Supporting Information for

A Green Tandem Cyclization Approach to Substituted 2-Aminothiazoles *via* Molecular Sieve/I_2 Catalysis: DFT, Molecular dockings, and Pharmacokinetic Profiles

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Table S1. The calculated and observed (in parentheses) frequencies (in cm^{-1})

	PhTA	**BFTA**	**FTA**	**ThTA**	**NapTA**
$\nu NH2_{(as.)}$	3529 (3430)	3531 (3435)	3528 (3431)	3531 (3342)	3530 (3421)
$\nu NH2_{(sym.)}$	3425 (3421	3426 (3289)	3424 (3268)	3426 (3260)	3426 (3244)
$\nu CH_{(ar.)}$	3129-3033 (3121)	3128-3038 (3119)	3147-3111 (2962)	3128-3065	3128-3029 (3121)
νCH2	---	2922-2854 (2923)	---	---	---
βNH2	1628 (1591)	1627 (1634)	1629 (1631)	1628 (1627)	1628 (1621)
βNH2+ νCC	1622 (1523)	1637 (1532)	1603 (1524)	1571,1550 (1554)	1620- 1558 (1589)
νCC	1599-1204	1600-1210 (1493)	1527-1220 (1452)	1514-1058 (1518)	1646- 1219 (1523)
νN=C	1559 (1477)	1560 (1480)	1555	1571,1550	1558 (1493)
νN-C	1347-1286 (1442)	1331-1286 (1443)	1330-1293 (1324)	1380-1289 (1360)	1372- 1286 (1358)
βNH2	1559-288 (1334)	1560-281 (1323)	1555-278 (1211)	1514-287 (1321)	1539- 275 (1180)
ipbHCC	1495-1029 (1301	1491-1038 (1296)	1487-1020 (1148)	1514-1015 (1283)	1646- 1027 (1327)
νC-O	---	1061,905 (1035)	1229, 1094 (1041)	---	
βCCC	1086-406 (1193)	1112-413 (1123)	1094-448 (1002)	1058-471 (1077)	1027- 455
opbHCC	988-406 (1068)	1010-413	866-504 (801)	896-471 (1048)	980- 400 (1031)
νS-C	827,671	808, 666	808, 663 (801)	787, 736, 671, 629	792, 667

* The abbreviations are defined as: ν, stretching; β, bending; ipb, in-plane bending; opb, out-of-pane bending.

