
| 2D ACQUISITION | | |
| sw1 4750.0 | | |
| ni 358 | | |
| phase arrayed | | |
| DISPLAY | | |
| sp 2085.0 | | |
| wp 366.8 | | |
| vs 2750 | | |
| sc 0 | | |
| wc 100 | | |
| hzmn 3.85 | | |
| is 33.57 | | |
| rfl1 3152.6 | | |
| rfpl 2661.4 | | |
| th 3 | | |
| ins 1.000 | | |
| at cdc ph | | |
| 2D DISPLAY | | |
| sp1 1005.3 | | |
| wp1 687.9 | | |
| sc2 0 | | |
| wc2 100 | | |
| rfl1 3152.6 | | |
| rfpl 2661.4 | | |

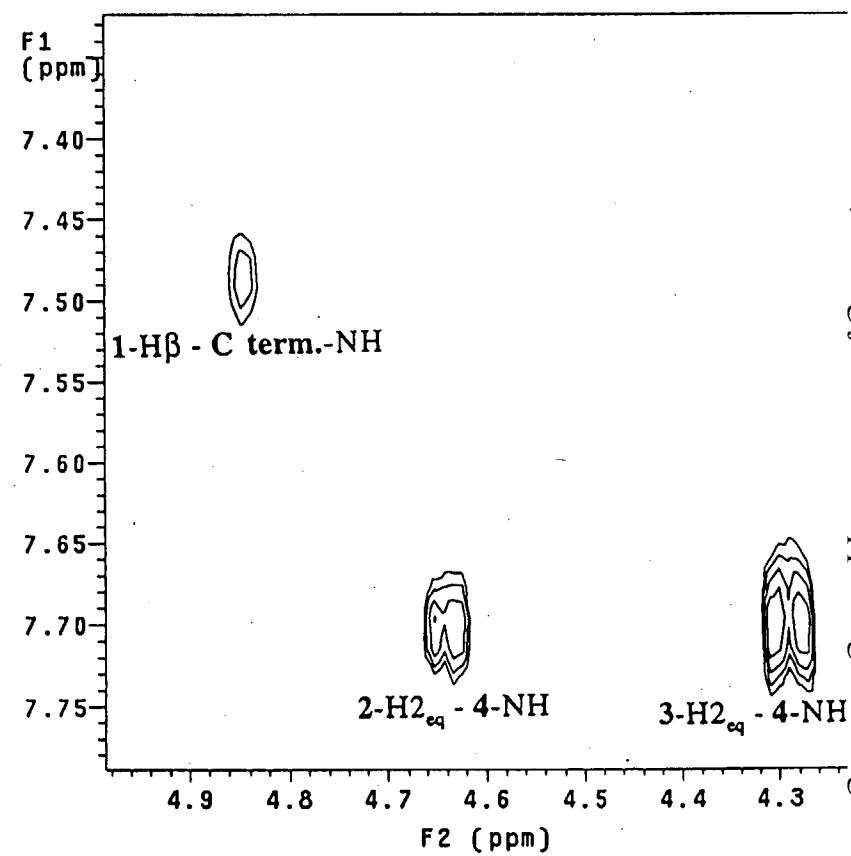


E8

Chung's JC-267 ROESY, 300msec mixing time
8

exp5 roesy

| SAMPLE | DEC. & VT | ACQUISITION ARRAYS |
|---------------------|---------------------|--------------------|
| date May 1 1998 | dfrq 500.254 | array H1 |
| solvent cd2c12 | dn | arraydim 716 |
| file /europa/stang~ | dpowr 0 | |
| er/Jc-267/CD2C12/j~ | dof 0 | i |
| c-267-1mH-roesy300~ | dm nnn 1 | phase 1 |
| -050198-wftbc~ | dmm c 2 | 2 |
| | 5 dmf 0 | |
| ACQUISITION | dseq | |
| sfrq 500.253 | dres 1.0 | |
| tn H1 | homo n | |
| at 0.216 | PROCESSING | |
| np 2048 | gf 0.100 | |
| sw 4750.0 | gfs not used | |
| fb 3000 | wtfile | |
| bs 4 | proc ft | |
| ss 8 | fn 2048 | |
| tpwr 54 | math f | |
| pw 3.1 | | |
| pi 9.2 | | |
| di 1.000 | wexp svf('/europa/~ | |
| presat 0 | stanger/lnova/chun~ | |
| tof -600.0 | g/jc-267-1mH-roesy~ | |
| ratio 8.0 | 300-050198') | |
| mix 0.300 | wbs | |
| nt 32 | wnt | |
| ct 32 | 2D PROCESSING | |
| alock n | gfi 0.025 | |
| gain 50 | gfsi not used | |
| FLAGS | wtfile1 | |
| fl n | proc1 ft | |
| in n | fn1 1024 | |
| dp y | | |
| hs yy | | |
| sspul y | | |
| rocomp y | | |
| 2D ACQUISITION | | |
| sw1 4750.0 | | |
| ni 358 | | |
| phase arrayed | | |
| DISPLAY | | |
| sp 2109.0 | | |
| wp 385.4 | | |
| vs 2500 | | |
| sc 0 | | |
| wc 100 | | |
| hzmm 3.85 | | |
| is 33.57 | | |
| rfl1 3152.6 | | |
| rfp 2661.4 | | |
| th 2 | | |
| ins 1.000 | | |
| at cdc ph | | |
| 2D DISPLAY | | |
| sp1 3663.9 | | |
| wpl1 232.4 | | |
| sc2 0 | | |
| wc2 100 | | |
| rfl1 3152.6 | | |
| rfp1 2661.4 | | |

