SUPLEMENTARY MATERIAL

Investigation on Molecular Structure, Vibrational Analysis and Thermodynamic Properties of 1-(2,6-dimethylmorpholine-4-yl-methyl)-3-methyl-4-[3-ethoxy-(4-benzenesulfonyloxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one

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Table 1. The calculated bond lengths (A^0) and bond angles (^{0}) of the title compound (6-31G(d,p) B3LYP)

	Bond Lengths	B3LYP 6-31G(d,p)		Bond Angels (^{0})	B3LYP 6-31G(d,p)
1	C(1)-N(58)	1.27	**1**	C(1)-N(58)-N(57)	105.315
2	C(1)-N(59)	1.39	**2**	C(1)-N(59)-N(60)	121.230
3	C(1)-C(16)	1.48	**3**	C(1)-N(59)-C(2)	108.100
4	C(16)-H(35)	1.09	**4**	C(1)-C(16)-H(35)	111.006
5	C(16)-H(36)	1.09	**5**	C(1)-C(16)-H(36)	111.021
6	C(16)-H(37)	1.09	**6**	C(1)-C(16)-H(37)	108.667
7	N(59)-C(2)	1.38	**7**	C(16)-C(1)-N(58)	125.330
8	C(2)-O(62)	1.21	**8**	C(16)-C(1)-N(59)	123.412
9	C(2)-N(57)	1.35	**9**	C(2)-N(59)-N(60)	130.667
10	N(57)-N(58)	1.38	**10**	C(2)-N(57)-N(58)	113.168
11	N(57)-C(17)	1.46	**11**	N(59)-C(2)-O(62)	128.572
12	C(17)-H(38)	1.08	**12**	O(62)-C(2)-N(57)	129.267
13	C(17)-H(39)	1.07	**13**	N(58)-N(57)-C(17)	121.497
14	C(17)-N(61)	1.42	**14**	C(2)-N(57)-C(17)	125.329
15	N(61)-C(18)	1.44	**15**	N(57)-C(17)-H(38)	106.173
16	C(18)-H(40)	1.07	**16**	N(57)-C(17)-H(39)	105.245
17	C(18)-H(41)	1.08	**17**	N(57)-C(17)-N(61)	117.141
18	C(18)-C(19)	1.50	**18**	H(38)-C(17)-H(39)	109.733
19	C(19)-H(42)	1.08	**19**	H(38)-C(17)-N(61)	109.217
20	C(19)-C(22)	1.51	**20**	H(39)-C(17)-N(61)	109.122
21	C(22)-H(46)	1.08	**21**	C(17)-N(61)-C(18)	114.917
22	C(22)-H(47)	1.07	**22**	C(17)-N(61)-C(21)	115.406
23	C(22)-H(48)	1.07	**23**	N(61)-C(18)-H(40)	108.913
24	C(19)-O(67)	1.39	**24**	N(61)-C(18)-H(41)	112.043
25	O(67)-C(20)	1.39	**25**	N(61)-C(18)-C(19)	109.587
26	C(20)-H(43)	1.08	**26**	H(40)-C(18)-C(19)	110.251
27	C(20)-C(23)	1.49	**27**	H(41)-C(18)-C(19)	108.523
28	C(23)-H(49)	1.08	**28**	C(18)-C(19)-O(67)	110.022
29	C(23)-H(50)	1.08	**29**	C(18)-C(19)-C(22)	112.808
30	C(23)-H(51)	1.07	**30**	C(18)-C(19)-H(42)	107.913
31	C(20)-C(21)	1.52	**31**	C(19)-C(22)-H(46)	110.760
32	C(21)-H(44)	1.08	**32**	C(19)-C(22)-H(47)	110.108
33	C(21)-H(45)	1.08	**33**	C(19)-C(22)-H(48)	110.499
34	C(21)-N(61)	1.43	**34**	H(42)-C(19)-C(22)	110.054
35	N(59)-N(60)	1.36	**35**	C(22)-C(19)-O(67)	107.154
36	N(60)-C(3)	1.24	**36**	H(42)-C(19)-O(67)	108.837
37	C(3)-H(26)	1.08	**37**	C(19)-O(67)-C(20)	112.838
38	C(3)-C(4)	1.47	**38**	O(67)-C(20)-C(23)	107.143
39	C(4)-C(5)	1.36	**39**	O(67)-C(20)-H(43)	108.873

