

# Supplementary Information

## Complete NMR assignment and conformational analysis of 17- $\alpha$ -ethinylestradiol by using RDCs obtained in grafted graphene oxide

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Griesinger\*<sup>5</sup>, Fernando Hallwass<sup>2\*</sup>

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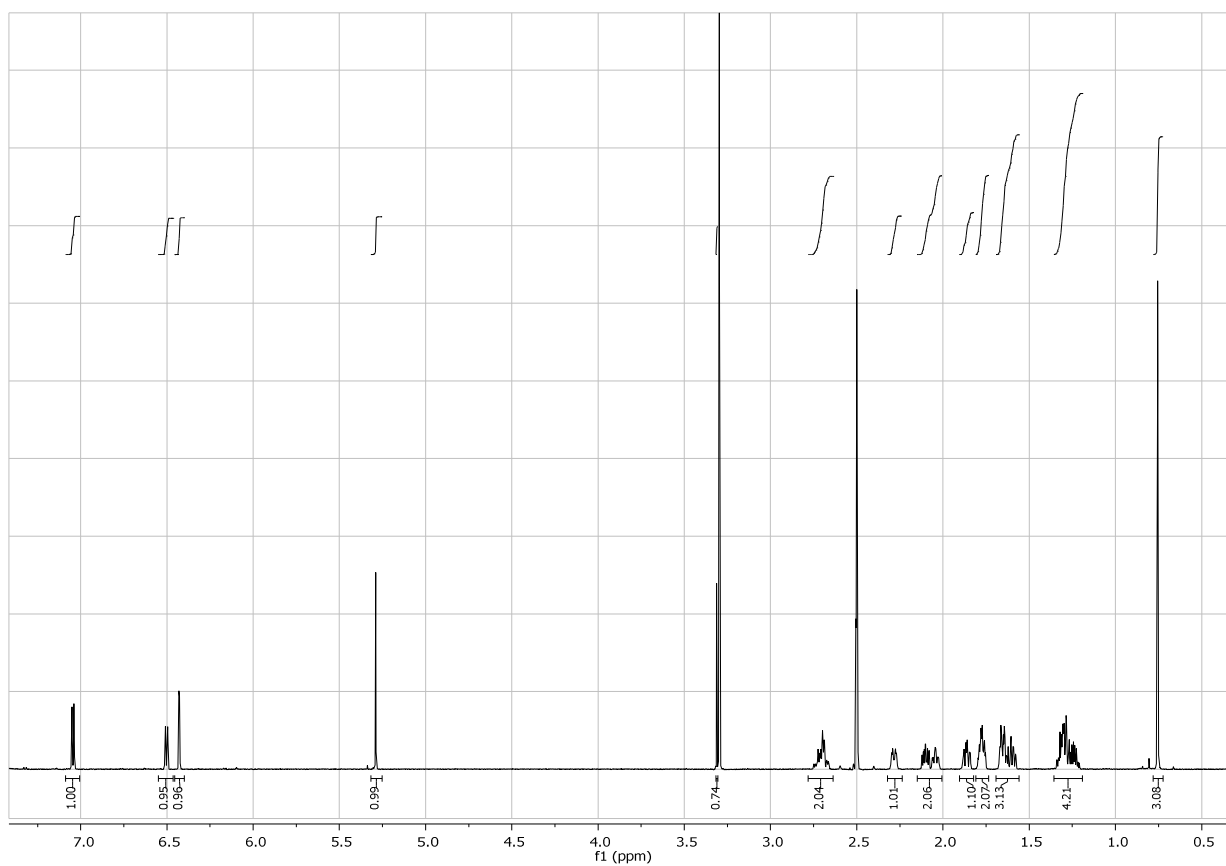


Figure S1.  $^1\text{H}$  NMR spectrum of **EE2** at 700 MHz in  $\text{DMSO-}d_6$ . Spectral width 7.0 kHz, 32 k data points, acquisition time 3.29 s, number of transients 8, relaxation delay 2 s and excitation pulse 90 degree.

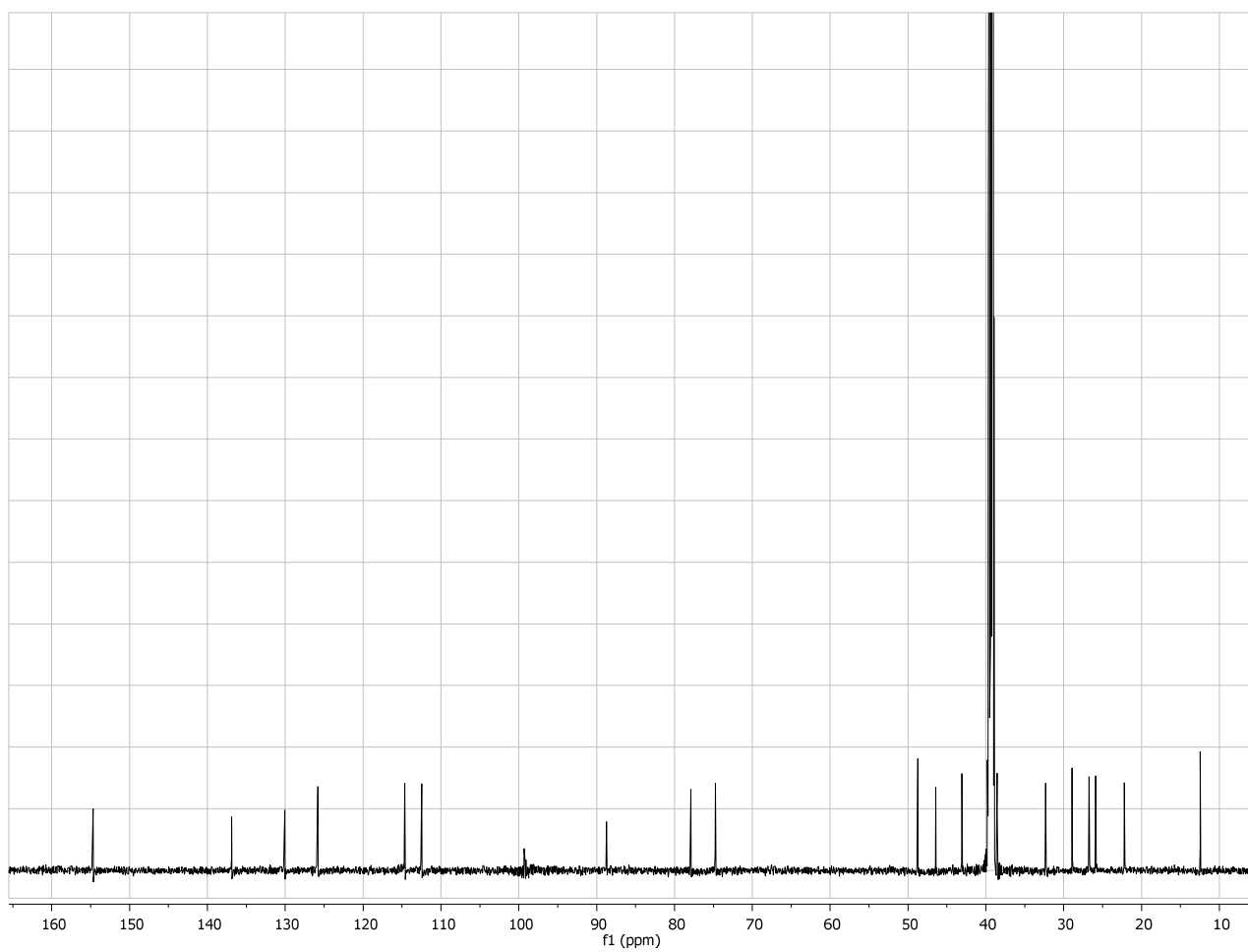


Figure S2.  $^{13}\text{C}$  NMR spectrum of **EE2** at 176 MHz in  $\text{DMSO-}d_6$ . Spectral width 34.7 kHz, 32 k data points, acquisition time 0.23 s, relaxation delay 1.5 s, excitation pulse 45 degree and number of transients 635.

