Supplementary Information

Enriching NLO Efficacy *via* Designing of Non-Fullerene Molecules with Modification of Acceptor Moieties into ICIF2F: An Emerging Theoretical Approach

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Table S1: Wave length, excitation energy and oscillator strength of reference compound (**NFAR1**) and investigated compound (**NFAD2-NFAD6**).

Compounds	λ (*nm*)	E (*eV*)	*f*	MO contributions
NFAR1	704.336	1.760	2.645	H→L (95%), H-1→L+1 (3%)
	555.137	2.233	0.216	H→L+1 (92%), H-1→L (2%)
	500.542	2.477	0.066	H-1→L (84%), H→L+1 (3%), H→L+2 (8%)
	496.354	2.498	0.024	H→L+2 (80%), H-1→L (9%), H-1→L+2 (4%)
	451.689	2.745	0.147	H→L+3 (84%), H-1→L+2 (2%), H-1→L+3 (6%)
	433.360	2.861	0.171	H-1→L+1 (87%), H→L (4%)
NFAD2	797.069	1.556	1.588	H→L (94%), H-1→LUMO (4%)
	597.313	2.076	0.500	H-1→L (89%), H-2→L (3%), H→L (5%)
	562.414	2.205	0.091	H-1→L+1 (11%), H→L+1 (85%)
	473.819	2.617	0.212	H→L+2 (82%), H-2→L (2%), H-1→L+1 (3%), H-1→L+2 (8%)

	461.302	2.688	0.017	H-1→L+1 (76%), H→L+1(12%), H-2→L+1 (6%), H→L+2 (3%)
	457.388	2.711	0.080	H-2→L (90%), H-1→L (2%), H→L+2 (3%)
NFAD3	810.301	1.530	1.578	H→L (95%), H-1→L (4%)
	605.658	2.047	0.525	H-1→L (89%), H-2→L (3%), H→L (5%)
	573.921	2.160	0.096	H-1→L+1 (10%) H→L+1 (86%), H-1→L (2%)
	474.272	2.614	0.175	H→L+2 (74%), H-2→L (5%), H-1→L+1 (8%), H-1→L+2 (7%)
	468.236	2.648	0.030	H-1→L+1 (72%) H→L+1 (11%) H-2→L+1 (5%), H→L+2 (8%)
	462.145	2.683	0.099	H-2→L (87%), H→L+2 (7%)
NFAD4	946.155	1.310	1.325	H→L (96%), H-1→L (3%)
	787.852	1.574	0.306	H→L+1 (92%), H-1→L+1 (7%)
	676.474	1.833	0.479	H-1→L (91%), H-2→L (3%), H→L (3%)
	594.563	2.085	0.124	H-1→L+1 (86%), H-2→L+1 (5%), H→L+1 (8%)
	562.899	2.203	0.307	H→L+2 (90%), H-1→L (3%), H-1→L+2 (5%)
	499.051	2.484	0.047	H-2→L (91%), H-1→L (2%)
NFAD5	936.861	1.323	0.872	H→L (95%), H-1→L (4%)
	864.785	1.434	0.716	H→L+1 (94%), H-1→L+1 (5%)
	673.864	1.840	0.294	H-1→L (89%), H-2→L (4%), H→L (4%)
	633.574	1.957	0.374	H-1→L+1 (87%), H-2→L+1 (4%), H→L+1 (5%)
	574.027	2.160	0.208	H→L+2 (90%), H-1→L+2 (4%)
	511.043	2.426	0.015	H→L+3 (86%), H-1→L+3 (4%), H→L+4 (6%)
NFAD6	868.662	1.427	1.533	H→L (96%), H-1→L (3%)
	653.822	1.896	0.243	H→L+1 (87%), H-1→L+1 (9%)
	635.230	1.952	0.440	H-1→L (90%), H-2→L (3%), H→L (3%), H→L+1 (2%)
	518.134	2.393	0.038	H-1→L+1 (83%), H→L+1 (10%), H-2→L+1 (5%)
	507.945	2.441	0.249	H→L+2 (88%), H-1→L (2%), H-1→L+2 (6%)
	479.982	2.583	0.066	H-2→L (91%), H-1→L (2%), H→L+2 (2%)

Table S2: Natural bond orbital (NBO) analysis of investigated compound **NFAR1**-NBO by using M06 6-311G(d,p).

