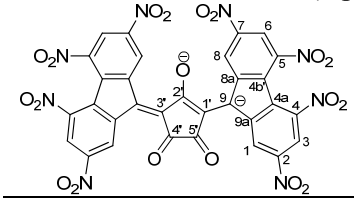
Supplementary data

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

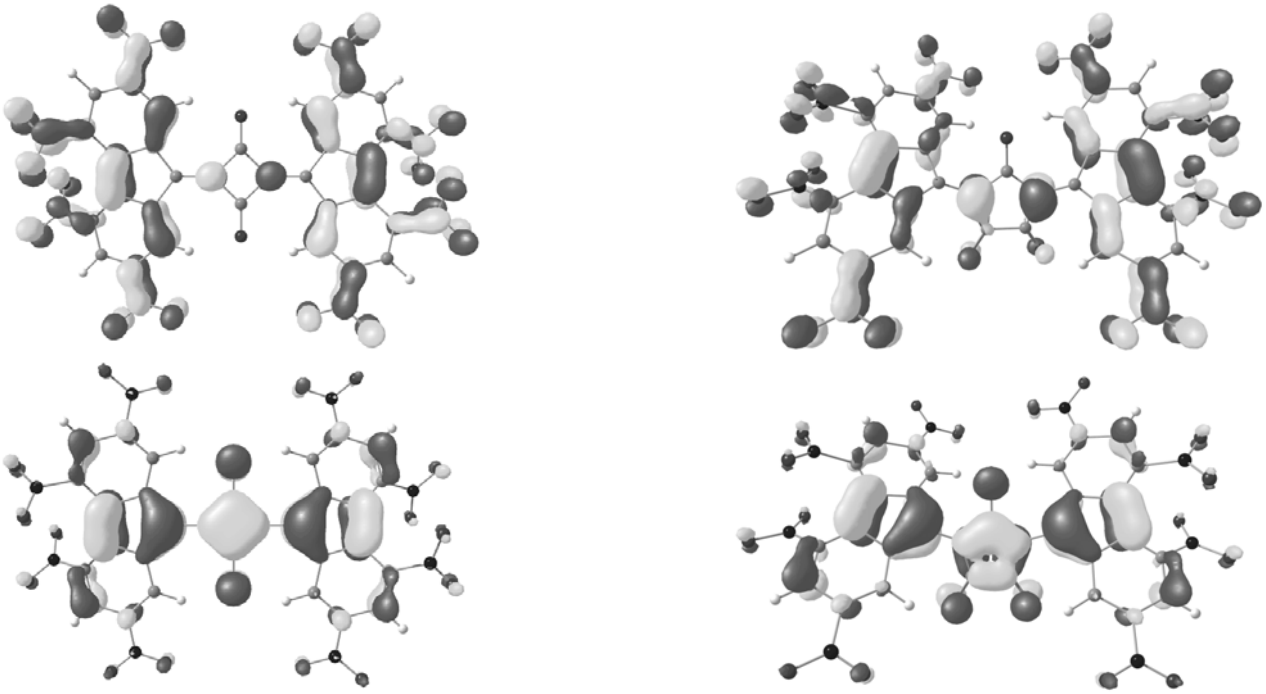
Dye	μ / D	μ^* / D [a]	E_{HOMO} / eV	E_{LUMO} / eV	ΔE / eV	$\lambda_{max,\ calc}$ / nm	f
3	0.001	0.045	–0.5470	0.7429	1.2898	1140.45 739.54 641.50 495.27	0.31 0.11 0.10 0.69
3 (PCM, DCM)	0.049	0.676	–4.2124	–2.9361	1.2762	1143.77 750.30 648.97 494.11	0.324 0.088 0.076 0.706
3 (PCM, DMSO)	0.047	0.768	–4.5688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

