Exploring the Photovoltaic Properties of Naphthalene-1,5-diamine Based Functionalized Materials in Aprotic Polar Medium: A Combine Experimental and DFT Approach

Iqra Shafiq,[1,2] Muhammad Khalid, *[1,2] Rifat Jawaria[1,2], Zahid Shafiq,[3] Shahzad Murtaza,[1,2] Ataualpa A. C. Braga,[4]

[1]Institute of Chemistry, Khwaja Fareed University of Engineering & Information Technology, Rahim Yar Khan, 64200, Pakistan

[2]Centre for Theoretical and Computational Research, Khwaja Fareed University of Engineering & Information Technology, Rahim Yar Khan, 64200, Pakistan

[3]Institute of Chemical Sciences, Bahauddin Zakariya University, Multan 60800, Pakistan

[4]Departamento de Química Fundamental, Instituto de Química,Universidade de São Paulo, Av. Prof. LineuPrestes, 748, São Paulo, 05508-000, Brazil

*Corresponding author's E-mail addresses:

Dr. Muhammad Khalid (muhammad.khalid@kfueit.edu.pk; Khalid@iq.usp.br).

Table S1: Calculated vibrational frequencies of **ND1**

Frequencies	*Experimental*	*Intensities*	*Vibrational assignments*
3239		2	υ(C-H)
3236		8	υ(s)+(as)C-H_{Ben}
3229		10	υ(s)C-H_{Ben}
3212		17	υ(s)+υ(as)C-H_{Ben}
3197		23	υ(as)C-H_{Ben}
3041	2861	26	υ(C-H)
1723		15	υ(C=N)
1719		200	β(C-H)+υ(C=N)
1678		40	υ(C=C-C=C_{Ben})+ (δ+ρ)C-H_{Ben}+υ(C-C_{CF3})
1659		22	υ(C=C-C=C_{Ben})+ (δ+ρ)C-H_{Ben}+υ(C-C_{CF3})
1641	1617	19	υ(C=C-C=C_{Ben})+(δ+ρ)C-H_{Ben}
1561		25	υ(C=C-C=C_{Ben}) +(δ+ρ)C-H_{Ben}
1530		14	υ(C=C-C=C_{Ben})+(ρ)C-H_{Ben}
1495		19	υ(C=C-C=C_{Ben})+(ρ)C-H_{Ben}
1453		50	υ(C=C-C=C_{Ben})+(δ+ρ)C-H_{Ben}
1367		13	υ(C=C-C=C_{Ben})+(δ+ρ)C-H_{Ben}
1357		228	υ(C=C-C=C_{Ben})+υ(ρ)C-H_{Ben}+υ(C-C_{CF3})
1356		308	υ(C=C-C=C_{Ben})+υ(ρ)C-H_{Ben}+υ(C-C_{CF3})+υ(C-F_{CF3})
1307	1320	114	υ(C=C-C=C_{Ben})+υ(ρ)C-H_{Ben}+υ(C-C_{CF3})
1250	1272	24	υ(ρ+δ)C-H_{Ben}+υ(C-H)

1232		42	$\upsilon(\rho)$C-H_{Ben}+υ(C-H)+υ(C-C_{CF3})+υ(C-F_{CF3})
1231		211	υ(ρ+δ)C-H_{Ben}+υ(C-H)+υ(C-C_{CF3})+υ(C-F_{CF3})
1214		390	υ(ρ+δ)C-H_{Ben}+υ(C-C_{CF3})+υ(C-F_{CF3})
1189		108	υ(ρ+δ)C-H_{Ben}+β(C-H)
1181	1152	307	υ(ρ+δ)C-H_{Ben}+υ(C-C_{CF3})+υ(C-F_{CF3})
1123	1115	39	υ(ρ+δ)C-H_{Ben}+υ(C-F_{CF3})
1098	1086	62	υ(ρ)C-H_{Ben}+υ(C-F_{CF3})+υ(C-C)
1015		10	υ(τ+γ)C-H_{Ben}+γ(C-H)
1014		19	υ(τ+γ)C-H_{Ben}+γ(C-H)+(ρ)C-H_{Ben}
967	961	28	υ(ρ)C-H_{Ben}+υ(τ+γ)C-H_{Ben}
947	912	42	$\upsilon(\delta+\rho)$C-H_{Ben}+υ(C-C)
822	892	31	υ(τ+*w*)C-H_{Ben}+υ(ρ)C-H
812	799	77	υ(τ+*w*)C-H_{Ben}+υ(C-F_{CF3})
717	782	28	υ(τ+*w*)C-H_{Ben}+υ(C-F_{CF3})
694	692	48	υ(ρ)C-H_{Ben}+(ρ)C-H+υ(C-F_{CF3})
666	674	8	υ(*w*)C-H_{CF3}+υ(C-H_{Ben})

Frequencies are given in cm^{-1}, υ=stretching, β=in-plane bending, γ=out-plane bending, δ=scissoring, ρ=rocking, *w*=wagging, s=symmetric, as=asymmetric, τ=twisting, Ben=benzene ring

Table S2: Calculated vibrational frequencies of **ND2**

Frequencies	***Experimental***	***Intensities***	***Vibrational assignments***
3238		7	υ(C-H)
3235		7	υ(s)(C-H)
3233		6	υ(s)(C-H)
3216		13	υ(s)+υ(as)C-H_{Ben}
3212		18	υ(s)+υ(as)C-H_{Ben}
3196		24	υ(as)C-H_{Ben}
3042	3054	33	υ(C-H)
1721		7	υ(C=N)+υ(C=C-C=C_{Ben})
1717		314	υ(C=N)+υ(C=C-C=C_{Ben})
1677		28	υ(C=N)+υ(C=C-C=C_{Ben})+(ρ)C-H_{Ben}
1656		54	υ(C=N)+υ(C=C-C=C_{Ben})+(ρ)C-H_{Ben}+υ(C-Cl)
1641	1613	23	υ(C=N)+υ(C=C-C=C_{Ben})+(δ+ρ)C-H_{Ben}
1562	1573	24	υ(C=C-C=C_{Ben})+(δ+ρ)C-H_{Ben}
1531		22	υ(C=C-C=C_{Ben})+(δ+ρ)C-H_{Ben}+υ(C-Cl)
1530		70	υ(C=C-C=C_{Ben})+(δ+ρ)C-H_{Ben}+υ(C-Cl)
1496		122	υ(C=C-C=C_{Ben})+(δ+ρ)C-H_{Ben}+υ(C-Cl)
1453	1444	42	υ(C=C-C=C_{Ben})+(δ+ρ)C-H_{Ben}+υ(C-Cl)
1406		12	β(C-H)+υ(C=C-C=C_{Ben})+(δ+ρ)C-H_{Ben}
1404	1401	36	β(C-H)+υ(C=C-C=C_{Ben})+(δ+ρ)C-H_{Ben}
1366	1356	39	υ(C=C-C=C_{Ben})+(δ+ρ)C-H_{Ben}
1306		96	υ(C=C-C=C_{Ben})+(δ+ρ)C-H_{Ben}+υ(C-Cl)
1298		74	υ(C=C-C=C_{Ben})+(ρ)C-H_{Ben}

1277	1259	38	$\upsilon(C=C\text{-}C=C_{Ben})+(\rho)C\text{-}H_{Ben}$
1247	1229	8	$\upsilon(C=C\text{-}C=C_{Ben})+(\delta+\rho)C\text{-}H_{Ben}$
1188		16	$\upsilon(C=C\text{-}C=C_{Ben})+(\delta+\rho)C\text{-}H_{Ben}$
1163		30	$\upsilon(C=C\text{-}C=C_{Ben})+(\delta+\rho)C\text{-}H_{Ben}+\upsilon(C\text{-}Cl)$
1157	1126	9	$\upsilon(C=C\text{-}C=C_{Ben})+(\delta+\rho)C\text{-}H_{Ben}+\upsilon(C\text{-}Cl)$
1098		19	$\upsilon(C=C\text{-}C=C_{Ben})+(\rho)C\text{-}H_{Ben}$
1011		9	$\gamma(C\text{-}H)+(\tau+\rho)C\text{-}H_{Ben}$
999		13	$\gamma(C\text{-}H)+(\tau+\rho)C\text{-}H_{Ben}$
960	967	67	$\upsilon(C=C\text{-}C=C_{Ben})+(\beta)C\text{-}H_{Ben}+(\rho)C\text{-}H_{Ben}$
910	918	9	$\upsilon(C=C\text{-}C=C_{Ben})+(\tau+w)C\text{-}H_{Ben}+\gamma(C\text{-}H)$
823	898	65	$\upsilon(C=C\text{-}C=C_{Ben})+(w)C\text{-}H_{Ben}+\upsilon(C\text{-}Cl)$
805	872	59	$\upsilon(C=C\text{-}C=C_{Ben})+(w)C\text{-}H_{Ben}+(\rho)C\text{-}H_{Ben}+\upsilon(C\text{-}Cl)$
791	774	57	$\upsilon(C=C\text{-}C=C_{Ben})+(\rho)C\text{-}H_{Ben}+\gamma(C\text{-}Cl)$
701		18	$\upsilon(C=C\text{-}C=C_{Ben})+(w)C\text{-}H_{Ben}$
692	695	11	$\upsilon(C=C\text{-}C=C_{Ben})+(w)C\text{-}H_{Ben}$

Frequencies are given in cm^{-1}, υ=stretching, β=in-plane bending, γ=out-plane bending, δ=scissoring, ρ=rocking, w=wagging, s=symmetric, as=asymmetric, τ=twisting, Ben=benzene ring

Table S3: Calculated vibrational frequencies of **ND3**

Frequencies	***Experimental***	***Intensities***	***Vibrational assignments***
3239		1	$\upsilon(C\text{-}H)$
3239		5	$\upsilon(C\text{-}H)$
3236		8	$\upsilon(s)(C\text{-}H)$
321		14	$\upsilon(s)+\upsilon(as)C\text{-}H_{Ben}$
3212		18	$\upsilon(s)+\upsilon(as)C\text{-}H_{Ben}$
3197		3	$\upsilon(s)+\upsilon(as)C\text{-}H_{Ben}$
3197		29	$\upsilon(s)+\upsilon(as)C\text{-}H_{Ben}$
3041	3047	39	$\upsilon(C\text{-}H)$
1721		5	$\upsilon(C=N)+\upsilon(C=C\text{-}C=C_{Ben})$
1716		316	$\upsilon(C=N)+\upsilon(C=C\text{-}C=C_{Ben})+(\rho)C\text{-}H$
1660		9	$\upsilon(C=C\text{-}C=C_{Ben})+(\delta+\rho)C\text{-}H_{Ben}$
1642		15	$\upsilon(C=C\text{-}C=C_{Ben})+(\delta+\rho)C\text{-}H_{Ben}$
1633		34	$\upsilon(C=C\text{-}C=C_{Ben})+(\delta+\rho)C\text{-}H_{Ben}$
1632	1611	29	$\upsilon(C=C\text{-}C=C_{Ben})+(\delta+\rho)C\text{-}H_{Ben}$
1562		26	$\upsilon(C=C\text{-}C=C_{Ben})+(\delta+\rho)C\text{-}H_{Ben}$
1514		42	$\upsilon(C=C\text{-}C=C_{Ben})+(\delta+\rho)C\text{-}H_{Ben}$
1470	1496	41	$\upsilon(C=C\text{-}C=C_{Ben})+(\delta+\rho)C\text{-}H_{Ben}$
1451	1421	38	$\upsilon(C=C\text{-}C=C_{Ben})+(\rho)C\text{-}H_{Ben}+\upsilon(C=N)$
1401	1399	34	$\upsilon(C=C\text{-}C=C_{Ben})+(\rho)C\text{-}H_{Ben}+(\rho)C\text{-}H$
1370		12	$\upsilon(C=C\text{-}C=C_{Ben})+(\delta+\rho)C\text{-}H_{Ben}+(\rho)C\text{-}H$
1362		14	$\upsilon(C=C\text{-}C=C_{Ben})+(\delta+\rho)C\text{-}H_{Ben}+(\rho)C\text{-}H$
1302		36	$\upsilon(C=C\text{-}C=C_{Ben})+(\rho)C\text{-}H_{Ben}+(\rho)C\text{-}H$

1293		5	$\upsilon(C=C-C=C_{Ben})+(\rho)C-H_{Ben}$
1252	1262	28	$\upsilon(C=C-C=C_{Ben})+\upsilon(C=N)+(\delta+\rho)C-H_{Ben}$
1239		122	$\upsilon(C=C-C=C_{Ben})+(\delta+\rho)C-H_{Ben}+(\rho)C-H$
1238	1194	7	$\upsilon(C=C-C=C_{Ben})+(\delta+\rho)C-H_{Ben}$
1190	1153	44	$\upsilon(C=C-C=C_{Ben})+(\delta+\rho)C-H_{Ben}$
1099		10	$\upsilon(C=C-C=C_{Ben})+\beta(C-H)+(\rho)C-H_{Ben}$
1097	1063	22	$\upsilon(C=C-C=C_{Ben})+(\rho)C-H_{Ben}+\beta(C-H)$
1018		6	$\upsilon(C=C-C=C_{Ben})+\beta(C-H)$
1013		10	$\upsilon(C=C-C=C_{Ben})+(\tau+w)C-H_{Ben}+\gamma(C-H)$
1012		10	$\upsilon(C=C-C=C_{Ben})+(\tau+\gamma)C-H_{Ben}+\gamma(C-H)$
964	962	52	$\upsilon(C=C-C=C_{Ben})+\beta(C-H)+(\rho)C-H_{Ben}$
935		9	$(\gamma)C-H_{Ben}+(\rho)C-H_{Ben}$
932	924	6	$(\gamma)C-H_{Ben}+(\rho)C-H_{Ben}$
930	895	11	$\upsilon(C=C-C=C_{Ben})+(\gamma)C-H_{Ben}+(\rho)C-H_{Ben}$
810		119	$(w)C-H_{Ben}+\beta(C-H)$
802		33	$(w)C-H_{Ben}+(\gamma)C-H$
799	779	14	$(w+\gamma)C-H_{Ben}+\beta(C-H)$
710	713	67	$\upsilon(C=C-C=C_{Ben})+(\rho)C-H_{Ben}+\upsilon(C-Br)$
695	677	10	$(w+\gamma)C-H_{Ben}+\upsilon(C-Br)$
681	663	8	$\upsilon(C=C-C=C_{Ben})+(\rho)C-H_{Ben}+\upsilon(C-Br)$

Frequencies are given in cm^{-1}, υ=stretching, β=in-plane bending, γ=out-plane bending, δ=scissoring, ρ=rocking, w=wagging, s=symmetric, as=asymmetric, τ=twisting, Ben=benzene ring

Table S4: Calculated vibrational frequencies of **ND4**

Frequencies	***Experimental***	***Intensities***	***Vibrational assignments***
3235		9	$\upsilon(s)(C-H)$
3214		2	$\upsilon(C-H)$
3211		20	$\upsilon(s)+\upsilon(as)C-H_{Ben}$
3197		24	$\upsilon(as)C-H_{Ben}$
3196		27	$\upsilon(as)C-H_{Ben}$
3153		11	$\upsilon(s)(as)C-H_{CH3}$
3153		12	$\upsilon(s)(as)C-H_{CH3}$
3120		11	$\upsilon(s)(as)C-H_{CH3}$
3120		10	$\upsilon(s)(as)C-H_{CH3}$
3060		55	$\upsilon(s)C-H_{CH3}$
3037		29	$\upsilon(s)C-H$
3037		41	$\upsilon(s)C-H$
1722		12	$\upsilon(C=N)+\upsilon(\rho)C-H$
1719		335	$\upsilon(C=N)+\upsilon(\rho)C-H$
1686		33	$\upsilon(C=C-C=C_{Ben})+\upsilon(\delta+\rho)C-H_{Ben}$
1642		138	$\upsilon(C=C-C=C_{Ben})+\upsilon(\delta+\rho)C-H_{Ben}$
1642		31	$\upsilon(C=C-C=C_{Ben})+(\delta+\rho)C-H_{Ben}+(\delta+\tau)C-H_{CH3}$
1640		94	$\upsilon(C=C-C=C_{Ben})+(\delta+\rho)C-H_{Ben}+(\delta+\tau)C-H_{CH3}$
1635		14	$\upsilon(C=C-C=C_{Ben})+(\delta+\rho)C-H_{Ben}$

1564	1567	83	$\upsilon(C=C\text{-}C=C_{Ben})+(\delta+\rho)C\text{-}H_{Ben}$
1557		25	$\upsilon(C=C\text{-}C=C_{Ben})+(\rho)C\text{-}H$
		13	$\upsilon(C=C\text{-}C=C_{Ben})+(\rho)C\text{-}H_{Ben}+(\delta+\tau)C\text{-}H_{CH3}$
1505			
1501		15	$(\delta+\tau)C\text{-}H_{CH3}$
1497		10	$(\delta+\tau)C\text{-}H_{CH3}$
1481		8	$(\delta+\tau)C\text{-}H_{CH3}$
1481		8	$(\delta+\tau)C\text{-}H_{CH3}$
		11	$\upsilon(C=C\text{-}C=C_{Ben})+(\rho)C\text{-}H_{Ben}+(\delta+\tau)C\text{-}H_{CH3}$
1463			
1445		66	$\upsilon(C=C\text{-}C=C_{Ben})+(\rho)C\text{-}H+\upsilon(C\text{-}F)$
1399	1398	27	$(\rho)C\text{-}H$
		33	$\upsilon(C=C\text{-}C=C_{Ben})+\upsilon(\delta+\rho)C\text{-}H_{Ben}+(\rho)C\text{-}H$
1358			
1321		27	$(\rho)C\text{-}H+\upsilon(C\text{-}F)$
		200	$\upsilon(C=C\text{-}C=C_{Ben})+\upsilon(\rho)C\text{-}H_{Ben}+(\rho)C\text{-}H+\upsilon(C\text{-}F)$
1320			
1300		14	$\upsilon(C=C\text{-}C=C_{Ben})+\upsilon(\rho)C\text{-}H_{Ben}$
1300		14	$\upsilon(C=C\text{-}C=C_{Ben})+\upsilon(\rho)C\text{-}H_{Ben}$
1293		122	$\upsilon(C=C\text{-}C=C_{Ben})+\upsilon(\rho)C\text{-}H_{Ben}$
1247	1262	15	$\upsilon(C=C\text{-}C=C_{Ben})+\upsilon(\delta+\rho)C\text{-}H_{Ben}$
1224	1234	39	$(w)C\text{-}H_{CH3}$
1193		32	$\upsilon(C=C\text{-}C=C_{Ben})+\upsilon(\delta+\rho)C\text{-}H_{Ben}$
		21	$\upsilon(C=C\text{-}C=C_{Ben})+\upsilon(\delta+\rho)C\text{-}H_{Ben}+(\upsilon)(C\text{-}F)$
1139			
	1113	25	$\upsilon(C=C\text{-}C=C_{Ben})+\upsilon(\delta+\rho)C\text{-}H_{Ben}+(\upsilon)(C\text{-}F)$
1136			
		18	$\upsilon(C=C\text{-}C=C_{Ben})+(\rho)C\text{-}H_{Ben}+\beta(C\text{-}H_{Ben})$
1099			
1059		4	$(\delta+\tau)C\text{-}H_{CH3}$
1022		46	$(\gamma)C\text{-}H_{CH3}$
1012		11	$(\gamma)C\text{-}H_{CH3}$
978		37	$(\gamma+\tau)C\text{-}H_{CH3}$
968		12	$(\gamma+\tau)C\text{-}H_{CH3}$
		60	$\upsilon(C=N)+\upsilon(C=C\text{-}C=C_{Ben})+(\gamma+\rho)C\text{-}H_{Ben}$
955			
885	874	18	$(\gamma)C\text{-}H$
884	823	14	$(\gamma)C\text{-}H$
852		18	$(w)C\text{-}H_{Ben}$
850		18	$\upsilon(C=C\text{-}C=C_{Ben})+(w)C\text{-}H_{Ben}$
812		40	$(\upsilon)(C\text{-}F)$
807		93	$\upsilon(C=C\text{-}C=C_{Ben})+(w)C\text{-}H_{Ben}$
800	796	17	$\upsilon(C=C\text{-}C=C_{Ben})+(\tau)C\text{-}H_{Ben}$
754	778	8	$\upsilon(C=C\text{-}C=C_{Ben})+(w)C\text{-}H_{Ben}$
641	604	8	$\upsilon(C=C\text{-}C=C_{Ben})+(w)C\text{-}H_{Ben}$

Frequencies are given in cm^{-1}, υ=stretching, β=in-plane bending, γ=out-plane bending, δ=scissoring, ρ=rocking, w=wagging, s=symmetric, as=asymmetric, τ=twisting, Ben=benzene ring

