Supporting Information

Synthesis, photophysical and biological properties of new oxazolone fluorescent probe for bioimaging: experimental and theoretical study

Przemysław Krawczyk[1*], Beata Jędrzejewska[2], Piotr Cysewski[1], Tomasz Janek[3]

[1] Nicolaus Copernicus University, Collegium Medicum, Faculty of Pharmacy, Department of Physical Chemistry, Kurpińskiego 5, 85-950 Bydgoszcz, Poland

[2] UTP University of Science and Technology, Faculty of Chemical Technology and Engineering, Seminaryjna 3, 85-326 Bydgoszcz, Poland

[3] Wroclaw Medical University, Department of Inorganic Chemistry, Faculty of Pharmacy, Borowska 211a, 50-556 Wroclaw, Poland

*Corresponding author: przemekk@cm.umk.pl; tel: +48 52 5853679

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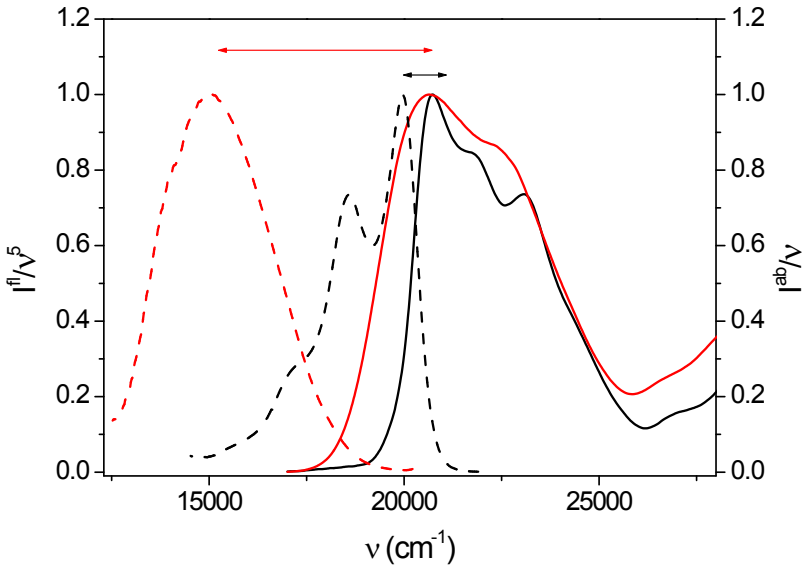

Figure S1. Normalized and sales electronic absorption and fluorescence spectra of PB3 in MCH (black) and DMF (red)

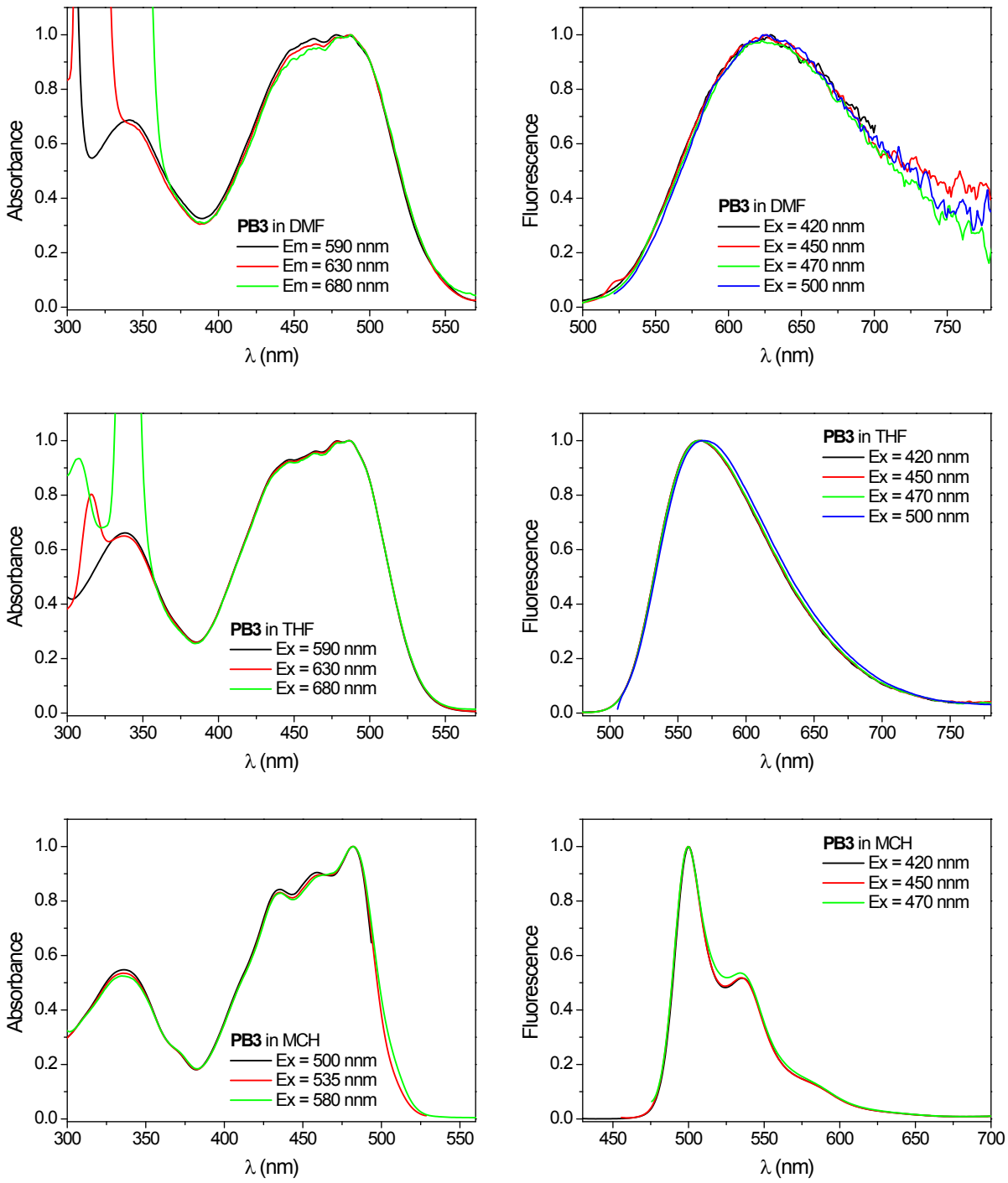

Figure S2. Fluorescence emission (left panel) and fluorescence excitation (right panel) spectra of P**K**3 in DMF, THF and MCH at room temperature

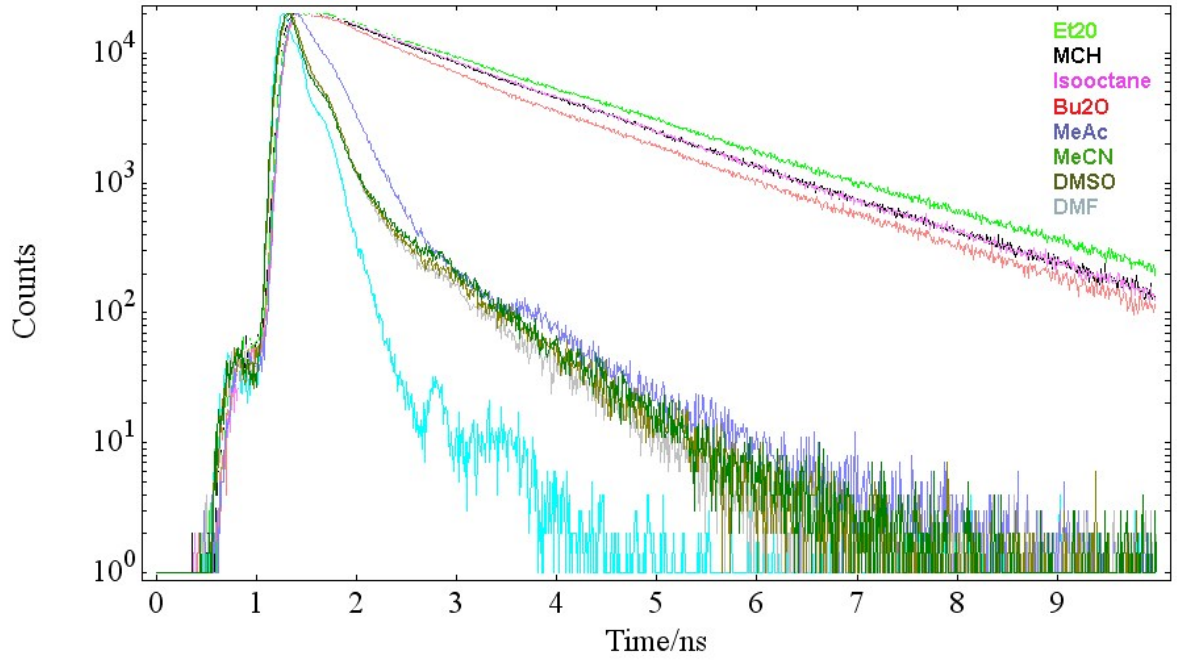

Figure S3. The fluorescence decay curves of compound PB3 recorded in solvents of different polarity; λ_{EX} = 466 nm; λ_{EM} = 560 or 630 nm, respectively. Cyan line is the instrument response function (IRF)

