Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Effect of Structural Fluctuations on Charge Carrier Mobility in Thiophene, Thiazole and Thiazolothiazole based Oligomers

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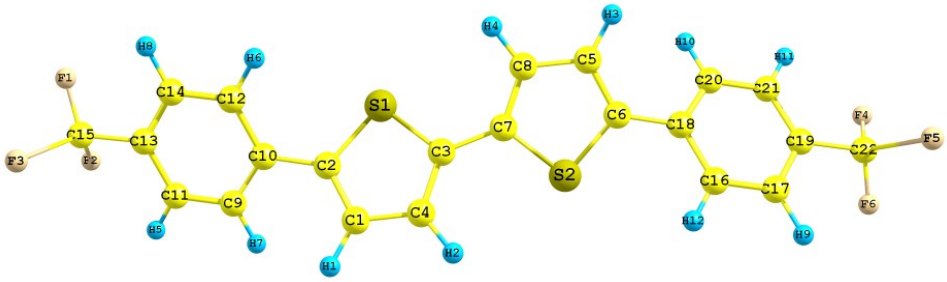
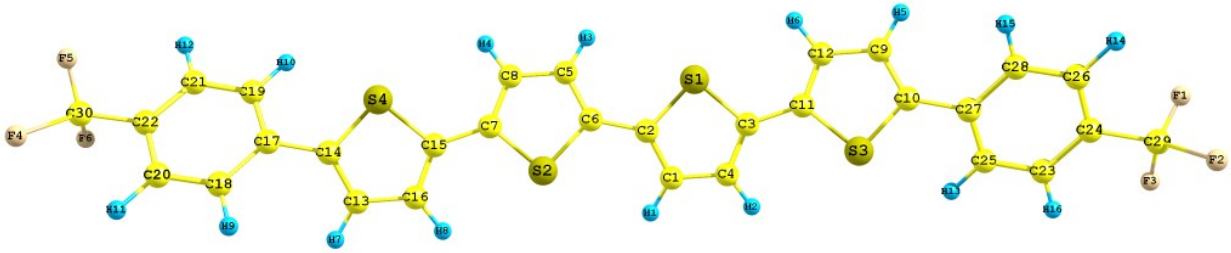
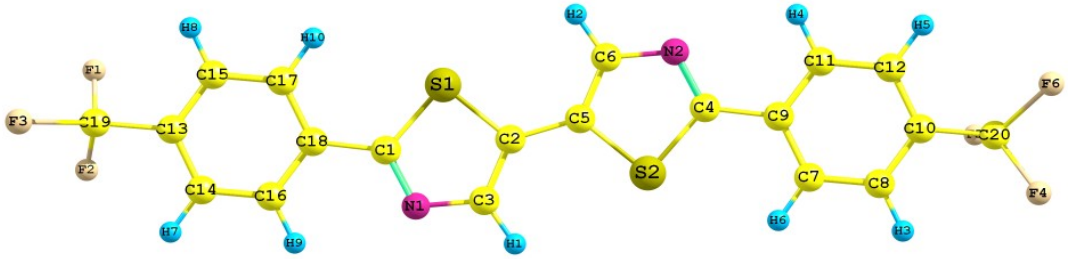
Fig. S1. The optimized structure of thiophene, thiazole and thiazolothiazole based oligomers.