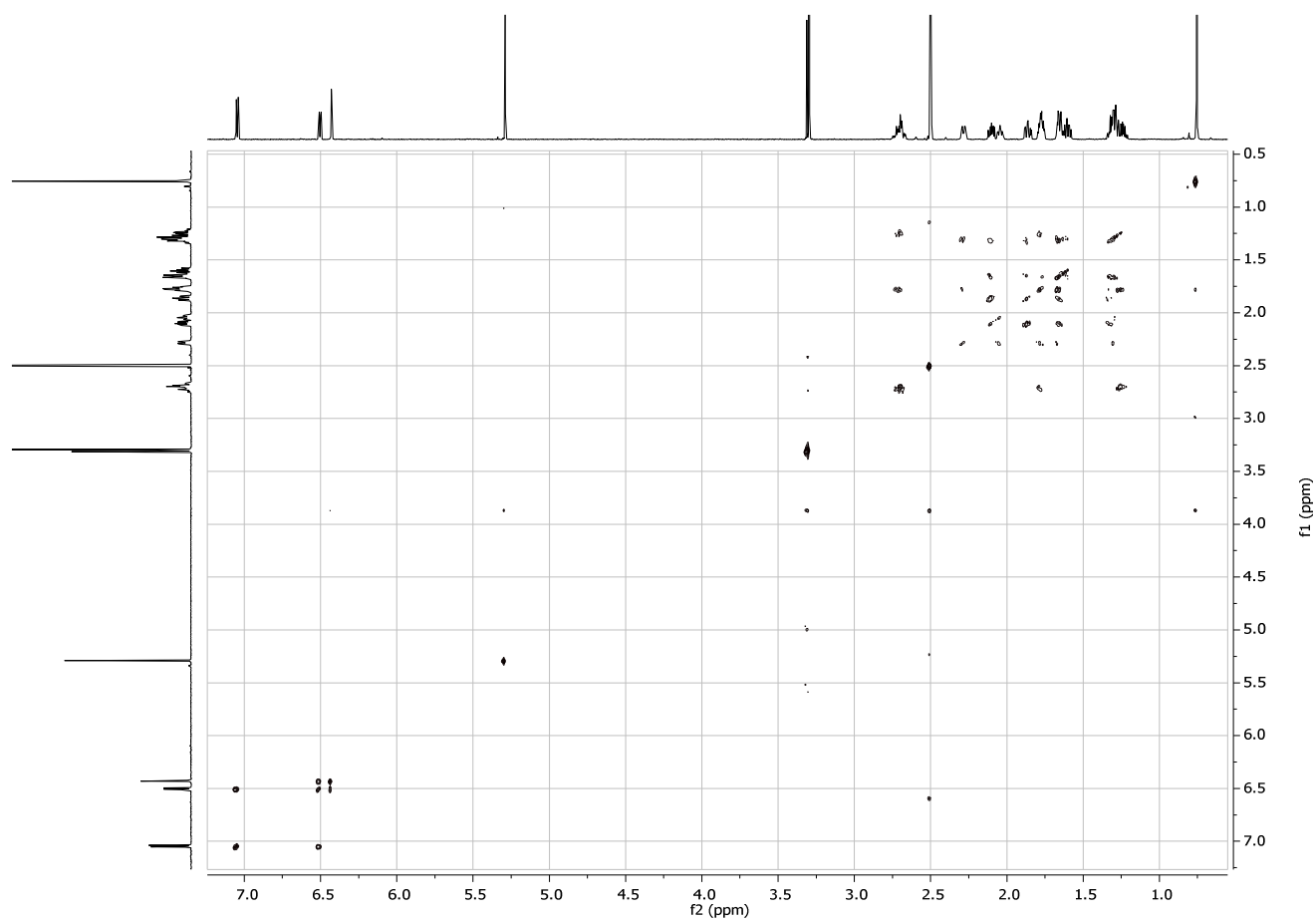


Figure S3. gCOSY45 H-H spectrum of **EE2** at 700 MHz in DMSO- $d_6$ . Spectral width 4.9 kHz in both dimensions, 512 ( $t_1$ ) x 4096 ( $t_2$ ) data points, relaxation delay 2 s and number of transients 4.

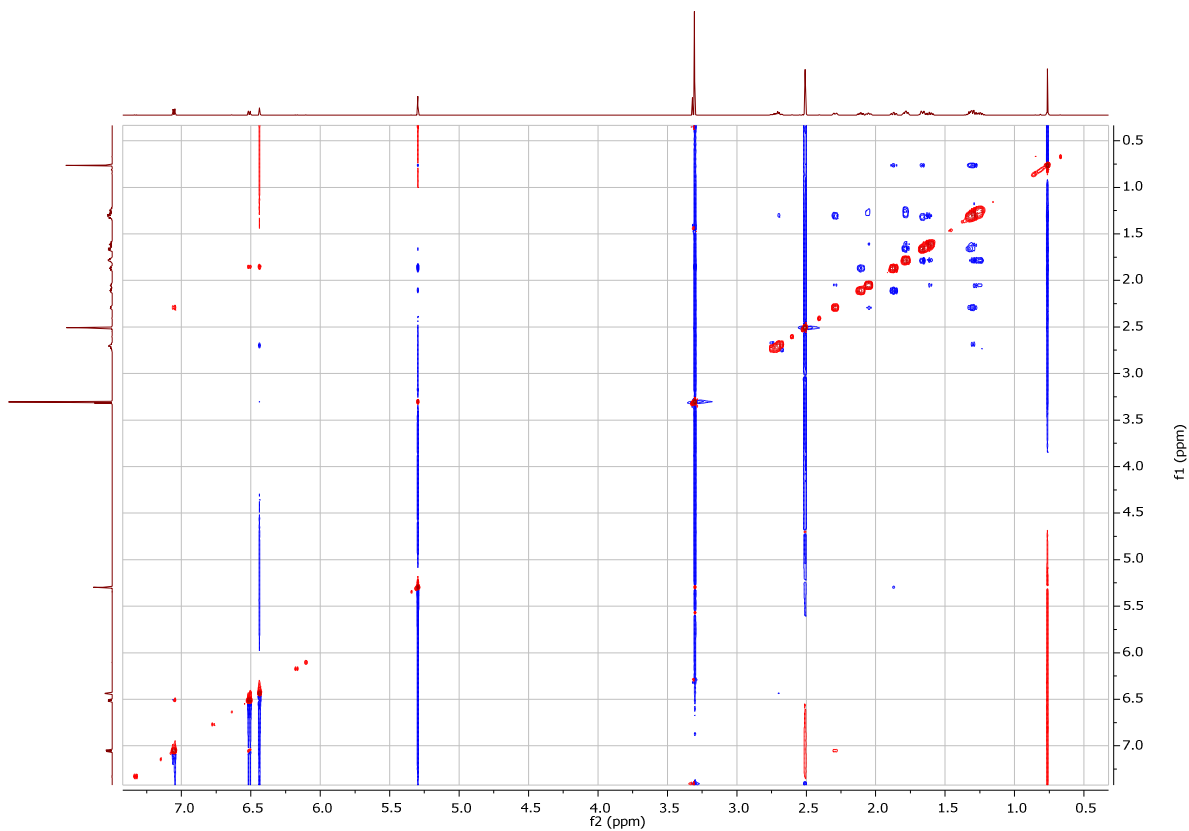


Figure S4. NOESY H-H NMR spectrum of **EE2** at 700 MHz in DMSO- $d_6$ . Spectral width 4.9 kHz in both dimensions, 512 ( $t_1$ ) x 4096 ( $t_2$ ) data points, relaxation delay 2 s, number of transients 8 and mixing time 0.7 s.

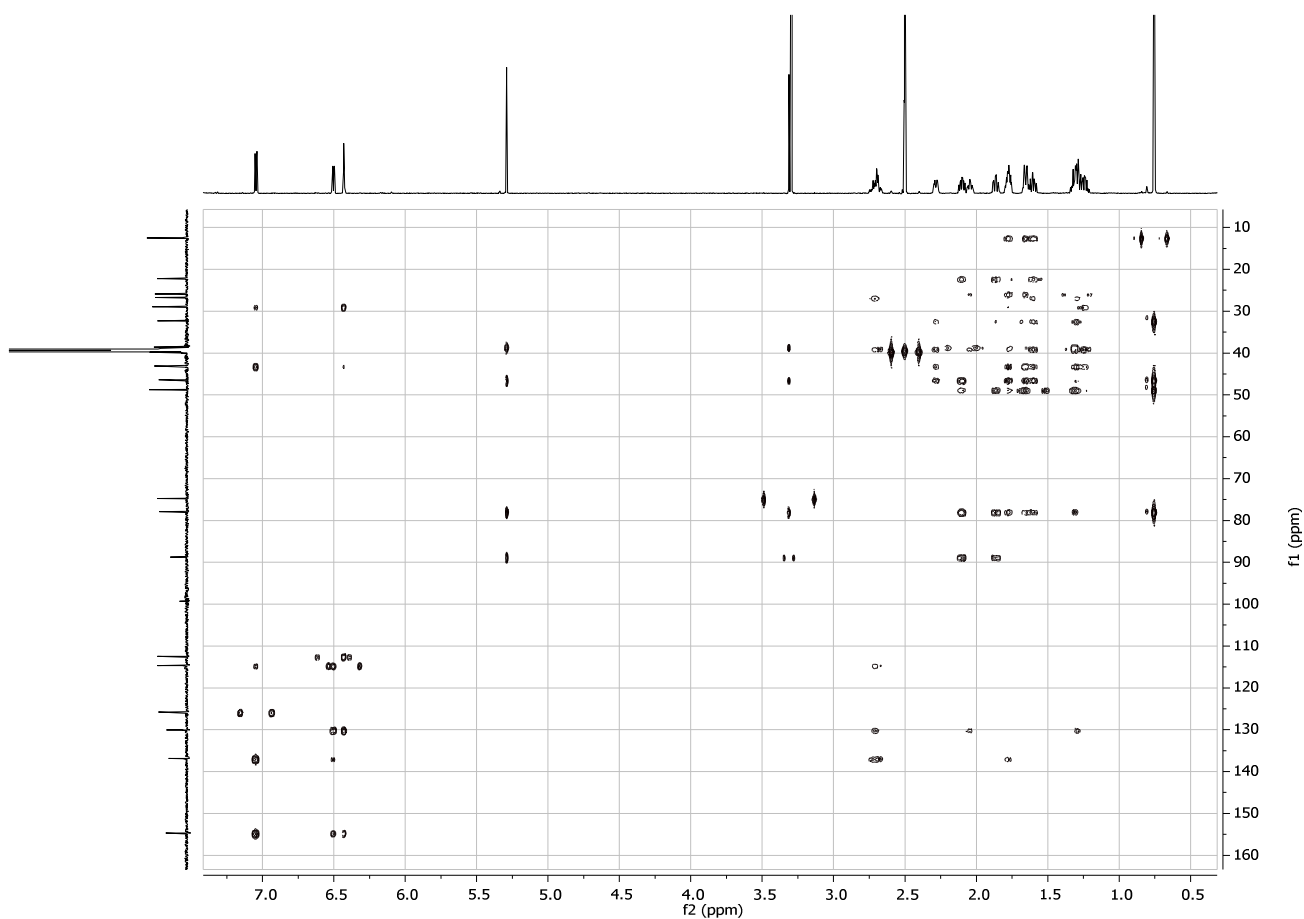


Figure S5. gHMBC NMR spectrum of **EE2** at 700 MHz in DMSO- $d_6$ . Pulse sequence hmbcetgpnrd, spectral width 4.9 kHz in F2 and 27.7 k Hz in F1, 512 ( $t_1$ ) x 8192 ( $t_2$ ) data points, relaxation delay 1.5 s and number of transients 16.

