Supplementary Material for Fluorescence quantum yield rationalized by the magnitude of the charge transfer in π-conjugated compounds

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Contents

1 Photophysical data[1]

Table S1: Photophysical data of π-conjugated hydrocarbons in $CHCl_3$. All spectra were measured for 10^{-6}M solution at 295 K. In the case of **C-3**, cyclohexane was used as solvent. Details of the photophysical measurements can be found in Ref 1.

cmpd	Φ_F	λ_{em} nm	ν_{em} s^{-1}	logε	λ_{abs} nm	τ ns	k_r s^{-1}	k_{nr} s^{-1}	A_π eq. xx	$h\nu/k_BT$	Molecular length in S_0 / Å
1	0.83	348	$8.61 \cdot 10^{14}$	4.59	328	5.51	$1.51 \cdot 10^{8}$	$3.09 \cdot 10^{7}$	-137.2	138.8	16.58
2	0.87	389	$7.71 \cdot 10^{14}$	4.77	343	6.01	$1.45 \cdot 10^{8}$	$2.16 \cdot 10^{7}$	-122.3	124.2	23.46
3	0.93	389	$7.71 \cdot 10^{14}$	5.13	354	6.27	$1.48 \cdot 10^{8}$	$1.12 \cdot 10^{7}$	-121.6	124.2	30.33
4	0.14	330	$9.08 \cdot 10^{14}$	4.70	302	5.46	$2.56 \cdot 10^{7}$	$1.58 \cdot 10^{8}$	-148.2	146.4	14.29
5	0.18	353	$8.49 \cdot 10^{14}$	4.93	305	18.78	$9.58 \cdot 10^{6}$	$4.37 \cdot 10^{7}$	-138.3	136.8	
6	0.57	391	$7.67 \cdot 10^{14}$	5.13	315	6.11	$9.33 \cdot 10^{7}$	$4.04 \cdot 10^{7}$	-123.2	123.5	
7	0.27	449	$6.68 \cdot 10^{14}$	5.07	349	21.64	$1.25 \cdot 10^{7}$	$3.37 \cdot 10^{7}$	-108.6	107.6	
P-0	0.02	314	$9.55 \cdot 10^{14}$	4.24	249	4.72	$4.24 \cdot 10^{6}$	$2.08 \cdot 10^{8}$	-157.7	153.8	7.20
P-1	0.49	342	$8.77 \cdot 10^{14}$	4.49	280	4.38	$1.12 \cdot 10^{8}$	$1.16 \cdot 10^{8}$	-141.3	141.2	11.59
P-2	0.86	369	$8.12 \cdot 10^{14}$	4.64	298	5.83	$1.48 \cdot 10^{8}$	$2.40 \cdot 10^{7}$	-129.1	130.9	15.99
P-3	0.91	386	$7.77 \cdot 10^{14}$	4.80	309	5.46	$1.67 \cdot 10^{8}$	$1.65 \cdot 10^{7}$	-122.8	125.1	20.38
C-1	0.02	323	$9.28 \cdot 10^{14}$	3.58	286	5.33	$3.75 \cdot 10^{6}$	$1.84 \cdot 10^{8}$	-153.4	149.5	4.86
C-2	0.13	383	$7.83 \cdot 10^{14}$	3.85	379	5.75	$2.26 \cdot 10^{7}$	$1.51 \cdot 10^{8}$	-128.0	126.1	7.31
C-3	0.26	373	$8.04 \cdot 10^{14}$	4.60	338	89.30	$2.91 \cdot 10^{6}$	$8.29 \cdot 10^{6}$	-132.7	129.5	7.04
C-4	0.90	448	$6.69 \cdot 10^{14}$	4.53	438	6.49	$1.39 \cdot 10^{8}$	$1.54 \cdot 10^{7}$	-107.4	107.8	7.55

[1] Yamaguchi *et al.*, *J. Am. Chem. Soc.*, **2008**, *130*, 13867

2 Method comparison

Table S2: Most intense excitation energies (eV) of compounds a-g as calculated with different methods using the gas phase CAM-B3LYP geometries

cmpd	CAM	CAM+PCM	CC2	ADC(2)	Experiment
a	4.2903	4.1941	4.3759	4.3607	4.2606
	(0.0297)	(-0.0665)	(0.1153)	(0.1001)	
b	4.3207	4.2262	4.4018	4.3864	4.3200
	(0.0007)	(-0.0938)	(0.0818)	(0.0664)	
c	4.5011	4.4619	4.3770	4.3771	4.2901
	(0.2110)	(0.1718)	(0.0869)	(0.0870)	
d	4.1471	4.0403	4.1472	4.1285	4.1605
	(-0.0134)	(-0.1202)	(-0.0133)	(-0.0320)	
e	4.1793	4.1455	3.8877	3.8649	3.7916
	(0.3877)	(0.3539)	(0.0961)	(0.0733)	
e	4.3927	4.2996	4.2275	4.2141	4.1887
	(0.2040)	(0.1109)	(0.0388)	(0.0254)	
f	4.2619	4.1928	4.2691	4.2664	3.7916
	(0.4703)	(0.4012)	(0.4775)	(0.4748)	
g	4.0193	3.9463	3.7662	3.7494	3.4633
	(0.5560)	(0.4830)	(0.3029)	(0.2861)	
g	4.4753	4.4325	4.3552	4.2923	4.3656
	(0.1097)	(0.0669)	(-0.0104)	(-0.0733)	

3 Gas phase CAM-B3LYP geometries

3.1 TDDFT/CAM-B3LYP

compound a

Table S3: Excitation energies of compound **a** obtained with TDDFT/CAM-B3LYP/cc-PVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
4.2903	34604	289	1.2672	101-102	87 %
4.3774	35307	283	0.1478	100-102	65%
				101-103	15%
4.6269	37319	268	0.0025	97-102	56%
				97-104	19%
4.7301	38152	262	0.0000	97-103	67%
				95-104	15 %

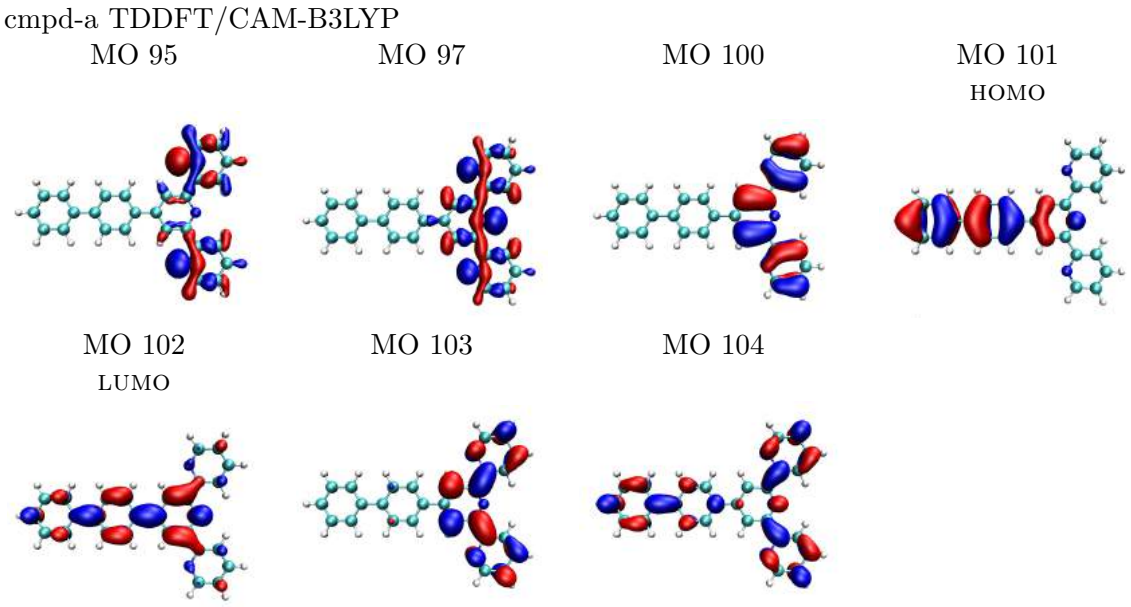


Figure S1: Pictures of orbitals involved in electronic transitions of cmpd-a computed using TDDFT/CAM-B3LYP

Table S4: ground and excited state dipole moments of compound a as calculated with TDDFT/CAM-B3LYP/cc-pVTZ using GAUSSIAN09

	μ_x (D)	μ_y (D)	μ_z (D)
GS	-1.4291	0.0000	0.0000
ES1 (GS geom)	2.6012	0.0000	0.0000
Δ_{ES-GS}	4.0303	0.0000	0.0000

compound b

Table S5: Excitation energies of compound **b** obtained with TDDFT/CAM-B3LYP/cc-PVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
4.3207	34850	287	1.2775	109-110	85%
4.3739	35279	283	0.1712	108-110	67%
				109-111	13%
4.6178	37246	268	0.0024	106-110	54%
				106-112	20%
4.7285	38139	262	0.0000	106-111	67 %
				104-112	14 %

cmpd-b TDDFT/CAM-B3LYP

MO 108 MO 109 MO 110 HOMO MO 111 LUMO

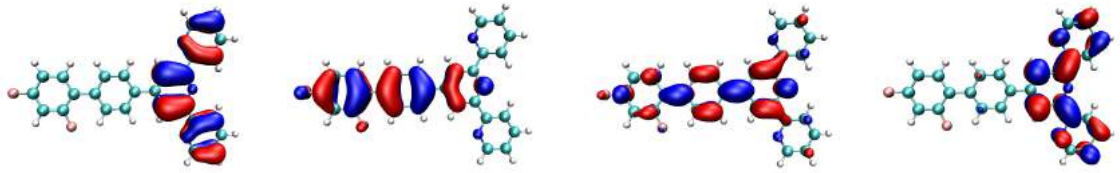


Figure S2: Pictures of orbitals involved in electronic transitions of cmpd-b computed using TDDFT/CAM-B3LYP

Table S6: ground and excited state dipole moments of compound b as calculated with TDDFT/CAM-B3LYP/cc-pVTZ using GAUSSIAN09

	μ_x (D)	μ_y (D)	μ_z (D)
GS	-2.5097	1.2496	0.0000
ES1 (GS geom)	0.8723	0.8080	0.0000
Δ_{ES-GS}	3.3820	-0.4416	0.0000

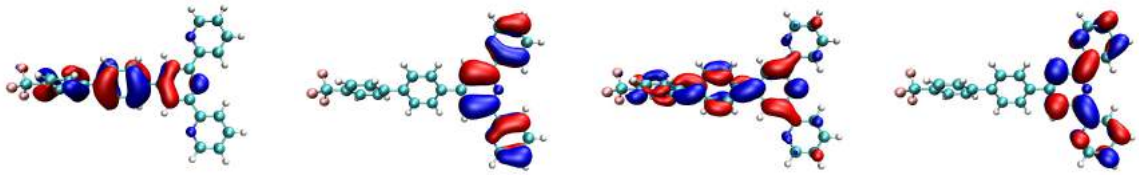
compound c

Table S7: Excitation energies of compound **c** obtained with TDDFT/CAM-B3LYP/cc-PVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
4.5011	36305	275	0.2262	117-118	70%
				117-120	13%
4.6478	37488	267	0.0032	114-118	46%
				114-120	19%
				112-119	15%
4.6953	37871	264	1.4779	116-118	70%
				117-119	14%
4.7186	38059	263	0.0018	114-119	63 %
				112-120	11 %

cmpd-c TDDFT/CAM-B3LYP

MO 116 MO 117 HOMO MO 118 LUMO MO 119



MO 120

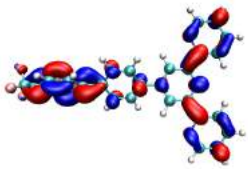


Figure S3: Pictures of orbitals involved in electronic transitions of cmpd-c computed using TDDFT/CAM-B3LYP

Table S8: ground and excited state dipole moments of compound c as calculated with TDDFT/CAM-B3LYP/cc-pVTZ using GAUSSIAN09

	μ_x (D)	μ_y (D)	μ_z (D)
GS	-5.0916	-0.0770	-0.0263
ES1 (GS geom)	7.0698	-0.707	0.0249
Δ_{ES-GS}	1.9782	0.0063	-0.0014

compound d

Table S9: Excitation energies of compound **a** obtained with TDDFT/CAM-B3LYP/cc-PVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
4.1471	33449	299	1.3697	109-110	82%
4.3672	35225	284	0.1120	108-110	58%
				109-111	19%
4.6367	37398	267	0.0025	105-110	58%
				105-112	16%
				102-111	12%
4.6479	37489	267	0.1341	109-114	35 %
				109-115	15 %
				108-110	14 %
				106-110	11 %

cmpd-d TDDFT/CAM-B3LYP

MO 108 MO 109 HOMO MO 110 LUMO MO 111

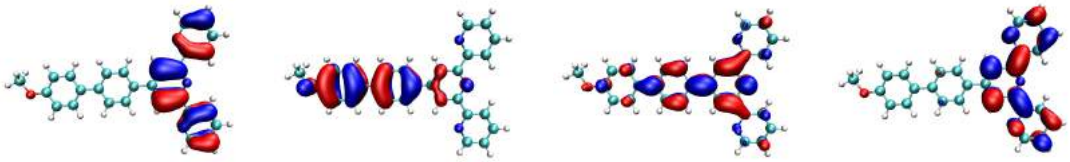


Figure S4: Pictures of orbitals involved in electronic transitions of cmpd-d computed using TDDFT/CAM-B3LYP

Table S10: ground and excited state dipole moments of compound d as calculated with TDDFT/CAM-B3LYP/cc-pVTZ using GAUSSIAN09

	μ_x (D)	μ_y (D)	μ_z (D)
GS	-0.4107	1.1398	0.0000
ES1 (GS geom)	6.7140	1.9648	0.0000
Δ_{ES-GS}	7.1247	0.8250	0.0000

compound e

Table S11: Excitation energies of compound **e** obtained with TDDFT/CAM-B3LYP/cc-PVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
4.1793	33709	297	0.0334	148-151	82%
4.3927	35430	282	1.3081	148-149	54%
				148-152	15%
4.5057	36342	275	0.1925	146-149	72%
4.6636	37615	266	0.0028	142-149	35 %
				144-149	26 %
				140-150	15 %