[a] A calculated dipole moment of excited state

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

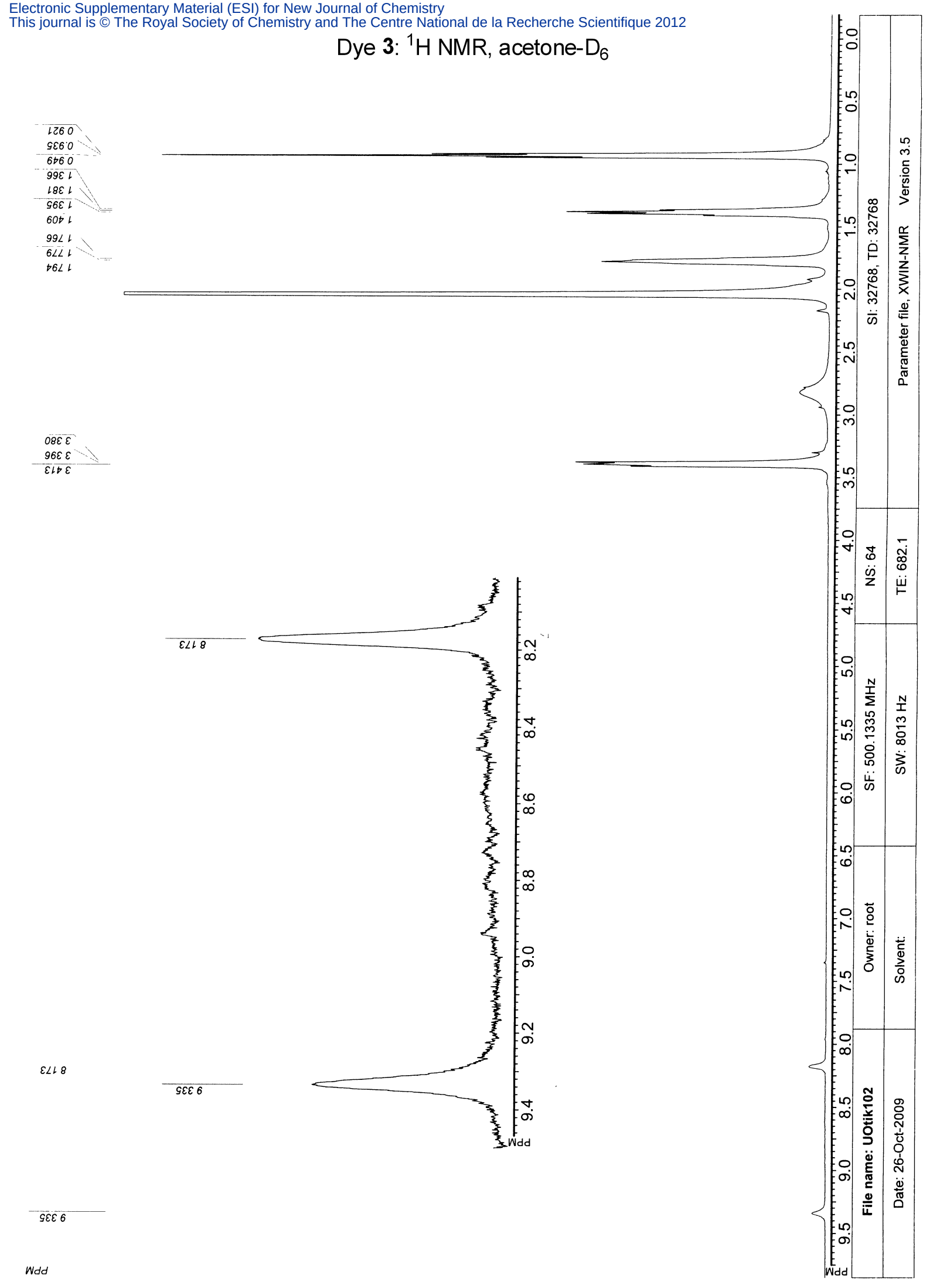


Atomic number	Charge	δ ^{13}C / ppm	Atomic number	Charge	δ ^{13}C / ppm
1	–0.046	127.8	8	–0.046	127.8
2	–0.019	144.4	8a	0.005	142.1
3	–0.097	113.1	9	–0.026	117.0
4	0.009	143.0	9a	0.003	142.1
4a	–0.015	122.4	1'	–0.063	140.7
4b	–0.015	122.4	2'	0.105	184.5
5	0.010	143.0	3'	–0.063	140.7
6	–0.097	113.1	4'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

