

### Supplementary material

#### **A Facile and Concise Route to Hydroxy Benzoyl Pyrido [2,3-d] Pyrimidine Heterocycles Derivatives: Synthesis, Structural, Spectral and Computational Exploration**

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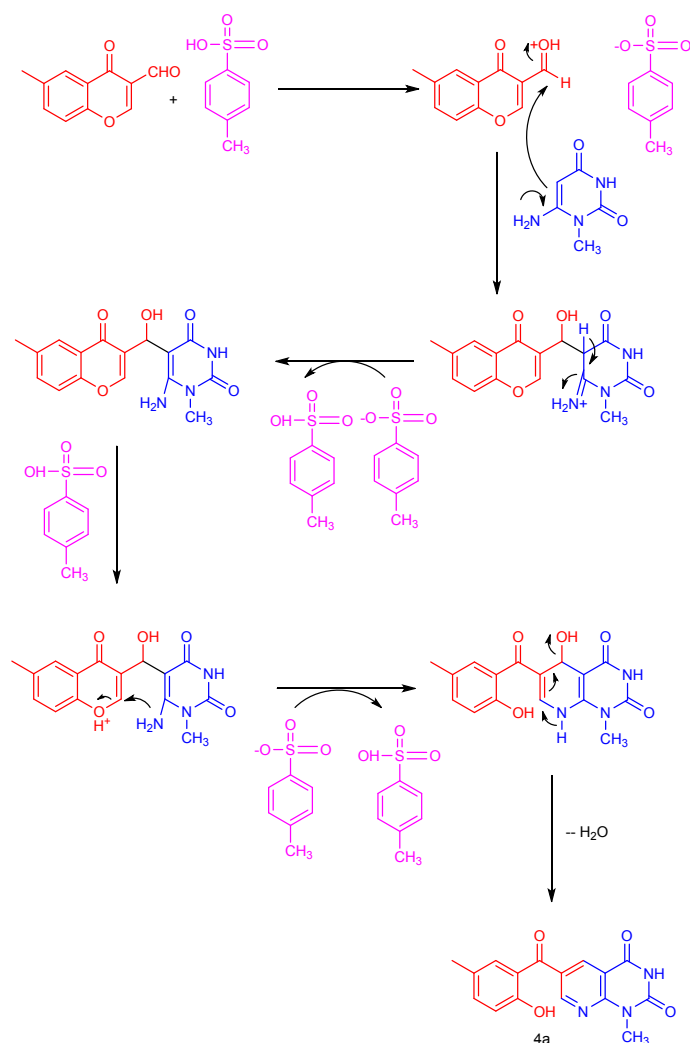
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**Scheme S1:** Plausible mechanism for the synthesis of pyrido[2,3-d]pyrimidines **6a**.

**Table S1** .Comparison of XRD and DFT values of selected bond lengths and bond angles of **4a**

Bond lengths			Bond angles		
	EXP	DFT		EXP	DFT
O1- C1	1.352 (2)	1.34	O1-C1-C2	117.46(15)	117.8
O2-C8	1.235(2)	1.239	O1-C1-C6	123.57(15)	122.9
O3- C14	1.222(2)	1.214	O2-C8-C6	120.79(15)	121.1
O4-C15	1.209 (2)	1.213	O2-C8-C9	121.91(14)	117.3
N1-C12	1.336(2)	1.336	O3-C14-N2	121.87(15)	121.7
N1-C13	1.334(2)	1.332	O3-C14-C11	124.43(15)	125.4
N2-C14	1.372 (2)	1.391	O4-C15-N2	121.25(16)	121.2
N2-C15	1.383(2)	1.393	O4-C15-N3	122.82(16)	123.6
N3-C12	1.385(2)	1.387	C12-N1-C13	117.29(14)	118
N3-C15	1.386(2)	1.395	N1-C12-N3	117.37(14)	116.9
N3-C16	1.464(2)	1.47	N1-C12-C11	123.07(15)	122.5
C1-C2	1.384(2)	1.402	N1-C13-C9	124.05(15)	124.3
C1-C6	1.415(2)	1.421	C14-N2-C15	127.54(14)	128.7

C2-C3	1.373(3)	1.382	N2-C14-C11	113.66(14)	113
C3-C4	1.395(3)	1.409	N2-C15-N3	115.93(14)	115.2
C4-C5	1.384(2)	1.385	C12-N3-C15	121.99(14)	122.2
C4-C7	1.504(3)	1.51	C12-N3-C16	120.49(14)	119.6
C5-C6	1.402(2)	1.414	N3-C12-C11	119.57(14)	120.6
C6-C8	1.461(2)	1.469	C15-N3-C16	117.50(14)	118.2
C8-C9	1.491(2)	1.496	C2-C1-C6	118.97(16)	119.3
C9-C10	1.382(2)	1.396	C1-C2-C3	120.63(16)	120.4
C9-C13	1.399(2)	1.402	C1-C6-C5	118.71(15)	118.4
C10-C11	1.381(2)	1.387	C1-C6-C8	119.76(14)	118.9
C11-C12	1.403(2)	1.411	C2-C3-C4	122.15(16)	121.9
C11-C14	1.460(2)	1.473	C3-C4-C5	117.24(16)	117.5

EXP=experiment, DFT=density functional theory

**Table S1** . Comparison of XRD and DFT values of selected bond angles of **4a**

	<b>Bond angles</b>	
	<b>EXP</b>	<b>DFT</b>
C3-C4-C7	121.45(17)	120.7
C5-C4-C7	121.28(17)	121.9
C4-C5-C6	122.20(16)	122.5
C5-C6-C8	121.40(14)	122.7
C6-C8-C9	121.91(14)	121.6
C8-C9-C10	117.72(14)	119.2
C8-C9-C13	124.85(15)	123.5
C10-C9-C13	117.40(14)	117
C9-C10-C11	119.83(15)	119.6
C10-C11-C12	118.11(14)	118.4
C10-C11-C14	121.21(14)	121.3
C12-C11-C14	120.62(14)	120.3

EXP=experiment, DFT=density functional theory

**Table S2**. Comparison of XRD and DFT values of selected bond lengths and bond angles of **4b**

	<b>Bond lengths</b>		<b>Bond angles</b>		
	<b>EXP</b>	<b>DFT</b>	<b>EXP</b>	<b>DFT</b>	
F1-C4	1.3613(17)	1.356	F1-C4-C3	118.16(13)	118.8
O1-C1	1.3508(18)	1.34	F1-C4-C5	118.84(13)	119.3
O2-C7	1.2420(16)	1.239	O2-C1-C2	117.6	117.4
O3-C15	1.2120(17)	1.215	O2-C1-C6	122.1	122.9
O4-C14	1.2217(17)	1.212	O2-C7-C6	120.79(12)	120.7
N1-C11	1.3361(18)	1.339	O2-C7-C8	116.68(13)	117.5
N1-C12	1.3241(19)	1.327	O3-C15-N3	121.22(12)	121.8
N2-C11	1.3844(17)	1.386	O3-C15-C10	124.86(13)	125.2
N2-C13	1.4670(18)	1.471	O4-C14-N2	122.28(13)	123.6
N2-C14	1.3677(19)	1.396	O4-C14-N3	120.85(13)	121.2
N3-C14	1.3754(18)	1.393	C11-N1-C12	116.98(12)	117.9

N3-C15	1.3776(18)	1.39	N1-C11-N2	116.70(11)	116.8
C1-C2	1.393(2)	1.403	N1-C11-C10	122.92(12)	122.5
C1-C6	1.4145(19)	1.423	N1-C12-C8	125.11(13)	124.5
C2-C3	1.365(2)	1.383	C11-N2-C13	120.38(12)	119.7
C3-C4	1.384(2)	1.394	C11-N2-C14	121.87(11)	122.1
C4-C5	1.360(2)	1.374	N2-C11-C10	120.38(12)	120.7
C5-C6	1.4091(19)	1.413	C13-N2-C14	117.75(12)	118.2
C6-C7	1.463(2)	1.472	N2-C14-N3	116.86(12)	115.2
C7-C8	1.4951(19)	1.493	C14-N3-C15	127.17(12)	128.6
C8-C9	1.3873(19)	1.393	N3-C15-C10	113.92(11)	113
C8-C12	1.3981(9)	1.406	C2-C1-C6	120.26(14)	119.7
C9-C10	1.3871(19)	1.39	C1-C2-C3	120.48(14)	120.7
C10-C11	1.4005(17)	1.409	C1-C6-C5	118.28(13)	118.6
C10-C15	1.4682(19)	1.472	C1-C6-C7	119.29(12)	119

EXP=experiment, DFT=density functional theory

**Table S2** . Comparison of XRD and DFT values of selected bond angles of **4b**

<b>Bond angles</b>		
	<b>EXP</b>	<b>DFT</b>
C2-C3-C4	118.88(14)	119.2
C3-C4-C5	123.00(14)	121.9
C4-C5-C6	119.02(13)	119.9
C5-C6-C7	122.42(12)	122.4
C6-C7-C8	122.53(12)	121.7
C7-C8-C9	125.98(12)	124.6
C7-C8-C12	116.77(12)	118.1
C9-C8-C12	117.11(13)	117.1
C8-C9-C10	119.04(12)	119.5
C9-C10-C11	118.8(12)	118.6
C9-C10-C15	121.49(12)	121

EXP=experiment, DFT=density functional theory

**Table S3** . Comparison of XRD and DFT values of selected bond lengths and bond angles of **4c**

<b>Bond lengths</b>			<b>Bond angles</b>		
	<b>EXP</b>	<b>DFT</b>		<b>EXP</b>	<b>DFT</b>
O1-C1	1.349(2)	1.349	O1-C1-C2	117.86(14)	117.9
O2-C9	1.2281(18)	1.228	O1-C1-C6	122.83(14)	122.8
O3-C15	1.2205(17)	1.22	O2-C9-C6	120.78(13)	120.8
O4-C16	1.2098(18)	1.21	O2-C9-C10	118.84(12)	118.8
N1-C11	1.3327(19)	1.333	O3-C15-N3	121.7	122
N1-C12	1.3368(17)	1.337	O3-C15-C13	124.13(13)	124.1
N2-C15	1.3710(19)	1.371	O4-C16-N2	121.05(13)	121
N2-C16	1.3800(19)	1.38	O4-C16-N3	122.76(14)	122.8
N3-C12	1.3826(18)	1.383	C11-N1-C12	117.24(12)	117.2

N3-C16	1.3803(18)	1.38	N1-C11-C10	124.69(12)	124.7
N3-C17	1.4680(18)	1.468	N1-C12-N3	116.82(12)	116.8
C1-C2	1.394(2)	1.394	N1-C12-C13	122.69(13)	122.7
C1-C6	1.408(2)	1.408	C15-N2-C16	127.74(12)	127.7
C2-C3	1.369(3)	1.369	N2-C15-C13	113.84(12)	113.8
C3-C4	1.393(2)	1.393	N2-C16-N3	116.20(13)	116.2
C4-C5	1.385(2)	1.385	C12-N3-C16	121.68(12)	121.7
C4-C7	1.502(2)	1.502	C12-N3-C17	120.79(11)	120.8
C5-C6	1.397(2)	1.397	N3-C12-C13	120.49(12)	120.5
C6-C9	1.4795(19)	1.479	C16-N3-C17	117.51(12)	117.5
C7-C8	1.507(2)	1.508	C2-C1-C6	119.29(15)	119.3
C9-C10	1.491(2)	1.49	C1-C2-C3	120.23(15)	120.2
C10-C11	1.394(2)	1.394	C1-C6-C5	118.40(13)	118.4
C10-C14	1.3903(18)	1.39	C1-C6-C9	118.98(13)	119
C12-C13	1.3999(19)	1.4	C2-C3-C4	122.24(14)	122.2
C13-C14	1.3821(19)	1.382	C3-C4-C5	117.13(14)	117.1
C13-C15	1.4638(18)	1.464	C3-C4-C7	121.93(14)	121.9

EXP=experiment, DFT=density functional theory

**Table S3** . Comparison of XRD and DFT values of selected bond angles of **4c**

<b>Bond angles</b>		
	<b>EXP</b>	<b>DFT</b>
C5-C6-C9	122.62(13)	122.6
C6-C9-C10	120.37(12)	120.4
C9-C10-C11	124.37(12)	124.4
C9-C10-C14	118.55(13)	118.5
C11-C10-C14	116.86(13)	116.9
C10-C14-C13	119.54(13)	119.5
C12-C13-C14	118.63(12)	118.6
C12-C13-C15	119.82(13)	119.8
C14-C13-C15	121.53(12)	121.5
C5-C6-C9	122.62(13)	122.6
C6-C9-C10	120.37(12)	120.4
C9-C10-C11	124.37(12)	124.4

EXP=experiment, DFT=density functional theory

**Table S4**. Comparison of XRD and DFT values of selected bond lengths and bond angles of **4d**

<b>Bond lengths</b>			<b>Bond angles</b>		
	<b>EXP</b>	<b>DFT</b>		<b>EXP</b>	<b>DFT</b>
O1-C2	1.352(2)	1.341	O1-C2-C1	122.48(16)	123
O2-C10	1.232 (2)	1.24	O1-C2-C3	118.26(16)	117.8
O3-C16	1.210 (2)	1.215	O2-C10-C1	121.55(16)	121.2
O4-C17	1.205(2)	1.213	O2-C10-C11	117.13(16)	117.2
N1-C14	1.332(2)	1.339	O3-C16-N2	121.78(17)	121.7
N1-C15	1.323(2)	1.328	O3-C16-C13	124.24(17)	125.3

N2-C16	1.368(2)	1.39	O4-C17-N2	121.46(18)	121.1
N2-C17	1.377(2)	1.394	O4-C17-N3	122.69(18)	123.7
N3-C14	1.384(2)	1.387	C14-N1-C15	116.70(15)	117.9
N3-C17	1.377(2)	1.395	N1-C14-N3	116.66(15)	116.8
N3-C18	1.462(2)	1.471	N1-C14-C13	123.26(16)	122.5
C1-C2	1.412(2)	1.421	N1-C15-C11	125.03(16)	124.5
C1-C6	1.399(2)	1.414	C16-N2-C17	127.81(16)	128.6
C1-C10	1.458(2)	1.468	N2-C16-C13	113.97(15)	113
C2-C3	1.378(3)	1.401	N2-C17-N3	115.83(15)	115.2
C3-C4	1.375(3)	1.382	C14-N3-C17	122.24(15)	122.1
C4-C5	1.397(3)	1.409	C14-N3-C18	120.25(16)	119.7
C5-C6	1.374(2)	1.385	N3-C14-C13	120.08(16)	120.7
C5-C7	1.517(2)	1.522	C17-N3-C18	117.44(16)	118.2
C7-C8	1.505(3)	1.54	C2-C1-C6	118.09(16)	118.3
C7-C9	1.502(3)	1.54	C2-C1-C10	119.45(16)	118.9
C10-C11	1.491(2)	1.496	C1-C2-C3	119.25(17)	119.2
C11-C12	1.376(2)	1.393	C6-C1-C10	122.49(15)	122.8
C11-C15	1.393(2)	1.406	C1-C6-C5	122.98(16)	122.7
C12-C13	1.380(2)	1.391	C1-C10-C11	121.329(15)	121.7
C13-C14	1.392(2)	1.409	C2-C3-C4	120.71(18)	120.5
C13-C16	1.463(2)	1.471	C3-C4-C5	121.71(18)	121.9