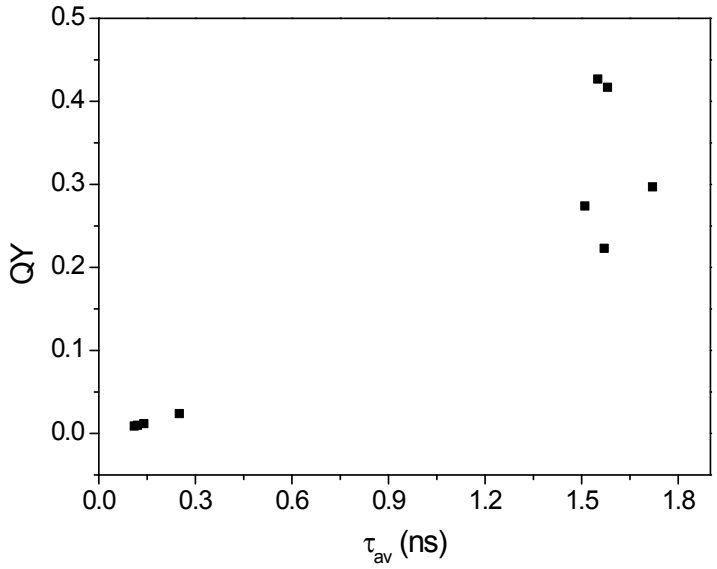

Figure S4. The fluorescence lifetime vs. its quantum yield for compound PB3 in solvents of different polarity

