Supporting Information to Accompany:

One probe, two-channel imaging of nuclear and cytosolic compartments with orange and red emissive dyes

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Figure S2. Absorption (solid line) and emission (dashed line) spectra of **1**-**4** in several protic (octanol, methanol) and aprotic (acetone, acetonitrile, THF) solvents. Emission intensity is highly sensitive to solvent polarity and viscosity with emission highest in octanol (red) and THF (green); this effect is consistent for both protic (octanol versus methanol) and aprotic solvents (THF versus acetone/acetonitrile).

Table S1. Summary of photophysical parameters in organic solvents.				
	1	2	3	4
acetone				
$\lambda_{ m max,abs}$ / nm	410	507	436	538
ϵ / cm ⁻¹ M ⁻¹	28,800	57,500	36,200	47,900
$\lambda_{max, em}$ / nm	552	624	585	661
φ	0.05	0.004	0.005	0.001
acetonitrile				
λ / nm	410	501	444	531
$\mathcal{N}_{\text{max, abs}}$ / IIII	33 300	54 000	35 600	49 500
$\epsilon / cm / nm$	570	627	613	652
$\Lambda_{\max, em} / \min$	0.02	0.001	0.002	~10 ⁻⁴
Ψ	0.02	0.001	0.002	-10
tetrahydrofuran				
$\lambda_{\max, abs}$ / nm	405	506	445	539
$\epsilon / cm^{-1} M^{-1}$	30,700	54,600	33,600	46,000
$\lambda_{max em} / nm$	558	602	598	638
φ	0.05	0.02	0.009	0.008
ootanol				
λ / nm	427	512	453	551
$\mathcal{N}_{\text{max, abs}}$ / IIII	30 300	55 300	33 100	48 200
$\frac{2}{n}$	556	609	580	675
$\Lambda_{\max, em} / \min$	0 14	0.04	0.03	0.01
Ψ	0.14	0.04	0.05	0.01
methanol				
$\lambda_{ m max, abs}$ / nm	438	521	478	572
(calculated)				
$\lambda_{max, abs}$ / nm	426	500	452	529
(observed)				
ϵ / cm ⁻¹ M ⁻¹	36,100	55,600	37,400	45,600
$\lambda_{\max,em}$	579	628	627	675
φ	0.01	0.003	0.001	~10-4



Figure S3. Determination of K_D values for a) 1 + DNA, b) 1 + RNA and c) 2 + DNA. Fluorescence was monitored at 550 nm for 1 and 625 nm for 2. Data was plotted and analyzed with Prism 5. No saturation was observed for 2 + RNA over the concentration range tested; inner filter effects preclude measurements for $[2] > 5 \mu M$, as A > 0.2.



Figure S5. ¹³C NMR of 1.



Figure S7. ¹³C NMR of **2**.



Figure S9. ¹³C NMR of **3**.





Figure S11. ¹³C NMR of 4.







Figure S13. ¹³C NMR of **5**.



Figure S15. ¹³C NMR of 6.



Figure S17. ¹³C NMR of **7**.

atom	nucleus	X	У	Z
1	С	1.118578	2.876965	-0.054545
2	С	1.091957	0.231865	-0.051602
3	Ν	2.31137	2.28752	-0.050583
4	Ν	-0.086373	2.317693	-0.06374
5	С	-0.105033	0.960143	-0.05851
6	С	2.307217	0.932631	-0.052363
7	Н	1.057243	-0.850346	-0.028719
8	С	-1.386476	0.268542	-0.052197
9	Н	-1.327674	-0.817389	-0.050921
10	С	-2.586279	0.900268	-0.045062
11	Н	-2.571886	1.989484	-0.048523
12	С	3.61825	0.260227	-0.045192
13	С	6.193375	-1.003255	-0.026707
14	С	4.797735	0.989234	0.202113
15	С	3.764016	-1.121115	-0.277688
16	С	5.004603	-1.740688	-0.268683
17	С	6.045364	0.386744	0.2227
18	Н	4.72511	2.054791	0.393501
19	Н	2.893845	-1.736455	-0.485791
20	Н	5.050628	-2.806856	-0.456195
21	Н	6.913052	0.999715	0.435754
22	С	-3.909888	0.303042	-0.032073
23	С	-6.57809	-0.75527	-0.007609
24	С	-4.154444	-1.088246	-0.009585
25	С	-5.04404	1.142097	-0.033034
26	С	-6.337412	0.643332	-0.017088
27	С	-5.438028	-1.606149	0.005463
28	Н	-3.320516	-1.785215	0.002447
29	Н	-4.899387	2.220522	-0.042515
30	Н	-7.165888	1.341612	-0.01271
31	Н	-5.562904	-2.682193	0.029927
32	Ν	7.431245	-1.604505	-0.045756
33	Ν	-7.854312	-1.266646	-0.016975
34	С	8.604672	-0.860547	0.398159
35	Н	8.545674	-0.57349	1.458918
36	Н	8.741869	0.049412	-0.196122
37	Н	9.49072	-1.482211	0.260228
38	С	7.529363	-3.057789	-0.117046
39	Н	7.078397	-3.554238	0.755448
40	Н	8.582471	-3.339734	-0.163259
41	Н	7.042308	-3.442812	-1.019892
42	С	-8.066889	-2.699693	0.143848
43	Н	-7.710796	-3.070933	1.116457
44	Н	-7.559431	-3.266055	-0.645692
45	Н	-9.134783	-2.910656	0.069667
46	С	-8.994688	-0.372908	0.144381
47	Н	-8.976244	0.159169	1.107022
48	Н	-9.914249	-0.957552	0.09396
49	Н	-9.029199	0.374445	-0.657105
50	0	1.168353	4.232076	-0.053062
51	Н	0.248144	4.555346	-0.058087

Table S2: Optimized geometry of **1**; B3LYP/6-31G(d), SMD solvent model (MeOH); E = -1146.955 a.u.