EXP=experiment, DFT=density functional theory

**Table S4** . Comparison of XRD and DFT values of selected bond angles of **4d**

Bond angles		
	EXP	DFT
C4-C5-C6	117.07(18)	117.3
C4-C5-C7	123.37(17)	121.6
C6-C5-C7	119.55(17)	121.1
C5-C7-C8	110.62(17)	112
C5-C7-C9	114.50(19)	111.9
C8-C7-C9	110.85(19)	111.1
C10-C11-C12	124.81(15)	124.5
C10-C11-C15	118.00(15)	118.3
C12-C11-C15	116.99(15)	117
C11-C12-C13	119.63(16)	119.5
C12-C13-C14	118.37(16)	118.6
C12-C13-C16	121.57(15)	121.1
C14-C13-C16	120.06(15)	120.4

EXP=experiment, DFT=density functional theory

**Table S5:** Experimental and DFT based vibrational frequencies of **6a**

Experimental	DFT	Intensity	Vibrational assignments
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Frequency	Frequency		
3217	3594	99.97	$\nu(\text{N-H})$
3092	3382	360.15	$\nu(\text{O-H})$
	3205	3.68	$\nu(\text{C-H}_{\text{Py}})$
	3197	4.26	$\nu_{\text{s}}(\text{C-H}_{\text{Ben}})$
	3170	11.73	$\nu(\text{C-H}_{\text{Py}})$
	3130	10.76	$\nu_{\text{as}}(\text{C-H}_{\text{CH}_3})$
	3102	14.08	$\nu_{\text{as}} + \nu(\text{C-H}_{\text{CH}_3})$
	3067	21.87	$\nu_{\text{s}}(\text{C-H}_{\text{CH}_3})$
	3023	34.24	$\nu_{\text{s}}(\text{C-H}_{\text{CH}_3})$
1717	1778	566.91	$\nu(\text{C=O})$
1697	1770	796.06	$\nu(\text{C=O})$
1625	1671	216.91	$\nu(\text{C=O})$
	1629	421.93	$\nu(\text{C=O})$
	1615	214.40	$\rho(\text{C-H}_{\text{Ben}}) + \rho(\text{O-H})$
1570	1595	78.49	$\rho(\text{C-H}_{\text{Py}}) + \nu(\text{C=C-C=N}_{\text{Py}})$
1474	1544	307.26	$\rho(\text{N-H})$
	1516	199.69	$\delta(\text{C-H}_{\text{CH}_3}) + \rho(\text{O-H})$
	1494	12.26	$\delta(\text{C-H}_{\text{CH}_3})$
	1438	10.39	$\delta_{\text{s}}(\text{C-H}_{\text{CH}_3})$
	1409	112.62	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{O-H})$
1373	1383	133.14	$\delta_{\text{s}}(\text{C-H}_{\text{CH}_3}) + \rho(\text{N-H})$
1329	1357	303.48	$\rho(\text{C-H}_{\text{Py}}) + \rho(\text{O-H})$
	1282	108.63	$\rho(\text{C-H}_{\text{Py}})$
	1276	142.38	$\rho(\text{C-H}_{\text{Py}}) + \rho(\text{C-H}_{\text{CH}_3})$
	1242	266.10	$\rho(\text{C-H}_{\text{Ben}}) + \rho(\text{O-H})$
1184	1227	29.69	$\rho(\text{C-H}_{\text{Ben}})$

	1179	50.46	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{N-H})$
	1166	16.40	$\rho + \delta(\text{C-H}_{\text{Ben}})$
	1138	4.88	$\rho(\text{C-H}_{\text{Py}})$
	1086	22.14	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{C-H}_{\text{Py}})$
	1066	2.42	$\rho(\text{C-H}_{\text{CH}_3})$
	1032	2.05	$\rho(\text{C-H}_{\text{CH}_3})$
	1003	30.67	$\rho(\text{C-H}_{\text{CH}_3})$
943	992	9.56	$\delta_{\text{as}}(\text{C-H}_{\text{Py}})$
	966	17.82	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{N-H})$
	925	4.84	$\rho(\text{C-H}_{\text{CH}_3}) + \nu(\text{C=C-C=C}_{\text{Ben}})$
	851	8.07	$\delta_{\text{s}}(\text{C-H}_{\text{Ben}})$
807	825	82.06	$\rho(\text{O-H})$
	800	19.00	$\rho(\text{C-H}_{\text{Ben}}) + \rho(\text{C-H}_{\text{CH}_3})$
	791	29.86	$\rho(\text{O-H})$
725	753	25.32	$\rho(\text{C=O})$
	707	15.56	$\delta_{\text{as}}(\text{C-H}_{\text{Ben}}) + \delta_{\text{s}}(\text{N-H})$
677	690	33.38	$\nu(\text{C=C-C=C}_{\text{Ben}})$
	661	54.60	$\delta_{\text{s}}(\text{N-H})$
	603	1.84	$\delta_{\text{s}}(\text{C-H}_{\text{Py}})$
	546	12.49	$\delta_{\text{s}}(\text{C-H}_{\text{Ben}}) + \delta_{\text{as}}(\text{C-H}_{\text{CH}_3})$
	515	49.64	$\rho(\text{O-H}) + \nu(\text{C=C-C=N}_{\text{Py}})$
	486	21.30	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{O-H})$
	402	22.45	$\rho(\text{C-O}) + \rho(\text{C-H}_{\text{CH}_3})$
	366	6.52	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{O-H})$
	337	6.77	$\delta_{\text{as}}(\text{C-H}_{\text{Ben}}) + \rho(\text{C-H}_{\text{CH}_3})$
	319	3.12	$\rho(\text{C-H}_{\text{CH}_3})$
	293	3.69	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{C-H}_{\text{Py}})$
	225	3.67	$\rho(\text{C-H}_{\text{CH}_3})$
	171	1.78	$\rho(\text{C-H}_{\text{CH}_3})$
	156	3.91	$\rho(\text{C-H}_{\text{CH}_3})$
	111	0.6	$\rho(\text{C-H}_{\text{CH}_3})$
	72	0.26	$\rho(\text{C-H}_{\text{CH}_3})$
	27	0.13	$\delta_{\text{s}}(\text{C-H}_{\text{CH}_3})$

$\delta$  Scissoring,  $\nu_{\text{s}}$  symmetric,  $\nu_{\text{as}}$  asymmetric,  $\rho$  rocking,  $\delta_{\text{s}}$  symmetric bending vibration (wagging),  $\delta_{\text{as}}$  asymmetric bending vibration (twisting),  $\nu$  is stretching vibration, in compound. (Ben) is benzene. Intensity in (km/mol) and Frequency in  $\nu(\text{cm}^{-1})$ .

**Table S6:** Experimental and DFT based vibrational frequencies of **6b**

Experimental Frequency	DFT Frequency	Intensity	Vibrational assignments
3119-3026	3592	96.83	$\nu(\text{N-H})$
3163	3395	333.11	$\nu(\text{O-H})$
	3207	0.82	$\nu(\text{C-H}_{\text{Ben}})$
	3194	1.59	$\nu_{\text{s}}(\text{C-H}_{\text{Ben}})$
	3179	2.01	$\nu(\text{C-H}_{\text{Py}})$
	3133	9.92	



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			$\nu_{as}(\text{C-H}_{\text{CH}_3})$
2837	3069	22.52	$\nu_s(\text{C-H}_{\text{CH}_3})$
1721	1780	633.13	$\nu(\text{C=O})$
1675-1589	1768	702.70	$\nu(\text{C=O}) + \rho(\text{N-H})$
	1672	91.51	$\rho(\text{H-O}) + \nu(\text{C=C-C=C}_{\text{Ben}})$
	1635	602.59	$\rho(\text{C-H}_{\text{Py}}) + \nu(\text{C=C-C=N}_{\text{Py}})$
	1615	118.24	$\rho(\text{C-H}_{\text{Ben}}) + \rho(\text{O-H})$
	1595	70.83	$\rho(\text{C-H}_{\text{Py}}) + \nu(\text{C=C-C=N}_{\text{Py}})$
	1523	265.78	$\rho(\text{C-H}_{\text{CH}_3})$
	1510	335.44	$\rho(\text{C-H}_{\text{Ben}}) + \rho(\text{O-H})$
1465	1495	13.17	$\rho(\text{C-H}_{\text{CH}_3})$
	1468	68.11	$\delta_s(\text{C-H}_{\text{CH}_3})$
	1404	114.37	$\rho(\text{C-H}_{\text{Ben}}) + \rho(\text{O-H})$
1326	1379	126.24	$\delta_s(\text{C-H}_{\text{CH}_3}) + \rho(\text{C-H}_{\text{Py}})$
	1346	290.29	$\rho(\text{C-H}_{\text{Py}}) + \rho(\text{O-H})$
	1284	48.64	$\rho(\text{C-H}_{\text{Py}})$
1280	1274	277.61	$\rho(\text{C-H}_{\text{Ben}}) + \rho(\text{C-H}_{\text{CH}_3})$
1222	1241	405.43	$\rho(\text{C-H}_{\text{Ben}}) + \rho(\text{O-H})$
	1211	36.72	$\rho + \delta(\text{C-H}_{\text{Ben}})$

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1172	1178	43.62	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{N-H})$
	1156	26.27	$\rho + \delta(\text{C-H}_{\text{Ben}})$
1069	1145	9.13	$\rho(\text{C-H}_{\text{Py}}) + \delta(\text{C-H}_{\text{Ben}})$
	1086	22.78	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{C-H}_{\text{Py}})$
988	1007	25.66	$\rho(\text{C-H}_{\text{Ben}})$
	998	19.25	$\delta_{\text{as}}(\text{C-H}_{\text{Py}})$
	968	20.66	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{N-H})$
869	941	10.02	$\rho(\text{N-H}) + \nu(\text{C=C-C=C}_{\text{Ben}})$
	851	22.84	$\delta_{\text{s}}(\text{C-H}_{\text{Ben}})$
834	844	63.69	$\rho(\text{N-H})$
	816	69.12	$\rho(\text{O-H})$
786	793	12.71	$\delta_{\text{s}}(\text{C-H}_{\text{Py}})$
	736	29.94	$\delta_{\text{s}}(\text{C=O})$
680	714	8.99	$\rho(\text{C-H}_{\text{Py}}) + \rho(\text{N-H})$
	691	34.52	$\nu(\text{C=C-C=C}_{\text{Ben}})$
	663	52.32	$\delta_{\text{s}}(\text{N-H})$
	610	15.02	$\delta_{\text{s}}(\text{C-H}_{\text{Py}})$
	551	5.27	$\delta_{\text{s}}(\text{C-H}_{\text{Ben}})$
	518	34.44	$\rho(\text{O-H}) + \rho(\text{C-H}_{\text{Ben}})$
	478	8.34	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{O-H})$
	408	20.46	$\rho(\text{C=O}) + \rho(\text{C-H}_{\text{CH}_3})$
	385	1.51	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{O-H})$
	324	7.42	$\rho(\text{C-H}_{\text{CH}_3})$
	312	3.69	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{C-H}_{\text{Ben}})$
	229	4.55	$\delta_{\text{as}}(\text{C-H}_{\text{CH}_3}) + \delta_{\text{as}}(\text{C-H}_{\text{Py}})$
	209	1.92	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{O-H})$
	171	2.61	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{C=O})$
	149	5.02	$\rho(\text{C-H}_{\text{CH}_3})$
	111	0.51	$\rho(\text{C-H}_{\text{CH}_3})$
	75	0.69	$\rho(\text{C-H}_{\text{CH}_3})$
	27	0.52	$\delta_{\text{s}}(\text{C-H}_{\text{CH}_3})$

$\delta$  Scissoring,  $\nu_{\text{s}}$  symmetric,  $\nu_{\text{as}}$  asymmetric,  $\rho$  rocking,  $\delta_{\text{s}}$  symmetric bending vibration (wagging),  $\delta_{\text{as}}$  asymmetric bending vibration (twisting),  $\nu$  is stretching vibration, in compound. (Ben) is benzene. Intensity in (km/mol) and Frequency in  $\nu(\text{cm}^{-1})$ .

**Table S7:** Experimental and DFT based vibrational frequencies of **6c**

Experimental Frequency	DFT Frequency	Intensity	Vibrational assignments
3168	3594	100.28	$\nu(\text{N-H})$
3131-3045	3385	365.09	$\nu(\text{O-H})$
	3207	3.72	$\nu(\text{C-H}_{\text{Py}})$
	3196	4.53	$\nu_{\text{s}}(\text{C-H}_{\text{Ben}})$
	3171	12.57	$\nu(\text{C-H}_{\text{Py}})$
	3159	12.71	$\nu_{\text{as}}(\text{C-H}_{\text{Ben}})$
	3130	10.74	$\nu_{\text{as}}(\text{C-H}_{\text{CH}_3})$
	3091	43.08	$\nu_{\text{s}} + \nu_{\text{as}}(\text{C-H}_{\text{CH}_3})$
	2936	3025	34.21

1720	1779	565.30	$\nu_s(\text{C-H}_{\text{CH}_3})$
1721-1685	1770	796.26	$\nu(\text{C=O})$
	1669	261.74	$\nu(\text{C=O}) + \rho(\text{N-H})$
1628	1628	417.69	$\rho(\text{O-H}) + \nu(\text{C=C-C=C}_{\text{Ben}})$
	1614	186.69	$\nu(\text{C=O}) + \nu(\text{C=C-C=N}_{\text{Py}})$
	1596	78.16	$\rho(\text{C-H}_{\text{Ben}}) + \rho(\text{O-H})$
			$\rho(\text{C-H}_{\text{Py}}) + \nu(\text{C=C-C=N}_{\text{Py}})$
	1523	190.75	$\delta(\text{C-H}_{\text{CH}_3})$
	1513	207.21	$\delta(\text{C-H}_{\text{CH}_3}) + \rho(\text{C-H}_{\text{Ben}})$
1478	1497	10.37	$\delta(\text{C-H}_{\text{CH}_3})$
	1424	26.51	$\delta_s(\text{C-H}_{\text{CH}_3}) + \rho(\text{N-H})$
	1407	127.73	$\rho(\text{C-H}_{\text{Ben}}) + \rho(\text{O-H})$
1376	1384	124.67	$\delta_s(\text{C-H}_{\text{CH}_3}) + \rho(\text{N-H})$
1329	1332	352.21	$\rho(\text{C-H}_{\text{Ben}}) + \rho(\text{C-H}_{\text{Py}})$
	1287	212.65	$\rho(\text{C-H}_{\text{CH}_3}) + \delta_{\text{as}}(\text{C-H}_{\text{CH}_2})$
1252	1267	102.21	$\delta_{\text{as}}(\text{C-H}_{\text{CH}_2}) + \delta_{\text{as}}(\text{C-H}_{\text{CH}_3}) + \rho(\text{O-H})$
	1240	265.88	$\rho(\text{C-H}_{\text{Ben}}) + \rho(\text{O-H})$
1205	1225	37.60	$\rho(\text{C-H}_{\text{Ben}}) + \delta_s(\text{C-H}_{\text{CH}_2})$