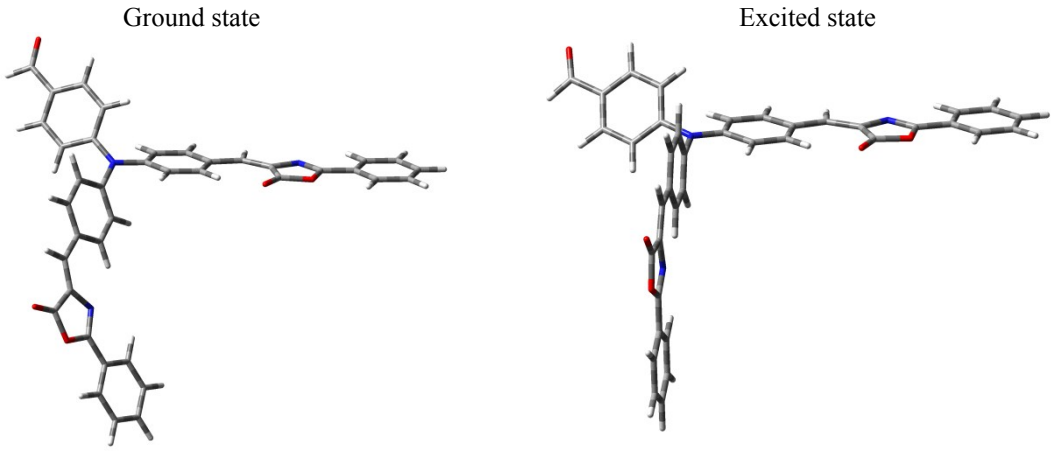

Figure S5. Optimized structures of PB3 in gas phase

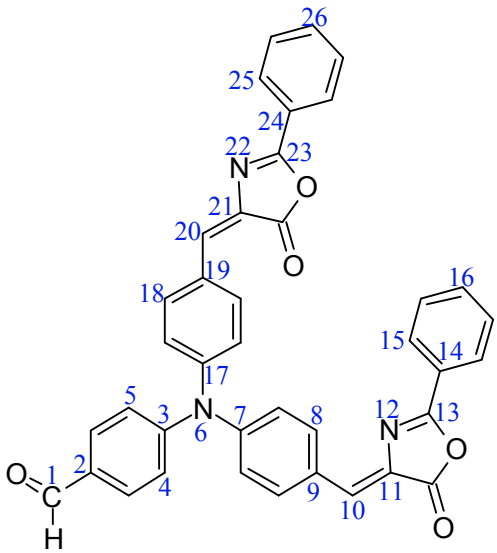

Figure S6. The scheme of atoms numbering

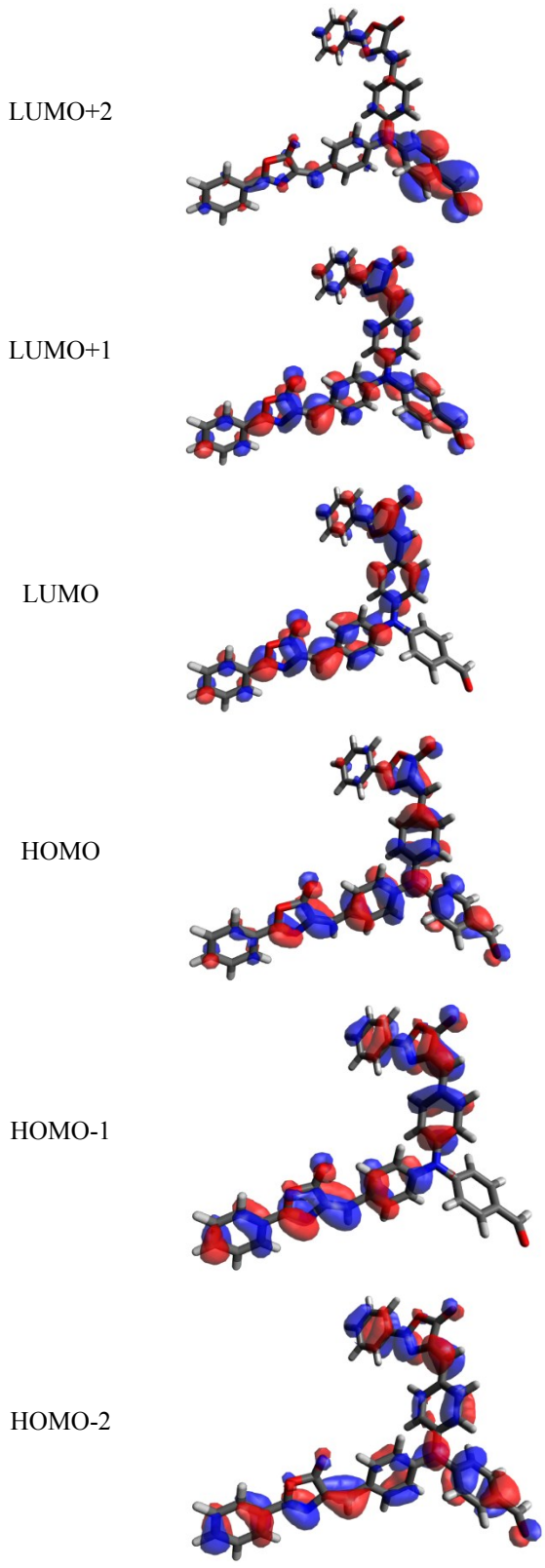

Figure S7. HOMO / LUMO plots for PB3 dyes

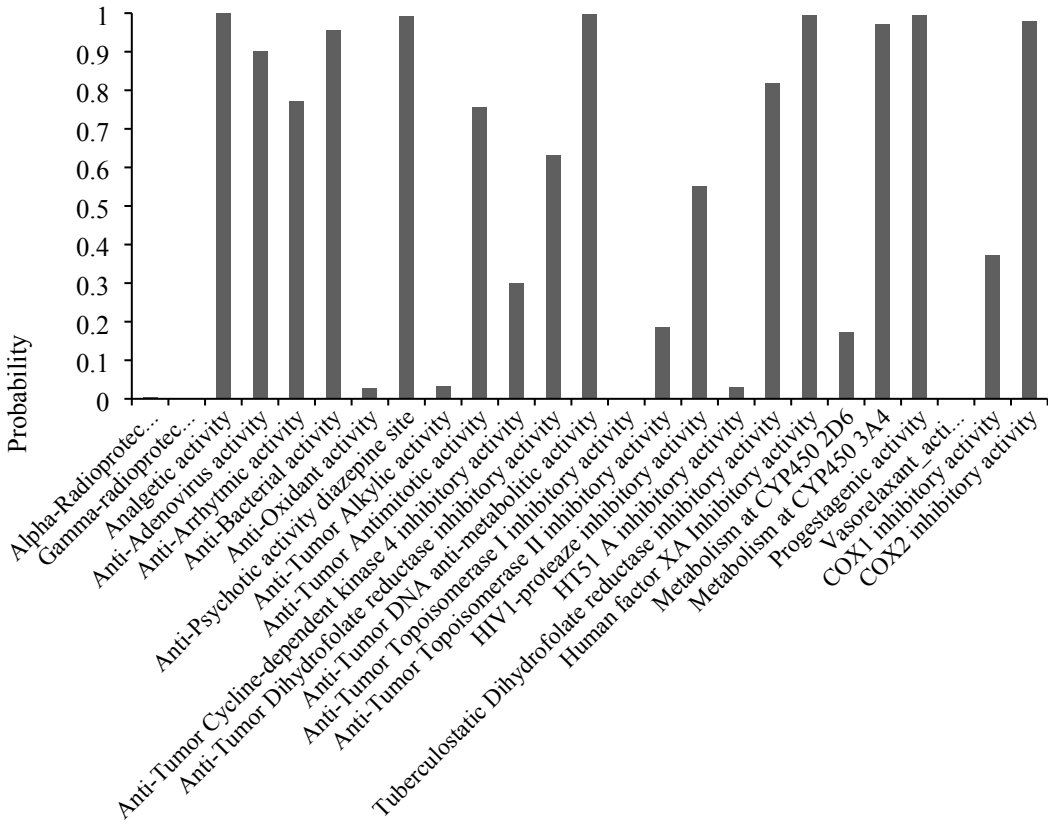

Figure S8. Calculated probability of the biological activity for the PB3 dye

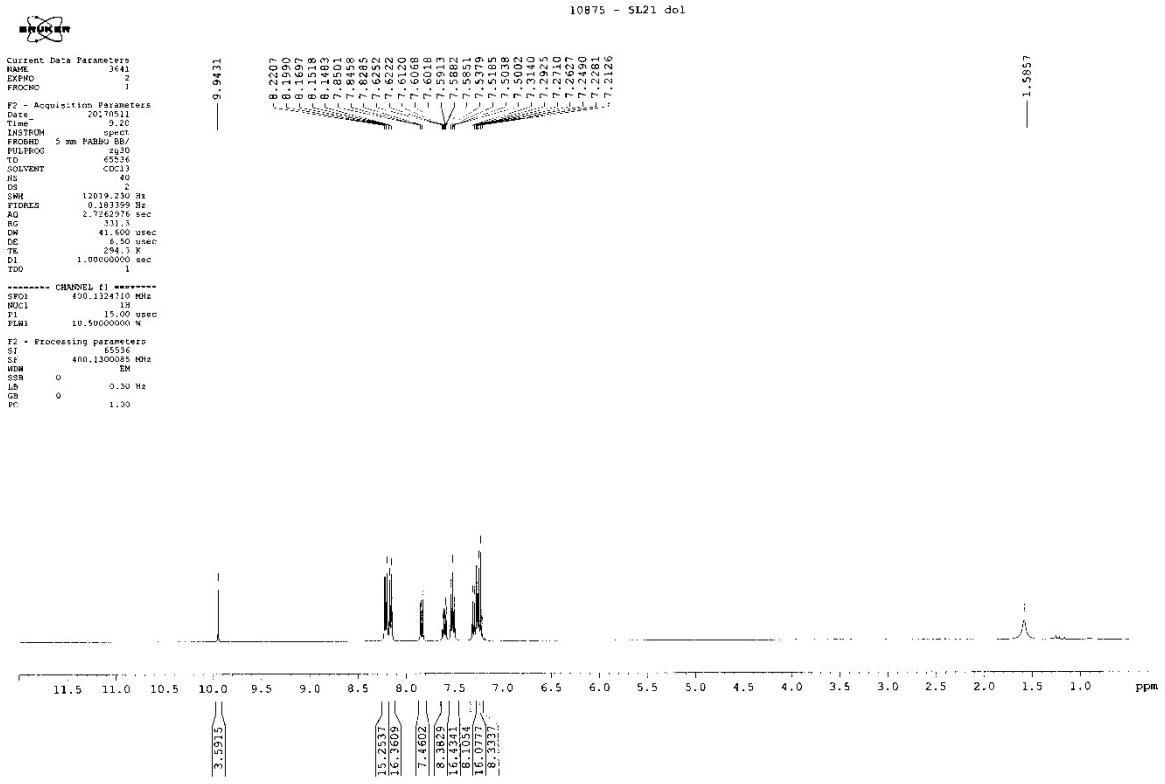

Figure S9. ^{1}H spectrum of PB3

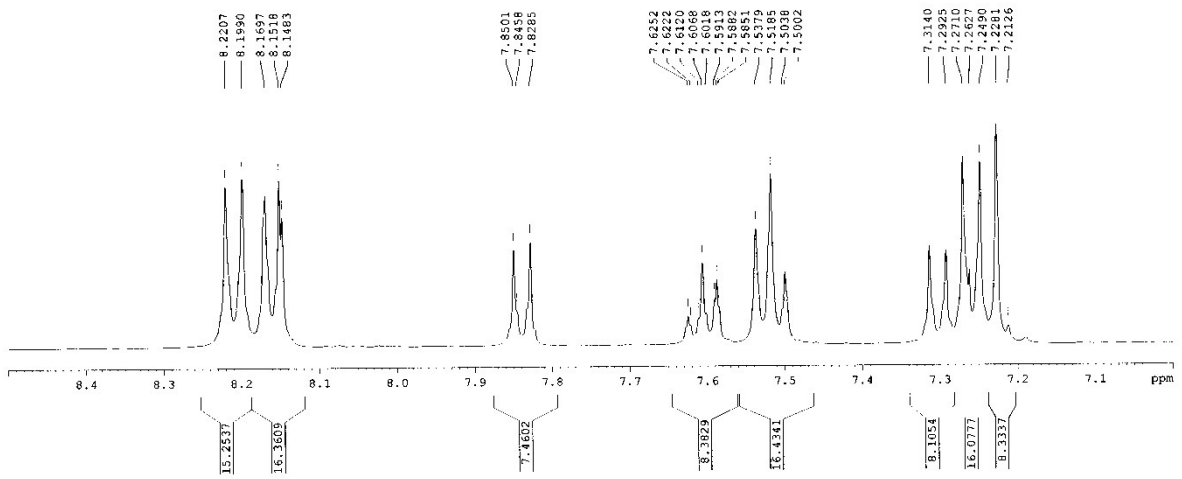

Figure S10. Enlarged spectrum in the range of 7.0 – 10.5 ppm

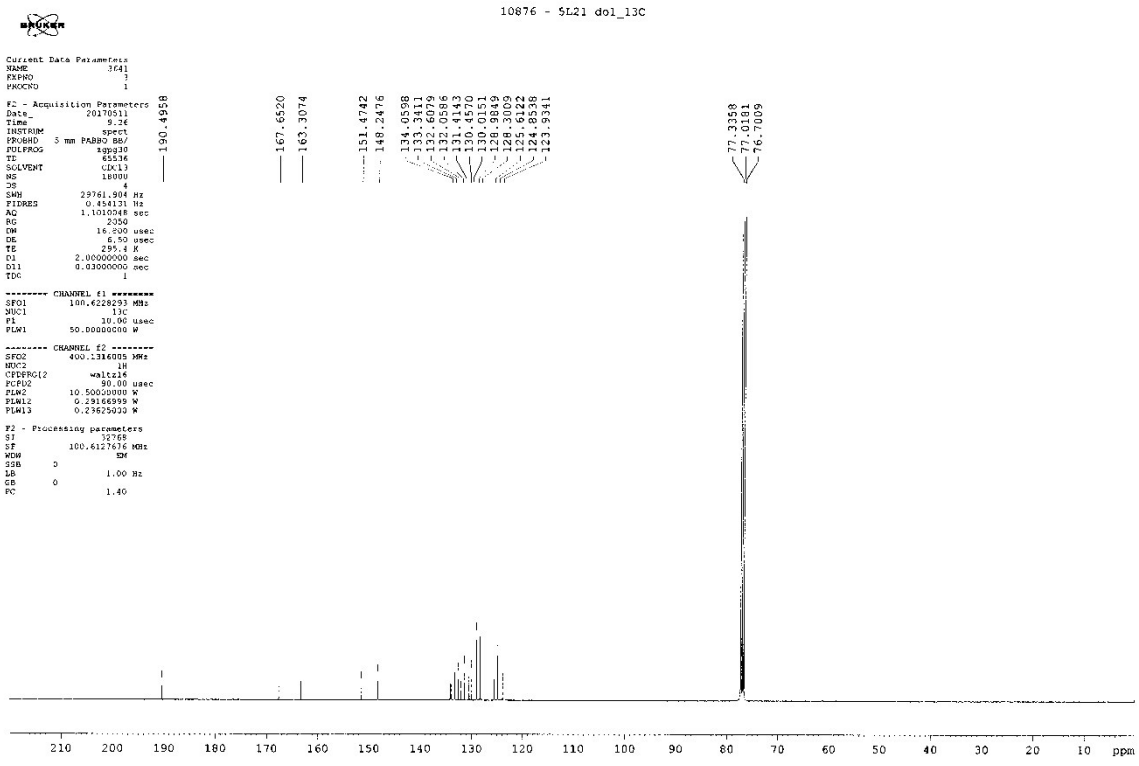

Figure S11. ^{13}C spectrum of PB3

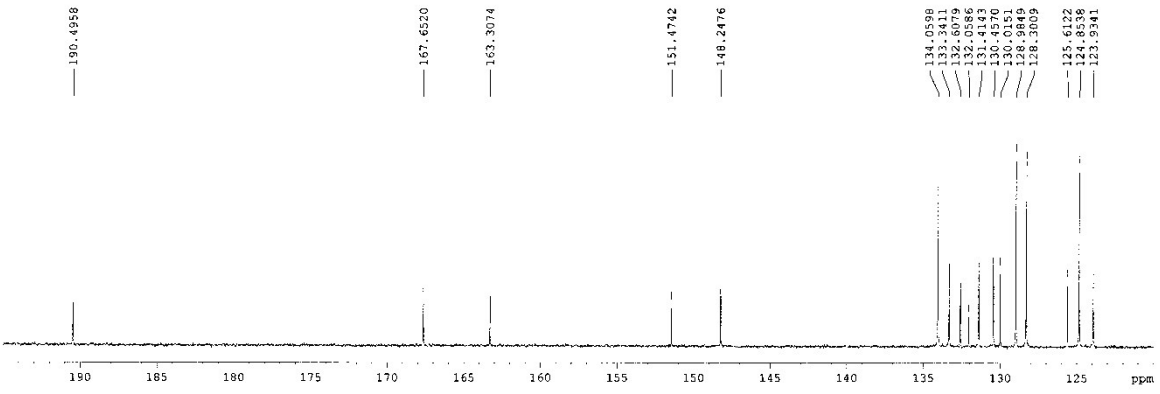

Figure S12. Enlarged spectrum in the range of 120 - 200 ppm

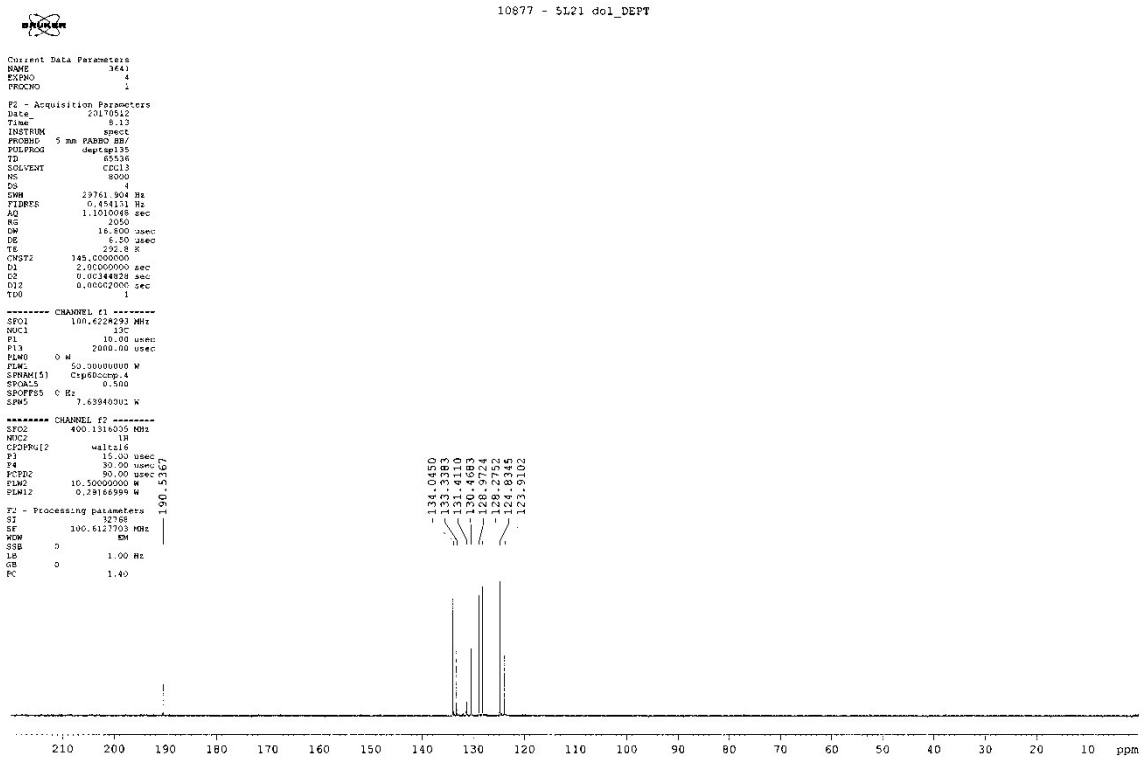

Figure S13. ^{13}C dept spectrum of PB3

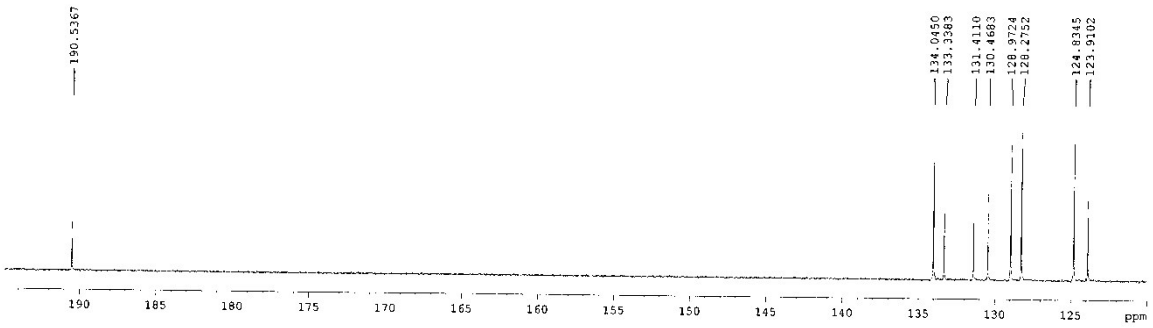

Figure S14. Enlarged spectrum in the range of 120 - 200 ppm

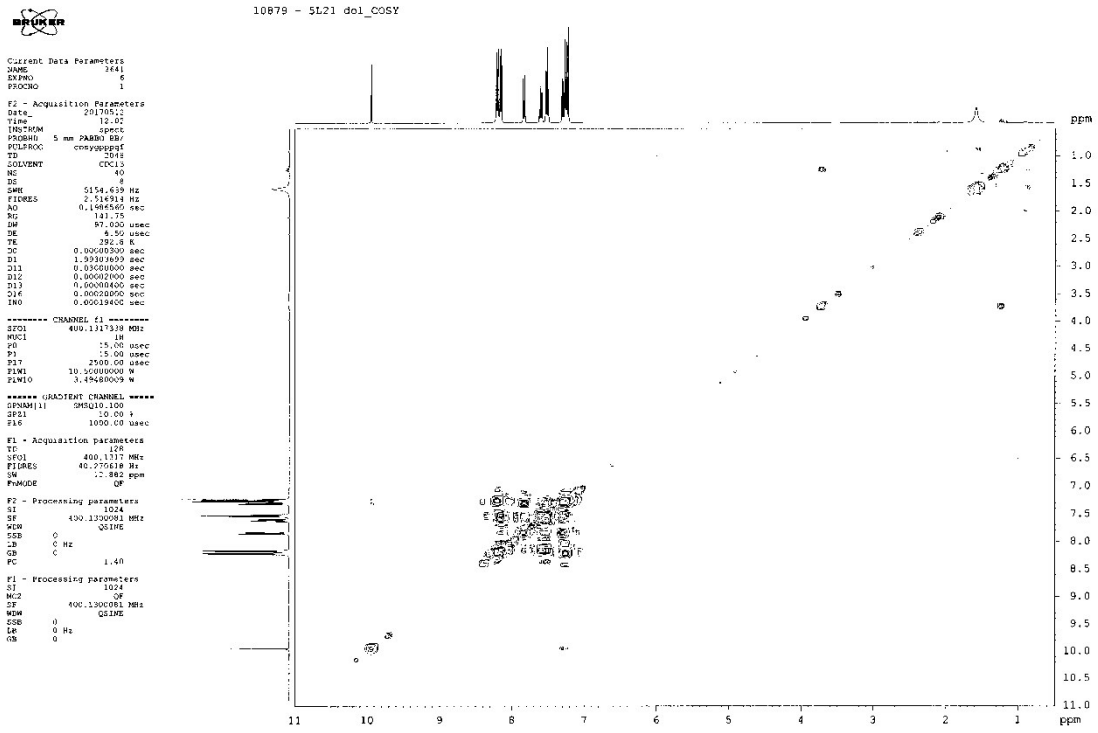

Figure S15. ^{1}H-^{1}H COSY spectrum of PB3

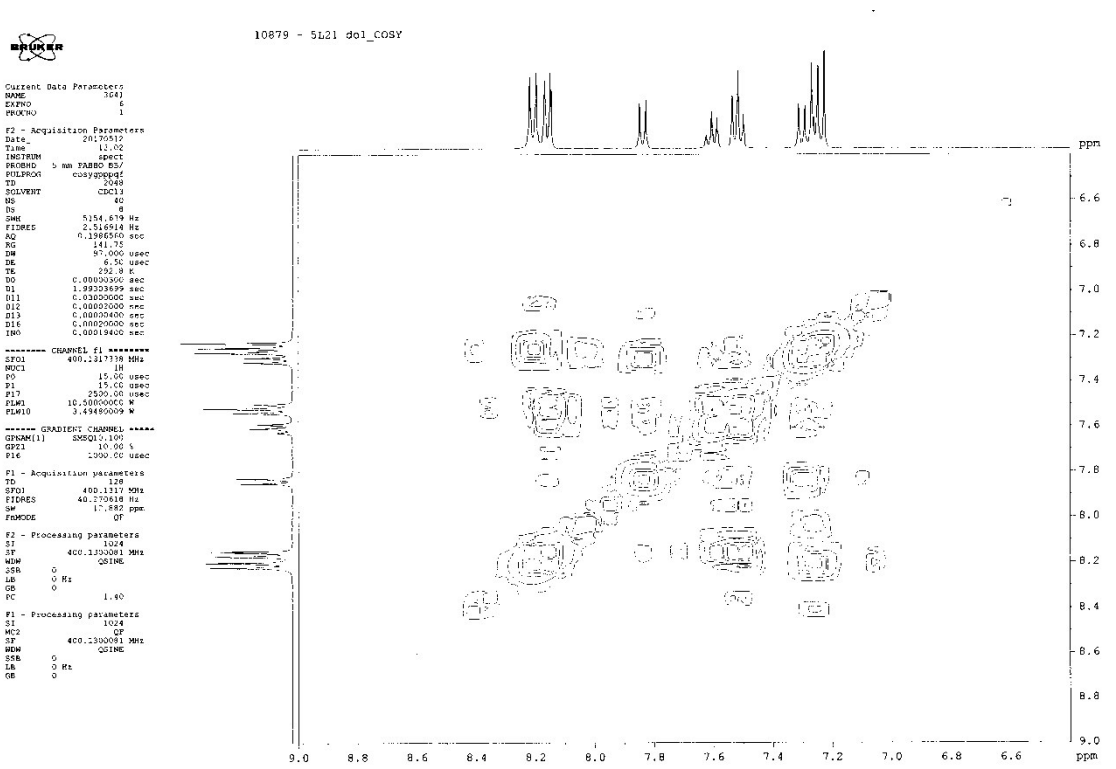

Figure S17. Enlarged spectrum in the range of 7 - 9 ppm

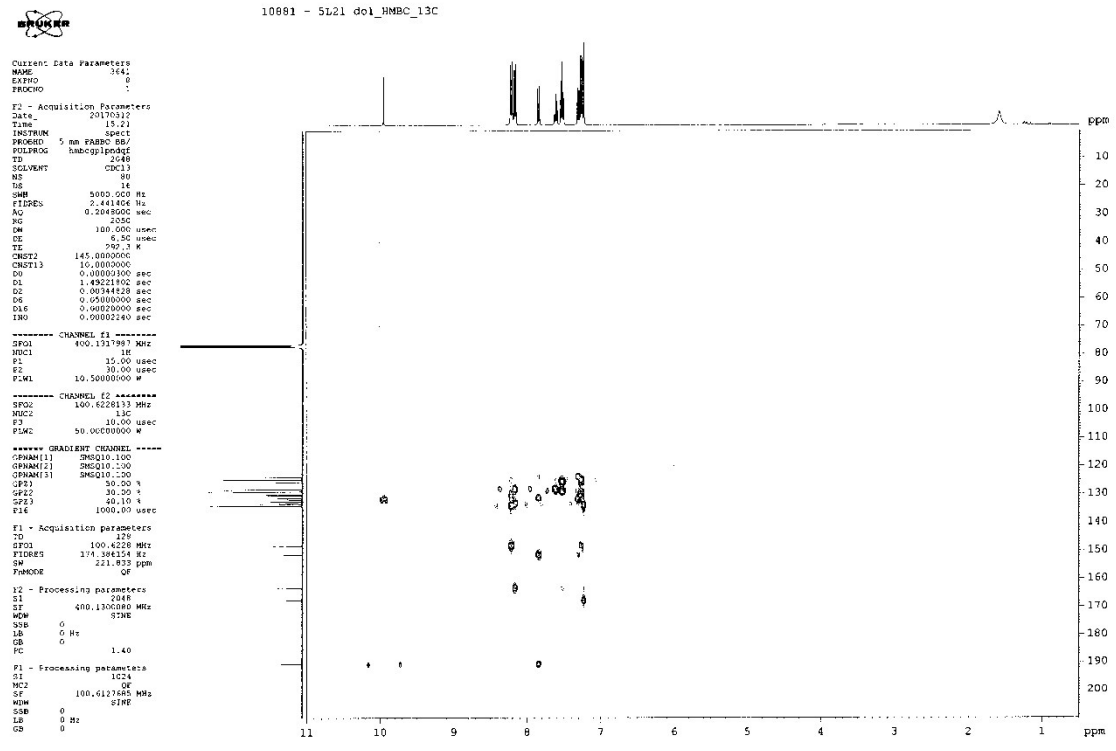

Figure S18. ^{1}H-^{13}C HMBC spectrum of PB3

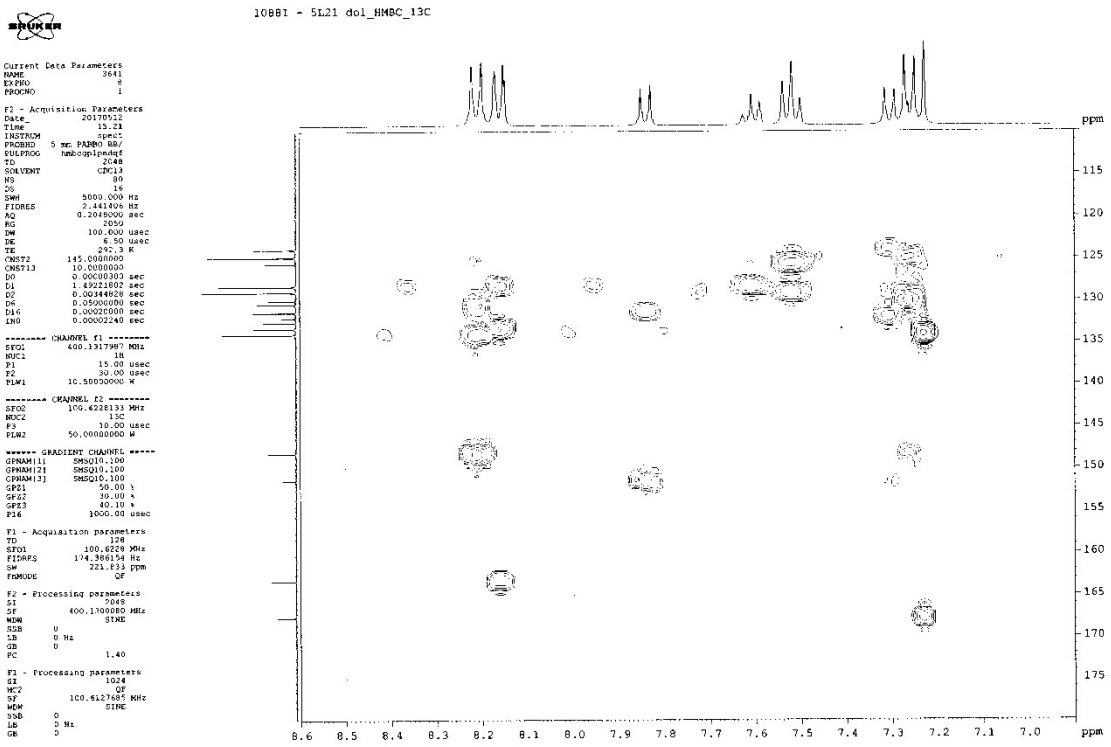

Figure S19. Enlarged spectrum in the range of 7 - 9 ppm

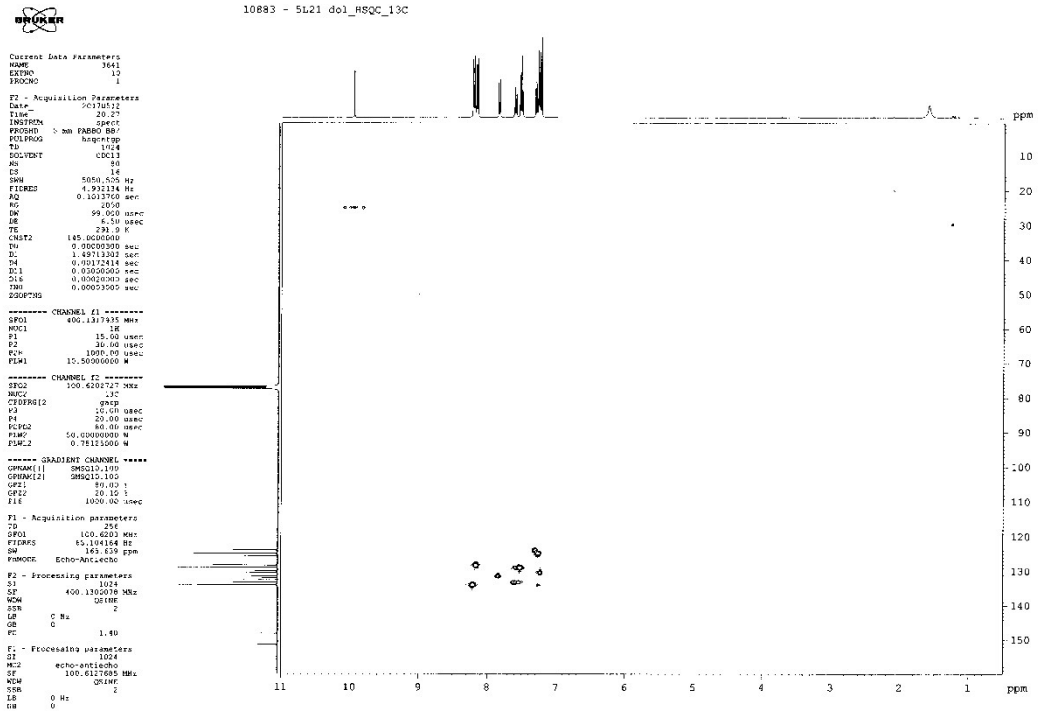

Figure S20. ^{1}H-^{13}C HMQC spectrum of PB3

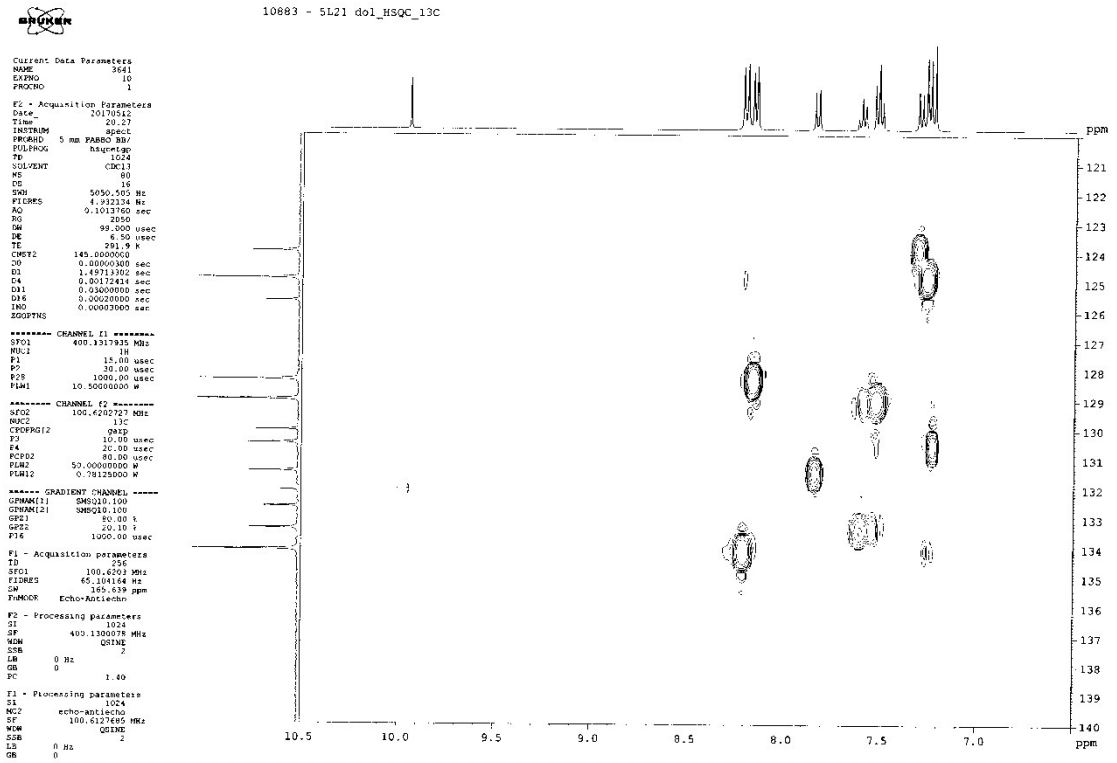

Figure S21. Enlarged spectrum in the range of 7 - 9 ppm

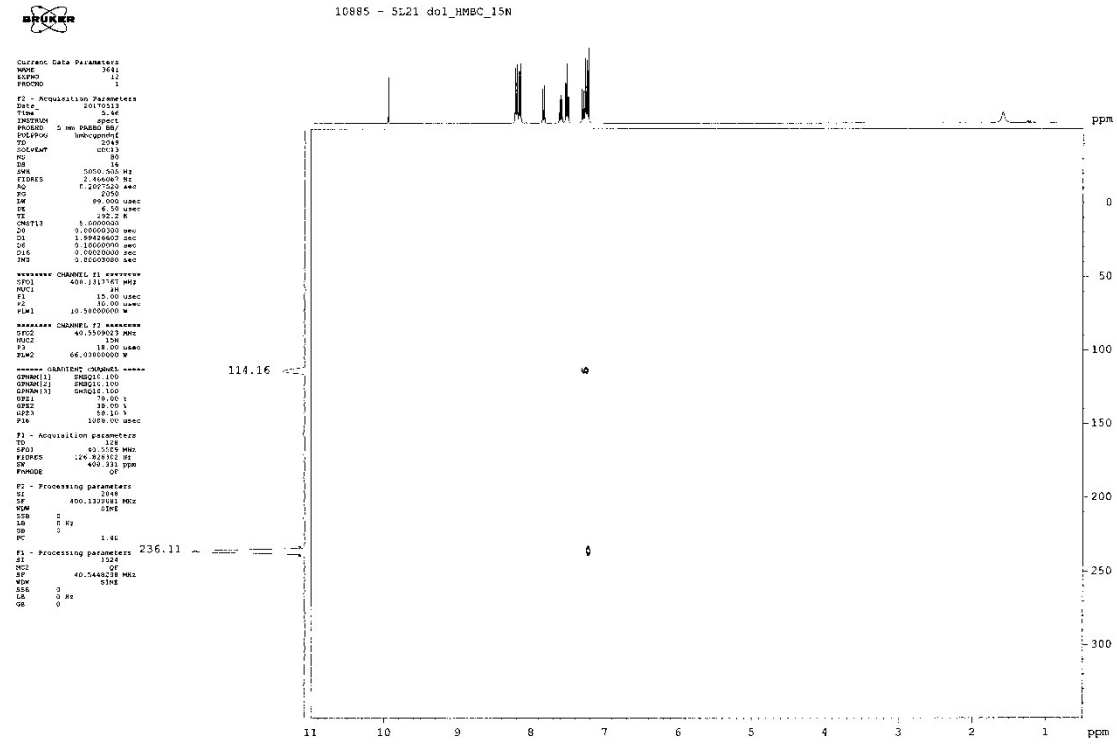

Figure S22. ^{1}H-^{15}N HMBC spectrum of PB3

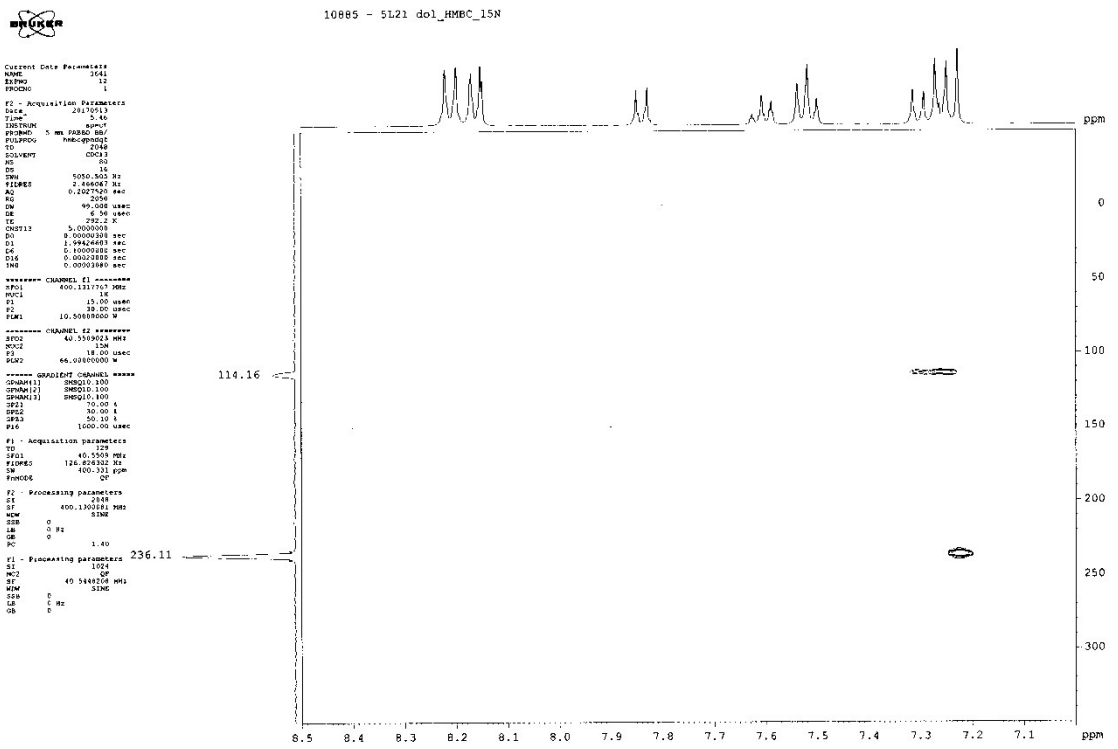

Figure S23. Enlarged spectrum in the range of 7 - 9 ppm

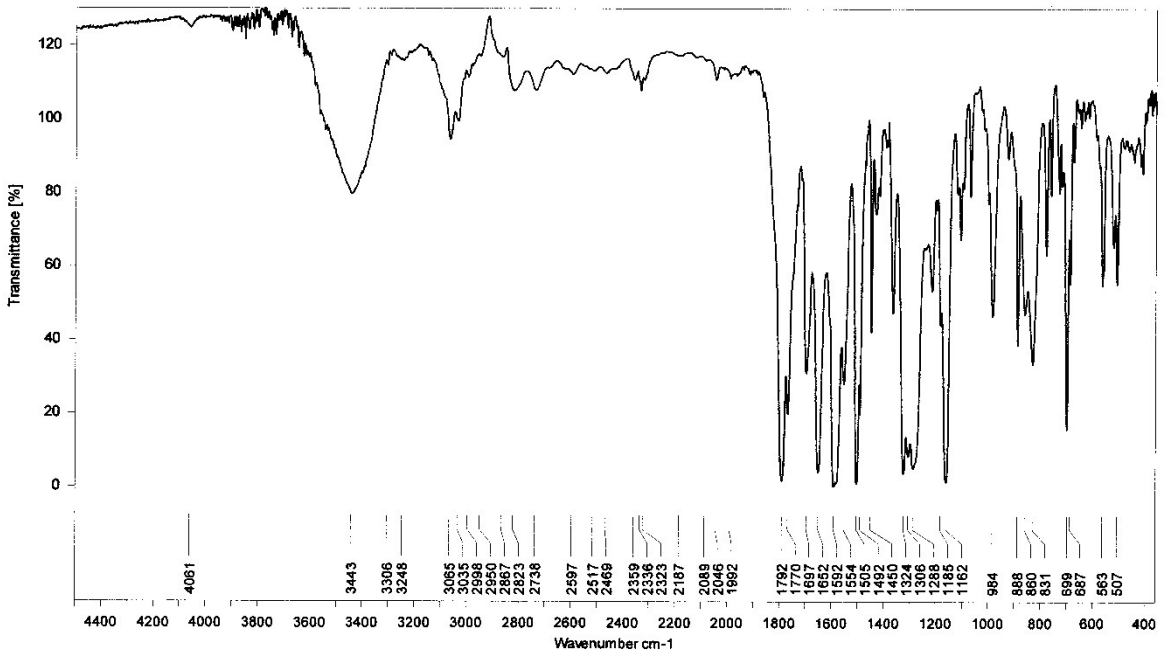

