10.000s

5.000s

2088.99

2089.05

12878.82

12878.68

170.653

170.651

2.0611e+08

2.9204e+08

1.4465e+08 1.2416e+08

```
Dataset : C:/Bruker/XWIN-NMR/data/guest/nmr/peptid-1/10/pdata/1
INTENSITY fit : I[t]=I[0]+P*exp(-t/T1)
8 points for Peak 1, Cursor Point = 1888, 13340.87 Hz, 176.776 ppm
Results
          Comp. 1
         7.217e-01
I[0] =
         -2.557e-01
     =
T1
         1.917s
SD
          1.291e-01
                                            integral
                                                       intensity
       tau
             cursor
                          freq
                                    ppm
  30.000s
          1891.77
                      13332.19
                                 176.661
                                          1.7837e+08
                                                      9.5971e+07
  20.000s
           1891.08
                                 176.682
                                                      9.9048e+07
                      13333.79
                                         9.6062e+07
                                                      1.7227e+08
  15.000s
           1890.01
                      13336.25
                                 176.715
                                          4.046e+08
  10.000s
           1890.02
                       13336.22
                                 176.714
                                          2.8596e+08
                                                      1.3498e+08
   5.000s
            1889.97
                       13336.34
                                 176.716
                                          3.0733e+08
                                                      1.1215e+08
           1890.02
   3.000s
                       13336.23
                                 176.714
                                          2.2336e+08
                                                      1.1906e+08
                      13337.04
   1.000s
          1889.66
                                 176.725
                                          2.9529e+08
                                                      9.8112e+07
 100.000m
          1889.27
                      13337.93
                               176.737
                                         1.5782e+08
                                                      8.2286e+07
______
8 points for Peak 2, Cursor Point = 2040, 12991.44 Hz, 172.145 ppm
          Comp. 1
Results
I[0] =
          8.882e-01
     =
         -4.028e-01
            4.075s
SD
         1.209e-01
       tau
            cursor
                          freq
                                    ppm
                                            integral
                                                      intensity
  30.000s
          2043.16
                      12984.17
                                172.049
                                         2.1207e+08
                                                      9.7273e+07
  20.000s
          2043.04
                      12984.44 172.053
                                         1.8969e+08
                                                      1.5357e+08
                               172.054
  15.000s
          2043.02
                      12984.50
                                         1.4039e+08
                                                      1.5584e+08
                                 172.055
  10.000s
           2042.98
                      12984.59
                                          3.0816e+08
                                                      1.499e+08
   5.000s
            2043.07
                       12984.37
                                 172.052
                                          1.7774e+08
                                                      1.1865e+08
   3.000s
            2043.06
                       12984.40
                                 172.052
                                          1.6069e+08
                                                      9.5906e+07
            2042.92
                                          1.5777e+08
   1.000s
                       12984.72
                                 172.056
                                                       8.393e+07
           2042.90
                                 172.057
                                                      8.5912e+07
 100.000m
                       12984.76
                                          1.5024e+08
______
8 points for Peak 3, Cursor Point = 2086, 12885.69 Hz, 170.744 ppm
Results
          Comp. 1
I[0] =
          8.911e-01
         -2.834e-01
T1
            3.485s
SD
          1.253e-01
             cursor
                          freq
                                            integral
                                                      intensity
                                    ppm
  30.000s
           2090.02
                      12876.44
                                 170.622
                                          1.5901e+08
                                                      1.2458e+08
  20.000s
          2089.27
                      12878.17
                                 170.645
                                          2.0118e+08
                                                      1.0398e+08
  15.000s
          2089.02
                      12878.75
                                 170.652
                                          2.398e+08
                                                      1.4197e+08
```

```
3.000s
         2089.05
                    12878.67
                            170.651 2.6769e+08
                                                1.1516e+08
   1.000s 2088.96
                   12878.88 170.654 2.0028e+08
                                                6.6252e+07
 100.000m 2088.29
                   12880.42 170.674 3.0747e+08 1.0974e+08
______
8 points for Peak 4, Cursor Point = 2104, 12844.31 Hz, 170.196 ppm
Results
        Comp. 1
I[0] =
        7.469e-01
       -1.919e-01
    =
           3.161s
SD
        1.312e-01
                       freq
                                       integral
                                                intensity
      tau
           cursor
                                ppm
                   12842.80 170.176 1.5977e+08 7.4987e+07
  30.000s 2104.66
  20.000s 2103.20
                   12846.15 170.220
                                    1.5915e+08
                                                1.1539e+08
  15.000s 2102.93
                                    2.5065e+08
                             170.228
                    12846.76
                                                1.5226e+08
  10.000s
          2102.99
                    12846.62
                             170.227
                                     2.6279e+08
                                                1.1271e+08
   5.000s
          2103.02
                    12846.57
                             170.226
                                     2.0968e+08
                                                1.0746e+08
         2102.68
                   12847.34
                             170.236
                                    1.6338e+08
   3.000s
                                                1.0465e+08
                   12847.79 170.242 1.9179e+08
   1.000s 2102.49
                                               8.1221e+07
 100.000m 2102.32
                   12848.18 170.247 2.0699e+08
                                                9.264e+07
______
8 points for Peak 5, Cursor Point = 2127, 12791.43 Hz, 169.495 ppm
         Comp. 1
Results
I[0] =
        9.184e-01
       -3.092e-01
          2.118s
SD
  = 5.926e-02
                                                intensity
      tau cursor
                      freq ppm
                                      integral
  30.000s 2128.98
                   12786.89 169.435 1.8765e+08 1.3666e+08
  20.000s 2128.32
                   12788.39 169.455 2.6897e+08 1.2059e+08
  15.000s 2128.11
                   12788.89 169.462 2.7224e+08
                                                1.2873e+08
  10.000s 2128.08
                   12788.95
                                                1.3942e+08
                            169.462 2.3014e+08
   5.000s
          2128.12
                    12788.85
                             169.461
                                      2.64e+08
                                                1.4492e+08
   3.000s
          2128.06
                    12789.00
                             169.463
                                      2.508e+08
                                                1.1281e+08
                                    2.2082e+08
                    12789.17
                             169.465
          2127.98
   1.000s
                                                1.0281e+08
         2102.32
                            170.247 1.0911e+08
                    12848.18
                                                9.264e+07
 100.000m
______
7 points for Peak 6, Cursor Point = 2611, 11678.78 Hz, 154.752 ppm
Results
        Comp. 1
I[0] =
       8.218e-01
        -4.110e-01
T1
          5.517s
SD
        1.144e-01
           cursor
                       freq
                                ppm
                                      integral
                                                intensity
```