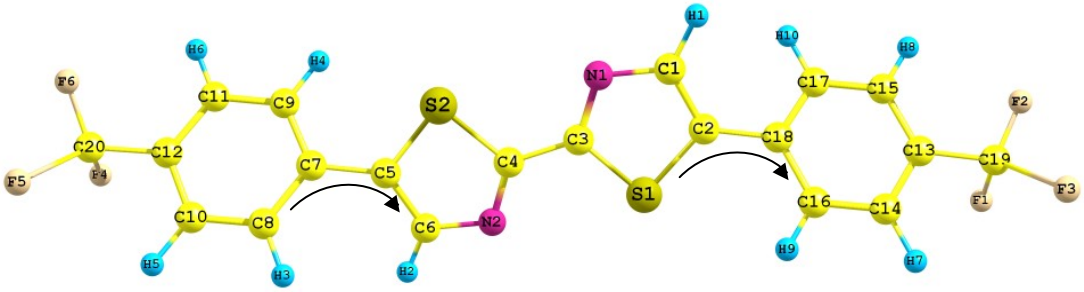
T1



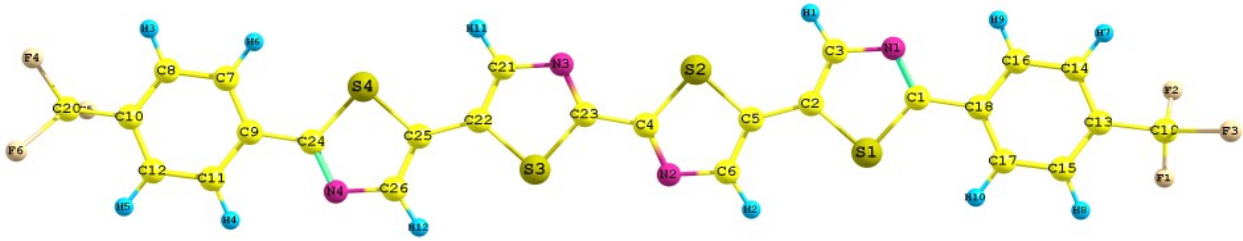
T2



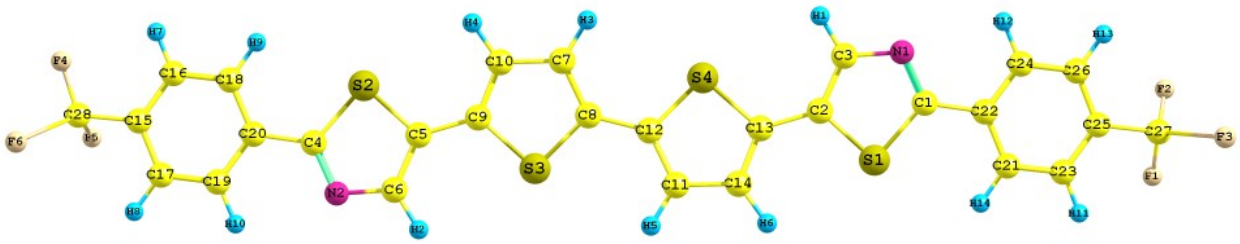
TZ1



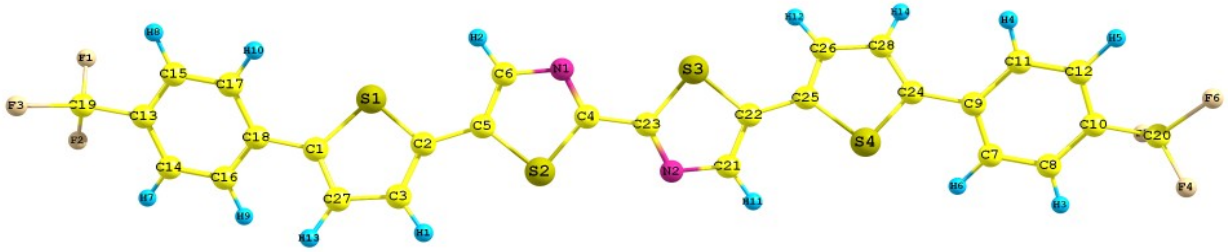
TZ2



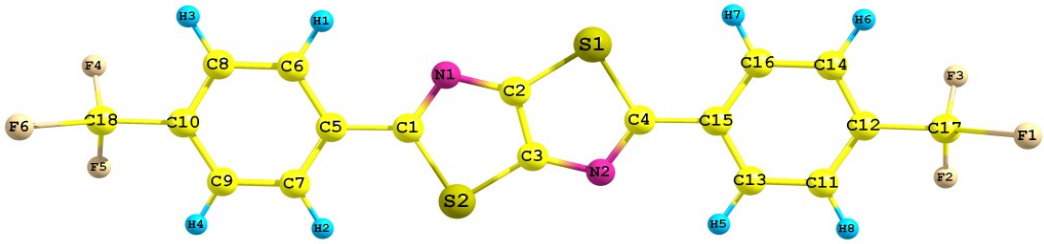
TZ3



TZ4



TZ5



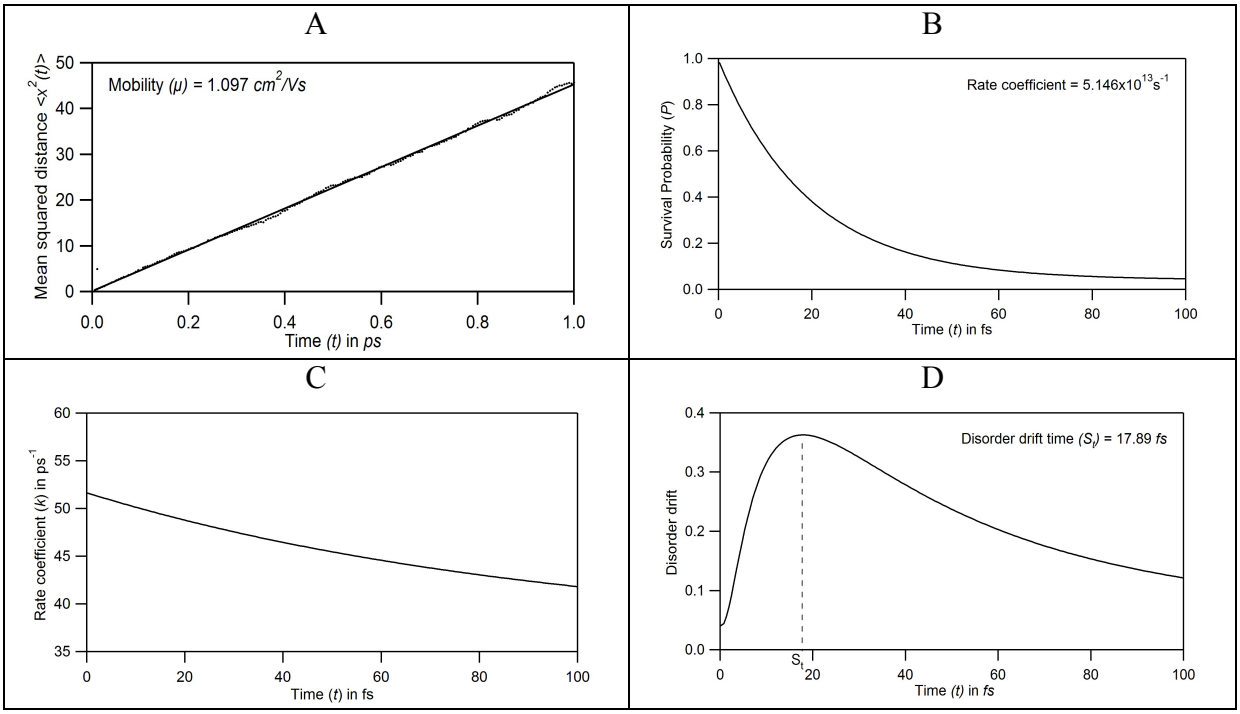
TZTZ1

TZTZ2

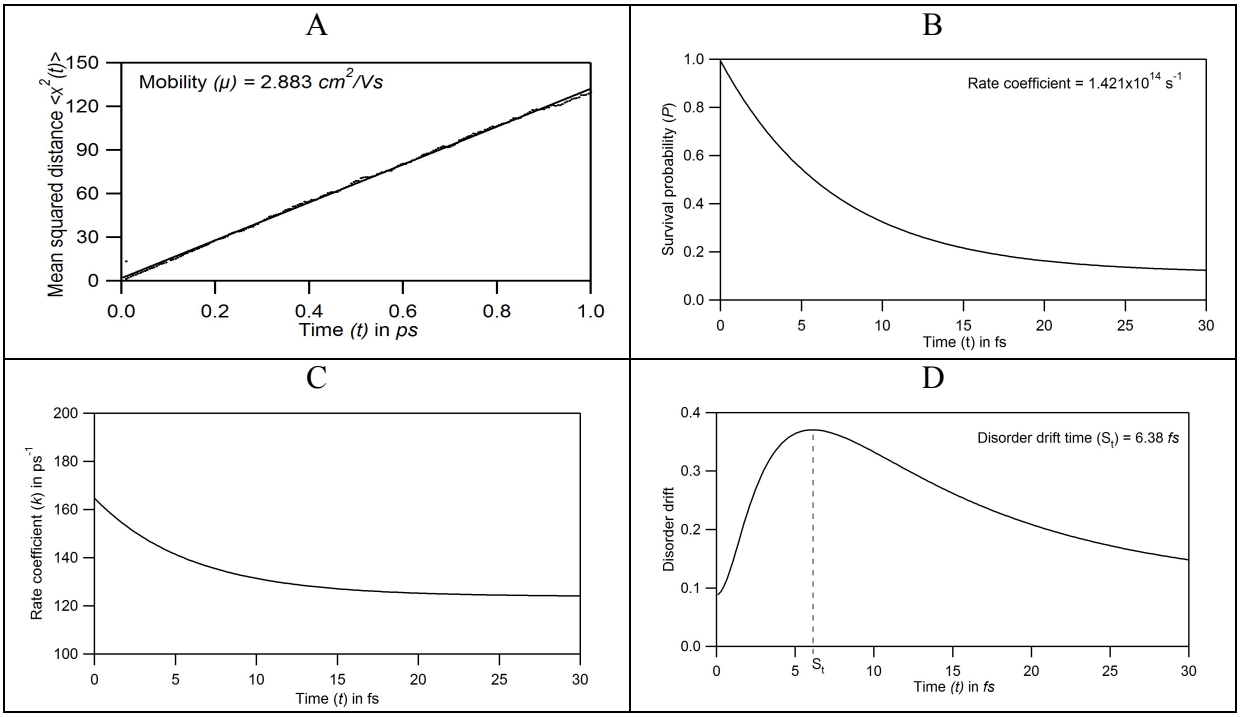
TZTZ3

Fig. S2. (a) A-The mean squared displacement, B-survival probability, C-time dependence of rate coefficient and D-disorder drift with the simulation time for hole transport in the studied thiophene (T1, T2), thiazole (TZ1-TZ5) and thiazolothiazole (TZTZ1-TZTZ3) oligomers.

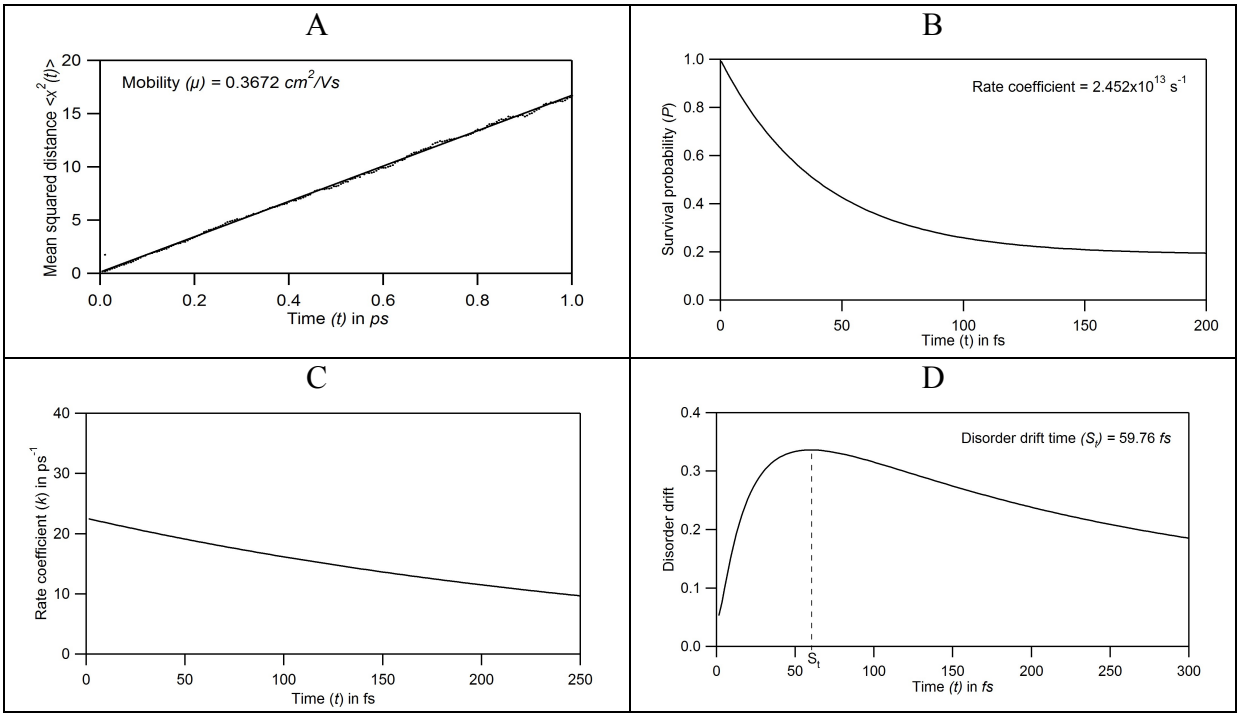
T1



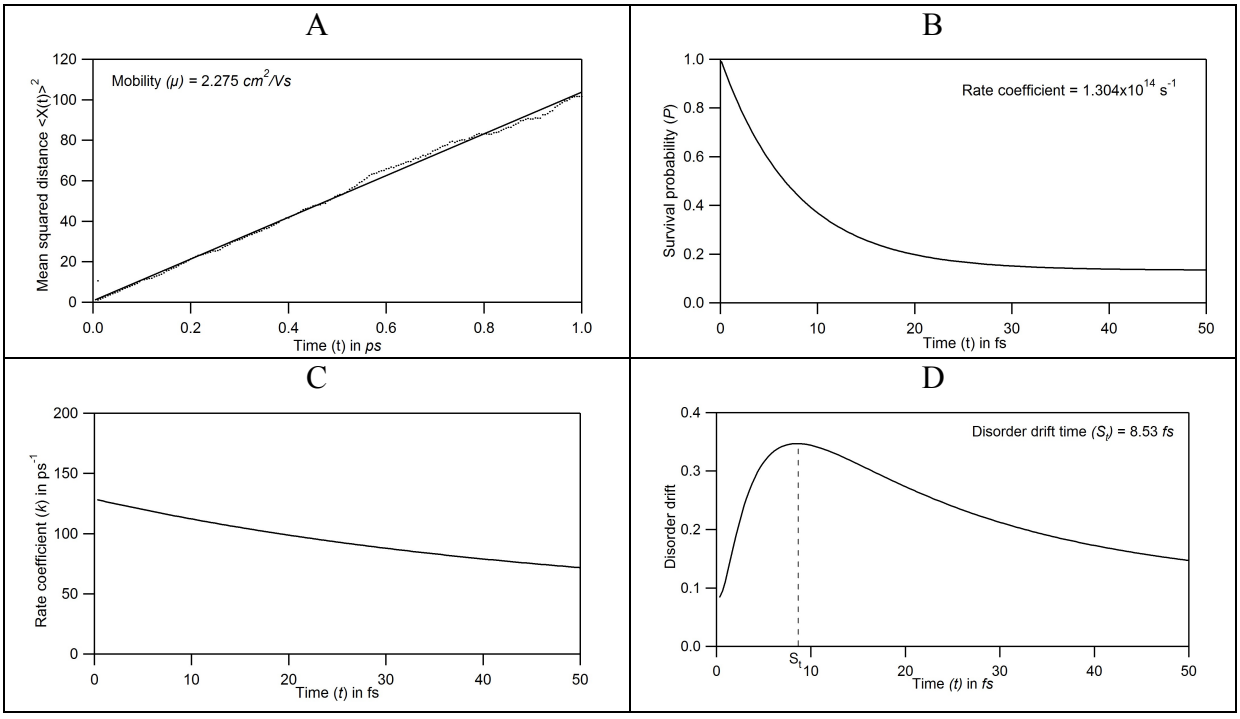
T2



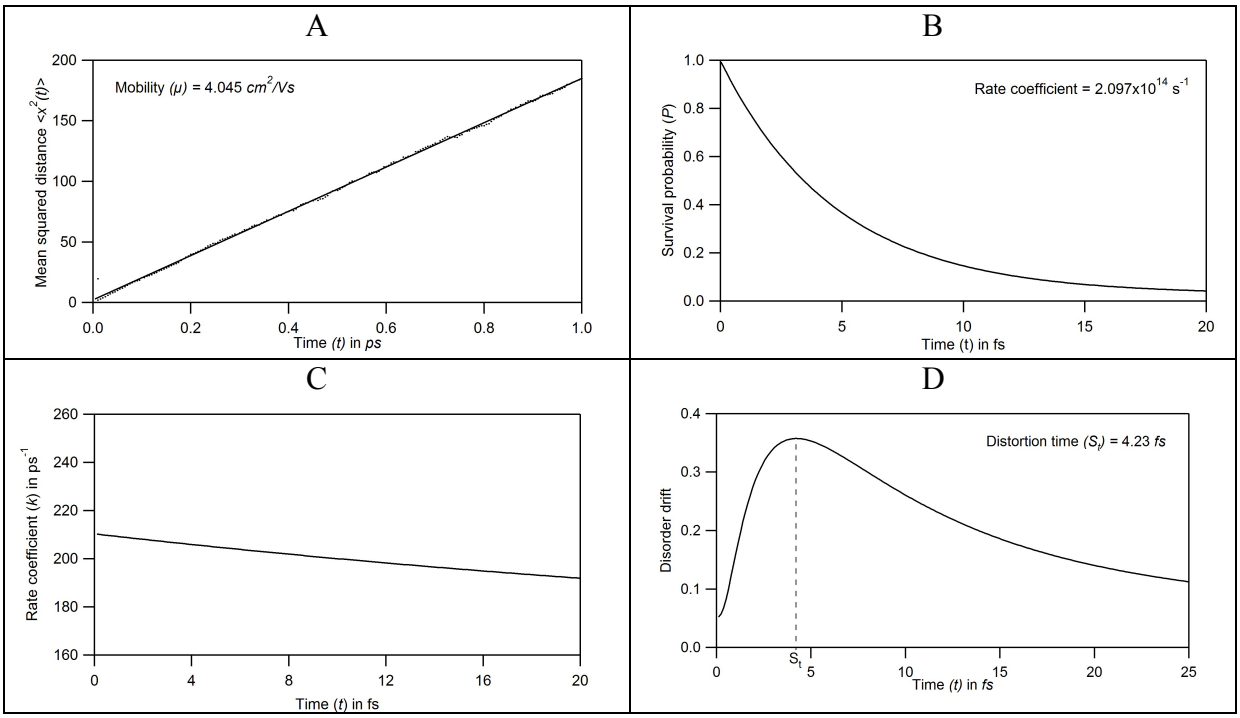
TZ2


A
Mobility (μ) = 0.3672 cm²/Vs
Mean squared distance <x²(t)>
Time (t) in ps
B
Rate coefficient = 2.452x10¹³ s⁻¹
Survival probability (P)
Time (t) in fs
C
Rate coefficient (k) in ps⁻¹
Time (t) in fs
D
Disorder drift time (S_t) = 59.76 fs
Disorder drift
S_t
Time (t) in fs

