Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Hyperbeanone A, a 5,6-*seco*-spirocyclic polycyclic polyprenylated acylphloroglucinol derivative with an unprecedented skeleton from *Hypericum beanii*

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CONTENTS

Figure S1. ^{1}H NMR spectrum of compound 1 (recorded in methanol-d_4)

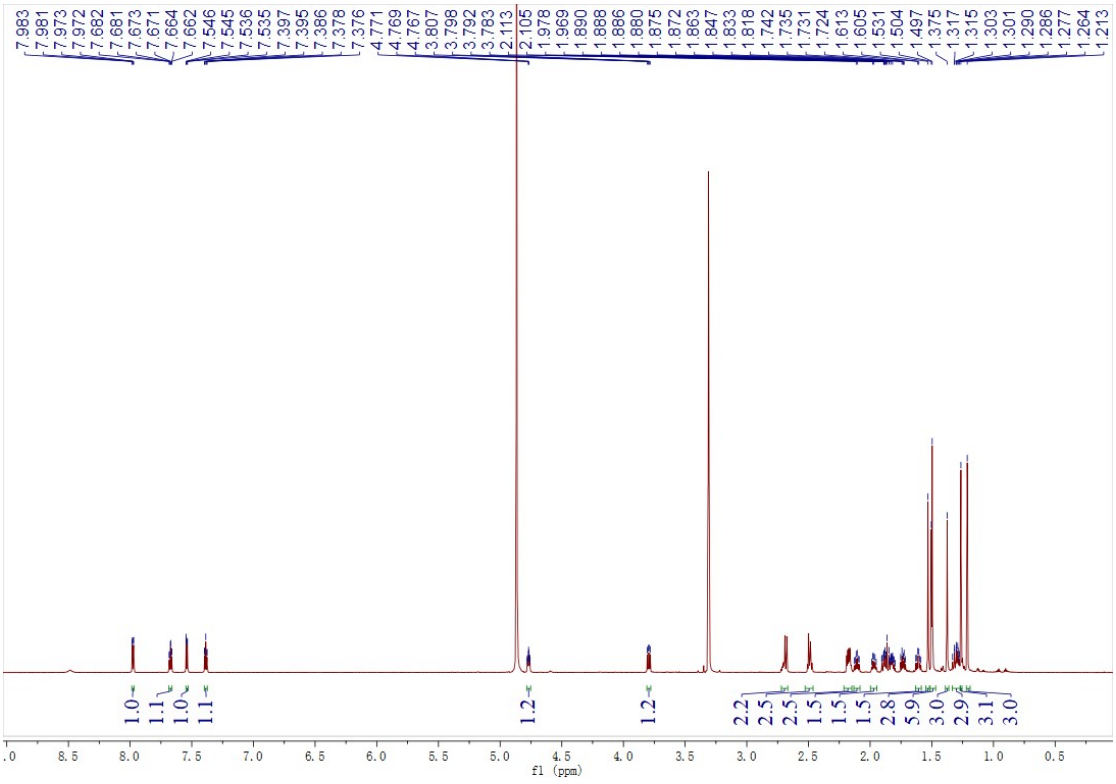


Figure S2. The partial enlargement ^{1}H NMR spectrum of compound 1 (recorded in methanol-d_4)

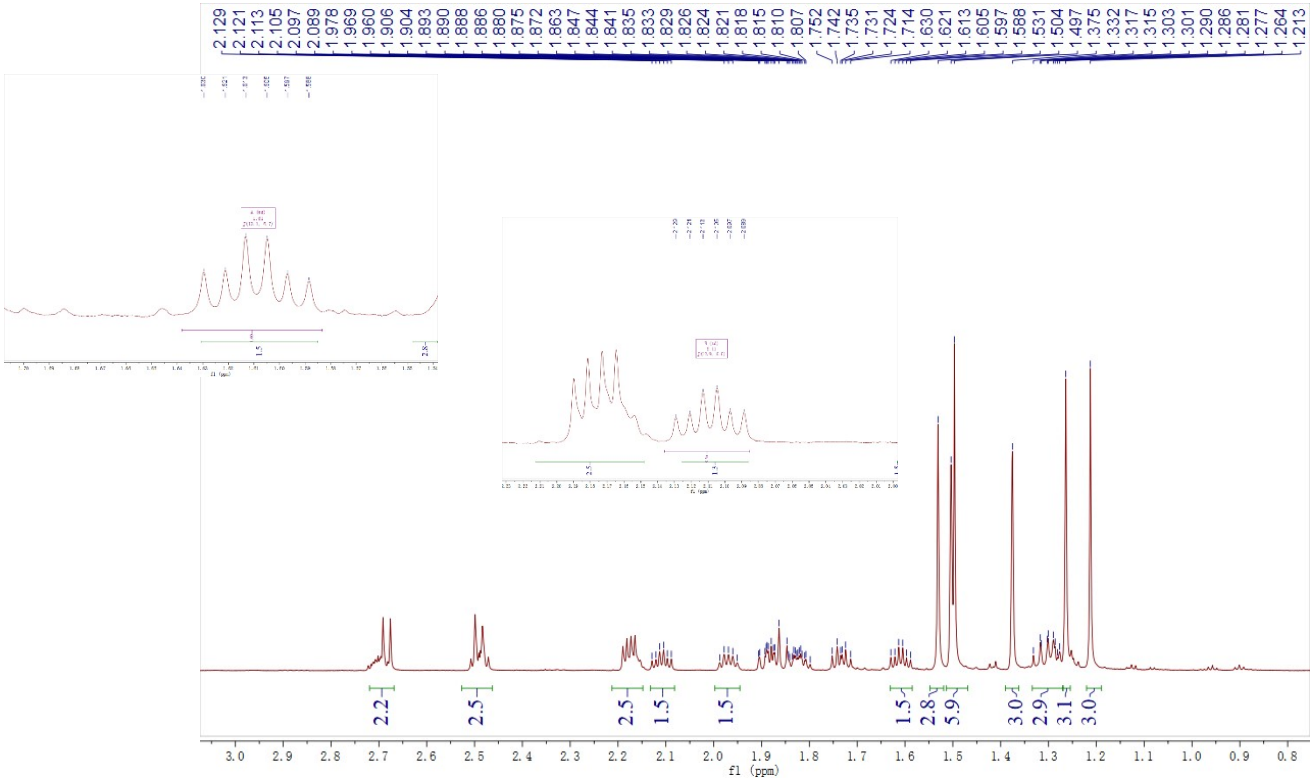


Figure S3. ^{13}C NMR spectrum of compound **1** (recorded in methanol-d_4)

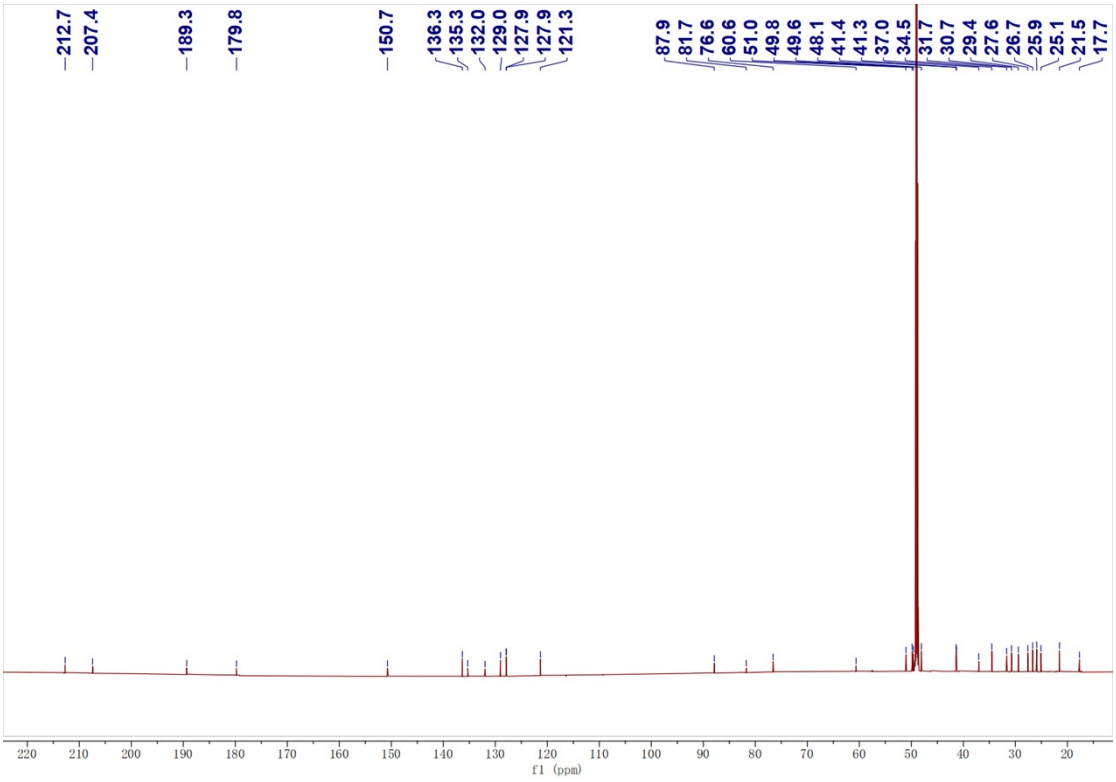


Figure S4. DEPT spectrum of compound **1** (recorded in methanol-d_4)

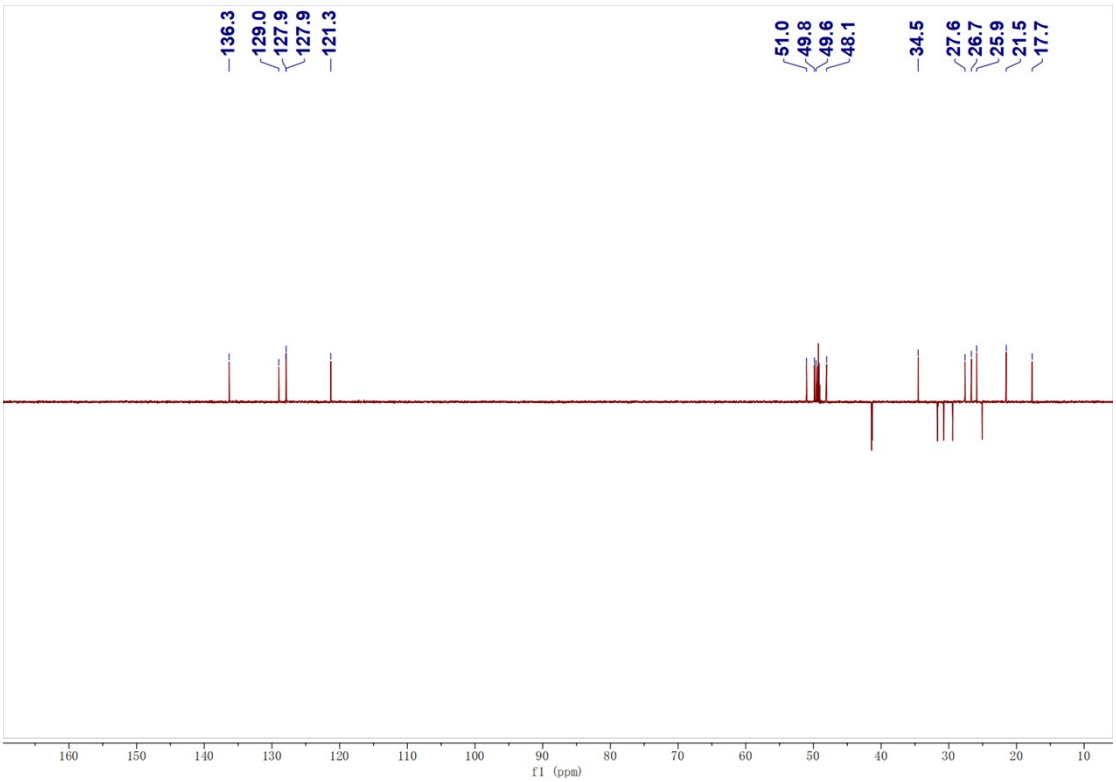


Figure S5. HSQC spectrum of compound **1** (recorded in methanol-d_4)

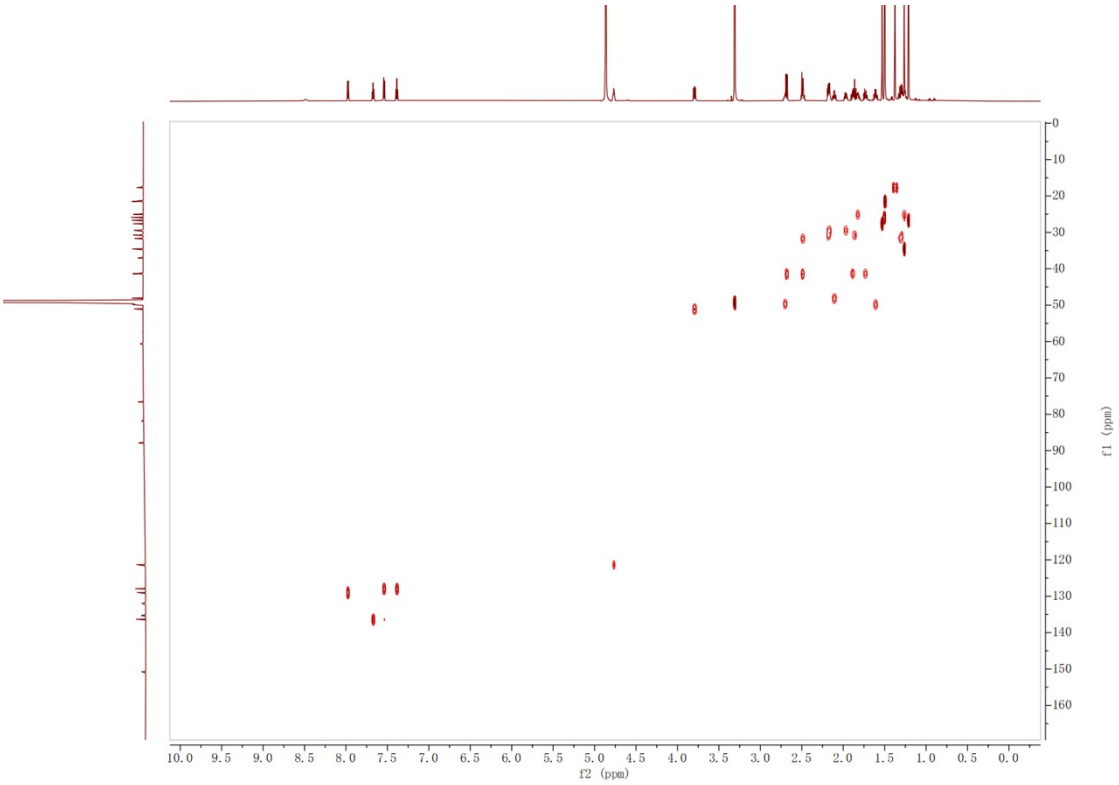


Figure S6. ^{1}H–^{1}H COSY spectrum of compound **1** (recorded in methanol-d_4)

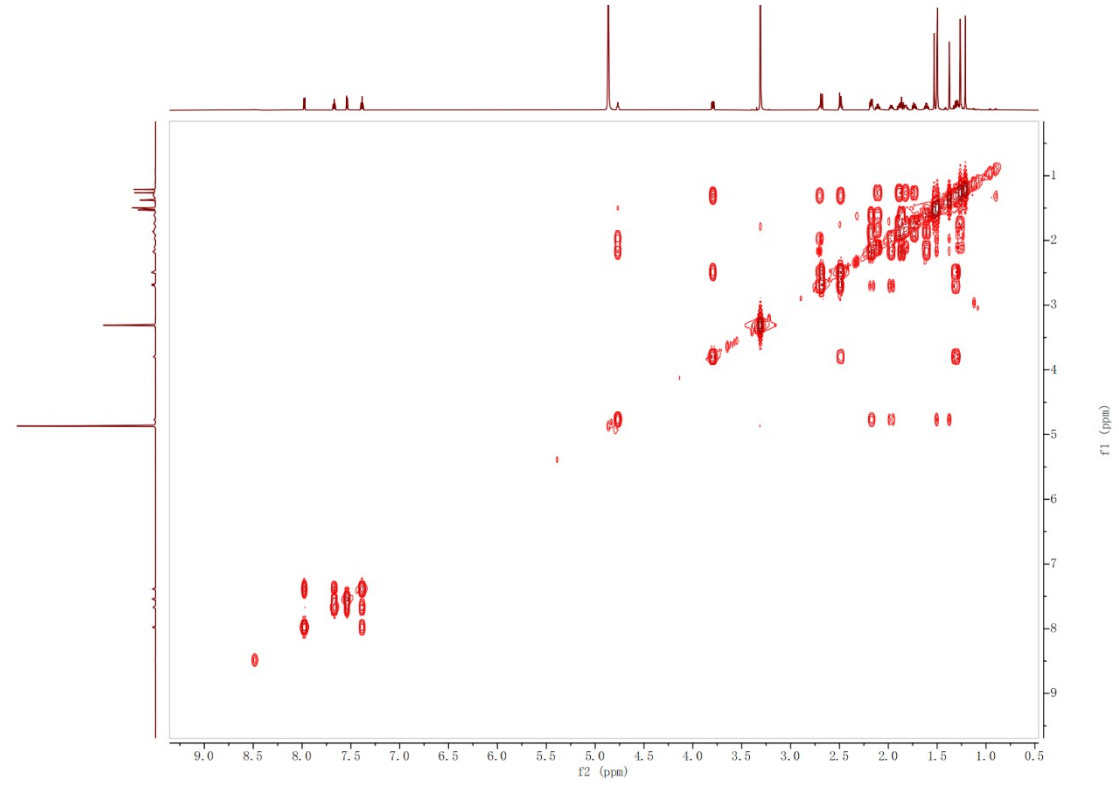


Figure S7. HMBC spectrum of compound **1** (recorded in methanol-d_4)

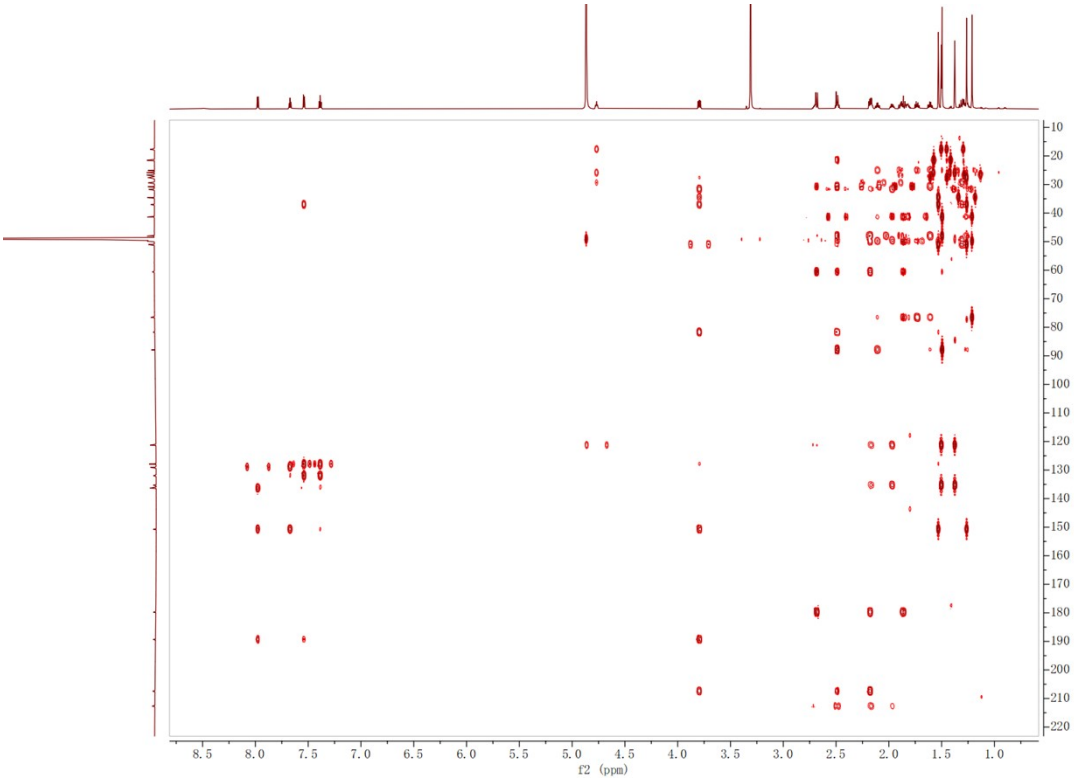


Figure S8. ROESY spectrum of compound **1** (recorded in methanol-d_4)

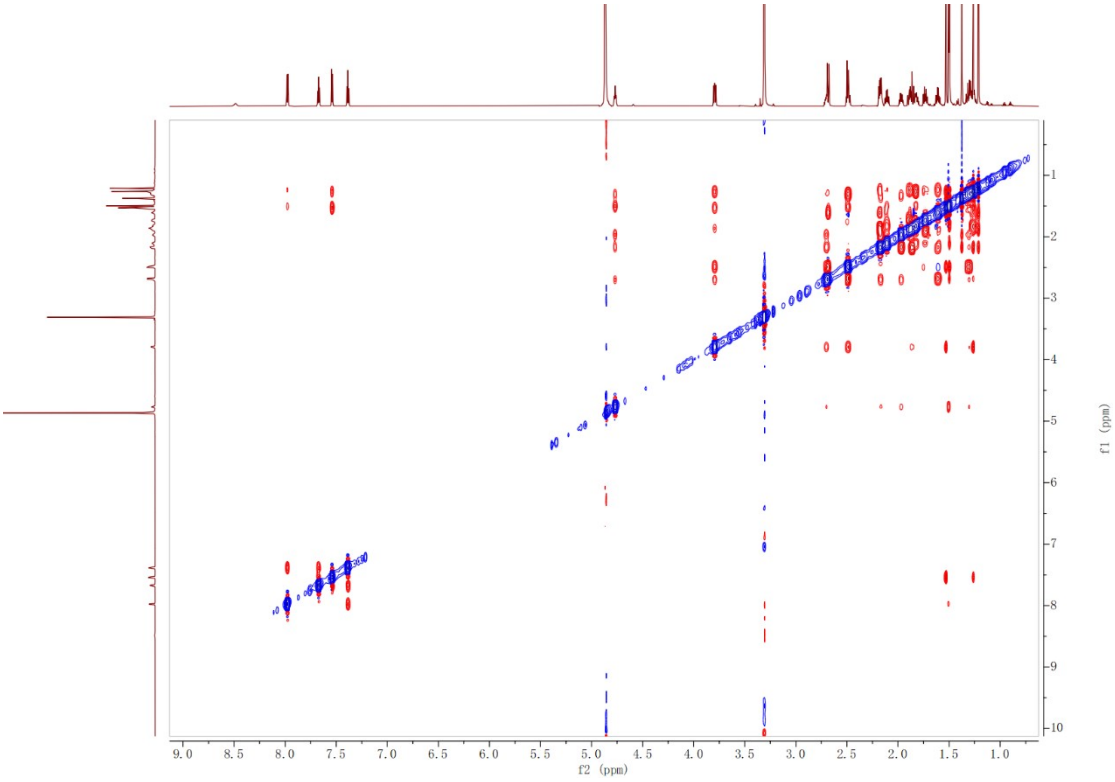


Figure S9. HRESIMS spectrum of compound **1**

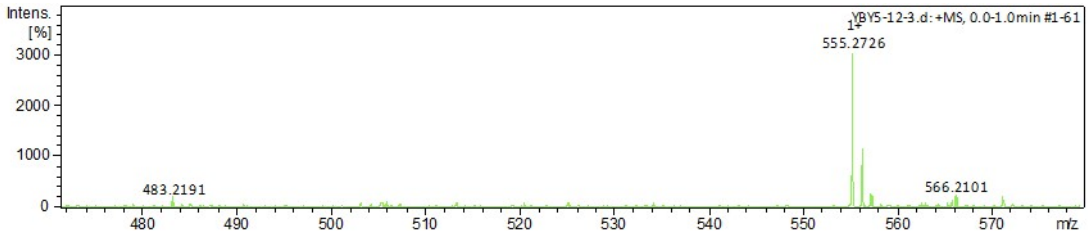


Figure S10. IR spectrum of compound **1**

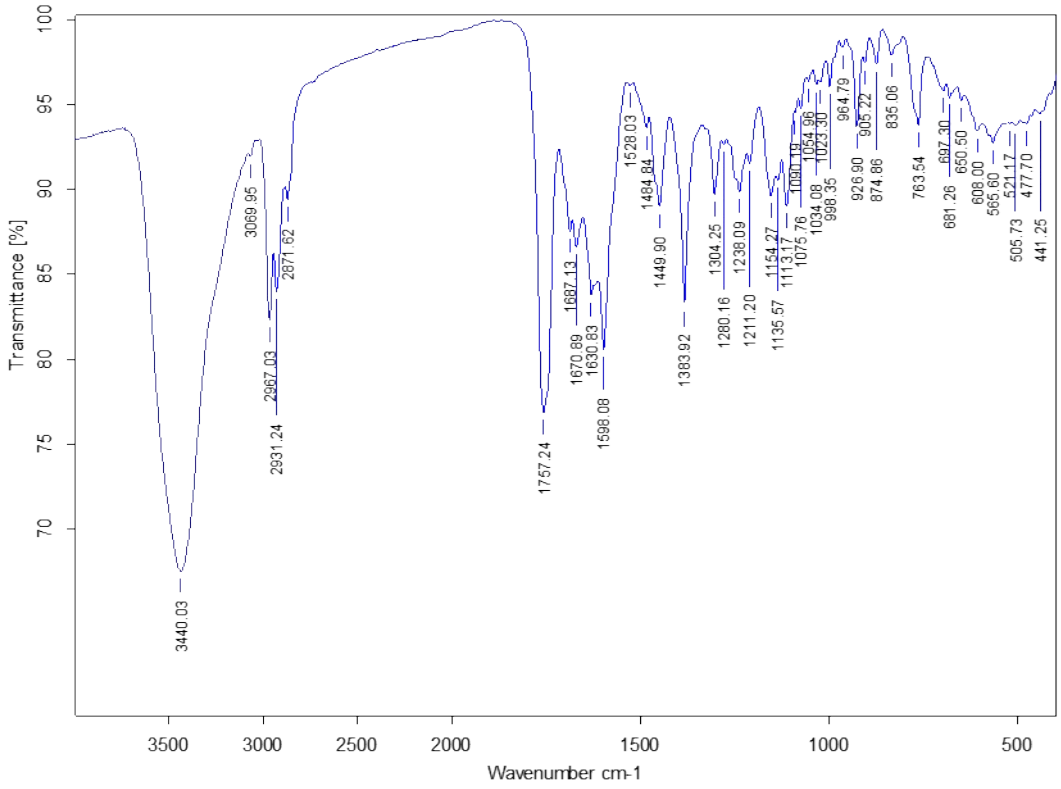


Figure S11. UV spectrum of compound **1**

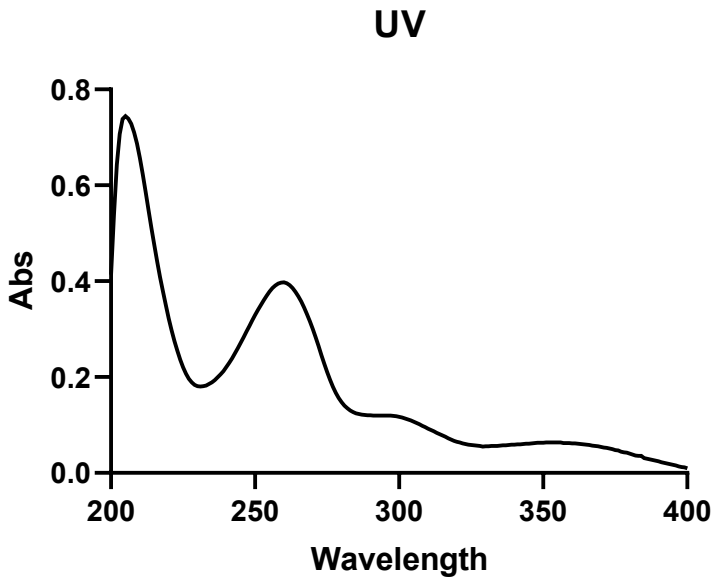


Figure S12. CD spectrum of compound **1**

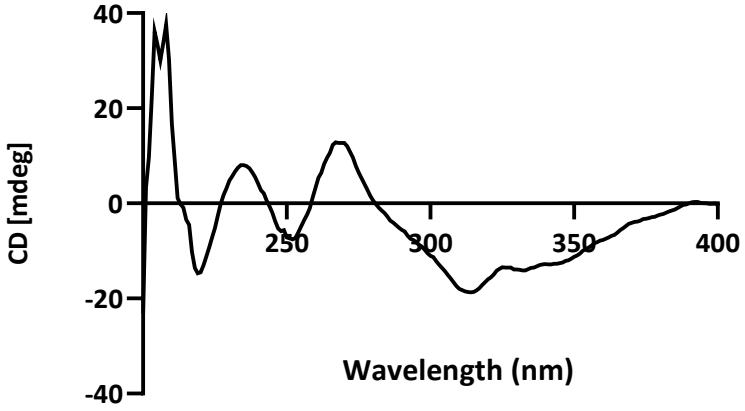


Figure S13. ^{1}H NMR spectrum of compound 2 (recorded in methanol-d_4)

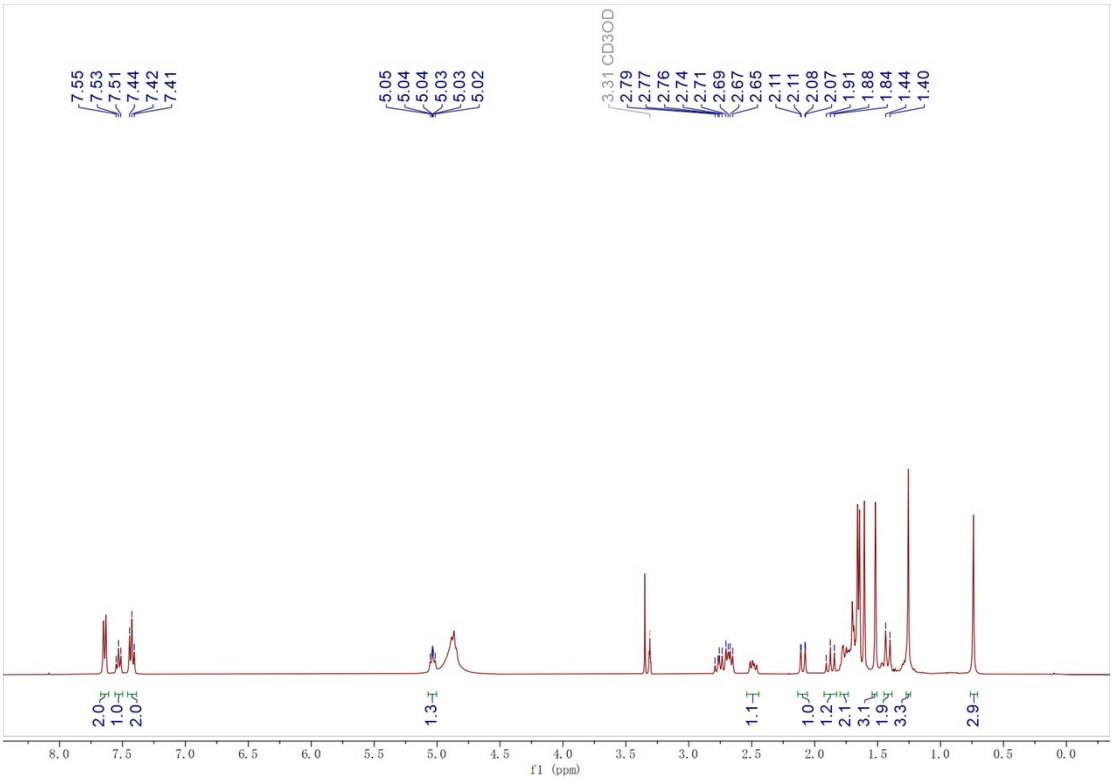


Figure S14. ^{13}C NMR spectrum of compound **2** (recorded in methanol-d_4)

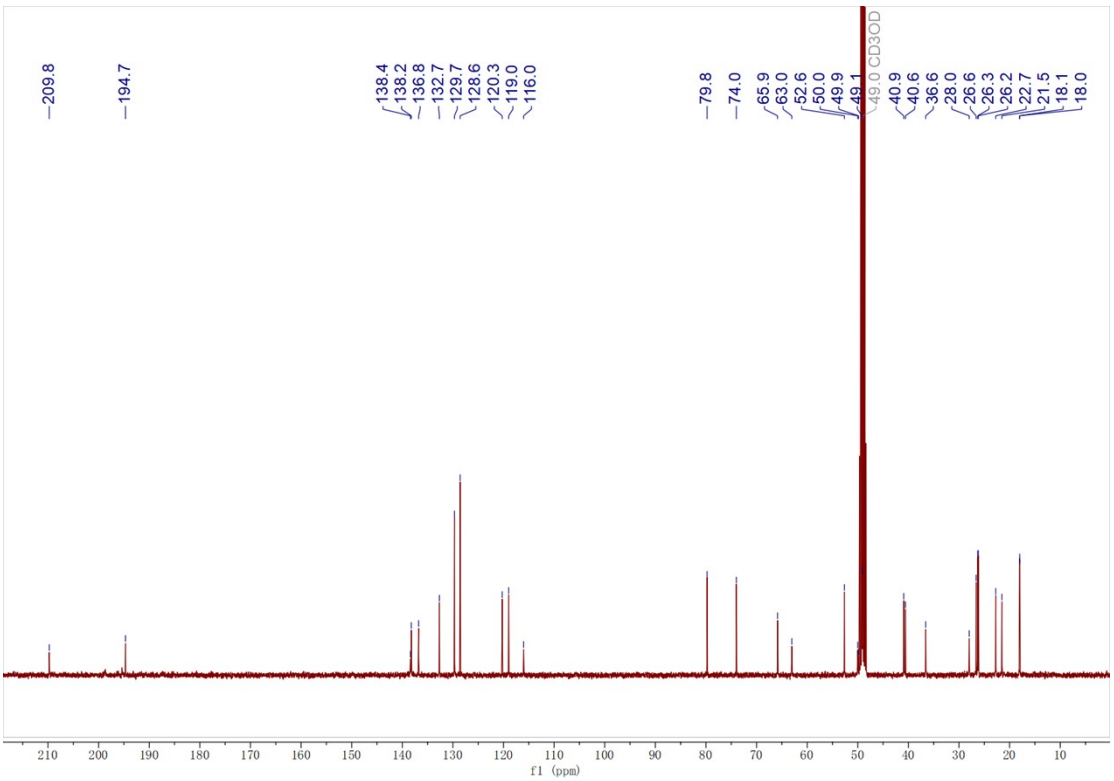


Figure S15. DEPT spectrum of compound **2** (recorded in methanol-d_4)

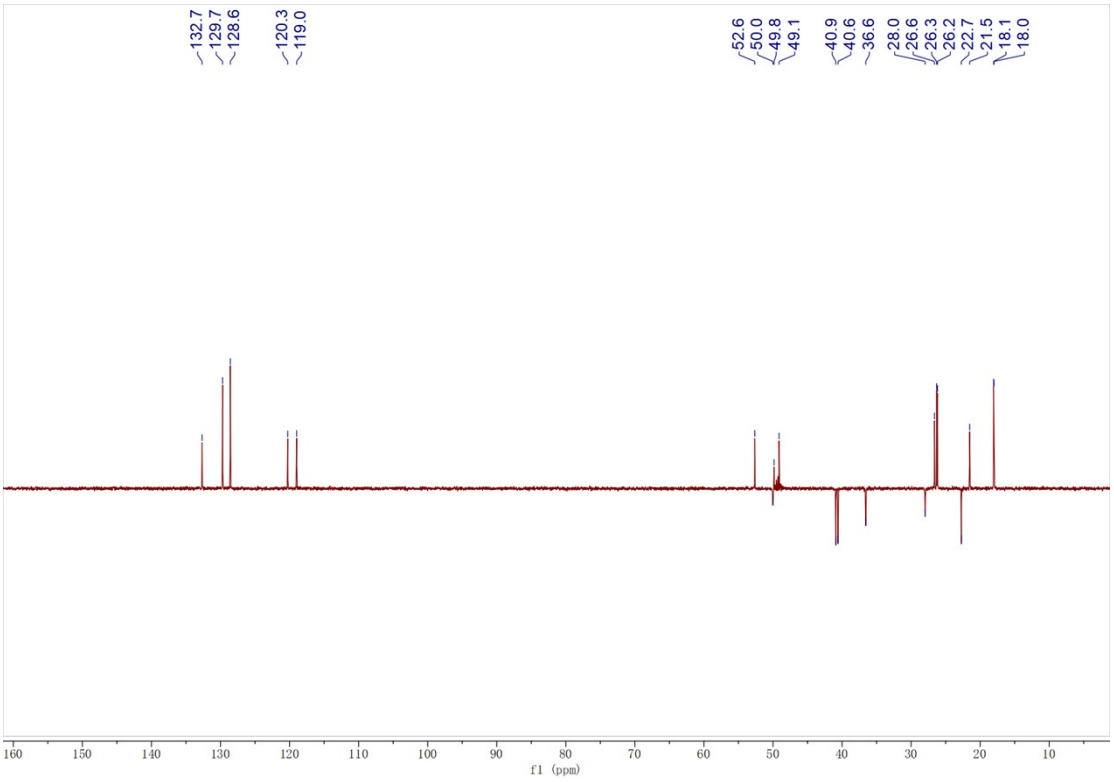


Figure S16. HSQC spectrum of compound **2** (recorded in methanol-d_4)