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)[a]**	**E(J)E(i)[b](a.u)**	**F(I,j)[c](a.u)**
C14-C15	π	C39-C47	π*	31.09	0.31	0.088
C61-C63	π	C74-C82	π*	29.1	0.33	0.087
C74-C82	π	C89-C90	π*	26.89	0.30	0.08
C42-C43	π	C44-C45	π*	20.76	0.30	0.072
C3-C4	π	C7-C18	π*	19.33	0.32	0.072
C60-C95	π	C62-C64	π*	14.97	0.32	0.067
C54-C55	π	C41-C46	π*	8.83	0.33	0.05
C87-O88	π	C74-C82	π*	3.65	0.43	0.038
C62-C64	π	C62-C64	π*	1.81	0.29	0.021
C12-C13	π	C12-C13	π*	0.97	0.30	0.016
C91-N92	π	C93-N94	π*	0.69	0.47	0.016
C74-H75	σ	C63-S65	σ*	10.37	0.72	0.077
C39-H40	σ	C14-S36	σ*	10.25	0.71	0.076
C90-C93	σ	C93-N94	σ*	8.21	1.61	0.103

C14-C15	σ	C9-C13	σ*	7.16	1.16	0.082
C14-C39	σ	C39-C47	σ*	6.56	1.35	0.084
C89-C90	σ	C90-C93	σ*	6.09	1.27	0.079
C1-C64	σ	C62-C64	σ*	5.95	1.29	0.079
C41-C54	σ	C54-C55	σ*	3.71	1.26	0.061
C5-C24	σ	C20-H23	σ*	1.66	1.01	0.037
C5-C24	σ	C6-C7	σ*	1.11	1.17	0.032
C5-C20	σ	C3-C4	σ*	0.92	1.19	0.03
C63-C74	σ	C63-S65	σ*	0.62	0.93	0.021
C14-S36	σ	C14-C39	σ*	0.50	1.21	0.022
O69	LP(2)	C67-O68	π*	49.01	0.37	0.121
S66	LP(2)	C61-C63	π*	32.64	0.24	0.084
S37	LP(2)	C3-C4	π*	27.16	0.28	0.079
S36	LP(2)	C14-C15	π*	22.64	0.26	0.069
S66	LP(2)	C60-C95	π*	21.56	0.27	0.068
F86	LP(3)	C79-C80	π*	20.69	0.44	0.093
O68	LP(2)	C67-O69	σ*	34.23	0.66	0.136
O88	LP(2)	C76-C87	σ*	21.31	0.76	0.115
N94	LP(1)	C90-C93	σ*	12.63	1.04	0.103
O69	LP(2)	C70-H72	σ*	4.89	0.72	0.056
S37	LP(1)	C4-C7	σ*	0.95	1.19	0.030
S65	LP(1)	C63-C74	σ*	0.51	1.22	0.022

Table S3: Natural bond orbital (NBO) analysis of investigated compound **NFAD2**-NBO by using M06 6-311G(d,p).

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)[a]**	**E(J)E(i)[b](a.u)**	**F(I,j)[c](a.u)**
C48-C50	π	C61-C69	π*	30.51	0.32	0.089
C41-C42	π	C39-C40	π*	28.44	0.30	0.082
C39-C40	π	C43-C84	π*	24.44	0.30	0.077
C1-C2	π	C49-C51	π*	21.93	0.28	0.075
C66-C67	π	C63-C68	π*	20.97	0.33	0.075
C10-C11	π	C12-C13	π*	15.51	0.29	0.061
C49-C51	π	C1-C2	π*	12.85	0.30	0.056
C76-C77	π	C61-C69	π*	8.06	0.33	0.047
C54-O55	π	C47-C82	π*	3.52	0.41	0.037
C78-N79	π	C80-N81	π*	0.71	0.47	0.016
C61-H62	σ	C50-S52	σ*	10.61	0.72	0.078
C77-C78	σ	C78-N79	σ*	8.21	1.61	0.103
C6-C7	σ	C4-S37	σ*	7.67	0.90	0.074
C47-S53	σ	C82-F83	σ*	6.62	0.95	0.071
C47-C82	σ	C49-C51	σ*	5.05	1.31	0.073