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40	C(5)-H(27)	1.08
41	C(5)-C(6)	1.39
42	C(6)-O(63)	1.35
43	C(6)-C(7)	1.38
44	C(7)-O(64)	1.38
45	C(7)-C(8)	1.38
46	C(8)-H(28)	1.07
47	C(8)-C(9)	1.38
48	C(9)-H(29)	1.08
49	C(9)-C(4)	1.39
50	O(63)-C(24)	1.41
51	C(24)-H(52)	1.08
52	C(24)-H(53)	1.08
53	C(24)-C(25)	1.50
54	C(25)-H(54)	1.08
55	C(25)-H(55)	1.08
56	C(25)-H(56)	1.08
57	O(64)-S(68)	1.61
58	O(65)-S(68)	1.41
59	O(66)-S(68)	1.41
60	S(68)-C(10)	1.77
61	C(10)-C(11)	1.38
62	C(11)-H(30)	1.07
63	C(11)-C(12)	1.38
64	C(12)-H(31)	1.07
65	C(12)-C(13)	1.39
66	C(13)-H(32)	1.07
67	C(13)-C(14)	1.39
68	C(14)-H(33)	1.07
69	C(14)-C(15)	1.38
70	C(15)-H(34)	1.07
71	C(15)-C(10)	1.39

40	O(67)-C(20)-C(21)	110.063
41	H(43)-C(20)-C(21)	110.002
42	H(43)-C(20)-C(23)	107.858
43	C(20)-C(23)-H(49)	110.772
44	C(20)-C(23)-H(50)	110.532
45	C(20)-C(23)-H(51)	110.099
46	H(49)-C(23)-H(50)	108.616
47	H(49)-C(23)-H(51)	108.569
48	H(50)-C(23)-H(51)	108.182
49	C(23)-C(20)-C(21)	112.851
50	C(20)-C(21)-H(44)	109.871
51	C(20)-C(21)-H(45)	108.950
52	H(44)-C(21)-H(45)	107.585
53	H(44)-C(21)-N(61)	107.585
54	H(45)-C(21)-N(61)	108.781
55	N(59)-N(60)-C(3)	118.769
56	N(60)-C(3)-H(26)	122.064
57	N(60)-C(3)-C(4)	119.927
58	H(26)-C(3)-C(4)	118.008
59	C(3)-C(4)-C(5)	118.311
60	C(3)-C(4)-C(9)	122.514
61	C(4)-C(5)-H(27)	120.710
62	C(4)-C(5)-C(6)	121.021
63	H(27)-C(5)-C(6)	118.261
64	C(5)-C(6)-O(63)	119.912
65	C(5)-C(6)-C(7)	118.803
66	C(6)-O(63)-C(24)	114.508
67	O(63)-C(24)-H(52)	108.059
68	O(63)-C(24)-H(53)	109.466
69	O(63)-C(24)-C(25)	108.930
70	H(52)-C(24)-C(25)	111.314
71	H(53)-C(24)-C(25)	110.874
72	H(52)-C(24)-H(53)	108.166
73	C(24)-C(25)-H(54)	109.906
74	C(24)-C(25)-H(55)	110.824
75	C(25)-C(25)-H(56)	110.688
76	H(54)-C(25)-H(55)	108.248
77	H(54)-C(25)-H(56)	108.530
78	H(55)-C(25)-H(56)	108.574
79	C(7)-O(64)-S(68)	117.018
80	O(64)-C(7)-C(8)	120.547
81	C(6)-C(7)-C(8)	120.853
82	C(7)-C(8)-H(28)	118.783
83	C(7)-C(8)-C(9)	119.904
84	H(28)-C(8)-C(9)	121.312
85	C(8)-C(9)-C(4)	120.239
86	H(29)-C(9)-C(4)	119.173
87	O(64)-S(68)-O(65)	105.967
88	O(64)-S(68)-O(66)	107.914
89	O(65)-S(68)-O(66)	121.264
90	O(64)-S(68)-C(10)	98.609
91	O(65)-S(68)-C(10)	109.399
92	O(66)-S(68)-C(10)	110.134
93	S(68)-C(10)-C(11)	119.036
94	S(68)-C(10)-C(15)	118.754
95	C(10)-C(11)-H(30)	119.821
96	C(10)-C(11)-C(12)	118.590
97	C(10)-C(15)-C(14)	118.462
98	H(30)-C(11)-C(12)	121.588
99	C(11)-C(12)-C(13)	120.104

100	C(11)-C(12)-H(31)	119.675
101	H(31)-C(12)-C(13)	120.220
102	C(12)-C(13)-C(14)	120.454
103	H(32)-C(13)-C(14)	119.748
104	C(13)-C(14)-H(33)	120.120
105	H(33)-C(14)-C(15)	119.672
106	H(34)-C(15)-C(10)	120.163