Table S3: O	ptimized geometr	y of 2	; B3LYP/6-31G(d)	, SMD solvent model	(MeOH); E = -129	8.708 a.u.
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atom	nucleus	X	y	Z
1	Н	-1.39568	-1.03525	0.11472
2	С	-2.63195	0.71106	-0.01575
3	Н	-2.5897	1.7975	-0.0772
4	С	3.55249	0.03624	0.0049
5	С	6.14009	-1.18453	-0.0129
6	С	4.73505	0.81096	0.02298
7	С	3.70386	-1.36925	-0.02873
8	С	4.9491	-1.96609	-0.03771
9	С	5.98753	0.23083	0.01678
10	Н	4.65852	1.89266	0.04856
11	Н	2.8317	-2.01436	-0.06171
12	Н	5.00784	-3.04736	-0.06967
13	Н	6.86025	0.87198	0.03717
14	С	-3.95812	0.1514	-0.00976
15	С	-6.64815	-0.83831	-0.00499
16	С	-4.23652	-1.23607	0.05518
17	С	-5.07225	1.02109	-0.07243
18	С	-6.37378	0.5562	-0.07114
19	С	-5.5291	-1.7203	0.05756
20	Н	-3.41926	-1.95052	0.10274
21	Н	-4.8972	2.09353	-0.12312
22	Н	-7.18634	1.2709	-0.12047
23	Н	-5.68462	-2.79126	0.10656
24	Ν	7.3738	-1.76527	-0.0193
25	Ν	-7.92825	-1.31459	-0.0021
26	С	8.57764	-0.93967	-0.01356
27	Н	8.63183	-0.31212	0.88533
28	Н	8.62385	-0.28638	-0.89446
29	Н	9.45341	-1.58877	-0.02666
30	С	7.50797	-3.21829	-0.05078
31	Н	7.02825	-3.68615	0.81809
32	Н	8.56694	-3.477	-0.03308
33	Н	7.06726	-3.64644	-0.96048
34	С	-8.18265	-2.75046	0.05581
35	Н	-7.76835	-3.19745	0.96853
36	Н	-7.75304	-3.27283	-0.80891
37	Н	-9.2594	-2.92157	0.0542
38	С	-9.05715	-0.39332	-0.08141
39	Н	-9.06601	0.30815	0.76267
40	Н	-9.98487	-0.9654	-0.05606
41	Н	-9.0396	0.18883	-1.01232
42	С	2.25414	0.68535	0.01241
43	С	1.03157	0.01486	0.10159
44	Н	0.99305	-1.0609	0.19919
45	С	-0.1734	0.72216	0.02688
46	0	2.27493	2.00536	-0.08205
47	0	-0.1788	2.04215	-0.0811
48	В	1.05837	2.8525	0.00779
49	F	1.07459	3.74964	-1.05208
50	F	1.07222	3.53006	1.22401

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20H6.639636-2.8097-0.03252821H8.2711.20307-0.01429622C-5.0011420.181282-0.01751223C-7.661968-0.895131-0.04292724C-5.23615-1.211923-0.02466125C-6.1410781.012623-0.01470626C-7.4309030.505045-0.02292427C-6.516187-1.738553-0.03348328H-4.397422-1.903205-0.0186429H-6.003772.091961-0.0021230H-8.2640121.197683-0.014606
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23C-7.661968-0.895131-0.04292724C-5.23615-1.211923-0.02466125C-6.1410781.012623-0.01470626C-7.4309030.505045-0.02292427C-6.516187-1.738553-0.03348328H-4.397422-1.903205-0.0186429H-6.003772.091961-0.0021230H-8.2640121.197683-0.014606
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26C-7.4309030.505045-0.02292427C-6.516187-1.738553-0.03348328H-4.397422-1.903205-0.0186429H-6.003772.091961-0.0021230H-8.2640121.197683-0.014606
27C-6.516187-1.738553-0.03348328H-4.397422-1.903205-0.0186429H-6.003772.091961-0.0021230H-8.2640121.197683-0.014606
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30 H -8.264012 1.197683 -0.014606
31 H -6.633972 -2.815694 -0.031786
32 N 8.940607 -1.409621 -0.079029
33 N -8.934314 -1.414721 -0.077049
34 C 10.089301 -0.526603 0.082813
35 H 10.09006 -0.014655 1.056492
36 H 10.115536 0.236779 -0.7036
37 H 11.004094 -1.115687 0.005119
38 C 9.145048 -2.846083 0.061431
39 H 8.79712 -3.227006 1.03321
40 H 10.21059 -3.063216 -0.027519
41 H 8.625243 -3.399175 -0.729466
42 C -9.139329 -2.851223 0.062375
43 H -8.789949 -3.23304 1.033237
44 H -8.621102 -3.403953 -0.729838
45 H -10.205132 -3.067687 -0.024861
46 C -10.08285 -0.531066 0.082372
47 H -10.083501 -0.016713 1.054763
48 H -10.997756 -1.120144 0.006177
49 H -10.108909 0.23043 -0.70591
50 O 0.029595 4.161592 0.030196
51 H -0.896616 4.467184 0.032748
52 C 2.483575 0.17399 -0.011485
53 H 2.414515 -0.911314 -0.0226
54 C 3.689088 0.795156 -0.007121
55 H 3.682583 1.884385 0.002866

Table S4: Optimized geometry of 3; B3LYP/6-31G(d), SMD solvent model (MeOH). -1224.371 a. u.