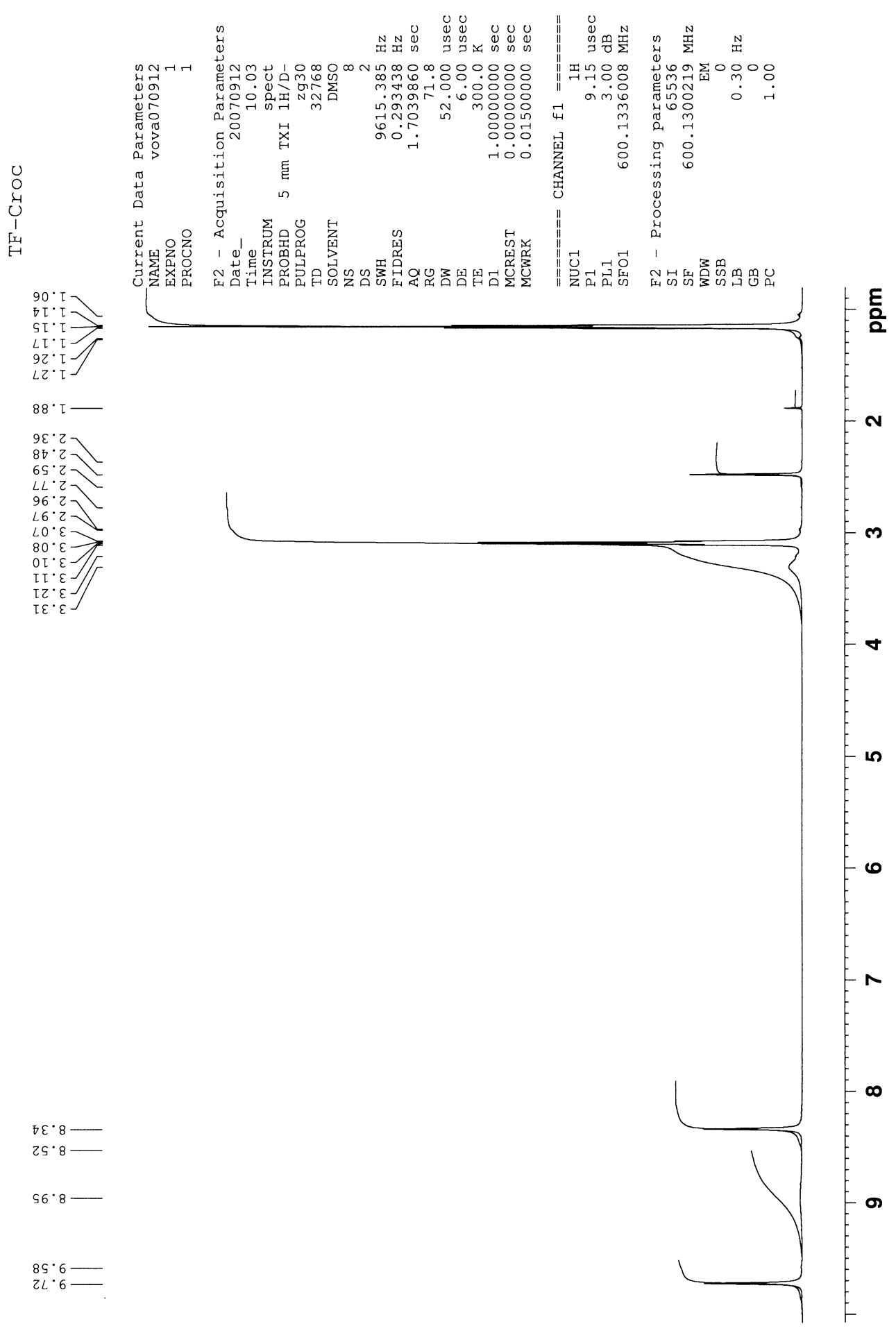


Supplementary figure. HOMOs (below) and LUMOs (above) of dyes **3** (left) and **4** (right).

