The Tandem of Full Spin Analysis and qHNMR for the Quality Control of Botanicals Exemplified with *Ginkgo biloba*

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■ Supporting Information

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S1. The ^{1}H Fingerprint of Ginkgolide A (**1**) in the PERCH .PMS file format.

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* NEW: the lines beginning by * are comment lines !
* To keep all the chemical shifts fixed during iteration
* replace "CHEMICAL SHIFTS(HZ):" by "..SHIFTS(HZ): fixed"
* The couplings can be fixed in the same way

NMR-data: C:\Users\jgnapo_2\Documents\jgnapo\perch\Ginkgolides\GA\ginkgoa
#$œ  Date  9. 3.2011;  Time 17: 5:18     ginkgoa.5TH

CHEMICAL SHIFTS(PPM):  Similarity% =  28.130
PROTON    2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 OH-3    / 1     6.378972  1*1*1  STAT=Y  PRED= 4.856 RANGE= 1.805 WIDTH(Y)= 1.273 RESP(Y)= 1.0000
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 H-7beta / 1     2.043863  1*1*1  STAT=Y  PRED= 2.070 RANGE= 0.557 WIDTH(Y)= 2.501 RESP(Y)= 0.8989 HSQC= C14
 H-1beta / 1     1.805711  1*1*1  STAT=Y  PRED= 1.401 RANGE= 0.302 WIDTH(Y)= 1.882 RESP(Y)= 0.9213 HSQC= C8
 H-1alpha/ 1     2.750139  1*1*1  STAT=Y  PRED= 2.169 RANGE= 0.387 WIDTH(Y)= 1.927 RESP(Y)= 0.9005 HSQC= C8
 H-2     / 1     4.833738  1*1*1  STAT=Y  PRED= 4.895 RANGE= 0.262 WIDTH(Y)= 1.798 RESP(Y)= 0.9709 HSQC= C9
 H-6     / 1     4.945707  1*1*1  STAT=Y  PRED= 4.760 RANGE= 0.247 WIDTH(Y)= 1.956 RESP(Y)= 0.9824 HSQC= C13
 H-7alpha/ 1     2.027505  1*1*1  STAT=Y  PRED= 2.025 RANGE= 0.472 WIDTH(Y)= 2.358 RESP(Y)= 0.8736 HSQC= C14
 H-8     / 1     1.710433  1*1*1  STAT=Y  PRED= 1.700 RANGE= 0.222 WIDTH(Y)= 2.173 RESP(Y)= 0.9339 HSQC= C15
 H-10    / 1     4.941390  1*1*1  STAT=Y  PRED= 4.165 RANGE= 0.392 WIDTH(Y)= 1.780 RESP(Y)= 0.9248 HSQC= C17
 H-12    / 1     6.023393  1*1*1  STAT=Y  PRED= 5.659 RANGE= 0.335 WIDTH(Y)= 1.498 RESP(Y)= 0.9865 HSQC= C19
 H-14    / 1     2.937891  1*1*1  STAT=Y  PRED= 2.949 RANGE= 0.387 WIDTH(Y)= 1.519 RESP(Y)= 0.9493 HSQC= C21
 H-16    / 1     1.117747  1*1*3  STAT=Y  PRED= 1.114 RANGE= 0.252 WIDTH(Y)= 1.687 RESP(Y)= 0.9350 HSQC= C23
 t-but   / 1     1.017131  1*1*9  STAT=Y  PRED= 0.928 RANGE= 0.227 WIDTH(Y)= 2.491 RESP(Y)= 0.9025 HSQC= C25-27

COUPLING CONSTANTS(HZ):  Similarity% =  35.913
 J6_29       5.1630   J OH-10    H-10       STAT=Y  PRED= 5.140 RANGE= 0.750
 J12_22      0.6218   J H-7beta  H-6        STAT=Y  PRED= 1.070 RANGE= 2.000
 J12_24    -13.7046   J H-7beta  H-7alpha   STAT=Y  PRED= -12.430 RANGE= 1.000
 J12_26      4.5778   J H-7beta  H-8        STAT=Y  PRED= 4.190 RANGE= 3.000
 J14_15    -15.1675   J H-1beta  H-1alpha   STAT=Y  PRED= -12.310 RANGE= 1.000
 J14_17      8.2624   J H-1beta  H-2        STAT=Y  PRED= 8.810 RANGE= 3.000
 J15_17      7.2878   J H-1alpha H-2        STAT=Y  PRED= 7.110 RANGE= 3.000
 J22_24      4.0483   J H-6      H-7alpha   STAT=Y  PRED= 4.830 RANGE= 3.000
 J24_26     14.3434   J H-7alpha H-8        STAT=Y  PRED= 13.120 RANGE= 2.200
 J35_38      7.1931   J H-14     H-16       STAT=Y  PRED= 6.640 RANGE= 0.250

CONTROL PARAMETERS:
       Solvent =  none (def. 99% enriched)
         1.000 =  Concentration (vol%, def=1.0%)
    0.00100000 =  Minimum line-intensity
    0.00100000 =  Diagonalization criterium (not in use)
    7.50126041 =  Left frequency (ppm)
    0.00000000 =  Right frequency (ppm)
        10.000 =  Acquisition time (s, for QMTLS)
         1.269 =  Line-width (for modes D, P & T, 0=use defaults)
   0.068609932 =  Data-point resolution (Hz)
        26.001 =  GAUSSIAN (%, 0=use default from INF)
         2.174 =  Dispersion contribution (%, 0=use default from INF)
    0.00000000 =  Decoupling frequency (for DORES)

CONSTRAINTS (in equations X0 = 1.0)...use no empty lines

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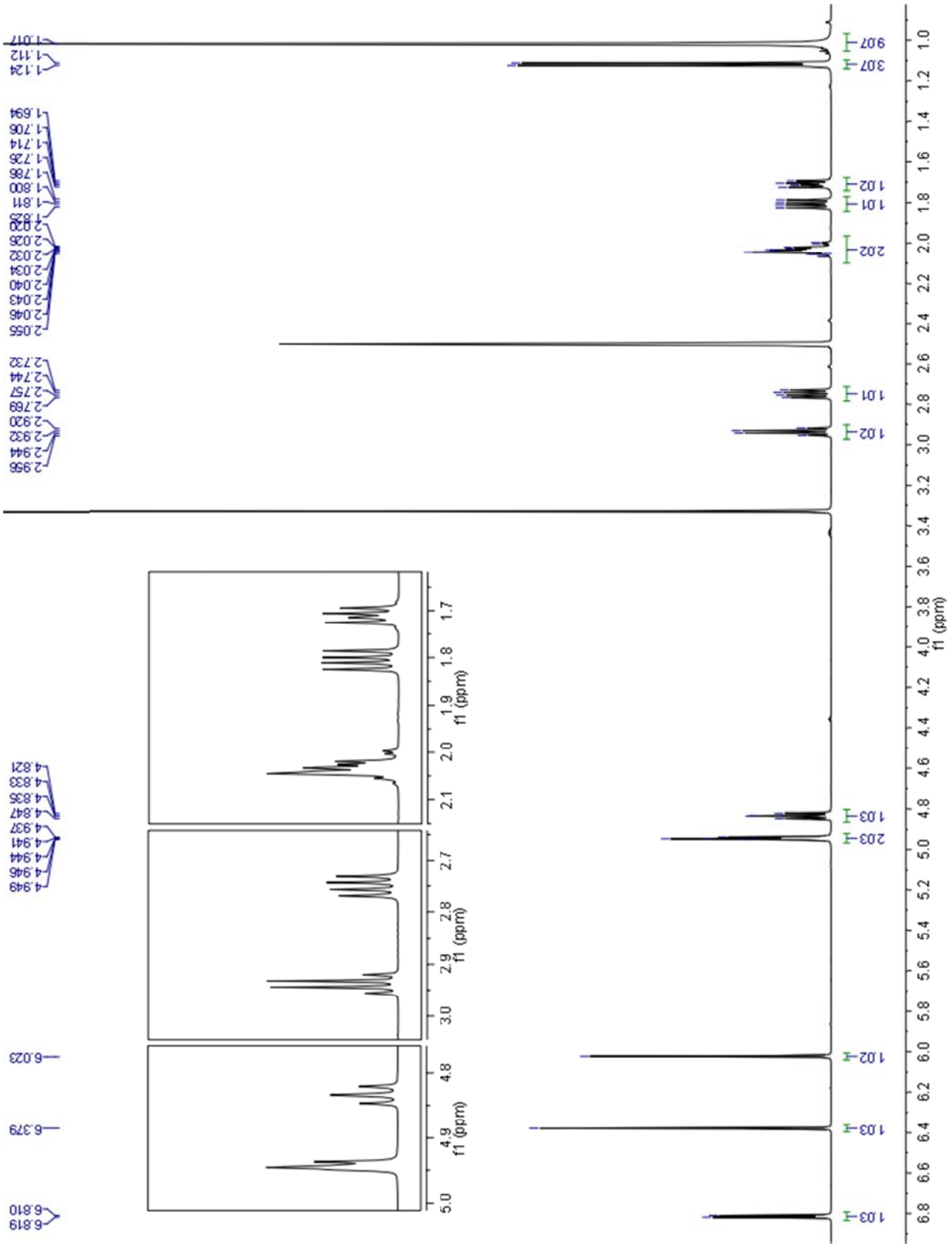
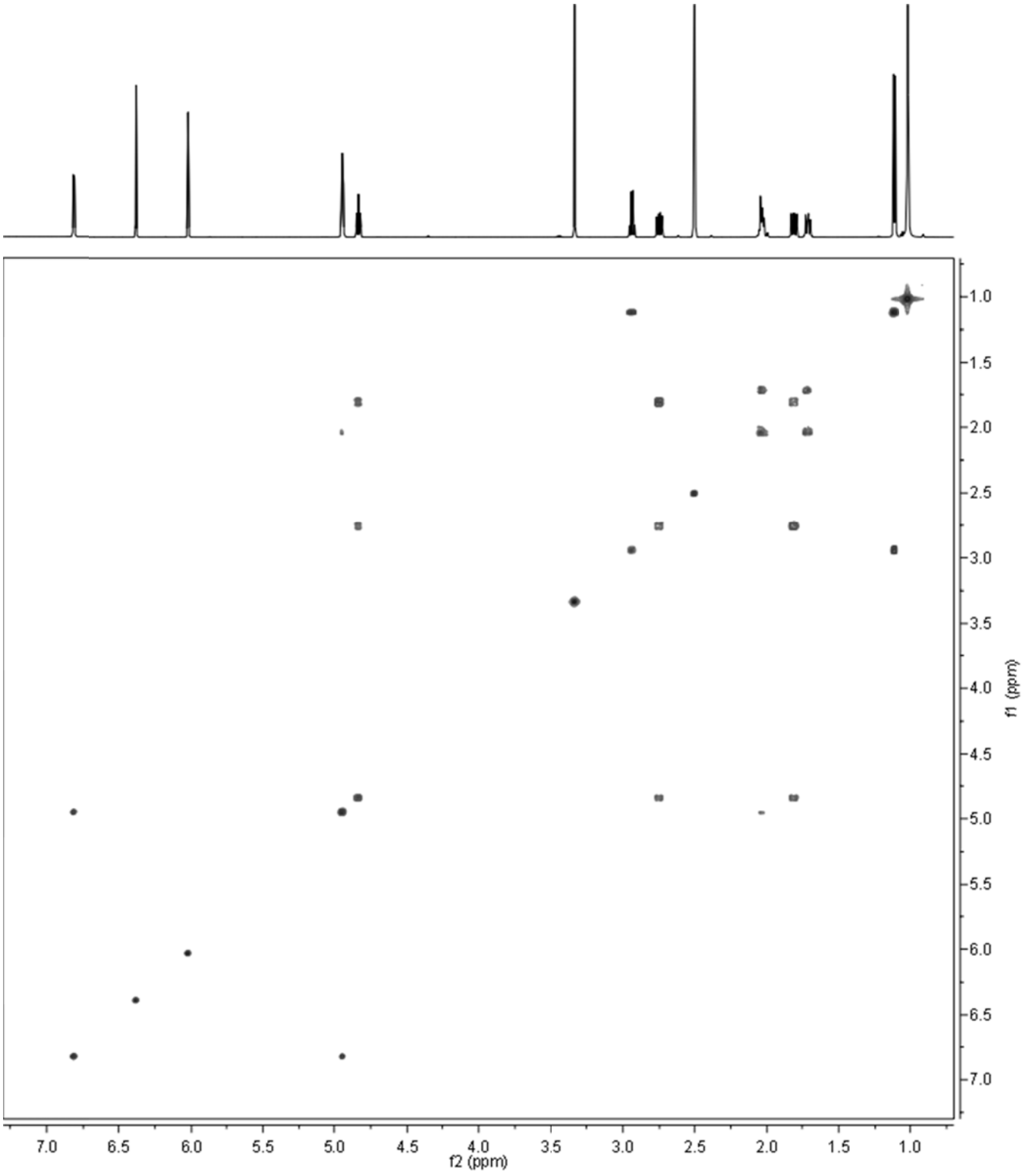
S2. ^{1}H NMR spectrum of Ginkgolide A (**1**, DMSO-d_6, 600 MHz).



S3. ^{1}H,^{1}H-COSY experiment of Ginkgolide A (**1**, DMSO-d_6, 600 MHz).



S4. The ^{1}H Fingerprint of Ginkgolide B (**2**) in the PERCH .PMS file format.

```
* NEW: the lines beginning by * are comment lines !
* To keep all the chemical shifts fixed during iteration
* replace "CHEMICAL SHIFTS(HZ):" by "..SHIFTS(HZ): fixed"
* The couplings can be fixed in the same way

NMR-data: C:\Users\jgnapo_2\Documents\jgnapo\perch\Ginkgolides\GB\ginkgob
#$œ  Date  9. 3.2011;  Time 17: 8:11     ginkgob.5TH

CHEMICAL SHIFTS(PPM):  Similarity% =  11.032
PROTON    2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 OH-3    / 1     6.471908  1*1*1  STAT=Y  PRED= 4.913 RANGE= 1.733 WIDTH(Y)= 1.525 RESP(Y)= 1.0000
 OH-10   / 1     7.462874  1*1*1  STAT=Y  PRED= 4.556 RANGE= 1.695 WIDTH(Y)= 1.929 RESP(Y)= 0.9612
 H-7beta / 1     2.137230  1*1*1  STAT=Y  PRED= 2.036 RANGE= 0.560 WIDTH(Y)= 2.168 RESP(Y)= 0.9003 HSQC= C14
 H-1     / 1     4.042104  1*1*1  STAT=Y  PRED= 3.762 RANGE= 0.100 WIDTH(Y)= 1.692 RESP(Y)= 0.9364 HSQC= C8
 H-2     / 1     4.642590  1*1*1  STAT=Y  PRED= 4.089 RANGE= 0.187 WIDTH(Y)= 1.644 RESP(Y)= 0.9775 HSQC= C9
 H-6     / 1     5.303773  1*1*1  STAT=Y  PRED= 4.895 RANGE= 0.237 WIDTH(Y)= 1.799 RESP(Y)= 0.9597 HSQC= C13
 H-7alpha/ 1     1.931786  1*1*1  STAT=Y  PRED= 2.041 RANGE= 0.477 WIDTH(Y)= 2.242 RESP(Y)= 0.8904 HSQC= C14
 H-8     / 1     1.724094  1*1*1  STAT=Y  PRED= 1.670 RANGE= 0.215 WIDTH(Y)= 2.358 RESP(Y)= 0.9326 HSQC= C15
 H-10    / 1     5.019748  1*1*1  STAT=Y  PRED= 4.165 RANGE= 0.380 WIDTH(Y)= 1.969 RESP(Y)= 0.9334 HSQC= C17
 H-12    / 1     6.074154  1*1*1  STAT=Y  PRED= 5.659 RANGE= 0.330 WIDTH(Y)= 1.664 RESP(Y)= 0.9898 HSQC= C19
 H-14    / 1     2.843287  1*1*1  STAT=Y  PRED= 2.949 RANGE= 0.367 WIDTH(Y)= 1.666 RESP(Y)= 0.9457 HSQC= C21
 H-16    / 1     1.106901  1*1*3  STAT=Y  PRED= 1.102 RANGE= 0.382 WIDTH(Y)= 1.848 RESP(Y)= 0.9294 HSQC= C23
 t-butyl / 1     1.028434  1*1*9  STAT=Y  PRED= 0.871 RANGE= 0.202 WIDTH(Y)= 2.590 RESP(Y)= 0.8997 HSQC= C25-27
 OH-1    / 1     4.918842  1*1*1  STAT=Y  PRED= 6.248 RANGE= 2.488 WIDTH(Y)= 1.544 RESP(Y)= 0.9556

COUPLING CONSTANTS(HZ):  Similarity% =  54.436
 J6_29       5.5557   J OH-10    H-10       STAT=Y  PRED= 5.110 RANGE= 0.750
 J12_22      0.8476   J H-7beta  H-6        STAT=Y  PRED= 1.140 RANGE= 2.200
 J12_24    -13.7414   J H-7beta  H-7alpha   STAT=Y  PRED= -12.420 RANGE= 1.000
 J12_26      4.6463   J H-7beta  H-8        STAT=Y  PRED= 4.190 RANGE= 3.000
 J14_17      7.4027   J H-1      H-2        STAT=Y  PRED= 7.800 RANGE= 3.000
 J14_54      3.5631   J H-1      OH-1       STAT=Y  PRED= 3.950 RANGE= 0.750
 J22_24      4.1428   J H-6      H-7alpha   STAT=Y  PRED= 4.630 RANGE= 3.000
 J24_26     14.3540   J H-7alpha H-8        STAT=Y  PRED= 13.130 RANGE= 2.200
 J35_38      7.0831   J H-14     H-16       STAT=Y  PRED= 6.640 RANGE= 0.250

CONTROL PARAMETERS:
       Solvent =  none (def. 99% enriched)
         1.000 =  Concentration (vol%, def=1.0%)
    0.00100000 =  Minimum line-intensity
    0.00100000 =  Diagonalization criterium (not in use)
    8.56788059 =  Left frequency (ppm)
   -0.17374428 =  Right frequency (ppm)
        10.000 =  Acquisition time (s, for QMTLS)
         1.426 =  Line-width (for modes D, P & T, 0=use defaults)
   0.068609932 =  Data-point resolution (Hz)
        26.703 =  GAUSSIAN (%, 0=use default from INF)
         3.021 =  Dispersion contribution (%, 0=use default from INF)
    0.00000000 =  Decoupling frequency (for DORES)

CONSTRAINTS (in equations X0 = 1.0)...use no empty lines

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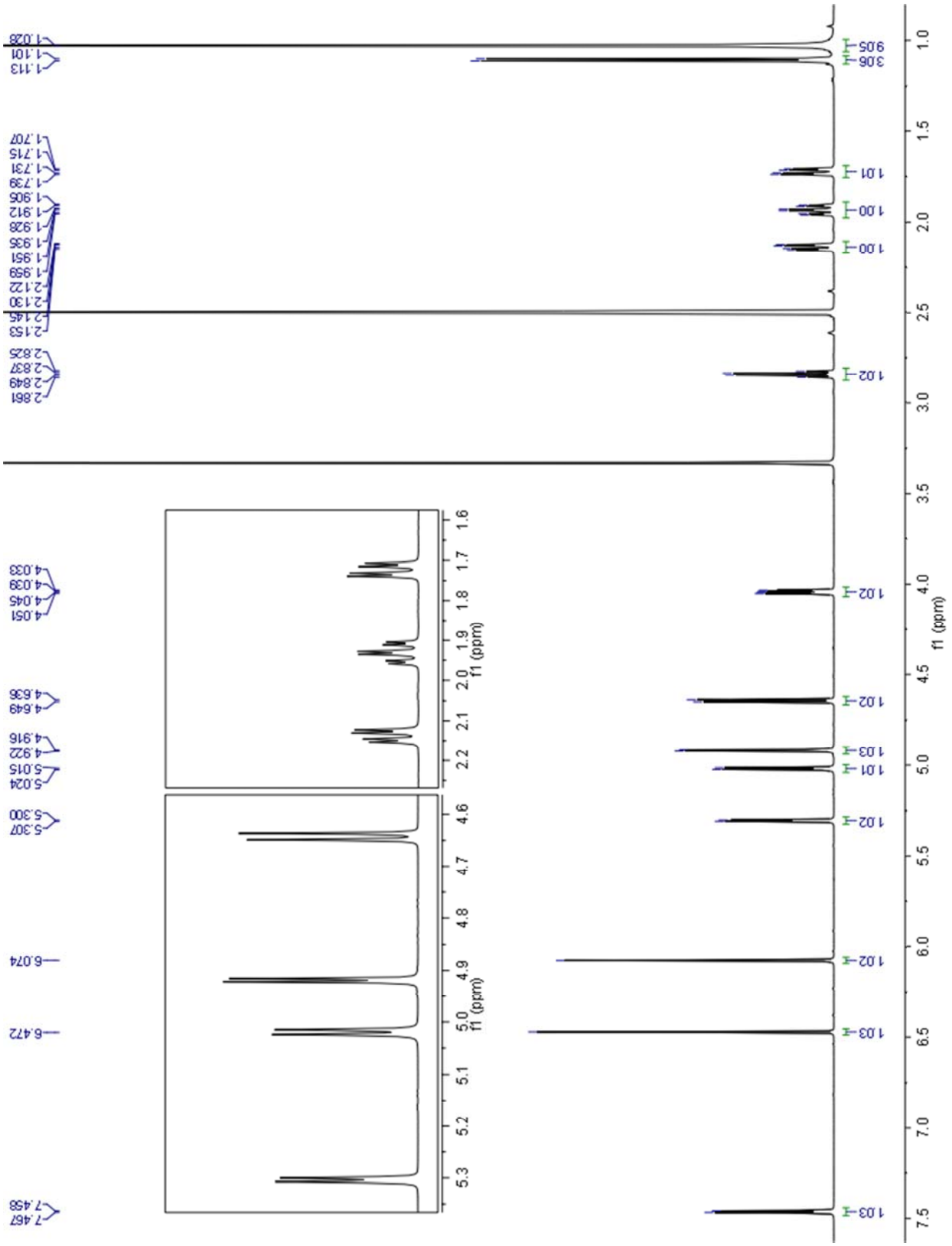
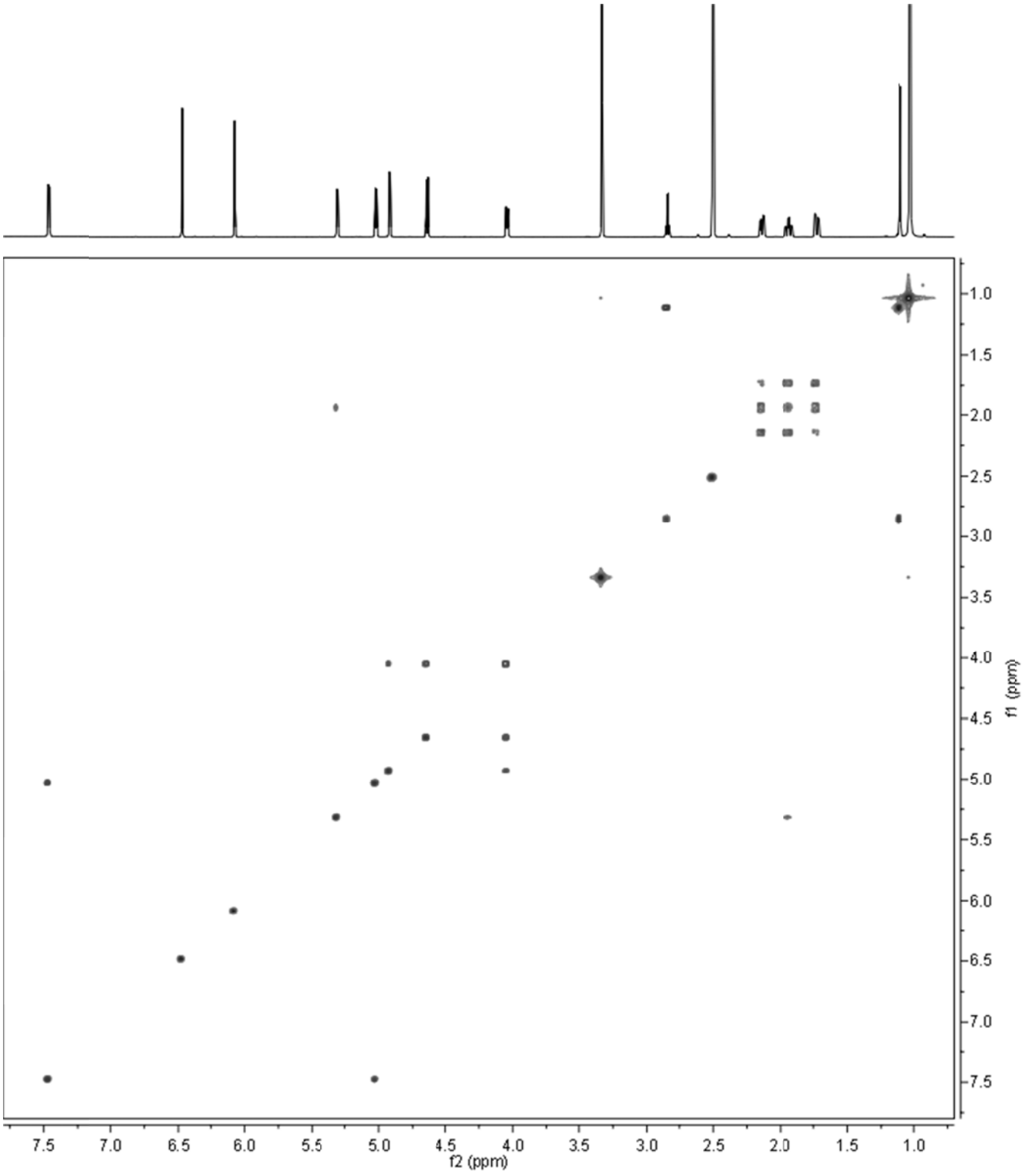
S5. ^{1}H NMR spectrum of Ginkgolide B (**2**, DMSO-d_6, 600 MHz).



S6. ^{1}H,^{1}H-COSY experiment of Ginkgolide B (**2**, DMSO-d_6, 600 MHz).



S7. The ^{1}H Fingerprint of Ginkgolide C (**3**) in the PERCH .PMS file format.