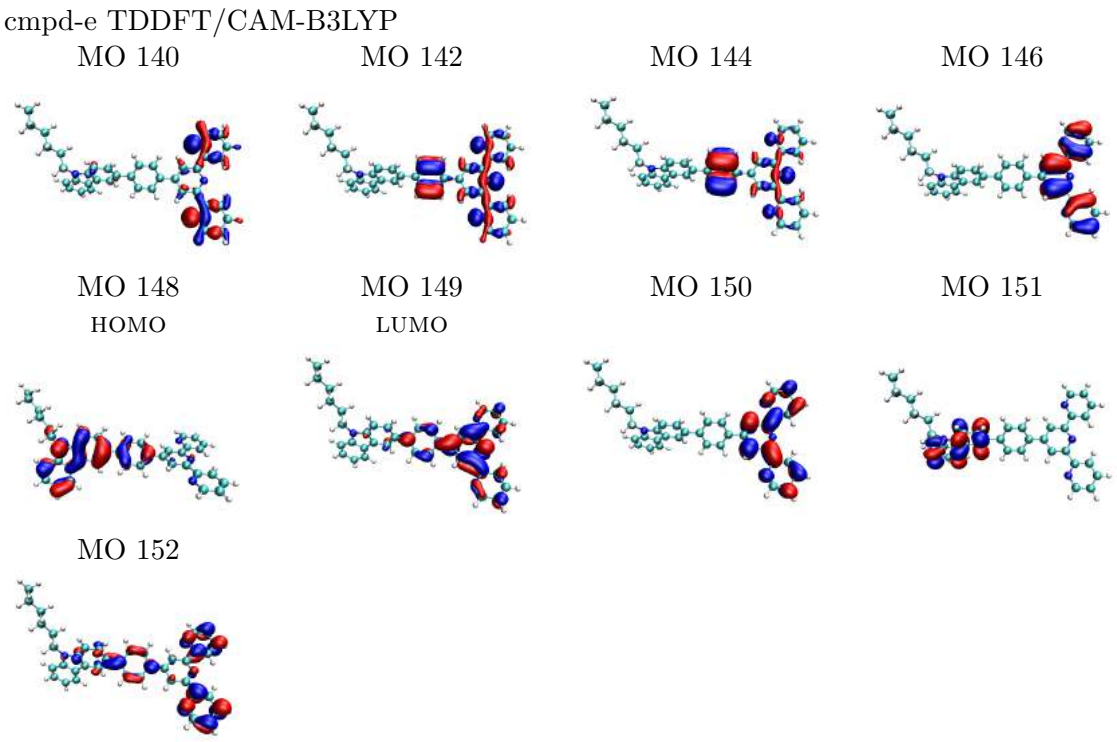


Figure S5: Pictures of orbitals involved in electronic transitions of cmpd-e computed using TDDFT/CAM-B3LYP

Table S12: ground and excited state dipole moments of compound e as calculated with TDDFT/CAM-B3LYP/cc-pVTZ using GAUSSIAN09

	μ_x (D)	μ_y (D)	μ_z (D)
GS	0.7354	1.0096	-0.9424
ES2 (GS geom)	11.8991	-0.4363	-0.4699
Δ_{ES-GS}	11.1637	-1.4459	0.4725

compound f

Table S13: Excitation energies of compound **a** obtained with TDDFT/CAM-B3LYP/cc-PVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
4.2619	34375	291	1.5642	172-173	63%
				172-175	26%
4.5057	36342	275	0.2062	171-173	65%
				171-175	13%
4.6581	37571	266	0.0030	167-173	34%
				165-173	17%
				164-174	16%
				167-175	12%
4.7216	38083	263	0.0005	167-174	41 %
				165-174	27 %
				164-176	11 %

cmpd-f TDDFT/CAM-B3LYP

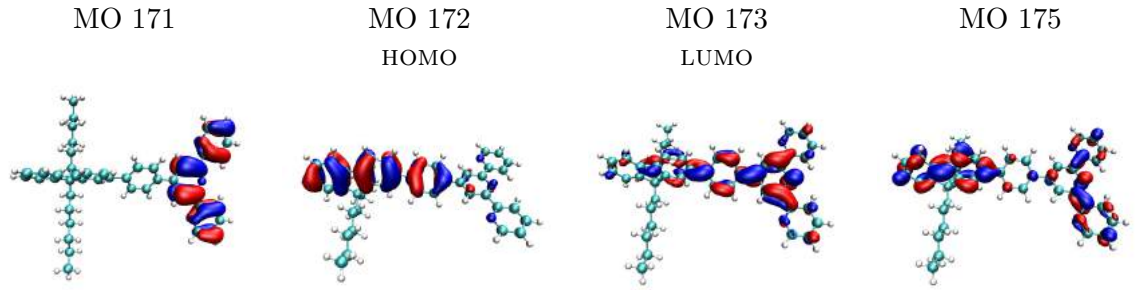


Figure S6: Pictures of orbitals involved in electronic transitions of cmpd-f computed using TDDFT/CAM-B3LYP

Table S14: ground and excited state dipole moments of compound f as calculated with TDDFT/CAM-B3LYP/cc-pVTZ using GAUSSIAN09

	μ_x (D)	μ_y (D)	μ_z (D)
GS	-1.3879	0.0605	-0.5848
ES1 (GS geom)	2.4521	-0.0189	-0.2653
Δ_{ES-GS}	3.8400	-0.0794	0.3195

compound g

Table S15: Excitation energies of compound **a** obtained with TDDFT/CAM-B3LYP/cc-PVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
4.0193	32419	308	1.2161	145-146	46%
				145-148	34%
4.2132	33983	294	0.0165	145-149	90%
4.4753	36097	277	0.2278	145-152	52%
				145-151	39%
4.5011	36305	275	0.2067	144-146	70 %

cmpd-d TDDFT/CAM-B3LYP

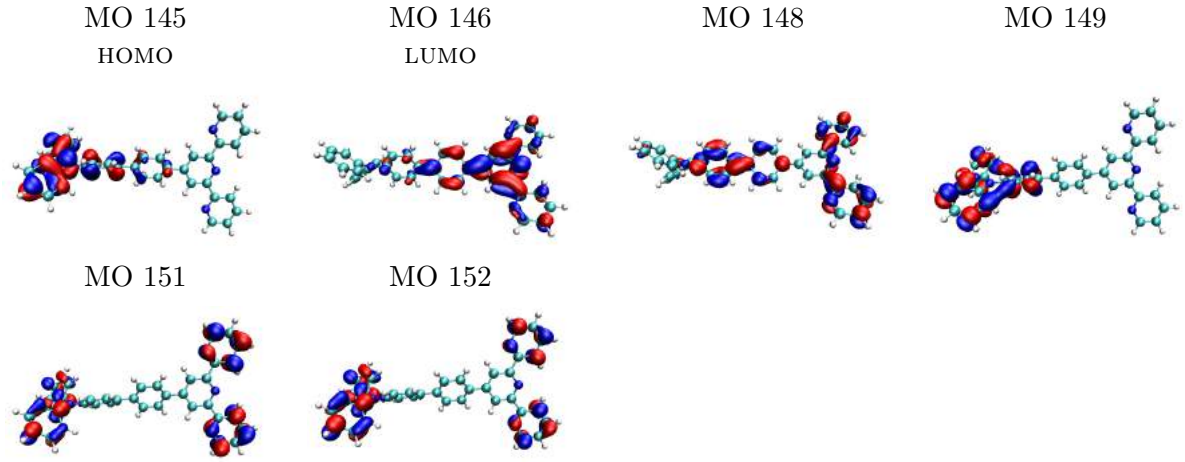


Figure S7: Pictures of orbitals involved in electronic transitions of cmpd-g computed using TDDFT/CAM-B3LYP

Table S16: ground and excited state dipole moments of compound g as calculated with TDDFT/CAM-B3LYP/cc-pVTZ using GAUSSIAN09

	μ_x (D)	μ_y (D)	μ_z (D)
GS	-1.1531	0.0000	0.0000
ES1 (GS geom)	9.2084	0.0000	0.0000
Δ_{ES-GS}	10.3615	0.0000	0.0000

3.2 TDDFT/CAM-B3LYP/PCM

compound a

Table S17: Excitation energies of compound **a** obtained with TDDFT/CAM-B3LYP/cc-PVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
4.1941	33828	296	1.4631	101-102	86 %
4.3450	35046	285	0.2317	100-102	70 %
				101-103	11 %
4.6422	37443	267	0.0029	97-102	57 %
				97-104	18 %
				95-103	10 %
4.7503	38315	261	0.1772	101-106	21 %
				101-103	21 %
				99-102	13 %
				96-102	11 %

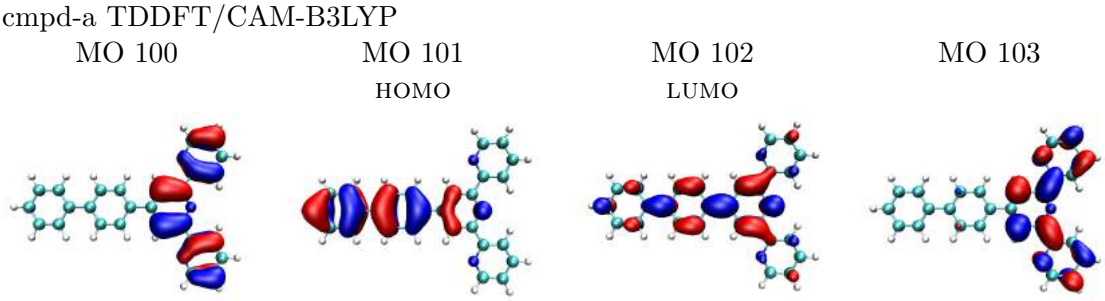


Figure S8: Pictures of orbitals involved in electronic transitions of cmpd-a computed using TDDFT/CAM-B3LYP/PCM

Table S18: ground and excited state dipole moments of compound a as calculated with TDDFT/CAM-B3LYP/cc-pVTZ using GAUSSIAN09

	μ_x (D)	μ_y (D)	μ_z (D)
GS	1.9894	0.0000	0.0000
ES1 (GS geom)	-3.3056	0.0000	0.0000
Δ_{ES-GS}	-5.2950	0.0000	0.0000

compound b

Table S19: Excitation energies of compound **b** obtained with TDDFT/CAM-B3LYP/cc-PVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
4.2262	34087	293	1.4892	109-110	86 %
4.3415	35017	286	0.2416	108-110	71 %
4.6359	37392	267	0.0028	105-110	56 %
				105-112	18 %
				100-110	10 %
4.7513	38323	261	0.2585	108-111	83 %

cmpd-b TDDFT/CAM-B3LYP

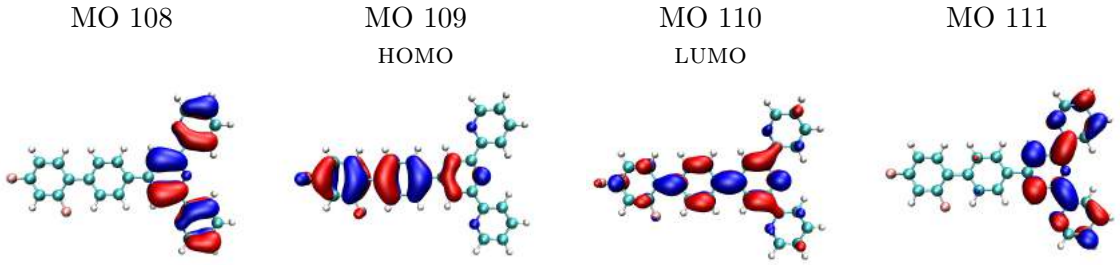


Figure S9: Pictures of orbitals involved in electronic transitions of cmpd-b computed using TDDFT/CAM-B3LYP/PCM

Table S20: ground and excited state dipole moments of compound b as calculated with TDDFT/CAM-B3LYP/cc-pVTZ using GAUSSIAN09

	μ_x (D)	μ_y (D)	μ_z (D)
GS	1.6848	-3.0909	0.0000
ES1 (GS geom)	1.1363	1.9170	0.0000
Δ_{ES-GS}	-0.5485	5.0079	0.0000

compound c

Table S21: Excitation energies of compound **c** obtained with TDDFT/CAM-B3LYP/cc-PVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
4.4619	35988	278	0.3374	117-118	73 %
				117-120	12 %
4.6115	37195	269	1.6825	116-118	70 %
				117-119	14 %
4.6707	37673	265	0.0038	114-118	39 %
				113-118	14 %
				111-119	13 %
				114-120	12 %
4.7502	38314	261	0.0013	114-119	45 %
				113-119	23 %

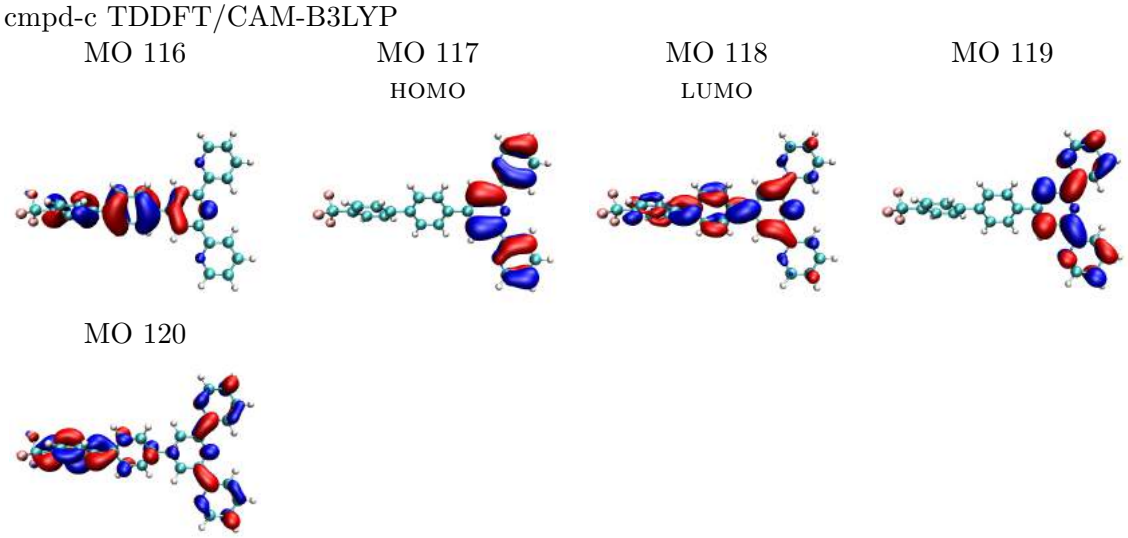


Figure S10: Pictures of orbitals involved in electronic transitions of cmpd-c computed using TDDFT/CAM-B3LYP/PCM

