SUPPLEMENTARY FILE INFORMATION

Table S1: Experimental and computed non-hydrogen atoms geometrical bond lengths of MK1

Atoms	Bond Length (Å)		Atoms	Bond Length (Å)	
	XRD	DFT		XRD	DFT
C1-O1	1.434(2)	1.4229	**C5-C4**	1.398(2)	1.3967
C23-O1	1.353(1)	1.3534	**C6-C5**	1.406(2)	1.4100
C24-O2	1.362(1)	1.3608	**C13-C5**	1.487(2)	1.4869
C2-O2	1.429(2)	1.4208	**C19-C6**	1.510(2)	1.5206
C19-O3	1.222(1)	1.2192	**C8-C7**	1.395(2)	1.4028
C2-N4	1.337(2)	1.3319	**C12-C7**	1.397(2)	1.4027
C6-N4	1.340(1)	1.3376	**C9-C8**	1.386(2)	1.3923
C3-C2	1.396(2)	1.4007	**C10-C9**	1.384(2)	1.3939
C4-C3	1.393(2)	1.3981	**C11-C10**	1.386(2)	1.3940
C7-C3	1.484(2)	1.4825	**C12-C11**	1.387(2)	1.3920
C15-C14	1.388(2)	1.3923	**C14-C13**	1.390(2)	1.4008
C16-C15	1.381(2)	1.3937	**C18-C13**	1.397(2)	1.4006
C17-C16	1.381(2)	1.3937	**C20-C19**	1.479(2)	1.4860
C18-C17	1.385(2)	1.3920	**C21-C20**	1.389(2)	1.3945
C22-C21	1.393(2)	1.3916	**C25-C20**	1.410(2)	1.4084
C23-C22	1.383(2)	1.3954			
C24-C23	1.418(2)	1.4184			
C25-C24	1.375(2)	1.3867			

Table S2: Experimental and computed non-hydrogen atoms geometrical bond angles of MK1

Atoms	Bond Angle (°)		Atoms	Bond Angle(°)	
	XRD	DFT		XRD	DFT
C1-O1-C23	116.9(1)	118.67	**C15-C16-C17**	119.6(1)	119.57
C24-O2-C26	117.0(1)	118.21	**C16-C17-C18**	120.2(1)	120.24
C2-N4-C6	117.9(1)	119.02	**C13-C18-C17**	120.6(1)	120.70
N4-C2-C3	124.3(1)	123.70	**O3-C19-C6**	119.1(1)	117.81
C2-C3-C4	116.6(1)	116.47	**O3-C19-C20**	122.3(1)	122.07
C2-C3-C7	120.7(1)	121.48	**C6-C19-C20**	118.56(9)	120.11
C4-C3-C7	122.6(1)	122.05	**C19-C20-C21**	122.1(1)	118.29
C3-C4-C5	120.9(1)	121.23	**C19-C20-C25**	118.2(1)	122.59
C4-C5-C6	116.9(1)	116.79	**C21-C20-C25**	119.7(1)	119.08
C4-C5-C13	120.3(1)	119.74	**C20-C21-C22**	120.2(1)	120.53
C6-C5-C13	122.8(1)	123.44	**C21-C22-C23**	120.2(1)	120.57
N4-C6-C5	123.4(1)	122.76	**O1-C23-C22**	124.7(1)	124.83
N4-C6-C19	114.82(9)	114.99	**O1-C23-C24**	115.3(1)	115.80
C5-C6-C19	121.74(9)	121.89	**C22-C23-C24**	120.0(1)	119.37
C3-C7-C8	121.0(1)	120.96	**O2-C24-C23**	114.7(1)	115.58
C3-C7-C12	120.9(1)	120.72	**O2-C24-C25**	125.7(1)	124.91
C7-C8-C9	121.1(1)	120.82	**C23-C24-C25**	119.6(1)	119.51
C8-C9-C10	120.1(1)	120.25	**C20-C25-C24**	120.3(1)	120.94
C9-C10-C11	119.5(1)	119.53			
C10-C11-C12	120.5(1)	120.23			
C7-C12-C11	120.6(1)	120.85			
C5-C13-C14	120.5(1)	120.31			
C5-C13-C18	120.7(1)	121.08			
C14-C13-C18	118.7(1)	118.29			
C13-C14-C15	120.3(1)	120.73			
C14-C15-C16	120.6(1)	120.19			

Table S3: Experimental and computed non-hydrogen atoms geometrical torsion angles of MK1

Atoms	Torsion Angles ()		Atoms	Torsion Angles ()	
	XRD	DFT		XRD	DFT
C1-O1-C23-C22	1.0(2)	-0.13	**C4-C5-C6-N4**	-1.0(2)	1.54
C1-O1-C23-C24	-178.0(1)	179.94	**C4-C5-C6-C19**	-177.3(1)	-171.27
C2-O2-C24-C23	-176.0(1)	178.60	**C13-C5-C6-N4**	-178.5(1)	-176.49
C2-O2-C24-C25	5.1(2)	-1.15	**C13-C5-C6-C19**	5.2(2)	10.70
C6-N4-C2-C3	0.3(2)	1.26	**C4-C5-C13-C14**	53.6(2)	51.41
C2-N4-C6-C5	1.3(2)	-2.31	**C4-C5-C13-C18**	-123.5(1)	-126.57
C2-N4-C6-C19	177.8(1)	170.95	**C6-C5-C13-C14**	-129.1(1)	-130.61
N4-C2-C3-C4	-2.1(2)	0.49	**C6-C5-C13-C18**	53.9(2)	51.41
N4-C2-C3-C7	175.2(1)	179.99	**N4-C6-C19-O3**	-120.3(1)	-120.52
C2-C3-C4-C5	2.3(2)	-1.24	**N4-C6-C19-C20**	58.3(1)	58.42
C7-C3-C4-C5	-175.0(1)	179.26	**C5-C6-C19-O3**	56.3(2)	52.82
C2-C3-C7-C8	28.9(2)	-39.38	**C5-C6-C19-C20**	-125.1(1)	-128.25
C2-C3-C7-C12	-150.1(1)	140.26	**C3-C7-C8-C9**	-178.1(1)	179.55
C4-C3-C7-C8	-154.0(1)	140.09	**C12-C7-C8-C9**	0.9(2)	-0.10
C4-C3-C7-C12	27.0(2)	-40.27	**C3-C7-C12-C11**	179.4(1)	-179.59
C3-C4-C5-C6	-0.8(2)	0.30	**C8-C7-C12-C11**	0.4(2)	0.07
C3-C4-C5-C13	176.6(1)	178.41	**C7-C8-C9-C10**	-1.5(2)	0.06
C5-C13-C14-C15	-177.5(1)	-178.65	**C8-C9-C10-C11**	0.9(2)	0.01
C18-C13-C14-C15	-0.4(2)	-0.36	**C9-C10-C11-C12**	0.3(2)	-0.05
C5-C13-C18-C17	177.2(1)	178.18	**C10-C11-C12-C7**	-1.0(2)	0.01
C14-C13-C18-C17	0.1(2)	0.15	**C23-C24-C25-C20**	0.7(2)	0.03
C13-C14-C15-C16	0.6(2)	0.34	**C19-C20-C21-C22**	178.0(1)	-177.99
C14-C15-C16-C17	-0.5(2)	-0.11	**C25-C20-C21-C22**	-0.8(2)	-0.16
C15-C16-C17-C18	0.1(2)	-0.10	**C19-C20-C25-C24**	-178.2(1)	177.78
C16-C17-C18-C13	0.0(2)	0.07	**C21-C20-C25-C24**	0.7(2)	0.04
O3-C19-C20-C21	-178.3(1)	2.88	**C20-C21-C22-C23**	-0.5(2)	0.19
O3-C19-C20-C25	0.5(2)	-174.87	**C21-C22-C23-O1**	-177.2(1)	179.95
C6-C19-C20-C21	3.1(2)	-176.01	**C21-C22-C23-C24**	1.8(2)	-0.24
C6-C19-C20-C25	-178.0(1)	6.23	**O1-C23-C24-O2**	-1.8(1)	0.17
O1-C23-C24-C25	177.2(1)	179.94			
C22-C23-C24-O2	179.1(1)	0.17			
C22-C23-C24-C25	-1.9(2)	0.00			
O2-C24-C25-C20	179.5(1)	179.77			

Table S4: Experimental and computed non-hydrogen atoms geometrical bond lengths of MK2

Atoms	Bond Length (Å)		Atoms	Bond Length (Å)	
	XRD	DFT		XRD	DFT
C24-Cl1	1.737(1)	1.7597	**C14-C13**	1.396(1)	1.4003
C22-Cl2	1.735(1)	1.7540	**C18-C13**	1.395(2)	1.4004
C1-O1	1.213(1)	1.2143	**C10-C9**	1.393(2)	1.3938
C2-N1	1.337(2)	1.3280	**C16-C15**	1.388(2)	1.3934
C6-N1	1.343(1)	1.3380	**C17-C16**	1.389(2)	1.3941
C6-C1	1.499(2)	1.5081	**C18-C17**	1.391(2)	1.3916
C19-C1	1.503(2)	1.5068	**C20-C19**	1.395(2)	1.4010
C11-C10	1.387(1)	1.3942	**C24-C19**	1.396(2)	1.3987
C3-C2	1.397(2)	1.4030	**C21-C20**	1.386(2)	1.3878
C4-C3	1.393(2)	1.3977	**C22-C21**	1.384(2)	1.3951
C7-C3	1.482(2)	1.4816	**C23-C22**	1.393(2)	1.3897
C12-C11	1.391(2)	1.3919	**C24-C23**	1.385(2)	1.3917
C5-C4	1.390(2)	1.3974			
C6-C5	1.405(2)	1.4095			
C13-C5	1.488(1)	1.4874			
C8-C7	1.401(1)	1.4029			
C12-C7	1.397(2)	1.4028			
C15-C14	1.395(2)	1.3927			
C9-C8	1.392(2)	1.3922			

Table S5: Experimental and computed non-hydrogen atoms geometrical bond angles of MK2

Atoms	Bond Angle (°)		Atoms	Bond Angle(°)	
	XRD	DFT		XRD	DFT
C2—N1—C6	117.69 (10)	119.13	**C24—C19—C1**	124.41 (10)	125.82
C18—C13—C14	119.43 (10)	118.76	**C8—C7—C3**	121.37 (10)	120.80
O1—C1—C6	120.42 (11)	120.89	**C21—C20—C19**	121.55 (11)	121.99
C18—C13—C5	119.71 (10)	120.99	**C9—C8—C7**	120.30 (11)	120.74
O1—C1—C19	119.84 (10)	119.77	**C24—C19—C1**	124.41 (10)	125.82
C14—C13—C5	120.81 (10)	120.19	**C8—C7—C3**	121.37 (10)	120.80
C6—C1—C19	119.36 (10)	119.01	**C21—C20—C19**	121.55 (11)	121.99
C15—C14—C13	120.26 (11)	120.64	**C9—C8—C7**	120.30 (11)	120.74
N1—C2—C3	123.66 (10)	123.44	**C22—C21—C20**	118.82 (11)	118.59
C16—C15—C14	119.85 (11)	120.14	**C8—C9—C10**	120.34 (11)	120.25
C4—C3—C2	117.25 (10)	116.59	**C21—C22—C23**	121.46 (11)	121.32
C4—C3—C7	121.90 (10)	122.01	**C11—C10—C9**	119.74 (11)	119.58
C2—C3—C7	120.80 (10)	121.39	**C21—C22—Cl2**	119.93 (9)	119.68
C15—C16—C17	120.17 (11)	119.63	**C23—C22—Cl2**	118.59 (9)	119
C5—C4—C3	120.83 (10)	121.34	**C24—C23—C22**	118.40 (11)	118.83
C16—C17—C18	120.08 (11)	120.25	**C10—C11—C12**	120.03 (11)	120.21
C4—C5—C6	116.72 (10)	116.43	**C23—C24—C19**	121.81 (11)	121.67
C4—C5—C13	120.37 (10)	119.34	**C11—C12—C7**	120.87 (10)	120.79
C6—C5—C13	122.85 (10)	124.17	**C23—C24—Cl1**	117.23 (9)	116.64
C17—C18—C13	120.21 (11)	120.57	**C19—C24—Cl1**	120.91 (9)	121.61
N1—C6—C5	123.72 (10)	123.04			
N1—C6—C1	113.73 (9)	113.57			
C5—C6—C1	122.09 (10)	123.06			
C20—C19—C24	117.94 (11)	117.55			
C12—C7—C8	118.69 (10)	118.43			
C20—C19—C1	117.61 (10)	116.59			
C12—C7—C3	119.92 (10)	120.77			

Table S6: Experimental and computed non-hydrogen atoms geometrical torsion angles of MK2

Atoms	Torsion Angles (°)		Atoms	Torsion Angles (°)	
	XRD	DFT		XRD	DFT
C6-N1-C2-C3	0.1(2)	0.93	**N1-C2 C3-C4**	-2.4(2)	0.19
C2-N1-C6-C1	-169.2(1)	171.96	**N1-C2-C3 C7**	175.2(1)	179.42
C2-N1-C6-C5	3.2(2)	-1.60	**C2-C3-C4-C5**	1.5(2)	-0.67
O1-C1-C6-N1	139.5(1)	-137.49	**C7-C3-C4-C5**	-176.0(1)	-179.90
O1-C1-C6-C5	-33.0(2)	36.07	**C2-C3-C7-C8**	40.3(2)	-39.75
C19-C1-C6-N1	-33.4(1)	35.88	**C2-C3-C7-C12**	-138.3(1)	140.19
C19-C1-C6-C5	154.0(1)	-150.55	**C4-C3-C7-C8**	-142.3(1)	139.44
O1-C1-C19-C20	-43.5(2)	38.96	**C4-C3-C7-C12**	39.1(2)	-40.62
O1-C1-C19-C24	134.5(1)	-138.51	**C3-C4-C5-C6**	1.4(2)	0.08
C6-C1-C19-C20	129.5(1)	-134.50	**C3-C4-C5-C13**	-175.9(1)	177.47
C6-C1-C19-C24	-52.6(2)	48.04	**C7-C8-C9-C10**	1.3(2)	-0.08
C4-C5-C6-N1	-3.9(2)	1.10	**C8-C9-C10-C11**	-1.3(2)	0.06
C4-C5-C6-C1	167.9(1)	-171.86	**C9-C10-C11-C12**	-0.2(2)	0.01
C13-C5-C6-N1	173.3(1)	-173.15	**C10-C11-C12-C7**	1.7(2)	-0.06
C13-C5-C6-C1	-14.9(2)	10.89	**C5-C13-C14-C15**	177.8(1)	-177.98
C4-C5-C13-C14	-61.5(2)	54.22	**C18-C13-C14-C15**	0.5(2)	-0.62
C4-C5-C3-C18	115.7(1)	-123.08	**C5-C13-C18-C17**	-177.4(1)	177.62
C6-C5-C13-C14	121.3(1)	-128.61	**C14-C13-C18-C17**	-0.1(2)	0.28
C6-C5-C13-C18	-61.4(2)	54.09	**C13-C14-C15-C16**	-0.8(2)	0.51
C3-C7-C8-C9	-178.4(1)	179.97	**C14-C15-C16-C17**	0.5(2)	-0.07
C12-C7-C8-C9	0.2(2)	0.03	**C15-C16-C17-C18**	-0.1(2)	-0.27
C3-C7-C12-C11	176.9(1)	-179.89	**C16-C17-C18-C13**	-0.1(2)	0.15
C8-C7-C12-C11	-1.7(2)	0.04	**C1-C19-C20-C21**	179.2(1)	-179.94
C24-C19-C20-C21	1.1(2)	-2.26			
C1-C19-C24 Cl1	-0.6(2)	178.84			
C1-C19-C24-C23	-178.0(1)	2.11			
C20-C19-C24-Cl1	177.36(9)	-175.34			
C22-C23-C24-Cl1	-178.70(9)	177.24			
C22-C23-C24-C19	-1.2(2)	0.35			
C20-C21 C22-Cl2	-179.3(1)	179.87			
C20-C21-C22-C23	-0.4(2)	0.52			
Cl2-C22 C23 C24	-179.67(9)	179.30			
C21-C22-C23-C24	1.4(2)	-1.35			
C20-C19-C24-C23	-0.0(2)	1.40			
C19-C20-C21-C22	-0.9(2)	1.33			

Table S7: Experimental and computed non-hydrogen atoms geometrical bond lengths of MK3

Atoms	Bond Length (Å)		Atoms	Bond Length (Å)	
	XRD	DFT		XRD	DFT
C13-S1	1.710(2)	1.724	**C19-C20**	1.380(4)	1.392
C16-S1	1.670(3)	1.754	**C1-C2**	1.380(5)	1.393
C7-C4	1.485(3)	1.489	**C19-C18**	1.376(4)	1.403
C5-C4	1.397(3)	1.420	**C16-C15**	1.354(5)	1.371
C3-C4	1.388(3)	1.399			
C12-O1	1.229(2)	1.220			
C11-N1	1.339(3)	1.387			
C10-N1	1.334(4)	1.328			
C11-C7	1.400(3)	1.412			
C8-C7	1.393(3)	1.397			
C12-C11	1.509(3)	1.510			
C9-C8	1.394(3)	1.398			
C6-C5	1.378(4)	1.391			
C13-C12	1.445(3)	1.479			
C14-C13	1.437(3)	1.387			
C10-C9	1.399(3)	1.402			
C17-C9	1.479(3)	1.482			
C22-C17	1.384(3)	1.403			
C18-C17	1.397(3)	1.403			
C2-C3	1.387(3)	1.393			
C21-C22	1.392(4)	1.392			
C1-C6	1.371(4)	1.394			
C20-C21	1.361(4)	1.394			
C15-C14	1.430(5)	1.414			