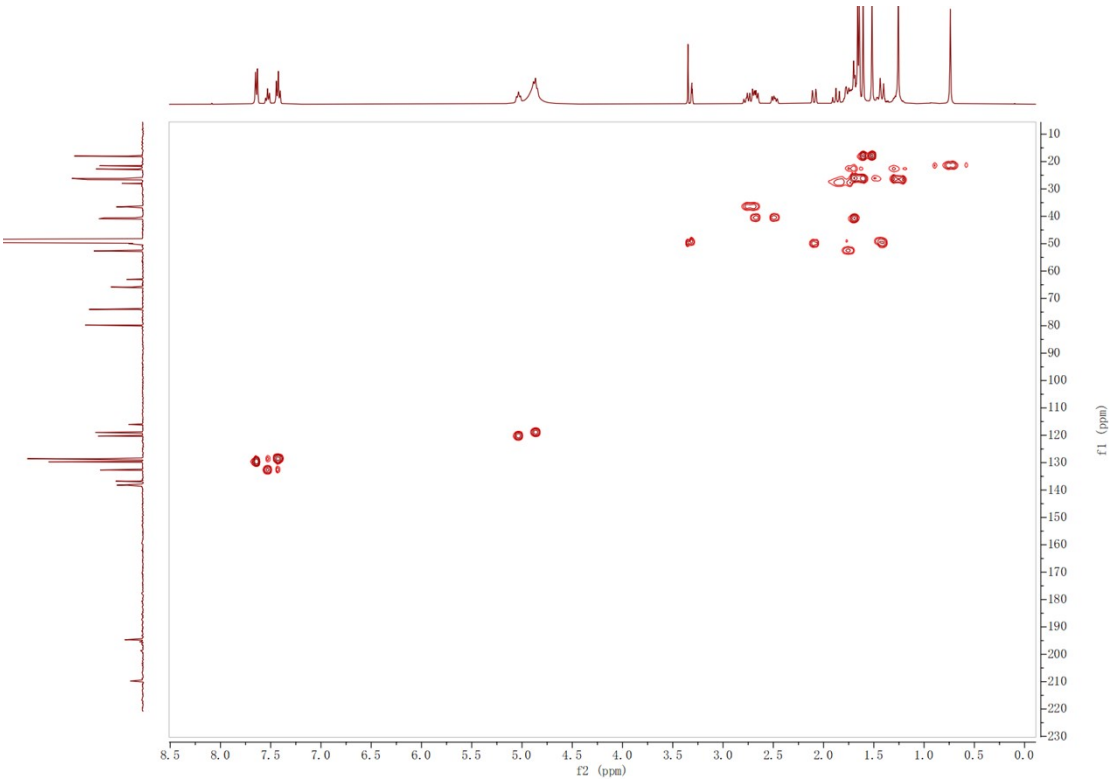


Figure S17. $^{1}H-^{1}H$ COSY spectrum of compound **2** (recorded in methanol-d_4)

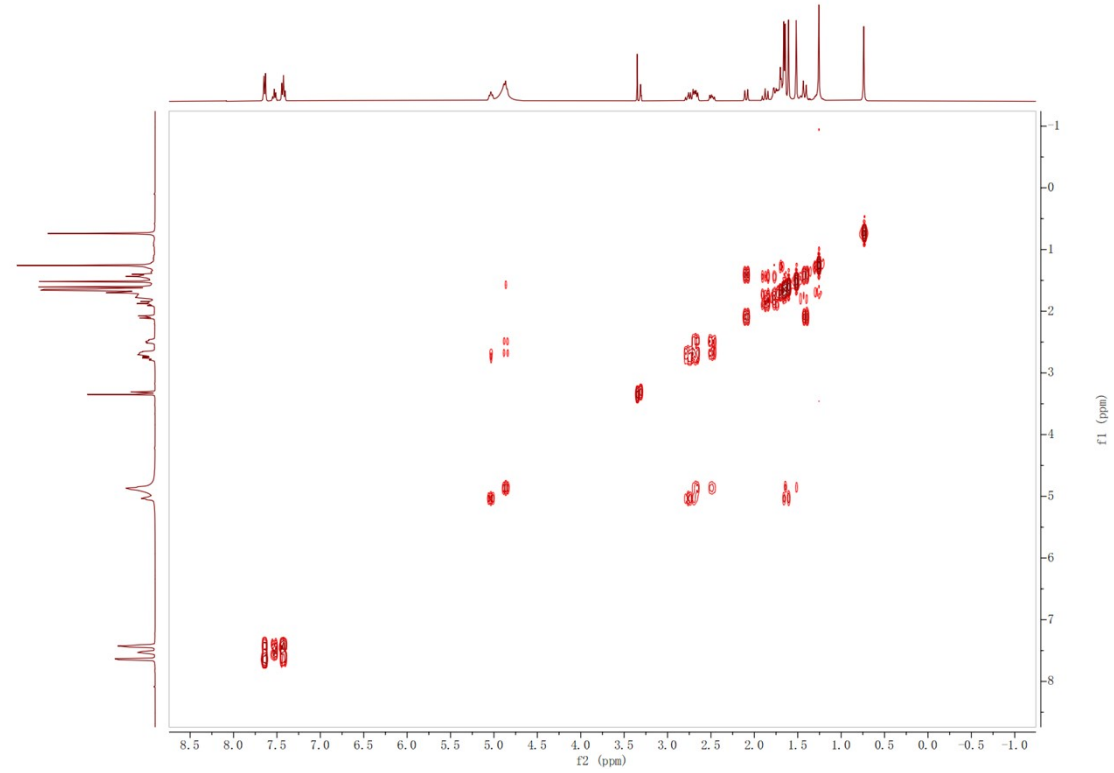


Figure S18. HMBC spectrum of compound **2** (recorded in methanol-d_4)

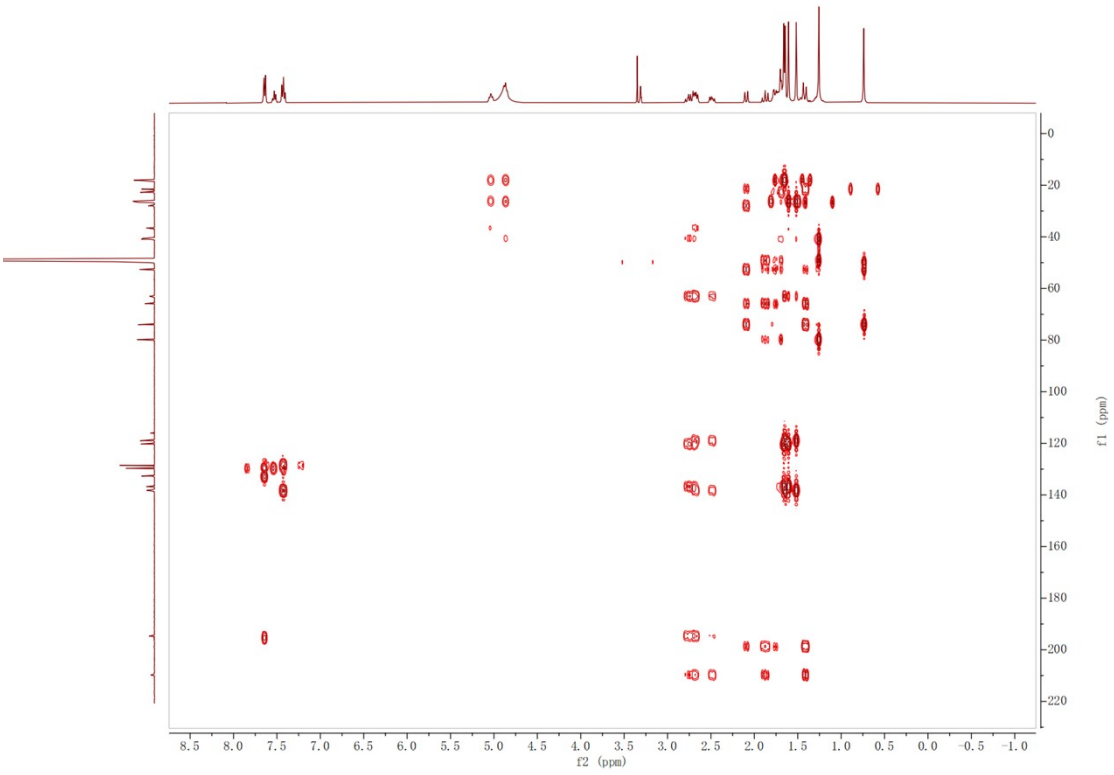
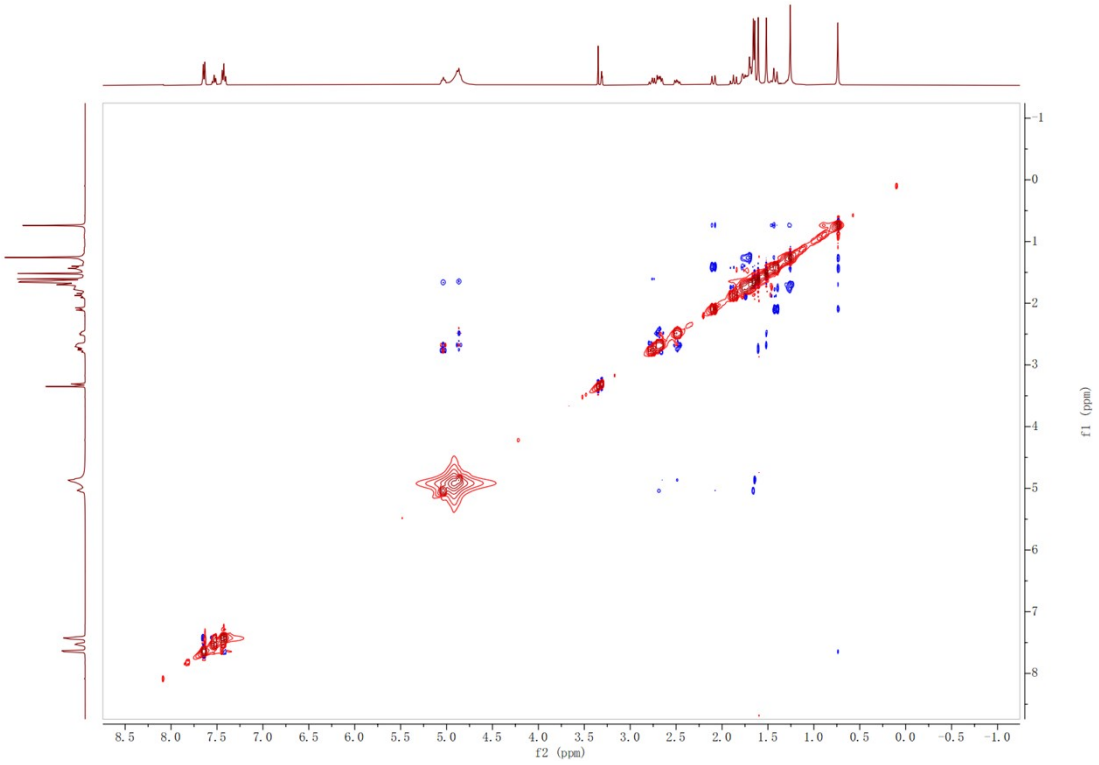


Figure S19. NOESY spectrum of compound **2** (recorded in methanol-d_4)



^{13}C NMR calculation details for 1a–1d

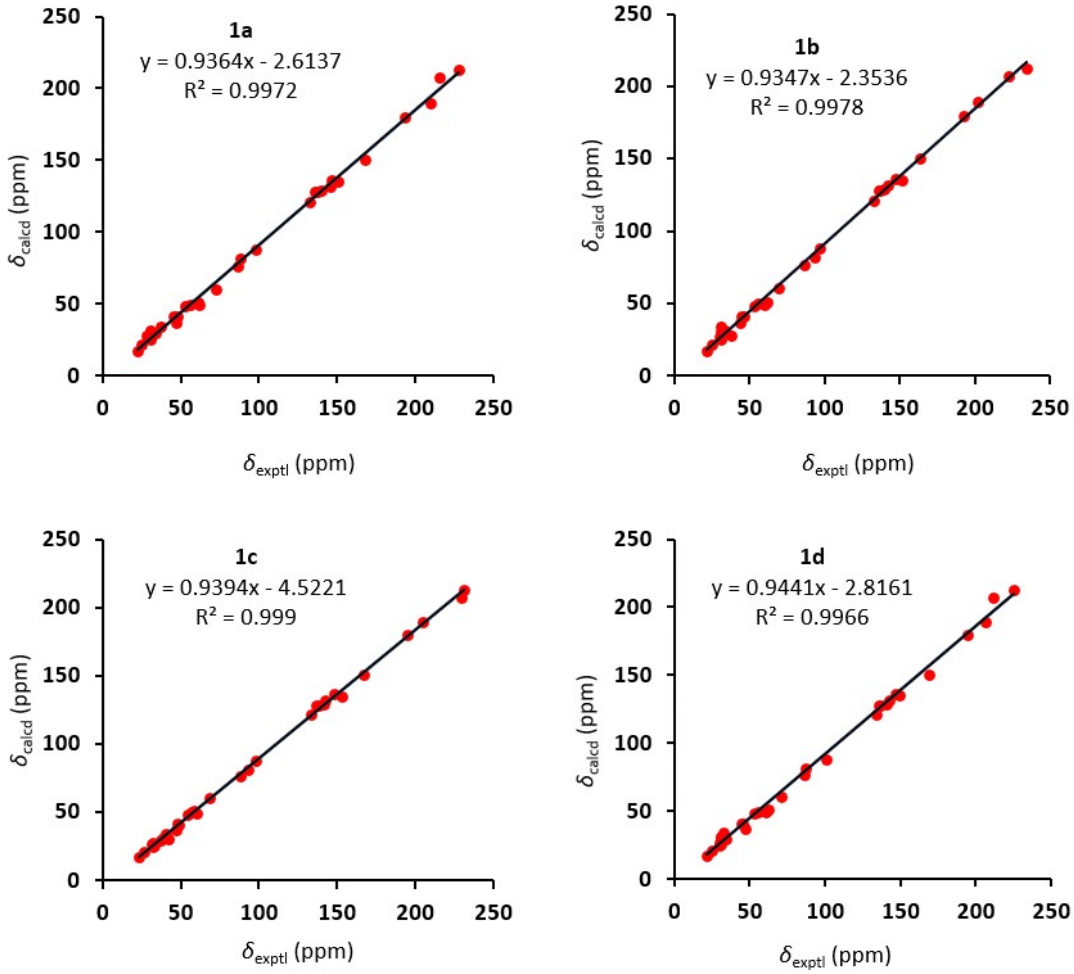


Figure S20. Regression analysis of experimental versus calculated ^{13}C NMR chemical shifts of **1a**–**1d** at the B972/pcSseg-2 level; linear fitting was shown as a line.

Table S1. Comparison of the experimental and computed ^{13}C NMR data for **1a**–**1d** (δ in ppm).

No.	δ_{expt}	δ_{calcd_corr} (**1a**)	δ_{calcd_corr} (**1b**)	δ_{calcd_corr} (**1c**)	δ_{calcd_corr} (**1d**)
1	212.7	210.8754701	216.5291906	212.4778998	209.6571619
2	81.7	79.72304757	84.60894326	83.16994785	79.71026474
3	207.4	199.4629832	205.400682	210.7977602	197.2682108
4	60.6	65.66144639	62.82989715	59.92361476	64.55358839
5	179.8	178.864248	178.0479	178.8683145	180.8977788
6	49.6	55.53756404	54.09522505	51.67850874	54.3314731
7	30.7	25.85026753	26.75116358	34.78421724	26.22776664
8	49.8	50.11921967	49.77261269	49.01956465	49.33730436
9	76.6	78.29847444	78.80204297	78.09228319	78.78027034
10	41.3	39.71649413	40.90217459	40.86708616	40.41647913

11	25.1	26.00897252	26.28927529	25.7517337	25.92011278
12	48.1	46.97375325	47.17819823	46.87581303	46.97298841
13	87.9	89.10396614	88.14191442	87.93791084	92.44850454
14	41.4	42.54931734	39.28673279	40.35212398	39.36334939
15	21.5	20.62641983	21.24198649	20.46634715	20.92668362
16	26.7	26.0219371	25.64167277	25.06532121	25.93245688
17	31.7	26.41237588	28.68147116	32.06278289	26.17347395
18	51	54.86688507	55.48396438	50.79914626	55.95205132
19	37	41.62602478	38.49092547	40.05625876	41.74759083
20	27.6	23.74214662	33.23736175	25.50349928	26.65976738
21	34.5	32.36794905	26.51839931	33.46789042	28.18081597
22	29.4	29.38589753	29.47591328	30.5927576	29.72001226
23	121.3	121.6767006	121.5011682	120.5406267	123.4805648
24	135.3	138.7590164	139.4336409	139.513663	138.4181507
25	17.7	18.03352496	18.04317855	17.503007	17.83715409
26	25.9	26.21074135	26.51817215	26.20699066	26.59474723
27	189.3	194.2116385	186.8883107	187.8669818	191.9499592
28	132	133.8415724	130.8828858	129.6600425	131.7848443
29	150.7	154.7866344	150.5247439	152.3876259	156.5348111
30	127.9	126.5374916	126.1310039	125.532056	126.49486
31	136.3	134.3423701	135.0407781	135.0671456	135.3653358
32	127.9	124.7522544	124.5750302	124.0753149	125.381246
33	129	128.5092424	128.5322635	128.5407279	130.3088068

Methods

In general, conformational analyses were carried out via random searching in the Sybyl-X 2.0 using the MMFF94S force field with an energy cutoff of 2.5 kcal/mol.[1] Subsequently, the lowest energy conformers were re-optimized using DFT at the B3LYP-D3(BJ)/6-31G** level in PCM methanol using Gaussian 09.[2] NMR shielding constants were computed using the GIAO method at the B972/pcSseg-2 level in PCM methanol using Gaussian 09.[2] Boltzmann weights were computed using relative free energies at the wB97M-V/def2-TZVP level in PCM methanol using ORCA.[3][4]

References:

[1] Sybyl Software, version X 2.0; Tripos Associates Inc.: St. Louis, MO, 2013.

[2] Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

[3] F. Neese, The ORCA program system, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2012, **2**, 73−78.

[4] F. Neese, Software update: the ORCA program system, version 4.0, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2017, **8**, e1327.

Table S2. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of yby5-12-3A (**1a**).

Conformers	ΔG (a.u.)	P(%)/100	G (a.u.)
yby5-12-3A000004_en_	0.00173	7.11	-1733.002478
yby5-12-3A000005_en_	6e-05	42.0	-1733.004153
yby5-12-3A000006_en_	0.0	44.52	-1733.004209
yby5-12-3A000007_en_	0.00183	6.37	-1733.002374

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15 K.

Table S3. Cartesian coordinates for the low-energy reoptimized random research conformers of yby5-12-3A at B3LYP-D3(BJ)/6-31G** level of theory in methanol.

yby5-12-3A000004_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.01561	1.725069	0.483128

1	6	0	-0.952199	0.825461	-1.328329
2	8	0	1.145234	1.75125	-1.117923
3	6	0	-1.32845	-1.345624	-3.224771
4	6	0	0.365441	-1.271594	-5.596861
5	6	0	-0.217437	0.825359	-7.502005
6	6	0	-3.006108	0.567201	-8.172826
7	6	0	-4.700739	-0.773837	-6.62701
8	6	0	-4.016458	-1.864355	-4.126826
9	8	0	-5.507752	-3.13489	-2.919741
10	6	0	-3.953219	1.688367	-10.356291
11	6	0	-6.468471	1.463461	-11.037794
12	6	0	-8.119676	0.084625	-9.53405
13	6	0	-7.231103	-1.013239	-7.347032
14	6	0	-0.045606	-3.635721	-1.810936
15	6	0	3.053914	-1.813853	-4.728649
16	6	0	2.708349	-3.78047	-2.6353
17	8	0	-1.064143	-5.058169	-0.363047
18	6	0	4.565804	-3.455523	-0.410717
19	6	0	4.372676	-5.423747	1.58823
20	6	0	3.375241	-5.18246	3.890113
21	6	0	3.277444	-7.377859	5.669062
22	6	0	-1.975087	3.581194	2.451594
23	6	0	-4.410108	4.843402	3.320548
24	6	0	-6.064747	2.972907	4.792869
25	6	0	-5.114325	0.280928	4.490018
26	6	0	-4.561889	-0.438994	1.788035
27	6	0	-6.384654	3.129218	7.648075
28	6	0	-7.499517	0.515049	8.32017
29	6	0	-7.016614	-1.259272	6.039508
30	8	0	-5.686869	5.246365	0.849665
31	6	0	-4.927055	3.476796	-0.818714
32	8	0	-5.702407	3.384103	-2.955542
33	8	0	-9.39271	-1.474776	4.7413
34	6	0	-6.061972	-3.859226	6.768535
35	6	0	-4.104205	7.401848	4.516127
36	1	0	-3.347124	0.14825	5.556892
37	1	0	-7.945562	3.080607	3.955347
38	1	0	-0.207722	-2.996468	-6.598871
39	1	0	2.944366	-5.688666	-3.39075
40	6	0	2.204508	-2.810306	4.886313
41	6	0	1.453244	0.363349	-9.822686
42	6	0	0.261539	3.510309	-6.53535
43	1	0	-2.705237	2.757493	-11.568172

44	1	0	-7.138132	2.361044	-12.749305
45	1	0	-10.086893	-0.102909	-10.056586
46	1	0	-8.480259	-2.047917	-6.108592
47	1	0	4.201447	-2.557055	-6.263459
48	1	0	3.972604	-0.135295	-3.99727
49	1	0	6.457017	-3.512138	-1.240309
50	1	0	4.332887	-1.563444	0.349396
51	1	0	5.088589	-7.273986	1.058501
52	1	0	4.219627	-6.939458	7.45302
53	1	0	1.32283	-7.850136	6.138145
54	1	0	4.161618	-9.053782	4.873707
55	1	0	-0.743477	4.951923	1.548207
56	1	0	-0.919011	2.689294	3.966214
57	1	0	-3.534728	-2.207963	1.68336
58	1	0	-6.299366	-0.736087	0.739292
59	1	0	-7.592634	4.678159	8.254302
60	1	0	-4.552707	3.383521	8.562522
61	1	0	-6.658547	-0.249654	10.033608
62	1	0	-9.527728	0.618167	8.629818
63	1	0	-9.172217	-2.645122	3.35965
64	1	0	-5.705728	-5.010906	5.096071
65	1	0	-4.301632	-3.734459	7.828933
66	1	0	-7.451989	-4.830678	7.932997
67	1	0	-3.067816	8.664732	3.268244
68	1	0	-5.932539	8.245088	4.929224
69	1	0	-3.062659	7.233022	6.280978
70	1	0	3.128805	-2.203631	6.628996
71	1	0	2.263645	-1.249769	3.55723
72	1	0	0.22698	-3.157684	5.3602
73	1	0	1.089745	1.727135	-11.313366
74	1	0	3.437806	0.545544	-9.315821
75	1	0	1.152137	-1.518247	-10.602428
76	1	0	-1.067708	4.043329	-5.069792
77	1	0	2.168751	3.713088	-5.798713
78	1	0	0.022248	4.848647	-8.079458

yby5-12-3A000005_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.165279	1.198578	0.844251
1	6	0	-1.104661	0.196396	-0.916848
2	8	0	0.94118	1.233649	-0.885368
3	6	0	-1.467526	-2.173868	-2.561267
4	6	0	0.338632	-2.390096	-4.84516
5	6	0	0.161442	-0.308853	-6.865894
6	6	0	-2.618334	0.364913	-7.231624
7	6	0	-4.56715	-0.798615	-5.853068
8	6	0	-4.073472	-2.551128	-3.731135
9	8	0	-5.566074	-4.176319	-3.083812
10	6	0	-3.307962	2.103485	-9.082714
11	6	0	-5.812665	2.683348	-9.558185
12	6	0	-7.726834	1.491134	-8.213693
13	6	0	-7.095615	-0.253977	-6.388115
14	6	0	-0.504624	-4.328266	-0.824739
15	6	0	2.862593	-3.215773	-3.737765
16	6	0	2.089726	-5.161751	-1.750028
17	8	0	-1.589039	-5.151286	1.005368
18	6	0	3.966234	-5.633248	0.409238
19	6	0	4.308487	-3.387007	2.07894
20	6	0	6.196311	-1.717557	2.083584
21	6	0	6.149877	0.509525	3.826487
22	6	0	-2.059833	2.130014	3.361849
23	6	0	-4.076406	4.033333	4.146318
24	6	0	-6.565798	2.68634	4.782911
25	6	0	-6.503	-0.062535	3.959326
26	6	0	-5.529866	-0.482729	1.305303
27	6	0	-7.512486	2.431217	7.488328
28	6	0	-9.548267	0.350076	7.27328
29	6	0	-9.116924	-1.040087	4.730689
30	8	0	-4.518287	5.352513	1.713026
31	6	0	-4.088139	3.75283	-0.224468
32	8	0	-4.429701	4.312673	-2.399672
33	8	0	-11.04164	-0.124626	3.041268
34	6	0	-9.26128	-3.892394	4.927022
35	6	0	-3.22722	5.993378	6.019582
36	1	0	-5.193665	-1.026952	5.236875
37	1	0	-8.035101	3.646235	3.701194
38	1	0	-0.383295	-4.075045	-5.81632
39	1	0	1.739436	-6.972009	-2.698433

40	6	0	8.454428	-1.83293	0.387603
41	6	0	1.169308	-1.458868	-9.338938
42	6	0	1.707966	2.07523	-6.304771
43	1	0	-1.862002	3.029443	-10.188551
44	1	0	-6.274006	4.067421	-10.990877
45	1	0	-9.686417	1.938904	-8.582387
46	1	0	-8.537671	-1.204338	-5.298146
47	1	0	4.10249	-4.033977	-5.159698
48	1	0	3.830306	-1.643885	-2.850578
49	1	0	3.256004	-7.20991	1.530811
50	1	0	5.744908	-6.251679	-0.421322
51	1	0	2.762383	-3.06057	3.386326
52	1	0	4.497631	0.491902	5.048538
53	1	0	7.834771	0.567417	5.017517
54	1	0	6.124507	2.271088	2.751301
55	1	0	-0.274488	3.082412	3.022144
56	1	0	-1.753214	0.639651	4.739578
57	1	0	-5.042346	-2.454879	1.065931
58	1	0	-6.970075	-0.023727	-0.093622
59	1	0	-8.258759	4.183145	8.26319
60	1	0	-5.982144	1.813719	8.726751
61	1	0	-9.458578	-0.965628	8.850804
62	1	0	-11.440989	1.148541	7.251167
63	1	0	-10.934385	-1.097774	1.503413
64	1	0	-7.854922	-4.616349	6.244188
65	1	0	-11.124089	-4.47172	5.580176
66	1	0	-8.910374	-4.782016	3.100589
67	1	0	-2.758364	5.096071	7.809613
68	1	0	-1.560108	6.977106	5.327807
69	1	0	-4.707746	7.376809	6.365747
70	1	0	8.527134	-0.163371	-0.824824
71	1	0	10.198144	-1.821494	1.490843
72	1	0	8.483851	-3.48683	-0.824986
73	1	0	1.08399	-0.105543	-10.882192
74	1	0	3.138252	-2.020449	-9.123018
75	1	0	0.079178	-3.114134	-9.895203
76	1	0	0.898909	3.200869	-4.802587
77	1	0	3.632191	1.581394	-5.778863
78	1	0	1.814769	3.254964	-7.985841

yby5-12-3A000006_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-2.018507	1.195453	0.543125
1	6	0	-0.685271	-0.485406	-1.39129
2	8	0	1.582019	-0.251912	-1.652711
3	6	0	-2.071533	-2.574607	-2.86253
4	6	0	-0.79664	-3.389014	-5.361901
5	6	0	-0.568241	-1.36613	-7.433915
6	6	0	-3.02459	0.142668	-7.492644
7	6	0	-5.013689	-0.292969	-5.789198
8	6	0	-4.800175	-2.064131	-3.635774
9	8	0	-6.629632	-3.080727	-2.681855
10	6	0	-3.394398	1.963172	-9.356485
11	6	0	-5.629587	3.30694	-9.540025
12	6	0	-7.601628	2.832145	-7.872931
13	6	0	-7.290569	1.025393	-6.024983
14	6	0	-1.647112	-4.93472	-1.180003
15	6	0	1.443345	-5.020869	-4.58229
16	6	0	0.379069	-6.576648	-2.391188
17	8	0	-2.704262	-5.37294	0.791824
18	6	0	2.255541	-7.624247	-0.447362
19	6	0	3.805277	-5.641527	0.826199
20	6	0	3.673016	-4.858858	3.220529
21	6	0	5.426376	-2.846996	4.166091
22	6	0	-0.327593	1.753442	2.833196
23	6	0	-1.471793	4.240508	3.729961
24	6	0	-4.150584	3.817187	4.764199
25	6	0	-5.110853	1.185919	4.132732
26	6	0	-4.713565	0.410697	1.410146
27	6	0	-4.7446	3.969582	7.576213
28	6	0	-7.352764	2.671376	7.764351
29	6	0	-7.765179	1.160495	5.288415
30	8	0	-1.792905	5.579111	1.286892
31	6	0	-2.186144	3.883617	-0.575244
32	8	0	-2.617578	4.474243	-2.726982
33	8	0	-9.498007	2.628719	3.794027
34	6	0	-8.807767	-1.473983	5.698237
35	6	0	0.224181	5.84765	5.34486
36	1	0	-4.030526	-0.134732	5.300723
37	1	0	-5.359974	5.18305	3.804471
38	1	0	-2.174935	-4.729035	-6.142936
39	1	0	-0.669258	-8.18251	-3.17933

40	6	0	1.878004	-5.859395	5.159876
41	6	0	-0.271622	-2.784263	-9.953069
42	6	0	1.684206	0.435231	-7.16172
43	1	0	-1.908417	2.348578	-10.704283
44	1	0	-5.836815	4.727816	-10.995985
45	1	0	-9.35202	3.877662	-8.012974
46	1	0	-8.781518	0.61736	-4.690709
47	1	0	2.096837	-6.22139	-6.117746
48	1	0	3.004362	-3.856574	-3.955072
49	1	0	1.2	-8.743657	0.914576
50	1	0	3.50792	-8.934344	-1.438553
51	1	0	5.201529	-4.729665	-0.366758
52	1	0	6.617857	-2.098077	2.669587
53	1	0	4.376821	-1.273406	4.989062
54	1	0	6.647376	-3.574792	5.663911
55	1	0	1.610063	2.030714	2.21926
56	1	0	-0.357257	0.279824	4.258358
57	1	0	-4.938409	-1.615512	1.236767
58	1	0	-6.106632	1.300272	0.182794
59	1	0	-4.771812	5.893084	8.301309
60	1	0	-3.340691	2.923621	8.668027
61	1	0	-7.465523	1.433656	9.402157
62	1	0	-8.868657	4.047467	7.932096
63	1	0	-9.968286	1.627744	2.34485
64	1	0	-10.639969	-1.386199	6.629805
65	1	0	-9.040869	-2.470416	3.908668
66	1	0	-7.53708	-2.598006	6.863879
67	1	0	0.630762	4.883007	7.115036
68	1	0	2.002473	6.216397	4.381431
69	1	0	-0.66586	7.647455	5.786093
70	1	0	0.561537	-7.243425	4.421849
71	1	0	2.910025	-6.702492	6.736919
72	1	0	0.757109	-4.321496	5.959622
73	1	0	-1.869634	-4.033609	-10.303979
74	1	0	-0.133584	-1.481898	-11.534726
75	1	0	1.446833	-3.9178	-9.93948
76	1	0	1.456107	1.753912	-5.616403
77	1	0	3.427873	-0.612046	-6.866926
78	1	0	1.909273	1.529853	-8.888536

yby5-12-3A000007_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-2.739278	1.691754	0.451338
1	6	0	-0.8705	0.546777	-1.431616
2	8	0	1.329775	1.214238	-1.311452
3	6	0	-1.577516	-1.570109	-3.293755
4	6	0	0.005428	-1.697101	-5.740184
5	6	0	-0.406237	0.457244	-7.625511
6	6	0	-3.234233	0.545203	-8.161782
7	6	0	-5.002886	-0.610015	-6.551036
8	6	0	-4.343561	-1.774615	-4.077781
9	8	0	-5.918301	-2.86114	-2.799543
10	6	0	-4.140425	1.803747	-10.286712
11	6	0	-6.691893	1.874857	-10.858092
12	6	0	-8.422532	0.664954	-9.299141
13	6	0	-7.572269	-0.553931	-7.161626
14	6	0	-0.506957	-3.987115	-1.920412
15	6	0	2.647947	-2.559714	-4.997122
16	6	0	2.173622	-4.449613	-2.858009
17	8	0	-1.614466	-5.279455	-0.416757
18	6	0	4.150441	-4.305242	-0.716697
19	6	0	3.769818	-6.148153	1.370814
20	6	0	2.98625	-5.671419	3.718625
21	6	0	2.629755	-7.76644	5.584092
22	6	0	-1.413281	3.442166	2.342686
23	6	0	-3.651211	4.981718	3.290066
24	6	0	-5.448865	3.32495	4.850141
25	6	0	-4.807313	0.542324	4.566034
26	6	0	-4.444463	-0.2783	1.859485
27	6	0	-5.649903	3.557547	7.710915
28	6	0	-7.02497	1.095651	8.467237
29	6	0	-6.801359	-0.762396	6.21301
30	8	0	-4.974175	5.503336	0.867307
31	6	0	-4.506312	3.628845	-0.794033
32	8	0	-5.395942	3.587592	-2.887141
33	8	0	-9.231221	-0.75913	4.999397
34	6	0	-6.086158	-3.43077	6.968526
35	6	0	-3.005155	7.496145	4.443176
36	1	0	-3.023538	0.240011	5.567835
37	1	0	-7.33433	3.626323	4.071584
38	1	0	-0.816503	-3.339396	-6.706559
39	1	0	2.162815	-6.382455	-3.586641

40	6	0	2.308048	-3.106821	4.694721
41	6	0	1.072797	-0.213655	-10.025119
42	6	0	0.458422	3.060196	-6.700572
43	1	0	-2.833509	2.750779	-11.537239
44	1	0	-7.328534	2.871268	-12.526923
45	1	0	-10.418508	0.706024	-9.737952
46	1	0	-8.876676	-1.45045	-5.873651
47	1	0	3.610512	-3.454225	-6.577834
48	1	0	3.807587	-1.002076	-4.342729
49	1	0	5.979467	-4.653539	-1.612562
50	1	0	4.205917	-2.371721	-0.035176
51	1	0	4.126011	-8.108735	0.874839
52	1	0	3.151081	-9.593286	4.800084
53	1	0	3.752701	-7.451719	7.287714
54	1	0	0.659305	-7.872762	6.191475
55	1	0	-0.076053	4.654409	1.365805
56	1	0	-0.396692	2.455967	3.825151
57	1	0	-3.605734	-2.144736	1.758982
58	1	0	-6.244808	-0.412821	0.886145
59	1	0	-6.653509	5.241468	8.330397
60	1	0	-3.770621	3.616214	8.560503
61	1	0	-6.230123	0.275213	10.176984
62	1	0	-9.020823	1.42813	8.821553
63	1	0	-9.166155	-1.945407	3.615408
64	1	0	-7.52592	-4.237722	8.196122
65	1	0	-5.900703	-4.643571	5.311862
66	1	0	-4.28758	-3.461094	7.970845
67	1	0	-1.89281	8.62833	3.136589
68	1	0	-4.704858	8.542169	4.934317
69	1	0	-1.905851	7.214088	6.157678
70	1	0	2.627429	-1.600518	3.341142
71	1	0	0.313594	-3.066659	5.224429
72	1	0	3.373873	-2.663182	6.405324
73	1	0	3.089751	-0.265397	-9.62782
74	1	0	0.508515	-2.053117	-10.757955
75	1	0	0.791696	1.170296	-11.51528
76	1	0	-0.730604	3.776416	-5.191819
77	1	0	2.400497	3.00465	-6.032055
78	1	0	0.348898	4.411831	-8.247593

Table S4. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of yby5-12-3B (**1b**).