Figure S24. IR spectrum of PB3

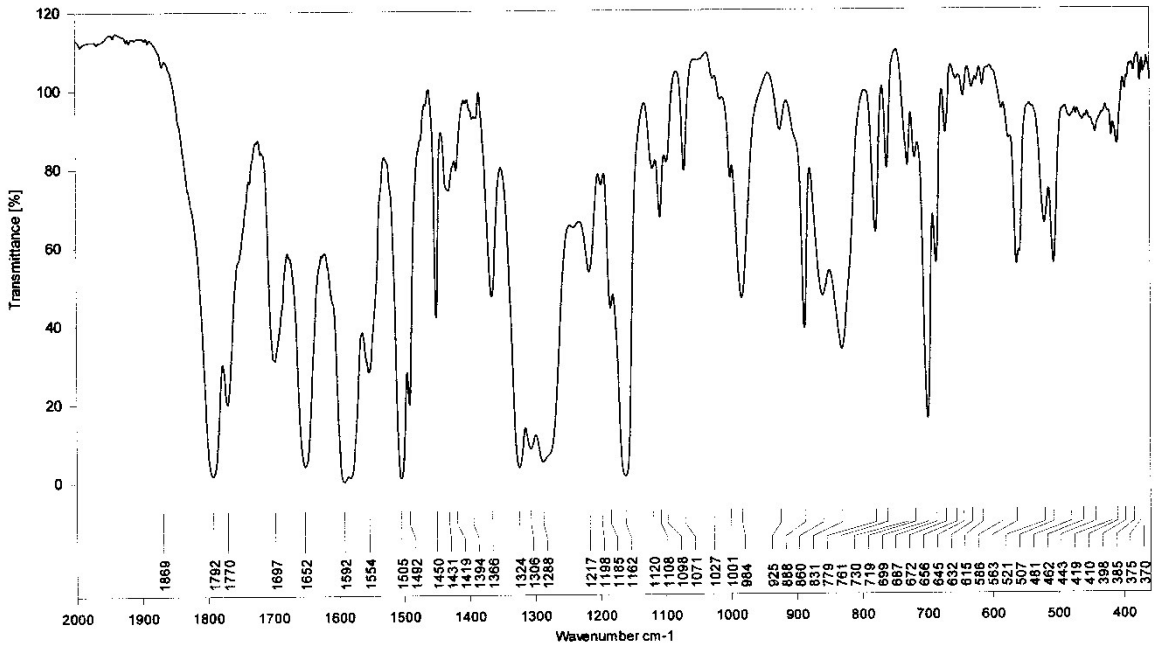

Figure S25. Enlarged spectrum in the range of 1900 - 400 cm^{-1}

Tables

Table S1. Solvent parameters and values of solvent polarity functions

Solvents	ε	n	E_T^N	SP	SdP	SA	SB	$f_{LM}(\varepsilon, n)$	$f_{MR}(\varepsilon, n)$	$f_B(\varepsilon, n)$
IsoOct	1.94	1.39145		0.618	0	0	0.044	0.0005	0.0007	0.0009
MCH	2.02	1.42312	0.006	0.675	0	0	0.069	-0.0006	-0.0010	-0.0012
Bu_2O	3.1	1.3992	0.071	0.672	0.175	0	0.637	0.0968	0.1698	0.2109
Et_2O	4.335	1.35243	0.117	0.617	0.385	0	0.562	0.1669	0.3099	0.3770
THF	7.58	1.40716	0.207	0.714	0.634	0	0.591	0.2096	0.4406	0.5491
MeAc	20.7	1.35868	0.355	0.651	0.907	0	0.475	0.2843	0.6479	0.7904
MeCN	35.94	1.34411	0.46	0.645	0.974	0.044	0.286	0.3046	0.7090	0.8593
DMF	36.71	1.43047	0.404	0.759	0.977	0.031	0.613	0.2744	0.6639	0.8356
DMSO	46.45	1.4793	0.444	0.83	1.000	0.072	0.647	0.2630	0.6544	0.8400

Table S2. Radiative (k_r) and non-radiative (k_{nr}) rate constants for **PB3** in different solvents

	k_r (10^8 s^{-1})	k_{nr} (10^8 s^{-1})	k_r / k_{nr}
IsoOct	2.75	3.69	0.745
MCH	2.63	3.68	0.715
Bu_2O	1.82	4.82	0.377
Et_2O	1.72	4.08	0.422
THF	1.42	4.94	0.287
MeAc	0.97	39.0	0.025
MeCN	0.83	82.3	0.010
DMF	0.78	86.6	0.009
DMSO	0.84	69.7	0.012

Table S3. Selected structural parameters of the PB3 compound in gas phase, IsoOct, MCH, Bu_2O and THF. Values are presented for the ground and CT excited state (Sg/S_{CT})

	Gas phase	IsoOct	MCH	Bu_2O	THF
bond lengths					
1-2	1.47112/ 1.47824	1.46894/ 1.47511	1.46884/ 1.47556	1.46782/ 1.47460	1.46633/ 1.47412
3-6	1.40709/ 1.42844	1.40808/ 1.41394	140815/ 1.41272	1.40827/ 1.41010	1.40846/ 1.41295
6-7	1.41020/ 1.44932	1.40993/ 1.36006	1.40998/ 1.36770	1.40969/ 1.39070	1.40935/ 1.39158