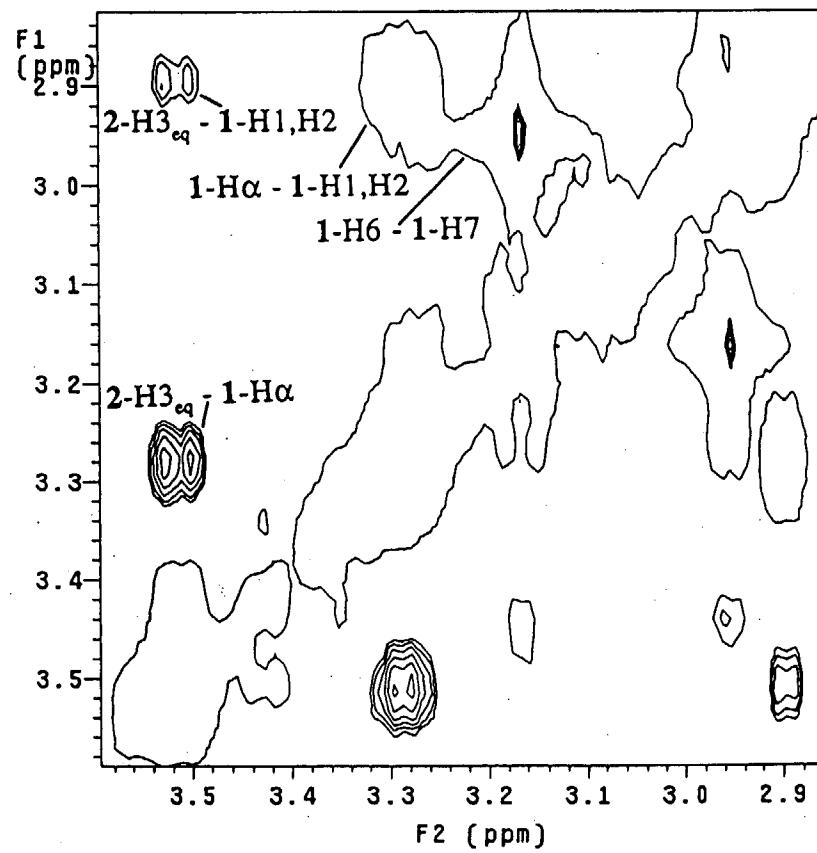


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Chung's JC-267 ROESY, 300msec mixing time