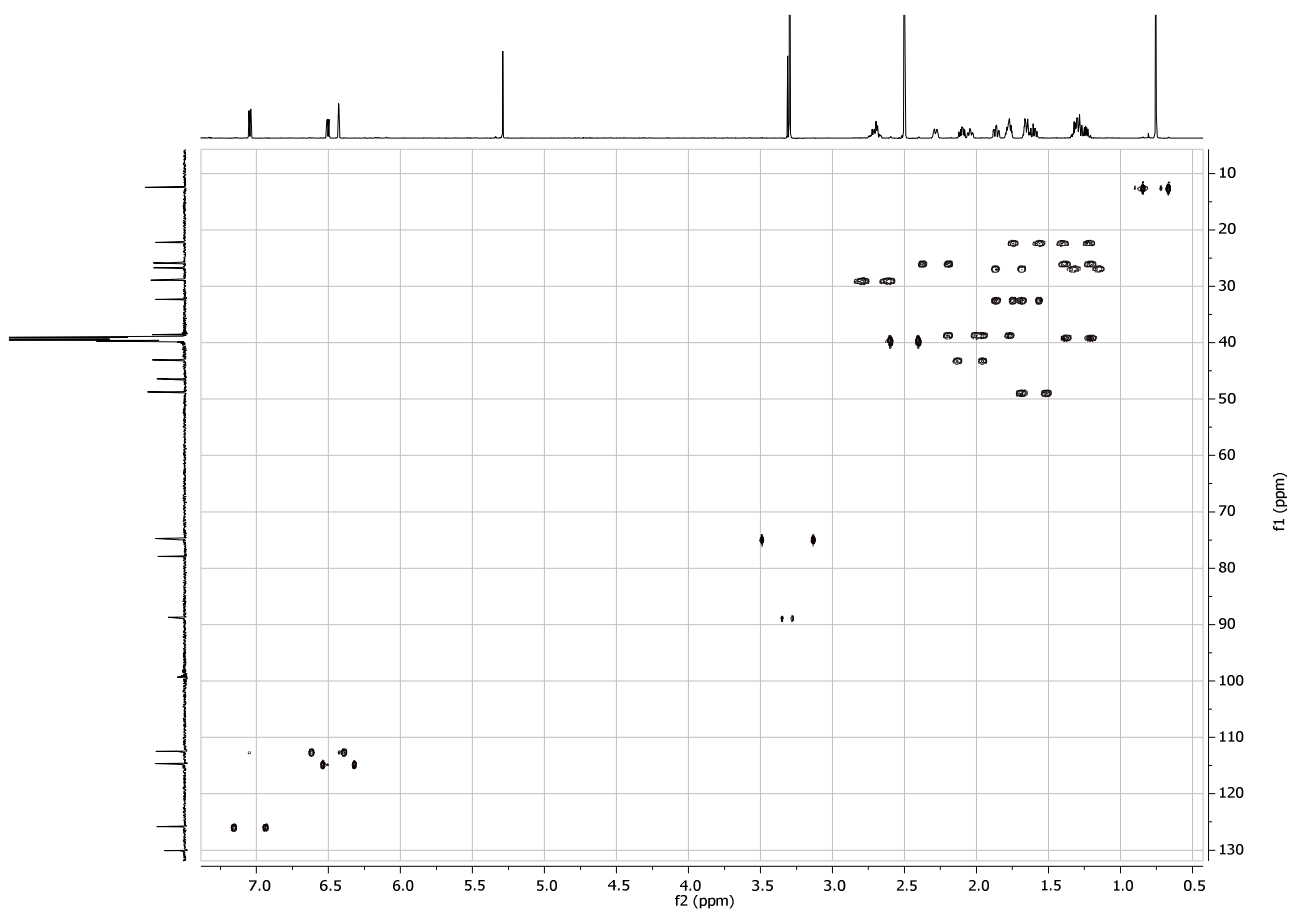


Figure S6. CLIP-HSQC coupled in F2 NMR spectrum of **EE2** at 700 MHz in DMSO-*d*<sub>6</sub>. Spectral width 4.9 kHz in F2 and 27.7 k Hz in F1, 512 (*t*<sub>1</sub>) x 8192 (*t*<sub>2</sub>) data points, relaxation delay 1.5 s and number of transients 16.



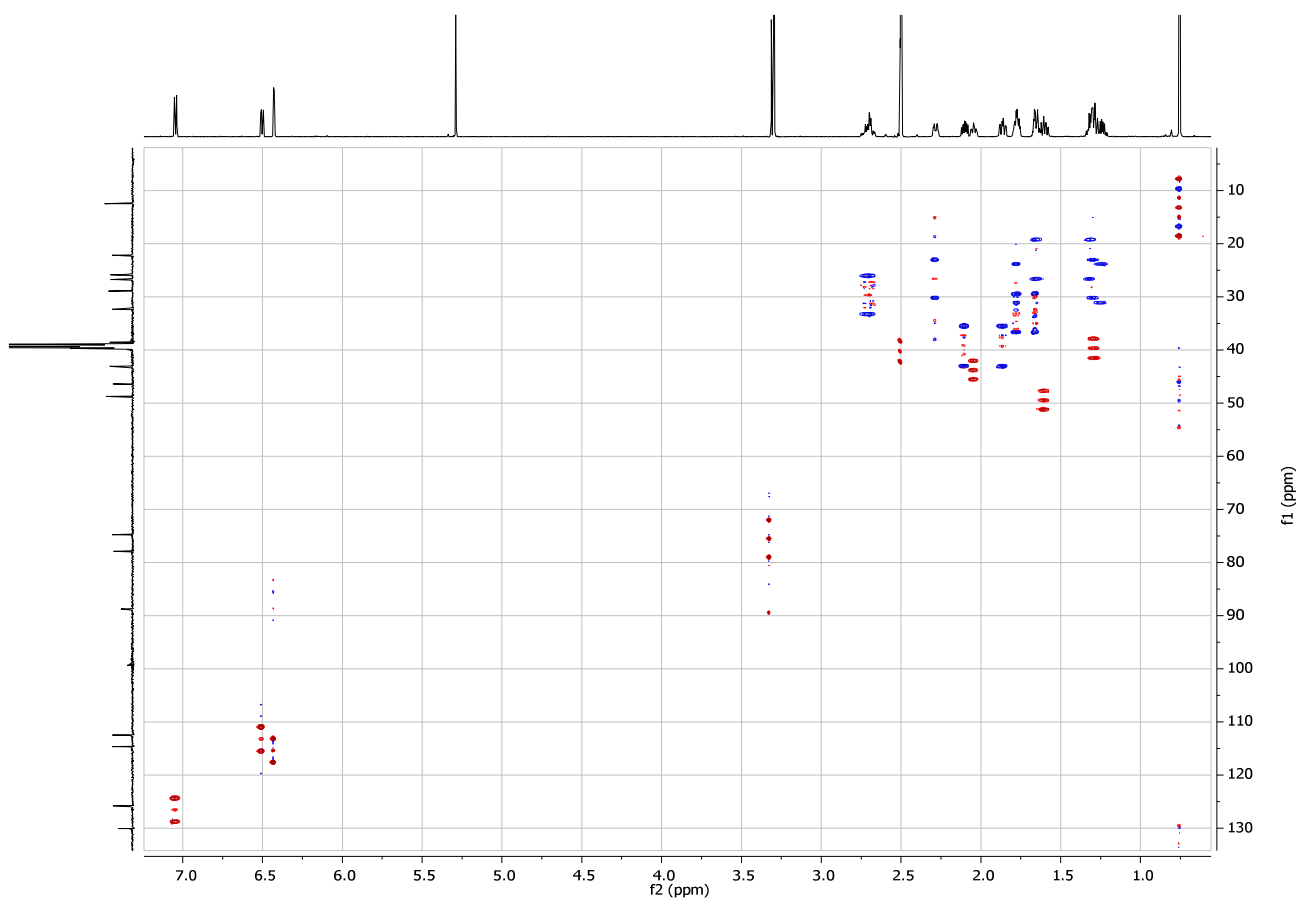


Figure S7. J-BIRD-HSQC coupled in F1 NMR spectrum of **EE2** at 700 MHz in DMSO- $d_6$ . Pulse sequence hsqcbietgpcsp.2, spectral width 5.2 kHz in F2 and 27.2 k Hz in F1, 1024 ( $t_1$ ) x 2048 ( $t_2$ ) data points, relaxation delay 1.5 s, number of transients 32 and  $J$  scale factor equal to 5.

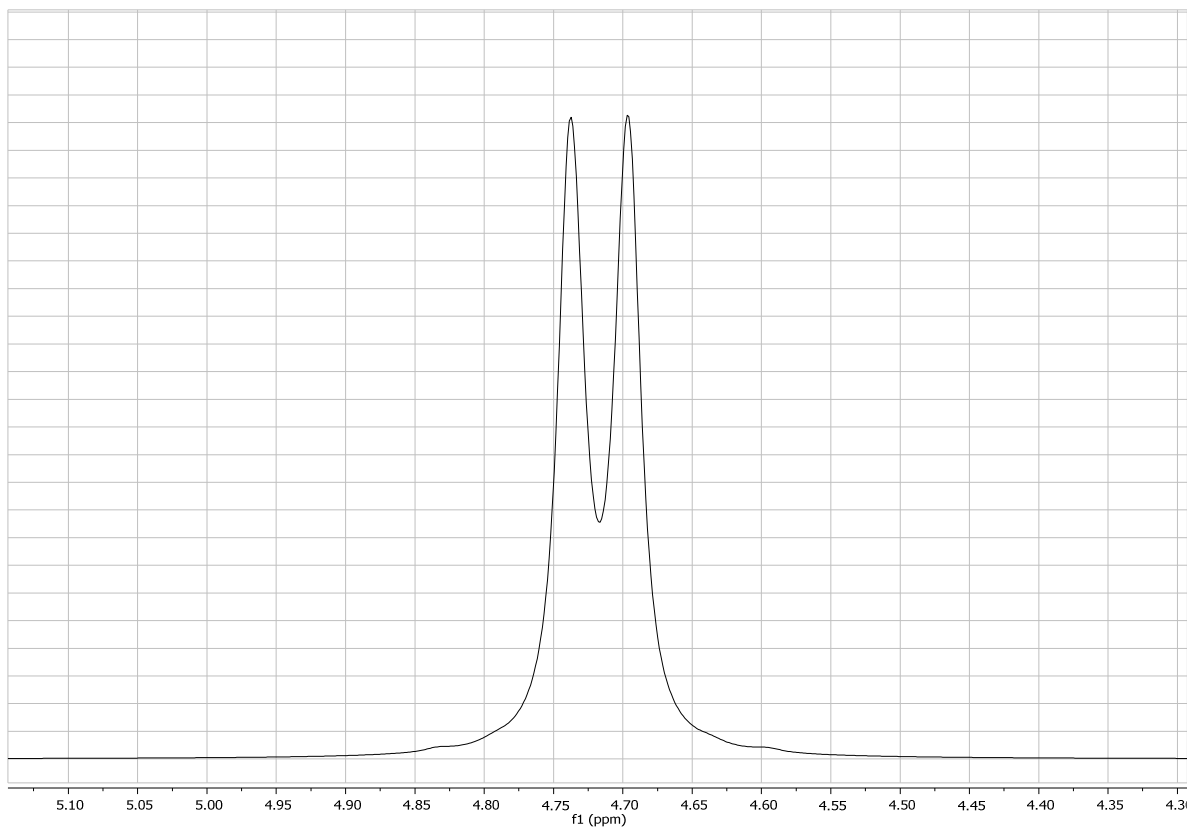


Figure S8.  $^2\text{H}$  NMR spectrum showing the quadrupole deuterium splitting of  $\text{DMSO-}d_6$  in GO-g-TFEMA alignment media at 107.5 MHz. Spectral width 2.1 kHz, 8 k data points, acquisition time 1.99 s and number of transients 16.