```
* NEW: the lines beginning by * are comment lines !
* To keep all the chemical shifts fixed during iteration
* replace "CHEMICAL SHIFTS(HZ):" by "..SHIFTS(HZ): fixed"
* The couplings can be fixed in the same way

NMR-data: C:\Users\jgnapo_2\Documents\jgnapo\perch\Ginkgolides\GC\ginkgoc
#$œ  Date  9. 3.2011;  Time 17:10:42     ginkgoc.5TH

CHEMICAL SHIFTS(PPM):  Similarity% =   7.110
PROTON    2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 OH-3   / 1     6.479066  1*1*1  STAT=Y  PRED= 5.334 RANGE= 1.700 WIDTH(Y)= 1.736 RESP(Y)= 1.0000
 OH-10  / 1     7.538812  1*1*1  STAT=Y  PRED= 4.347 RANGE= 1.768 WIDTH(Y)= 2.242 RESP(Y)= 0.9489
 OH-7   / 1     5.658435  1*1*1  STAT=Y  PRED= 4.985 RANGE= 1.620 WIDTH(Y)= 1.944 RESP(Y)= 0.9704
 H-1beta/ 1     3.986275  1*1*1  STAT=Y  PRED= 4.316 RANGE= 0.100 WIDTH(Y)= 1.907 RESP(Y)= 0.9449 HSQC= C8
 H-2    / 1     4.626842  1*1*1  STAT=Y  PRED= 4.089 RANGE= 0.170 WIDTH(Y)= 1.789 RESP(Y)= 0.9761 HSQC= C9
 H-6    / 1     4.966384  1*1*1  STAT=Y  PRED= 4.852 RANGE= 0.122 WIDTH(Y)= 1.940 RESP(Y)= 0.9965 HSQC= C13
 H-7    / 1     4.053494  1*1*1  STAT=Y  PRED= 4.559 RANGE= 0.317 WIDTH(Y)= 1.975 RESP(Y)= 0.9273 HSQC= C14
 H-8    / 1     1.551161  1*1*1  STAT=Y  PRED= 1.808 RANGE= 0.222 WIDTH(Y)= 2.077 RESP(Y)= 0.9481 HSQC= C15
 H-10   / 1     4.998365  1*1*1  STAT=Y  PRED= 4.165 RANGE= 0.367 WIDTH(Y)= 2.302 RESP(Y)= 0.9280 HSQC= C17
 H-12   / 1     6.099451  1*1*1  STAT=Y  PRED= 5.659 RANGE= 0.325 WIDTH(Y)= 1.837 RESP(Y)= 0.9848 HSQC= C19
 H-14   / 1     2.813690  1*1*1  STAT=Y  PRED= 2.949 RANGE= 0.342 WIDTH(Y)= 1.804 RESP(Y)= 0.9418 HSQC= C21
 H-16   / 1     1.107483  1*1*3  STAT=Y  PRED= 1.103 RANGE= 0.377 WIDTH(Y)= 1.979 RESP(Y)= 0.8915 HSQC= C23
 t-butyl/ 1     1.091336  1*1*9  STAT=Y  PRED= 0.887 RANGE= 0.225 WIDTH(Y)= 2.733 RESP(Y)= 0.8975 HSQC= C25-27
 OH-1   / 1     4.971784  1*1*1  STAT=Y  PRED= 5.998 RANGE= 1.965 WIDTH(Y)= 1.840 RESP(Y)= 0.8956

COUPLING CONSTANTS(HZ):  Similarity% =  28.377
 J6_30       5.6531   J OH-10   H-10      STAT=Y  PRED= 4.950 RANGE= 0.750
 J13_25      6.2720   J OH-7    H-7       STAT=Y  PRED= 4.300 RANGE= 0.500
 J15_18      7.2205   J H-1beta H-2       STAT=Y  PRED= 7.910 RANGE= 3.000
 J15_55      3.6847   J H-1beta OH-1      STAT=Y  PRED= 4.300 RANGE= 0.500
 J23_25      4.1999   J H-6     H-7       STAT=Y  PRED= 4.670 RANGE= 3.000
 J25_27     12.3964   J H-7     H-8       STAT=Y  PRED= 11.070 RANGE= 2.200
 J36_39      7.0914   J H-14    H-16      STAT=Y  PRED= 6.640 RANGE= 0.250

CONTROL PARAMETERS:
       Solvent =  none (def. 99% enriched)
         1.000 =  Concentration (vol%, def=1.0%)
    0.00100000 =  Minimum line-intensity
    0.00100000 =  Diagonalization criterium (not in use)
    8.89596571 =  Left frequency (ppm)
    0.00000000 =  Right frequency (ppm)
        10.000 =  Acquisition time (s, for QMTLS)
         1.640 =  Line-width (for modes D, P & T, 0=use defaults)
   0.068609932 =  Data-point resolution (Hz)
        33.440 =  GAUSSIAN (%, 0=use default from INF)
        -0.834 =  Dispersion contribution (%, 0=use default from INF)
    0.00000000 =  Decoupling frequency (for DORES)

CONSTRAINTS (in equations X0 = 1.0)...use no empty lines

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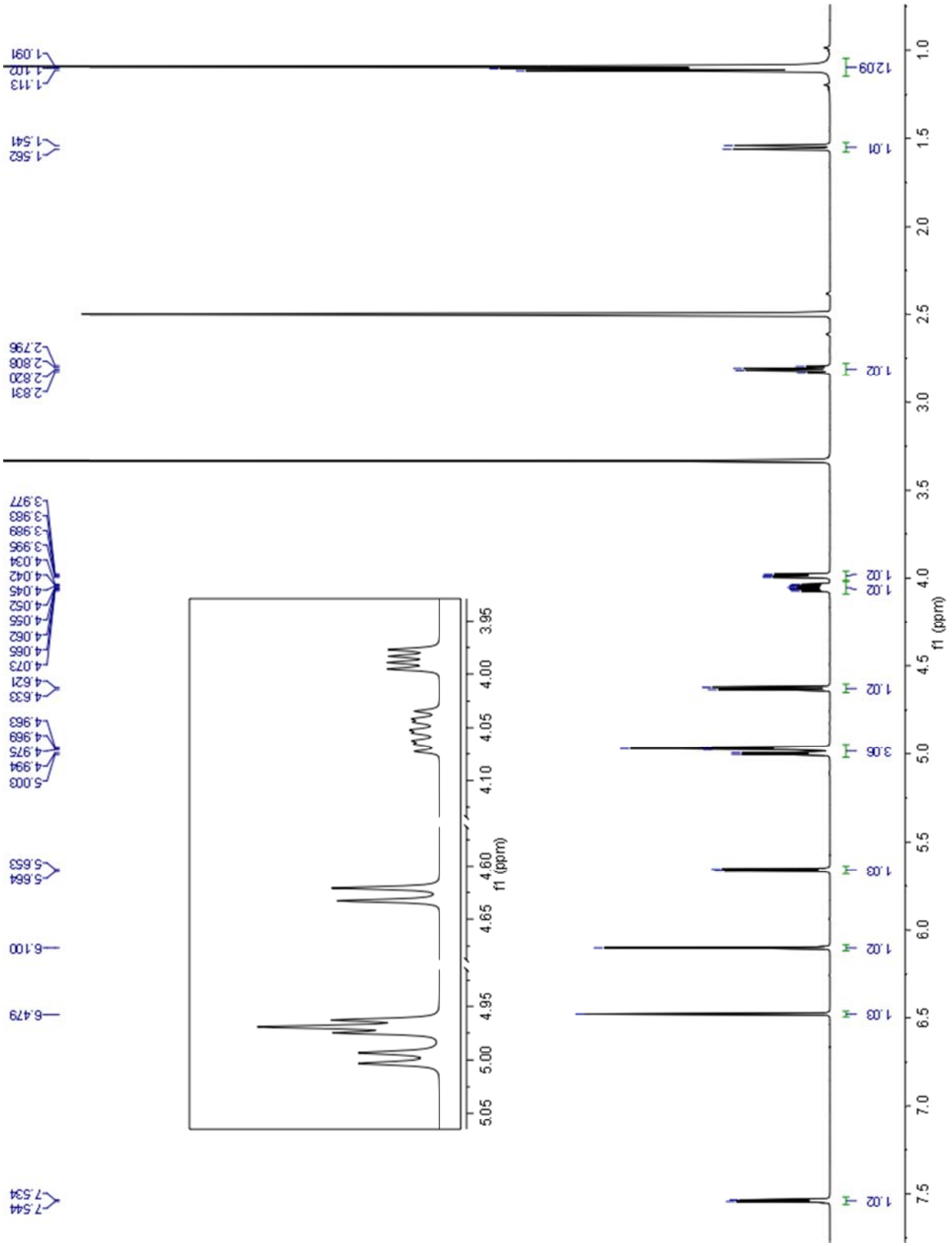
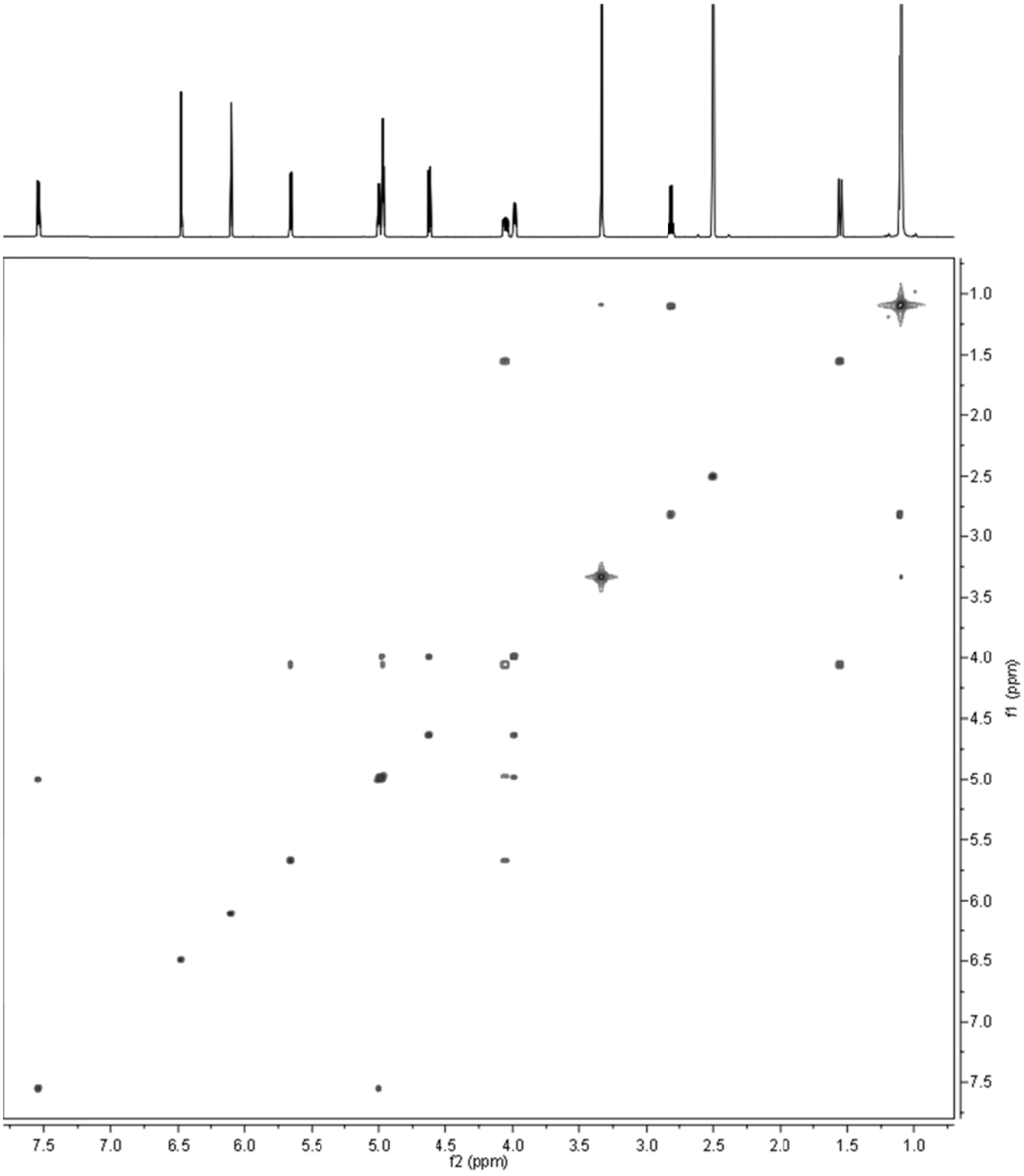
S8. ^{1}H NMR spectrum of Ginkgolide C (**3**, DMSO-d_6, 600 MHz).



S9. ^{1}H,^{1}H-COSY experiment of Ginkgolide C (**3**, DMSO-d_6, 600 MHz).



S10. The ^{1}H Fingerprint of Ginkgolide J (**4**) in the PERCH .PMS file format.