Table 2. The calculated Mulliken atomic charges of the title compound

Atoms	DFT	Atoms	DFT
C1	0.52	**H35**	0.14
C2	0.85	**H36**	0.14
C3	0.12	**H37**	0.14
C4	0.09	**H38**	0.13
C5	-0.16	**H39**	0.14
C6	0.33	**H40**	0.11
C7	0.29	**H41**	0.09
C8	-0.09	**H42**	0.08
C9	-0.16	**H43**	0.08
C10	-0.19	**H44**	0.10
C11	-0.08	**H45**	0.10
C12	-0.09	**H46**	0.12
C13	-0.07	**H47**	0.10
C14	-0.09	**H48**	0.12
C15	-0.07	**H49**	0.10
C16	-0.36	**H50**	0.11
C17	0.08	**H51**	0.12
C18	-0.03	**H52**	0.12
C19	0.18	**H53**	0.10
C20	0.18	**H54**	0.11
C21	-0.02	**H55**	0.12
C22	-0.33	**H56**	0.13
C23	-0.33	**N57**	-0.39
C24	0.06	**N58**	-0.34
C25	-0.34	**N59**	-0.43
H26	0.16	**N60**	-0.32
H27	0.11	**N61**	-0.43
H28	0.13	**O62**	-0.56
H29	0.11	**O63**	-0.55
H30	0.14	**O64**	-0.62
H31	0.11	**O65**	-0.51
H32	0.10	**O66**	-0.45
H33	0.11	**O67**	-0.51
H34	0.15	**S68**	1.25

Table 3. All calculated and selected IR frequencies of the title compound (6-31G(d,p))

Vibrational Frequencies (%PED)	Experimental	Scaled DFT
τ CCCC(10), τ NCNN(23), τ COSC(14)		10
τ COSC(44), τ NCCC(21)		12
τ COSC(19), τ NCCC(11), τ CNCN(28), τ CNNC(11)		16
τ CCOS(17), τ OSCC(10)		20
τ CNCN(34), τ CCNN(16)		26
τ OSCC(53)		31
τ CCNN(27)		33
τ CCOS(39), τ CNCN(19)		41
τ COCC(47)		51
τ COCC(18), τ NCNN(12)		57
τ CCOS(16), τ CNCN(14)		60
τ OSCC(11), τ CCOC(37)		70
τ CCOC(17), τ SCCC(18)		79
τ CNNC(11), τ CCNC(10)		93
δ COC(23), τ OCCC(27)		107
τ CNNC(12), τ CCNC(13)		120
τ COCC(16)		141
δ COC(11), τ COCC(15), τ HCCC(10), τ CCOC(22)		149
τ HCCC(50)		153
τ COCC(31)		157
δ SCC(21), τ CNNC(10)		169
δ SCC(27)		170
τ CNNC(12)		177
δ CCN(18)		188
τ NCCC(11)		196
τ HCCC(60)		199
τ HCCC(22)		209
τ HCCC(20)		217
δ CCO(18), δ OCC(12), δ OSO(11)		222
δ CCO(16)		234
δ CCO(43)		244
τ HCOC(26), τ HCCO(10)		253
τ CCCC(19), τ NCNN(20)		267
ν SC(35), δ OSO(14)		295
δ CCN(17), δ CCO(18)		301
δ CCO(12)		312
δ COC(12), τ CCCC(17)		316
δ CCN(10), δ OCN(12)		328
τ CNNC(19)		334
δ OSO(10)		350
δ CNC(12), τ CCCN(10)		371
τ CCOC(18)		387

δ OCN(13), δ NNC(14)		390
τ HCCS(14), τ CCCC(73)		397
δ OSO(22), τ OCOS(16), τ CCCC(10)		419
δ COC(16), δ CCO(20), τ HCNC(10)		426
δ CNC(20), δ CCO(22)		434
τ CCCC(10)		446
τ CCCC(19)		457
ν OC(11), ν CC(13), δ COC(13), τ CCOC(17)		463
τ CCOC(42)		473
δ COC(22)		486
δ OCC(16), τ SCCC(10)		493
δ OSO(31)		513
δ NCN(10)		549
δ CCC(12)		569
δ CCC(15)		579
δ CCC(14)		587
δ CCC(74)		602
ν CC(10)		604
τ NNCN(24), τ CNNC(11)		614
ν SO(32)		625
δ CCC(10), τ CCCC(18)		633
ν SO(10)		648
τ SCCC(13), τ CCCC(52), τ HCCC(20)	605	671
τ ONNC(43)		680
δ CNN(15), τ ONNC(31)		699
ν SC(23), δ CCC(14)		704
τ CCCC(22)		720
τ HCCS(62), τ HCCC(17)		736
τ HCCC(16)		754
ν OC(11), τ HCOC(13)		793
τ HCOC(26)		795
δ NCC(12)		810
ν OC(31)		815
τ HCCC(62)	754	826
τ HCCS(98)		827
ν NC(34), τ HCCC(10)		834
ν CC(21), δ CCN(20), τ HCCC(12)		843
ν OC(21), ν CC(10), τ HCCC(10)		854
τ OCCC(10), τ HCCC(27)		876
τ HCCC(11), τ HCNC(25)		891
ν NC(10), ν CC(19), τ HCCC(10)		905
τ HCCS(34), τ CCCC(11)		909
ν NC(12), ν NN(16), δ NNC(12)		914
ν CC(18), δ CNC(18), τ HCNC(12)		928

