Supplementary Materials for

Electric-Field-Induced Covalent Condensation of Boronic Acids in Water Microdroplets

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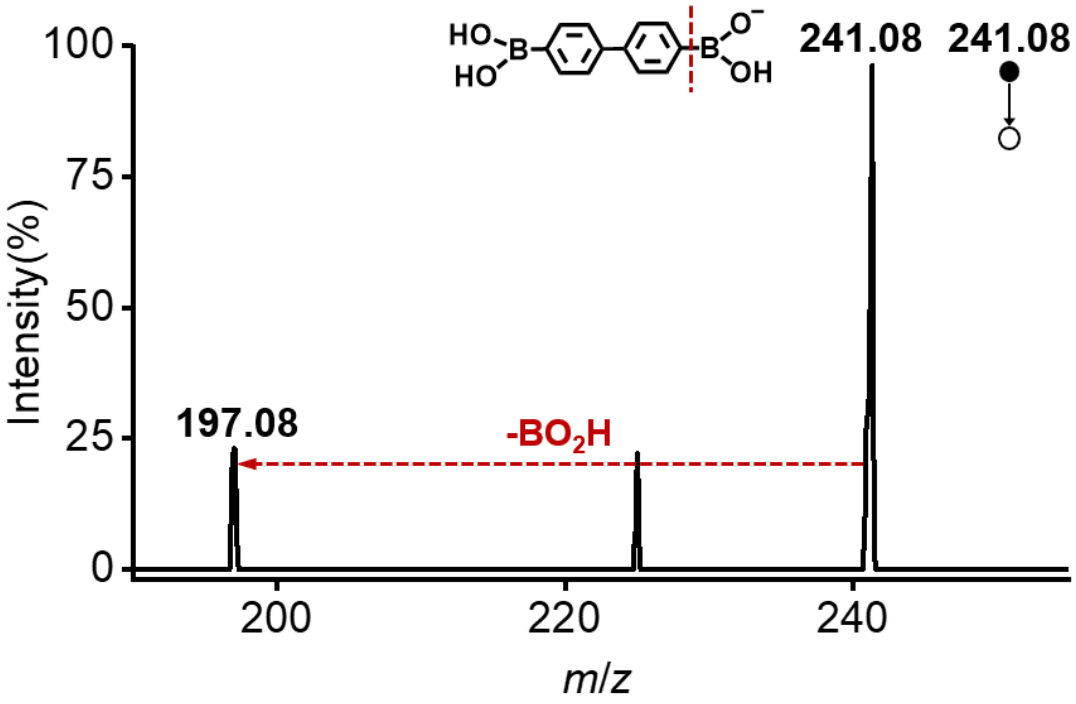

Figure S1. MS^2 spectrum of the peak at m/z of 241.08 shown in Fig. 2a.

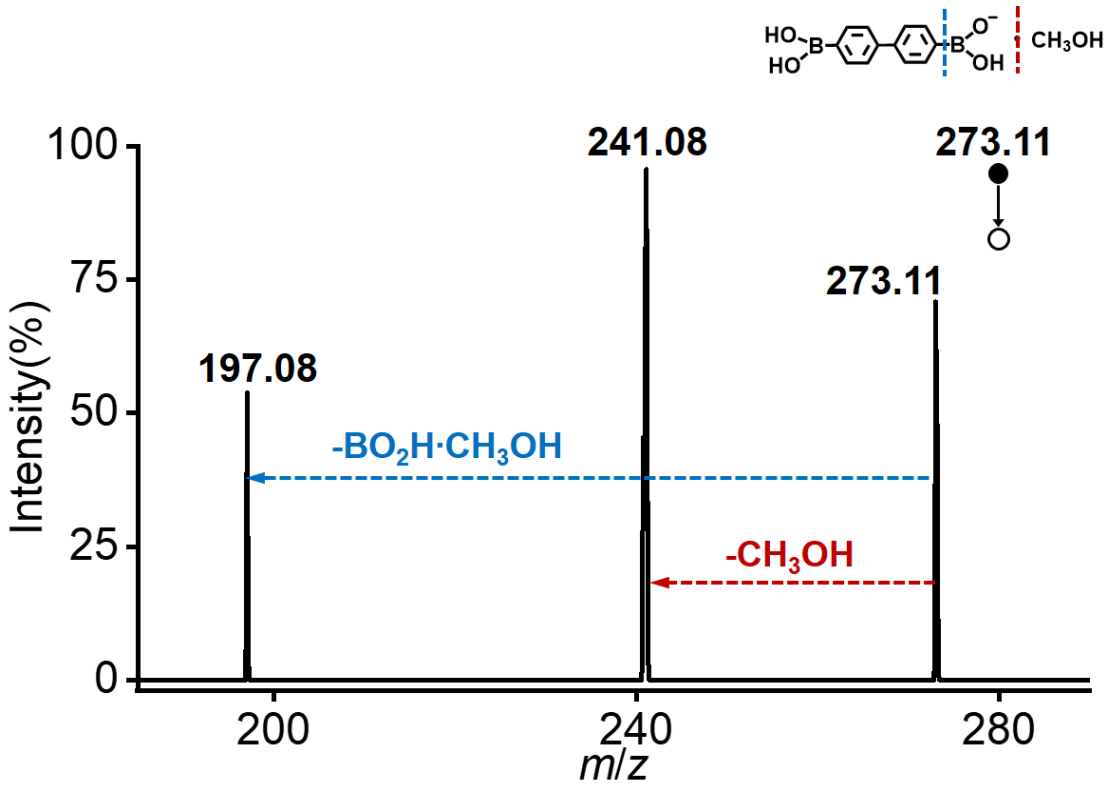

Figure S2. MS^2 spectrum of the peak at m/z of 273.11 shown in Figure 2a.