Conformers	ΔG (a.u.)	P(%)/100	G (a.u.)
yby5-12-3B000001_en_	0.0	49.07	-1733.016719
yby5-12-3B000003_en_	0.00157	9.3	-1733.015149
yby5-12-3B000004_en_	0.00018	40.36	-1733.016534
yby5-12-3B000007_en_	0.00345	1.26	-1733.013267

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15 K.

Table S5. Cartesian coordinates for the low-energy reoptimized random research conformers of yby5-12-3B at B3LYP-D3(BJ)/6-31G** level of theory in methanol.

yby5-12-3B000001_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-5.744291	1.589254	-2.709327
1	6	0	-7.444533	1.826771	-0.393932
2	8	0	-9.228643	3.267896	-0.508617
3	6	0	-7.196537	0.23486	2.040561
4	6	0	-7.920985	1.769656	4.413883
5	6	0	-5.776206	3.329655	5.57638
6	6	0	-3.519297	1.635876	6.05938
7	6	0	-3.06918	-0.495212	4.545685
8	6	0	-4.729849	-1.242031	2.432156
9	8	0	-4.248564	-3.062464	1.100566
10	6	0	-1.784915	2.189809	7.958014
11	6	0	0.31448	0.682831	8.376861
12	6	0	0.73561	-1.436564	6.886365
13	6	0	-0.949143	-2.006569	4.983194
14	6	0	-4.969799	5.462647	3.787344
15	6	0	-6.768943	4.546226	8.009004
16	6	0	-9.344504	-1.795616	1.957821
17	6	0	-9.07932	-0.181182	6.211793
18	6	0	-10.56677	-1.975452	4.542514
19	8	0	-9.994522	-2.977956	0.124721
20	6	0	-10.811299	-4.721889	5.451528
21	6	0	-8.325323	-5.948744	5.993325
22	6	0	-7.052714	-7.569108	4.537562
23	6	0	-4.520172	-8.540515	5.339247
24	6	0	-7.931224	-8.526838	2.030216
25	6	0	-6.394803	3.590354	-4.701848
26	6	0	-4.0573	3.442466	-6.369688

27	6	0	-3.976676	0.916912	-7.791015
28	6	0	-5.887212	-0.944578	-6.72824
29	6	0	-5.829322	-1.141518	-3.884617
30	6	0	-4.526453	0.731555	-10.610001
31	6	0	-4.995194	-2.125248	-10.996914
32	6	0	-5.461688	-3.303141	-8.356695
33	8	0	-2.039653	3.30716	-4.415545
34	6	0	-2.957488	2.242563	-2.29067
35	8	0	-1.667853	1.910571	-0.442545
36	8	0	-3.147702	-4.5581	-7.682687
37	6	0	-7.643248	-5.156331	-8.279114
38	6	0	-3.517514	5.743206	-7.945751
39	1	0	-7.760978	-0.264507	-7.276455
40	1	0	-2.093876	0.136539	-7.479016
41	1	0	-9.407654	3.070977	3.833103
42	1	0	-12.474848	-1.222532	4.258129
43	1	0	-2.070489	3.826975	9.142339
44	1	0	1.62365	1.165301	9.872225
45	1	0	2.371288	-2.620047	7.205272
46	1	0	-0.664692	-3.621042	3.769055
47	1	0	-3.528266	6.625454	4.682937
48	1	0	-4.156978	4.735439	2.053364
49	1	0	-6.576709	6.664095	3.322587
50	1	0	-8.557459	5.493788	7.630951
51	1	0	-7.074917	3.167692	9.501607
52	1	0	-5.476445	5.974613	8.723718
53	1	0	-10.269496	0.710459	7.627924
54	1	0	-7.588921	-1.187017	7.208668
55	1	0	-11.962085	-4.711289	7.165379
56	1	0	-11.874975	-5.76811	4.037807
57	1	0	-7.449252	-5.4104	7.767587
58	1	0	-3.090576	-8.041361	3.938771
59	1	0	-3.932045	-7.77375	7.153376
60	1	0	-4.521991	-10.600495	5.474453
61	1	0	-9.78509	-7.838043	1.496178
62	1	0	-6.610897	-7.937742	0.560652
63	1	0	-7.96264	-10.59042	2.016007
64	1	0	-6.5325	5.442586	-3.822716
65	1	0	-8.150534	3.243314	-5.69903
66	1	0	-7.467403	-2.140522	-3.163324
67	1	0	-4.183936	-2.175415	-3.23007
68	1	0	-2.999904	1.444978	-11.787556
69	1	0	-6.222444	1.80492	-11.086024

70	1	0	-6.595204	-2.467795	-12.241809
71	1	0	-3.363411	-3.052422	-11.832427
72	1	0	-3.392418	-5.348235	-6.05752
73	1	0	-7.278296	-6.745689	-9.532768
74	1	0	-7.922842	-5.891489	-6.373485
75	1	0	-9.402416	-4.258289	-8.860575
76	1	0	-1.73939	5.540943	-8.957525
77	1	0	-5.013619	6.017182	-9.329582
78	1	0	-3.411264	7.421907	-6.76392

yby5-12-3B000003_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-5.139409	1.920635	-3.053545
1	6	0	-6.651138	2.330952	-0.636045
2	8	0	-7.896518	4.249138	-0.442603
3	6	0	-6.885016	0.384755	1.517911
4	6	0	-7.131588	1.644619	4.13271
5	6	0	-4.62248	2.39153	5.37523
6	6	0	-2.900032	0.105853	5.476536
7	6	0	-3.09457	-1.824096	3.666532
8	6	0	-4.978482	-1.796141	1.607319
9	8	0	-5.153958	-3.542881	0.105033
10	6	0	-1.035624	-0.112763	7.31819
11	6	0	0.578545	-2.172795	7.39459
12	6	0	0.361881	-4.085459	5.610046
13	6	0	-1.464581	-3.899145	3.761932
14	6	0	-3.291239	4.483491	3.873057
15	6	0	-5.207472	3.432478	8.015233
16	6	0	-9.53761	-0.896825	1.254276
17	6	0	-8.687971	-0.239807	5.696596
18	6	0	-10.497645	-1.527311	3.871194
19	8	0	-10.658018	-1.298195	-0.686211
20	6	0	-10.670913	-4.42197	4.176841
21	6	0	-11.458506	-5.150546	6.776866
22	6	0	-10.033655	-6.187407	8.583788
23	6	0	-11.125123	-6.775891	11.127406
24	6	0	-7.300041	-6.85744	8.296336
25	6	0	-5.195255	4.268048	-4.750544
26	6	0	-3.013474	3.67681	-6.525139
27	6	0	-3.674059	1.438387	-8.244961
28	6	0	-6.038488	0.082696	-7.339271
29	6	0	-6.02806	-0.490372	-4.545944
30	6	0	-4.264704	1.787447	-11.04137
31	6	0	-5.578948	-0.721844	-11.756589
32	6	0	-6.326577	-2.062698	-9.263989
33	8	0	-1.106082	2.718198	-4.690648
34	6	0	-2.282431	1.677213	-2.687254
35	8	0	-1.142395	0.722226	-0.960484
36	8	0	-4.455683	-3.993389	-8.869476
37	6	0	-8.942761	-3.225054	-9.308651
38	6	0	-1.847613	5.915163	-7.829019
39	1	0	-7.634264	1.340898	-7.718186

40	1	0	-2.097564	0.117419	-8.10719
41	1	0	-8.242065	3.356368	3.856163
42	1	0	-12.399681	-0.740587	4.011045
43	1	0	-0.833229	1.345732	8.732009
44	1	0	2.006425	-2.284373	8.854808
45	1	0	1.618158	-5.697072	5.661077
46	1	0	-1.671413	-5.343851	2.335313
47	1	0	-2.694036	3.836676	2.022972
48	1	0	-4.53112	6.109813	3.642869
49	1	0	-1.595578	5.090765	4.867121
50	1	0	-6.676616	4.868702	7.887688
51	1	0	-5.849816	1.967823	9.304152
52	1	0	-3.561069	4.331055	8.853721
53	1	0	-9.685573	0.691418	7.22879
54	1	0	-7.451211	-1.634137	6.56361
55	1	0	-12.024268	-5.123123	2.78889
56	1	0	-8.854205	-5.24803	3.686029
57	1	0	-13.414607	-4.725247	7.239696
58	1	0	-10.96187	-8.788702	11.55572
59	1	0	-10.101667	-5.781556	12.619861
60	1	0	-13.109573	-6.256198	11.257224
61	1	0	-7.001271	-8.866283	8.661495
62	1	0	-6.538865	-6.433627	6.440857
63	1	0	-6.15502	-5.841731	9.680688
64	1	0	-4.782947	5.949023	-3.642581
65	1	0	-6.986175	4.575056	-5.698595
66	1	0	-7.887753	-1.048043	-3.887654
67	1	0	-4.757954	-2.039549	-4.102874
68	1	0	-2.59753	2.155355	-12.186615
69	1	0	-5.5566	3.37228	-11.311104
70	1	0	-7.236709	-0.39802	-12.929139
71	1	0	-4.324552	-1.966269	-12.804844
72	1	0	-4.893806	-4.893184	-7.345027
73	1	0	-10.385726	-1.796536	-9.650139
74	1	0	-9.069637	-4.645908	-10.790619
75	1	0	-9.381817	-4.132823	-7.510613
76	1	0	-1.268231	7.329523	-6.454554
77	1	0	-0.203019	5.356676	-8.928524
78	1	0	-3.211988	6.772683	-9.1065

yby5-12-3B000004_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-5.424904	1.469819	-3.007297
1	6	0	-7.390224	1.470896	-0.896127
2	8	0	-9.219109	2.840652	-1.130379
3	6	0	-7.346707	-0.271521	1.440806
4	6	0	-8.43953	1.043743	3.801939
5	6	0	-6.54744	2.620838	5.322911
6	6	0	-4.266529	1.017603	5.970755
7	6	0	-3.495558	-0.95304	4.372599
8	6	0	-4.862398	-1.649158	2.040002
9	8	0	-4.135375	-3.360808	0.679632
10	6	0	-2.818617	1.513969	8.109966
11	6	0	-0.681179	0.109518	8.670304
12	6	0	0.069628	-1.839677	7.080652
13	6	0	-1.334395	-2.354999	4.947055
14	6	0	-5.655952	4.912971	3.788445
15	6	0	-7.89597	3.610464	7.686902
16	6	0	-9.347436	-2.398486	0.951882
17	6	0	-9.678328	-1.096559	5.305921
18	6	0	-10.839036	-2.842425	3.356833
19	8	0	-9.696473	-3.483006	-1.017539
20	6	0	-10.938578	-5.655542	4.073753
21	6	0	-8.371967	-6.797742	4.342877
22	6	0	-7.085388	-7.260102	6.462366
23	6	0	-4.483414	-8.364043	6.357988
24	6	0	-8.039814	-6.745508	9.074396
25	6	0	-5.967223	3.576951	-4.923521
26	6	0	-3.454053	3.684853	-6.310317
27	6	0	-3.070188	1.288658	-7.89919
28	6	0	-4.949314	-0.763362	-7.174652
29	6	0	-5.20362	-1.169934	-4.364861
30	6	0	-3.332894	1.293192	-10.764638
31	6	0	-3.539678	-1.548016	-11.403166
32	6	0	-4.23074	-2.968044	-8.912053
33	8	0	-1.66026	3.491404	-4.161333
34	6	0	-2.753669	2.237242	-2.221192
35	8	0	-1.659494	1.854151	-0.262251
36	8	0	-2.118009	-4.369426	-7.955076
37	6	0	-6.317135	-4.891691	-9.236424
38	6	0	-2.886053	6.126327	-7.648455
39	1	0	-6.782773	-0.131653	-7.890361

40	1	0	-1.150679	0.654132	-7.452678
41	1	0	-9.92282	2.307138	3.135093
42	1	0	-12.760724	-2.218882	2.909116
43	1	0	-3.361494	3.023616	9.371765
44	1	0	0.402348	0.542076	10.350119
45	1	0	1.741557	-2.936694	7.504391
46	1	0	-0.795072	-3.845205	3.662578
47	1	0	-7.262753	6.05539	3.195566
48	1	0	-4.409557	6.087403	4.92801
49	1	0	-4.591245	4.352876	2.130358
50	1	0	-9.68887	4.470781	7.154291
51	1	0	-8.279366	2.11959	9.047849
52	1	0	-6.790797	5.061151	8.633785
53	1	0	-11.082354	-0.388436	6.626775
54	1	0	-8.260303	-2.108454	6.397914
55	1	0	-12.046734	-5.831327	5.798828
56	1	0	-11.972821	-6.650919	2.595426
57	1	0	-7.441664	-7.223101	2.567115
58	1	0	-3.843027	-8.631376	4.424584
59	1	0	-3.129973	-7.135324	7.314383
60	1	0	-4.412266	-10.186896	7.325452
61	1	0	-9.940477	-5.973694	9.113165
62	1	0	-8.030114	-8.46963	10.208629
63	1	0	-6.798202	-5.409996	10.042753
64	1	0	-6.31801	5.34929	-3.944791
65	1	0	-7.577016	3.213805	-6.137804
66	1	0	-6.855214	-2.299703	-3.925267
67	1	0	-3.600861	-2.198664	-3.608796
68	1	0	-1.770439	2.213271	-11.734227
69	1	0	-5.060236	2.277422	-11.311777
70	1	0	-4.9406	-1.893159	-12.869305
71	1	0	-1.755279	-2.298486	-12.09916
72	1	0	-0.770286	-3.201156	-7.582646
73	1	0	-5.74876	-6.343685	-10.57796
74	1	0	-6.741834	-5.807628	-7.445988
75	1	0	-8.030283	-3.993781	-9.936609
76	1	0	-3.026737	7.712443	-6.348643
77	1	0	-0.992955	6.107361	-8.450261
78	1	0	-4.22927	6.418981	-9.177043

yby5-12-3B000007_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-5.055307	1.636055	-3.040373
1	6	0	-6.472929	1.658388	-0.530918
2	8	0	-8.259925	3.081036	-0.300929
3	6	0	-5.928373	-0.141135	1.702085
4	6	0	-6.403917	1.131664	4.281826
5	6	0	-4.196621	2.688945	5.326308
6	6	0	-1.813948	1.105649	5.339771
7	6	0	-1.485606	-0.875905	3.608535
8	6	0	-3.406896	-1.581887	1.710809
9	8	0	-3.086269	-3.355984	0.270888
10	6	0	0.151354	1.627937	7.007657
11	6	0	2.368868	0.237647	6.988756
12	6	0	2.674206	-1.733609	5.282645
13	6	0	0.753831	-2.276463	3.608806
14	6	0	-3.728776	5.033589	3.68504
15	6	0	-4.918154	3.595474	7.981143
16	6	0	-8.039677	-2.214399	1.655231
17	6	0	-7.269914	-1.042418	5.985522
18	6	0	-8.972295	-2.643088	4.327372
19	8	0	-8.844422	-3.275442	-0.190828
20	6	0	-9.154905	-5.455622	4.984445
21	6	0	-10.294382	-5.885917	7.528014
22	6	0	-12.67193	-6.549791	8.049007
23	6	0	-13.536053	-6.875295	10.723952
24	6	0	-14.66459	-7.02245	6.099237
25	6	0	-6.001875	3.72166	-4.815806
26	6	0	-3.848777	3.800505	-6.719152
27	6	0	-3.800308	1.377162	-8.308502
28	6	0	-5.497613	-0.648097	-7.183039
29	6	0	-5.141308	-1.016454	-4.378294
30	6	0	-4.641581	1.340431	-11.061488
31	6	0	-5.023059	-1.50607	-11.590891
32	6	0	-5.138964	-2.872959	-9.003292
33	8	0	-1.631505	3.648574	-4.994394
34	6	0	-2.269665	2.394648	-2.872376
35	8	0	-0.777746	1.985767	-1.199716
36	8	0	-2.70739	-4.038515	-8.666192
37	6	0	-7.205695	-4.846785	-8.825114
38	6	0	-3.586633	6.2221	-8.180756
39	1	0	-7.448612	-0.036972	-7.492468

40	1	0	-1.859648	0.684004	-8.248879
41	1	0	-8.001628	2.406197	4.025756
42	1	0	-10.886387	-1.855658	4.350345
43	1	0	-0.04211	3.146955	8.357492
44	1	0	3.859882	0.69382	8.312376
45	1	0	4.402657	-2.824353	5.257869
46	1	0	0.940943	-3.783487	2.245368
47	1	0	-3.072953	4.532779	1.809409
48	1	0	-5.449594	6.149933	3.510698
49	1	0	-2.269815	6.20876	4.534629
50	1	0	-6.786684	4.460225	7.937378
51	1	0	-4.951732	2.05914	9.344885
52	1	0	-3.613381	5.024286	8.673733
53	1	0	-8.241088	-0.364151	7.660106
54	1	0	-5.651121	-2.149397	6.625566
55	1	0	-10.212304	-6.398254	3.496933
56	1	0	-7.249308	-6.24937	4.936137
57	1	0	-9.03556	-5.568586	9.117659
58	1	0	-15.113055	-5.614163	11.154114
59	1	0	-14.222671	-8.794409	11.053539
60	1	0	-12.030398	-6.498425	12.071702
61	1	0	-14.007911	-6.750816	4.175148
62	1	0	-15.398411	-8.945318	6.255269
63	1	0	-16.275532	-5.766996	6.397389
64	1	0	-6.131723	5.505962	-3.805883
65	1	0	-7.835624	3.343619	-5.649368
66	1	0	-6.654847	-2.136215	-3.570005
67	1	0	-3.396082	-2.01178	-3.965912
68	1	0	-3.285992	2.204349	-12.342735
69	1	0	-6.424989	2.353006	-11.281129
70	1	0	-6.737209	-1.850584	-12.67274
71	1	0	-3.457143	-2.295718	-12.660536
72	1	0	-2.746436	-4.973106	-7.100631
73	1	0	-9.059224	-4.013004	-9.152304
74	1	0	-6.902277	-6.327987	-10.220096
75	1	0	-7.237932	-5.719667	-6.958186
76	1	0	-3.439543	7.826821	-6.90442
77	1	0	-1.91695	6.183134	-9.379633
78	1	0	-5.231803	6.498176	-9.382656

Table S6. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of yby5-12-3C (**1c**).

Conformers	ΔG (a.u.)	P(%)/100	G (a.u.)
yby5-12-3C5000002_en_	0.00198	8.20	-1733.02374
yby5-12-3C5000003_en_	0.00256	4.44	-1733.02316
yby5-12-3C5000005_en_	0.00000	66.95	-1733.02572
yby5-12-3C5000009_en_	0.00197	8.32	-1733.02375
yby5-12-3C5000014_en_	0.00189	9.04	-1733.02383
yby5-12-3C5000021_en_	0.00292	3.04	-1733.02281

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15 K.

Table S7. Cartesian coordinates for the low-energy reoptimized random research conformers of yby5-12-3C at B3LYP-D3(BJ)/6-31G** level of theory in methanol.

yby5-12-3C5000002_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.661286	-0.484268	-2.973349
1	6	0	-6.966171	-0.244977	-1.944491
2	8	0	-5.366841	0.452507	-3.42591
3	6	0	-6.300659	-0.883368	0.805423
4	6	0	-6.224295	-3.767796	1.309147
5	6	0	-3.593661	-4.993833	0.970144
6	6	0	-1.712536	-3.62223	2.645876
7	6	0	-1.824524	-0.970061	2.800824
8	6	0	-3.845712	0.502638	1.53679
9	8	0	-3.671039	2.768159	1.199342
10	6	0	0.223148	-4.863595	3.933972
11	6	0	1.999015	-3.520564	5.332928
12	6	0	1.894115	-0.892793	5.452136
13	6	0	-0.008365	0.373103	4.177431
14	6	0	-3.816525	-7.821607	1.588105
15	6	0	-2.684968	-4.755843	-1.788687
16	6	0	-8.299583	0.149007	2.71238
17	6	0	-7.304736	-4.143187	4.024314
18	6	0	-8.564634	-1.683507	4.893728
19	8	0	-9.304142	2.181416	2.50614
20	6	0	-7.294931	-0.562335	7.296904
21	6	0	-8.64156	1.694189	8.329325
22	6	0	-7.860464	4.097167	8.31842
23	6	0	-9.510112	6.165517	9.351077
24	6	0	-5.397623	4.994449	7.232356
25	6	0	-9.657225	-1.592393	-5.670487

26	6	0	-12.469568	-2.165359	-5.982799
27	6	0	-13.997844	0.308529	-6.138856
28	6	0	-12.405067	2.598587	-5.37646
29	6	0	-10.947165	2.223685	-2.932668
30	6	0	-15.116614	1.226955	-8.646348
31	6	0	-15.722033	4.052526	-8.101698
32	6	0	-14.294662	4.792534	-5.64143
33	8	0	-13.056594	-3.287687	-3.466458
34	6	0	-11.515161	-2.292036	-1.698129
35	8	0	-11.722114	-2.808043	0.516267
36	8	0	-16.149817	4.724075	-3.654993
37	6	0	-13.059977	7.387253	-5.748694
38	6	0	-13.138152	-4.136329	-7.9329
39	1	0	-11.01827	2.909336	-6.898177
40	1	0	-15.557559	0.12718	-4.780939
41	1	0	-7.490076	-4.699394	-0.041198
42	1	0	-10.586024	-1.917933	5.261628
43	1	0	0.360665	-6.907468	3.852933
44	1	0	3.478935	-4.535484	6.330709
45	1	0	3.287825	0.153028	6.535717
46	1	0	-0.146258	2.420036	4.219942
47	1	0	-2.08263	-8.833528	1.091908
48	1	0	-4.221787	-8.170645	3.584368
49	1	0	-5.349136	-8.647354	0.467111
50	1	0	-0.878403	-5.73812	-2.020469
51	1	0	-4.062462	-5.625504	-3.072146
52	1	0	-2.420241	-2.788988	-2.354698
53	1	0	-8.638532	-5.720015	4.044614
54	1	0	-5.754971	-4.620634	5.315019
55	1	0	-7.303204	-2.085202	8.7103
56	1	0	-5.303287	-0.167674	6.887259
57	1	0	-10.513144	1.303275	9.102345
58	1	0	-9.918204	7.565833	7.875263
59	1	0	-11.304975	5.435754	10.067864
60	1	0	-8.554336	7.182096	10.886466
61	1	0	-5.737662	6.080034	5.498774
62	1	0	-4.434613	6.257486	8.565623
63	1	0	-4.105569	3.461146	6.751334
64	1	0	-8.558451	-3.349805	-5.7066
65	1	0	-8.883432	-0.324432	-7.097728
66	1	0	-9.475033	3.657577	-2.701987
67	1	0	-12.170798	2.337272	-1.269038
68	1	0	-16.786343	0.162056	-9.238554

69	1	0	-13.705745	1.073726	-10.159538
70	1	0	-15.137629	5.264355	-9.671891
71	1	0	-17.74292	4.35704	-7.795901
72	1	0	-15.344815	5.256798	-2.107364
73	1	0	-14.490586	8.843689	-6.082007
74	1	0	-12.094603	7.823392	-3.966428
75	1	0	-11.656249	7.477727	-7.266501
76	1	0	-12.627654	-3.460372	-9.81903
77	1	0	-12.11744	-5.895081	-7.561456
78	1	0	-15.16805	-4.528432	-7.907552

yby5-12-3C5000003_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.690151	-0.335887	-2.953074
1	6	0	-6.982168	-0.066618	-1.966244
2	8	0	-5.426247	0.702769	-3.458826
3	6	0	-6.251424	-0.766917	0.751093
4	6	0	-6.160001	-3.659456	1.195705
5	6	0	-3.535031	-4.872129	0.777601
6	6	0	-1.623214	-3.533438	2.444761
7	6	0	-1.738379	-0.885868	2.65929
8	6	0	-3.78759	0.609235	1.465781
9	8	0	-3.62127	2.881806	1.175646
10	6	0	0.339463	-4.797906	3.66788
11	6	0	2.139251	-3.481123	5.061325
12	6	0	2.030519	-0.857048	5.239835
13	6	0	0.100695	0.431351	4.030111
14	6	0	-3.738831	-7.713335	1.336073
15	6	0	-2.685456	-4.568343	-1.993369
16	6	0	-8.218286	0.223025	2.716481
17	6	0	-7.183718	-4.091168	3.925123
18	6	0	-8.437128	-1.654323	4.865841
19	8	0	-9.230938	2.254259	2.564875
20	6	0	-7.133875	-0.574204	7.269185
21	6	0	-8.471437	1.661278	8.357763
22	6	0	-7.70077	4.067478	8.366606
23	6	0	-9.348091	6.116304	9.440956
24	6	0	-5.259621	4.990689	7.253913
25	6	0	-9.697671	-1.429726	-5.657871
26	6	0	-12.503742	-2.038883	-5.947628
27	6	0	-14.063376	0.416396	-6.086557
28	6	0	-12.488013	2.719289	-5.314705
29	6	0	-11.020687	2.350929	-2.874365
30	6	0	-15.191032	1.330833	-8.593833
31	6	0	-15.763927	4.171489	-8.078676
32	6	0	-14.384596	4.887255	-5.567923
33	8	0	-13.057589	-3.17441	-3.433229
34	6	0	-11.502918	-2.177335	-1.67152
35	8	0	-11.678472	-2.722824	0.53751
36	8	0	-16.07216	4.666139	-3.449374
37	6	0	-13.188525	7.50139	-5.611486
38	6	0	-13.162442	-4.013219	-7.898801
39	1	0	-11.114063	3.049054	-6.843148

40	1	0	-15.614957	0.203501	-4.726325
41	1	0	-7.450698	-4.569504	-0.14553
42	1	0	-10.451381	-1.905419	5.260625
43	1	0	0.479551	-6.839281	3.540295
44	1	0	3.640106	-4.513809	6.008385
45	1	0	3.442345	0.168818	6.319135
46	1	0	-0.041641	2.476437	4.12062
47	1	0	-2.01286	-8.709131	0.782634
48	1	0	-4.103372	-8.108003	3.331855
49	1	0	-5.292266	-8.517715	0.228241
50	1	0	-0.8767	-5.530555	-2.285649
51	1	0	-4.08338	-5.420261	-3.266507
52	1	0	-2.447629	-2.587333	-2.521512
53	1	0	-8.511272	-5.673439	3.941149
54	1	0	-5.605987	-4.587588	5.174435
55	1	0	-7.117705	-2.121241	8.656173
56	1	0	-5.149334	-0.166857	6.837182
57	1	0	-10.331028	1.252381	9.150025
58	1	0	-8.370308	7.140709	10.957085
59	1	0	-9.802821	7.512793	7.97518
60	1	0	-11.119896	5.36618	10.193225
61	1	0	-4.282351	6.242861	8.587035
62	1	0	-3.967184	3.470429	6.733771
63	1	0	-5.633203	6.094058	5.5384
64	1	0	-8.576321	-3.172281	-5.716046
65	1	0	-8.952755	-0.143915	-7.084713
66	1	0	-9.569733	3.805477	-2.644807
67	1	0	-12.253374	2.4575	-1.221338
68	1	0	-16.871263	0.273062	-9.169181
69	1	0	-13.791935	1.155074	-10.114931
70	1	0	-15.108764	5.362025	-9.639707
71	1	0	-17.794035	4.505963	-7.858958
72	1	0	-17.278959	6.027336	-3.543829
73	1	0	-14.623865	8.958614	-5.952637
74	1	0	-12.273457	7.90477	-3.801027
75	1	0	-11.776402	7.645399	-7.117385
76	1	0	-12.668416	-3.330474	-9.786911
77	1	0	-12.121523	-5.761613	-7.534679
78	1	0	-15.187831	-4.428114	-7.862952

yby5-12-3C5000005_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.292921	0.151749	-2.942034
1	6	0	-6.878977	-0.26595	-1.401075
2	8	0	-4.900659	0.052336	-2.517168
3	6	0	-6.890318	-1.00636	1.40026
4	6	0	-7.616914	-3.789511	1.966086
5	6	0	-5.482747	-5.748034	1.637305
6	6	0	-3.166138	-4.932302	3.122421
7	6	0	-2.596744	-2.351877	3.426195
8	6	0	-4.25468	-0.302177	2.474937
9	8	0	-3.609313	1.899593	2.526222
10	6	0	-1.474237	-6.701792	4.107613
11	6	0	0.71376	-5.952724	5.352311
12	6	0	1.27558	-3.395383	5.629129
13	6	0	-0.374057	-1.614003	4.66161
14	6	0	-6.500434	-8.330873	2.505972
15	6	0	-4.717863	-5.992497	-1.166535
16	6	0	-8.814157	0.547326	2.984269
17	6	0	-8.669378	-3.690923	4.699303
18	6	0	-9.945652	-1.120038	5.033079
19	8	0	-9.243548	2.760737	2.670041
20	6	0	-9.690384	0.111675	7.665725
21	6	0	-7.003997	0.464966	8.516784
22	6	0	-5.657488	2.607846	8.473565
23	6	0	-2.962352	2.643649	9.369458
24	6	0	-6.593342	5.11171	7.52919
25	6	0	-8.993552	-0.930744	-5.634691
26	6	0	-11.736519	-0.832338	-6.524342
27	6	0	-12.591342	1.931591	-6.865024
28	6	0	-10.699526	3.784879	-5.694742
29	6	0	-9.88778	3.089738	-3.028703
30	6	0	-12.931572	3.080415	-9.502092
31	6	0	-12.923222	5.975541	-8.976318
32	6	0	-11.93254	6.348507	-6.218674
33	8	0	-13.069045	-1.777161	-4.234834
34	6	0	-11.746693	-1.141062	-2.145781
35	8	0	-12.541169	-1.542376	-0.04601
36	8	0	-14.005295	6.559837	-4.474135
37	6	0	-10.156486	8.590255	-5.922431
38	6	0	-12.425617	-2.594022	-8.6594
39	1	0	-9.008417	3.76604	-6.908457

40	1	0	-14.392512	2.117399	-5.852489
41	1	0	-9.153443	-4.344366	0.695309
42	1	0	-11.959907	-1.25721	4.565519
43	1	0	-1.862634	-8.704749	3.906417
44	1	0	1.988564	-7.37515	6.105967
45	1	0	2.988226	-2.805213	6.593304
46	1	0	0.003874	0.392867	4.834606
47	1	0	-5.239368	-9.866557	1.936571
48	1	0	-6.749509	-8.426305	4.555392
49	1	0	-8.334616	-8.684764	1.611322
50	1	0	-3.368864	-7.545006	-1.395453
51	1	0	-6.385963	-6.414448	-2.325675
52	1	0	-3.827931	-4.273533	-1.878246
53	1	0	-9.975907	-5.251497	5.053208
54	1	0	-7.087967	-3.879121	6.025628
55	1	0	-10.695566	1.917832	7.611886
56	1	0	-10.694571	-1.093222	9.02561
57	1	0	-6.053756	-1.216768	9.235864
58	1	0	-2.286014	0.758106	9.878605
59	1	0	-1.728889	3.411781	7.889245
60	1	0	-2.756178	3.886759	11.018265
61	1	0	-8.608253	5.132644	7.102441
62	1	0	-6.178028	6.599796	8.912837
63	1	0	-5.591939	5.59887	5.779365
64	1	0	-8.338913	-2.894521	-5.537964
65	1	0	-7.679177	0.123689	-6.819811
66	1	0	-8.194267	4.132214	-2.464587
67	1	0	-11.357821	3.52907	-1.64705
68	1	0	-14.655181	2.448789	-10.452118
69	1	0	-11.327007	2.575851	-10.715787
70	1	0	-11.724092	6.980666	-10.331058
71	1	0	-14.825904	6.774378	-9.127719
72	1	0	-14.805674	8.174433	-4.739629
73	1	0	-8.488442	8.376798	-7.128452
74	1	0	-11.103862	10.353483	-6.463968
75	1	0	-9.538219	8.763855	-3.956398
76	1	0	-11.39648	-2.062897	-10.37226
77	1	0	-11.936414	-4.542425	-8.171935
78	1	0	-14.452274	-2.500366	-9.058816

yby5-12-3C5000009_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.246425	-0.3639	-2.91442
1	6	0	-6.600949	-0.300842	-1.734057
2	8	0	-4.876467	0.270189	-3.125812
3	6	0	-6.139682	-0.959681	1.053757
4	6	0	-6.312288	-3.836088	1.577398
5	6	0	-3.765097	-5.258389	1.407583
6	6	0	-1.893264	-4.016097	3.191122
7	6	0	-1.811288	-1.361252	3.318256
8	6	0	-3.632342	0.244448	1.918874
9	8	0	-3.263456	2.485176	1.573518
10	6	0	-0.145212	-5.385315	4.611038
11	6	0	1.636739	-4.163189	6.109979
12	6	0	1.727602	-1.533866	6.200444
13	6	0	0.012248	-0.142543	4.796753
14	6	0	-4.238751	-8.054969	2.022339
15	6	0	-2.671053	-5.112798	-1.290357
16	6	0	-8.160659	0.240909	2.833737
17	6	0	-7.581999	-4.103499	4.222188
18	6	0	-8.706107	-1.548575	4.998828
19	8	0	-8.98598	2.34509	2.560489
20	6	0	-7.513782	-0.512593	7.4782
21	6	0	-8.725333	1.86327	8.404489
22	6	0	-7.740755	4.190211	8.420671
23	6	0	-9.268179	6.408414	9.32128
24	6	0	-5.147038	4.856167	7.481218
25	6	0	-9.163097	-1.4664	-5.61181
26	6	0	-11.981751	-1.895149	-6.066389
27	6	0	-13.378514	0.65255	-6.269549
28	6	0	-11.710583	2.862675	-5.434485
29	6	0	-10.362209	2.416691	-2.938774
30	6	0	-14.360344	1.634779	-8.809086
31	6	0	-14.884052	4.472899	-8.250513
32	6	0	-13.492103	5.141416	-5.748117
33	8	0	-12.748509	-2.999533	-3.590927
34	6	0	-11.273933	-2.052953	-1.74131
35	8	0	-11.650435	-2.514283	0.462834
36	8	0	-15.403163	5.153434	-3.814988
37	6	0	-12.13689	7.676743	-5.812099
38	6	0	-12.651556	-3.81628	-8.064611
39	1	0	-10.258755	3.119711	-6.904577