30.000s 2613.08 11673.99 154.688 2.3013e+08 1.3545e+08 20.000s 2611.21 11678.30 154.745 2.1455e+08 9.7598e+07 15.000s 2610.97 11678.84 154.753 1.769e+08 1.5834e+08 10.000s 2611.05 11678.67 154.750 1.4322e+08 1.1847e+08 8.9737e+07 5.000s 2610.97 11678.84 154.753 1.7336e+08

```
3.000s 2610.15 11680.73 154.778 1.9039e+08 1.0025e+08 1.000s 2610.20 11680.63 154.776 1.4179e+08 7.5748e+07 100.000m 2611.00 11678.78 154.752 5.3744e+07 ********
```

7 points for Peak 7, Cursor Point = 3233, 10248.88 Hz, 135.805 ppm

Results Comp. 1

I[0] = 8.715e-01
P = -5.389e-01
T1 = 2.013s

SD = 7.533e - 02

	tau	cursor	freq	ppm	integral	intensity
20. 15. 10. 5. 3.	000s 000s 000s 000s 000s 000s 000s	3234.13 3232.40 3232.00 3231.28 3231.31 3231.12 3230.92 3233.00	10246.28 10250.25 10251.17 10252.84 10252.76 10253.21 10253.65 10248.88	135.770 135.823 135.835 135.857 135.856 135.862 135.868 135.805	1.9243e+08 2.7441e+08 2.72e+08 2.65e+08 2.1432e+08 1.4337e+08 1.4714e+08 4.3815e+07	1.1691e+08 1.1485e+08 1.379e+08 1.1669e+08 9.8222e+07 1.1522e+08 7.2785e+07 *******