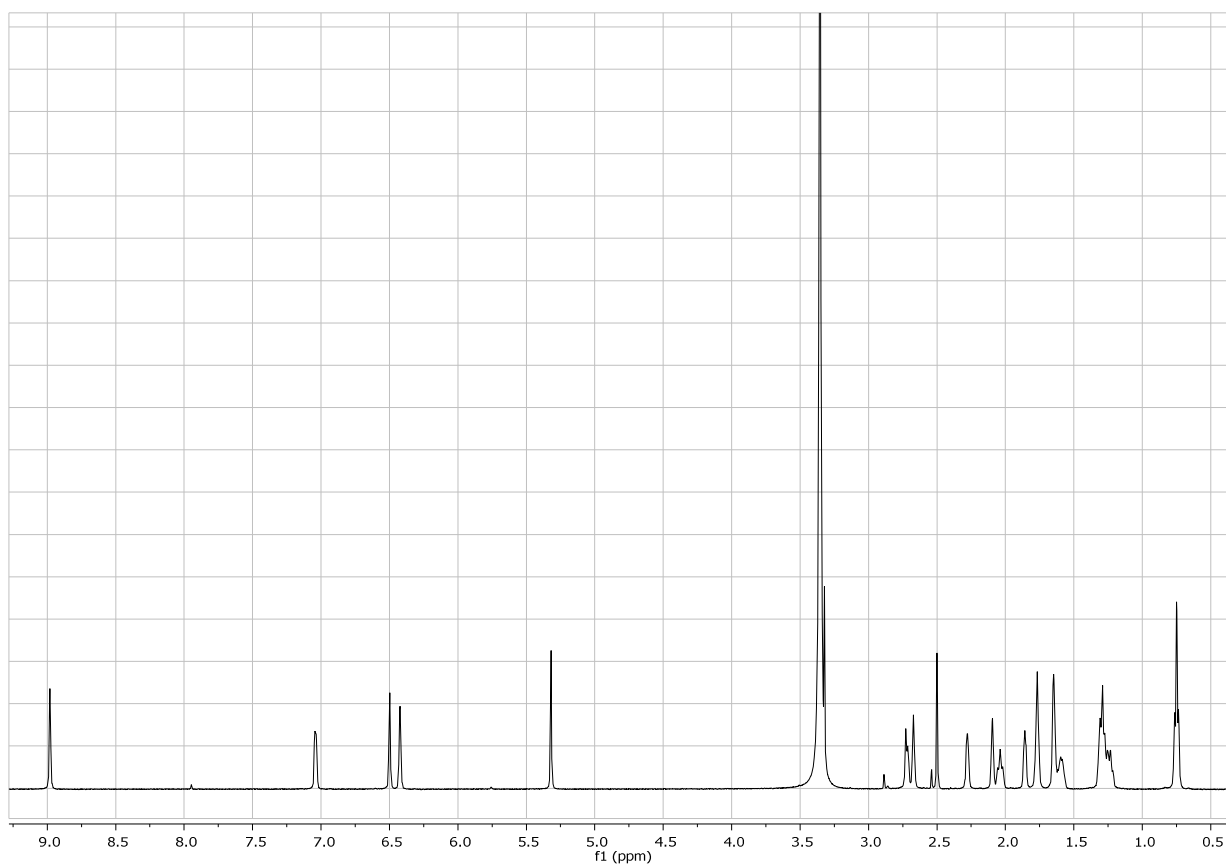


Figure S9.  $^1\text{H}$  NMR spectrum of **EE2** at 700 MHz in  $\text{DMSO-}d_6$  in GO-g-TFEMA. Spectral width 7.0 kHz, 32 k data points, acquisition time 3.29 s, number of transients 8, relaxation delay 2 s and excitation pulse 90 degree.

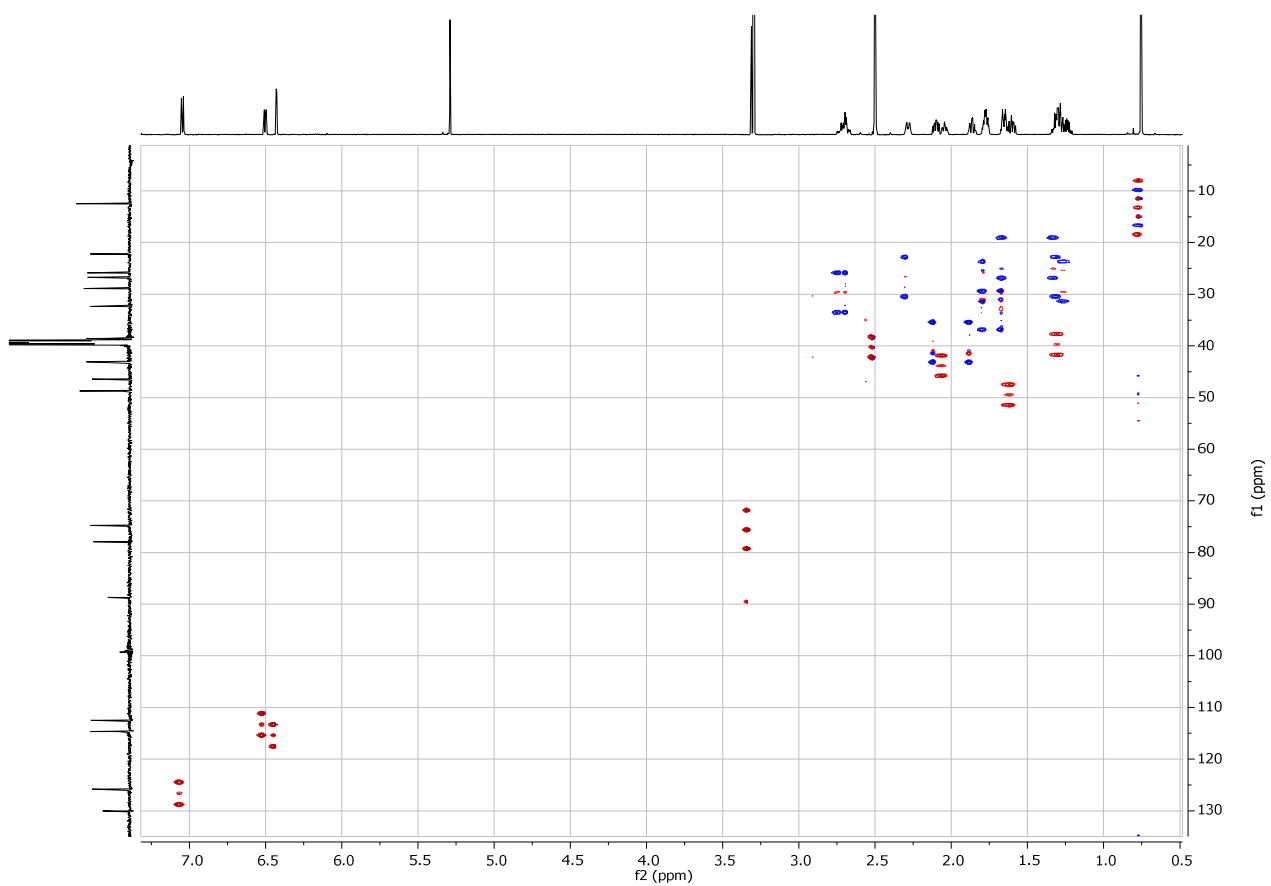


Figure S10. J-BIRD-HSQC coupled in F1 NMR spectrum of **EE2** in DMSO- $d_6$  in GO-g-TFEMA. Pulse sequence hsqcbietgpjpcsp.2, spectral width 5.2 kHz in F2 and 27.2 k Hz in F1, 1024 ( $t_1$ ) x 2048 ( $t_2$ ) data points, relaxation delay 1.5 s, number of transients 32 and  $J$  scale factor equal to 5.