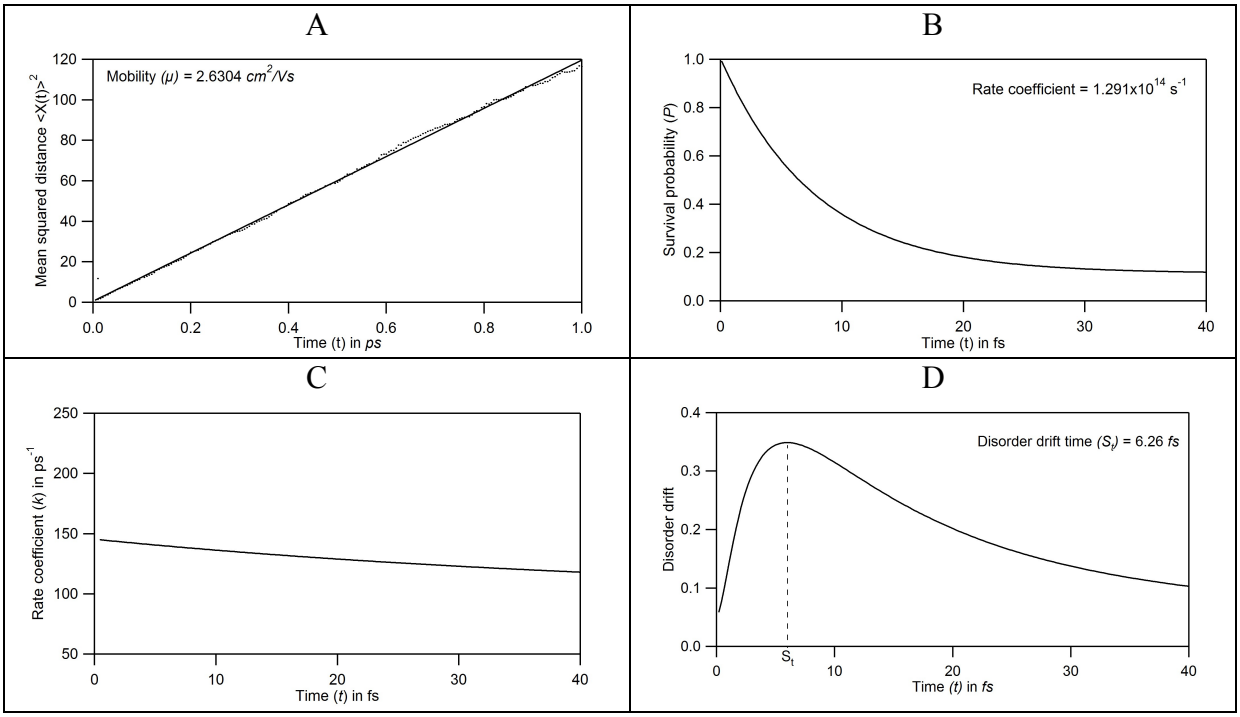
TZ3


A
Mobility (μ) = 2.275 cm²/Vs
Mean squared distance <X(t)>²
Time (t) in ps
B
Rate coefficient = 1.304x10¹⁴ s⁻¹
Survival probability (P)
Time (t) in fs
C
Rate coefficient (k) in ps⁻¹
Time (t) in fs
D
Disorder drift time (S_t) = 8.53 fs
Disorder drift
S_t
Time (t) in fs

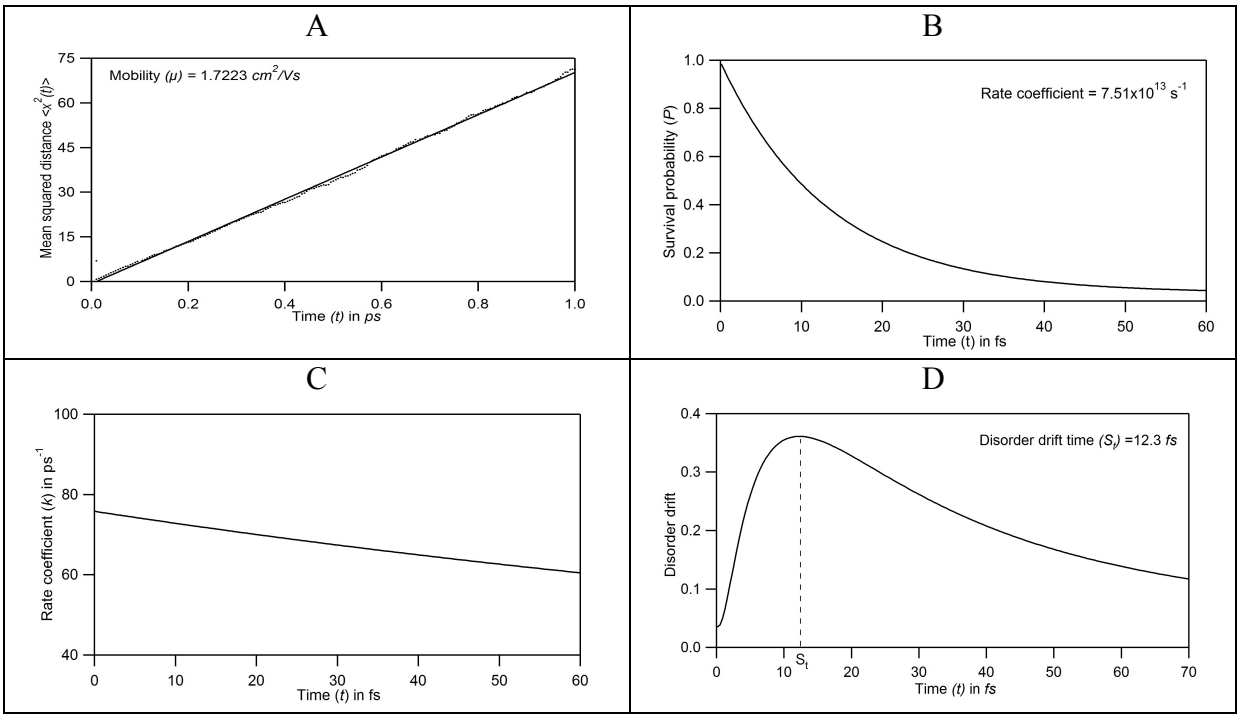
TZ4


A
Mobility (μ) = 4.045 cm²/Vs
Mean squared distance <x²(t)>
Time (t) in ps
B
Rate coefficient = 2.097x10¹⁴ s⁻¹
Survival probability (P)
Time (t) in fs
C
Rate coefficient (k) in ps⁻¹
Time (t) in fs
D
Distortion time (St) = 4.23 fs
Disorder drift
St
Time (t) in fs

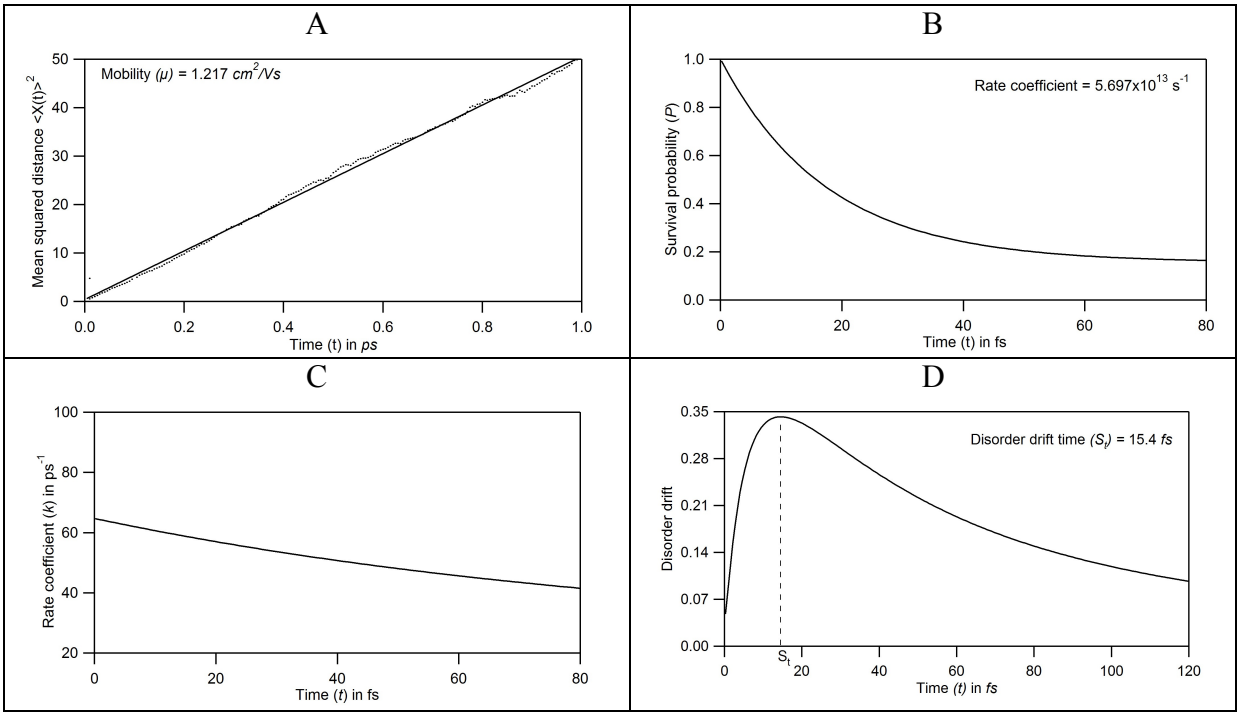
TZ5


A
Mobility (μ) = 2.6304 cm²/Vs
Mean squared distance <X(t)>²
Time (t) in ps
B
Rate coefficient = 1.291x10¹⁴ s⁻¹
Survival probability (P)
Time (t) in fs
C
Rate coefficient (k) in ps⁻¹
Time (t) in fs
D
Disorder drift time (St) = 6.26 fs
Disorder drift
St
Time (t) in fs

TZTZ1


A
Mobility (μ) = 1.7223 cm²/Vs
Mean squared distance <x²(t)>
Time (t) in ps
B
Rate coefficient = 7.51x10¹³ s⁻¹
Survival probability (P)
Time (t) in fs
C
Rate coefficient (k) in ps⁻¹
Time (t) in fs
D
Disorder drift time (S_t) =12.3 fs
Disorder drift
S_t
Time (t) in fs

