

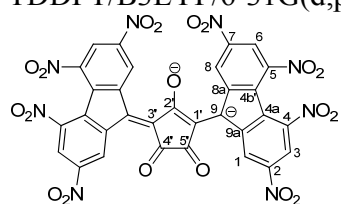
## Supplementary data

**Supplementary table 1.** Some results of TDDFT/B3LYP/6-31G(d,p) quantum chemical calculation of dyes **3** and **4**.

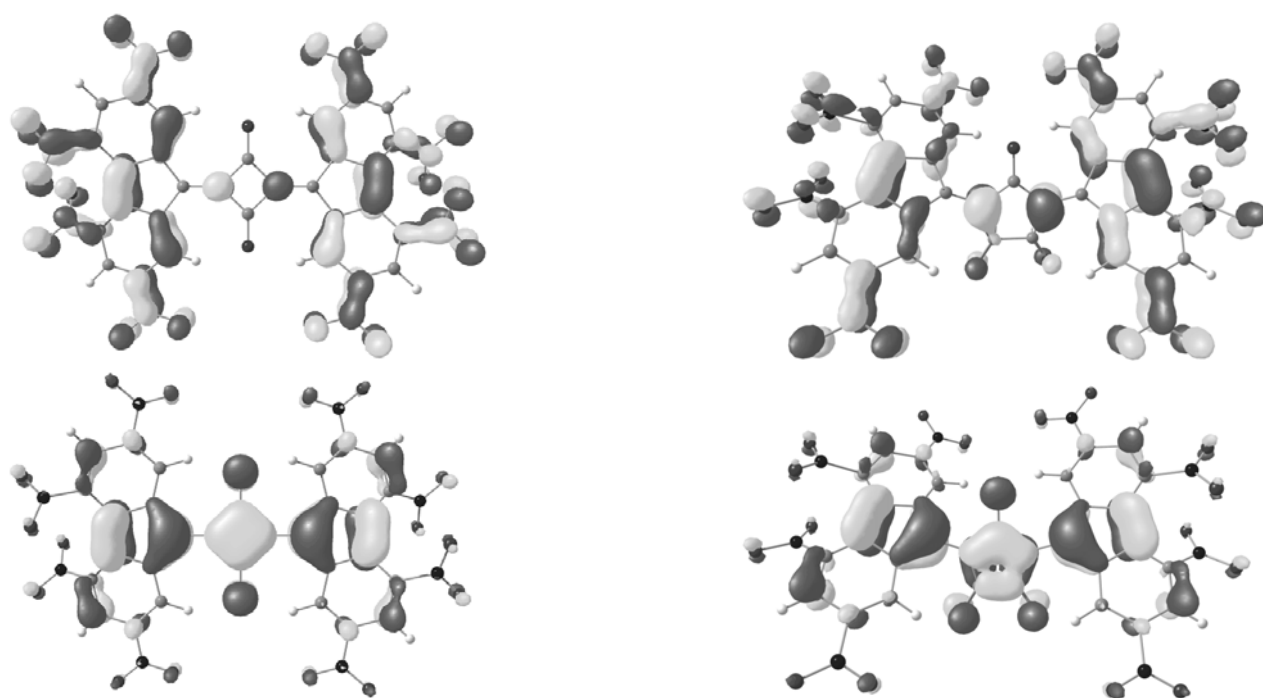
Dye	$\mu / \text{D}$	$\mu^* / \text{D}^{[a]}$	$E_{\text{HOMO}} / \text{eV}$	$E_{\text{LUMO}} / \text{eV}$	$\Delta E / \text{eV}$	$\lambda_{\text{max, calc}} / \text{nm}$	f
<b>3</b>	0.001	0.045	-0.5470	0.7429	1.2898	1140.45	0.31
						739.54	0.11
						641.50	0.10
						495.27	0.69
<b>3 (PCM, DCM)</b>	0.049	0.676	-4.2124	-2.9361	1.2762	1143.77	0.324
						750.30	0.088
						648.97	0.076
						494.11	0.706
<b>3 (PCM, DMSO)</b>	0.047	0.768	-4.5688	-3.2981	1.2708	1146.39	0.326
						753.67	0.084
						651.10	0.073
						493.97	0.705
<b>3 (PCM, acetone)</b>	0.054	0.939	-4.4627	-3.1892	1.2735	1145.43	0.325
						752.67	0.085
						650.52	0.073
						493.97	0.705
<b>3 (PCM, methanol)</b>	0.099	0.691	-4.5362	-3.2627	1.2735	1144.43	0.326
						752.23	0.086
						649.56	0.073
						493.87	0.706
<b>4</b>	1.233	1.891	-0.7129	0.4653	1.1783	1165.83	0.321
						768.41	0.175
						641.35	0.033
						640.83	0.047
						621.41	0.087
						598.68	0.239
<b>4 (PCM, DCM)</b>	2.408	0.971	-4.3266	-3.1429	1.1837	460.43	0.049
						1148.00	0.340
						765.25	0.169
						633.13	0.035
						604.47	0.322
<b>3 (PCM, DMSO)</b>	3.079	1.613	-4.6396	-3.4695	1.1701	453.61	0.032
						1161.06	0.340
						775.02	0.160
						608.12	0.303
						589.20	0.049
<b>3 (PCM, acetone)</b>	2.792	0.461	-4.5579	-3.3797	1.1783	456.95	0.040
						455.04	0.039
						1150.11	0.342
						768.33	0.165
						605.31	0.327
<b>3 (PCM, methanol)</b>	2.454	0.989	-4.6614	-3.4722	1.1892	455.26	0.039
						454.68	0.036
						1141.58	0.343
						761.61	0.169
						602.09	0.356
						453.83	0.042
						453.37	0.041

