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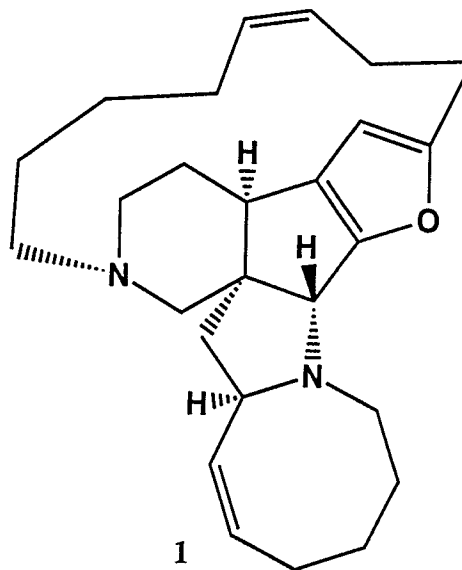
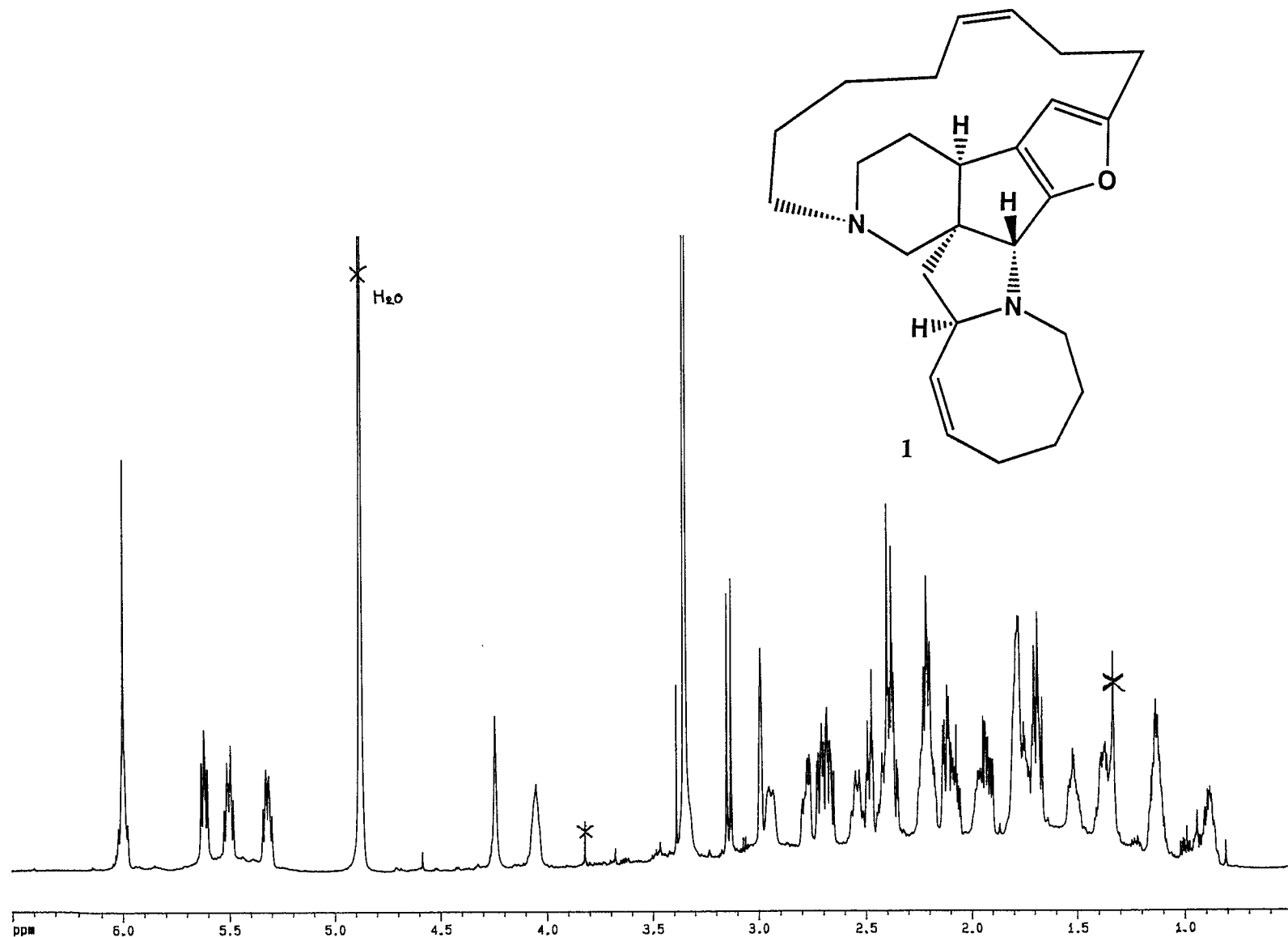


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Figure 4

$^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) Spectrum of Nakadomarin A (1).



Current Data Parameters  
 NAME sho  
 EXPNO 2270  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 970611  
 Time 19.01  
 PULPROG zg  
 SOLVENT CDCl3  
 AQ 1.5073479 sec  
 FIDRES 0.331713 Hz  
 DW 92.0 usec  
 RG 256  
 NUCLEUS 1H  
 D1 2.000000 sec  
 P1 10.5 usec  
 DE 115.0 usec  
 SF01 600.1399811 MHz  
 SWH 5434.78 Hz  
 TD 16384  
 NS 32  
 DS 0

F2 - Processing parameters  
 SI 32768  
 SF 600.1378808 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 30.00 cm  
 F1P 6.500 ppm  
 F1 3900.90 Hz  
 F2P 0.500 ppm  
 F2 300.07 Hz  
 PPMCM 0.20000 ppm/cm  
 HZCM 120.02757 Hz/cm

Figure 5

<sup>13</sup>C NMR (125 MHz, CD<sub>3</sub>OD) Spectrum of Nakadomin A (1).