Table S8: Experimental and computed non-hydrogen atoms geometrical bond angles of MK3

Atoms	Bond Angle (°)		Atoms	Bond Angle(°)	
	XRD	DFT		XRD	DFT
C13-S1-C16	92.3(1)	91.33	**C4-C3-C2**	120.5(2)	120.61
C7-C4-C5	120.3(2)	120.79	**C17-C22-C21**	120.5(2)	120.75
C7-C4-C3	121.4(2)	120.32	**C5-C6-C1**	120.1(3)	120.23
C5-C4-C3	118.2(2)	118.78	**C22-C21-C20**	120.9(3)	120.24
C11-N1-C10	117.4(2)	119.80	**C13-C14-C15**	107.8(2)	113.64
C4-C7-C11	121.8(2)	124.61	**C21-C20-C19**	119.4(3)	120.21
C4-C7-C8	121.3(2)	120.59	**C3-C2-C1**	120.2(3)	120.16
C11-C7-C8	116.9(2)	116.59	**C6-C1-C2**	120.0(3)	119.60
N1-C11-C7	123.8(2)	122.32	**C17-C18-C19**	121.1(3)	120.79
N1-C11-C12	114.9(2)	115.04	**C14-C15-C16**	114.6(3)	112.15
C7-C11-C12	121.0(2)	122.47	**S1-C16-C15**	113.1(2)	112.45
C7-C8-C9	120.9(2)	121.52	**C20-C19-C18**	120.3(3)	120.21
C4-C5-C6	121.0(2)	120.59			
O1-C12-C11	118.4(2)	119.92			
O1-C12-C13	122.6(2)	120.04			
C11-C12-C13	119.0(2)	120.02			
S1-C13-C12	119.4(2)	127.07			
S1-C13-C14	112.2(2)	110.39			
C12-C13-C14	128.4(2)	122.45			
C8-C9-C10	116.4(2)	116.42			
C8-C9-C17	122.7(2)	122.07			
C10-C9-C17	120.9(2)	121.49			
N1-C10-C9	124.5(2)	123.25			
C9-C17-C22	121.1(2)	120.88			
C9-C17-C18	121.1(2)	120.69			
C22-C17-C18	117.8(2)	118.42			

Table S9: Experimental and computed non-hydrogen atoms geometrical torsion angles of MK3

Atoms	Torsion Angles (°)		Atoms	Torsion Angles (°)	
	XRD	DFT		XRD	DFT
C16-S1-C13-C12	178.2(2)	176.25	**C7-C11-C12-C13**	125.1(2)	-152.90
C16-S1-C13-C14	0.4(2)	-0.72	**C7-C8-C9-C10**	0.5(3)	-1.23
C13-S1-C16-C15	-0.7(3)	0.84	**C7-C8-C9-C17**	179.6(2)	179.63
C5-C4-C7-C11	-51.1(3)	58.14	**C4-C5-C6-C1**	-0.4(4)	0.18
C5-C4-C7-C8	127.6(2)	-118.67	**O1-C12-C13-S1**	-3.4(3)	176.26
C3-C4-C7-C11	128.8(2)	-125.46	**O1-C12-C13-C14**	174.0(2)	-7.09
C3-C4-C7-C8	-52.5(3)	57.71	**C11-C12-C13-S1**	175.4(2)	-3.31
C7-C4-C5-C6	179.9(2)	176.80	**C11-C12-C13-C14**	-7.2(3)	173.31
C3-C4-C5-C6	-0.0(3)	0.36	**S1-C13-C14-C15**	-0.1(3)	0.44
C7-C4-C3-C2	-179.3(2)	-177.25	**C12-C13-C14-C15**	-177.7(2)	-176.69
C5-C4-C3-C2	0.6(3)	-0.79	**C8-C9-C10-N1**	-2.0(3)	1.50
C10-N1-C11-C7	2.2(3)	-2.52	**C17-C9-C10-N1**	178.9(2)	-179.36
C10-N1-C11-C12	-171.4(2)	173.12	**C8-C9-C17-C22**	149.5(2)	139.48
C11-N1-C10-C9	0.7(4)	0.33	**C8-C9-C17-C18**	-31.8(3)	-40.75
C4-C7-C11-N1	175.3(2)	-174.20	**C10-C9-C17-C22**	-31.4(3)	-39.68
C4-C7-C11-C12	-11.5(3)	10.47	**C10-C9-C17-C18**	147.3(2)	140.15
C8-C7-C11-N1	-3.5(3)	2.68	**C9-C17-C22-C21**	178.9(2)	179.81
C8-C7-C11-C12	169.7(2)	-172.64	**C18-C17-C22-C21**	0.2(4)	0.009
C4-C7-C8-C9	-176.8(2)	176.35	**C9-C17-C18-C19**	-179.3(2)	-179.73
C11-C7-C8-C9	2.0(3)	-0.72	**C22-C17-C18-C19**	-0.6(4)	0.07
N1-C11-C12-O1	117.8(2)	-147.91	**C4-C3-C2-C1**	-0.9(4)	0.67
N1-C11-C12-C13	-61.1(3)	31.67	**C17-C22-C21-C20**	0.6(4)	-0.08
C7-C11-C12-O1	-56.0(3)	27.72	**C5-C6-C1-C2**	0.1(4)	-0.30
C22-C21-C20-C19	-0.9(4)	0.07			
C13-C14-C15-C16	-0.4(4)	0.17			
C21-C20-C19-C18	0.4(4)	-0.07			
C3-C2-C1-C6	0.5(4)	-0.12			
C17-C18-C19-C20	0.3(4)	-0.07			
C14-C15-C16-S1	0.7(4)	-0.73			

Table S10: Experimental and computed non-hydrogen atoms geometrical bond lengths of MK4

Atoms	Bond Length (Å)		Atoms	Bond Length (Å)	
	XRD	DFT		XRD	DFT
C18-O1	1.219(2)	1.218	**C22-C23**	1.409(2)	1.419
C9-N1	1.341(2)	1.337	**C28-C23**	1.428(2)	1.419
C8-N1	1.338(2)	1.330	**C26-C25**	1.378(2)	1.376
C12-C10	1.489(2)	1.487	**C21-C20**	1.412(2)	1.372
C9-C10	1.401(2)	1.410	**C1-C2**	1.391(2)	1.392
C11-C10	1.397(1)	1.397	**C15-C16**	1.384(2)	1.394
C13-C12	1.393(2)	1.400	**C5-C4**	1.387(2)	1.392
C17-C12	1.403(2)	1.401	**C15-C14**	1.385(2)	1.394
C24-C19	1.446(2)	1.440	**C6-C1**	1.370(2)	1.394
C18-C19	1.495(2)	1.493	**C5-C6**	1.377(2)	1.394
C20-C19	1.382(2)	1.385	**C27-C26**	1.404(2)	1.412
C23-C24	1.435(2)	1.435	**C21-C22**	1.362(2)	1.372
C25-C24	1.418(2)	1.421	**C27-C28**	1.357(2)	1.373
C18-C9	1.522(2)	1.493			
C7-C11	1.390(2)	1.398			
C3-C7	1.487(2)	1.482			
C8-C7	1.392(2)	1.402			
C2-C3	1.387(2)	1.403			
C4-C3	1.390(2)	1.403			
C14-C13	1.387(2)	1.392			
C16-C17	1.385(2)	1.392			

Table S11: Experimental and computed non-hydrogen atoms geometrical bond angles of MK4

Atoms	Bond Angle (°)		Atoms	Bond Angle(°)	
	XRD	DFT		XRD	DFT
C9-N1-C8	117.7(1)	119.07	**C12-C13-C14**	120.2(1)	120.70
C12-C10-C9	123.8(1)	123.75	**C12-C17-C16**	120.3(1)	120.72
C12-C10-C11	119.4(1)	119.51	**C24-C23-C22**	120.5(1)	119.80
C9-C10-C11	116.7(1)	116.68	**C24-C23-C28**	119.0(1)	119.06
C10-C12-C13	120.9(1)	121.20	**C22-C23-C28**	120.5(1)	120.53
C10-C12-C7	120.1(1)	121.25	**C24-C25-C26**	120.9(1)	120.93
C13-C12-C17	119.0(1)	118.58	**N1-C8-C7**	124.5(1)	123.61
C24-C19-C18	123.0(1)	122.49	**C19-C20-C21**	122.5(1)	121.89
C24-C19-C20	118.9(1)	119.48	**C3-C2-C1**	120.7(1)	120.79
C18-C19-C20	118.0(1)	117.95	**C17-C16-C15**	120.2(1)	120.17
C19-C24-C23	117.7(1)	118.14	**C3-C4-C5**	121.1(1)	120.83
C19-C24-C25	124.4(1)	124.02	**C13-C14-C15**	120.4(1)	120.22
C23-C24-C25	117.9(1)	117.80	**C2-C1-C6**	120.7(1)	120.25
N1-C9-C10	123.4(1)	122.83	**C16-C15-C14**	119.9(1)	119.58
N1-C9-C18	114.0(1)	114.52	**C1-C6-C5**	119.4(1)	119.55
C10-C9-C18	122.4(1)	122.21	**C25-C26-C27**	121.0(1)	121.04
C10-C11-C7	121.3(1)	121.25	**C23-C22-C21**	121.0(1)	120.93
C11-C7-C3	122.5(1)	122.03	**C23-C28-C27**	121.2(1)	120.89
C11-C7-C8	116.3(1)	116.50	**C4-C5-C6**	120.3(1)	120.21
C3-C7-C8	121.1(1)	121.46	**C20-C21-C22**	119.4(1)	119.70
O1-C18-C19	124.7(1)	123.55	**C26-C27-C28**	120.0(1)	119.64
O1-C18-C9	117.2(1)	117.86			
C19-C18-C9	118.1(1)	118.56			
C7-C3-C2	121.8(1)	120.90			
C7-C3-C4	120.3(1)	120.74			
C2-C3-C4	117.9(1)	118.35			

Table S12: Experimental and computed non-hydrogen atoms geometrical torsion angles of MK4

Atoms	Torsion Angles (°)		Atoms	Torsion Angles (°)	
	XRD	DFT		XRD	DFT
C8-N1-C9-C10	1.2(2)	-1.82	**N1-C9-C18-C19**	67.3(1)	53.03
C8-N1-C9-C18	176.2(1)	170.83	**C10-C9-C18-O1**	64.0(2)	47.15
C9-N1-C8-C7	1.3(2)	1.21	**C10-C9-C18-C19**	-117.6(1)	-134.26
C9-C10-C12-C13	53.7(2)	51.91	**C10-C11-C7-C3**	-173.4(1)	179.45
C9-C10-C12-C17	-129.9(1)	-130.32	**C10-C11-C7-C8**	2.4(2)	-1.06
C11-C10-C12-C13	-123.6(1)	-125.85	**C11-C7-C3-C2**	-152.5(1)	139.98
C11-C10-C12-C17	52.8(2)	51.90	**C11-C7-C3-C4**	30.4(2)	-40.24
C12-C10-C9-N1	-179.1(1)	-176.86	**C8-C7-C3-C2**	31.9(2)	-39.47
C12-C10-C9-C18	6.3(2)	11.04	**C8-C7-C3-C4**	-145.2(1)	140.30
C11-C10-C9-N1	-1.7(2)	0.96	**C11-C7-C8-N1**	-3.0(2)	0.204
C11-C10-C9-C18	-176.3(1)	-171.12	**C3-C7-C8-N1**	172.8(1)	179.68
C12-C10-C11-C7	177.3(1)	178.44	**C7-C3-C2-C1**	-175.8(1)	179.71
C9-C10-C11-C7	-0.2(2)	0.513	**C4-C3-C2-C1**	1.4(2)	-0.01
C10-C12-C13-C14	175.2(1)	178.03	**C7-C3-C4-C5**	176.3(1)	-179.77
C17-C12-C13-C14	-1.2(2)	0.24	**C2-C3-C4-C5**	-0.9(2)	0.004
C10-C12-C17-C16	-176.8(1)	-178.26	**C12-C13-C14-C15**	1.4(2)	0.02
C13-C12-C17-C16	-0.4(2)	-0.44	**C12-C17-C16-C15**	1.8(2)	0.383
C18-C19-C24-C23	-178.0(1)	-176.58	**C24-C23-C22-C21**	0.8(2)	-1.04
C18-C19-C24-C25	0.8(2)	5.10	**C28-C23-C22-C21**	-177.5(1)	178.83
C20-C19-C24-C23	-0.5(2)	0.249	**C24-C23-C28-C27**	0.5(2)	0.410
C20-C19-C24-C25	178.3(1)	-178.06	**C22-C23-C28-C27**	178.8(1)	-179.47
C24-C19-C18-O1	4.4(2)	22.70	**C24-C25-C26-C27**	-0.0(2)	0.301
C24-C19-C18-C9	-173.9(1)	-155.78	**C19-C20-C21-C22**	-1.1(2)	1.39
C20-C19-C18-O1	-173.1(1)	-154.16	**C3-C2-C1-C6**	-0.7(2)	0.01
C20-C19-C18-C9	8.6(2)	27.33	**C17-C16-C15-C14**	-1.6(2)	-0.107
C24-C19-C20-C21	1.4(2)	-1.44	**C3-C4-C5-C6**	-0.3(2)	0.008
C18-C19-C20-C21	178.9(1)	175.52	**C13-C14-C15-C16**	-0.0(2)	-0.09
C19-C24-C23-C22	-0.5(2)	0.969	**C2-C1-C6-C5**	-0.5(2)	0.0003
C19-C24-C23-C28	177.8(1)	-178.91	**C1-C6-C5-C4**	1.0(2)	-0.0011
C25-C24-C23-C22	-179.4(1)	179.38	**C25-C26-C27-C28**	-0.7(2)	-0.399
C25-C24-C23-C28	-1.1(2)	-0.49	**C23-C22-C21-C20**	-0.0(2)	-0.116
C19-C24-C25-C26	-177.9(1)	178.46	**C23-C28-C27-C26**	0.4(2)	0.037
C23-C24-C25-C26	0.9(2)	0.14			
N1-C9-C18-O1	-111.1(1)	-125.54			

Table S13: Prominent X-H...Cg (Pi-Ring) Interaction Analysis

Molecule	X-H	Cg(J)	H…Cg (A˚)	H⊥ (A˚)	γ (°)	X-H…Cg (°)	X...Cg (A˚)	X-H…π (°)
MK1	C10-H10	Cg3^{i}	2.98	2.76	22.18	160	3.8721(16)	50
	C12-H12	Cg4^{ii}	2.88	-2.78	15.08	167	3.7937(15)	66
	C26-H26B	Cg1^{iii}	3.00	2.97	8.68	162	3.9237(15)	63
MK2	C10-H10	Cg3^{i}	2.73	-2.72	3.33	137	3.4701(13)	46
MK3	No interactions found							
MK4	C6-H6	Cg3^{i}	2.81	2.77	9.57	154	3.6643(19)	54
	C22-H22	Cg2^{ii}	2.87	2.79	13.27	175	3.7932(19)	74

MK1 i: X,-1+Y, Z **ii:** 1-X, 1-Y, 1-Z **iii:** 3/2-X, 1/2+Y, 3/2-Z **Cg1:** N4-C2-C3-C4-C5-C6. **Cg3:** C13-C14-C15-C16-C17-C18, **Cg4:** C20-C21-C22-C23-C24-C25
MK2 i: 1-X,-Y, 1-Z **Cg3:** C13-C14-C15-C16-C17-C18
MK4 i: -1+X, Y,-1+**Z ii:** -X,1-Y,1-Z **Cg2:** C1-C2-C3-C4-C5-C6, **Cg3:** C13-C14-C15-C16-C17-C12

Table S14: Prominent Cg-Cg Interaction Analysis of Rings

Molecule	CgI	CgJ	CgI -CgJ	α(°)	β(°)	γ(°)	CgI⊥ (Å)	CgJ⊥ (Å)	Slippage (Å)
MK1	Cg1	Cg3^{i}	4.7885(7)	54.47(6)	17.7	63.4	-2.1437(4)	-4.5616(6)	-
	Cg3	Cg4^{i}	4.9502(7)	58.92(6)	20.1	78.7	-0.9662(6)	-4.6475(5)	-
MK2	Cg2	Cg2^{i}	3.7548(7)	0.00(6)	25.2	25.2	-3.3983(5)	-3.3984(5)	1.597
	Cg3	Cg2^{i}	4.7141(7)	46.75(6)	20.9	67.3	-1.8157(5)	-4.4038(5)	-
	Cg4	Cg4^{ii}	4.0402(7)	0.00(6)	27	27	-3.6006(5)	-3.6006(5)	1.833
MK3	Cg4	Cg4^{i}	3.8405(16)	0.02(13)	14.5	14.5	3.7181(11)	3.7181(11)	0.962
	Cg4	Cg1^{ii}	3.8746(15)	4.72(13)	23.5	27.1	3.4484(11)	3.5532(11)	1.545
	Cg2	Cg3^{iii}	4.7608(14)	49.14(12)	10.5	59.2	2.4411(9)	4.6809(11)	-
	Cg4	Cg4^{iv}	3.8405(16)	0.02(13)	14.5	14.5	3.7181(11)	3.7181(11)	0.962
MK4	Cg2	Cg2^{i}	3.6838(19)	0	11.8	11.8	3.6061(1)	3.6061(1)	0.752
	Cg4	Cg5^{ii}	3.8076(19)	2	25.8	27.7	3.3721(1)	3.4272(1)	1.659
	Cg5	Cg5^{ii}	3.7811(19)	0	25.6	25.6	3.4093(1)	3.4093(1)	1.635
	Cg5	Cg6^{ii}	3.5863(18)	1	19.2	18.8	3.3953(1)	3.3871(1)	1.179
	Cg6	Cg6^{ii}	3.7980(19)	0	26.7	26.7	3.3920(1)	3.3920(1)	1.709