40	1	0	-14.996417	0.543986	-4.972857
41	1	0	-7.5554	-4.68684	0.15529
42	1	0	-10.7593	-1.625694	5.232547
43	1	0	-0.161132	-7.434629	4.556109
44	1	0	2.967742	-5.274971	7.209154
45	1	0	3.126662	-0.583585	7.362333
46	1	0	0.029311	1.909276	4.81433
47	1	0	-5.755396	-8.775513	0.810743
48	1	0	-2.557942	-9.198763	1.644121
49	1	0	-4.794928	-8.352789	3.990466
50	1	0	-0.939319	-6.239838	-1.407112
51	1	0	-4.031828	-5.874963	-2.657155
52	1	0	-2.210645	-3.177975	-1.842158
53	1	0	-9.024419	-5.580534	4.171358
54	1	0	-6.150114	-4.674363	5.607527
55	1	0	-7.74996	-2.014033	8.894835
56	1	0	-5.471738	-0.296373	7.204475
57	1	0	-10.66839	1.64381	9.059824
58	1	0	-9.456074	7.814835	7.807263
59	1	0	-11.162814	5.847323	9.924293
60	1	0	-8.330279	7.363842	10.906121
61	1	0	-4.177097	6.086143	8.83976
62	1	0	-3.952032	3.210815	7.138172
63	1	0	-5.284432	5.902324	5.696154
64	1	0	-8.154824	-3.277112	-5.603648
65	1	0	-8.259704	-0.233462	-6.993008
66	1	0	-8.812849	3.759108	-2.666879
67	1	0	-11.631475	2.618243	-1.318826
68	1	0	-16.042566	0.638151	-9.479277
69	1	0	-12.895753	1.447245	-10.266522
70	1	0	-14.23081	5.681473	-9.795737
71	1	0	-16.90089	4.835179	-7.983143
72	1	0	-14.621785	5.656702	-2.245573
73	1	0	-11.192958	8.058968	-4.006097
74	1	0	-10.696957	7.708983	-7.297986
75	1	0	-13.490631	9.199458	-6.16957
76	1	0	-12.02487	-3.148832	-9.91845
77	1	0	-11.732165	-5.624329	-7.665913
78	1	0	-14.696517	-4.112827	-8.135228

yby5-12-3C5000014_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.708918	-0.189256	-2.681325
1	6	0	-6.922409	-0.408734	-1.919819
2	8	0	-5.383088	-0.074237	-3.579876
3	6	0	-6.110801	-1.050441	0.790341
4	6	0	-6.54395	-3.865116	1.471798
5	6	0	-4.248491	-5.60216	0.971864
6	6	0	-1.982922	-4.56384	2.391697
7	6	0	-1.563124	-1.938174	2.38917
8	6	0	-3.372355	-0.151199	1.209993
9	8	0	-2.792354	2.015254	0.713489
10	6	0	-0.2141	-6.107879	3.588702
11	6	0	1.911876	-5.083403	4.74898
12	6	0	2.330891	-2.484796	4.712204
13	6	0	0.599834	-0.922809	3.52353
14	6	0	-4.955544	-8.301653	1.770537
15	6	0	-3.587639	-5.659314	-1.865935
16	6	0	-7.66915	0.446109	2.798337
17	6	0	-7.388237	-3.891871	4.29413
18	6	0	-8.06052	-1.193771	5.109787
19	8	0	-8.279047	2.624981	2.547873
20	6	0	-6.36881	-0.227135	7.311923
21	6	0	-7.162616	2.288371	8.31878
22	6	0	-5.969209	4.500361	8.060083
23	6	0	-7.086001	6.886621	9.120524
24	6	0	-3.530507	4.871176	6.658871
25	6	0	-10.171929	-1.38967	-5.297823
26	6	0	-13.057206	-1.481509	-5.30491
27	6	0	-14.158049	1.211758	-5.442484
28	6	0	-12.131964	3.224593	-4.979827
29	6	0	-10.483611	2.703863	-2.686654
30	6	0	-15.378927	2.215415	-7.86746
31	6	0	-15.473072	5.115549	-7.397771
32	6	0	-13.65304	5.697086	-5.163118
33	8	0	-13.55844	-2.3894	-2.685625
34	6	0	-11.713404	-1.572021	-1.129647
35	8	0	-11.796476	-1.908236	1.127054
36	8	0	-15.238401	6.027981	-2.979744
37	6	0	-12.027941	8.035285	-5.564014
38	6	0	-14.248097	-3.377759	-7.070919
39	1	0	-10.89834	3.237864	-6.656707

40	1	0	-15.566385	1.354286	-3.923767
41	1	0	-8.096889	-4.589808	0.307931
42	1	0	-10.042616	-1.009829	5.66999
43	1	0	-0.485881	-8.139571	3.625266
44	1	0	3.253083	-6.326499	5.682679
45	1	0	3.996308	-1.690051	5.609427
46	1	0	0.868087	1.110308	3.450788
47	1	0	-3.507155	-9.657886	1.188009
48	1	0	-5.229421	-8.483345	3.811029
49	1	0	-6.719117	-8.849539	0.834235
50	1	0	-2.036672	-6.988453	-2.19882
51	1	0	-5.226452	-6.290201	-2.969517
52	1	0	-3.003706	-3.808691	-2.568888
53	1	0	-8.988587	-5.173381	4.543764
54	1	0	-5.831175	-4.60108	5.463759
55	1	0	-6.515706	-1.654553	8.814338
56	1	0	-4.38877	-0.23687	6.70276
57	1	0	-8.97104	2.289842	9.310245
58	1	0	-7.42983	8.258704	7.602351
59	1	0	-8.873869	6.535678	10.094474
60	1	0	-5.778396	7.790576	10.45362
61	1	0	-2.178595	5.929071	7.822754
62	1	0	-2.63891	3.105508	6.077007
63	1	0	-3.862225	5.986429	4.942778
64	1	0	-9.390011	-3.308662	-5.341272
65	1	0	-9.355365	-0.327368	-6.862481
66	1	0	-8.765351	3.854359	-2.715346
67	1	0	-11.460353	3.116813	-0.910971
68	1	0	-17.247357	1.414493	-8.24158
69	1	0	-14.17392	1.792248	-9.502409
70	1	0	-14.918751	6.173362	-9.085642
71	1	0	-17.369733	5.738401	-6.863903
72	1	0	-14.172811	6.467393	-1.566108
73	1	0	-10.828696	7.827366	-7.237729
74	1	0	-13.227779	9.701905	-5.812481
75	1	0	-10.790122	8.366442	-3.934067
76	1	0	-13.502389	-5.271241	-6.707345
77	1	0	-16.300723	-3.414669	-6.825485
78	1	0	-13.834534	-2.868712	-9.031698

yby5-12-3C5000021_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.565952	-0.456904	-2.990599
1	6	0	-6.856018	-0.228086	-1.993066
2	8	0	-5.284772	0.510336	-3.484559
3	6	0	-6.14692	-0.930413	0.728163
4	6	0	-6.098767	-3.822691	1.181969
5	6	0	-3.491182	-5.075037	0.772502
6	6	0	-1.563378	-3.759476	2.440142
7	6	0	-1.640781	-1.110023	2.649133
8	6	0	-3.664304	0.411871	1.447441
9	8	0	-3.466013	2.680865	1.152257
10	6	0	0.378153	-5.049459	3.670105
11	6	0	2.193507	-3.755667	5.064952
12	6	0	2.121811	-1.129989	5.238519
13	6	0	0.213358	0.183614	4.022029
14	6	0	-3.738484	-7.910938	1.341074
15	6	0	-2.630918	-4.793858	-1.997425
16	6	0	-8.105665	0.093374	2.683535
17	6	0	-7.132577	-4.229363	3.911346
18	6	0	-8.356632	-1.772701	4.838974
19	8	0	-9.093908	2.135485	2.518207
20	6	0	-7.048596	-0.701089	7.243999
21	6	0	-8.366274	1.550158	8.324409
22	6	0	-7.577248	3.950511	8.317764
23	6	0	-9.205594	6.017774	9.385
24	6	0	-5.130858	4.847992	7.194916
25	6	0	-9.578894	-1.5563	-5.692788
26	6	0	-12.39015	-2.135359	-5.991021
27	6	0	-13.923995	0.33998	-6.137267
28	6	0	-12.332539	2.629401	-5.361211
29	6	0	-10.852555	2.251478	-2.931222
30	6	0	-15.049787	1.276057	-8.634114
31	6	0	-15.702068	4.080518	-8.04635
32	6	0	-14.197407	4.847351	-5.615761
33	8	0	-12.969758	-3.254614	-3.478777
34	6	0	-11.410079	-2.266164	-1.710015
35	8	0	-11.61603	-2.795624	0.499173
36	8	0	-15.828292	5.049897	-3.458708
37	6	0	-12.915293	7.40558	-5.818096
38	6	0	-13.067839	-4.098344	-7.946451
39	1	0	-10.962923	2.923357	-6.900905

40	1	0	-15.487565	0.08652	-4.784763
41	1	0	-7.400649	-4.718386	-0.15873
42	1	0	-10.375272	-1.995436	5.228517
43	1	0	0.489096	-7.092882	3.547219
44	1	0	3.677464	-4.807718	6.017279
45	1	0	3.545504	-0.122356	6.319319
46	1	0	0.099866	2.230682	4.109021
47	1	0	-2.025875	-8.934143	0.796392
48	1	0	-4.11382	-8.292123	3.337439
49	1	0	-5.300491	-8.69697	0.232069
50	1	0	-0.838718	-5.788506	-2.282368
51	1	0	-4.040234	-5.625515	-3.271465
52	1	0	-2.356667	-2.819086	-2.5311
53	1	0	-8.478487	-5.795995	3.933489
54	1	0	-5.562463	-4.738773	5.164987
55	1	0	-7.051835	-2.245743	8.633589
56	1	0	-5.059032	-0.314814	6.815941
57	1	0	-10.226606	1.159288	9.124002
58	1	0	-8.216171	7.041586	10.893879
59	1	0	-9.651986	7.410366	7.913085
60	1	0	-10.981932	5.286156	10.144655
61	1	0	-5.499712	5.94352	5.473448
62	1	0	-4.142732	6.101416	8.518633
63	1	0	-3.850208	3.314921	6.682766
64	1	0	-8.480988	-3.313753	-5.744985
65	1	0	-8.813223	-0.282325	-7.118957
66	1	0	-9.377313	3.68492	-2.727524
67	1	0	-12.063216	2.401886	-1.263645
68	1	0	-16.693833	0.189504	-9.259927
69	1	0	-13.620886	1.169793	-10.133427
70	1	0	-15.222376	5.316107	-9.634197
71	1	0	-17.722901	4.332733	-7.679267
72	1	0	-16.758155	3.495168	-3.265098
73	1	0	-14.325661	8.88512	-6.132421
74	1	0	-11.902689	7.842576	-4.068708
75	1	0	-11.572163	7.422777	-7.390048
76	1	0	-12.567371	-3.414693	-9.832554
77	1	0	-12.042617	-5.856643	-7.586472
78	1	0	-15.096783	-4.495762	-7.912364

Table S8. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of yby5-12-3D (**1d**).

Conformers	ΔG (a.u.)	P(%)/100	G (a.u.)
yby5-12-3D000001_en_	0.00148	14.73	-1733.007018
yby5-12-3D000002_en_	0.00189	9.52	-1733.006606
yby5-12-3D000003_en_	0.00253	4.85	-1733.005969
yby5-12-3D2000016_en_	0.0	70.89	-1733.0085

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15 K.

Table S9. Cartesian coordinates for the low-energy reoptimized random research conformers of yby5-12-3D at B3LYP-D3(BJ)/6-31G** level of theory in methanol.

yby5-12-3D000001_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.473393	-1.188351	-0.236629
1	6	0	-5.409778	0.934276	0.013176
2	8	0	-6.476336	1.271739	2.011311
3	6	0	-6.148044	2.600007	-2.279409
4	6	0	-7.424951	5.131474	-1.619578
5	6	0	-5.776057	7.147374	-0.354678
6	6	0	-3.420712	7.435437	-1.987758
7	6	0	-2.6968	5.604753	-3.774299
8	6	0	-4.006613	3.146682	-4.118
9	8	0	-3.378685	1.667495	-5.771016
10	6	0	-1.885976	9.556575	-1.715851
11	6	0	0.260022	9.901059	-3.169164
12	6	0	0.937423	8.108152	-4.963272
13	6	0	-0.533129	5.980287	-5.247849
14	6	0	-4.951626	6.578803	2.362276
15	6	0	-7.31874	9.602776	-0.344667
16	6	0	-8.45229	1.157427	-3.450611
17	6	0	-10.05203	4.455397	-0.654081
18	6	0	-10.872605	2.399687	-2.506287
19	8	0	-8.367576	-0.624764	-4.861254
20	6	0	-12.81815	0.464312	-1.55693
21	6	0	-11.805984	-1.281651	0.410409
22	6	0	-12.154	-1.199947	2.904623
23	6	0	-10.894473	-3.083219	4.597655
24	6	0	-13.717066	0.731919	4.250437
25	6	0	-3.752998	-3.033552	-2.457052
26	6	0	-1.075888	-4.109999	-2.549464

27	6	0	-0.548939	-5.760843	-0.223333
28	6	0	-2.567122	-5.386661	1.791188
29	6	0	-3.20717	-2.652337	2.31358
30	6	0	-0.458432	-8.63292	-0.389005
31	6	0	-0.745646	-9.470289	2.395958
32	6	0	-1.70743	-7.136846	3.911103
33	8	0	0.463866	-1.790468	-2.184156
34	6	0	-0.845378	-0.103694	-0.80896
35	8	0	0.015145	1.880028	-0.093277
36	8	0	0.349098	-5.878562	5.161588
37	6	0	-3.764467	-7.768752	5.802731
38	6	0	-0.317141	-5.219234	-5.051421
39	1	0	-4.278334	-6.284903	1.059406
40	1	0	1.253062	-5.120655	0.542616
41	1	0	-7.770436	5.946263	-3.498319
42	1	0	-11.67156	3.307359	-4.188139
43	1	0	-2.371248	10.982537	-0.337878
44	1	0	1.406716	11.573019	-2.899856
45	1	0	2.614723	8.362418	-6.103183
46	1	0	-0.026117	4.524002	-6.584057
47	1	0	-3.606727	5.03782	2.457407
48	1	0	-4.036683	8.242061	3.157893
49	1	0	-6.568371	6.110027	3.540844
50	1	0	-8.996188	9.376465	0.823238
51	1	0	-6.25381	11.173997	0.436525
52	1	0	-7.9162	10.125865	-2.244459
53	1	0	-11.33666	6.058796	-0.712741
54	1	0	-9.995993	3.72846	1.258136
55	1	0	-14.460298	1.504916	-0.882783
56	1	0	-13.44542	-0.641846	-3.179422
57	1	0	-10.583185	-2.759834	-0.317006
58	1	0	-9.618319	-2.134969	5.913036
59	1	0	-12.273385	-4.107042	5.742806
60	1	0	-9.800135	-4.458792	3.531326
61	1	0	-14.635404	2.063706	2.988923
62	1	0	-15.177342	-0.172191	5.394618
63	1	0	-12.544896	1.815483	5.558898
64	1	0	-4.181424	-2.055619	-4.198445
65	1	0	-5.190998	-4.469882	-2.173312
66	1	0	-4.976004	-2.4913	3.338515
67	1	0	-1.771217	-1.759538	3.482228
68	1	0	1.262059	-9.346555	-1.258818
69	1	0	-2.044869	-9.334662	-1.504307

70	1	0	-2.046147	-11.05517	2.578206
71	1	0	1.057645	-10.078476	3.180537
72	1	0	0.99712	-7.003071	6.43972
73	1	0	-3.097976	-9.143529	7.18853
74	1	0	-4.356756	-6.080616	6.816535
75	1	0	-5.410388	-8.580691	4.868434
76	1	0	-0.562632	-3.831174	-6.545954
77	1	0	1.647138	-5.826825	-5.025168
78	1	0	-1.489068	-6.853003	-5.484264

yby5-12-3D000002_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-2.901142	-1.362568	-0.421559
1	6	0	-5.171621	0.338131	0.091758
2	8	0	-6.282573	0.196407	2.097362
3	6	0	-6.28624	2.051334	-1.999117
4	6	0	-7.683619	4.440094	-1.092144
5	6	0	-6.030853	6.499275	0.081434
6	6	0	-3.973022	7.0953	-1.843046
7	6	0	-3.370102	5.423008	-3.820046
8	6	0	-4.479823	2.857709	-4.082781
9	8	0	-3.952111	1.493814	-5.866725
10	6	0	-2.606855	9.336909	-1.671348
11	6	0	-0.747267	9.950512	-3.405314
12	6	0	-0.201322	8.316897	-5.386152
13	6	0	-1.502374	6.070441	-5.574416
14	6	0	-4.781974	5.768474	2.587656
15	6	0	-7.720254	8.809876	0.528694
16	6	0	-8.599279	0.425266	-2.895663
17	6	0	-10.111357	3.554245	0.166346
18	6	0	-10.939402	1.337217	-1.488546
19	8	0	-8.552363	-1.280342	-4.397853
20	6	0	-12.236092	-0.848018	-0.085208
21	6	0	-14.619261	-0.013497	1.159263
22	6	0	-15.036898	0.338977	3.622613
23	6	0	-17.563942	1.209011	4.553533
24	6	0	-13.115446	-0.080502	5.655479
25	6	0	-3.234777	-3.222113	-2.631832
26	6	0	-0.470138	-3.86836	-3.151379
27	6	0	0.644803	-5.42612	-0.973913
28	6	0	-1.07481	-5.380384	1.331923
29	6	0	-2.050916	-2.782445	2.019556
30	6	0	1.161123	-8.246072	-1.227976
31	6	0	1.434949	-9.123473	1.545799
32	6	0	0.373115	-6.970625	3.249721
33	8	0	0.737825	-1.34227	-2.950274
34	6	0	-0.577701	0.104371	-1.328837
35	8	0	0.101897	2.170898	-0.65315
36	8	0	2.377943	-5.400357	4.193547
37	6	0	-1.232364	-7.924067	5.421989
38	6	0	0.061654	-4.836734	-5.767634
39	1	0	-2.717132	-6.542968	0.857616

40	1	0	2.421579	-4.514915	-0.467508
41	1	0	-8.310668	5.288241	-2.880605
42	1	0	-12.226321	2.007865	-2.962451
43	1	0	-2.998259	10.645227	-0.153517
44	1	0	0.276771	11.710069	-3.209997
45	1	0	1.250058	8.785164	-6.746807
46	1	0	-1.077529	4.728294	-7.051595
47	1	0	-3.336292	4.336542	2.345646
48	1	0	-3.862763	7.420126	3.400588
49	1	0	-6.173172	5.081546	3.93568
50	1	0	-6.660521	10.390389	1.298559
51	1	0	-8.616908	9.435056	-1.216475
52	1	0	-9.194878	8.357956	1.888315
53	1	0	-11.535396	5.032915	0.189818
54	1	0	-9.798801	2.944742	2.094273
55	1	0	-12.637563	-2.332769	-1.458693
56	1	0	-10.907718	-1.630878	1.271655
57	1	0	-16.166203	0.393167	-0.13073
58	1	0	-18.375665	-0.152656	5.87629
59	1	0	-17.399643	2.990233	5.584808
60	1	0	-18.901234	1.480555	3.016454
61	1	0	-11.273243	-0.62943	4.944335
62	1	0	-12.869	1.638407	6.77167
63	1	0	-13.753679	-1.534653	6.974637
64	1	0	-4.068272	-2.307901	-4.260064
65	1	0	-4.375128	-4.864512	-2.172786
66	1	0	-3.661155	-2.914528	3.284586
67	1	0	-0.613928	-1.682822	2.996061
68	1	0	2.823511	-8.670414	-2.35941
69	1	0	-0.441422	-9.191072	-2.117435
70	1	0	0.431817	-10.888892	1.880176
71	1	0	3.407689	-9.450906	2.033038
72	1	0	3.373891	-6.398907	5.34612
73	1	0	-2.854672	-8.988383	4.733546
74	1	0	-0.145533	-9.176846	6.648335
75	1	0	-1.913114	-6.353248	6.560662
76	1	0	-0.90572	-6.62701	-6.068213
77	1	0	-0.606893	-3.492653	-7.169385
78	1	0	2.076201	-5.140785	-6.047289

yby5-12-3D000003_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-2.94643	-1.478224	-0.50607
1	6	0	-5.200443	0.222749	0.083398
2	8	0	-6.305524	0.00287	2.085059
3	6	0	-6.311105	2.020608	-1.933854
4	6	0	-7.665061	4.393239	-0.928215
5	6	0	-5.963498	6.387707	0.28534
6	6	0	-3.956221	7.042369	-1.673488
7	6	0	-3.401199	5.422778	-3.708762
8	6	0	-4.514567	2.863364	-4.009381
9	8	0	-3.990893	1.523639	-5.813425
10	6	0	-2.584724	9.278007	-1.47385
11	6	0	-0.768526	9.939291	-3.23659
12	6	0	-0.272049	8.360236	-5.273832
13	6	0	-1.576043	6.117652	-5.489434
14	6	0	-4.642783	5.538494	2.717911
15	6	0	-7.621194	8.684903	0.886002
16	6	0	-8.661808	0.459879	-2.860647
17	6	0	-10.088514	3.497899	0.332023
18	6	0	-10.970957	1.356875	-1.39401
19	8	0	-8.655317	-1.19118	-4.422404
20	6	0	-12.291147	-0.856943	-0.05906
21	6	0	-14.640074	-0.029342	1.25236
22	6	0	-15.014161	0.23872	3.733359
23	6	0	-17.512873	1.113505	4.734094
24	6	0	-13.07076	-0.281819	5.721454
25	6	0	-3.367841	-3.304919	-2.730366
26	6	0	-0.629831	-3.981856	-3.337949
27	6	0	0.526577	-5.584834	-1.210905
28	6	0	-1.112823	-5.539437	1.152661
29	6	0	-2.055047	-2.945701	1.891756
30	6	0	1.010737	-8.4068	-1.492287
31	6	0	1.446436	-9.270745	1.261876
32	6	0	0.377308	-7.167233	3.029359
33	8	0	0.623686	-1.481655	-3.131077
34	6	0	-0.628001	-0.036	-1.452796
35	8	0	0.116002	2.002204	-0.760491
36	8	0	2.365876	-5.768326	4.230358
37	6	0	-1.217531	-8.181431	5.171899
38	6	0	-0.183847	-4.928699	-5.977543
39	1	0	-2.773004	-6.684953	0.699622

40	1	0	2.342838	-4.68271	-0.801812
41	1	0	-8.306467	5.310144	-2.676883
42	1	0	-12.25905	2.104137	-2.82941
43	1	0	-2.936023	10.543249	0.089427
44	1	0	0.259776	11.693811	-3.019833
45	1	0	1.144116	8.866818	-6.65765
46	1	0	-1.186993	4.815731	-7.011885
47	1	0	-3.213979	4.112334	2.362793
48	1	0	-3.687188	7.146845	3.574472
49	1	0	-5.992679	4.794163	4.076936
50	1	0	-6.527882	10.229927	1.680223
51	1	0	-8.580095	9.384487	-0.796806
52	1	0	-9.045248	8.17934	2.280229
53	1	0	-11.487746	4.997338	0.428112
54	1	0	-9.764439	2.811566	2.23148
55	1	0	-12.739613	-2.278999	-1.483458
56	1	0	-10.959487	-1.718417	1.245479
57	1	0	-16.201314	0.446291	0.004059
58	1	0	-18.329597	-0.285545	6.014123
59	1	0	-17.303729	2.849388	5.831952
60	1	0	-18.867224	1.467559	3.229009
61	1	0	-12.767668	1.397802	6.882892
62	1	0	-13.721764	-1.758722	7.008562
63	1	0	-11.251917	-0.851306	4.967032
64	1	0	-4.229416	-2.353634	-4.322803
65	1	0	-4.520341	-4.935087	-2.259312
66	1	0	-3.639323	-3.086047	3.187524
67	1	0	-0.593425	-1.871321	2.864155
68	1	0	2.596884	-8.847095	-2.723364
69	1	0	-0.653022	-9.332637	-2.28347
70	1	0	0.546831	-11.081732	1.639106
71	1	0	3.447806	-9.51378	1.673337
72	1	0	3.485547	-5.134004	2.941317
73	1	0	-2.823597	-9.23856	4.441262
74	1	0	-0.105695	-9.431521	6.368181
75	1	0	-1.920923	-6.643672	6.342071
76	1	0	-1.173462	-6.708849	-6.264475
77	1	0	-0.883401	-3.56592	-7.345544
78	1	0	1.819041	-5.245031	-6.320513

yby5-12-3D2000016_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.60708	-0.829523	0.05576
1	6	0	-5.624149	1.215988	0.322091
2	8	0	-6.424706	1.76188	2.39881
3	6	0	-6.791075	2.507657	-2.027713
4	6	0	-8.055522	5.086326	-1.550346
5	6	0	-6.301084	7.289262	-0.880318
6	6	0	-4.290325	7.390887	-2.939994
7	6	0	-3.797477	5.325005	-4.539728
8	6	0	-5.019347	2.811703	-4.273484
9	8	0	-4.608087	1.106053	-5.768346
10	6	0	-2.842286	9.56451	-3.26133
11	6	0	-1.002982	9.73251	-5.11274
12	6	0	-0.558765	7.702562	-6.716635
13	6	0	-1.945605	5.520815	-6.41669
14	6	0	-4.97527	7.098299	1.687817
15	6	0	-7.920215	9.692786	-0.897726
16	6	0	-9.192902	0.861575	-2.573069
17	6	0	-10.466892	4.53272	-0.07785
18	6	0	-11.476999	2.179573	-1.417396
19	8	0	-9.263171	-1.097487	-3.723462
20	6	0	-13.125012	0.34479	0.111039
21	6	0	-11.759558	-0.90812	2.234524
22	6	0	-11.097669	-3.334437	2.431222
23	6	0	-9.685464	-4.254033	4.704962
24	6	0	-11.658331	-5.336021	0.515988
25	6	0	-4.166628	-3.028576	-1.748799
26	6	0	-1.48585	-4.009435	-2.183575
27	6	0	-0.430154	-5.224846	0.228218
28	6	0	-2.061369	-4.60157	2.510337
29	6	0	-2.791313	-1.845457	2.704767
30	6	0	-0.157174	-8.074804	0.50678
31	6	0	0.20121	-8.416226	3.383836
32	6	0	-0.687066	-5.942101	4.677698
33	8	0	-0.063457	-1.606186	-2.491581
34	6	0	-1.196673	0.230121	-1.158752
35	8	0	-0.336211	2.32531	-0.908605
36	8	0	1.578976	-4.61401	5.378168
37	6	0	-2.32079	-6.373139	6.990128
38	6	0	-1.126784	-5.496347	-4.575641
39	1	0	-3.812975	-5.674966	2.271426

40	1	0	1.43255	-4.395351	0.530378
41	1	0	-8.727062	5.599185	-3.446815
42	1	0	-12.594409	2.792013	-3.049868
43	1	0	-3.148085	11.17313	-2.041379
44	1	0	0.086608	11.452792	-5.302877
45	1	0	0.879057	7.819623	-8.164624
46	1	0	-1.603339	3.88799	-7.591382
47	1	0	-3.549038	5.628154	1.70928
48	1	0	-4.02808	8.878177	2.099627
49	1	0	-6.32415	6.727034	3.192934
50	1	0	-8.899847	9.931006	-2.692957
51	1	0	-9.32373	9.607405	0.602351
52	1	0	-6.794167	11.375736	-0.566289
53	1	0	-11.81159	6.082056	-0.195726
54	1	0	-10.071114	4.166383	1.895981
55	1	0	-14.7224	1.424828	0.852363
56	1	0	-13.908114	-1.038926	-1.188831
57	1	0	-11.203322	0.332576	3.766365
58	1	0	-9.239673	-2.729254	6.008133
59	1	0	-10.768033	-5.683893	5.727986
60	1	0	-7.915189	-5.159696	4.152877
61	1	0	-9.913396	-6.241285	-0.112817
62	1	0	-12.81868	-6.828754	1.345226
63	1	0	-12.609263	-4.630178	-1.155071
64	1	0	-4.974733	-2.37	-3.505665
65	1	0	-5.428226	-4.43861	-0.957125
66	1	0	-4.349958	-1.577035	4.010945
67	1	0	-1.231828	-0.690464	3.40011
68	1	0	1.404466	-8.854848	-0.578876
69	1	0	-1.877341	-9.024247	-0.121439
70	1	0	-0.849397	-10.034412	4.095177
71	1	0	2.175923	-8.712624	3.866424
72	1	0	1.086936	-3.08144	6.2341
73	1	0	-4.002729	-7.465015	6.524713
74	1	0	-1.263831	-7.392642	8.430347
75	1	0	-2.947008	-4.584835	7.804198
76	1	0	-1.756012	-4.399925	-6.194806
77	1	0	0.849124	-5.999727	-4.842106
78	1	0	-2.226058	-7.232509	-4.497614

Calculated $^{1}H/^{13}C$ NMR-DP4+ probability analysis for 1a–1d

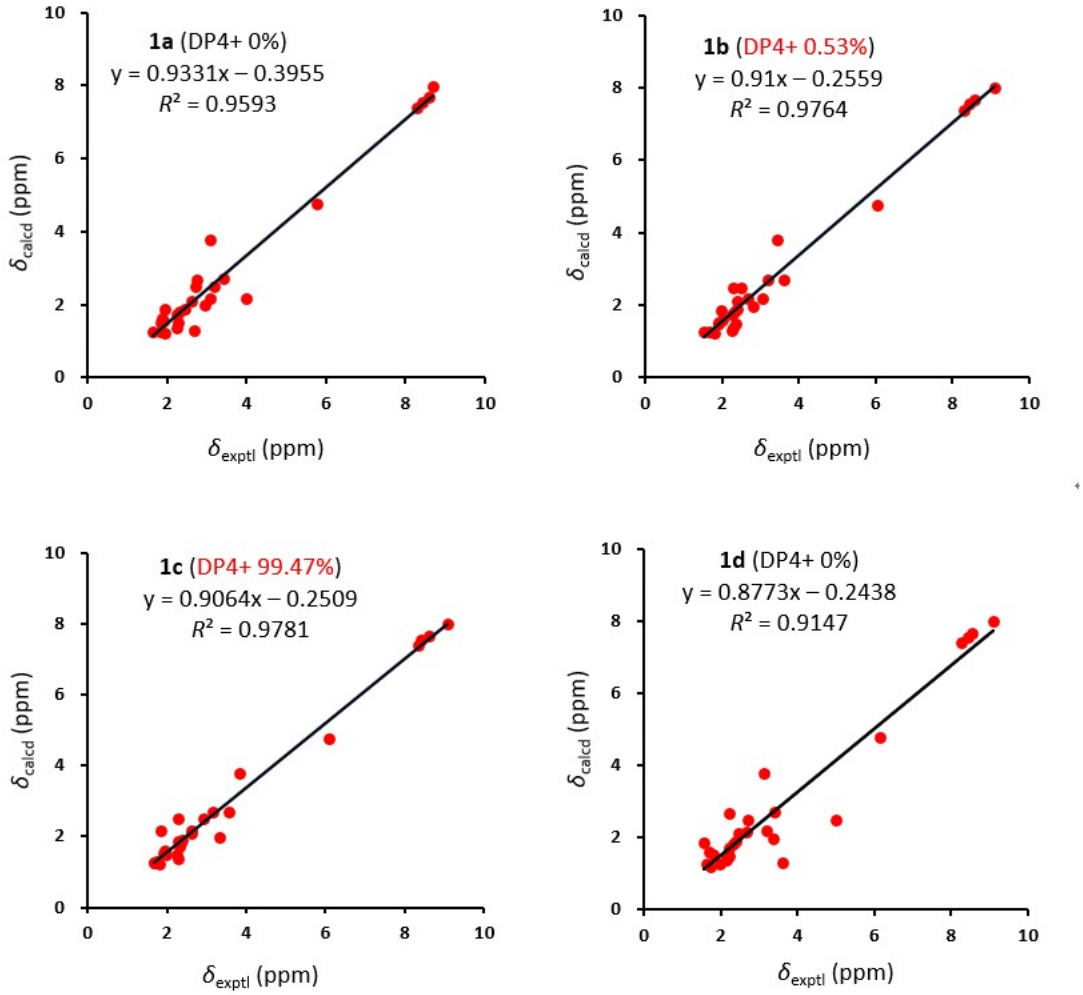


Figure S21. Correlation coefficients and DP4+ probability analyses between the calculated and experimental ^{1}H NMR chemical shifts for **1a**–**1d**.

Table S10. Comparison of the experimental and computed ^{1}H NMR data for **1a**–**1d** (δ in ppm).

No.	δ_{expt}	δ_{calcd} (**1a**)	δ_{calcd} (**1b**)	δ_{calcd} (**1c**)	δ_{calcd} (**1d**)
6	2.70	3.431626979	3.605400777	3.563660043	3.416915244
7a	1.86	1.932879575	1.980570241	2.271951702	1.563394443
7b	2.18	4.006110214	2.675208128	2.606232885	3.179357489
8	1.61	1.892045025	2.01728215	1.961218531	1.696677969
10a	1.73	2.242979173	2.242786755	2.319851178	2.218230194
10b	1.89	2.451169743	2.395249472	2.374111872	2.383018775
11a	1.26	1.654168473	1.674031689	1.684623295	1.639756187
11b	1.82	2.304811683	2.307335631	2.353956005	2.321599025
12	2.10	2.628410313	2.385446483	2.633082817	2.473384136

14a	2.49	2.720125911	2.286220102	2.286528259	5.010735292
14b	2.68	2.743559247	3.20677115	3.162326035	2.220873729
15	1.50	1.852171571	1.915648042	1.966762101	2.147715392
16	1.21	1.930467173	1.788609733	1.806526657	1.725798072
17a	1.30	2.664920085	2.252723116	1.758460858	3.618952628
17b	2.49	3.182611581	2.492216206	2.912320829	2.68956878
18	3.79	3.079790418	3.435300501	3.820884279	3.139160818
20	1.53	1.897621012	1.901730349	1.91015503	1.786370476
21	1.26	1.852425197	1.519948524	1.685177425	1.988976307
22a	1.97	2.941101949	2.815276364	3.316771672	3.376464822
22b	2.17	3.082188168	3.051601944	1.836942483	2.666712313
23	4.77	5.778792746	6.049811858	6.06944368	6.139139929
25	1.38	2.23035164	2.283307069	2.27951546	2.157985135
26	1.50	2.273878692	2.341445903	2.245121056	2.226503522
30	7.54	8.434850056	8.436153899	8.397427648	8.442405359
31	7.67	8.590831403	8.583030581	8.620180713	8.52908089
32	7.38	8.286247194	8.305969773	8.337038599	8.276026796
33	7.98	8.688422511	9.097668855	9.083886007	9.101031134

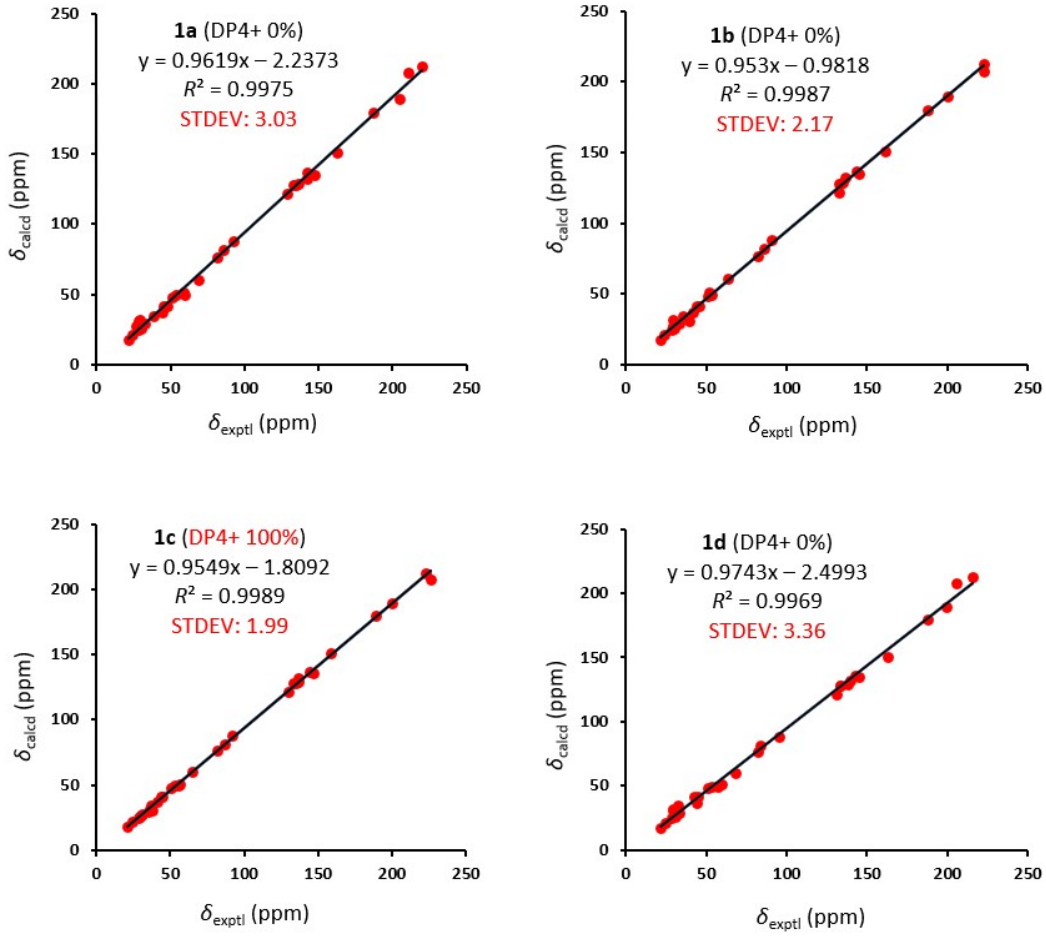


Figure S22. Correlation coefficients and DP4+ probability analyses between the calculated and experimental ^{13}C NMR chemical shifts for **1a**–**1d**.