C10-C18	σ	C7-C18	σ*	4.96	1.29	0.072
C67-C68	σ	C66-C67	σ*	3.82	1.27	0.063
C42-N86	σ	C41-C42	σ*	2.35	1.38	0.051
C10-C11	σ	C9-C10	σ*	2.27	1.11	0.045
C48-S53	σ	C48-C50	σ*	1.75	1.24	0.042
C67-F72	σ	C63-C68	σ*	1.11	1.68	0.039
C14-S36	σ	C9-C13	σ*	0.52	1.11	0.022
N86	LP(1)	C41-C42	π*	48.70	0.29	0.109
O56	LP(2)	C54-O55	π*	48.64	0.37	0.121
S53	LP(2)	C48-C50	π*	32.63	0.24	0.084
S52	LP(2)	C49-C51	π*	28.74	0.26	0.079
S37	LP(2)	C1-C2	π*	22.23	0.27	0.069
F73	LP(3)	C66-C67	π*	20.55	0.44	0.093
O55	LP(2)	C54-O56	σ*	34.33	0.66	0.136
O75	LP(2)	C63-C74	σ*	21.38	0.76	0.115
F72	LP(2)	C67-C68	σ*	6.33	1.01	0.072
O55	LP(1)	C54-O56	σ*	1.65	1.09	0.039
O56	LP(1)	C47-C82	σ*	0.56	1.16	0.023
S52	LP(1)	C50-C61	σ*	0.52	1.23	0.023

Table S4: Natural bond orbital (NBO) analysis of investigated compound **NFAD3**-NBO by using M06 6-311G(d,p).

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)[a]**	**E(J)E(i)[b](a.u)**	**F(I,j)[c](a.u)**
C48-C50	π	C61-C69	π*	31.03	0.32	0.089
C61-C69	π	C75-C76	π*	28.91	0.29	0.083
C61-C69	π	C73-O74	π*	24.74	0.30	0.079
C66-C67	π	C64-C65	π*	19.05	0.33	0.071
C47-C81	π	C49-C51	π*	14.59	0.32	0.067
C75-C76	π	C61-C69	π*	8.22	0.33	0.048
C73-O74	π	C63-C68	π*	4.15	0.41	0.041
C79-N80	π	C77-N78	π*	0.75	0.47	0.017
C77-N78	π	C79-N80	π*	0.72	0.47	0.017
C61-H62	σ	C50-S52	σ*	10.69	0.72	0.078
C76-C77	σ	C77-N78	σ*	8.21	1.61	0.103
C49-C81	σ	C49-C51	σ*	7.02	1.25	0.084
C47-S53	σ	C81-F82	σ*	6.62	0.95	0.071
C14-S36	σ	C11-C12	σ*	5.61	1.19	0.073
C2-C3	σ	C3-C5	σ*	5.03	1.16	0.068
C12-C13	σ	C11-C12	σ*	4.95	1.23	0.07
C11-C12	σ	C10-C18	σ*	3.77	1.30	0.063
C63-C64	σ	C64-C75	σ*	2.51	1.17	0.049
C68-F94	σ	C63-C64	σ*	1.57	1.65	0.046