MK1 i: 1-X, 1-Y, 1-Z **Cg1:** N4-C2-C3-C4-C5-C6. **Cg3:** C13-C14-C15-C16-C17-C18, **Cg4:** C20-C21-C22-C23-C24-C25
MK2 i: 1-X,-Y, 1-Z **ii:** 1-X, 1-Y,1-Z **Cg2:** C7-C8-C9-C10-C11-C12, **Cg3:** C13-C14-C15-C16-C17-C18 **Cg4:** C19-C20-C21-C22-C23-C24
MK3 i: 2-X, 2-Y,-Z **ii:** 1/2+X, 3/2-Y,-1/2+Z **iii:** 3/2-X,1/2+Y,1/2-Z **iv:** 1-X,1-Y,-Z **Cg1:** S1-C13-C14-C15-C16, **Cg2:** N1-C8-C7-C11-C10-C9, **Cg3:** C1-C2-C3-C4-C5-C6, **Cg4:** C17-C18-C19-C20-C21-C22
MK4 i: -X,-Y,-Z **ii:** 1-X, 1-Y,2-Z **Cg1:** N1-C8-C7-C11-C10-C9, **Cg2:** C1-C2-C3-C4-C5-C6, **Cg4:** C19-C20-C21-C22-C23-C24, **Cg5:** C23-C24-C25-C26-C27-C28, **Cg6:** C19-C20-C21-C22-C23-C28-C27-C26

Table S15: Prominent Y-X...Cg (Pi-Ring) Interaction Analysis

Molecule	X-H	Cg(J)	X…Cg (A˚)	H⊥ (A˚)	γ (°)	Y-X…Cg (°)	Y...Cg (A˚)	X-H…π (°)
MK1	No interactions found							
MK2	C24-Cl1	Cg1[i]	3.4527(6)	-3.331	16.99	144.30(4)	4.9972(12)	58.75
MK3	No interactions found							
MK4	No interactions found							

MK2 i: X, 1/2-Y, 1/2+Z **Cg1:** N1-C2-C3-C4-C5-C6

Table S16: The molecular pairs with interaction energies calculated using energy framework analysis

	N	Symmetry operations	R	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
MK1								
	2	x, y, z	11.02	-5.6	-2.2	-19.1	11.2	-17.2
	2	-x+1/2, y+1/2, -z+1/2	11.32	-4.2	-2.0	-16.6	7.8	-15.6
	2	x, y, z	11.99	-8.9	-0.6	-24.9	17.1	-21.0
	2	-x+1/2, y+1/2, -z+1/2	8.14	-13.6	-1.7	-39.8	27.7	-33.2
	2	x+1/2, -y+1/2, z+1/2	12.23	0.3	-0.6	-10.0	0.0	-8.8
	1	-x, -y, -z	3.83	-24.2	-3.7	-119.3	75.9	-85.3
	1	-x, -y, -z	9.65	-8.3	-2.3	-22.4	9.2	-24.3
	2	x+1/2, -y+1/2, z+1/2	11.52	-10.9	-3.3	-8.3	12.4	-13.5
	1	-x, -y, -z	11.90	0.2	-0.2	-7.2	0.9	-5.6
	1	-x, -y, -z	14.83	-10.2	-4.8	-16.8	0.0	-28.9

	N	Symmetry operations	R	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
MK2								
	1	x, -y+1/2, z+1/2	9.15	-8.8	-1.7	-25.0	16.0	-22.5
	2	x, -y+1/2, z+1/2	5.64	-10.3	-0.6	-52.7	35.7	-35.1
	2	x, y, z	9.00	-4.8	-0.8	-17.5	9.8	-14.8
	1	-x, -y, -z	10.71	-17.0	-2.9	-55.8	45.0	-41.0
	2	-x, y+1/2, -z+1/2	10.87	-12.3	-3.0	-22.9	24.9	-19.7
	1	-x, -y, -z	9.57	-6.7	-4.8	-47.2	29.0	-33.8
	1	-x, -y, -z	13.01	6.0	-0.7	-29.5	0.0	-19.9
	2	-x, y+1/2, -z+1/2	13.27	2.7	-0.5	-11.2	0.0	-7.2
	1	x, -y+1/2, z+1/2	9.15	-8.8	-3.7	-25.0	16.0	-23.9

	N	Symmetry operations	R	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
MK3								
	2	-x+1/2, y+1/2, -z+1/2	10.68	-15.4	-3.4	-22.5	21.9	-24.8
	2	x, y, z	9.69	-6.3	-2.1	-14.2	9.9	-14.5
	2	-x+1/2, y+1/2, -z+1/2	7.06	-4.4	-1.1	-36.6	17.2	-26.8
	2	x, y, z	10.02	0.3	-0.6	-11.3	5.0	-6.8
	2	x+1/2, -y+1/2, z+1/2	11.42	-2.8	-0.9	-29.3	19.1	-17.3
	1	-x, -y, -z	5.67	-9.8	-5.4	-49.3	21.9	-43.8
	1	-x, -y, -z	10.42	-2.5	-0.6	-23.8	13.4	-15.5
	1	-x, -y, -z	7.36	-16.5	-3.5	-34.2	29.2	-31.8
	1	-x, -y, -z	11.43	-0.1	-0.5	-27.1	10.7	-17.5

	N	Symmetry operations	R	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
MK4								
	2	x, y, z	9.77	-3.4	-1.5	-18.1	12.1	-13.0
	2	x, y, z	11.15	-8.5	-1.5	-33.6	19.9	-27.1
	1	-x, -y, -z	10.45	-7.8	-2.6	-66.1	43.7	-40.7
	2	x, y, z	11.65	-7.3	-2.1	-28.7	18.6	-22.9
	1	-x, -y, -z	7.13	-11.2	-1.6	-46.6	28.6	-35.9
	1	-x, -y, -z	6.78	-3.0	-0.5	-35.9	12.9	-26.8
	1	-x, -y, -z	10.87	-2.0	-1.4	-7.4	1.0	-8.9
	1	-x, -y, -z	6.89	-5.9	-3.1	-38.8	18.8	-30.7
	1	-x, -y, -z	7.26	-15.5	-5.5	-42.0	23.9	-42.2
	1	-x, -y, -z	12.10	13.3	-1.0	-38.6	0.0	-20.2

Table S17: **The interaction energy calculated for components selected molecular pairs C1-H1A…O3, C26-H26A…O1 interactions in MK1 and C16-H16…O1, C19-H19…O1 interactions in MK2 using energy framework analysis.**

MK1

	N	Symmetry operations	R	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	1	x+1/2, -y+1/2, z+1/2	11.52	-10.9	-3.3	-8.3	12.4	-13.5
	1	-x, -y, -z	14.83	-10.2	-4.8	-16.8	0.0	-28.9

MK3

	N	Symmetry operations	R	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	1	-x+1/2, y+1/2, -z+1/2	10.68	-15.4	-3.4	-22.5	21.9	-24.8
	1	x, y, z	9.69	-6.3	-2.1	-14.2	9.9	-14.5

Table S18: Selected Lewis and non-Lewis interactions via a second order natural bond orbital perturbation theory corresponding to the fock matrix.

Donor (i)	ED (i)(e)	Acceptor(j)	ED (j)(e)	E^2 kJ/mol	$\Delta E^{a.}$	F(i,j)[b] a.u.
MK1						
π(C3-C2)	1.60	π*(N4-C6)	0.40	92.18	0.26	0.064
		π*(C5-C4)	0.31	97.72	0.28	0.069
π(N4-C6)	1.71	π*(C3-C2)	0.33	118.47	0.32	0.081
		π*(C5-C4)	0.31	63.44	0.33	0.059
π(C5-C4)	1.62	π*(C3-C2)	0.33	93.24	0.28	0.066
		π*(N4-C6)	0.40	126.12	0.26	0.075
π(C7-C8)	1.63	π*(C9-C10)	0.33	98.59	0.28	0.068
		π*(C11-C12)	0.32	91.17	0.28	0.066
π(C13-C14)	1.64	π*(C15-C16)	0.33	98.92	0.28	0.068
		π*(C17-C18)	0.32	93.53	0.28	0.066
π(C20-C25)	1.64	π*(C19-O3)	0.16	99.12	0.27	0.070
		π*(C24-C23)	0.38	87.03	0.26	0.062
		π*(C22-C21)	0.35	99.93	0.27	0.067
π(C25-C24)	1.66	π*(C20-C25)	0.37	102.92	0.30	0.072
		π*(C22-C21)	0.35	77.60	0.29	0.061
π(C22-C21)	1.70	π*(C20-C25)	0.37	80.24	0.30	0.064
		π*(C24-C23)	0.38	90.02	0.28	0.066
π(C15-C16)	1.65	π*(C13-C14)	0.35	95.84	0.28	0.068
		π*(C17-C18)	0.32	96.08	0.28	0.067
π(C17-C18)	1.66	π*(C13-C14)	0.35	97.43	0.28	0.067
		π*(C15-C16)	0.33	96.71	0.28	0.067
π(C9-C10)	1.65	π*(C7-C8)	0.36	96.52	0.28	0.067
		π*(C10-C11)	0.32	95.41	0.28	0.067
π(C11-C12)	1.66	π*(C7-C8)	0.36	96.90	0.28	0.067
		π*(C9-C10)	0.33	95.60	0.28	0.067
σ(C1-H1C)	1.99	σ*(C1-H1C)	0.01	52.13	3.60	0.177
LP (1) N4	1.91	σ*(C3-C2)	0.03	49.00	0.89	0.086
		σ*(C6-C5)	0.04	52.13	0.91	0.089
LP (2)O 3	1.88	π*(C6-C19)	0.07	99.98	0.66	0.106
		π*(C19-C20)	0.06	88.43	0.71	0.104
LP (2)O 2	1.82	π*(C25-C24)	0.38	154.04	0.34	0.098
LP (2)O 1	1.84	π*(C23-C22)	0.35	142.63	0.34	0.094

Donor (i)	ED (i)(e)	Acceptor(j)	ED (j)(e)	E^2 kJ/mol	$\Delta E^{a.}$	F(i,j)[b] a.u.
MK2						
π(C3-C4)	1.61	π*(C2-N1)	0.36	107.23	0.27	0.074
		π*(C6-C5)	0.35	85.35	0.29	0.069
π(C2-N1)	1.72	π*(C3-C4)	0.33	57.19	0.33	0.061
		π*(C6-C5)	0.35	98.07	0.33	0.081
π(C6-C5)	1.58	π*(C3-C4)	0.33	84.26	0.28	0.069
		π*(C2-N1)	0.36	82.25	0.26	0.065
π(C7-C8)	1.64	π*(C9-C10)	0.33	84.14	0.28	0.067
π(C13-C14)	1.96	σ*(C11-H11)	0.01	125.14	4.97	0.346
		σ*(C12-H12)	0.01	105.06	3.09	0.250
π(C13-C14)	1.64	π*(C15-C16)	0.33	86.35	0.28	0.068
		π*(C17-C18)	0.01	80.75	0.28	0.067
π(C19-C24)	1.65	π*(C20-C21)	0.29	79.70	0.30	0.068
		π*(C14-C15)	0.38	86.02	0.28	0.068
π(C20-C21)	1.65	π*(C11-C16)	0.41	82.71	0.27	0.067

		π^*(C14-C15)	0.38	96.73	0.27	0.071
π(C22-C23)	1.67	π^*(C11-C16)	0.41	80.37	0.29	0.068
		π^*(C12-C13)	0.29	71.71	0.30	0.065
π(C15-C16)	1.65	π^*(C13-C14)	0.35	84.76	0.28	0.068
		π^*(C17-C16)	0.31	83.21	0.28	0.068
π(C17-C18)	1.66	π^*(C13-C14)	0.35	87.06	0.28	0.069
		π^*(C15-C16)	0.33	85.64	0.28	0.068
π(C9-C10)	1.65	π^*(C7-C22)	0.36	85.93	0.28	0.068
σ (C11-C12)	1.97	σ^*(C25-H42)	0.01	91.75	5.00	0.296
π(C11-C12)	1.66	π^*(C7-C8)	0.36	85.35	0.28	0.069
		π^*(C9-C10)	0.33	85.43	0.29	0.068
σ (C12-H12)	1.97	σ^*(C11-H11)	0.01	288.61	4.80	0.515
		σ^*(C12-H12)	0.01	127.69	2.92	0.267
LP (1) N1	1.910	π^*(C6-C5)	0.04	42.50	0.89	0.086
LP (2) O1	1.879	σ^*(C6-C1)	0.07	81.29	0.68	0.103
		σ^*(C1-C19)	0.06	84.26	0.68	0.106
LP (2) Cl 2	1.92	π^*(C22-C23)	0.38	54.55	0.32	0.063
LP (2) Cl 1	1.92	π^*(C19-C24)	0.41	53.80	0.33	0.064

Donor (i)	**ED (i)(e)**	**Acceptor(j)**	**ED (j)(e)**	**E^2 kJ/mol**	**$\Delta E^{a.}$**	**F(i,j)[b] a.u.**
MK3						
π(C7-C8)	1.610	π^*(C10-N1)	0.371	104.99	0.26	0.074
		π^*(C10-C9)	0.354	79.91	0.28	0.068
π(C10-N1)	1.730	π^*(C7-C8)	0.332	52.67	0.33	0.060
		π^*(C9-C10)	0.354	91.57	0.33	0.079
π(C11-7)	1.579	π^*(C7-C8)	0.332	81.44	0.28	0.069
		π^*(C2-N3)	0.371	81.20	0.26	0.065
		π^*(C12-O1)	0.199	49.22	0.28	0.055
π(C4-C5)	1.638	π^*(C6-C1)	0.330	81.44	0.28	0.068
		π^*(C2-C3)	0.320	77.38	0.28	0.066
π(C17-C18)	1.650	π^*(C19-C20)	0.331	82.48	0.28	0.068
		π^*(C21-C22)	0.317	77.22	0..28	0.066
π(C13-C14)	1.780	π^*(C12-O1)	0.199	89.19	0.28	0.07
		π^*(C15-C16)	0.312	63.28	0.28	0.06
π(C19-C20)	1.662	π^*(C17-C18)	0.355	79.27	0.28	0.067
		π^*(C21-C22)	0.317	79.51	0.28	0.067
π(C21-C22)	1.664	π^*(C17-C18)	0.355	81.88	0.28	0.068
		π^*(C19-C20)	0.331	80.84	0.28	0.067
π(C6-C1)	1.652	π^*(C1-C6)	0.365	81.36	0.28	0.067
		π^*(C2-C3)	0.320	80.60	0.28	0.067
π(C2-C3)	1.666	π^*(C4-C5)	0.365	80.72	0.28	0.067
		π^*(C6-C1)	0.330	79.87	0.28	0.067
π(C15-C16)	1.819	π^*(C13-C14)	0.342	72.88	0.28	0.068
LP (1) N1	1.902	π^*(C10-C9)	0.039	43.11	0.89	0.089
LP (2) O1	1.878	σ^*(C7-C5)	0.071	80.11	0.67	0.104
		σ^*(C12-C13)	0.062	78.51	0.70	0.106
LP (2) S1	1.599	σ^*(C13-C14)	0.342	80.52	0.26	0.066
		σ^*(C15-C16)	0.312	96.47	0.25	0.071