TZTZ2


A
Mobility (μ) = 1.217 cm²/Vs
Mean squared distance <X(t)>²
Time (t) in ps
B
Rate coefficient = 5.697x10¹³ s⁻¹
Survival probability (P)
Time (t) in fs
C
Rate coefficient (k) in ps⁻¹
Time (t) in fs
D
Disorder drift time (S_t) = 15.4 fs
Disorder drift
S_t
Time (t) in fs

TZTZ3

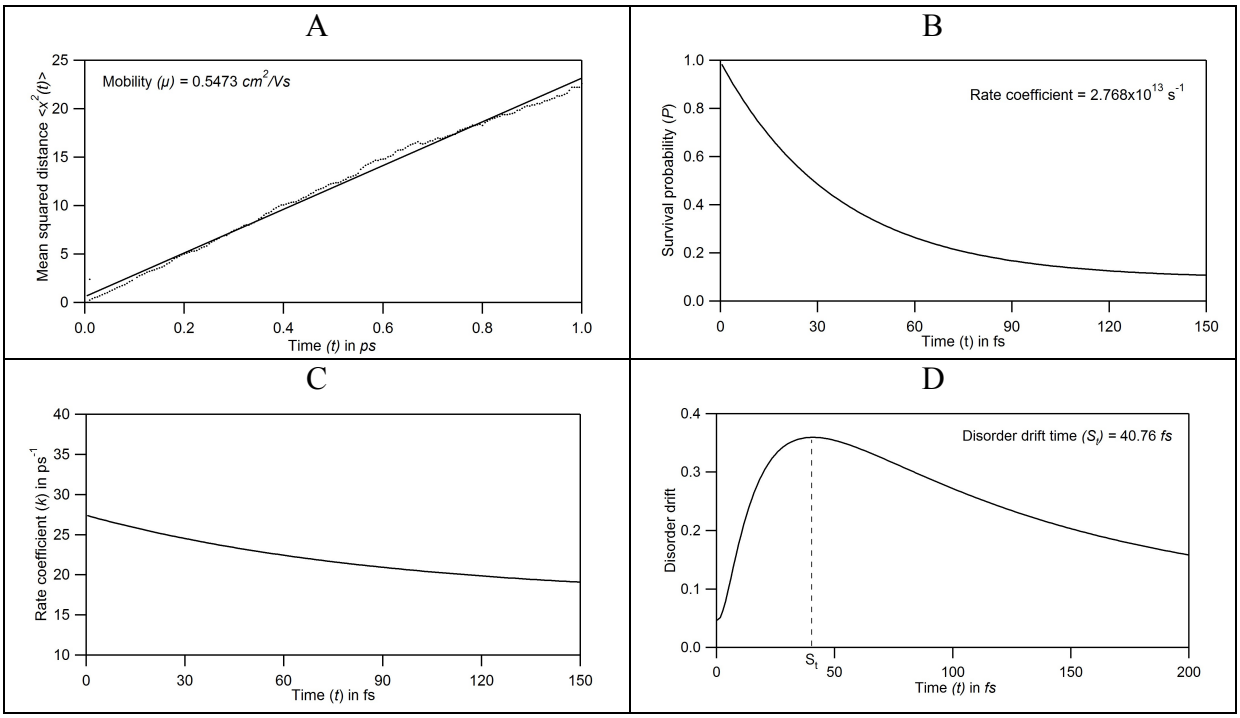
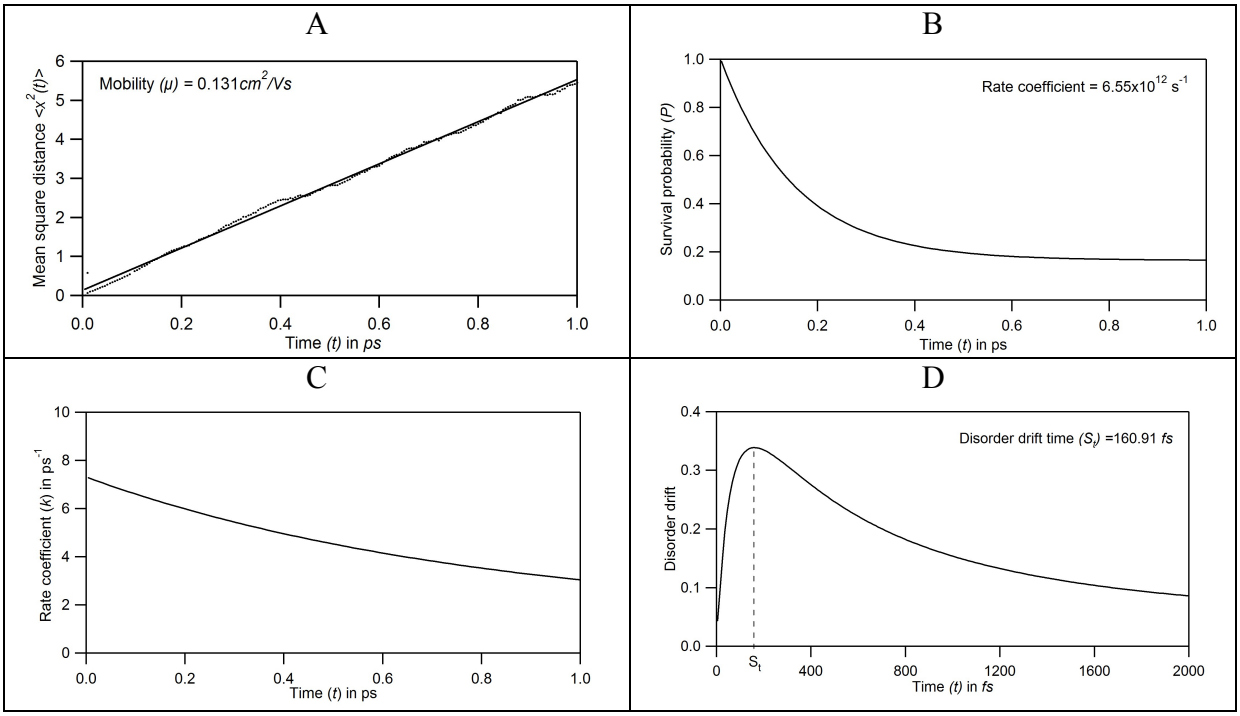
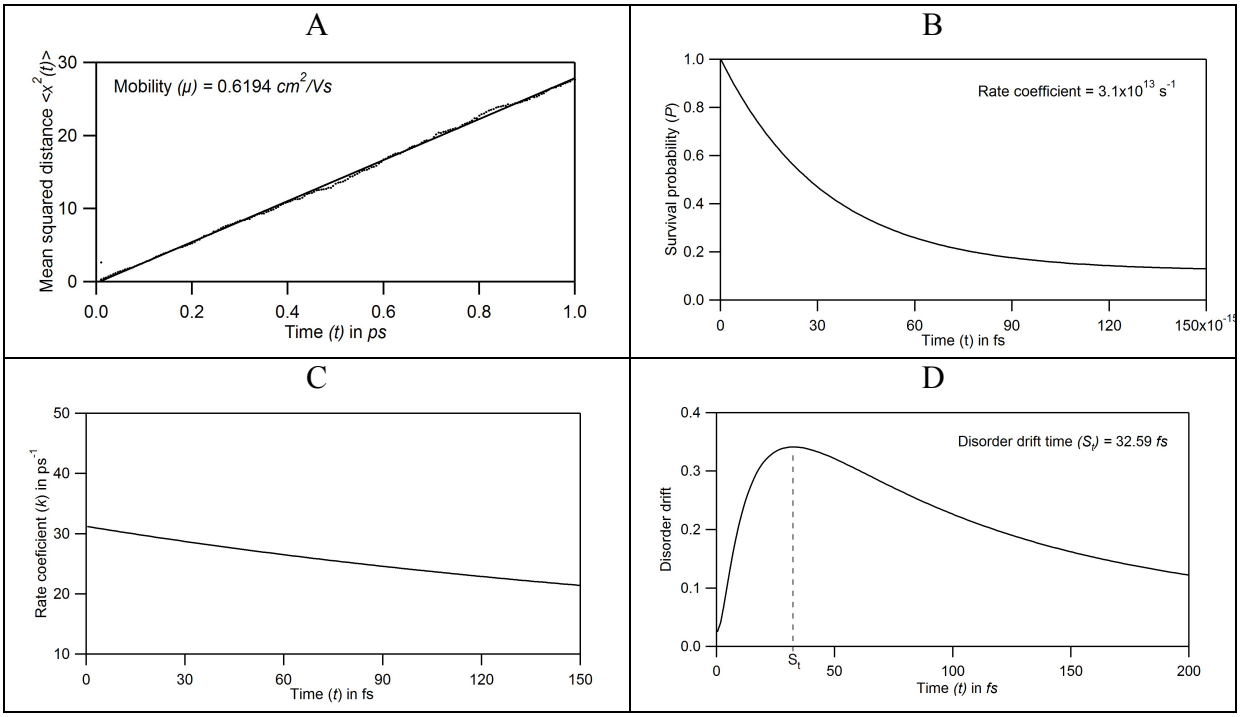

A
Mobility (μ) = 0.5473 cm²/Vs
Mean squared distance <x²(t)>
Time (t) in ps
B
Rate coefficient = 2.768x10¹³ s⁻¹
Survival probability (P)
Time (t) in fs
C
Rate coefficient (k) in ps⁻¹
Time (t) in fs
D
Disorder drift time (S_t) = 40.76 fs
Disorder drift
S_t
Time (t) in fs

Fig. S2. (b) A-The mean squared displacement, B-survival probability, C-time dependence of rate coefficient and D-disorder drift with the simulation time for electron transport in the studied thiophene (T1, T2), thiazole (TZ1-TZ5) and thiazolothiazole (TZTZ1-TZTZ3) oligomers.