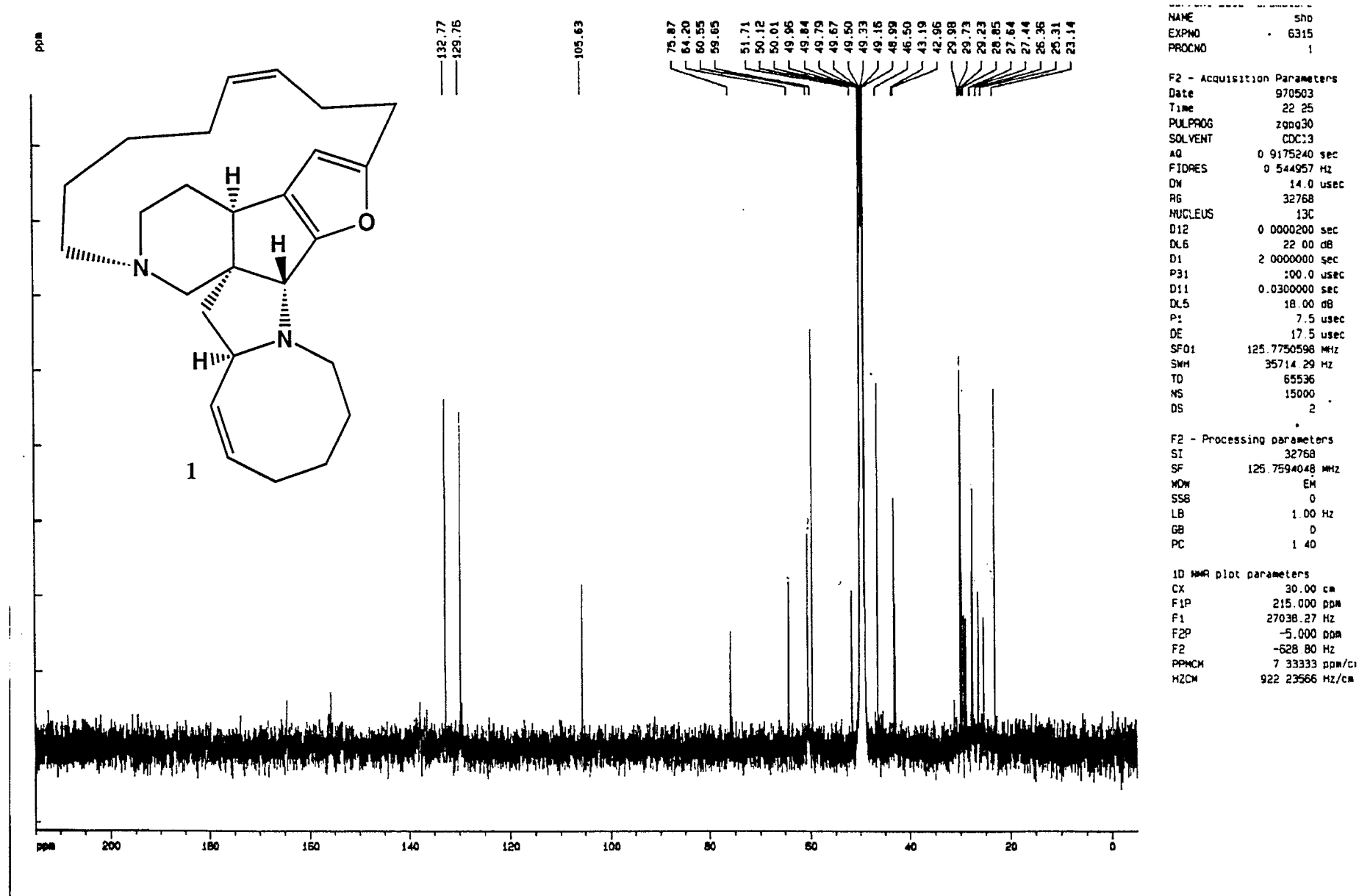
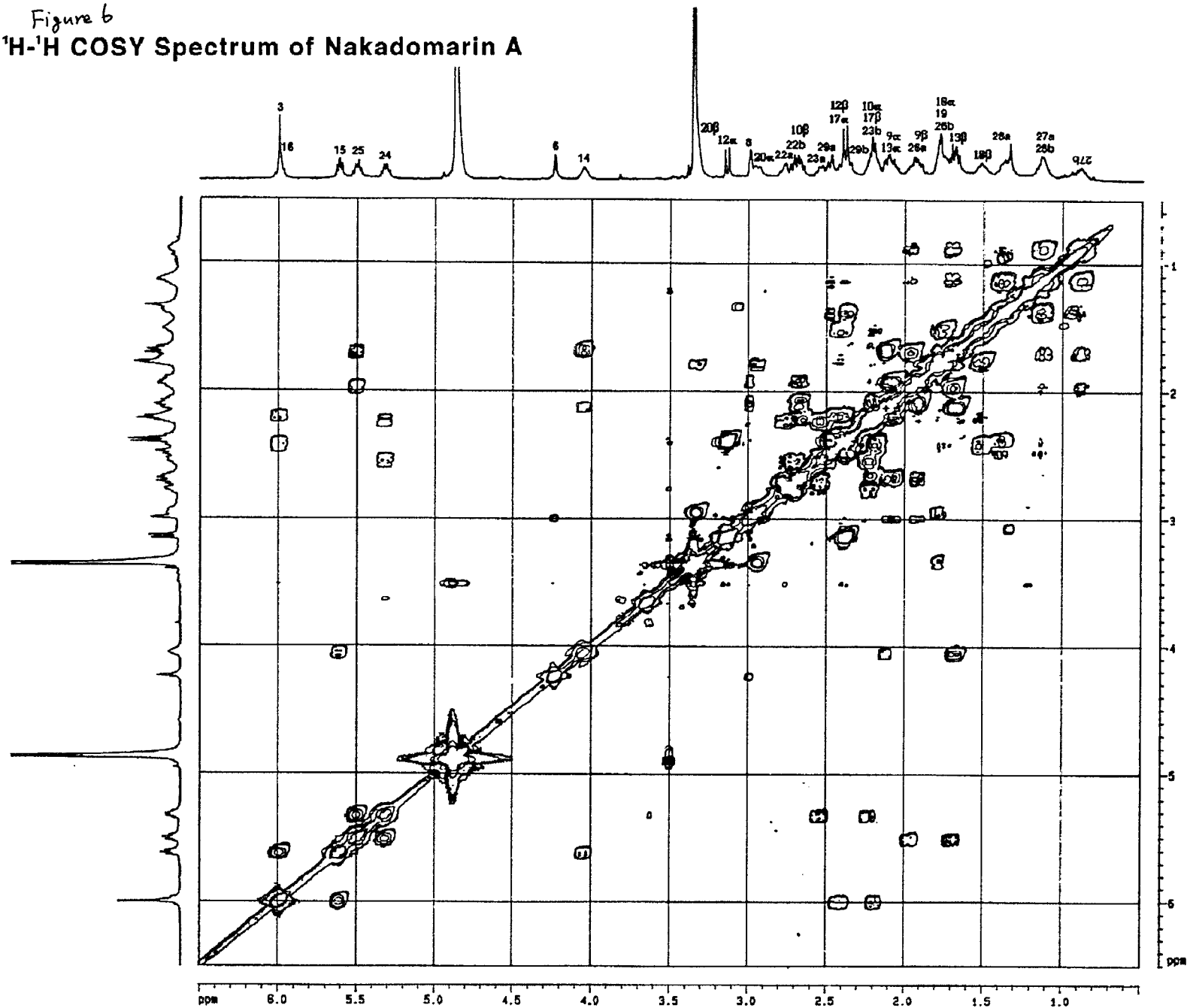