$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	atom	nucleus	X	У	Z
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1	С	-2.473583	-0.057153	0.000288
3 C -3.672809 0.596578 -0.040753 4 H -3.671105 -0.85006 -0.040753 5 C 4.991166 0.023759 -0.000845 6 C 7.674167 -0.990387 0.01049 7 C 5.254469 -1.37678 0.021273 8 C 6.115814 0.884664 -0.019976 9 C 7.122978 0.407941 -0.03333 10 C 6.54655 -1.863574 0.02375 11 H 4.343485 -2.075768 0.03303 12 H 5.950943 1.959721 -0.03853 13 H 8.23231 1.16347 -0.0224468 17 C -5.258301 -1.367287 -0.019574 18 C -7.413411 0.407912 -0.023175 20 C -5.258307 -1.16169 -0.0221769 21 H	2	Н	-2.418108	-1.141475	0.024229
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3	С	-3.672809	0.596578	-0.024001
5 C 4.993166 0.023759 -0.000545 6 C 7.76167 0.990387 0.01049 7 C 5.258469 -1.367678 0.021273 8 C 6.115814 0.884664 -0.010975 9 C 7.12278 0.407941 -0.014976 10 C 6.546565 -1.863574 0.023382 11 H 4.434385 -2.075768 0.03303 12 H 5.950943 1.959721 -0.03853 13 H 8.23231 1.116347 -0.032375 14 H 6.691784 -2.937002 0.039913 15 C -4.993448 0.024376 -0.024468 17 C -5.258301 -1.367287 -0.019574 18 C -6.116382 0.885082 -0.03131 19 C -7.413411 0.407912 -0.028127 20 C -6.546242 -1.863603 -0.018531 <	4	Н	-3.641105	1.685006	-0.040753
6 C 7.74167 -0.990387 0.01049 7 C 5.258469 -1.367678 0.021273 8 C 6.115814 0.884664 -0.019095 9 C 7.412978 0.407941 -0.014976 10 C 6.545655 -1.863574 0.03333 12 H 5.950943 1.959721 -0.03853 13 H 8.23231 1.116347 -0.023575 14 H 6.691784 -2.937002 0.039913 15 C -4.993448 0.022476 -0.024168 16 C -7.67411 -0.990706 -0.024468 17 C -5.258301 -1.367287 -0.019574 18 C -6.116382 0.885082 -0.03131 19 C -7.413411 0.407912 -0.022177 20 C 6.4591082 -2.937155 -0.0116035 21 H -4.934034 -2.075522 -0.015031 <td>5</td> <td>С</td> <td>4.993166</td> <td>0.023759</td> <td>-0.000545</td>	5	С	4.993166	0.023759	-0.000545
7 C 5258469 -1.367678 0.021273 8 C 6.115814 0.884664 -0.019095 9 C 7.412978 0.407941 0.014976 10 C 6.546565 -1.863574 0.023303 11 H 4.34385 -2.075768 0.03303 12 H 5.950943 1.959721 -0.032375 14 H 6.691784 -2.937002 0.039913 15 C -4.993448 0.024376 -0.024168 16 C -7.67411 0.499706 -0.024168 17 C -5.258301 -1.367287 -0.018714 18 C -6.16822 -9.03653 -0.018008 21 H -4.34034 -2.075252 -0.015631 22 H -5.951882 1.960365 -0.034574 23 H 8.94996 -1.47848 0.020627 26 N	6	С	7.674167	-0.990387	0.01049
8 C 6.118144 0.884664 -0.019095 9 C 7.412978 0.407941 -0.019095 10 C 6.544565 1.863574 0.025382 11 H 4.434385 -2.075768 0.03303 12 H 5.999721 -0.03853 13 H 8.23231 1.116347 -0.032375 14 H 6.691784 -0.024176 -0.024118 15 C -4.993448 0.024376 -0.024118 16 C -7.67411 0.990706 0.024468 17 C 5.53301 -1.367287 -0.019574 18 C -6.116382 0.885082 -0.03131 19 C -7.413411 0.407912 -0.028127 20 C 6.54242 -1.863603 -0.015631 21 H -4.691082 -2.937155 -0.01631 22 H -5.94981 </td <td>7</td> <td>С</td> <td>5.258469</td> <td>-1.367678</td> <td>0.021273</td>	7	С	5.258469	-1.367678	0.021273
9C $7,412978$ 0.407941 -0.014976 10C 6.546565 -1.863574 0.02382 11H 4.434385 -2.075768 0.03303 12H 5.950943 1.959721 -0.033853 13H 8.23231 1.116347 -0.032375 14H 6.691784 -2.937002 0.039913 15C -4.993448 0.024376 -0.026118 16C -7.67411 -0.990706 -0.024468 17C -5.258301 -1.367287 -0.018574 18C -6.116322 0.885082 -0.03131 19C -7.413411 0.407912 -0.028127 20C -6.546242 -1.863603 -0.018008 21H -4.34034 -2.075252 -0.015631 22H -5.951882 1.960365 -0.034574 23H -8.233067 1.116169 -0.027769 24H -6.691082 -2.937155 -0.011635 25N 8.94996 -1.47848 0.002627 26N -8.94981 -1.47848 0.002627 26N -8.94986 -3.098388 0.005278 31C 10.088021 -0.57203 -0.03868 32H 10.0255698 -3.098388 0.005278 33H 11.01071 -1.147363 0.004876 34H 10.0285698 -0.33755 0.03868 <t< td=""><td>8</td><td>С</td><td>6.115814</td><td>0.884664</td><td>-0.019095</td></t<>	8	С	6.115814	0.884664	-0.019095