9-10	1.44161/ 1.42076	1.44106/ 1.41430	1.44101/ 1.41927	1.44069/ 1.42092	1.44015/ 1.41973
10-11	1.35418/ 1.38756	1.35496/ 1.37525	1.35502/ 1.37697	1.35544/ 1.37666	1.35611/ 1.37909
11-12	1.38732/ 1.37289	1.38780/ 1.36458	1.38781/ 1.36837	1.38806/ 1.37074	1.38844/ 1.37162
12-13	1.28949/ 1.30501	1.28910/ 1.30506	1.28908/ 1.30700	1.28886/ 1.30312	1.28857/ 1.30271
13-14	1.45249/ 1.44135	1.45207/ 1.44025	1.45205/ 1.44222	1.45188/ 1.44013	1.45170/ 1.44027
6-17	1.40717/ 1.33838	1.40668/ 1.43470	1.40662/ 1.43075	1.40629/ 1.40010	1.40572/ 1.39433
19-20	1.44106/ 1.40069	1.44038/ 1.42282	1.44033/ 1.42553	1.43992/ 1.42128	1.43923/ 1.41985
20-21	1.36043/ 1.39193	1.36119/ 1.39403	1.36124/ 1.39576	1.36166/ 1.38679	1.36234/ 1.38710
21-22	1.39327/ 1.36031	1.39414/ 1.38233	1.39418/ 1.38312	1.39460/ 1.37789	1.39520/ 1.37836
22-23	1.28403/ 1.30768	1.28410/ 1.29567	1.28411/ 1.29953	1.28411/ 1.29776	1.28410/ 1.29753
23-24	1.45254/ 1.43790	1.45249/ 1.44569	1.45248/ 1.44657	1.45248/ 1.44212	1.45251/ 1.44231
bond angles					
3-6-7	119.85962/ 116.11975	119.83760/ 122.40698	119.83009/ 122.15412	119.81632/ 120.18268	119.79236/ 119.78710
3-6-17	120.08748/ 122.39636	120.08248/ 117.22777	120.07854/ 117.60381	120.07741/ 119.38608	120.07969/ 119.48543
7-6-17	120.05132/ 121.47791	120.07894/ 120.36440	120.09047/ 120.24150	120.10552/ 120.43124	120.12725/ 120.72741
5-3-6	120.21712/ 119.94983	120.18438/ 119.24677	120.18136/ 119.32965	120.16290/ 119.69754	120.13330/ 119.65650
4-3-6	120.35048/ 119.40771	120.31348/ 120.34567	120.30830/ 120.31127	120.28937/ 119.94839	120.26356/ 119.78304
9-10-11	129.51822/ 128.18115	129.58065/ 128.80887	129.58321/ 128.78203	129.61555/ 128.81737	129.65756/ 128.91551