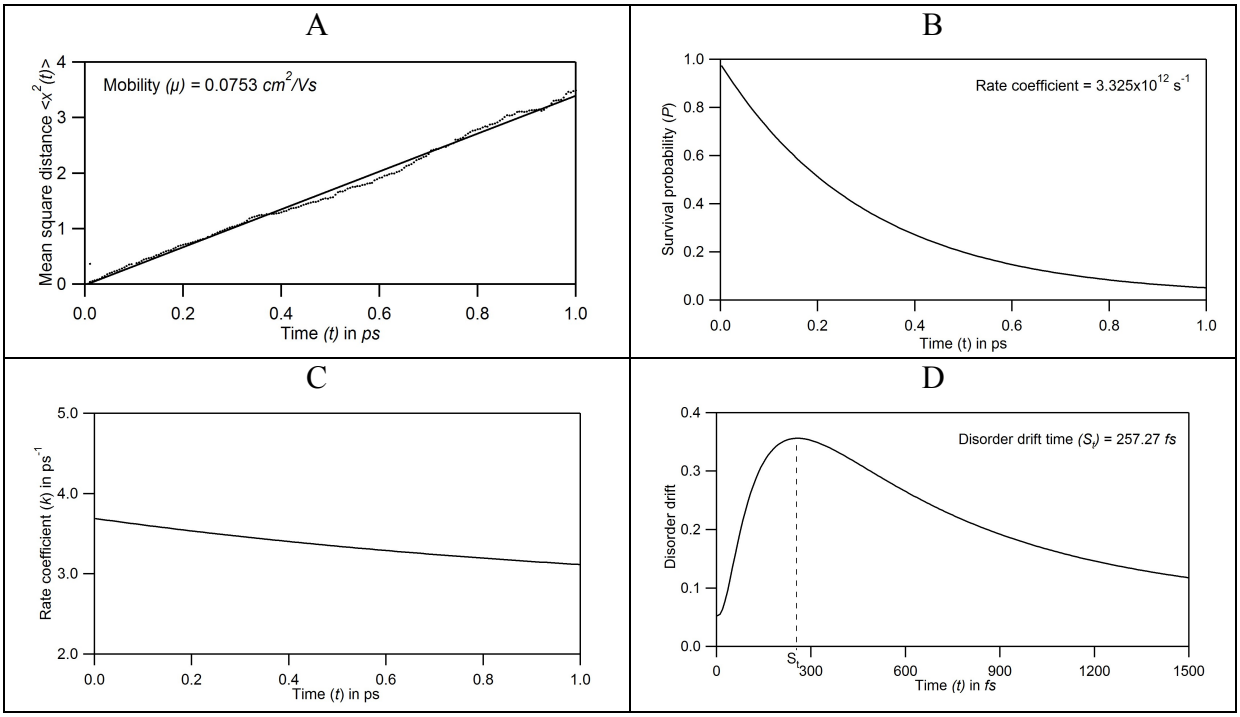
T1



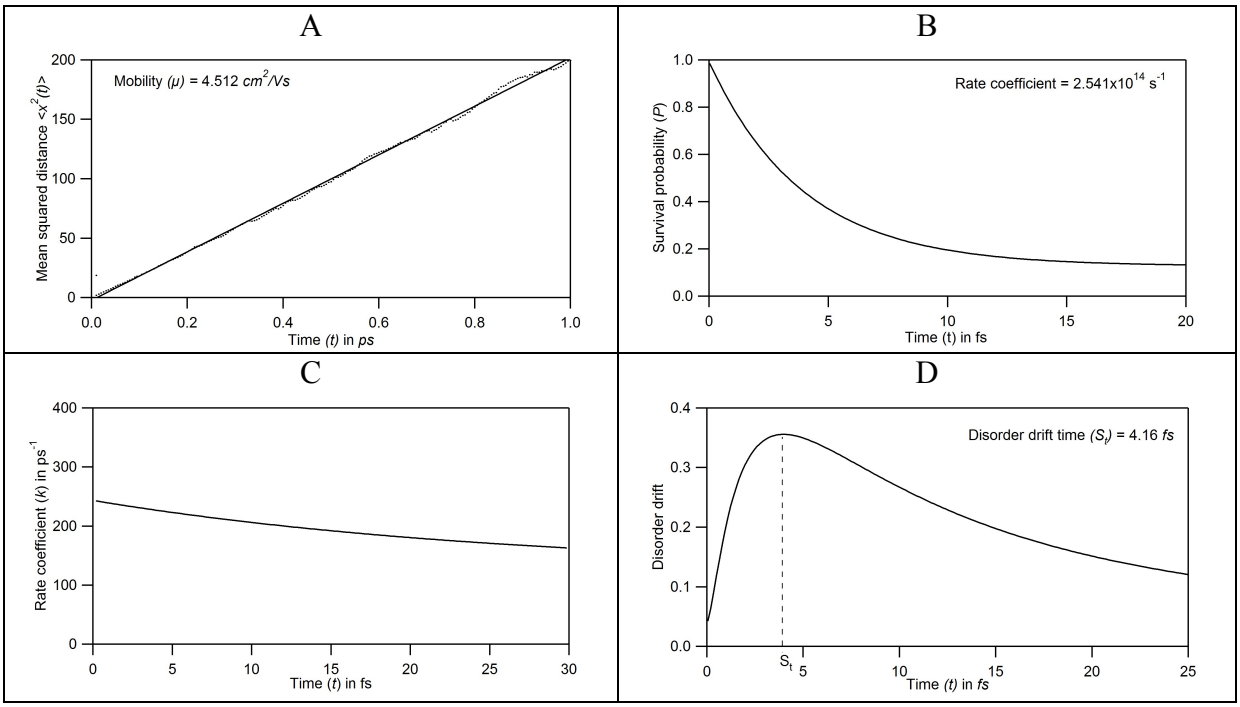
T2



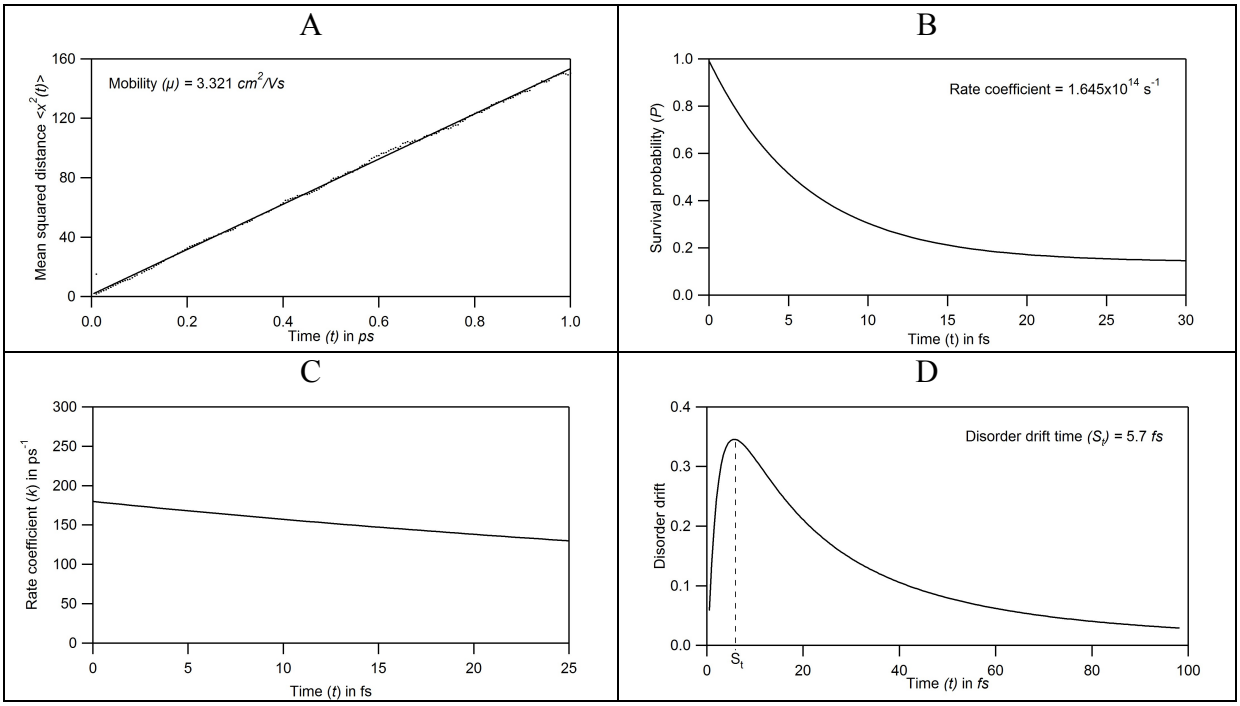
TZ2


A
Mobility (μ) = 0.0753 cm²/Vs
Mean square distance <x²(t)>
Time (t) in ps
B
Rate coefficient = 3.325x10¹² s⁻¹
Survival probability (P)
Time (t) in ps
C
Rate coefficient (k) in ps⁻¹
Time (t) in ps
D
Disorder drift time (S_t) = 257.27 fs
Disorder drift
Time (t) in fs

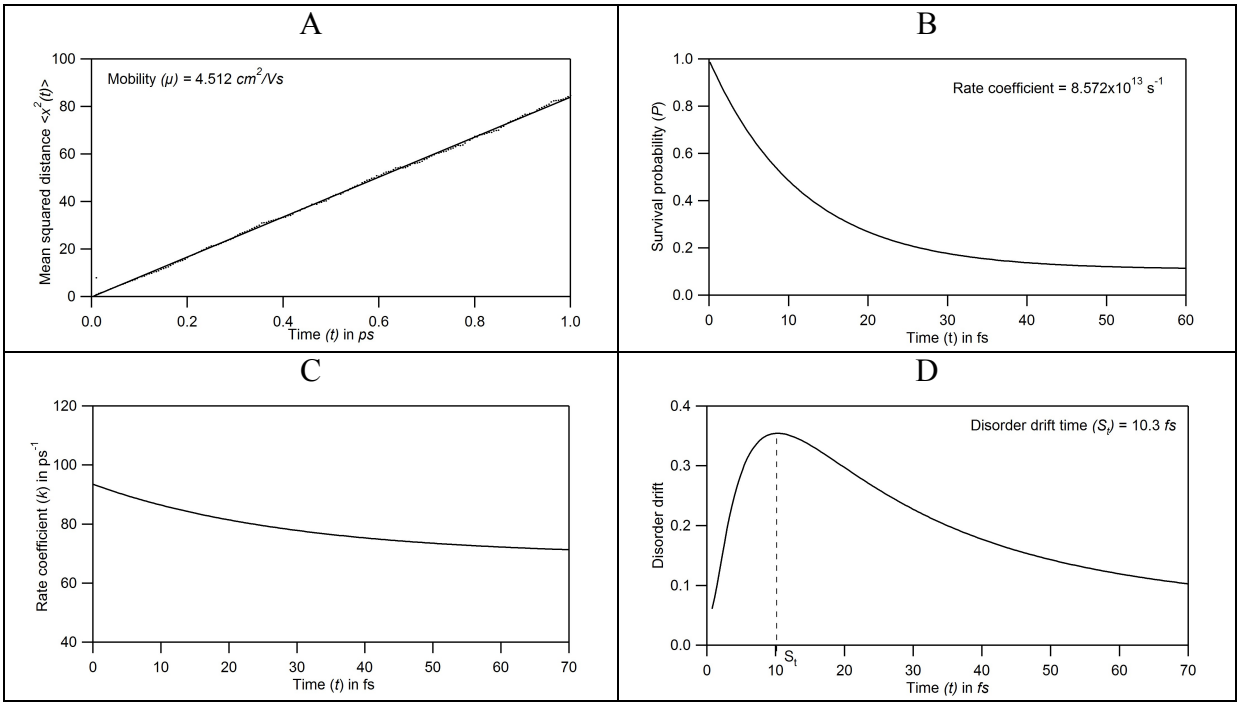
TZ3


A
Mobility (μ) = 4.512 cm²/Vs
Mean squared distance <x²(t)>
Time (t) in ps
B
Rate coefficient = 2.541x10¹⁴ s⁻¹
Survival probability (P)
Time (t) in fs
C
Rate coefficient (k) in ps⁻¹
Time (t) in fs
D
Disorder drift time (S_t) = 4.16 fs
Disorder drift
Time (t) in fs