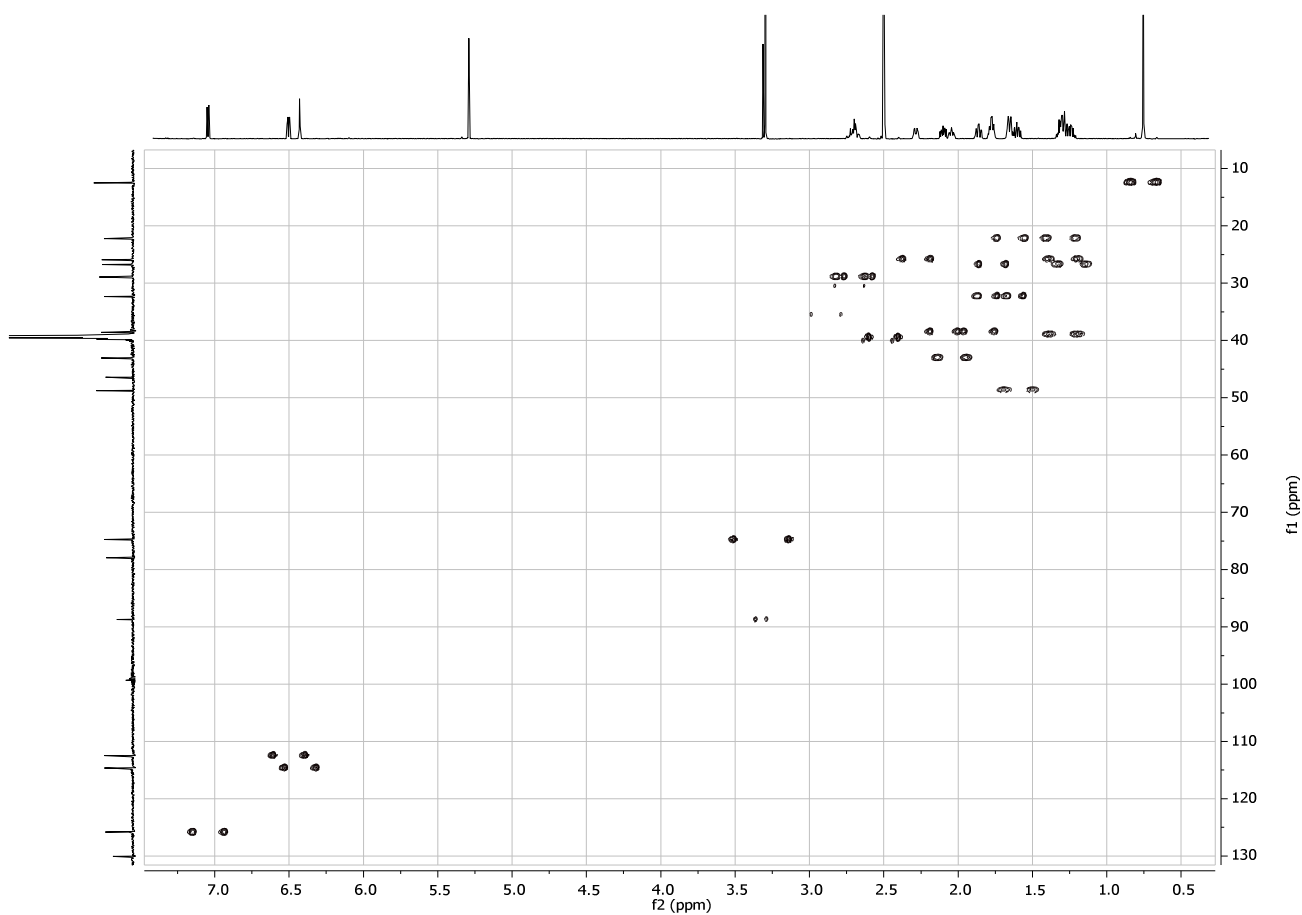


Figure S11. CLIP-HSQC coupled in F2 NMR spectrum of **EE2** in DMSO- $d_6$  in GO-g-TFEMA. Spectral width 4.9 kHz in F2 and 27.7 k Hz in F1, 512 ( $t_1$ ) x 8192 ( $t_2$ ) data points, relaxation delay 1.5 s and number of transients 16.

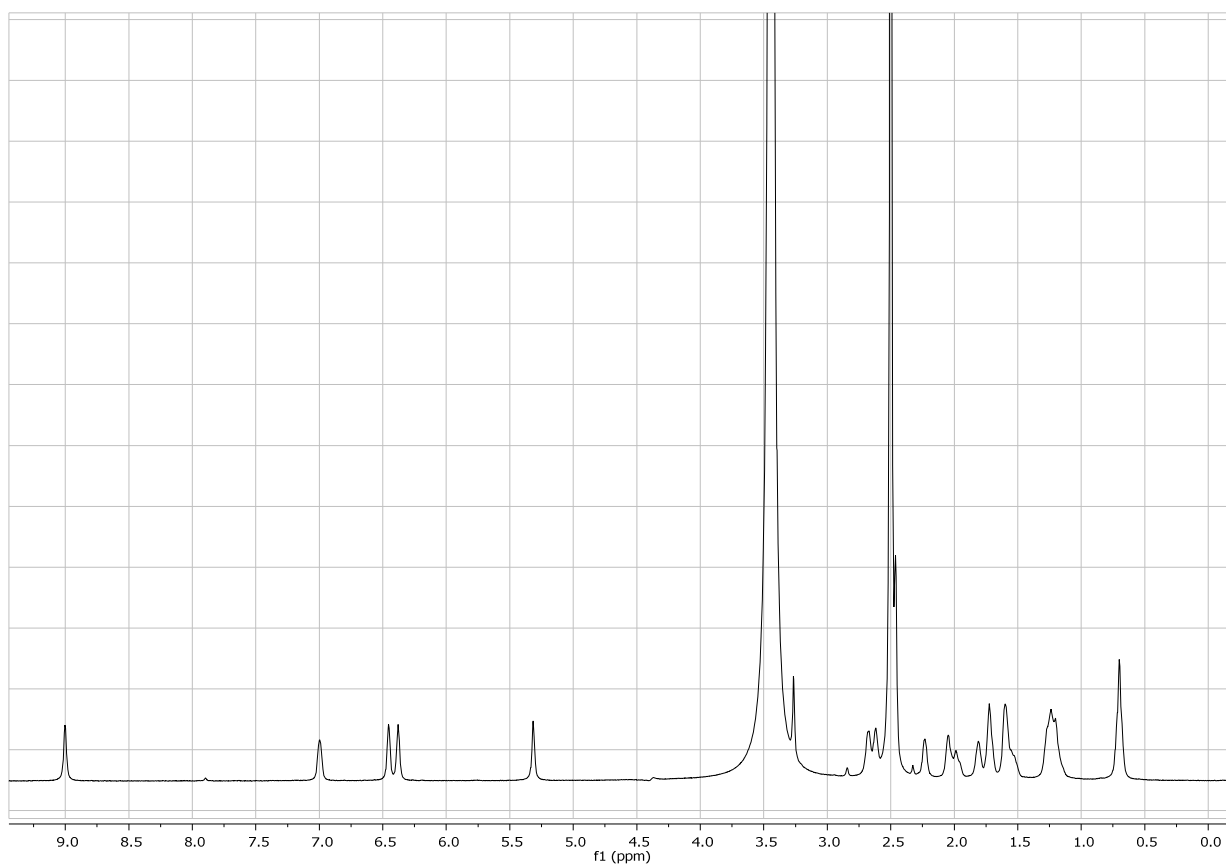


Figure S12. <sup>1</sup>H NMR spectrum of **EE2** at 400 MHz in DMSO-*d*<sub>6</sub> in GO-g-TFEMA. Spectral width 4.2 kHz, 32 k data points, acquisition time 3.9 s, number of transients 32, relaxation delay 2 s and excitation pulse 90 degree.

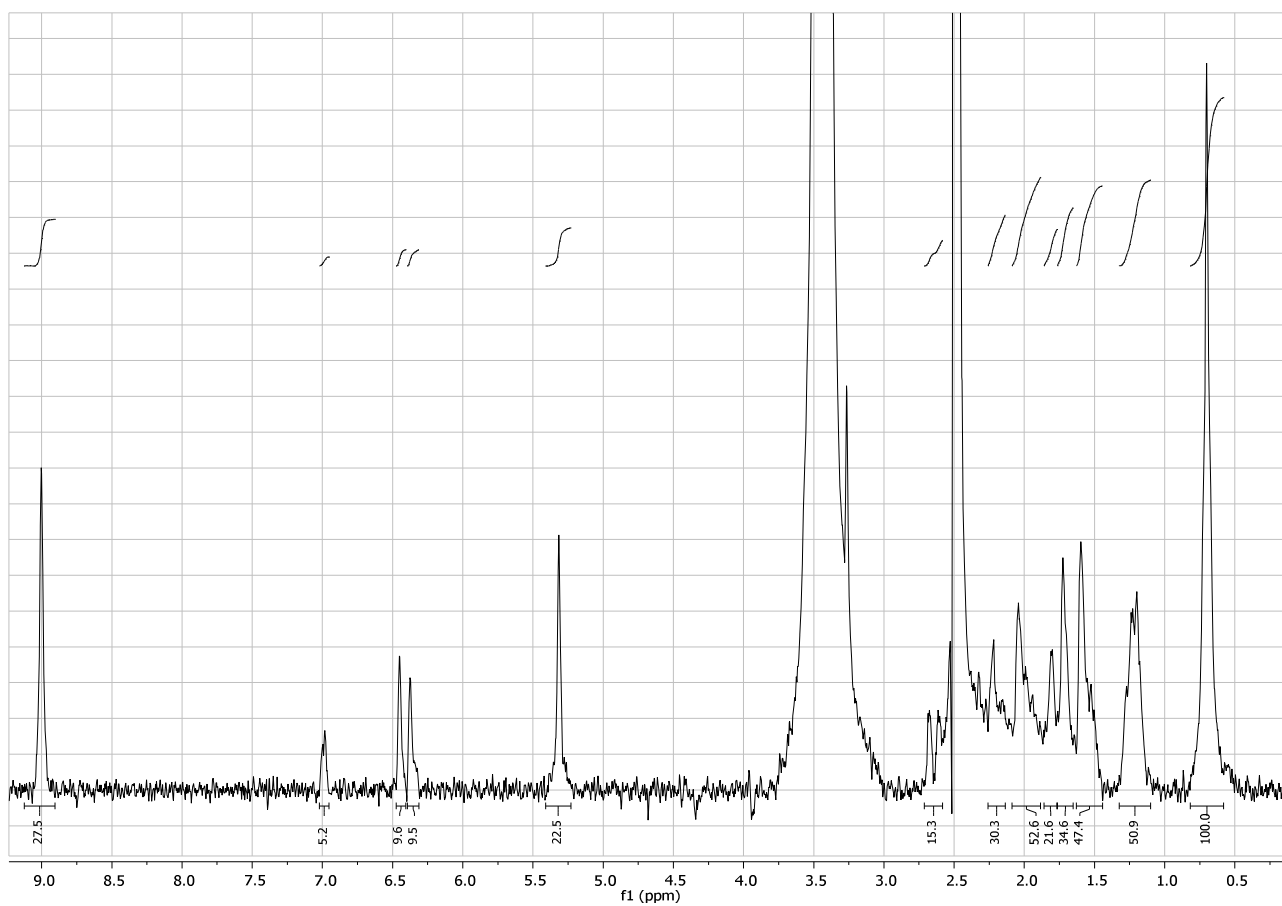


Figure S13. STD NMR spectrum of **EE2** at 400 MHz in DMSO- $d_6$  in GO-g-TFEMA. Spectral width 4.2 kHz, 32 k data points, acquisition time 3.9 s, number of transients 512, relaxation delay 2 s, saturation transfer 1.5 s, irradiation at -0.5 ppm and 35 ppm.