Table S5: Calculated vibrational frequencies of **ND5**

Frequencies	***Experimental***	***Intensities***	***Vibrational assignments***

3239		3	υ(s)(C-H)
3236		8	υ(s)(C-H)
3216		1	υ(C-H)
3213		17	υ(s)+υ(as)C-H_{Ben}
3197		24	υ(s)+υ(as)C-H_{Ben}
3043		30	υ(C-H)
3043		36	υ(C-H)
1721		10	υ(C=N)
1717		251	υ(C=N)+υ(C=C-C=C_{Ben})+(ρ)C-H
1672		9	υ(C=C-C=C_{Ben})+υ(δ+ρ)C-H_{Ben}
1671		18	υ(C=C-C=C_{Ben})+υ(δ+ρ)C-H_{Ben}
164		31	υ(C=C-C=C_{Ben})+υ(δ+ρ)C-H_{Ben}
1642		138	υ(C=C-C=C_{Ben})+υ(δ+ρ)C-H_{Ben}
1641		62	υ(C=C-C=C_{Ben})+υ(δ+ρ)C-H_{Ben}
	1613	9	υ(C=C-C=C_{Ben})+υ(δ+ρ)C-H_{Ben}+υ(C=N)
1633			
1562	1567	45	υ(C=C-C=C_{Ben})+υ(δ+ρ)C-H_{Ben}
1538		34	υ(C=C-C=C_{Ben})+(ρ)C-H_{Ben}
1537		189	υ(C=C-C=C_{Ben})+(ρ)C-H_{Ben}
1504		4	υ(C=C-C=C_{Ben})+υ(ρ)C-H_{Ben}+(ρ)C-H
	1474	15	υ(C=C-C=C_{Ben})+υ(ρ)C-H_{Ben}+(ρ)C-H+υ(C-Cl)
1476			
		30	υ(C=C-C=C_{Ben})+υ(ρ)C-H_{Ben}+(ρ)C-H+υ(C-Cl)
1470			
		7	υ(C=C-C=C_{Ben})+υ(δ+ρ)C-H_{Ben}+(ρ)C-H+υ(C-Cl)
1449			
1444	1416	50	υ(C=C-C=C_{Ben})+(ρ)C-H_{Ben}
1397		43	(ρ)C-H
1395		3	(ρ)C-H
1372		26	υ(C=C-C=C_{Ben})+υ(δ+ρ)C-H_{Ben}
		11	υ(C=C-C=C_{Ben})+υ(δ+ρ)C-H_{Ben}+(ρ)C-H
1355			
1326		23	υ(C=C-C=C_{Ben})+(ρ)C-H+υ(C-Cl)
1325		209	υ(C=C-C=C_{Ben})+(ρ)C-H+υ(C-Cl)
1295	1288	167	υ(C=C-C=C_{Ben})+(ρ)C-H+υ(C-Cl)
1272		14	υ(C=C-C=C_{Ben})+(ρ)C-H+υ(C-Cl)
1272		49	υ(C=C-C=C_{Ben})+(ρ)C-H+υ(C-Cl)
1248	1233	11	υ(C=C-C=C_{Ben})+υ(δ+ρ)C-H_{Ben}
		17	υ(C=C-C=C_{Ben})+υ(δ+ρ)C-H_{Ben}+(ρ)C-H
1197			
		4	υ(C=C-C=C_{Ben})+υ(δ+ρ)C-H_{Ben}+(ρ)C-H+υ(C-Cl)
1187			
1185		7	υ(C=C-C=C_{Ben})+υ(δ+ρ)C-H_{Ben}
1160		5	υ(C=C-C=C_{Ben})+υ(δ+ρ)C-H_{Ben}
1100		16	υ(C=C-C=C_{Ben})+υ(δ+ρ)C-H_{Ben}
		164	υ(C=C-C=C_{Ben})+υ(δ)C-H_{Ben}+β(C-H)+υ(C-Cl)
1087			
	1052	12	υ(C=C-C=C_{Ben})+υ(δ)C-H_{Ben}+β(C-H)+υ(C-Cl)
1087			
1011		8	(γ)C-H
1011		10	(γ)C-H

993		3	(τ)C-H+(γ)C-H
988		63	υ(C=C-C=C_{Ben})+$\upsilon(\rho)$C-H_{Ben}+β(C-H)+υ(C-Cl)
982		21	υ(C=C-C=C_{Ben})+$\upsilon(\rho)$C-H_{Ben}+β(C-H)+υ(C-Cl)
960	969	72	υ(C=C-C=C_{Ben})+$\upsilon(\rho)$C-H_{Ben}+γ(C-H)+υ(C-Cl)
886	920	22	(γ)C-H_{Ben}
885	874	17	(γ)C-H_{Ben}
850		19	(w)C-H_{Ben}
849		19	(w)C-H_{Ben}
811	813	42	υ(C-Cl)
843		1	τ(C-Cl)
808		93	υ(C=C-C=C_{Ben})+(w)C-H_{Ben}
800	774	15	υ(C=C-C=C_{Ben})+(τ)C-H_{Ben}
755	695	10	(w)C-H_{Ben}
641	608	10	υ(C=C-C=C_{Ben})+(w)C-H_{Ben}

Frequencies are given in cm^{-1}, υ=stretching, β=in-plane bending, γ=out-plane bending, δ=scissoring, ρ=rocking, w=wagging, s=symmetric, as=asymmetric, τ=twisting, Ben=benzene ring

Table S6: Calculated vibrational frequencies of compound **ND6**

DFT Freq. (*cm^{-1}*)	**XRD**	**Intensities (*Km/mol*)**	**Vibrational assignments**
3696.48		31	υ(N-H_{Pyr})
3696.47		381	υ(N-H_{Pyr})
3308.0	3365	42	υ(C-H_{Pyr})
3231.34		22	υ_s(C-H_{Ben})
3223.95		15	υ_s(C-H_{Ben})
3223.94		47	υ_s(C-H_{Ben})
3212.5		30	υ_s+υ_{as}(C-H_{Ben})
3209.2		8	υ_s+υ_{as}(C-H_{Ben})
3209.1		9	υ_s+υ_{as}(C-H_{Ben})
3197.90		39	υ_{as}(C-H_{Ben})
3194.63		6	υ_s+υ_{as}(C-H_{Ben})
3194.63		12	υ_s+υ_{as}(C-H_{Ben})
3043.59		66	υ(C-H)
3043.50		80	υ(C-H)
1700.17		30	υ(C-N)+ρ(C-H)
1695.32		926	υ(C-N)+ρ(C-H)
1675.12		5	υ(C=C-C=C_{Ben})+δ(C-H_{Ben})+ρ(C-H_{Pyr})+ρ(N-H_{Pyr})
1674.3		99	υ(C=C-C=C_{Ben})+δ(C-H_{Ben})+ρ(C-H_{Pyr})+ρ(N-H_{Pyr})+ υ(C-N)
1636.7	1612	41	υ(C=C-C=C_{Ben})+ρ+δ(C-H_{Ben})
1626.13		312	υ(C=C-C=C_{Ben})+δ(C-H_{Ben})+ρ(C-H_{Pyr})+ρ(N-H_{Pyr})
1560.6		24	υ(C=C-C=C_{Ben})+ρ+δ(C-H_{Ben})+ρ(N-H_{Pyr})
1554.1		13	υ(C-N_{Pyr})+ρ(C-H)
1552.05		12	υ(C=C-C=C_{Ben})+ρ+δ(C-H_{Ben})+υ(C-

			N_{Pyr})+ρ(N-H_{Pyr})+δ(C-H_{Pyr})
1546.29		10	υ(C=C-C=C_{Ben})+ρ(C-H_{Ben})+υ(C-N_{Pyr})+δ(C-H_{Pyr})
1543.6		263	υ(C=C-C=C_{Ben})+ρ+δ(C-H_{Ben})+υ(C-N_{Pyr})+ρ(N-H_{Pyr})+δ(C-H_{Pyr})
1482.8		74	υ(C=C-C=C_{Ben})+ρ(C-H_{Ben})+υ(C-N_{Pyr})
1481.8		21	υ(C=C-C=C_{Ben})+ρ(C-H_{Ben})+υ(C-N_{Pyr})+ρ(N-H_{Pyr})
1473.67		219	υ(C=C-C=C_{Ben})+ρ(C-H_{Ben})+υ(C-N_{Pyr})+ρ(N-H_{Pyr})+υ(C-H_{Pyr})
1448.79		130	υ(C=C-C=C_{Ben})+ρ(C-H_{Ben})+υ(C-N)
1445.29		8	υ(C=C-C=C_{Ben})+ρ+δ(C-H_{Ben})
1408.48	1429	61	ρ(C-H)
1406.64		116	ρ(C-H)
1400.99		87.9	υ(C=C-C=C_{Ben})+ρ+δ(C-H_{Ben})+υ(C-N_{Pyr})+ρ(N-H_{Pyr})+ρ(C-H_{Pyr})
1400.75		84.4	υ(C=C-C=C_{Ben})+ρ+δ(C-H_{Ben})+υ(C-N_{Pyr})+ρ(N-H_{Pyr})+ρ(C-H_{Pyr})
1362.54	1336	15	υ(C=C-C=C_{Ben})+ρ+δ(C-H_{Ben})
1304.34		59	υ(C=C-C=C_{Ben})+ρ+δ(C-H_{Ben})+υ(C-N_{Pyr})+ρ(N-H_{Pyr})
1297.16		127	υ(C=C-C=C_{Ben})+ρ(C-H_{Ben})+υ(C-N_{Pyr})+ρ(N-H_{Pyr})
1264.07		74	υ(C=C-C=C_{Ben})+ρ(C-H_{Ben})+υ(C-N_{Pyr})+ρ(N-H_{Pyr})+ρ(C-H_{Pyr})
1241.61		18	υ(C=C-C=C_{Ben})+ρ(C-H_{Ben})+ρ(N-H_{Pyr})+ρ(C-H_{Pyr})
1239.45		37	ρ(C-H)+ρ(N-H_{Pyr})+ρ(C-H_{Pyr})
1193.03		73	δ(C-H_{Ben})
1182.67		52	δ(C-H_{Ben})
1141.87		301	δ(C-H_{Ben})+ρ(N-H_{Pyr})+δ(C-H)$_{Pyr}$
1141.63		11	δ(C-H_{Ben})+ρ(N-H_{Pyr})+δ(C-H)$_{Pyr}$
1115.40		33	δ(C-H_{Ben})+ρ(N-H_{Pyr})+ρ(C-H)$_{Pyr}$
1115.25	1108	27	δ(C-H_{Ben})+ρ(N-H_{Pyr})+ρ(C-H)$_{Pyr}$
1096.86		18	ρ(C-H_{Ben})
1091.03		36	ρ(C-H_{Ben})
1090.42		8	ρ(C-H_{Ben})
1049.17		42	δ(C-H_{Ben})
1049.08		9.8	δ(C-H_{Ben})
1015.13		11	γ(C-H)+τ(C-H_{Ben})
1014.40		42	γ(C-H)+τ(C-H_{Ben})
956	966	125	υ(C=C-C=C_{Ben})+ρ+γ(C-H_{Ben})+υ(C-N)
915.34	920	22	υ(C-N)+ρ+γ(C-H_{Pyr})+ρ(C-N)
915.25		26	υ(C-N)+ρ+γ(C-H_{Pyr})+ρ(C-N)
810.43		59	*w*(C-H_{Ben})
797.54		29	υ(C=C-C=C_{Ben})+τ(C-H_{Ben})
780.7	780	158	υ(C=C-C=C_{Ben})+*w*(C-H_{Ben})+*w*(C-H_{Pyr})
780.6		190	υ(C=C-C=C_{Ben})+*w*(C-H_{Ben})+*w*(C-H_{Pyr})
756.8	750	5.3	*w*(C-H_{Ben})
743.78		81	*w*(C-H_{Ben})
644.1		21	υ(C-N)+γ(N-H_{Pyr})+γ(C-H_{Pyr})

641.17		5	$\gamma(N\text{-}H_{Pyr})+\gamma(C\text{-}H_{Pyr})$
617.07	626	5	$\gamma(N\text{-}H_{Pyr})+\tau(C\text{-}H_{Pyr})$

Frequencies are given in cm^{-1}, υ=stretching, *β*=in-plane bending, γ=out-plane bending, δ=scissoring, *ρ*=rocking, *w*= wagging, s =symmetric stretching, as=asymmetric stretching, τ=twisting, Ben=benzene ring.

Table S7: Calculated vibrational frequencies of compound **ND7**

DFT unscaled Freq. (*cm*$^{-1}$)	**Experimental**	**Intensities (*Km/mol*)**	**Vibrational assignments**
3693.56		217	$\upsilon(N\text{-}H_{Pyr})$
3692.49		229	$\upsilon(N\text{-}H_{Pyr})$
3288.66		3	$\upsilon_s(C\text{-}H_{Pyr})$
3231.77		17	$\upsilon_s(C\text{-}H_{Ben})$
3226.98		9	$\upsilon_s(C\text{-}H_{Ben})$
3220.85		18	$\upsilon_s(C\text{-}H_{Ben})$
3212.04		31	$\upsilon_s+\upsilon_{as}(C\text{-}H_{Ben})$
3209.04		6	$\upsilon_s+\upsilon_{as}(C\text{-}H_{Ben})$
3197.40		43	$\upsilon_{as}(C\text{-}H_{Ben})$
3195.64	3165	13	$\upsilon(C\text{-}H_{Ben})$
3046.14		25	υ(C-H)
3045.99		114	υ(C-H)
1708.38		115	υ(C-N)+ρ(C-H)
1701.18		707	υ(C-N)+ρ(C-H)
1677.41		254	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{pyr})+\rho(C\text{-}H_{Pyr})+\rho(N\text{-}H_{Pyr})$
1671.96		32	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})$
1665.72		716	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})+\rho(C\text{-}H_{Pyr})+\rho(N\text{-}H_{Pyr})+\upsilon(C\text{-}N)$
1643.5		7	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\delta+\rho(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{pyr})+\delta(C\text{-}H_{Pyr})+\rho(N\text{-}H_{Pyr})$
1638.8		53	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\delta+\rho(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{pyr})+\delta(C\text{-}H_{Pyr})+\rho(N\text{-}H_{Pyr})$
1636.54	1603	120	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})$
1565.76	1570	21	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{pyr})+\rho(C\text{-}H_{Pyr})+\rho(N\text{-}H_{Pyr})$
1556.99		210	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})$
1529.10		47	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{pyr})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H_{Pyr})$
1527.94		42	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{pyr})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H_{Pyr})$
1501.78		67	$\rho(C\text{-}H_{Ben})+\rho(N\text{-}H_{Pyr})$
1481.49	1495	54	$\upsilon(C\text{-}N_{pyr})+\rho(C\text{-}H_{Ben})+\rho(N\text{-}H_{Pyr})$
1476.85		97	$\upsilon(C\text{-}N_{pyr})+\rho(C\text{-}H_{Ben})+\rho(N\text{-}H_{Pyr})$
1448.45		161	$\rho(C\text{-}H_{Ben})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H)$
1413.70		91	ρ(C-H)
1410.41		53	ρ(C-H)
1394.25		140	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho(C\text{-}H_{Ben})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H)$

1389.43		12	$\upsilon(C\text{-}N_{Pyr})+\rho(C\text{-}H_{Pyr})+\rho(C\text{-}H)$
1368.84		111	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{Pyr})+\rho(N\text{-}H_{Pyr})+\delta(C\text{-}H_{Pyr})$
1362.33		80	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{Pyr})+\rho(N\text{-}H_{Pyr})+\delta(C\text{-}H_{Pyr})$
1353.34		59	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho(C\text{-}H_{Ben})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H)$
1339.79		205	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho(C\text{-}H_{Ben})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H)$
1313.12		205	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{Pyr})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H)$
1294.76		114	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{Pyr})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H_{Pyr})$
1281.18	1294	7	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho(C\text{-}H_{Ben})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H_{Pyr})$
1275.42		10	$\rho(C\text{-}H_{Ben})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H_{Pyr})+\rho(C\text{-}H_{Ben})$
1256.17		60	$\rho(C\text{-}H_{Ben})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H_{Pyr})$
1247.12		7	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H_{Pyr})+\ \rho(C\text{-}H)$
1241.04	1224	54	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})$
1179.78		19	$\rho+\delta(C\text{-}H_{Ben})$
1174.32		49	$\rho+\delta(C\text{-}H_{Ben})$
1160.67		8	$\delta(C\text{-}H_{Ben})$
1153.01		107	$\rho+\delta(C\text{-}H_{Ben})+\rho(N\text{-}H_{Pyr})$
1139.86		48	$\rho+\delta(C\text{-}H_{Ben})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H_{Pyr})$
1120.91	1121	66	$\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H_{Pyr})$
1116.59		90	$\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H_{Pyr})$
1094.84		19	$\rho(C\text{-}H_{Ben})+\delta(C\text{-}H_{Pyr})$
1094.01		13	$\delta(C\text{-}H_{Pyr})$
1093.82	1092	26	$\delta(C\text{-}H_{Pyr})$
1019.84		37	$\gamma(C\text{-}H)$
987.21		11	$\rho+\gamma(C\text{-}H_{Ben})$
970.22	975	41	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\rho+\gamma(C\text{-}H_{Ben})+\rho(C\text{-}H_{Pyr})$
955.02		120	$\upsilon(C{=}C\text{-}C{=}C_{Ben})\rho+\gamma(C\text{-}H_{Ben})$
931.37		15	$\gamma(C\text{-}H_{Ben})$
923.11	923	16	$\tau(C\text{-}H_{Ben})$
916.35		15	$\tau(C\text{-}H_{Pyr})+\gamma(N\text{-}H_{Pyr})$
914.33		17	$\gamma(C\text{-}H)$
912.81		9	$\upsilon(C\text{-}N)+\tau(C\text{-}H_{Pyr})+\gamma(N\text{-}H_{Pyr})$
846.7	880	7	$w(C\text{-}H_{Ben})$
834.90		23	$w(C\text{-}H_{Ben})$
832.35		28	$w(C\text{-}H_{Ben})$
826.89		26	$w(C\text{-}H_{Ben})$
806.12	805	156	$w(C\text{-}H_{Ben})$
798.28		35	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\tau(C\text{-}H_{Ben})$
795.68		9	$\upsilon(C{=}C\text{-}C{=}C_{Ben})+\tau(C\text{-}H_{Ben})$
788.16		22	$w(C\text{-}H_{Pyr})+\gamma(N\text{-}H_{Pyr})$
787.78	780	12	$w(C\text{-}H_{Pyr})+\gamma(N\text{-}H_{Pyr})$
745.88	764	165	$w(C\text{-}H_{Pyr})$

745.58	724	19	w(C-H_{Pyr})
626.71		10	γ(C-H_{Pyr})+ γ(N-H_{Pyr})
617.84	618	22	w(C-H_{Ben})+γ(C-H_{Pyr})+γ(N-H_{Pyr})

Frequencies are given in cm^{-1}, υ=stretching, β=in-plane bending, γ=out-plane bending, δ=scissoring, ρ=rocking, w= wagging, s =symmetric stretching, as=asymmetric stretching, τ=twisting, Ben=benzene ring.

Table S8: Calculated vibrational frequencies of compound **ND8**

DFT Freq. (*cm^{-1}*)	**Exp**	**Intensities (*Km/mol*)**	**Vibrational assignments**
3690.85		252	υ(N-H_{Pyz})
3690.19		248	υ(N-H_{Pyz})
3266.80		8	υ(C-H_{Pyz})
3232.10	3232	16	υ_s(C-H_{Ben})
3231.53		9	υ_s(C-H_{Ben})
3229.20		10	υ_s(C-H_{Ben})
3213.07		29	υ_s+υ_{as}(C-H_{Ben})
3206.09		7	υ_s+υ_{as}(C-H_{Ben})
3198.72		37	υ_{as}(C-H_{Ben})
3052.88		51	υ(C-H)
3052.06		76	υ(C-H)
1713.86		95	υ(C=C-C=C_{Ben})+ρ+δ(C-H_{Ben})+υ(C-N=N)+ρ(N-H)
1706.72		404	υ(C=C-C=C_{Ben})+ρ+δ(C-H_{Ben})+υ(C-N=N)+ρ(N-H)
1684.01		357	υ(C=C-C=C_{Ben})+ρ+δ(C-H_{Ben})+ρ(N-H)
1673.86		443	υ(C=C-C=C_{Ben})+ρ+δ(C-H_{Ben})+υ(C-$N=N_{pyz}$)+ρ(C-H_{Pyz})+ρ(N-H_{Pyz})
1671.70		279	υ(C=C-C=C_{Ben})+ρ+δ(C-H_{Ben})+υ(C-$N=N_{pyz}$)+ρ(C-H_{Pyz})+ρ(N-H_{Pyz})
1647.50		8	υ(C=C-C=C_{Ben})+ρ(C-H_{Ben})+υ(C-$N=N_{pyz}$)+ρ(C-H_{Pyz})+ρ(N-H_{Pyz})
1643.62		63	υ(C=C-C=C_{Ben})+ρ(C-H_{Ben})+υ(C-$N=N_{pyz}$)+ρ(C-H_{Pyz})+ρ(N-H_{Pyz})
1637.54	1605	75	υ(C=C-C=C_{Ben})+δ+ρ(C-H_{Ben})
1567.72	1572	74	υ(C=C-C=C_{Ben})+ρ(C-H_{Ben})+υ(C-$N=N_{pyz}$)+ρ(C-H_{Pyz})+ρ(N-H_{Pyz})
1564.21		132	υ(C=C-C=C_{Ben})+ρ(C-H_{Ben})+υ(C-$N=N_{pyz}$)+ρ(C-H_{Pyz})+ρ(N-H_{Pyz})
1555.62		55	υ(C=C-C=C_{Ben})+ρ+δ(C-H_{Ben})
1519.96		33	υ(C=C-C=C_{Ben})+δ+ρ(C-H_{Ben})+υ(C-$N=N_{pyz}$)+ρ(C-H_{Pyz})+ρ(N-H_{Pyz})
1519.52	1500	37	υ(C=C-C=C_{Ben})+δ+ρ(C-H_{Ben})+υ(C-$N=N_{pyz}$)+ρ(C-H_{Pyz})+ρ(N-H_{Pyz})
1484.75		10	υ(C=C-C=C_{Ben})+δ+ρ(C-H_{Ben})+υ(C-$N=N_{pyz}$)+ρ(C-H_{Pyz})+ρ(N-H_{Pyz})
1462.83		36	υ(C=C-C=C_{Ben})+ρ(C-H_{Ben})+υ(C-$N=N_{pyz}$)+ρ(C-H_{Pyz})+ρ(N-H_{Pyz})
1454.17		17	υ(C=C-C=C_{Ben})+ρ(C-H_{Ben})+υ(C-