[a] A calculated dipole moment of excited state

**Supplementary table 2.** Correlation between the  $^{13}\text{C}$  NMR chemical shifts Some results of TDDFT/B3LYP/6-31G(d,p) quantum chemical calculation of dye **4**.

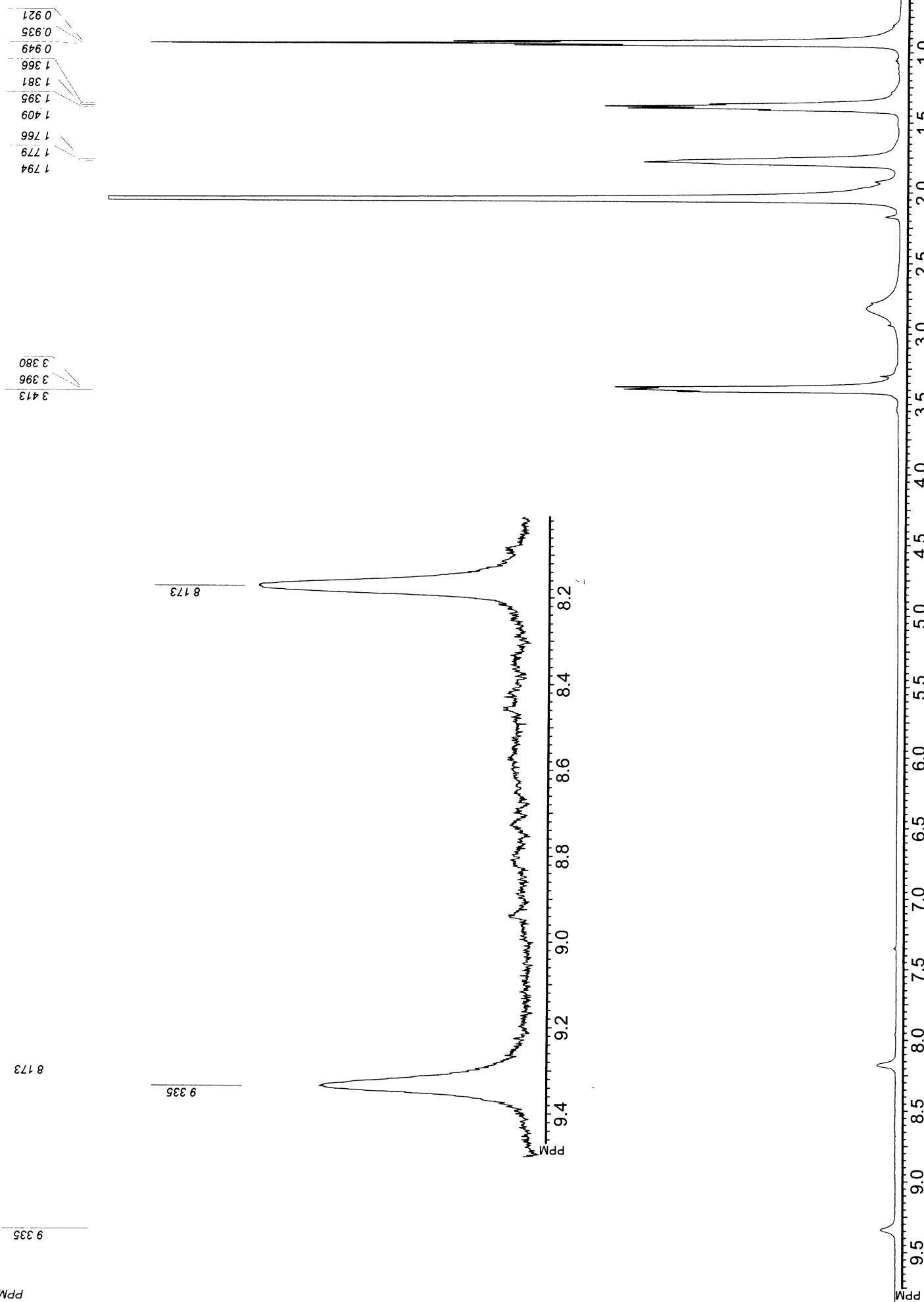


Atomic number	Charge	$\delta^{13}\text{C}$ / ppm	Atomic number	Charge	$\delta^{13}\text{C}$ / ppm
1	-0.046	127.8	8	-0.046	127.8
2	-0.019	144.4	8a	0.005	142.1
3	-0.097	113.1	9	-0.026	117.0
4	0.009	143.0	9a	0.003	142.1
4a	-0.015	122.4	1'	-0.063	140.7
4b	-0.015	122.4	2'	0.105	184.5
5	0.010	143.0	3'	-0.063	140.7
6	-0.097	113.1	4'	0.097	187.2
7	-0.019	144.4	5'	0.097	187.2



**Supplementary figure.** HOMOs (below) and LUMOs (above) of dyes **3** (left) and **4** (right).

### Dye 3: $^1\text{H}$ NMR, acetone- $\text{D}_6$



File name: UOtik102	Owner: root	SF: 500.1335 MHz	NS: 64	SI: 32768, TD: 32768
Date: 26-Oct-2009	Solvent:	SW: 8013 Hz	TE: 682.1	Parameter file: XWIN-NMR Version 3.5

### Dye 4: <sup>1</sup>H NMR, DMSO-D<sub>6</sub>

TF-Croc

1.06  
1.14  
1.15  
1.17  
1.26  
1.27  
1.88  
2.36  
2.48  
2.59  
2.77  
2.96  
2.97  
3.07  
3.08  
3.10  
3.11  
3.21  
3.31

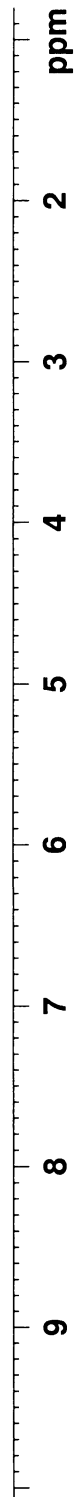
8.34  
8.52  
8.95  
9.58  
9.72

Current Data Parameters  
NAME vova070912  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070912  
Time 10.03  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30  
TD 32768  
SOLVENT DMSO  
NS 8  
DS 2  
SWH 9615.385 Hz  
FIDRES 0.293438 Hz  
AQ 1.7039860 sec  
RG 71.8  
DW 52.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec