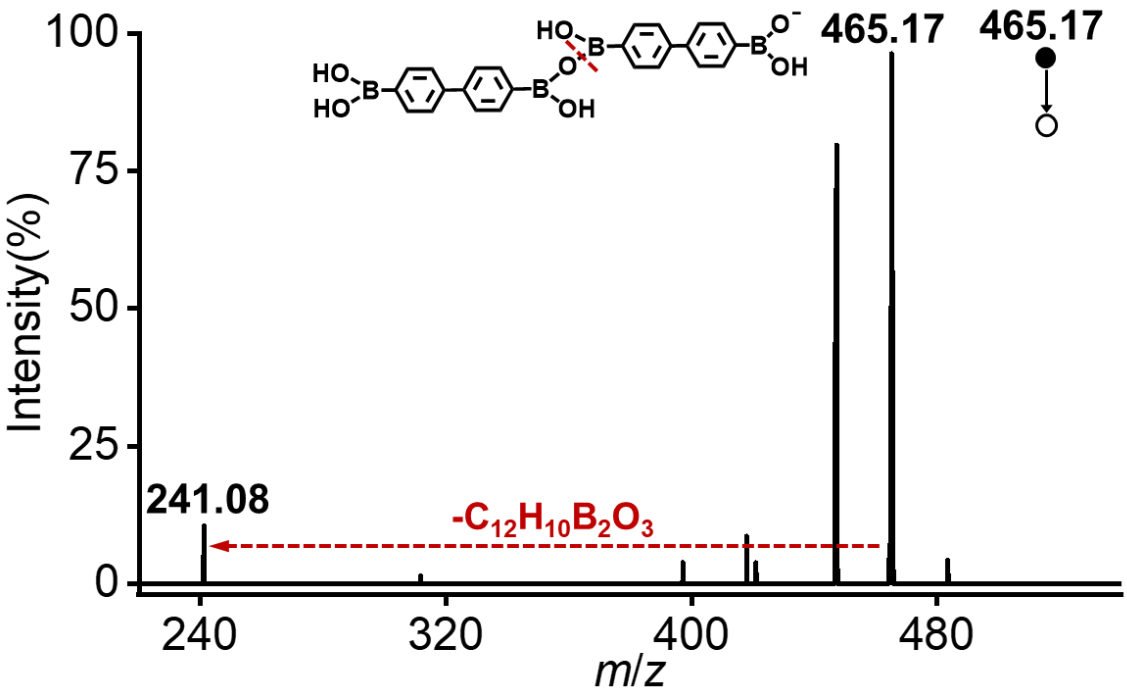

Figure S3. MS^2 spectrum of the peak at m/z of 465.17 shown in Figure 2b.

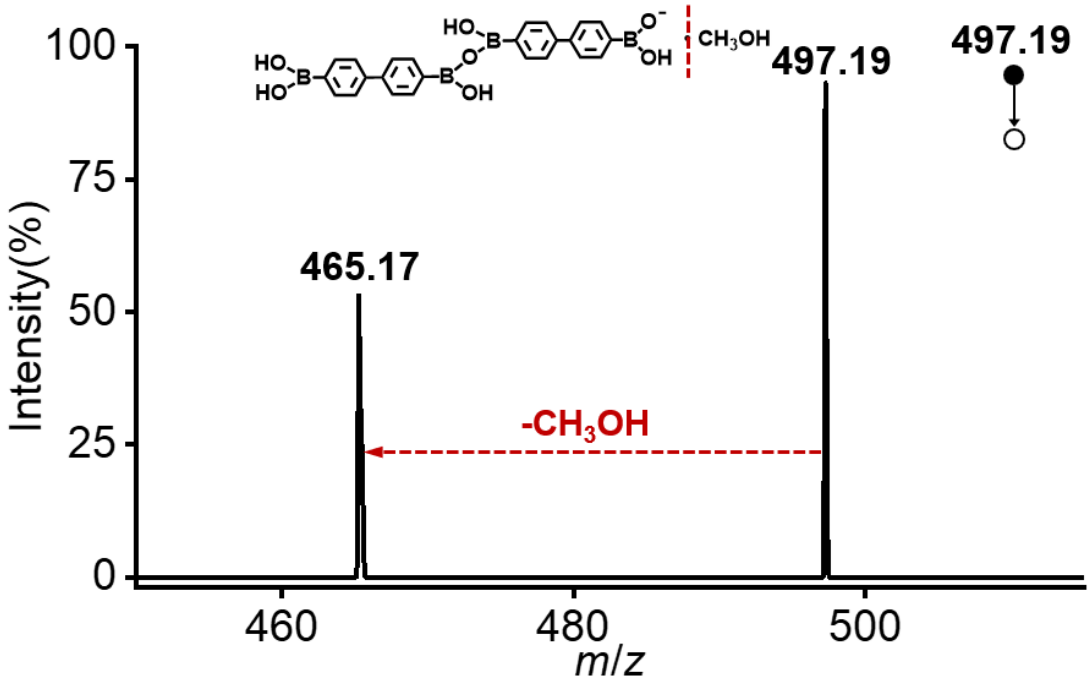

Figure S4. MS^2 spectrum of the peak at m/z of 497.19 shown in Figure 2b.

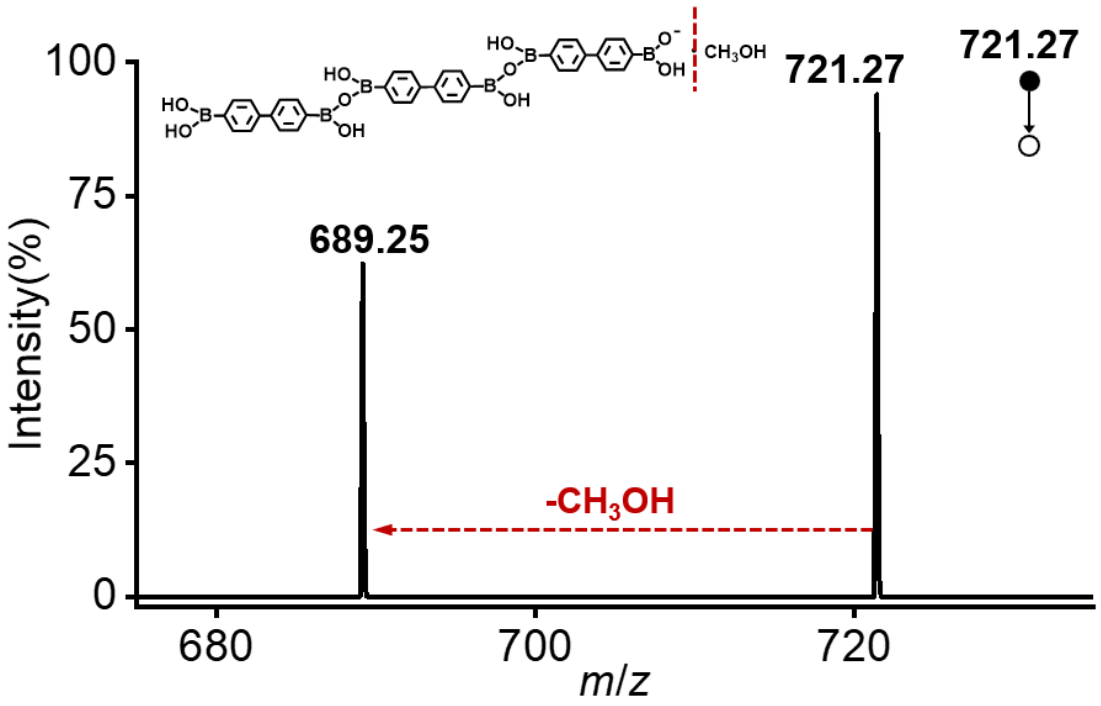

Figure S5. MS^2 spectrum of the peak at m/z of 721.27 shown in Figure 2c.