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* NEW: the lines beginning by * are comment lines !
* To keep all the chemical shifts fixed during iteration
* replace "CHEMICAL SHIFTS(HZ):" by "..SHIFTS(HZ): fixed"
* The couplings can be fixed in the same way

NMR-data: C:\Users\jgnapo_2\Documents\jgnapo\perch\Ginkgolides\GJ\ginkgoj
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CHEMICAL SHIFTS(PPM):  Similarity% =  13.626
PROTON    2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 OH-3    / 1     6.393136  1*1*1  STAT=Y  PRED= 4.925 RANGE= 1.775 WIDTH(Y)= 1.498 RESP(Y)= 1.0000
 OH-10   / 1     6.908209  1*1*1  STAT=Y  PRED= 4.324 RANGE= 1.710 WIDTH(Y)= 1.844 RESP(Y)= 0.9617
 OH-7    / 1     5.545649  1*1*1  STAT=Y  PRED= 4.759 RANGE= 1.580 WIDTH(Y)= 1.670 RESP(Y)= 0.9709
 H-1beta / 1     1.752901  1*1*1  STAT=Y  PRED= 1.338 RANGE= 0.287 WIDTH(Y)= 2.106 RESP(Y)= 0.9100 HSQC= C8
 H-1alpha/ 1     2.717097  1*1*1  STAT=Y  PRED= 2.169 RANGE= 0.377 WIDTH(Y)= 2.200 RESP(Y)= 0.8989 HSQC= C8
 H-2     / 1     4.832003  1*1*1  STAT=Y  PRED= 4.895 RANGE= 0.232 WIDTH(Y)= 1.942 RESP(Y)= 0.9577 HSQC= C9
 H-6     / 1     4.645476  1*1*1  STAT=Y  PRED= 4.895 RANGE= 0.110 WIDTH(Y)= 1.872 RESP(Y)= 0.9688 HSQC= C13
 H-7     / 1     4.171447  1*1*1  STAT=Y  PRED= 4.559 RANGE= 0.325 WIDTH(Y)= 1.862 RESP(Y)= 0.9203 HSQC= C14
 H-8     / 1     1.537556  1*1*1  STAT=Y  PRED= 1.768 RANGE= 0.212 WIDTH(Y)= 1.979 RESP(Y)= 0.9531 HSQC= C15
 H-10    / 1     4.928198  1*1*1  STAT=Y  PRED= 4.165 RANGE= 0.390 WIDTH(Y)= 2.064 RESP(Y)= 0.9291 HSQC= C17
 H-12    / 1     6.046780  1*1*1  STAT=Y  PRED= 5.659 RANGE= 0.332 WIDTH(Y)= 1.684 RESP(Y)= 0.9761 HSQC= C19
 H-14    / 1     2.906534  1*1*1  STAT=Y  PRED= 2.949 RANGE= 0.362 WIDTH(Y)= 1.711 RESP(Y)= 0.9406 HSQC= C21
 H-16    / 1     1.117886  1*1*3  STAT=Y  PRED= 1.135 RANGE= 0.260 WIDTH(Y)= 1.906 RESP(Y)= 0.9293 HSQC= C23
 t-butyl / 1     1.081520  1*1*9  STAT=Y  PRED= 0.894 RANGE= 0.230 WIDTH(Y)= 2.587 RESP(Y)= 0.9000 HSQC= C25-27

COUPLING CONSTANTS(HZ):  Similarity% =  17.523
 J6_30       5.3487   J OH-10    H-10       STAT=Y  PRED= 5.040 RANGE= 0.750
 J13_25      6.8614   J OH-7     H-7        STAT=Y  PRED= 4.300 RANGE= 0.500
 J15_16    -15.1380   J H-1beta  H-1alpha   STAT=Y  PRED= -12.310 RANGE= 1.000
 J15_18      8.1701   J H-1beta  H-2        STAT=Y  PRED= 9.280 RANGE= 3.000
 J16_18      7.2493   J H-1alpha H-2        STAT=Y  PRED= 7.040 RANGE= 3.000
 J23_25      4.1855   J H-6      H-7        STAT=Y  PRED= 4.830 RANGE= 3.000
 J25_27     12.2977   J H-7      H-8        STAT=Y  PRED= 11.060 RANGE= 2.200
 J36_39      7.2044   J H-14     H-16       STAT=Y  PRED= 6.640 RANGE= 0.250

CONTROL PARAMETERS:
       Solvent =  none (def. 99% enriched)
         1.000 =  Concentration (vol%, def=1.0%)
    0.00100000 =  Minimum line-intensity
    0.00100000 =  Diagonalization criterium (not in use)
    7.83034303 =  Left frequency (ppm)
   -0.20624264 =  Right frequency (ppm)
        10.000 =  Acquisition time (s, for QMTLS)
         1.433 =  Line-width (for modes D, P & T, 0=use defaults)
   0.068609932 =  Data-point resolution (Hz)
        25.038 =  GAUSSIAN (%, 0=use default from INF)
        -2.507 =  Dispersion contribution (%, 0=use default from INF)
    0.00000000 =  Decoupling frequency (for DORES)

CONSTRAINTS (in equations X0 = 1.0)...use no empty lines
 EQUAL H-2      = H-6

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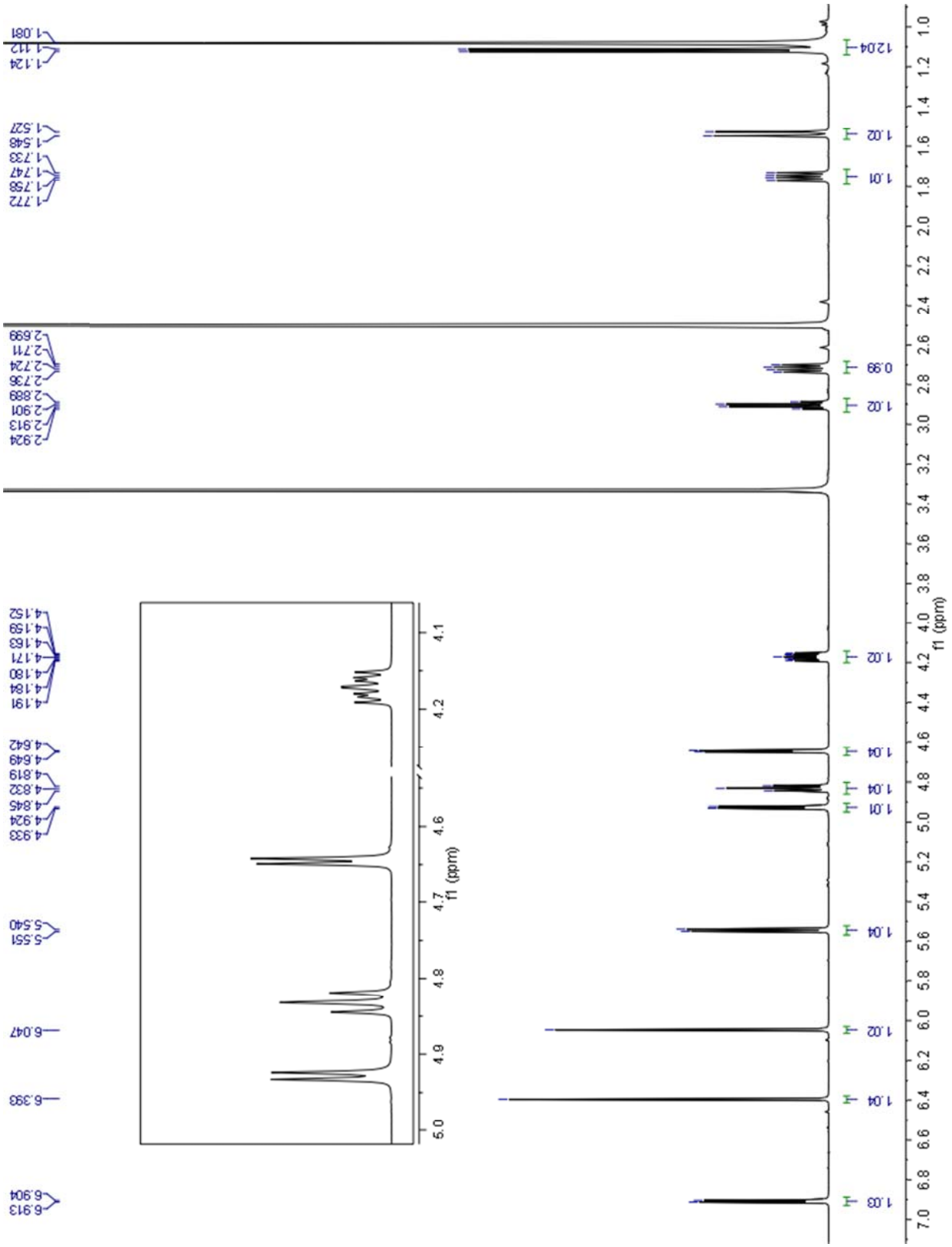
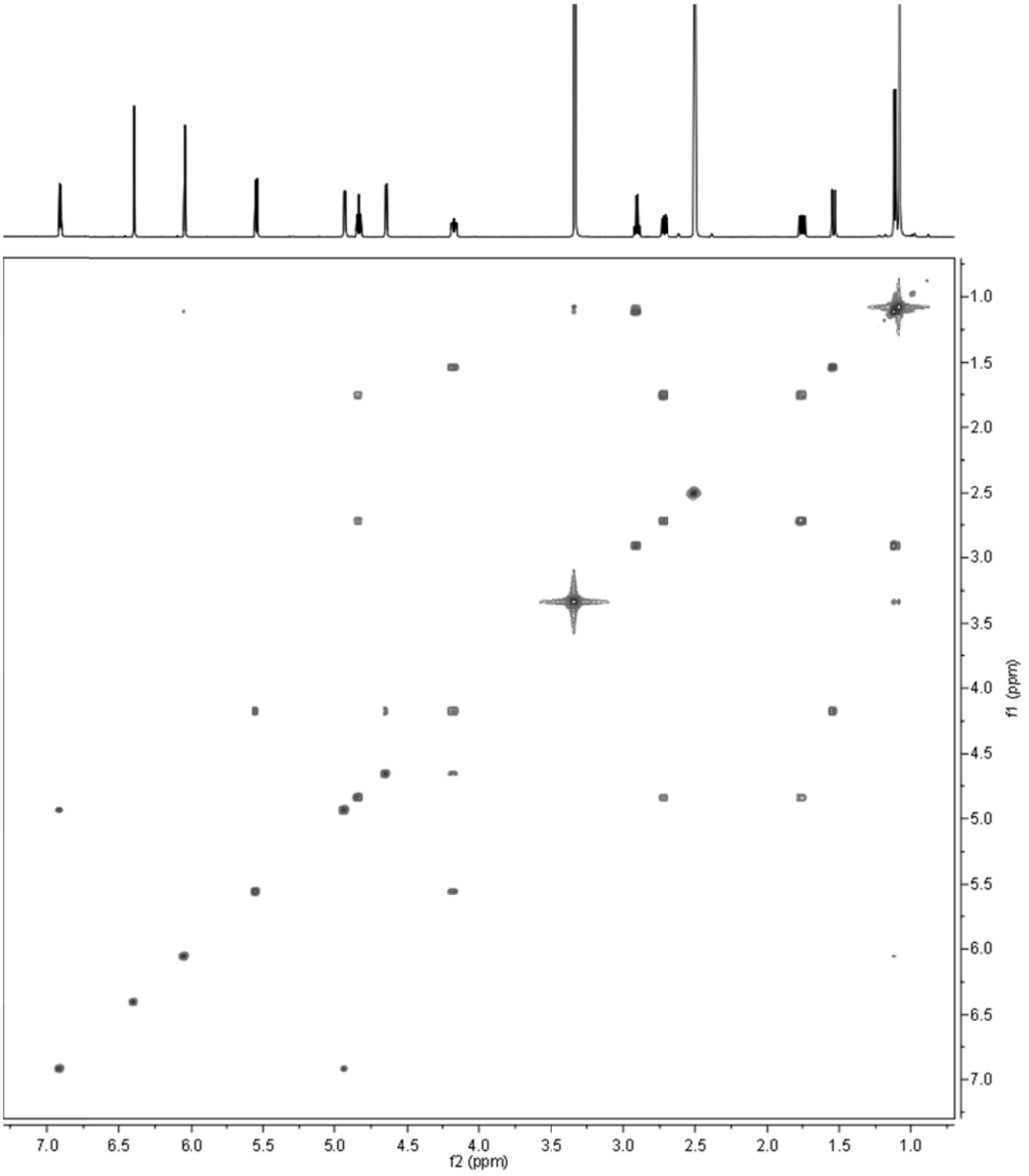
S11. ^{1}H NMR spectrum of Ginkgolide J (**4**, DMSO-d_6, 600 MHz).



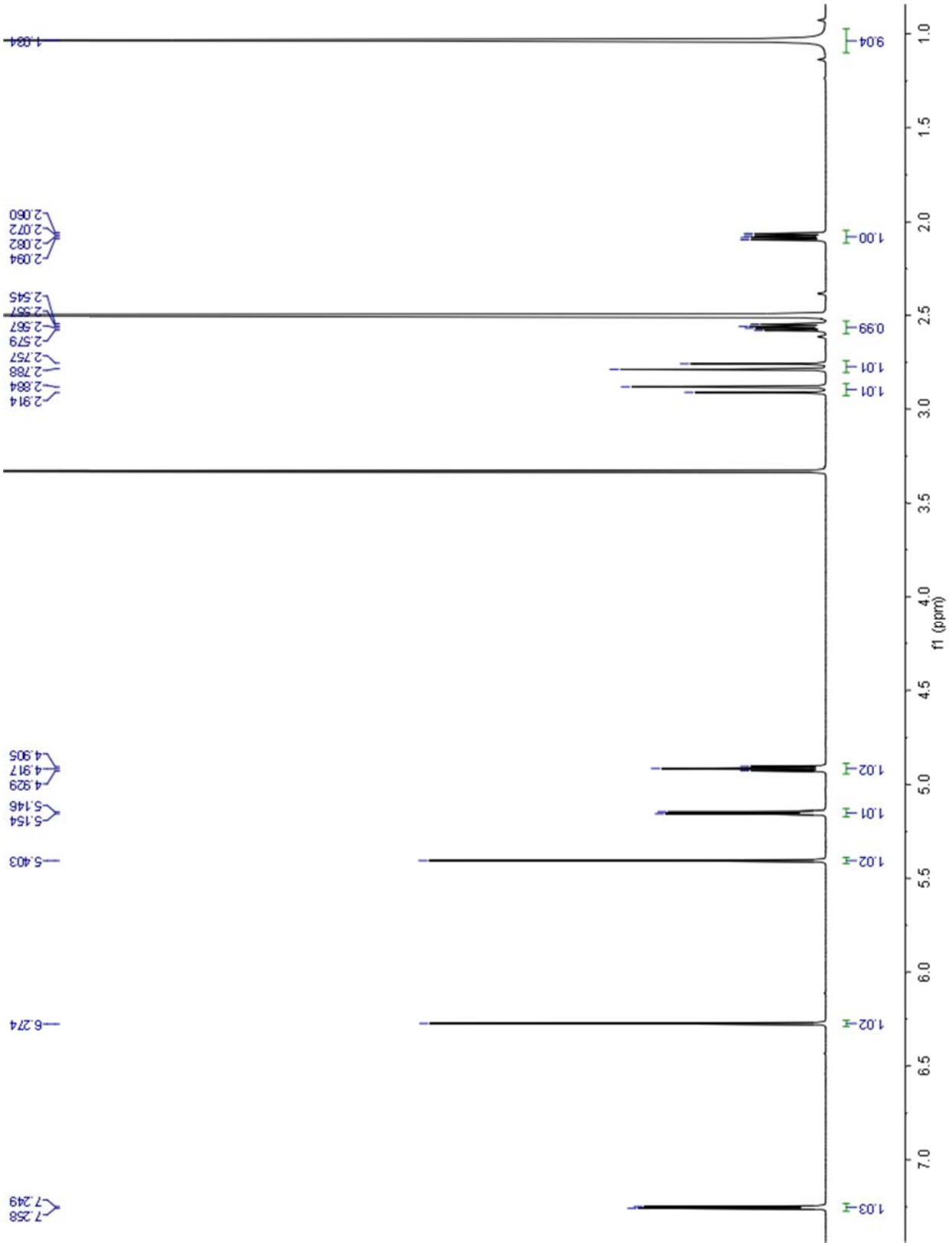
S12. ^{1}H,^{1}H-COSY experiment of Ginkgolide J (**4**, DMSO-d_6, 600 MHz).



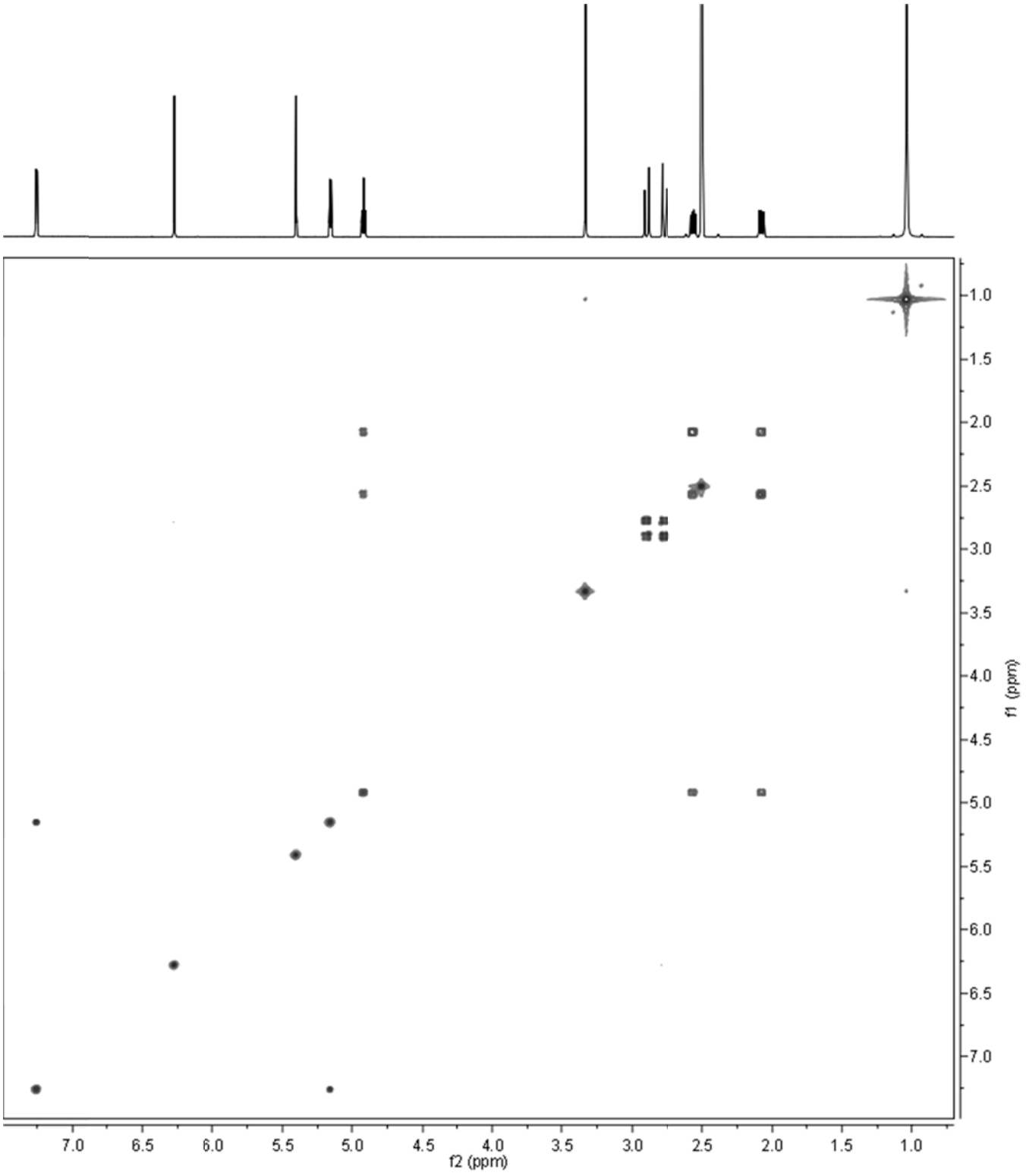
S13. The ^{1}H Fingerprint of Bilobalide (**5**) in the PERCH .PMS file format.

```
* NEW: the lines beginning by * are comment lines !
* To keep all the chemical shifts fixed during iteration
* replace "CHEMICAL SHIFTS(HZ):" by "..SHIFTS(HZ): fixed"
* The couplings can be fixed in the same way

NMR-data: C:\Users\jgnapo_2\Documents\jgnapo\perch\Ginkgolides\BB\bb
#$œ  Date  9. 3.2011;  Time 17: 1:31     bb.5TH

CHEMICAL SHIFTS(PPM):  Similarity% =  12.410
PROTON    2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 OH-10   / 1     7.253250  1*1*1  STAT=Y  PRED= 4.828 RANGE= 1.750 WIDTH(Y)= 1.600 RESP(Y)= 0.9729
 H-7beta / 1     2.077084  1*1*1  STAT=Y  PRED= 1.896 RANGE= 0.357 WIDTH(Y)= 1.891 RESP(Y)= 0.9170 HSQC= C14
 H-6     / 1     4.916794  1*1*1  STAT=Y  PRED= 4.888 RANGE= 0.282 WIDTH(Y)= 1.768 RESP(Y)= 0.9697 HSQC= C13
 H-7alpha/ 1     2.561866  1*1*1  STAT=Y  PRED= 2.518 RANGE= 0.282 WIDTH(Y)= 1.976 RESP(Y)= 0.8993 HSQC= C14
 H-10    / 1     5.149952  1*1*1  STAT=Y  PRED= 4.165 RANGE= 0.370 WIDTH(Y)= 1.774 RESP(Y)= 0.9421 HSQC= C17
 H-12    / 1     6.274102  1*1*1  STAT=Y  PRED= 5.659 RANGE= 0.102 WIDTH(Y)= 1.500 RESP(Y)= 1.0000 HSQC= C19
 t-Butyl / 1     1.034063  1*1*9  STAT=Y  PRED= 0.914 RANGE= 0.237 WIDTH(Y)= 2.678 RESP(Y)= 0.9023 HSQC= C25-27
 OH-8    / 1     5.403089  1*1*1  STAT=Y  PRED= 3.979 RANGE= 1.923 WIDTH(Y)= 1.508 RESP(Y)= 0.9843
 H-1beta / 1     2.774028  1*1*1  STAT=Y  PRED= 2.359 RANGE= 0.370 WIDTH(Y)= 1.686 RESP(Y)= 0.9603 HSQC= #27
 H-1alpha/ 1     2.897044  1*1*1  STAT=Y  PRED= 2.405 RANGE= 0.462 WIDTH(Y)= 1.740 RESP(Y)= 0.9580 HSQC= #27

COUPLING CONSTANTS(HZ):  Similarity% =  64.488
 J4_18       5.1195   J OH-10    H-10       STAT=Y  PRED= 4.890 RANGE= 0.750
 J7_11       6.8503   J H-7beta  H-6        STAT=Y  PRED= 9.550 RANGE= 3.000
 J7_13     -13.3259   J H-7beta  H-7alpha   STAT=Y  PRED= -12.140 RANGE= 1.000
 J11_13      7.0969   J H-6      H-7alpha   STAT=Y  PRED= 6.600 RANGE= 3.000
 J40_41    -18.1406   J H-1beta  H-1alpha   STAT=Y  PRED= -15.860 RANGE= 2.000

CONTROL PARAMETERS:
       Solvent =  none (def. 99% enriched)
         1.000 =  Concentration (vol%, def=1.0%)
    0.00100000 =  Minimum line-intensity
    0.00100000 =  Diagonalization criterium (not in use)
    8.04426687 =  Left frequency (ppm)
    0.00000000 =  Right frequency (ppm)
        10.000 =  Acquisition time (s, for QMTLS)
         1.505 =  Line-width (for modes D, P & T, 0=use defaults)
   0.068609932 =  Data-point resolution (Hz)
        25.060 =  GAUSSIAN (%, 0=use default from INF)
         2.716 =  Dispersion contribution (%, 0=use default from INF)
    0.00000000 =  Decoupling frequency (for DORES)

CONSTRAINTS (in equations X0 = 1.0)...use no empty lines

END of FILE
```

S14. ^{1}H NMR spectrum of Bilobalide (**5**, DMSO-d_6, 600 MHz).