	1180	51.63	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{N-H})$
	1166	18.80	$\rho + \delta(\text{C-H}_{\text{Ben}})$
	1139	5.31	$\rho(\text{C-H}_{\text{Py}})$
1067	1087	13.70	$\delta_{\text{as}}(\text{C-H}_{\text{CH}_3}) + \delta_{\text{as}}(\text{C-H}_{\text{CH}_2}) + \rho(\text{C-H}_{\text{Py}})$
	1087	11.19	$\rho(\text{C-H}_{\text{CH}_3}) + \delta_{\text{as}}(\text{C-H}_{\text{CH}_2})$
	1075	6.59	$\delta_{\text{as}}(\text{C-H}_{\text{CH}_3}) + \delta_{\text{as}}(\text{C-H}_{\text{CH}_2})$
	1013	22.26	$\rho(\text{C-H}_{\text{Ben}})$
	996	9.40	$\delta_{\text{as}}(\text{C-H}_{\text{Py}})$
940	967	19.23	$\rho(\text{C-H}_{\text{CH}_3})$
862	912	9.72	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{N-H})$
	857	12.03	$\delta_{\text{s}}(\text{C-H}_{\text{Ben}})$
821	833	71.68	$\rho(\text{O-H}) + \nu(\text{C=C-C=C}_{\text{Ben}})$
	823	70.95	$\rho(\text{O-H})$
786	799	17.75	$\rho(\text{C-H}_{\text{CH}_3})$
750	752	24.30	$\nu(\text{C=O})$
710	710	18.98	$\delta_{\text{s}}(\text{C-H}_{\text{Ben}}) + \delta_{\text{s}}(\text{N-H})$
672	690	24.21	$\nu(\text{C=C-C=C}_{\text{Ben}}) + \delta_{\text{as}}(\text{C-H}_{\text{CH}_3})$
	663	58.04	$\delta_{\text{s}}(\text{N-H})$
	612	5.92	$\delta_{\text{s}}(\text{C-H}_{\text{Ben}}) + \delta_{\text{s}}(\text{N-H})$
	563	7.91	$\delta_{\text{s}}(\text{C-H}_{\text{Ben}}) + \delta_{\text{as}}(\text{C-H}_{\text{Py}})$
	515	48.97	$\rho(\text{O-H}) + \nu(\text{C=C-C=N}_{\text{Py}})$
	483	16.37	$\rho(\text{C-H}_{\text{Ben}}) + \rho(\text{O-H})$
	404	23.46	$\rho(\text{C=O}) + \rho(\text{C-H}_{\text{CH}_3})$
	367	5.79	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{O-H})$
	326	3.15	$\rho(\text{C-H}_{\text{Py}}) + \rho(\text{C-H}_{\text{CH}_3})$
	301	7.21	$\rho(\text{C-H}_{\text{CH}_3})$
	246	0.37	$\rho(\text{C-H}_{\text{CH}_3})$
	214	3.92	$\rho(\text{C-H}_{\text{CH}_3})$
	166	2.41	$\rho(\text{C-H}_{\text{CH}_3}) + \delta_{\text{as}}(\text{C-H}_{\text{Py}})$
	146	1.96	$\rho(\text{C-H}_{\text{CH}_3})$
	109	0.53	$\rho(\text{C-H}_{\text{CH}_3})$
	74	0.79	$\rho(\text{C-H}_{\text{CH}_3})$
	25	0.14	$\rho(\text{C-H}_{\text{CH}_3})$

$\delta$  Scissoring,  $\nu_{\text{s}}$  symmetric,  $\nu_{\text{as}}$  asymmetric,  $\rho$  rocking,  $\delta_{\text{s}}$  symmetric bending vibration (wagging),  $\delta_{\text{as}}$  asymmetric bending vibration (twisting),  $\nu$  is stretching vibration, in compound. (Ben) is benzene. Intensity in (km/mol) and Frequency in  $\nu(\text{cm}^{-1})$ .

**Table S8:** Experimental and DFT based vibrational frequencies of **6d**

Experimental Frequency	DFT Frequency	Intensity	Vibrational assignments
3051-2963	3594	93.38	$\nu(\text{N-H})$
3168-3051	3391	343.14	$\nu(\text{O-H})$
2950	3204	1.20	$\nu(\text{C-H}_{\text{Py}})$
	3196	5.31	$\nu_{\text{s}}(\text{C-H}_{\text{Ben}})$
	3183	5.98	$\nu(\text{C-H}_{\text{Ben}})$
	3168	10.34	$\nu_{\text{as}}(\text{C-H}_{\text{Ben}})$
	3132	10.16	$\nu_{\text{as}}(\text{C-H}_{\text{CH}_3})$
	3096	33.63	$\nu_{\text{s}} + \nu_{\text{as}}(\text{C-H}_{\text{CH}_3})$

	3093	22.21	$\nu_s + \nu_{as}(\text{C-H}_{\text{CH}_3})$
	3087	65.57	$\nu_{as}(\text{C-H}_{\text{CH}_3})$
	3068	23.42	$\nu_s(\text{C-H}_{\text{CH}_3})$
	3025	35.50	$\nu_s(\text{C-H}_{\text{CH}_3})$
	3020	23.61	$\nu_s(\text{C-H}_{\text{CH}_3})$
	3017	7.72	$\nu(\text{C-H})$
1717	1778	655.11	$\nu(\text{C=O})$
1677	1765	691.36	$\nu(\text{C=O}) + \rho(\text{N-H})$
	1667	225.78	$\rho(\text{O-H}) + \nu(\text{C=C-C=C}_{\text{Ben}}) + \delta(\text{C-H}_{\text{Ben}})$
1571	1646	117.34	$\nu(\text{C=O}) + \nu(\text{C=C-C=N}_{\text{Py}})$
	1632	464.76	$\nu(\text{C-O}) + \nu(\text{C=C-C=N}_{\text{Py}})$
	1613	163.26	$\rho(\text{C-H}_{\text{Ben}}) + \rho(\text{O-H})$
	1596	76.87	$\rho(\text{C-H}_{\text{Py}}) + \nu(\text{C=C-C=N}_{\text{Py}})$
	1522	262.94	$\delta(\text{C-H}_{\text{CH}_3})$
	1515	187.88	$\delta(\text{C-H}_{\text{CH}_3}) + \rho(\text{C-H}_{\text{Ben}}) + \rho(\text{O-H})$
	1507	33.06	$\delta(\text{C-H}_{\text{CH}_3})$
1474	1502	22.99	$\delta(\text{C-H}_{\text{CH}_3})$
	1495	12.51	$\delta(\text{C-H}_{\text{CH}_3})$
	1468	63.58	$\delta(\text{C-H}_{\text{CH}_3})$
	1422	10.66	$\delta_s(\text{C-H}_{\text{CH}_3})$
1336	1408	172.16	$\rho(\text{O-H}) + \rho(\text{C-H}_{\text{Ben}})$
	1386	37.70	$\rho(\text{N-H}) + \rho(\text{C-H})$
	1379	108.49	$\delta_s(\text{C-H}_{\text{CH}_3}) + \rho(\text{N-H})$
	1369	38.10	$\rho(\text{C-H}_{\text{Py}}) + \rho(\text{C-H})$
	1331	380.88	$\rho(\text{C-H}_{\text{Ben}}) + \nu(\text{C=C-C=C}_{\text{Ben}}) + \rho(\text{C-H}_{\text{Py}})$
	1315	78.81	$\nu(\text{C=C-C=N}_{\text{Py}}) + \rho(\text{C-H}_{\text{Py}})$
	1284	60.75	$\rho(\text{C-H}_{\text{Py}})$
1209	1280	294.05	$\rho(\text{C-H}_{\text{Ben}}) + \delta(\text{C-H}_{\text{Ben}})$
	1245	257.10	$\rho(\text{C-H}_{\text{Ben}}) + \rho(\text{O-H})$
	1232	97.28	$\rho(\text{C-H}_{\text{Ben}})$
	1177	29.39	$\rho(\text{N-H}) + \rho(\text{C-H}_{\text{CH}_3})$
1072	1169	21.90	$\rho + \delta(\text{C-H}_{\text{Ben}})$
998	1087	20.48	$\rho(\text{C-H}_{\text{Py}}) + \rho(\text{C-H}_{\text{CH}_3})$
	999	30.34	$\delta_{as}(\text{C-H}_{\text{Ben}}) + \delta_s(\text{C-H}_{\text{Py}})$
	968	19.89	$\rho(\text{C-H}_{\text{CH}_3}) + \rho(\text{N-H})$
	919	6.79	$\delta_s(\text{C-H}_{\text{Ben}})$
833	885	21.85	$\rho(\text{C-H}_{\text{CH}_3})$
	836	35.03	$\nu(\text{C=C-C=C}_{\text{Ben}}) + \rho(\text{N-H})$
789	819	81.40	$\delta_s(\text{O-H})$
	788	32.59	$\delta_s(\text{O-H})$
750	766	21.77	$\delta_s(\text{C-H}_{\text{CH}_3})$
	752	30.46	$b(\text{N-H})$
672	690	33.01	$\nu(\text{C=C-C=C}_{\text{Ben}}) + \delta_{as}(\text{C-H}_{\text{CH}_3})$
	662	63.22	$\delta_s(\text{N-H})$

614	16.54	$\delta_s$ (N-H)+ $\delta_s$ (C-H <sub>py</sub> )
593	11.39	$\delta_s$ (C-H <sub>Ben</sub> )
521	35.09	$\delta_s$ (N-H <sub>py</sub> )
499	7.04	$\rho$ (O-H)+ $\rho$ (C-H <sub>Ben</sub> )
451	22.62	$\rho$ (O-H)+ $\delta_s$ (C-H <sub>Ben</sub> )
409	24.02	$\rho$ (C=O) + $\rho$ (C-H <sub>CH3</sub> )
399	2.53	$\rho$ (C-H <sub>CH3</sub> )+ $\rho$ (C=O)
322	7.60	$\rho$ (C-H <sub>CH3</sub> )+ $\rho$ (C-H <sub>Py</sub> )
289	0.80	$\rho$ (C-H <sub>CH3</sub> )
211	4.25	$\rho$ (C-H <sub>CH3</sub> )+ $\rho$ (O-H)
148	1.70	$\delta_s$ (C-H <sub>Ben</sub> )+ $\rho$ (C-H <sub>CH3</sub> )
147	3.42	$\rho$ (C-H <sub>CH3</sub> )
101	0.40	$\rho$ (C-H <sub>CH3</sub> )
69	0.55	$\rho$ (C-H <sub>CH3</sub> )
31	0.51	$\delta_s$ (C-H <sub>CH3</sub> )

$\delta$  Scissoring ,  $\nu_s$  symmetric ,  $\nu_{as}$  asymmetric ,  $\rho$  rocking ,  $\delta_s$  symmetric bending vibration (wagging),  $\delta_{as}$  asymmetric bending vibration(twisting),  $\nu$  is stretching vibration, b is bending vibration, in compound. (Ben) is benzene. Intensity in (km/mol) and Frequency in  $\nu$ (cm<sup>-1</sup>).

**Table S9:** Natural bond orbital (NBO) analysis of **6a**

Donor(i)	Type	Acceptor(j)	Type	E (2) <sup>a</sup> [kJ/mol]	E(j)-E(i) <sup>b</sup> [a.u.]	F(i,j) <sup>c</sup> [a.u.]
O <sub>1</sub> -H <sub>2</sub>	$\sigma$	C <sub>10</sub> -C <sub>11</sub>	$\sigma^*$	6.07	1.44	0.084
N <sub>6</sub> -C <sub>28</sub>	$\pi$	C <sub>24</sub> -C <sub>29</sub>	$\pi^*$	43.15	0.41	0.119
N <sub>6</sub> -C <sub>28</sub>	$\pi$	C <sub>25</sub> -C <sub>27</sub>	$\pi^*$	14.04	0.42	0.068
C <sub>10</sub> -C <sub>18</sub>	$\pi$	O <sub>3</sub> -C <sub>23</sub>	$\pi^*$	31.62	0.33	0.096
C <sub>10</sub> -C <sub>18</sub>	$\pi$	C <sub>11</sub> -C <sub>13</sub>	$\pi^*$	18.62	0.36	0.076
C <sub>10</sub> -C <sub>18</sub>	$\pi$	C <sub>15</sub> -C <sub>16</sub>	$\pi^*$	30.00	0.37	0.096
C <sub>11</sub> -C <sub>13</sub>	$\pi$	C <sub>10</sub> -C <sub>18</sub>	$\pi^*$	32.30	0.34	0.098
C <sub>11</sub> -C <sub>13</sub>	$\pi$	C <sub>15</sub> -C <sub>16</sub>	$\pi^*$	21.28	0.37	0.081
C <sub>15</sub> -C <sub>16</sub>	$\pi$	C <sub>10</sub> -C <sub>18</sub>	$\pi^*$	20.41	0.34	0.077
C <sub>15</sub> -C <sub>16</sub>	$\pi$	C <sub>11</sub> -C <sub>13</sub>	$\pi^*$	29.57	0.37	0.093
C <sub>24</sub> -C <sub>29</sub>	$\pi$	O <sub>3</sub> -C <sub>23</sub>	$\pi^*$	16.01	0.36	0.071
C <sub>24</sub> -C <sub>29</sub>	$\pi$	N <sub>6</sub> -C <sub>28</sub>	$\pi^*$	20.26	0.32	0.073
C <sub>24</sub> -C <sub>29</sub>	$\pi$	C <sub>25</sub> -C <sub>27</sub>	$\pi^*$	37.06	0.36	0.105
C <sub>25</sub> -C <sub>27</sub>	$\pi$	O <sub>4</sub> -C <sub>31</sub>	$\pi^*$	27.46	0.37	0.092
C <sub>25</sub> -C <sub>27</sub>	$\pi$	N <sub>6</sub> -C <sub>28</sub>	$\pi^*$	42.80	0.33	0.108
C <sub>29</sub> -H <sub>30</sub>	$\sigma$	N <sub>6</sub> -C <sub>28</sub>	$\sigma^*$	5.70	1.19	0.074
C <sub>13</sub> -C <sub>15</sub>	$\sigma$	C <sub>12</sub> -C <sub>13</sub>	$\sigma^*$	4.68	1.37	0.072
LP-O <sub>1</sub>	$\sigma$	C <sub>10</sub> -C <sub>18</sub>	$\sigma^*$	9.12	1.24	0.095
LP-O <sub>1</sub>	$\pi$	C <sub>10</sub> -C <sub>18</sub>	$\pi^*$	48.09	0.42	0.135
LP-O <sub>3</sub>	$\pi$	O <sub>1</sub> -H <sub>2</sub>	$\sigma^*$	5.80	1.30	0.078
LP-O <sub>3</sub>	$\pi$	C <sub>13</sub> -C <sub>15</sub>	$\sigma^*$	5.53	1.30	0.076
LP-O <sub>3</sub>	$\pi$	O <sub>1</sub> -H <sub>2</sub>	$\sigma^*$	21.88	0.92	0.129
LP-O <sub>3</sub>	$\pi$	C <sub>18</sub> -C <sub>23</sub>	$\sigma^*$	13.13	0.92	0.100
LP-O <sub>3</sub>	$\pi$	C <sub>23</sub> -C <sub>24</sub>	$\sigma^*$	21.12	0.88	0.123
LP-O <sub>4</sub>	$\pi$	N <sub>7</sub> -C <sub>31</sub>	$\sigma^*$	34.49	0.81	0.151
LP-O <sub>4</sub>	$\pi$	C <sub>27</sub> -C <sub>31</sub>	$\sigma^*$	24.00	0.83	0.128
LP-O <sub>5</sub>	$\pi$	N <sub>7</sub> -C <sub>32</sub>	$\sigma^*$	31.82	0.80	0.145
LP-O <sub>5</sub>	$\pi$	N <sub>9</sub> -C <sub>32</sub>	$\sigma^*$	33.26	0.79	0.147
LP-N <sub>6</sub>	$\sigma$	N <sub>9</sub> -C <sub>28</sub>	$\sigma^*$	5.53	0.93	0.065