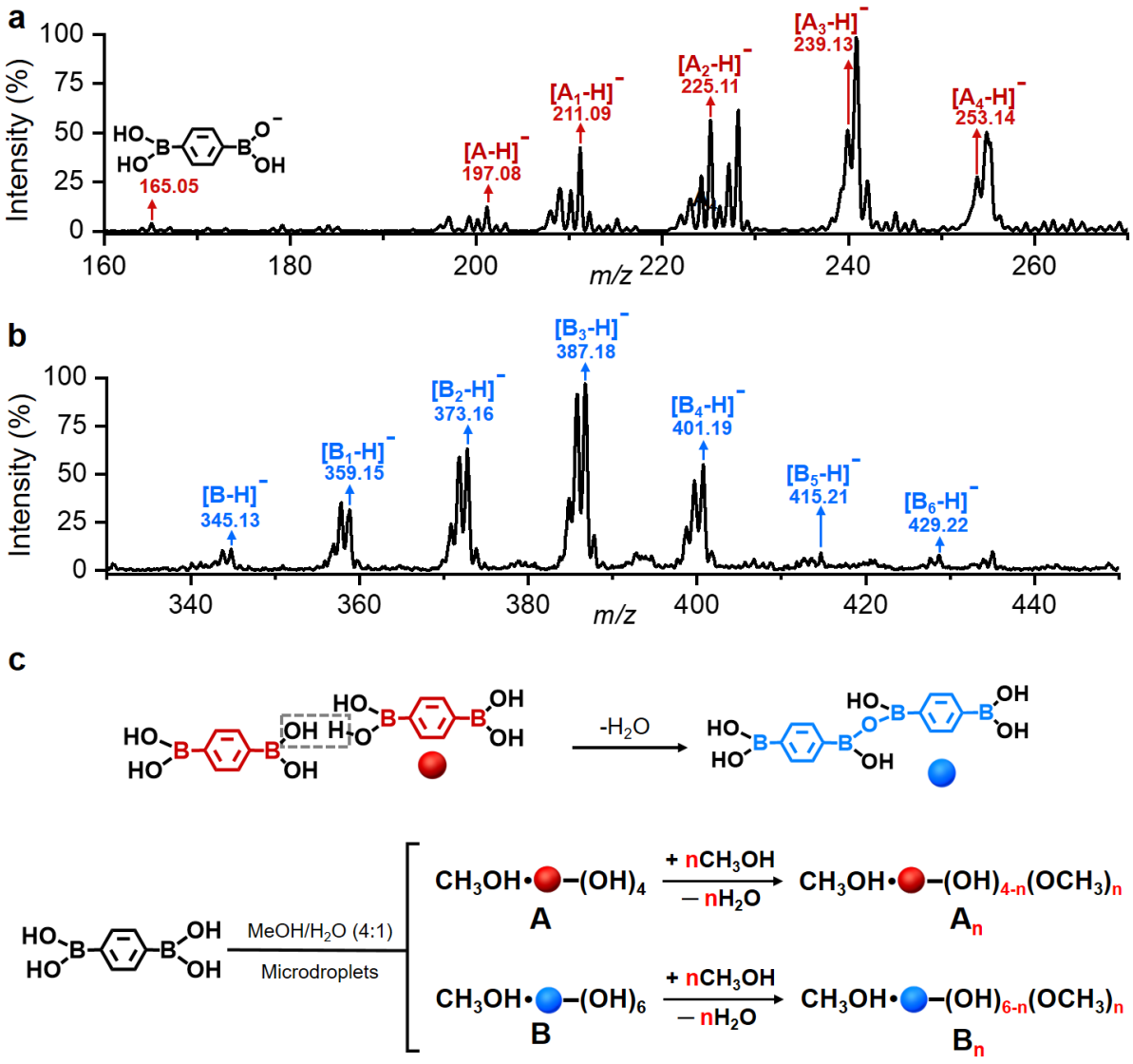

Figure S6. Spontaneous condensation of BDBA in MeOH/H_2O (4:1) microdroplets.

a-b, Mass spectrum of BDBA in microdroplets of MeOH/H_2O (4:1) using N_2 as the nebulizing gas with m/z range 160-270 and 330-450. **c**, Proposed reaction scheme.

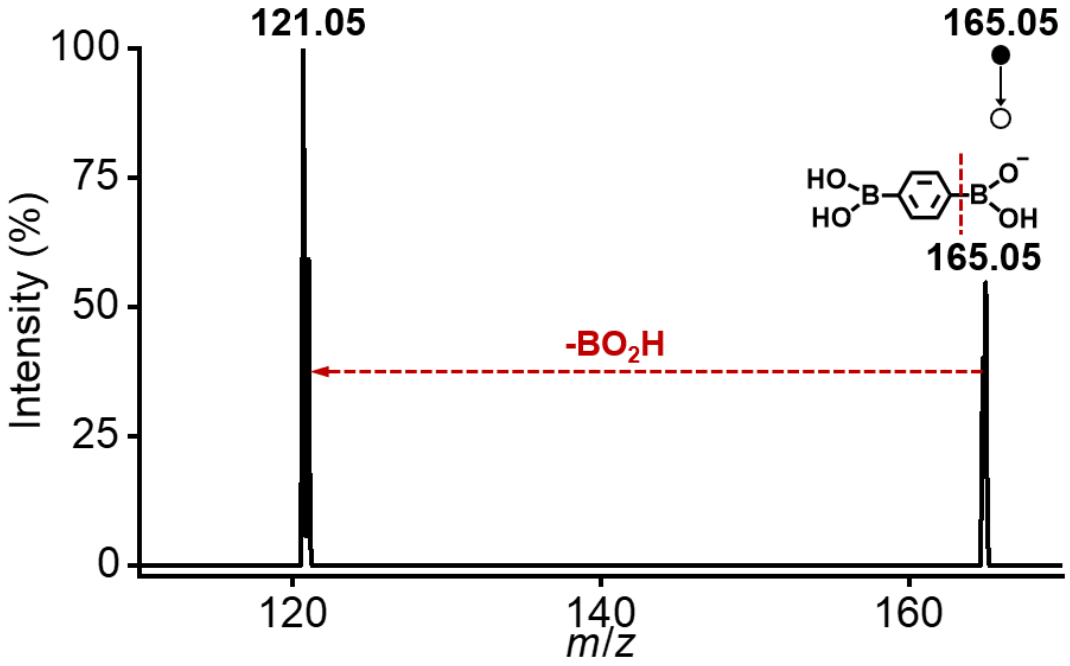

Figure S7. MS^2 spectrum of the peak at m/z of 165.05 shown in Figure S6a.