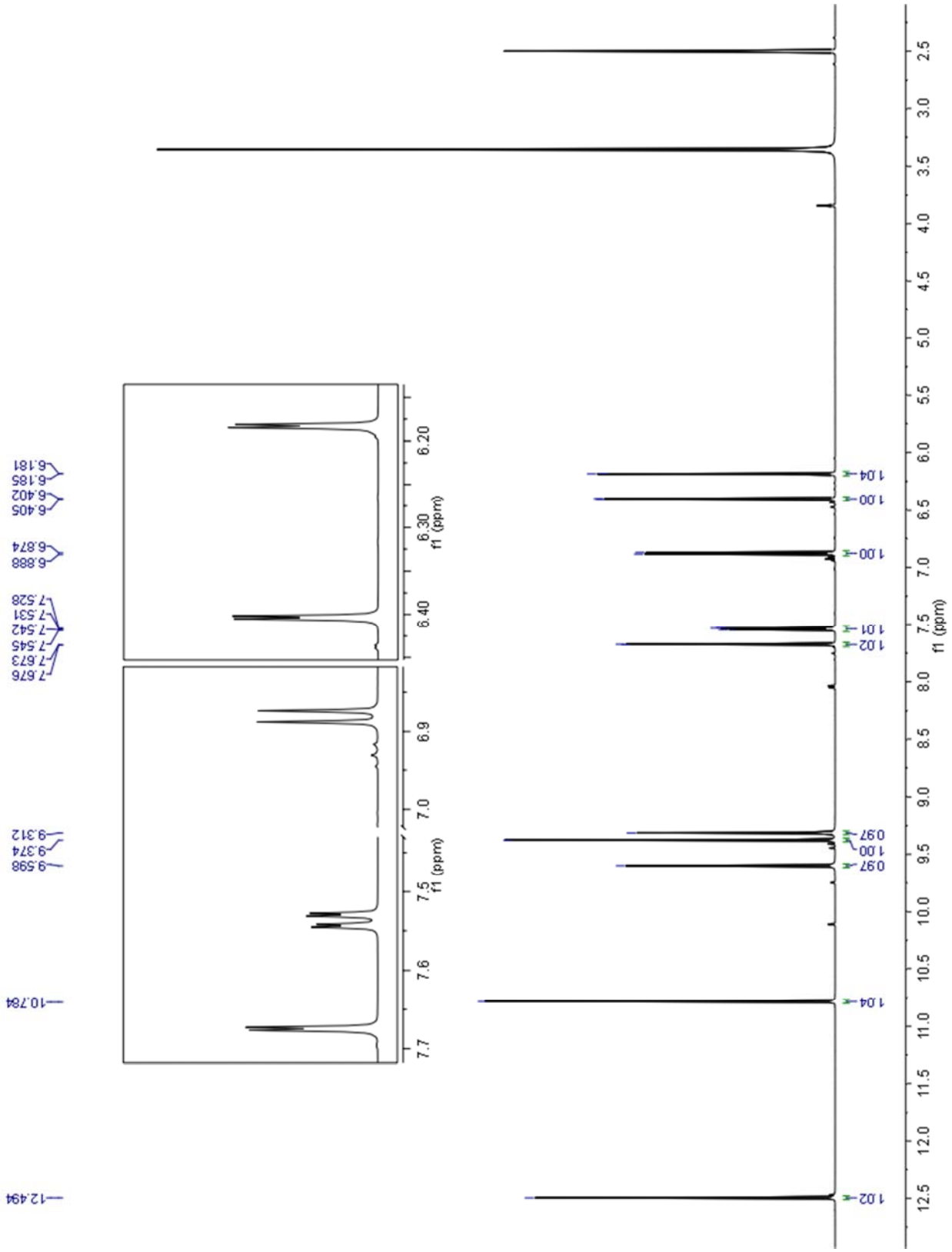
S15. ^{1}H,^{1}H-COSY experiment of Bilobalide (**5**, DMSO-d_6, 600 MHz).



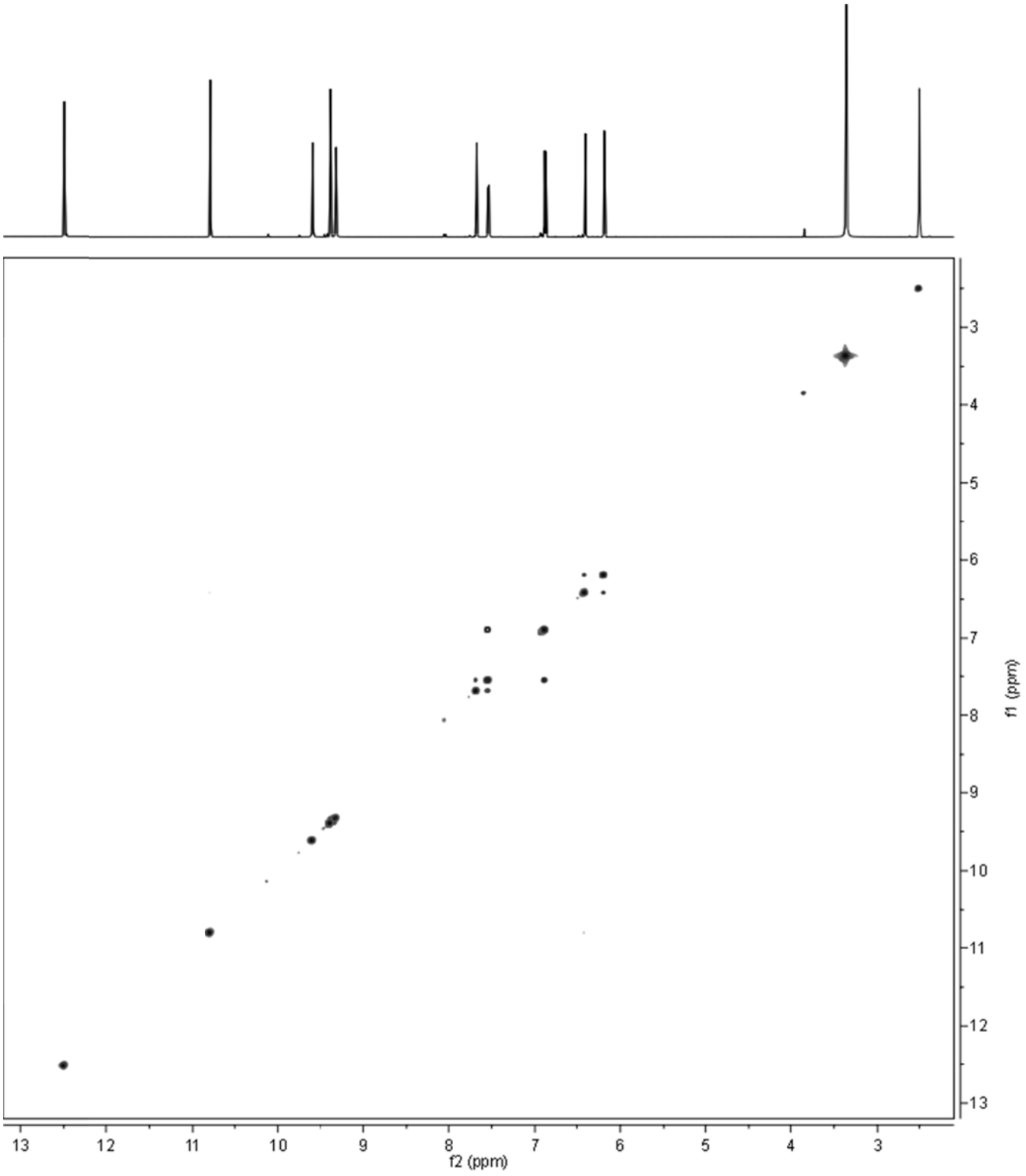
S16. The ^{1}H Fingerprint of Quercetin (**6**) in the PERCH .PMS file format.

```
* NEW: the lines beginning by * are comment lines !
* To keep all the chemical shifts fixed during iteration
* replace "CHEMICAL SHIFTS(HZ):" by "..SHIFTS(HZ): fixed"
* The couplings can be fixed in the same way

NMR-data: C:\Users\jgnapo_2\Documents\users\jgnapo\perch\Ginkgo\Flavonoids\
#$œ  Date 20.10.2011;  Time 16: 2:48     perch.3rd

CHEMICAL SHIFTS(PPM):
PROTON    2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 H6  / 1     6.183050  1*1*1  STAT=Y  PRED= 6.298 RANGE= 0.242 WIDTH(Y)= 1.416 RESP(Y)= 1.0000 HSQC= C2
 H8  / 1     6.403402  1*1*1  STAT=Y  PRED= 6.461 RANGE= 0.172 WIDTH(Y)= 1.407 RESP(Y)= 0.9861 HSQC= C4
 OH7 / 1    10.783504  1*1*1  STAT=Y  PRED= 10.896 RANGE= 1.000 WIDTH(Y)= 1.739 RESP(Y)= 0.9816
 OH5 / 1    12.494440  1*1*1  STAT=Y  PRED= 13.379 RANGE= 0.850 WIDTH(Y)= 1.942 RESP(Y)= 0.9532
 H6' / 1     7.536549  1*1*1  STAT=Y  PRED= 7.627 RANGE= 0.265 WIDTH(Y)= 1.496 RESP(Y)= 0.9718 HSQC= C14
 H5' / 1     6.880921  1*1*1  STAT=Y  PRED= 6.929 RANGE= 0.197 WIDTH(Y)= 1.406 RESP(Y)= 0.9618 HSQC= C15
 H2' / 1     7.674662  1*1*1  STAT=Y  PRED= 7.698 RANGE= 0.247 WIDTH(Y)= 1.416 RESP(Y)= 0.9741 HSQC= C18
 OH3'/ 1     9.374357  1*1*1  STAT=Y  PRED= 9.494 RANGE= 1.215 WIDTH(Y)= 1.780 RESP(Y)= 0.9566
 OH4'/ 1     9.311783  1*1*1  STAT=Y  PRED= 9.682 RANGE= 1.315 WIDTH(Y)= 2.880 RESP(Y)= 0.9305
 OH3 / 1     9.597692  1*1*1  STAT=Y  PRED= 9.115 RANGE= 1.115 WIDTH(Y)= 2.732 RESP(Y)= 0.9341

COUPLING CONSTANTS(HZ):
 J22_23      2.0315   J H6   H8     STAT=Y  PRED= 2.110 RANGE= 0.890
 J27_28      8.4728   J H6'  H5'    STAT=Y  PRED= 8.380 RANGE= 0.500
 J27_29      2.2019   J H6'  H2'    STAT=Y  PRED= 2.080 RANGE= 0.800
 J28_29      0.4659   J H5'  H2'    STAT=Y  PRED= 0.460 RANGE= 0.320

CONTROL PARAMETERS:
       Solvent =  none (def. 99% enriched)
         1.000 =  Concentration (vol%, def=1.0%)
    0.00100000 =  Minimum line-intensity
    0.00100000 =  Diagonalization criterium (not in use)
   14.00343391 =  Left frequency (ppm)
    0.00000000 =  Right frequency (ppm)
         0.000 =  Acquisition time (s, for QMTLS)
         1.402 =  Line-width (for modes D, P & T, 0=use defaults)
   0.068609932 =  Data-point resolution (Hz)
        37.540 =  GAUSSIAN (%, 0=use default from INF)
         5.203 =  Dispersion contribution (%, 0=use default from INF)
    0.00000000 =  Decoupling frequency (for DORES)

CONSTRAINTS (in equations X0 = 1.0)...use no empty lines

END of FILE
```

S17. ^{1}H NMR spectrum of Quercetin (**6**, DMSO-d_6, 600 MHz).



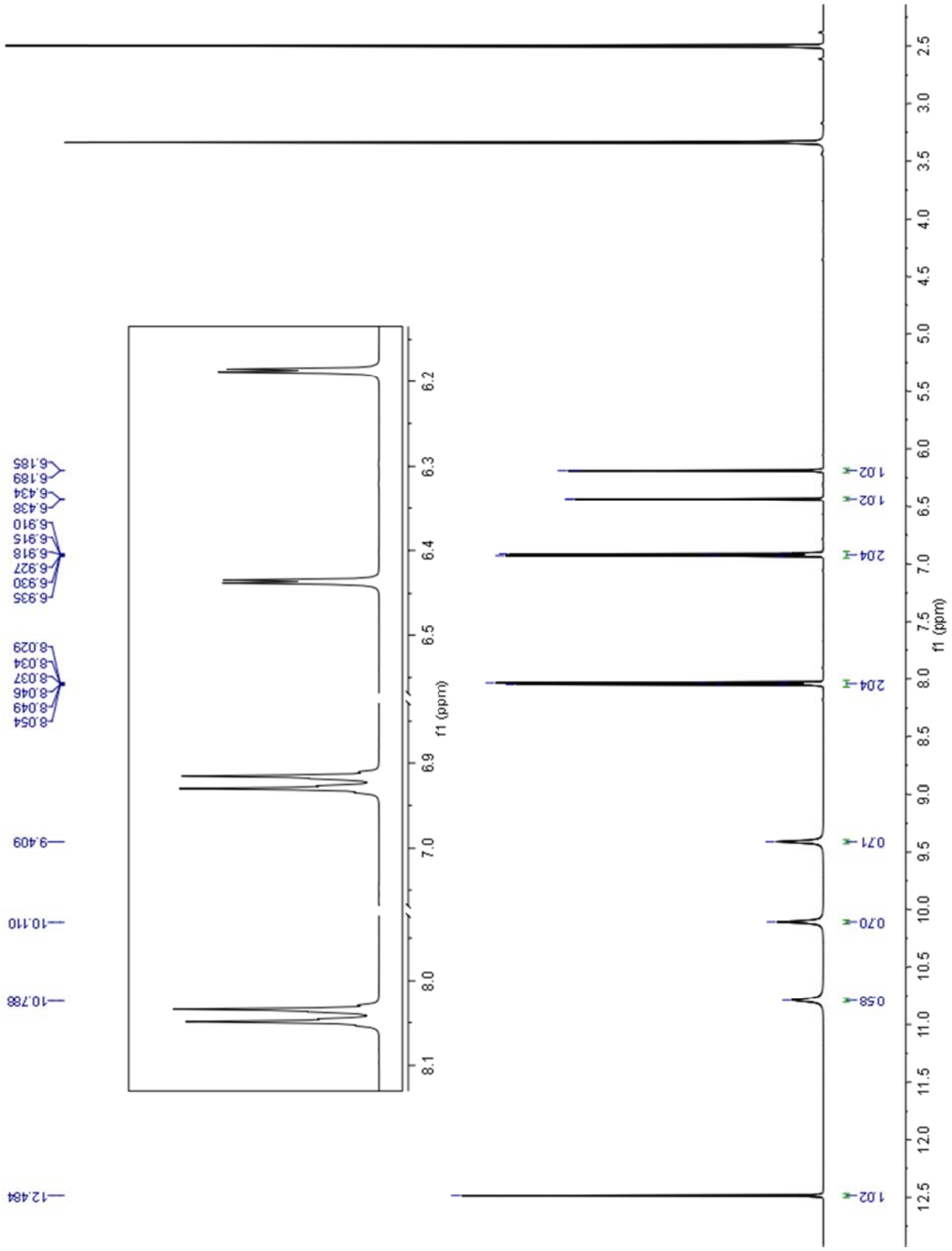
S18. ^{1}H,^{1}H-COSY experiment of Quercetin (**6**, DMSO-d_6, 600 MHz).