Table S11. Comparison of the experimental and computed ^{13}C NMR data for **1a**–**1d** (δ in ppm).

No.	δ_{expt}	δ_{calcd_corr} (**1a**)	δ_{calcd_corr} (**1b**)	δ_{calcd_corr} (**1c**)	δ_{calcd_corr} (**1d**)
1	212.7	209.6999222	211.4172427	210.6766496	207.6865248
2	81.7	80.21937646	81.14706847	81.33092005	79.2784491
3	207.4	200.7562307	211.4116626	214.4102653	197.8474109
4	60.6	63.87702013	59.3638767	60.1326376	63.47036153
5	179.8	177.2601147	178.1431417	178.3924441	180.0941139
6	49.6	55.2276603	49.34833881	51.35273894	53.28483905
7	30.7	24.73251579	36.59440011	34.51645391	25.66457678
8	49.8	49.35762519	49.76573899	48.95866065	49.46386502
9	76.6	76.3436524	77.11555515	76.52236	77.12006432
10	41.3	41.43742513	40.91215655	39.75200725	41.28766681
11	25.1	25.12907388	26.35216221	25.61518944	25.53627574
12	48.1	47.40539646	47.25216144	46.21456801	47.49196476
13	87.9	86.53366013	85.64261793	86.05831763	90.1113569

14	41.4	43.94944335	42.30295743	40.62813031	38.82952118
15	21.5	20.92618965	22.01882775	21.44741673	21.3309557
16	26.7	26.31754492	26.85174714	26.57716833	26.45473857
17	31.7	26.19760466	26.94445478	32.59693288	25.82800436
18	51	54.14888316	48.31054737	51.85953495	55.87114086
19	37	40.37466237	38.70738152	37.18876496	40.68284112
20	27.6	23.82691676	27.13855026	27.93190594	26.99625898
21	34.5	34.83677116	32.78318773	33.20114961	28.79686319
22	29.4	29.40218446	30.37585866	32.00055282	29.63137781
23	121.3	121.8671353	125.1058924	122.0934505	125.0704938
24	135.3	139.7816989	137.0508543	138.2468459	138.4438138
25	17.7	18.25174938	19.64203022	17.80858137	18.22254874
26	25.9	26.86638615	27.65778259	26.48189121	27.42803657
27	189.3	194.8519734	189.9967951	189.4174354	191.9906349
28	132	134.9066503	129.331736	128.3774952	133.1261885
29	150.7	153.9906027	152.5379482	149.3219347	156.1962845
30	127.9	126.9833225	125.839487	126.7205136	127.2932616
31	136.3	134.7042939	135.4135982	135.5191396	136.0834539
32	127.9	126.089315	125.6574557	125.6789812	127.0606825
33	129	129.0263649	127.3548521	128.3022696	131.7903652

Methods

In general, conformational analyses were carried out via random searching in the Sybyl-X 2.0 using the MMFF94S force field with an energy cutoff of 2.5 kcal/mol.[1] Subsequently, the lowest energy conformers were re-optimized using DFT at the B3LYP-D3(BJ)/6-31G** level in PCM methanol by the Gaussian 09 program.[2] NMR shielding constants were computed using the GIAO method at the mPW1PW91/6-311G** level in PCM methanol using Gaussian 09.[2] Boltzmann weights were computed using relative free energies at the wB97M-V/def2-TZVP level in PCM methanol using ORCA.[3][4] Shielding constants were used to calculate DP4+ probability analysis.[5]

References:

[1] Sybyl Software, version X 2.0; Tripos Associates Inc.: St. Louis, MO, 2013.

[2] Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

[3] F. Neese, The ORCA program system, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2012, **2**, 73−78.

[4] F. Neese, Software update: the ORCA program system, version 4.0, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2017, **8**, e1327.

[5] N. Grimblat, M. M. Zanardi and A. M. Sarotti, Beyond DP4: an improved probability for the stereochemical assignment of isomeric compounds using quantum chemical calculations of NMR shifts, *J. Org. Chem.*, 2015, **80**, 12526−12534.

Table S12. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of yby5-12-3A (**1a**).

Conformers	ΔG (a.u.)	P(%)/100	G (a.u.)
yby5-12-3A2000003_en_	0.0032	2.7	-1733.00147
yby5-12-3A2000005_en_	0.00536	0.27	-1732.999311
yby5-12-3A2000006_en_	0.00218	7.98	-1733.002493
yby5-12-3A2000008_en_	0.00296	3.48	-1733.001711
yby5-12-3A2000011_en_	0.00256	5.32	-1733.002111
yby5-12-3A2000019_en_	0.0	80.24	-1733.004671

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15 K.

Table S13. Cartesian coordinates for the low-energy reoptimized random research conformers of yby5-12-3A at B3LYP-D3(BJ)/6-31G** level of theory in methanol.

yby5-12-3A2000003_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.484255	2.564956	0.425027
1	6	0	-1.321474	1.259533	-0.978835
2	8	0	0.709064	2.32714	-1.097946
3	6	0	-1.543346	-1.442348	-2.037233
4	6	0	0.184922	-2.052277	-4.311656
5	6	0	-0.296558	-0.544431	-6.742113
6	6	0	-3.14677	-0.421596	-7.158231
7	6	0	-4.891848	-1.373562	-5.398175
8	6	0	-4.132061	-2.368557	-2.896072
9	8	0	-5.418387	-3.874579	-1.724452
10	6	0	-4.09777	0.599404	-9.38848
11	6	0	-6.664748	0.685188	-9.875799
12	6	0	-8.373995	-0.300319	-8.14322
13	6	0	-7.479153	-1.337549	-5.929438
14	6	0	-0.280873	-3.003379	0.107846
15	6	0	2.829401	-2.374204	-3.226078
16	6	0	2.353574	-3.779985	-0.747796
17	8	0	-1.1997	-3.442187	2.147524
18	6	0	4.335853	-3.429856	1.327807
19	6	0	6.865931	-4.425658	0.572747
20	6	0	7.849698	-6.680364	1.132309
21	6	0	10.417936	-7.420775	0.202534
22	6	0	-2.523146	4.333029	2.515046
23	6	0	-4.756848	6.139498	2.734151
24	6	0	-7.085639	4.774965	3.80093
25	6	0	-6.694932	1.933055	3.857281
26	6	0	-5.647477	0.847046	1.431668
27	6	0	-8.060806	5.256268	6.464365
28	6	0	-9.856493	2.998427	6.911616
29	6	0	-9.197961	0.944189	4.92783
30	8	0	-5.312925	6.602692	0.023606
31	6	0	-4.664544	4.556293	-1.348667
32	8	0	-5.008905	4.403963	-3.590414
33	8	0	-11.167533	1.045919	3.055137
34	6	0	-9.012307	-1.699775	6.009087
35	6	0	-4.176147	8.659593	3.908888
36	1	0	-5.308932	1.553574	5.342951
37	1	0	-8.63282	5.178331	2.499136
38	1	0	-0.40355	-3.977656	-4.81345
39	1	0	2.200881	-5.806698	-1.146565

40	6	0	6.541625	-8.651205	2.682152
41	6	0	0.927061	-2.035931	-8.913474
42	6	0	0.802896	2.135545	-6.752742
43	1	0	-2.809234	1.35648	-10.780285
44	1	0	-7.335723	1.518853	-11.618417
45	1	0	-10.382	-0.239613	-8.519064
46	1	0	-8.758674	-2.108123	-4.536972
47	1	0	4.053597	-3.445126	-4.480579
48	1	0	3.707599	-0.560992	-2.852787
49	1	0	4.48108	-1.411894	1.732335
50	1	0	3.64076	-4.320885	3.043606
51	1	0	7.986746	-3.172557	-0.603693
52	1	0	11.679278	-7.850276	1.779454
53	1	0	10.326419	-9.13167	-0.949314
54	1	0	11.287785	-5.937024	-0.923466
55	1	0	-0.85398	5.334775	1.867294
56	1	0	-2.063173	3.372734	4.269028
57	1	0	-4.931853	-1.039944	1.773661
58	1	0	-7.122757	0.705461	0.00371
59	1	0	-9.01034	7.067556	6.674161
60	1	0	-6.507492	5.214577	7.820767
61	1	0	-9.682188	2.256254	8.82084
62	1	0	-11.820406	3.537305	6.642099
63	1	0	-10.932649	-0.367164	1.92726
64	1	0	-10.817628	-2.274295	6.811311
65	1	0	-8.489036	-3.063089	4.553195
66	1	0	-7.583346	-1.800577	7.487173
67	1	0	-5.814869	9.898908	3.843969
68	1	0	-3.640086	8.409357	5.878385
69	1	0	-2.622791	9.57826	2.924591
70	1	0	4.695224	-8.06802	3.35954
71	1	0	6.289327	-10.380143	1.582605
72	1	0	7.685081	-9.173831	4.318956
73	1	0	0.595818	-1.134769	-10.728385
74	1	0	2.964837	-2.147364	-8.649804
75	1	0	0.18121	-3.952065	-9.018443
76	1	0	-0.216533	3.402332	-5.512217
77	1	0	2.779058	2.11794	-6.188437
78	1	0	0.705153	2.924266	-8.650142

yby5-12-3A2000005_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.597776	2.097576	0.39997
1	6	0	-1.364669	1.302107	-1.252317
2	8	0	0.486908	2.659306	-1.30173
3	6	0	-1.288677	-1.240411	-2.662172
4	6	0	0.484885	-1.336325	-4.978577
5	6	0	-0.12692	0.472186	-7.168317
6	6	0	-2.990347	0.575547	-7.485876
7	6	0	-4.649512	-0.815475	-5.949207
8	6	0	-3.778357	-2.241391	-3.707461
9	8	0	-4.89116	-4.078868	-2.885771
10	6	0	-4.036669	1.976872	-9.451843
11	6	0	-6.614002	2.017161	-9.888102
12	6	0	-8.234764	0.59949	-8.385528
13	6	0	-7.243874	-0.823067	-6.443146
14	6	0	0.106741	-2.965939	-0.745223
15	6	0	3.136545	-1.563233	-3.892235
16	6	0	2.793138	-3.397921	-1.682421
17	8	0	-0.7804	-3.718831	1.217757
18	6	0	4.80937	-3.194112	0.392666
19	6	0	4.858171	-5.379841	2.171742
20	6	0	6.684239	-7.09692	2.45849
21	6	0	6.398888	-9.195515	4.33822
22	6	0	-2.71709	3.446702	2.814534
23	6	0	-5.057078	5.015957	3.41945
24	6	0	-7.265857	3.305755	4.199927
25	6	0	-6.70125	0.549661	3.631298
26	6	0	-5.628939	0.068433	1.026771
27	6	0	-8.168767	3.123634	6.926191
28	6	0	-9.815353	0.713395	6.901928
29	6	0	-9.106728	-0.807806	4.498996
30	8	0	-5.703427	5.990724	0.870161
31	6	0	-4.94687	4.329413	-0.908517
32	8	0	-5.337219	4.618221	-3.128173
33	8	0	-11.140521	-0.419151	2.735536
34	6	0	-8.73384	-3.608038	4.9616
35	6	0	-4.611378	7.274789	5.084297
36	1	0	-5.258352	-0.043968	4.987728
37	1	0	-8.878409	3.884114	3.052313
38	1	0	0.084078	-3.213366	-5.765104
39	1	0	2.805153	-5.336331	-2.411151

40	6	0	9.120854	-7.14551	1.022133
41	6	0	1.021724	-0.699126	-9.568293
42	6	0	0.954245	3.143838	-6.882145
43	1	0	-2.816468	3.062619	-10.678597
44	1	0	-7.362239	3.153652	-11.414335
45	1	0	-10.249746	0.623407	-8.725934
46	1	0	-8.452631	-1.941914	-5.235524
47	1	0	4.482304	-2.283783	-5.269955
48	1	0	3.816365	0.244507	-3.206011
49	1	0	6.624835	-2.953117	-0.543436
50	1	0	4.470746	-1.443366	1.436055
51	1	0	3.174311	-5.580501	3.318113
52	1	0	4.606168	-9.093742	5.337343
53	1	0	6.514645	-11.039323	3.416049
54	1	0	7.917512	-9.150435	5.736651
55	1	0	-1.126555	4.669315	2.384923
56	1	0	-2.170506	2.16907	4.323636
57	1	0	-4.784797	-1.794372	0.980118
58	1	0	-7.103779	0.124103	-0.408433
59	1	0	-9.206508	4.77952	7.564443
60	1	0	-6.560638	2.877047	8.194443
61	1	0	-9.536233	-0.416684	8.59691
62	1	0	-11.814968	1.17265	6.798217
63	1	0	-10.857347	-1.525714	1.31468
64	1	0	-8.199466	-4.582302	3.224941
65	1	0	-7.23822	-3.939387	6.336145
66	1	0	-10.469294	-4.456923	5.668458
67	1	0	-6.331923	8.378703	5.302369
68	1	0	-4.000469	6.665394	6.950654
69	1	0	-3.154856	8.486218	4.286665
70	1	0	10.728343	-7.019628	2.310924
71	1	0	9.330764	-8.934604	0.014409
72	1	0	9.300947	-5.631414	-0.350933
73	1	0	3.061727	-0.891437	-9.36927
74	1	0	0.225294	-2.559241	-9.945085
75	1	0	0.670782	0.480704	-11.213003
76	1	0	0.007391	4.227036	-5.429406
77	1	0	2.958674	3.069702	-6.432872
78	1	0	0.762435	4.167433	-8.655321

yby5-12-3A2000006_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-2.96973	1.852042	0.45944
1	6	0	-0.910684	0.782527	-1.262782
2	8	0	1.24152	1.545745	-0.967544
3	6	0	-1.370542	-1.37166	-3.160501
4	6	0	0.404083	-1.433023	-5.474447
5	6	0	0.026364	0.683296	-7.408234
6	6	0	-2.744522	0.587333	-8.185644
7	6	0	-4.575	-0.628725	-6.691785
8	6	0	-4.056903	-1.711185	-4.147653
9	8	0	-5.676575	-2.841113	-2.966336
10	6	0	-3.536184	1.732008	-10.418215
11	6	0	-6.03126	1.642034	-11.198779
12	6	0	-7.818168	0.381435	-9.747386
13	6	0	-7.084092	-0.73161	-7.51106
14	6	0	-0.292883	-3.728821	-1.688541
15	6	0	3.018932	-2.148983	-4.515271
16	6	0	2.470622	-4.066673	-2.420487
17	8	0	-1.451744	-5.067624	-0.266782
18	6	0	4.278406	-3.850579	-0.142162
19	6	0	3.850607	-5.741781	1.893094
20	6	0	2.839894	-5.348081	4.168031
21	6	0	2.485662	-7.480837	5.990421
22	6	0	-1.87237	3.696097	2.408771
23	6	0	-4.250098	5.118929	3.180857
24	6	0	-6.048117	3.38437	4.651326
25	6	0	-5.246669	0.635745	4.442055
26	6	0	-4.66772	-0.188131	1.775243
27	6	0	-6.430449	3.63339	7.492303
28	6	0	-7.718103	1.109288	8.196141
29	6	0	-7.27188	-0.752915	5.978961
30	8	0	-5.438472	5.531489	0.668639
31	6	0	-4.744863	3.675704	-0.933805
32	8	0	-5.477004	3.570221	-3.085043
33	8	0	-9.620885	-0.878055	4.621609
34	6	0	-6.478574	-3.377282	6.807793
35	6	0	-3.826784	7.684029	4.325165
36	1	0	-3.517533	0.432069	5.558527
37	1	0	-7.897745	3.577246	3.761196
38	1	0	-0.252801	-3.12264	-6.484513
39	1	0	2.59634	-5.9934	-3.155033

40	6	0	1.899716	-2.848011	5.093229
41	6	0	1.754464	0.107525	-9.660009
42	6	0	0.634229	3.338225	-6.430165
43	1	0	-2.181263	2.711394	-11.590616
44	1	0	-6.579166	2.551675	-12.946804
45	1	0	-9.770176	0.298576	-10.348192
46	1	0	-8.440665	-1.67079	-6.31024
47	1	0	4.160694	-2.983783	-6.006917
48	1	0	4.028272	-0.531027	-3.766115
49	1	0	6.182382	-4.091385	-0.907501
50	1	0	4.187624	-1.926052	0.564128
51	1	0	4.386013	-7.666588	1.418214
52	1	0	3.197764	-9.258354	5.244369
53	1	0	3.444864	-7.103666	7.779344
54	1	0	0.486182	-7.733404	6.439028
55	1	0	-0.541275	4.968424	1.502476
56	1	0	-0.905526	2.787853	3.972423
57	1	0	-3.738534	-2.013866	1.745797
58	1	0	-6.389415	-0.418531	0.684471
59	1	0	-7.556379	5.267664	8.028307
60	1	0	-4.60984	3.800385	8.448678
61	1	0	-6.978871	0.344626	9.956092
62	1	0	-9.745251	1.339347	8.436908
63	1	0	-9.413599	-2.066479	3.253283
64	1	0	-4.740844	-3.313018	7.910293
65	1	0	-7.947992	-4.237515	7.961989
66	1	0	-6.143483	-4.597617	5.18024
67	1	0	-2.695226	8.857788	3.072971
68	1	0	-5.612949	8.637461	4.67932
69	1	0	-2.833568	7.498447	6.116017
70	1	0	-0.121605	-2.968114	5.490302
71	1	0	2.8148	-2.327056	6.868287
72	1	0	2.185635	-1.318659	3.757983
73	1	0	1.525896	1.479223	-11.169732
74	1	0	3.725941	0.178703	-9.07997
75	1	0	1.374545	-1.759931	-10.439286
76	1	0	-0.735319	3.974381	-5.044291
77	1	0	2.504061	3.410315	-5.582599
78	1	0	0.578713	4.677586	-7.990695

yby5-12-3A2000008_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-2.490627	1.775152	-0.076582
1	6	0	-0.781865	0.134477	-1.732035
2	8	0	1.360163	0.863521	-2.146761
3	6	0	-1.58099	-2.482916	-2.679225
4	6	0	-0.264403	-3.406476	-5.11697
5	6	0	-0.766254	-1.861982	-7.525354
6	6	0	-3.566942	-1.178386	-7.594991
7	6	0	-5.231195	-1.771873	-5.61524
8	6	0	-4.371078	-2.952642	-3.22946
9	8	0	-5.741738	-4.278781	-1.947204
10	6	0	-4.571614	0.014052	-9.714961
11	6	0	-7.109929	0.620251	-9.87441
12	6	0	-8.744203	0.0049	-7.913966
13	6	0	-7.803628	-1.20704	-5.809837
14	6	0	-0.377026	-4.24774	-0.658364
15	6	0	2.408082	-4.140131	-4.343502
16	6	0	2.110299	-5.265554	-1.692669
17	8	0	-1.260501	-4.680039	1.39507
18	6	0	4.373775	-4.688613	0.044907
19	6	0	4.302599	-5.955759	2.554132
20	6	0	3.882582	-4.898729	4.802662
21	6	0	3.827042	-6.464276	7.156329
22	6	0	-0.978377	3.255081	1.909609
23	6	0	-2.768972	5.457524	2.395124
24	6	0	-5.179386	4.539652	3.726564
25	6	0	-5.357047	1.670693	3.688325
26	6	0	-4.82521	0.477666	1.145713
27	6	0	-5.691628	5.092171	6.506296
28	6	0	-7.755315	3.144108	7.208271
29	6	0	-7.845687	1.155446	5.042213
30	8	0	-3.531851	6.100083	-0.222774
31	6	0	-3.444961	4.010682	-1.684943
32	8	0	-4.054196	4.00192	-3.873604
33	8	0	-9.8187	1.75594	3.271498
34	6	0	-8.135376	-1.540669	5.95994
35	6	0	-1.565344	7.778855	3.50738
36	1	0	-3.914578	0.979588	4.998162
37	1	0	-6.757019	5.297087	2.640066
38	1	0	-1.224315	-5.209123	-5.48051
39	1	0	1.870779	-7.316094	-1.800687

40	6	0	3.343162	-2.15375	5.201769
41	6	0	-0.140456	-3.588323	-9.774996
42	6	0	0.820316	0.549279	-7.780839
43	1	0	-3.351059	0.487537	-11.283146
44	1	0	-7.817682	1.574724	-11.538763
45	1	0	-10.728215	0.481804	-8.030311
46	1	0	-9.022198	-1.702838	-4.247987
47	1	0	3.235139	-5.495487	-5.650143
48	1	0	3.630841	-2.49781	-4.264295
49	1	0	6.056622	-5.311972	-0.979938
50	1	0	4.539058	-2.647738	0.217705
51	1	0	4.592362	-7.988523	2.50252
52	1	0	5.197969	-5.784664	8.542644
53	1	0	1.974363	-6.354798	8.061614
54	1	0	4.231082	-8.443179	6.775991
55	1	0	0.777692	3.928754	1.090158
56	1	0	-0.534705	2.174338	3.595559
57	1	0	-4.455106	-1.519277	1.400061
58	1	0	-6.459001	0.650174	-0.087183
59	1	0	-6.280992	7.030145	6.857613
60	1	0	-3.994373	4.75615	7.628501
61	1	0	-7.355156	2.244801	9.015339
62	1	0	-9.601905	4.036369	7.373768
63	1	0	-11.41305	1.387288	4.07088
64	1	0	-9.879221	-1.765344	7.039398
65	1	0	-8.189765	-2.844752	4.372309
66	1	0	-6.574847	-2.077762	7.190415
67	1	0	-2.924235	9.31372	3.662123
68	1	0	-0.846529	7.365266	5.389042
69	1	0	0.003269	8.41031	2.338213
70	1	0	1.44999	-1.922964	5.990963
71	1	0	4.656222	-1.33049	6.564416
72	1	0	3.437364	-1.045395	3.478486
73	1	0	-1.256193	-5.318021	-9.727011
74	1	0	-0.508129	-2.653108	-11.56551
75	1	0	1.852214	-4.101918	-9.75089
76	1	0	0.265538	1.996173	-6.446875
77	1	0	2.818428	0.147034	-7.515617
78	1	0	0.595507	1.332941	-9.669253

yby5-12-3A2000011_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.070226	1.671049	0.590555
1	6	0	-1.300318	0.142224	-1.10632
2	8	0	0.843287	0.905912	-1.394126
3	6	0	-2.072979	-2.397301	-2.288145
4	6	0	-0.488837	-3.219158	-4.596811
5	6	0	-0.562092	-1.485764	-6.928907
6	6	0	-3.253056	-0.496809	-7.23961
7	6	0	-5.220436	-1.155913	-5.582711
8	6	0	-4.786404	-2.610575	-3.234766
9	8	0	-6.409791	-3.909257	-2.252584
10	6	0	-3.857984	1.01725	-9.305591
11	6	0	-6.298826	1.854189	-9.726702
12	6	0	-8.23908	1.154015	-8.102536
13	6	0	-7.694175	-0.360318	-6.056262
14	6	0	-1.249664	-4.341151	-0.261087
15	6	0	1.991711	-4.192534	-3.507543
16	6	0	1.144863	-5.65474	-1.16641
17	8	0	-2.280789	-4.692386	1.743799
18	6	0	3.114353	-5.979556	0.937003
19	6	0	3.90084	-3.530454	2.091477
20	6	0	5.98995	-2.190332	1.652849
21	6	0	6.390079	0.309537	2.915187
22	6	0	-1.666767	2.767582	2.882312
23	6	0	-3.326094	5.052112	3.465444
24	6	0	-5.935735	4.209049	4.414093
25	6	0	-6.331809	1.393451	4.019383
26	6	0	-5.60542	0.444653	1.421375
27	6	0	-6.729088	4.501549	7.165109
28	6	0	-9.055464	2.748375	7.362036
29	6	0	-9.005229	0.959088	5.041294
30	8	0	-3.742247	6.065279	0.885269
31	6	0	-3.696258	4.157233	-0.804673
32	8	0	-4.118484	4.444184	-3.018698
33	8	0	-10.877873	1.916714	3.3176
34	6	0	-9.557909	-1.777764	5.670654
35	6	0	-2.076094	7.105994	4.979122
36	1	0	-5.100433	0.433574	5.375423
37	1	0	-7.319039	5.217675	3.265717
38	1	0	-1.485252	-4.926125	-5.227466
39	1	0	0.514271	-7.541669	-1.748437

40	6	0	8.059438	-2.958376	-0.112575
41	6	0	0.082063	-3.155146	-9.22034
42	6	0	1.315015	0.72	-6.883092
43	1	0	-2.395566	1.561462	-10.623505
44	1	0	-6.691216	3.054143	-11.33515
45	1	0	-10.14917	1.803254	-8.428756
46	1	0	-9.15595	-0.927022	-4.747675
47	1	0	2.997775	-5.398951	-4.835169
48	1	0	3.225584	-2.652115	-2.959649
49	1	0	2.287937	-7.181313	2.393693
50	1	0	4.713327	-7.013289	0.157749
51	1	0	2.532591	-2.730926	3.3931
52	1	0	4.872705	0.756969	4.226769
53	1	0	8.173594	0.349498	3.953237
54	1	0	6.484692	1.823777	1.516051
55	1	0	0.211132	3.375145	2.321203
56	1	0	-1.491427	1.45962	4.453895
57	1	0	-5.406206	-1.590091	1.47993
58	1	0	-7.061375	0.888509	0.035207
59	1	0	-7.161697	6.442062	7.689204
60	1	0	-5.22847	3.847345	8.420627
61	1	0	-9.050505	1.674541	9.115178
62	1	0	-10.80914	3.816581	7.305026
63	1	0	-11.068573	0.699959	1.973888
64	1	0	-11.434894	-1.960239	6.492642
65	1	0	-9.472662	-2.960322	3.983892
66	1	0	-8.18459	-2.521111	7.011541
67	1	0	-1.625605	6.414491	6.862425
68	1	0	-0.333227	7.713264	4.073884
69	1	0	-3.315133	8.73444	5.1747
70	1	0	9.875723	-3.001375	0.86604
71	1	0	7.764402	-4.795451	-0.976377
72	1	0	8.258168	-1.576822	-1.634136
73	1	0	-1.244327	-4.718408	-9.40493
74	1	0	0.030162	-2.079659	-10.969277
75	1	0	1.978597	-3.933873	-9.031552
76	1	0	3.187005	0.071907	-6.33835
77	1	0	1.473038	1.543399	-8.760535
78	1	0	0.750673	2.20361	-5.595259

yby5-12-3A2000019_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-2.801586	1.473866	0.480365
1	6	0	-1.152046	-0.157026	-1.239578
2	8	0	1.000923	0.530871	-1.63074
3	6	0	-2.054611	-2.709539	-2.285473
4	6	0	-0.540982	-3.71514	-4.571305
5	6	0	-0.534365	-2.07057	-6.97414
6	6	0	-3.098004	-0.767797	-7.211765
7	6	0	-5.106704	-1.26587	-5.547228
8	6	0	-4.77084	-2.801618	-3.237443
9	8	0	-6.444787	-4.070421	-2.307262
10	6	0	-3.574563	0.839471	-9.239728
11	6	0	-5.926333	1.923985	-9.606127
12	6	0	-7.907457	1.386767	-7.969933
13	6	0	-7.494997	-0.221172	-5.963032
14	6	0	-1.332313	-4.603798	-0.186402
15	6	0	1.891823	-4.761669	-3.444585
16	6	0	0.982097	-6.086071	-1.044601
17	8	0	-2.368297	-4.806598	1.83732
18	6	0	2.94184	-6.430015	1.064247
19	6	0	3.811974	-3.983343	2.165889
20	6	0	5.927619	-2.704774	1.674056
21	6	0	6.407246	-0.196015	2.890681
22	6	0	-1.323809	2.342426	2.826768
23	6	0	-2.747283	4.765126	3.47123
24	6	0	-5.440191	4.16138	4.370169
25	6	0	-6.118956	1.416109	3.855654
26	6	0	-5.452094	0.47577	1.237845
27	6	0	-6.222887	4.422636	7.130477
28	6	0	-8.669207	2.826825	7.289322
29	6	0	-8.823266	1.229194	4.824102
30	8	0	-3.032664	5.901396	0.928548
31	6	0	-3.163324	4.055467	-0.830652
32	8	0	-3.546645	4.460213	-3.031556
33	8	0	-10.385884	2.464861	2.973612
34	6	0	-9.729177	-1.453859	5.242496
35	6	0	-1.31205	6.628804	5.065022
36	1	0	-5.024877	0.282479	5.194932
37	1	0	-6.693691	5.357123	3.256708
38	1	0	-1.633424	-5.390893	-5.116204
39	1	0	0.248287	-7.957278	-1.551874

40	6	0	7.950752	-3.55522	-0.106381
41	6	0	-0.239021	-3.889001	-9.226094
42	6	0	1.620265	-0.141762	-7.1156
43	1	0	-2.085594	1.260562	-10.573526
44	1	0	-6.215786	3.192594	-11.183498
45	1	0	-9.744905	2.235179	-8.253375
46	1	0	-8.987589	-0.662898	-4.640637
47	1	0	2.844352	-6.061492	-4.72334
48	1	0	3.186965	-3.251327	-2.957287
49	1	0	2.078562	-7.569411	2.549228
50	1	0	4.504522	-7.534151	0.307335
51	1	0	2.487507	-3.128274	3.477156
52	1	0	8.201147	-0.186078	3.911392
53	1	0	6.527085	1.292213	1.465783
54	1	0	4.914646	0.310437	4.209504
55	1	0	0.614044	2.774552	2.308088
56	1	0	-1.312294	0.970682	4.352386
57	1	0	-5.436067	-1.568055	1.269623
58	1	0	-6.853673	1.07332	-0.140434
59	1	0	-6.511598	6.373462	7.711417
60	1	0	-4.777535	3.625687	8.366733
61	1	0	-8.660038	1.609059	8.948142
62	1	0	-10.339673	4.020335	7.423706
63	1	0	-12.116512	2.317441	3.521135
64	1	0	-11.613124	-1.470668	6.083687
65	1	0	-9.810459	-2.476966	3.461868
66	1	0	-8.472111	-2.470855	6.515985
67	1	0	-0.936822	5.826153	6.920742
68	1	0	0.484649	7.099924	4.183891
69	1	0	-2.38894	8.361287	5.320204
70	1	0	8.157571	-2.21018	-1.658913
71	1	0	9.780171	-3.622283	0.846242
72	1	0	7.597915	-5.402344	-0.926261
73	1	0	-0.212081	-2.864647	-11.007145
74	1	0	1.52959	-4.934436	-9.079427
75	1	0	-1.788988	-5.241132	-9.297348
76	1	0	1.353324	1.429513	-5.835653
77	1	0	3.417659	-1.035641	-6.674512
78	1	0	1.772024	0.607378	-9.023972

Table S14. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of yby5-12-3B (**1b**).

Conformers	ΔG (a.u.)	P(%)/100	G (a.u.)
yby5-12-3B2000002_en_	0.00559	0.2	-1733.003854
yby5-12-3B2000009_en_	0.0	73.4	-1733.00944
yby5-12-3B2000010_en_	0.00444	0.66	-1733.004996
yby5-12-3B2000015_en_	0.001	25.54	-1733.008444
yby5-12-3B2000017_en_	0.00553	0.21	-1733.003909

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15 K.