## DFT Structures

	E(SCF) <sup>a</sup> (a.u)	E(SCF)+ZPVE <sup>a</sup> (a.u)	$\Delta H_0^a$ (kcal/mol)	E(SCF) <sup>b</sup> (a.u)
<b>EE2-(a)</b>	-926.14084	-925.74341	0	-925.96192
<b>EE2-(b)</b>	-926.13815	-925.74051	1.8	-925.95916
<b>EE2-(c)</b>	-926.12147	-925.72403	12.2	---
<b>TS(1-2)</b>	-926.13703	-925.74000	2.1	---

a) PBE0/IEFPCM(DMSO)/6-311+G\*\* b) PBE0/pcj-2006-1//PBE0/IEFPCM(DMSO)/6-311+G\*\*

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EE2 a

C	-2.915197	-1.551374	0.192943
H	-2.430588	-2.517916	0.275951
C	-4.299120	-1.528456	0.079551
H	-4.864576	-2.456339	0.071879
C	-4.952939	-0.304278	-0.020496
C	-4.210586	0.868728	-0.003340
H	-4.731276	1.819586	-0.077170
C	-2.820307	0.844011	0.108554
C	-2.080958	2.160359	0.096656
H	-2.095109	2.552214	-0.929612
H	-2.629703	2.889281	0.702254
C	-0.637984	2.048166	0.562255
H	-0.106431	2.977245	0.333110
H	-0.596728	1.918746	1.652381
C	0.036334	0.858300	-0.106751
H	-0.121673	0.954584	-1.191857
C	-0.634051	-0.440531	0.375237
H	-0.432593	-0.493811	1.459151
C	-2.144911	-0.385044	0.206515
C	0.019040	-1.680969	-0.250304
H	-0.230580	-1.721425	-1.317654
H	-0.398932	-2.589856	0.192046
C	1.537989	-1.714900	-0.047217
H	1.960630	-2.583577	-0.564941
H	1.749143	-1.844971	1.020909
C	2.195060	-0.424973	-0.530439
C	1.527480	0.769727	0.172126
H	1.630452	0.580723	1.252504
C	2.432036	1.960672	-0.162335



H	2.128535	2.427997	-1.104881
H	2.389004	2.735275	0.606487
C	3.843410	1.345637	-0.288650
H	4.270538	1.515041	-1.280218
H	4.547364	1.749220	0.441914
C	3.674706	-0.192150	-0.108411
C	2.116849	-0.338107	-2.059780
H	2.662221	-1.171952	-2.506813
H	1.082773	-0.391962	-2.403237
H	2.545772	0.586945	-2.451385
C	3.912484	-0.559911	1.294481
C	4.169187	-0.853973	2.434563
H	4.386982	-1.115303	3.445116
O	4.547577	-0.951170	-0.936793
H	5.446323	-0.826178	-0.617586
O	-6.306711	-0.199114	-0.132719
H	-6.699607	-1.076893	-0.123224

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TS 1-2

C	-2.860058	-1.526961	0.259997
H	-2.365001	-2.486508	0.359887
C	-4.222440	-1.519867	-0.022000
H	-4.764059	-2.455292	-0.133328
C	-4.881716	-0.305038	-0.173269
C	-4.174273	0.883522	-0.029303
H	-4.700273	1.826539	-0.149326
C	-2.814062	0.873018	0.269732
C	-2.095645	2.175197	0.499389
H	-2.595731	2.961967	-0.072493
H	-2.241635	2.444790	1.552935
C	-0.582969	2.161087	0.196419
H	-0.357314	2.886803	-0.590406
H	-0.040288	2.499887	1.086847
C	-0.019470	0.797203	-0.205085
H	-0.292369	0.593797	-1.250444
C	-0.640303	-0.315899	0.667546
H	-0.474162	-0.011764	1.715343
C	-2.132543	-0.346643	0.410573
C	0.039034	-1.675881	0.474814
H	-0.252907	-2.090491	-0.497143
H	-0.334838	-2.379025	1.226883
C	1.565626	-1.618885	0.573271
H	1.984258	-2.610628	0.367207
H	1.853923	-1.355395	1.597652
C	2.134946	-0.577774	-0.386320
C	1.494844	0.781111	-0.065149
H	1.703489	0.962553	1.001600
C	2.325225	1.792656	-0.861722
H	1.926508	1.907560	-1.874914
H	2.317319	2.783119	-0.401068
C	3.741223	1.177682	-0.900397
H	4.083130	1.013293	-1.925266

H	4.487401	1.802487	-0.405474
C	3.638567	-0.215877	-0.211829
C	1.913728	-1.011828	-1.840568
H	2.331145	-0.300883	-2.557144
H	2.389036	-1.978847	-2.019971
H	0.850104	-1.112956	-2.062377
C	4.018829	-0.102769	1.203194
C	4.392039	-0.006282	2.344923
H	4.712817	0.078529	3.358245
O	4.453424	-1.205493	-0.829058
H	5.373748	-0.980565	-0.662686
O	-6.210642	-0.219682	-0.464291
H	-6.580049	-1.104206	-0.543059

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EE2 b

C	-2.876508	-1.533277	0.126571
H	-2.390527	-2.503260	0.123525
C	-4.250259	-1.478931	-0.102298
H	-4.812308	-2.392295	-0.278169
C	-4.897896	-0.248691	-0.110079
C	-4.172455	0.919438	0.115947
H	-4.690211	1.874270	0.107749
C	-2.804601	0.858218	0.350922
C	-1.977072	2.075784	0.630472
H	-2.556800	2.988019	0.466253
H	-1.710748	2.066780	1.696167
C	-0.682729	2.102652	-0.197798
H	-0.892123	2.538961	-1.179169
H	0.023474	2.780021	0.294279
C	-0.032008	0.713895	-0.385195
H	-0.244624	0.372421	-1.406598
C	-0.643619	-0.336229	0.577443
H	-0.467764	0.043910	1.598603
C	-2.136149	-0.377644	0.355353
C	0.051414	-1.694073	0.480830
H	-0.189314	-2.162970	-0.480610
H	-0.348190	-2.362410	1.251643
C	1.570385	-1.595376	0.645981
H	2.022988	-2.586344	0.526608
H	1.800023	-1.258291	1.663804
C	2.164628	-0.605538	-0.352976
C	1.474921	0.757955	-0.178911
H	1.628986	1.041281	0.874933
C	2.320659	1.714855	-1.025561
H	1.983157	1.710903	-2.066965
H	2.254776	2.746280	-0.672063
C	3.754173	1.150817	-0.915560
H	4.174485	0.917446	-1.896957
H	4.442129	1.840944	-0.423110
C	3.645803	-0.185828	-0.121591
C	2.044939	-1.155933	-1.779870
H	2.474922	-0.483615	-2.525393

H	2.568388	-2.111463	-1.855240
H	1.001629	-1.321754	-2.052564
C	3.936002	0.052050	1.299227
C	4.235051	0.252153	2.449303
H	4.490338	0.428339	3.469451
O	4.522674	-1.195887	-0.606775
H	5.425095	-0.926283	-0.411289
O	-6.236983	-0.124607	-0.333571
H	-6.621380	-0.994726	-0.475391

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EE2 c

C	2.757457	-1.580885	-0.188279
H	2.243906	-2.529561	-0.298470
C	4.110182	-1.611304	0.131401
H	4.619714	-2.560888	0.269847
C	4.803201	-0.413949	0.269238
C	4.132826	0.789060	0.085197
H	4.685744	1.717981	0.196881
C	2.776091	0.820519	-0.233141
C	2.121703	2.180308	-0.380625
H	2.202473	2.686680	0.590003
H	2.709633	2.787332	-1.077620
C	0.650487	2.154867	-0.800658
H	0.170724	3.090269	-0.494478
H	0.558881	2.092974	-1.892488
C	-0.029085	0.952390	-0.168897
H	0.214314	0.978532	0.903218
C	0.599839	-0.321315	-0.774187
H	0.600084	-0.147004	-1.861207
C	2.061939	-0.386077	-0.372063
C	-0.284571	-1.575553	-0.564826
H	0.322116	-2.480145	-0.478585
H	-0.881624	-1.718411	-1.470246
C	-1.237883	-1.510609	0.631929
H	-0.654300	-1.591091	1.555710
H	-1.896886	-2.385954	0.617785
C	-2.065649	-0.209269	0.701309
C	-1.532446	0.820315	-0.314296
H	-1.711579	0.391123	-1.312023
C	-2.512182	1.982825	-0.196888
H	-2.284242	2.618182	0.664156
H	-2.505237	2.622754	-1.082468
C	-3.869578	1.260589	-0.011614
H	-4.423182	1.642965	0.849385
H	-4.514218	1.368058	-0.886351
C	-3.554036	-0.249359	0.257995
C	-2.031910	0.306383	2.147795
H	-2.394183	-0.475509	2.819089
H	-1.008351	0.549912	2.444370
H	-2.651838	1.190356	2.310153
C	-3.736548	-1.045280	-0.962816
C	-3.936882	-1.709163	-1.948338

H	-4.104718	-2.294556	-2.823558
O	-4.359835	-0.808192	1.289528
H	-5.260578	-0.878764	0.959518
O	6.129092	-0.360435	0.580848
H	6.471567	-1.253160	0.684940