19-20-21	134.08770/ 133.69116	134.13078/ 132.98770	134.13388/ 132.93313	134.15593/ 133.40817	134.18642/ 133.51157
16-6-26	84.65062/ 103.51726	84.65317/ 78.70485	84.65864/ 78.87594	84.65805/ 80.80130	84.67332/ 81.64738
torsion angles					
4-3-6-7	-39.00702/ -50.89284	-39.27440/ -44.43110	-39.34327/ -42.92863	-39.49179/ -40.84104	-39.67481/ -42.17427
5-3-6-17	-39.63987/ -53.82017	-39.83658/ -40.98986	-39.89839/ -39.76674	-40.02483/ -40.33211	-40.21255/ -42.09839
8-9-10-11	1.20533/ -0.18927	1.21459/ 1.17933	1.20695/ 1.23187	1.20363/ 1.46525	1.18594/ 1.11103
9-10-11-12	0.44761/ -0.32355	0.45121/ 0.66629	0.45151/ 0.64175	0.44481/ 0.59652	0.41107/ 0.51640

18-19-20-21	179.49278/ 179.86173	179.39969/ -178.49863	179.40180/ -178.59147	179.39864/ -179.62679	179.44788/ -179.78314
19-20-21-22	-179.83670/ 179.70264	-179.89770/ -178.89536	-179.90296/ -179.02467	-179.92038/ -179.58396	-179.92557/ -179.64631
12-13-14-15	1.26750/ -0.14534	1.31714/ 0.81438	1.30927/ 0.64158	1.29301/ 0.98290	1.19590/ 0.97763
22-23-24-25	0.47191/ -0.06494	0.52285/ 0.11685	0.51998/ 0.11622	0.54611/ 0.31404	0.60094/ 0.21378

Table S4. Selected structural parameters of the PB3 compound in MeCN, DMF, DMSO and water. Values are presented for the ground and CT excited state (Sg/S_{CT})

	MeCN	DMF	DMSO	Water
bond lengths				
1-2	1.46528/ 1.47365	1.46533/ 1.47364	1.46522/ 1.45808	1.46513/ 1.47358
3-6	1.40864/ 1.41458	1.40868/ 1.41460	1.40865/ 1.39566	1.40866/ 1.41482
6-7	1.40904/ 1.39057	1.40903/ 1.39056	1.40902/ 1.40143	1.40899/ 1.39037
9-10	1.43974/ 1.41889	1.43973/ 1.41888	1.43971/ 1.42882	1.43967/ 1.41875
10-11	1.35662/ 1.38043	1.35661/ 1.38045	1.35665/ 1.37365	1.35670/ 1.38064
11-12	1.38870/ 1.37220	1.38870/ 1.37221	1.38872/ 1.37292	1.38874/ 1.37230