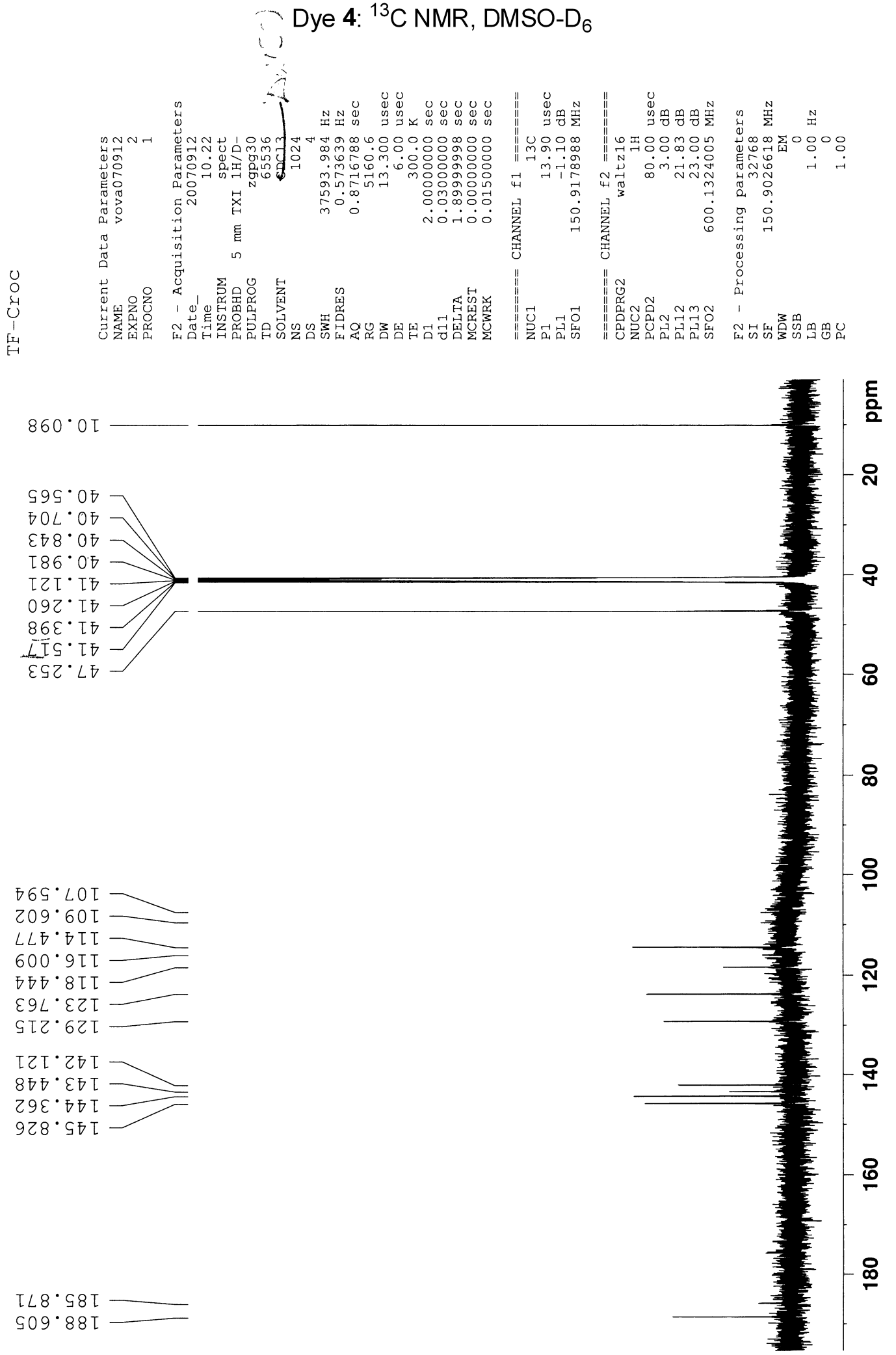
Dye **3**: ^{1}H NMR, acetone-D_6