C41-C42	σ	C41-H45	σ*	1.29	1.12	0.034
C12-C13	σ	C9-C32	σ*	0.97	1.10	0.029
C14-S36	σ	C9-C13	σ*	0.52	1.11	0.022
N85	LP(1)	C41-C42	π*	48.92	0.29	0.11
O56	LP(2)	C54-O55	π*	48.65	0.37	0.121
S53	LP(2)	C48-C50	π*	32.79	0.24	0.085
S52	LP(2)	C49-C51	π*	28.75	0.26	0.079
S53	LP(2)	C47-C81	π*	21.45	0.26	0.067
F71	LP(3)	C66-C67	π*	20.24	0.44	0.093
O55	LP(2)	C54-O56	σ*	34.33	0.66	0.136
O74	LP(2)	C63-C73	σ*	23.02	0.74	0.119
O74	LP(2)	C69-C73	σ*	17.98	0.76	0.106
F82	LP(2)	C47-C81	σ*	7.97	1.04	0.081
S53	LP(1)	C48-C49	σ*	2.96	1.19	0.053
F94	LP(1)	C67-C68	σ*	1.05	1.6	0.037
S52	LP(1)	C50-C61	σ*	0.53	1.23	0.023

Table S5: Natural bond orbital (NBO) analysis of investigated compound **NFAD4**-NBO by using M06 6-311G(d,p).

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)[a]**	**E(J)E(i)[b](a.u)**	**F(I,j)[c](a.u)**
C48-C49	π	C1-C51	π*	28.81	0.27	0.083
C11-C16	π	C6-C7	π*	28.61	0.29	0.082
C14-C15	π	C12-C13	π*	20.31	0.32	0.075
C6-C7	π	C11-C16	π*	19.29	0.30	0.068
C63-C68	π	C71-O72	π*	14.14	0.32	0.062
C11-C16	π	C12-C13	π*	13.18	0.30	0.056
C47-C79	π	C48-C49	π*	11.14	0.31	0.058
C73-C74	π	C64-C65	π*	9.86	0.31	0.051
C71-O72	π	C63-C68	π*	4.78	0.42	0.043
C54-O55	π	C47-C79	π*	3.52	0.41	0.037
C61-H62	σ	C50-S52	σ*	11.02	0.72	0.079
C67-C94	σ	C94-N95	σ*	8.95	1.62	0.108
C10-C11	σ	C12-S36	σ*	7.71	0.90	0.075
C48-C50	σ	C50-C61	σ*	6.19	1.32	0.081
C49-C51	σ	C1-C51	σ*	5.59	1.29	0.076
C11-C16	σ	C5-C6	σ*	4.89	1.14	0.067
C1-C2	σ	C49-C51	σ*	4.19	1.25	0.065
C47-C54	σ	C47-C79	σ*	3.45	1.29	0.06
C10-C11	σ	C18-H19	σ*	2.93	1.07	0.05
C14-C39	σ	C40-C41	σ*	1.96	1.31	0.045
C10-C11	σ	C9-C32	σ*	0.83	1.07	0.027

C71-O72	σ	C63-C64	σ*	0.67	1.66	0.03
C14-S36	σ	C9-C13	σ*	0.52	1.11	0.022
O56	LP(2)	C54-O55	π*	48.91	0.37	0.121
S53	LP(2)	C48-C49	π*	29.67	0.26	0.081
S37	LP(2)	C1-C51	π*	20.85	0.24	0.065
O55	LP(2)	C54-O56	σ*	34.26	0.66	0.136
O72	LP(2)	C63-C71	σ*	22.77	0.73	0.117
O72	LP(2)	C69-C71	σ*	17.91	0.77	0.107
N76	LP(1)	C74-C75	σ*	12.57	1.04	0.102
N83	LP(1)	C88-H91	σ*	5.59	0.63	0.057
S37	LP(1)	C3-C4	σ*	2.89	1.22	0.053
S52	LP(1)	C50-C61	σ*	0.54	1.24	0.023

Table S6: Natural bond orbital (NBO) analysis of investigated compound **NFAD5**-NBO by using M06 6-311G(d,p).