12-13	1.28839/ 1.30233	1.28837/ 1.30232	1.28838/ 1.30217	1.28837/ 1.30225
13-14	1.45260/ 1.44050	1.45160/ 1.44051	1.45159/ 1.43999	1.45159/ 1.44055
6-17	1.40529/ 1.39211	1.40521/ 1.39209	1.40525/ 1.40277	1.40521/ 1.39180
19-20	1.43870/ 1.41904	1.43867/ 1.41903	1.43866/ 1.42972	1.43861/ 1.41891
20-21	1.36286/ 1.38776	1.36286/ 1.38777	1.36289/ 1.37934	1.36294/ 1.38787
21-22	1.39559/ 1.37849	1.39558/ 1.37895	1.39562/ 1.38084	1.39565/ 1.37905
22-23	1.28408/ 1.29729	1.28407/ 1.29729	1.28408/ 1.29575	1.28408/ 1.29724
23-24	1.45255/ 1.44261	1.45256/ 1.44261	1.45256/ 1.44326	1.45257/ 1.44266
bond angles				
3-6-7	119.77937/ 119.65969	119.77053/ 119.65846	119.77853/ 120.23095	119.77749/ 119.64355
3-6-17	120.08041/ 119.45580	120.07965/ 119.45547	120.08052/ 120.01093	120.08066/ 119.44941
7-6-17	120.13936/ 120.88443	120.14898/ 120.88599	120.14007/ 119.75693	120.14094/ 120.90697
5-3-6	120.10952/ 119.59712	120.10853/ 119.59646	120.10767/ 120.07969	120.10522/ 119.58690
4-3-6	120.24698/ 119.70444	120.24293/ 119.70355	120.24590/ 120.24115	120.24448/ 119.62248
9-10-11	129.68634/ 128.97013	129.68506/ 128.97070	129.68829/ 128.66287	129.69075/ 128.79820
19-20-21	134.20691/ 133.56161	134.20717/ 133.56188	134.20761/ 133.51342	134.20846/ 133.56697
16-6-26	84.69551/ 82.00947	84.69728/ 82.01375	84.69603/ 84.04379	84.69639/ 82.05815
torsion angles				
4-3-6-7	-39.78706/ -43.07903	-39.83961/ -43.08979	-39.79467/ -37.05629	-39.80439/ -43.22120
5-3-6-17	-40.36393/ -43.08861	-40.41710/ -43.10001	-40.37585/ -37.34660	-40.39161/ -43.23993
8-9-10-11	1.13310/ 0.96936	1.14260/ 0.96770	1.13116/ 0.31809	1.12899/ 0.95790
9-10-11-12	0.37255/ 0.49563	0.36695/ 0.49539	0.36937/ 0.13667	0.36513/ 0.49547