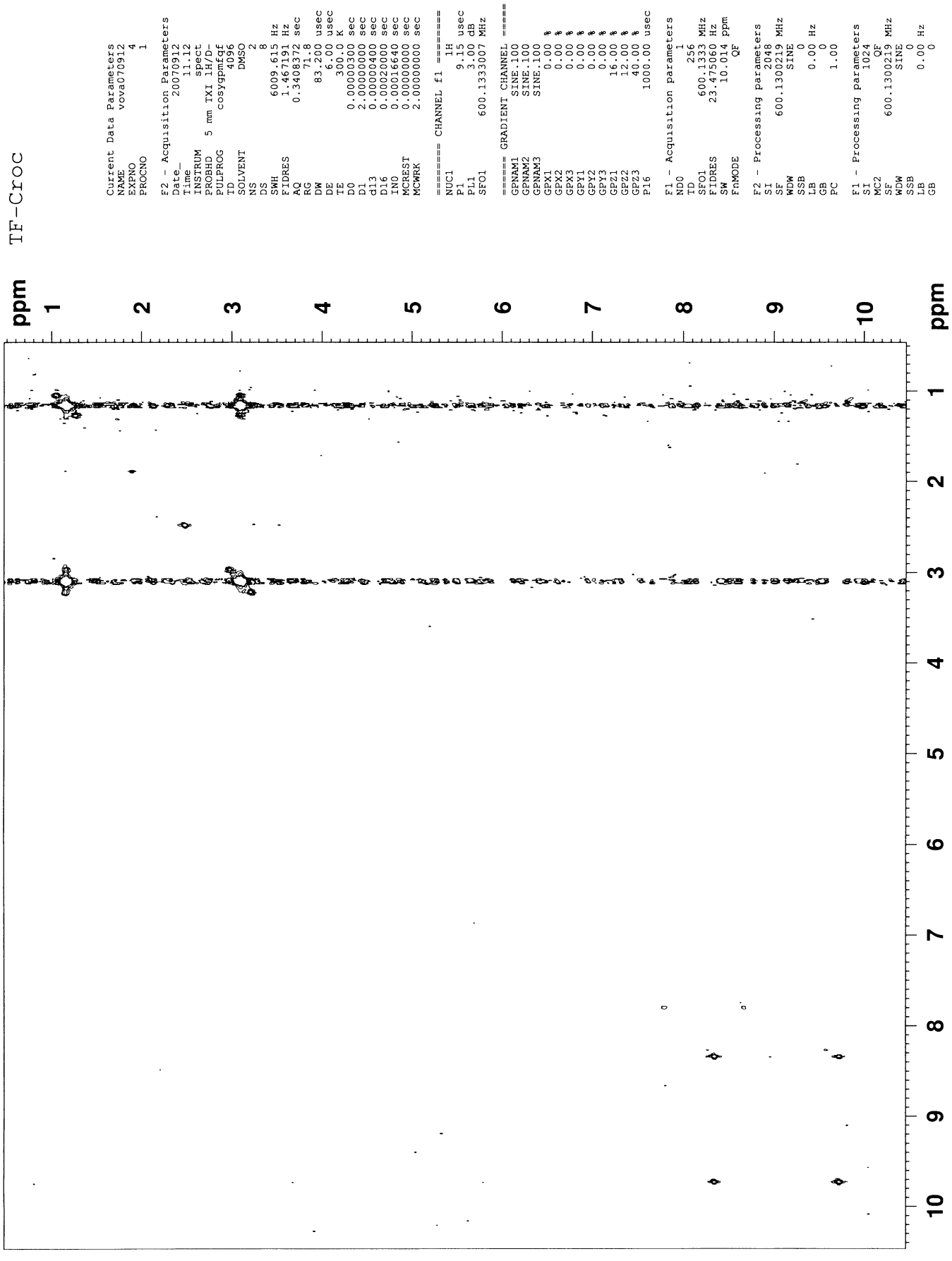
Dye **4**: ^{1}H NMR, DMSO-D$_6$



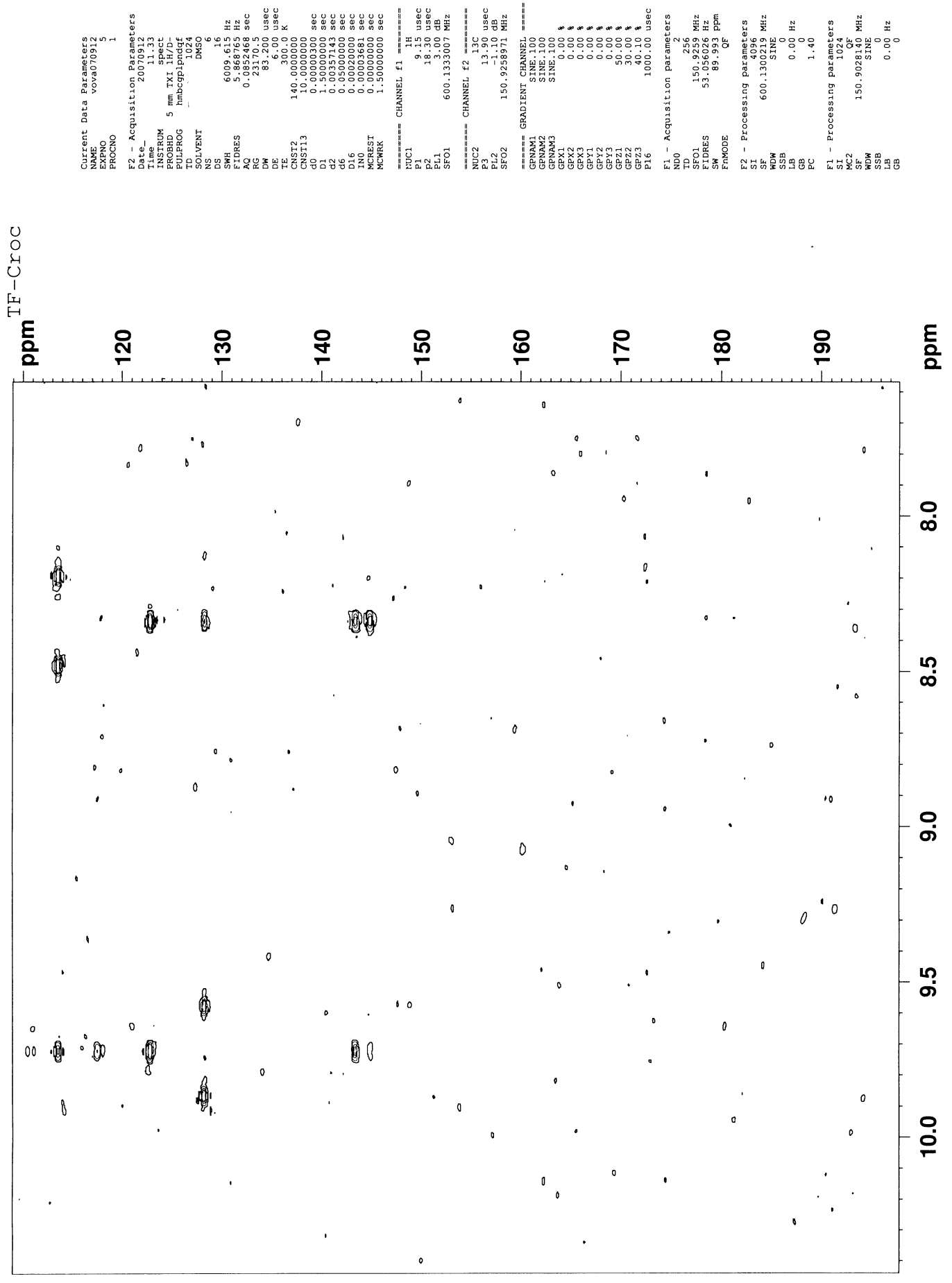
Dye **4**: ^{13}C NMR, DMSO-D$_6$



Dye **4**: H-H COSY



Dye **4**: HMBC



Dye **4**: HSQC