LP-N <sub>6</sub>	$\sigma$	C <sub>24</sub> -C <sub>29</sub>	$\sigma^*$	11.39	1.03	0.098
LP-N <sub>6</sub>	$\sigma$	C <sub>27</sub> -C <sub>28</sub>	$\sigma^*$	12.21	1.01	0.100
LP-N <sub>7</sub>	$\sigma$	O <sub>4</sub> -C <sub>31</sub>	$\pi^*$	65.27	0.38	0.143
LP-N <sub>7</sub>	$\sigma$	O <sub>5</sub> -C <sub>32</sub>	$\pi^*$	68.70	0.36	0.141
LP-N <sub>9</sub>	$\sigma$	O <sub>5</sub> -C <sub>32</sub>	$\pi^*$	70.39	0.36	0.142
LP-N <sub>9</sub>	$\sigma$	N <sub>6</sub> -C <sub>28</sub>	$\pi^*$	64.20	0.33	0.133
N <sub>6</sub> -C <sub>28</sub>	$\pi$	C <sub>24</sub> -C <sub>29</sub>	$\pi^*$	165.36	0.03	0.096
N <sub>6</sub> -C <sub>28</sub>	$\pi$	C <sub>25</sub> -C <sub>27</sub>	$\pi^*$	120.98	0.04	0.095
C <sub>10</sub> -C <sub>18</sub>	$\pi$	C <sub>11</sub> -C <sub>13</sub>	$\pi^*$	167.00	0.02	0.096
C <sub>10</sub> -C <sub>18</sub>	$\pi$	C <sub>15</sub> -C <sub>16</sub>	$\pi^*$	134.44	0.03	0.088

**Table S10:** Natural bond orbital (NBO) analysis of **6b**

Donor(i)	Type	Acceptor(j)	Type	E (2) <sup>a</sup> [kJ/mol]	E(j)-E(i) <sup>b</sup> [a.u.]	F(i,j) <sup>c</sup> [a.u.]
O <sub>5</sub> - C <sub>33</sub>	$\sigma$	C <sub>24</sub> - C <sub>33</sub>	$\sigma^*$	65.09	4.11	0.469
O <sub>5</sub> - C <sub>33</sub>	$\sigma$	C <sub>28</sub> - H <sub>30</sub>	$\sigma^*$	21.55	4.07	0.265
N <sub>7</sub> - C <sub>26</sub>	$\pi$	C <sub>21</sub> - C <sub>22</sub>	$\pi^*$	9.53	0.34	0.051
N <sub>7</sub> - C <sub>26</sub>	$\pi$	C <sub>24</sub> - C <sub>25</sub>	$\pi^*$	29.05	0.32	0.090
N <sub>9</sub> - H <sub>10</sub>	$\sigma$	C <sub>24</sub> - C <sub>33</sub>	$\sigma^*$	15.93	3.72	0.220
N <sub>9</sub> - H <sub>10</sub>	$\sigma$	C <sub>28</sub> - H <sub>30</sub>	$\sigma^*$	12.09	3.69	0.189
N <sub>9</sub> - C <sub>32</sub>	$\sigma$	C <sub>28</sub> - H <sub>30</sub>	$\sigma^*$	13.09	3.85	0.201
N <sub>9</sub> - C <sub>33</sub>	$\sigma$	C <sub>28</sub> - H <sub>30</sub>	$\sigma^*$	58.20	3.84	0.422
C <sub>11</sub> - C <sub>19</sub>	$\pi$	O <sub>4</sub> - C <sub>20</sub>	$\pi^*$	25.60	0.25	0.075
C <sub>11</sub> - C <sub>19</sub>	$\pi$	C <sub>12</sub> - C <sub>14</sub>	$\pi^*$	14.59	0.29	0.059
C <sub>11</sub> - C <sub>19</sub>	$\pi$	C <sub>16</sub> - C <sub>17</sub>	$\pi^*$	22.31	0.28	0.072
C <sub>12</sub> - C <sub>14</sub>	$\pi$	C <sub>11</sub> - C <sub>19</sub>	$\pi^*$	22.39	0.28	0.073
C <sub>12</sub> - C <sub>14</sub>	$\pi$	C <sub>16</sub> - C <sub>17</sub>	$\pi^*$	18.22	0.28	0.065
C <sub>16</sub> - C <sub>17</sub>	$\pi$	C <sub>11</sub> - C <sub>19</sub>	$\pi^*$	14.86	0.29	0.061
C <sub>16</sub> - C <sub>17</sub>	$\pi$	C <sub>12</sub> - C <sub>14</sub>	$\pi^*$	20.42	0.30	0.070
C <sub>21</sub> - C <sub>22</sub>	$\pi$	O <sub>4</sub> - C <sub>20</sub>	$\pi^*$	14.75	0.27	0.058
C <sub>21</sub> - C <sub>22</sub>	$\pi$	N <sub>7</sub> - C <sub>26</sub>	$\pi^*$	30.31	0.27	0.081
C <sub>21</sub> - C <sub>22</sub>	$\pi$	C <sub>24</sub> - C <sub>25</sub>	$\pi^*$	15.19	0.28	0.059
C <sub>24</sub> - C <sub>25</sub>	$\pi$	O <sub>5</sub> - C <sub>33</sub>	$\pi^*$	24.56	0.29	0.078
C <sub>24</sub> - C <sub>25</sub>	$\pi$	N <sub>7</sub> - C <sub>26</sub>	$\pi^*$	12.58	0.28	0.054
C <sub>24</sub> - C <sub>25</sub>	$\pi$	C <sub>21</sub> - C <sub>22</sub>	$\pi^*$	25.56	0.30	0.080
LP-F <sub>1</sub>	$\pi$	C <sub>14</sub> - C <sub>16</sub>	$\sigma^*$	6.06	0.96	0.068
LP-F <sub>1</sub>	$\pi$	C <sub>16</sub> - C <sub>17</sub>	$\sigma^*$	5.88	0.99	0.068
LP-F <sub>1</sub>	$\pi$	C <sub>16</sub> - C <sub>17</sub>	$\pi^*$	17.63	0.43	0.083
LP-O <sub>2</sub>	$\pi$	C <sub>11</sub> - C <sub>19</sub>	$\pi^*$	37.71	0.32	0.105
LP-O <sub>4</sub>	$\pi$	C <sub>19</sub> - C <sub>20</sub>	$\sigma^*$	11.23	0.78	0.085
LP-O <sub>4</sub>	$\pi$	C <sub>20</sub> - C <sub>21</sub>	$\sigma^*$	18.11	0.71	0.103
LP-O <sub>5</sub>	$\sigma$	C <sub>24</sub> - C <sub>33</sub>	$\sigma^*$	40.60	3.72	0.351
LP-O <sub>5</sub>	$\sigma$	C <sub>28</sub> - H <sub>30</sub>	$\sigma^*$	15.52	3.69	0.214
LP-O <sub>5</sub>	$\pi$	N <sub>9</sub> - C <sub>33</sub>	$\sigma^*$	33.40	0.67	0.136
LP-O <sub>5</sub>	$\pi$	C <sub>24</sub> - C <sub>33</sub>	$\sigma^*$	16.66	3.31	0.214
LP-O <sub>5</sub>	$\pi$	C <sub>28</sub> - H <sub>30</sub>	$\sigma^*$	26.19	3.28	0.271
LP-O <sub>6</sub>	$\pi$	N <sub>8</sub> - C <sub>32</sub>	$\sigma^*$	26.30	0.65	0.119
LP-O <sub>6</sub>	$\pi$	N <sub>9</sub> - C <sub>32</sub>	$\sigma^*$	25.66	0.66	0.119
LP-N <sub>7</sub>	$\sigma$	C <sub>21</sub> - C <sub>26</sub>	$\sigma^*$	11.48	0.89	0.092
LP-N <sub>7</sub>	$\sigma$	C <sub>24</sub> - C <sub>25</sub>	$\sigma^*$	9.61	0.86	0.082
LP-N <sub>7</sub>	$\sigma$	C <sub>24</sub> - C <sub>33</sub>	$\sigma^*$	6.82	3.39	0.137
LP-N <sub>7</sub>	$\sigma$	C <sub>28</sub> - H <sub>30</sub>	$\sigma^*$	11.10	3.35	0.176

LP-N <sub>8</sub>	$\sigma$	C <sub>24</sub> -C <sub>25</sub>	$\pi^*$	47.19	0.28	0.103
LP-N <sub>9</sub>	$\sigma$	O <sub>5</sub> -C <sub>33</sub>	$\pi^*$	51.05	0.28	0.109
O <sub>4</sub> -C <sub>20</sub>	$\pi^*$	C <sub>11</sub> -C <sub>19</sub>	$\pi^*$	113.58	0.02	0.071
N <sub>7</sub> -C <sub>26</sub>	$\pi^*$	C <sub>21</sub> -C <sub>22</sub>	$\pi^*$	135.27	0.02	0.084
C <sub>11</sub> -C <sub>19</sub>	$\pi^*$	C <sub>12</sub> -C <sub>14</sub>	$\pi^*$	260.90	0.01	0.083
C <sub>24</sub> -C <sub>25</sub>	$\pi^*$	C <sub>21</sub> -C <sub>22</sub>	$\pi^*$	249.85	0.01	0.086

**Table S11:** Natural bond orbital (NBO) analysis of **6c**

Donor(i)	Type	Acceptor(j)	Type	E (2) <sup>a</sup> [kJ/mol]	E(j)-E(i) <sup>b</sup> [a.u.]	F(i,j) <sup>c</sup> [a.u.]
N <sub>6</sub> -C <sub>30</sub>	$\pi$	C <sub>27</sub> -C <sub>28</sub>	$\pi^*$	30.14	0.33	0.090
N <sub>6</sub> -C <sub>30</sub>	$\pi$	C <sub>31</sub> -C <sub>32</sub>	$\pi^*$	9.83	0.34	0.051
N <sub>9</sub> -C <sub>36</sub>	$\sigma$	C <sub>15</sub> -C <sub>16</sub>	$\pi^*$	5.18	0.94	0.067
N <sub>9</sub> -C <sub>36</sub>	$\sigma$	C <sub>19</sub> -H <sub>20</sub>	$\sigma^*$	9.92	1.57	0.112
N <sub>9</sub> -C <sub>36</sub>	$\sigma$	C <sub>36</sub> -H <sub>39</sub>	$\sigma^*$	25.55	6.12	0.353
C <sub>11</sub> -C <sub>13</sub>	$\pi$	C <sub>15</sub> -C <sub>16</sub>	$\pi^*$	10.84	0.45	0.063
C <sub>15</sub> -C <sub>16</sub>	$\pi$	C <sub>11</sub> -C <sub>13</sub>	$\pi^*$	20.76	0.29	0.070
C <sub>27</sub> -C <sub>28</sub>	$\pi$	O <sub>3</sub> -C <sub>26</sub>	$\pi^*$	14.28	0.27	0.058
C <sub>27</sub> -C <sub>28</sub>	$\pi$	N <sub>6</sub> -C <sub>30</sub>	$\pi^*$	14.22	0.25	0.054
C <sub>27</sub> -C <sub>28</sub>	$\pi$	C <sub>31</sub> -C <sub>32</sub>	$\pi^*$	26.15	0.29	0.079
C <sub>31</sub> -C <sub>32</sub>	$\pi$	O <sub>4</sub> -C <sub>34</sub>	$\pi^*$	23.69	0.28	0.074
C <sub>31</sub> -C <sub>32</sub>	$\pi$	N <sub>6</sub> -C <sub>30</sub>	$\pi^*$	33.01	0.26	0.084
C <sub>31</sub> -C <sub>32</sub>	$\pi$	C <sub>27</sub> -C <sub>28</sub>	$\pi^*$	14.23	0.28	0.057
C <sub>36</sub> -H <sub>37</sub>	$\sigma$	C <sub>36</sub> -H <sub>39</sub>	$\sigma^*$	16.75	5.90	0.281
C <sub>36</sub> -H <sub>38</sub>	$\sigma$	C <sub>36</sub> -H <sub>39</sub>	$\sigma^*$	10.19	5.90	0.219
C <sub>36</sub> -H <sub>39</sub>	$\sigma$	C <sub>36</sub> -H <sub>39</sub>	$\sigma^*$	53.30	5.89	0.500
LP-O <sub>1</sub>	$\sigma$	C <sub>10</sub> -C <sub>18</sub>	$\sigma^*$	6.91	1.11	0.078
LP-O <sub>1</sub>	$\pi$	C10 LP	$\sigma^*$	69.67	0.19	0.128
LP-O <sub>3</sub>	$\pi$	O <sub>1</sub> -H <sub>2</sub>	$\sigma^*$	17.30	0.72	0.102
LP-O <sub>3</sub>	$\pi$	C <sub>18</sub> -C <sub>26</sub>	$\sigma^*$	11.93	0.77	0.087
LP-O <sub>3</sub>	$\pi$	C <sub>26</sub> -C <sub>27</sub>	$\sigma^*$	17.69	0.73	0.103
LP-O <sub>4</sub>	$\pi$	N <sub>7</sub> -C <sub>34</sub>	$\sigma^*$	27.75	0.68	0.124
LP-O <sub>4</sub>	$\pi$	C <sub>31</sub> -C <sub>34</sub>	$\sigma^*$	18.45	0.71	0.104
LP-O <sub>5</sub>	$\pi$	N <sub>7</sub> -C <sub>35</sub>	$\sigma^*$	25.49	0.66	0.118
LP-O <sub>5</sub>	$\pi$	N <sub>9</sub> -C <sub>35</sub>	$\sigma^*$	26.18	0.66	0.119
LP-N <sub>6</sub>	$\pi$	N <sub>9</sub> -C <sub>30</sub>	$\sigma^*$	5.48	0.78	0.059
LP-N <sub>6</sub>	$\sigma$	C <sub>27</sub> -C <sub>28</sub>	$\sigma^*$	8.92	0.90	0.081
LP-N <sub>6</sub>	$\sigma$	C <sub>30</sub> -C <sub>31</sub>	$\sigma^*$	9.77	0.88	0.084
LP-N <sub>7</sub>	$\sigma$	O <sub>4</sub> -C <sub>34</sub>	$\pi^*$	51.60	0.29	0.111
LP-N <sub>7</sub>	$\sigma$	O <sub>5</sub> -C <sub>35</sub>	$\pi^*$	54.94	0.28	0.111
LP-N <sub>9</sub>	$\sigma$	O <sub>5</sub> -C <sub>35</sub>	$\pi^*$	55.52	0.27	0.111
LP-N <sub>9</sub>	$\sigma$	N <sub>6</sub> -C <sub>30</sub>	$\pi^*$	52.49	0.26	0.106
LP-C <sub>10</sub>	$\sigma$	C <sub>11</sub> -C <sub>13</sub>	$\pi^*$	48.29	0.16	0.101
LP-C <sub>18</sub>	$\pi$	O <sub>3</sub> -C <sub>26</sub>	$\pi^*$	78.19	0.12	0.104
LP-C <sub>18</sub>	$\pi$	C <sub>15</sub> -C <sub>16</sub>	$\pi^*$	30.44	0.32	0.105
N <sub>6</sub> -C <sub>30</sub>	$\pi^*$	C <sub>27</sub> -C <sub>28</sub>	$\pi^*$	113.08	0.03	0.079
N <sub>6</sub> -C <sub>30</sub>	$\pi^*$	C <sub>31</sub> -C <sub>32</sub>	$\pi^*$	100.04	0.03	0.083
C <sub>11</sub> -C <sub>13</sub>	$\pi^*$	C <sub>15</sub> -C <sub>16</sub>	$\pi^*$	28.64	0.16	0.111
C <sub>15</sub> -C <sub>16</sub>	$\pi^*$	C <sub>16</sub> -H <sub>17</sub>	$\sigma^*$	11.03	0.37	0.143