			$N=N_{pyz})+\rho(C-H_{Pyz})+\rho(N-H_{Pyz})$
1446.79		67	$\upsilon(C=C-C=C_{Ben})+\rho(C-H_{Ben})$
1444.11		21	$\upsilon(C=C-C=C_{Ben})+\delta+\rho(C-H_{Ben})$
1418.28		118	$\rho(C-H)+\rho(N-H_{Pyz})$
1410.78		6	$\rho(C-H)+\rho(N-H_{Pyz})$
1394.67		206	$\upsilon(C=C-C=C_{Ben})+\upsilon(C-N=N_{pyz})+\rho(N-H_{Pyz})$
1377.98		32	$\rho(C-H)$
1361.81	1360	8	$\upsilon(C=C-C=C_{Ben})+\delta+\rho(C-H_{Ben})+\rho(C-H)$
1345.56		96	$\upsilon(C=C-C=C_{Ben})+\rho(C-H_{Ben})+\upsilon(C-N=N_{pyz})+\rho(C-H_{Pyz})+\rho(N-H_{Pyz})$
1316.38		39	$\upsilon(C=C-C=C_{Ben})+\rho(C-H_{Ben})+\upsilon(C-N=N_{pyz})+\rho(C-H_{Pyz})+\rho(N-H_{Pyz})$
1296.20	1298	59	$\rho(C-H_{Ben})+\rho(N-H_{Pyz})+\rho(C-H_{Pyz})$
1278.70		8	$\rho(C-H_{Ben})+\rho(N-H_{Pyz})+\rho(C-H_{Pyz})$
1265.13		9	$\rho(C-H_{Ben})+\rho(N-H_{Pyz})$
1260.33		35	$\rho(C-H_{Ben})+\rho(N-H_{Pyz})$
1204.72		9	$\upsilon(C=C-C=C_{Ben})+\delta+\rho(C-H_{Ben})+\rho(C-H)$
1189		12	$\upsilon(C=C-C=C_{Ben})+\rho+\delta(C-H_{Ben})+\rho(C-H_{Pyz})$
1179.96		43	$\upsilon(C=C-C=C_{Ben})+\rho+\delta(C-H_{Ben})+\rho(C-H_{Pyz})$
1173.25		63	$\rho+\delta(C-H_{Ben})$
1163.83		45	$\rho+\delta(C-H_{Ben})$
1156.79		127	$\delta(C-H_{Ben})$
1143.07	1142	99	$\rho+\delta(C-H_{Ben})$
1133.52		21	$\upsilon(C-N=N_{pyz})+\rho(C-H_{Pyz})+\rho(N-H_{Pyz})$
1130.27	1116	30	$\upsilon(C-N=N_{pyz})+\rho(C-H_{Pyz})+\rho(N-H_{Pyz})$
1095.16		38	$\delta(C-H_{Ben})$
1022.23	1056	19	$\gamma(C-H)$
1020.51		31	$\gamma(C-H)$
988.92		8.2	$\rho+\gamma(C-H_{Ben})$
972.80	977	21	$\rho+\gamma(C-H_{Ben})$
964.06		39	$\upsilon(C-N=N_{pyz})+\rho(C-H_{Pyz})+\rho(N-H_{Pyz})$
960.37		81	$\upsilon(C-N=N_{pyz})+\rho(C-H_{Pyz})+\rho(N-H_{Pyz})$
955.03	953	116	$\upsilon(C=C-C=C_{Ben})+\rho+\gamma(C-H_{Ben})+\upsilon(C-N)+\rho(C-H_{Pyz})$
942.60		14	$\gamma(C-H_{Ben})+\gamma(C-H_{Pyz})$
926.73		16	$\tau+\gamma(C-H_{Ben})$
923.53	921	13	$\tau+\gamma(C-H_{Ben})$
876.82	881	32	$\gamma(C-H_{Pyz})$
841.63		35	$w(C-H_{Ben})$
837.96		36	$w(C-H_{Ben})$
833.04	832	33	$w(C-H_{Ben})$
807.69	811	124	$w(C-H_{Ben})$
803.62		49	$w(C-H_{Ben})$
797.41		19	$\upsilon(C=C-C=C_{Ben})+\tau(C-H_{Ben})$
781.59	788	10	$\upsilon(C=C-C=C_{Ben})+w(C-H_{Ben})$
685.22	718	48	$\gamma(C-H_{Pyz})+\gamma(N-H_{Pyz})$
684.00		10	$\gamma(C-H_{Pyz})+\gamma(N-H_{Pyz})$
679.36		30	$\gamma(N-H_{Pyz})$
629.58	622	52	$w(C-H_{Ben})+\gamma(C-H_{Pyz})+\gamma(N-H_{Pyz})$

Frequencies are given in cm^{-1}, υ=stretching, *β*=in-plane bending, γ=out-plane bending, δ=scissoring, *ρ*=rocking, *w*= wagging, s =symmetric stretching, as=asymmetric stretching, τ=twisting, Ben=benzene ring, Pyr=Pyrole, Pyz=Pyrazole .

Table S9:. Calculated vibrational frequencies of compound **ND9**

DFT Freq. (*cm^{-1}*)		**Intensities (*Km/mol*)**	**Vibrational assignments**
3683.19		176	$\upsilon(N\text{-}H_{Pyr})$
3683.13	3417	183	$\upsilon(N\text{-}H_{Pyr})$
3232.61		21	$\upsilon_s(C\text{-}H_{Ben})$
3223.77		64	$\upsilon_s(C\text{-}H_{Ben})$
3215.86		53	$\upsilon_s(C\text{-}H_{Ben})$
3213.84		28	$\upsilon_s+\upsilon_{as}(C\text{-}H_{Ben})$
3205.37		8	$\upsilon_s+\upsilon_{as}(C\text{-}H_{Ben})$
3205.37		11	$\upsilon_s+\upsilon_{as}(C\text{-}H_{Ben})$
3199.64		41	$\upsilon_{as}(C\text{-}H_{Ben})$
3087.76		37	υ(C-H)
3087.71		62	υ(C-H)
1695.27		24	$\upsilon(C\text{-}N)+\rho(C\text{-}H)+\rho(N\text{-}H_{Pyr})$
1690.63		788	$\upsilon(C\text{=}C\text{-}C\text{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{Pyr})+\rho(N\text{-}H_{Pyr})+\upsilon(C\text{-}N)$
1678.44		1221	$\upsilon(C\text{=}C\text{-}C\text{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{Pyr})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H_{Pyr})$
1640.64		28	$\upsilon(C\text{=}C\text{-}C\text{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})+\rho(C\text{-}H_{Pyr})+\rho(N\text{-}H_{Pyr})$
1636.90	1604	49	$\upsilon(C\text{=}C\text{-}C\text{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})$
1596.39		21	$\upsilon(C\text{=}C\text{-}C\text{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{Pyr})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H_{Pyr})+\upsilon(C\text{-}N)$
1595.36		10	$\upsilon(C\text{=}C\text{-}C\text{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{Pyr})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H_{Pyr})+\upsilon(C\text{-}N)$
1554.82		181	$\upsilon(C\text{=}C\text{-}C\text{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})$
1492.39	1493	15	$\upsilon(C\text{=}C\text{-}C\text{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})$
1489.33		9	$\upsilon(C\text{=}C\text{-}C\text{=}C_{Ben})+\rho(C\text{-}H_{Ben})$
1471.30		49	$\upsilon(C\text{-}N_{Pyr})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H)+\rho(C\text{-}H_{Ben})$
1471.03		183	$\upsilon(C\text{-}N_{Pyr})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H)+\rho(C\text{-}H_{Ben})$
1441.99	1439	221	$\upsilon(C\text{=}C\text{-}C\text{=}C_{Ben})+\rho(C\text{-}H_{Ben})$
1418.5	1396	7	$\upsilon(C\text{=}C\text{-}C\text{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{Pyr})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H_{Pyr})$
1382.21		266	$\upsilon(C\text{=}C\text{-}C\text{=}C_{Ben})+\rho(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{Pyr})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H_{Pyr})$
1378.80		52	ρ(C-H)
1355.80		81	$\upsilon(C\text{=}C\text{-}C\text{=}C_{Ben})+\rho(C\text{-}H_{Ben})$
1339.49		37	ρ(C-H)
1295.17		68	ρ(C-H)
1262.14		8	$\rho(C\text{-}H_{Ben})$
1247.07	1249	122	$\upsilon(C\text{=}C\text{-}C\text{=}C_{Ben})+\rho+\delta(C\text{-}H_{Ben})+\rho(N\text{-}H_{Pyr})$
1176.33		16	$\upsilon(C\text{=}C\text{-}C\text{=}C_{Ben})+\delta(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{Pyr})+\rho(C\text{-}H_{Pyr})$
1154.43		373	$\upsilon(C\text{=}C\text{-}C\text{=}C_{Ben})+\delta(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{Pyr})+\rho(C\text{-}$

			H_{Pyr})
1143.97	1104	23	$\upsilon(C=C\text{-}C=C_{Ben})+\rho+\delta(C\text{-}H_{Ben})$
1096.67		41	$\upsilon(C=C\text{-}C=C_{Ben})+\rho+\delta(C\text{-}H_{Ben})$
1044.69		12	$\upsilon(C=C\text{-}C=C_{Ben})+\rho+\delta(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{Pyr})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H_{Pyr})$
1026.35		10	$\upsilon(C=C\text{-}C=C_{Ben})+\rho+\delta(C\text{-}H_{Ben})+\upsilon(C\text{-}N_{Pyr})+\rho(N\text{-}H_{Pyr})+\rho(C\text{-}H_{Pyr})$
996.58		11	$\gamma(C\text{-}H_{Ben})$
962.29	971	153	$\upsilon(C=C\text{-}C=C_{Ben})+\rho+\gamma(C\text{-}H_{Ben})$
930.76	923	7	$\tau(C\text{-}H_{Ben})$
829.03		72	$w(C\text{-}H_{Ben})+\gamma(C\text{-}H_{Pyr})$
828.42	821	60	$w+\tau(C\text{-}H_{Ben})+\gamma(C\text{-}H_{Pyr})$
811.08	803	143	$w(C\text{-}H_{Ben})$
799.04		14	$w(C\text{-}H_{Ben})$
797		35	$\upsilon(C=C\text{-}C=C_{Ben})+\tau(C\text{-}H_{Ben})$
774.63		26	$w+\tau(C\text{-}H_{Ben})$
774.37	768	27	$w+\tau(C\text{-}H_{Ben})$
758.48		60	$w(C\text{-}H_{Ben})$
758.42		50	$w(C\text{-}H_{Ben})$
668.04		29	$\gamma(C\text{-}H_{Pyr})+\gamma(N\text{-}H_{Pyr})$

Frequencies are given in cm^{-1}, υ =stretching, β=in-plane bending, γ=out-plane bending, δ=scissoring, ρ=rocking, w= wagging, s =symmetric stretching, as=asymmetric stretching, τ=twisting, Pyr=Pyrole, Ben=benzene ring.

Table S10: Energies of frontier molecular orbitals and band gaps of entitled compounds.

Compounds	E_{HOMO}	E_{LUMO}	ΔE	E_{opt}	$\lambda_{onset\ (nm)}$
ND1	-6.070	-2.232	3.838	3.850	322
ND2	-6.042	-2.175	3.867	3.916	317
ND3	-6.060	-2.208	3.852	4.065	305
ND4	-5.994	-2.094	3.900	3.936	315
ND5	-6.071	-2.267	3.804	3.850	322
ND6	-5.783	-2.003	3.780	3.647	340
ND7	-5.811	-1.830	3.981	3.875	320
ND8	-5.904	-1.970	3.934	3.815	325
ND9	-5.836	-2.133	3.703	3.792	327

Band gap = $E_{LUMO}-E_{HOMO}$, units in *eV*; E_{opt} is the optical band gap calculated through onset wavelength of experimental UV-Vis spectrum

Table S11: Wave length, excitation energy and oscillator strength of investigated chromophores in acetonitrile phase

Compounds	λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
ND1	399.112	3.107	0.686	H→L (97%)
	370.633	3.345	0.005	H→L+1 (95%)
	304.899	4.066	0.002	H-4→L (11%), H-1→L (76%), H-7→L+1 (6%), H→L+1 (2%)
	298.218	4.158	0.000	H-2→L (56%), H→L+5 (25%), H-7→L (2%), H-4→L+1 (3%), H-2→L+4 (2%), H-1→L+1 (8%)
	294.331	4.212	0.001	H-4→L+1 (12%), H-3→L (11%), H-1→L+1 (36%), H→L+4

				(12%), H-7→L (8%), H-2→L (6%), H→L+5 (9%)
	275.001	4.509	0.001	H→L+3 (88%), H-6→L (4%), H-5→L+1 (3%), H-1→L+2 (3%)
ND2	396.052	3.131	0.690	H→L (97%)
	367.274	3.376	0.006	H→L+1 (95%)
	304.047	4.078	0.003	H-6→L (11%), H-1→L (74%), H-7→L+1 (6%), H-4→L (4%), H→L+1 (2%)
	297.125	4.173	0.001	H-2→L (55%), H→L+3 (28%), H-7→L (2%), H-6→L+1 (3%), H-2→L+2 (2%), H-1→L+1 (6%)
	293.447	4.225	0.001	H-6→L+1 (12%), H-1→L+1 (32%), H→L+2 (13%), H-7→L (8%), H-5→L (7%), H-4→L+1 (3%), H-3→L (5%), H-2→L (4%), H→L+3 (9%)
	277.233	4.472	0.596	H-3→L (21%), H-1→L+1 (29%), H→L+2 (41%), H-4→L+1 (3%)
ND3	398.253	3.113	0.711	H→L (97%)
	369.429	3.356	0.004	H→L+1 (95%)
	304.869	4.067	0.002	H-6→L (10%), H-1→L (71%), H-7→L+1 (6%), H-4→L (7%), H→L+1 (2%)
	297.774	4.164	0.001	H-3→L (29%), H-2→L (26%), H→L+5 (26%), H-7→L (2%), H-6→L+1 (3%), H-1→L+1 (7%)
	294.129	4.215	0.001	H-6→L+1 (11%), H-1→L+1 (30%), H→L+2 (12%), H-7→L (8%), H-5→L (9%), H-4→L+1 (6%), H-3→L (8%), H→L+5 (9%)
	283.256	4.377	0.224	H-4→L+1 (16%), H-3→L (23%), H-2→L (32%), H-1→L+1 (14%), H-1→L+3 (2%), H→L+4 (6%)
ND4	392.367	3.160	0.799	H→L (97%)
	361.639	3.428	0.006	H→L+1 (94%)
	304.248	4.075	0.002	H-4→L (11%), H-1→L (73%), H-7→L+1 (5%), H-6→L (6%), H→L+1 (2%)
	295.884	4.190	0.010	H-3→L (40%), H-2→L (12%), H→L+3 (30%), H-7→L (3%), H-6→L+1 (2%), H-4→L+1 (4%), H-3→L+2 (2%), H-1→L+1 (3%)
	292.650	4.237	0.005	H-4→L+1 (14%), H-3→L (12%), H-2→L (10%), H-1→L+1 (17%), H→L+2 (14%), H→L+3 (12%), H-7→L (9%), H-6→L+1 (7%)
	282.418	4.390	0.811	H-2→L (35%), H-1→L+1 (50%), H-3→L (4%), H→L+2 (5%)
ND5	403.686	3.071	0.784	H→L (97%)
	374.281	3.313	0.005	H→L+1 (95%)
	308.303	4.022	0.002	H-4→L (16%), H-1→L (71%), H-7→L+1 (6%), H→L+1 (2%)
	299.602	4.138	0.001	H-2→L (46%), H-1→L+1 (11%), H→L+5 (18%), H-7→L (5%), H-4→L+1 (8%), H-3→L (3%)
	296.329	4.184	0.001	H-4→L+1 (14%), H-3→L (21%), H-1→L+1 (22%), H→L+5 (15%), H-7→L (8%), H-2→L (5%), H→L+2 (9%)
	283.250	4.377	1.061	H-3→L (26%), H-1→L+1 (42%), H→L+2 (18%), H-2→L (8%)
ND6	405.320	3.059	0.949	H→L (95%), H-1→L+1 (3%)
	370.133	3.350	0.000	H→L+1 (91%), H-1→L (4%)
	345.830	3.585	0.016	H-2→L+1 (10%), H-1→L (87%), H→L+1 (2%)
	334.665	3.705	0.181	H-2→L (68%), H-1→L+1 (27%),
	315.126	3.934	0.099	H-2→L (20%), H-1→L+1 (64%), H-7→L (2%), H-5→L+1 (5%), H→L (4%), H→L+2 (2%)

	309.788	4.002	0.039	H-5→L (19%), H-3→L (14%), H-2→L+1 (51%), H-7→L+1 (3%), H-1→L (4%), H→L+1 (4%)
ND7	383.138	3.236	1.005	H→L (96%)
	347.360	3.569	0.018	H→L+1 (93%)
	327.496	3.786	0.018	H-1→L (74%), H-1→L+1 (12%), H-2→L (6%), H-2→L+1 (3%)
	319.429	3.881	0.016	H-2→L (65%), H-2→L+1 (18%), H-1→L (6%), H-1→L+1 (4%)
	307.598	4.031	0.002	H-3→L (79%), H-6→L (7%), H-2→L+1 (3%), H-1→L (3%)
	293.883	4.219	0.084	H-5→L (34%), H-4→L (10%), H→L+4 (47%)
ND8	388.054	3.195	0.866	H→L (96%)
	355.620	3.486	0.043	H→L+1 (93%)
	311.359	3.982	0.042	H-1→L (87%), H-6→L (2%), H-2→L+1 (2%)
	300.413	4.127	0.154	H-2→L (49%), H→L+2 (14%), H-6→L (4%), H-3→L (8%), H-3→L+1 (5%), H-1→L+1 (7%)
	294.204	4.214	0.003	H-4→L (40%), H→L+4 (39%), H-5→L (3%), H→L+2 (6%), H→L+5 (3%)
	292.634	4.237	0.009	H-3→L (26%), H-2→L+1 (11%), H→L+2 (31%), H-7→L+1 (3%), H-6→L (8%), H-4→L (3%), H-3→L+1 (3%), H-1→L+1 (2%), H→L+4 (3%)
ND9	411.113	3.016	1.350	H→L (96%)
	369.449	3.356	0.004	H→L+1 (93%), H-2→L+1 (2%)
	341.938	3.626	0.015	H-1→L (94%), H-2→L+1 (4%)
	332.904	3.724	0.089	H-2→L (79%), H-1→L+1 (10%), H-3→L+1 (8%)
	323.556	3.832	0.013	H-3→L (71%), H-2→L+1 (19%), H-4→L+1 (3%)
	314.543	3.942	0.571	H-1→L+1 (82%), H-6→L+1 (3%), H-3→L+1 (4%), H-2→L (6%), H→L (3%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength=λ (nm)

Table S112: Hole-electron analysis indices for $S_0 \rightarrow S_1$ excitation (with highest f_{osc}) of compounds **ND1** to **ND9.**

Compound	Excitation	E (eV)	D (Å)	E_{Coul} (eV)	S_r	H (Å)	t (Å)	HDI	EDI
ND1	$S_0 \rightarrow S_1$	3.107	0.328	3.8702	0.6931	4.027	-0.511	6.15	5.17
ND2	$S_0 \rightarrow S_1$	3.131	0.301	3.9519	0.7010	3.999	-0.539	6.12	5.18
ND3	$S_0 \rightarrow S_1$	3.113	0.311	3.8703	0.6960	4.016	-0.528	6.13	5.17
ND4	$S_0 \rightarrow S_1$	3.160	0.296	3.9206	0.7213	4.068	-0.543	5.95	5.19
ND5	$S_0 \rightarrow S_1$	3.071	0.323	3.8697	0.6951	4.152	-0.513	6.06	5.18
ND6	$S_0 \rightarrow S_1$	3.059	0.314	3.5747	0.7439	4.756	-0.691	4.91	4.98
ND7	$S_0 \rightarrow S_1$	3.236	0.564	3.7819	0.7474	4.234	-3.297	5.46	5.20
ND8	$S_0 \rightarrow S_1$	3.195	1.296	3.7668	0.7226	4.169	-2.486	5.68	5.32
ND9	$S_0 \rightarrow S_1$	3.016	0.148	3.4318	0.7504	4.926	-0.725	4.91	5.03

Table S13. AIM properties of the main intra- and intermolecular interactions for **MK19**. Electronic density (ρ), Laplacian of density ($\nabla^2\rho$), ellipticity (ε) and density of potential energy (V).