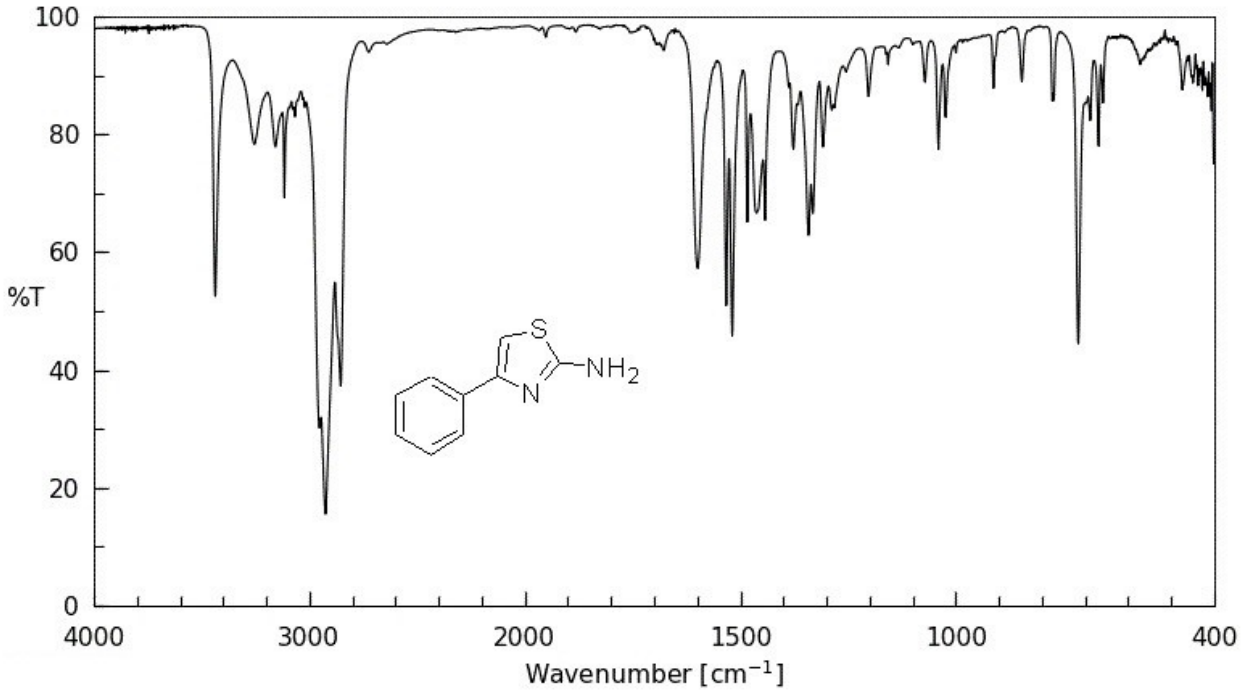

Fig. S1a. The recorded *FT-IR* spectrum of the compound PhTA

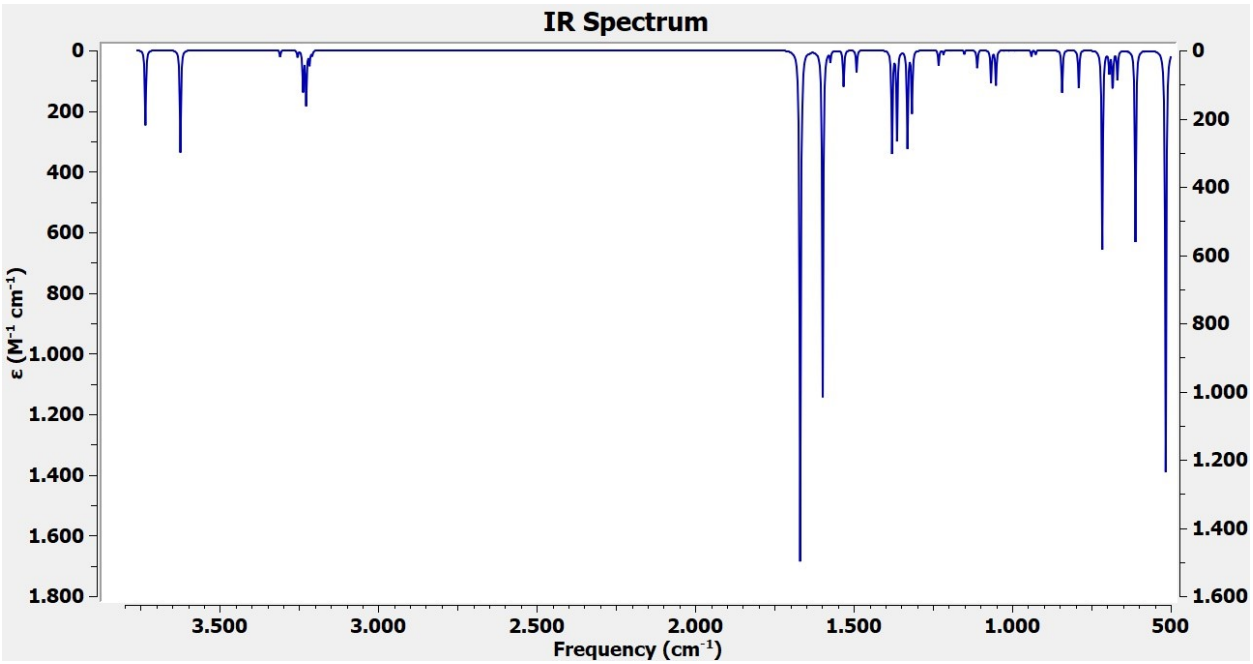