Table S22: ground and excited state dipole moments of compound c as calculated with TDDFT/CAM-B3LYP/cc-pVTZ using GAUSSIAN09

	μ_x (D)	μ_y (D)	μ_z (D)
GS	6.0049	-0.0885	0.0294
ES1 (GS geom)	8.2668	-0.0817	0.0276
Δ_{ES-GS}	2.2619	0.0068	-0.0018

compound d

Table S23: Excitation energies of compound **a** obtained with TDDFT/CAM-B3LYP/cc-PVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
4.0403	32588	307	1.5433	109-110	81 %
				109-112	10 %
4.3394	35000	286	0.1863	108-110	64 %
				109-111	15 %
4.6289	37335	268	0.1863	109-114	33 %
				109-111	16 %
				108-110	12 %
				109-115	12 %
4.6526	37527	266	0.0030	105-110	60 %
				105-112	15 %
				102-111	11 %

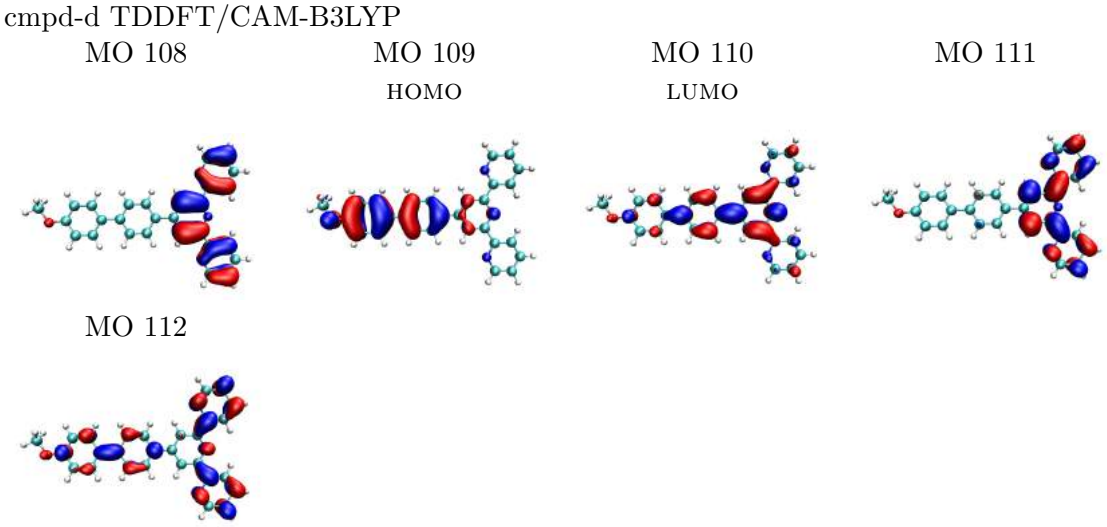


Figure S11: Pictures of orbitals involved in electronic transitions of cmpd-d computed using TDDFT/CAM-B3LYP/PCM

Table S24: ground and excited state dipole moments of compound d as calculated with TDDFT/CAM-B3LYP/cc-pVTZ using GAUSSIAN09

	μ_x (D)	μ_y (D)	μ_z (D)
GS	1.4445	-0.9362	0.0000
ES1 (GS geom)	2.4919	8.1495	0.0000
Δ_{ES-GS}	1.0474	9.0857	0.0000

compound e

Table S25: Excitation energies of compound **e** obtained with TDDFT/CAM-B3LYP/cc-PVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
4.1455	33436	299	0.0723	148-151	82 %
4.2996	34679	288	1.5039	148-149	51 %
				148-152	15 %
				145-149	10 %
4.4661	36022	278	0.2995	146-149	76 %
4.6574	37565	266	0.6408	147-151	76 %

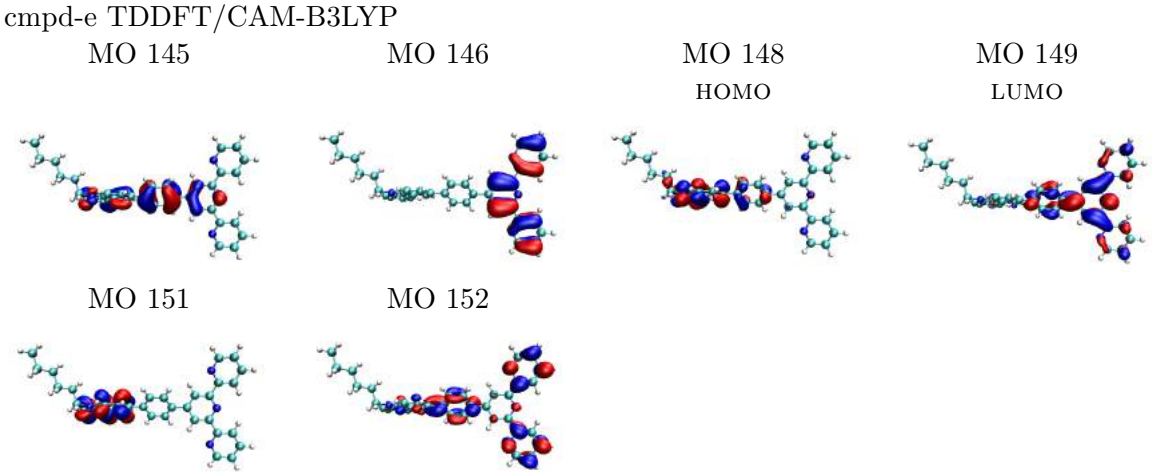


Figure S12: Pictures of orbitals involved in electronic transitions of cmpd-e computed using TDDFT/CAM-B3LYP/PCM

Table S26: ground and excited state dipole moments of compound e as calculated with TDDFT/CAM-B3LYP/cc-pVTZ using GAUSSIAN09

	μ_x (D)	μ_y (D)	μ_z (D)
GS	0.4405	1.2134	-1.2892
ES2 (GS geom)	12.6307	-0.4852	-0.7973
Δ_{ES-GS}	12.1902	-1.6986	0.4919

compound f

Table S27: Excitation energies of compound **a** obtained with TDDFT/CAM-B3LYP/cc-PVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
4.1928	33818	296	1.7730	172-173	60 %
				172-175	28 %
4.4652	36015	278	0.3152	171-173	70 %
				171-175	12 %
4.6787	37737	265	0.0036	165-173	29 %
				167-173	24 %
				164-174	14 %
				165-175	11 %
4.7512	38322	261	0.0325	165-174	39 %
				167-174	23 %

cmpd-f TDDFT/CAM-B3LYP

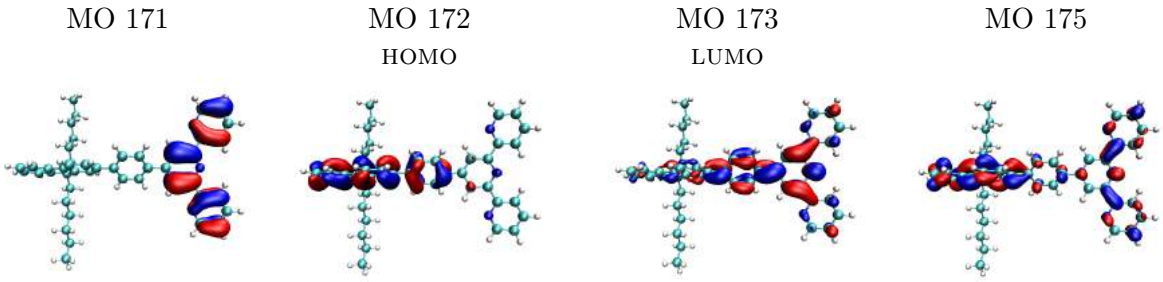


Figure S13: Pictures of orbitals involved in electronic transitions of cmpd-f computed using TDDFT/CAM-B3LYP/PCM

Table S28: ground and excited state dipole moments of compound f as calculated with TDDFT/CAM-B3LYP/cc-pVTZ using GAUSSIAN09

	μ_x (D)	μ_y (D)	μ_z (D)
GS	-2.003	0.1267	-1.0486
ES1 (GS geom)	2.9328	0.0134	-0.5153
Δ_{ES-GS}	4.9358	-0.1133	0.5333

compound g

Table S29: Excitation energies of compound **a** obtained with TDDFT/CAM-B3LYP/cc-PVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
3.9463	31830	314	1.3326	145-146	45 %
				145-148	34 %
4.2136	33986	294	0.0227	145-149	90 %
4.4325	35751	280	0.3043	145-152	91 %
4.4612	35983	278	0.3122	144-146	73 %

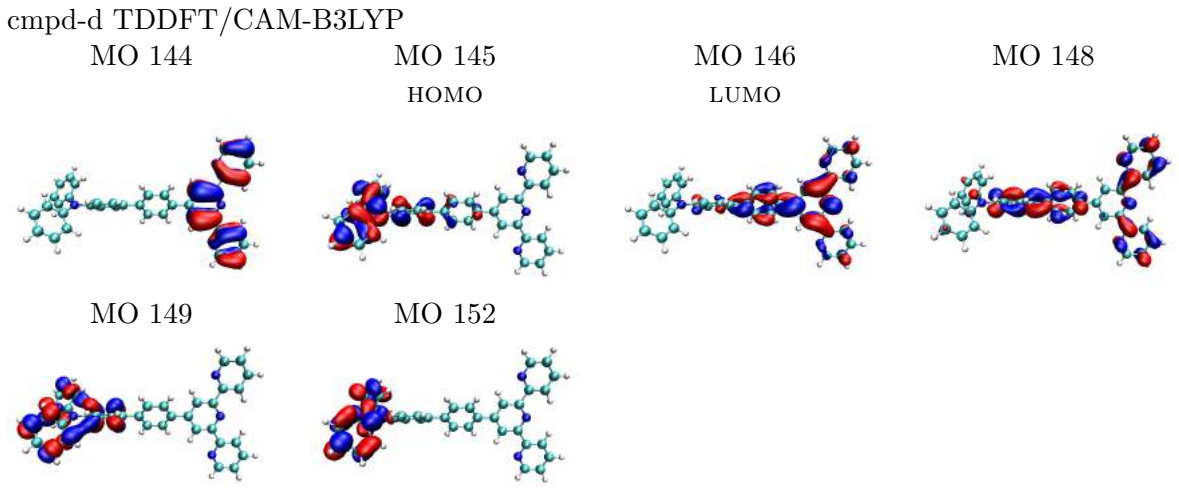


Figure S14: Pictures of orbitals involved in electronic transitions of cmpd-g computed using TDDFT/CAM-B3LYP/PCM

Table S30: ground and excited state dipole moments of compound g as calculated with TDDFT/CAM-B3LYP/cc-pVTZ using GAUSSIAN09

	μ_x (D)	μ_y (D)	μ_z (D)
GS	1.7778	0.0000	0.0000
ES1 (GS geom)	-10.5284	0.0000	0.0000
Δ_{ES-GS}	-12.3062	0.0000	0.0000

3.3 CC2

cmpd a

Table S31: Excitation energies of compound **a** obtained with CC2/cc-pVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
4.2261	34086	293	0.0752	100-102	54 %
				101-103	19 %
4.3759	35295	283	1.4181	101-102	91 %
4.5982	37087	270	0.0665	101-105	31 %
				98-102	23 %
4.8460	39087	256	0.1632	100-103	67 %

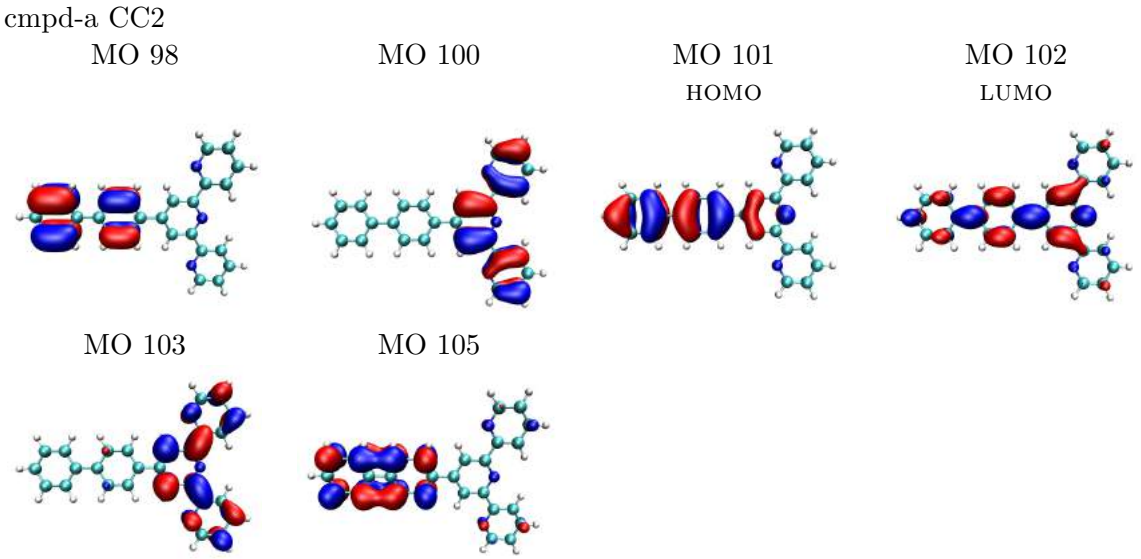


Figure S15: Pictures of orbitals involved in electronic transitions of cmpd-a computed using CC2

Table S32: ground and excited state dipole moments of compound a as calculated with CC2/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	-1.1931	0.6888	0.0000
ES2 (GS geom)	5.1076	-2.9489	0.0000
Δ_{ES-GS}	6.3007	-3.6377	0.0000

cmpd b

Table S33: Excitation energies of compound **b** obtained with CC2/cc-pVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
4.2256	34082	293	0.0843	108-110	57%
				109-111	17%
4.4018	35504	282	1.4155	109-110	87%
4.6360	37393	267	0.1236	106-110	34%
				109-113	20%
4.8491	39111	256	0.1440	108-111	66%