C <sub>15</sub> -C <sub>16</sub>	$\pi^*$	C <sub>18</sub> -C <sub>26</sub>	$\sigma^*$	0.51	0.26	0.025
C <sub>15</sub> -C <sub>16</sub>	$\pi^*$	C <sub>19</sub> -H <sub>20</sub>	$\sigma^*$	17.78	0.63	0.238
C <sub>15</sub> -C <sub>16</sub>	$\pi^*$	C <sub>36</sub> -H <sub>37</sub>	$\sigma^*$	5.95	0.24	0.086
C <sub>15</sub> -C <sub>16</sub>	$\pi^*$	C <sub>36</sub> -H <sub>38</sub>	$\sigma^*$	5.84	0.26	0.089
C <sub>15</sub> -C <sub>16</sub>	$\pi^*$	C <sub>36</sub> -H <sub>39</sub>	$\sigma^*$	30.04	5.18	0.890

**Table S12:** Natural bond orbital (NBO) analysis of **6d**

Donor(i)	Type	Acceptor(j)	Type	E (2) <sup>a</sup> [kJ/mol]	E(j)-E(i) <sup>b</sup> [a.u.]	F(i,j) <sup>c</sup> [a.u.]
N <sub>61</sub> -C <sub>35</sub>	$\pi$	C <sub>33</sub> -C <sub>34</sub>	$\pi^*$	29.69	0.32	0.090
N <sub>9</sub> -C <sub>39</sub>	$\sigma$	C <sub>39</sub> -H <sub>42</sub>	$\sigma^*$	24.55	6.07	0.345
C <sub>10</sub> -C <sub>11</sub>	$\pi$	O <sub>3</sub> -C <sub>29</sub>	$\pi^*$	26.96	0.25	0.076
C <sub>10</sub> -C <sub>11</sub>	$\pi$	C <sub>12</sub> -C <sub>14</sub>	$\pi^*$	13.38	0.29	0.057
C <sub>10</sub> -C <sub>11</sub>	$\pi$	C <sub>16</sub> -C <sub>17</sub>	$\pi^*$	17.65	0.36	0.073
C <sub>12</sub> -C <sub>14</sub>	$\pi$	C <sub>10</sub> -C <sub>11</sub>	$\pi^*$	23.77	0.27	0.074
C <sub>12</sub> -C <sub>14</sub>	$\pi$	C <sub>16</sub> -C <sub>17</sub>	$\pi^*$	13.80	0.36	0.063
C <sub>16</sub> -C <sub>17</sub>	$\pi$	C <sub>10</sub> -C <sub>11</sub>	$\pi^*$	15.57	0.27	0.060
C <sub>16</sub> -C <sub>17</sub>	$\pi$	C <sub>12</sub> -C <sub>14</sub>	$\pi^*$	21.01	0.29	0.070
C <sub>30</sub> -C <sub>31</sub>	$\pi$	O <sub>3</sub> -C <sub>29</sub>	$\pi^*$	14.37	0.27	0.058
C <sub>30</sub> -C <sub>31</sub>	$\pi$	N <sub>6</sub> -C <sub>35</sub>	$\pi^*$	30.65	0.27	0.082
C <sub>30</sub> -C <sub>31</sub>	$\pi$	C <sub>33</sub> -C <sub>34</sub>	$\pi^*$	15.82	0.27	0.059
C <sub>33</sub> -C <sub>34</sub>	$\pi$	O <sub>4</sub> -C <sub>37</sub>	$\pi^*$	23.48	0.29	0.076
C <sub>33</sub> -C <sub>34</sub>	$\pi$	N <sub>6</sub> -C <sub>35</sub>	$\pi^*$	12.18	0.28	0.053
C <sub>33</sub> -C <sub>34</sub>	$\pi$	C <sub>30</sub> -C <sub>31</sub>	$\pi^*$	25.04	0.30	0.079
C <sub>39</sub> -H <sub>40</sub>	$\sigma$	C <sub>39</sub> -H <sub>42</sub>	$\sigma^*$	17.37	5.85	0.285
C <sub>39</sub> -H <sub>42</sub>	$\sigma$	C <sub>19</sub> -H <sub>20</sub>	$\sigma^*$	15.60	1.18	0.121
C <sub>39</sub> -H <sub>42</sub>	$\sigma$	C <sub>21</sub> -H <sub>22</sub>	$\sigma^*$	20.74	1.31	0.147
C <sub>39</sub> -H <sub>42</sub>	$\sigma$	C <sub>39</sub> -H <sub>42</sub>	$\sigma^*$	51.83	5.84	0.491
LP-O <sub>1</sub>	$\pi$	C <sub>10</sub> -C <sub>11</sub>	$\pi^*$	37.59	0.33	0.106
LP-O <sub>3</sub>	$\pi$	C <sub>10</sub> -C <sub>29</sub>	$\sigma^*$	11.76	0.77	0.087

LP-O <sub>3</sub>	$\pi$	C <sub>29</sub> -C <sub>30</sub>	$\sigma^*$	17.05	0.75	0.103
LP-O <sub>4</sub>	$\pi$	N <sub>7</sub> -C <sub>37</sub>	$\sigma^*$	27.70	0.67	0.124
LP-O <sub>4</sub>	$\pi$	C <sub>33</sub> -C <sub>37</sub>	$\sigma^*$	17.97	0.71	0.103
LP-O <sub>5</sub>	$\pi$	N <sub>7</sub> -C <sub>38</sub>	$\sigma^*$	25.57	0.66	0.118
LP-O <sub>5</sub>	$\pi$	N <sub>9</sub> -C <sub>38</sub>	$\sigma^*$	26.12	0.66	0.119
LP-N <sub>6</sub>	$\sigma$	C <sub>30</sub> -C <sub>35</sub>	$\sigma^*$	8.79	0.89	0.08
LP-N <sub>6</sub>	$\sigma$	C <sub>33</sub> -C <sub>34</sub>	$\sigma^*$	10.04	0.89	0.086
LP-N <sub>7</sub>	$\sigma$	O <sub>4</sub> -C <sub>37</sub>	$\pi^*$	52.43	0.29	0.111
LP-N <sub>9</sub>	$\sigma$	C <sub>33</sub> -C <sub>34</sub>	$\pi^*$	47.08	0.27	0.103
LP-N <sub>9</sub>	$\sigma$	C <sub>39</sub> -C <sub>40</sub>	$\sigma^*$	5.06	0.77	0.062
O <sub>3</sub> -C <sub>29</sub>	$\pi$	C <sub>10</sub> -C <sub>11</sub>	$\pi^*$	99.51	0.02	0.072
O <sub>3</sub> -C <sub>29</sub>	$\pi$	C <sub>30</sub> -C <sub>31</sub>	$\pi^*$	76.04	0.01	0.056
N <sub>6</sub> -C <sub>35</sub>	$\pi$	C <sub>30</sub> -C <sub>31</sub>	$\pi^*$	145.81	0.02	0.084
C <sub>10</sub> -C <sub>11</sub>	$\pi$	C <sub>12</sub> -C <sub>14</sub>	$\pi^*$	170.92	0.02	0.083
C <sub>10</sub> -C <sub>11</sub>	$\pi$	C <sub>16</sub> -C <sub>17</sub>	$\pi^*$	31.26	0.09	0.077
C <sub>12</sub> -C <sub>14</sub>	$\pi$	C <sub>16</sub> -C <sub>17</sub>	$\pi^*$	34.29	0.07	0.080
C <sub>16</sub> -C <sub>17</sub>	$\pi$	C <sub>19</sub> -H <sub>20</sub>	$\sigma^*$	5.65	0.56	0.126
C <sub>16</sub> -C <sub>17</sub>	$\pi$	C <sub>21</sub> -H <sub>22</sub>	$\sigma^*$	5.79	0.69	0.145
C <sub>16</sub> -C <sub>17</sub>	$\pi$	C <sub>39</sub> -H <sub>42</sub>	$\sigma^*$	10.90	5.22	0.545
C <sub>33</sub> -C <sub>34</sub>	$\pi$	C <sub>30</sub> -C <sub>31</sub>	$\pi^*$	183.60	0.02	0.081

**Table S13:** TD-DFT analysis of FMOs

Com.	No	DFT $\lambda$ (nm)	E (cm <sup>-1</sup> )	<i>f</i>	MO contributions
<b>6a</b>	1	364.466438392	27437.3685657	0.1403	H→L (97%)
	2	342.545083609	29193.2375577	0.0017	H→L (99%)
	3	327.627812309	30522.4392566	0.013	H-4→L (27%), H-3→L (29%), H-2→L (15%), H-1→L (23%)
<b>6b</b>	4	364.466438392	27437.3685657	0.1403	H→L (97%)
	5	342.545083609	29193.2375577	0.0017	H→L +1(99%)
	6	327.627812309	30522.4392566	0.013	H-4→L (27%), H-3→L (29%), H-2→L (15%), H-

					1→L (23%)
<b>6c</b>	7	365.670362214	27347.0344697	0.1357	H→L (97%)
	8	342.990464237	29155.3294995	0.0018	H→L +1(99%)
	9	327.749062921	30511.1474946	0.0131	H-4→L (26%), H-3→L (33%), H-2→L (13%), H-1→L (22%)
<b>6d</b>	10	368.200614772	27159.1072877	0.1197	H→L (96%)
	11	350.277412737	28548.8005689	0.0021	H→L+1 (98%)
	12	327.394225012	30544.2162262	0.0196	H-4→L (20%), H-3→L (38%), H-1→L (28%), H-2→L (8%)

Com. = compound MO=molecular orbital, H=HOMO, L=LUMO,  $f$ = oscillator strength

**Table S13:** UV-Vis experimental data in different solvents of **6a-d**

Solvent	<b>6a</b>		<b>6c</b>	
	$\lambda_{\max}$	Absorbance	$\lambda_{\max}$	Absorbance
<b>1,4-dioxane</b>	300	2.5850	305	2.3565
<b>Acetone</b>	332	1.4814	332	1.5702
<b>DMSO</b>	305	2.3979	311	2.1135
Solvent	<b>6b</b>		<b>6d</b>	
	$\lambda_{\max}$	Absorbance	$\lambda_{\max}$	Absorbance
<b>1,4-dioxane</b>	373	2.0000	372	1.9281
<b>Acetone</b>	377	2.5086	365	1.8297
<b>DMSO</b>	300	1.8477	313	1.8827

**Table S15.** Dipole polarizability and major contributing tensor (au) of the studied **6a-d**

Polarizability	Compounds			
	<b>6a</b>	<b>6b</b>	<b>6c</b>	<b>6d</b>
$\alpha_{xx}$	346	331	355	355
$\alpha_{yy}$	230	213	241	263
$\alpha_{zz}$	137	126	156	166
$\alpha_{total}$	238	223	251	261

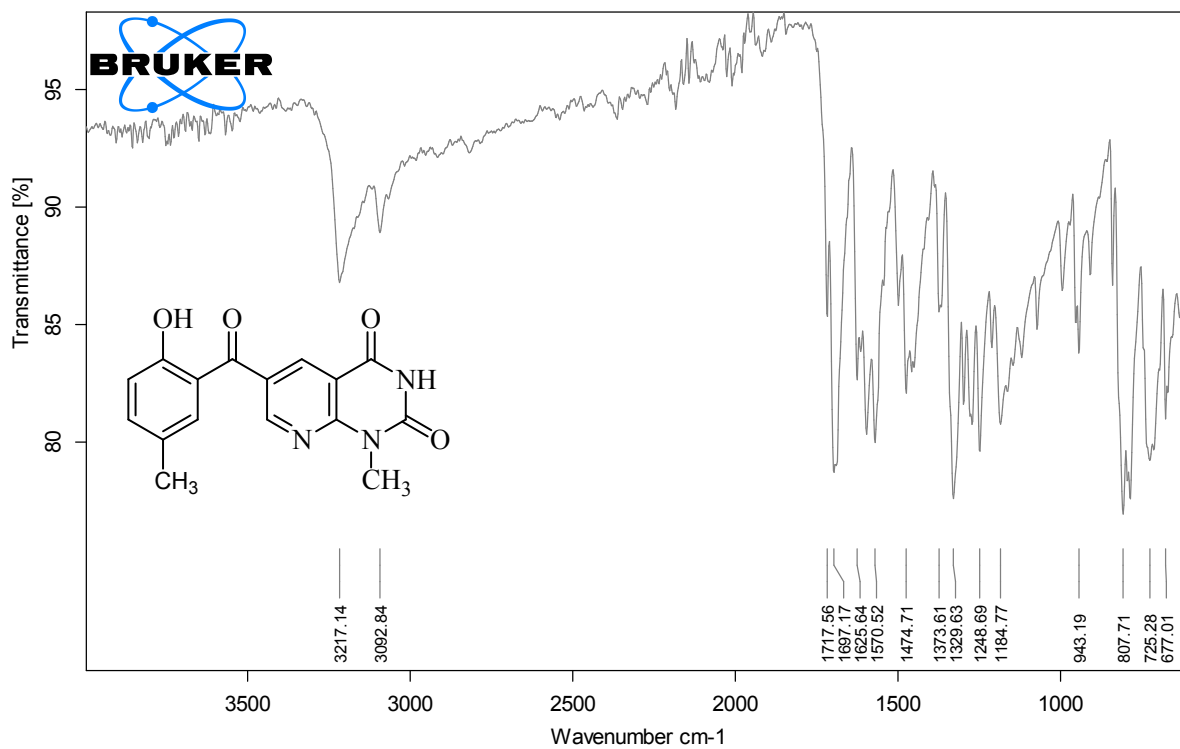
**Table S16:** Computed first hyperpolarizabilities ( $\beta_{tot}$ ) and major contributing tensor (au) of the studied **6a-d**