==== CHANNEL f1 =====  
NUC1 1H  
P1 9.15 usec  
PL1 3.00 dB  
SFO1 600.1336008 MHz

F2 - Processing parameters  
SI 65536  
SF 600.1300219 MHz  
EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Dye 4: <sup>13</sup>C NMR, DMSO-D<sub>6</sub>

TF-CrOC

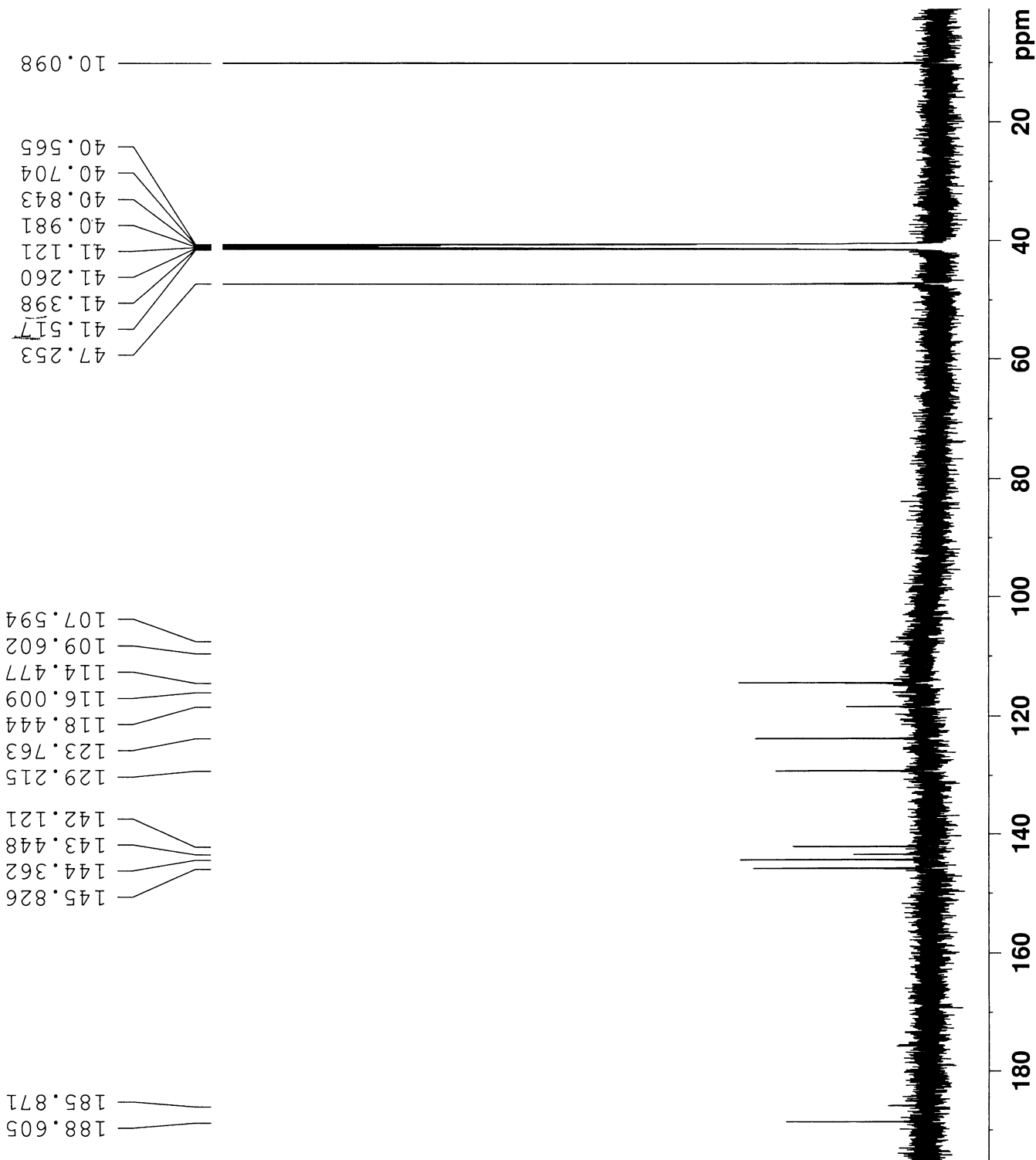
Current Data Parameters  
NAME vova070912  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070912  
Time 10.22  
INSTRUM spect  
PROBHD 5 mm TXI IH/D-  
PULPROG zgpg30  
ID 65536  
SOLVENT ~~CDCl3~~  
NS 1024  
DS 4  
SWH 37593.984 Hz  
FIDRES 0.573639 Hz  
AQ 0.8716788 sec  
RG 5160.6  
DW 13.300 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec