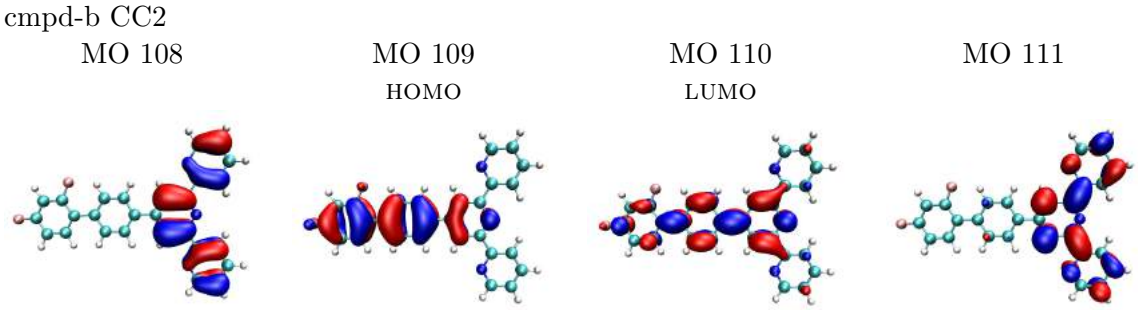


Figure S16: Pictures of orbitals involved in electronic transitions of cmpd-b computed using CC2

Table S34: ground and excited state dipole moments of compound b as calculated with CC2/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	-2.5299	0.4488	0.0000
ES2 (GS geom)	2.5186	-2.1955	0.0000
Δ_{ES-GS}	5.0485	-2.6443	0.0000

cmpd-c

Table S35: Excitation energies of compound **c** obtained with CC2/cc-pVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
4.3770	35303	283	0.1258	117-118	60%
				116-119	11%
				117-120	10%
4.4692	36048	277	0.0029	108-118	51%
				108-120	16%
4.4888	36205	276	0.2481 10^{-04}	108-119	68 %
				109-119	10%
4.7775	38534	260	1.5199	116-118	63%
				117-119	21%

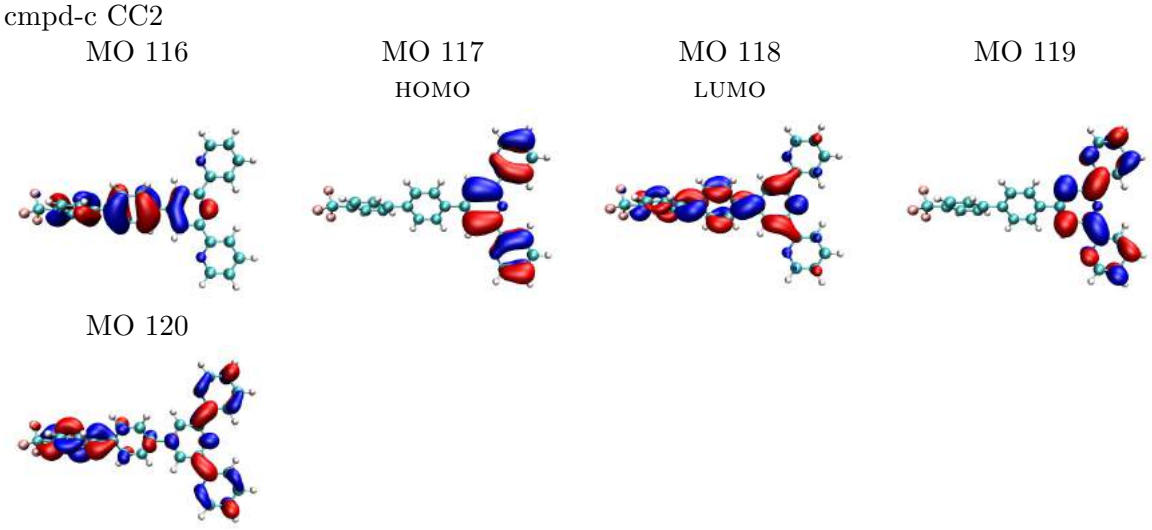


Figure S17: Pictures of orbitals involved in electronic transitions of cmpd-c computed using CC2

Table S36: ground and excited state dipole moments of compound c as calculated with CC2/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	4.8573	-0.0730	0.0250
ES1 (GS geom)	6.9900	-0.0660	0.0233
Δ_{ES-GS}	2.1327	0.0070	-0.0017

cmpd d

Table S37: Excitation energies of compound **a** obtained with CC2/cc-pVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
4.1472	33451	299	1.4648	109-110	90%
4.2068	33931	295	0.0519	108-110	46%
				109-111	26%
4.4905	36219	276	0.0919	109-113	45%
				108-110	15%
				106-110	14%
4.8408	39044	256	0.2077	108-111	66%

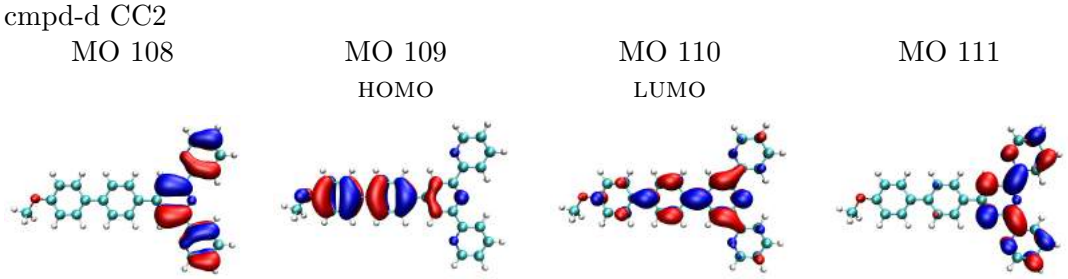


Figure S18: Pictures of orbitals involved in electronic transitions of cmpd-d computed using CC2

Table S38: ground and excited state dipole moments of compound d as calculated with CC2/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	1.1086	-0.1223	0.0000
ES1 (GS geom)	2.4892	12.0296	0.0000
Δ_{ES-GS}	1.3806	12.1519	0.0000

cmpd e

Table S39: Excitation energies of compound **a** obtained with CC2/cc-pVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
3.8877	31357	319	0.0236	148-151	70%
4.2275	34098	293	1.1497	148-149	71%
				148-152	12%
4.3667	35220	284	0.0902	146-149	56%
				148-150	15%
4.6267	37318	268	0.4968	147-151	54%

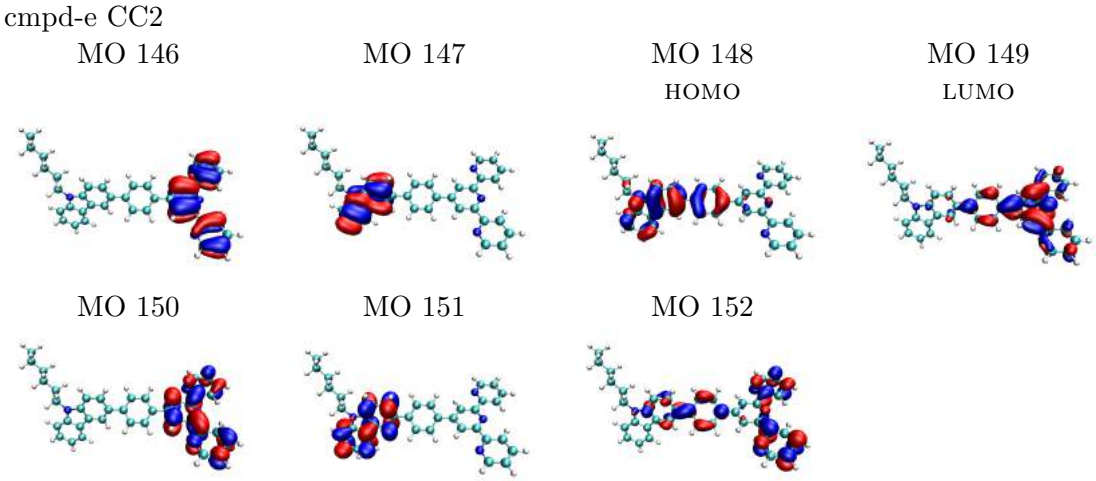


Figure S19: Pictures of orbitals involved in electronic transitions of cmpd-e computed using CC2

Table S40: ground and excited state dipole moments of compound e as calculated with CC2/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	1.0272	1.0818	-1.0116
ES2 (GS geom)	19.8715	-1.5634	-0.0751
Δ_{ES-GS}	18.8443	-2.6452	0.9365

cmpd-f

Table S41: Excitation energies of compound **f** obtained with ADC(2)/cc-pVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
4.2691	34434	290	1.5431	172-173	73%
				172-175	13%
4.3723	35266	284	0.1069	171-173	52%
				171-175	13%
				170-174	11%
4.4906	36220	276	0.5537 10^{-04}	161-174	54%
				162-174	25%
4.5575	36759	272	0.1556	172-177	29%
				172-176	18%
				168-173	10%

Table S42: ground and excited state dipole moments of compound f as calculated with CC2/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	-1.3181	0.0526	-0.5436
ES1 (GS geom)	5.7918	-0.0990	0.0625
Δ_{ES-GS}	7.1099	-0.1516	0.6061

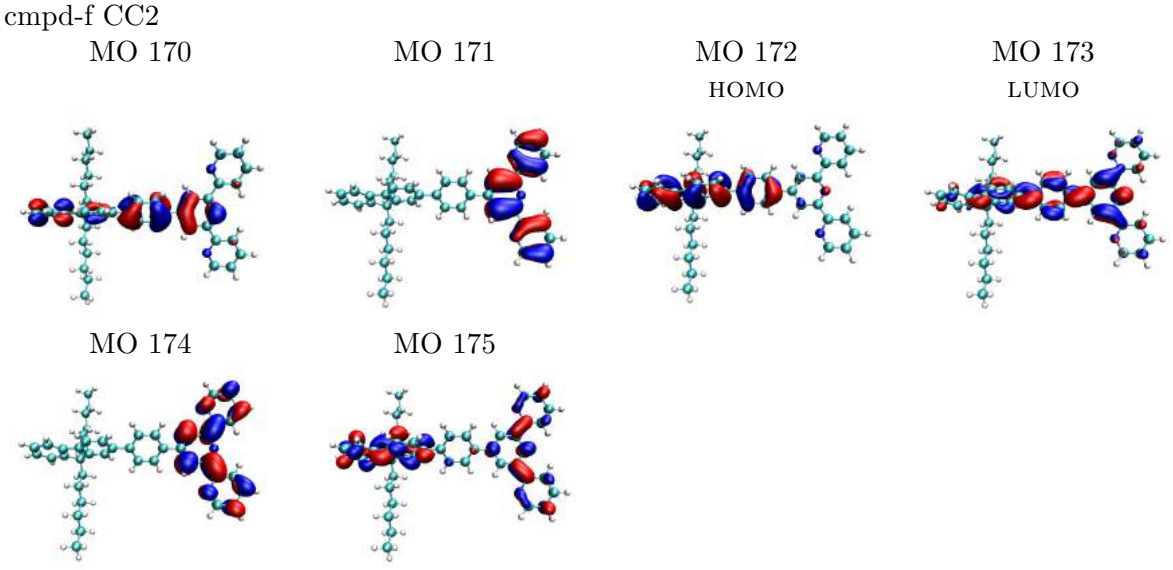


Figure S20: Pictures of orbitals involved in electronic transitions of cmpd-f computed using CC2

cmpd g

Table S43: Excitation energies of compound **g** obtained with CC2/cc-pVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
3.7662	30377	329	1.0523	145-146	59%
				145-148	27%
3.9397	31777	315	0.0131	145-149	81%
4.3552	35128	285	0.0986	144-146	51%
				145-147	16%
				143-147	10%
4.4907	36221	276	0.0156 10^{-04}	132-147	50%
				133-147	29%

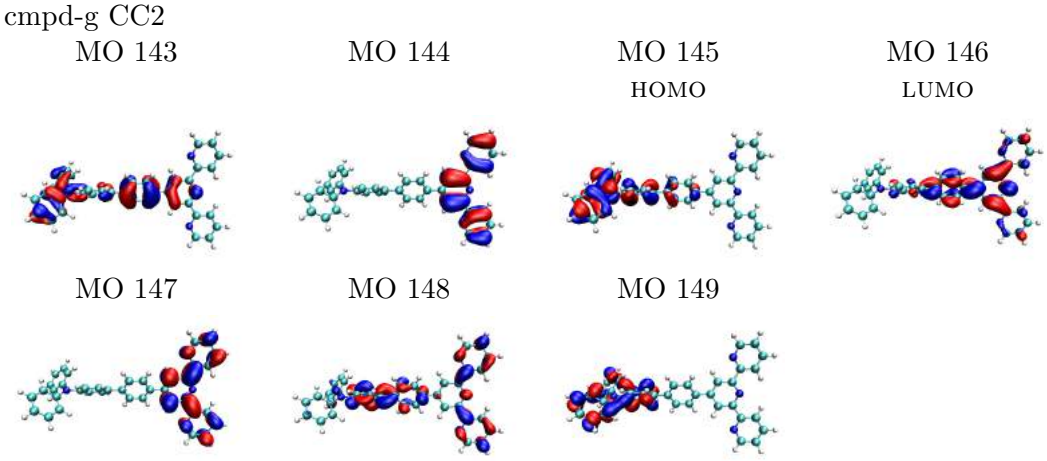


Figure S21: Pictures of orbitals involved in electronic transitions of cmpd-g computed using CC2

Table S44: ground and excited state dipole moments of compound g as calculated with CC2/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	-0.9811	0.0000	0.0000
ES1 (GS geom)	16.4623	0.0000	0.0000
Δ_{ES-GS}	17.4434	0.0000	0.0000

3.4 ADC(2)

cmpd-a

Table S45: Excitation energies of compound **a** obtained with ADC(2)/cc-pVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
4.2307	34124	293	0.0827	100-102	55 %
				101-103	18 %
4.3607	35172	284	1.4539	101-102	91 %
4.6046	37139	269	0.0747	101-105	31 %
				98-102	24 %
				97-102	10 %
4.8402	39040	256	0.2025	100-103	69 %

Table S46: ground and excited state dipole moments of compound a as calculated with ADC(2)/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	-1.1957	0.6903	0.0000
ES2 (GS geom)	5.0850	-2.9358	0.0000
Δ_{ES-GS}	6.2807	-3.6261	0.0000

cmpd-b

Table S47: Excitation energies of compound **b** obtained with ADC(2)/cc-pVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
4.2289	34109	293	0.0936	108-110	58%
				109-111	16%
4.3864	35380	283	1.4374	109-110	87%
4.6378	37407	267	0.1275	106-110	35%
				109-113	20%
4.8432	39064	256	0.1814	108-111	68%