Polarizability	Compounds			
	<b>6a</b>	<b>6b</b>	<b>6c</b>	<b>6d</b>
$\beta_{xxx}$	836	1777	646	1180
$\beta_{xxy}$	-1070	-461	-1089	-801
$\beta_{xyy}$	-33	-372	144	-162
$\beta_{yyy}$	194	66	282	350
$\beta_{xxz}$	93	-207	253	-139
$\beta_{yyz}$	24	-66	33	-43
$\beta_{xzz}$	-14	-11	-27	2
$\beta_{yzz}$	55	-0.43	63	69
$\beta_{zzz}$	2	35	-1.35	66

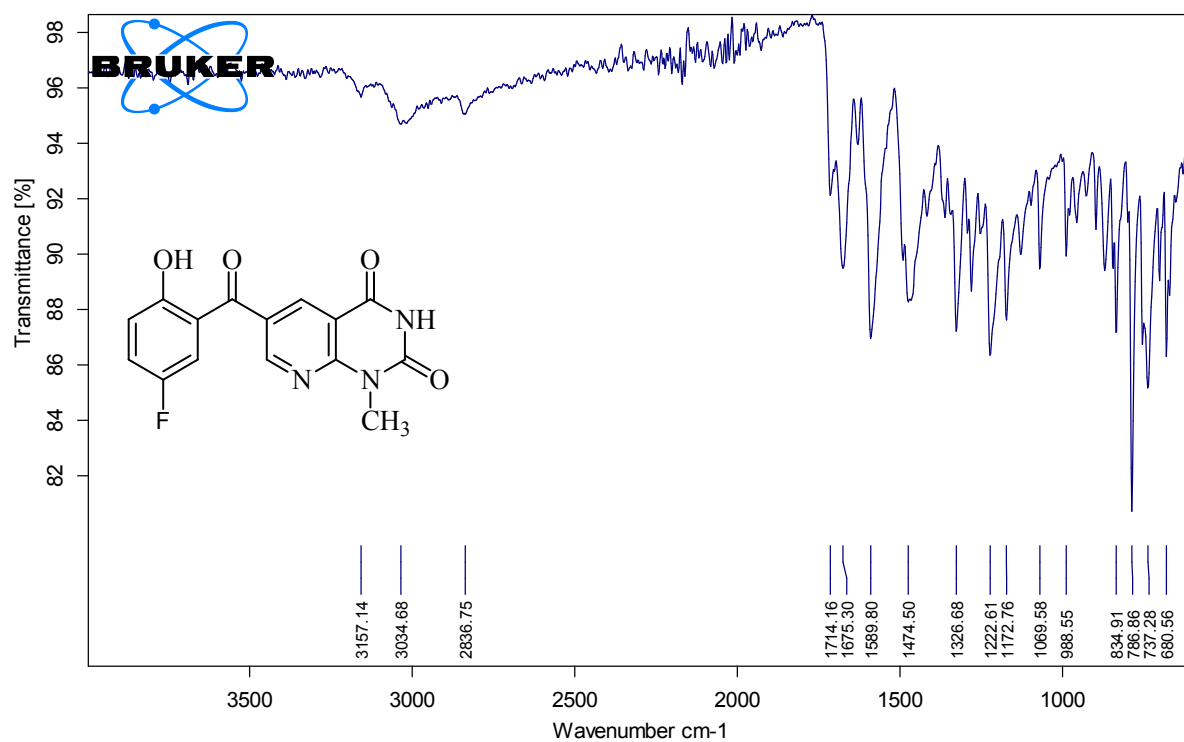
$\beta_{total}$	1144.868	1468.416	1103.055	1095.345
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**Table S17.** X-ray crystallographic data of **6a-d**

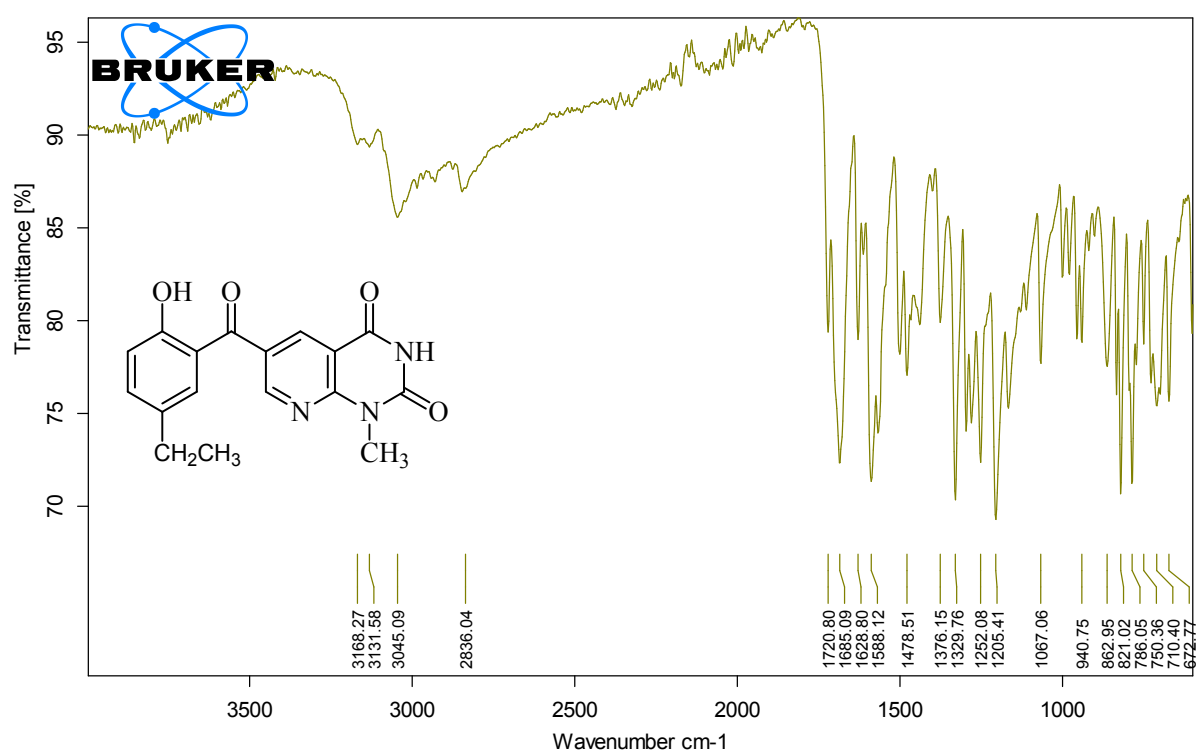
Crystal data	<b>6a</b>	<b>6b</b>	<b>6c</b>	<b>6d</b>
Diffractometer	Bruker Kappa APEXII CCD	Bruker Kappa APEXII CCD	Bruker Kappa APEXII CCD	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2005)	Multi-scan ( <i>SADABS</i> ; Bruker, 2005)	Multi-scan ( <i>SADABS</i> ; Bruker, 2005)	Multi-scan ( <i>SADABS</i> ; Bruker, 2005)
<b>Refinement</b>				
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained



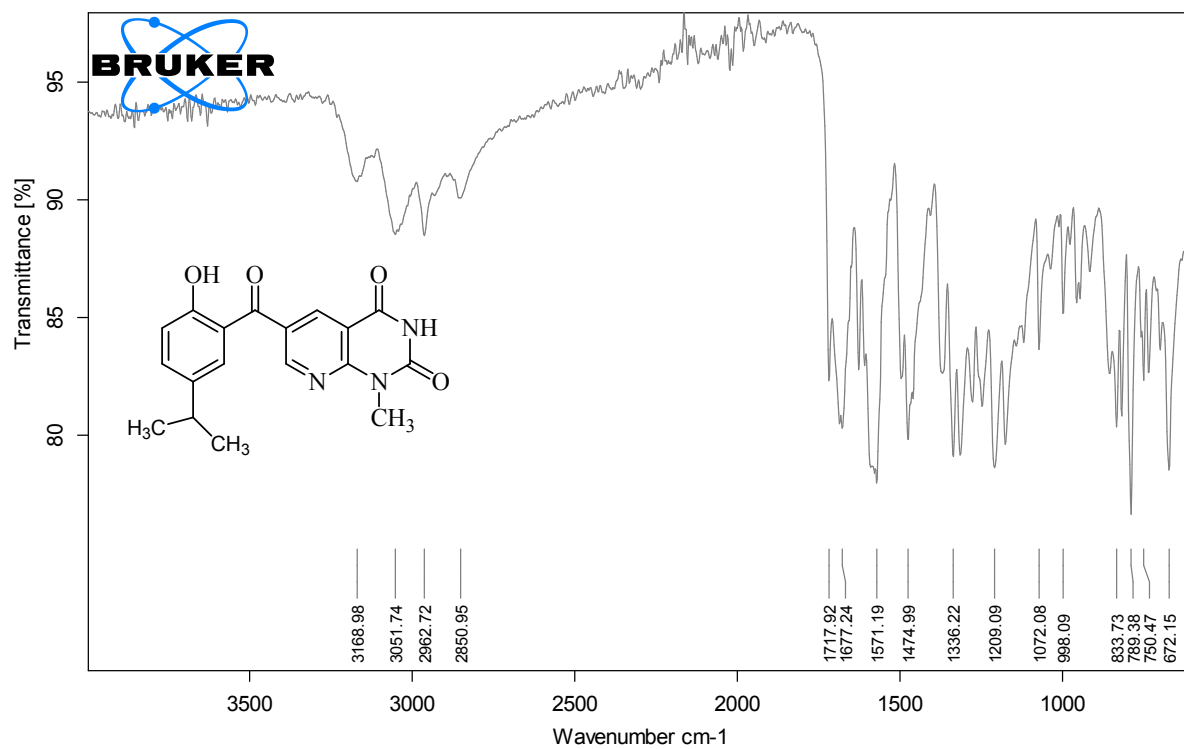
**Figure S1:** Experimental FT-IR spectrum of **6a**



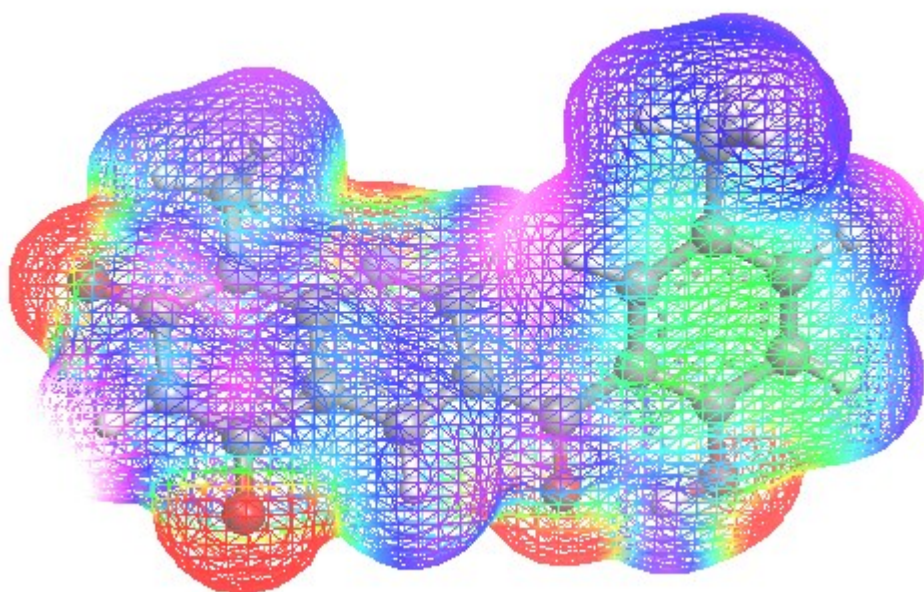
**Figure S2:** Experimental FT-IR spectrum of **6b**



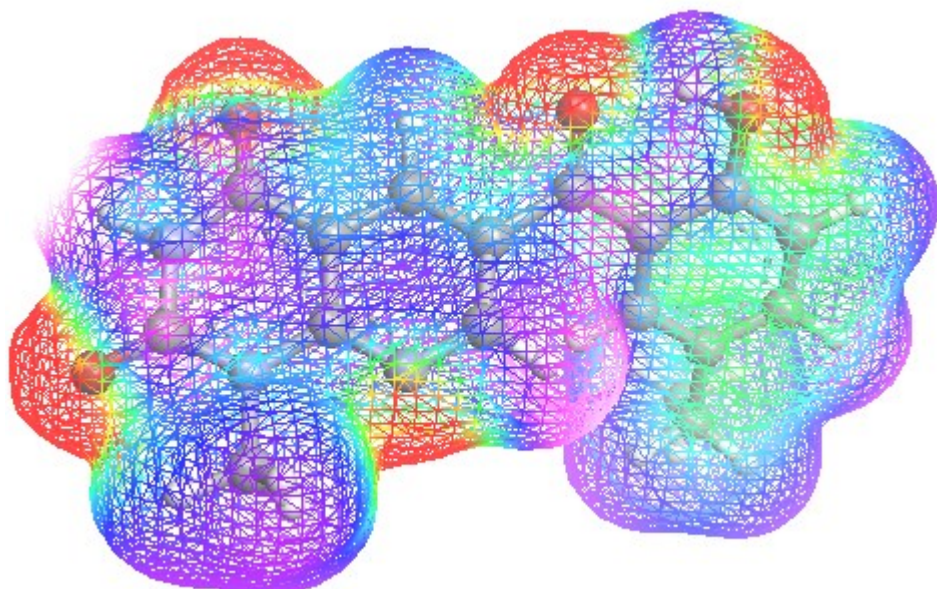
**Figure S3:** Experimental FT-IR spectrum of **6c**