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)**	**E(J)E(i)[b](a.u)**	**F(I,j)[c](a.u)**
C48-C50	π	C61-C69	π*	33.72	0.31	0.092
C61-C69	π	C73-C74	π*	30.79	0.29	0.084
C41-C42	π	C39-C40	π*	28.82	0.29	0.083
C49-C51	π	C48-C50	π*	27.04	0.45	0.079
C39-C40	π	C43-C81	π*	24.40	0.30	0.077
C43-C81	π	C41-C42	π*	22.13	0.30	0.075
C14-C15	π	C12-C13	π*	20.31	0.32	0.075
C47-C79	π	C54-O55	π*	19.90	0.34	0.075
C39-C40	π	C41-C42	π*	18.41	0.29	0.066
C43-C81	π	C39-C40	π*	16.41	0.30	0.066
C14-C15	π	C39-C40	π*	10.56	0.32	0.055
C73-C74	π	C64-C65	π*	9.91	0.31	0.051
N98-O99	π	C66-C67	π*	3.22	0.48	0.039
C61-H62	σ	C50-S52	σ*	11.02	0.71	0.079
C74-C77	σ	C77-N78	σ*	8.26	1.61	0.104
C50-S52	σ	C48-S53	σ*	7.77	0.87	0.073
C14-C15	σ	C9-C13	σ*	6.72	1.17	0.080
C47-S53	σ	C79-F80	σ*	6.64	0.95	0.071
C48-C50	σ	C50-C61	σ*	6.16	1.32	0.081
C14-S36	σ	C11-C12	σ*	5.60	1.19	0.073
C47-S53	σ	C48-C50	σ*	5.52	1.20	0.073
C39-C81	σ	C14-C39	σ*	5.13	1.21	0.071
C14-C15	σ	C13-C15	σ*	5.05	1.30	0.072
C13-C15	σ	C9-C13	σ*	4.52	1.14	0.064
C13-C15	σ	C11-C12	σ*	3.30	1.22	0.057
C48-C50	σ	C49-C79	σ*	2.73	1.24	0.052
C13-C15	σ	C15-H38	σ*	1.82	1.10	0.040
C14-S36	σ	C9-C13	σ*	0.53	1.11	0.022
N92-O93	σ	N92-O94	σ*	0.50	1.59	0.026
N83	LP(1)	C41-C42	π*	49.79	0.29	0.110

O56	LP(2)	C54-O55	π*	48.97	0.37	0.121
S53	LP(2)	C48-C50	π*	33.61	0.24	0.085
F80	LP(3)	C47-C79	π*	25.52	0.46	0.103
O55	LP(2)	C54-O56	σ*	34.25	0.66	0.136
O72	LP(2)	C63-C71	σ*	24.16	0.72	0.12
O96	LP(2)	N95-O97	σ*	20.77	0.76	0.114
O100	LP(2)	N98-O99	σ*	20.48	0.77	0.113
O56	LP(1)	C47-C54	σ*	0.50	1.03	0.020

Table S7: Natural bond orbital (NBO) analysis of investigated compound **NFAD6**-NBO by using M06 6-311G(d,p).

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)**	**E(J)E(i)[b](a.u)**	**F(I,j)[c](a.u)**
C61-C69	π	C73-C74	π*	30.71	0.29	0.084
C41-C42	π	C39-C40	π*	28.67	0.29	0.083
C10-C11	π	C7-C18	π*	25.43	0.28	0.076
C39-C40	π	C43-C81	π*	24.43	0.30	0.077
C6-C16	π	C10-C11	π*	23.38	0.30	0.077
C7-C18	π	C6-C16	π*	21.35	0.30	0.074
C14-C15	π	C12-C13	π*	20.07	0.32	0.075
C39-C40	π	C14-C15	π*	16.63	0.28	0.061
C47-C79	π	C49-C51	π*	14.46	0.31	0.066
C14-C15	π	C39-C40	π*	10.64	0.32	0.055
C71-O72	π	C63-C68	π*	4.36	0.42	0.042
C54-O55	π	C47-C79	π*	3.52	0.41	0.037
C61-H62	σ	C50-S52	σ*	10.96	0.71	0.079
C74-C77	σ	C77-N78	σ*	8.22	1.61	0.103
C47-S53	σ	C79-F80	σ*	6.61	0.95	0.071
C49-C51	σ	C48-C49	σ*	6.14	1.26	0.079
C14-S36	σ	C11-C12	σ*	5.60	1.19	0.073
C49-C51	σ	C1-C51	σ*	5.56	1.28	0.076
C43-C81	σ	C42-C43	σ*	4.15	1.28	0.065
C3-C4	σ	C2-H8	σ*	3.97	1.11	0.059
C10-C11	σ	C9-C10	σ*	2.27	1.11	0.045
C1-C2	σ	C2-H8	σ*	1.39	1.12	0.035
C3-C4	σ	C5-C20	σ*	2.80	0.67	0.042
C14-S36	σ	C9-C13	σ*	0.53	1.11	0.022
C77-N78	σ	C73-C74	σ*	0.50	1.65	0.026
N83	LP(1)	C41-C42	π*	49.41	0.29	0.110
O56	LP(2)	C54-O55	π*	48.88	0.37	0.12
F80	LP (3)	C47-C79	π*	25.55	0.46	0.103
S36	LP(2)	C14-C15	π*	24.78	0.28	0.074
S36	LP(2)	C12-C13	π*	23.69	0.29	0.074
O55	LP(2)	C54-O56	σ*	34.25	0.66	0.136
O72	LP(2)	C63-C71	σ*	24.00	0.72	0.119
O55	LP(1)	C47-C54	σ*	19.78	0.73	0.110
O72	LP(1)	C69-C71	σ*	17.64	0.77	0.106
S52	LP(1)	C49-C51	σ*	3.11	1.20	0.055
S52	LP(1)	C50-C61	σ*	0.55	1.24	0.023