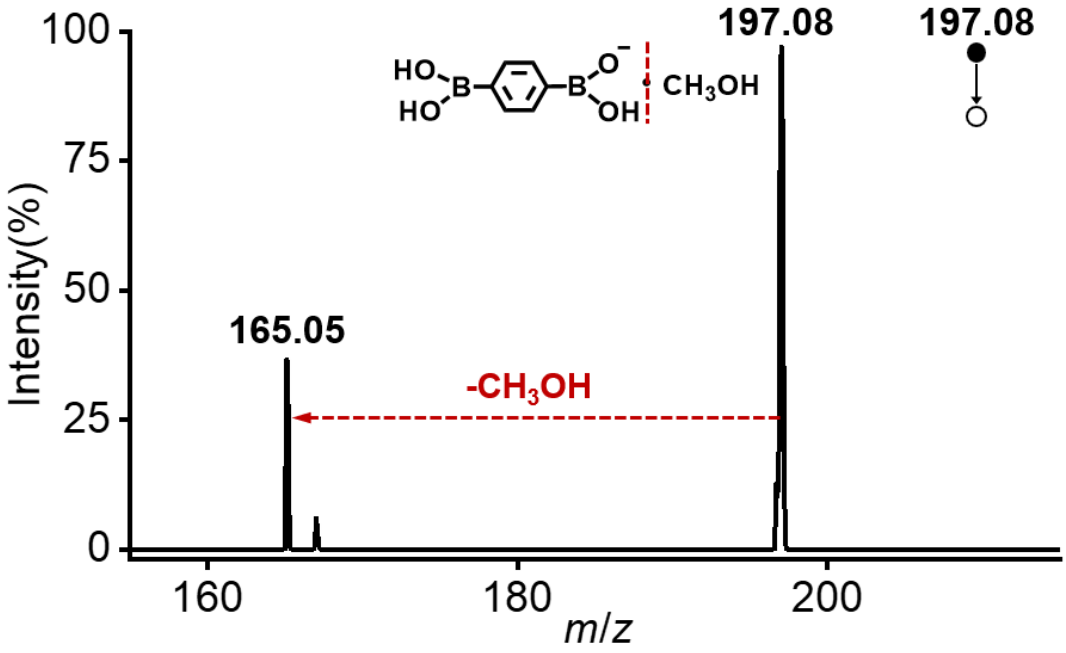

Figure S8. MS^2 spectrum of the peak at m/z of 197.08 shown in Figure S6a.

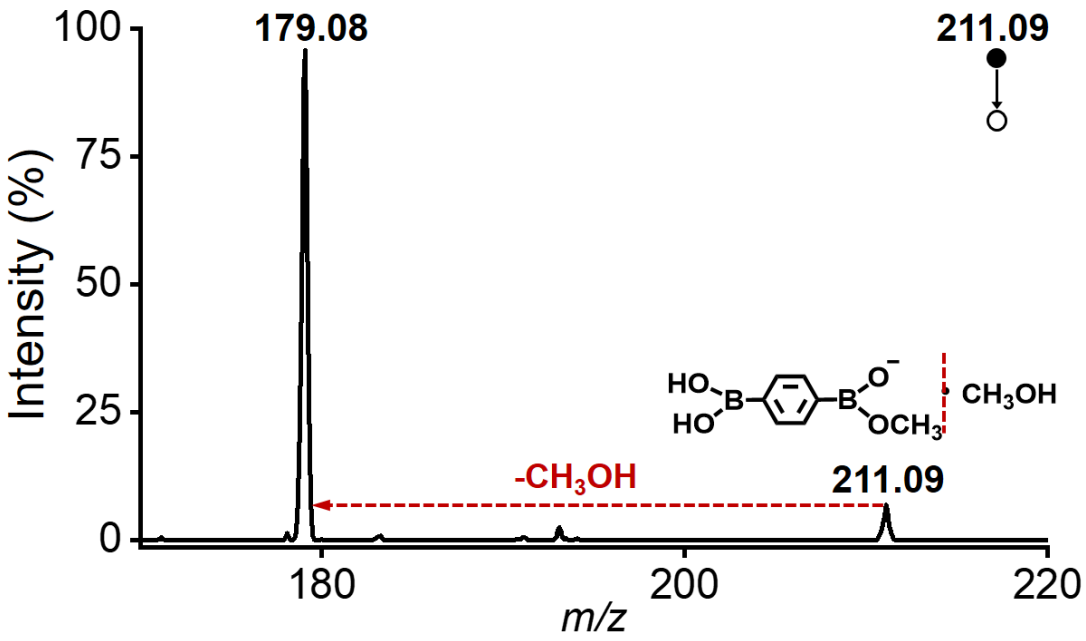

Figure S9. MS^2 spectrum of the peak at m/z of 211.09 shown in Figure S6a.

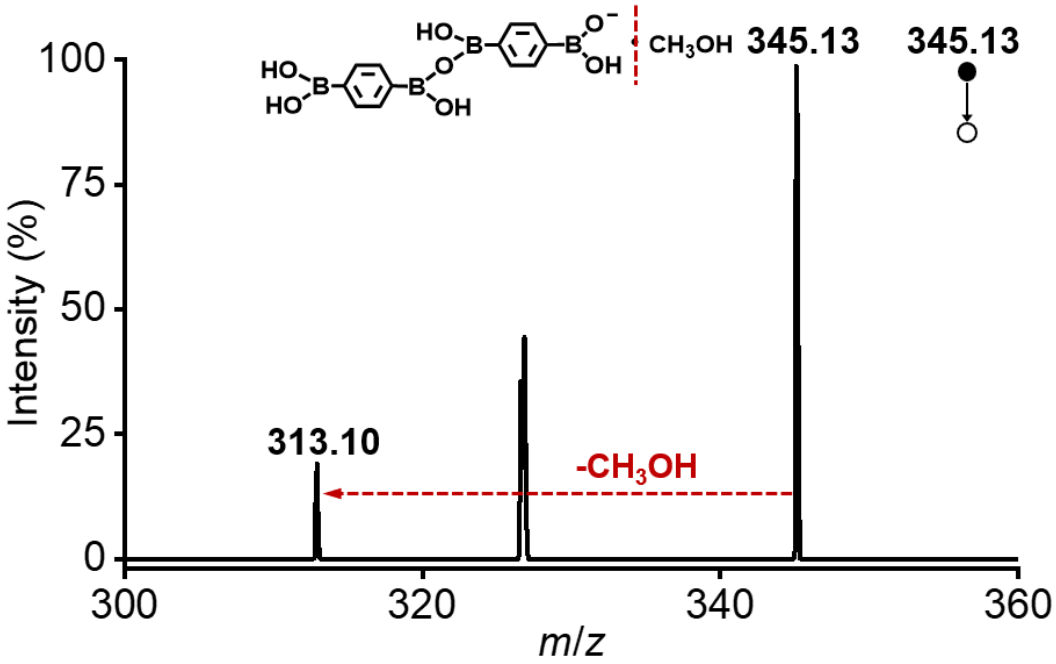

Figure S10. MS^2 spectrum of the peak at m/z of 345.13 shown in Figure S6b.