7 points for Peak 8, Cursor Point = 3408, 9846.57 Hz, 130.474 ppm

Results Comp. 1 I[0] = 9.062e-01 P = -3.272e-01 T1 = 1.580s

SD = 4.865e-02

tau	cursor	freq	ppm	integral	intensity
30.000s 20.000s 15.000s 10.000s 5.000s 3.000s 1.000s	3413.00 3411.42 3411.04 3410.93 3410.98 3410.83 3410.34 3408.00	9835.07 9838.71 9839.59 9839.84 9839.72 9840.07 9841.19 9846.57	130.321 130.370 130.381 130.385 130.383 130.388 130.402 130.474	5.4298e+08 6.7578e+08 7.0401e+08 5.748e+08 7.1193e+08 7.0157e+08 7.2657e+08 1.4567e+08	2.8276e+08 2.8521e+08 3.3468e+08 3.0574e+08 3.0784e+08 2.8147e+08 2.4593e+08 ********

7 points for Peak 9, Cursor Point = 3464, 9717.84 Hz, 128.768 ppm

Results Comp. 1 I[0] = -2.061e+03 P = 2.062e+03 T1 = 428958.561s

SD = 6.545e - 02

tau	cursor	freq	ppm	integral	intensity
30.000s	3465.21	9715.06	128.731	6.406e+08	2.5347e+08
20.000s	3464.03	9717.77	128.767	7.522e+08	2.7849e+08
15.000s	3463.26	9719.53	128.790	6.7713e+08	2.8919e+08
10.000s	3463.16	9719.77	128.794	7.674e+08	3.286e+08
5.000s	3463.16	9719.76	128.794	7.294e+08	2.9638e+08

```
3.000s 3463.08
                  9719.96 128.796 7.0942e+08 3.3035e+08
  1.000s 3463.01
                 9720.11 128.798 7.2975e+08 2.7166e+08
 100.000m 3464.00
                 9717.84 128.768 2.0596e+08
______
7 points for Peak 10, Cursor Point = 3482, 9676.46 Hz, 128.220 ppm
Results
       Comp. 1
I[0] = 8.879e-01
```

-2.205e-01

1.406s

SD = 6.185e-02

=

20.000s 3481.15 9678.42 128.246 7.4178e+08 2.9116e 15.000s 3480.84 9679.12 128.255 7.3866e+08 2.6014e 10.000s 3480.62 9679.64 128.262 7.3429e+08 2.5581e	ta	tau cursor	freq	ppm	integral	intensity
1.000s 3480.17 9680.66 128.275 6.7331e+08 2.2722e	20.000s 15.000s 10.000s 5.000s 3.000s 1.000s	00s 3481.15 00s 3480.84 00s 3480.62 00s 3480.63 00s 3480.57 00s 3480.17	9678.42 9679.12 9679.64 9679.60 9679.73 9680.66	128.246 128.255 128.262 128.261 128.263 128.275	7.4178e+08 7.3866e+08 7.3429e+08 7.4053e+08 7.0136e+08 6.7331e+08	2.2428e+08 2.9116e+08 2.6014e+08 2.5581e+08 2.6105e+08 2.4887e+08 2.2722e+08 *******

7 points for Peak 11, Cursor Point = 3533, 9559.21 Hz, 126.666 ppm

Comp. 1 Results

I[0] = -2.843e+03= 2.844e+03= 563954.941s

SD = 9.972e-02

30.000s 3534.09 9556.71 126.633 2.2758e+08 1.2323e+08 20.000s 3532.97 9559.29 126.667 3.152e+08 1.1923e+08 15.000s 3532.14 9561.18 126.692 3.0029e+08 1.3737e+08 10.000s 3532.15 9561.17 126.692 4.4253e+08 1.8562e+08 5.000s 3532.21 9561.04 126.690 3.5819e+08 1.3898e+08 3.000s 3532.07 9561.36 126.695 3.6253e+08 1.5244e+08 1.000s 3532.02 9561.48 126.696 2.4352e+08 1.3439e+08 100.000m 3533.00 9559.21 126.666 1.2975e+08 ********	tau	cursor	freq	ppm	integral	intensity
	20.000s	3532.97	9559.29	126.667	3.152e+08	1.1923e+08
	15.000s	3532.14	9561.18	126.692	3.0029e+08	1.3737e+08
	10.000s	3532.15	9561.17	126.692	4.4253e+08	1.8562e+08
	5.000s	3532.21	9561.04	126.690	3.5819e+08	1.3898e+08
	3.000s	3532.07	9561.36	126.695	3.6253e+08	1.5244e+08
	1.000s	3532.02	9561.48	126.696	2.4352e+08	1.3439e+08