### Computed $^1J_{CH}$ couplings for the C6-H6 $\beta$ and C6H6 $\alpha$ couplings.

Coupling	J (Hz) <sup>a</sup>	FC (Hz) <sup>a</sup>	SD (Hz) <sup>b</sup>	DSO (Hz) <sup>c</sup>	PSO(Hz) <sup>d</sup>
$^1J_{C6H6\beta}$	122.99	121.13	0.07	1.06	0.73
$^1J_{C6H6\alpha}$	127.47	125.67	0.10	1.02	0.69

a) Fermi Contact term b) Spin-dipole term c) diamagnetic spin orbit term d) paramagnetic spin orbit term

### MSpin RDC fitting

Superimposed geometries

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EE2 a

C	-2.769640	-1.622092	0.336137
H	-2.285032	-2.588634	0.419145
C	-4.153563	-1.599174	0.222745
H	-4.719019	-2.527057	0.215073
C	-4.807383	-0.374996	0.122698
C	-4.065030	0.798010	0.139854
H	-4.585720	1.748868	0.066024
C	-2.674751	0.773293	0.251748
C	-1.935401	2.089641	0.239850
H	-1.949553	2.481496	-0.786418
H	-2.484147	2.818563	0.845448
C	-0.492428	1.977448	0.705449
H	0.039125	2.906527	0.476304
H	-0.451172	1.848028	1.795575
C	0.181890	0.787582	0.036443
H	0.023883	0.883866	-1.048663
C	-0.488495	-0.511249	0.518431
H	-0.287037	-0.564529	1.602345
C	-1.999355	-0.455762	0.349709

C	0.164596	-1.751687	-0.107110
H	-0.085024	-1.792143	-1.174460
H	-0.253376	-2.660574	0.335240
C	1.683545	-1.785618	0.095977
H	2.106186	-2.654295	-0.421747
H	1.894699	-1.915689	1.164103
C	2.340616	-0.495691	-0.387245
C	1.673036	0.699009	0.315320
H	1.776008	0.510005	1.395698
C	2.577592	1.889954	-0.019141
H	2.274091	2.357279	-0.961687
H	2.534560	2.664557	0.749681
C	3.988966	1.274919	-0.145456
H	4.416094	1.444323	-1.137024
H	4.692921	1.678502	0.585108
C	3.820262	-0.262868	0.034783
C	2.262405	-0.408825	-1.916586
H	2.807777	-1.242670	-2.363619
H	1.228329	-0.462680	-2.260043
H	2.691329	0.516227	-2.308191
C	4.058041	-0.630629	1.437675
C	4.314744	-0.924691	2.577757
H	4.532538	-1.186021	3.588310
O	4.693133	-1.021888	-0.793599
H	5.591879	-0.896896	-0.474392
O	-6.161155	-0.269832	0.010475
H	-6.554050	-1.147611	0.019970

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EE2 b

C	-2.711250	-1.563373	-0.129467
H	-2.216081	-2.505405	-0.340271
C	-4.082219	-1.468140	-0.361627
H	-4.633126	-2.323133	-0.744447
C	-4.741348	-0.270961	-0.106095
C	-4.030171	0.822314	0.384678
H	-4.556815	1.751871	0.580669
C	-2.665116	0.718985	0.621175
C	-1.853062	1.849212	1.176671
H	-2.439145	2.771499	1.210145
H	-1.601164	1.605435	2.217745
C	-0.547902	2.067429	0.394996
H	-0.748082	2.709463	-0.468150
H	0.145086	2.623005	1.035929
C	0.118466	0.759057	-0.085959
H	-0.077004	0.651615	-1.160818
C	-0.496162	-0.482420	0.610078
H	-0.337811	-0.337454	1.692718
C	-1.985076	-0.482802	0.361449
C	0.212986	-1.780535	0.225174
H	-0.010196	-2.025709	-0.819939

H	-0.190685	-2.605843	0.822189
C	1.728568	-1.711493	0.431412
H	2.192142	-2.648361	0.102026
H	1.941148	-1.607429	1.502068
C	2.326895	-0.520838	-0.313682
C	1.621968	0.765618	0.148069
H	1.759006	0.808796	1.240751
C	2.470000	1.891906	-0.451984
H	2.146727	2.117212	-1.473345
H	2.389527	2.818642	0.120574
C	3.907180	1.326488	-0.447925
H	4.342981	1.319516	-1.450069
H	4.581798	1.894306	0.195922
C	3.800737	-0.153750	0.027801
C	2.231832	-0.741352	-1.828813
H	2.665495	0.082411	-2.399823
H	2.765308	-1.652997	-2.106345
H	1.193944	-0.848988	-2.147495
C	4.069339	-0.235529	1.470261
C	4.350826	-0.293960	2.640517
H	4.590547	-0.347130	3.678120
O	4.693672	-1.025345	-0.655950
H	5.590754	-0.800254	-0.391669
O	-6.078393	-0.108710	-0.317002
H	-6.452547	-0.927991	-0.654299

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EE2 c

C	-2.649246	-1.644503	0.429678
H	-2.149587	-2.581400	0.649743
C	-3.999383	-1.693363	0.101456
H	-4.520489	-2.646016	0.064014
C	-4.674874	-0.510178	-0.175526
C	-3.989914	0.697368	-0.119244
H	-4.529190	1.614959	-0.339005
C	-2.635743	0.747063	0.207571
C	-1.964322	2.106544	0.209961
H	-2.029649	2.502912	-0.811646
H	-2.550109	2.794538	0.829203
C	-0.497353	2.109565	0.645328
H	-0.002277	2.999097	0.242181
H	-0.416241	2.168219	1.738166
C	0.171421	0.835955	0.157937
H	-0.062123	0.745858	-0.912903
C	-0.480022	-0.354667	0.894339
H	-0.487507	-0.060677	1.955240
C	-1.939257	-0.445449	0.486874
C	0.389130	-1.635341	0.834567
H	-0.228970	-2.536271	0.843013
H	0.976173	-1.684163	1.756339
C	1.353768	-1.715664	-0.352137
H	0.777331	-1.890990	-1.267232

H	2.000702	-2.592176	-0.234162
C	2.199668	-0.440523	-0.556991
C	1.671512	0.702096	0.332545
H	1.835994	0.384207	1.373528
C	2.667905	1.832045	0.096932
H	2.456207	2.370601	-0.831601
H	2.661808	2.566437	0.905907
C	4.016975	1.076809	0.006921
H	4.583292	1.354220	-0.885456
H	4.655261	1.272742	0.870910
C	3.683401	-0.449688	-0.096685
C	2.185695	-0.088388	-2.052037
H	2.543258	-0.944482	-2.628652
H	1.168189	0.133440	-2.384315
H	2.818951	0.764267	-2.305109
C	3.844324	-1.107264	1.206725
C	4.026934	-1.659993	2.261842
H	4.179087	-2.146573	3.198300
O	4.490636	-1.129679	-1.051489
H	5.387391	-1.174388	-0.706441
O	-5.997114	-0.475070	-0.504767
H	-6.350718	-1.369488	-0.512661

### F1-coupled RDC file. MSpin input file

```

rdc_data {
#C1-H1
1 2 -6.2
#C2-H2
3 4 -7.9
#C4-H4
6 7 -6.3
#C6-H6 alfa
9 10 8.3
#C6-H6 beta
9 11 8.3
#C7-H7 alfa
12 13 6.3
#C7-H7 beta
12 14 6.3
#C8-H8
15 16 14.5
#C9-H9
17 18 14.8
#C11-H11 alfa
20 21 8.1
#C11-H11 beta
20 22 8.1
#C12-H12 alfa

```

```

23 24 4.6
#C12-H12 beta
23 25 4.6
#C14-H14
27 28 14.8
#C15 H15 alfa
29 30 5.8
#C15-H15 beta
29 31 5.8
#C16-H16 alfa
32 33 5.1
#C16-H16 beta
32 34 5.1
#CH3
36 37 -4.2
36 38 -4.2
36 39 -4.2
#C19-H20
40 42 1.8
#C20-H20
41 42 11.9
}

superimpose {
true
}

superimpose_atoms {
1,3,5,6,8,9,12,15,17,19,20,23,26,27,29,32,35,36,43
}

average_methylene_groups {
true
}

single_tensor {
true
}

optimize_populations {
true
}

scale_rdc {
false
}

```

## Output

```

!* MagNes-RDC Plugin *!
*****
SpinBatch-RDC job started at qua mai 4 18:59:41 2016
*****

```



```

!* File info *!
Directory:
/Users/armando/research/adonias/dynamics/magnes_results/estradiol_pbe6311+
Conformer #1 : 4_JF_A_pbe06311+.out
Conformer #2 : 4_JF_B1_pbe06311+.out
Input file: RDC_Estradiol_G0pol_F1.txt
*****
!* Computation flags *!
Method: SVD
Scale RDCs: False
Scale SVD with errors: False
CSA weight: 1
Scale QCSA with axial component: False
Single Tensor: True
Optimize populations: True
Grid search points: 16
Average methyl groups: True
Average methylene groups: True
Average phenyl groups: False
Bootstrapping: False
RDC Std. Error [ppm]: 1
CSA Std. Error [ppm]: 0.01
PCS Std. Error [ppm]: 0.01
DQ Std. Error [Hz]: 1
*****
!* Permutations *!
There are no permutations on the original data set
*****
Data set: #1
Computed data for frame #1
RDC Data:

```

I	J	Exp. [Hz]	Comp. [Hz]
C1	H2	-6.20	-6.74
C3	H4	-7.90	-7.13
C6	H7	-6.30	-7.01
C9	H10	8.30	9.98
C9	H11	8.30	9.98
C12	H13	6.30	7.21
C12	H14	6.30	7.21
C15	H16	14.50	14.33
C17	H18	14.80	13.02
C20	H21	8.10	7.05
C20	H22	8.10	7.05
C23	H24	4.60	6.97
C23	H25	4.60	6.97
C27	H28	14.80	15.56
C29	H30	5.80	6.48
C29	H31	5.80	6.48
C32	H33	5.10	6.18
C32	H34	5.10	6.18
C36	H37	-4.20	-5.16
C36	H38	-4.20	-5.16