Bond	ρ (e/a^3)	$\nabla^2\rho$ (e/a^5)	ε	V (hartree.e/a^3)

C1 - C2	+0.320434	-0.923135	+0.238782	-0.455390
C3 - C4	+0.293330	-0.787165	+0.172781	-0.374279
C2 - C3	+0.297389	-0.813355	+0.165985	-0.385532
C2 - H8	+0.284081	-0.990531	+0.019517	-0.322614
C1 - C6	+0.301014	-0.832658	+0.173419	-0.396535
C4 - C5	+0.291219	-0.784410	+0.180977	-0.364023
C5 - N17	+0.302935	-0.904809	+0.034566	-0.546007
C5 - C6	+0.315301	-0.889524	+0.259981	-0.441548
C1 - H7	+0.282583	-0.982260	+0.016081	-0.320960
C3 - C9	+0.291219	-0.784411	+0.180977	-0.364024
C9 - N18	+0.302935	-0.904809	+0.034566	-0.546008
C4 - C10	+0.297389	-0.813356	+0.165985	-0.385533
C10 - H14	+0.284081	-0.990526	+0.019517	-0.322612
C6 - H11	+0.281659	-0.972441	+0.022137	-0.320350
C10 - C12	+0.320434	-0.923137	+0.238782	-0.455391
C12 - C13	+0.301014	-0.832662	+0.173419	-0.396537
C9 - C13	+0.315301	-0.889524	+0.259981	-0.441548
C12 - H15	+0.282583	-0.982256	+0.016081	-0.320959
C13 - H16	+0.281659	-0.972440	+0.022137	-0.320350
N17 - C19	+0.373373	-0.796462	+0.169141	-0.981490
C19 - C26	+0.281325	-0.753120	+0.125008	-0.333399
N18 - C20	+0.373374	-0.796462	+0.169141	-0.981492
C20 - C21	+0.281324	-0.753116	+0.125007	-0.333397
C21 - C23	+0.308027	-0.856032	+0.223573	-0.417950
C21 - C22	+0.294638	-0.798093	+0.172685	-0.378432
C23 - C31	+0.304898	-0.846671	+0.196201	-0.408554
C24 - C31	+0.311361	-0.874882	+0.229401	-0.430572
C24 - H25	+0.282084	-0.980441	+0.016791	-0.319340
C24 - C46	+0.307550	-0.865705	+0.207443	-0.417211
C26 - C28	+0.308026	-0.856031	+0.223573	-0.417950
C26 - C27	+0.294638	-0.798091	+0.172685	-0.378431
C28 - C32	+0.304898	-0.846671	+0.196201	-0.408554
C29 - C32	+0.311361	-0.874885	+0.229401	-0.430573
C29 - H30	+0.282084	-0.980441	+0.016791	-0.319340
C29 - C39	+0.307550	-0.865704	+0.207442	-0.417211
C19 - H33	+0.279097	-0.956747	+0.016614	-0.308087
C28 - H37	+0.281735	-0.973412	+0.018740	-0.320422
C20 - H34	+0.279098	-0.956749	+0.016614	-0.308087
C23 - H36	+0.281735	-0.973410	+0.018740	-0.320421
C31 - H35	+0.282636	-0.980718	+0.021518	-0.321763
C32 - H38	+0.282636	-0.980717	+0.021518	-0.321763
C27 - C39	+0.300342	-0.821067	+0.202866	-0.394350
C27 - C41	+0.286848	-0.738680	+0.183276	-0.368142
C39 - N40	+0.306073	-0.707242	+0.115480	-0.694032
N17 - H44	+0.010474	+0.035922	+0.358304	-0.006093
N40 - H43	+0.342367	-1.794849	+0.043663	-0.544339

N40 - C42	+0.305584	-0.647432	+0.116594	-0.717106
C41 - C42	+0.320927	-0.907585	+0.315610	-0.470805
C41 - H44	+0.284716	-0.997836	+0.031549	-0.324100
C42 - H45	+0.286970	-1.020784	+0.033503	-0.322896
C22 - C46	+0.300342	-0.821067	+0.202865	-0.394350
C22 - C48	+0.286847	-0.738677	+0.183276	-0.368141
C46 - N47	+0.306073	-0.707244	+0.115480	-0.694028
N18 - H51	+0.010474	+0.035921	+0.358313	-0.006093
N47 - H50	+0.342367	-1.794845	+0.043664	-0.544338
N47 - C49	+0.305584	-0.647431	+0.116594	-0.717109
C48 - C49	+0.320927	-0.907585	+0.315610	-0.470805
C48 - H51	+0.284716	-0.997839	+0.031549	-0.324101
C49 - H52	+0.286970	-1.020785	+0.033503	-0.322896