Donor (i)	ED (i)(e)	Acceptor(j)	ED (j)(e)	E^2 kJ/mol	$\Delta E^{a.}$	F(i,j)[b] a.u.
MK4						
π(C6-C1)	1.654	π^*(C5-C4)	0.321	84.14	0.28	0.067
		π^*(C3-C2)	0.364	84.14	0.28	0.067
π(C5-C4)	1.667	π^*(C6-C1)	0.331	83.05	0.28	0.067
		π^*(C3-C2)	0.364	84.01	0.28	0.067
π(C7-C11)	1.616	π^*(C3-C2)	0.364	39.07	0.29	0.046
		π^*(C8-N1)	0.372	109.83	0.26	0.074
		π^*(C9-C10)	0.355	81.83	0.29	0.067
π(C8-N1)	1.722	π^*(C7-C11)	0.337	55.81	0.33	0.060
		π^*(C9-C10)	0.355	98.70	0.33	0.080
π(C9-C10)	1.588	π^*(C7-C11)	0.337	86.48	0.28	0.069
		π^*(C8-N1)	0.372	80.87	0.26	0.064
π(C12-C13)	1.644	π^*(C16-C15)	0.332	85.81	0.28	0.068
		π^*(C14-C13)	0.320	81.12	0.28	0.066
π(C16-C15)	1.657	π^*(C12-C17)	0.358	83.38	0.28	0.068
		π^*(C14-C13)	0.320	83.59	0.28	0.067
π(C14-C13)	1.663	π^*(C18-C17)	0.358	84.85	0.28	0.067
		π^*(C16-C15)	0.332	83.80	0.28	0.067
π(C19-C20)	1.690	π^*(C18-O1)	0.153	78.86	0.27	0.066
		π^*(C21-C22)	0.250	65.47	0.29	0.061
		π^*(C23-C24)	0.453	67.32	0.29	0.063
π(C21-C22)	1.720	π^*(C19-C20)	0.289	81.96	0.29	0.068
		π^*(C30-C29)	0.453	63.26	0.29	0.062
π(C23-C24)	1.528	π^*(C19-C20)	0.289	65.39	0.27	0.061
		π^*(C21-C22)	0.250	73.38	0.27	0.065
		π^*(C28-C27)	0.254	67.48	0.27	0.063
		π^*(C26-C25)	0.241	60.96	0.30	0.063
π(C28-C27)	1.736	π^*(C23-C24)	0.453	68.19	0.28	0.064
		π^*(C26-C25)	0.241	65.64	0.29	0.063
π(C26-C25)	1.714	π^*(C23-C24)	0.453	71.37	0.28	0.064
		π^*(C28-C27)	0.254	75.85	0.29	0.065
LP (1) N1	1.916	σ^*(C7-C8)	0.033	42.59	0.89	0.086
		σ^*(C9-C10)	0.040	45.39	0.89	0.089
LP (2) O1	1.881	σ^*(C11-C18)	0.073	85.60	0.66	0.105
		σ^*(C18-C19)	0.062	77.11	0.70	0.103

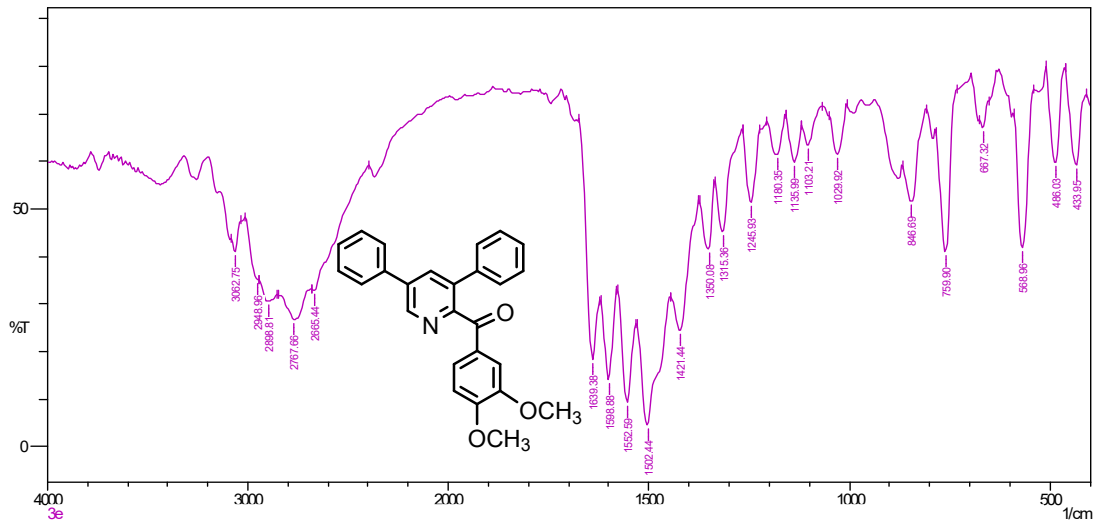


Figure S1: FT-IR Spectrum of (3,4-dimethoxyphenyl)(3,5-diphenylpyridin-2-yl)methanone [MK1]

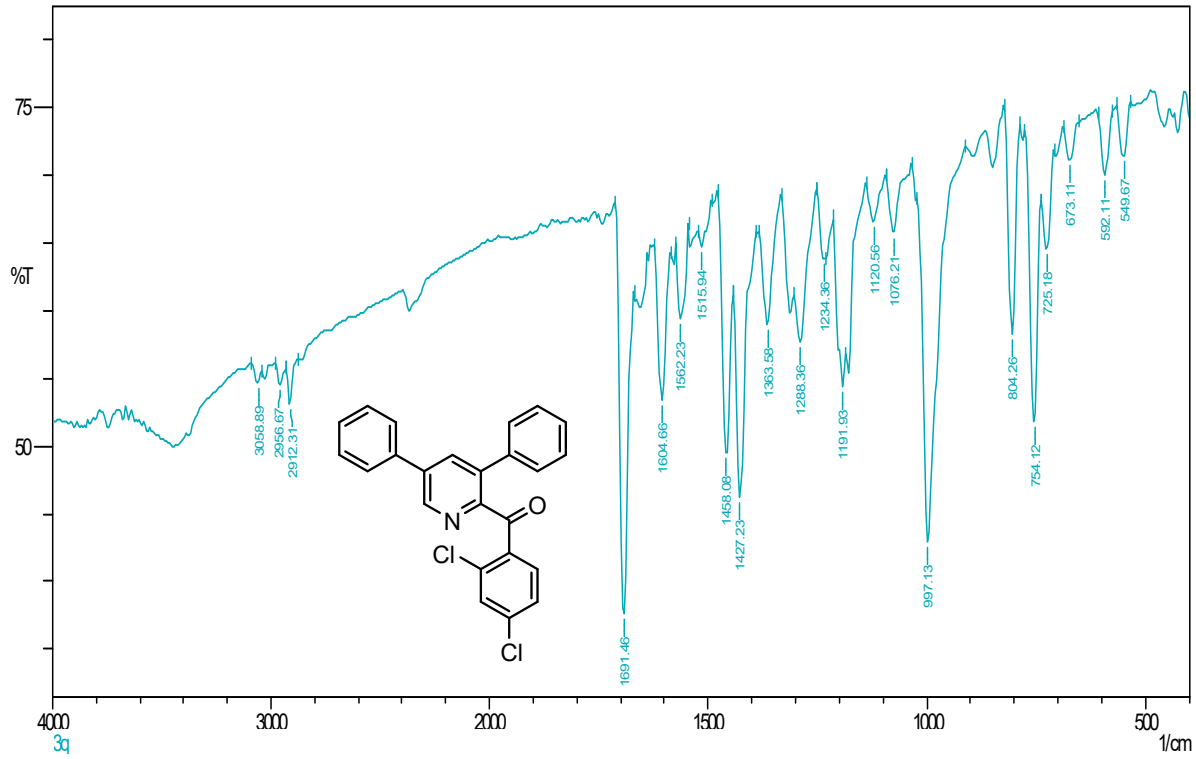


Figure S2: FT-IR Spectrum of(2, 4-dichlorophenyl)(3,5-diphenylpyridin-2-yl)methanone [MK2]

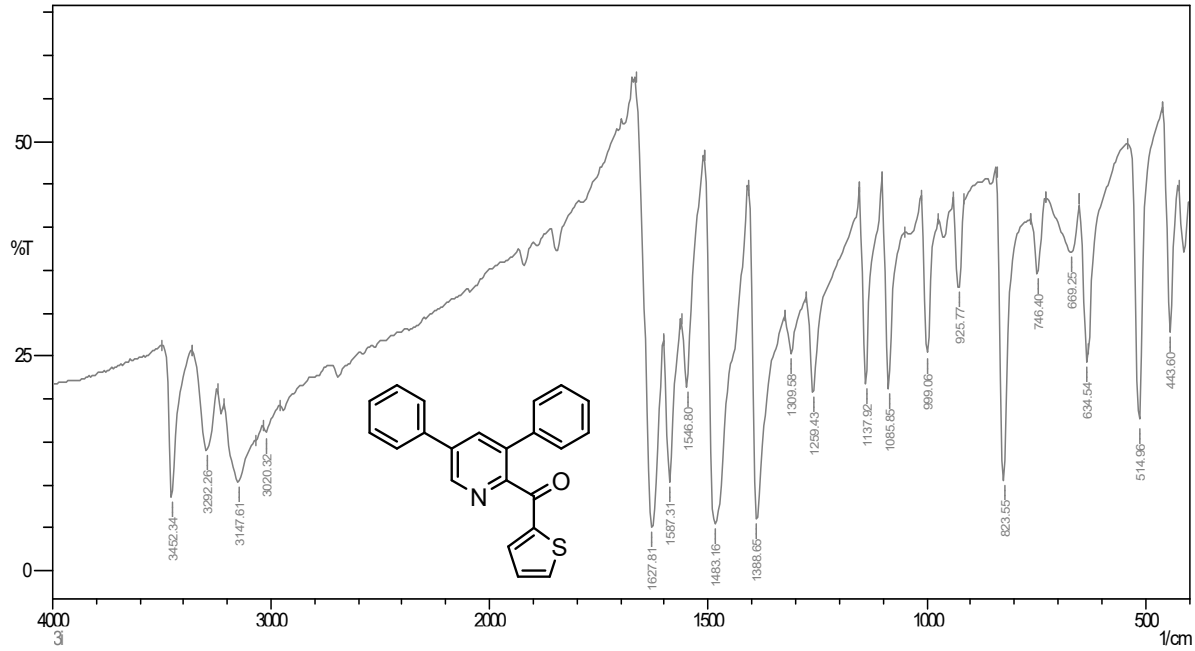


Figure S3: FT-IR Spectrum of (3,5-diphenylpyridin-2-yl)(thiophen-2-yl)methanone [MK3]

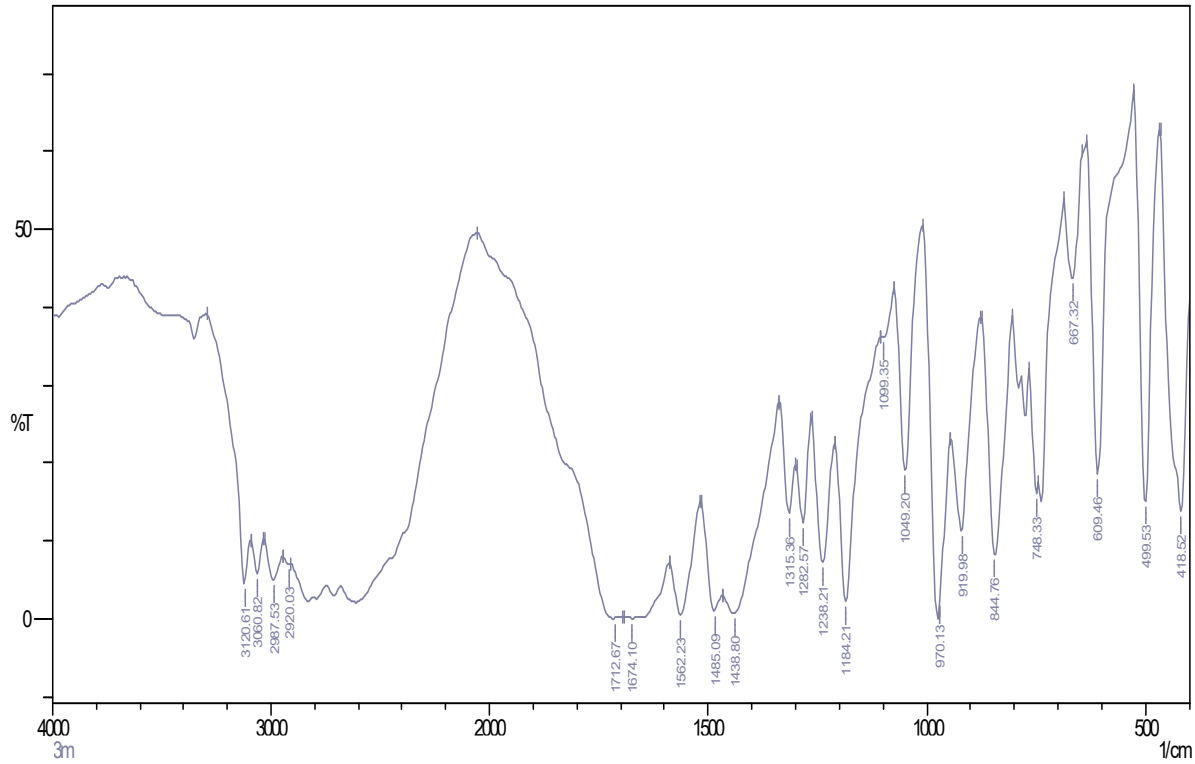
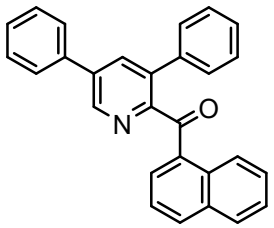


Figure S4: FT-IR Spectrum of (3,5-diphenylpyridin-2-yl)(naphthalen-1-yl)methanone [MK4]


N
O

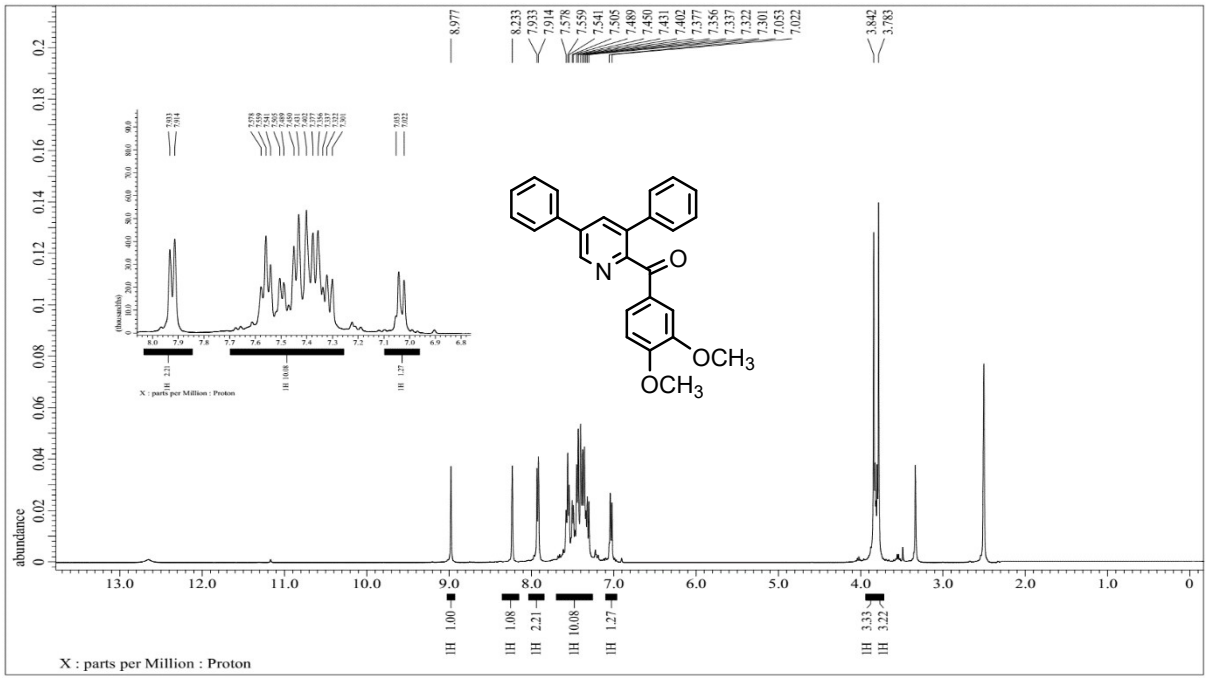


Figure S5: 400MHz ^{1}H-NMR spectrum of (3, 4-dimethoxyphenyl)(3,5-diphenylpyridin-2-yl)methanone [MK1]