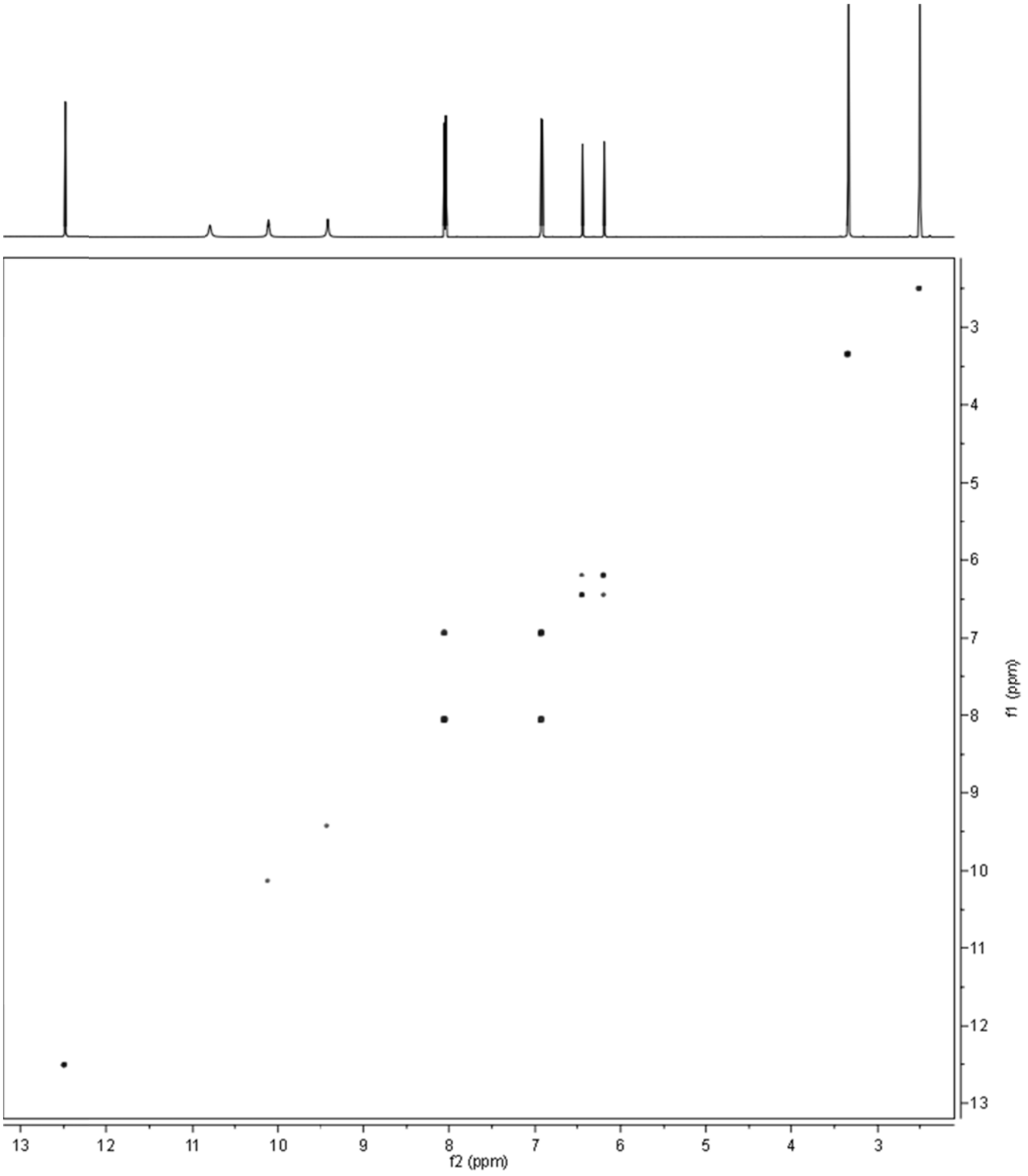
S19. The ^{1}H Fingerprint of Kaempferol (**7**) in the PERCH .PMS file format.

```
* NEW: the lines beginning by * are comment lines !
* To keep all the chemical shifts fixed during iteration
* replace "CHEMICAL SHIFTS(HZ):" by "..SHIFTS(HZ): fixed"
* The couplings can be fixed in the same way

NMR-data: C:\Users\jgnapo_2\Documents\users\jgnapo\perch\Ginkgo\Flavonoids\
#$œ  Date 20.10.2011;  Time 17: 5:18     perch.3rd

CHEMICAL SHIFTS(PPM):
PROTON    2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 H3'_5'/ 1     6.922821  1*2*1  STAT=Y  PRED= 6.925 RANGE= 0.177 WIDTH(Y)= 1.511 RESP(Y)= 0.9770 HSQC= C15_17
 H6    / 1     6.186969  1*1*1  STAT=Y  PRED= 6.295 RANGE= 0.252 WIDTH(Y)= 1.406 RESP(Y)= 1.0000 HSQC= C2
 H8    / 1     6.435905  1*1*1  STAT=Y  PRED= 6.468 RANGE= 0.172 WIDTH(Y)= 1.404 RESP(Y)= 0.9947 HSQC= C4
 OH7   / 1    10.788285  1*1*1  STAT=Y  PRED= 10.903 RANGE= 0.985 WIDTH(Y)= 17.150 RESP(Y)= 0.8071
 OH5   / 1    12.484003  1*1*1  STAT=Y  PRED= 13.446 RANGE= 0.850 WIDTH(Y)= 1.739 RESP(Y)= 0.9625
 H2'_6'/ 1     8.041525  1*2*1  STAT=Y  PRED= 8.080 RANGE= 0.252 WIDTH(Y)= 1.495 RESP(Y)= 0.9722 HSQC= C14_18
 OH4'  / 1     9.408526  1*1*1  STAT=Y  PRED= 9.807 RANGE= 1.500 WIDTH(Y)= 11.480 RESP(Y)= 0.8274
 OH3   / 1    10.109684  1*1*1  STAT=Y  PRED= 9.155 RANGE= 1.070 WIDTH(Y)= 11.760 RESP(Y)= 0.8250

COUPLING CONSTANTS(HZ):
 J21_28      2.4778   J H3'_5' H3'_5'   STAT=Y  PRED= 2.710 RANGE= 0.700
 J21_27      0.2690   J H2'_6' H3'_5'   STAT=Y  PRED= 0.460 RANGE= 0.320
 J21_29      8.7801   J H3'_5' H2'_6'   STAT=Y  PRED= 8.530 RANGE= 0.440
 J22_23      2.0325   J H6     H8       STAT=Y  PRED= 2.110 RANGE= 0.890
 J29_27      2.4747   J H2'_6' H2'_6'   STAT=Y  PRED= 2.380 RANGE= 0.700

CONTROL PARAMETERS:
       Solvent =  none (def. 99% enriched)
         1.000 =  Concentration (vol%, def=1.0%)
    0.00100000 =  Minimum line-intensity
    0.00100000 =  Diagonalization criterium (not in use)
   13.07908736 =  Left frequency (ppm)
    0.00000000 =  Right frequency (ppm)
         0.000 =  Acquisition time (s, for QMTLS)
         1.391 =  Line-width (for modes D, P & T, 0=use defaults)
   0.068609932 =  Data-point resolution (Hz)
        47.309 =  GAUSSIAN (%, 0=use default from INF)
         6.174 =  Dispersion contribution (%, 0=use default from INF)
    0.00000000 =  Decoupling frequency (for DORES)

CONSTRAINTS (in equations X0 = 1.0)...use no empty lines

END of FILE
```

S20. ^{1}H NMR spectrum of Kaempferol (**7**, DMSO-d_6, 600 MHz).



S21. ^{1}H,^{1}H-COSY experiment of Kaempferol (**7**, DMSO-d_6, 600 MHz).



S22. The ^{1}H Fingerprint of Isorhamnetin (**8**) in the PERCH .PMS file format.

```
* NEW: the lines beginning by * are comment lines !
* To keep all the chemical shifts fixed during iteration
* replace "CHEMICAL SHIFTS(HZ):" by "..SHIFTS(HZ): fixed"
* The couplings can be fixed in the same way

NMR-data: c:\users\jgnapo_2\documents\users\jgnapo\perch\ginkgo\flavonoids\
#$œ  Date 20.10.2011;  Time 16:43:26     perch.3rd

CHEMICAL SHIFTS(PPM):
PROTON    2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 H6  / 1     6.192379  1*1*1  STAT=Y  PRED= 6.306 RANGE= 0.242 WIDTH(Y)= 1.456 RESP(Y)= 0.9979 HSQC= C2
 H8  / 1     6.476736  1*1*1  STAT=Y  PRED= 6.462 RANGE= 0.182 WIDTH(Y)= 1.446 RESP(Y)= 0.9882 HSQC= C4
 OH7 / 1    10.773796  1*1*1  STAT=Y  PRED= 10.912 RANGE= 1.015 WIDTH(Y)= 2.985 RESP(Y)= 0.9504
 OH5 / 1    12.467391  1*1*1  STAT=Y  PRED= 13.376 RANGE= 0.855 WIDTH(Y)= 1.433 RESP(Y)= 1.0000
 H6' / 1     7.687450  1*1*1  STAT=Y  PRED= 7.638 RANGE= 0.297 WIDTH(Y)= 1.538 RESP(Y)= 0.9733 HSQC= C14
 H5' / 1     6.936966  1*1*1  STAT=Y  PRED= 6.904 RANGE= 0.242 WIDTH(Y)= 1.475 RESP(Y)= 0.9759 HSQC= C15
 H2' / 1     7.752072  1*1*1  STAT=Y  PRED= 7.676 RANGE= 0.305 WIDTH(Y)= 1.697 RESP(Y)= 0.9921 HSQC= C18
 OH4'/ 1     9.445056  1*1*1  STAT=Y  PRED= 9.712 RANGE= 0.752 WIDTH(Y)= 2.159 RESP(Y)= 0.9537
 OH3 / 1     9.747292  1*1*1  STAT=Y  PRED= 9.072 RANGE= 1.125 WIDTH(Y)= 2.173 RESP(Y)= 0.9713
 OMe / 1     3.840464  1*1*3  STAT=Y  PRED= 3.899 RANGE= 0.132 WIDTH(Y)= 1.727 RESP(Y)= 0.9945 HSQC= H20

COUPLING CONSTANTS(HZ):
 J22_23      2.0139   J H6   H8     STAT=Y  PRED= 2.110 RANGE= 0.890
 J27_28      8.4712   J H6'  H5'    STAT=Y  PRED= 8.340 RANGE= 0.500
 J27_29      2.0570   J H6'  H2'    STAT=Y  PRED= 2.080 RANGE= 0.800
 J28_29      0.2967   J H5'  H2'    STAT=Y  PRED= 0.460 RANGE= 0.320

CONTROL PARAMETERS:
       Solvent =  none (def. 99% enriched)
         1.000 =  Concentration (vol%, def=1.0%)
    0.00100000 =  Minimum line-intensity
    0.00100000 =  Diagonalization criterium (not in use)
   13.09593996 =  Left frequency (ppm)
    0.00000000 =  Right frequency (ppm)
        10.000 =  Acquisition time (s, for QMTLS)
         0.000 =  Line-width (for modes D, P & T, 0=use defaults)
   0.071649999 =  Data-point resolution (Hz)
        30.935 =  GAUSSIAN (%, 0=use default from INF)
        -0.908 =  Dispersion contribution (%, 0=use default from INF)
    0.00000000 =  Decoupling frequency (for DORES)

CONSTRAINTS (in equations X0 = 1.0)...use no empty lines

END of FILE
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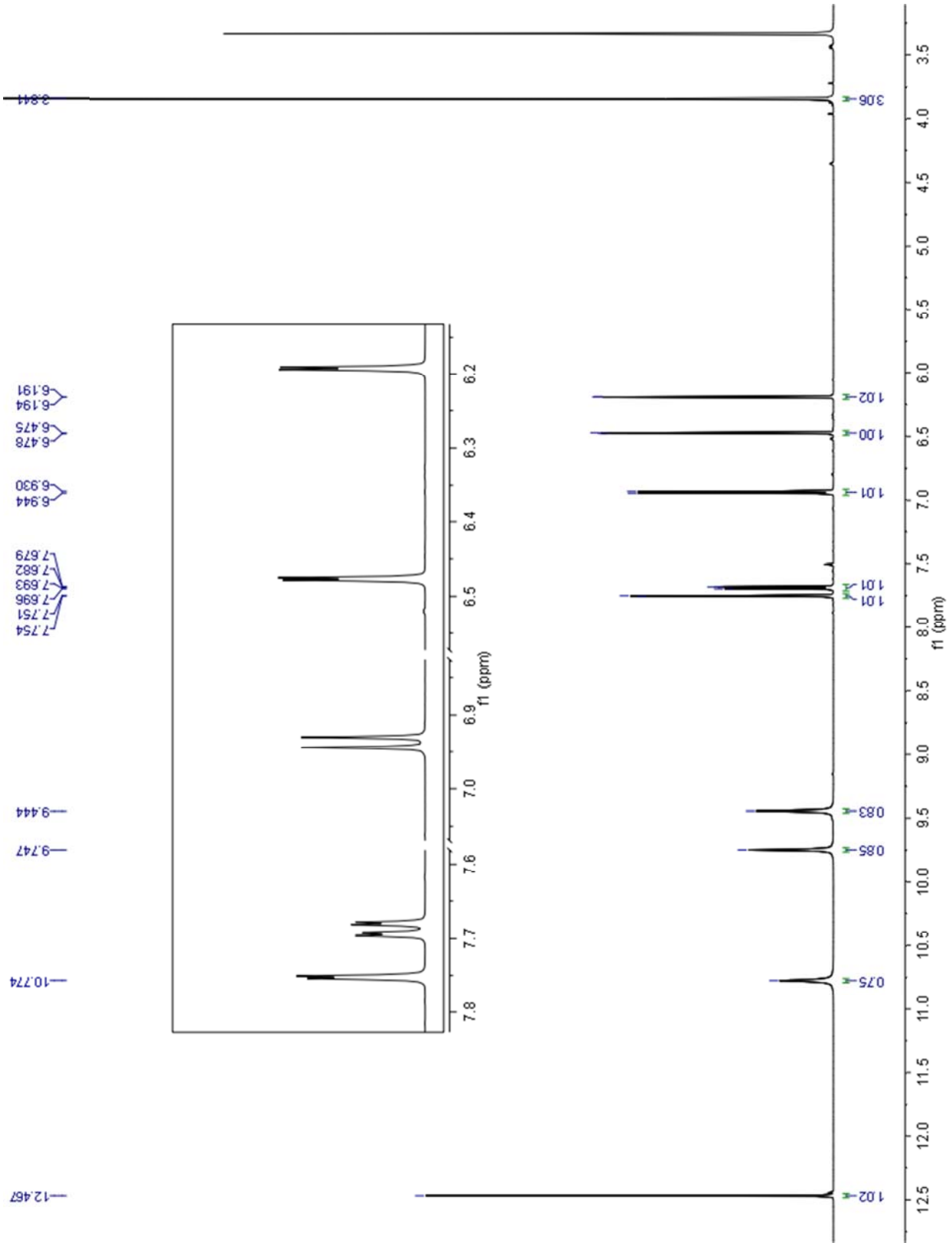
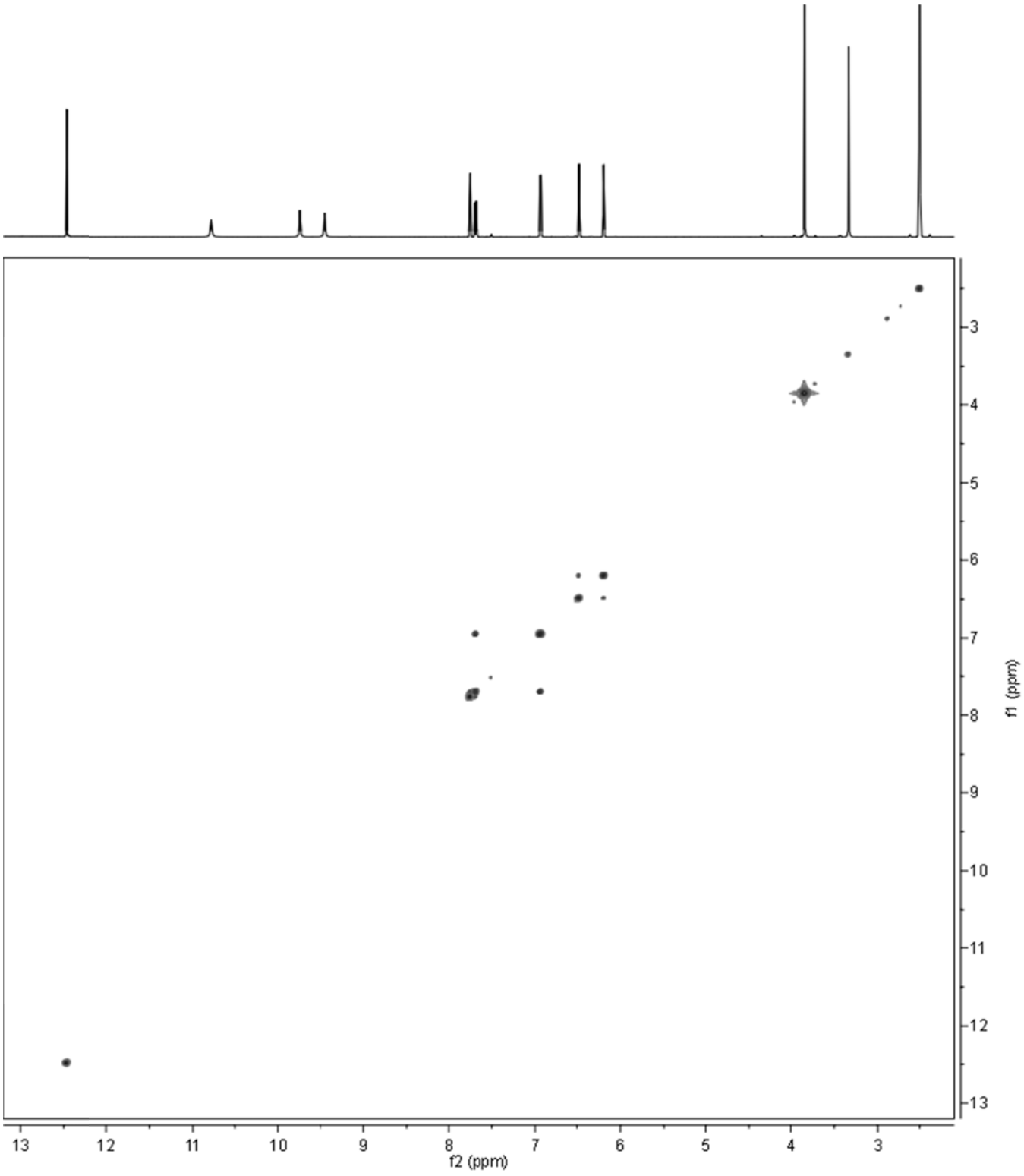
S23. ^{1}H NMR spectrum of Isorhamnetin (**8**, DMSO-d_6, 600 MHz).



S24. ^{1}H,^{1}H-COSY experiment of Isorhamnetin (**8**, DMSO-d_6, 600 MHz).



S25. The ^{1}H Fingerprint of Rutin (**9**) in the PERCH .PMS file format.

```
* NEW: the lines beginning by * are comment lines !
* To keep all the chemical shifts fixed during iteration
* replace "CHEMICAL SHIFTS(HZ):" by "..SHIFTS(HZ): fixed"
* The couplings can be fixed in the same way

NMR-data: c:\users\jgnapo_2\documents\users\jgnapo\perch\ginkgo\flavonoids\
#$œ  Date 21.10.2011;  Time  0:33:18     perch.5TH

CHEMICAL SHIFTS(PPM):  Similarity% =  16.777
PROTON    2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 H6      / 1     6.190056  1*1*1  STAT=Y  PRED= 6.412 RANGE= 0.305 WIDTH(Y)= 1.062 RESP(Y)= 0.9766 HSQC= C2
 H8      / 1     6.380863  1*1*1  STAT=Y  PRED= 6.581 RANGE= 0.362 WIDTH(Y)= 1.055 RESP(Y)= 0.9738 HSQC= C4
 OH7     / 1    10.829194  1*1*1  STAT=Y  PRED= 10.802 RANGE= 1.260 WIDTH(Y)= 6.056 RESP(Y)= 0.7582
 OH5     / 1    12.599850  1*1*1  STAT=Y  PRED= 13.831 RANGE= 0.985 WIDTH(Y)= 1.142 RESP(Y)= 1.0000
 H6'     / 1     7.537800  1*1*1  STAT=Y  PRED= 7.839 RANGE= 0.327 WIDTH(Y)= 1.146 RESP(Y)= 0.9079 HSQC= C14
 H5'     / 1     6.836057  1*1*1  STAT=Y  PRED= 7.028 RANGE= 0.445 WIDTH(Y)= 1.149 RESP(Y)= 0.9452 HSQC= C15
 H2'     / 1     7.525994  1*1*1  STAT=Y  PRED= 7.813 RANGE= 0.392 WIDTH(Y)= 1.146 RESP(Y)= 0.9585 HSQC= C18
 OH3'    / 1     9.671753  1*1*1  STAT=Y  PRED= 9.599 RANGE= 1.830 WIDTH(Y)= 9.146 RESP(Y)= 0.7385
 OH4'    / 1     9.182772  1*1*1  STAT=Y  PRED= 9.443 RANGE= 1.775 WIDTH(Y)= 6.955 RESP(Y)= 0.7480
 Glc-1   / 1     5.341488  1*1*1  STAT=Y  PRED= 5.565 RANGE= 0.342 WIDTH(Y)= 1.356 RESP(Y)= 0.9078 HSQC= H21
 Glc-2   / 1     3.219724  1*1*1  STAT=Y  PRED= 3.526 RANGE= 0.200 WIDTH(Y)= 1.897 RESP(Y)= 0.9171 HSQC= C23
 Glc-5   / 1     3.238384  1*1*1  STAT=Y  PRED= 3.485 RANGE= 0.247 WIDTH(Y)= 2.050 RESP(Y)= 0.8314 HSQC= C25
 Glc-3   / 1     3.204949  1*1*1  STAT=Y  PRED= 3.317 RANGE= 0.155 WIDTH(Y)= 2.091 RESP(Y)= 0.8548 HSQC= C26
 Glc-4   / 1     3.047931  1*1*1  STAT=Y  PRED= 3.387 RANGE= 0.287 WIDTH(Y)= 2.008 RESP(Y)= 0.8374 HSQC= C27
 OH-Glc-2/ 1     5.286398  1*1*1  STAT=Y  PRED= 5.633 RANGE= 1.215 WIDTH(Y)= 1.765 RESP(Y)= 0.8978
 Glc-6   / 1     3.281188  1*1*1  STAT=Y  PRED= 3.351 RANGE= 0.450 WIDTH(Y)= 2.220 RESP(Y)= 0.8318 HSQC= C29
 Glc-6'  / 1     3.701113  1*1*1  STAT=Y  PRED= 3.509 RANGE= 0.232 WIDTH(Y)= 2.257 RESP(Y)= 0.8536 HSQC= C29
 OH-Glc-3/ 1     5.115871  1*1*1  STAT=Y  PRED= 4.296 RANGE= 1.420 WIDTH(Y)= 2.048 RESP(Y)= 0.8798
 OH-Glc-4/ 1     5.074713  1*1*1  STAT=Y  PRED= 4.702 RANGE= 1.568 WIDTH(Y)= 2.000 RESP(Y)= 0.8679
 Rh-1    / 1     4.376166  1*1*1  STAT=Y  PRED= 4.453 RANGE= 0.300 WIDTH(Y)= 1.672 RESP(Y)= 0.9527 HSQC= C33
 Rh-5    / 1     3.265194  1*1*1  STAT=Y  PRED= 2.961 RANGE= 0.627 WIDTH(Y)= 1.684 RESP(Y)= 0.9335 HSQC= C36
 Rh-Me   / 1     0.987386  1*1*3  STAT=Y  PRED= 0.586 RANGE= 0.262 WIDTH(Y)= 1.730 RESP(Y)= 0.8538 HSQC= C40
 Rh-4    / 1     3.067177  1*1*1  STAT=Y  PRED= 2.968 RANGE= 0.287 WIDTH(Y)= 3.477 RESP(Y)= 0.9349 HSQC= C37
 Rh-2    / 1     3.383564  1*1*1  STAT=Y  PRED= 3.609 RANGE= 0.242 WIDTH(Y)= 2.395 RESP(Y)= 0.9502 HSQC= C38
 Rh-3    / 1     3.275197  1*1*1  STAT=Y  PRED= 3.082 RANGE= 0.582 WIDTH(Y)= 2.131 RESP(Y)= 0.8779 HSQC= C39
 OH-Rh-2 / 1     4.350559  1*1*1  STAT=Y  PRED= 4.719 RANGE= 1.395 WIDTH(Y)= 4.049 RESP(Y)= 0.7880
 OH-Rh-3 / 1     4.400478  1*1*1  STAT=Y  PRED= 4.127 RANGE= 1.613 WIDTH(Y)= 3.183 RESP(Y)= 0.8379
 OH-Rh-4 / 1     4.534535  1*1*1  STAT=Y  PRED= 4.732 RANGE= 1.673 WIDTH(Y)= 10.065 RESP(Y)= 0.8554