Table S48: ground and excited state dipole moments of compound b as calculated with ADC(2)/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	-2.9151	0.3413	0.0000
ES2 (GS geom)	1.9175	-2.0203	0.0000
Δ_{ES-GS}	4.8326	-2.3643	0.0000

cmpd-c

Table S49: Excitation energies of compound **c** obtained with ADC(2)/cc-pVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
4.3771	35305	283	0.1379	117-118	60%
				116-119	10%
				117-120	10%
4.4583	35959	278	0.0032	108-118	50%
				108-120	16%
4.4866	36188	276	0.0953 10^{-04}	108-119	68 %
				109-119	10%
4.7710	38481	260	1.6113	116-118	65%
				117-119	20%

Table S50: ground and excited state dipole moments of compound c as calculated with ADC(2)/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	5.2791	-0.0811	0.0278
ES1 (GS geom)			
Δ_{ES-GS}			

cmpd-d

Table S51: Excitation energies of compound **a** obtained with ADC(2)/cc-pVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
4.1285	33299	300	1.4241	109-110	89%
4.2128	33979	294	0.0560	108-110	47%
				109-111	24%
4.4920	36232	276	0.0983	109-113	45%
				106-110	15%
				108-110	14%
4.8356	39002	256	0.2405	108-111	68%

Table S52: ground and excited state dipole moments of compound d as calculated with ADC(2)/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	1.1630	-0.5375	0.0000
ES1 (GS geom)	2.5241	11.7932	0.0000
Δ_{ES-GS}	1.3611	12.3307	0.0000

cmpd-e

Table S53: Excitation energies of compound **e** obtained with ADC(2)/cc-pVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
3.8649	31173	321	0.0253	148-151	69%
				147-151	10%
4.2141	33990	294	1.0744	148-149	69%
				148-152	13%
4.3698	35246	284	0.1004	146-149	57%
				148-150	13%
4.6242	37298	268	0.5565	147-151	55%

Table S54: ground and excited state dipole moments of compound e as calculated with ADC(2)/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	0.6311	0.9533	-0.8864
ES1 (GS geom)	19.8717	-1.8426	-0.033
Δ_{ES-GS}	19.2406	-2.7959	0.8534

cmpd-f

Table S55: Excitation energies of compound **f** obtained with ADC(2)/cc-pVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
4.2664	34412	291	1.5744	172-173	73%
				172-175	14%
4.3747	35285	283	0.1175	171-173	52%
				171-175	13%
				170-174	10%
4.4885	36203	276	0.0001	161-174	53%
				162-174	25%
4.5646	36817	272	0.1363	172-177	29%
				172-176	18%
				168-173	10%

Table S56: ground and excited state dipole moments of compound f as calculated with ADC(2)/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	-1.3687	0.0570	-0.5673
ES1 (GS geom)	5.8189	-0.1082	0.1559
Δ_{ES-GS}	7.1876	-0.1652	0.7232

cmpd-g

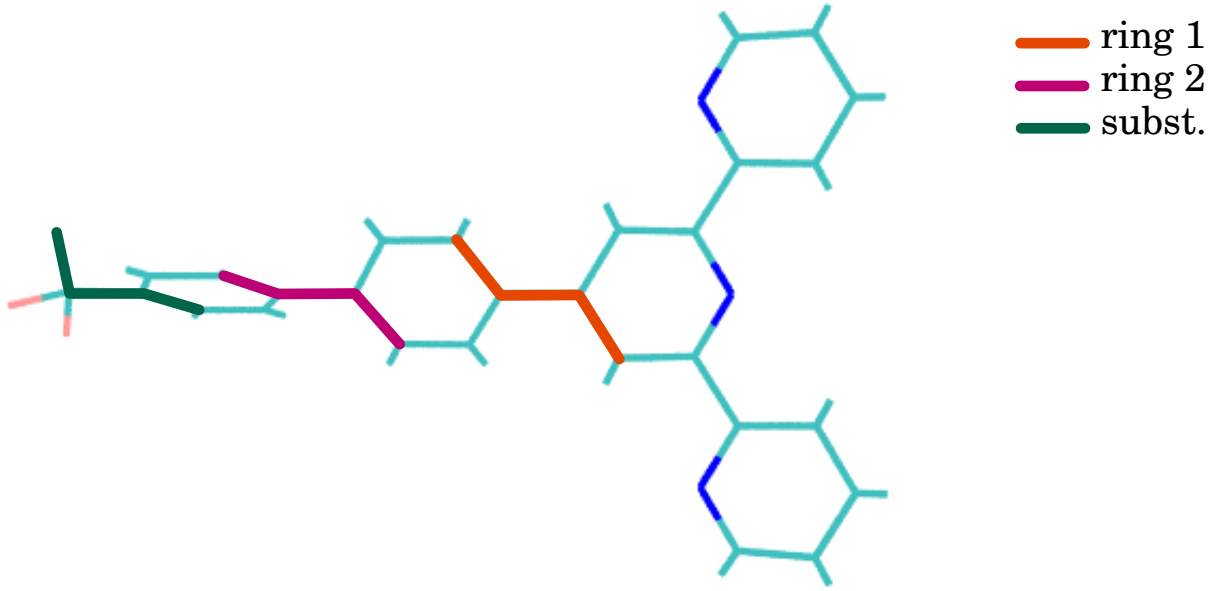
Table S57: Excitation energies of compound **g** obtained with ADC(2)/cc-pVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
3.7494	30241	331	0.8602	145-146	57%
				145-148	28%
3.9426	31800	314	0.0154	145-149	80%
4.2923	34620	289	0.2422	145-151	80%
4.3610	35175	284	0.1036	144-146	53%
				145-147	14%
				143-147	10%

Table S58: ground and excited state dipole moments of compound g as calculated with ADC(2)/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	-1.1557	0.0000	0.0000
ES1 (GS geom)	16.4836	0.0000	0.0000
Δ_{ES-GS}	17.6393	0.0000	0.0000

4 Structural parameters



Compd	geometry	ring 1	ring 2	subst.
cmpd-a	CAM-B3LYP	180.0	180.0	n/a
	MP2	-142.9	138.0	n/a
cmpd-b	CAM-B3LYP	180.0	180.0	n/a
	MP2	-142.8	135.8	n/a
cmpd-c	CAM-B3LYP	144.7	140.7	89.3
		144.7	140.7	96.4
		144.7	140.7	162.9
		144.7	140.7	-58.1
		144.7	-127.4	89.3
		144.7	-178.2	89.3
		144.7	-98.8	89.3
	MP2	-142.7	138.3	120.1
cmpd-d	CAM-B3LYP	180.0	180.0	180.0
	MP2	-143.0	139.1	-179.6
cmpd-e	CAM-B3LYP	145.2	140.8	n/a
	MP2	142.9	138.2	n/a
cmpd-f	CAM-B3LYP	145.1	141.1	n/a
	MP2	142.8	138.9	n/a
cmpd-g	CAM-B3LYP	145.1	142.1	140.2
	MP2	142.9	139.6	142.6

5 cmpd-c structure

5.1 Rotation of CF_3

Dihedral : 89.3 (CAM-B3LYP optimized)

Table S59: Excitation energies of compound **c** obtained with CC2/cc-pVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
4.3770	35303	283	0.1258	117-118	60%
				116-119	11%
				117-120	10%
4.4692	36048	277	0.0029	108-118	51%
				108-120	16%
4.4888	36205	276	0.2481 10^{-04}	108-119	68 %
				109-119	10%
4.7775	38534	260	1.5199	116-118	63%
				117-119	21%

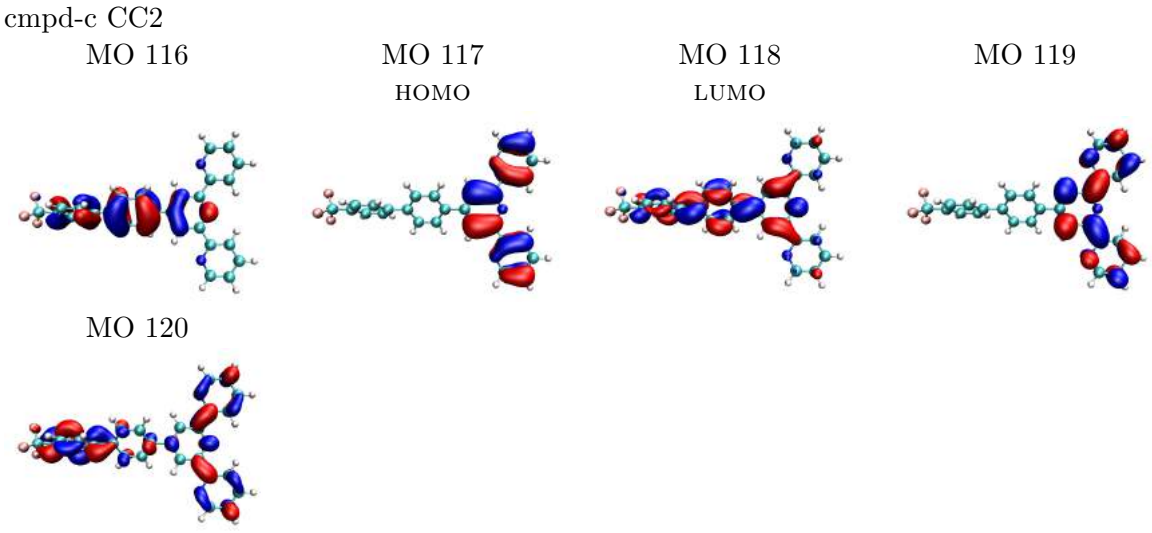


Figure S22: Pictures of orbitals involved in electronic transitions of *modified* cmpd-c computed using CC2

Table S60: ground and excited state dipole moments of compound c as calculated with CC2/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	4.8573	-0.0730	0.0250
ES1 (GS geom)	6.9900	-0.0660	0.0233
Δ_{ES-GS}	2.1327	0.0070	-0.0017

Dihedral : 96.4

Table S61: Excitation energies of compound **c** with dihedral(CF_3) = 96.4, obtained with CC2/cc-pVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
4.3773	35306	283	0.1259	117-118	60%
				116-119	11%
				117-120	10%
4.4695	36049	277	0.0029	108-118	51%
				108-120	16%
4.4888	36205	276	0.2442 10^{-04}	108-119	68%
				109-119	10%
4.7789	38545	259	1.5169	116-118	63%
				117-119	21%

cmpd-c CC2

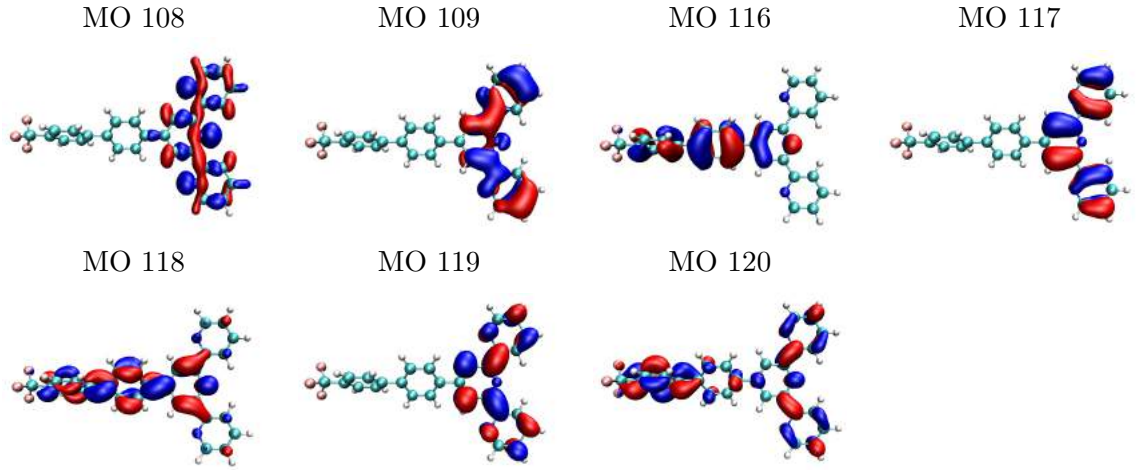


Figure S23: Pictures of orbitals involved in electronic transitions of *modified* cmpd-c computed using CC2

Table S62: ground and excited state dipole moments of compound c as calculated with CC2/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	4.8650	-0.0448	0.0341
ES1 (GS geom)	6.9849	-0.0380	0.0336
Δ_{ES-GS}	2.1199	0.0068	-0.0005

Dihedral : 162.9

Table S63: Excitation energies of compound **c** with dihedral(CF_3) = 96.4, obtained with CC2/cc-pVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
4.3766	35300	283	0.1259	117-118	59%
				117-120	11%
				116-119	11%
4.4688	36044	277	0.0029	108-118	50%
				108-120	17%
4.4888	36205	276	0.2597 10^{-04}	108-119	68%
				109-119	10%
4.7715	38485	260	1.5251	116-118	66%
				117-119	19%

cmpd-c CC2

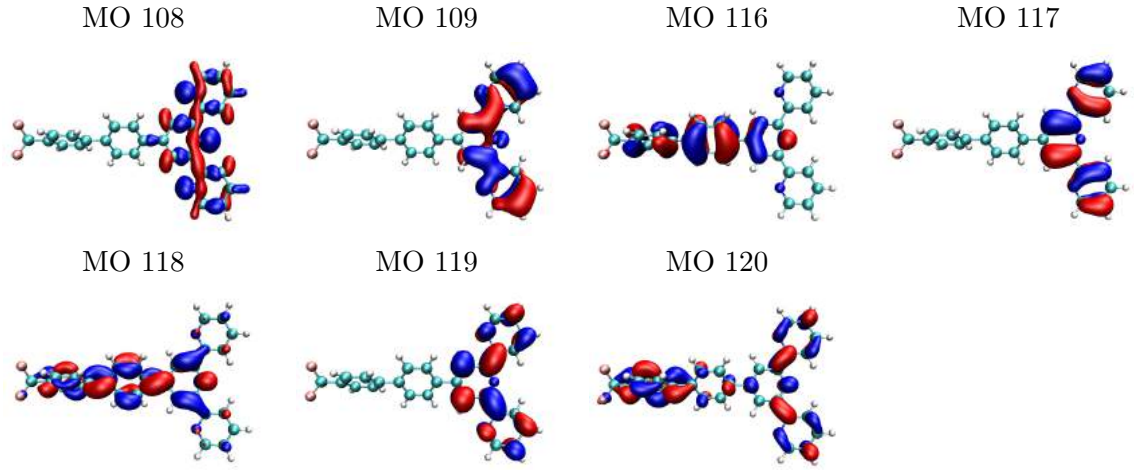


Figure S24: Pictures of orbitals involved in electronic transitions of *modified* cmpd-c computed using CC2