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	9	С	7.412978	0.407941	-0.014976
11H 4.434385 -2.075768 0.03303 12H 5.950943 1.959721 -0.03853 13H 8.23231 1.116347 -0.032375 14H 6.691784 -2.937002 0.039913 15C -4.993448 0.024376 -0.026118 16C -7.67411 -0.990706 -0.024468 17C -5.258301 -1.367287 -0.019574 18C -6.116382 0.885082 -0.03131 19C -7.413411 0.407912 -0.028127 20C -6.546242 -1.863603 -0.015631 21H -4.434034 -2.075252 -0.015631 22H -5.951882 1.960365 -0.027769 23H -8.94981 -1.47844 -0.0228233 24H -6.691082 -2.937155 -0.011635 25N 8.94996 -1.47844 -0.0228283 27C 9.190727 -2.917292 -0.015116 28H 8.78377 -3.376175 -0.926081 29H 8.78377 -3.376175 -0.926081 29H 8.78377 -3.375175 0.03868 31C 10.093796 0.017444 -0.968736 33H 11.010071 -1.47363 0.004876 34H 10.086598 -0.095757 0.018737 36H -8.737795 -3.437554 -0.817253	10	С	6.546565	-1.863574	0.025382
12H 5.950943 1.959721 -0.03853 13H 8.23231 1.116347 -0.032375 14H 6.691784 -2.937002 0.039913 15C -4.993448 0.024376 -0.026118 16C -7.67411 0.099706 0.024468 17C -5.258301 -1.367287 -0.019574 18C -6.116382 0.885082 -0.03131 19C -7.413411 0.407912 -0.0228127 20C -6.546242 -1.863603 -0.018008 21H -4.343034 -2.075252 -0.034574 23H -8.233067 1.116169 -0.027769 24H -6.691082 -2.937155 -0.024683 25N 8.94986 -1.47848 0.020627 26N -8.94981 -1.479344 -0.022833 27C 9.190727 -2.917222 -0.015116 28H 8.78377 -3.376175 -0.926081 29H 8.78377 -3.398188 0.005278 31C 10.088021 -0.567203 -0.03868 32H 10.093796 0.017444 -0.968736 33H 10.093796 0.017444 -0.968736 34H 10.092399 0.030945 0.035931 36H -8.737795 -3.3437554 -0.817253 38H -10.088046 -0.567575 0.118737 </td <td>11</td> <td>Н</td> <td>4.434385</td> <td>-2.075768</td> <td>0.03303</td>	11	Н	4.434385	-2.075768	0.03303
13H 8.23231 1.116347 -0.032375 14H 6.691784 -2.937002 0.039913 15C -4.993448 0.024376 -0.024468 16C -7.67411 -0.990706 -0.024468 17C -5.258301 -1.367287 -0.019574 18C -6.116382 0.885082 -0.03131 19C -7.413411 0.407912 -0.028127 20C -6.546242 -1.863603 -0.018008 21H -4.434034 -2.075252 -0.015631 22H -5.951882 1.960365 -0.027769 24H -6.691082 -2.937155 -0.011635 25N 8.94996 -1.47848 0.020627 26N -8.94981 -1.479344 -0.028283 27C 9.190727 -2.917292 -0.015116 28H 8.745603 -3.420558 0.852122 30H 10.265698 -3.098388 0.005278 31C 10.093796 0.017444 -0.968736 33H 11.010071 -1.147363 0.004876 34H 10.086598 0.309515 0.01374 35C -9.190152 -2.917235 0.035931 36H -8.737795 -3.437554 -0.817253 38H -10.0264826 -3.099501 0.010479 39C -1.008046 -0.05775 0.011877 <td>12</td> <td>Н</td> <td>5.950943</td> <td>1.959721</td> <td>-0.03853</td>	12	Н	5.950943	1.959721	-0.03853
14H 6.691784 -2.937002 0.039913 15C -4.993448 0.024376 -0.026118 16C -7.67411 -0.990706 -0.024468 17C -5.258301 -1.367287 -0.019574 18C -6.116382 0.885082 -0.03131 19C -7.413411 0.407912 -0.028127 20C -6.546242 -1.863603 -0.018008 21H -4.34034 2.075252 -0.015631 22H -5.951882 1.960365 -0.034574 23H -8.233067 1.116169 -0.0227769 24H -6.691082 -2.937155 -0.011635 25N 8.94996 -1.47848 0.020627 26N -8.94981 -1.479344 -0.028283 27C 9.190727 -2.917292 -0.015116 28H 8.78377 -3.376175 -0.926081 29H 8.745603 -3.420558 0.852122 30H 10.025698 -3.098388 0.005278 31C 10.088021 -0.567203 -0.03868 32H 10.025698 -3.099501 0.010479 34H 10.086598 0.131826 0.035931 35C -9.190152 -2.917235 0.035931 36H -8.79725 -3.357388 0.95924 37H -8.79725 -3.39754 -0.817253 <td>13</td> <td>Н</td> <td>8.23231</td> <td>1.116347</td> <td>-0.032375</td>	13	Н	8.23231	1.116347	-0.032375