Table S15. Cartesian coordinates for the low-energy reoptimized random research conformers of yby5-12-3B at B3LYP-D3(BJ)/6-31G** level of theory in methanol.

yby5-12-3B2000002_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-5.099018	1.906465	-2.57695
1	6	0	-5.983592	1.764687	0.171611
2	8	0	-7.545521	3.291218	0.881228
3	6	0	-5.065013	-0.234221	2.131189
4	6	0	-5.721616	0.765348	4.808248
5	6	0	-3.934225	-0.188853	6.91727
6	6	0	-1.236018	0.389334	6.15088
7	6	0	-0.491018	-0.134251	3.670476
8	6	0	-2.318571	-1.052652	1.782383
9	8	0	-1.66585	-2.407974	0.042225
10	6	0	0.592337	1.233045	7.841708
11	6	0	3.08115	1.559777	7.087173
12	6	0	3.804781	1.013687	4.624711
13	6	0	2.020898	0.152717	2.928051
14	6	0	-4.637869	1.162633	9.371084
15	6	0	-4.134052	-3.054131	7.333667
16	6	0	-6.9642	-2.491603	1.814358
17	6	0	-8.518522	0.063922	5.279175
18	6	0	-9.33398	-1.818356	3.253744
19	8	0	-6.616107	-4.40896	0.642285
20	6	0	-10.816613	-4.125255	4.151952
21	6	0	-13.281579	-3.424447	5.336661
22	6	0	-15.555978	-3.41985	4.246503
23	6	0	-17.861417	-2.64086	5.690517
24	6	0	-16.037251	-4.158468	1.559528
25	6	0	-6.73506	3.735525	-4.128901

26	6	0	-4.940796	4.335327	-6.298238
27	6	0	-4.540212	2.008915	-7.978059
28	6	0	-5.568597	-0.362781	-6.732708
29	6	0	-4.768577	-0.661029	-4.01153
30	6	0	-5.691334	1.80457	-10.608171
31	6	0	-5.478201	-1.04908	-11.194835
32	6	0	-4.937363	-2.42562	-8.666435
33	8	0	-2.542116	4.71149	-4.887139
34	6	0	-2.576805	3.352833	-2.732157
35	8	0	-0.862056	3.363132	-1.239362
36	8	0	-2.278842	-2.981	-8.674325
37	6	0	-6.439793	-4.83769	-8.312939
38	6	0	-5.472212	6.757636	-7.684983
39	1	0	-7.631686	-0.220873	-6.783235
40	1	0	-2.501329	1.782692	-8.181459
41	1	0	-5.53306	2.809332	4.777301
42	1	0	-10.500948	-0.831083	1.858132
43	1	0	0.094209	1.64326	9.776863
44	1	0	4.460845	2.241379	8.434304
45	1	0	5.74431	1.273915	4.034625
46	1	0	2.514997	-0.257977	0.992361
47	1	0	-4.311216	3.189085	9.228542
48	1	0	-6.616439	0.876635	9.840583
49	1	0	-3.546991	0.444313	10.958777
50	1	0	-6.003351	-3.594396	8.001955
51	1	0	-3.731571	-4.125598	5.625428
52	1	0	-2.772473	-3.650808	8.755181
53	1	0	-9.695202	1.741083	5.249383
54	1	0	-8.749265	-0.792459	7.129772
55	1	0	-11.066792	-5.39756	2.558207
56	1	0	-9.662196	-5.150227	5.521096
57	1	0	-13.176799	-2.810682	7.292241
58	1	0	-17.41619	-2.121923	7.628688
59	1	0	-18.794263	-1.031945	4.79401
60	1	0	-19.252906	-4.165087	5.739584
61	1	0	-16.911028	-2.59733	0.529704
62	1	0	-14.337938	-4.700618	0.54727
63	1	0	-17.368881	-5.732291	1.45829
64	1	0	-7.126864	5.431723	-3.044062
65	1	0	-8.530537	2.948041	-4.733217
66	1	0	-5.850102	-2.133368	-3.088098
67	1	0	-2.809758	-1.243902	-3.876416
68	1	0	-4.737989	2.967668	-12.009693

69	1	0	-7.670339	2.385327	-10.57302
70	1	0	-7.194517	-1.773681	-12.064941
71	1	0	-3.927427	-1.444002	-12.482787
72	1	0	-1.893315	-3.90303	-7.14857
73	1	0	-8.464967	-4.467806	-8.358489
74	1	0	-5.992008	-6.18239	-9.80366
75	1	0	-6.006409	-5.723585	-6.50251
76	1	0	-4.022597	7.132093	-9.093695
77	1	0	-7.284806	6.631515	-8.648292
78	1	0	-5.538416	8.343145	-6.378385

yby5-12-3B2000009_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-5.267889	0.529554	-3.030237
1	6	0	-6.652303	-1.376126	-1.361583
2	8	0	-8.511578	-2.361202	-2.278855
3	6	0	-5.80139	-2.045651	1.34299
4	6	0	-6.435304	0.106227	3.194381
5	6	0	-4.884091	0.052847	5.686987
6	6	0	-2.124703	-0.624801	5.247422
7	6	0	-1.367858	-2.208858	3.26671
8	6	0	-3.102743	-2.949038	1.236597
9	8	0	-2.459643	-4.278672	-0.544785
10	6	0	-0.286387	0.136613	6.971698
11	6	0	2.201966	-0.644517	6.759259
12	6	0	2.925601	-2.242942	4.806486
13	6	0	1.140863	-3.007657	3.071661
14	6	0	-5.158902	2.685799	6.860574
15	6	0	-5.862921	-1.912427	7.585507
16	6	0	-7.637324	-4.17722	2.237665
17	6	0	-9.324892	-0.134531	3.574225
18	6	0	-10.059046	-2.895802	3.075025
19	8	0	-7.18406	-6.40246	2.287485
20	6	0	-11.47979	-4.3121	5.152871
21	6	0	-13.971391	-3.117094	5.690142
22	6	0	-14.812821	-2.129043	7.852897
23	6	0	-17.392152	-0.971616	8.009275
24	6	0	-13.362568	-2.073849	10.280398
25	6	0	-7.161433	2.328909	-4.300406
26	6	0	-5.371408	4.346597	-5.289538
27	6	0	-3.704861	3.272817	-7.409022
28	6	0	-3.908626	0.409746	-7.588886
29	6	0	-3.700931	-0.943023	-5.081148
30	6	0	-4.07652	4.029193	-10.161177
31	6	0	-2.583176	1.982238	-11.612123
32	6	0	-2.083108	-0.220813	-9.750558
33	8	0	-3.676515	4.665904	-3.073896
34	6	0	-3.467824	2.443642	-1.835678
35	8	0	-1.992489	2.150054	-0.126184
36	8	0	0.500549	0.050114	-8.955834
37	6	0	-2.493729	-2.814941	-10.890041
38	6	0	-6.536997	6.8819	-5.817124
39	1	0	-5.785548	-0.002859	-8.352417

40	1	0	-1.76201	3.737231	-6.90177
41	1	0	-6.004393	1.909527	2.316137
42	1	0	-11.23725	-2.974254	1.382603
43	1	0	-0.789431	1.358953	8.526296
44	1	0	3.579892	-0.002908	8.127686
45	1	0	4.865549	-2.865316	4.640481
46	1	0	1.637861	-4.214947	1.50255
47	1	0	-4.147657	4.09294	5.753094
48	1	0	-7.140698	3.231501	6.934604
49	1	0	-4.458344	2.75251	8.790013
50	1	0	-7.766482	-1.470688	8.21282
51	1	0	-5.840915	-3.816297	6.813066
52	1	0	-4.652957	-1.925114	9.247258
53	1	0	-10.288	1.108234	2.247919
54	1	0	-9.917174	0.473305	5.442895
55	1	0	-11.755236	-6.245819	4.486325
56	1	0	-10.320554	-4.458643	6.83726
57	1	0	-15.231992	-3.028246	4.069077
58	1	0	-18.380309	-1.044869	6.208462
59	1	0	-18.555984	-1.935242	9.416084
60	1	0	-17.285079	1.004004	8.601038
61	1	0	-11.526527	-2.979873	10.162604
62	1	0	-13.073724	-0.130227	10.914989
63	1	0	-14.425328	-3.013992	11.778839
64	1	0	-8.430888	3.135721	-2.893756
65	1	0	-8.30417	1.434746	-5.744294
66	1	0	-4.426948	-2.857379	-5.218245
67	1	0	-1.758765	-1.089147	-4.422477
68	1	0	-3.414881	5.930016	-10.578788
69	1	0	-6.074945	3.94873	-10.664937
70	1	0	-3.614833	1.319732	-13.262225
71	1	0	-0.769411	2.689506	-12.267663
72	1	0	0.898583	-1.347799	-7.854716
73	1	0	-4.428566	-3.036914	-11.557118
74	1	0	-1.219915	-3.106536	-12.478094
75	1	0	-2.137561	-4.300203	-9.504738
76	1	0	-7.893357	6.731428	-7.35493
77	1	0	-7.517362	7.588402	-4.153754
78	1	0	-5.10345	8.251849	-6.358658

yby5-12-3B2000010_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-5.344877	2.074078	-2.84194
1	6	0	-6.494803	1.748913	-0.206832
2	8	0	-8.08613	3.262473	0.466631
3	6	0	-5.814678	-0.413249	1.672146
4	6	0	-6.701799	0.402119	4.346682
5	6	0	-5.156059	-0.783774	6.528335
6	6	0	-2.381317	-0.230834	6.074819
7	6	0	-1.410131	-0.569054	3.641165
8	6	0	-3.064254	-1.280134	1.516141
9	8	0	-2.278054	-2.508729	-0.259275
10	6	0	-0.707208	0.418024	7.996137
11	6	0	1.849378	0.733514	7.510653
12	6	0	2.796187	0.372601	5.090288
13	6	0	1.166635	-0.293444	3.165488
14	6	0	-6.064559	0.369355	9.015217
15	6	0	-5.470812	-3.664584	6.66571
16	6	0	-7.712789	-2.591284	1.007038
17	6	0	-9.551604	-0.221076	4.476458
18	6	0	-10.187957	-2.004354	2.303812
19	8	0	-7.297931	-4.410897	-0.291669
20	6	0	-11.674372	-4.379305	3.003216
21	6	0	-14.223244	-3.749819	4.016938
22	6	0	-15.150528	-4.187877	6.321219
23	6	0	-17.774592	-3.374917	7.005455
24	6	0	-13.752828	-5.490051	8.40699
25	6	0	-6.785178	4.084003	-4.368243
26	6	0	-4.792839	4.79389	-6.317669
27	6	0	-4.341922	2.60469	-8.159974
28	6	0	-5.53513	0.176838	-7.192724
29	6	0	-4.947647	-0.378105	-4.455343
30	6	0	-5.317163	2.671996	-10.86958
31	6	0	-5.247344	-0.137128	-11.679355
32	6	0	-4.847096	-1.731932	-9.239608
33	8	0	-2.5112	4.946712	-4.693614
34	6	0	-2.782467	3.435554	-2.656045
35	8	0	-1.211423	3.281458	-1.020487
36	8	0	-2.216982	-2.30942	-8.89679
37	6	0	-6.400872	-4.1354	-9.161772
38	6	0	-5.118586	7.348875	-7.519349
39	1	0	-7.581804	0.404514	-7.381031

40	1	0	-2.302124	2.327859	-8.236864
41	1	0	-6.447175	2.433734	4.50264
42	1	0	-11.269364	-0.970735	0.871551
43	1	0	-1.381159	0.68197	9.902992
44	1	0	3.106333	1.261084	9.035457
45	1	0	4.788723	0.625105	4.710648
46	1	0	1.833147	-0.557865	1.256355
47	1	0	-5.684203	2.389978	9.089199
48	1	0	-8.084523	0.09991	9.263506
49	1	0	-5.150569	-0.518783	10.628346
50	1	0	-7.416104	-4.188175	7.079088
51	1	0	-4.912569	-4.59341	4.918591
52	1	0	-4.288097	-4.431356	8.163696
53	1	0	-10.651507	1.503158	4.359274
54	1	0	-10.045927	-1.113232	6.256349
55	1	0	-11.848624	-5.541436	1.307891
56	1	0	-10.572667	-5.484002	4.341183
57	1	0	-15.447262	-2.773292	2.685593
58	1	0	-18.717691	-2.421691	5.44766
59	1	0	-18.932617	-4.990679	7.561793
60	1	0	-17.754187	-2.091047	8.622289
61	1	0	-13.53204	-4.233094	10.030244
62	1	0	-14.817126	-7.123274	9.083772
63	1	0	-11.888181	-6.146866	7.861311
64	1	0	-7.227628	5.695981	-3.180033
65	1	0	-8.539852	3.413034	-5.193093
66	1	0	-6.131264	-1.888827	-3.744718
67	1	0	-3.023768	-1.041937	-4.252324
68	1	0	-4.203312	3.879961	-12.104954
69	1	0	-7.256269	3.371336	-10.917141
70	1	0	-6.984658	-0.684163	-12.637475
71	1	0	-3.69821	-0.507301	-12.98214
72	1	0	-1.748055	-3.542956	-10.152043
73	1	0	-8.414825	-3.725147	-9.286826
74	1	0	-5.922887	-5.372709	-10.742211
75	1	0	-6.050416	-5.163325	-7.416029
76	1	0	-3.558291	7.770907	-8.789626
77	1	0	-6.863062	7.399044	-8.607283
78	1	0	-5.206517	8.817058	-6.083403

yby5-12-3B2000015_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-5.265123	0.546491	-2.978072
1	6	0	-6.673905	-1.367386	-1.337479
2	8	0	-8.545131	-2.312677	-2.271759
3	6	0	-5.836305	-2.087142	1.357549
4	6	0	-6.436285	0.046862	3.241123
5	6	0	-4.879812	-0.067932	5.729054
6	6	0	-2.127178	-0.756965	5.26421
7	6	0	-1.395524	-2.32259	3.259322
8	6	0	-3.151727	-3.032251	1.236666
9	8	0	-2.53885	-4.363107	-0.552564
10	6	0	-0.270858	-0.026829	6.982448
11	6	0	2.211566	-0.818641	6.738835
12	6	0	2.910481	-2.395677	4.760029
13	6	0	1.107108	-3.131343	3.031527
14	6	0	-5.130029	2.541977	6.957901
15	6	0	-5.869687	-2.063232	7.59011
16	6	0	-7.706058	-4.202096	2.220754
17	6	0	-9.328622	-0.155108	3.624504
18	6	0	-10.107516	-2.894436	3.076318
19	8	0	-7.289221	-6.434608	2.238802
20	6	0	-11.554601	-4.318843	5.129719
21	6	0	-14.043464	-3.112931	5.655684
22	6	0	-14.886875	-2.109748	7.810657
23	6	0	-17.463389	-0.944425	7.954989
24	6	0	-13.441883	-2.045039	10.240936
25	6	0	-7.14859	2.37443	-4.224458
26	6	0	-5.351779	4.401308	-5.177327
27	6	0	-3.689325	3.352658	-7.318263
28	6	0	-3.895657	0.489545	-7.533723
29	6	0	-3.703615	-0.905221	-5.049201
30	6	0	-4.049102	4.144232	-10.06174
31	6	0	-2.53334	2.127679	-11.53005
32	6	0	-2.080031	-0.140889	-9.704752
33	8	0	-3.651668	4.676752	-2.967771
34	6	0	-3.454655	2.428768	-1.756886
35	8	0	-1.972657	2.112072	-0.059612
36	8	0	0.495117	-0.243124	-8.867111
37	6	0	-2.573844	-2.686538	-10.903436
38	6	0	-6.508536	6.947187	-5.673472
39	1	0	-5.776366	0.120583	-8.308743

40	1	0	-1.757674	3.859821	-6.776587
41	1	0	-5.978723	1.857189	2.391285
42	1	0	-11.283093	-2.925198	1.380625
43	1	0	-0.753707	1.17893	8.556281
44	1	0	3.604442	-0.200726	8.103182
45	1	0	4.845971	-3.02461	4.568579
46	1	0	1.584368	-4.32018	1.442304
47	1	0	-4.113629	3.964815	5.875329
48	1	0	-7.107205	3.1003	7.054095
49	1	0	-4.41929	2.562495	8.884655
50	1	0	-7.765316	-1.613935	8.236483
51	1	0	-5.871662	-3.950582	6.777533
52	1	0	-4.651516	-2.12462	9.244724
53	1	0	-10.276864	1.128531	2.326726
54	1	0	-9.904975	0.423722	5.507454
55	1	0	-11.837824	-6.244851	4.444609
56	1	0	-10.40875	-4.48582	6.821253
57	1	0	-15.299692	-3.029268	4.030896
58	1	0	-18.448135	-1.026495	6.152691
59	1	0	-18.632431	-1.896336	9.365485
60	1	0	-17.35211	1.034517	8.534749
61	1	0	-11.603958	-2.947953	10.129777
62	1	0	-13.157766	-0.099056	10.870385
63	1	0	-14.505947	-2.982671	11.740152
64	1	0	-8.418901	3.166737	-2.810693
65	1	0	-8.290863	1.506869	-5.68434
66	1	0	-4.450093	-2.807936	-5.226264
67	1	0	-1.757352	-1.096987	-4.424711
68	1	0	-3.408083	6.058912	-10.449978
69	1	0	-6.045025	4.051441	-10.569458
70	1	0	-3.526678	1.523813	-13.226372
71	1	0	-0.704928	2.846749	-12.139473
72	1	0	0.931304	1.361924	-8.123962
73	1	0	-4.512432	-2.807172	-11.580043
74	1	0	-1.307873	-2.982702	-12.49668
75	1	0	-2.255307	-4.200438	-9.549374
76	1	0	-7.866245	6.819205	-7.212139
77	1	0	-7.486316	7.634342	-4.000853
78	1	0	-5.072616	8.321833	-6.197533

yby5-12-3B2000017_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-5.141896	1.7678	-2.568535
1	6	0	-5.999727	1.626511	0.187817
2	8	0	-7.592974	3.119572	0.898939
3	6	0	-5.016821	-0.335607	2.154219
4	6	0	-5.663348	0.675092	4.829467
5	6	0	-3.836303	-0.228264	6.926878
6	6	0	-1.155905	0.386185	6.126245
7	6	0	-0.427819	-0.146748	3.642769
8	6	0	-2.260036	-1.10526	1.779308
9	8	0	-1.603631	-2.45689	0.037651
10	6	0	0.676902	1.270033	7.791878
11	6	0	3.153331	1.625282	7.010446
12	6	0	3.860725	1.068837	4.545548
13	6	0	2.072699	0.16947	2.873561
14	6	0	-4.535172	1.13429	9.375964
15	6	0	-3.9818	-3.092445	7.373547
16	6	0	-6.870207	-2.636869	1.881822
17	6	0	-8.441821	-0.074184	5.335533
18	6	0	-9.235925	-2.004856	3.346891
19	8	0	-6.494941	-4.556027	0.721212
20	6	0	-10.644706	-4.337829	4.297193
21	6	0	-13.128597	-3.68821	5.470507
22	6	0	-15.408354	-3.820607	4.399008
23	6	0	-17.734226	-3.075439	5.828246
24	6	0	-15.877788	-4.689561	1.749092
25	6	0	-6.813161	3.571498	-4.112884
26	6	0	-5.052326	4.167043	-6.310972
27	6	0	-4.655262	1.830786	-7.977909
28	6	0	-5.649125	-0.538419	-6.700434
29	6	0	-4.809741	-0.808454	-3.988313
30	6	0	-5.840261	1.596611	-10.590507
31	6	0	-5.608775	-1.258987	-11.158647
32	6	0	-5.030245	-2.612508	-8.62605
33	8	0	-2.639157	4.573747	-4.934334
34	6	0	-2.637039	3.237713	-2.764763
35	8	0	-0.907879	3.286114	-1.289408
36	8	0	-2.368942	-3.153758	-8.662508
37	6	0	-6.51486	-5.029664	-8.233547
38	6	0	-5.620605	6.573753	-7.710316
39	1	0	-7.71353	-0.41063	-6.723292

40	1	0	-2.617477	1.618987	-8.206269
41	1	0	-5.512638	2.721936	4.779875
42	1	0	-10.450266	-1.071961	1.954687
43	1	0	0.192008	1.688624	9.72859
44	1	0	4.536398	2.337022	8.338397
45	1	0	5.790697	1.350761	3.934445
46	1	0	2.553451	-0.250432	0.936501
47	1	0	-4.243574	3.164447	9.211558
48	1	0	-6.503477	0.820245	9.870259
49	1	0	-3.41548	0.447999	10.957667
50	1	0	-5.832386	-3.65673	8.072831
51	1	0	-3.583858	-4.174216	5.670814
52	1	0	-2.591358	-3.650853	8.782553
53	1	0	-9.651265	1.578946	5.286626
54	1	0	-8.641779	-0.904581	7.201476
55	1	0	-10.857467	-5.649685	2.730549
56	1	0	-9.456656	-5.297312	5.684504
57	1	0	-13.037153	-2.988754	7.397849
58	1	0	-17.299835	-2.473354	7.744568
59	1	0	-18.72852	-1.533135	4.882018
60	1	0	-19.069273	-4.646157	5.937706
61	1	0	-17.128858	-6.33112	1.725086
62	1	0	-16.838609	-3.21646	0.668553
63	1	0	-14.163372	-5.186371	0.739251
64	1	0	-7.202616	5.274209	-3.037058
65	1	0	-8.611621	2.766681	-4.684497
66	1	0	-5.86872	-2.280471	-3.038515
67	1	0	-2.845281	-1.376017	-3.872249
68	1	0	-4.9172	2.757747	-12.013831
69	1	0	-7.823782	2.159994	-10.531888
70	1	0	-7.326122	-2.0043	-12.009152
71	1	0	-4.066003	-1.648991	-12.457709
72	1	0	-1.958352	-4.057125	-7.132043
73	1	0	-8.542602	-4.672155	-8.261845
74	1	0	-6.074484	-6.386395	-9.71548
75	1	0	-6.056808	-5.894241	-6.419002
76	1	0	-4.192344	6.946826	-9.140965
77	1	0	-7.444528	6.425954	-8.648813
78	1	0	-5.681992	8.169542	-6.416037

Table S16. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of yby5-12-3C (**1c**).

Conformers	ΔG (a.u.)	P(%)/100	G (a.u.)
yby5-12-3C2000001_en_	0.01068	0.0	-1733.004597
yby5-12-3C2000002_en_	0.00586	0.11	-1733.00942
yby5-12-3C2000003_en_	0.01163	0.0	-1733.003656
yby5-12-3C2000004_en_	0.00548	0.16	-1733.009804
yby5-12-3C2000005_en_	0.00015	44.67	-1733.015127
yby5-12-3C2000006_en_	0.00553	0.15	-1733.009747
yby5-12-3C2000007_en_	0.00731	0.02	-1733.007971
yby5-12-3C2000008_en_	0.0	52.59	-1733.015281
yby5-12-3C2000009_en_	0.00306	2.05	-1733.012218
yby5-12-3C2000010_en_	0.0052	0.21	-1733.010077
yby5-12-3C2000011_en_	0.00656	0.05	-1733.008722

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15 K.

Table S17. Cartesian coordinates for the low-energy reoptimized random research conformers of yby5-12-3C at B3LYP-D3(BJ)/6-31G** level of theory in methanol.

yby5-12-3C2000001_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.492786	-1.535939	-2.049878
1	6	0	-7.359995	-3.099889	-0.886637
2	8	0	-7.064398	-5.237038	-1.650664
3	6	0	-5.516141	-2.045867	1.158162
4	6	0	-4.443496	-4.282411	2.695172
5	6	0	-1.710812	-3.874026	3.637656
6	6	0	-0.076648	-3.170415	1.388574
7	6	0	-0.996132	-1.449521	-0.408469
8	6	0	-3.606989	-0.496999	-0.317515
9	8	0	-4.27391	1.36932	-1.5094
10	6	0	2.398552	-4.016372	1.123757
11	6	0	3.91342	-3.201803	-0.853718
12	6	0	2.992966	-1.48725	-2.614616
13	6	0	0.548511	-0.611948	-2.378916
14	6	0	-1.467621	-1.712706	5.560446
15	6	0	-0.837095	-6.333874	4.873469
16	6	0	-6.951319	-0.607676	3.266145
17	6	0	-6.411299	-4.744147	4.825975
18	6	0	-8.390984	-2.630129	4.652225
19	8	0	-6.688213	1.576029	3.852917

20	6	0	-9.648856	-1.779781	7.095232
21	6	0	-12.066222	-0.414598	6.580953
22	6	0	-12.596363	2.032278	6.874027
23	6	0	-15.122655	3.05581	6.11085
24	6	0	-10.807657	3.965382	7.89546
25	6	0	-9.239916	-1.458457	-4.945975
26	6	0	-11.99219	-1.063244	-5.702751
27	6	0	-12.907787	1.571299	-4.891363
28	6	0	-11.054155	2.812027	-3.079651
29	6	0	-10.082963	1.132547	-0.983621
30	6	0	-13.342182	3.70201	-6.778217
31	6	0	-13.461325	6.073912	-5.075384
32	6	0	-12.314098	5.342106	-2.462114
33	8	0	-13.283163	-2.860106	-3.985253
34	6	0	-11.950694	-3.089005	-1.823207
35	8	0	-12.704845	-4.258887	-0.024738
36	8	0	-14.243538	5.080838	-0.570155
37	6	0	-10.501025	7.284462	-1.414604
38	6	0	-12.643595	-1.818314	-8.362905
39	1	0	-9.414909	3.331062	-4.227033
40	1	0	-14.702111	1.224938	-3.921706
41	1	0	-4.383187	-5.908267	1.443589
42	1	0	-9.863481	-3.259142	3.336699
43	1	0	3.179493	-5.328081	2.475456
44	1	0	5.824818	-3.910645	-1.015655
45	1	0	4.175244	-0.849381	-4.154867
46	1	0	-0.23072	0.720448	-3.715327
47	1	0	-2.613984	-2.052575	7.233028
48	1	0	0.489507	-1.545739	6.17119
49	1	0	-2.020248	0.098031	4.768098
50	1	0	1.001136	-6.128483	5.771162
51	1	0	-2.146072	-6.907149	6.34871
52	1	0	-0.720614	-7.865316	3.504126
53	1	0	-7.285845	-6.593024	4.645775
54	1	0	-5.527758	-4.669842	6.680111
55	1	0	-10.042199	-3.463985	8.225375
56	1	0	-8.323363	-0.637003	8.176959
57	1	0	-13.533955	-1.606129	5.777735
58	1	0	-16.037378	4.035296	7.681389
59	1	0	-14.917801	4.431853	4.588016
60	1	0	-16.385682	1.570083	5.458144
61	1	0	-8.998079	3.185437	8.455627
62	1	0	-10.436343	5.411742	6.472233

63	1	0	-11.636724	4.931615	9.520334
64	1	0	-8.577923	-3.275304	-5.637083
65	1	0	-7.978885	0.009809	-5.62065
66	1	0	-8.374285	1.967997	-0.247994
67	1	0	-11.439613	1.00396	0.558344
68	1	0	-15.03652	3.457022	-7.917277
69	1	0	-11.743886	3.828623	-8.074706
70	1	0	-12.44074	7.651769	-5.911285
71	1	0	-15.396958	6.708416	-4.78635
72	1	0	-15.473843	3.871715	-1.155312
73	1	0	-8.925656	7.568452	-2.705093
74	1	0	-11.454706	9.085609	-1.136762
75	1	0	-9.749778	6.668645	0.39706
76	1	0	-12.101436	-3.770245	-8.710784
77	1	0	-14.66053	-1.627618	-8.711773
78	1	0	-11.644273	-0.616471	-9.699302

yby5-12-3C2000002_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.970941	-0.976044	-3.043354
1	6	0	-7.877757	-2.61126	-1.878743
2	8	0	-7.615124	-4.741982	-2.672707
3	6	0	-6.109373	-1.78803	0.321468
4	6	0	-5.440832	-4.085265	2.043132
5	6	0	-2.722079	-5.104117	1.761513
6	6	0	-0.914543	-2.90604	2.038293
7	6	0	-1.450983	-0.695292	0.680625
8	6	0	-3.789068	-0.506732	-0.818155
9	8	0	-3.897921	0.709077	-2.77509
10	6	0	1.315272	-2.998454	3.420281
11	6	0	2.956277	-0.95137	3.468865
12	6	0	2.414098	1.223774	2.104856
13	6	0	0.21914	1.34003	0.692859
14	6	0	-2.291953	-7.172958	3.72834
15	6	0	-2.310958	-6.292919	-0.851205
16	6	0	-7.284781	0.162205	2.215689
17	6	0	-6.031394	-3.247514	4.760328
18	6	0	-8.075011	-1.249889	4.544785
19	8	0	-7.338137	2.421834	1.91578
20	6	0	-8.51856	0.415672	6.846535
21	6	0	-9.443595	-1.058989	9.074645
22	6	0	-11.839143	-1.641697	9.607318
23	6	0	-12.491631	-3.18333	11.88828
24	6	0	-14.048487	-0.863387	8.023923
25	6	0	-10.735001	-1.927745	-5.674261
26	6	0	-13.430297	-0.930633	-5.836329
27	6	0	-13.446168	1.962536	-5.994688
28	6	0	-10.862089	3.054781	-5.385218
29	6	0	-9.658786	1.956533	-3.040818
30	6	0	-14.078906	3.351605	-8.434517
31	6	0	-13.090555	6.052105	-7.922026
32	6	0	-11.307744	5.908271	-5.602745
33	8	0	-14.370715	-1.564809	-3.258962
34	6	0	-12.439987	-1.544654	-1.611652
35	8	0	-12.713934	-1.886422	0.626147
36	8	0	-12.747146	6.84378	-3.495192
37	6	0	-8.900891	7.43007	-5.895723
38	6	0	-15.124663	-2.265033	-7.68432
39	1	0	-9.631722	2.604943	-6.984435

40	1	0	-14.767787	2.613386	-4.55288
41	1	0	-6.71415	-5.613355	1.52821
42	1	0	-9.845668	-2.179501	4.027544
43	1	0	1.797734	-4.680776	4.469736
44	1	0	4.673786	-1.062819	4.57323
45	1	0	3.69722	2.814221	2.145344
46	1	0	-0.25358	3.002703	-0.394807
47	1	0	-3.767774	-8.598072	3.568565
48	1	0	-0.494407	-8.124703	3.421266
49	1	0	-2.308932	-6.45963	5.654671
50	1	0	-0.370263	-6.958128	-1.020405
51	1	0	-3.581975	-7.885634	-1.118734
52	1	0	-2.657581	-4.968839	-2.380579
53	1	0	-6.620615	-4.824609	5.933805
54	1	0	-4.359361	-2.411764	5.634429
55	1	0	-6.749676	1.364696	7.32097
56	1	0	-9.835499	1.907012	6.32558
57	1	0	-7.992092	-1.76949	10.339287
58	1	0	-13.766155	-2.149749	13.141151
59	1	0	-13.481686	-4.915284	11.356579
60	1	0	-10.821773	-3.705881	12.967775
61	1	0	-15.011332	-2.521081	7.259653
62	1	0	-15.443777	0.143519	9.163726
63	1	0	-13.540318	0.327359	6.434146
64	1	0	-10.729482	-3.978066	-5.710861
65	1	0	-9.51426	-1.258308	-7.180369
66	1	0	-7.669605	2.423281	-2.963917
67	1	0	-10.528863	2.724955	-1.346039
68	1	0	-16.081471	3.319955	-8.898889
69	1	0	-13.065353	2.509167	-10.021777
70	1	0	-12.098874	6.814025	-9.554439
71	1	0	-14.621473	7.347749	-7.477351
72	1	0	-11.653888	6.855126	-2.03565
73	1	0	-7.798658	6.77855	-7.508051
74	1	0	-9.342354	9.420507	-6.169054
75	1	0	-7.709613	7.262023	-4.221656
76	1	0	-15.150996	-4.287079	-7.315998
77	1	0	-17.04869	-1.550511	-7.567877
78	1	0	-14.445215	-1.962402	-9.601228

yby5-12-3C2000003_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.257617	-1.3181	-2.469326
1	6	0	-7.035923	-2.892153	-1.501031
2	8	0	-6.502995	-4.810062	-2.628267
3	6	0	-5.393368	-2.127319	0.834701
4	6	0	-4.385571	-4.553926	2.091065
5	6	0	-1.79494	-4.226262	3.402057
6	6	0	0.041276	-3.077684	1.518689
7	6	0	-0.765577	-1.14007	-0.105959
8	6	0	-3.42423	-0.3388	-0.228511
9	8	0	-4.073337	1.618785	-1.27623
10	6	0	2.583778	-3.747668	1.455826
11	6	0	4.271677	-2.555032	-0.154778
12	6	0	3.459873	-0.629811	-1.742764
13	6	0	0.949991	0.071761	-1.706582
14	6	0	-1.874617	-2.454222	5.700436
15	6	0	-0.931815	-6.842848	4.273482
16	6	0	-6.985145	-1.024706	3.026021
17	6	0	-6.553495	-5.41106	3.870244
18	6	0	-8.464839	-3.232914	4.028972
19	8	0	-6.836111	1.076866	3.894815
20	6	0	-9.77774	-2.797014	6.551081
21	6	0	-12.042725	-1.136196	6.265706
22	6	0	-12.40644	1.181513	7.185486
23	6	0	-14.770969	2.616839	6.582636
24	6	0	-10.527831	2.593471	8.763628
25	6	0	-9.042681	-0.8415	-5.327175
26	6	0	-11.822258	-0.497095	-6.012285
27	6	0	-12.884461	1.933309	-4.841556
28	6	0	-11.074474	3.039997	-2.906601
29	6	0	-9.958256	1.158068	-1.065048
30	6	0	-13.4933	4.265159	-6.418107
31	6	0	-13.684672	6.384899	-4.411716
32	6	0	-12.51605	5.34985	-1.935405
33	8	0	-12.98468	-2.59409	-4.548586
34	6	0	-11.629248	-3.022576	-2.446699
35	8	0	-12.288092	-4.473036	-0.81831
36	8	0	-14.612711	4.60456	-0.371492
37	6	0	-10.87513	7.233191	-0.540326
38	6	0	-12.468261	-0.929633	-8.743646
39	1	0	-9.489582	3.824693	-3.975655

40	1	0	-14.617318	1.391355	-3.867554
41	1	0	-4.102088	-5.94594	0.609128
42	1	0	-9.91697	-3.587252	2.59416
43	1	0	3.281815	-5.225283	2.675245
44	1	0	6.232545	-3.135566	-0.16693
45	1	0	4.775927	0.303041	-2.997848
46	1	0	0.248954	1.556098	-2.920216
47	1	0	-3.22471	-3.103103	7.111516
48	1	0	-0.023247	-2.397989	6.595406
49	1	0	-2.3665	-0.530929	5.184727
50	1	0	-0.621349	-8.1005	2.674956
51	1	0	0.803821	-6.749189	5.370352
52	1	0	-2.345149	-7.704404	5.489773
53	1	0	-7.447305	-7.119098	3.162418
54	1	0	-5.849617	-5.839856	5.751347
55	1	0	-10.369485	-4.642376	7.269843
56	1	0	-8.426057	-2.036058	7.902513
57	1	0	-13.524534	-1.936908	5.088988
58	1	0	-14.328986	4.469214	5.779145
59	1	0	-15.981315	1.604526	5.263777
60	1	0	-15.870788	2.994995	8.288193
61	1	0	-11.480228	3.828777	10.108973
62	1	0	-9.271496	1.358935	9.817492
63	1	0	-9.342132	3.781195	7.566301
64	1	0	-8.286832	-2.507106	-6.259206
65	1	0	-7.869583	0.772726	-5.798502
66	1	0	-8.271248	1.976308	-0.258083
67	1	0	-11.262599	0.73516	0.471073
68	1	0	-15.214519	4.071259	-7.525169
69	1	0	-11.958357	4.666542	-7.736648
70	1	0	-12.694305	8.081461	-5.017882
71	1	0	-15.634329	6.912204	-4.037358
72	1	0	-13.948625	4.043926	1.231476
73	1	0	-9.304537	7.86234	-1.713114
74	1	0	-11.979652	8.879868	0.008373
75	1	0	-10.074163	6.396221	1.164995
76	1	0	-11.823155	-2.782318	-9.357927
77	1	0	-14.49745	-0.80603	-9.046886
78	1	0	-11.558645	0.497288	-9.911457

yby5-12-3C2000004_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.794028	-0.869448	-3.1748
1	6	0	-7.611329	-2.317751	-1.931584
2	8	0	-6.995104	-4.323465	-2.845949
3	6	0	-6.171	-1.462243	0.484637
4	6	0	-5.324379	-3.790333	2.082058
5	6	0	-2.473667	-4.403389	1.976566
6	6	0	-1.027435	-2.01633	2.596953
7	6	0	-1.764018	0.217181	1.378451
8	6	0	-3.969255	0.221626	-0.320345
9	8	0	-4.079315	1.582724	-2.178714
10	6	0	1.070797	-1.932168	4.172412
11	6	0	2.386866	0.307393	4.544333
12	6	0	1.648477	2.506947	3.318167
13	6	0	-0.415205	2.453059	1.717077
14	6	0	-1.913435	-6.563925	3.806937
15	6	0	-1.681432	-5.277655	-0.67254
16	6	0	-7.77473	0.13085	2.398988
17	6	0	-6.236607	-3.277046	4.787806
18	6	0	-8.523505	-1.568314	4.547127
19	8	0	-8.138879	2.376958	2.260578
20	6	0	-9.315385	-0.163765	6.928253
21	6	0	-10.239438	-1.92965	8.920385
22	6	0	-9.106837	-2.590525	11.074467
23	6	0	-10.319376	-4.442247	12.839798
24	6	0	-6.599261	-1.614088	11.946806
25	6	0	-10.20191	-1.700665	-5.924317
26	6	0	-12.976644	-1.020186	-6.275781
27	6	0	-13.337114	1.855493	-6.251544
28	6	0	-10.969562	3.189921	-5.326896
29	6	0	-9.871687	2.071285	-2.942859
30	6	0	-13.919469	3.336988	-8.650521
31	6	0	-13.278112	6.087621	-7.901134
32	6	0	-11.731402	5.981958	-5.417953
33	8	0	-14.048902	-1.956971	-3.846309
34	6	0	-12.280493	-1.851042	-2.02746
35	8	0	-12.692843	-2.418615	0.141787
36	8	0	-13.476303	6.594092	-3.425626
37	6	0	-9.505747	7.78262	-5.35841
38	6	0	-14.321208	-2.404418	-8.359718
39	1	0	-9.548569	2.996071	-6.815724

40	1	0	-14.849833	2.239909	-4.905021
41	1	0	-6.323622	-5.424987	1.341367
42	1	0	-10.111365	-2.6767	3.823191
43	1	0	1.703129	-3.623205	5.124009
44	1	0	4.005493	0.329173	5.794033
45	1	0	2.679211	4.247491	3.610471
46	1	0	-1.033111	4.129872	0.728459
47	1	0	-3.154524	-8.154967	3.403275
48	1	0	0.019804	-7.230937	3.589307
49	1	0	-2.183552	-6.032073	5.772702
50	1	0	0.345203	-5.637766	-0.713983
51	1	0	-2.668917	-7.006254	-1.185115
52	1	0	-2.099802	-3.879715	-2.115739
53	1	0	-6.672723	-5.00984	5.795091
54	1	0	-4.777165	-2.292392	5.861422
55	1	0	-7.733836	0.977725	7.582207
56	1	0	-10.808342	1.165774	6.422402
57	1	0	-12.049716	-2.806801	8.503463
58	1	0	-9.109855	-6.090592	13.131759
59	1	0	-10.619782	-3.60741	14.704089
60	1	0	-12.135765	-5.100823	12.137779
61	1	0	-5.745704	-0.271579	10.652045
62	1	0	-6.774086	-0.695369	13.786664
63	1	0	-5.26973	-3.172712	12.205107
64	1	0	-9.938237	-3.726924	-6.094932
65	1	0	-8.952507	-0.776763	-7.26307
66	1	0	-7.979838	2.773279	-2.614008
67	1	0	-11.003817	2.590629	-1.309593
68	1	0	-15.862816	3.12484	-9.28704
69	1	0	-12.69947	2.713248	-10.191768
70	1	0	-12.20632	7.03588	-9.377679
71	1	0	-14.969619	7.202361	-7.560839
72	1	0	-12.547058	6.613073	-1.856673
73	1	0	-8.174176	7.366609	-6.872186
74	1	0	-10.147834	9.725818	-5.565558
75	1	0	-8.482581	7.629722	-3.575739
76	1	0	-14.131818	-4.437195	-8.120027
77	1	0	-16.321081	-1.929376	-8.390127
78	1	0	-13.512692	-1.887907	-10.17864

yby5-12-3C2000005_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-8.927943	-0.095521	-3.074233
1	6	0	-6.356763	0.04688	-1.779221
2	8	0	-4.559791	0.569742	-3.117707
3	6	0	-5.985249	-0.330462	1.04063
4	6	0	-6.186753	-3.06179	2.053813
5	6	0	-4.007174	-4.850279	1.378719
6	6	0	-1.470235	-3.615325	1.852781
7	6	0	-1.205241	-0.979736	1.958714
8	6	0	-3.353565	0.784476	1.693827
9	8	0	-3.105729	3.051319	1.971767
10	6	0	0.700639	-5.085698	2.106266
11	6	0	3.055268	-4.003038	2.457735
12	6	0	3.302627	-1.390555	2.573054
13	6	0	1.18094	0.099103	2.328621
14	6	0	-4.334809	-7.270832	2.940911
15	6	0	-4.138167	-5.600918	-1.423125
16	6	0	-7.902287	1.1292	2.696547
17	6	0	-6.592679	-2.631708	4.897566
18	6	0	-8.337537	-0.35816	5.103128
19	8	0	-8.792919	3.165853	2.198098
20	6	0	-8.012082	1.276648	7.469039
21	6	0	-8.551184	-0.154264	9.844338
22	6	0	-10.779412	-0.390661	11.002178
23	6	0	-11.045991	-1.938246	13.355575
24	6	0	-13.171817	0.808436	10.089809
25	6	0	-8.739829	-1.41936	-5.647902
26	6	0	-11.524716	-1.80915	-6.232169
27	6	0	-12.821007	0.736515	-6.736021
28	6	0	-11.147183	2.949461	-5.986911
29	6	0	-9.963457	2.682862	-3.403672
30	6	0	-13.635522	1.523285	-9.381932
31	6	0	-14.071546	4.397201	-9.109996
32	6	0	-12.796976	5.247998	-6.614694
33	8	0	-12.465832	-2.669523	-3.724363
34	6	0	-11.065587	-1.613963	-1.875677
35	8	0	-11.596809	-1.865063	0.328878
36	8	0	-14.807788	5.535718	-4.811112
37	6	0	-11.325299	7.692991	-6.846282
38	6	0	-12.119947	-3.873605	-8.089071
39	1	0	-9.606867	3.025117	-7.363116