==== CHANNEL f1 =====  
NUC1 13C  
P1 13.90 usec  
PL1 -1.10 dB  
SFO1 150.9178988 MHz

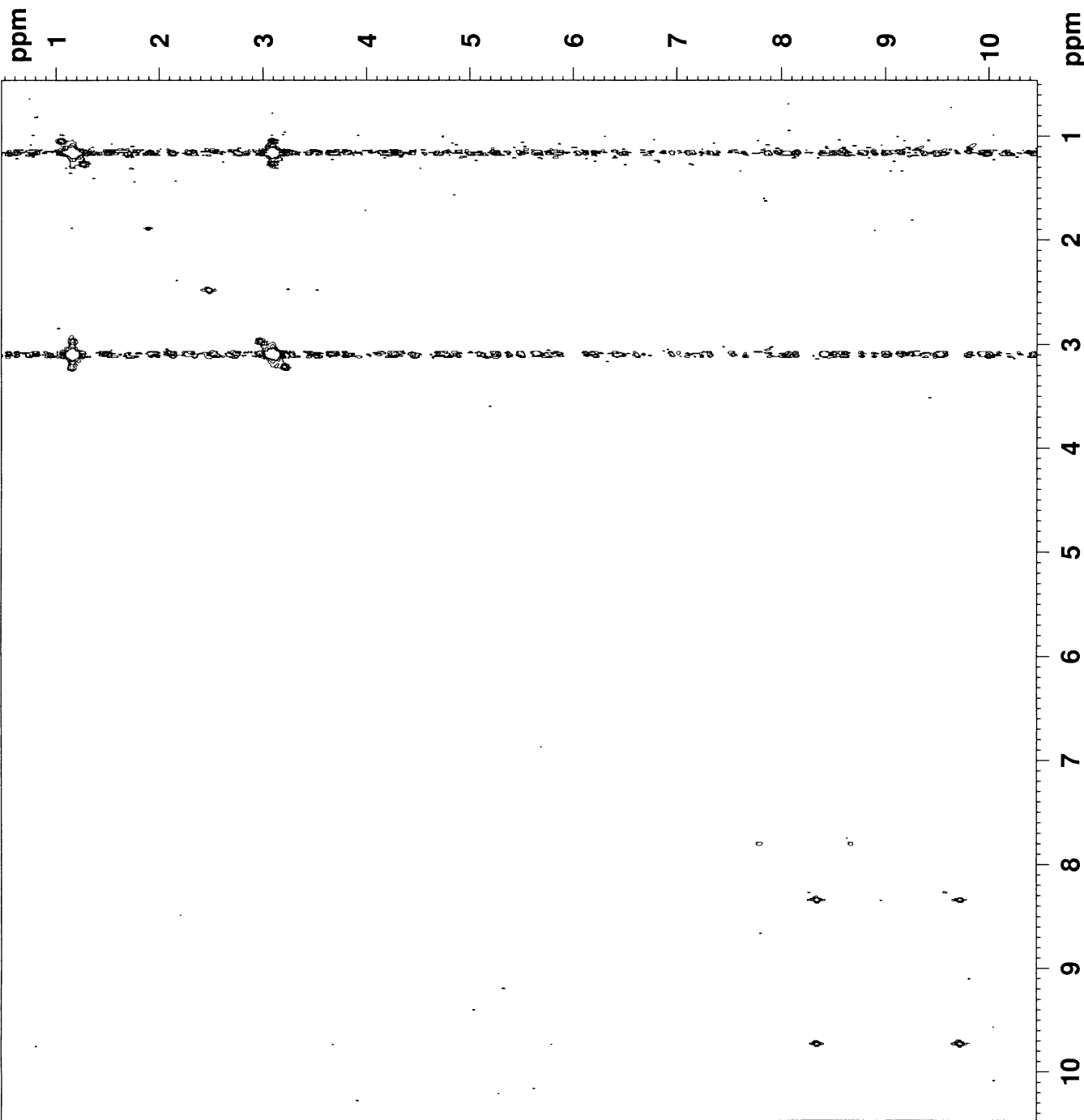
==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 3.00 dB  
PLI2 21.83 dB  
PLI3 23.00 dB  
SFO2 600.1324005 MHz