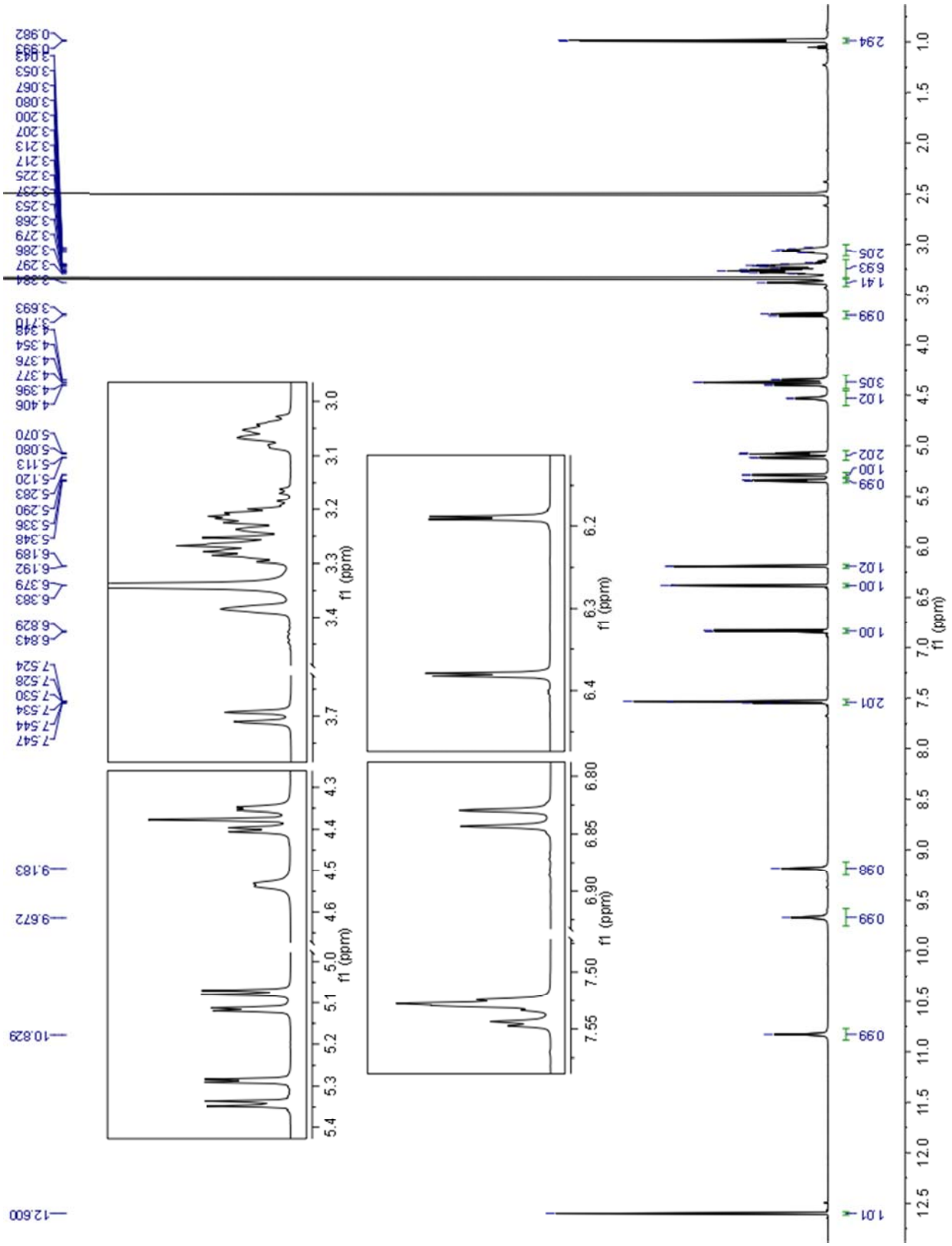
COUPLING CONSTANTS(HZ):  Similarity% =  36.900
 J22_23      2.0571   J H6       H8         STAT=Y  PRED= 2.110 RANGE= 1.790
 J27_28      8.4604   J H6'      H5'        STAT=Y  PRED= 8.380 RANGE= 1.000
 J27_29      2.2300   J H6'      H2'        STAT=Y  PRED= 2.080 RANGE= 1.600
 J28_29      0.2251   J H5'      H2'        STAT=Y  PRED= 0.460 RANGE= 0.640
 J38_40      7.7199   J Glc-1    Glc-2      STAT=Y  PRED= 7.190 RANGE= 3.580
 J40_43      9.0266   J Glc-2    Glc-3      STAT=Y  PRED= 8.920 RANGE= 3.580
 J40_48      4.7130   J Glc-2    OH-Glc-2   STAT=Y  PRED= 4.300 RANGE= 1.000
 J41_46      9.8132   J Glc-5    Glc-4      STAT=Y  PRED= 10.550 RANGE= 2.560
 J41_49      6.9219   J Glc-5    Glc-6      STAT=Y  PRED= 2.700 RANGE= 3.000
 J41_50      1.7617   J Glc-5    Glc-6'     STAT=Y  PRED= 1.280 RANGE= 3.000
 J43_46      8.7207   J Glc-3    Glc-4      STAT=Y  PRED= 9.140 RANGE= 3.580
 J43_51      4.8865   J Glc-3    OH-Glc-3   STAT=Y  PRED= 4.300 RANGE= 1.000
 J46_52      5.8261   J Glc-4    OH-Glc-4   STAT=Y  PRED= 4.300 RANGE= 1.000
 J49_50    -11.2374   J Glc-6    Glc-6'     STAT=Y  PRED= -12.300 RANGE= 0.800
 J56_68      1.5856   J Rh-1     Rh-2       STAT=Y  PRED= 2.330 RANGE= 2.800
 J57_59      6.2129   J Rh-5     Rh-Me      STAT=Y  PRED= 6.250 RANGE= 0.600
 J57_66      9.2814   J Rh-5     Rh-4       STAT=Y  PRED= 9.940 RANGE= 3.580
 J66_69      9.5011   J Rh-4     Rh-3       STAT=Y  PRED= 9.590 RANGE= 3.580
 J66_73      3.6210   J Rh-4     OH-Rh-4    STAT=Y  PRED= 4.300 RANGE= 1.000
 J68_69      3.0081   J Rh-2     Rh-3       STAT=Y  PRED= 3.420 RANGE= 3.800
 J68_71      4.0866   J Rh-2     OH-Rh-2    STAT=Y  PRED= 4.440 RANGE= 1.500
 J69_72      5.6937   J Rh-3     OH-Rh-3    STAT=Y  PRED= 4.300 RANGE= 1.000

CONTROL PARAMETERS:
       Solvent =  none (def. 99% enriched)
         1.000 =  Concentration (vol%, def=1.0%)
    0.00100000 =  Minimum line-intensity
    0.00100000 =  Diagonalization criterium (not in use)
   13.25602790 =  Left frequency (ppm)
    0.00000000 =  Right frequency (ppm)
        10.000 =  Acquisition time (s, for QMTLS)
         1.046 =  Line-width (for modes D, P & T, 0=use defaults)
   0.068609922 =  Data-point resolution (Hz)
        70.615 =  GAUSSIAN (%, 0=use default from INF)
        -1.053 =  Dispersion contribution (%, 0=use default from INF)
    0.00000000 =  Decoupling frequency (for DORES)

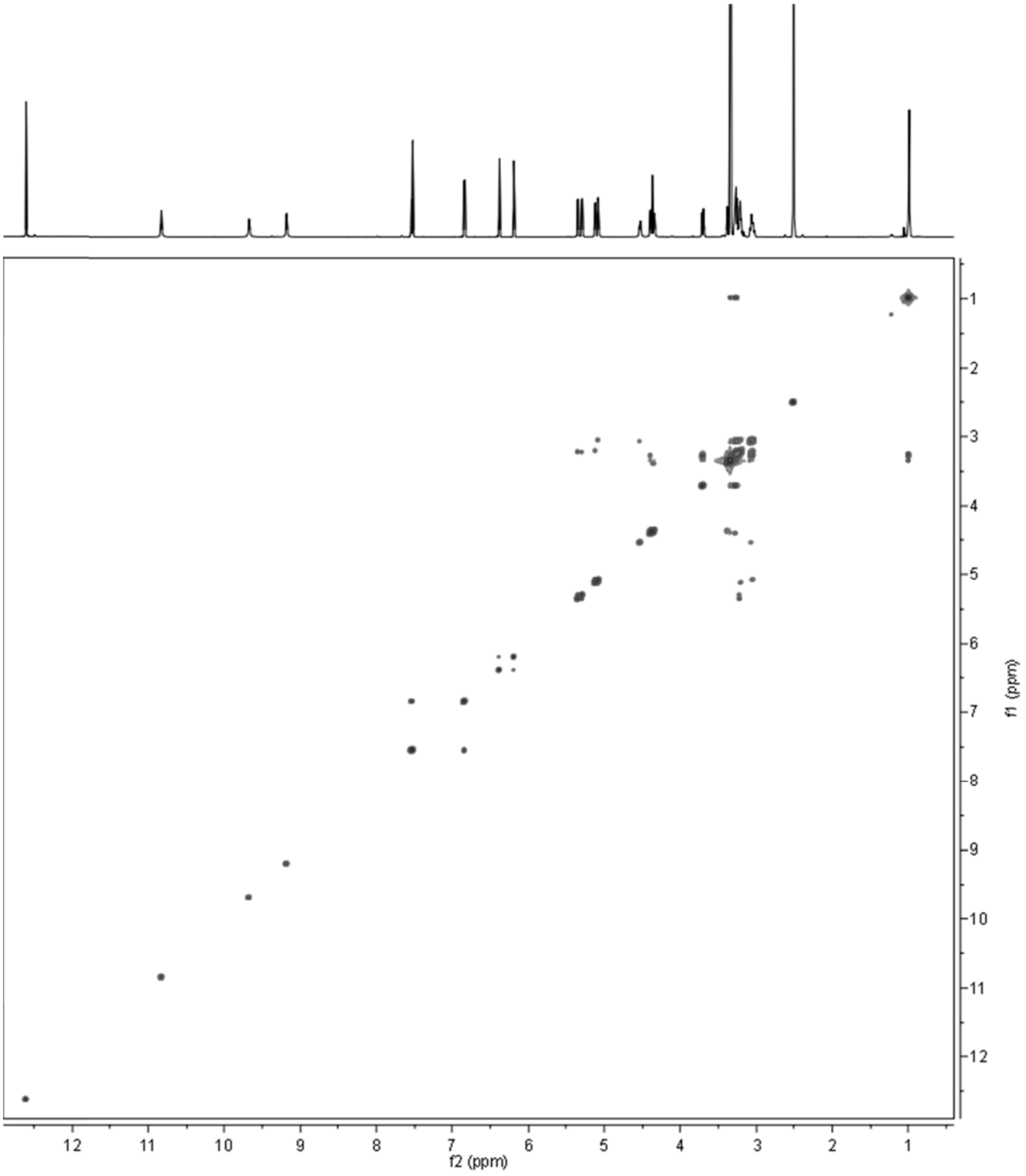
CONSTRAINTS (in equations X0 = 1.0)...use no empty lines

END of FILE
```

S26. ^{1}H NMR spectrum of Rutin (**9**, DMSO-d_6, 600 MHz).



S27. ^{1}H,^{1}H-COSY experiment of Rutin (**9**, DMSO-d_6, 600 MHz).



S28. Combined ^{1}H Fingerprints of nine *Ginkgo biloba* constituents (**1**–**9**) in the PERCH .PMS file format.

```
* NEW: the lines beginning by * are comment lines !
* To keep all the chemical shifts fixed during iteration
* replace "CHEMICAL SHIFTS(HZ):" by "..SHIFTS(HZ): fixed"
* The couplings can be fixed in the same way

NMR-data: C:\Users\jgnapo_2\Documents\jgnapo\perch\Ginkgo\
#$œ  Date  10. 15.2011;  Time 15: 5:45     Ginkgo.5TH