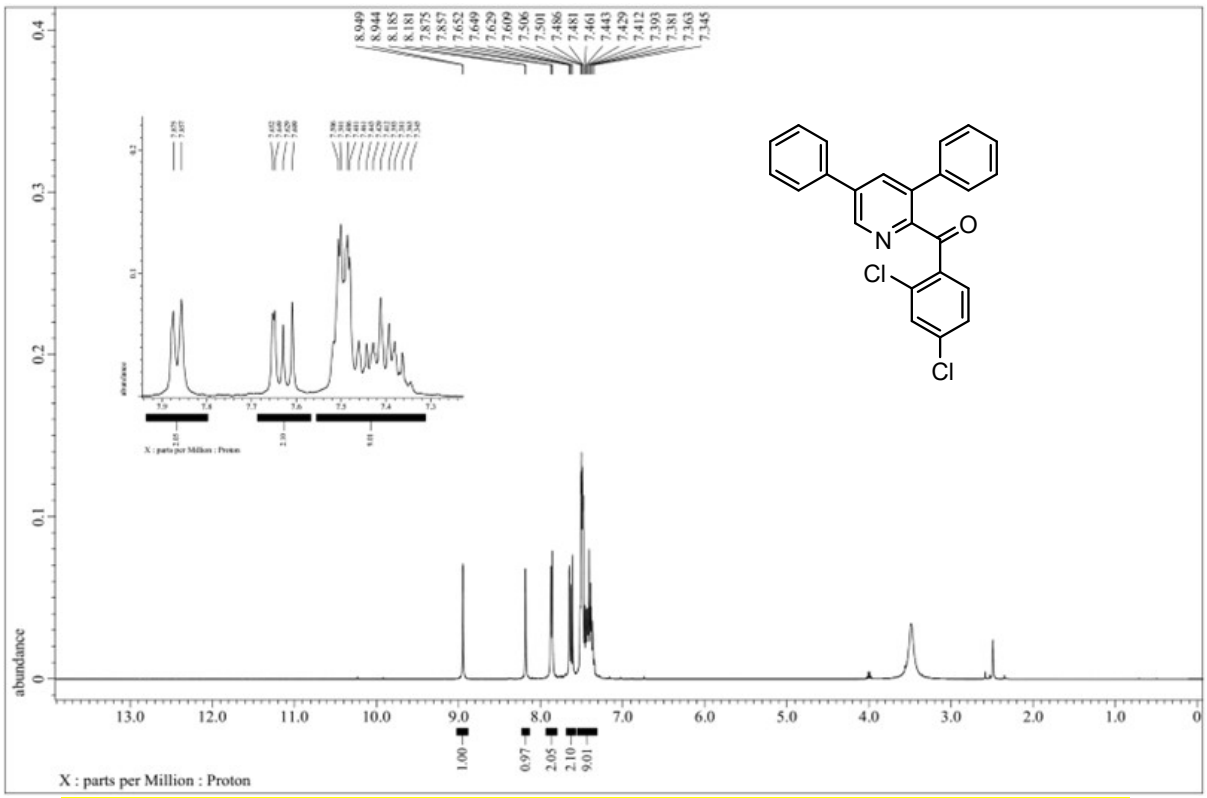


Figure S6: 400MHz ^{1}H-NMR spectrum of (2,4-dichlorophenyl)(3,5-diphenylpyridin-2-yl)methanone [MK2]

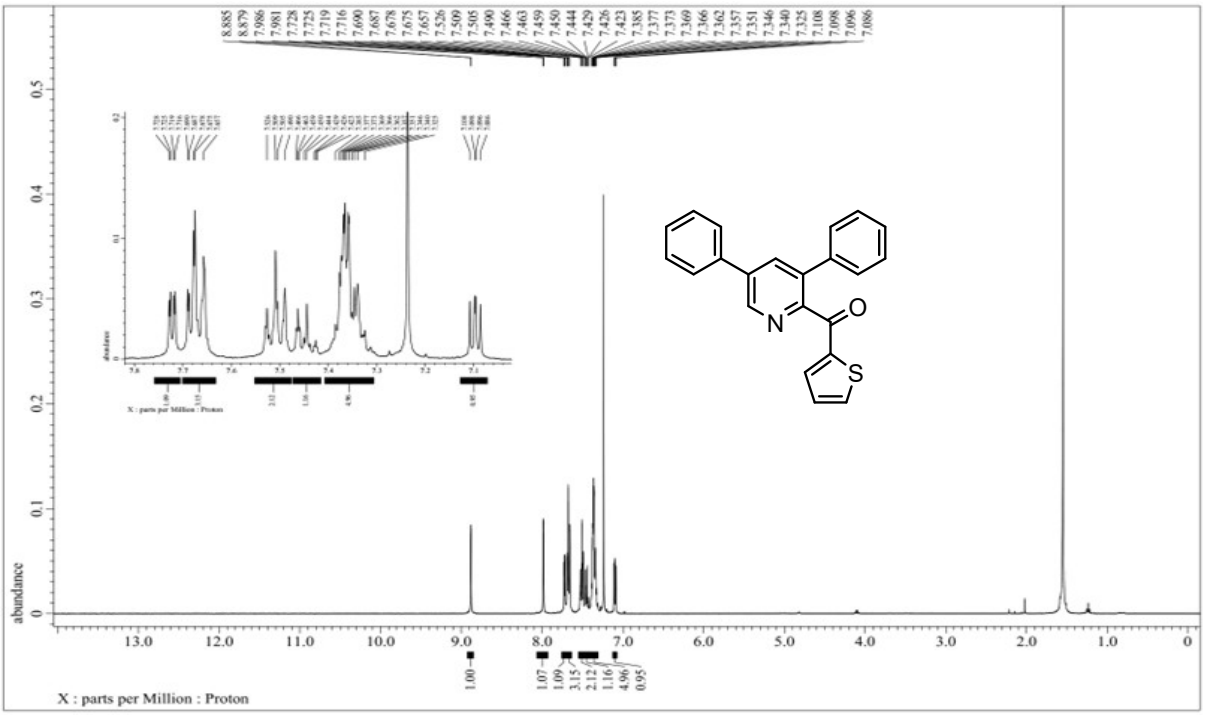


Figure S7: 400MHz ^{1}H-NMR spectrum of (3,5-diphenylpyridin-2-yl)(thiophen-2-yl)methanone [MK3]

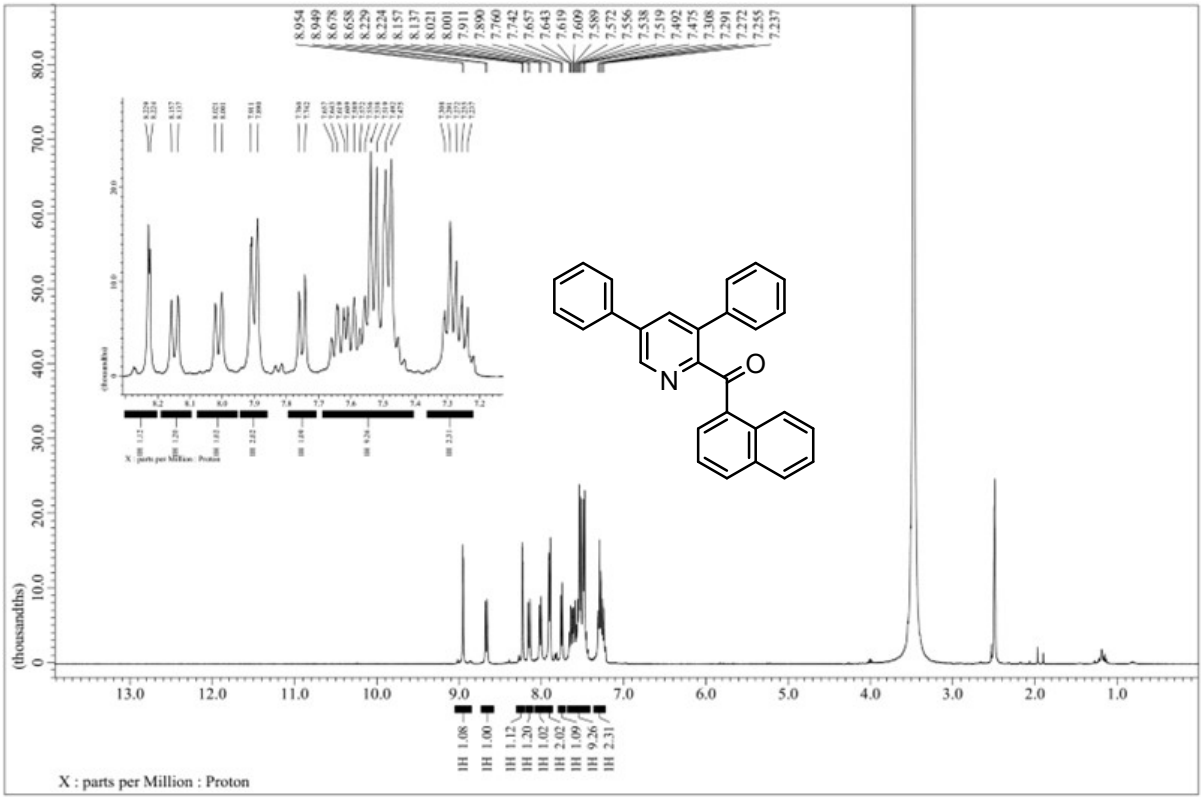


Figure S8: 400MHz 1H-NMR spectrum of (3,5-diphenylpyridin-2-yl)(naphthalen-1-yl)methanone [MK4]

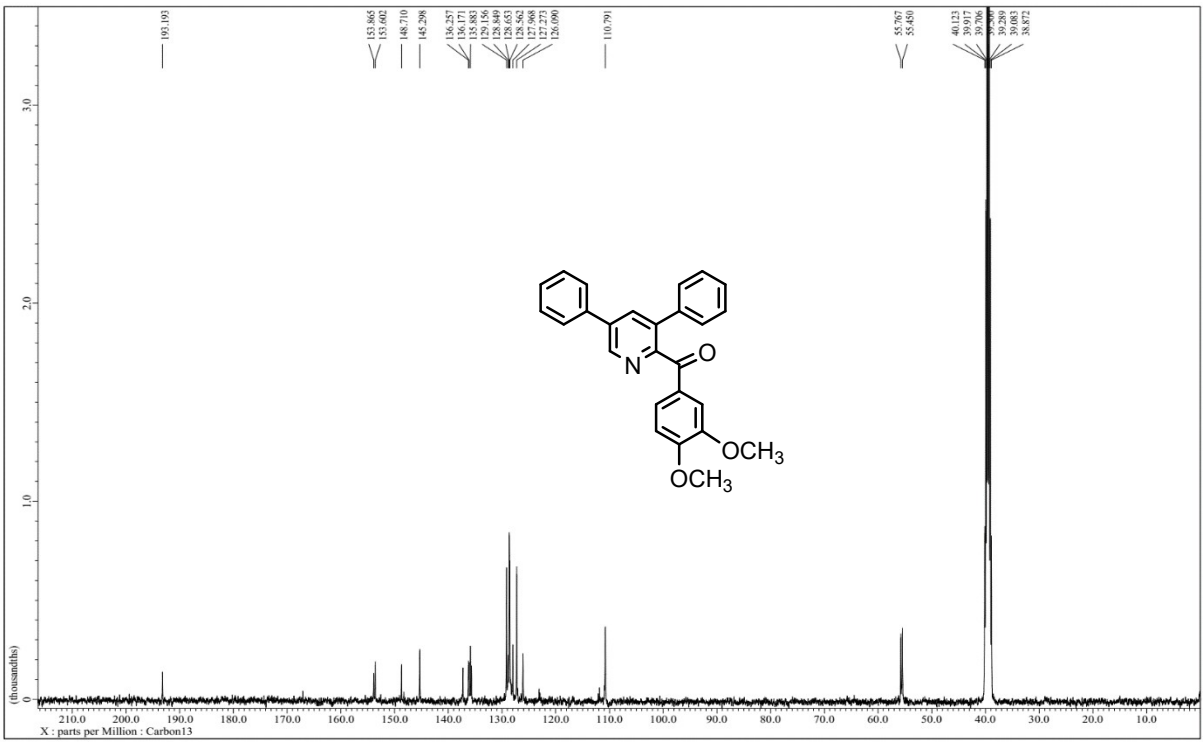


Figure S9*:* 101MHz 13C-NMR spectrum of (3,4-dimethoxyphenyl)(3,5-diphenylpyridin-2-yl)methanone [MK1]

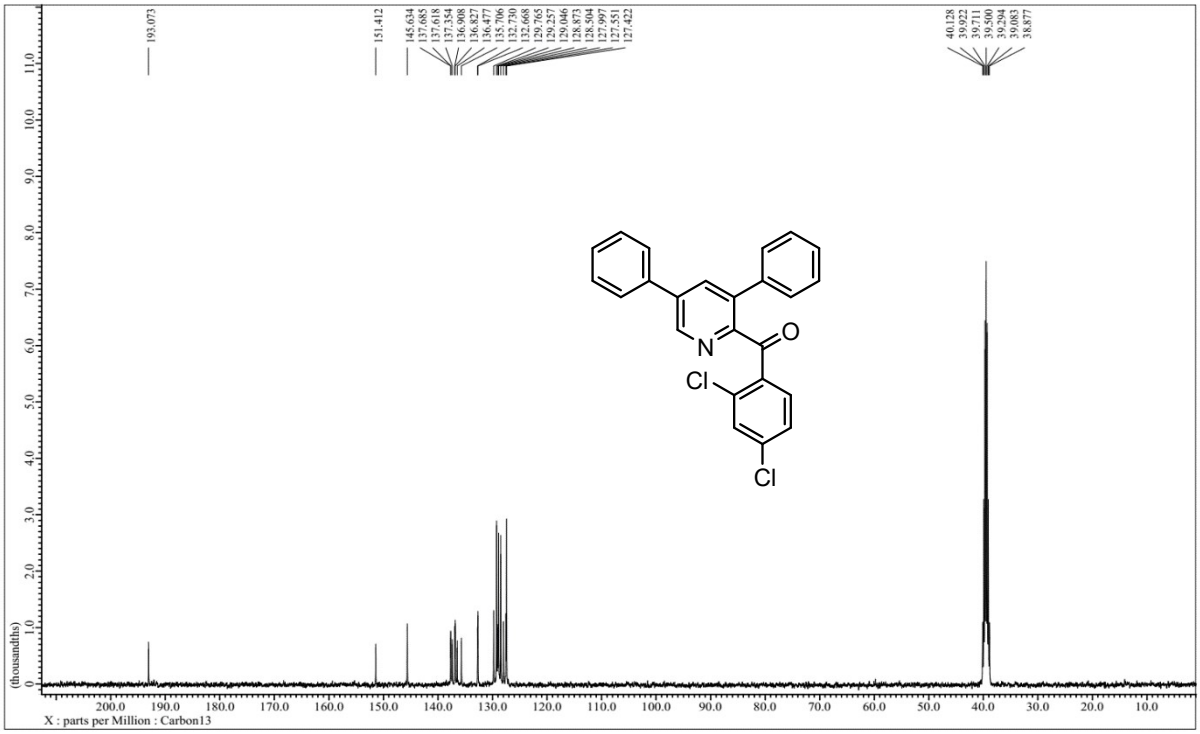


Figure S10*:* 101MHz 13C-NMR spectrum of (2,4-dichlorophenyl)(3,5-diphenylpyridin-2-yl)methanone [MK2]

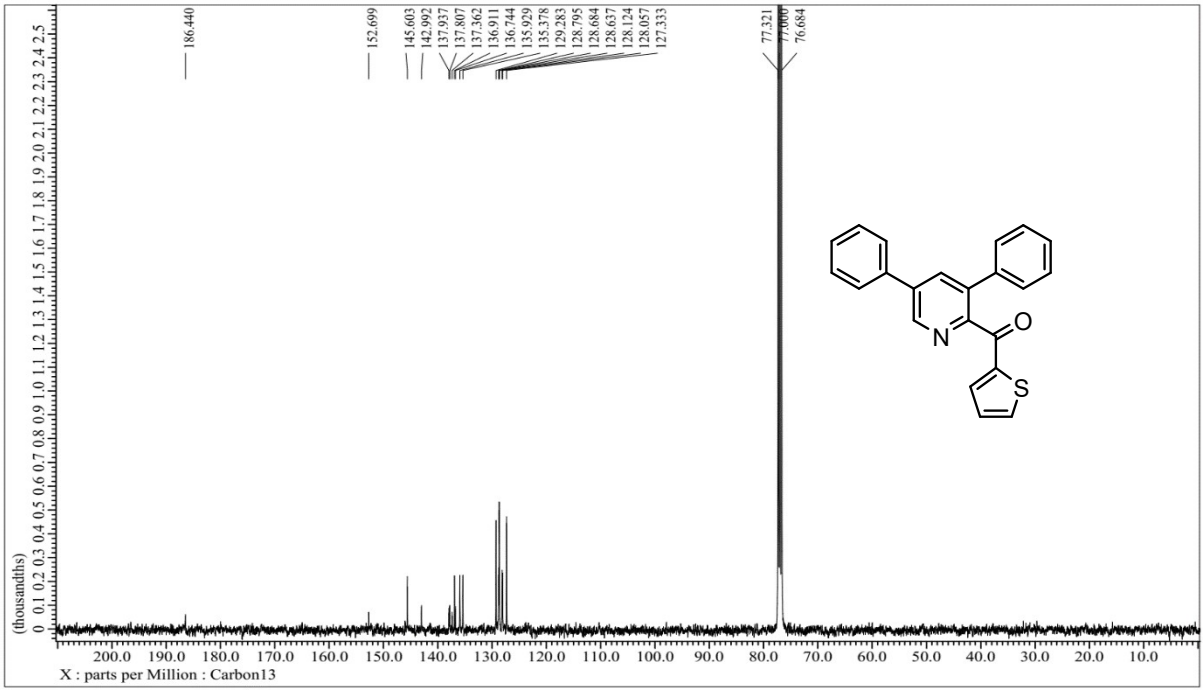


Figure S11: 101MHz 13C--NMR spectrum of (3,5-diphenylpyridin-2-yl)(thiophen-2-yl)methanone [MK3]