Fig. S1b. The calculated *FT-IR* spectrum of the compound PhTA

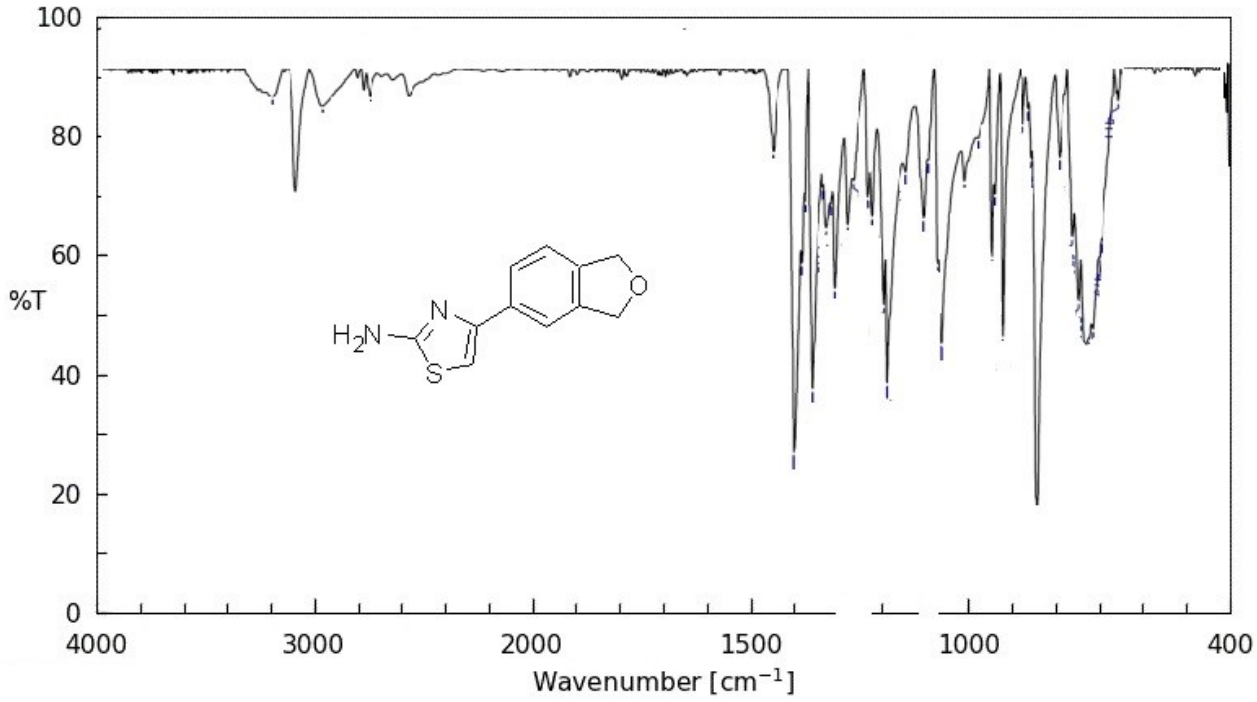

Fig. S2a. The recorded *FT-IR* spectrum of the compound BFTA

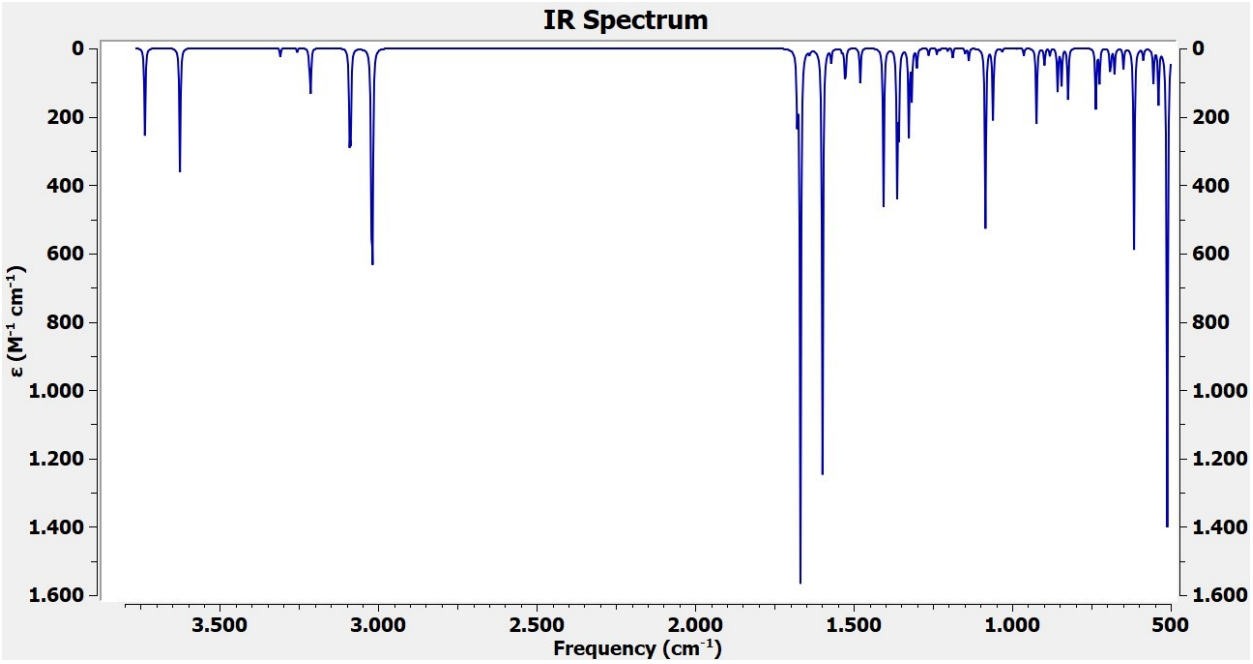