exp5 roesy

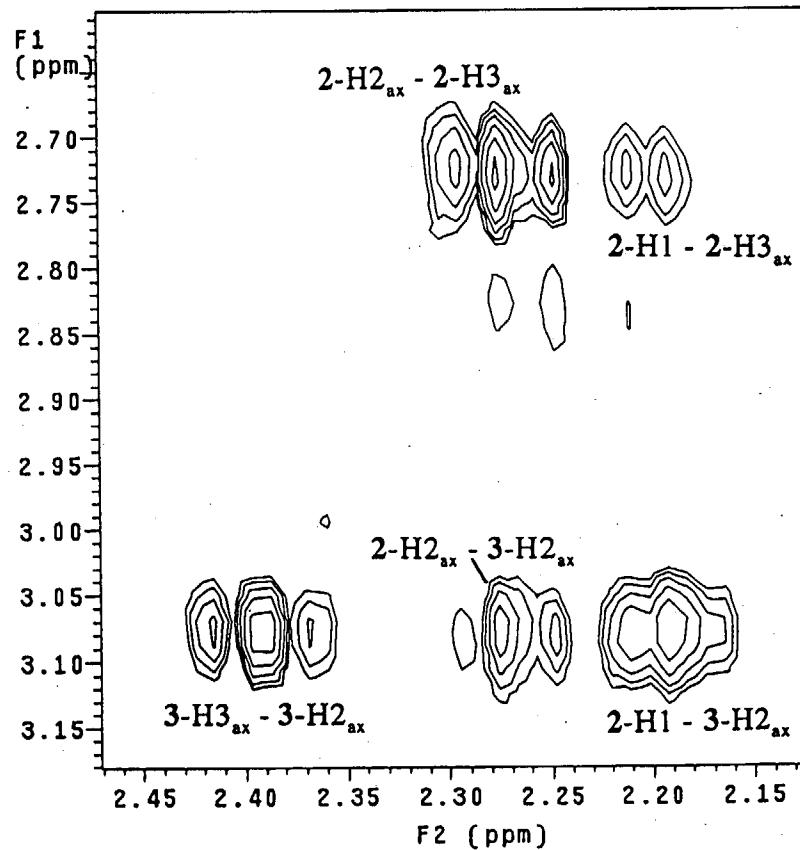
| SAMPLE | DEC. & VT | ACQUISITION ARRAYS |
|---------------------|---------------------|--------------------|
| date May 1 1998 | dfrq 500.254 | array H1 |
| solvent cd2c12 | dn | arraydim 716 |
| file /europa/stang~ | dpwr 0 | |
| er/Jc-267/CD2C12/j~ | dof 0 | phase 1 |
| c-267-1mM-roesy300~ | dm nnn | 1 |
| -050198-wkup-wftbc~ | dmm c | 2 |
| | dmf 0 | 2 |
| ACQUISITION | dseq | |
| sfrq 500.253 | dres 1.0 | |
| tn H1 | homo n | |
| at 0.216 | PROCESSING | |
| np 2048 | gf 0.100 | |
| sw 4750.0 | gfs not used | |
| fb 3000 | wtfile | |
| bs 4 | proc ft | |
| ss 8 | fn 2048 | |
| tpwr 54 | math | |
| pw 3.1 | | |
| pi 9.2 | | |
| d1 1.000 | werr | |
| presat 0 | wexp svf('/europa/~ | |
| tof -600.0 | stanger/lnova/chun~ | |
| ratio 8.0 | g/jc-267-1mM-roesy~ | |
| mix 0.300 | 300-050198') | |
| nt 32 | wbs | |
| ct 32 | wnt | |
| alock n | 2D PROCESSING | |
| gain 50 | gfl 0.025 | |
| FLAGS | gfs1 not used | |
| fl n | wtfile1 | |
| in n | proc1 ft | |
| dp y | fn1 1024 | |
| hs yy | | |
| sspu1 yy | | |
| rocomp y | | |
| 2D ACQUISITION | | |
| sw1 4750.0 | | |
| ni 358 | | |
| phase arrayed | | |
| DISPLAY | | |
| sp 1412.5 | | |
| wp 385.4 | | |
| ve 1500 | | |
| sc 0 | | |
| wc 100 | | |
| hzmn 3.86 | | |
| ls 33.57 | | |
| rfl 3152.6 | | |
| rfp 2661.4 | | |
| th 3 | | |
| ins 1.000 | | |
| ai cdc ph | | |
| 2D DISPLAY | | |
| sp1 1414.3 | | |
| wpl 381.1 | | |
| sc2 0 | | |
| wc2 100 | | |
| rfl1 3152.6 | | |
| rfp1 2661.4 | | |