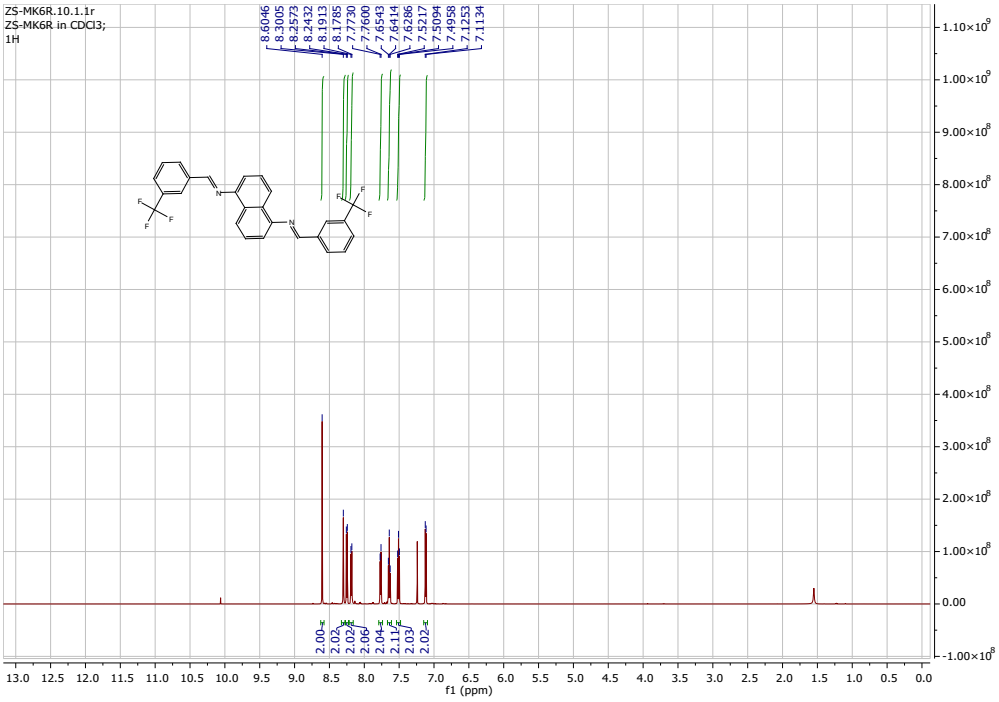


Figure S1: [1]HNMR of **ND1**

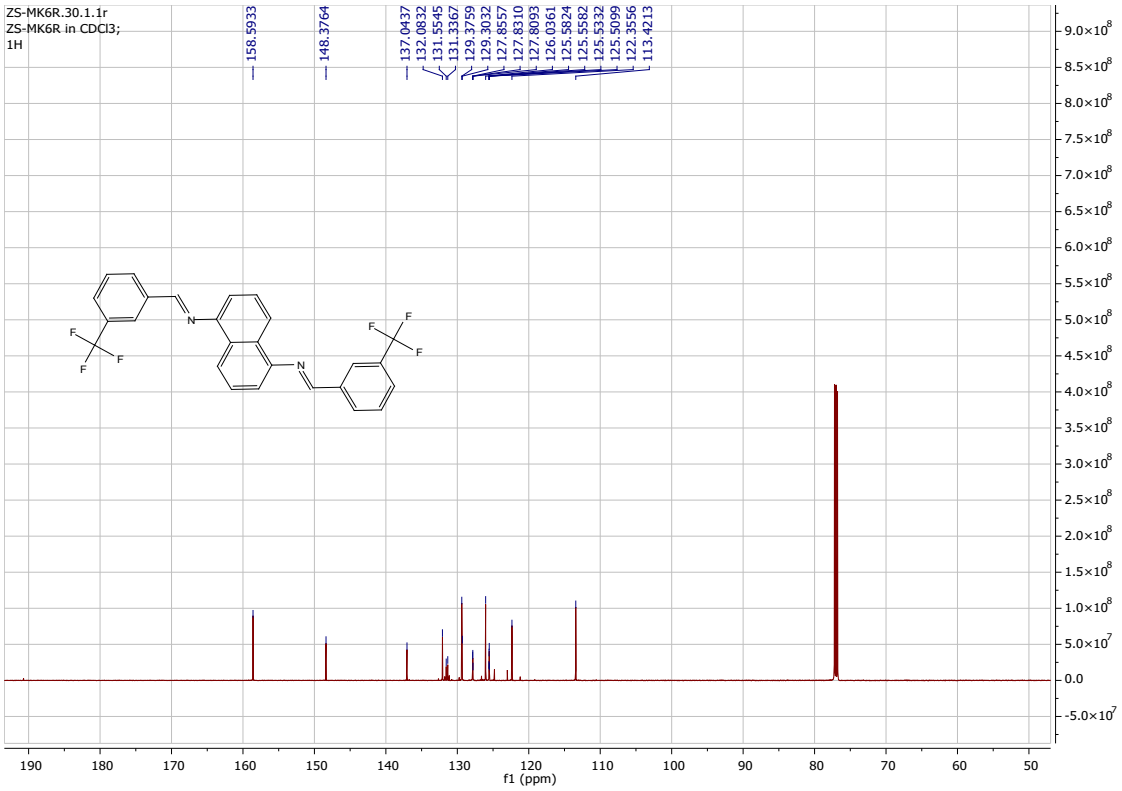


Figure S2: ^{13}CNMR of **ND1**

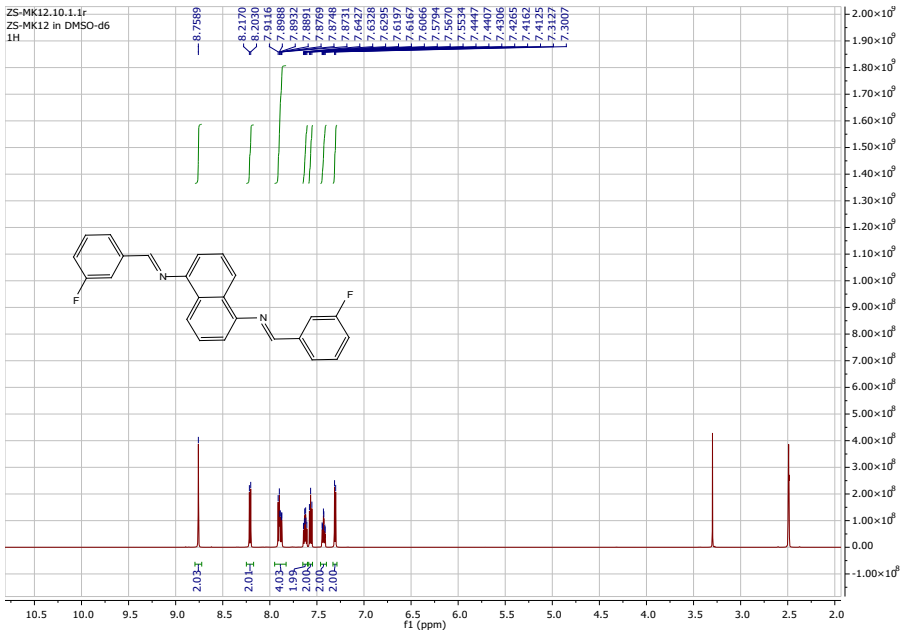


Figure S3: ^{1}HNMR of **ND2**

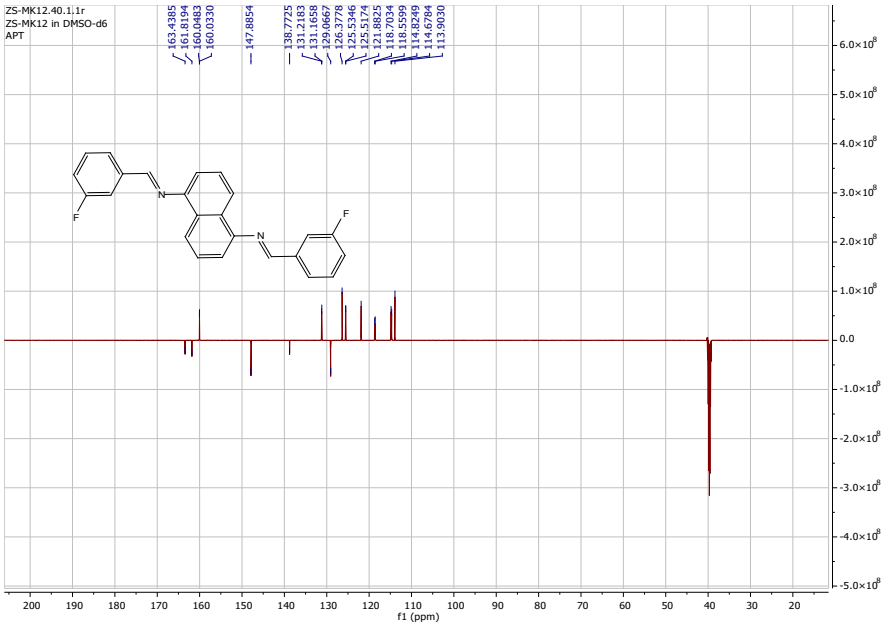


Figure S4: ^{13}CNMR of **ND2**

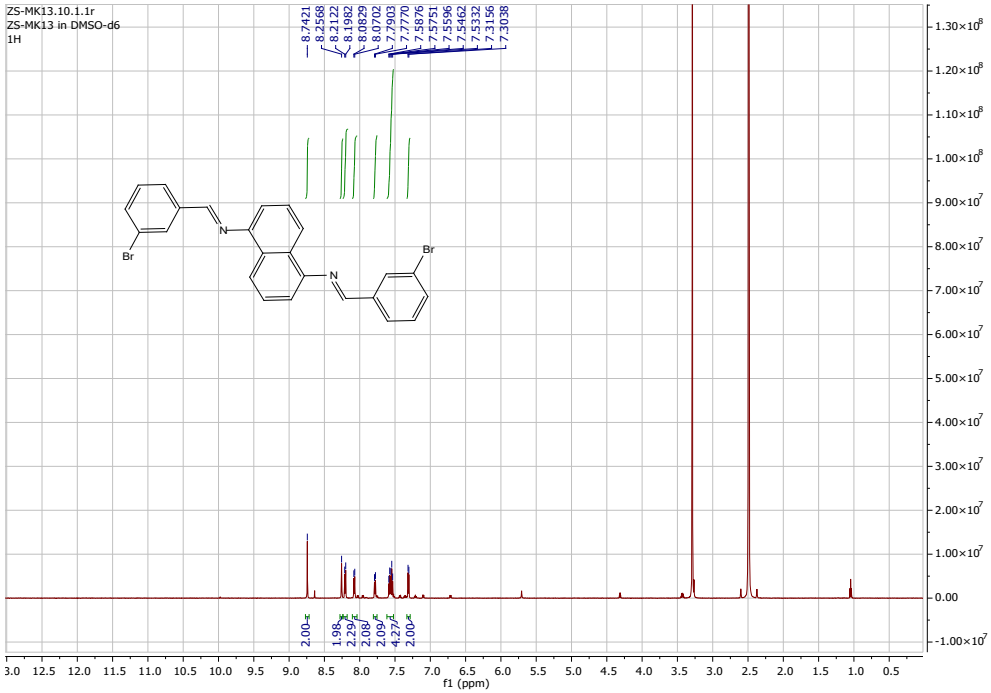


Figure S5: ^{1}HNMR of **ND3**

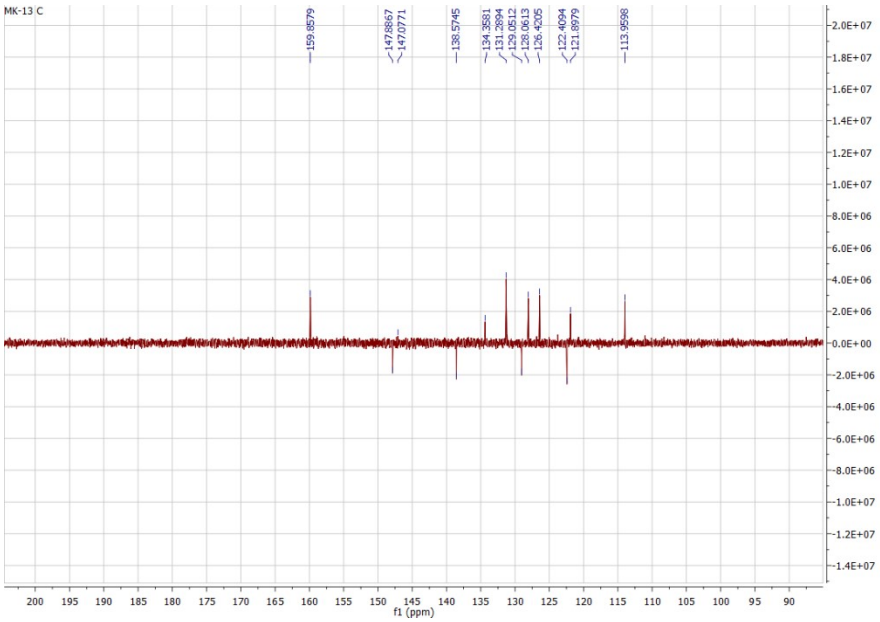


Figure S6: ^{13}CNMR of **ND3**

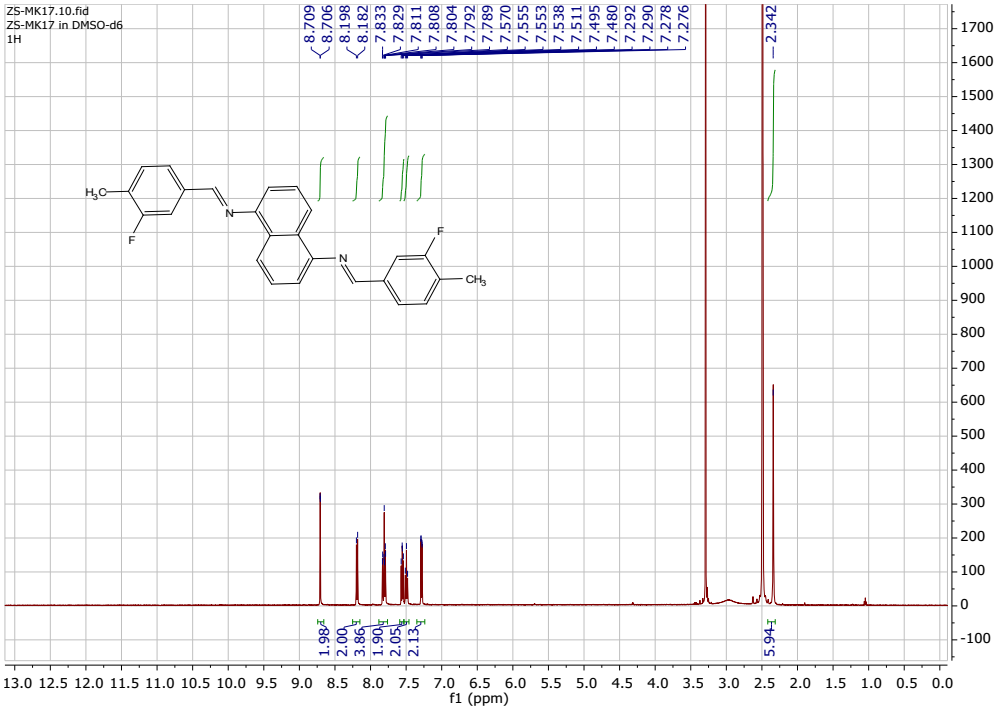


Figure S7: ^{1}HNMR of **ND4**

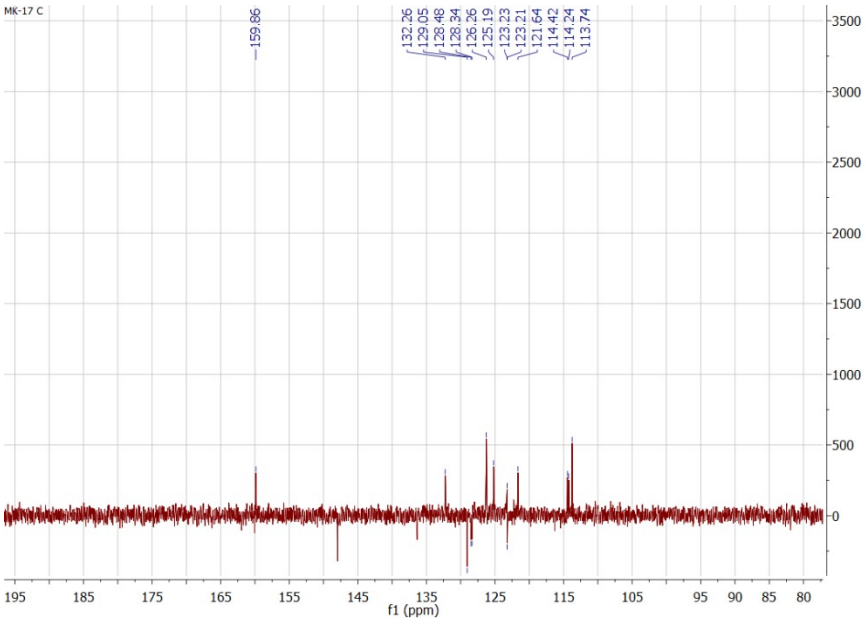


Figure S8: ^{13}CNMR of **ND4**

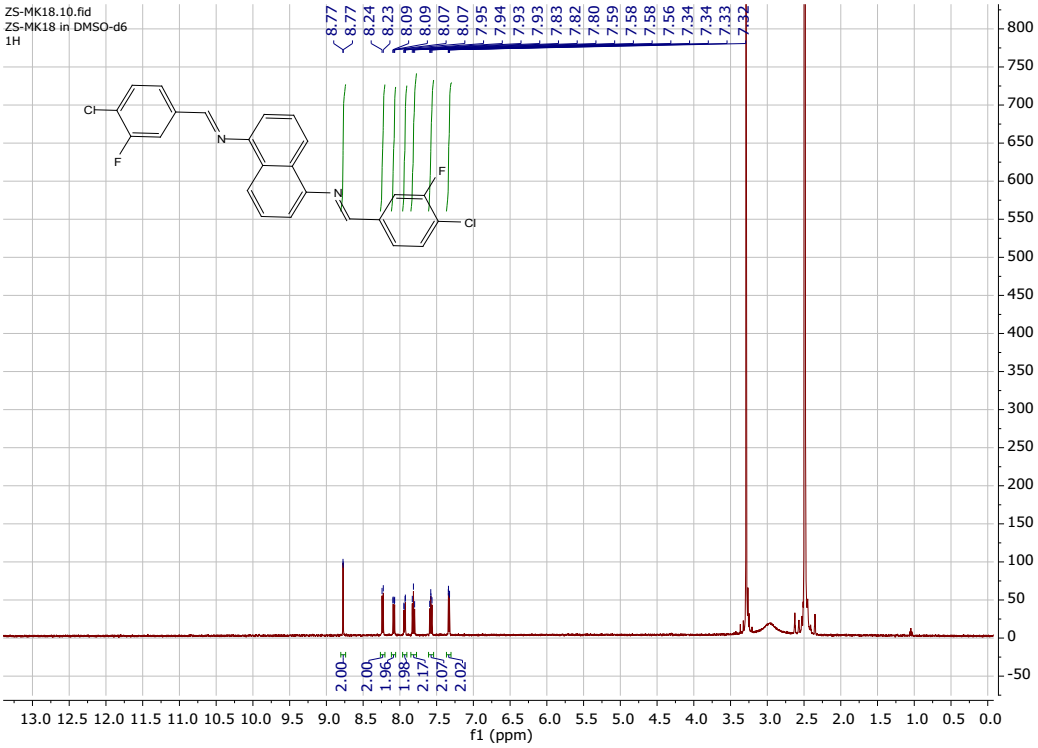


Figure S9: ^{1}HNMR of **ND5**

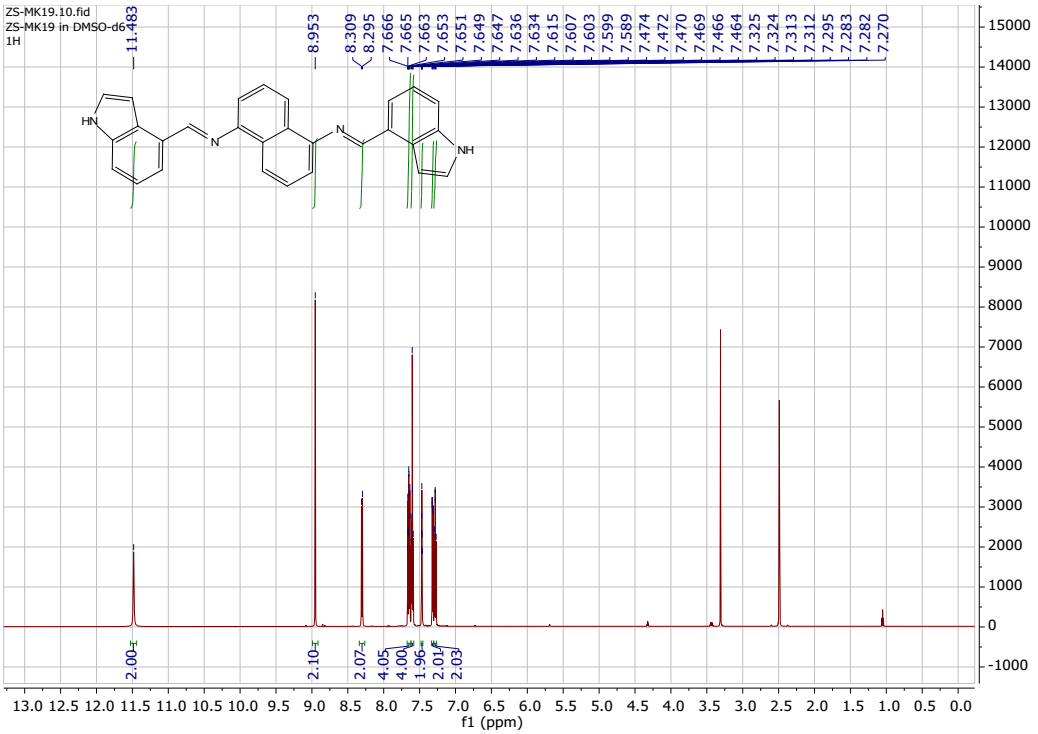


Figure S10: [1]HNMR of **ND6**

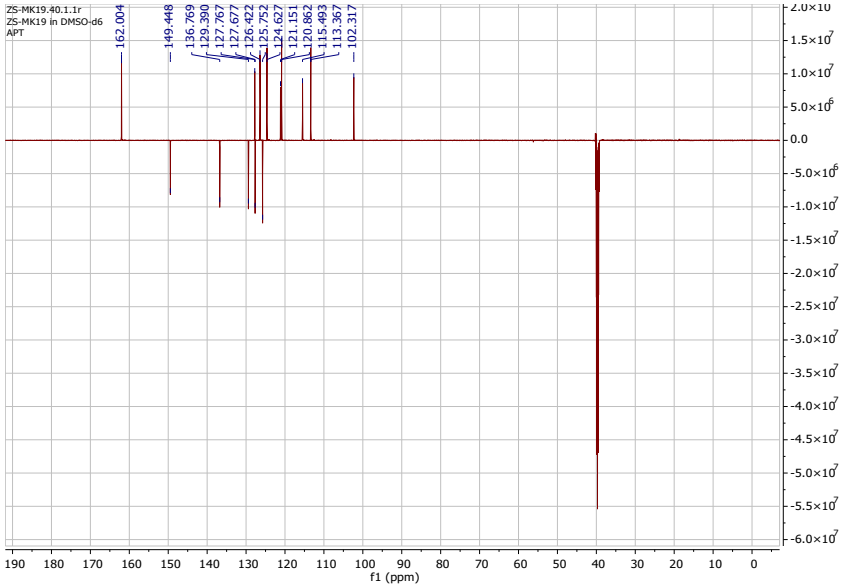


Figure S11: [13]CNMR of **ND6**

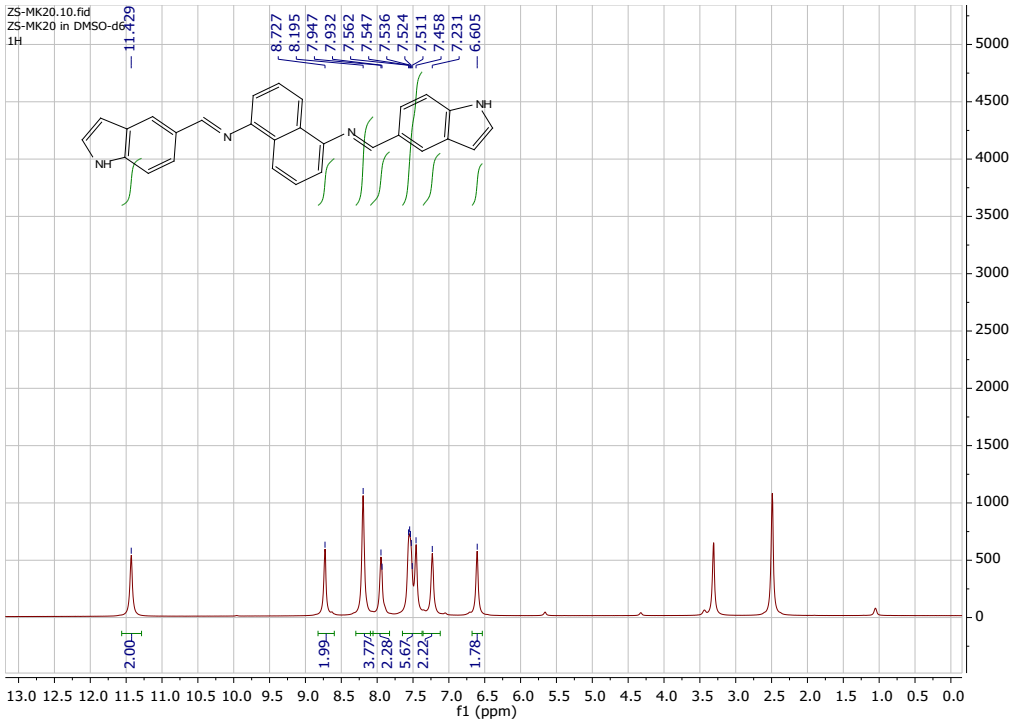


Figure S12: [1]HNMR of **ND7**

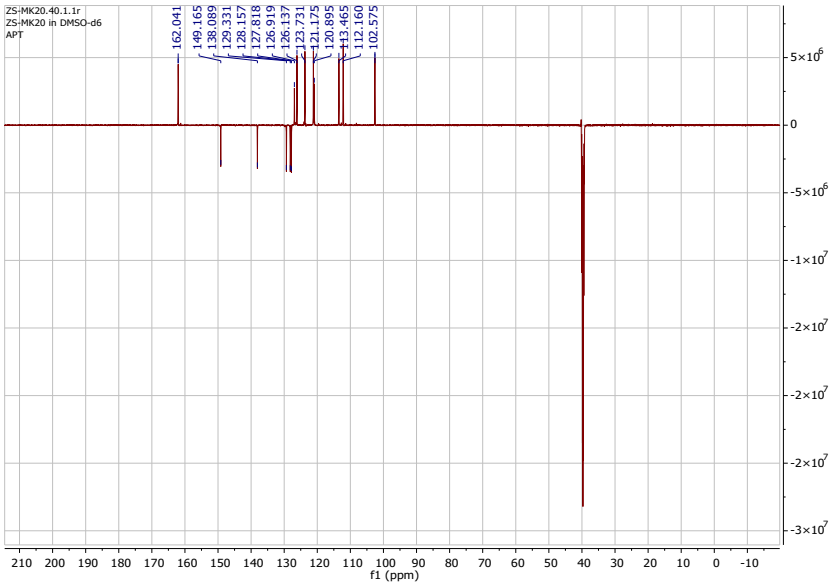


Figure S13: [13]CNMR of **ND7**

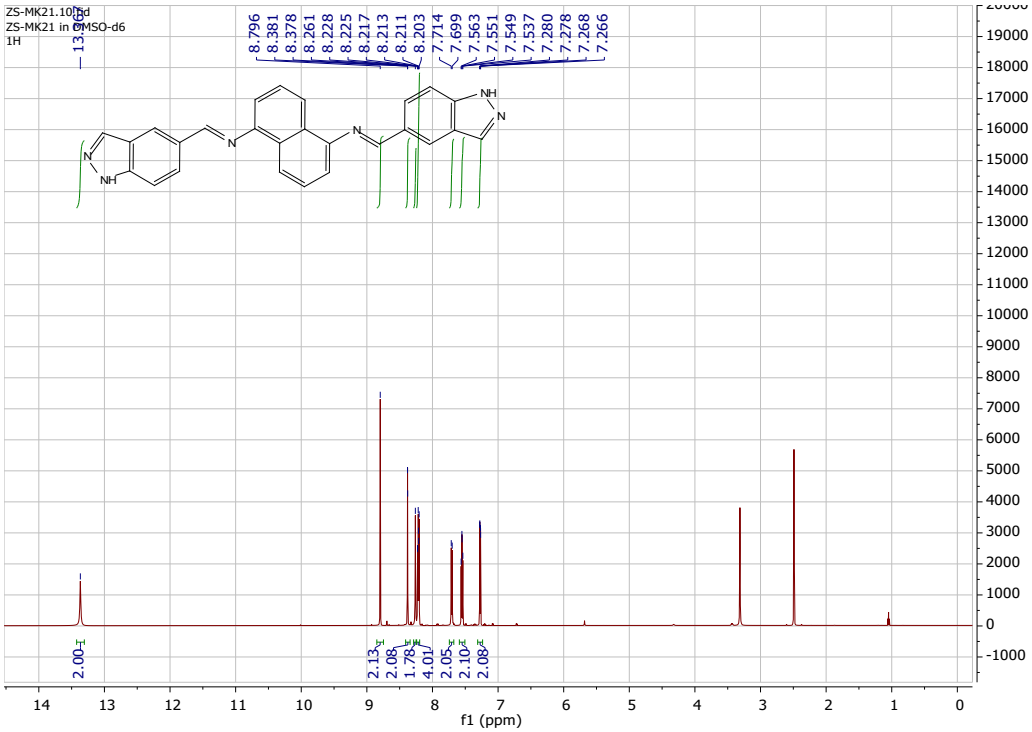


Figure S14: [1]HNMR of **ND8**

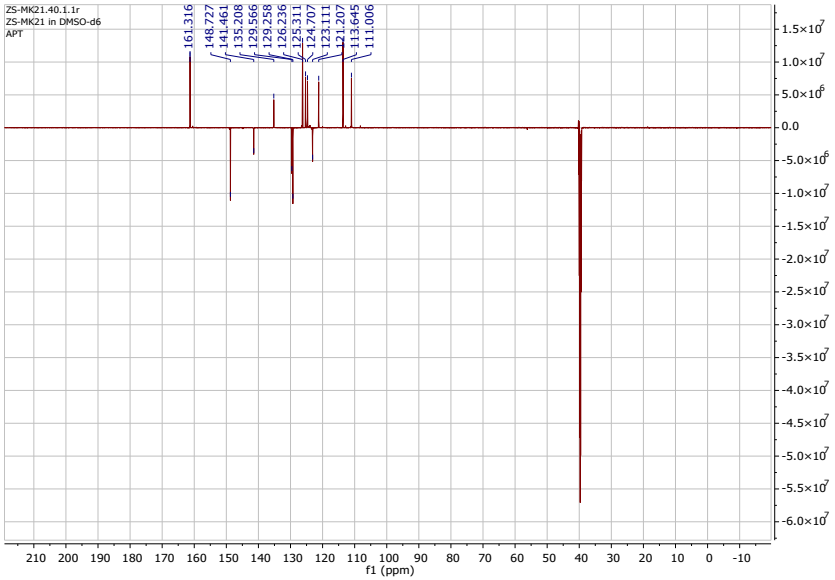


Figure S15: [13]CNMR of **ND8**

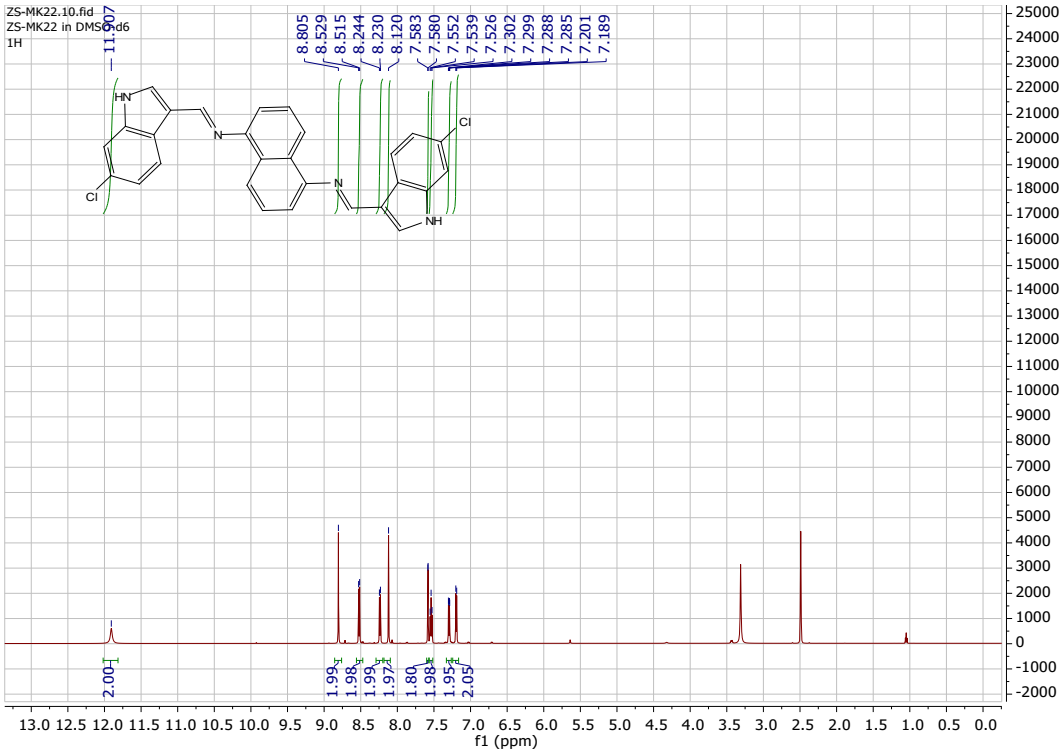


Figure S16: [1]HNMR of **ND9**

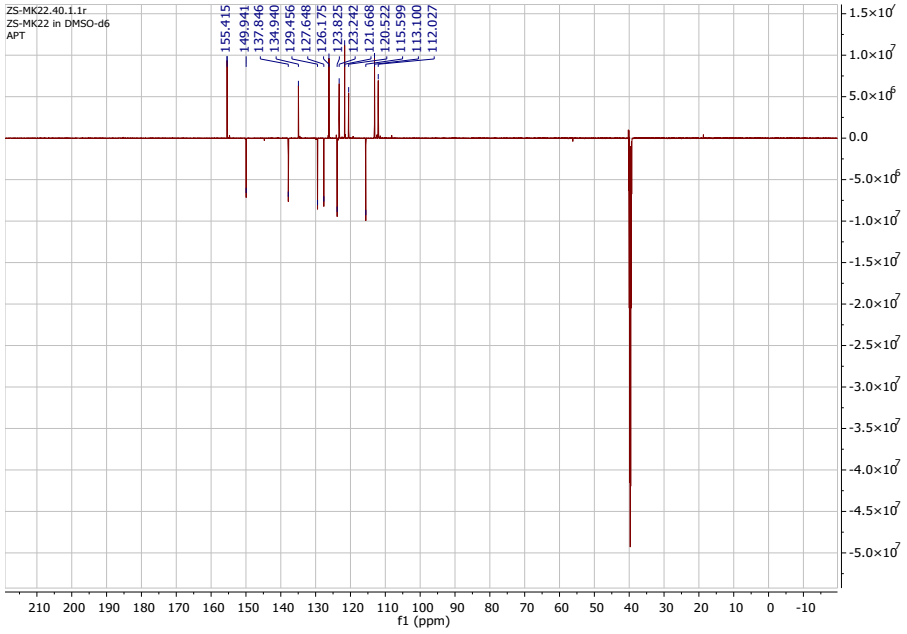


Figure S17: [13]CNMR of **ND9**

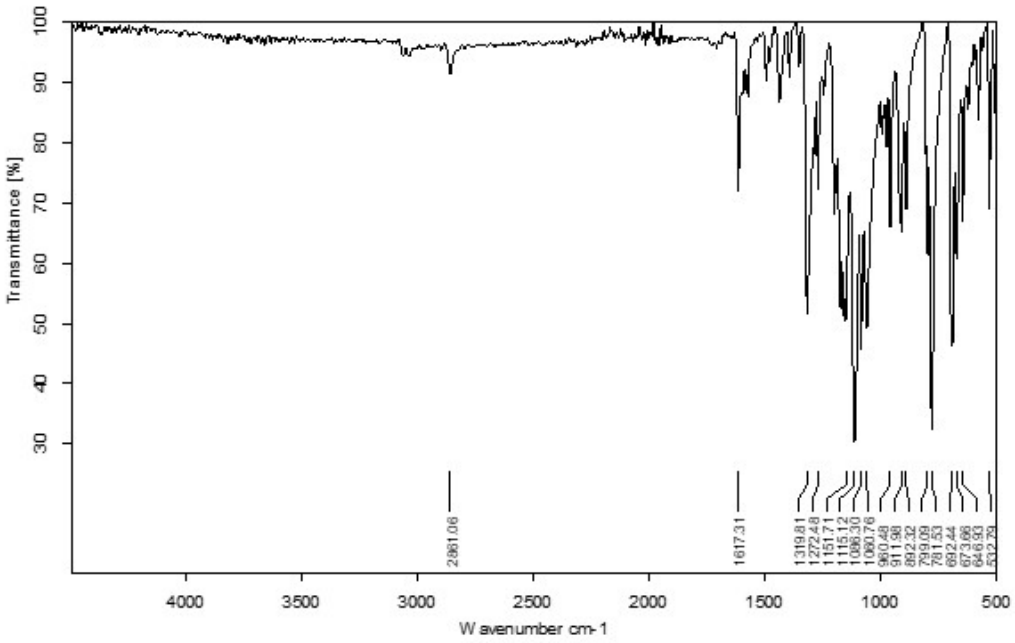


Figure S18: IR Spectrum of **ND1**