Fig. S2b. The calculated *FT-IR* spectrum of the compound BFTA

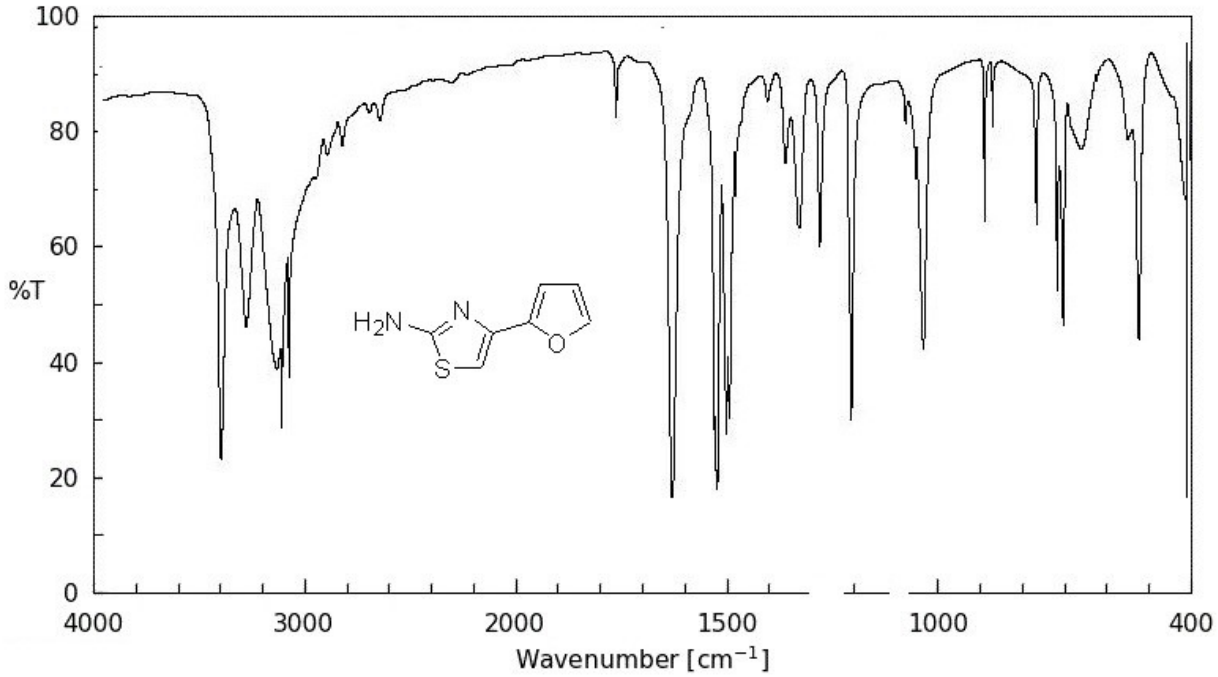

Fig. S3a. The recorded *FT-IR* spectrum of the compound FTA