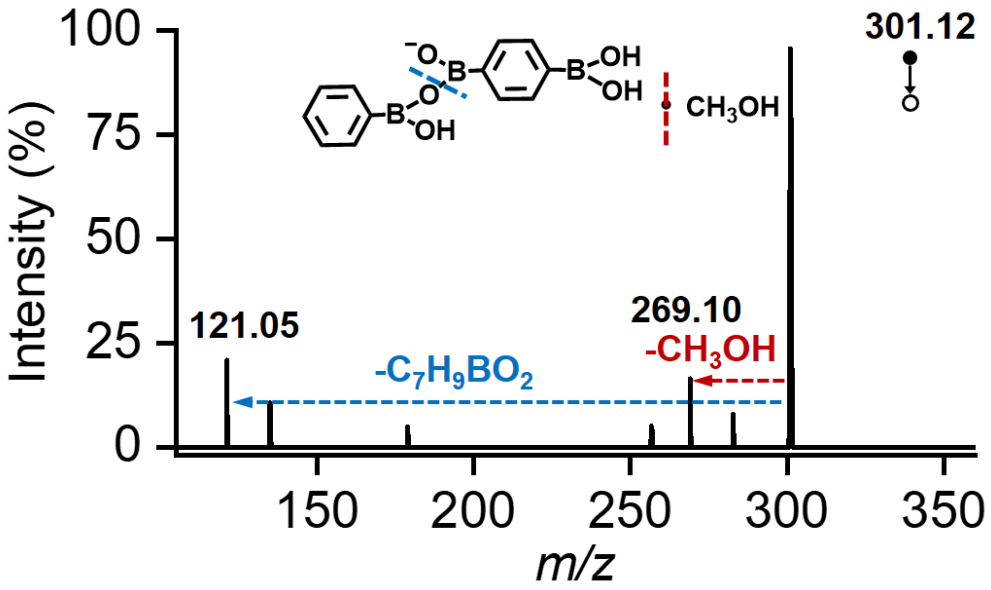

Figure S11. MS^2 spectrum of the peak at m/z of 301.12 shown in Figure 3a.

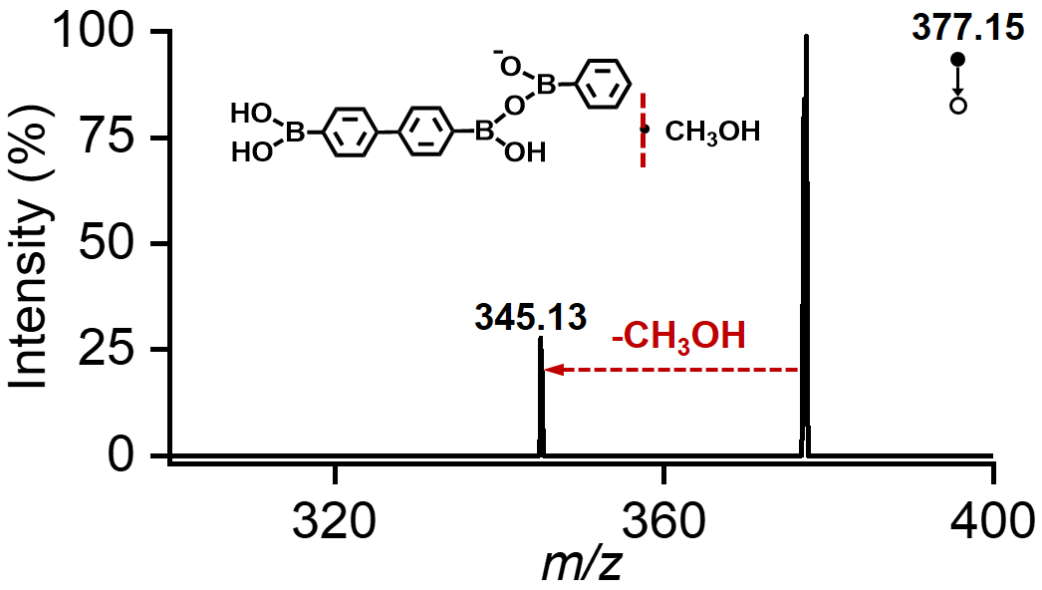

Figure S12. MS^2 spectrum of the peak at m/z of 377.15 shown in Figure 3b.