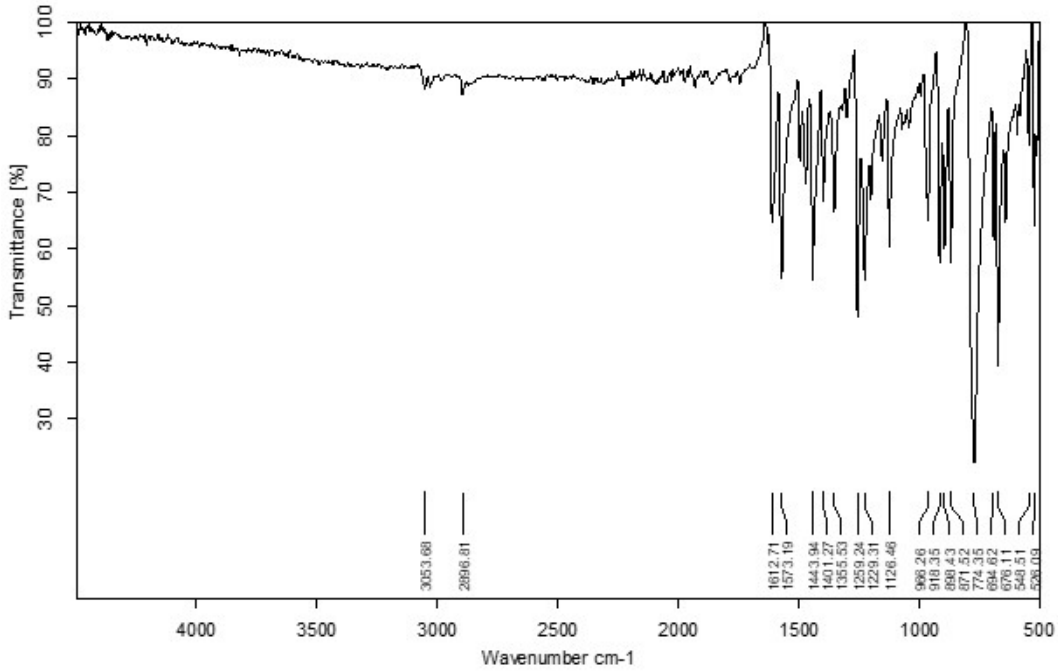


Figure S19: IR Spectrum of **ND2**

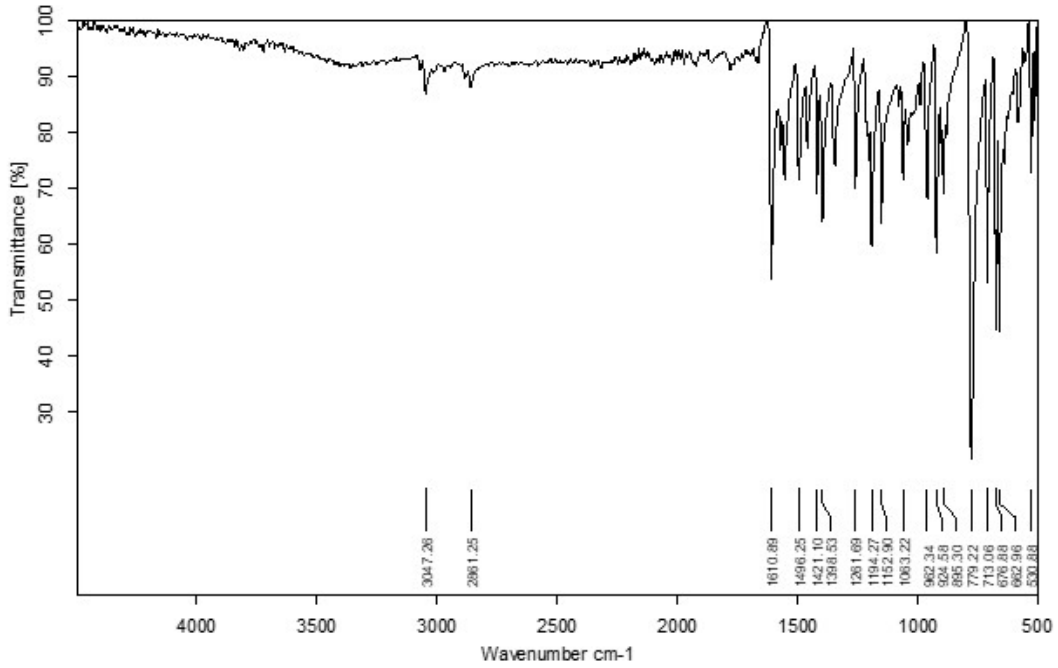


Figure S20: IR Spectrum of **ND3**

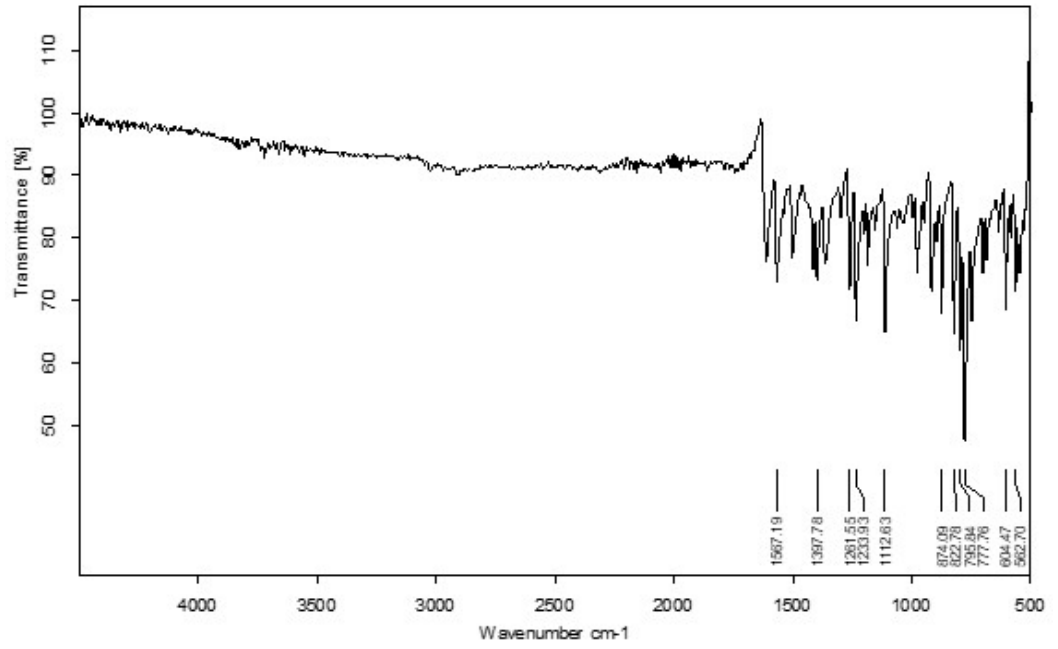


Figure S21: IR Spectrum of **ND4**

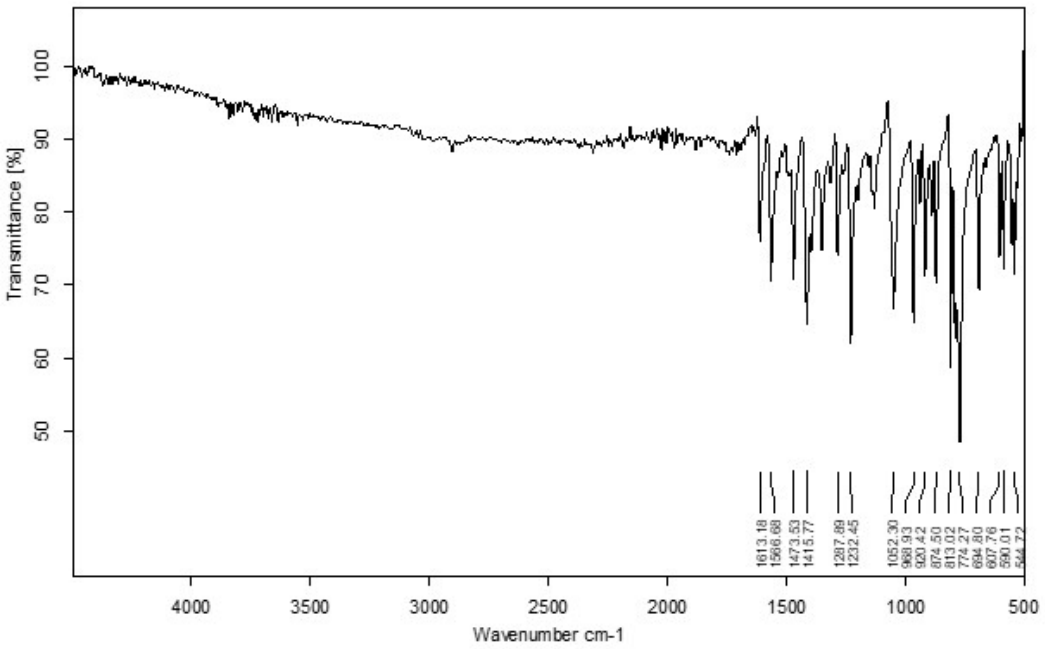


Figure S22: IR Spectrum of **ND5**

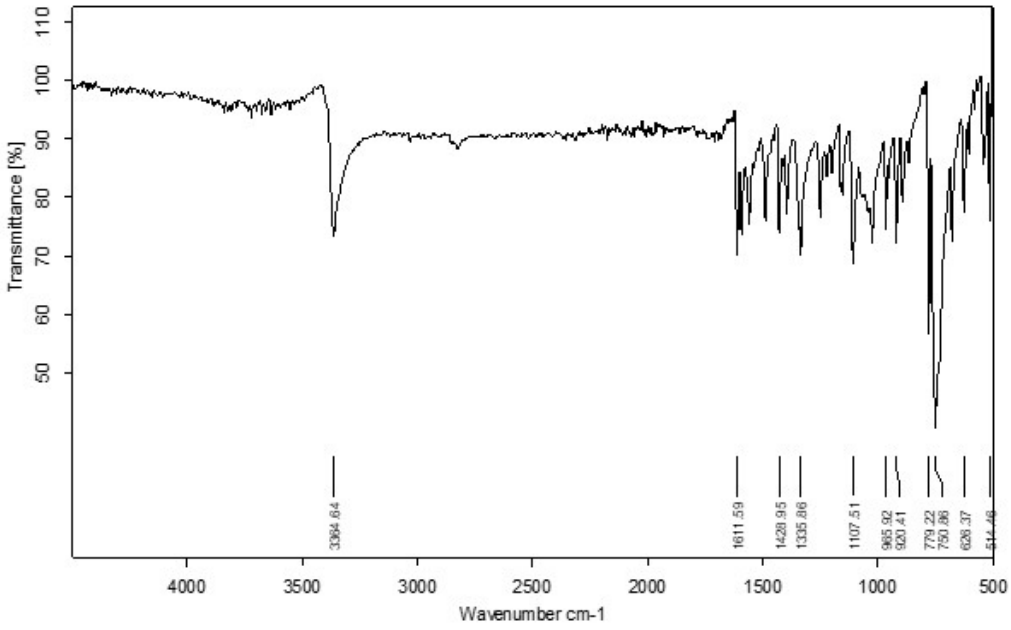


Figure S23: IR Spectrum of **ND6**

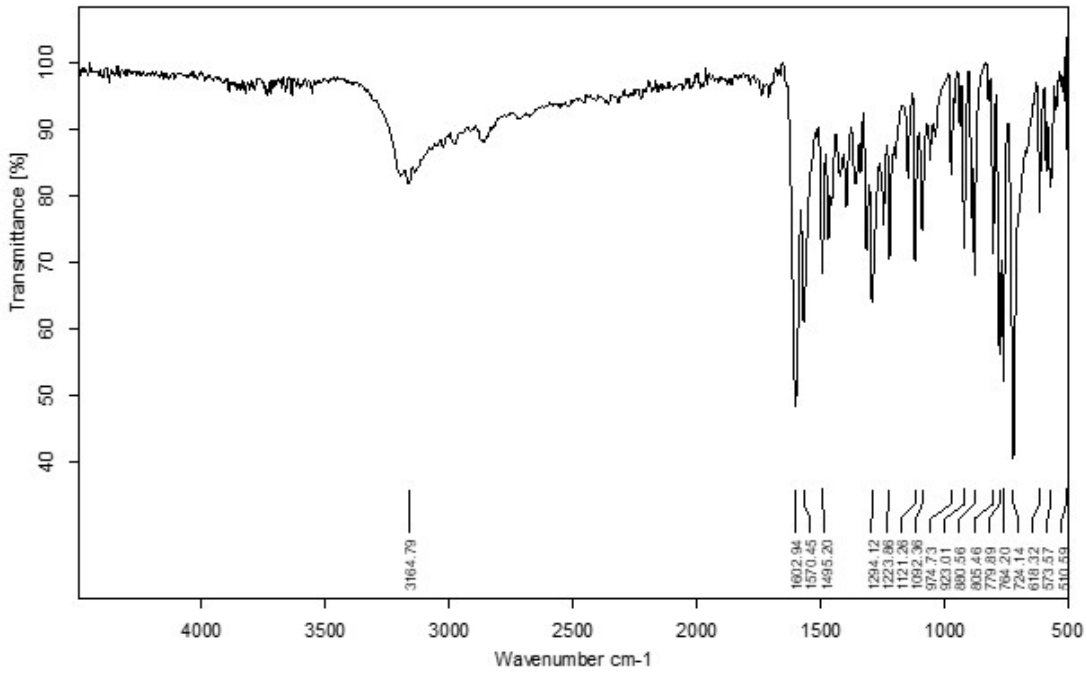


Figure S24: IR Spectrum of **ND7**

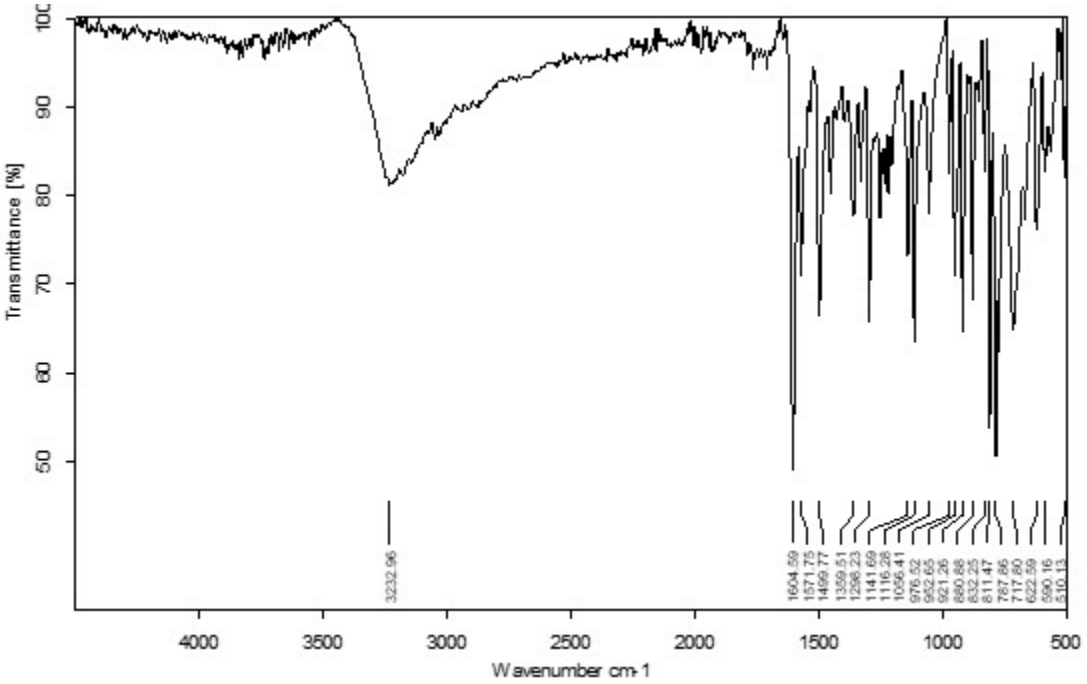


Figure S25: IR Spectrum of **ND8**

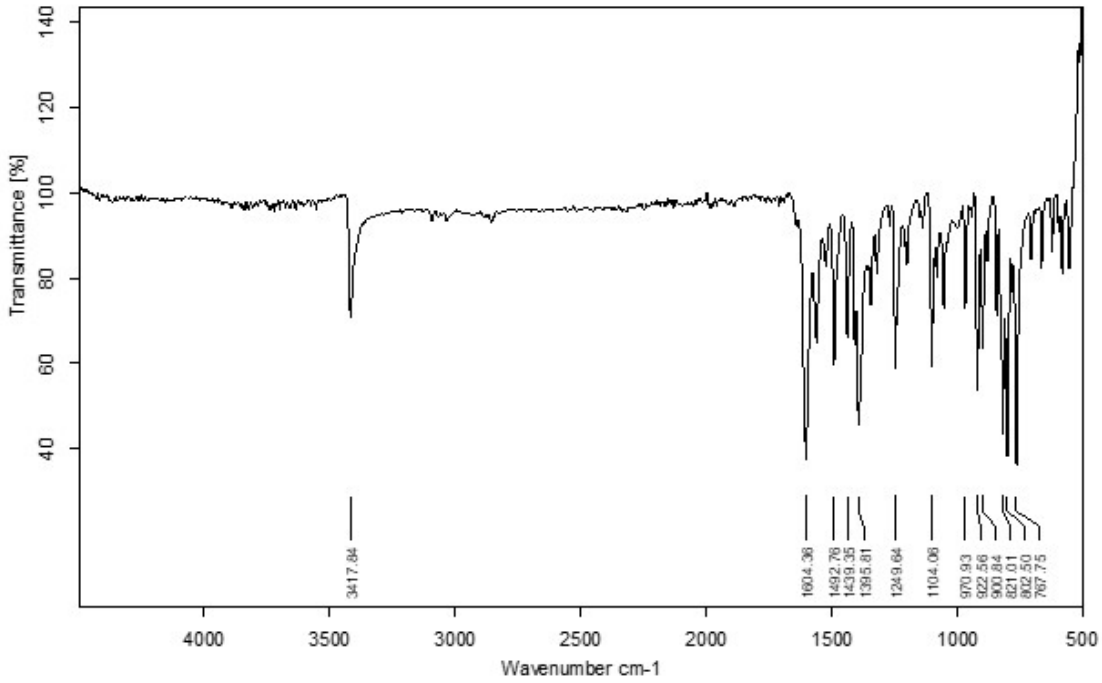


Figure S26: IR Spectrum of **ND9**

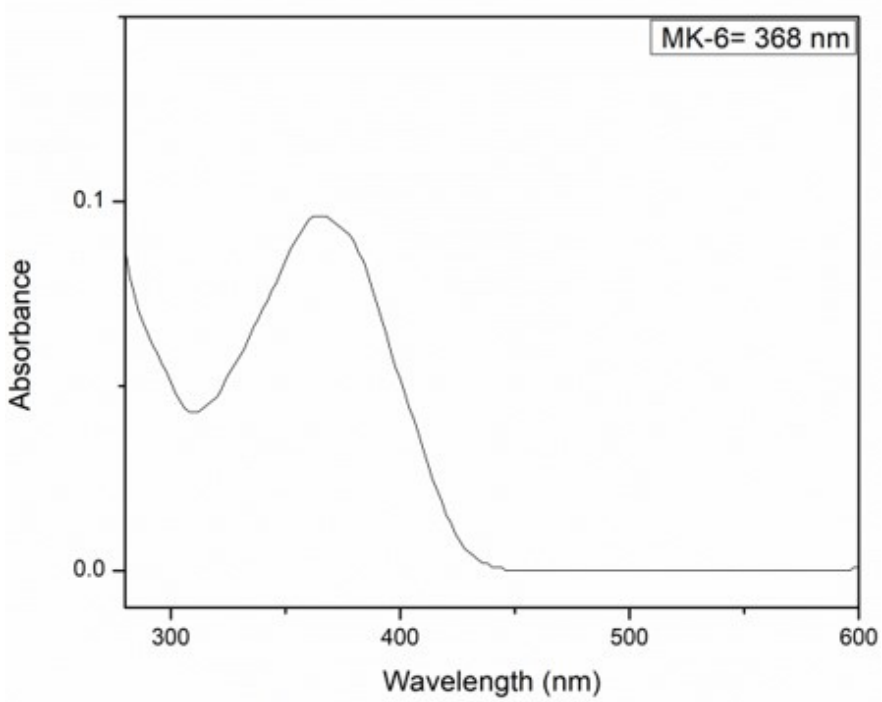


Figure S27: UV-Visible Spectra of **ND1**

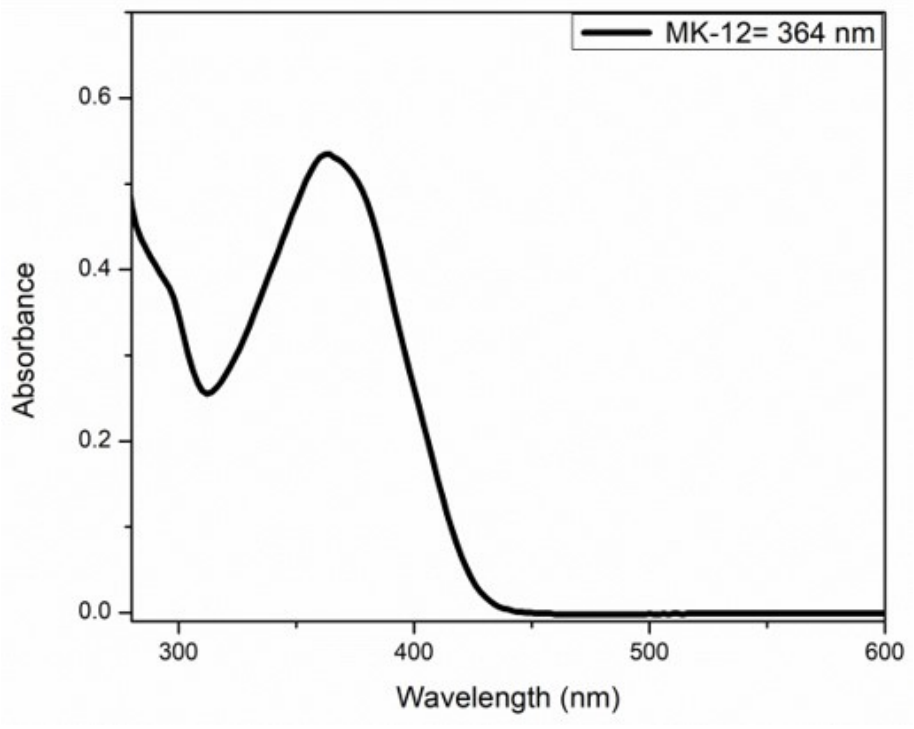


Figure S28: UV-Visible Spectra of **ND2**

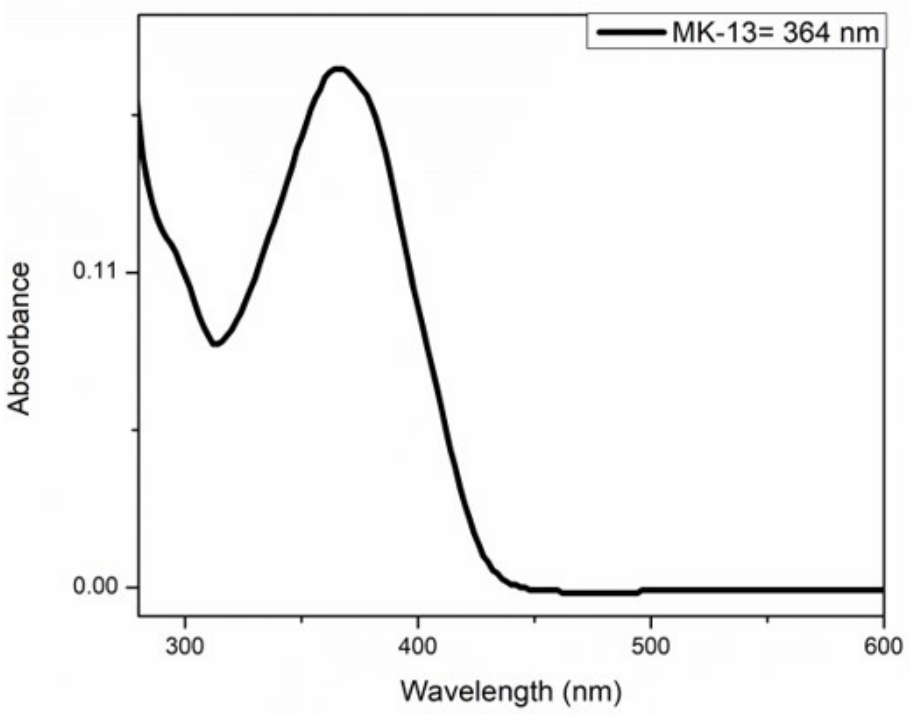


Figure S29: UV-Visible Spectra of **ND3**

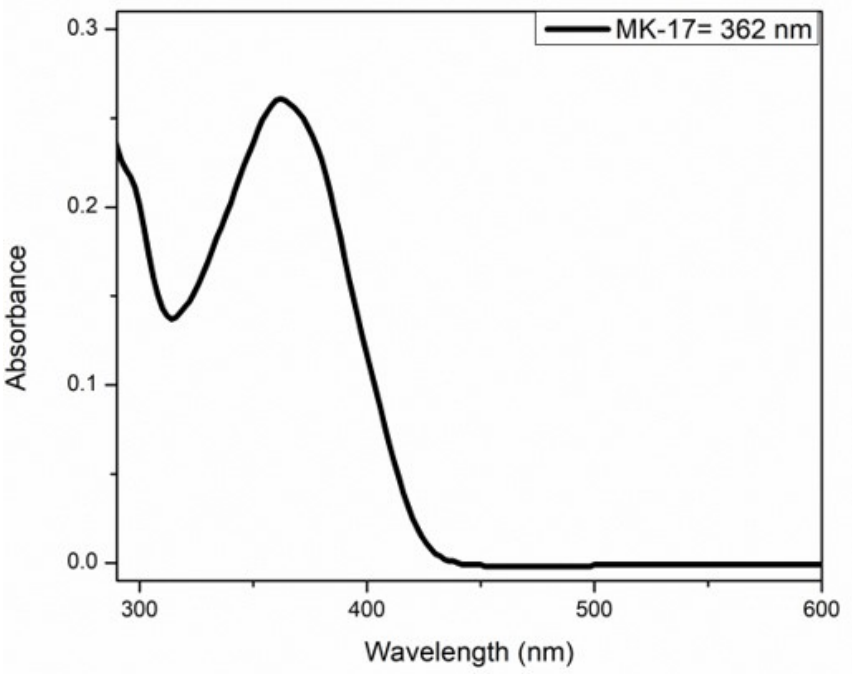


Figure S30: UV-Visible Spectra of **ND4**

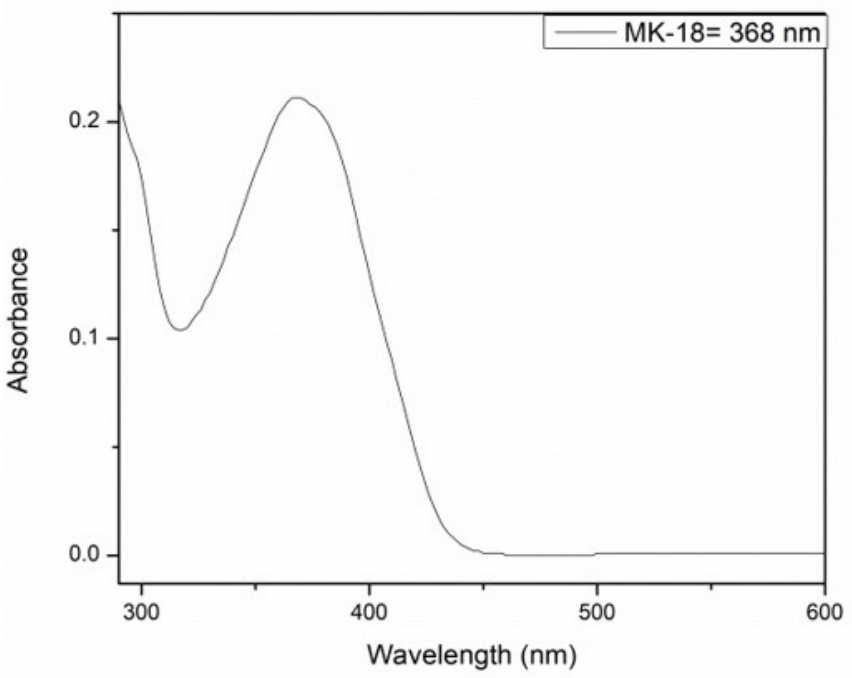


Figure S31: UV-Visible Spectra of **ND5**

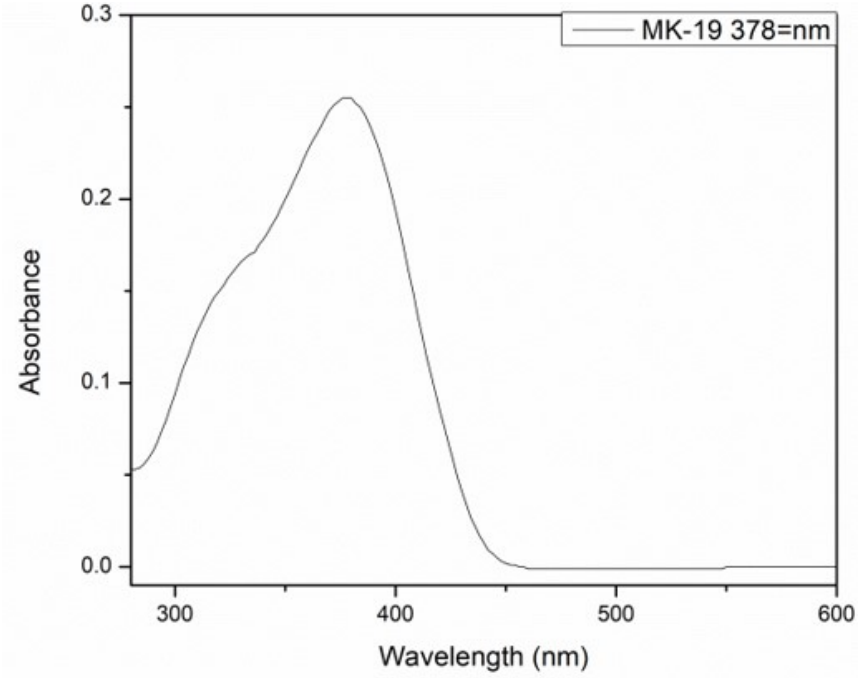


Figure S32: UV-Visible Spectra of **ND6**

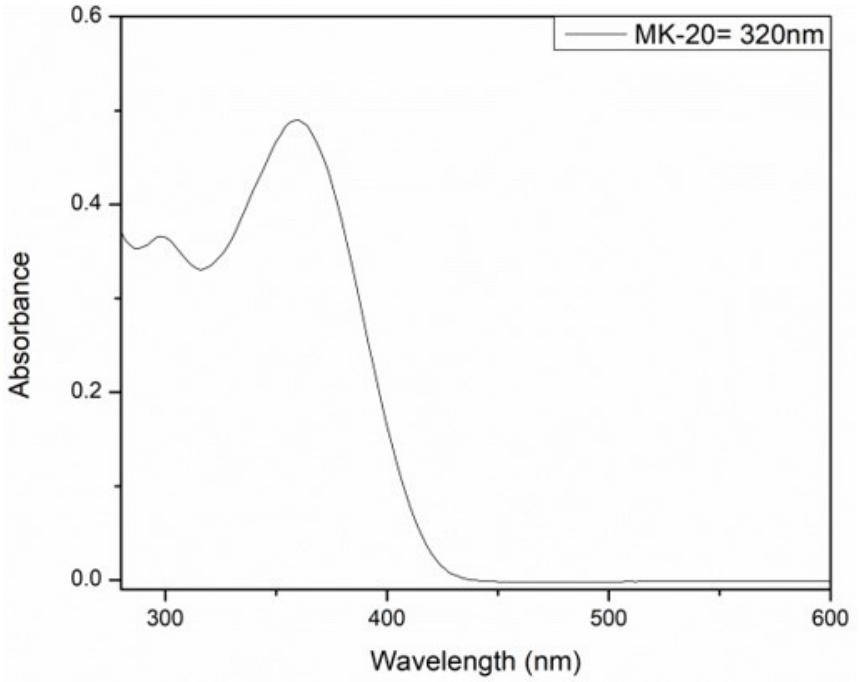


Figure S33: UV-Visible Spectra of **ND7**

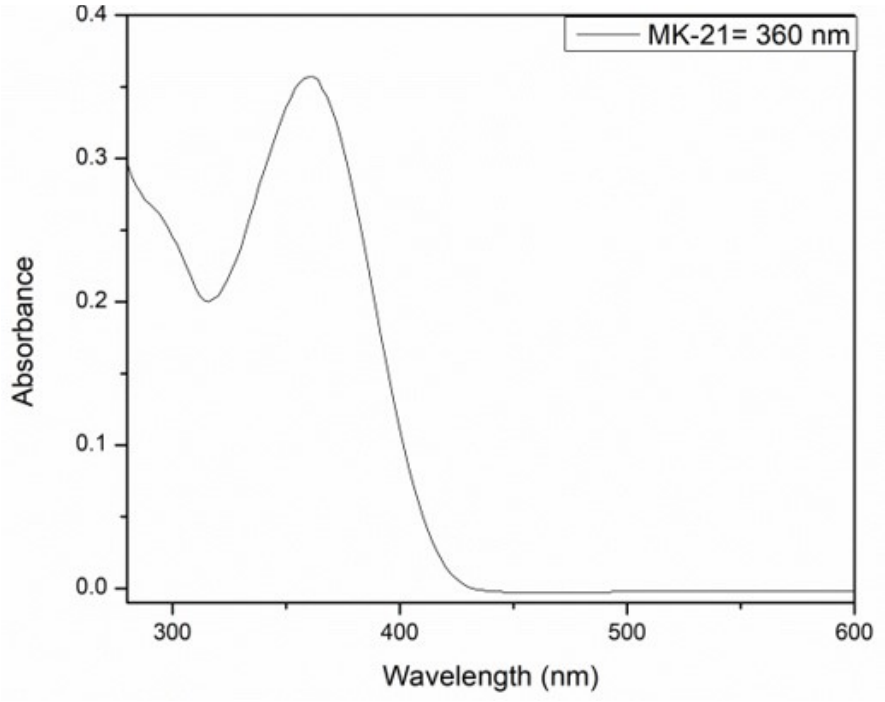


Figure S34: UV-Visible Spectra of **ND8**

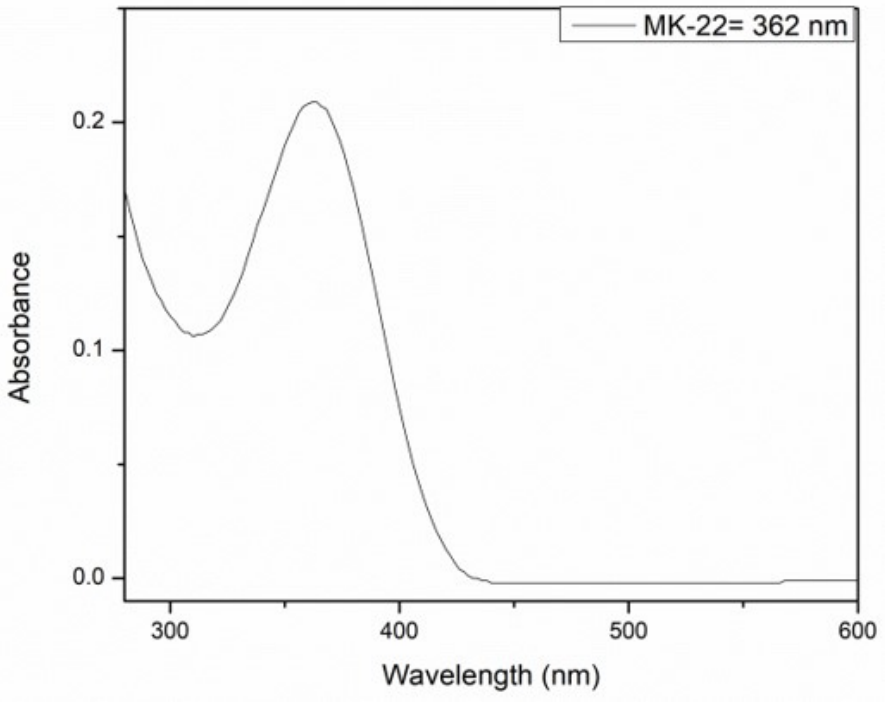