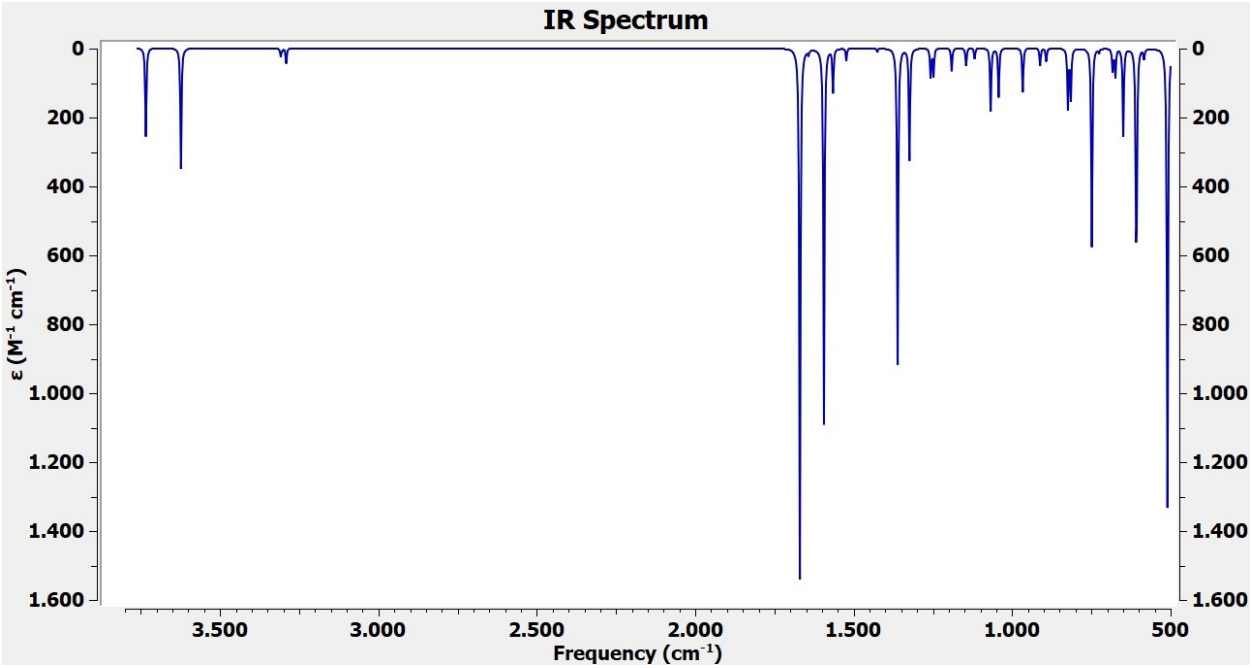

Fig. S3b. The calculated *FT-IR* spectrum of the compound FTA

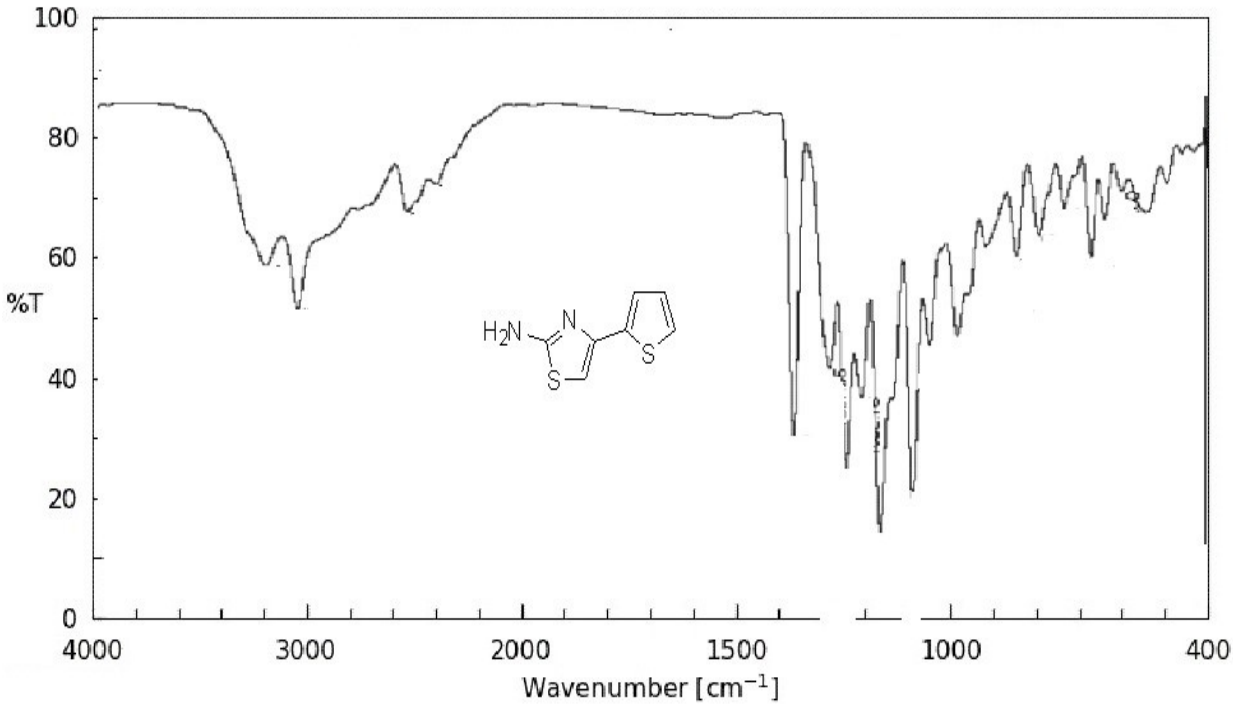