15C-4.993448 0.024376 -0.02611816C-7.67411-0.990706-0.02446817C-5.258301-1.367287-0.01957418C-6.1163820.885082-0.0313119C-7.4134110.407912-0.02812720C-6.546242-1.863603-0.01800821H-4.434034-2.075252-0.01563122H-5.9518821.960365-0.03457423H-8.2330671.116169-0.02776924H-6.691082-2.937155-0.01163525N8.94996-1.478480.02062726N-8.94981-1.479344-0.02828327C9.190727-2.917292-0.01511628H8.78377-3.376175-0.92608129H8.745603-3.4205580.85212230H10.265698-3.0983880.00527831C10.088021-0.567203-0.0386832H10.0937960.017444-0.96873633H-11.02658980.1318260.80680435C-9.190152-2.9172350.03593136H-8.79023-3.3573880.95929437H-8.79023-3.357354-0.81725338H-10.264826-3.0995010.01047939C1.2140420.620610.00896244C-0.000408	14	Н	6.691784	-2.937002	0.039913
16C -7.67411 -0.990706 -0.024468 17C -5.258301 -1.367287 -0.019574 18C -6.116382 0.0885082 -0.03131 19C -7.413411 0.407912 -0.028127 20C -6.546242 -1.863603 -0.018008 21H -4.434034 -2.075252 -0.015631 22H -5.951882 1.960365 -0.0287769 23H -8.233067 1.116169 -0.027769 24H -6.691082 -2.937155 -0.011635 25N 8.94996 -1.47848 0.020627 26N -8.94981 -1.479344 -0.028283 27C 9.190727 -2.917292 -0.015116 28H 8.78377 -3.376175 -0.926081 29H 8.78377 -3.376175 -0.926081 29H 0.017444 -0.968736 31C 10.088021 -0.567203 -0.03868 32H 10.026598 0.3131826 0.806804 35C -9.190152 -2.917235 0.035931 36H -8.737795 -3.337388 0.959294 37H -8.737795 -3.357384 -0.817253 38H -10.264826 -3.099501 0.010479 39C -10.088046 -0.567575 0.018737 41H -10.088012 0.118494 -0.337275 <t< td=""><td>15</td><td>С</td><td>-4.993448</td><td>0.024376</td><td>-0.026118</td></t<>	15	С	-4.993448	0.024376	-0.026118
17C -5.258301 -1.367287 -0.019574 18C -6.116382 0.885082 -0.03131 19C -7.413411 0.407912 -0.028127 20C -6.546242 -1.863603 -0.018008 21H -4.434034 -2.075252 -0.015631 22H -5.951882 1.960365 -0.034574 23H -8.233067 1.116169 -0.027769 24H -6.691082 -2.937155 -0.011635 25N 8.94996 -1.47848 0.020627 26N -8.94981 -1.479344 -0.028283 27C 9.190727 -2.917292 -0.015116 28H 8.78377 -3.376175 -0.926081 29H 8.745603 -3.420558 0.852122 30H 10.0265698 -3.098388 0.005278 31C 10.088021 -0.567203 -0.03868 32H 10.093796 0.017444 -0.968736 33H 11.010071 -1.147363 0.04876 34H 10.086598 -3.357384 0.035931 36H -8.79023 -3.357384 0.04876 37H -8.79795 -3.437554 -0.817253 38H -10.264826 -3.099501 0.010479 39C -1.0088012 0.118494 -0.837275 43C 1.214042 0.629601 0.008962 <td>16</td> <td>С</td> <td>-7.67411</td> <td>-0.990706</td> <td>-0.024468</td>	16	С	-7.67411	-0.990706	-0.024468
18C-6.1163820.885082-0.0313119C-7.4134110.407912-0.02812720C-6.546242-1.863603-0.01800821H-4.434034-2.075252-0.01563122H-5.9518821.960365-0.03457423H-8.2330671.116169-0.02776924H-6.691082-2.937155-0.01163525N8.94986-1.478480.02062726N-8.94981-1.479344-0.02828327C9.190727-2.917292-0.01511628H8.78377-3.376175-0.92608129H8.745603-3.4205580.85212230H10.265698-3.0983880.00527831C10.088021-0.567203-0.0386832H10.0937960.017444-0.96873633H11.010071-1.1473630.00487634H10.0865980.1318260.80680435C-9.190152-2.9172350.03593136H-8.7307795-3.437554-0.81725338H-10.264826-3.0995010.01047939C-10.088046-0.5675750.01873740H-10.082046-0.5675750.01873741H-11.008914-1.1482570.08346842H-0.00816-1.1452570.08246843C1.214042 <t< td=""><td>17</td><td>С</td><td>-5.258301</td><td>-1.367287</td><td>-0.019574</td></t<>	17	С	-5.258301	-1.367287	-0.019574
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	18	С	-6.116382	0.885082	-0.03131
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	19	С	-7.413411	0.407912	-0.028127
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	20	С	-6.546242	-1.863603	-0.018008
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	21	Н	-4.434034	-2.075252	-0.015631