Chung's JC-267 ROESY, 300msec mixing time

exp5 roesy

| SAMPLE | DEC. & VT | ACQUISITION ARRAYS |
|---------------------|---------------------|--------------------|
| date May 1 1998 | dfrq 500.254 | array H1 |
| solvent cd2c12 | dn | arraydim 716 |
| f11 /europa/stang~ | dpwr 0 | |
| er/Jc-267/CD2C12/1~ | dof 0 | |
| c-267-1mH-roesy300~ | dm nnn 1 | phase 1 |
| -050198-wftbc- | dmm c 2 | 2 |
| | dmf 0 | |
| ACQUISITION | dseq | |
| sfrq 500.253 | dres 1.0 | |
| tn H1 | homo n | |
| at 0.216 | PROCESSING | |
| np 2048 | gf 0.100 | |
| sw 4750.0 | gfs not used | |
| fb 3000 | wtfile | |
| bs 4 | proc ft | |
| ss 8 | fn 2048 | |
| tpwr 54 | math f | |
| pw 3.1 | | |
| p1 9.2 | | |
| d1 1.000 | wexp svf('/europa/~ | |
| presat 0 | stanger/lnova/chun~ | |
| tof -600.0 | g/Jc-267-1mH-roesy~ | |
| ratio 8.0 | 300-050198') | |
| mix 0.300 | wbs | |
| nt 32 | wnt | |
| ct 32 | 2D PROCESSING | |
| clock n | gf1 0.025 | |
| gain 50 | gfs1 not used | |
| FLAGS | wtfile1 | |
| ii n | proc1 ft | |
| in n | fn1 1024 | |
| dp y | | |
| hs yy | | |
| sspul y | | |
| rocomp y | | |
| 2D ACQUISITION | | |
| sw1 4750.0 | | |
| ni 358 | | |
| phase arrayed | | |
| DISPLAY | | |
| sp 1050.3 | | |
| wp 185.7 | | |
| vs 4000 | | |
| sc 0 | | |
| wc 100 | | |
| h2ma 3.86 | | |
| is 33.57 | | |
| rfl 3152.6 | | |
| rfp 2661.4 | | |
| th 3 | | |
| ins 1.000 | | |
| ai cdc ph | | |
| 2D DISPLAY | | |
| spi 1302.8 | | |
| wpi 288.2 | | |
| sc2 0 | | |
| wc2 100 | | |
| rfl1 3152.6 | | |
| rfp1 2661.4 | | |

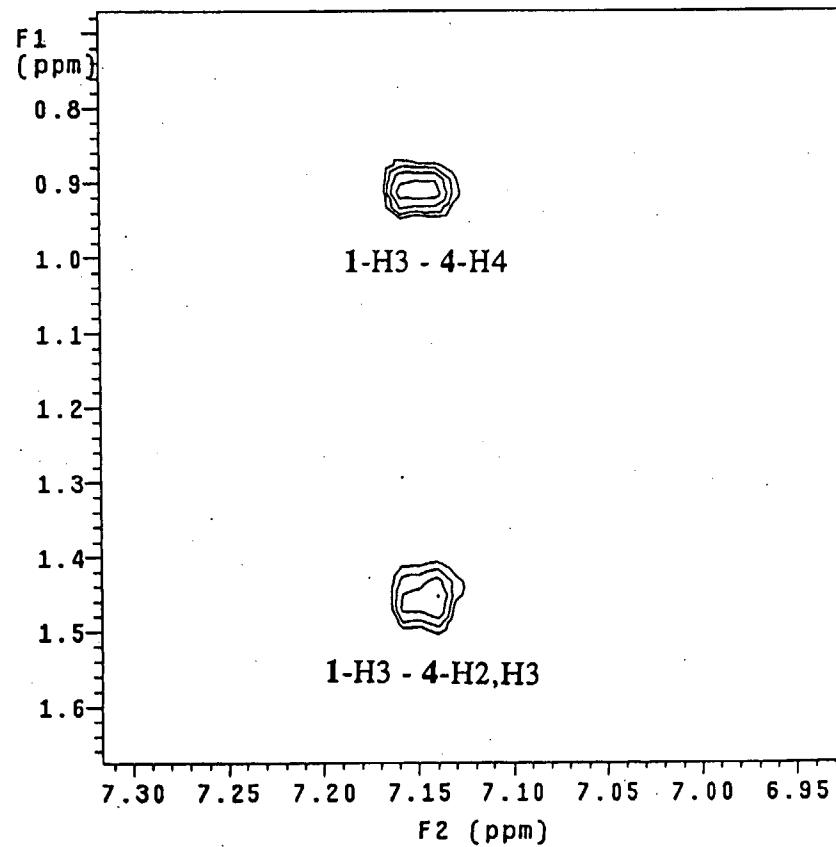


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Chung's JC-267 ROESY, 300msec mixing time