F101	LP(1)	C66-C94	σ*	0.51	1.44	0.025

Table S8: Dipole polarizabilities and major contributing tensors (*a.u.*) of the studied compounds (**NFAR1)** and (**NFAD2- NFAD6**).

Compounds	μ_x	μ_y	μ_z	α_{xx}	α_{yy}	α_{zz}
NFAR1	-1.38	-1.91	-0.33	2582.24	1358.45	429.88
NFAD2	6.47	-1.09	0.01	2218.58	1173.29	411.23
NFAD3	6.23	-0.76	0.05	2253.28	1167.94	409.17
NFAD4	8.10	2.87	0.02	2542.74	1346.96	423.98
NFAD5	8.31	1.95	-0.06	2498.13	1272.01	473.41
NFAD6	7.48	-0.22	-0.05	2410.34	1235.42	438.85

Table S9: The computed second-order polarizabilities (β_{tot}) and major contributing tensors (*a.u*) of (**NFAR1**) and (**NFAD2- NFAD6**).

Compounds	β_{xxx}	β_{xxy}	β_{XYY}	β_{yyy}	β_{xxz}	β_{yyz}	β_{xzz}	β_{yzz}	β_{zzz}
NFAR1	-71130.50	19364.10	-3925.58	-4632.56	-89.24	72.02	-40.60	-122.37	-32.38
NFAD2	143018.00	7718.59	823.93	-3983.63	1581.05	-42.58	-307.97	-16.50	39.46
NFAD3	148227.00	5309.55	265.29	-3864.88	1195.51	-12.95	-313.78	-19.74	34.77
NFAD4	200741.00	14538.50	11077.30	10739.70	2615.29	212.42	-298.23	-26.67	29.35
NFAD5	194095.00	112.96	9044.79	7596.66	-1972.04	-162.72	-441.28	-3.11	-38.09
NFAD6	172101.00	-11250.60	4221.77	841.05	1873.49	174.06	-356.95	-13.59	38.40

Table S10: The computed third-order polarizabilities <γ> and major contributing tensors (*a.u*) of (**NFAR1)** and (**NFAD2- NFAD6**).

Compounds	γ_X	γ_Y	γ_Z
NFAR1	1.03×10^{7}	6.01×10^{5}	2.40×10^{4}
NFAD2	1.55×10^{7}	4.76×10^{5}	1.97×10^{4}
NFAD3	1.66×10^{7}	4.32×10^{5}	1.91×10^{4}
NFAD4	3.77×10^{7}	1.93×10^{6}	2.00×10^{4}
NFAD5	3.41×10^{7}	1.76×10^{6}	1.96×10^{4}
NFAD6	2.38×10^{7}	1.03×10^{6}	1.76×10^{4}