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	22	Н	-5.951882	1.960365	-0.034574
24H -6.691082 -2.937155 -0.011635 25N 8.94996 -1.47848 0.020627 26N -8.94981 -1.479344 -0.028283 27C 9.190727 -2.917292 -0.015116 28H 8.78377 -3.376175 -0.926081 29H 8.745603 -3.420558 0.852122 30H 10.265698 -3.098388 0.005278 31C 10.088021 -0.567203 -0.03868 32H 10.093796 0.017444 -0.968736 33H 11.010071 -1.147363 0.004876 34H 10.086598 0.131826 0.806804 35C -9.190152 -2.917235 0.035931 36H -8.79023 -3.357388 0.959294 37H -8.737795 -3.437554 -0.817253 38H -10.264826 -3.099501 0.010479 39C -10.088046 -0.567575 0.018737 40H -10.092939 0.030945 0.939955 41H -11.0088012 0.118494 -0.8372755 43C -2.124313 0.629661 0.008962 44C -0.0000408 -0.663096 0.043228 45H -0.0003877 3.646778 -1.074078 47O 1.230441 1.95358 -0.041331 48O -1.23004 1.95358 0.013684 <td>23</td> <td>Н</td> <td>-8.233067</td> <td>1.116169</td> <td>-0.027769</td>	23	Н	-8.233067	1.116169	-0.027769
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	24	Н	-6.691082	-2.937155	-0.011635
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	25	Ν	8.94996	-1.47848	0.020627
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	26	Ν	-8.94981	-1.479344	-0.028283
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	27	С	9.190727	-2.917292	-0.015116
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	28	Н	8.78377	-3.376175	-0.926081
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	29	Н	8.745603	-3.420558	0.852122
31C 10.088021 -0.567203 -0.03868 32H 10.093796 0.017444 -0.968736 33H 11.010071 -1.147363 0.004876 34H 10.086598 0.131826 0.806804 35C -9.190152 -2.917235 0.035931 36H -8.79023 -3.357388 0.959294 37H -8.737795 -3.437554 -0.817253 38H -10.264826 -3.099501 0.010479 39C -10.088046 -0.567575 0.018737 40H -10.099239 0.030945 0.939955 41H -11.009944 -1.148656 -0.015074 42H -10.088012 0.118494 -0.837275 43C 1.214042 0.629061 0.008962 44C -0.0000408 -0.063096 0.043228 45H -0.000816 -1.145257 0.082468 46C -1.214313 0.629569 0.000539 47O 1.230461 1.95358 -0.041331 48O -1.23004 1.95358 0.013684 50F 0.003278 2.780985 0.013684 51F -0.003292 3.497997 1.207496 52C 3.672458 0.595648 -0.0058 53H 3.6466778 -1.074078 54C 2.417389 -1.142168 0.045137	30	Н	10.265698	-3.098388	0.005278
32H 10.093796 0.017444 -0.968736 33H 11.010071 -1.147363 0.004876 34H 10.086598 0.131826 0.806804 35C -9.190152 -2.917235 0.035931 36H -8.79023 -3.357388 0.959294 37H -8.737795 -3.437554 -0.817253 38H -10.264826 -3.099501 0.010479 39C -10.088046 -0.567575 0.018737 40H -10.092939 0.30945 0.939955 41H -11.009944 -1.148656 -0.015074 42H -10.088012 0.118494 -0.837275 43C 1.214042 0.629061 0.008962 44C -0.000408 -0.063096 0.043228 45H -0.000816 -1.145257 0.082468 46C -1.214313 0.629569 0.000539 47O 1.23044 1.953058 -0.041331 48O -1.23004 1.95358 0.013684 50F 0.003877 3.646778 -1.074078 51F -0.003292 3.497997 1.207496 52C 3.672458 0.595648 -0.0029418 54C 2.473104 -0.05794 0.017523 55H 2.417389 -1.142168 0.045137	31	С	10.088021	-0.567203	-0.03868
33H 11.010071 -1.147363 0.004876 34H 10.086598 0.131826 0.806804 35C -9.190152 -2.917235 0.035931 36H -8.79023 -3.357388 0.959294 37H -8.737795 -3.437554 -0.817253 38H -10.264826 -3.099501 0.010479 39C -10.088046 -0.567575 0.018737 40H -10.092939 0.030945 0.939955 41H -11.009944 -1.148656 -0.015074 42H -10.088012 0.118494 -0.837275 43C 1.214042 0.629061 0.008962 44C -0.000408 -0.063096 0.043228 45H -0.000816 -1.145257 0.082468 46C -1.214313 0.629569 0.000539 47O 1.23004 1.95358 -0.041331 48O -1.23004 1.95358 -0.041331 48O -1.23004 1.95358 0.013684 50F 0.003877 3.646778 -1.074078 51F -0.003292 3.497997 1.207496 52C 3.672458 0.595648 -0.0029418 54C 2.473104 -0.05794 0.017523 55H 2.417389 -1.142168 0.045137	32	Н	10.093796	0.017444	-0.968736