exp5 roesy

| SAMPLE | DEC. & VT | ACQUISITION ARRAYS |
|---------------------|---------------------|--------------------|
| date May 1 1998 | dfrq 500.254 | array H1 |
| solvent cd2c12 | dn | arraydim 716 |
| file /europa/stang~ | dpwr 0 | |
| er/jc-267/CD2C12/ | dof 0 | phase 1 |
| c-267-1mM-roesy300~ | dm nnn 1 | phase 1 |
| -050198-wkup-wftbc~ | dmm c 2 | 2 |
| | 5 dmf 0 | |
| ACQUISITION | | |
| sfrq 500.253 | dseq | 1.0 |
| tn H1 | homo | n |
| at 0.216 | PROCESSING | |
| np 2048 | gf 0.100 | |
| sw 4750.0 | gfs not used | |
| fb 3000 | wtfille | |
| bs 4 | proc ft | |
| ss 8 | fn 2048 | |
| tpwr 54 | math f | |
| pw 3.1 | | |
| pi 9.2 | | |
| d1 1.000 | werr | |
| presat 0 | wexp svf('/europa/~ | |
| tof -600.0 | stanger/1nova/chun~ | |
| ratio 8.0 | g/jc-267-1mM-roesy~ | |
| mix 0.300 | 300-050198") | |
| nt 32 | wbs | |
| ct 32 | wnt | |
| alock 50 | 2D PROCESSING | |
| gain 50 | gfi 0.025 | |
| FLAGS | gfsi not used | |
| ii n | wtfille1 | |
| in n | proc1 ft | |
| dp y | fni 1024 | |
| hs yy | | |
| sspul yy | | |
| rocomp y | | |
| 2D ACQUISITION | | |
| sw1 4750.0 | | |
| n1 358 | | |
| phase arrayed | | |
| DISPLAY | | |
| sp 3460.1 | | |
| wp 199.7 | | |
| vs 3500 | | |
| sc 0 | | |
| wc 100 | | |
| hzmm 47.50 | | |
| is 33.57 | | |
| rfl1 3152.6 | | |
| rfp 2661.4 | | |
| th 3 | | |
| ins 1.000 | | |
| ai cdc ph | | |
| 2D DISPLAY | | |
| spi 336.1 | | |
| wpi 502.0 | | |
| sc2 0 | | |
| wc2 100 | | |
| rfl1 3152.6 | | |
| rfp1 2661.4 | | |



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Chung's JC-267 ROESY, 300msec mixing time

exp5 roesy

| SAMPLE | DEC. & VT | ACQUISITION ARRAYS |
|---------------------|---------------------|--------------------|
| date May 1 1998 | dfrq 500.254 | array H1 |
| solvent cd2c12 | dn | arraydim 716 |
| file /europa/stang~ | dpwr 0 | |
| er/Jc-267/CD2C12/J~ | dof 0 | phase 1 |
| C-267-1mH-roesy300~ | dm nnn 1 | 1 |
| -050198-wkup-wftbc~ | dmm c 2 | 2 |
| | 5 dmf 0 | |
| ACQUISITION | dseq | |
| sfrq 500.253 | dres 1.0 | |
| tn H1 | homo n | |
| at 0.216 | PROCESSING | |
| np 2048 | gf 0.100 | |
| sw 4750.0 | gfs not used | |
| fb 3000 | wf file | |
| bs 4 | proc ft | |
| ss 8 | fn 2048 | |
| tpwr 54 | math f | |
| pw 3.1 | | |
| p1 9.2 | | |
| d1 1.000 | wexp svf('/europa/~ | |
| presat 0 | stanger/lnova/chun~ | |
| tof -600.0 | g/Jc-267-1mH-roesy~ | |
| ratio 8.0 | 300-050198') | |
| mix 0.300 | wbs | |
| nt 32 | wnt | |
| ct 32 | 2D PROCESSING | |
| clock n | gfi 0.025 | |
| gain 50 | gfsi not used | |
| FLAGS | wf file1 | |
| ii n | proc1 ft | |
| in n | fni 1024 | |
| dp y | | |
| hs y | | |
| sspul y | | |
| rocomp y | | |
| 2D ACQUISITION | | |
| sw1 4750.0 | | |
| ni 358 | | |
| phase arrayed | | |
| DISPLAY | | |
| sp 2057.9 | | |
| wp 311.1 | | |
| vs 4000 | | |
| sc 0 | | |
| wc 100 | | |
| hzma 3.86 | | |
| is 33.57 | | |
| rfl1 3152.6 | | |
| rfp 2661.4 | | |
| th 4 | | |
| ins 1.000 | | |
| ai cdc ph | | |
| 2D DISPLAY | | |
| sp1 2055.7 | | |
| wp1 316.0 | | |
| sc2 0 | | |
| wc2 100 | | |
| rfl1 3152.6 | | |
| rfp1 2661.4 | | |