Table S64: ground and excited state dipole moments of compound c as calculated with CC2/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	4.8879	-0.0420	-0.0400
ES1 (GS geom)	7.0511	-0.0339	-0.0433
Δ_{ES-GS}	2.1632	0.0081	-0.0033

Dihedral : -58.1

Table S65: Excitation energies of compound **c** with dihedral(CF_3) = 96.4, obtained with CC2/cc-pVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
4.3769	35302	283	0.1258	117-118	59%
				117-120	11%
				116-119	11%
4.4691	36046	277	0.0029	108-118	50%
				108-120	16%
4.4888	36205	276	0.2532 10^{-04}	108-119	68%
				109-119	10%
4.7742	38507	260	1.5169	116-118	65%
				117-119	20%

cmpd-c CC2

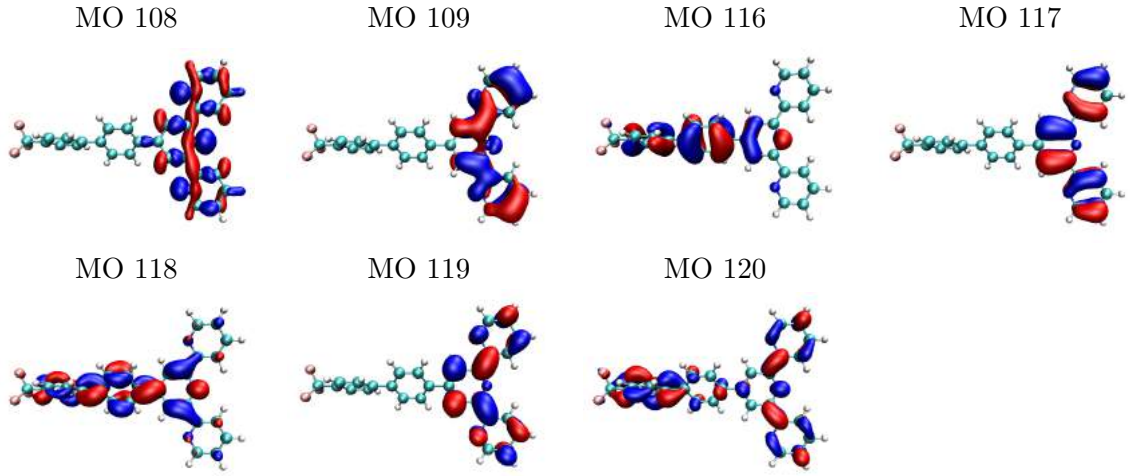


Figure S25: Pictures of orbitals involved in electronic transitions of *modified* cmpd-c computed using CC2

Table S66: ground and excited state dipole moments of compound c as calculated with CC2/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	4.8318	-0.0410	-0.0642
ES1 (GS geom)	6.9757	-0.0346	-0.0670
Δ_{ES-GS}	2.1439	0.0064	-0.0028

5.2 Dihedral angle between rings

Dihedral : 140.7 (CAM-B3LYP optimized)

Table S67: Excitation energies of compound **c** obtained with CC2/cc-pVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
4.3770	35303	283	0.1258	117-118	60%
				116-119	11%
				117-120	10%
4.4692	36048	277	0.0029	108-118	51%
				108-120	16%
4.4888	36205	276	0.2481 10^{-04}	108-119	68 %
				109-119	10%
4.7775	38534	260	1.5199	116-118	63%
				117-119	21%

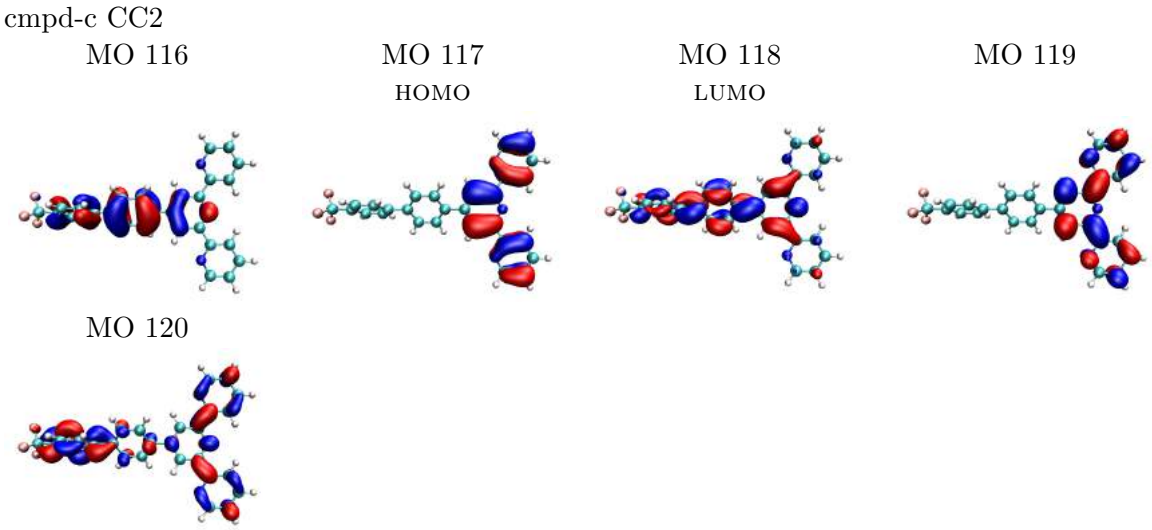


Figure S26: Pictures of orbitals involved in electronic transitions of *modified* cmpd-c computed using CC2

Table S68: ground and excited state dipole moments of compound c as calculated with CC2/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	4.8573	-0.0730	0.0250
ES1 (GS geom)	6.9900	-0.0660	0.0233
Δ_{ES-GS}	2.1327	0.0070	-0.0017

Dihedral : -98.8

Table S69: Excitation energies of compound **c** with dihedral2 = -98.8, obtained with CC2/cc-pVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
4.4025	35509	282	0.1322	117-118	70%
				116-119	13%
4.4874	36194	276	0.0033	108-118	63%
4.8623	39218	255	0.3329	117-119	67%
4.9856	40212	249	0.3398	117-122	18%
				115-119	15%
				116-119	14%

cmpd-c CC2

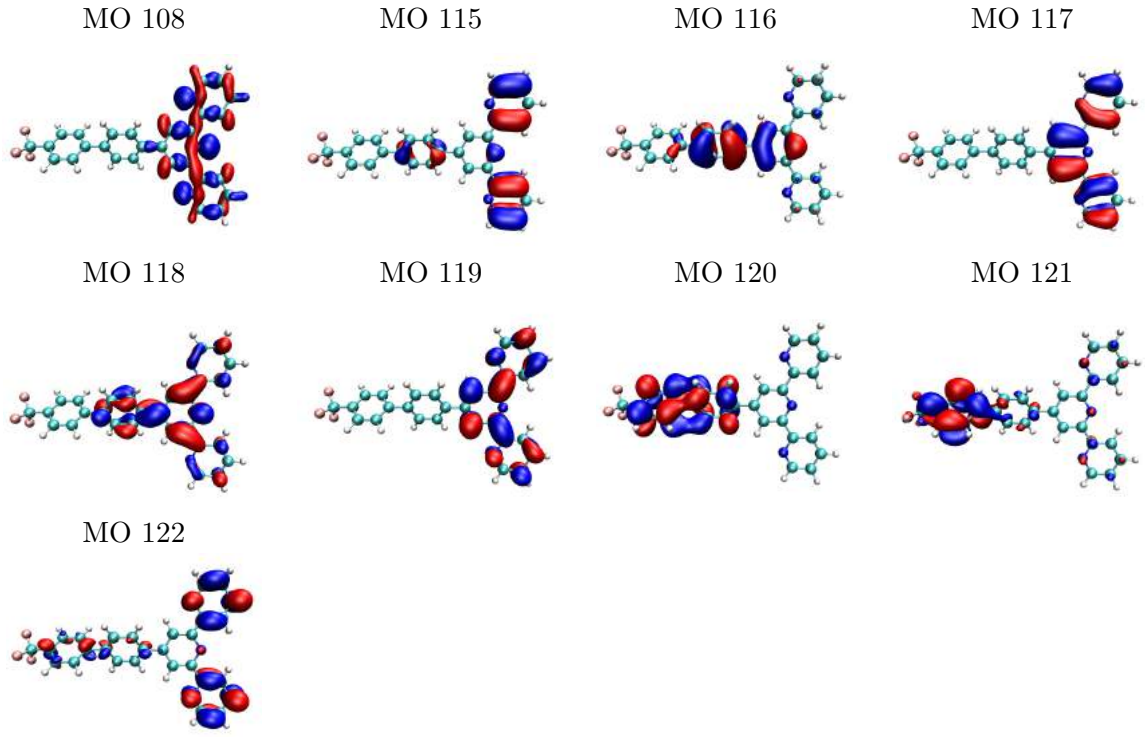


Figure S27: Pictures of orbitals involved in electronic transitions of *modified* cmpd-c computed using CC2

Table S70: ground and excited state dipole moments of compound c as calculated with CC2/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	4.7468	0.0820	0.0572
ES1 (GS geom)	6.2645	0.0860	0.0561
Δ_{ES-GS}	1.5177	0.0040	-0.0011

Dihedral : -127.4

Table S71: Excitation energies of compound **c** with dihedral2 = -127.4, obtained with CC2/cc-pVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
4.3885	35397	283	0.1287	117-118	64%
				116-119	11%
4.4775	36114	277	0.0031	108-118	55%
				108-120	11%
4.4898	36213	276	0.0573 10^{-04}	108-119	68%
				109-119	10%
4.8467	39092	256	0.7241	117-119	60%

cmpd-c CC2

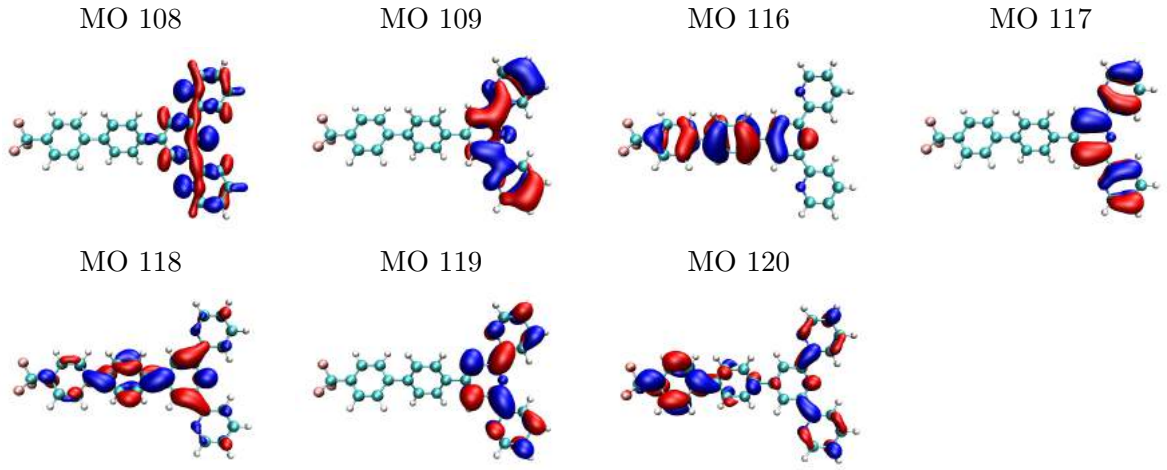


Figure S28: Pictures of orbitals involved in electronic transitions of *modified* cmpd-c computed using CC2

Table S72: ground and excited state dipole moments of compound c as calculated with CC2/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	4.8175	0.0446	0.0829
ES1 (GS geom)	6.7011	0.0501	0.0817
Δ_{ES-GS}	1.8836	0.0055	-0.0012

Dihedral : -178.8

Table S73: Excitation energies of compound **c** with dihedral2 = -178.2, obtained with CC2/cc-pVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
4.3563	35137	285	0.1193	116-118	54%
				116-120	16%
				117-119	10%
4.4530	35917	278	0.0023	108-118	44%
				108-120	22%
4.5498	36698	273	1.5602	117-118	88%
4.6281	37329	268	0.0059	117-121	44%
				114-118	33%

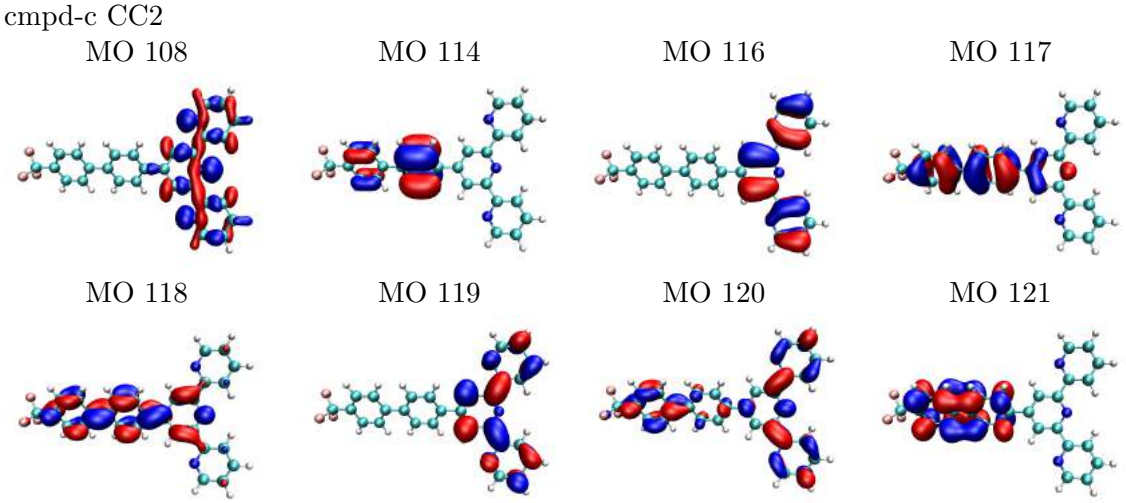


Figure S29: Pictures of orbitals involved in electronic transitions of *modified* cmpd-c computed using CC2

Table S74: ground and excited state dipole moments of compound c as calculated with CC2/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	4.9238	0.0618	-0.0845
ES1 (GS geom)	7.5844	0.0696	-0.0871
Δ_{ES-GS}	2.6606	0.0078	-0.0026

Table S75: Excitation details and relative total energies for different conformations of compound-c as calculated with CC2/cc-pVTZ