Figure 6  
<sup>1</sup>H-<sup>1</sup>H COSY Spectrum of Nakadomin A



Current Data Parameters

NAME	sho
EXPNO	6341
PROCNO	1

F2 - Acquisition Parameters

Date	970512
Time	0.39
PULPROG	coesy90
SOLVENT	CDCL3
AQ	0.1136840 sec
FIDRES	4.396930 Hz
DN	111.0 usec
RG	715
NUCLEUS	1H
D1	1.6000000 sec
P1	7.2 USEC
DD	0.0000030 sec
DE	136.7 usec
SF01	500.138195 MHz
SNH	4904.50 Hz
TD	1024
NS	16
DS	2
IN0	0.0002220 sec

F1 - Acquisition parameters

MD0	1
TD	256
SF01	500.1381 MHz
FIDRES	17.585718 Hz
SN	9.007 ppm

F2 - Processing parameters

SI	1024
SF	500.1373669 MHz
MDN	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

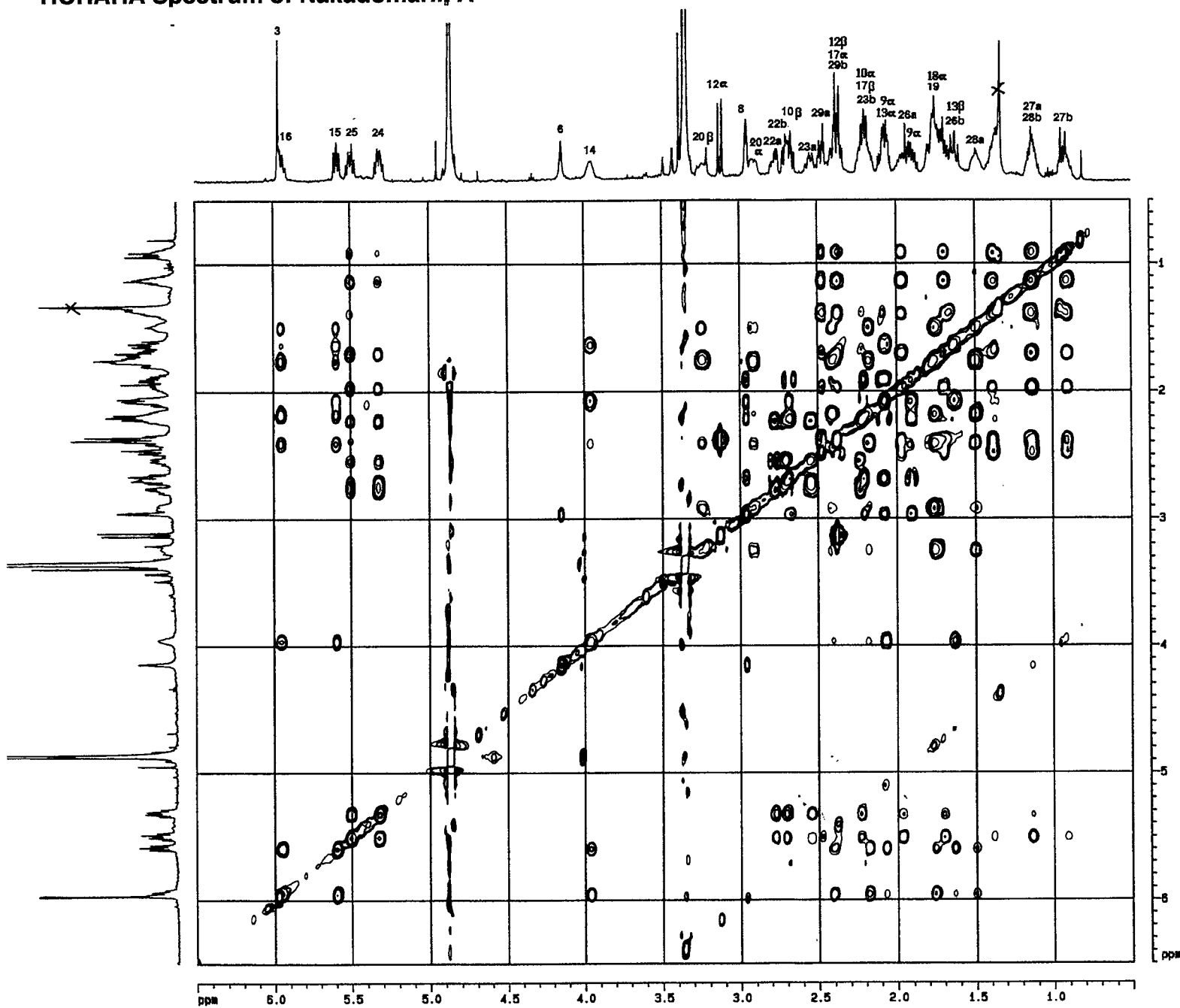
F1 - Processing parameters

SI	1024
MC2	OF
SF	500.1373673 MHz
MDN	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	25.00 cm
CX1	20.00 cm
F2PL0	6.504 ppm
F2L0	3252.65 Hz
F2PHI	0.496 ppm
F2HI	248.18 Hz
F1PL0	6.503 ppm
F1L0	3252.25 Hz
F1PHI	0.500 ppm
F1HI	250.07 Hz
F2PPMCH	0.24029 ppm/cm
F2HZCM	120.17877 Hz/cm
F1PPMCH	0.30014 ppm/cm
F1HZCM	150.10064 Hz/cm

Figure 7  
HOHAHA Spectrum of Nakadomarin A



Current Data Parameters

NAME	..ho
EXPNO	2101
PROCNO	1

F2 - Acquisition Parameters

File	..ho
Time	..ho
PROCNO	1
SOLVENT	F..
AQ	0.121 sec
FIDRES	0.4297 Hz
DW	87.0 usec
RG	..30
NUCLEUS	1H
D1	2.000000 sec
D12	0.000200 sec
TL0	1.00 dB
P1	7.0 usec
D13	0.000030 sec
D0	0.000030 sec
TL3	14.00 dB
P17	2500.0 usec
P6	32.0 usec
P7	64.0 usec
L1	28
P5	22.0 usec
DE	103.8 usec
SFO1	500.136987 MHz
SWH	6024.10 Hz
TD	1024
NS	32
DS	4
IN0	0.000030 sec