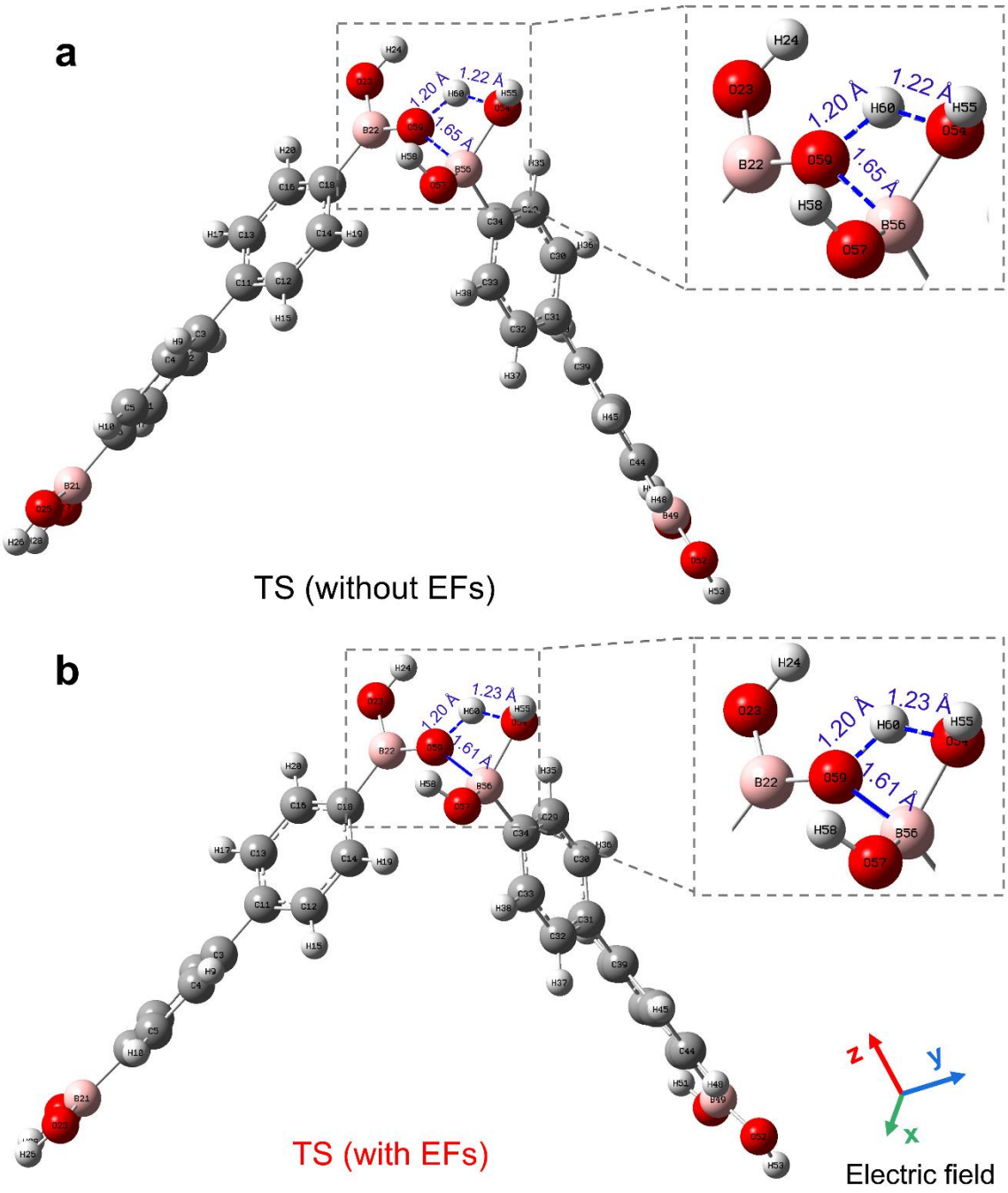

Figure S13. Transition states of BPBA dimer with and without the presence of external electric field.

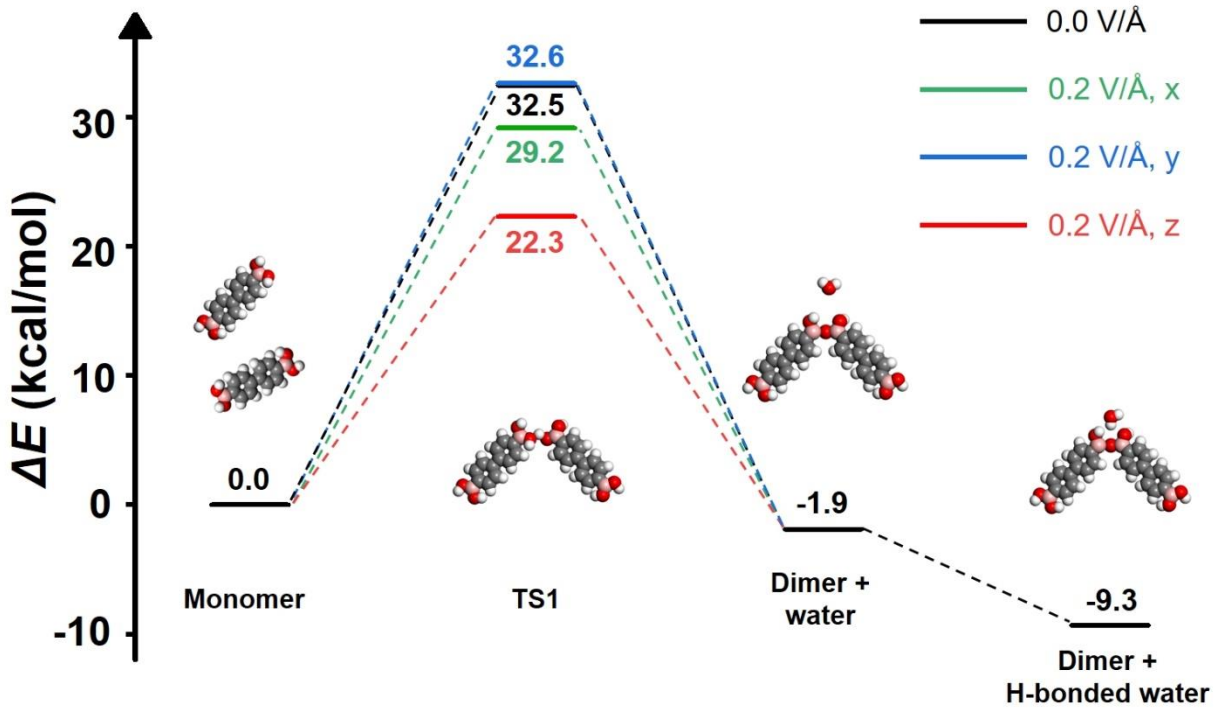

Figure S14. Potential energy profile of BPBA condensation.

Potential energy profile of BPBA condensation without the presence of external electric field (black trace). Potential energy profile of the transition state under external EFs of x-axes (green trace), y-axes (blue trace), and z-axes (red trace).