F2 - Processing parameters  
SI 32768  
SF 150.9026618 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.00



# Dye 4: H-H COSY

TF-C1OC



```
Current Data Parameters
NAME vova070912
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070912
Time 11.12
INSTRUM spect
PROBHD 5 mm TXI 1H/D
PULPROG cosygprgf
TD 4096
SOLVENT DMSO
NS 2
DS 6
SWH 6009.615 Hz
FIDRES 1.467191 Hz
AQ 0.3406372 sec
RG 71.8
WDW 83.200 usec
DE 6.00 usec
TE 300.0 K
D0 0.00000300 sec
d1 2.00000000 sec
d13 0.00000400 sec
d16 0.00020000 sec
IN0 0.00016640 sec
MCREST 0.00000000 sec
MCWRK 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.15 usec
PL1 3.00 dB
SF01 600.1333007 MHz

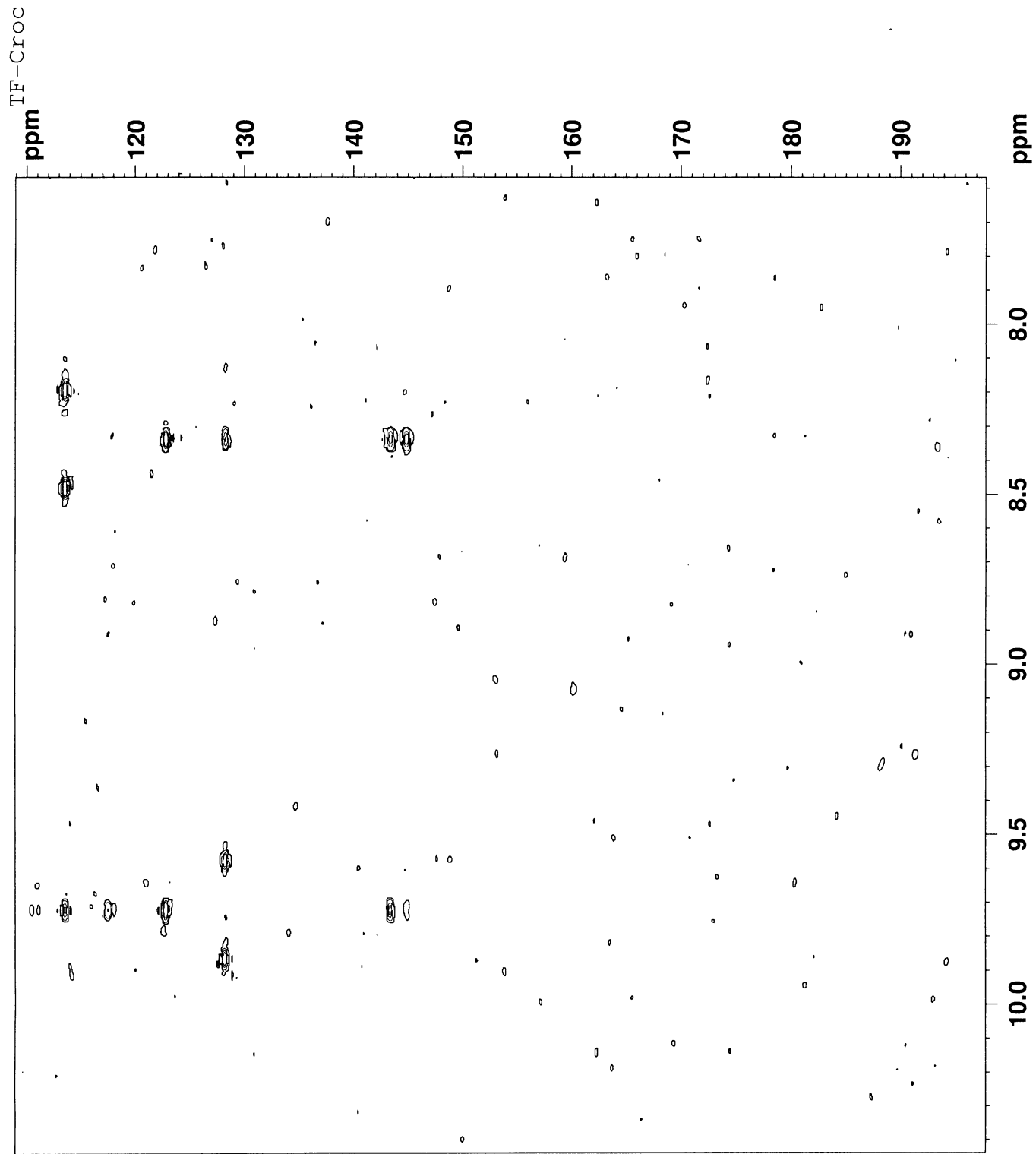
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
TD 256
SF01 600.1333 MHz
FIDRES 23.475060 Hz
SW 10.014 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 600.1300219 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
SF 600.1300219 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
```