6 points for Peak 12, Cursor Point = 3588, 9432.78 Hz, 124.991 ppm

Results Comp. 1

I[0] = 7.861e-01-1.821e+01 = 783.817m T1

SD = 1.109e-01

intensity	integral	ppm	freq	cursor	tau
1.3824e+08	2.4312e+08	124.926	9427.86	3590.14	30.000s
1.1682e+08	2.9871e+08	124.964	9430.72	3588.89	20.000s
1.8688e+08	3.0836e+08	124.988	9432.55	3588.10	15.000s
1.4569e+08	3.3876e+08	124.989	9432.63	3588.07	10.000s
1.4115e+08	1.9999e+08	124.986	9432.40	3588.17	5.000s

7 points for Peak 13, Cursor Point = 3902, 8710.93 Hz, 115.426 ppm

Results Comp. 1

I[0] = 9.743e-01 P = -1.002e-01T1 = 66.015s

SD = 5.914e-02

tau	u cursor	freq	ppm	integral	intensity
30.000s 20.000s 15.000s 10.000s 5.000s 3.000s 1.000s	3904.01 3902.30 3901.90 3901.59 3901.70 3901.35 3901.13 3902.00	8706.31 8710.25 8711.16 8711.86 8711.62 8712.42 8712.92 8710.93	115.365 115.417 115.429 115.438 115.435 115.446 115.452	5.6102e+08 7.2465e+08 7.5972e+08 6.0912e+08 8.8313e+08 8.3006e+08 6.8058e+08 2.9358e+07	3.0655e+08 2.8518e+08 3.3496e+08 2.6874e+08 2.9426e+08 3.1225e+08 2.8463e+08 *******

8 points for Peak 14, Cursor Point = 5915, 4083.29 Hz, 54.106 ppm

Results Comp. 1

I[0] = 8.856e-01 P = -2.752e-01T1 = 436.962m

SD = 1.011e-01

30.000s 5917.84 4076.77 54.020 2.3511e+08 1.0211e+08 20.000s 5916.94 4078.84 54.047 3.5084e+08 7.8342e+07 15.000s 5916.14 4080.68 54.072 3.9039e+08 1.1379e+08 10.000s 5909.08 4096.91 54.287 3.481e+08 1.1248e+08 5.000s 5915.90 4081.22 54.079 3.5211e+08 9.2041e+07 3.000s 5909.03 4097.01 54.288 4.1825e+08 1.1555e+08 1.000s 5908.75 4097.67 54.297 5.4112e+08 9.8667e+07 100.000m 5908.95 4097.20 54.291 2.9297e+08 7.7067e+07	tau	cursor	freq	ppm	integral	intensity
	20.000s	5916.94	4078.84	54.047	3.5084e+08	7.8342e+07
	15.000s	5916.14	4080.68	54.072	3.9039e+08	1.1379e+08
	10.000s	5909.08	4096.91	54.287	3.481e+08	1.1248e+08
	5.000s	5915.90	4081.22	54.079	3.5211e+08	9.2041e+07
	3.000s	5909.03	4097.01	54.288	4.1825e+08	1.1555e+08
	1.000s	5908.75	4097.67	54.297	5.4112e+08	9.8667e+07