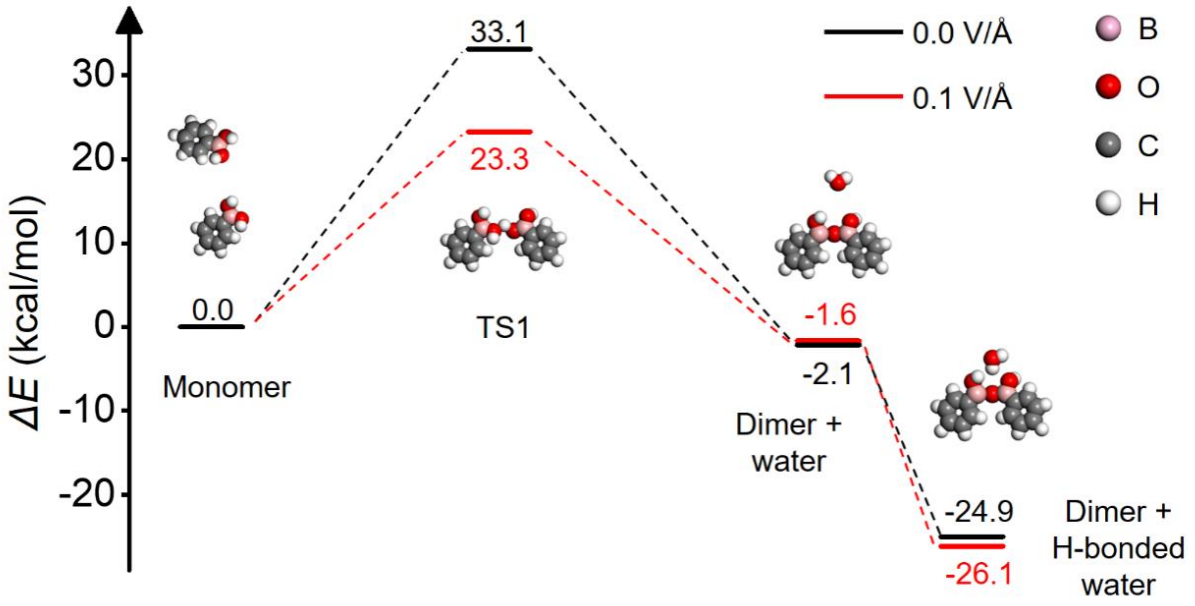

Figure S15. Potential energy profile of PBA condensation.

Potential energy profile of PBA condensation with (red trace) and without (black trace) the presence of external electric field.

Table S1 Mulliken charge of TS.

ATOM	0.0 V/Å	0.1 V/Å, z	0.2 V/Å, z	0.3 V/Å, z	0.2 V/Å, x	0.2 V/Å, y
C1	-0.42290	-0.36762	-0.48075	-0.40409	-0.44297	-0.43911
C2	-0.53437	-0.55872	-0.49068	-0.53667	-0.54339	-0.54788
C3	1.58631	1.55494	1.68744	1.66252	1.68954	1.68655
C4	-0.62247	-0.58588	-0.74026	-0.56464	-0.68932	-0.69303
C5	-0.41895	-0.43776	-0.31706	-0.40499	-0.35869	-0.35328
C6	-0.41949	-0.43311	-0.49613	-0.49335	-0.50035	-0.49932
H7	0.14176	0.15140	0.15475	0.18439	0.14245	0.13392
H8	0.12263	0.12577	0.12684	0.14689	0.12288	0.11577
H9	0.12241	0.11686	0.11417	0.08997	0.12084	0.12953
H10	0.14142	0.13883	0.13729	0.12285	0.14217	0.14895
C11	1.10581	1.17894	1.15787	0.92942	1.17813	1.17140
C12	-0.54140	-0.54571	-0.67283	-0.60257	-0.62949	-0.63001
C13	-0.60207	-0.60982	-0.68051	-0.76656	-0.68987	-0.70067
C14	-0.08151	-0.11729	-0.01985	0.09317	-0.05756	-0.05853
H15	0.12174	0.11528	0.10551	0.11223	0.12606	0.12507
C16	-0.15320	-0.19723	-0.04377	-0.25637	-0.06911	-0.04621
H17	0.12206	0.13530	0.14514	0.15824	0.11647	0.11723
C18	-0.63286	-0.63640	-0.64764	-0.43761	-0.64025	-0.63977
H19	0.14503	0.13836	0.12531	0.16599	0.15152	0.15127
H20	0.14368	0.15409	0.15748	0.16866	0.13480	0.13575
B21	0.50503	0.50820	0.50937	0.51204	0.50752	0.50543
B22	0.85197	0.86685	0.80885	0.72907	0.82865	0.82680
O23	-0.39130	-0.37450	-0.36361	-0.35790	-0.39707	-0.39097
H24	0.28597	0.28864	0.27695	0.29670	0.28152	0.28189
O25	-0.33391	-0.34363	-0.32856	-0.35890	-0.32314	-0.31549
H26	0.26169	0.26709	0.26424	0.27349	0.26089	0.25882
O27	-0.33162	-0.32484	-0.31979	-0.29712	-0.32899	-0.33400
H28	0.26173	0.27058	0.26527	0.29254	0.26148	0.25902
C29	-0.33555	-0.34902	-0.39833	-0.15585	-0.33141	-0.34644
C30	-0.62828	-0.58505	-0.58387	-0.52939	-0.63313	-0.62555
C31	1.02532	1.06603	0.90210	0.94996	0.89550	0.90227
C32	-0.54603	-0.58701	-0.57312	-0.61990	-0.55642	-0.54026

C33	-0.28719	-0.32318	-0.13478	-0.21697	-0.16969	-0.16665
C34	-0.06839	-0.02008	-0.13877	-0.34306	-0.14239	-0.15331
H35	0.11287	0.11478	0.12085	0.15429	0.11176	0.11575
H36	0.11701	0.11736	0.11386	0.12571	0.11670	0.10969
H37	0.11864	0.11379	0.11419	0.09075	0.12363	0.12134
H38	0.13714	0.13469	0.13164	0.12355	0.13240	0.14116
C39	1.53450	1.51634	1.64094	1.47374	1.64237	1.63945
C40	-0.59545	-0.65737	-0.62327	-0.57309	-0.62171	-0.64118
C41	-0.59492	-0.59078	-0.80064	-0.55934	-0.76788	-0.78006
C42	-0.30380	-0.27489	-0.26732	-0.32826	-0.27959	-0.26572
H43	0.12451	0.13538	0.14344	0.15677	0.11725	0.12133
C44	-0.39615	-0.34075	-0.29433	-0.48129	-0.30883	-0.30055
H45	0.12534	0.11704	0.11186	0.10642	0.12947	0.13409
C46	-0.46687	-0.46443	-0.44376	-0.37018	-0.43963	-0.43912
H47	0.08256	0.09187	0.10439	0.10070	0.08838	0.08061
H48	0.14641	0.13382	0.12280	0.10545	0.15279	0.14642
B49	0.50699	0.50471	0.49321	0.51482	0.49588	0.49283
O50	-0.35375	-0.35799	-0.34948	-0.38041	-0.33822	-0.35485
H51	0.24682	0.25472	0.25485	0.26881	0.24624	0.24694
O52	-0.35451	-0.36790	-0.35272	-0.39847	-0.34122	-0.34197
H53	0.29095	0.28390	0.27374	0.27004	0.28955	0.27822
O54	-0.59982	-0.58238	-0.62275	-0.49517	-0.62229	-0.62221
H55	0.29194	0.27875	0.29078	0.27641	0.30605	0.31035
B56	0.84901	0.84851	0.83714	0.80181	0.84229	0.84391
O57	-0.32690	-0.36744	-0.31053	-0.42629	-0.28956	-0.28756
H58	0.26180	0.27161	0.26288	0.30251	0.25046	0.26138
O59	-0.97629	-1.02803	-0.89361	-0.81299	-0.91313	-0.90282
H60	0.42891	0.43438	0.43359	0.41156	0.41966	0.42341
Total	0	0	0	0	0	0

Table S2 Bond length of TS (Å).