Dihedral angle (°)	Excitation number	Excitation energy (eV)	Oscillator strength	Orbitals involved	Weight	ΔE_{tot} kcal/mol
140.7 (opt)	1	4.3770	0.1258	117-118	60%	
	4	4.7775	1.5199	116-118	63%	
-98.8	1	4.4025	0.1322	117-118	70%	2.4143
	> 4					
-127.4	1	4.3885	0.1287	117-118	64%	0.7096
	> 4					
-178.8	1	4.3563	0.1193	116-118	54%	2.4649
	3	4.5498	1.5602	117-118	88%	

6 cmpd-f structure

6.1 Planar arrangement of the rings

Table S76: Excitation energies of compound **f** obtained with ADC(2)/cc-pVTZ

Excitation energy			Oscillator	Orbitals	
eV	cm^{-1}	nm	strength	involved	
4.0280	32489	308	1.6670	172-173	85%
4.3379	34988	286	0.0902	171-173	24%
				172-176	22%
4.3712	35257	284	0.0818	172-176	29%
				171-173	20%
4.4682	36039	277	0.0035	161-173	30%
				161-175	19%
				162-173	14%

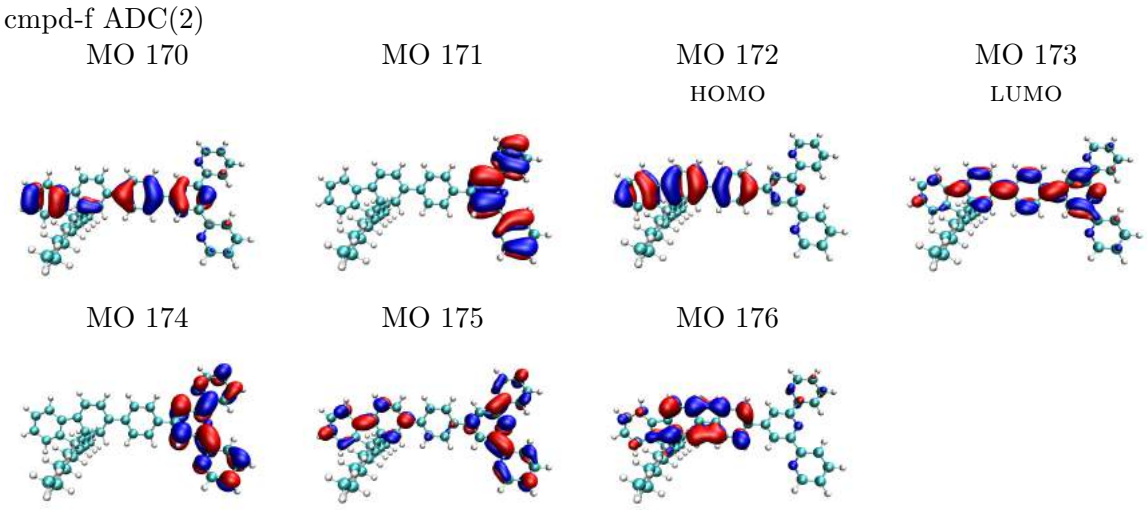


Figure S30: Pictures of orbitals involved in electronic transitions of *modified* cmpd-f computed using CC2

Table S77: ground and excited state dipole moments of compound f as calculated with ADC(2)/cc-pVTZ using TURBOMOLE v6.6

	μ_x (D)	μ_y (D)	μ_z (D)
GS	-1.3287	0.2522	-0.4421
ES1 (GS geom)	5.6312	0.2672	0.4858
Δ_{ES-GS}	6.9599	0.015	0.9279

6.2 Perpendicular arrangement of the rings

Table S78: Excitation energies of compound **f** obtained with ADC(2)/cc-pVTZ

Excitation energy eV	cm^{-1}	nm	Oscillator strength	Orbitals involved	
4.4050	35530	281	0.1350	171-173	68%
				170-174	15%
4.4898	36213	276	0.0141 10^{-04}	160-174	55%
				162-174	23%
4.5861	36990	270	0.3071	172-175	45%
				172-176	16%
				168-175	14%
4.8491	39112	256	0.6411	171-174	64%

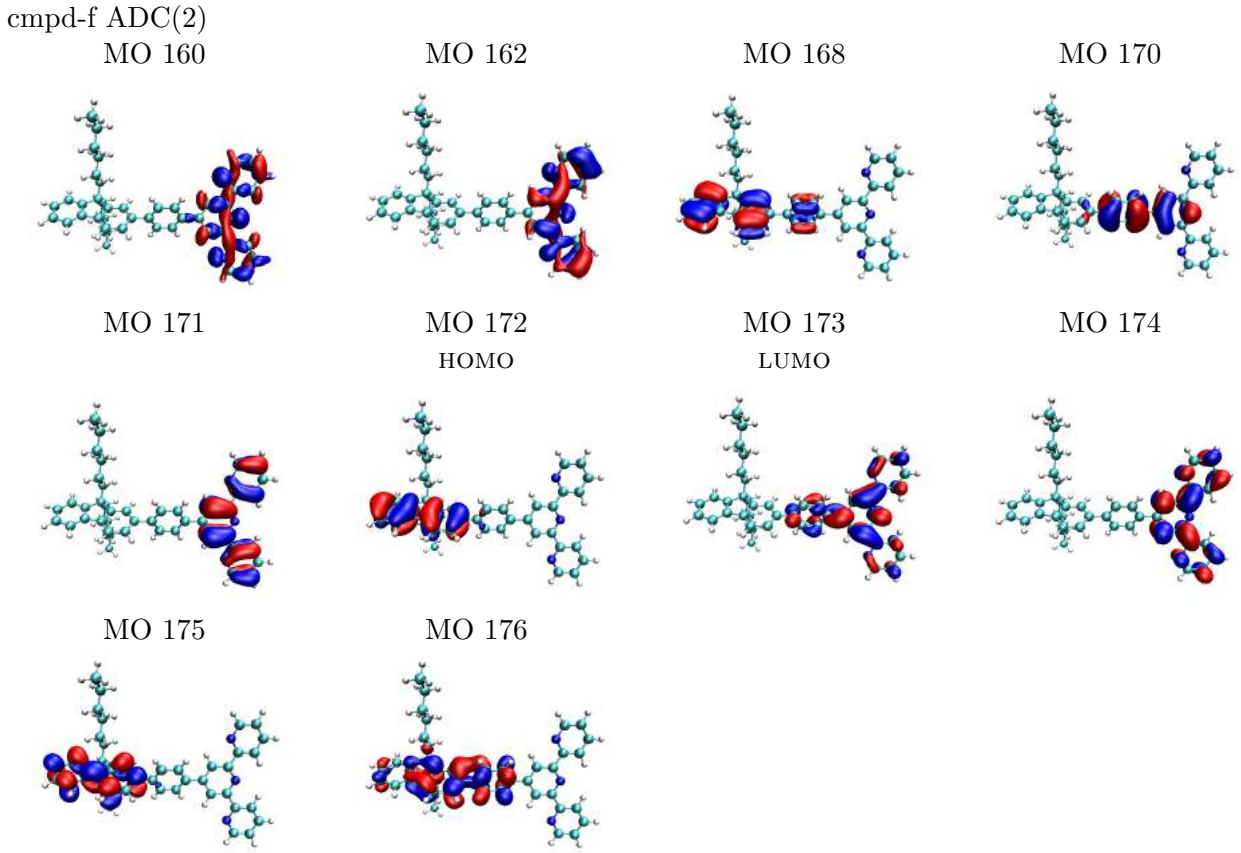


Figure S31: Pictures of orbitals involved in electronic transitions of *modified* cmpd-f computed using CC2

Energy comparison

Table S79: Excitation details and relative total MP2 energies for different conformations of compound-f as calculated with ADC(2)/cc-pVTZ

Orientation	Excitation number	Excitation energy (eV)	Oscillator strength	Orbitals involved	Weight	ΔE_{tot} kcal/mol
OPT	1	4.2664	1.5744	172-173	73 %	
				172-175	14%	
Planar	1	4.0280	1.6670	172-173	85%	2.5893
Perpendicular	> 4	n/a			%	2.7373

7 Cartesian structures of compounds

7.1 compound a

Table S80: Cartesian coordinates of compound **a** optimized with CAM-B3LYP/cc-pVTZ using GAUSSIAN09

N	-2.834403	1.636443	0.000000
C	-2.813199	0.308230	0.000000
C	-1.634581	-0.420626	0.000000
C	-0.410036	0.236734	0.000000
C	-0.453018	1.625901	0.000000
C	-1.673535	2.282186	0.000000
C	-4.126982	-0.393679	0.000000
H	-1.717693	-1.493260	0.000000
C	0.875637	-0.505549	0.000000
H	0.434355	2.234195	0.000000
C	-1.722555	3.770911	0.000000
C	-2.938437	4.444743	0.000000
C	-2.936237	5.824532	0.000000
C	-1.726160	6.494227	0.000000
C	-0.566314	5.740463	0.000000
N	-0.557754	4.416121	0.000000
H	-3.854108	3.876422	0.000000
H	-3.868732	6.372135	0.000000
H	-1.676923	7.573272	0.000000
H	0.403013	6.224986	0.000000
N	-4.103350	-1.725031	0.000000
C	-5.254544	-2.379789	0.000000
C	-6.487246	-1.752214	0.000000
C	-6.512312	-0.369410	0.000000
C	-5.318479	0.322390	0.000000
H	-5.189490	-3.461512	0.000000
H	-7.397107	-2.334377	0.000000
H	-7.452797	0.164353	0.000000
H	-5.284134	1.399545	0.000000
C	2.101525	0.153770	0.000000
C	3.295781	-0.536619	0.000000
C	3.341708	-1.929336	0.000000
C	2.112616	-2.585921	0.000000
C	0.917593	-1.896859	0.000000
H	2.140557	1.231963	0.000000
H	4.207009	0.040290	0.000000
C	4.629986	-2.673124	0.000000
H	2.068612	-3.663522	0.000000
H	0.003366	-2.469758	0.000000
C	4.665900	-4.067460	0.000000
C	5.861990	-4.760387	0.000000
C	7.066091	-4.079609	0.000000
C	7.053611	-2.696438	0.000000

C	5.855473	-2.007058	0.000000
H	3.749525	-4.636304	0.000000
H	5.849843	-5.841574	0.000000
H	8.002144	-4.620039	0.000000
H	7.983873	-2.145324	0.000000
H	5.889919	-0.929032	0.000000

7.2 compound b

Table S81: Cartesian coordinates of compound **b** optimized with CAM-B3LYP/cc-pVTZ using GAUSSIAN09

N	-2.842528	1.641320	0.000000
C	-2.811320	0.313401	0.000000
C	-1.626888	-0.406154	0.000000
C	-0.408117	0.261386	0.000000
C	-0.461221	1.649979	0.000000
C	-1.687003	2.296609	0.000000
C	-4.119478	-0.398821	0.000000
H	-1.701523	-1.479437	0.000000
C	0.883381	-0.470803	0.000000
H	0.421627	2.264877	0.000000
C	-1.747674	3.784850	0.000000
C	-2.968499	4.449494	0.000000
C	-2.976348	5.829324	0.000000
C	-1.771221	6.507797	0.000000
C	-0.605746	5.762655	0.000000
N	-0.587621	4.438442	0.000000
H	-3.880082	3.874627	0.000000
H	-3.912796	6.370118	0.000000
H	-1.729919	7.587168	0.000000
H	0.360015	6.254177	0.000000
N	-4.085067	-1.729962	0.000000
C	-5.231027	-2.393883	0.000000
C	-6.468677	-1.776130	0.000000
C	-6.504841	-0.393586	0.000000
C	-5.316569	0.307754	0.000000
H	-5.157420	-3.475049	0.000000
H	-7.373854	-2.365535	0.000000
H	-7.449559	0.132620	0.000000
H	-5.290879	1.385153	0.000000
C	2.103881	0.193709	0.000000
C	3.308310	-0.482553	0.000000
C	3.365690	-1.877321	0.000000
C	2.136342	-2.539929	0.000000
C	0.936958	-1.861960	0.000000
H	2.136974	1.272110	0.000000
H	4.209743	0.100921	0.000000
C	4.640140	-2.646723	0.000000
H	2.089592	-3.616649	0.000000

H	0.028518	-2.443879	0.000000
C	4.636695	-4.046602	0.000000
C	5.781911	-4.814672	0.000000
C	7.001130	-4.174994	0.000000
C	7.086137	-2.804946	0.000000
C	5.914028	-2.077939	0.000000
H	3.695897	-4.570445	0.000000
H	5.736451	-5.893036	0.000000
F	8.128048	-4.896992	0.000000
H	8.037789	-2.296687	0.000000
F	6.076619	-0.743803	0.000000

7.3 compound c

Table S82: Cartesian coordinates of compound **c** optimized with CAM-B3LYP/cc-pVTZ using GAUSSIAN09

N	4.472790	0.005393	-0.000916
C	3.791980	1.146004	-0.035181
C	2.405736	1.184871	-0.036377
C	1.690217	-0.003305	0.001485
C	2.413215	-1.186985	0.038120
C	3.799182	-1.139451	0.034528
C	4.578971	2.409166	-0.081527
H	1.916274	2.143801	-0.085729
C	0.211332	-0.007910	0.002697
H	1.929845	-2.148959	0.088302
C	4.594146	-2.397662	0.079482
C	5.982443	-2.364181	0.137621
C	6.676531	-3.556163	0.177717
C	5.970504	-4.745183	0.158985
C	4.589794	-4.680933	0.101320
N	3.914381	-3.542438	0.062442
H	6.485531	-1.411165	0.151529
H	7.756912	-3.557831	0.223845
H	6.472358	-5.701216	0.188886
H	3.998248	-5.588734	0.085535
N	3.892075	3.549655	-0.063173
C	4.560258	4.692365	-0.103252
C	5.940431	4.765270	-0.163479
C	6.653863	3.580703	-0.183571
C	5.967339	2.384388	-0.142238
H	3.963059	5.596437	-0.086331
H	6.436223	5.724432	-0.194275
H	7.734125	3.589148	-0.231708
H	6.476369	1.434548	-0.157122
C	-0.502269	-1.004416	-0.655152
C	-1.882934	-1.005972	-0.657906
C	-2.602447	-0.016575	0.004828
C	-1.888015	0.977219	0.666526