F1 - Acquisition parameters

MD0	2
TD	256
SFO1	500.1394 MHz
FIDRES	23.533945 Hz
SW	12.045 ppm

F2 - Processing parameters

SI	1024
SF	500.1373639 MHz
WDW	OSINE
SSB	3
LB	0.00 Hz
GB	0
PC	1.00

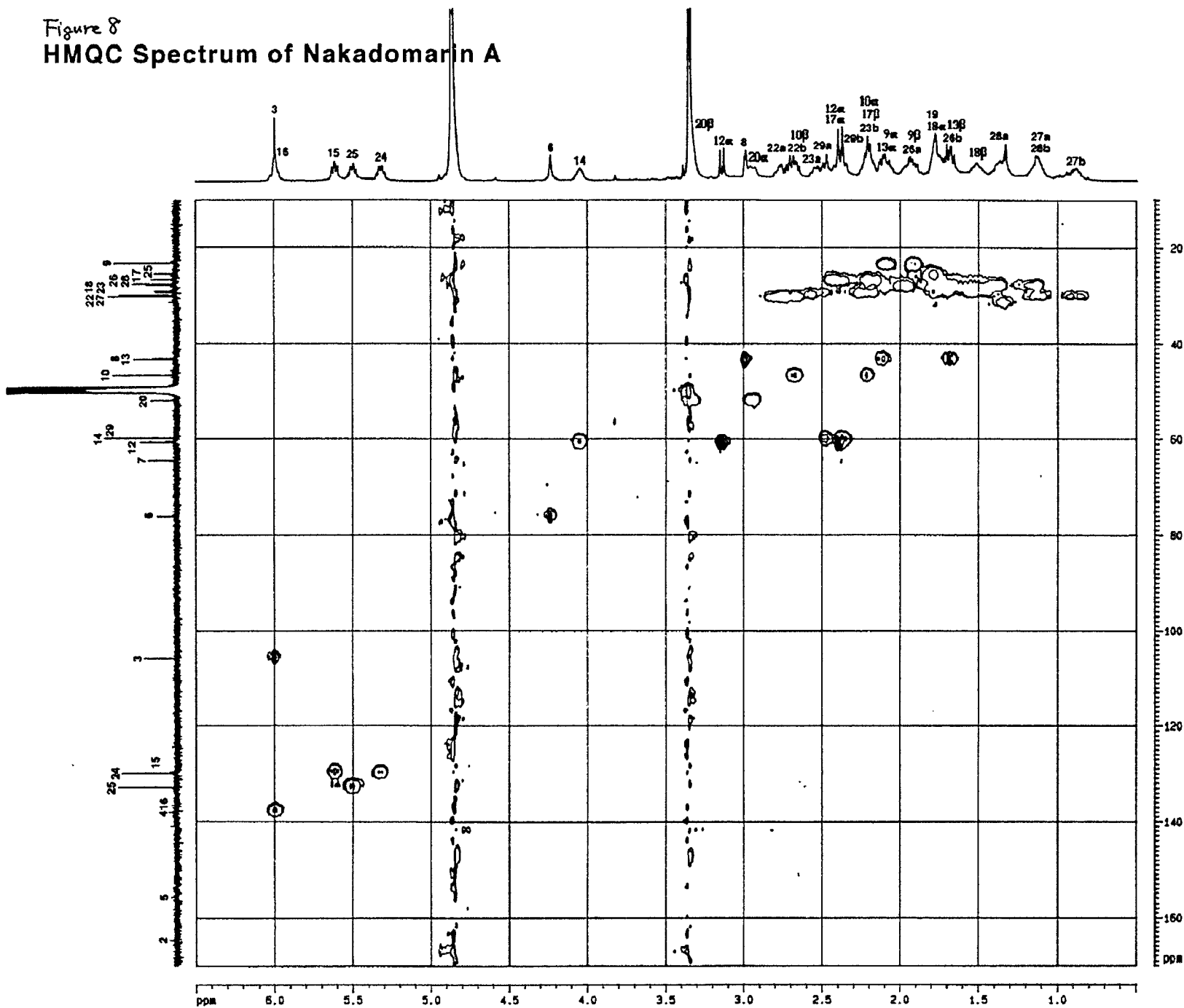
F1 - Processing parameters

SI	1024
MC2	TPPI
SF	500.1373628 MHz
WDW	OSINE
SSB	3
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	25.00 cm
CX1	20.00 cm
F2PLO	6.500 ppm
F2L0	3250.89 Hz
F2PHI	0.500 ppm
F2H1	250.07 Hz
F1PLO	6.500 ppm
F1L0	3250.89 Hz
F1PHI	0.500 ppm
F1H1	250.07 Hz
F2PPNCH	0.24000 ppm/cm
F2HZCH	120.03297 Hz/cm
F1PPNCH	0.30000 ppm/cm
F1HZCH	150.04121 Hz/cm

Figure 8  
 HMQC Spectrum of Nakadomin A



Current Data Parameters

NAME	886
EXPNO	6342
PROCNO	1

F2 - Acquisition Parameters

Date_	870612
Time	2.41
PULPROG	invzga
SOLVENT	CDCl3
AS	0.2273489 sec
FIDRES	2.198485 Hz
DS	111.0 usec
MS	715
NUCLEUS	1H
D1	2.0000000 sec
P1	7.2 usec
D2	0.0034800 sec
P2	14.4 usec
P4	23.0 usec
SFO2	125.7732386 MHz
D7	0.4840000 sec
P3	11.5 usec
D8	0.0000000 sec
D13	0.0000000 sec
DE	138.7 usec
SFO1	500.1361195 MHz
SNH	4004.50 Hz
TD	2848
P31	78.8 usec
MS	48
DS	4
IN0	0.0000000 sec