ATOM	0.0 V/Å	0.1 V/Å, z	0.2 V/Å, z	0.3 V/Å, z	0.2 V/Å, x	0.2 V/Å, y
R(1,2)	1.3900	1.3899	1.3896	1.3893	1.3904	1.3903
R(1,6)	1.4039	1.4037	1.4034	1.4033	1.4039	1.4038
R(1,7)	1.0843	1.084	1.0836	1.0835	1.0846	1.0843
R(2,3)	1.4035	1.4033	1.403	1.4033	1.4037	1.4035
R(2,8)	1.0842	1.0841	1.0838	1.0837	1.0845	1.0843
R(3,4)	1.4036	1.4036	1.4038	1.4043	1.4034	1.4035
R(3,11)	1.4834	1.4832	1.4828	1.4817	1.4834	1.4835
R(4,5)	1.3900	1.3905	1.3914	1.392	1.3897	1.3900
R(4,9)	1.0842	1.0845	1.0853	1.0859	1.0840	1.0843
R(5,6)	1.4040	1.4036	1.4033	1.4033	1.4039	1.4039
R(5,10)	1.0843	1.0844	1.0849	1.0851	1.0840	1.0843
R(6,21)	1.5590	1.5623	1.5663	1.571	1.5595	1.5602
R(11,12)	1.4028	1.4036	1.4047	1.406	1.4027	1.4028
R(11,13)	1.4040	1.4042	1.4043	1.4053	1.4041	1.4042
R(12,14)	1.3903	1.3904	1.3915	1.3919	1.3902	1.3901
R(12,15)	1.0841	1.0842	1.0844	1.0844	1.0839	1.0839
R(13,16)	1.3888	1.3879	1.3879	1.3865	1.3890	1.3892
R(13,17)	1.0842	1.0837	1.0835	1.0832	1.0843	1.0844
R(14,18)	1.4044	1.4053	1.4068	1.4084	1.4046	1.4044
R(14,19)	1.0834	1.0837	1.0861	1.0873	1.0833	1.0834
R(16,18)	1.4063	1.4072	1.4068	1.4084	1.4064	1.4062
R(16,20)	1.0841	1.0837	1.0837	1.0835	1.0842	1.0844
R(18,22)	1.5556	1.5514	1.5528	1.5479	1.5555	1.5558
R(21,25)	1.3752	1.3752	1.3775	1.3779	1.3724	1.3742
R(21,27)	1.3752	1.3712	1.3644	1.3591	1.3775	1.3747
R(22,23)	1.3707	1.3665	1.3625	1.3585	1.3724	1.3752
R(22,59)	1.3875	1.3972	1.4013	1.4128	1.3861	1.3832
R(23,24)	0.9616	0.9613	0.9614	0.9611	0.9617	0.9617
R(25,26)	0.9610	0.9613	0.9618	0.9623	0.9609	0.9611
R(27,28)	0.9610	0.9612	0.9614	0.9619	0.9611	0.9611
R(29,30)	1.3903	1.3901	1.3915	1.3917	1.3904	1.3904
R(29,34)	1.4031	1.4030	1.4025	1.4022	1.4028	1.4033

R(29,35)	1.0854	1.0853	1.0841	1.084	1.0855	1.0856
R(30,31)	1.4033	1.4032	1.4025	1.4029	1.4033	1.4035
R(30,36)	1.0845	1.0845	1.0845	1.0845	1.0848	1.0844
R(31,32)	1.4016	1.4015	1.4030	1.4041	1.4014	1.4019
R(31,39)	1.4835	1.4833	1.4825	1.4808	1.4832	1.4837
R(32,33)	1.3919	1.3925	1.3919	1.3916	1.3920	1.3914
R(32,37)	1.0844	1.0848	1.0853	1.0859	1.0844	1.0842
R(33,34)	1.4017	1.4014	1.4033	1.4035	1.4016	1.4021
R(33,38)	1.0843	1.0844	1.0857	1.0856	1.0841	1.0843
R(34,56)	1.5792	1.5841	1.5952	1.6009	1.5821	1.5740
R(39,40)	1.4030	1.4032	1.4039	1.4053	1.4034	1.4027
R(39,41)	1.4037	1.4041	1.4053	1.407	1.4039	1.4033
R(40,42)	1.3903	1.3901	1.3895	1.3887	1.3899	1.3907
R(40,43)	1.0841	1.0838	1.0835	1.0833	1.0841	1.0843
R(41,44)	1.3897	1.3896	1.3892	1.3888	1.3897	1.3898
R(41,45)	1.0842	1.0845	1.0846	1.0847	1.0840	1.0842
R(42,46)	1.4036	1.4041	1.405	1.4066	1.4042	1.4032
R(42,47)	1.0876	1.0872	1.0871	1.0872	1.0882	1.0876
R(44,46)	1.4050	1.4052	1.4058	1.4067	1.4053	1.4047
R(44,48)	1.0841	1.0844	1.085	1.0857	1.0841	1.0839
R(46,49)	1.5638	1.5610	1.5566	1.5512	1.5608	1.5677
R(49,50)	1.3758	1.3744	1.3742	1.3754	1.3798	1.3748
R(49,52)	1.3686	1.3738	1.3803	1.3873	1.3682	1.3648
R(50,51)	0.9602	0.9607	0.9612	0.9617	0.9604	0.9599
R(52,53)	0.9631	0.9632	0.9631	0.9631	0.9628	0.9634
R(54,55)	0.9634	0.9634	0.9666	0.9668	0.9638	0.9634
R(54,56)	1.5961	1.6096	1.5881	1.6061	1.5927	1.5954
R(54,60)	1.2221	1.2336	1.2240	1.2310	1.2235	1.2142
R(56,57)	1.3978	1.4027	1.4077	1.4085	1.3937	1.3956
R(56,59)	1.6526	1.6125	1.5974	1.5705	1.6550	1.6781
R(57,58)	0.9611	0.9611	0.9623	0.9642	0.9611	0.9608
R(59,60)	1.2026	1.1956	1.2198	1.2165	1.2013	1.2069