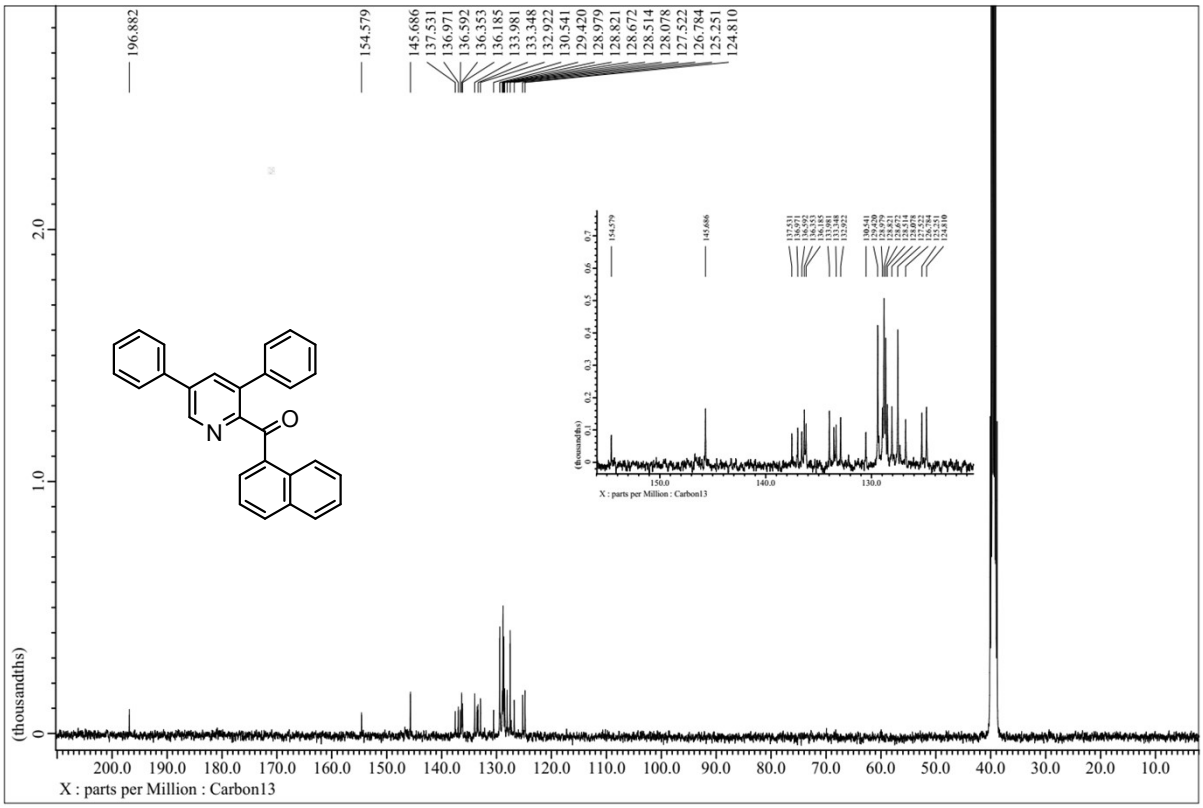


Figure S12: 101MHz 13C-NMR spectrum of (3,5-diphenylpyridin-2-yl)(naphthalen-1-yl)methanone [MK4]

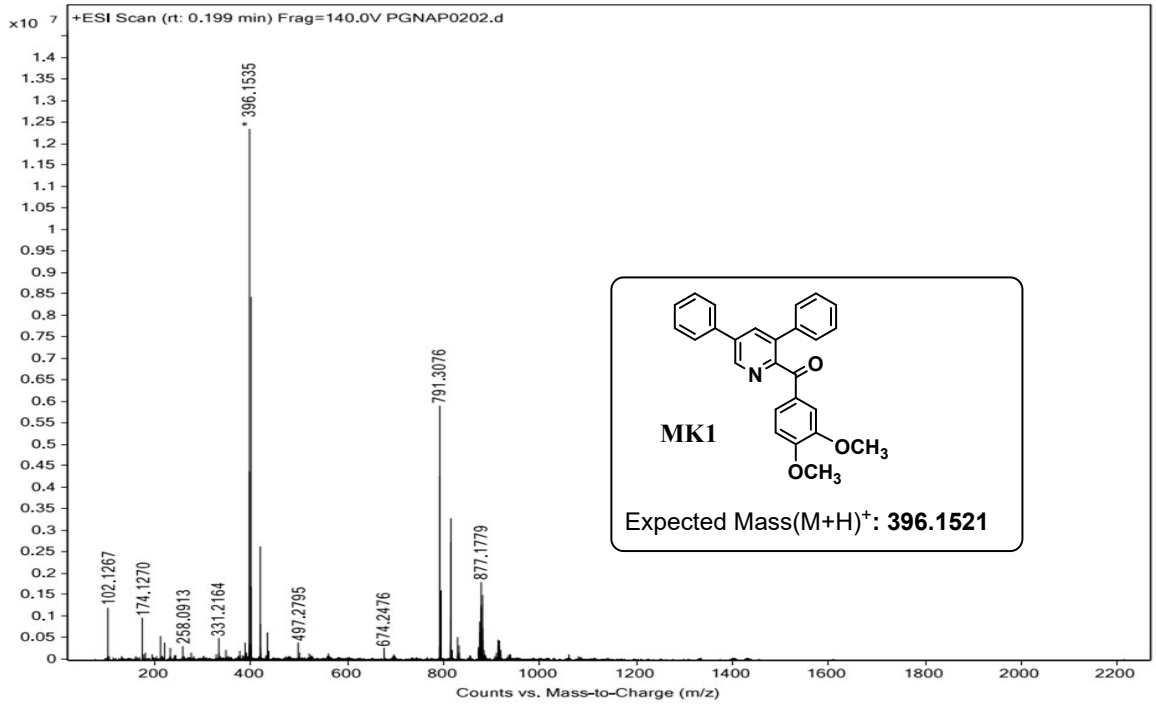


Figure S13: HRMS spectrum of (3,4-dimethoxyphenyl)(3,5-diphenylpyridin-2-yl)methanone [MK1]

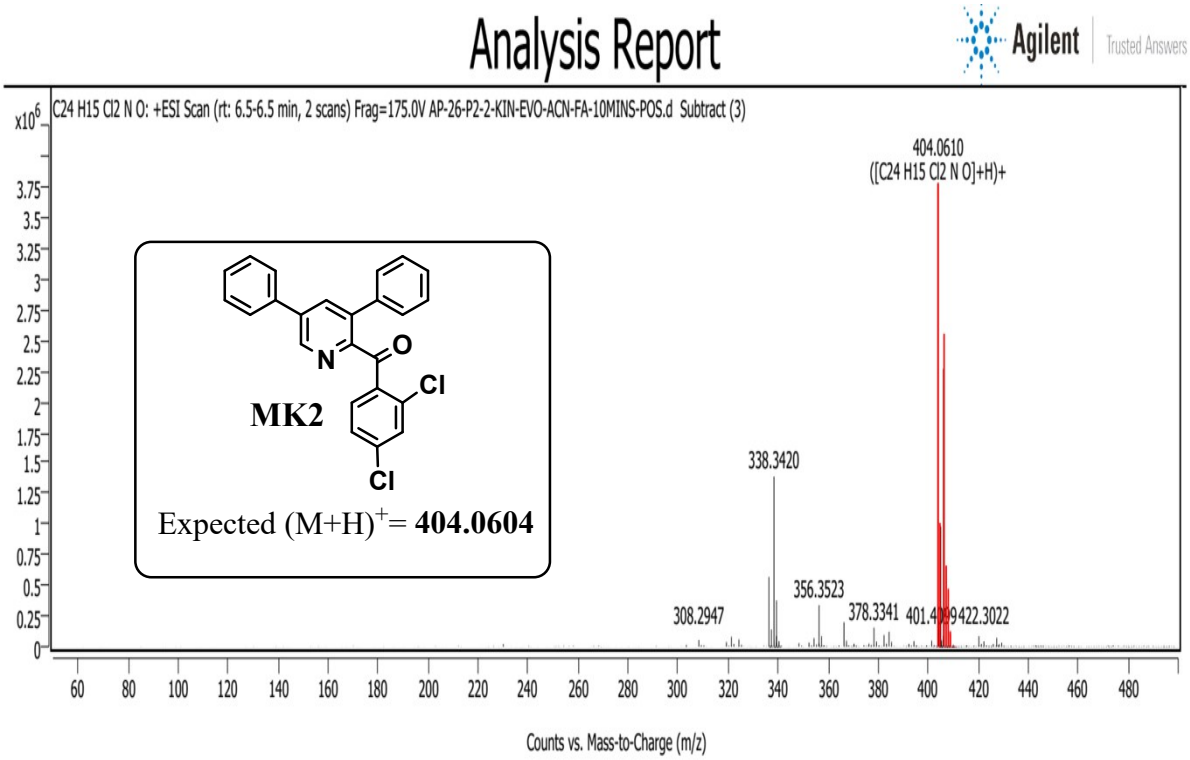


Figure S14: HRMS spectrum of (2,4-dichlorophenyl)(3,5-diphenylpyridin-2-yl)methanone [MK2]

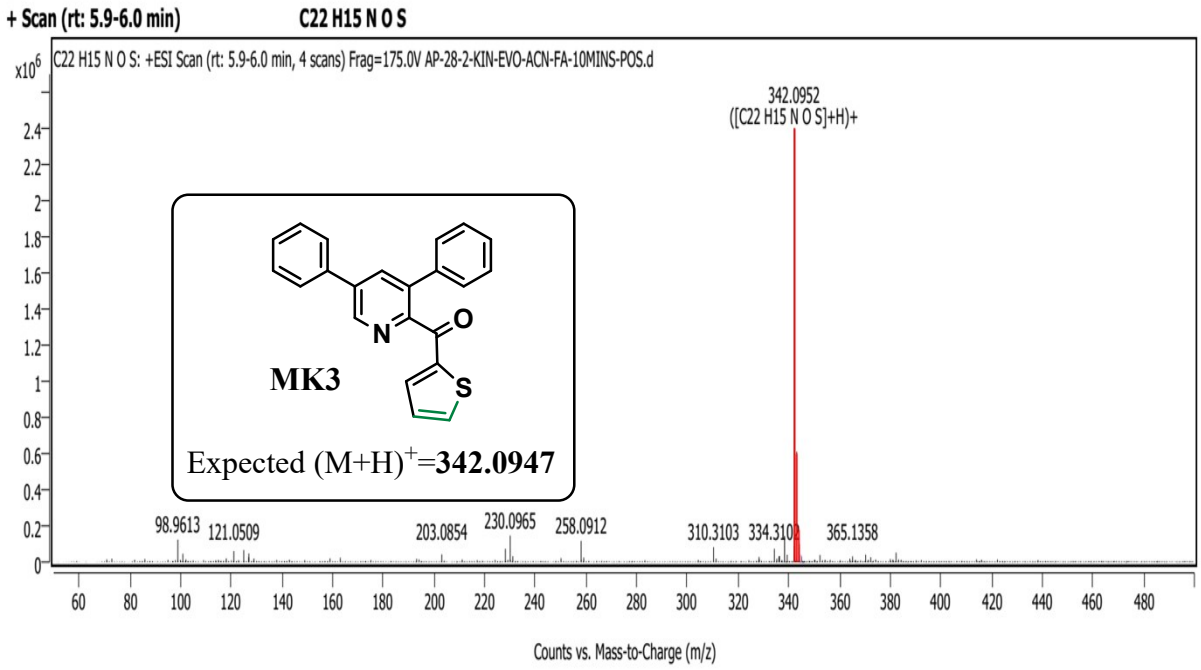


Figure S15: HRMS spectrum of (3,5-diphenylpyridin-2-yl)(thiophen-2-yl)methanone [MK3]

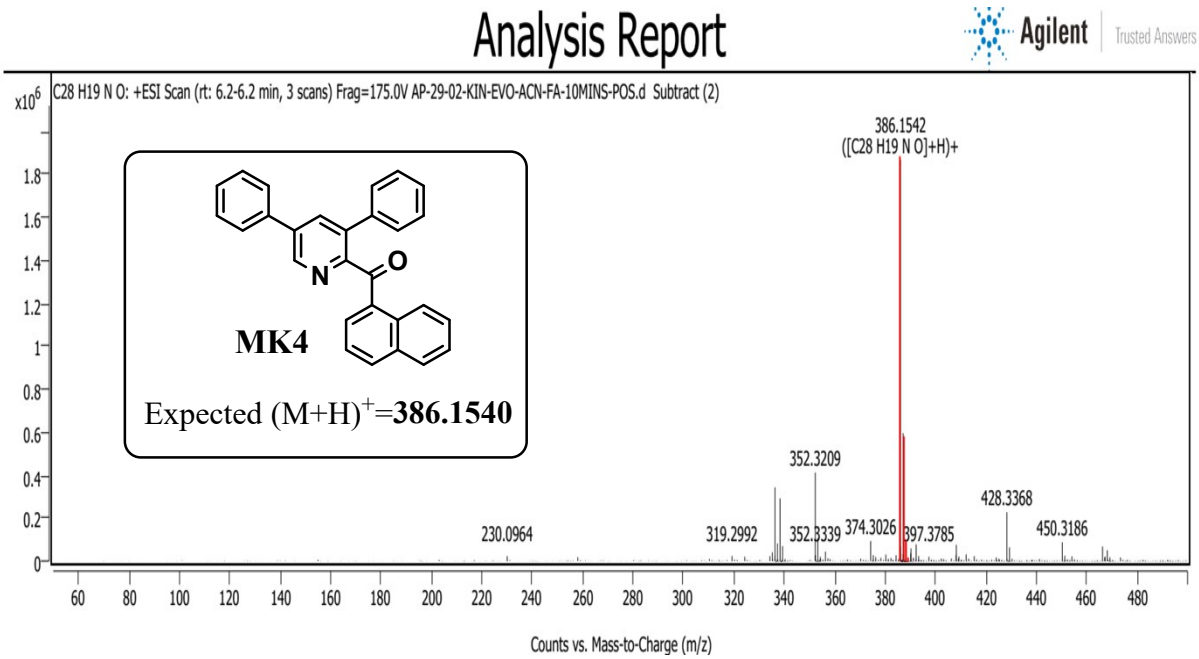


Figure S16: HRMS spectrum of (3,5-diphenylpyridin-2-yl)(naphthalen-1-yl)methanone [MK4]

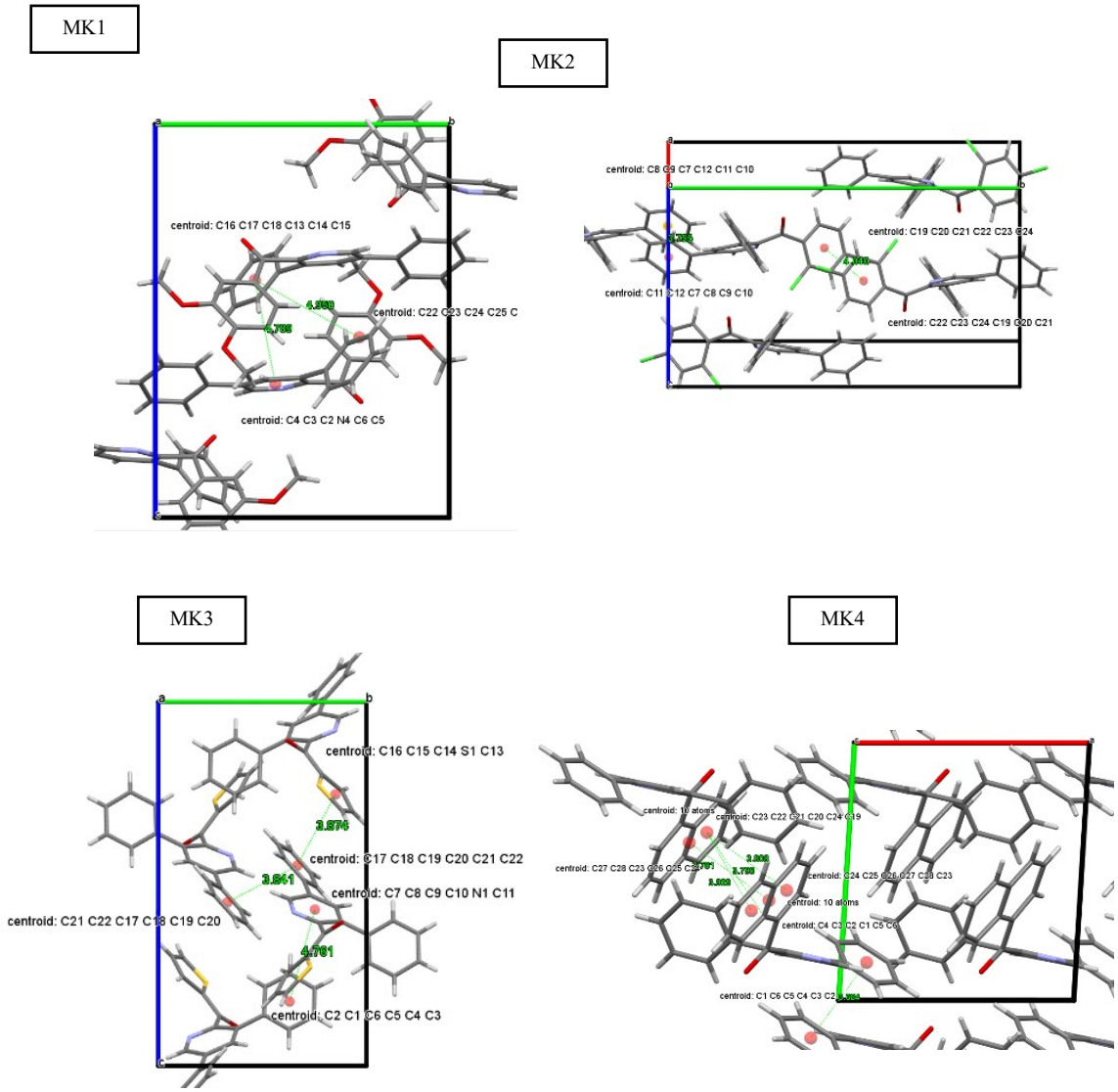


Figure S17: Three dimensional crystal packing interactions revealing prominent Cg-Cg intermolecular interactions (Green lines)