# Dye 4: HMBC



Current Data Parameters  
NAME vova070912  
EXPNO 5  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070912  
Time 11.33  
INSTRUM spect  
PROBHD 5 mm TXI 1H/1D-  
TUPROG hmbcggp1pro04  
PULPROG zgpg30  
SOLVENT DMSO  
NS 16  
DS 16  
SWH 6009.615 Hz  
FIDRES 5.868765 Hz  
AQ 0.0952468 sec  
RG 23.200  
DQ 83.200  
DE 6.00 usec  
TE 300.0 K  
CNS12 140.0000000  
CNS13 10.0000000  
d0 0.00000300 sec  
d1 1.50000000 sec  
d2 0.00000000 sec  
d6 0.03000000 sec  
d16 0.00020000 sec  
IN0 0.00003681 sec  
MCREST 0.00000000 sec  
MCWRK 1.50000000 sec

==== CHANNEL f1 =====  
NUC1 1H  
P1 9.15 usec  
P2 18.30 usec  
PL1 3.00 dB  
SFO1 600.1333007 MHz

==== CHANNEL f2 =====  
NUC2 13C  
P1 13.90 usec  
P2 -1.10 dB  
SFO2 150.9258971 MHz

==== GRADIENT CHANNEL =====  
GPMAM1 SINE.100  
GPMAM2 SINE.100  
GPMAM3 SINE.100  
GFX2 0.00  
GFX3 0.00  
GPY1 0.00  
GPY2 0.00  
GPY3 0.00  
GZ1 30.00  
GZ2 40.00  
GZ3 40.00  
P16 1000.00 usec

F1 - Acquisition parameters  
ND0 2  
TD 256  
SFO1 150.9259 MHz  
SFO2 600.1333007 MHz  
SF 89.99 Ppm  
FRMODE QF

F2 - Processing parameters  
SI 4096  
SF 600.1300219 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
SF 150.9028100 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

# Dye 4: HSQC

TF-Croc  
 ppm