40	1	0	-14.498164	0.773742	-5.537789
41	1	0	-7.906727	-3.903815	1.315485
42	1	0	-10.299466	-0.984157	5.008412
43	1	0	0.557806	-7.120966	2.02784
44	1	0	4.702062	-5.201502	2.644368
45	1	0	5.13845	-0.535025	2.84714
46	1	0	1.305272	2.13504	2.406247
47	1	0	-6.276617	-7.938722	2.787427
48	1	0	-3.124581	-8.781714	2.253443
49	1	0	-3.910273	-6.975878	4.928192
50	1	0	-2.702905	-7.011802	-1.846586
51	1	0	-5.977619	-6.42397	-1.857146
52	1	0	-3.809808	-4.00681	-2.667194
53	1	0	-7.376621	-4.289914	5.815443
54	1	0	-4.788461	-2.225309	5.812735
55	1	0	-6.073927	1.982595	7.513388
56	1	0	-9.220257	2.928547	7.27433
57	1	0	-6.953583	-1.152895	10.658305
58	1	0	-11.765445	-0.795377	14.917337
59	1	0	-12.402096	-3.472307	13.087428
60	1	0	-9.256449	-2.763404	13.941271
61	1	0	-14.007495	1.989376	11.562022
62	1	0	-12.91426	1.963996	8.415214
63	1	0	-14.577016	-0.635966	9.640209
64	1	0	-7.796034	-3.236595	-5.445522
65	1	0	-7.725471	-0.341955	-7.061973
66	1	0	-8.414034	4.007992	-3.161147
67	1	0	-11.302577	3.060544	-1.893629
68	1	0	-15.310069	0.531697	-10.043884
69	1	0	-12.125664	1.149033	-10.736045
70	1	0	-13.299904	5.432348	-10.710049
71	1	0	-16.070653	4.854351	-8.995225
72	1	0	-14.089847	6.189901	-3.268042
73	1	0	-9.818278	7.52324	-8.238229
74	1	0	-12.571778	9.225418	-7.419351
75	1	0	-10.458749	8.214671	-5.049436
76	1	0	-11.285615	-5.652713	-7.483778
77	1	0	-14.150418	-4.134282	-8.275398
78	1	0	-11.361195	-3.396298	-9.93926

yby5-12-3C2000006_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.652059	-0.936285	-3.301305
1	6	0	-7.447438	-2.320082	-2.024844
2	8	0	-6.74587	-4.296362	-2.941707
3	6	0	-6.087109	-1.439786	0.429535
4	6	0	-5.21302	-3.753585	2.032707
5	6	0	-2.346819	-4.296251	1.981675
6	6	0	-0.971557	-1.877157	2.637746
7	6	0	-1.740562	0.344705	1.417393
8	6	0	-3.915877	0.308363	-0.319042
9	8	0	-4.031111	1.685383	-2.165422
10	6	0	1.096061	-1.750538	4.250482
11	6	0	2.351679	0.517577	4.656118
12	6	0	1.582244	2.705221	3.427819
13	6	0	-0.45161	2.610357	1.791008
14	6	0	-1.771813	-6.448487	3.817783
15	6	0	-1.47993	-5.144396	-0.652731
16	6	0	-7.774746	0.100029	2.315532
17	6	0	-6.190557	-3.276949	4.722382
18	6	0	-8.514221	-1.623567	4.446761
19	8	0	-8.203805	2.334404	2.173146
20	6	0	-9.377096	-0.244528	6.818005
21	6	0	-10.295135	-2.034934	8.790912
22	6	0	-9.199314	-2.652864	10.976424
23	6	0	-10.403017	-4.530529	12.720387
24	6	0	-6.746923	-1.595162	11.90911
25	6	0	-9.982817	-1.764783	-6.06252
26	6	0	-12.770747	-1.17568	-6.460842
27	6	0	-13.226548	1.685903	-6.431088
28	6	0	-10.923818	3.094399	-5.452478
29	6	0	-9.831895	1.999398	-3.054704
30	6	0	-13.804939	3.16002	-8.835297
31	6	0	-13.290581	5.926878	-8.049521
32	6	0	-11.782049	5.858432	-5.540794
33	8	0	-13.855707	-2.159134	-4.055274
34	6	0	-12.124573	-2.005936	-2.20431
35	8	0	-12.556083	-2.600097	-0.045878
36	8	0	-13.582183	6.392228	-3.574396
37	6	0	-9.626393	7.739328	-5.428296
38	6	0	-14.032347	-2.592568	-8.574585
39	1	0	-9.469574	2.956335	-6.915105

40	1	0	-14.779657	2.01294	-5.115942
41	1	0	-6.156784	-5.409638	1.266666
42	1	0	-10.062837	-2.768699	3.695764
43	1	0	1.751804	-3.430832	5.205357
44	1	0	3.947206	0.571391	5.93425
45	1	0	2.565661	4.468379	3.746408
46	1	0	-1.092444	4.277142	0.800065
47	1	0	-2.969978	-8.065418	3.388262
48	1	0	0.179296	-7.072529	3.634025
49	1	0	-2.089565	-5.92738	5.779344
50	1	0	0.553479	-5.466371	-0.649491
51	1	0	-2.423563	-6.889173	-1.191837
52	1	0	-1.892056	-3.749147	-2.100071
53	1	0	-6.604539	-5.024567	5.713382
54	1	0	-4.777357	-2.262908	5.830022
55	1	0	-7.833261	0.930051	7.502318
56	1	0	-10.891277	1.052819	6.291104
57	1	0	-12.066548	-2.967878	8.330145
58	1	0	-9.149337	-6.134853	13.064895
59	1	0	-10.789056	-3.689968	14.566381
60	1	0	-12.174399	-5.254602	11.969522
61	1	0	-7.001477	-0.656842	13.729605
62	1	0	-5.382764	-3.111975	12.228013
63	1	0	-5.893494	-0.246817	10.620395
64	1	0	-9.647095	-3.780078	-6.237999
65	1	0	-8.741391	-0.792361	-7.374199
66	1	0	-7.970213	2.761065	-2.688752
67	1	0	-11.009658	2.470437	-1.439566
68	1	0	-15.721066	2.878694	-9.524955
69	1	0	-12.519593	2.59623	-10.34619
70	1	0	-12.238143	6.936901	-9.498686
71	1	0	-15.033726	6.963601	-7.723985
72	1	0	-12.679635	6.439757	-1.990539
73	1	0	-8.255516	7.391737	-6.924298
74	1	0	-10.338591	9.658951	-5.626085
75	1	0	-8.626383	7.606418	-3.630864
76	1	0	-13.779635	-4.619278	-8.341999
77	1	0	-16.046002	-2.183448	-8.636648
78	1	0	-13.210854	-2.038619	-10.37663

yby5-12-3C2000007_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.65959	-0.925057	-3.175539
1	6	0	-7.420663	-2.320599	-1.972937
2	8	0	-6.768789	-4.305714	-2.907352
3	6	0	-5.966638	-1.443887	0.426762
4	6	0	-5.036275	-3.759527	1.994545
5	6	0	-2.175047	-4.306527	1.832429
6	6	0	-0.768939	-1.890461	2.431484
7	6	0	-1.580573	0.333032	1.24181
8	6	0	-3.825134	0.302922	-0.404577
9	8	0	-4.015272	1.684065	-2.241801
10	6	0	1.363775	-1.769697	3.957519
11	6	0	2.642224	0.494668	4.309143
12	6	0	1.829433	2.684049	3.112205
13	6	0	-0.270439	2.594835	1.560766
14	6	0	-1.534899	-6.459139	3.645996
15	6	0	-1.41266	-5.155968	-0.833637
16	6	0	-7.58097	0.094137	2.378305
17	6	0	-5.911903	-3.279849	4.718068
18	6	0	-8.254609	-1.640976	4.521254
19	8	0	-7.999028	2.33241	2.26894
20	6	0	-9.054863	-0.279606	6.924632
21	6	0	-9.90712	-2.090654	8.908391
22	6	0	-8.732523	-2.744435	11.041868
23	6	0	-9.872976	-4.649536	12.79834
24	6	0	-6.243717	-1.70842	11.898863
25	6	0	-10.055137	-1.716813	-5.938256
26	6	0	-12.858005	-1.148058	-6.255414
27	6	0	-13.336906	1.708895	-6.171346
28	6	0	-11.021708	3.12502	-5.231896
29	6	0	-9.854758	2.004179	-2.881337
30	6	0	-13.994106	3.212435	-8.536841
31	6	0	-13.470081	5.972429	-7.731142
32	6	0	-11.911811	5.880413	-5.25471
33	8	0	-13.871709	-2.17465	-3.837255
34	6	0	-12.095441	-2.027076	-2.029112
35	8	0	-12.466398	-2.644951	0.133898
36	8	0	-13.677971	6.359374	-3.243765
37	6	0	-9.777967	7.786344	-5.151984
38	6	0	-14.161418	-2.545545	-8.356684
39	1	0	-9.604946	3.025614	-6.733539

40	1	0	-14.8575	2.002415	-4.811027
41	1	0	-6.012002	-5.413671	1.265468
42	1	0	-9.816829	-2.793977	3.811047
43	1	0	2.053303	-3.452004	4.884667
44	1	0	4.289578	0.544329	5.519909
45	1	0	2.83103	4.444121	3.388384
46	1	0	-0.946553	4.263098	0.596118
47	1	0	-2.754125	-8.072508	3.264588
48	1	0	0.40535	-7.089925	3.387292
49	1	0	-1.773708	-5.935173	5.617885
50	1	0	0.619228	-5.478825	-0.911574
51	1	0	-2.377366	-6.900149	-1.336661
52	1	0	-1.880335	-3.76007	-2.263645
53	1	0	-6.27755	-5.02485	5.731974
54	1	0	-4.46431	-2.249355	5.764924
55	1	0	-7.495977	0.897665	7.569701
56	1	0	-10.589121	1.01426	6.450423
57	1	0	-11.696972	-3.012864	8.500635
58	1	0	-8.610322	-6.261621	13.066735
59	1	0	-10.185956	-3.84137	14.672285
60	1	0	-11.672918	-5.358846	12.103416
61	1	0	-5.452886	-0.310246	10.623429
62	1	0	-6.419138	-0.836742	13.76137
63	1	0	-4.861105	-3.228623	12.101728
64	1	0	-9.706914	-3.72641	-6.149965
65	1	0	-8.857628	-0.714414	-7.26815
66	1	0	-7.99045	2.777373	-2.556374
67	1	0	-10.990541	2.441987	-1.22686
68	1	0	-15.928703	2.928572	-9.17167
69	1	0	-12.753011	2.6753	-10.09358
70	1	0	-12.443655	6.99659	-9.189027
71	1	0	-15.206605	7.006317	-7.364109
72	1	0	-12.743057	6.39465	-1.678509
73	1	0	-8.429359	7.480469	-6.677137
74	1	0	-10.518458	9.699188	-5.307687
75	1	0	-8.745089	7.640476	-3.374265
76	1	0	-16.179699	-2.15464	-8.360336
77	1	0	-13.392214	-1.95764	-10.171012
78	1	0	-13.88457	-4.573013	-8.160874

yby5-12-3C2000008_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-8.65082	-0.262854	-2.88348
1	6	0	-6.095495	-0.001572	-1.573976
2	8	0	-4.311941	0.574345	-2.908165
3	6	0	-5.730168	-0.330303	1.252814
4	6	0	-5.848969	-3.058107	2.290557
5	6	0	-3.598694	-4.77445	1.659971
6	6	0	-1.11404	-3.446531	2.161738
7	6	0	-0.942703	-0.801777	2.235424
8	6	0	-3.146329	0.882727	1.914146
9	8	0	-2.978833	3.161298	2.155501
10	6	0	1.102437	-4.835645	2.47233
11	6	0	3.411266	-3.665684	2.847807
12	6	0	3.565415	-1.044916	2.930248
13	6	0	1.397447	0.365585	2.629564
14	6	0	-3.863071	-7.192892	3.236468
15	6	0	-3.661358	-5.549904	-1.137136
16	6	0	-7.711626	1.078599	2.876923
17	6	0	-6.304645	-2.619807	5.125571
18	6	0	-8.118306	-0.397783	5.294845
19	8	0	-8.668955	3.077018	2.347962
20	6	0	-7.858969	1.269189	7.647004
21	6	0	-8.395036	-0.151715	10.029356
22	6	0	-10.63878	-0.456313	11.140664
23	6	0	-10.903362	-1.987645	13.504672
24	6	0	-13.050997	0.646047	10.161144
25	6	0	-8.388215	-1.617091	-5.434899
26	6	0	-11.14962	-2.132224	-6.031915
27	6	0	-12.546811	0.349987	-6.580968
28	6	0	-10.973491	2.644454	-5.853874
29	6	0	-9.78925	2.466175	-3.262263
30	6	0	-13.373766	1.066553	-9.242153
31	6	0	-13.955173	3.917417	-9.001189
32	6	0	-12.723729	4.858326	-6.516207
33	8	0	-12.072528	-2.994264	-3.518214
34	6	0	-10.737238	-1.845208	-1.676742
35	8	0	-11.282362	-2.074754	0.526615
36	8	0	-14.748129	5.080884	-4.718517
37	6	0	-11.362504	7.363348	-6.779622
38	6	0	-11.645153	-4.244522	-7.864048
39	1	0	-9.432982	2.772053	-7.225378

40	1	0	-14.233277	0.334839	-5.395484
41	1	0	-7.529441	-3.964255	1.538074
42	1	0	-10.060273	-1.081522	5.194116
43	1	0	1.033375	-6.875536	2.421183
44	1	0	5.095439	-4.802703	3.0794
45	1	0	5.365098	-0.121513	3.223201
46	1	0	1.448365	2.405492	2.681343
47	1	0	-5.772591	-7.941269	3.050547
48	1	0	-2.57998	-8.659914	2.587287
49	1	0	-3.490954	-6.86519	5.229136
50	1	0	-2.175783	-6.917757	-1.52741
51	1	0	-5.466313	-6.435209	-1.592286
52	1	0	-3.364901	-3.956461	-2.390139
53	1	0	-7.050744	-4.295166	6.043851
54	1	0	-4.524098	-2.157753	6.060216
55	1	0	-5.938909	2.021383	7.706863
56	1	0	-9.103167	2.889889	7.419865
57	1	0	-6.781186	-1.083602	10.888909
58	1	0	-11.69059	-0.853275	15.039765
59	1	0	-12.204509	-3.566641	13.225434
60	1	0	-9.100859	-2.749303	14.134968
61	1	0	-13.962219	1.811215	11.600982
62	1	0	-12.797006	1.793618	8.48056
63	1	0	-14.394118	-0.851412	9.695752
64	1	0	-7.3682	-3.387877	-5.196438
65	1	0	-7.410657	-0.518131	-6.858241
66	1	0	-8.290597	3.852214	-3.039796
67	1	0	-11.145553	2.819333	-1.761667
68	1	0	-14.99165	-0.011018	-9.91103
69	1	0	-11.833209	0.755313	-10.577496
70	1	0	-13.242682	4.97426	-10.614285
71	1	0	-15.975476	4.26887	-8.885078
72	1	0	-14.060824	5.781082	-3.181731
73	1	0	-9.861937	7.249168	-8.184192
74	1	0	-12.680212	8.83437	-7.354191
75	1	0	-10.504572	7.9378	-4.994616
76	1	0	-10.744129	-5.980136	-7.228684
77	1	0	-13.661704	-4.590236	-8.062787
78	1	0	-10.891785	-3.760905	-9.714924

yby5-12-3C2000009_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-10.123905	-0.832446	-3.229266
1	6	0	-7.936928	-2.335368	-2.072674
2	8	0	-7.039771	-4.047287	-3.299477
3	6	0	-6.807248	-1.904092	0.606409
4	6	0	-6.117753	-4.46996	1.874701
5	6	0	-3.262274	-5.09664	1.953067
6	6	0	-1.9327	-2.877492	3.172475
7	6	0	-2.556432	-0.454559	2.305307
8	6	0	-4.533765	-0.128522	0.372157
9	8	0	-4.436245	1.543279	-1.211157
10	6	0	-0.047556	-3.096333	4.985522
11	6	0	1.168591	-0.97019	5.925905
12	6	0	0.541941	1.42158	5.04813
13	6	0	-1.307623	1.67453	3.220966
14	6	0	-2.889986	-7.564211	3.403594
15	6	0	-2.150348	-5.472076	-0.69704
16	6	0	-8.58303	-0.573413	2.560992
17	6	0	-7.227426	-4.376732	4.55919
18	6	0	-9.328935	-2.438406	4.572373
19	8	0	-9.123415	1.64198	2.525031
20	6	0	-9.879595	-1.206093	7.134382
21	6	0	-7.659073	0.169775	8.200994
22	6	0	-6.075451	-0.586439	10.012466
23	6	0	-3.904667	1.044623	10.808698
24	6	0	-6.255179	-3.049266	11.390216
25	6	0	-10.520233	-1.508775	-6.022005
26	6	0	-13.258157	-0.694914	-6.376711
27	6	0	-13.49924	2.188568	-6.224635
28	6	0	-11.093381	3.37446	-5.20484
29	6	0	-10.106731	2.102055	-2.850383
30	6	0	-13.978658	3.803677	-8.558554
31	6	0	-13.239721	6.486588	-7.668161
32	6	0	-11.727561	6.200561	-5.178209
33	8	0	-14.401221	-1.706821	-4.009505
34	6	0	-12.644703	-1.810525	-2.176246
35	8	0	-13.100361	-2.559744	-0.071876
36	8	0	-13.464042	6.805408	-3.177092
37	6	0	-9.422904	7.892334	-5.020022
38	6	0	-14.631118	-1.923952	-8.538671
39	1	0	-9.654836	3.184306	-6.677178

40	1	0	-15.014271	2.575839	-4.881151
41	1	0	-7.040452	-5.952494	0.792298
42	1	0	-11.065732	-3.287952	3.847893
43	1	0	0.495165	-4.937849	5.679224
44	1	0	2.620795	-1.18686	7.349671
45	1	0	1.489741	3.07371	5.789273
46	1	0	-1.831239	3.508759	2.4909
47	1	0	-4.032112	-9.049403	2.551801
48	1	0	-0.930173	-8.1808	3.314323
49	1	0	-3.418657	-7.414358	5.382717
50	1	0	-2.396007	-3.823459	-1.892987
51	1	0	-0.132167	-5.855166	-0.557047
52	1	0	-3.056957	-7.055325	-1.643343
53	1	0	-7.881022	-6.227331	5.166039
54	1	0	-5.779644	-3.762019	5.884384
55	1	0	-11.435827	0.119729	6.876081
56	1	0	-10.55864	-2.669105	8.411431
57	1	0	-7.286831	1.985786	7.327218
58	1	0	-3.815817	2.785071	9.720765
59	1	0	-4.03953	1.53699	12.809571
60	1	0	-2.111412	0.054215	10.563458
61	1	0	-4.552958	-4.175169	11.072162
62	1	0	-6.36808	-2.742467	13.428088
63	1	0	-7.868419	-4.188388	10.83344
64	1	0	-10.337999	-3.533955	-6.291768
65	1	0	-9.208762	-0.583598	-7.298109
66	1	0	-8.202178	2.711613	-2.413974
67	1	0	-11.271462	2.57682	-1.229444
68	1	0	-15.917307	3.704821	-9.23589
69	1	0	-12.758185	3.204431	-10.108972
70	1	0	-12.118968	7.465966	-9.08689
71	1	0	-14.892626	7.646014	-7.289108
72	1	0	-12.561705	6.680496	-1.597283
73	1	0	-8.095547	7.483192	-6.539561
74	1	0	-9.974195	9.870045	-5.146945
75	1	0	-8.425743	7.617069	-3.236954
76	1	0	-13.775573	-1.364324	-10.32269
77	1	0	-14.534275	-3.971702	-8.387536
78	1	0	-16.608417	-1.361838	-8.571677

yby5-12-3C2000010_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.714841	-1.626476	-2.246545
1	6	0	-7.287938	-3.03549	-1.559558
2	8	0	-6.930246	-5.089587	-2.502813
3	6	0	-5.26346	-2.038504	0.313961
4	6	0	-4.13633	-4.251818	1.902496
5	6	0	-1.352898	-4.880915	1.307379
6	6	0	0.166618	-2.456362	1.274059
7	6	0	-0.794809	-0.405474	-0.104855
8	6	0	-3.339008	-0.546204	-1.217832
9	8	0	-3.952976	0.598759	-3.124636
10	6	0	2.541607	-2.203426	2.364579
11	6	0	3.917513	0.015959	2.102776
12	6	0	2.957592	2.023565	0.712838
13	6	0	0.60498	1.803355	-0.401544
14	6	0	-0.388948	-6.790574	3.242696
15	6	0	-1.139604	-6.106462	-1.313896
16	6	0	-6.208638	-0.198353	2.424196
17	6	0	-4.607492	-3.547823	4.689325
18	6	0	-6.889242	-1.787223	4.665697
19	8	0	-6.033136	2.076206	2.361984
20	6	0	-7.456837	-0.306176	7.062545
21	6	0	-9.68139	1.424605	6.776578
22	6	0	-12.115351	0.786478	6.941199
23	6	0	-14.153154	2.695612	6.484226
24	6	0	-13.038224	-1.820842	7.523114
25	6	0	-10.525262	-2.098226	-4.989868
26	6	0	-13.37097	-1.693621	-4.770756
27	6	0	-13.975209	1.080343	-4.178019
28	6	0	-11.608897	2.543383	-3.471037
29	6	0	-9.91056	1.224299	-1.58709
30	6	0	-15.153689	2.846046	-6.120254
31	6	0	-14.703108	5.483959	-4.950698
32	6	0	-12.636641	5.187848	-2.895319
33	8	0	-13.914233	-3.102234	-2.397265
34	6	0	-11.891775	-2.99426	-0.868622
35	8	0	-11.885735	-3.835241	1.249985
36	8	0	-13.942313	5.2308	-0.510418
37	6	0	-10.638839	7.237542	-2.954724
38	6	0	-14.937826	-2.875948	-6.822538
39	1	0	-10.514929	2.772264	-5.209981

40	1	0	-15.225725	1.057521	-2.539474
41	1	0	-5.230934	-5.932836	1.458894
42	1	0	-8.55125	-2.886096	4.117994
43	1	0	3.349371	-3.747415	3.427208
44	1	0	5.755856	0.170224	2.985008
45	1	0	4.035616	3.748163	0.51099
46	1	0	-0.204817	3.335801	-1.481413
47	1	0	-1.656166	-8.410825	3.313464
48	1	0	1.470543	-7.496521	2.721005
49	1	0	-0.261443	-6.005241	5.136872
50	1	0	-2.198269	-7.868761	-1.365826
51	1	0	-1.883331	-4.903868	-2.801586
52	1	0	0.831668	-6.505891	-1.750066
53	1	0	-4.919845	-5.209042	5.856249
54	1	0	-2.986767	-2.5307	5.461851
55	1	0	-7.754983	-1.656433	8.592182
56	1	0	-5.790257	0.794325	7.572435
57	1	0	-9.226938	3.358831	6.28392
58	1	0	-15.346006	2.141758	4.892858
59	1	0	-15.403871	2.856486	8.118637
60	1	0	-13.386397	4.56349	6.091318
61	1	0	-13.957575	-2.644449	5.871818
62	1	0	-11.536419	-3.100687	8.090551
63	1	0	-14.444301	-1.778684	9.032357
64	1	0	-10.118625	-4.038521	-5.518836
65	1	0	-9.618245	-0.847835	-6.339028
66	1	0	-8.048268	2.068572	-1.641489
67	1	0	-10.631272	1.4314	0.330652
68	1	0	-17.144378	2.469536	-6.468956
69	1	0	-14.171541	2.684615	-7.926776
70	1	0	-14.128687	6.855172	-6.370807
71	1	0	-16.401159	6.209531	-4.0504
72	1	0	-12.693536	5.105934	0.812983
73	1	0	-9.213995	6.92952	-1.496759
74	1	0	-9.669883	7.274686	-4.770825
75	1	0	-11.495101	9.080402	-2.635649
76	1	0	-14.525231	-1.972606	-8.622881
77	1	0	-14.521371	-4.881795	-6.990578
78	1	0	-16.944931	-2.652384	-6.43961

yby5-12-3C2000011_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.583127	-1.59233	-2.579502
1	6	0	-7.137602	-3.010589	-1.984327
2	8	0	-6.604589	-4.835774	-3.257943
3	6	0	-5.304656	-2.292959	0.190741
4	6	0	-4.154497	-4.719039	1.415273
5	6	0	-1.29819	-5.07425	0.957649
6	6	0	0.053556	-2.615966	1.520081
7	6	0	-0.937566	-0.388816	0.478194
8	6	0	-3.372297	-0.443967	-0.863678
9	8	0	-3.904291	1.008454	-2.57637
10	6	0	2.316262	-2.45962	2.842339
11	6	0	3.553596	-0.163054	3.129588
12	6	0	2.56663	2.025193	2.070185
13	6	0	0.326491	1.905365	0.731618
14	6	0	-0.359507	-7.27862	2.564811
15	6	0	-0.813163	-5.745833	-1.824222
16	6	0	-6.519558	-0.964672	2.533336
17	6	0	-4.900648	-4.615937	4.228825
18	6	0	-7.30106	-3.019844	4.318707
19	8	0	-6.449831	1.27415	2.963846
20	6	0	-8.214697	-2.107932	6.88172
21	6	0	-10.75354	-0.883618	6.712228
22	6	0	-11.396653	1.484067	7.290437
23	6	0	-14.074592	2.359716	6.999601
24	6	0	-9.616949	3.450768	8.26432
25	6	0	-10.189052	-1.582927	-5.414585
26	6	0	-13.05524	-1.291914	-5.334764
27	6	0	-13.801922	1.315158	-4.301004
28	6	0	-11.541637	2.681582	-3.180935
29	6	0	-9.931171	1.087678	-1.439827
30	6	0	-14.91914	3.372942	-5.973356
31	6	0	-14.633466	5.769776	-4.328359
32	6	0	-12.686681	5.162869	-2.226321
33	8	0	-13.703856	-3.120154	-3.300231
34	6	0	-11.793031	-3.249333	-1.633919
35	8	0	-11.902993	-4.470298	0.28738
36	8	0	-14.131397	4.763154	0.041289
37	6	0	-10.745861	7.22417	-1.797959
38	6	0	-14.43394	-2.121488	-7.674599
39	1	0	-10.341311	3.240347	-4.769017

40	1	0	-15.152387	0.96621	-2.782852
41	1	0	-5.095835	-6.328986	0.554286
42	1	0	-8.804166	-4.076205	3.370258
43	1	0	3.145742	-4.13869	3.653762
44	1	0	5.305921	-0.087705	4.181125
45	1	0	3.537352	3.809713	2.295239
46	1	0	-0.50214	3.574934	-0.103037
47	1	0	-1.524039	-8.938661	2.213764
48	1	0	1.573887	-7.781666	2.077353
49	1	0	-0.419318	-6.876533	4.578592
50	1	0	-1.710057	-7.536053	-2.295147
51	1	0	-1.560529	-4.330959	-3.110087
52	1	0	1.20876	-5.908123	-2.172186
53	1	0	-5.191234	-6.493494	5.009468
54	1	0	-3.431016	-3.690524	5.342639
55	1	0	-8.337326	-3.754541	8.126609
56	1	0	-6.805791	-0.855283	7.701714
57	1	0	-12.230385	-2.113553	5.988596
58	1	0	-14.193154	4.078198	5.861417
59	1	0	-15.267055	0.931706	6.126902
60	1	0	-14.894475	2.84261	8.832453
61	1	0	-10.29047	4.218128	10.058212
62	1	0	-7.706614	2.761072	8.536257
63	1	0	-9.511121	5.038817	6.950165
64	1	0	-9.676467	-3.388857	-6.243297
65	1	0	-9.236172	-0.093995	-6.454303
66	1	0	-8.099895	1.96806	-1.212107
67	1	0	-10.782424	0.932142	0.429196
68	1	0	-16.87043	3.017781	-6.514009
69	1	0	-13.823642	3.561041	-7.710523
70	1	0	-14.029767	7.386792	-5.445419
71	1	0	-16.408254	6.280488	-3.42829
72	1	0	-12.959146	4.384969	1.386463
73	1	0	-9.407014	6.678964	-0.32771
74	1	0	-9.667296	7.596328	-3.511361
75	1	0	-11.666995	8.967681	-1.212224
76	1	0	-13.920298	-0.90835	-9.253057
77	1	0	-13.943688	-4.058417	-8.157416
78	1	0	-16.469587	-2.005316	-7.413358

Table S18. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of yby5-12-3D (**1d**).

Conformers	ΔG (a.u.)	P(%)/100	G (a.u.)
yby5-12-3D2000002_en_	0.0	43.19	-1733.008597
yby5-12-3D2000003_en_	0.00173	6.9	-1733.006866
yby5-12-3D2000004_en_	0.00514	0.19	-1733.003454
yby5-12-3D2000005_en_	0.00522	0.17	-1733.003376
yby5-12-3D2000006_en_	0.00233	3.65	-1733.006265
yby5-12-3D2000008_en_	0.00232	3.71	-1733.006282
yby5-12-3D2000009_en_	0.00647	0.05	-1733.002129
yby5-12-3D2000010_en_	0.00246	3.18	-1733.006135
yby5-12-3D2000016_en_	0.0001	38.97	-1733.0085

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15 K.