34H 10.086598 0.131826 0.806804 35 C -9.190152 -2.917235 0.035931 36 H -8.79023 -3.357388 0.959294 37 H -8.737795 -3.437554 -0.817253 38 H -10.264826 -3.099501 0.010479 39 C -10.088046 -0.567575 0.018737 40 H -10.092939 0.030945 0.939955 41 H -11.009944 -1.148656 -0.015074 42 H -10.088012 0.118494 -0.837275 43 C 1.0214042 0.629061 0.008962 44 C -0.000408 -0.063096 0.043228 45 H -0.000816 -1.145257 0.082468 46 C -1.214313 0.629569 0.000539 47 O 1.230461 1.953058 -0.041331 48 O -1.23004 1.95358 -0.049079 49 B 0.000258 2.780985 0.013684 50 F 0.003877 3.646778 -1.074078 51 F -0.003292 3.497997 1.207496 52 C 3.672458 0.595648 -0.0058 53 H 3.64069 1.683941 -0.029418 54 C 2.473104 -0.05794 0.017523 55 H 2.417389 -1.142168 0.045137	33	Н	11.010071	-1.147363	0.004876
35C -9.190152 -2.917235 0.035931 36H -8.79023 -3.357388 0.959294 37H -8.737795 -3.437554 -0.817253 38H -10.264826 -3.099501 0.010479 39C -10.088046 -0.567575 0.018737 40H -10.092939 0.030945 0.939955 41H -11.009944 -1.148656 -0.015074 42H -10.088012 0.118494 -0.837275 43C 1.214042 0.629061 0.008962 44C -0.000408 -0.063096 0.043228 45H -0.00816 -1.145257 0.082468 46C -1.214313 0.629569 0.000539 47O 1.230461 1.953058 -0.041331 48O -1.23004 1.95358 0.049079 49B 0.000258 2.780985 0.013684 50F 0.003292 3.497997 1.207496 51F -0.003292 3.497997 1.207496 52C 3.64069 1.683941 -0.029418 54C 2.473104 -0.05794 0.017523 55H 2.417389 -1.142168 0.045137	34	Н	10.086598	0.131826	0.806804
36H -8.79023 -3.357388 0.959294 37 H -8.737795 -3.437554 -0.817253 38 H -10.264826 -3.099501 0.010479 39 C -10.088046 -0.567575 0.018737 40 H -10.092939 0.030945 0.939955 41 H -11.009944 -1.148656 -0.015074 42 H -10.088012 0.118494 -0.837275 43 C 1.214042 0.629061 0.008962 44 C -0.000408 -0.063096 0.043228 45 H -0.000816 -1.145257 0.082468 46 C -1.214313 0.629569 0.000539 47 O 1.230461 1.953058 -0.041331 48 O -1.23004 1.95358 -0.049079 49 B 0.000258 2.780985 0.013684 50 F 0.003877 3.646778 -1.074078 51 F -0.03292 3.497997 1.207496 52 C 3.672458 0.595648 -0.029418 54 C 2.473104 -0.05794 0.017523 55 H 2.417389 -1.142168 0.045137	35	С	-9.190152	-2.917235	0.035931
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	36	Н	-8.79023	-3.357388	0.959294
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	37	Н	-8.737795	-3.437554	-0.817253
39C -10.088046 -0.567575 0.018737 40H -10.092939 0.030945 0.939955 41H -11.009944 -1.148656 -0.015074 42H -10.088012 0.118494 -0.837275 43C 1.214042 0.629061 0.008962 44C -0.000408 -0.063096 0.043228 45H -0.000816 -1.145257 0.082468 46C -1.214313 0.629569 0.000539 47O 1.230461 1.953058 -0.0413311 48O -1.23004 1.95358 -0.049079 49B 0.000258 2.780985 0.013684 50F 0.003877 3.646778 -1.074078 51F -0.003292 3.497997 1.207496 52C 3.672458 0.595648 -0.0058 53H 3.64069 1.683941 -0.029418 54C 2.473104 -0.05794 0.017523 55H 2.417389 -1.142168 0.045137	38	Н	-10.264826	-3.099501	0.010479
40H -10.092939 0.030945 0.939955 41 H -11.009944 -1.148656 -0.015074 42 H -10.088012 0.118494 -0.837275 43 C 1.214042 0.629061 0.008962 44 C -0.000408 -0.063096 0.043228 45 H -0.000816 -1.145257 0.082468 46 C -1.214313 0.629569 0.000539 47 O 1.230461 1.953058 -0.041331 48 O -1.23004 1.95358 -0.049079 49 B 0.000258 2.780985 0.013684 50 F 0.003877 3.646778 -1.074078 51 F -0.003292 3.497997 1.207496 52 C 3.672458 0.595648 -0.0058 53 H 3.64069 1.683941 -0.029418 54 C 2.473104 -0.05794 0.017523 55 H 2.417389 -1.142168 0.045137	39	С	-10.088046	-0.567575	0.018737