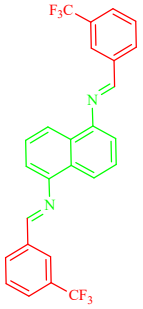
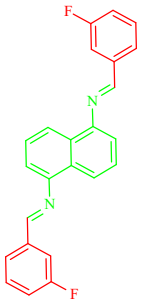


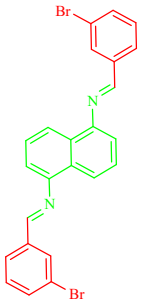
Figure S35: UV-Visible Spectra of **ND9**



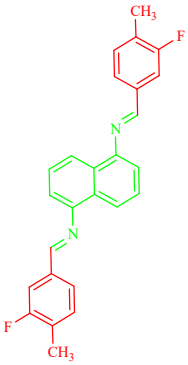
ND1



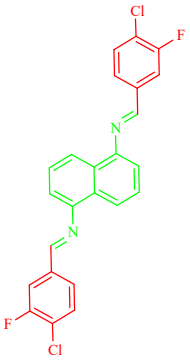
ND2



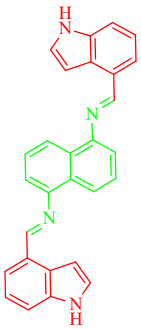
ND3



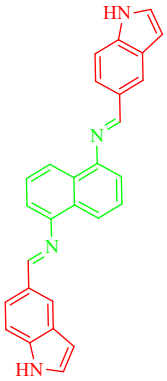
ND4



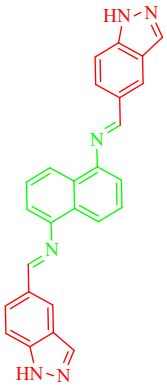
ND5



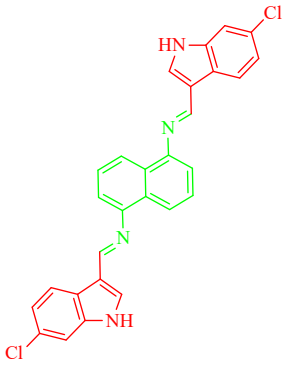
ND6



ND7

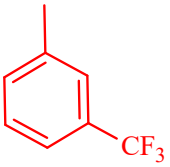


ND8

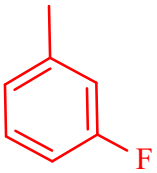


ND9

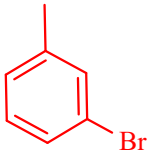
Figure S36: ChemDraw sketches of **ND1-ND9** compounds.



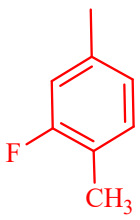
1-methyl-3-(trifluoromethyl)benzene
A1



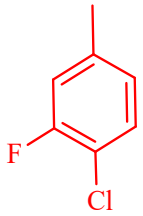
1-fluoro-3-methylbenzene
A2



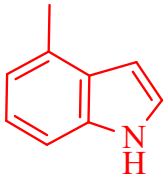
1-bromo-3-methylbenzene
A3



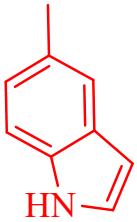
2-fluoro-1,4-dimethylbenzene
A4



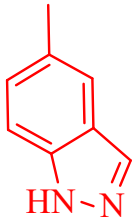
1-chloro-2-fluoro-4-methylbenzene
A5



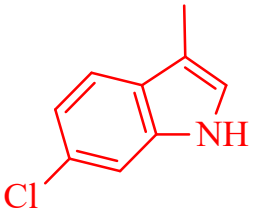
4-methyl-1H-indole
A6



5-methyl-1H-indole
A7

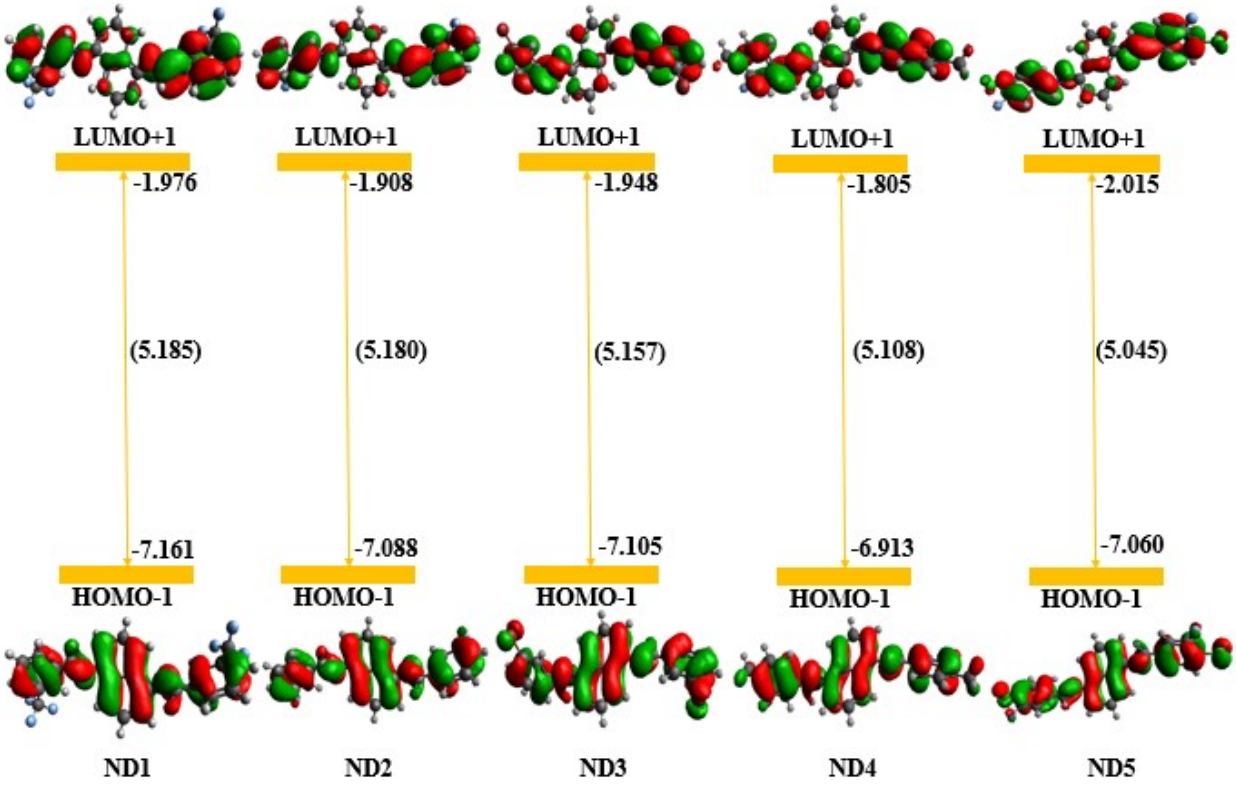


5-methyl-1H-indazole
A8



6-chloro-3-methyl-1H-indole
A9

Figure S37: The structures of various acceptors with IUPAC names used in the synthesized chromophores.