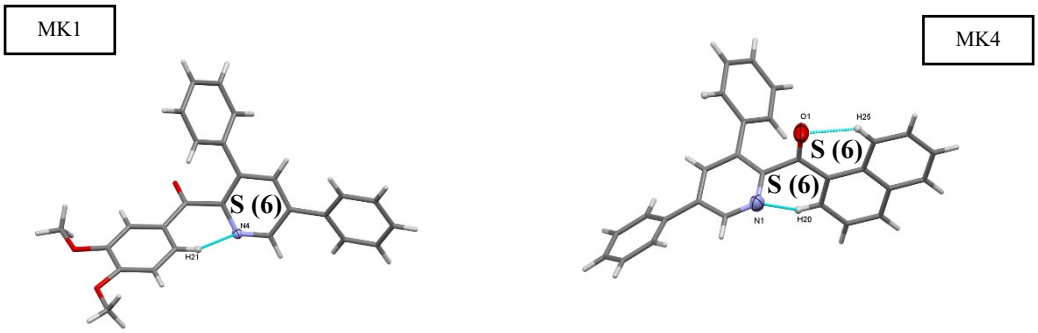


Figure S18: Formation of ring motifs through short contact interactions within the molecule

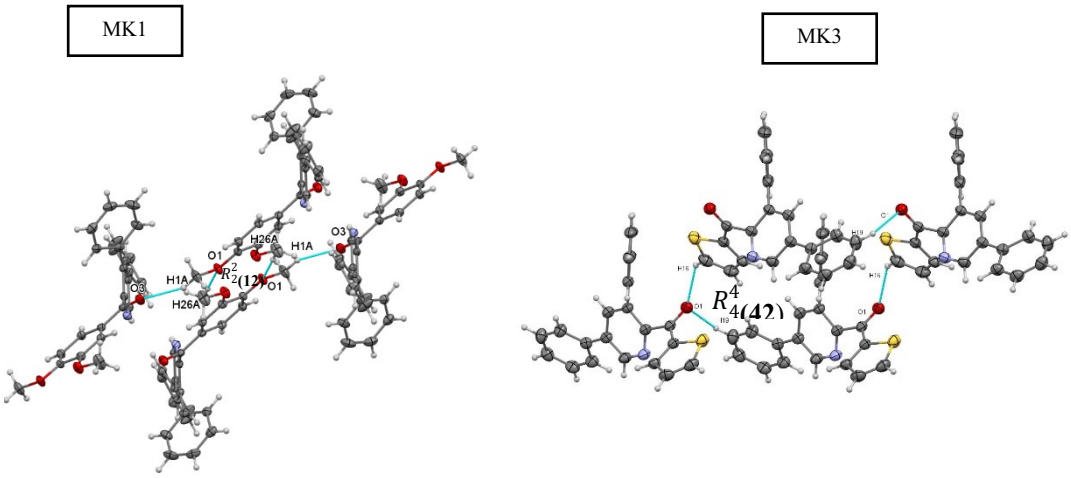


Figure S19: Formation of supramolecular synthon through intermolecular interactions within the molecule

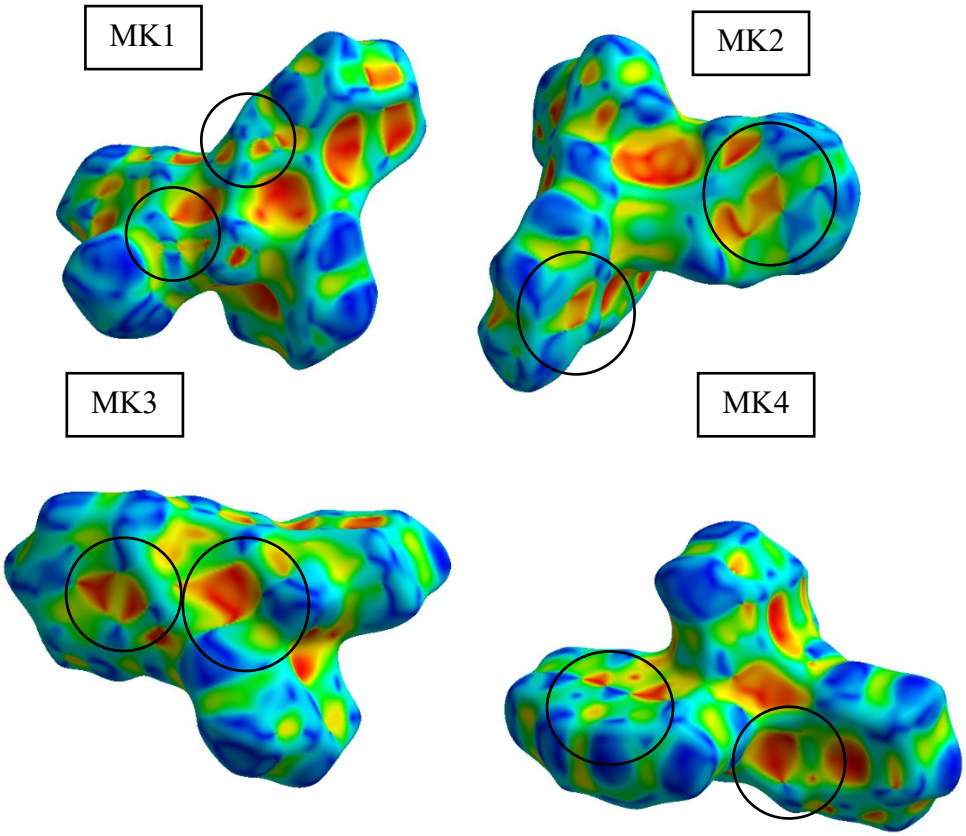


Figure S20: Shape index surface showing complementary red and blue triangular patches indicative of π···π interactions (encircled in black)

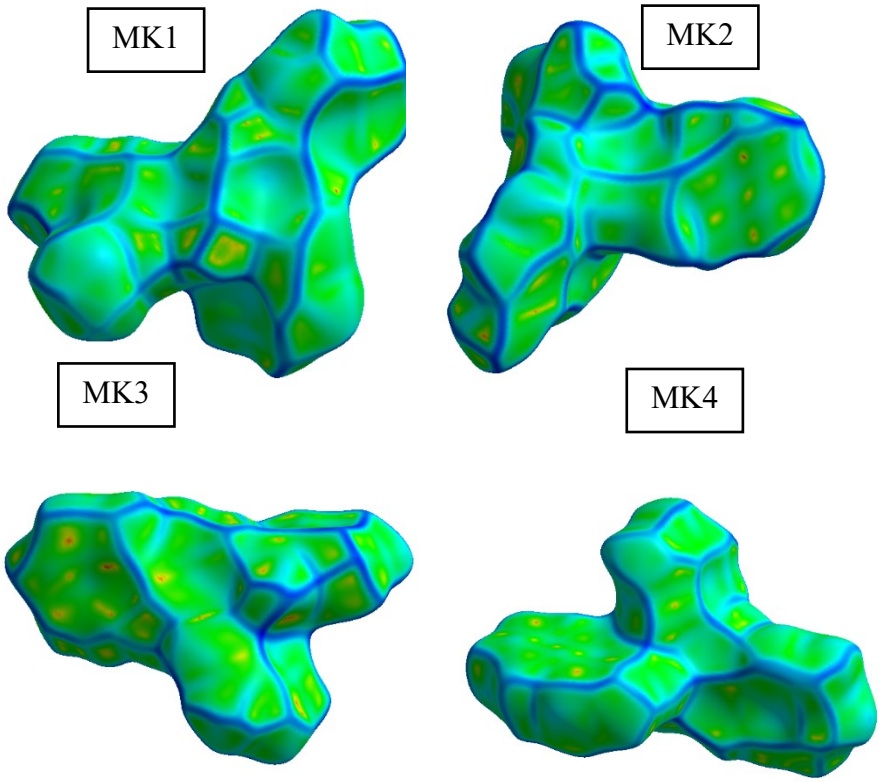


Figure S21: Curvedness surface map to delineate the planar stacking interactions within the crystal lattice.

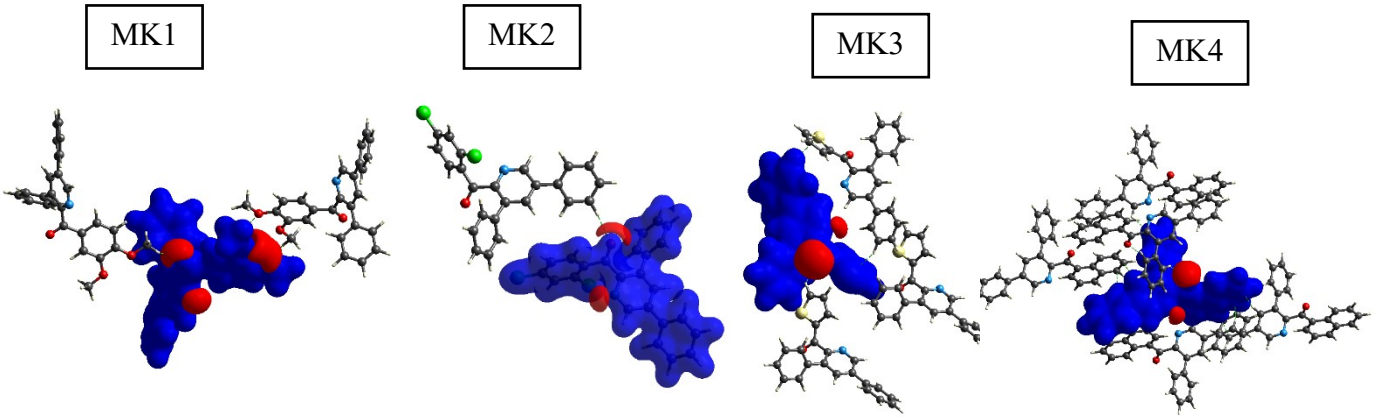


Figure S22: Electrostatic potential surface plot indicating nucleophile attack regions

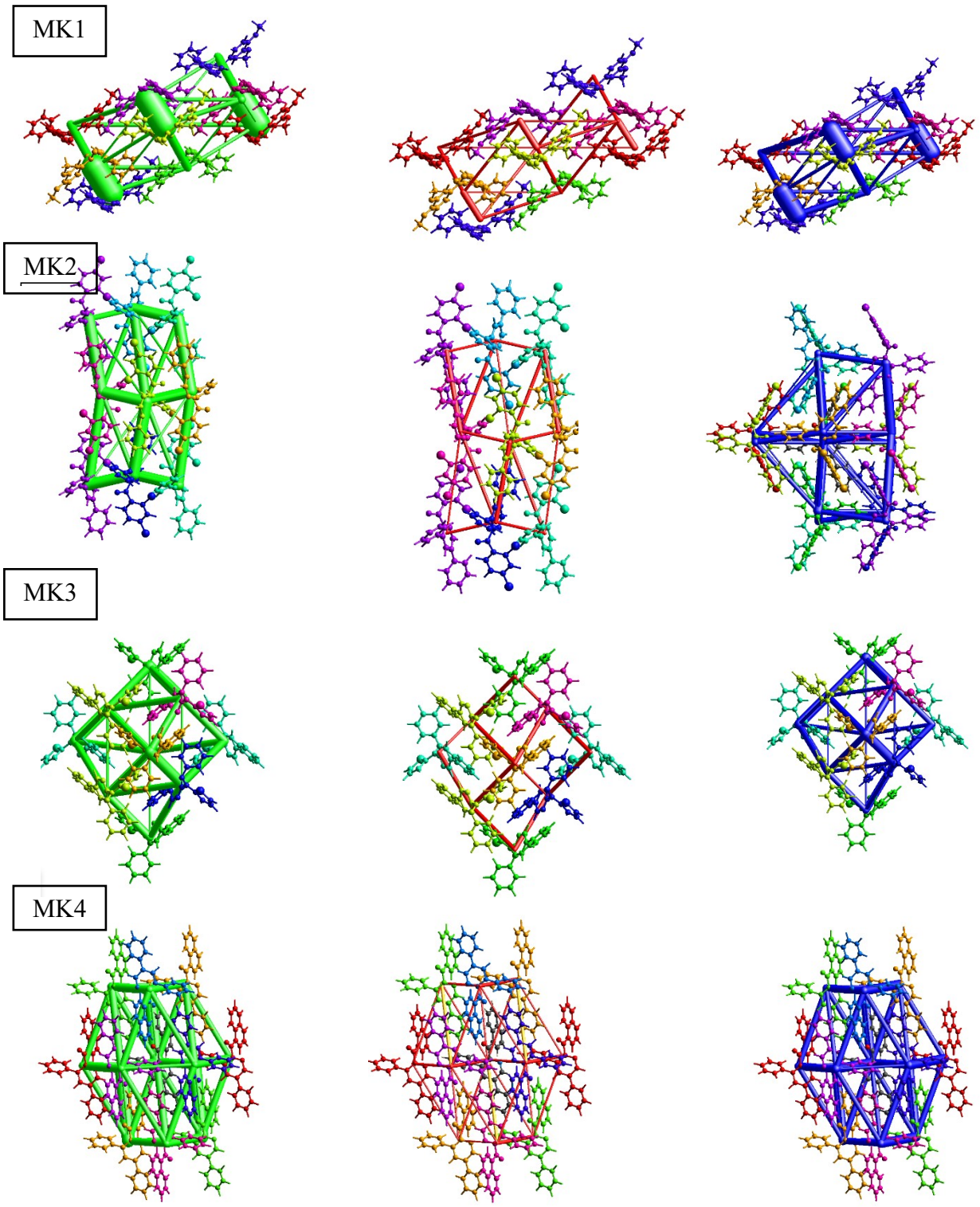


Figure S23: Molecular packing with energy framework of MK series of molecule representing to coulomb energy (red), dispersion energy (green), and total energy (blue) components with respect to unit cell axis respectively

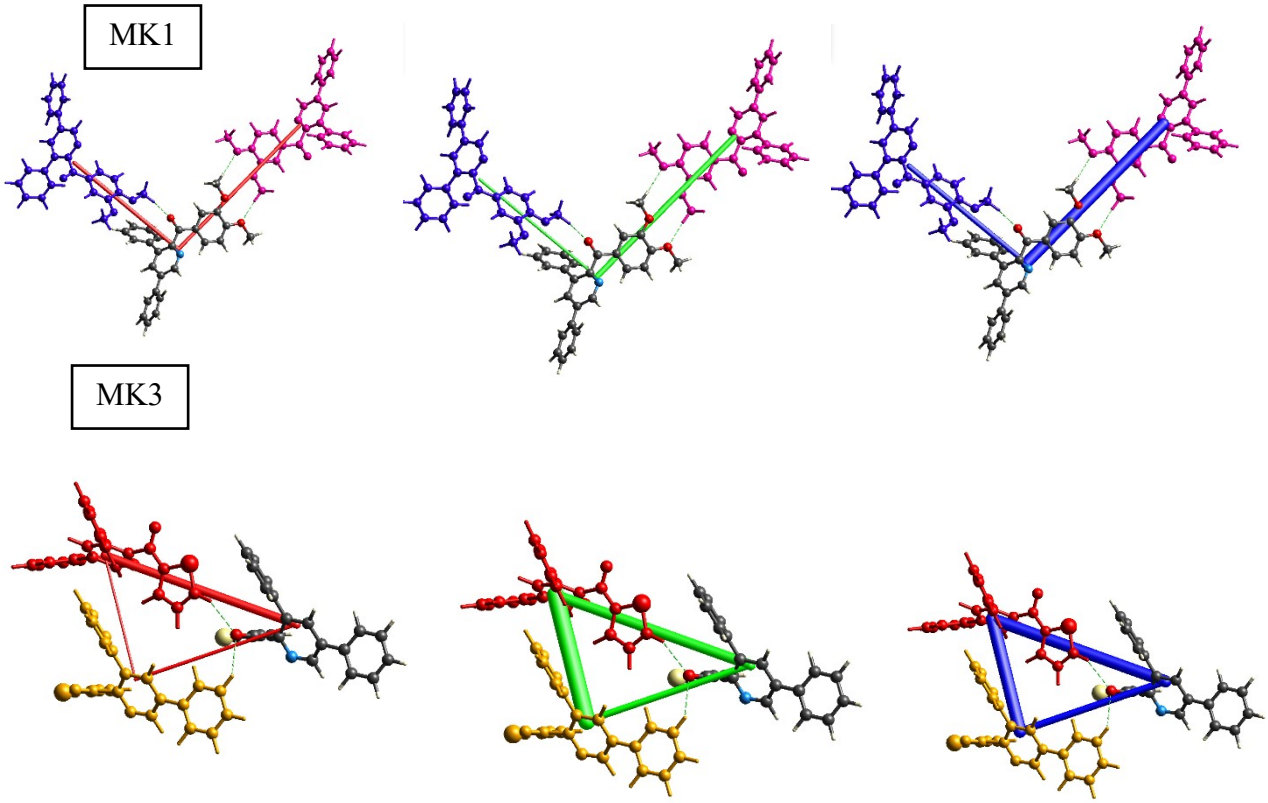


Figure S24: Energy framework diagrams for selected intermolecular molecular pairs involving C1–H1A···O3 and C26–H26A···O1 interactions in MK1, and C16–H16···O1 and C19–H19···O1 interactions in MK3, generated using energy framework analysis. The interaction energies are represented as cylindrical tubes having coulomb energy (red), dispersion energy (green), and total energy (blue) components with respect to unit cell axis respectively, respectively.