41H-11.009944-1.148656-0.01507442H-10.0880120.118494-0.83727543C1.2140420.6290610.00896244C-0.000408-0.0630960.04322845H-0.000816-1.1452570.08246846C-1.2143130.6295690.00053947O1.2304611.953058-0.04133148O-1.230041.95358-0.04907949B0.0002582.7809850.01368450F0.0038773.646778-1.07407851F-0.0032923.4979971.20749652C3.6724580.595648-0.005853H3.640691.683941-0.02941854C2.473104-0.057940.01752355H2.417389-1.1421680.045137	40	Н	-10.092939	0.030945	0.939955
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	41	Н	-11.009944	-1.148656	-0.015074
43C1.2140420.6290610.00896244C-0.000408-0.0630960.04322845H-0.000816-1.1452570.08246846C-1.2143130.6295690.00053947O1.2304611.953058-0.04133148O-1.230041.95358-0.04907949B0.0002582.7809850.01368450F0.0038773.646778-1.07407851F-0.0032923.4979971.20749652C3.6724580.595648-0.005853H3.640691.683941-0.02941854C2.473104-0.057940.01752355H2.417389-1.1421680.045137	42	Н	-10.088012	0.118494	-0.837275
44C-0.000408-0.0630960.04322845H-0.000816-1.1452570.08246846C-1.2143130.6295690.00053947O1.2304611.953058-0.04133148O-1.230041.95358-0.04907949B0.0002582.7809850.01368450F0.0038773.646778-1.07407851F-0.0032923.4979971.20749652C3.6724580.595648-0.005853H3.640691.683941-0.02941854C2.473104-0.057940.01752355H2.417389-1.1421680.045137	43	С	1.214042	0.629061	0.008962
45H-0.000816-1.1452570.08246846C-1.2143130.6295690.00053947O1.2304611.953058-0.04133148O-1.230041.95358-0.04907949B0.0002582.7809850.01368450F0.0038773.646778-1.07407851F-0.0032923.4979971.20749652C3.6724580.595648-0.005853H3.640691.683941-0.02941854C2.473104-0.057940.01752355H2.417389-1.1421680.045137	44	С	-0.000408	-0.063096	0.043228
46C-1.2143130.6295690.00053947O1.2304611.953058-0.04133148O-1.230041.95358-0.04907949B0.0002582.7809850.01368450F0.0038773.646778-1.07407851F-0.0032923.4979971.20749652C3.6724580.595648-0.005853H3.640691.683941-0.02941854C2.473104-0.057940.01752355H2.417389-1.1421680.045137	45	Н	-0.000816	-1.145257	0.082468
47O1.2304611.953058-0.04133148O-1.230041.95358-0.04907949B0.0002582.7809850.01368450F0.0038773.646778-1.07407851F-0.0032923.4979971.20749652C3.6724580.595648-0.005853H3.640691.683941-0.02941854C2.473104-0.057940.01752355H2.417389-1.1421680.045137	46	С	-1.214313	0.629569	0.000539
48 O -1.23004 1.95358 -0.049079 49 B 0.000258 2.780985 0.013684 50 F 0.003877 3.646778 -1.074078 51 F -0.003292 3.497997 1.207496 52 C 3.672458 0.595648 -0.0058 53 H 3.64069 1.683941 -0.029418 54 C 2.473104 -0.05794 0.017523 55 H 2.417389 -1.142168 0.045137	47	0	1.230461	1.953058	-0.041331
49 B 0.000258 2.780985 0.013684 50 F 0.003877 3.646778 -1.074078 51 F -0.003292 3.497997 1.207496 52 C 3.672458 0.595648 -0.0058 53 H 3.64069 1.683941 -0.029418 54 C 2.473104 -0.05794 0.017523 55 H 2.417389 -1.142168 0.045137	48	Õ	-1.23004	1.95358	-0.049079
50 F 0.003877 3.646778 -1.074078 51 F -0.003292 3.497997 1.207496 52 C 3.672458 0.595648 -0.0058 53 H 3.64069 1.683941 -0.029418 54 C 2.473104 -0.05794 0.017523 55 H 2.417389 -1.142168 0.045137	49	B	0.000258	2.780985	0.013684
51 F -0.003292 3.497997 1.207496 52 C 3.672458 0.595648 -0.0058 53 H 3.64069 1.683941 -0.029418 54 C 2.473104 -0.05794 0.017523 55 H 2.417389 -1.142168 0.045137	50	F	0.003877	3.646778	-1.074078
52 C 3.672458 0.595648 -0.0058 53 H 3.64069 1.683941 -0.029418 54 C 2.473104 -0.05794 0.017523 55 H 2.417389 -1.142168 0.045137	51	F	-0.003292	3.497997	1.207496
53 H 3.64069 1.683941 -0.029418 54 C 2.473104 -0.05794 0.017523 55 H 2.417389 -1.142168 0.045137	52	Ĉ	3.672458	0.595648	-0.0058
54 C 2.473104 -0.05794 0.017523 55 H 2.417389 -1.142168 0.045137	53	Ĥ	3.64069	1.683941	-0.029418
55 H 2.417389 -1.142168 0.045137	54	C	2.473104	-0.05794	0.017523
	55	Ĥ	2.417389	-1.142168	0.045137

Table S5: Optimized geometry of 4; B3LYP/6-31G(d), SMD solvent model (MeOH); E = -1376.125 a. u.