7 points for Peak 15, Cursor Point = 5985, 3922.37 Hz, 51.974 ppm

Results Comp. 1

I[0] = 8.307e-01 P = 7.553e-02T1 = 3.158s

SD = 1.062e-01

tau	cursor	freq	ppm	integral	intensity
30.000s	5988.95	3913.29	51.854	2.8208e+08	9.9024e+07
20.000s	5987.23	3917.25	51.906	2.3669e+08	6.9562e+07
15.000s	5986.01	3920.06	51.943	4.6107e+08	8.8891e+07
10.000s	5985.96	3920.17	51.945	3.6422e+08	6.8912e+07
5.000s	5985.75	3920.64	51.951	3.2552e+08	8.1018e+07

```
3.000s 5985.86 3920.40 51.948 3.3548e+08 9.4273e+07
1.000s 5985.63 3920.91 51.955 3.8529e+08 8.4385e+07
100.000m 5985.00 3922.37 51.974 4.6377e+08 ********
```

8 points for Peak 16, Cursor Point = 6312, 3170.64 Hz, 42.013 ppm

Results Comp. 1

I[0] = -2.336e+03 P = 2.337e+03 T1 = 381745.930s

SD = 7.705e-02

intensity	integral	ppm	freq	cursor	tau
6.5946e+07 6.7238e+07 8.3895e+07 7.5786e+07 8.02e+07 9.8994e+07 7.5965e+07 7.8985e+07	5.6481e+08 5.2469e+08 5.4946e+08 4.8364e+08 5.3637e+08 5.4198e+08 6.5287e+08 4.3717e+08	41.619 41.947 41.707 41.981 41.980 41.705 41.709	3140.93 3165.67 3147.50 3168.23 3168.13 3147.42 3147.69 3148.82	6324.92 6314.16 6322.06 6313.05 6313.09 6322.10 6321.98 6321.49	30.000s 20.000s 15.000s 10.000s 5.000s 3.000s 1.000s 100.000m

8 points for Peak 17, Cursor Point = 6321, 3149.95 Hz, 41.739 ppm

Results Comp. 1

I[0] = -2.550e+03 P = 2.551e+03T1 = 483557.906s

SD = 7.547e - 02

tau	cursor	freq	ppm	integral	intensity
30.000s	6324.92	3140.93	41.619	* * * * * * *	6.5946e+07
20.000s	6323.62	3143.92	41.659	*****	7.2342e+07
15.000s	6322.06	3147.50	41.707	*****	8.3895e+07
10.000s	6322.34	3146.86	41.698	*****	7.6191e+07
5.000s	6322.57	3146.33	41.691	*****	7.717e+07
3.000s	6322.10	3147.42	41.705	*****	9.8994e+07
1.000s	6321.98	3147.69	41.709	* * * * * * *	7.5965e+07
100.000m	6321.49	3148.82	41.724	* * * * * * *	7.8985e+07

8 points for Peak 18, Cursor Point = 6395, 2979.83 Hz, 39.485 ppm

Results Comp. 1

I[0] = -7.711e+02 P = 7.719e+02 $T_1 = 376761.719s$

SD = 8.521e-02

tau	cursor	freq	ppm	integral	intensity
30.000s	6397.96	2973.02	39.395	2.34e+08	1.2035e+08
20.000s	6395.99	2977.56	39.455	2.2777e+08	1.1034e+08
15.000s	6395.08	2979.64	39.482	3.0398e+08	1.4982e+08
10.000s	6394.73	2980.44	39.493	3.0181e+08	1.1649e+08
5.000s	6394.79	2980.32	39.491	4.0649e+08	1.2951e+08

```
3.000s 6394.40 2981.22 39.503 3.3081e+08 1.3657e+08
1.000s 6394.10 2981.89 39.512 2.3103e+08 1.3894e+08
100.000m 6394.04 2982.05 39.514 3.191e+08 1.1345e+08
```

8 points for Peak 19, Cursor Point = 6492, 2756.84 Hz, 36.530 ppm

Results Comp. 1

I[0] = 8.991e-01 P = -2.667e-01 T1 = 653.522m

SD = 6.182e-02

tau	cursor	freq	ppm	integral	intensity
30.000s 20.000s 15.000s 10.000s 5.000s 3.000s 1.000s	6493.23 6492.07 6491.41 6491.31 6491.41 6491.21 6491.51	2754.01 2756.68 2758.20 2758.42 2758.20 2758.66 2757.97	36.493 36.528 36.548 36.551 36.548 36.554 36.554	3.1784e+08 2.9545e+08 2.6002e+08 3.7934e+08 3.2174e+08 2.8975e+08 3.0881e+08	9.1112e+07 1.0986e+08 9.353e+07 1.0201e+08 1.1384e+08 1.0379e+08 9.5383e+07
100.000m	6491.01	2759.12	36.560	2.4317e+08	7.6376e+07