Table S19. Cartesian coordinates for the low-energy reoptimized random research conformers of yby5-12-3D at B3LYP-D3(BJ)/6-31G** level of theory in methanol.

yby5-12-3D2000002_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.487808	-0.793796	0.141549
1	6	0	-5.544444	1.221568	0.305266
2	8	0	-6.454373	1.762355	2.337183
3	6	0	-6.616591	2.491233	-2.103781
4	6	0	-7.917265	5.063495	-1.694809
5	6	0	-6.209127	7.280384	-0.956719
6	6	0	-4.096576	7.37873	-2.911172
7	6	0	-3.531839	5.317134	-4.49174
8	6	0	-4.751819	2.798386	-4.271943
9	8	0	-4.264492	1.090207	-5.741059
10	6	0	-2.628034	9.549107	-3.151971
11	6	0	-0.706022	9.721472	-4.916528
12	6	0	-0.196808	7.699545	-6.511441
13	6	0	-1.597863	5.518312	-6.283299
14	6	0	-5.022581	7.117545	1.680014
15	6	0	-7.838671	9.674721	-1.082085
16	6	0	-8.980038	0.829037	-2.748634
17	6	0	-10.388825	4.502087	-0.328317
18	6	0	-11.322902	2.133759	-1.696126
19	8	0	-8.987804	-1.133666	-3.895366
20	6	0	-13.013972	0.29224	-0.222932
21	6	0	-11.70374	-0.964546	1.932655
22	6	0	-11.033748	-3.388222	2.131714
23	6	0	-9.656681	-4.311325	4.425278
24	6	0	-11.540232	-5.38282	0.19449
25	6	0	-3.94809	-3.010105	-1.672268
26	6	0	-1.239994	-3.956741	-1.997307
27	6	0	-0.262721	-5.14635	0.460395
28	6	0	-1.998542	-4.53287	2.670967
29	6	0	-2.767517	-1.784066	2.826612
30	6	0	0.033141	-7.993093	0.759096
31	6	0	0.228085	-8.337786	3.653524
32	6	0	-0.703916	-5.833613	4.891933
33	8	0	0.16275	-1.54064	-2.261906
34	6	0	-1.046715	0.290607	-0.982954
35	8	0	-0.221766	2.396983	-0.717496
36	8	0	1.397506	-4.256287	5.581712

37	6	0	-2.401361	-6.244171	7.161671
38	6	0	-0.771954	-5.452618	-4.365431
39	1	0	-3.718338	-5.639792	2.36506
40	1	0	1.573808	-4.288296	0.826011
41	1	0	-8.50819	5.564636	-3.621325
42	1	0	-12.377658	2.727845	-3.37595
43	1	0	-2.981385	11.149805	-1.934114
44	1	0	0.39758	11.438518	-5.046094
45	1	0	1.304713	7.820818	-7.893032
46	1	0	-1.202116	3.8886	-7.445593
47	1	0	-3.581156	5.665925	1.787684
48	1	0	-4.123809	8.911194	2.137929
49	1	0	-6.447363	6.732257	3.109493
50	1	0	-8.739271	9.879067	-2.922439
51	1	0	-9.306481	9.6027	0.356238
52	1	0	-6.737744	11.369968	-0.729818
53	1	0	-11.736805	6.041673	-0.51782
54	1	0	-10.081623	4.152607	1.66458
55	1	0	-14.634161	1.367424	0.474756
56	1	0	-13.754582	-1.089121	-1.549728
57	1	0	-11.188375	0.271584	3.481957
58	1	0	-10.746262	-5.755591	5.420502
59	1	0	-7.870017	-5.199426	3.896685
60	1	0	-9.2425	-2.792172	5.744975
61	1	0	-9.771593	-6.231943	-0.445886
62	1	0	-12.6598	-6.914762	1.007993
63	1	0	-12.511489	-4.686112	-1.468703
64	1	0	-4.692815	-2.37583	-3.465754
65	1	0	-5.222596	-4.433203	-0.924333
66	1	0	-4.383343	-1.537643	4.06556
67	1	0	-1.252108	-0.633814	3.605918
68	1	0	1.6607	-8.752185	-0.241433
69	1	0	-1.636382	-8.966193	0.038752
70	1	0	-0.882914	-9.944222	4.301877
71	1	0	2.173884	-8.678111	4.231242
72	1	0	2.278527	-5.067707	6.954067
73	1	0	-4.066072	-7.34808	6.663805
74	1	0	-1.403321	-7.269863	8.647534
75	1	0	-3.019248	-4.443381	7.93818
76	1	0	-1.347042	-4.370221	-6.013834
77	1	0	1.21725	-5.939463	-4.552442
78	1	0	-1.858704	-7.198011	-4.322503

yby5-12-3D2000003_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-2.693604	-0.82702	0.176224
1	6	0	-5.392366	0.159252	-0.078167
2	8	0	-6.904311	-0.200779	1.614564
3	6	0	-6.345749	1.343939	-2.572835
4	6	0	-8.476448	3.312355	-2.324339
5	6	0	-7.719377	5.817967	-1.098029
6	6	0	-5.507399	6.834567	-2.638929
7	6	0	-4.041695	5.251481	-4.19459
8	6	0	-4.342955	2.461424	-4.301395
9	8	0	-3.044156	1.158439	-5.692518
10	6	0	-4.855592	9.379064	-2.513738
11	6	0	-2.870108	10.359591	-3.907015
12	6	0	-1.468556	8.798667	-5.484108
13	6	0	-2.052317	6.264715	-5.608216
14	6	0	-6.896134	5.607035	1.668794
15	6	0	-10.005007	7.587295	-1.261585
16	6	0	-7.881199	-0.919206	-3.729279
17	6	0	-10.84101	1.885415	-1.530504
18	6	0	-10.652144	-0.579632	-3.024826
19	8	0	-7.030635	-2.65542	-4.923946
20	6	0	-11.694978	-2.932108	-1.686174
21	6	0	-14.438522	-2.666859	-1.118611
22	6	0	-15.523637	-2.295116	1.128422
23	6	0	-18.333566	-2.04461	1.354366
24	6	0	-14.124329	-2.098198	3.577918
25	6	0	-1.997243	-2.914729	-1.722912
26	6	0	0.881235	-2.78324	-1.564006
27	6	0	1.807926	-3.720076	1.019973
28	6	0	-0.356245	-3.948866	2.898037
29	6	0	-2.122987	-1.701051	2.935199
30	6	0	3.096351	-6.270954	1.347071
31	6	0	2.978171	-6.692216	4.233559
32	6	0	0.972119	-4.847621	5.309444
33	8	0	1.309013	-0.007628	-1.537459
34	6	0	-0.673366	1.146237	-0.453716
35	8	0	-0.718425	3.370544	0.041168
36	8	0	2.36814	-2.830342	6.480165
37	6	0	-0.792461	-6.05325	7.215848
38	6	0	2.257018	-3.817268	-3.822378
39	1	0	-1.475368	-5.58064	2.298296

40	1	0	3.11112	-2.28355	1.717593
41	1	0	-8.828316	3.835915	-4.301633
42	1	0	-11.642241	-0.375559	-4.82999
43	1	0	-5.91335	10.637979	-1.303455
44	1	0	-2.418306	12.34897	-3.761259
45	1	0	0.084799	9.554082	-6.576713
46	1	0	-0.954863	4.987311	-6.76068
47	1	0	-5.117119	4.605591	1.859651
48	1	0	-6.613706	7.49104	2.44509
49	1	0	-8.320703	4.650594	2.80091
50	1	0	-9.589205	9.447708	-0.500559
51	1	0	-10.637303	7.822198	-3.207094
52	1	0	-11.567261	6.826743	-0.162724
53	1	0	-12.548246	2.917159	-2.015611
54	1	0	-10.879238	1.515169	0.481261
55	1	0	-11.37774	-4.557413	-2.915132
56	1	0	-10.59765	-3.250015	0.020453
57	1	0	-15.669947	-2.743603	-2.76234
58	1	0	-18.85141	-0.226907	2.185936
59	1	0	-19.271088	-2.203294	-0.467888
60	1	0	-19.110662	-3.494543	2.601566
61	1	0	-14.544084	-0.301557	4.503645
62	1	0	-14.733097	-3.574907	4.885689
63	1	0	-12.088339	-2.228248	3.375547
64	1	0	-2.63606	-2.44789	-3.608815
65	1	0	-2.750512	-4.757307	-1.228552
66	1	0	-3.900724	-2.170571	3.84706
67	1	0	-1.31706	-0.113041	3.972992
68	1	0	5.021033	-6.309534	0.627025
69	1	0	2.040166	-7.742477	0.360173
70	1	0	2.50963	-8.639057	4.699687
71	1	0	4.777248	-6.267045	5.129238
72	1	0	1.172832	-1.698676	7.263549
73	1	0	0.271329	-6.771725	8.823235
74	1	0	-2.171613	-4.691838	7.921825
75	1	0	-1.836177	-7.615935	6.375062
76	1	0	1.908638	-5.83658	-3.992103
77	1	0	1.602191	-2.89642	-5.537738
78	1	0	4.284895	-3.527298	-3.646213

yby5-12-3D2000004_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-2.828149	-0.712501	0.424758
1	6	0	-5.294726	0.767226	0.624201
2	8	0	-6.459014	0.7852	2.604794
3	6	0	-6.533158	1.988781	-1.724733
4	6	0	-8.149095	4.356525	-1.23112
5	6	0	-6.684291	6.717959	-0.43672
6	6	0	-4.736964	7.186387	-2.50685
7	6	0	-3.978836	5.258309	-4.174902
8	6	0	-4.78095	2.577772	-3.921615
9	8	0	-4.048958	0.95539	-5.388681
10	6	0	-3.629287	9.555747	-2.779678
11	6	0	-1.880673	10.046009	-4.662929
12	6	0	-1.188431	8.152698	-6.343346
13	6	0	-2.225004	5.778774	-6.081038
14	6	0	-5.305727	6.484756	2.09834
15	6	0	-8.577615	8.901832	-0.274654
16	6	0	-8.681632	0.021735	-2.322424
17	6	0	-10.495136	3.473701	0.169448
18	6	0	-11.126107	0.960669	-1.115216
19	8	0	-8.433416	-1.894585	-3.518265
20	6	0	-12.381359	-0.990196	0.638378
21	6	0	-13.369679	-3.286145	-0.661905
22	6	0	-15.778112	-3.859213	-1.148043
23	6	0	-16.4437	-6.25821	-2.494992
24	6	0	-18.00004	-2.251508	-0.454497
25	6	0	-2.979928	-3.023303	-1.335063
26	6	0	-0.166354	-3.491178	-1.774383
27	6	0	1.101838	-4.444667	0.652199
28	6	0	-0.606059	-4.072961	2.939972
29	6	0	-1.822821	-1.490369	3.087431
30	6	0	1.880332	-7.195924	0.981812
31	6	0	2.240968	-7.443619	3.871952
32	6	0	1.002168	-5.078084	5.109092
33	8	0	0.784477	-0.875903	-2.130848
34	6	0	-0.670265	0.747665	-0.825421
35	8	0	-0.194331	2.965557	-0.613047
36	8	0	2.864271	-3.170738	5.631909
37	6	0	-0.480368	-5.676872	7.484965
38	6	0	0.448171	-4.936431	-4.140774
39	1	0	-2.12648	-5.461747	2.757456

40	1	0	2.785818	-3.28818	0.914164
41	1	0	-8.83394	4.83209	-3.131273
42	1	0	-12.402535	1.295202	-2.706892
43	1	0	-4.136591	11.063743	-1.500045
44	1	0	-1.058983	11.912383	-4.819275
45	1	0	0.175631	8.524907	-7.819317
46	1	0	-1.668965	4.247246	-7.30991
47	1	0	-3.727929	5.179686	1.99432
48	1	0	-4.53388	8.316396	2.630163
49	1	0	-6.581173	5.8675	3.587102
50	1	0	-9.972296	8.521749	1.188024
51	1	0	-7.664244	10.672874	0.218193
52	1	0	-9.568523	9.174275	-2.058572
53	1	0	-12.042946	4.811117	-0.032029
54	1	0	-10.137395	3.195653	2.167398
55	1	0	-11.000078	-1.52813	2.071018
56	1	0	-13.88418	-0.002311	1.638773
57	1	0	-11.93871	-4.597111	-1.313135
58	1	0	-17.484981	-5.869415	-4.234809
59	1	0	-14.773072	-7.350647	-2.981923
60	1	0	-17.673055	-7.445197	-1.335375
61	1	0	-17.489582	-0.515298	0.512341
62	1	0	-19.073058	-1.736081	-2.14101
63	1	0	-19.304589	-3.29092	0.761528
64	1	0	-3.905877	-2.560207	-3.098176
65	1	0	-3.947689	-4.629553	-0.503581
66	1	0	-3.400434	-1.494124	4.399461
67	1	0	-0.485137	-0.080401	3.75724
68	1	0	3.573592	-7.695604	-0.071385
69	1	0	0.371952	-8.450293	0.34591
70	1	0	1.392531	-9.176001	4.589229
71	1	0	4.236028	-7.494581	4.37482
72	1	0	3.93127	-3.785102	6.974148
73	1	0	-2.006456	-7.002851	7.095435
74	1	0	0.733281	-6.532573	8.916942
75	1	0	-1.293225	-3.963263	8.279318
76	1	0	-0.366777	-4.000384	-5.777658
77	1	0	2.481655	-5.08914	-4.405853
78	1	0	-0.328906	-6.836717	-4.021965

yby5-12-3D2000005_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-2.730943	-0.705803	0.428524
1	6	0	-5.190733	0.785025	0.641523
2	8	0	-6.32481	0.832895	2.639662
3	6	0	-6.449461	1.983559	-1.703745
4	6	0	-8.078632	4.343439	-1.214715
5	6	0	-6.626581	6.721653	-0.445971
6	6	0	-4.691597	7.188557	-2.527593
7	6	0	-3.92579	5.254059	-4.184622
8	6	0	-4.710492	2.570925	-3.91242
9	8	0	-3.973351	0.943489	-5.370927
10	6	0	-3.601074	9.56357	-2.820641
11	6	0	-1.861035	10.052097	-4.712246
12	6	0	-1.160295	8.151496	-6.380877
13	6	0	-2.180324	5.772683	-6.099295
14	6	0	-5.231551	6.519811	2.08326
15	6	0	-8.535595	8.891946	-0.289973
16	6	0	-8.59186	0.002518	-2.283938
17	6	0	-10.410984	3.453995	0.205716
18	6	0	-11.029501	0.924332	-1.052406
19	8	0	-8.343337	-1.908472	-3.487401
20	6	0	-12.23362	-1.031575	0.733805
21	6	0	-13.185902	-3.360751	-0.532924
22	6	0	-15.583191	-3.96623	-1.033488
23	6	0	-16.211299	-6.392204	-2.349646
24	6	0	-17.82741	-2.369646	-0.390511
25	6	0	-2.890873	-3.025968	-1.316314
26	6	0	-0.079819	-3.496109	-1.769786
27	6	0	1.204222	-4.432697	0.653699
28	6	0	-0.479333	-4.047699	2.953649
29	6	0	-1.711336	-1.471499	3.089197
30	6	0	1.992352	-7.179289	1.000172
31	6	0	2.392384	-7.393664	3.887512
32	6	0	1.172569	-5.03466	5.116538
33	8	0	0.86622	-0.8779	-2.1486
34	6	0	-0.576715	0.747938	-0.838913
35	8	0	-0.097262	2.965834	-0.624898
36	8	0	3.222737	-3.33116	5.649376
37	6	0	-0.277133	-5.600679	7.519667
38	6	0	0.521716	-4.953262	-4.131421
39	1	0	-2.003709	-5.436628	2.8014

40	1	0	2.891206	-3.276209	0.901204
41	1	0	-8.778122	4.80192	-3.113624
42	1	0	-12.33386	1.227097	-2.627199
43	1	0	-4.115462	11.077296	-1.550685
44	1	0	-1.052822	11.92291	-4.884334
45	1	0	0.197433	8.522114	-7.862978
46	1	0	-1.617901	4.236773	-7.319701
47	1	0	-3.641591	5.229545	1.977166
48	1	0	-4.475103	8.362643	2.598293
49	1	0	-6.491424	5.899031	3.583649
50	1	0	-9.91887	8.5131	1.183853
51	1	0	-7.633148	10.673827	0.183388
52	1	0	-9.539184	9.143071	-2.069908
53	1	0	-11.969259	4.778273	-0.001547
54	1	0	-10.043046	3.199208	2.204919
55	1	0	-10.831913	-1.526037	2.161529
56	1	0	-13.747329	-0.060591	1.73481
57	1	0	-11.736855	-4.669591	-1.148047
58	1	0	-17.221344	-6.038769	-4.115265
59	1	0	-14.526968	-7.484428	-2.786901
60	1	0	-17.457032	-7.565145	-1.193408
61	1	0	-17.344831	-0.611737	0.551481
62	1	0	-18.887393	-1.894607	-2.096892
63	1	0	-19.133921	-3.401404	0.829812
64	1	0	-3.826846	-2.570073	-3.07611
65	1	0	-3.853762	-4.628268	-0.471686
66	1	0	-3.281173	-1.468186	4.410973
67	1	0	-0.388143	-0.023519	3.724517
68	1	0	3.676741	-7.681286	-0.065794
69	1	0	0.482041	-8.444651	0.390348
70	1	0	1.551579	-9.113805	4.637572
71	1	0	4.385665	-7.422005	4.383465
72	1	0	2.519766	-1.825958	6.400015
73	1	0	0.965714	-6.434242	8.930673
74	1	0	-1.084862	-3.880385	8.320405
75	1	0	-1.82892	-6.906147	7.163175
76	1	0	-0.304089	-4.028508	-5.769319
77	1	0	2.553535	-5.106683	-4.407104
78	1	0	-0.252102	-6.853756	-3.996383

yby5-12-3D2000006_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.338876	-0.552366	0.429172
1	6	0	-5.572417	1.270259	0.443947
2	8	0	-6.762937	1.605331	2.381886
3	6	0	-6.521005	2.505856	-2.014886
4	6	0	-8.028419	4.977524	-1.718634
5	6	0	-6.504551	7.288825	-0.880409
6	6	0	-4.342349	7.567495	-2.760795
7	6	0	-3.534204	5.53731	-4.275802
8	6	0	-4.550166	2.928112	-4.060296
9	8	0	-3.821022	1.236783	-5.447508
10	6	0	-3.071374	9.859117	-2.992504
11	6	0	-1.101308	10.17221	-4.68467
12	6	0	-0.344309	8.17476	-6.210032
13	6	0	-1.551918	5.878992	-5.990364
14	6	0	-5.377575	7.106341	1.78048
15	6	0	-8.282246	9.57207	-0.980537
16	6	0	-8.749072	0.686351	-2.777902
17	6	0	-10.532048	4.290553	-0.47523
18	6	0	-11.170003	1.697805	-1.596479
19	8	0	-8.592112	-1.157743	-4.092083
20	6	0	-12.321106	-0.149203	0.342909
21	6	0	-12.887683	-2.718005	-0.643526
22	6	0	-11.880911	-4.906571	0.101301
23	6	0	-12.672456	-7.345556	-1.092702
24	6	0	-9.911148	-5.175822	2.11466
25	6	0	-3.560518	-2.80721	-1.3893
26	6	0	-0.787036	-3.590171	-1.546207
27	6	0	0.102829	-4.718067	0.971981
28	6	0	-1.782723	-4.185541	3.073762
29	6	0	-2.705258	-1.482233	3.158788
30	6	0	0.511469	-7.545987	1.308727
31	6	0	0.593294	-7.853788	4.210845
32	6	0	-0.552501	-5.425167	5.381542
33	8	0	0.484022	-1.093118	-1.741691
34	6	0	-0.911681	0.670723	-0.567103
35	8	0	-0.233891	2.826119	-0.269868
36	8	0	1.557832	-3.9665	6.28106
37	6	0	-2.38325	-5.92592	7.526242
38	6	0	-0.09842	-5.065098	-3.873313
39	1	0	-3.431162	-5.369697	2.679111

40	1	0	1.874436	-3.77476	1.440779
41	1	0	-8.533637	5.423854	-3.681549
42	1	0	-12.495343	1.886884	-3.169096
43	1	0	-3.62299	11.444889	-1.830494
44	1	0	-0.155699	11.98112	-4.812551
45	1	0	1.195645	8.407297	-7.533783
46	1	0	-0.966612	4.272533	-7.104365
47	1	0	-6.814142	6.623843	3.168439
48	1	0	-3.872563	5.717939	1.8824
49	1	0	-4.56225	8.922436	2.301357
50	1	0	-7.322202	11.313127	-0.470779
51	1	0	-9.089819	9.819067	-2.858269
52	1	0	-9.821971	9.324369	0.359906
53	1	0	-11.988391	5.670663	-0.919569
54	1	0	-10.361402	4.174866	1.563439
55	1	0	-11.074788	-0.222246	1.968456
56	1	0	-14.071856	0.735307	0.996562
57	1	0	-14.27482	-2.783133	-2.155622
58	1	0	-11.070607	-8.261562	-2.019558
59	1	0	-13.369265	-8.67843	0.321809
60	1	0	-14.146492	-7.074114	-2.498492
61	1	0	-8.313797	-6.273397	1.404776
62	1	0	-9.185733	-3.38734	2.808567
63	1	0	-10.6524	-6.226738	3.729824
64	1	0	-4.229926	-2.222009	-3.228762
65	1	0	-4.79118	-4.298135	-0.706098
66	1	0	-4.393252	-1.305958	4.312129
67	1	0	-1.294394	-0.219691	3.973829
68	1	0	2.216371	-8.239025	0.393133
69	1	0	-1.079518	-8.595426	0.519505
70	1	0	-0.436858	-9.522481	4.829426
71	1	0	2.521645	-8.041901	4.894037
72	1	0	0.902687	-2.481756	7.111483
73	1	0	-3.955198	-7.099799	6.902324
74	1	0	-1.43052	-6.884759	9.076524
75	1	0	-3.172553	-4.16363	8.25258
76	1	0	-1.095476	-6.863468	-3.877803
77	1	0	-0.630546	-4.021347	-5.560621
78	1	0	1.920387	-5.449397	-3.936634

yby5-12-3D2000008_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.360517	-0.964631	-0.0477
1	6	0	-5.739078	0.670455	-0.121813
2	8	0	-7.027077	0.888442	1.75886
3	6	0	-6.632798	1.940044	-2.602627
4	6	0	-8.417499	4.215361	-2.273665
5	6	0	-7.276518	6.607778	-1.110957
6	6	0	-4.909191	7.216556	-2.6358
7	6	0	-3.740636	5.428926	-4.219901
8	6	0	-4.530164	2.741114	-4.393449
9	8	0	-3.528451	1.281423	-5.870819
10	6	0	-3.81817	9.605427	-2.468561
11	6	0	-1.686102	10.24544	-3.840349
12	6	0	-0.57454	8.488559	-5.443344
13	6	0	-1.597849	6.10207	-5.615525
14	6	0	-6.555034	6.419869	1.687221
15	6	0	-9.246166	8.714195	-1.409036
16	6	0	-8.523765	-0.049445	-3.714514
17	6	0	-10.933349	3.125053	-1.401524
18	6	0	-11.202218	0.789199	-3.073904
19	8	0	-7.985	-1.930673	-4.873933
20	6	0	-12.848145	-1.376224	-2.058563
21	6	0	-11.71634	-2.716759	0.147406
22	6	0	-12.261949	-2.445913	2.592466
23	6	0	-10.836386	-3.897523	4.557723
24	6	0	-14.224672	-0.69183	3.619432
25	6	0	-3.086956	-3.036367	-2.058841
26	6	0	-0.234665	-3.46944	-1.946207
27	6	0	0.524491	-4.698764	0.57244
28	6	0	-1.635901	-4.613101	2.469341
29	6	0	-2.957731	-2.087514	2.649021
30	6	0	1.322586	-7.456057	0.766094
31	6	0	1.147586	-7.987704	3.631484
32	6	0	-0.508536	-5.861002	4.825881
33	8	0	0.718872	-0.835465	-1.790231
34	6	0	-1.00459	0.622262	-0.61747
35	8	0	-0.62864	2.793793	-0.04425
36	8	0	0.989831	-4.12792	6.275471
37	6	0	-2.484341	-6.84047	6.643521
38	6	0	0.891116	-4.633329	-4.278114
39	1	0	-3.020857	-5.986819	1.784177

40	1	0	2.095527	-3.548873	1.271854
41	1	0	-8.764698	4.785905	-4.239572
42	1	0	-11.998378	1.373911	-4.895131
43	1	0	-4.647729	11.010686	-1.241225
44	1	0	-0.891663	12.121134	-3.658302
45	1	0	1.092696	8.975845	-6.52031
46	1	0	-0.739874	4.674115	-6.794051
47	1	0	-8.117622	5.693176	2.805589
48	1	0	-4.926012	5.214777	1.982625
49	1	0	-6.073402	8.290274	2.39713
50	1	0	-9.825838	8.932626	-3.372796
51	1	0	-10.913172	8.29403	-0.280625
52	1	0	-8.527054	10.524573	-0.761343
53	1	0	-12.488431	4.434816	-1.702492
54	1	0	-10.891355	2.600827	0.575394
55	1	0	-14.6998	-0.596151	-1.615533
56	1	0	-13.128495	-2.725921	-3.591611
57	1	0	-10.212523	-4.025157	-0.338632
58	1	0	-12.111618	-4.994996	5.753119
59	1	0	-9.475648	-5.188821	3.718461
60	1	0	-9.810996	-2.613333	5.805638
61	1	0	-13.349609	0.718364	4.847393
62	1	0	-15.268226	0.309696	2.164569
63	1	0	-15.583497	-1.714512	4.787973
64	1	0	-3.616788	-2.360655	-3.912567
65	1	0	-4.185056	-4.723238	-1.662103
66	1	0	-4.791028	-2.284062	3.547425
67	1	0	-1.887835	-0.763137	3.804461
68	1	0	3.196697	-7.823585	0.003677
69	1	0	-0.002923	-8.648818	-0.269738
70	1	0	0.351742	-9.846878	4.008776
71	1	0	2.999492	-7.948527	4.526917
72	1	0	2.279037	-3.432357	5.191625
73	1	0	-1.595283	-7.805968	8.227134
74	1	0	-3.609876	-5.291137	7.393841
75	1	0	-3.741322	-8.164241	5.695495
76	1	0	2.938086	-4.760906	-4.129658
77	1	0	0.145246	-6.53105	-4.54544
78	1	0	0.413376	-3.508546	-5.929294

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Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-2.943159	-0.620241	0.422401
1	6	0	-5.336753	0.988102	0.479616
2	8	0	-6.596515	1.098011	2.396296
3	6	0	-6.352322	2.280359	-1.938307
4	6	0	-7.9676	4.664558	-1.530891
5	6	0	-6.541693	6.991875	-0.576632
6	6	0	-4.417781	7.462057	-2.465052
7	6	0	-3.545106	5.550122	-4.094567
8	6	0	-4.413569	2.881955	-3.971565
9	8	0	-3.591117	1.278961	-5.411046
10	6	0	-3.257184	9.818285	-2.601206
11	6	0	-1.342909	10.31061	-4.314765
12	6	0	-0.531258	8.43298	-5.959467
13	6	0	-1.62242	6.072843	-5.830711
14	6	0	-5.390057	6.716625	2.064496
15	6	0	-8.411425	9.203732	-0.547375
16	6	0	-8.479286	0.382383	-2.774865
17	6	0	-10.434222	3.797382	-0.337032
18	6	0	-10.989564	1.295863	-1.679678
19	8	0	-8.189327	-1.463867	-4.067768
20	6	0	-12.268745	-0.684927	-0.008426
21	6	0	-13.208877	-2.974935	-1.384913
22	6	0	-14.61457	-4.804276	-0.371033
23	6	0	-15.514993	-6.996382	-1.911518
24	6	0	-15.434896	-4.783065	2.342216
25	6	0	-2.997928	-2.860146	-1.427673
26	6	0	-0.167902	-3.393669	-1.637399
27	6	0	0.861737	-4.472254	0.850512
28	6	0	-1.032229	-4.135649	2.988532
29	6	0	-2.20352	-1.53134	3.131691
30	6	0	1.551702	-7.255063	1.133649
31	6	0	1.538719	-7.668837	4.03101
32	6	0	0.339164	-5.280525	5.247313
33	8	0	0.881838	-0.796656	-1.799925
34	6	0	-0.639957	0.819282	-0.571118
35	8	0	-0.137219	3.017161	-0.239335
36	8	0	2.243263	-3.488745	5.983329
37	6	0	-1.35614	-5.865772	7.48221
38	6	0	0.617872	-4.760971	-3.999822
39	1	0	-2.565436	-5.471211	2.613526

40	1	0	2.541541	-3.367467	1.295401
41	1	0	-8.491146	5.186727	-3.470179
42	1	0	-12.198575	1.636362	-3.322066
43	1	0	-3.854954	11.314858	-1.347663
44	1	0	-0.48426	12.166126	-4.366459
45	1	0	0.961423	8.80744	-7.30457
46	1	0	-0.986336	4.5525	-7.034161
47	1	0	-6.801828	6.119856	3.433998
48	1	0	-3.836052	5.380203	2.093603
49	1	0	-4.633346	8.531679	2.670384
50	1	0	-9.938697	8.82304	0.775652
51	1	0	-7.517864	10.949645	0.058817
52	1	0	-9.230093	9.525063	-2.408931
53	1	0	-11.943188	5.154559	-0.661122
54	1	0	-10.248235	3.514206	1.683549
55	1	0	-10.947583	-1.211509	1.488565
56	1	0	-13.833368	0.260452	0.953377
57	1	0	-12.67269	-3.136497	-3.353379
58	1	0	-17.575481	-7.134151	-1.876151
59	1	0	-14.918672	-6.85003	-3.87304
60	1	0	-14.800515	-8.780274	-1.155279
61	1	0	-15.556023	-6.696639	3.094764
62	1	0	-14.159422	-3.714404	3.548958
63	1	0	-17.317476	-3.95484	2.543208
64	1	0	-3.755634	-2.315976	-3.2457
65	1	0	-4.06994	-4.465729	-0.734241
66	1	0	-3.897747	-1.556676	4.289757
67	1	0	-0.916322	-0.175504	3.988046
68	1	0	3.361553	-7.718229	0.276229
69	1	0	0.128201	-8.448771	0.240785
70	1	0	0.447188	-9.34016	4.531381
71	1	0	3.437617	-7.959564	4.773126
72	1	0	3.327981	-4.295776	7.203644
73	1	0	-2.158607	-4.133579	8.245421
74	1	0	-2.895042	-7.12466	6.946868
75	1	0	-0.289438	-6.787637	8.987177
76	1	0	-0.04257	-3.748529	-5.660633
77	1	0	2.664123	-4.93924	-4.100383
78	1	0	-0.195187	-6.649297	-4.018238

yby5-12-3D2000010_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.302963	-1.007776	0.03114
1	6	0	-5.678727	0.632385	-0.017887
2	8	0	-6.950363	0.847304	1.87421
3	6	0	-6.591183	1.910782	-2.487117
4	6	0	-8.364751	4.191204	-2.135285
5	6	0	-7.20292	6.576782	-0.979038
6	6	0	-4.853291	7.183211	-2.532215
7	6	0	-3.70674	5.39418	-4.130789
8	6	0	-4.503989	2.708217	-4.297463
9	8	0	-3.520233	1.2469	-5.785301
10	6	0	-3.75629	9.570051	-2.376741
11	6	0	-1.639372	10.207016	-3.773288
12	6	0	-0.549757	8.448855	-5.389835
13	6	0	-1.579149	6.064154	-5.550951
14	6	0	-6.445242	6.37708	1.808765
15	6	0	-9.170463	8.689317	-1.243991
16	6	0	-8.499952	-0.070124	-3.584612
17	6	0	-10.875719	3.107703	-1.24106
18	6	0	-11.169001	0.777387	-2.916893
19	8	0	-7.978748	-1.951081	-4.752411
20	6	0	-12.814456	-1.384073	-1.893008
21	6	0	-11.663844	-2.742585	0.292566
22	6	0	-12.168315	-2.47214	2.746461
23	6	0	-10.728636	-3.944375	4.686117
24	6	0	-14.095845	-0.700581	3.808758
25	6	0	-3.055684	-3.077717	-1.985229
26	6	0	-0.20371	-3.519362	-1.901612
27	6	0	0.577139	-4.753902	0.607822
28	6	0	-1.564492	-4.664881	2.525706
29	6	0	-2.876182	-2.135392	2.722163
30	6	0	1.369457	-7.513901	0.789282
31	6	0	1.215604	-8.052624	3.654698
32	6	0	-0.417316	-5.919617	4.868826
33	8	0	0.758867	-0.888203	-1.752419
34	6	0	-0.948679	0.573173	-0.561239
35	8	0	-0.56078	2.743284	0.009659
36	8	0	1.10528	-4.194312	6.3027
37	6	0	-2.376959	-6.890902	6.708073
38	6	0	0.895413	-4.683478	-4.246099
39	1	0	-2.959926	-6.033239	1.851316

40	1	0	2.157661	-3.608808	1.293678
41	1	0	-8.72998	4.767735	-4.096123
42	1	0	-11.978856	1.37082	-4.729306
43	1	0	-4.568908	10.976025	-1.138963
44	1	0	-0.839679	12.08131	-3.6
45	1	0	1.10543	8.93366	-6.486322
46	1	0	-0.737558	4.635265	-6.740078
47	1	0	-7.994969	5.650891	2.945298
48	1	0	-4.815345	5.166869	2.078843
49	1	0	-5.94895	8.243776	2.518424
50	1	0	-9.776592	8.915225	-3.198894
51	1	0	-10.822954	8.270309	-0.094002
52	1	0	-8.437805	10.495857	-0.600887
53	1	0	-12.428491	4.424198	-1.524149
54	1	0	-10.817699	2.578767	0.734114
55	1	0	-14.657	-0.596602	-1.424916
56	1	0	-13.120534	-2.724947	-3.428754
57	1	0	-10.182288	-4.066093	-0.219776
58	1	0	-9.67438	-2.67436	5.92436
59	1	0	-11.997266	-5.034611	5.895119
60	1	0	-9.391503	-5.24496	3.823257
61	1	0	-15.149426	0.318744	2.373534
62	1	0	-15.448585	-1.712312	4.993821
63	1	0	-13.186574	0.694484	5.029053
64	1	0	-3.601439	-2.397402	-3.832598
65	1	0	-4.155607	-4.761454	-1.580241
66	1	0	-4.700829	-2.327524	3.639102
67	1	0	-1.790033	-0.816124	3.868172
68	1	0	3.236475	-7.884439	0.011119
69	1	0	0.032909	-8.700687	-0.239122
70	1	0	0.410619	-9.907642	4.032988
71	1	0	3.074866	-8.02811	4.5352
72	1	0	2.388799	-3.50805	5.206187
73	1	0	-1.47524	-7.867234	8.277845
74	1	0	-3.482044	-5.335782	7.476677
75	1	0	-3.655224	-8.203035	5.772275
76	1	0	0.141273	-6.578564	-4.509132
77	1	0	0.405049	-3.55498	-5.891018
78	1	0	2.943311	-4.817839	-4.117804

yby5-12-3D2000016_en_		Standard Orientation (a.u.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.60708	-0.829523	0.05576
1	6	0	-5.624149	1.215988	0.322091
2	8	0	-6.424706	1.76188	2.39881
3	6	0	-6.791075	2.507657	-2.027713
4	6	0	-8.055522	5.086326	-1.550346
5	6	0	-6.301084	7.289262	-0.880318
6	6	0	-4.290325	7.390887	-2.939994
7	6	0	-3.797477	5.325005	-4.539728
8	6	0	-5.019347	2.811703	-4.273484
9	8	0	-4.608087	1.106053	-5.768346
10	6	0	-2.842286	9.56451	-3.26133
11	6	0	-1.002982	9.73251	-5.11274
12	6	0	-0.558765	7.702562	-6.716635
13	6	0	-1.945605	5.520815	-6.41669
14	6	0	-4.97527	7.098299	1.687817
15	6	0	-7.920215	9.692786	-0.897726
16	6	0	-9.192902	0.861575	-2.573069
17	6	0	-10.466892	4.53272	-0.07785
18	6	0	-11.476999	2.179573	-1.417396
19	8	0	-9.263171	-1.097487	-3.723462
20	6	0	-13.125012	0.34479	0.111039
21	6	0	-11.759558	-0.90812	2.234524
22	6	0	-11.097669	-3.334437	2.431222
23	6	0	-9.685464	-4.254033	4.704962
24	6	0	-11.658331	-5.336021	0.515988
25	6	0	-4.166628	-3.028576	-1.748799
26	6	0	-1.48585	-4.009435	-2.183575
27	6	0	-0.430154	-5.224846	0.228218
28	6	0	-2.061369	-4.60157	2.510337
29	6	0	-2.791313	-1.845457	2.704767
30	6	0	-0.157174	-8.074804	0.50678
31	6	0	0.20121	-8.416226	3.383836
32	6	0	-0.687066	-5.942101	4.677698
33	8	0	-0.063457	-1.606186	-2.491581
34	6	0	-1.196673	0.230121	-1.158752
35	8	0	-0.336211	2.32531	-0.908605
36	8	0	1.578976	-4.61401	5.378168
37	6	0	-2.32079	-6.373139	6.990128
38	6	0	-1.126784	-5.496347	-4.575641
39	1	0	-3.812975	-5.674966	2.271426

40	1	0	1.43255	-4.395351	0.530378
41	1	0	-8.727062	5.599185	-3.446815
42	1	0	-12.594409	2.792013	-3.049868
43	1	0	-3.148085	11.17313	-2.041379
44	1	0	0.086608	11.452792	-5.302877
45	1	0	0.879057	7.819623	-8.164624
46	1	0	-1.603339	3.88799	-7.591382
47	1	0	-3.549038	5.628154	1.70928
48	1	0	-4.02808	8.878177	2.099627
49	1	0	-6.32415	6.727034	3.192934
50	1	0	-8.899847	9.931006	-2.692957
51	1	0	-9.32373	9.607405	0.602351
52	1	0	-6.794167	11.375736	-0.566289
53	1	0	-11.81159	6.082056	-0.195726
54	1	0	-10.071114	4.166383	1.895981
55	1	0	-14.7224	1.424828	0.852363
56	1	0	-13.908114	-1.038926	-1.188831
57	1	0	-11.203322	0.332576	3.766365
58	1	0	-9.239673	-2.729254	6.008133
59	1	0	-10.768033	-5.683893	5.727986
60	1	0	-7.915189	-5.159696	4.152877
61	1	0	-9.913396	-6.241285	-0.112817
62	1	0	-12.81868	-6.828754	1.345226
63	1	0	-12.609263	-4.630178	-1.155071
64	1	0	-4.974733	-2.37	-3.505665
65	1	0	-5.428226	-4.43861	-0.957125
66	1	0	-4.349958	-1.577035	4.010945
67	1	0	-1.231828	-0.690464	3.40011
68	1	0	1.404466	-8.854848	-0.578876
69	1	0	-1.877341	-9.024247	-0.121439
70	1	0	-0.849397	-10.034412	4.095177
71	1	0	2.175923	-8.712624	3.866424
72	1	0	1.086936	-3.08144	6.2341
73	1	0	-4.002729	-7.465015	6.524713
74	1	0	-1.263831	-7.392642	8.430347
75	1	0	-2.947008	-4.584835	7.804198
76	1	0	-1.756012	-4.399925	-6.194806
77	1	0	0.849124	-5.999727	-4.842106
78	1	0	-2.226058	-7.232509	-4.497614

ECD calculation data for 1c

Methods

In general, conformational analyses were carried out via random searching in the Sybyl-X 2.0 using the MMFF94S force field with an energy cutoff of 2.5 kcal/mol.[1] The results showed six lowest energy conformer for model molecule **1c** (calculated data were the same as those in Tables S6 and S7). Subsequently, the conformers were re-optimized using DFT at the B3LYP-D3(BJ)/6-31G** level in PCM methanol using Gaussian 09.[2] The excitation energies, oscillator strengths, and rotational strengths (velocity) of the first 60 electronic excitations were calculated using the TDDFT methodology at the CAM-B3LYP/def2-TZVP level in MeOH using ORCA.[3][4] Boltzmann weights were computed using relative free energies at the wB97M-V/def2-TZVP level in PCM methanol using ORCA.[3][4] The ECD spectra (red shift 26 nm) were simulated by the overlapping Gaussian function (half the bandwidth at 1/e peak height, sigma = 0.30 for all).[4] To get the final spectra, the simulated spectra of the conformers were averaged according to the Boltzmann distribution theory and their relative Gibbs free energy (ΔG). After comparing the calculated UV spectrum with the experimental UV spectrum, the UV correction value was determined to be 26 nm. By comparing the experiment spectrum with the calculated model molecules, the absolute configuration of **1** (**1c**) was determined.

References:

[1] Sybyl Software, version X 2.0; Tripos Associates Inc.: St. Louis, MO, 2013.

[2] F. Neese, The ORCA program system, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2012, **2**, 73−78.

[3] F. Neese, Software update: the ORCA program system, version 4.0, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2017, **8**, e1327.

[4] P. J. Stephens and N. Harada, ECD cotton effect approximated by the Gaussian curve and other methods, *Chirality*, 2010, **22**, 229–233.