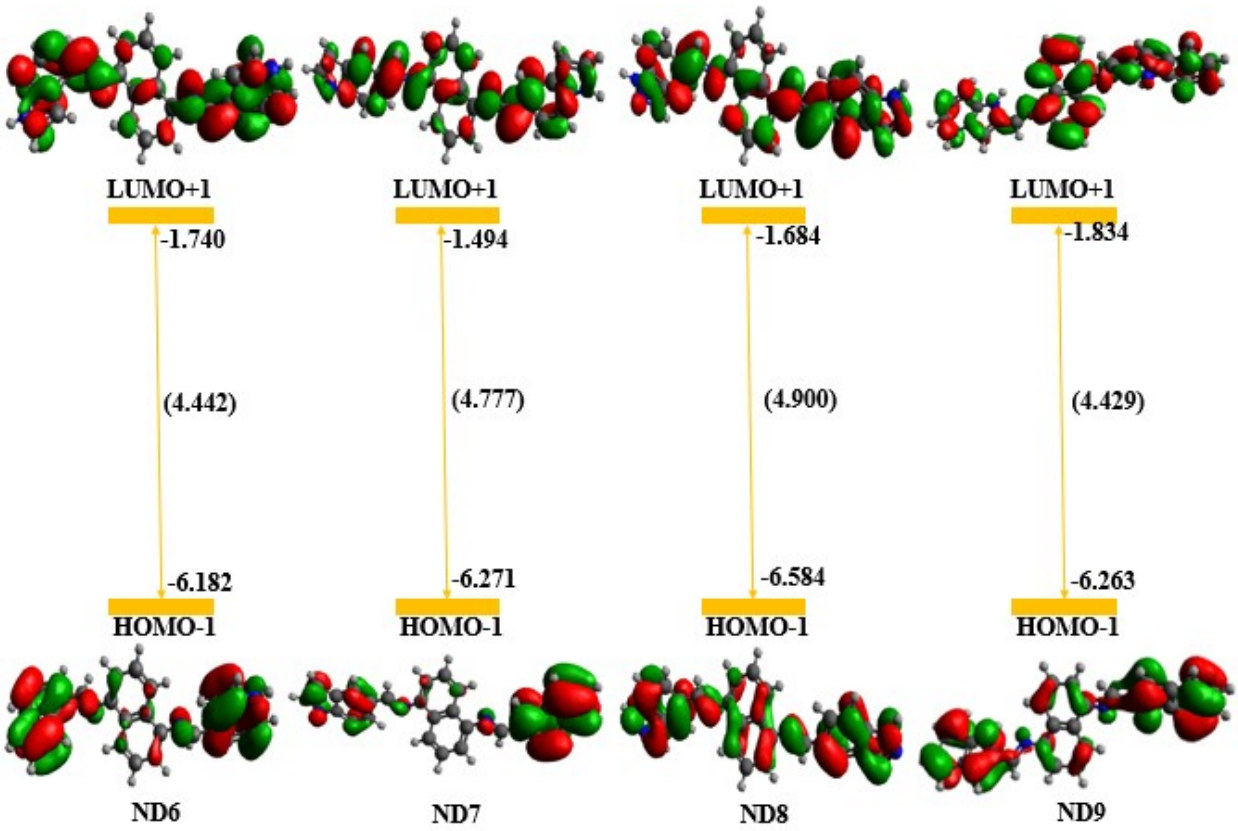
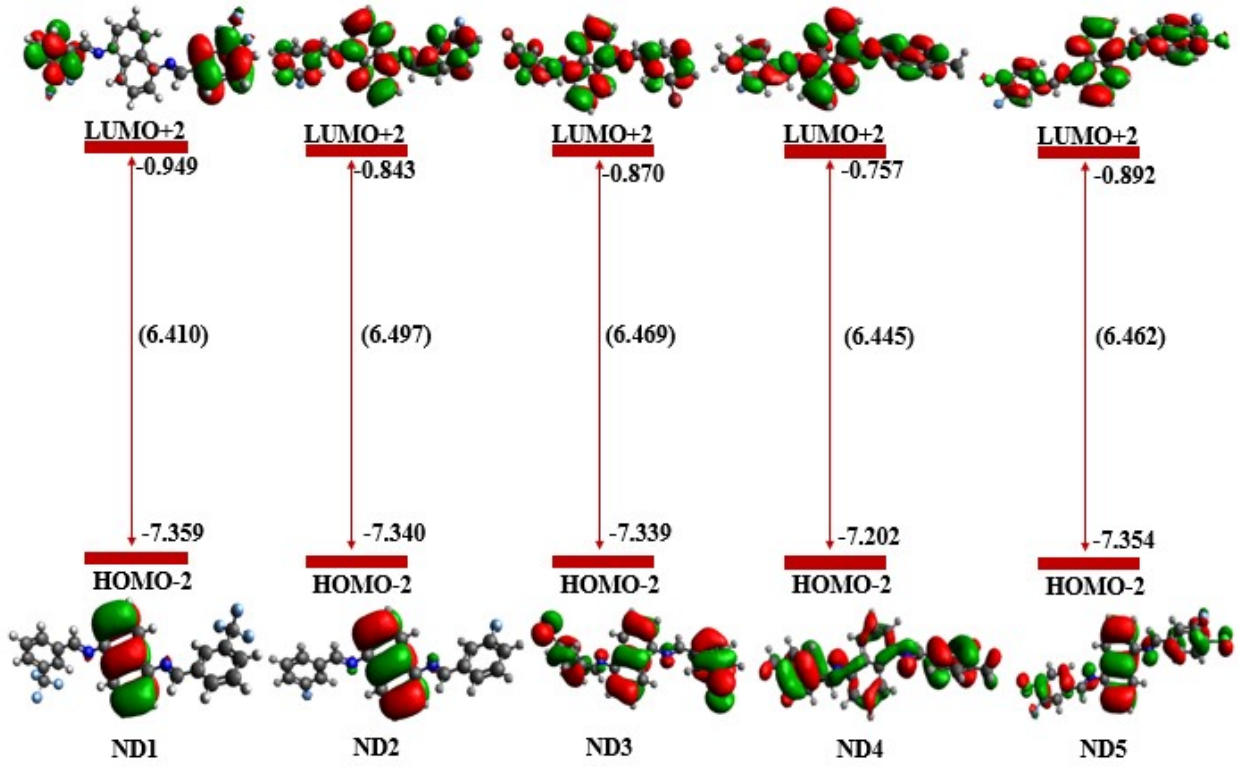


Figure S38: Frontier molecular orbitals HOMO+1/LUMO+1 of all synthesized chromophores.



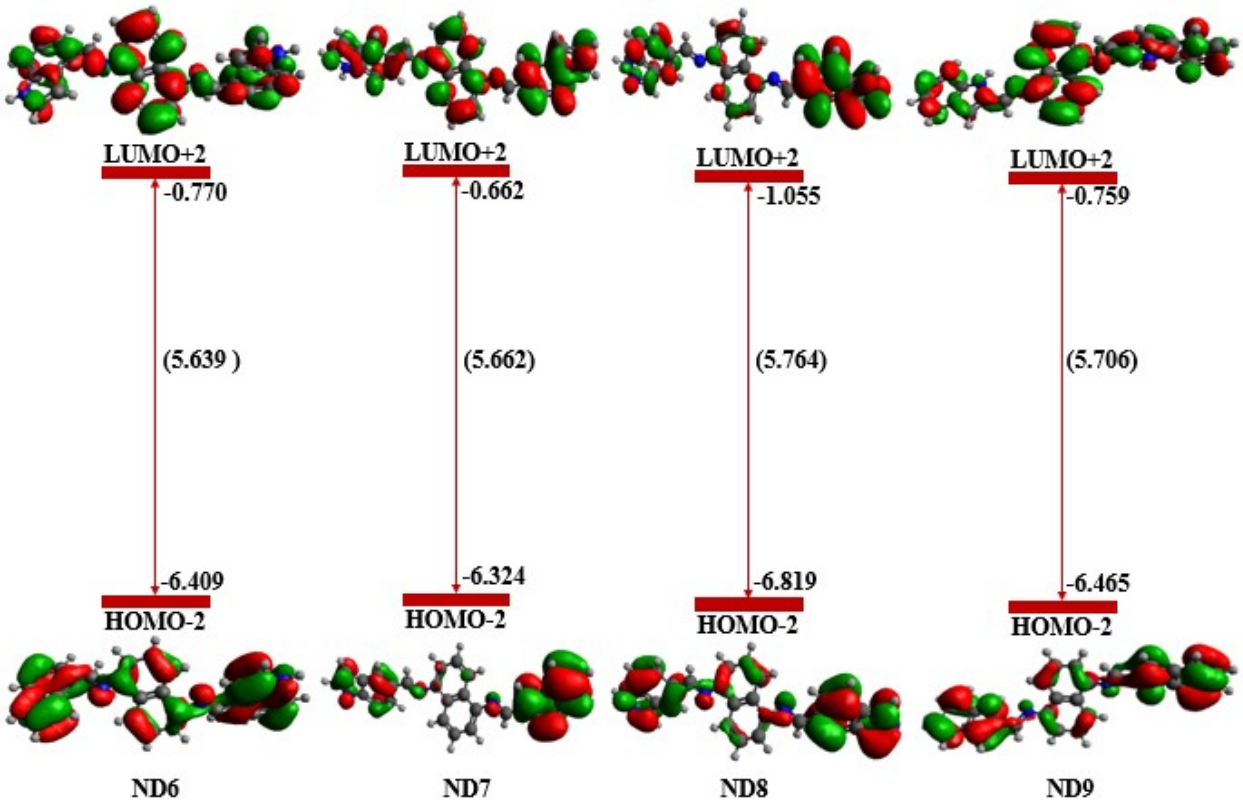
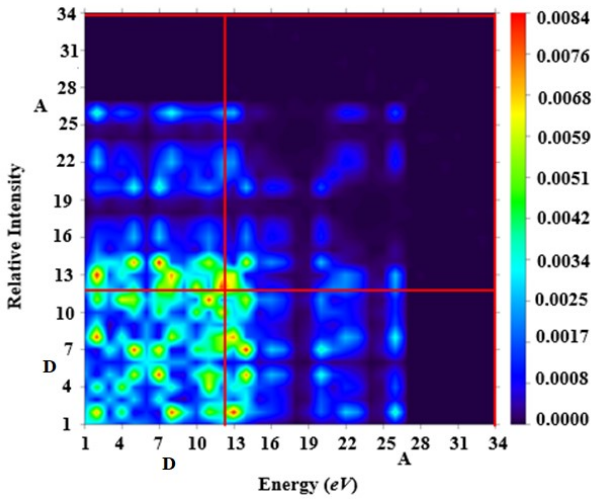
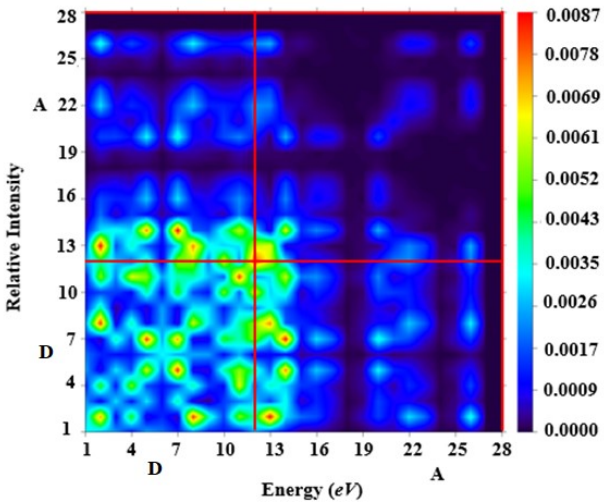


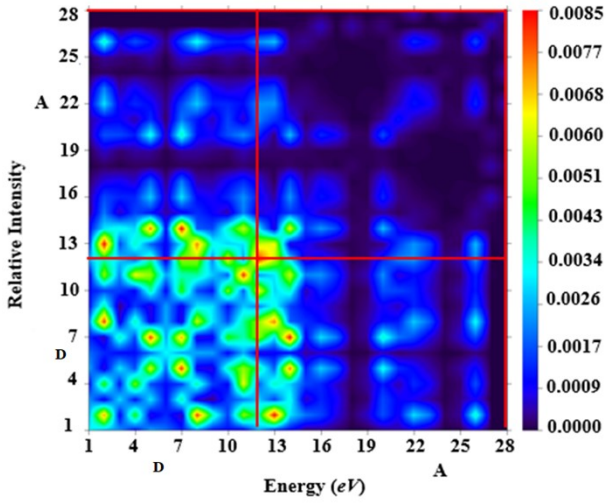
Figure S39: Frontier molecular orbitals HOMO+2/LUMO+2 of all synthesized chromophores.

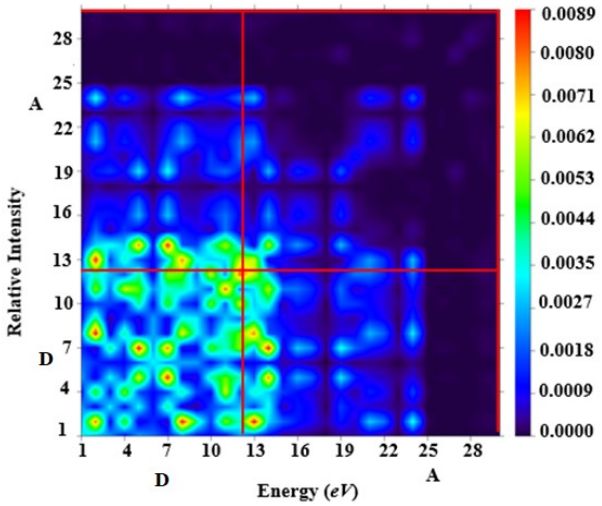


ND1



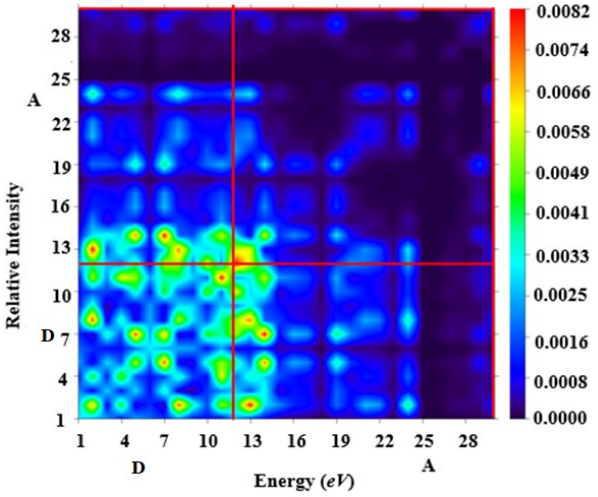
ND2

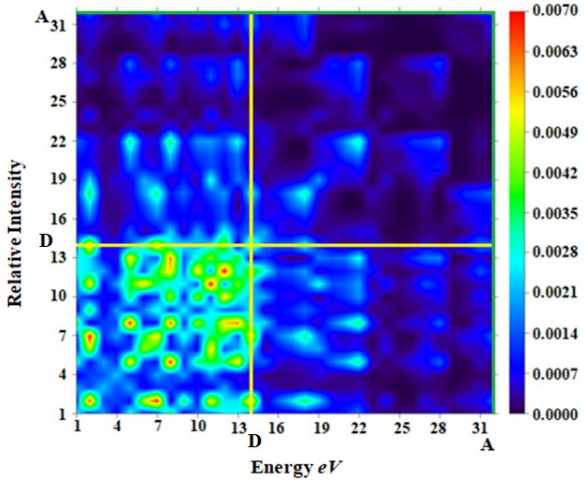




ND3

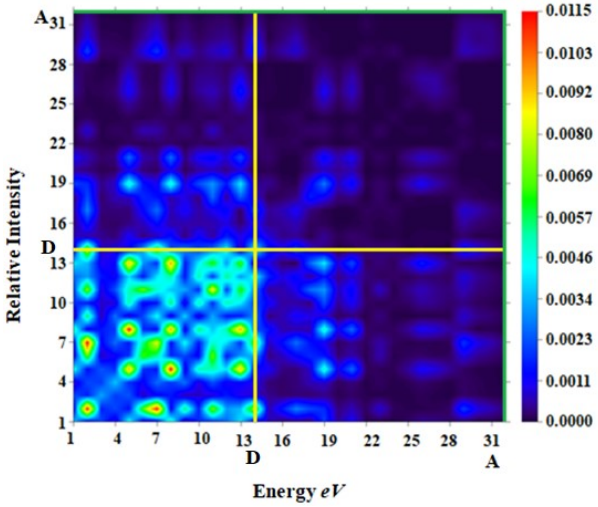
ND4

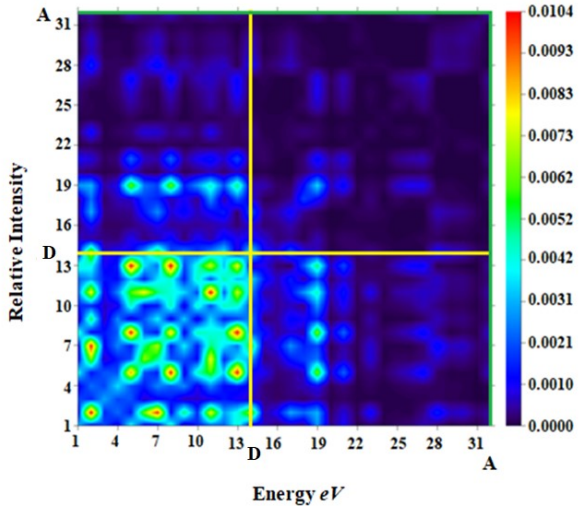




ND5

ND6





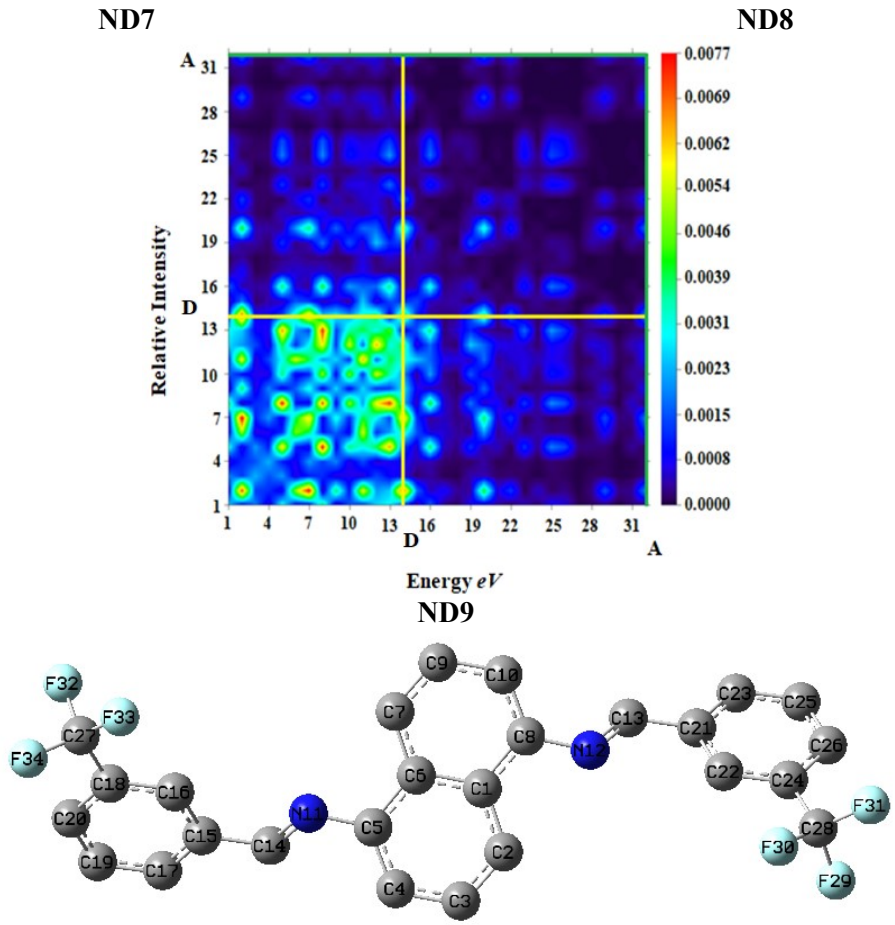


Figure S40: Transition density maps of all synthesized chromophores **ND1**-**ND9**.

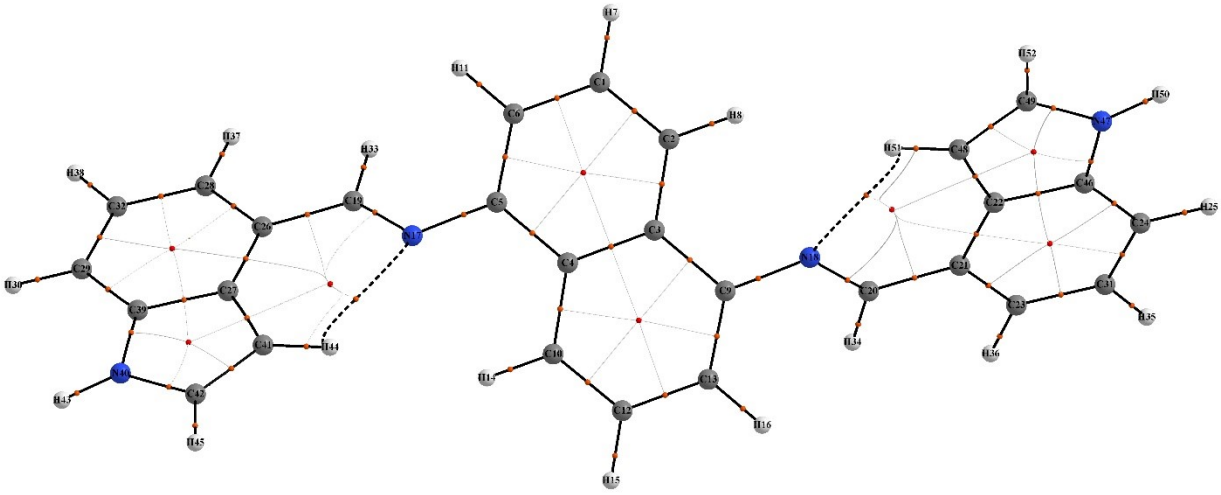


Figure S41. Schematic structure of AIM analysis of **MN6**.