F1 - Acquisition parameters

MD	4
TD	256
SFO1	125.7732 MHz
FIDRES	100.511177 Hz
SN	220.865 ppm

F2 - Processing parameters

SI	2048
SF	500.1373863 MHz
MDW	881INE
SGB	2
LB	0.00 Hz
GB	0
PC	1.48

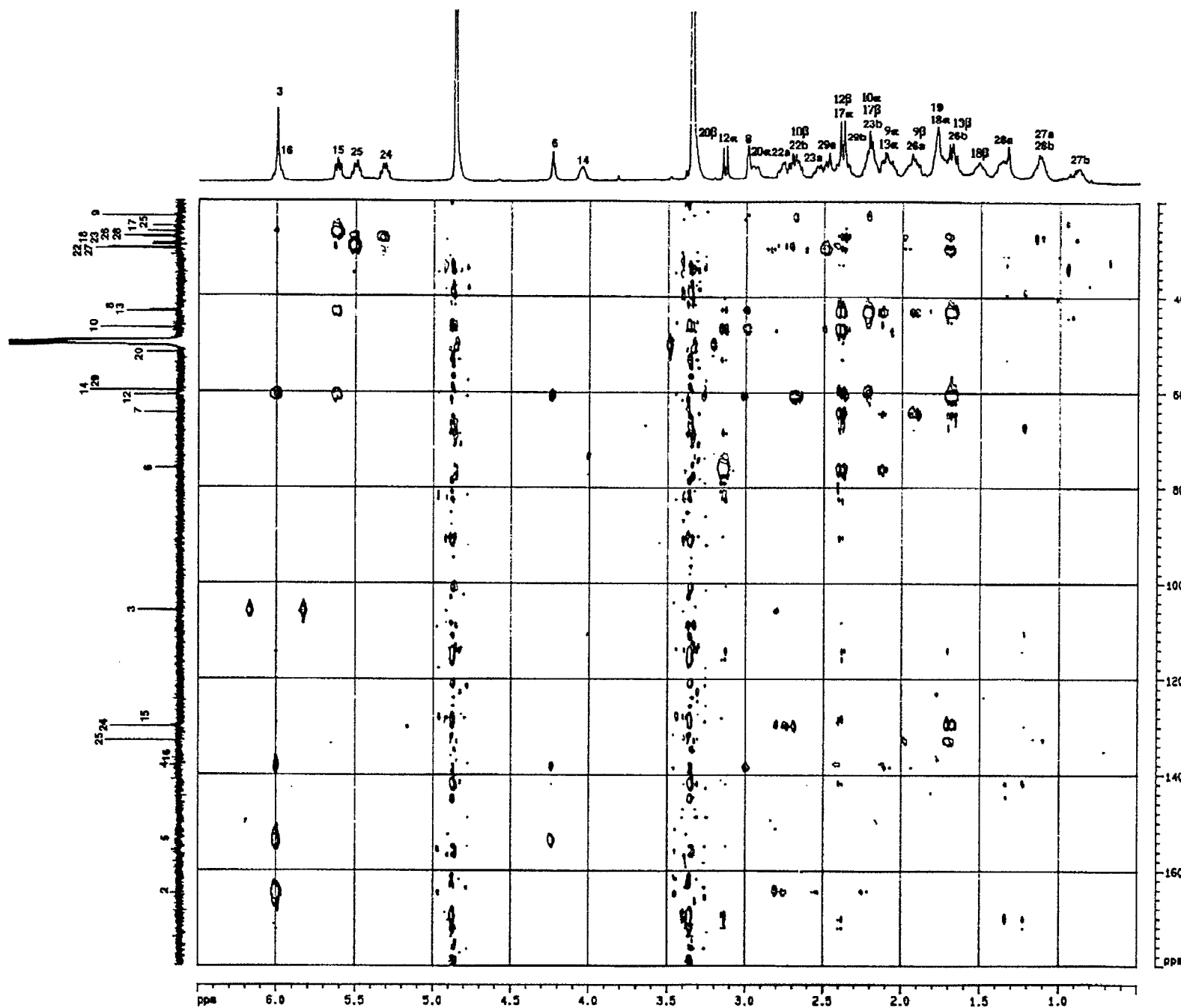
F1 - Processing parameters

SI	512
MC2	TPPI
SF	125.7584411 MHz
MDW	881INE
SGB	2
LB	0.00 Hz
GB	0

2D NMR plot parameters

CSZ	25.00 cm
CSX	20.00 cm
F2PLD	6.500 ppm
F2LO	3251.68 Hz
F2FHI	0.487 ppm
F2HI	248.82 Hz
F2PLD	178.000 ppm
F2LO	21379.10 Hz
F2FHI	10.000 ppm
F2HI	1257.58 Hz
F2PPHCH	0.24012 ppm/ca
F2FZCH	120.99079 Hz/ca
F2PPHCH	8.00000 ppm/ca
F2FZCH	1006.07350 Hz/ca

Figure 9  
HMBC Spectrum of Nakadomarin A