C	-0.507396	0.984171	0.661691
H	0.029512	-1.782761	-1.183803
H	-2.410233	-1.800101	-1.167742
C	-4.081201	-0.020481	0.005845
H	-2.419519	1.768025	1.177179
H	0.020386	1.765798	1.189508
C	-4.795663	0.324680	1.149845
C	-6.176614	0.320644	1.154657
C	-6.869828	-0.031878	0.009228
C	-6.176423	-0.377927	-1.138168
C	-4.795577	-0.372163	-1.136273
H	-4.263087	0.575763	2.055876
H	-6.716842	0.576924	2.054037
C	-8.366969	0.009213	-0.004392
H	-6.716632	-0.651474	-2.032517
H	-4.263071	-0.625643	-2.041679
F	-8.888588	-0.885722	-0.856259
F	-8.890037	-0.240080	1.204970
F	-8.828910	1.214655	-0.382559

7.4 compound d

Table S83: Cartesian coordinates of compound **d** optimized with CAM-B3LYP/cc-pVTZ using GAUSSIAN09

N	-0.439725	-3.829803	0.000000
C	-1.503134	-3.033559	0.000000
C	-1.402642	-1.651555	0.000000
C	-0.152264	-1.044225	0.000000
C	0.947747	-1.894109	0.000000
C	0.763859	-3.267504	0.000000
C	-2.841953	-3.686542	0.000000
H	-2.320255	-1.089912	0.000000
C	0.000000	0.431908	0.000000
H	1.960726	-1.531732	0.000000
C	1.941034	-4.180239	0.000000
C	1.773562	-5.560332	0.000000
C	2.892145	-6.368062	0.000000
C	4.144483	-5.781080	0.000000
C	4.214419	-4.399635	0.000000
N	3.146997	-3.615650	0.000000
H	0.776067	-5.968304	0.000000
H	2.788465	-7.444491	0.000000
H	5.047208	-6.374269	0.000000
H	5.175497	-3.898890	0.000000
N	-3.907022	-2.887355	0.000000
C	-5.112172	-3.436532	0.000000
C	-5.326083	-4.803120	0.000000
C	-4.220195	-5.633714	0.000000
C	-2.960092	-5.071713	0.000000

H	-5.950564	-2.749877	0.000000
H	-6.331003	-5.199242	0.000000
H	-4.338767	-6.708604	0.000000
H	-2.067074	-5.675004	0.000000
C	1.252762	1.039316	0.000000
C	1.393743	2.411226	0.000000
C	0.292625	3.266390	0.000000
C	-0.959737	2.654391	0.000000
C	-1.101951	1.282209	0.000000
H	2.149332	0.438991	0.000000
H	2.395665	2.811054	0.000000
C	0.444513	4.743267	0.000000
H	-1.858836	3.250310	0.000000
H	-2.102301	0.877849	0.000000
C	-0.663345	5.596929	0.000000
C	-0.530040	6.965399	0.000000
C	0.731798	7.549037	0.000000
C	1.849324	6.729368	0.000000
C	1.693549	5.352748	0.000000
H	-1.663168	5.191908	0.000000
H	-1.397741	7.609171	0.000000
O	0.767564	8.902492	0.000000
H	2.844749	7.144545	0.000000
H	2.591072	4.754078	0.000000
C	2.025731	9.539752	0.000000
H	1.825302	10.606706	0.000000
H	2.603624	9.282657	0.890298
H	2.603624	9.282657	-0.890298

7.5 compound e

Table S84: Cartesian coordinates of compound **e** optimized with CAM-B3LYP/cc-pVTZ using GAUSSIAN09

C	-7.874028	2.725646	0.902262
C	-6.489363	2.628713	0.824814
N	-5.690264	3.635599	1.171999
C	-6.239400	4.761178	1.602623
C	-7.605563	4.948805	1.711810
C	-8.435887	3.902830	1.352048
C	-5.835384	1.379483	0.346113
C	-4.452940	1.274436	0.330871
C	-3.861220	0.099935	-0.113103
C	-4.703505	-0.924112	-0.523651
C	-6.076889	-0.739911	-0.474947
N	-6.630519	0.390590	-0.048829
C	-6.997087	-1.824080	-0.916810
C	-8.373814	-1.631404	-0.929974
C	-9.187658	-2.664525	-1.347225
C	-8.609742	-3.858367	-1.739231

C	-7.230807	-3.958588	-1.694077
N	-6.440994	-2.973203	-1.295189
C	-2.391459	-0.054175	-0.147428
C	-1.563726	1.022853	-0.447421
C	-0.191079	0.877635	-0.482266
C	0.412249	-0.348110	-0.213747
C	-0.418897	-1.423720	0.087623
C	-1.791881	-1.280954	0.118436
C	1.882817	-0.502647	-0.245707
C	2.534466	-1.291546	0.691531
C	3.913445	-1.424493	0.648537
C	4.649941	-0.762945	-0.349674
C	4.015845	0.032515	-1.294575
C	2.643416	0.149586	-1.227014
N	5.990274	-1.051904	-0.197017
C	6.137238	-1.876608	0.901773
C	4.871846	-2.140045	1.457133
C	4.767719	-2.961266	2.571641
C	5.914263	-3.503199	3.116950
C	7.162756	-3.230172	2.557795
C	7.293799	-2.416511	1.449526
H	-4.320816	-1.858858	-0.899458
H	-3.867765	2.107496	0.684434
H	-8.476891	1.880947	0.611474
H	-9.510333	4.003398	1.422165
H	-8.001606	5.888037	2.069316
H	-5.553001	5.554483	1.874563
H	-6.737081	-4.875793	-1.993047
H	-9.207978	-4.693537	-2.073031
H	-10.261677	-2.539835	-1.367246
H	-8.774405	-0.681379	-0.616128
H	-1.999744	1.986953	-0.668728
H	0.425605	1.737342	-0.704338
H	0.016479	-2.393747	0.283177
H	-2.407403	-2.134985	0.364082
H	1.966617	-1.782830	1.469853
H	4.569132	0.545948	-2.067697
H	2.134382	0.747576	-1.969733
H	8.268543	-2.209342	1.031889
H	8.048514	-3.662418	3.002298
H	5.847991	-4.142923	3.985284
H	3.801224	-3.173237	3.008499
C	7.063701	-0.526734	-1.006756
H	7.851771	-1.278994	-1.055077
H	6.693042	-0.406947	-2.025356
C	7.629061	0.792957	-0.495944
C	8.757131	1.317482	-1.371362
H	6.823709	1.528822	-0.445730
H	7.985002	0.654851	0.527174

C	9.337493	2.635710	-0.879894
H	9.554809	0.570334	-1.423710
H	8.394287	1.443685	-2.395902
C	10.466405	3.163972	-1.753410
H	8.541410	3.384018	-0.827751
H	9.701766	2.510915	0.143903
C	11.039190	4.481581	-1.253512
H	11.261287	2.415571	-1.804807
H	10.101356	3.288314	-2.776078
H	11.844278	4.837078	-1.895696
H	10.272366	5.256705	-1.223123
H	11.440936	4.377557	-0.244777

7.6 compound f

Table S85: Cartesian coordinates of compound **f** optimized with CAM-B3LYP/cc-pVTZ using GAUSSIAN09

C	4.912986	0.020060	-0.537586
C	3.775200	-0.075520	0.464343
C	4.262937	-0.230435	1.761418
C	5.726283	-0.241201	1.709314
C	6.119088	-0.096777	0.378172
C	3.386389	-0.345940	2.825891
C	2.024976	-0.307487	2.583160
C	1.520770	-0.153213	1.291724
C	2.418733	-0.035929	0.229315
C	7.458480	-0.075993	0.048506
C	8.405542	-0.200128	1.056309
C	8.012884	-0.343476	2.379267
C	6.669006	-0.365256	2.715718
C	0.061734	-0.114495	1.053173
C	-0.491708	0.752017	0.114648
C	-1.853991	0.790619	-0.106755
C	-2.718292	-0.041712	0.597023
C	-2.167424	-0.911047	1.532996
C	-0.805717	-0.943926	1.758570
C	-4.176769	-0.003498	0.357909
C	-4.949110	-1.154365	0.429933
C	-6.314309	-1.075748	0.200297
N	-6.923610	0.068464	-0.092095
C	-6.195353	1.177622	-0.165412
C	-4.826060	1.184607	0.052930
C	-7.159525	-2.299874	0.267017
C	-8.518669	-2.246150	-0.019763
C	-9.262111	-3.406141	0.055288
C	-8.633156	-4.584883	0.412767
C	-7.276373	-4.542852	0.679226
N	-6.554023	-3.435000	0.610167
C	-6.911635	2.442661	-0.487786

N	-6.171084	3.542185	-0.612444
C	-6.776329	4.684841	-0.898669
C	-8.143510	4.798598	-1.076135
C	-8.913039	3.656835	-0.945724
C	-8.292414	2.461085	-0.647543
H	-4.515926	-2.118059	0.642302
H	-4.299230	2.123163	-0.002002
H	-8.846950	1.543966	-0.533949
H	-9.985968	3.698160	-1.074330
H	-8.586808	5.755785	-1.308670
H	-6.136617	5.554658	-0.991205
H	-6.744418	-5.443628	0.962066
H	-9.175664	-5.516225	0.484030
H	-10.321050	-3.391325	-0.163469
H	-8.960866	-1.302655	-0.295086
H	-2.251031	1.470189	-0.847681
H	0.152852	1.420687	-0.438538
H	-0.406189	-1.639529	2.483137
H	-2.814292	-1.563088	2.102922
H	1.335969	-0.374658	3.413301
H	2.038740	0.061744	-0.779247
H	7.776187	0.035147	-0.980212
H	9.458006	-0.185127	0.809045
H	8.762273	-0.438921	3.152719
H	6.367278	-0.477370	3.748438
C	4.897253	1.361362	-1.298996
C	4.864781	-1.122356	-1.572905
H	3.751520	-0.458019	3.837906
H	5.744943	1.366315	-1.989288
H	4.000757	1.382976	-1.924376
C	4.941665	2.620719	-0.445353
C	4.921272	3.892858	-1.282007
H	4.094012	2.629491	0.242907
H	5.839923	2.613071	0.175269
C	4.964991	5.164837	-0.447852
H	5.769294	3.886526	-1.973456
H	4.022945	3.902854	-1.906747
C	4.944872	6.439001	-1.280192
H	4.117366	5.172973	0.243725
H	5.863133	5.156697	0.176711
C	4.988828	7.703931	-0.436124
H	5.792242	6.430518	-1.970592
H	4.047168	6.446650	-1.903748
H	4.973413	8.600261	-1.055599
H	4.134865	7.753770	0.240773
H	5.892778	7.737534	0.173554
H	5.715575	-0.999802	-2.248394
C	4.870948	-2.538144	-1.014285
H	3.971057	-0.983179	-2.186891

C	4.825500	-3.595867	-2.108767
H	5.764046	-2.689556	-0.404650
H	4.017297	-2.674572	-0.347323
C	4.829741	-5.019997	-1.572624
H	3.932462	-3.445196	-2.722727
H	5.679411	-3.461313	-2.779635
C	4.785331	-6.080469	-2.663553
H	5.722020	-5.172375	-0.958212
H	3.975654	-5.156478	-0.902790
C	4.789829	-7.500018	-2.116474
H	3.893464	-5.927840	-3.276690
H	5.638977	-5.943737	-3.332410
H	4.757702	-8.238553	-2.917062
H	5.686965	-7.689997	-1.525661
H	3.928582	-7.673980	-1.470001

7.7 compound g

Table S86: Cartesian coordinates of compound **g** optimized with CAM-B3LYP/cc-pVTZ using GAUSSIAN09

C	-1.454820	-0.825642	0.859488
C	-2.172323	0.000000	0.000000
C	-1.454820	0.825642	-0.859488
C	-0.074190	0.823134	-0.861110
C	0.646312	0.000000	0.000000
C	-0.074190	-0.823133	0.861110
C	-3.650680	0.000000	0.000000
C	-4.371379	-1.163223	0.232031
C	-5.757291	-1.120580	0.224992
N	-6.435289	0.000000	0.000000
C	-5.757291	1.120580	-0.224992
C	-4.371379	1.163223	-0.232031
C	-6.548765	-2.358579	0.466427
N	-5.866654	-3.469432	0.737779
C	-6.539630	-4.588628	0.957795
C	-7.920267	-4.666597	0.920919
C	-8.629000	-3.513068	0.638255
C	-7.937538	-2.341580	0.407256
C	-6.548765	2.358579	-0.466427
C	-7.937538	2.341580	-0.407256
C	-8.629000	3.513068	-0.638255
C	-7.920267	4.666597	-0.920920
C	-6.539630	4.588628	-0.957794
N	-5.866654	3.469432	-0.737779
H	-3.884811	-2.109924	0.400738
H	-3.884811	2.109924	-0.400738
H	-8.442678	1.416678	-0.181643
H	-9.709554	3.526613	-0.597588
H	-8.419991	5.605750	-1.108184

H	-5.945808	5.468757	-1.174903
H	-5.945808	-5.468757	1.174903
H	-8.419990	-5.605750	1.108184
H	-9.709554	-3.526613	0.597588
H	-8.442678	-1.416679	0.181643
H	-1.983755	1.471238	-1.546411
H	0.454431	1.486166	-1.531622
C	2.124153	0.000000	0.000000
H	0.454431	-1.486166	1.531622
H	-1.983755	-1.471238	1.546411
C	2.847055	-0.120707	1.183359
C	4.227316	-0.127542	1.187821
C	4.940870	0.000000	0.000000
C	4.227316	0.127542	-1.187821
C	2.847055	0.120707	-1.183359
H	2.320607	-0.200476	2.124299
H	4.761143	-0.223447	2.121940
N	6.351820	0.000000	0.000000
H	4.761143	0.223447	-2.121940
H	2.320607	0.200477	-2.124298
C	7.060592	-0.678304	-1.018227
C	7.060592	0.678303	1.018227
C	6.645169	-1.932530	-1.454943
C	7.337275	-2.589074	-2.455607
C	8.461815	-2.016833	-3.026069
C	8.882832	-0.772588	-2.587921
C	8.186606	-0.102831	-1.598897
H	5.775077	-2.389657	-1.006609
H	6.999830	-3.563004	-2.782478
H	9.004362	-2.535136	-3.803694
H	9.755688	-0.310094	-3.027793
H	8.514508	0.872174	-1.268944
C	8.186606	0.102830	1.598897
C	8.882832	0.772588	2.587921
C	8.461815	2.016833	3.026069
C	7.337275	2.589074	2.455607
C	6.645169	1.932530	1.454942
H	8.514508	-0.872175	1.268944
H	9.755688	0.310094	3.027794
H	9.004362	2.535136	3.803694
H	6.999830	3.563004	2.782478
H	5.775077	2.389657	1.006609