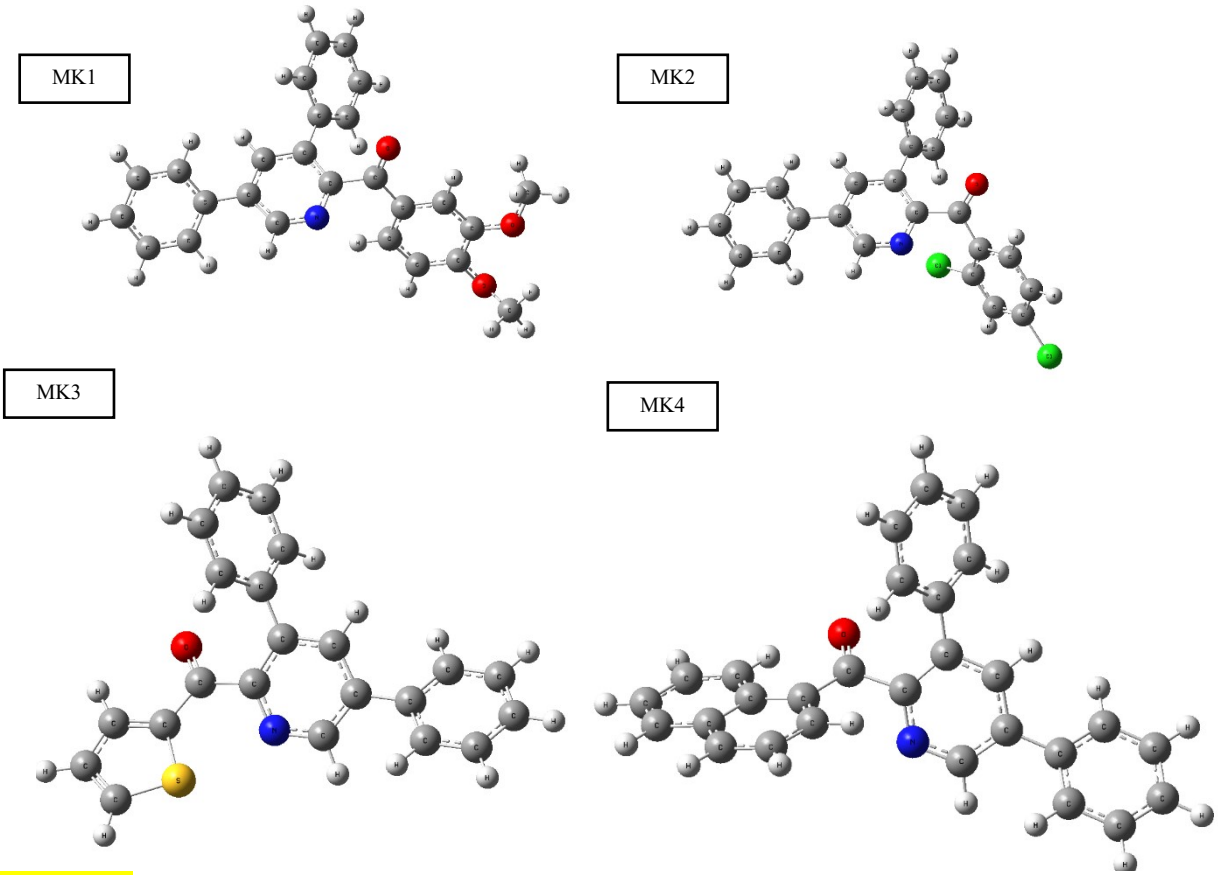


Figure S25: Three dimensional optimized geometries using B3LYP/6-311++G (d, p) level of theory

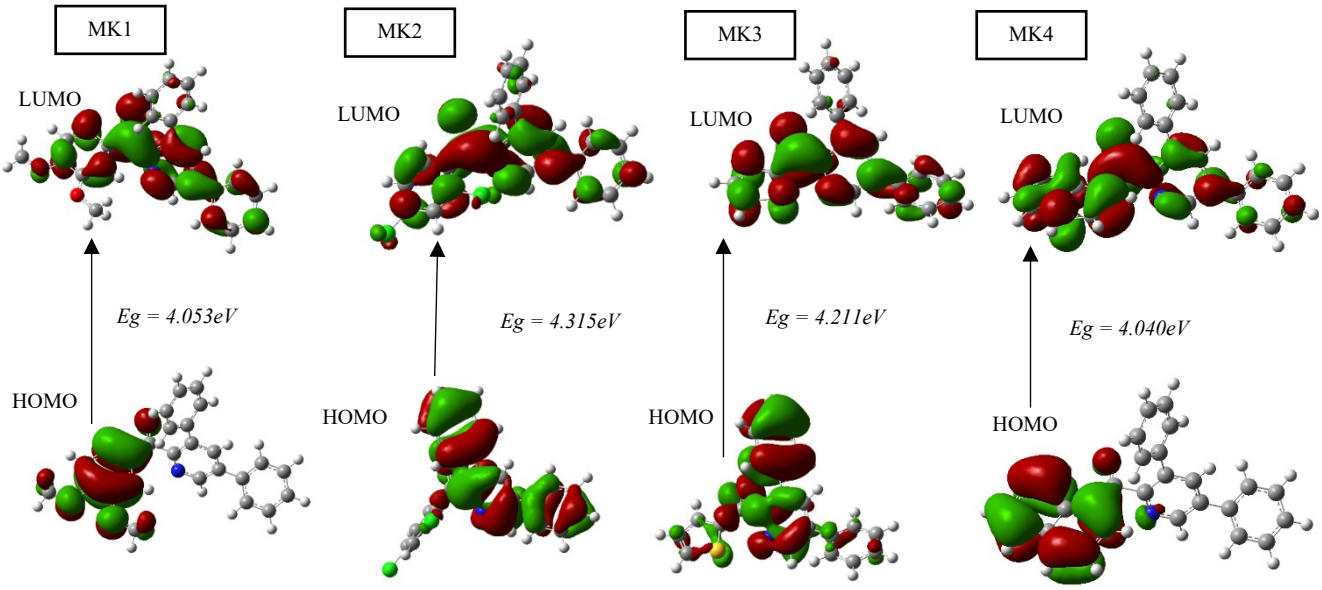


Figure S26: The frontier molecular orbital (FMO) plot of the optimized compounds

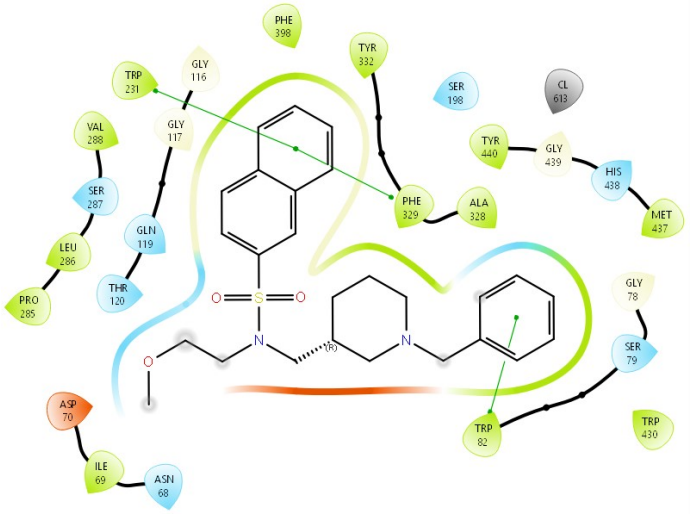


Figure S27: Two dimensional protein-cocrystal ligand (5HF) interaction plot interacting with neighboring amino acid residues of hBChE target

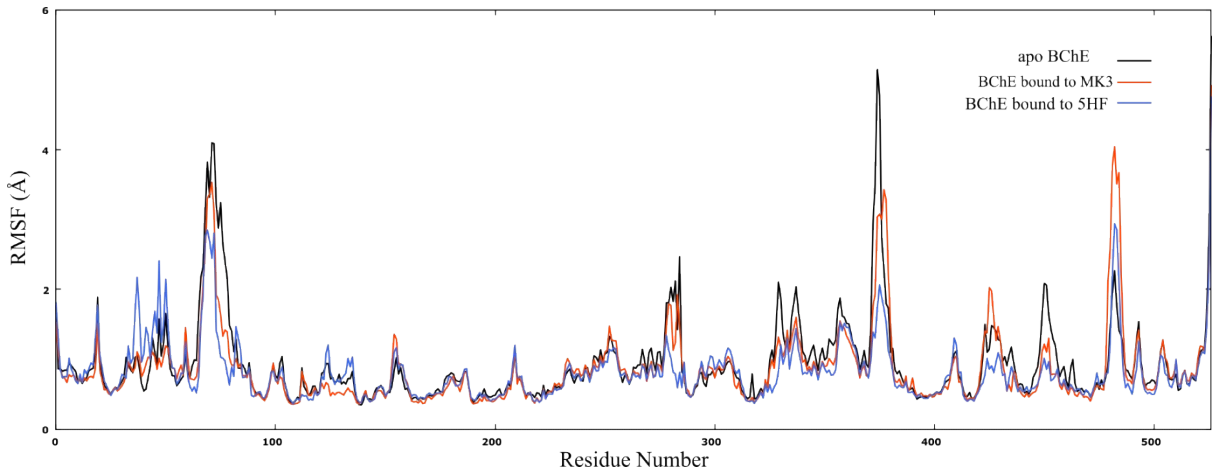


Figure S28: The RMSF plot shows residue-level flexibility across the hBChE structure in its apo form (black), MK3-bound complex (orange), and 5HF-bound complex (blue)

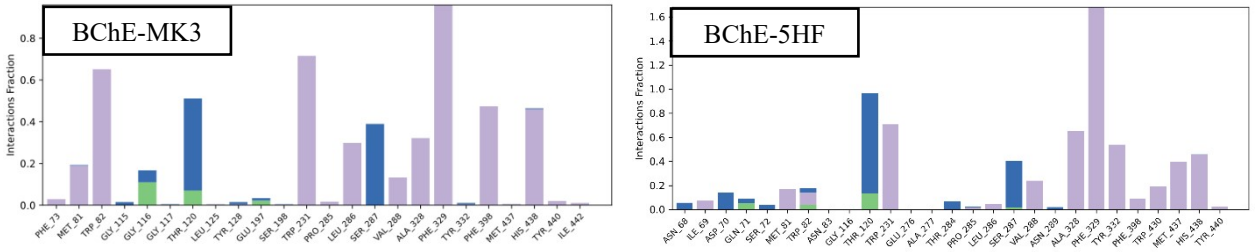


Figure S29: Protein-Ligand complex interaction profile highlights key residues involved in stabilising MK3 and 5HF relies predominantly on hydrophobic interactions along with a strong water-mediated bridge illustrating distinct binding mechanisms and stabilisation strategies for each ligand.

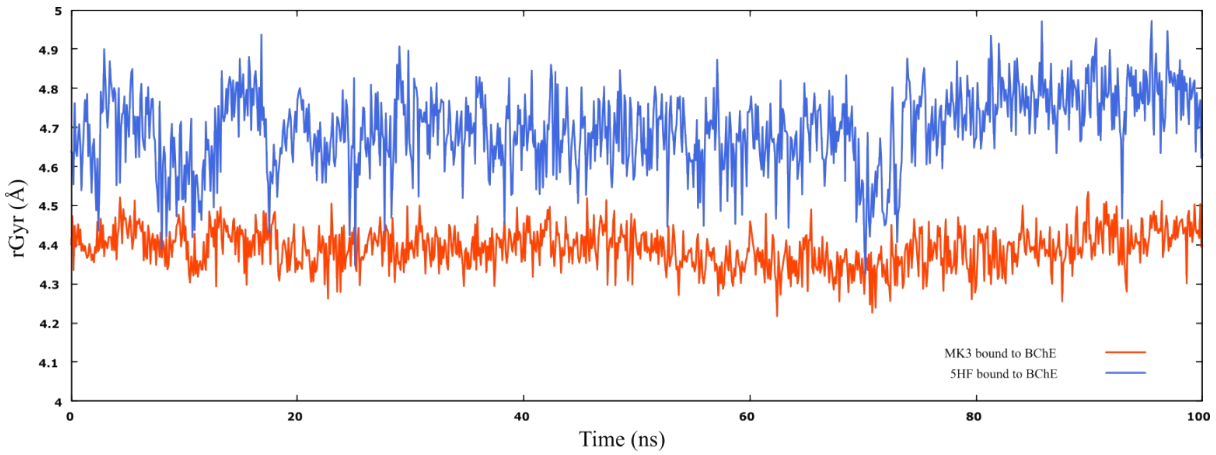


Figure S30: Radius of gyration (Rg) plots for MK3 (orange) and 5HF (bluee) show their conformational rigidity during the simulation.

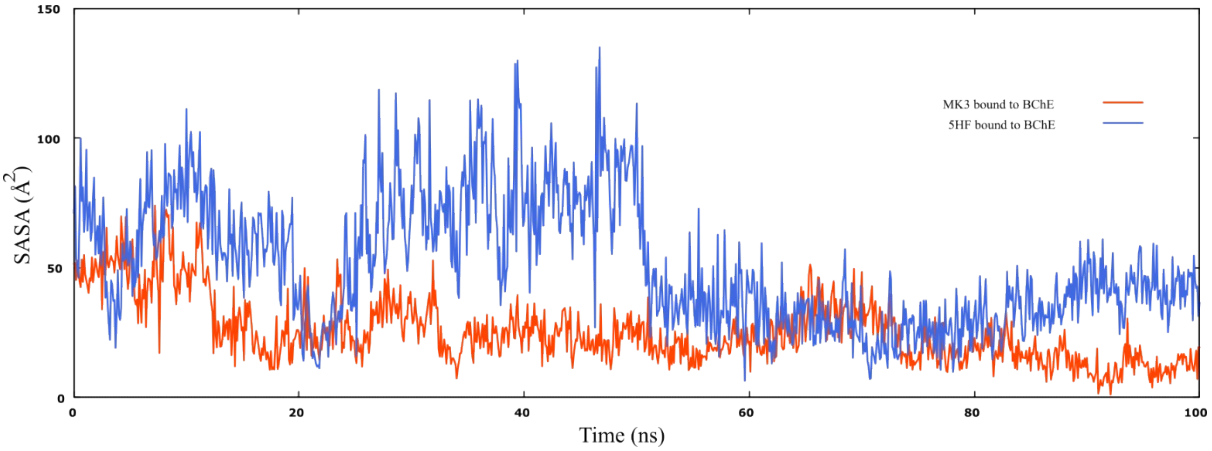


Figure S31: The SASA plots for MK3 and 5HF (co crystal ligand) revealing differences in solvent exposure over the simulation.

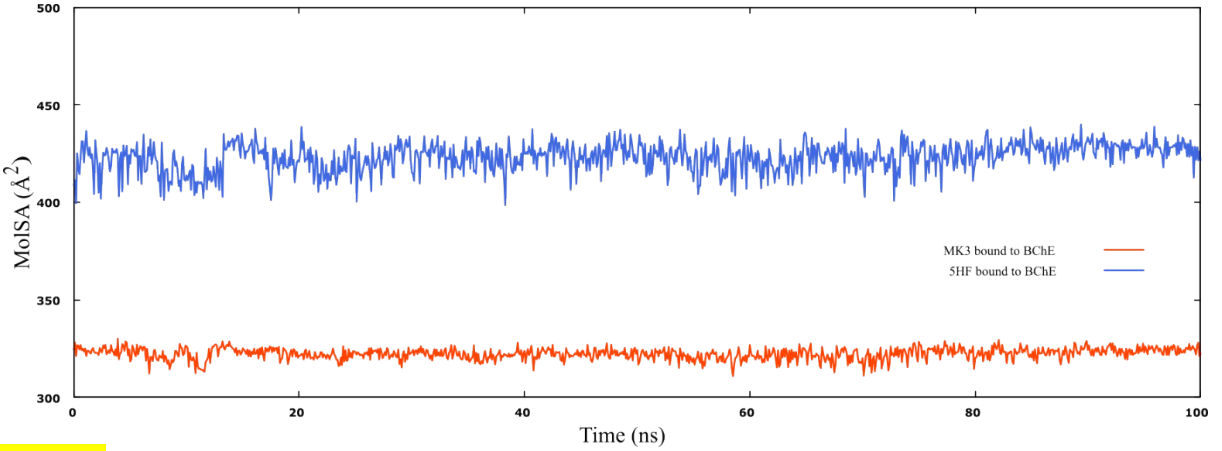


Figure S32: The Molecular Surface Area (MolSA) plots for MK3 and 5HF (co crystal ligand) revealing differences in total surface area of a molecule based on its van der Waals surface.