18-19-20-21	179.45405/ -179.84943	179.53650/ -179.85042	179.55296/ -179.30226	179.56354/ -179.86202
19-20-21-22	-179.91190/ -179.58325	-179.91316/ -179.58188	-179.91013/ -179.41122	-179.90765/ -179.56881
12-13-14-15	0.99429/ 0.84600	0.99168/ 0.84393	0.97765/ 0.73423	0.95558/ 0.81604
22-23-24-25	0.64756/ 0.16299	0.65699/ 0.16238	0.65174/ 0.52421	0.65733/ 0.15324

Table S5. The frontier orbital energies in selected solvents. All values are given in eV

	Gas phase	IsoOct	MCH	Bu2O	THF	MeCN	DMF	DMSO	water
E_{HOMO}	-5.7707	-5.8869	-5.8858	-5.8782	-5.8692	-5.8635	-5.8632	-5.8630	-5.8627
E_{LUMO}	-3.7340	-2.9418	-2.9424	-2.9497	-2.9655	-2.9788	-2.9772	-2.9796	-2.9810
E_{GAP}	2.0367	2.9451	2.9434	2.9285	2.9037	2.8847	2.8860	2.8833	2.8817
η	1.0183	1.4725	1.4717	1.4642	1.4519	1.4423	1.4430	1.4417	1.4408
μ	-4.7524	-4.4144	-4.4141	-4.4139	-4.4174	-4.4212	-4.4202	-4.4213	-4.4218
χ	4.7524	4.4144	4.4141	4.4139	4.4174	4.4212	4.4202	4.4213	4.4218

Table S6. The vertical and cLR corrected excitation energies (in nm)

	B3LYP		CAM-B3LYP		HSEH1PBE		OHSE1PBE		OHSE2PBE		PBE0		mPW1PBE		mPW3PBE	
	$\lambda_{ABS}^{vertical}$	λ_{ABS}^{cLR}	$\lambda_{ABS}^{vertical}$	λ_{ABS}^{cLR}	$\lambda_{ABS}^{vertical}$	λ_{ABS}^{cLR}	$\lambda_{ABS}^{vertical}$	λ_{ABS}^{cLR}	$\lambda_{ABS}^{vertical}$	λ_{ABS}^{cLR}	$\lambda_{ABS}^{vertical}$	λ_{ABS}^{cLR}	$\lambda_{ABS}^{vertical}$	λ_{ABS}^{cLR}	$\lambda_{ABS}^{vertical}$	λ_{ABS}^{cLR}
Gas phase	523.63	---	423.98	---	526.67	---	526.66	---	524.19	---	489.26		488.59	---	522.77	---
IsoOct	544.43	534.42	439.39	430.20	546.83	537.31	546.83	---	544.28	---	508.60	500.01	507.89	---	543.40	---
MCH	545.67	535.16	440.31	430.64	548.04	538.01	548.04	---	545.48	---	509.75	500.68	509.04	---	544.63	---
Bu_2O	548.41	538.85	442.08	433.04	550.60	541.54	550.59	---	548.05	---	512.17	502.99	511.45	---	547.25	---
THF	552.44	545.61	445.89	437.23	556.13	547.98	556.12	---	553.57	---	517.37	509.03	516.62	---	552.90	---
MeCN	556.79	549.85	447.36	439.99	558.44	551.95	558.44	---	555.90	---	519.54	512.77	518.80	---	555.27	---
DMF	559.50	551.36	449.33	440.73	561.12	553.48	561.11	---	558.55	---	522.05	514.12	521.31	---	557.96	---
DMSO	559.37	551.49	449.19	440.80	560.98	553.55	560.97	---	558.41	---	521.92	514.23	521.17	---	557.84	---
Water	557.17	550.53	447.57	440.44	558.78	552.57	558.78	---	556.24	---	**519.86**	513.36	519.12	---	555.62	---

Table S7. Calculated values of dipole moments (in D) for the ground and CT excited state.

	B3LYP		CAM-B3LYP		HSEH1PBE		OHSE1PBE		OHSE2PBE		PBE0		mPW1PBE		mPW3PBE	
	μ_g	μ_{CT}	μ_g	μ_{CT}	μ_g	μ_{CT}	μ_g	μ_{CT}	μ_g	μ_{CT}	μ_g	μ_{CT}	μ_g	μ_{CT}	μ_g	μ_{CT}
Gas phase	5.85	6.61	5.91	6.53	5.87	6.94	5.87	6.94	5.89	6.89	5.88	6.23	5.90	6.23	5.85	6.54
IsoOct	6.38	7.36	6.44	7.12	6.40	7.59	6.40	7.59	6.42	7.56	6.41	7.02	6.43	6.90	6.37	7.28
MCH	6.41	7.42	6.47	7.15	6.43	7.64	6.43	7.64	6.44	7.61	6.43	7.08	6.45	7.08	6.40	7.34
Bu_2O	6.64	7.99	6.70	7.43	6.66	8.19	6.66	8.19	6.68	8.16	6.67	7.64	6.69	7.64	6.63	7.34
THF	6.97	8.90	7.03	7.75	6.98	9.33	6.98	9.07	7.00	9.04	6.99	8.52	7.01	8.52	6.95	8.79
MeCN	7.20	9.60	7.26	7.98	7.20	9.74	7.20	9.74	7.22	9.72	7.21	9.20	7.23	9.21	7.17	9.48
DMF	7.20	9.61	7.26	7.99	7.20	9.74	7.20	9.74	7.22	9.72	7.21	9.20	7.23	9.21	7.17	9.48
DMSO	7.21	9.64	7.28	8.00	7.22	9.77	7.22	9.77	7.24	9.75	7.22	9.28	7.25	9.24	7.19	9.51
Water	7.23	9.72	7.30	8.02	7.24	9.06	7.24	9.86	7.26	9.83	7.24	9.32	7.27	9.32	7.21	9.59

Table S8. The vertical and cLR corrected de-excitation energies (in nm)

	B3LYP		CAM-B3LYP		HSEH1PBE		OHSE1PBE		OHSE2PBE		PBE0		mPW1PBE		mPW3PBE	
	$\lambda_{Fl}^{vertical}$	λ_{Fl}^{cLR}	$\lambda_{Fl}^{vertical}$	λ_{Fl}^{cLR}	$\lambda_{Fl}^{vertical}$	λ_{Fl}^{cLR}	$\lambda_{Fl}^{vertical}$	λ_{Fl}^{cLR}	$\lambda_{Fl}^{vertical}$	λ_{Fl}^{cLR}	$\lambda_{Fl}^{vertical}$	λ_{Fl}^{cLR}	$\lambda_{Fl}^{vertical}$	λ_{Fl}^{cLR}	$\lambda_{Fl}^{vertical}$	λ_{Fl}^{cLR}
Gas phase	759.56	---	443.89	---	806.78	---	806.77	---	798.31	---	644.37	---	642.72	---	760.57	---
IsoOct	651.85	720.72	475.26	464.90	668.37	748.25	668.36	---	663.83	---	516.41	619.21	565.38	---	651.17	---
MCH	638.43	688.12	480.37	468.65	651.79	712.35	651.78	---	647.70	---	507.56	592.9	556.61	---	637.55	---
Bu_2O	594.64	580.26	486.24	473.82	597.47	583.73	597.47	---	594.86	---	537.97	534.27	547.24	---	593.24	---
THF	600.44	586.86	492.67	481.89	602.65	588.92	602.64	---	600.09	---	573.81	561.42	573.06	---	598.81	---
MeCN	602.76	594.45	495.38	488.42	604.63	596.08	604.62	---	602.10	---	626.12	608.76	615.37	---	600.98	---
DMF	606.62	594.54	498.13	488.49	608.46	596.17	608.45	---	605.90	---	629.69	608.87	618.93	---	604.82	---
DMSO	590.74	590.69	476.71	471.55	593.29	593.23	593.28	---	590.61	---	612.49	602.21	601.72	---	589.07	---
Water	603.07	595.79	495.76	489.52	604.88	597.34	604.88	---	602.36	---	**626.43**	610.05	615.69	---	601.26	---

Table S9. Binding free energies (ΔG_b, kcal/mol) and values of the inhibitor constants (K_i in mM) obtained during AutoDock simulations.

Lysine residues	ΔG_b	K_i
LYS30	-3.0	73.82
LYS35	-5.2	7.58
LYS36	-4.8	4.52
LYS39	-3.8	19.95
LYS46	-5.7	0.31
LYS59	-4.3	16.63
LYS101	-5.4	0.73
LYS114	-5.0	3.74
LYS116	-6.2	1.09
LYS135	-3.8	65.55
LYS138	-4.1	15.60
LYS200	-4.1	15.04
LYSTer	-2.8	310.47