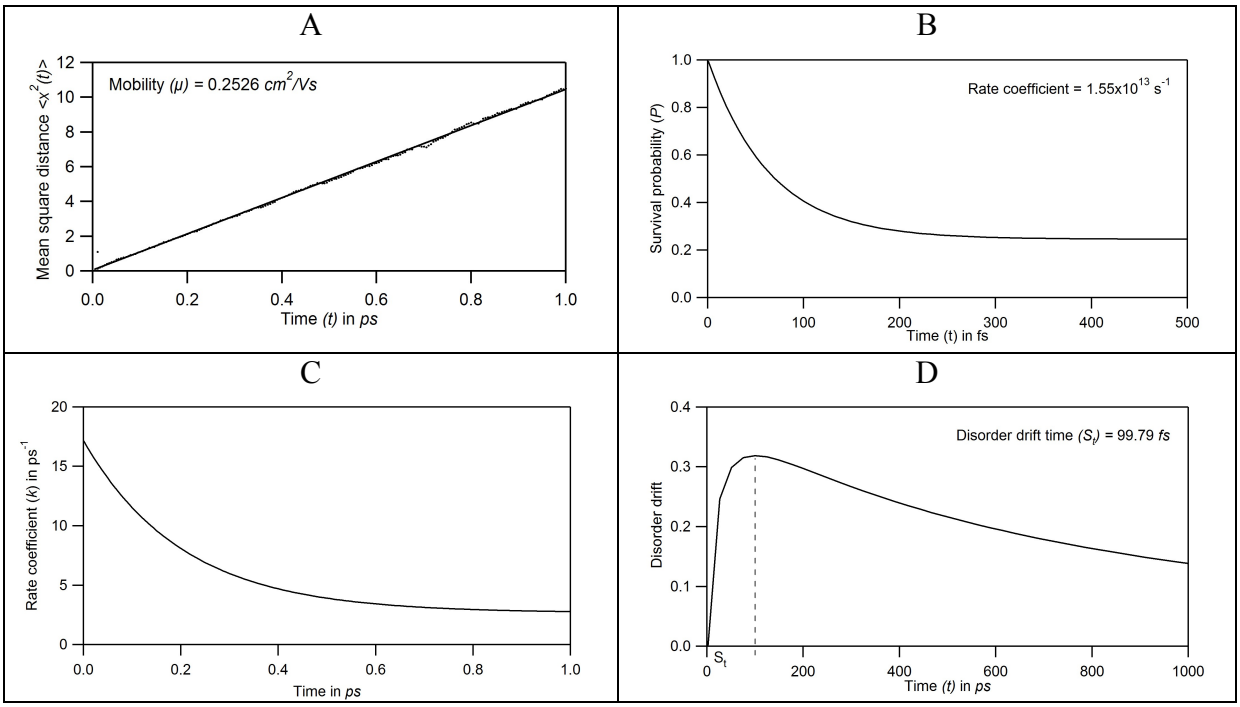
TZ4


A
Mobility (μ) = 3.321 cm²/Vs
Mean squared distance <x²(t)>
Time (t) in ps
B
Rate coefficient = 1.645x10¹⁴ s⁻¹
Survival probability (P)
Time (t) in fs
C
Rate coefficient (k) in ps⁻¹
Time (t) in fs
D
Disorder drift time (St) = 5.7 fs
Disorder drift
St
Time (t) in fs

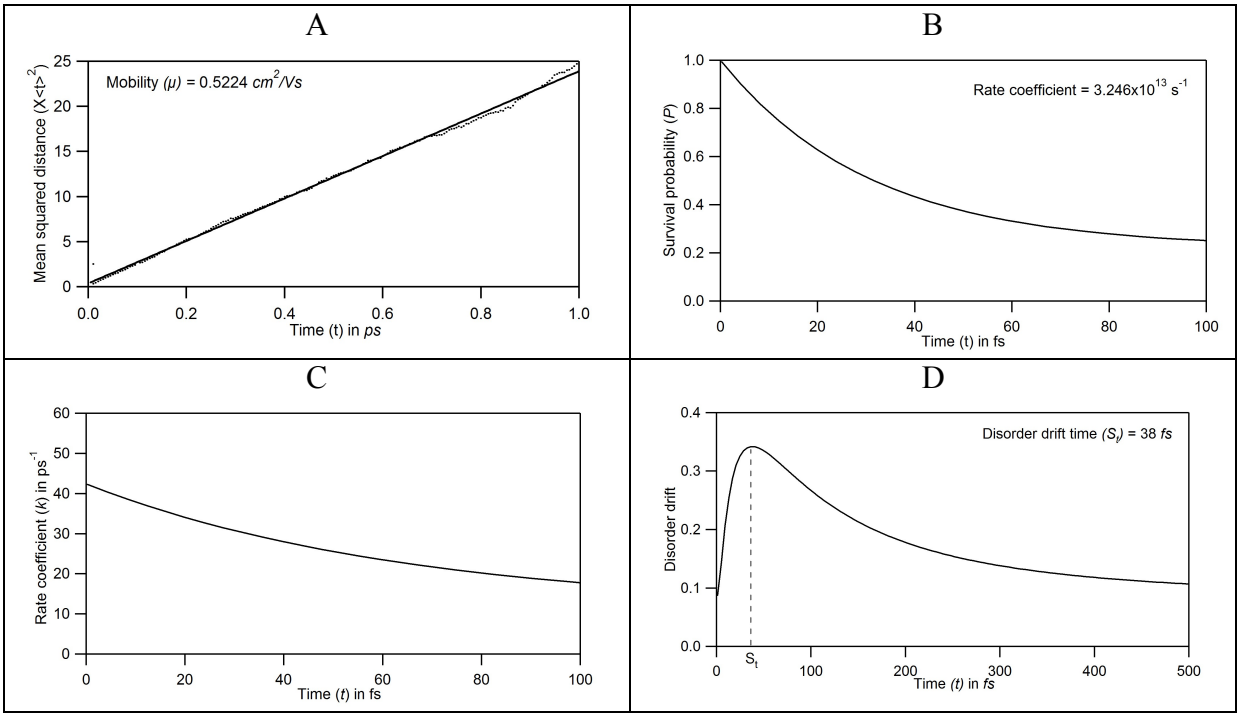
TZ5


A
Mobility (μ) = 4.512 cm²/Vs
Mean squared distance <x²(t)>
Time (t) in ps
B
Rate coefficient = 8.572x10¹³ s⁻¹
Survival probability (P)
Time (t) in fs
C
Rate coefficient (k) in ps⁻¹
Time (t) in fs
D
Disorder drift time (St) = 10.3 fs
Disorder drift
St
Time (t) in fs

TZTZ1


A
Mobility (μ) = 0.2526 cm²/Vs
Mean square distance <x²(t)>
Time (t) in ps
B
Rate coefficient = 1.55x10¹³ s⁻¹
Survival probability (P)
Time (t) in fs
C
Rate coefficient (k) in ps⁻¹
Time in ps
D
Disorder drift time (S_t) = 99.79 fs
Disorder drift
Time (t) in ps

TZTZ2


A
Mobility (μ) = 0.5224 cm²/Vs
Mean squared distance (X<t>²)
Time (t) in ps
B
Rate coefficient = 3.246x10¹³ s⁻¹
Survival probability (P)
Time (t) in fs
C
Rate coefficient (k) in ps⁻¹
Time (t) in fs
D
Disorder drift time (S_t) = 38 fs
Disorder drift
Time (t) in fs

TZTZ3

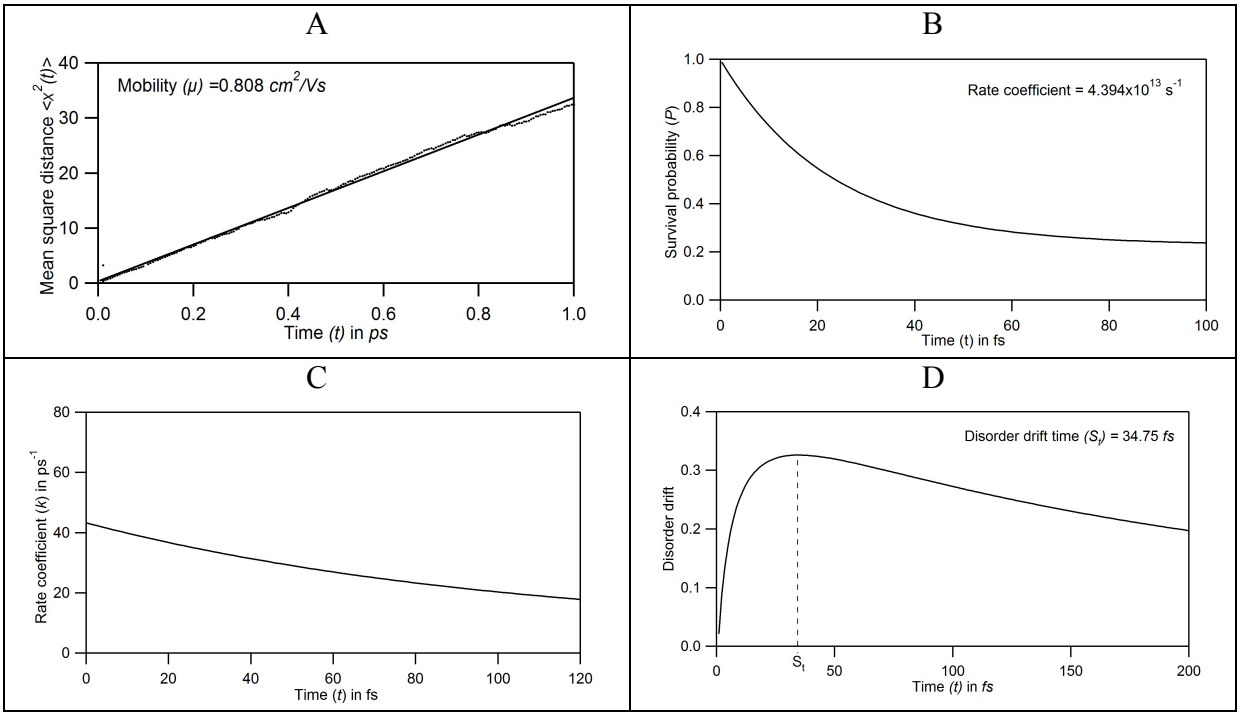

A
Mobility (μ) =0.808 cm²/Vs
Mean square distance <x²(t)>
Time (t) in ps
B
Rate coefficient = 4.394x10¹³ s⁻¹
Survival probability (P)
Time (t) in fs
C
Rate coefficient (k) in ps⁻¹
Time (t) in fs
D
Disorder drift time (S_t) = 34.75 fs
Disorder drift
Time (t) in fs

Table S1: Calculated effective charge transfer integral (J_{eff}, in eV) of the T2, TZ1 and TZTZ2 oligomers using statistical average of orbital potentials (SAOP) exchange correlation functional method for hole transport.