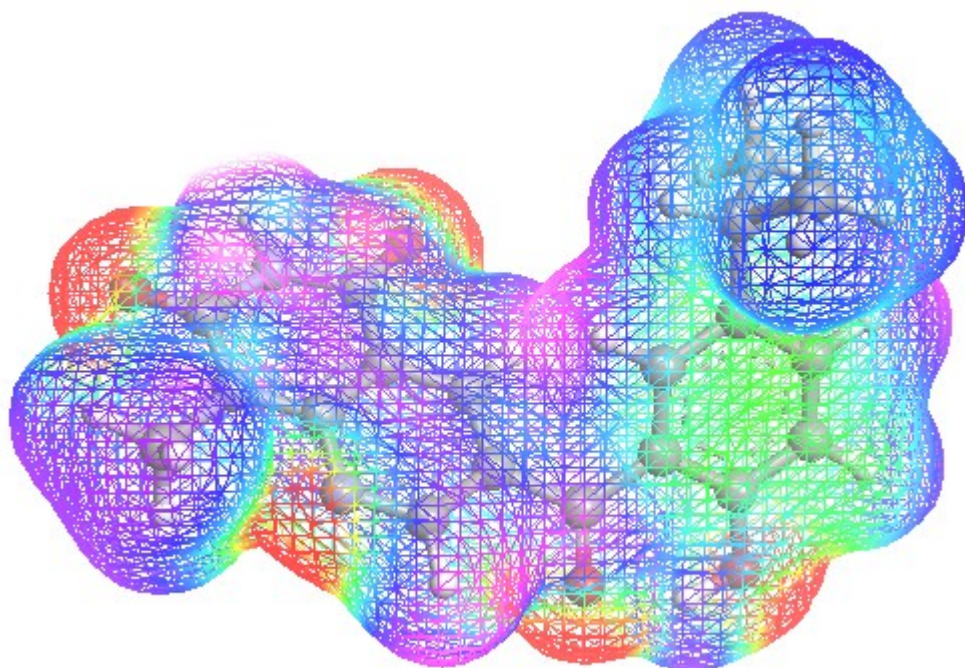
**Figure S4:** Experimental FT-IR spectrum of **6d**



**6a**



6c

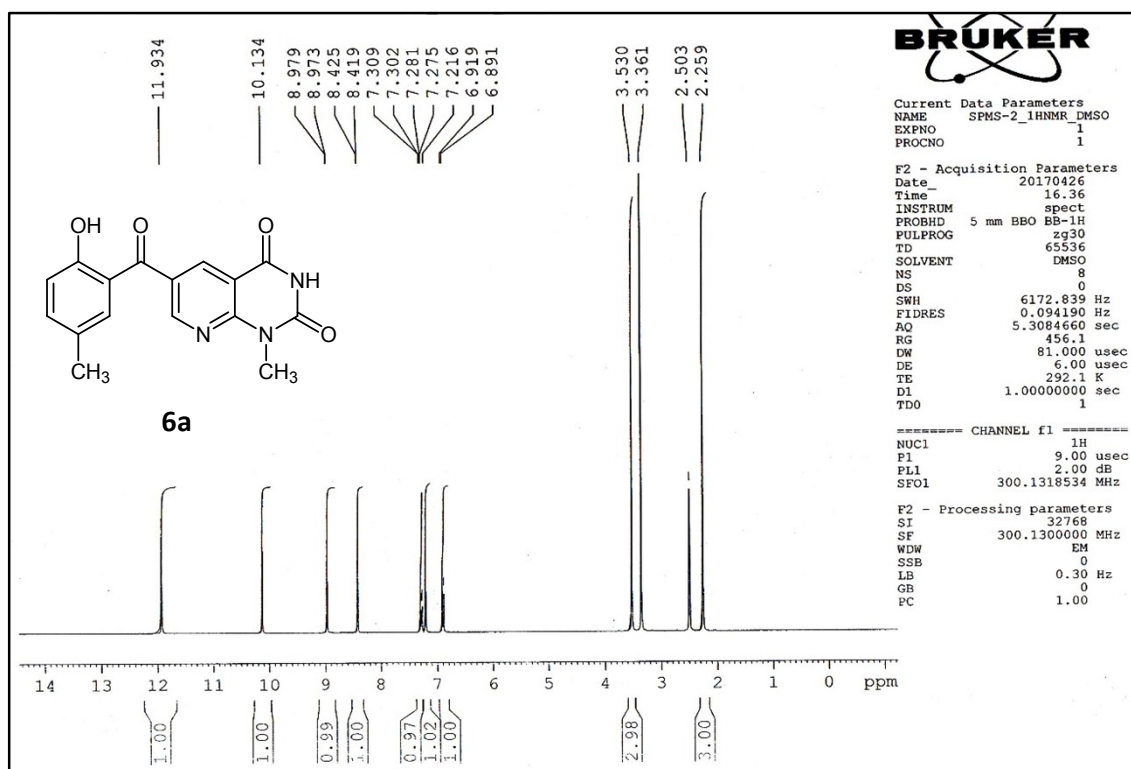


6d

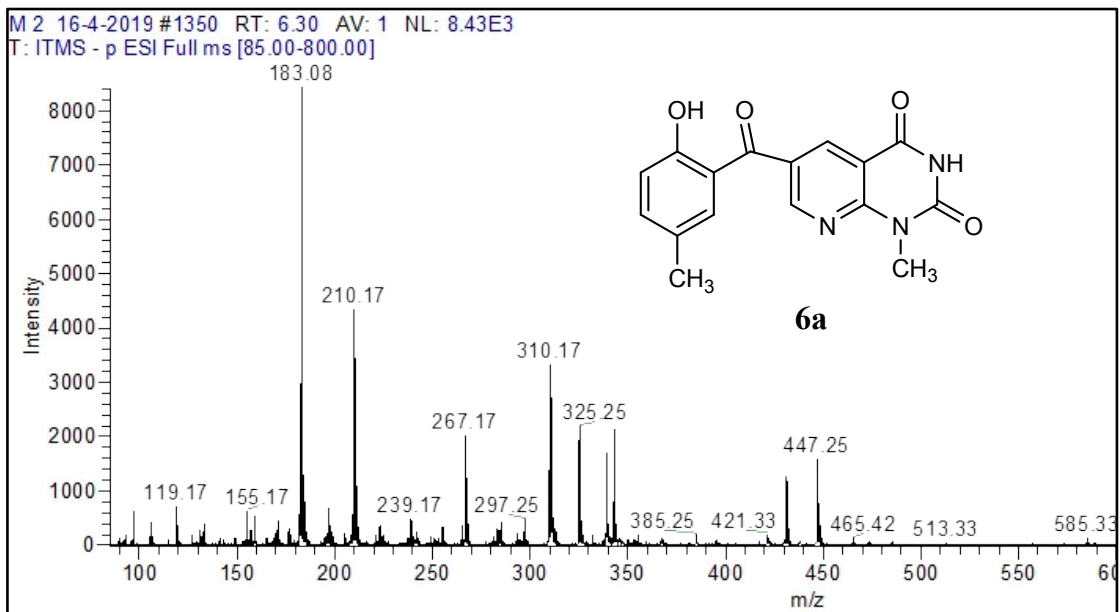
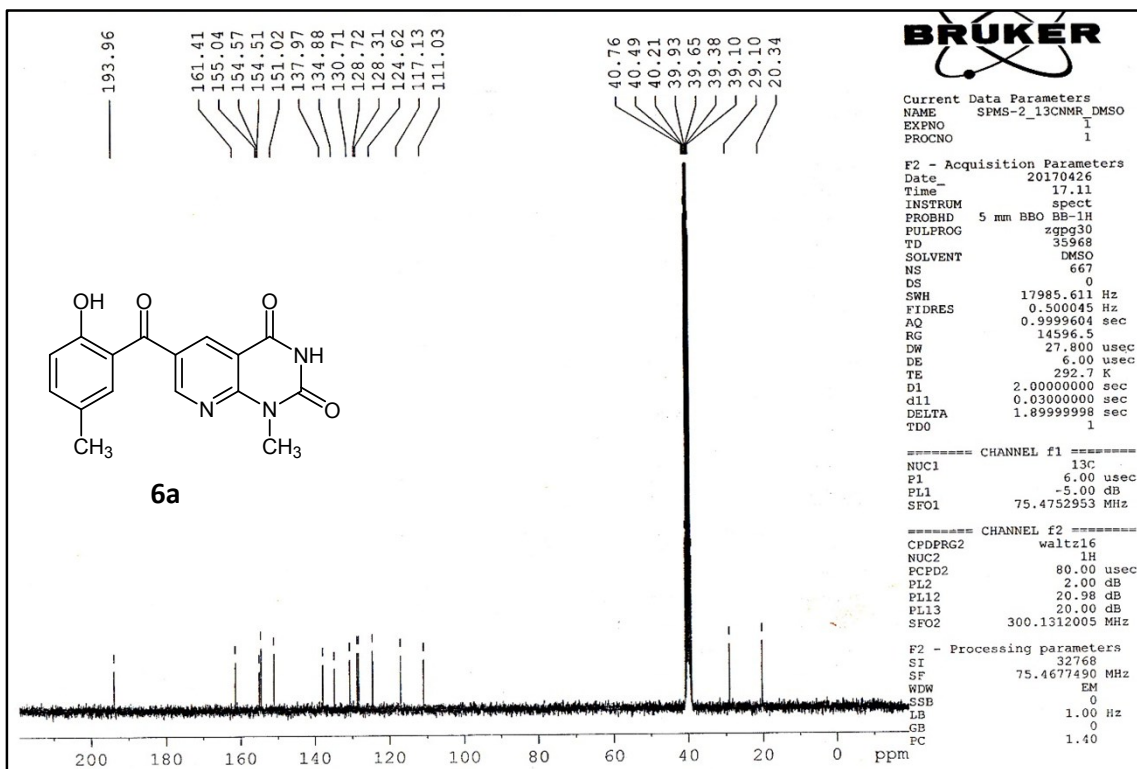


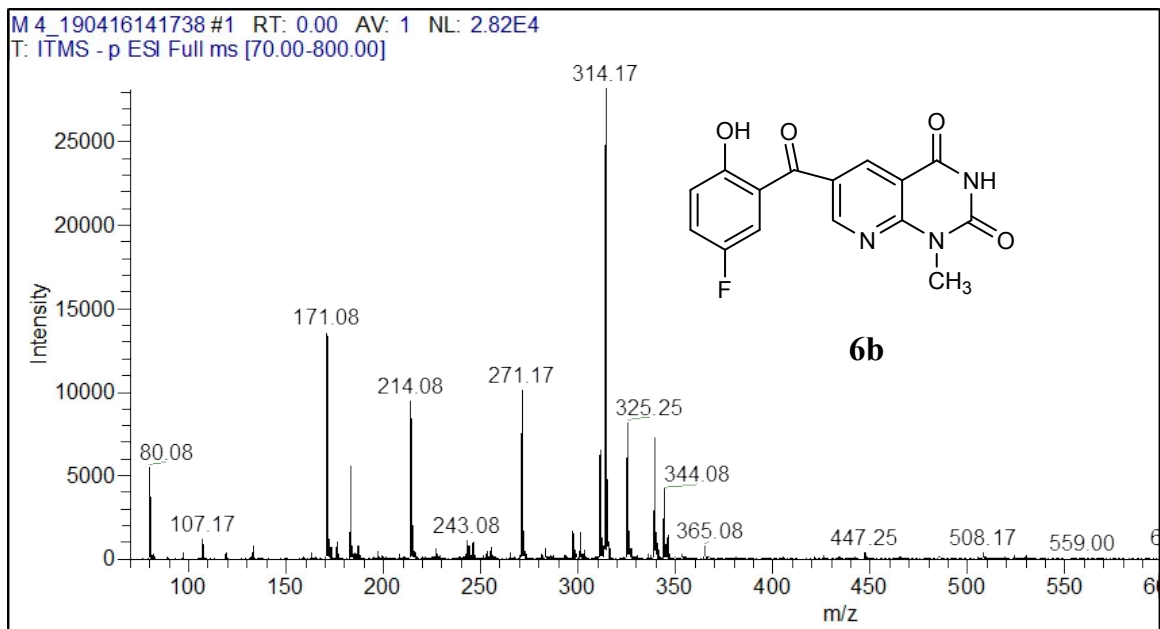
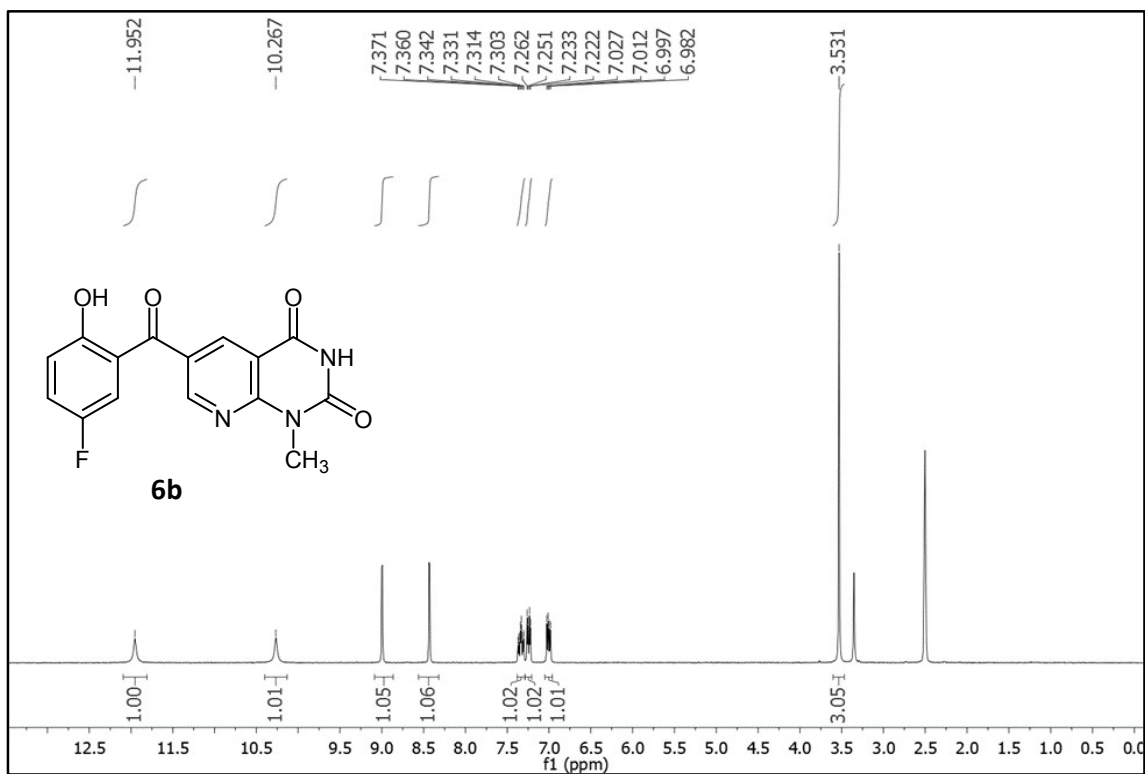