CHEMICAL SHIFTS(PPM):
BILOBALIDE    2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 BB-OH-10   / 1     7.253250  1*1*1  STAT=Y  PRED= 4.828 RANGE= 1.750 WIDTH(Y)= 1.600 RESP(Y)= 0.9729
 BB-H-7beta / 1     2.077084  1*1*1  STAT=Y  PRED= 1.896 RANGE= 0.357 WIDTH(Y)= 1.891 RESP(Y)= 0.9170 HSQC= C14
 BB-H-6     / 1     4.916794  1*1*1  STAT=Y  PRED= 4.888 RANGE= 0.282 WIDTH(Y)= 1.768 RESP(Y)= 0.9697 HSQC= C13
 BB-H-7alpha/ 1     2.561866  1*1*1  STAT=Y  PRED= 2.518 RANGE= 0.282 WIDTH(Y)= 1.976 RESP(Y)= 0.8993 HSQC= C14
 BB-H-10    / 1     5.149952  1*1*1  STAT=Y  PRED= 4.165 RANGE= 0.370 WIDTH(Y)= 1.774 RESP(Y)= 0.9421 HSQC= C17
 BB-H-12    / 1     6.274102  1*1*1  STAT=Y  PRED= 5.659 RANGE= 0.102 WIDTH(Y)= 1.500 RESP(Y)= 1.0000 HSQC= C19
 BB-t-Butyl / 1     1.034063  1*1*9  STAT=Y  PRED= 0.914 RANGE= 0.237 WIDTH(Y)= 2.678 RESP(Y)= 0.9023 HSQC= C25-27
 BB-OH-8    / 1     5.403089  1*1*1  STAT=Y  PRED= 3.979 RANGE= 1.923 WIDTH(Y)= 1.508 RESP(Y)= 0.9843
 BB-H-1beta / 1     2.774028  1*1*1  STAT=Y  PRED= 2.359 RANGE= 0.370 WIDTH(Y)= 1.686 RESP(Y)= 0.9603 HSQC= #27
 BB-H-1alpha/ 1     2.897044  1*1*1  STAT=Y  PRED= 2.405 RANGE= 0.462 WIDTH(Y)= 1.740 RESP(Y)= 0.9580 HSQC= #27
GINKGOLIDE_A   2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 GA-OH-3    / 2     6.378972  1*1*1  STAT=Y  PRED= 4.856 RANGE= 1.805 WIDTH(Y)= 1.273 RESP(Y)= 1.0000
 GA-OH-10   / 2     6.814323  1*1*1  STAT=Y  PRED= 4.509 RANGE= 1.630 WIDTH(Y)= 1.565 RESP(Y)= 0.9632
 GA-H-7beta / 2     2.043863  1*1*1  STAT=Y  PRED= 2.070 RANGE= 0.557 WIDTH(Y)= 2.501 RESP(Y)= 0.8989 HSQC= C14
 GA-H-1beta / 2     1.805711  1*1*1  STAT=Y  PRED= 1.401 RANGE= 0.302 WIDTH(Y)= 1.882 RESP(Y)= 0.9213 HSQC= C8
 GA-H-1alpha/ 2     2.750139  1*1*1  STAT=Y  PRED= 2.169 RANGE= 0.387 WIDTH(Y)= 1.927 RESP(Y)= 0.9005 HSQC= C8
 GA-H-2     / 2     4.833738  1*1*1  STAT=Y  PRED= 4.895 RANGE= 0.262 WIDTH(Y)= 1.798 RESP(Y)= 0.9709 HSQC= C9
 GA-H-6     / 2     4.945707  1*1*1  STAT=Y  PRED= 4.760 RANGE= 0.247 WIDTH(Y)= 1.956 RESP(Y)= 0.9824 HSQC= C13
 GA-H-7alpha/ 2     2.027505  1*1*1  STAT=Y  PRED= 2.025 RANGE= 0.472 WIDTH(Y)= 2.358 RESP(Y)= 0.8736 HSQC= C14
 GA-H-8     / 2     1.710433  1*1*1  STAT=Y  PRED= 1.700 RANGE= 0.222 WIDTH(Y)= 2.173 RESP(Y)= 0.9339 HSQC= C15
 GA-H-10    / 2     4.941390  1*1*1  STAT=Y  PRED= 4.165 RANGE= 0.392 WIDTH(Y)= 1.780 RESP(Y)= 0.9248 HSQC= C17
 GA-H-12    / 2     6.023393  1*1*1  STAT=Y  PRED= 5.659 RANGE= 0.335 WIDTH(Y)= 1.498 RESP(Y)= 0.9865 HSQC= C19
 GA-H-14    / 2     2.937891  1*1*1  STAT=Y  PRED= 2.949 RANGE= 0.387 WIDTH(Y)= 1.519 RESP(Y)= 0.9493 HSQC= C21
 GA-H-16    / 2     1.117747  1*1*3  STAT=Y  PRED= 1.114 RANGE= 0.252 WIDTH(Y)= 1.687 RESP(Y)= 0.9350 HSQC= C23
 GA-t-but   / 2     1.017131  1*1*9  STAT=Y  PRED= 0.928 RANGE= 0.227 WIDTH(Y)= 2.491 RESP(Y)= 0.9025 HSQC= C25-27
GINKGOLIDE_B    2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 GB-OH-3    / 3     6.471908  1*1*1  STAT=Y  PRED= 4.913 RANGE= 1.733 WIDTH(Y)= 1.525 RESP(Y)= 1.0000
 GB-OH-10   / 3     7.462874  1*1*1  STAT=Y  PRED= 4.556 RANGE= 1.695 WIDTH(Y)= 1.929 RESP(Y)= 0.9612
 GB-H-7beta / 3     2.137230  1*1*1  STAT=Y  PRED= 2.036 RANGE= 0.560 WIDTH(Y)= 2.168 RESP(Y)= 0.9003 HSQC= C14
 GB-H-1     / 3     4.042104  1*1*1  STAT=Y  PRED= 3.762 RANGE= 0.100 WIDTH(Y)= 1.692 RESP(Y)= 0.9364 HSQC= C8
 GB-H-2     / 3     4.642590  1*1*1  STAT=Y  PRED= 4.089 RANGE= 0.187 WIDTH(Y)= 1.644 RESP(Y)= 0.9775 HSQC= C9
 GB-H-6     / 3     5.303773  1*1*1  STAT=Y  PRED= 4.895 RANGE= 0.237 WIDTH(Y)= 1.799 RESP(Y)= 0.9597 HSQC= C13
 GB-H-7alpha/ 3     1.931786  1*1*1  STAT=Y  PRED= 2.041 RANGE= 0.477 WIDTH(Y)= 2.242 RESP(Y)= 0.8904 HSQC= C14
 GB-H-8     / 3     1.724094  1*1*1  STAT=Y  PRED= 1.670 RANGE= 0.215 WIDTH(Y)= 2.358 RESP(Y)= 0.9326 HSQC= C15
 GB-H-10    / 3     5.019748  1*1*1  STAT=Y  PRED= 4.165 RANGE= 0.380 WIDTH(Y)= 1.969 RESP(Y)= 0.9334 HSQC= C17
 GB-H-12    / 3     6.074154  1*1*1  STAT=Y  PRED= 5.659 RANGE= 0.330 WIDTH(Y)= 1.664 RESP(Y)= 0.9898 HSQC= C19
 GB-H-14    / 3     2.843287  1*1*1  STAT=Y  PRED= 2.949 RANGE= 0.367 WIDTH(Y)= 1.666 RESP(Y)= 0.9457 HSQC= C21
 GB-H-16    / 3     1.106901  1*1*3  STAT=Y  PRED= 1.102 RANGE= 0.382 WIDTH(Y)= 1.848 RESP(Y)= 0.9294 HSQC= C23
 GB-t-butyl / 3     1.028434  1*1*9  STAT=Y  PRED= 0.871 RANGE= 0.202 WIDTH(Y)= 2.590 RESP(Y)= 0.8997 HSQC= C25-27
 GB-OH-1    / 3     4.918842  1*1*1  STAT=Y  PRED= 6.248 RANGE= 2.488 WIDTH(Y)= 1.544 RESP(Y)= 0.9556
GINKGOLIDE_C    2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 GC-OH-3    / 4     6.479066  1*1*1  STAT=Y  PRED= 5.334 RANGE= 1.700 WIDTH(Y)= 1.736 RESP(Y)= 1.0000
 GC-OH-10   / 4     7.538812  1*1*1  STAT=Y  PRED= 4.347 RANGE= 1.768 WIDTH(Y)= 2.242 RESP(Y)= 0.9489
 GC-OH-7    / 4     5.658435  1*1*1  STAT=Y  PRED= 4.985 RANGE= 1.620 WIDTH(Y)= 1.944 RESP(Y)= 0.9704
 GC-H-1beta / 4     3.986275  1*1*1  STAT=Y  PRED= 4.316 RANGE= 0.100 WIDTH(Y)= 1.907 RESP(Y)= 0.9449 HSQC= C8
 GC-H-2     / 4     4.626842  1*1*1  STAT=Y  PRED= 4.089 RANGE= 0.170 WIDTH(Y)= 1.789 RESP(Y)= 0.9761 HSQC= C9
 GC-H-6     / 4     4.966384  1*1*1  STAT=Y  PRED= 4.852 RANGE= 0.122 WIDTH(Y)= 1.940 RESP(Y)= 0.9965 HSQC= C13
 GC-H-7     / 4     4.053494  1*1*1  STAT=Y  PRED= 4.559 RANGE= 0.317 WIDTH(Y)= 1.975 RESP(Y)= 0.9273 HSQC= C14
 GC-H-8     / 4     1.551161  1*1*1  STAT=Y  PRED= 1.808 RANGE= 0.222 WIDTH(Y)= 2.077 RESP(Y)= 0.9481 HSQC= C15
 GC-H-10    / 4     4.998365  1*1*1  STAT=Y  PRED= 4.165 RANGE= 0.367 WIDTH(Y)= 2.302 RESP(Y)= 0.9280 HSQC= C17
 GC-H-12    / 4     6.099451  1*1*1  STAT=Y  PRED= 5.659 RANGE= 0.325 WIDTH(Y)= 1.837 RESP(Y)= 0.9848 HSQC= C19
 GC-H-14    / 4     2.813690  1*1*1  STAT=Y  PRED= 2.949 RANGE= 0.342 WIDTH(Y)= 1.804 RESP(Y)= 0.9418 HSQC= C21
 GC-H-16    / 4     1.107483  1*1*3  STAT=Y  PRED= 1.103 RANGE= 0.377 WIDTH(Y)= 1.979 RESP(Y)= 0.8915 HSQC= C23
 GC-t-butyl / 4     1.091336  1*1*9  STAT=Y  PRED= 0.887 RANGE= 0.225 WIDTH(Y)= 2.733 RESP(Y)= 0.8975 HSQC= C25-27
 GC-OH-1    / 4     4.971784  1*1*1  STAT=Y  PRED= 5.998 RANGE= 1.965 WIDTH(Y)= 1.840 RESP(Y)= 0.8956
GINKGOLIDE_J    2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 GJ-OH-3    / 5     6.393136  1*1*1  STAT=Y  PRED= 4.925 RANGE= 1.775 WIDTH(Y)= 1.498 RESP(Y)= 1.0000
 GJ-OH-10   / 5     6.908209  1*1*1  STAT=Y  PRED= 4.324 RANGE= 1.710 WIDTH(Y)= 1.844 RESP(Y)= 0.9617
 GJ-OH-7    / 5     5.545649  1*1*1  STAT=Y  PRED= 4.759 RANGE= 1.580 WIDTH(Y)= 1.670 RESP(Y)= 0.9709
 GJ-H-1beta / 5     1.752901  1*1*1  STAT=Y  PRED= 1.338 RANGE= 0.287 WIDTH(Y)= 2.106 RESP(Y)= 0.9100 HSQC= C8
 GJ-H-1alpha/ 5     2.717097  1*1*1  STAT=Y  PRED= 2.169 RANGE= 0.377 WIDTH(Y)= 2.200 RESP(Y)= 0.8989 HSQC= C8
 GJ-H-2     / 5     4.832003  1*1*1  STAT=Y  PRED= 4.895 RANGE= 0.232 WIDTH(Y)= 1.942 RESP(Y)= 0.9577 HSQC= C9
 GJ-H-6     / 5     4.645476  1*1*1  STAT=Y  PRED= 4.895 RANGE= 0.110 WIDTH(Y)= 1.872 RESP(Y)= 0.9688 HSQC= C13
 GJ-H-7     / 5     4.171447  1*1*1  STAT=Y  PRED= 4.559 RANGE= 0.325 WIDTH(Y)= 1.862 RESP(Y)= 0.9203 HSQC= C14
 GJ-H-8     / 5     1.537556  1*1*1  STAT=Y  PRED= 1.768 RANGE= 0.212 WIDTH(Y)= 1.979 RESP(Y)= 0.9531 HSQC= C15
 GJ-H-10    / 5     4.928198  1*1*1  STAT=Y  PRED= 4.165 RANGE= 0.390 WIDTH(Y)= 2.064 RESP(Y)= 0.9291 HSQC= C17
 GJ-H-12    / 5     6.046780  1*1*1  STAT=Y  PRED= 5.659 RANGE= 0.332 WIDTH(Y)= 1.684 RESP(Y)= 0.9761 HSQC= C19
 GJ-H-14    / 5     2.906534  1*1*1  STAT=Y  PRED= 2.949 RANGE= 0.362 WIDTH(Y)= 1.711 RESP(Y)= 0.9406 HSQC= C21
 GJ-H-16    / 5     1.117886  1*1*3  STAT=Y  PRED= 1.135 RANGE= 0.260 WIDTH(Y)= 1.906 RESP(Y)= 0.9293 HSQC= C23
 GJ-t-butyl / 5     1.081520  1*1*9  STAT=Y  PRED= 0.894 RANGE= 0.230 WIDTH(Y)= 2.587 RESP(Y)= 0.9000 HSQC= C25-27
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QUERCETIN    2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 Q-H6       / 6     6.183050  1*1*1  STAT=Y  PRED= 6.298 RANGE= 0.242 WIDTH(Y)= 1.416 RESP(Y)= 1.0000 HSQC= C2
 Q-H8       / 6     6.403402  1*1*1  STAT=Y  PRED= 6.461 RANGE= 0.172 WIDTH(Y)= 1.407 RESP(Y)= 0.9861 HSQC= C4
 Q-OH7      / 6    10.783504  1*1*1  STAT=Y  PRED= 10.896 RANGE= 1.000 WIDTH(Y)= 1.739 RESP(Y)= 0.9816
 Q-OH5      / 6    12.494440  1*1*1  STAT=Y  PRED= 13.379 RANGE= 0.850 WIDTH(Y)= 1.942 RESP(Y)= 0.9532
 Q-H6'      / 6     7.536549  1*1*1  STAT=Y  PRED= 7.627 RANGE= 0.265 WIDTH(Y)= 1.496 RESP(Y)= 0.9718 HSQC= C14
 Q-H5'      / 6     6.880921  1*1*1  STAT=Y  PRED= 6.929 RANGE= 0.197 WIDTH(Y)= 1.406 RESP(Y)= 0.9618 HSQC= C15
 Q-H2'      / 6     7.674662  1*1*1  STAT=Y  PRED= 7.698 RANGE= 0.247 WIDTH(Y)= 1.416 RESP(Y)= 0.9741 HSQC= C18
 Q-OH3'     / 6     9.374357  1*1*1  STAT=Y  PRED= 9.494 RANGE= 1.215 WIDTH(Y)= 1.780 RESP(Y)= 0.9566
 Q-OH4'     / 6     9.311783  1*1*1  STAT=Y  PRED= 9.682 RANGE= 1.315 WIDTH(Y)= 2.880 RESP(Y)= 0.9305
 Q-OH3      / 6     9.597692  1*1*1  STAT=Y  PRED= 9.115 RANGE= 1.115 WIDTH(Y)= 2.732 RESP(Y)= 0.9341
KAEMPFEROL    2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 H3'_5'     / 7     6.922821  1*2*1  STAT=Y  PRED= 6.925 RANGE= 0.177 WIDTH(Y)= 1.511 RESP(Y)= 0.9770 HSQC= C15_17
 K-H6       / 7     6.186969  1*1*1  STAT=Y  PRED= 6.295 RANGE= 0.252 WIDTH(Y)= 1.406 RESP(Y)= 1.0000 HSQC= C2
 K-H8       / 7     6.435905  1*1*1  STAT=Y  PRED= 6.468 RANGE= 0.172 WIDTH(Y)= 1.404 RESP(Y)= 0.9947 HSQC= C4
 K-OH7      / 7    10.788285  1*1*1  STAT=Y  PRED= 10.903 RANGE= 0.985 WIDTH(Y)= 17.150 RESP(Y)= 0.8071
 K-OH5      / 7    12.484003  1*1*1  STAT=Y  PRED= 13.446 RANGE= 0.850 WIDTH(Y)= 1.739 RESP(Y)= 0.9625
 H2'_6'     / 7     8.041525  1*2*1  STAT=Y  PRED= 8.080 RANGE= 0.252 WIDTH(Y)= 1.495 RESP(Y)= 0.9722 HSQC= C14_18
 K-OH4'     / 7     9.408526  1*1*1  STAT=Y  PRED= 9.807 RANGE= 1.500 WIDTH(Y)= 11.480 RESP(Y)= 0.8274
 K-OH3      / 7    10.109684  1*1*1  STAT=Y  PRED= 9.155 RANGE= 1.070 WIDTH(Y)= 11.760 RESP(Y)= 0.8250
ISORHAMNETIN    2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 I-H6       / 8     6.192379  1*1*1  STAT=Y  PRED= 6.306 RANGE= 0.242 WIDTH(Y)= 1.456 RESP(Y)= 0.9979 HSQC= C2
 I-H8       / 8     6.476736  1*1*1  STAT=Y  PRED= 6.462 RANGE= 0.182 WIDTH(Y)= 1.446 RESP(Y)= 0.9882 HSQC= C4
 I-OH7      / 8    10.773796  1*1*1  STAT=Y  PRED= 10.912 RANGE= 1.015 WIDTH(Y)= 2.985 RESP(Y)= 0.9504
 I-OH5      / 8    12.467391  1*1*1  STAT=Y  PRED= 13.376 RANGE= 0.855 WIDTH(Y)= 1.433 RESP(Y)= 1.0000
 I-H6'      / 8     7.687450  1*1*1  STAT=Y  PRED= 7.638 RANGE= 0.297 WIDTH(Y)= 1.538 RESP(Y)= 0.9733 HSQC= C14
 I-H5'      / 8     6.936966  1*1*1  STAT=Y  PRED= 6.904 RANGE= 0.242 WIDTH(Y)= 1.475 RESP(Y)= 0.9759 HSQC= C15
 I-H2'      / 8     7.752072  1*1*1  STAT=Y  PRED= 7.676 RANGE= 0.305 WIDTH(Y)= 1.697 RESP(Y)= 0.9921 HSQC= C18
 I-OH4'     / 8     9.445056  1*1*1  STAT=Y  PRED= 9.712 RANGE= 0.752 WIDTH(Y)= 2.159 RESP(Y)= 0.9537
 I-OH3      / 8     9.747292  1*1*1  STAT=Y  PRED= 9.072 RANGE= 1.125 WIDTH(Y)= 2.173 RESP(Y)= 0.9713
 I-OMe      / 8     3.840464  1*1*3  STAT=Y  PRED= 3.899 RANGE= 0.132 WIDTH(Y)= 1.727 RESP(Y)= 0.9945 HSQC= H20
RUTIN     2*SPIN= 1 SPECIES=1H    POPULATION(Y)=   1.00000
 R-H6       / 9     6.190056  1*1*1  STAT=Y  PRED= 6.412 RANGE= 0.305 WIDTH(Y)= 1.062 RESP(Y)= 0.9766 HSQC= C2
 R-H8       / 9     6.380863  1*1*1  STAT=Y  PRED= 6.581 RANGE= 0.362 WIDTH(Y)= 1.055 RESP(Y)= 0.9738 HSQC= C4
 R-OH7      / 9    10.829194  1*1*1  STAT=Y  PRED= 10.802 RANGE= 1.260 WIDTH(Y)= 6.056 RESP(Y)= 0.7582
 R-OH5      / 9    12.599850  1*1*1  STAT=Y  PRED= 13.831 RANGE= 0.985 WIDTH(Y)= 1.142 RESP(Y)= 1.0000
 R-H6'      / 9     7.537800  1*1*1  STAT=Y  PRED= 7.839 RANGE= 0.327 WIDTH(Y)= 1.146 RESP(Y)= 0.9079 HSQC= C14
 R-H5'      / 9     6.836057  1*1*1  STAT=Y  PRED= 7.028 RANGE= 0.445 WIDTH(Y)= 1.149 RESP(Y)= 0.9452 HSQC= C15
 R-H2'      / 9     7.525994  1*1*1  STAT=Y  PRED= 7.813 RANGE= 0.392 WIDTH(Y)= 1.146 RESP(Y)= 0.9585 HSQC= C18
 R-OH3'     / 9     9.671753  1*1*1  STAT=Y  PRED= 9.599 RANGE= 1.830 WIDTH(Y)= 9.146 RESP(Y)= 0.7385
 R-OH4'     / 9     9.182772  1*1*1  STAT=Y  PRED= 9.443 RANGE= 1.775 WIDTH(Y)= 6.955 RESP(Y)= 0.7480
 R-Glc-1    / 9     5.341488  1*1*1  STAT=Y  PRED= 5.565 RANGE= 0.342 WIDTH(Y)= 1.356 RESP(Y)= 0.9078 HSQC= H21
 R-Glc-2    / 9     3.219724  1*1*1  STAT=Y  PRED= 3.526 RANGE= 0.200 WIDTH(Y)= 1.897 RESP(Y)= 0.9171 HSQC= C23
 R-Glc-5    / 9     3.238384  1*1*1  STAT=Y  PRED= 3.485 RANGE= 0.247 WIDTH(Y)= 2.050 RESP(Y)= 0.8314 HSQC= C25
 R-Glc-3    / 9     3.204949  1*1*1  STAT=Y  PRED= 3.317 RANGE= 0.155 WIDTH(Y)= 2.091 RESP(Y)= 0.8548 HSQC= C26
 R-Glc-4    / 9     3.047931  1*1*1  STAT=Y  PRED= 3.387 RANGE= 0.287 WIDTH(Y)= 2.008 RESP(Y)= 0.8374 HSQC= C27
 R-OH-Glc-2 / 9     5.286398  1*1*1  STAT=Y  PRED= 5.633 RANGE= 1.215 WIDTH(Y)= 1.765 RESP(Y)= 0.8978
 R-Glc-6    / 9     3.281188  1*1*1  STAT=Y  PRED= 3.351 RANGE= 0.450 WIDTH(Y)= 2.220 RESP(Y)= 0.8318 HSQC= C29
 R-Glc-6'   / 9     3.701113  1*1*1  STAT=Y  PRED= 3.509 RANGE= 0.232 WIDTH(Y)= 2.257 RESP(Y)= 0.8536 HSQC= C29
 R-OH-Glc-3 / 9     5.115871  1*1*1  STAT=Y  PRED= 4.296 RANGE= 1.420 WIDTH(Y)= 2.048 RESP(Y)= 0.8798
 R-OH-Glc-4 / 9     5.074713  1*1*1  STAT=Y  PRED= 4.702 RANGE= 1.568 WIDTH(Y)= 2.000 RESP(Y)= 0.8679
 R-Rh-1     / 9     4.376166  1*1*1  STAT=Y  PRED= 4.453 RANGE= 0.300 WIDTH(Y)= 1.672 RESP(Y)= 0.9527 HSQC= C33
 R-Rh-5     / 9     3.265194  1*1*1  STAT=Y  PRED= 2.961 RANGE= 0.627 WIDTH(Y)= 1.684 RESP(Y)= 0.9335 HSQC= C36
 R-Rh-Me    / 9     0.987386  1*1*3  STAT=Y  PRED= 0.586 RANGE= 0.262 WIDTH(Y)= 1.730 RESP(Y)= 0.8538 HSQC= C40
 R-Rh-4     / 9     3.067177  1*1*1  STAT=Y  PRED= 2.968 RANGE= 0.287 WIDTH(Y)= 3.477 RESP(Y)= 0.9349 HSQC= C37
 R-Rh-2     / 9     3.383564  1*1*1  STAT=Y  PRED= 3.609 RANGE= 0.242 WIDTH(Y)= 2.395 RESP(Y)= 0.9502 HSQC= C38
 R-Rh-3     / 9     3.275197  1*1*1  STAT=Y  PRED= 3.082 RANGE= 0.582 WIDTH(Y)= 2.131 RESP(Y)= 0.8779 HSQC= C39
 R-OH-Rh-2  / 9     4.350559  1*1*1  STAT=Y  PRED= 4.719 RANGE= 1.395 WIDTH(Y)= 4.049 RESP(Y)= 0.7880
 R-OH-Rh-3  / 9     4.400478  1*1*1  STAT=Y  PRED= 4.127 RANGE= 1.613 WIDTH(Y)= 3.183 RESP(Y)= 0.8379
 R-OH-Rh-4  / 9     4.534535  1*1*1  STAT=Y  PRED= 4.732 RANGE= 1.673 WIDTH(Y)= 10.065 RESP(Y)= 0.8554