Stacking angle (θ) in deg.	Effective charge transfer integral (J_{eff}) in eV		
	Oligomer T2	Oligomer TZ1	Oligomer TZTZ2
0	0.332	0.326	0.249
15	0.236	0.260	0.175
30	0.098	0.165	0.096
45	0.042	0.088	0.065
60	0.021	0.040	0.045
75	0.018	0.015	0.034
90	0.017	0.0002	0.032

Table S2: Calculated effective charge transfer integral (J_{eff}, in eV) of the T2, TZ1 and TZTZ2 oligomers using statistical average of orbital potentials (SAOP) exchange correlation functional method for electron transport.

Stacking angle (θ) in deg.	Effective charge transfer integral (J_{eff}) in eV		
	Oligomer T2	Oligomer TZ1	Oligomer TZTZ2
0	0.322	0.382	0.273
15	0.155	0.220	0.136
30	0.033	0.089	0.042
45	0.073	0.045	0.005
60	0.128	0.081	0.044
75	0.153	0.138	0.036
90	0.138	0.162	0.002

Table S3. (a) Contribution of HOMO of monomer 1 (M1) and monomer 2 (M2) for charge transfer integral corresponding to hole transport in thiophene (T1, T2) oligomers.

Stacking angle *(θ)* in deg.	Contribution of HOMO of each monomer for charge transfer integral (in %)			
	T1		T2	
	M1	M2	M1	M2
0	50	49	50	49
15	59	40	55	44
30	74	25	67	31
45	86	13	73	25
60	84	14	86	12
75	92	7	92	6
90	93	7	95	4

Table S3. (b) Contribution of HOMO of monomer 1 (M1) and monomer 2 (M2) for charge transfer integral corresponding to hole transport in thiazole (TZ1-TZ5) oligomers**.**

Stacking angle *(θ)* in deg.	Contribution of HOMO of each monomer for charge transfer integral (in %)									
	TZ1		TZ2		TZ3		TZ4		TZ5	
	M1	M2	M1	M2	M1	M2	M1	M2	M1	M2
0	50	50	50	50	50	50	50	50	50	50
15	53	49	50	49	54	45	52	47	53	46
30	58	42	50	48	61	38	55	43	61	38
45	70	30	78	20	81	18	52	47	95	4
60	82	17	90	7	52	48	93	7	94	5
75	85	14	94	3	66	33	97	2	89	10
90	98	1	97	1	99	1	94	3	92	8

Table S3. (c) Contribution of HOMO of monomer 1 (M1) and monomer 2 (M2) for charge transfer integral corresponding to hole transport in thiazolothiazole (TZTZ1-TZTZ3) oligomers**.**

Stacking angle *(θ)* in deg.	Contribution of HOMO of each monomer for charge transfer integral (in %)					
	TZTZ1		TZTZ2		TZTZ3	
	M1	M2	M1	M2	M1	M2
0	52	48	50	49	50	50
15	52	48	51	48	50	49
30	56	43	50	49	60	39
45	62	37	52	47	60	39
60	63	36	61	38	62	37
75	65	34	66	33	61	38
90	51	49	61	38	50	49

Table S4. (a) Contribution of LUMO of monomer 1 (M1) and monomer 2 (M2) for charge transfer integral corresponding to electron transport in thiophene (T1, T2) oligomers.

Stacking angle *(θ)* in *deg.*	Contribution of LUMO of each monomer for charge transfer integral (in %)			
	T1		T2	
	M1	M2	M1	M2
0	51	48	51	48
15	61	38	58	41
30	93	6	80	19
45	85	14	63	37
60	64	36	58	41
75	66	33	63	36
90	68	33	68	31

Table S4. (b) Contribution of LUMO of monomer 1 (M1) and monomer 2 (M2) for charge transfer integral corresponding to electron transport in thiazole (TZ1-TZ5) oligomers**.**

Stacking angle *(θ)* in deg.	Contribution of LUMO of each monomer for charge transfer integral (in %)									
	TZ1		TZ2		TZ3		TZ4		TZ5	
	M1	M2	M1	M2	M1	M2	M1	M2	M1	M2
0	50	50	56	42	50	50	53	44	50	50
15	55	44	50	49	56	42	56	42	52	47
30	73	26	60	39	62	37	59	40	61	38
45	88	11	61	38	59	40	50	49	76	24
60	75	24	54	45	50	49	64	35	65	35
75	60	39	52	47	52	48	66	33	55	44
90	50	49	54	45	50	50	65	33	50	49

Table S4. (c) Contribution of LUMO of monomer 1 (M1) and monomer 2 (M2) for charge transfer integral corresponding to electron transport for thiazolothiazole (TZTZ1-TZTZ3) oligomers.

Stacking angle *(θ)* in deg.	Contribution of LUMO of each monomer for charge transfer Integral (in %)					
	TZTZ1		TZTZ2		TZTZ3	
	M1	M2	M1	M2	M1	M2
0	51	48	50	49	50	50
15	53	46	49	49	52	47
30	76	24	53	46	74	25
45	81	18	94	5	99	1
60	66	33	67	33	65	35
75	64	35	70	30	62	37
90	85	15	87	13	100	0

Table S5. (a) Calculated bond lengths for neutral, cationic and anionic geometries for the studied oligomers.

Molecules	Atomic specification	Bond length in Å		
		Neutral geometry	Cationic geometry	Anionic geometry
T1	F1-C15	1.347	1.342	1.355
	C15-C13	1.502	1.512	1.484
	C13-C11	1.394	1.393	1.402
	C11-C9	1.383	1.381	1.376
	C9-C10	1.404	1.41	1.421
	C10-C2	1.462	1.445	1.429
	C2-S1	1.747	1.742	1.776
	S1-C3	1.747	1.753	1.772
	C3-C7	1.443	1.404	1.405
	C7-C8	1.375	1.405	1.400
	C8-C5	1.411	1.38	1.389
	C5-C6	1.373	1.403	1.394
	C6-C18	1.472	1.445	1.429
T2	F6-C30	1.352	1.347	1.361
	C30-C22	1.502	1.509	1.49
	C22-C20	1.394	1.391	1.400
	C20-C18	1.383	1.384	1.380
	C18-C17	1.404	1.404	1.416
	C17-C14	1.461	1.455	1.440
	C14-C13	1.373	1.389	1.385
	C13-C16	1.410	1.392	1.396
	C16-C15	1.376	1.392	1.394
	C15-C7	1.440	1.414	1.412
	C7-S2	1.750	1.749	1.771
	S2-C6	1.750	1.755	1.771
	C6-C2	1.440	1.407	1.409
TZ1	F1-C19	1.347	1.341	1.355
	C19-C13	1.504	1.514	1.487
	C13-C15	1.391	1.40	1.397
	C15-C17	1.385	1.38	1.38
	C17-C18	1.4	1.408	1.414
	C18-C1	1.463	1.439	1.433
	C1-N1	1.304	1.331	1.324
	N1-C3	1.357	1.323	1.337
	C3-C2	1.374	1.412	1.398
	C2-C5	1.439	1.403	1.407
	C5-S2	1.746	1.746	1.767
	S2-C4	1.762	1.761	1.788
TZ2	F4-C20	1.351	1.344	1.364
	C20-C12	1.503	1.513	1.487
	C12-C10	1.393	1.394	1.4
	C10-C8	1.383	1.38	1.377
	C8-C7	1.404	1.411	1.418

	C7-C5	1.462	1.441	1.433
	C5-C6	1.374	1.415	1.391
	C6-N2	1.358	1.325	1.336
	N2-C4	1.306	1.330	1.335
	C4-C3	1.443	1.406	1.4
	C3-S1	1.749	1.755	1.779
	S1-C2	1.744	1.731	1.771
	C2-C18	1.462	1.441	1.433
TZ3	F4-C20	1.348	1.343	1.352
	C20-C10	1.504	1.511	1.494
	C10-C8	1.391	1.394	1.394
	C8-C7	1.385	1.382	1.383
	C7-C9	1.4	1.403	1.407
	C9-C24	1.463	1.45	1.446
	C24-S4	1.762	1.758	1.777
	S4-C25	1.746	1.748	1.76
	C25-C22	1.439	1.414	1.416
	C22-C21	1.377	1.408	1.39
	C21-N3	1.356	1.328	1.338
	N3-C23	1.306	1.327	1.327
	C23-C4	1.439	1.41	1.407
TZ4	F4-C28	1.346	1.343	1.351
	C28-C15	1.503	1.51	1.492
	C15-C16	1.389	1.391	1.393
	C16-C18	1.387	1.384	1.384
	C18-C20	1.398	1.4	1.407
	C20-C4	1.463	1.452	1.443
	C4-N2	1.304	1.319	1.316
	N2-C6	1.357	1.337	1.343
	C6-C5	1.375	1.393	1.393
	C5-S2	1.746	1.748	1.76
	C5-C9	1.439	1.415	1.414
	C9-S3	1.75	1.749	1.77
	S3-C8	1.75	1.755	1.769
	C8-C12	1.439	1.407	1.411
TZ5	F2-C19	1.348	1.344	1.355
	C19-C13	1.502	1.509	1.491
	C13-C14	1.392	1.392	1.398
	C14-C16	1.385	1.383	1.379
	C16-C18	1.403	1.403	1.414
	C18-C1	1.462	1.453	1.442
	C1-S1	1.747	1.74	1.766
	S1-C2	1.747	1.753	1.763
	C2-C5	1.44	1.414	1.415
	C5-C6	1.377	1.408	1.392
	C6-N1	1.356	1.328	1.337
	N1-C4	1.306	1.327	1.329
	C4-C23	1.439	1.41	1.405

TZTZ1	F4-C18	1.347	1.34	1.356
	C18-C10	1.504	1.515	1.484
	C10-C9	1.392	1.397	1.4
	C9-C7	1.385	1.378	1.379
	C7-C5	1.399	1.411	1.417
	C5-C1	1.462	1.432	1.426
	C1-S2	1.783	1.8	1.809
	S2-C3	1.737	1.724	1.753
	C3-N2	1.348	1.318	1.324
	N2-C4	1.309	1.331	1.336
	C4-C15	1.462	1.432	1.426
TZTZ2	F4-C26	1.352	1.346	1.361
	C26-C16	1.502	1.51	1.49
	C16-C18	1.392	1.392	1.4
	C18-C17	1.384	1.383	1.379
	C17-C15	1.403	1.406	1.416
	C15-C7	1.461	1.451	1.438
	C7-S3	1.746	1.742	1.767
	S3-C6	1.742	1.746	1.757
	C6-C4	1.441	1.409	1.412
	C4-N2	1.313	1.336	1.335
	N2-C3	1.345	1.318	1.326
	C3-S2	1.739	1.733	1.751
	S2-C1	1.783	1.792	1.802
	C1-C11	1.44	1.409	1.412
TZTZ3	H2-C6	1.076	1.077	1.076
	C6-S3	1.727	1.715	1.74
	S3-C7	1.75	1.753	1.764
	C7-C10	1.442	1.423	1.426
	C10-S4	1.748	1.746	1.767
	C10-C9	1.377	1.398	1.387
	C9-C12	1.406	1.384	1.395
	C12-C11	1.376	1.398	1.394
	C11-C1	1.439	1.409	1.411
	C1-N1	1.313	1.335	1.335
	N1-C2	1.345	1.32	1.326
	C2-S1	1.740	1.735	1.753
	C2-C3	1.385	1.418	1.402
	S1-C4	1.785	1.791	1.804
	C4-C14	1.439	1.409	1.411

Table S5. (b) Calculated bond angles for neutral, cationic and anionic geometries for the studied oligomers.