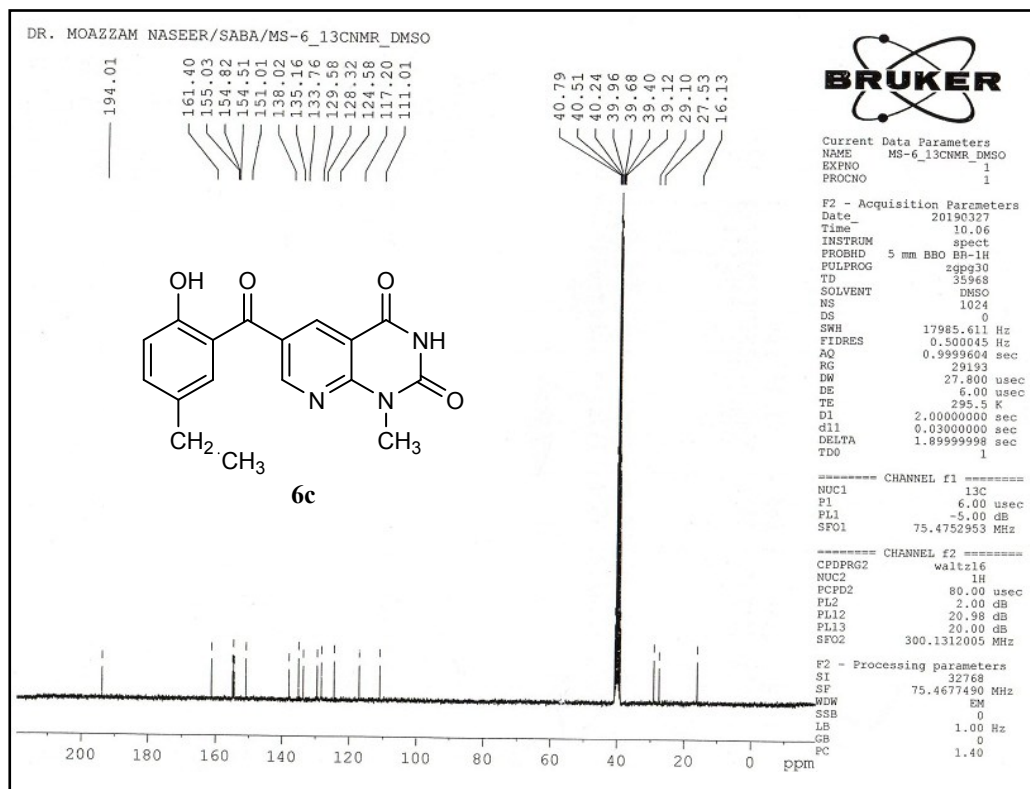
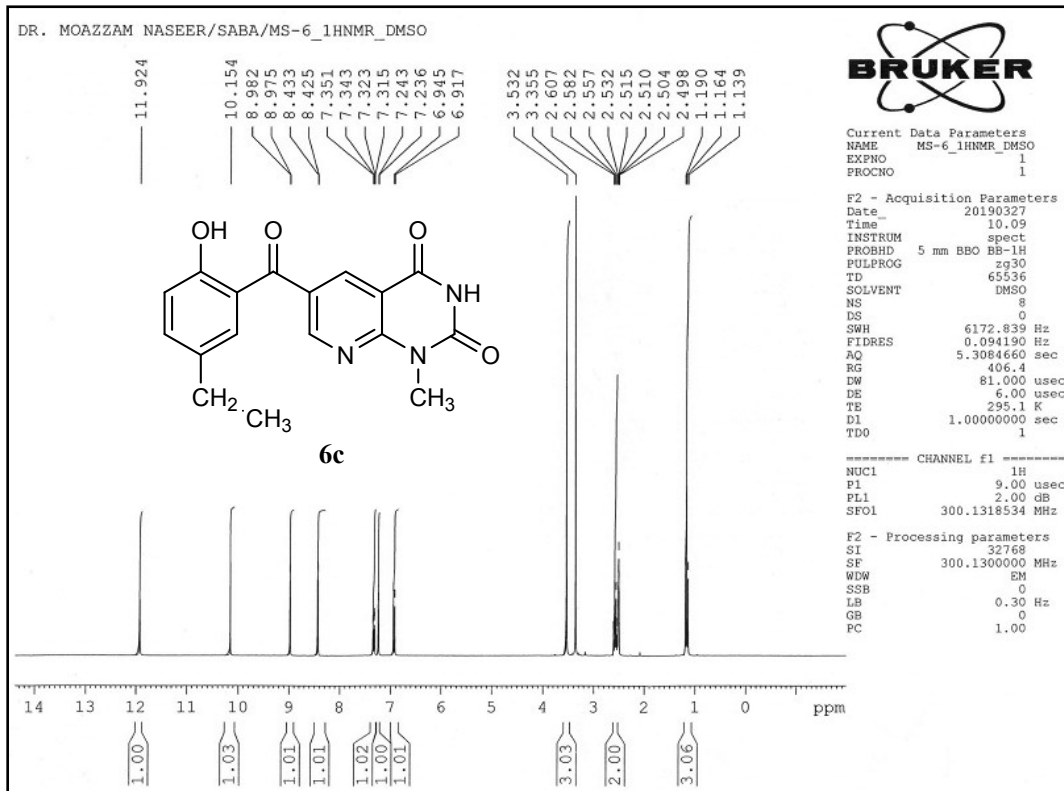
Figure S5: MEP surfaces of 6a-d



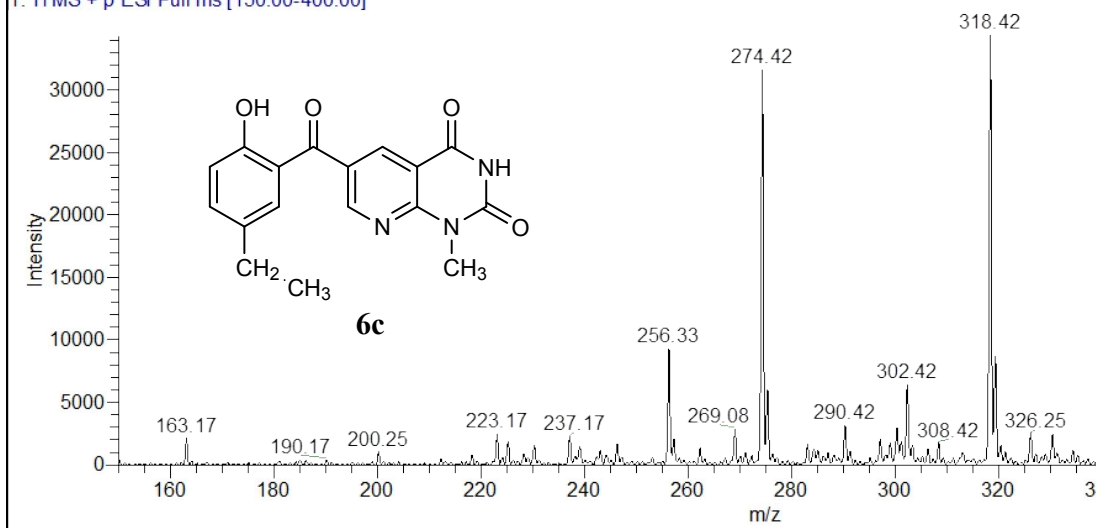




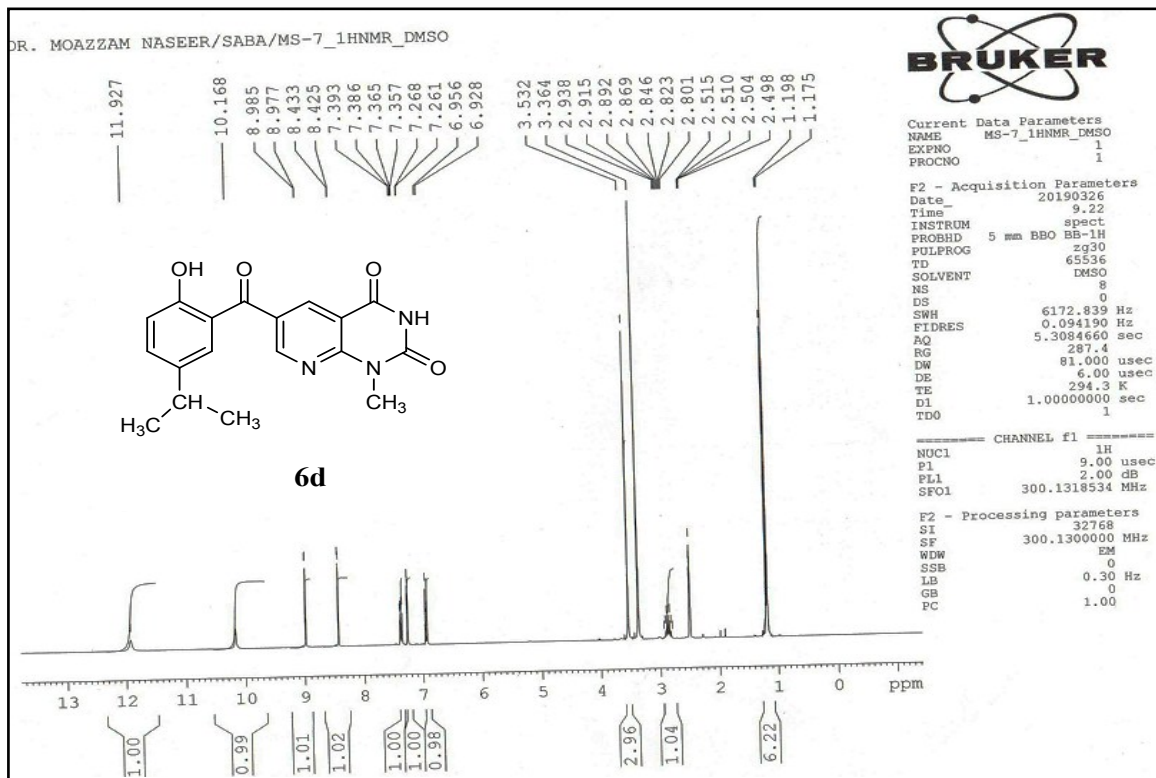




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DR. MOAZZAM NASEER/SABA/MS-7\_1HNMR\_DMSO



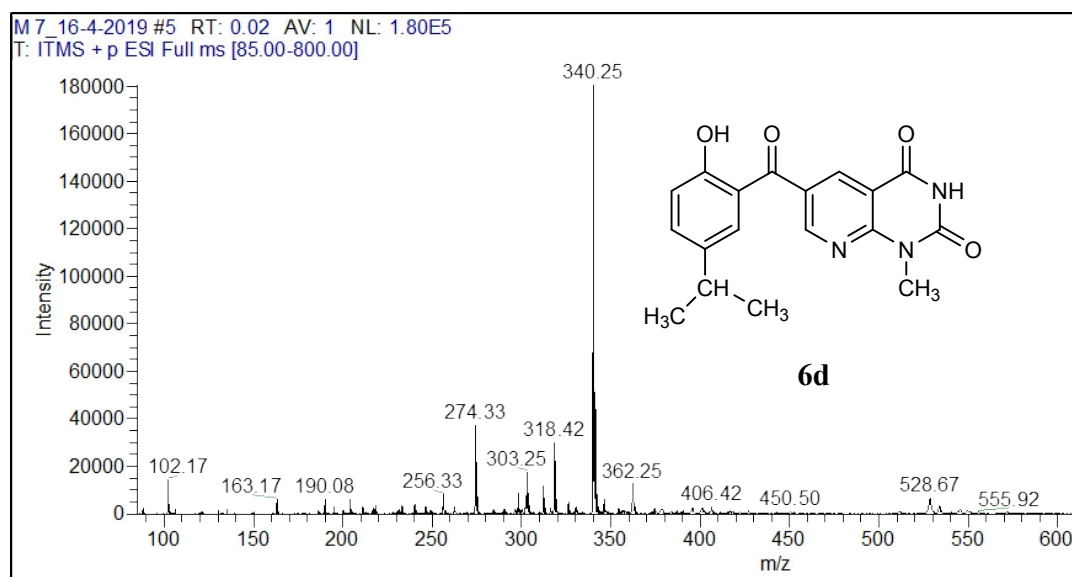
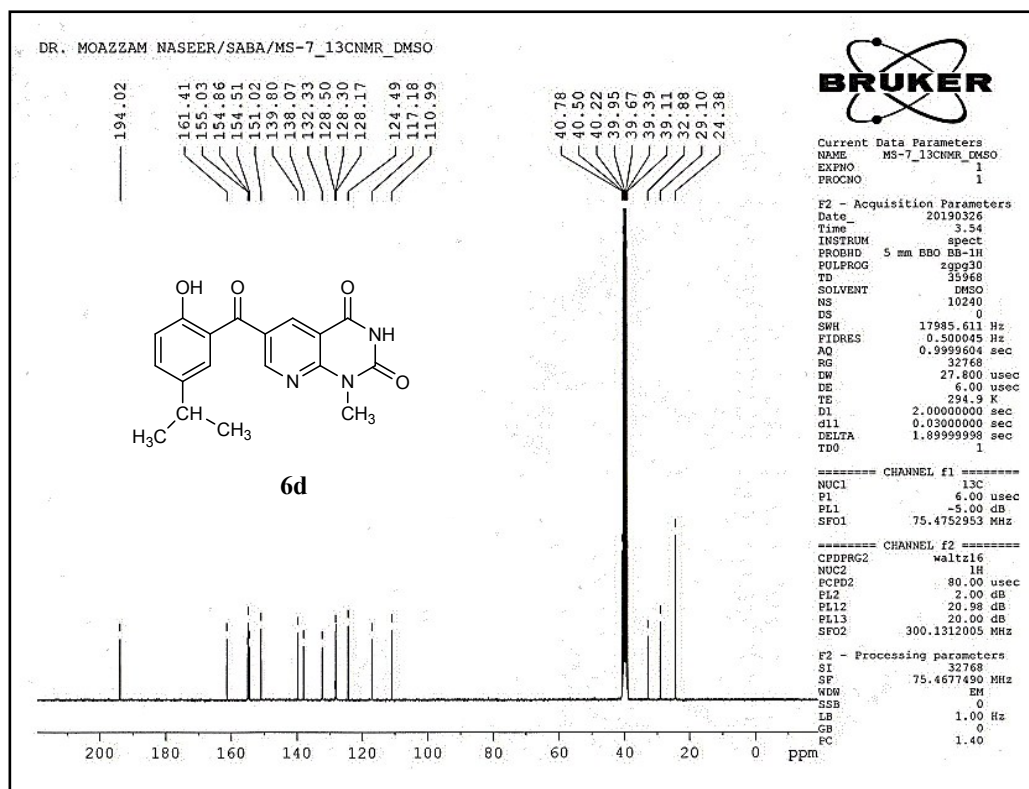


Figure S6: Spectroscopic spectra of 6a-d