Current Data Parameters  
NAME sho  
EXPNO 6312  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 970427  
Time 0.26  
PULPROG inv4iprmd  
SOLVENT CDC13  
AQ 0.2027720 sec  
FIDRES 2.464047 Hz  
AQ 09.0 usec  
RG 715  
NUCLEUS 1H  
D1 2.0000000 sec  
P1 6.8 usec  
D2 0.034500 sec  
P2 11.5 usec  
SFO2 125.7732066 MHz  
D3 0.0500000 sec  
D4 0.0000000 sec  
P2 13.5 usec  
DE 123.7 usec  
SFO1 500.1373653 MHz  
SH 5090.50 Hz  
TD 2048  
HE 64  
DE 4  
AQ 0.0000100 sec

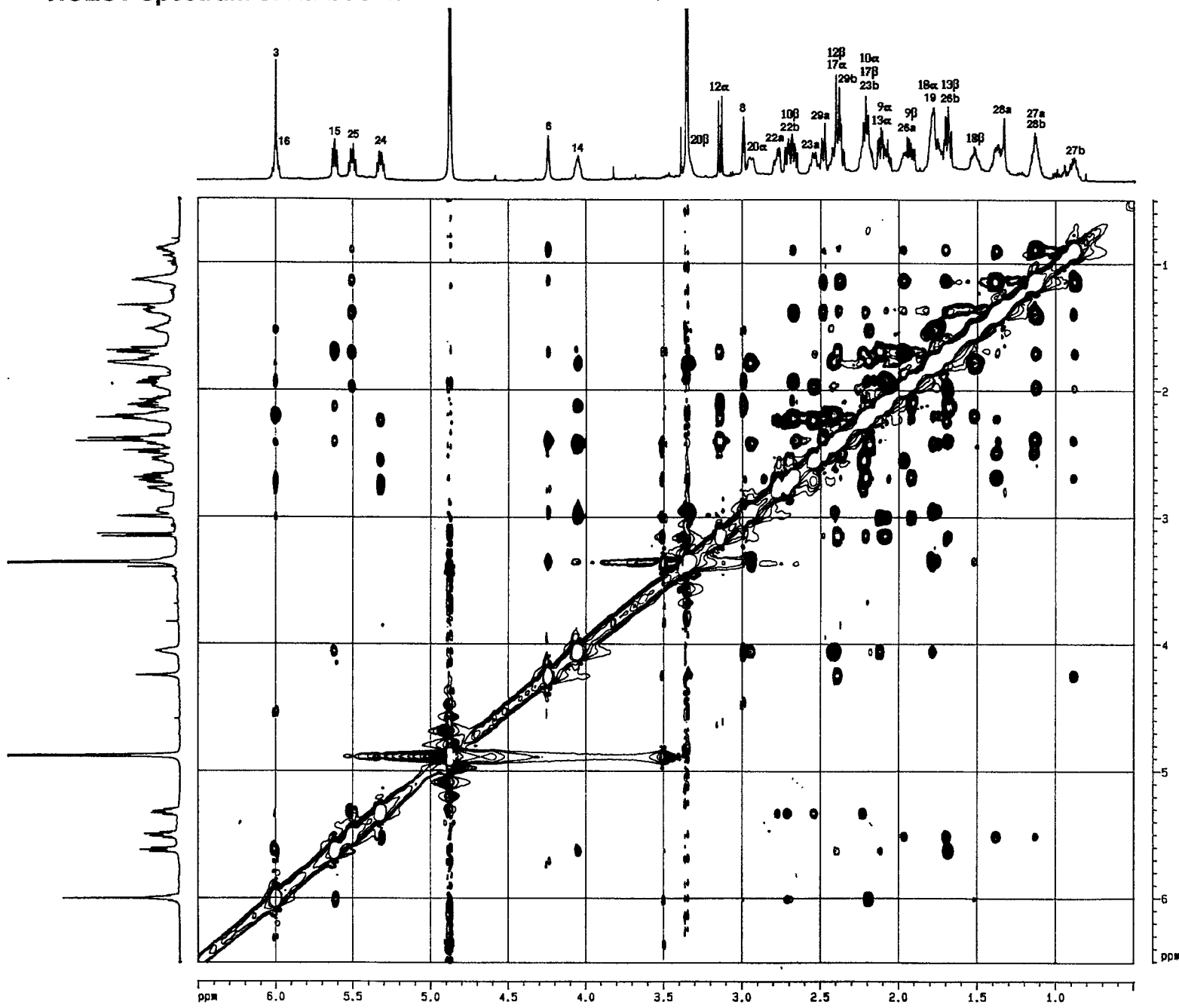
F1 - acquisition parameters  
MD 2  
TD 256  
SFO1 125.7732 MHz  
FIDRES 168.588331 Hz  
SH 220.861 ppm