Molecules	Atomic specification	Bond angle *(θ)* in degree		
		Neutral geometry	Cationic geometry	Anionic geometry
T1	C15-C13-C11	119.23	119.71	120.31
	C13-C11-C9	120.16	120.03	120.90
	C9-C10-C2	120.20	120.37	121.60
	C10-C2-C1	128.44	128.00	129.34
	C10-C2-S1	121.57	121.78	121.95
	C4-C3-C7	129.03	128.23	129.42
T2	C30-C22-C20	119.44	120.58	120.07
	C18-C17-C14	120.18	120.06	121.45
	C17-C14-S4	121.76	121.68	121.82
	C16-C15-C7	128.98	128.55	129.21
	C15-C7-S2	120.77	121.57	121.33
	C6-C2-C1	129.08	128.36	129.31
TZ1	C19-C13-C14	119.84	119.60	120.25
	C18-C1-N1	123.92	123.32	124.57
	C1-N1-C3	112.11	112.28	112.85
	C2-C5-S2	122.53	124.10	123.23
TZ2	C20-C12-C11	121.08	119.87	121.01
	C7-C5-C6	128.28	127.58	128.92
	C7-C5-S2	123.05	123.88	123.47
	C4-C3-S1	121.17	121.85	121.53
	N2-C4-C3	124.21	123.55	125.02
	S1-C2-C18	123.02	123.75	123.47
TZ3	C20-C10-C12	119.79	119.61	119.97
	C9-C24-N4	123.99	123.61	124.34
	C25-C22-S3	122.41	123.66	122.95
	S3-C23-C4	121.05	121.78	121.39
	C23-C4-N2	124.35	123.69	124.90
TZ4	C28-C15-C17	118.87	118.66	119.15
	C20-C4-N2	123.97	123.67	124.43
	S2-C5-C9	122.48	123.36	123.04
	C8-C12-C11	129.11	128.35	129.35
TZ5	C19-C13-C15	119.80	119.73	121.05
	C18-C1-C27	128.48	128.07	129.17
	C18-C1-S1	121.52	121.61	121.78
	C2-C5-C6	129.07	127.83	129.16
	N1-C4-C23	124.35	123.72	124.91
	C4-C23-S3	121.11	121.81	121.46
TZTZ1	C18-C10-C8	120.05	119.76	120.69
	C5-C1-S2	121.68	121.71	122.06
	C15-C4-N2	123.49	123.36	124.59
	S1-C2-N1	133.07	133.10	132.84

TZTZ2	C26-C16-C14	120.29	119.55	121.07
	C15-C7-C8	128.50	128.14	129.28
	C15-C7-S3	121.44	121.46	121.74
	C6-C4-N2	122.84	122.35	123.66
	N2-C3-S2	132.89	132.90	132.75
	C1-C11-S4	123.06	123.78	123.16
	C1-C11-C12	126.36	125.63	127.06
TZTZ3	C5-C6-S3	111.68	112.40	111.12
	C7-C10-C9	129.09	128.24	129.54
	C7-C10-S4	120.76	121.36	121.12
	C11-C1-N1	122.90	122.33	123.69
	C11-C1-S2	122.20	122.77	122.55
	S2-C3-N2	132.88	132.90	132.73

Table S5. (c) Calculated dihedral angle *(φ)* in neutral, cationic and anionic geometries of the studied oligomers.

Molecules	Atomic specification of adjacent rings	Torsion angle *(φ)* in degree		
		Neutral geometry	Cationic geometry	Anionic geometry
T1	C9-C10-C2-C1	27.25	1.58	0.27
	C4-C3-C7-S2	21.41	0.17	0.33
	S2-C6-C18-C16	27.02	1.80	0.04
T2	C18-C17-C14-C13	24.52	19.54	0.79
	C16-C15-C7-S2	15.02	2.00	0.12
	S2-C6-C2-C1	22.6	0.86	0.00
	C4-C3-C11-S3	16.75	2.26	0.13
	S3-C10-C27-C25	23.23	21.14	0.6
TZ1	C17-C18-C1-S1	0.365	0.04	0.11
	S1-C2-C5-C6	0.24	0.00	0.02
	N2-C4-C9-C11	0.18	0.19	0.09
TZ2	C8-C7-C5-C6	27.94	0.91	0.4
	N2-C4-C3-S1	0.14	0.10	0.16
	S1-C2-C18-C16	28.46	2.15	0.10
TZ3	C7-C9-C24-S4	0.36	0.18	0.05
	S4-C25-C22-C21	3.19	0.12	0.10
	N3-C23-C4-S2	0.02	0.00	0.01
	S2-C5-C2-C3	3.15	0.14	0.09
	N1-C1-C16-C18	0.13	0.40	0.14
TZ4	C18-C20-C4-S2	2.01	0.02	0.10
	S2-C5-C9-C10	9.76	0.13	0.01
	C7-C8-C12-S4	15.5	0.13	0.05
	S4-C13-C2-C3	13.08	0.39	0.02
	N1-C1-C22-C24	1.44	0.39	0.24
TZ5	C16-C18-C1-C27	24.66	15.16	1.18
	C3-C2-C5-S2	14.75	2.32	0.36
	S2-C4-C23-N2	0.04	0.05	0.01
	C21-C23-C25-S4	15.02	2.54	0.45

	S4-C24-C9-C7	25.06	15.24	0.94
TZTZ1	C7-C5-C1-S2	2.04	0.42	0.78
	C1-S2-C3-N2	0.23	0.21	0.14
	N2-C4-C15-C13	1.37	0.16	0.42
TZTZ2	C17-C15-C7-C8	22.93	12.33	0.06
	C5-C6-C4-N2	0.62	0.53	0.03
	C4-N2-C3-S2	0.12	0.14	0.00
	S2-C1-C11-S4	1.62	0.65	0.05
	S4-C10-C21-C19	21.9	13.45	0.13
TZTZ3	C8-C7-C10-S4	18.0	0.01	0.01
	S4-C11-C1-S2	2.78	0.00	0.00
	C1-S2-C3-N2	0.02	0.00	0.00
	N2-C4-C14-C13	2.30	0.00	0.00
	C16-C15-C18-S6	17.96	0.02	0.01

Table S6. Calculated hole mobility *(μ)* at different stacking angles *(θ)* for thiophene (T1, T2), thiazole (TZ1-TZ5) and thiazolothiazole (TZTZ1-TZTZ3) oligomers.

Stacking angle (θ) in degree	Mobility *(μ)* in cm^2/Vs									
	Thiophene derivatives		Thiazole derivatives					Thiazolothiazole derivatives		
	T1	T2	TZ1	TZ2	TZ3	TZ4	TZ5	TZTZ1	TZTZ2	TZTZ3
0	2.753	7.518	5.203	3.113	7.647	8.442	8.944	3.945	4.069	4.308
15	1.433	3.775	3.279	1.675	3.203	4.077	3.616	2.803	1.901	1.624
30	0.443	0.638	1.284	0.437	0.490	1.255	0.468	1.413	0.565	0.315
45	0.096	0.110	0.352	0.025	0.010	0.179	0.014	0.688	0.243	0.131
60	0.059	0.026	0.070	0.001	0.013	0.005	0.011	0.530	0.200	0.120
75	0.027	0.018	0.010	0.001	0.010	0.007	0.009	0.142	0.066	0.041
90	0.027	0.015	0.000	0.0002	0.000	0.018	0.000	0.103	0.054	0.037

Table S7. Calculated electron mobility *(μ)* at different stacking angles *(θ)* for thiophene (T1, T2), thiazole (TZ1-TZ5) and thiazolothiazole (TZTZ1-TZTZ3) oligomers.

Stacking angle (θ) in degree	Mobility *(μ)* in cm^2/Vs									
	Thiophene derivatives		Thiazole derivatives					Thiazolothiazole derivatives		
	T1	T2	TZ1	TZ2	TZ3	TZ4	TZ5	TZTZ1	TZTZ2	TZTZ3
0	0.558	3.437	9.197	0.755	23.44	15.686	5.616	3.338	4.424	13.951
15	0.205	0.862	3.071	0.260	5.502	2.637	2.185	1.267	1.064	3.698
30	0.009	0.042	0.507	0.074	1.560	2.186	0.600	0.070	0.136	0.258
45	0.051	0.174	0.137	0.065	0.512	0.629	0.116	0.081	0.0005	0.003
60	0.404	0.554	0.454	0.191	0.938	0.189	0.280	0.506	0.230	0.629
75	0.258	0.792	1.329	0.337	2.367	1.105	0.771	0.170	0.067	0.238
90	0.230	0.667	1.794	0.340	3.212	1.920	1.026	0.000	0.002	0.000

Table S8. Site energy difference (Δε) at different stacking angles for hole transport in thiophene (T1, T2), thiazole (TZ1-TZ5) and thiazolothiazole (TZTZ1-TZTZ3) oligomers.

Stacking angle (θ) in deg.	Thiophene derivatives		Thiazole derivatives					Thiazolothiazole derivatives		
	T1	T2	TZ1	TZ2	TZ3	TZ4	TZ5	TZTZ1	TZTZ2	TZTZ3
0	0.005	0.004	0.002	0.072	0.002	0.052	0.001	0.114	0.004	0
15	0.062	0.046	0.051	0.001	0.047	0.038	0.026	0.026	0.002	0.006
30	0.104	0.050	0.083	0.029	0.049	0.042	0.051	0.054	0.011	0.046
45	0.106	0.037	0.104	0.057	0.017	0.004	0.081	0.069	0.017	0.032
60	0.073	0.040	0.081	0.042	0.002	0.023	0.055	0.043	0.038	0.032
75	0.095	0.055	0.042	0.035	0.005	0.034	0.018	0.036	0.025	0.015
90	0.084	0.062	0.002	0.030	0.004	0.048	0.001	0	0.014	0

Table S9. Site energy difference (Δε) at different stacking angles for electron transport in thiophene (T1, T2), thiazole (TZ1-TZ5) and thiazolothiazole (TZTZ1-TZTZ3) oligomers.

Stacking angle (θ) in deg.	Thiophene derivatives		Thiazole derivatives					Thiazolothiazole derivatives		
	T1	T2	TZ1	TZ2	TZ3	TZ4	TZ5	TZTZ1	TZTZ2	TZTZ3
0	0.015	0.023	0.001	0.036	0.001	0.040	0	0.008	0.006	0
15	0.073	0.055	0.028	0.022	0.056	0.031	0.006	0.017	0.006	0.007
30	0.104	0.060	0.059	0.027	0.077	0.044	0.010	0.041	0.001	0.039
45	0.099	0.040	0.084	0.026	0.049	0.006	0.031	0.047	0.003	0.025
60	0.080	0.048	0.081	0.031	0.024	0.043	0.021	0.061	0.017	0.021
75	0.102	0.079	0.046	0.016	0.011	0.064	0.075	0.030	0.015	0.011
90	0.105	0.101	0.001	0.021	0.021	0.078	0.001	0.002	0.012	0