ν NC(11), ν CC(10), ν OC(14), τ HCNC(10)		939
τ HCCC(49), τ CCCC(11)		940
ν CC(14), δ CCC(19)		947
τ HCCS(80), τ CCCC(14)		950
ν OC(10), τ HCNC(11)		957
τ HCCS(51), τ HCCC(31), τ CCCC(10)		973
ν CC(20), δ CCC(32)		975
τ HCNN(88)		977
τ HCCC(20)		995
ν CC(20), δ CCC(43)		1008
ν OC(40), ν CC(42)		1020
τ HCCC(49)		1028
ν NC(11)		1049
ν SO(15)		1051
ν NC(11), ν CC(13)		1056
ν CC(30), ν OC(18), δ HCC(22)		1067
ν CC(20), δ HCC(11)		1067
δ HCC(15)		1085
δ HCN(11)		1086
ν CC(11), δ CCO(12), τ HCCO(18)		1097
ν NC(13)		1099
ν SO(63)	1171	1114
ν CC(15), τ HCCC(20)		1122
ν OC(28)		1122
δ HCO(36), τ HCOC(19)		1139
ν CC(18)		1144
ν CC(11), δ HCC(33)		1145
ν CC(10), δ HCC(30)		1146
ν CC(16), δ HCC(67)		1161
ν OC(16), τ CCOC(11)		1165
ν OC(19), δ HCC(17)		1168
δ HCN(16)		1194
ν NN(15), δ HCN(21)		1217
ν OC(15), δ HCC(38)		1230
ν NN(14), δ HCN(10), δ NCN(12)		1239
δ HCO(53), τ HCOC(16)		1255
ν CC(12), ν OC(11), δ HCC(10)		1268
τ HCNC(16)		1271
τ HCNC(21)		1284
ν CC(14), δ HCC(56)		1292
ν CC(27)		1293
ν SO(70), δ HCC(11)		1296
ν NC(12), δ HCN(12)		1297
δ HCC(60)		1311

ν NC(12), δ HCN(15), δ HCC(10), τ HCNC(14)		1314
ν CC(52), ν SO(16), δ HCC(12)		1315
δ HCN(37)		1334
δ HCN(12), τ HCNC(30)		1348
δ HCH(43), τ HCOC(17)		1351
δ HCH(11), δ HCC(13), τ HCNC(12)		1360
δ HCH(13), δ HCN(10), τ HCNC(16)		1362
δ HCN(15), τ HCNC(16)		1365
δ HCH(36)		1367
δ HCH(15)		1371
δ HCH(10), τ HCNC(37)		1377
δ HCH(17), τ HCOC(10)		1379
ν CC(11), δ HCC(32), ν SO(42)	1375	1386
ν NC(10)		1395
δ HCH(19)		1410
δ HCN(12)		1415
δ HCH(12), τ HCCC(12)		1428
ν CC(19), δ HCC(31)		1432
δ HCH(29)		1434
δ HCH(22), τ HCCC(16)		1439
δ HCH(39), τ HCOC(12)		1441
δ HCH(33), τ HCOC(10)		1442
δ HCH(23), τ HCCC(13)		1443
δ HCH(31)		1452
δ HCH(31)		1455
δ HCH(57), τ HCCO(13)		1458
δ HCH(30)		1458
δ HCC(71)		1464
δ HCH(29)		1479
δ HCC(42), δ CCO(10)		1481
ν CC(33)		1557
ν CC(32), δ CCC(11), δ HCC(16)		1578
ν CC(31)		1580
ν CC(30), δ HCC(11)		1588
ν NC(46)	1575	1592
ν NC(57)	1603	1611
ν OC(75), ν NC(11)	1705	1724
ν CH(44)		2843
ν CH(29)		2854
ν CH(42)		2862
ν CH(50)		2867
ν CH(50)		2907
ν CH(55)		2936
ν CH(51)		2936

ν CH(38)	2941
ν CH(92)	2944
ν CH(56)	2955
ν CH(49)	2959
ν CH(40)	2962
ν CH(35)	2973
ν CH(99)	3002
ν CH(61)	3007
ν CH(31)	3007
ν CH(44)	3012
ν CH(18)	3015
ν CH(16)	3016
ν CH(51)	3019
ν CH(57)	3021
ν CH(91)	3044
ν CH(28)	3052
ν CH(53)	3068
ν CH(30)	3079
ν CH(71)	3080
ν CH(48)	3088
ν CH(47)	3089
ν CH(44)	3103
ν CH(44)	3105
ν CH(47)	3107