F2 - Processing parameters  
SI 2048  
SF 500.1373653 MHz  
WDW 65TIME  
SSB 2  
LB 0.60 Hz  
GB 0  
PC 1.00

F1 - Processing parameters  
SI 256  
MC 0F  
SF 125.7584109 MHz  
WDW 65TIME  
SSB 2  
LB 0.04 Hz  
GB 0

2D NMR plot parameters  
C12 25.00 cm  
C11 20.00 cm  
F2PL0 8.504 ppm  
F2D0 3230.89 Hz  
F2PHI 0.500 ppm  
F2M1 236.87 Hz  
F1PL0 180.000 ppm  
F1D0 22436.70 Hz  
F1PHI 20.000 ppm  
F1M1 2515.19 Hz  
F2PPMCH 0.24000 ppm/cm  
F1PPMCH 120.03287 Hz/cm  
F1PPMCH 8.00000 ppm/cm

Figure 10  
NOESY Spectrum of Nakadomarin A



Current Data Parameters  
 NAME sho  
 EXPNO 2271  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 970511  
 Time 18.08  
 PULPROG noesytp  
 SOLVENT C5D8  
 AQ 0.0942280 sec  
 FIDRES 5.307405 Hz  
 DW 92.0 usec  
 RG 256  
 NUCLEUS 1H  
 ML1 3 dB  
 O1 2.0000000 sec  
 P1 10.5 usec  
 O0 0.0000030 sec  
 O8 0.0000000 sec  
 DE 131.4 usec  
 SFO1 500.1399811 MHz  
 SWH 5434.78 Hz  
 TD 1024  
 NS 56  
 DS 2  
 INO 0.0000260 sec

F1 - Acquisition parameters  
 NDD 2  
 TD 256  
 SFO1 500.14 MHz  
 FIDRES 21.229622 Hz  
 SW 9.056 ppm

F2 - Processing parameters  
 SI 1024  
 SF 500.1378782 MHz  
 MVM GSINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0  
 PC 1.00

F1 - Processing parameters  
 SI 1024  
 MC2 TPPI  
 SF 500.1378762 MHz  
 MVM GSINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0

2D NMR plot parameters  
 CX2 25.00 cm  
 CX1 20.00 cm  
 F2PL0 5.502 ppm  
 F2L0 3902.17 Hz  
 F2PHI 0.467 ppm  
 F2HI 298.44 Hz  
 F1PL0 6.505 ppm  
 F1L0 3904.11 Hz  
 F1PHI 0.492 ppm  
 F1HI 295.07 Hz  
 F2PPMCH 0.24019 ppm/cm  
 F2HZCH 144.14911 Hz/cm  
 F1PPMCH 0.30058 ppm/cm