8 points for Peak 20, Cursor Point = 6528, 2674.08 Hz, 35.433 ppm

Results Comp. 1

I[0] = -2.822e+03 P = 2.823e+03T1 = 618496.031s

SD = 9.748e - 02

tau	cursor	freq	ppm	integral	intensity
30.000s 20.000s 15.000s 10.000s 5.000s 3.000s	6528.92 6527.75 6527.05 6527.05 6526.99 6527.02 6526.95 6526.22	2671.98 2674.66 2676.26 2676.28 2676.40 2676.32 2676.50 2678.18	35.406 35.441 35.462 35.462 35.464 35.463 35.465	2.5558e+08 2.8172e+08 3.2261e+08 4.0212e+08 3.4274e+08 3.8087e+08 4.565e+08	9.6259e+07 9.7052e+07 1.1792e+08 1.3475e+08 1.3722e+08 1.0542e+08 1.1532e+08
100.000m	0520.22	26/8.18	35.488	3.4/390+08	1.0539e+08

8 points for Peak 21, Cursor Point = 6906, 1805.11 Hz, 23.919 ppm

Results Comp. 1

I[0] = 6.557e-01 P = 2.316e-01T1 = 43.743s

SD = 7.040e-02

intensity	integral	ppm	freq	cursor	tau
1.0718e+08	2.0118e+08	23.833	1798.61	6908.82	30.000s
1.0891e+08	2.3436e+08	23.886	1802.59	6907.09	20.000s
1.1648e+08	3.4539e+08	23.900	1803.70	6906.61	15.000s
1.1325e+08	3.4141e+08	23.908	1804.25	6906.37	10.000s
1.271e+08	2.8197e+08	23.910	1804.44	6906.29	5.000s

```
3.000s 6906.17 1804.72 23.914 3.7511e+08 1.1963e+08
1.000s 6906.25 1804.53 23.911 3.2371e+08 1.0132e+08
100.000m 6905.92 1805.28 23.921 4.4754e+08 1.3836e+08
```

8 points for Peak 22, Cursor Point = 6975, 1646.48 Hz, 21.817 ppm

Results Comp. 1

I[0] = 8.403e-01 P = -1.193e-01T1 = 847.408m

SD = 9.218e-02

	tau	cursor	freq	ppm	integral	intensity
3.0	000s 000s 000s 000s 000s	6979.02 6977.85 6977.14 6977.03 6977.05 6977.07 6976.87 6976.61	1637.25 1639.93 1641.57 1641.81 1641.78 1641.71 1642.19 1642.78	21.695 21.730 21.752 21.755 21.755 21.754 21.760 21.768	2.9811e+08 2.6965e+08 2.7413e+08 3.2506e+08 3.503e+08 3.2505e+08 3.3561e+08 4.5125e+08	1.2028e+08 1.0583e+08 1.3966e+08 1.4146e+08 1.5908e+08 1.3692e+08 1.2545e+08 1.1743e+08

8 points for Peak 23, Cursor Point = 7026, 1529.24 Hz, 20.263 ppm

Results Comp. 1

I[0] = 7.829e-01 P = 1.881e-01T1 = 7.704s

SD = 1.185e-01

tau	cursor	freq	ppm	integral	intensity
30.000s 20.000s 15.000s 10.000s 5.000s 3.000s 1.000s	7027.99 7025.87 7025.11 7024.83 7024.82 7024.75 7024.17	1524.66 1529.54 1531.28 1531.92 1531.96 1532.12 1533.45	20.203 20.268 20.290 20.299 20.300 20.302 20.319	3.2012e+08 2.8372e+08 2.8204e+08 2.4065e+08 4.1341e+08 3.4499e+08 3.4963e+08 2.7776e+08	1.193e+08 7.1652e+07 1.0938e+08 1.1035e+08 1.2819e+08 1.0086e+08 1.2802e+08
		1333.71	23.323	2.7.700.00	