C36	H39	-4.20	-5.16
C40	H42	1.80	1.38
C41	H42	11.90	13.45

Cornilescu Quality factor: 0.130858

Computed data for frame #2

RDC Data:

I	J	Exp. [Hz]	Comp. [Hz]
C1	H2	-6.20	-4.76
C3	H4	-7.90	-9.14
C6	H7	-6.30	-5.06
C9	H10	8.30	2.36
C9	H11	8.30	2.36
C12	H13	6.30	-0.38
C12	H14	6.30	-0.38
C15	H16	14.50	12.52
C17	H18	14.80	12.98
C20	H21	8.10	8.68
C20	H22	8.10	8.68
C23	H24	4.60	4.62
C23	H25	4.60	4.62
C27	H28	14.80	14.32
C29	H30	5.80	4.82
C29	H31	5.80	4.82
C32	H33	5.10	5.65
C32	H34	5.10	5.65
C36	H37	-4.20	-4.60
C36	H38	-4.20	-4.60
C36	H39	-4.20	-4.60
C40	H42	1.80	1.33
C41	H42	11.90	13.01

Cornilescu Quality factor: 0.281629

!Conformationally averaged data

!Populations

Frame #1: 76.5%

Frame #2: 23.5%

RDC Data:

I	J	Exp. [Hz]	Comp. [Hz]
C1	H2	-6.20	-6.28
C3	H4	-7.90	-7.60
C6	H7	-6.30	-6.55
C9	H10	8.30	8.19
C9	H11	8.30	8.19
C12	H13	6.30	5.43
C12	H14	6.30	5.43
C15	H16	14.50	13.91
C17	H18	14.80	13.01
C20	H21	8.10	7.43
C20	H22	8.10	7.43
C23	H24	4.60	6.42

C23	H25	4.60	6.42
C27	H28	14.80	15.27
C29	H30	5.80	6.09
C29	H31	5.80	6.09
C32	H33	5.10	6.06
C32	H34	5.10	6.06
C36	H37	-4.20	-5.03
C36	H38	-4.20	-5.03
C36	H39	-4.20	-5.03
C40	H42	1.80	1.36
C41	H42	11.90	13.35

Cornilescu Quality factor: 0.101516

Alignment tensor information:

A'x= 6.903e-05

A'y= 2.344e-04

A'z=-3.035e-04

Saupe tensor

S'x= 1.036e-04

S'y= 3.516e-04

S'z=-4.552e-04

Alignment tensor eigenvectors

e[x]=( 0.082, -0.994, -0.074)

e[y]=( 0.957, 0.057, 0.286)

e[z]=(-0.280, -0.094, 0.955)

Alignment tensor in laboratory coordinates:

[ 1.912e-04, -6.938e-07, 1.449e-04]

[-6.938e-07, 6.630e-05, 3.611e-05]

[ 1.449e-04, 3.611e-05, -2.575e-04]

SVD condition number is 7.169e+00

Axial component Aa = -4.552e-04

Rhombic component Ar = -1.654e-04

rhombicity R = 0.363

Asimmetry parameter etha =5.450e-01

GDO = 5.633e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(-161.5, 17.2, 75.6)

Set 2

(18.5, -17.2, -104.4)

\*\*\*\*\*

MagNes-RDC job finished at qua mai 4 18:59:46 2016

Job Wall clock time: 0:0:4.222

\*\*\*\*\*

## F2-coupled RDCs. Input file

```
rdc_data {  
#C1-H1  
1 2 -6.6  
#C2-H2  
3 4 -8.9  
#C4-H4  
6 7 -6.2  
#C6-H6 alfa  
#9 10 0.00  
#C6-H6 beta  
9 11 6.1  
9 10 9.2  
#C7-H7 alfa  
12 14 12.9  
#C7-H7 beta  
12 13 -1.5  
#C8-H8  
15 16 13.8  
#C9-H9  
17 18 14.3  
#C11-H11 alfa  
20 22 4.6  
#C11-H11 beta  
20 21 10.5  
#C12-H12 alfa  
23 25 13.3  
#C12-H12 beta  
23 24 -2.6  
#C14-H14  
27 28 14.0  
#C15 H15 alfa  
29 31 -0.5  
#C15-H15 beta  
29 30 11.2  
#C16-H16 alfa  
32 34 -3.3  
#C16-H16 beta  
32 33 14.7  
#CH3  
36 37 -4.4  
36 38 -4.4  
36 39 -4.4  
#C19-H20  
40 42 2.7  
#C20-H20  
41 42 12.1  
}
```

```
permutations {  
#C12  
#24 25
```

```

#C15
#30 31
#C6
#10 11
#C7
#13 14
#C11
#21 22
#C16
#33 34
}

superimpose {
true
}

superimpose_atoms {
1,3,5,6,8,9,12,15,17,19,20,23,26,27,29,32,35,36,43
}

single_tensor {
true
}

optimize_populations {
true
}

scale_rdc {
false
}

!* MagNes-RDC Plugin *!
*****
MagNes-RDC job started at seg jun 6 18:12:36 2016
*****
!* File info *!
Directory:
/Users/armando/research/adonias/dynamics/magnes_results/f2/estra
diol_pbe6311+
Conformer #1 : 4_JF_A_pbe06311+.out
Conformer #2 : 4_JF_B1_pbe06311+.out
Input file: RDCs_F2_best.txt
*****
!* Computation flags *!
Method: SVD
Scale RDCs: False
Scale SVD with errors: False
CSA weight: 1
Scale QCSA with axial component: False
Single Tensor: True

```

Optimize populations: True  
Grid search points: 16  
Average methyl groups: True  
Average methylene groups: False  
Average phenyl groups: False  
Bootstrapping: False  
RDC Std. Error [ppm]: 1  
CSA Std. Error [ppm]: 0.01  
PCS Std. Error [ppm]: 0.01  
DQ Std. Error [Hz]: 1

\*\*\*\*\*

!\* Permutations \*!

There are no permutations on the original data set

\*\*\*\*\*

Data set: #1

Computed data for frame #1

RDC Data:

I	J	Exp. [Hz]	Comp. [Hz]
C1	H2	-6.60	-6.23
C3	H4	-8.90	-7.55
C6	H7	-6.20	-6.38
C9	H11	6.10	0.16
C9	H10	9.20	15.17
C12	H14	12.90	15.81
C12	H13	-1.50	-3.93
C15	H16	13.80	14.13
C17	H18	14.30	13.18
C20	H22	4.60	0.77
C20	H21	10.50	11.96
C23	H25	13.30	13.50
C23	H24	-2.60	-2.19
C27	H28	14.00	15.00
C29	H31	-0.50	1.70
C29	H30	11.20	10.24
C32	H34	-3.30	-4.12
C32	H33	14.70	15.91
C36	H37	-4.40	-4.74
C36	H38	-4.40	-4.74
C36	H39	-4.40	-4.74
C40	H42	2.70	1.47
C41	H42	12.10	14.32

Cornilescu Quality factor: 0.253476

Computed data for frame #2

RDC Data:

I	J	Exp. [Hz]	Comp. [Hz]
C1	H2	-6.60	-6.03
C3	H4	-8.90	-8.44
C6	H7	-6.20	-6.13
C9	H11	6.10	12.67
C9	H10	9.20	-6.68
C12	H14	12.90	-6.10
C12	H13	-1.50	9.47

C15	H16	13.80	12.30
C17	H18	14.30	12.32
C20	H22	4.60	4.70
C20	H21	10.50	10.18
C23	H25	13.30	12.08
C23	H24	-2.60	-4.86
C27	H28	14.00	13.64
C29	H31	-0.50	-2.61
C29	H30	11.20	11.35
C32	H34	-3.30	-5.97
C32	H33	14.70	15.39
C36	H37	-4.40	-4.09
C36	H38	-4.40	-4.09
C36	H39	-4.40	-4.09
C40	H42	2.70	1.41
C41	H42	12.10	13.72

Cornilescu Quality factor: 0.654503  
!Conformationally averaged data

!Populations

Frame #1: 75.4%

Frame #2: 24.6%

RDC Data:

I	J	Exp. [Hz]	Comp. [Hz]
C1	H2	-6.60	-6.18
C3	H4	-8.90	-7.77
C6	H7	-6.20	-6.32
C9	H11	6.10	3.24
C9	H10	9.20	9.79
C12	H14	12.90	10.41
C12	H13	-1.50	-0.63
C15	H16	13.80	13.68
C17	H18	14.30	12.96
C20	H22	4.60	1.74
C20	H21	10.50	11.52
C23	H25	13.30	13.15
C23	H24	-2.60	-2.85
C27	H28	14.00	14.66
C29	H31	-0.50	0.64
C29	H30	11.20	10.52
C32	H34	-3.30	-4.57
C32	H33	14.70	15.78
C36	H37	-4.40	-4.58
C36	H38	-4.40	-4.58
C36	H39	-4.40	-4.58
C40	H42	2.70	1.46
C41	H42	12.10	14.17

Cornilescu Quality factor: 0.143737

Alignment tensor information:

A'x= 8.812e-05

A'y= 1.618e-04

A'z=-2.499e-04

Saupe tensor

S'x= 1.322e-04

S'y= 2.427e-04

S'z=-3.749e-04

Alignment tensor eigenvectors

e[x]=( 0.229, -0.968, -0.104)

e[y]=( 0.958, 0.205, 0.202)

e[z]=(-0.174, -0.146, 0.974)

Alignment tensor in laboratory coordinates:

[ 1.454e-04, 5.838e-06, 7.162e-05]

[ 5.838e-06, 8.398e-05, 5.117e-05]

[ 7.162e-05, 5.117e-05, -2.294e-04]

SVD condition number is 2.327e+00

Axial component Aa = -3.749e-04

Rhombic component Ar = -7.369e-05

rhombicity R = 0.197

Asimmetry parameter etha =2.948e-01

GDO = 4.422e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(-140.0, 13.1, 62.7)

Set 2

(40.0, -13.1, -117.3)

\*\*\*\*\*

MagNes-RDC job finished at seg jun 6 18:12:37 2016

Job Wall clock time: 0:0:0.948

\*\*\*\*\*