Figure 11. PDB file of 5/5/15/6-tetracyclic system in nakadomarin A (1) calculated by Macromodel ver. 5.0.

```
HETATM 1 C -1.945 -0.664 -2.360
HETATM 2 C -1.544 -1.855 -1.485
HETATM 3 C -2.495 -2.005 -0.257
HETATM 4 C -3.232 -0.678 0.011
HETATM 5 N -2.274 0.437 -0.144
HETATM 6 C -1.898 0.649 -1.564
HETATM 7 C -2.622 1.683 0.578
HETATM 8 C -1.608 -2.382 0.981
HETATM 9 C -0.247 -1.973 0.491
HETATM 10 C -0.219 -1.717 -0.816
HETATM 11 C 1.761 -1.300 0.053
HETATM 12 C 1.108 -1.281 -1.170
HETATM 13 O 0.965 -1.744 1.129
HETATM 14 C -1.378 2.567 0.753
HETATM 15 C 3.195 -0.854 0.236
HETATM 16 C -0.305 1.871 1.607
HETATM 17 C 3.249 0.527 0.902
HETATM 18 C 1.026 2.630 1.604
HETATM 19 C 2.705 1.606 -0.039
HETATM 20 C 1.724 2.482 0.248
HETATM 21 H -1.271 -0.589 -3.215
HETATM 22 H -2.955 -0.830 -2.739
HETATM 23 H -1.550 -2.774 -2.073
HETATM 24 H -3.238 -2.785 -0.432
HETATM 25 H -4.059 -0.554 -0.691
HETATM 26 H -3.652 -0.700 1.017
HETATM 27 H -2.564 1.370 -2.041
HETATM 28 H -0.879 1.036 -1.602
HETATM 29 H -3.393 2.230 0.033
HETATM 30 H -3.005 1.442 1.570
HETATM 31 H -1.885 -1.845 1.888
HETATM 32 H -1.623 -3.459 1.151
HETATM 33 H 1.481 -0.963 -2.133
HETATM 34 H -0.976 2.833 -0.224
HETATM 35 H -1.674 3.490 1.254
HETATM 36 H 3.700 -1.575 0.879
HETATM 37 H 3.710 -0.826 -0.726
HETATM 38 H -0.672 1.805 2.633
HETATM 39 H -0.117 0.861 1.246
HETATM 40 H 2.700 0.476 1.840
HETATM 41 H 4.290 0.763 1.125
HETATM 42 H 0.843 3.687 1.800
HETATM 43 H 1.654 2.254 2.410
HETATM 44 H 3.134 1.652 -1.033
HETATM 45 H 1.433 3.176 -0.531
CONNECT 1 2 6 21 22
CONNECT 2 1 3 10 23
CONNECT 3 2 4 8 24
CONNECT 4 3 5 25 26
CONNECT 5 4 6 7
CONNECT 6 1 5 27 28
CONNECT 7 5 14 29 30
CONNECT 8 3 9 31 32
```

CONNECT 9 8 10 13  
CONNECT 10 2 9 12  
CONNECT 11 12 13 15  
CONNECT 12 10 11 33  
CONNECT 13 9 11  
CONNECT 14 7 16 34 35  
CONNECT 15 11 17 36 37  
CONNECT 16 14 18 38 39  
CONNECT 17 15 19 40 41  
CONNECT 18 16 20 42 43  
CONNECT 19 17 20 44  
CONNECT 20 18 19 45  
CONNECT 21 1  
CONNECT 22 1  
CONNECT 23 2  
CONNECT 24 3  
CONNECT 25 4  
CONNECT 26 4  
CONNECT 27 6  
CONNECT 28 6  
CONNECT 29 7  
CONNECT 30 7  
CONNECT 31 8  
CONNECT 32 8  
CONNECT 33 12  
CONNECT 34 14  
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CONNECT 36 15  
CONNECT 37 15  
CONNECT 38 16  
CONNECT 39 16  
CONNECT 40 17  
CONNECT 41 17  
CONNECT 42 18  
CONNECT 43 18  
CONNECT 44 19  
CONNECT 45 20  
END

Figure 12. PDB file of 8/5-bicyclic system in nakadomarin A (1) calculated by Macromodel ver. 5.0.

```

HETATM  1  C      1.568 -0.231  0.554
HETATM  2  C      1.415 -1.581 -0.174
HETATM  3  C      0.292 -2.494  0.355
HETATM  4  C     -1.142 -2.037  0.054
HETATM  5  C     -1.565 -0.837  0.862
HETATM  6  C     -1.231  0.434  0.592
HETATM  7  C     -0.350  0.857 -0.559
HETATM  8  N      1.052  0.916 -0.180
HETATM  9  C      1.198  2.166  0.550
HETATM 10  C      0.275  3.172 -0.156
HETATM 11  C     -0.644  2.295 -1.022
HETATM 12  H      2.657 -0.044  0.718
HETATM 13  H      1.122 -0.298  1.573
HETATM 14  H      2.371 -2.145 -0.048
HETATM 15  H      1.310 -1.430 -1.274
HETATM 16  H      0.413 -2.651  1.453
HETATM 17  H      0.427 -3.497 -0.117
HETATM 18  H     -1.855 -2.866  0.278
HETATM 19  H     -1.258 -1.842 -1.037
HETATM 20  H     -2.171 -1.038  1.763
HETATM 21  H     -1.580  1.226  1.276
HETATM 22  H     -0.483  0.163 -1.420
HETATM 24  H      2.263  2.500  0.557
HETATM 25  H      0.868  2.043  1.610
HETATM 26  H      0.857  3.885 -0.788
HETATM 27  H     -0.311  3.766  0.586
HETATM 28  H     -0.347  2.405 -2.094
HETATM 29  H     -1.723  2.568 -0.942
CONNECT  1  2  8 12 13
CONNECT  2  1  3 14 15
CONNECT  3  2  4 16 17
CONNECT  4  3  5 18 19
CONNECT  5  4  6 20
CONNECT  6  5  7 21
CONNECT  7  6  8 11 22
CONNECT  8  1  7  9
CONNECT  9  8 10 24 25
CONNECT 10  9 11 26 27
CONNECT 11  7 10 28 29
CONNECT 12  1
CONNECT 13  1
CONNECT 14  2
CONNECT 15  2
CONNECT 16  3
CONNECT 17  3
CONNECT 18  4
CONNECT 19  4
CONNECT 20  5
CONNECT 21  6
CONNECT 22  7
CONNECT 24  9
CONNECT 25  9
CONNECT 26 10

```

CONECT 27 10  
CONECT 28 11  
CONECT 29 11  
END