COUPLING CONSTANTS(HZ):
 J1_2       5.1195    J BB-OH-10    BB-H-10       STAT=Y  PRED= 4.890 RANGE= 0.750
 J3_4       6.8503    J BB-H-7beta  BB-H-6        STAT=Y  PRED= 9.550 RANGE= 3.000
 J3_4     -13.3259    J BB-H-7beta  BB-H-7alpha   STAT=Y  PRED= -12.140 RANGE= 1.000
 J4_5       7.0969    J BB-H-6      BB-H-7alpha   STAT=Y  PRED= 6.600 RANGE= 3.000
 J6_7     -18.1406    J BB-H-1beta  BB-H-1alpha   STAT=Y  PRED= -15.860 RANGE= 2.000
 J8_9       5.1630    J GA-OH-10    GA-H-10       STAT=Y  PRED= 5.140 RANGE= 0.750
 J10_11     0.6218    J GA-H-7beta  GA-H-6        STAT=Y  PRED= 1.070 RANGE= 2.000
 J10_12   -13.7046    J GA-H-7beta  GA-H-7alpha   STAT=Y  PRED= -12.430 RANGE= 1.000
 J10_13     4.5778    J GA-H-7beta  GA-H-8        STAT=Y  PRED= 4.190 RANGE= 3.000
 J14_15   -15.1675    J GA-H-1beta  GA-H-1alpha   STAT=Y  PRED= -12.310 RANGE= 1.000
 J14_16     8.2624    J GA-H-1beta  GA-H-2        STAT=Y  PRED= 8.810 RANGE= 3.000
 J15_16     7.2878    J GA-H-1alpha GA-H-2        STAT=Y  PRED= 7.110 RANGE= 3.000
 J11_12     4.0483    J GA-H-6      GA-H-7alpha   STAT=Y  PRED= 4.830 RANGE= 3.000
 J12_13    14.3434    J GA-H-7alpha GA-H-8        STAT=Y  PRED= 13.120 RANGE= 2.200
 J17_18     7.1931    J GA-H-14     GA-H-16       STAT=Y  PRED= 6.640 RANGE= 0.250
 J19_20     5.5557    J GB-OH-10    GB-H-10       STAT=Y  PRED= 5.110 RANGE= 0.750
 J21_22     0.8476    J GB-H-7beta  GB-H-6        STAT=Y  PRED= 1.140 RANGE= 2.200
 J21_23   -13.7414    J GB-H-7beta  GB-H-7alpha   STAT=Y  PRED= -12.420 RANGE= 1.000
 J21_24     4.6463    J GB-H-7beta  GB-H-8        STAT=Y  PRED= 4.190 RANGE= 3.000
 J25_26     7.4027    J GB-H-1      GB-H-2        STAT=Y  PRED= 7.800 RANGE= 3.000
 J25_27     3.5631    J GB-H-1      GB-OH-1       STAT=Y  PRED= 3.950 RANGE= 0.750
 J22_23     4.1428    J GB-H-6      GB-H-7alpha   STAT=Y  PRED= 4.630 RANGE= 3.000
 J23_24    14.3540    J GB-H-7alpha GB-H-8        STAT=Y  PRED= 13.130 RANGE= 2.200
 J28_29     7.0831    J GB-H-14     GB-H-16       STAT=Y  PRED= 6.640 RANGE= 0.250
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 J30_31      5.6531   J GC-OH-10    GC-H-10       STAT=Y  PRED= 4.950 RANGE= 0.750
 J32_33      6.2720   J GC-OH-7     GC-H-7        STAT=Y  PRED= 4.300 RANGE= 0.500
 J34_35      7.2205   J GC-H-1beta  GC-H-2        STAT=Y  PRED= 7.910 RANGE= 3.000
 J34_36      3.6847   J GC-H-1beta  GC-OH-1       STAT=Y  PRED= 4.300 RANGE= 0.500
 J37_33      4.1999   J GC-H-6      GC-H-7        STAT=Y  PRED= 4.670 RANGE= 3.000
 J33_38     12.3964   J GC-H-7      GC-H-8        STAT=Y  PRED= 11.070 RANGE= 2.200
 J39_40      7.0914   J GC-H-14     GC-H-16       STAT=Y  PRED= 6.640 RANGE= 0.250
 J41_42      5.3487   J GJ-OH-10    GJ-H-10       STAT=Y  PRED= 5.040 RANGE= 0.750
 J43_44      6.8614   J GJ-OH-7     GJ-H-7        STAT=Y  PRED= 4.300 RANGE= 0.500
 J45_46    -15.1380   J GJ-H-1beta  GJ-H-1alpha   STAT=Y  PRED= -12.310 RANGE= 1.000
 J45_48      8.1701   J GJ-H-1beta  GJ-H-2        STAT=Y  PRED= 9.280 RANGE= 3.000
 J46_48      7.2493   J GJ-H-1alpha GJ-H-2        STAT=Y  PRED= 7.040 RANGE= 3.000
 J47_44      4.1855   J GJ-H-6      GJ-H-7        STAT=Y  PRED= 4.830 RANGE= 3.000
 J44_49     12.2977   J GJ-H-7      GJ-H-8        STAT=Y  PRED= 11.060 RANGE= 2.200
 J50_51      7.2044   J GJ-H-14     GJ-H-16       STAT=Y  PRED= 6.640 RANGE= 0.250
 J52_53      2.0315   J Q-H6        Q-H8          STAT=Y  PRED= 2.110 RANGE= 0.890
 J54_55      8.4728   J Q-H6'       Q-H5'         STAT=Y  PRED= 8.380 RANGE= 0.500
 J54_56      2.2019   J Q-H6'       Q-H2'         STAT=Y  PRED= 2.080 RANGE= 0.800
 J55_56      0.4659   J Q-H5'       Q-H2'         STAT=Y  PRED= 0.460 RANGE= 0.320
 J57_58      2.4778   J H3'_5'      H3'_5'        STAT=Y  PRED= 2.710 RANGE= 0.700
 J57_59      0.2690   J H2'_6'      H3'_5'        STAT=Y  PRED= 0.460 RANGE= 0.320
 J57_60      8.7801   J H3'_5'      H2'_6'        STAT=Y  PRED= 8.530 RANGE= 0.440
 J61_62      2.0325   J K-H6        K-H8          STAT=Y  PRED= 2.110 RANGE= 0.890
 J60_59      2.4747   J H2'_6'      H2'_6'        STAT=Y  PRED= 2.380 RANGE= 0.700
 J64_63      2.0139   J I-H6        I-H8          STAT=Y  PRED= 2.110 RANGE= 0.890
 J65_66      8.4712   J I-H6'       I-H5'         STAT=Y  PRED= 8.340 RANGE= 0.500
 J65_67      2.0570   J I-H6'       I-H2'         STAT=Y  PRED= 2.080 RANGE= 0.800
 J66_67      0.2967   J I-H5'       I-H2'         STAT=Y  PRED= 0.460 RANGE= 0.320
 J68_69      2.0571   J R-H6        R-H8          STAT=Y  PRED= 2.110 RANGE= 1.790
 J70_71      8.4604   J R-H6'       R-H5'         STAT=Y  PRED= 8.380 RANGE= 1.000
 J70_72      2.2300   J R-H6'       R-H2'         STAT=Y  PRED= 2.080 RANGE= 1.600
 J71_72      0.2251   J R-H5'       R-H2'         STAT=Y  PRED= 0.460 RANGE= 0.640
 J73_74      7.7199   J R-Glc-1     R-Glc-2       STAT=Y  PRED= 7.190 RANGE= 3.580
 J74_75      9.0266   J R-Glc-2     R-Glc-3       STAT=Y  PRED= 8.920 RANGE= 3.580
 J74_80      4.7130   J R-Glc-2     R-OH-Glc-2    STAT=Y  PRED= 4.300 RANGE= 1.000
 J77_76      9.8132   J R-Glc-5     R-Glc-4       STAT=Y  PRED= 10.550 RANGE= 2.560
 J77_78      6.9219   J R-Glc-5     R-Glc-6       STAT=Y  PRED= 2.700 RANGE= 3.000
 J77_79      1.7617   J R-Glc-5     R-Glc-6'      STAT=Y  PRED= 1.280 RANGE= 3.000
 J75_76      8.7207   J R-Glc-3     R-Glc-4       STAT=Y  PRED= 9.140 RANGE= 3.580
 J75_81      4.8865   J R-Glc-3     R-OH-Glc-3    STAT=Y  PRED= 4.300 RANGE= 1.000
 J76_82      5.8261   J R-Glc-4     R-OH-Glc-4    STAT=Y  PRED= 4.300 RANGE= 1.000
 J78_79    -11.2374   J R-Glc-6     R-Glc-6'      STAT=Y  PRED= -12.300 RANGE= 0.800
 J83_84      1.5856   J R-Rh-1      R-Rh-2        STAT=Y  PRED= 2.330 RANGE= 2.800
 J87_88      6.2129   J R-Rh-5      R-Rh-Me       STAT=Y  PRED= 6.250 RANGE= 0.600
 J87_86      9.2814   J R-Rh-5      R-Rh-4        STAT=Y  PRED= 9.940 RANGE= 3.580
 J86_85      9.5011   J R-Rh-4      R-Rh-3        STAT=Y  PRED= 9.590 RANGE= 3.580
 J86_91      3.6210   J R-Rh-4      R-OH-Rh-4     STAT=Y  PRED= 4.300 RANGE= 1.000
 J84_85      3.0081   J R-Rh-2      R-Rh-3        STAT=Y  PRED= 3.420 RANGE= 3.800
 J84_89      4.0866   J R-Rh-2      R-OH-Rh-2     STAT=Y  PRED= 4.440 RANGE= 1.500
 J85_90      5.6937   J R-Rh-3      R-OH-Rh-3     STAT=Y  PRED= 4.300 RANGE= 1.000

CONTROL PARAMETERS:
       Solvent =  none (def. 99% enriched)
         1.000 =  Concentration (vol%, def=1.0%)
    0.00100000 =  Minimum line-intensity
    0.00100000 =  Diagonalization criterium (not in use)
    8.04426687 =  Left frequency (ppm)
    0.00000000 =  Right frequency (ppm)
        10.000 =  Acquisition time (s, for QMTLS)
         1.505 =  Line-width (for modes D, P & T, 0=use defaults)
   0.068609932 =  Data-point resolution (Hz)
        25.060 =  GAUSSIAN (%, 0=use default from INF)
         2.716 =  Dispersion contribution (%, 0=use default from INF)
    0.00000000 =  Decoupling frequency (for DORES)

CONSTRAINTS (in equations X0 = 1.0)...use no empty lines

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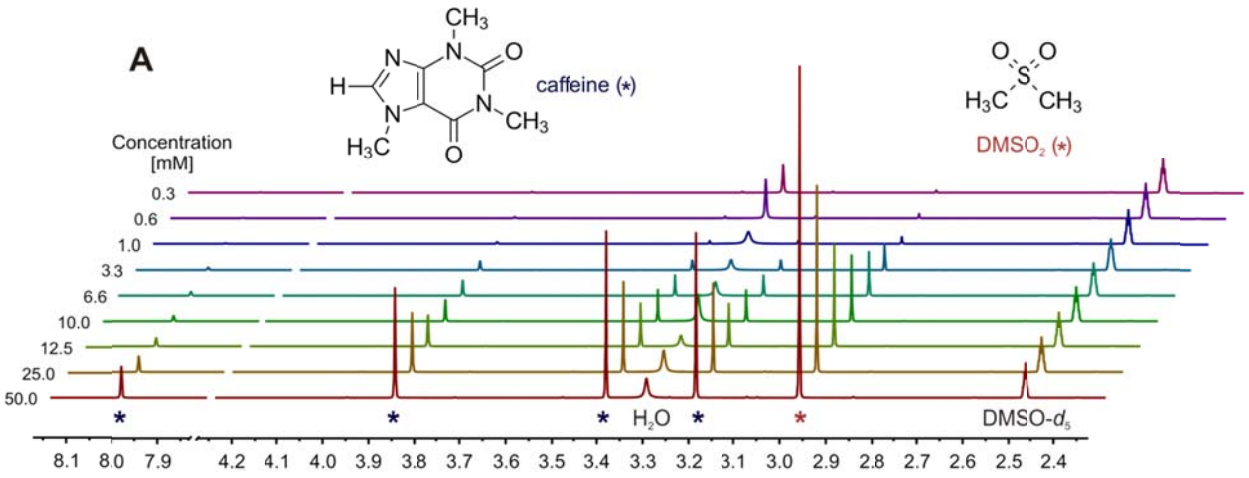
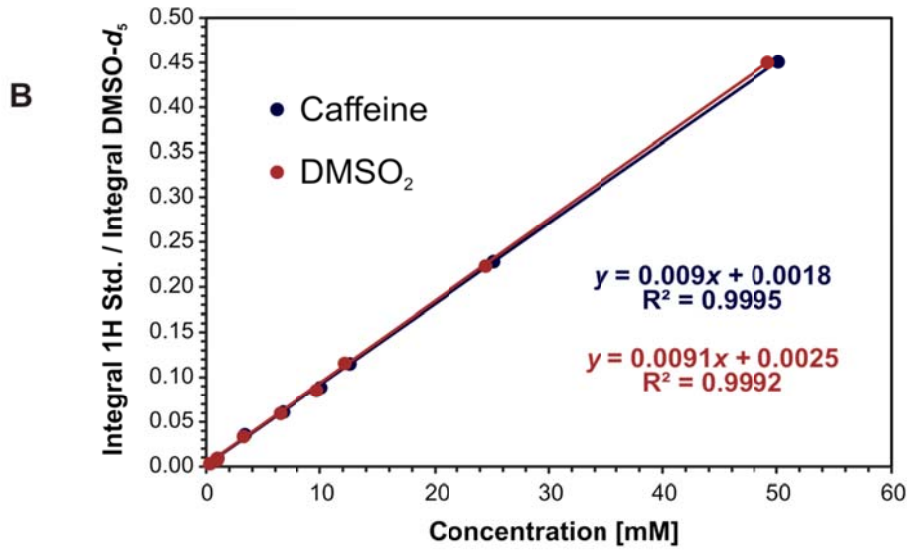
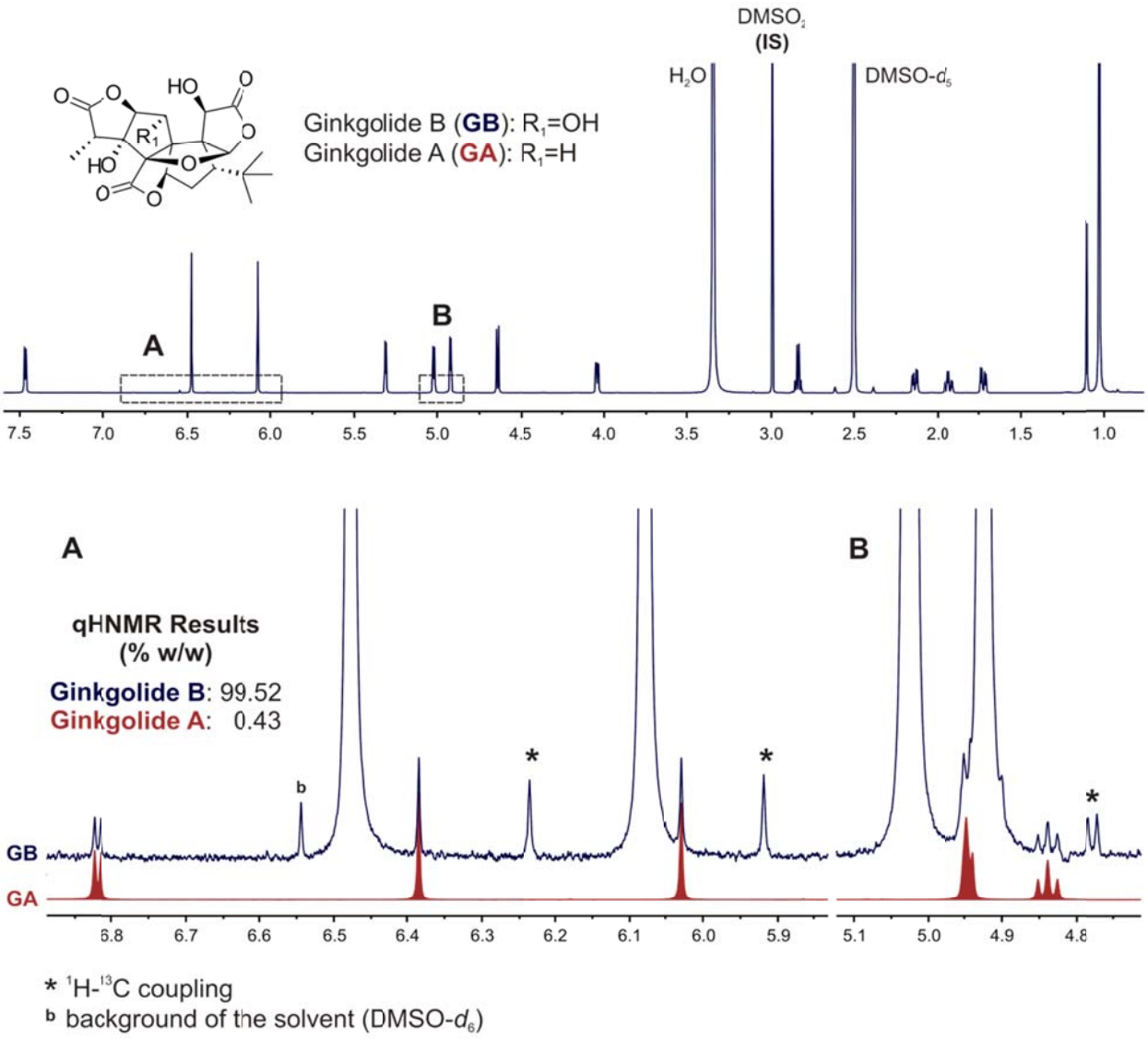
S29. Calibration of residual solvent signals using primary reference standards of $DMSO_2$ and caffeine as internal calibrants. (**A**) qHNMR spectra of stock solutions of caffeine and $DMSO_2$ in DMSO-d_6 (600 MHz). (**B**) Calibration curves for the determination of residual DMSO-d_5 content in DMSO-d_6 lot B.





S30. The qHNMR analysis of a ginkgolide B reference material (DMSO-d_6, 600 MHz). $DMSO_2$ was used as Internal Standard (IS) for quantitative calibration. Using qHNMR, ginkgolide A was readily detected as a very minor (0.43 %) impurity, present at an abundance level where intensities/integrals are comparable to those of ^{13}C satellite signals of the major component (see also reference #17 in the main text).



* ^{1}H-^{13}C coupling
ᵇ background of the solvent (DMSO-d_6)

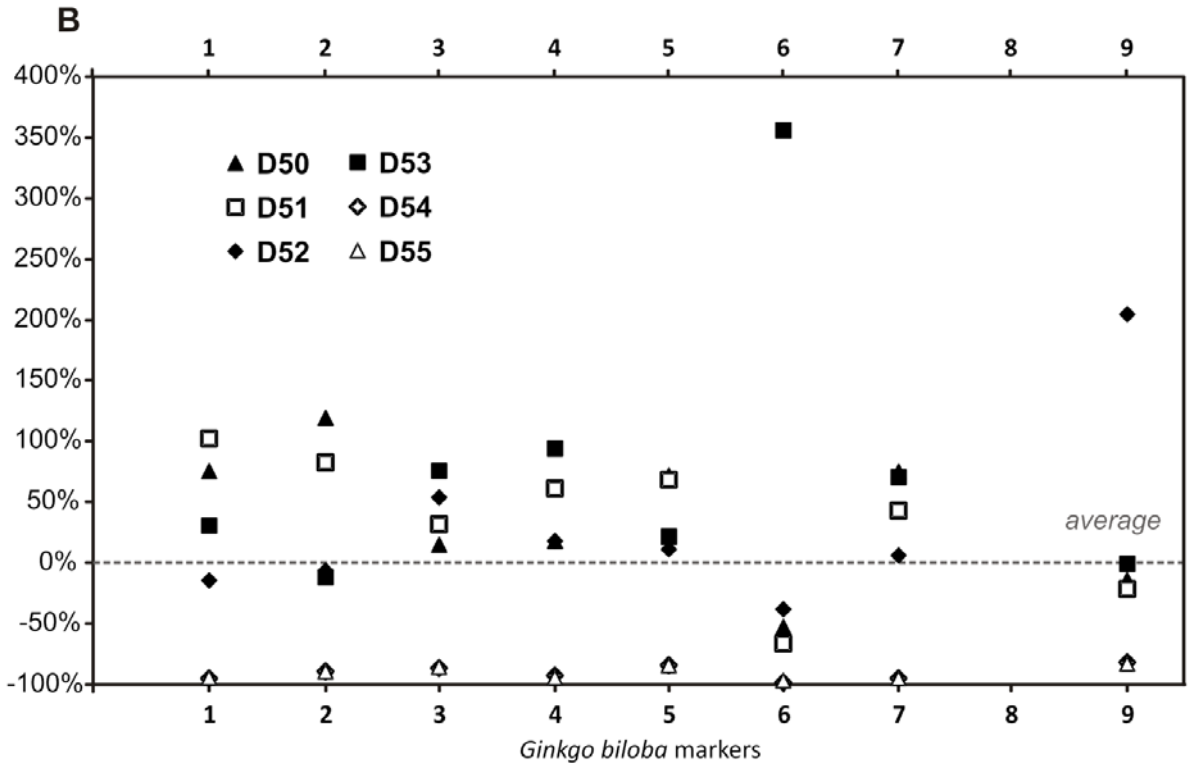
S31. (**A**) Weight percentage of compounds **1-9** in six Ginkgo samples according to qHNMR measurements. (**B**) Variability of selected botanical markers in commercially available *Ginkgo biloba* preparations, expressed as deviation (*y*-axis, in %) from the *average* percent content (set to 0% deviation, dotted line) of each of the compounds, **1-9**.

A

	***Ginkgo biloba* markers**								
	concentration, % (w/w)								
sample	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
D50	2.34	1.92	1.15	0.68	4.03	0.73	0.38	Ø[a]	3.33
D51	2.70	1.60	1.32	0.93	3.95	0.52	0.31	Ø	3.05
D52	1.14	0.81	1.54	0.68	2.60	0.96	0.23	Ø	11.91
D53	1.74	0.77	1.76	1.12	2.85	7.14	0.37	Ø	3.86
D54	0.06	0.09	0.13	0.04	0.36	0.02	<0.01	Ø	0.70
D55	0.07	0.09	0.14	0.03	0.36	0.04	<0.01	Ø	0.65

[a] Ø denotes values below the calculated limit of detection (LOD).

B



S32. The effect of random noise on iterative fitting with PERCH in qHNMR analysis. (**A**) Sections of the qHNMR spectra of caffeine (DMSO-d_6, 600 MHz), showing the olefinic proton signals (δ_H 8.01 ppm). The six qHNMR spectra were acquired using a different number of scans to reach the indicated signal-to-noise ratio (S/N) values. (**B**) Fitting of the signals of the olefinic proton of caffeine at the various S/N levels shown in **A**: comparison of experimental (*Exp*) and calculated (*Calc*) qHNMR spectra. While the root mean square (RMS) deviations for the iterative fits increase with decreasing S/N, the errors always remain <0.1%, even at a S/N level of ~11:1.