Fig. S4a. The recorded *FT-IR* spectrum of the compound THTA

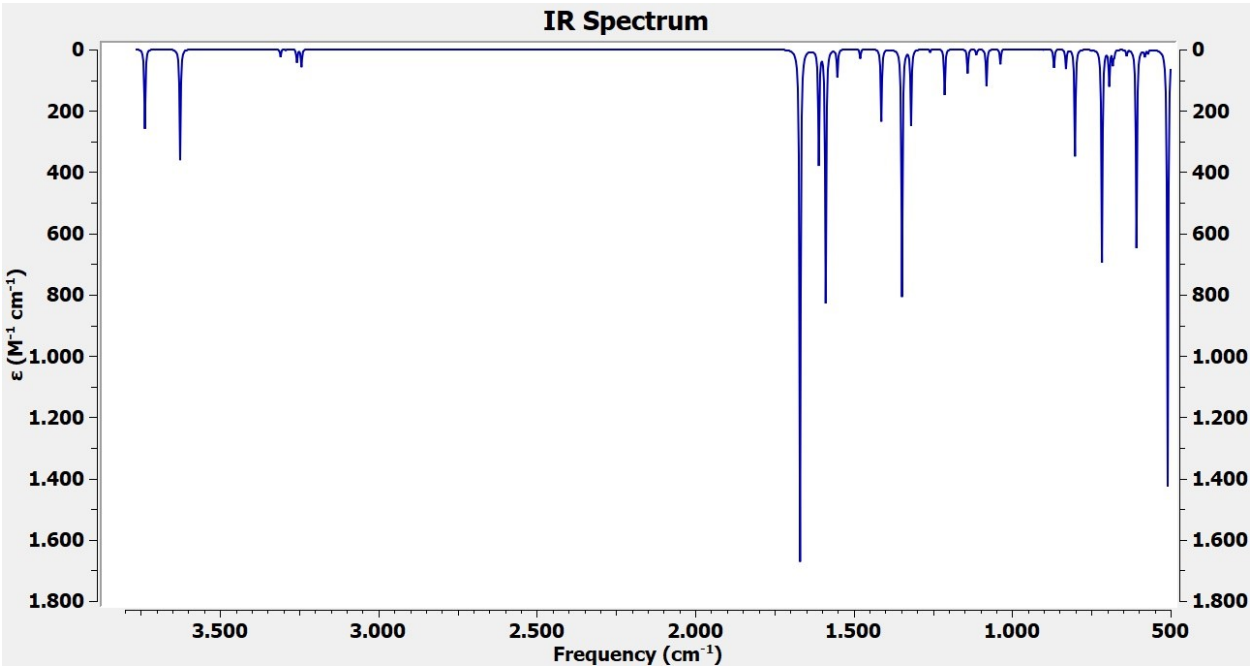

Fig. S4b. The calculated *FT-IR* spectrum of the compound THTA

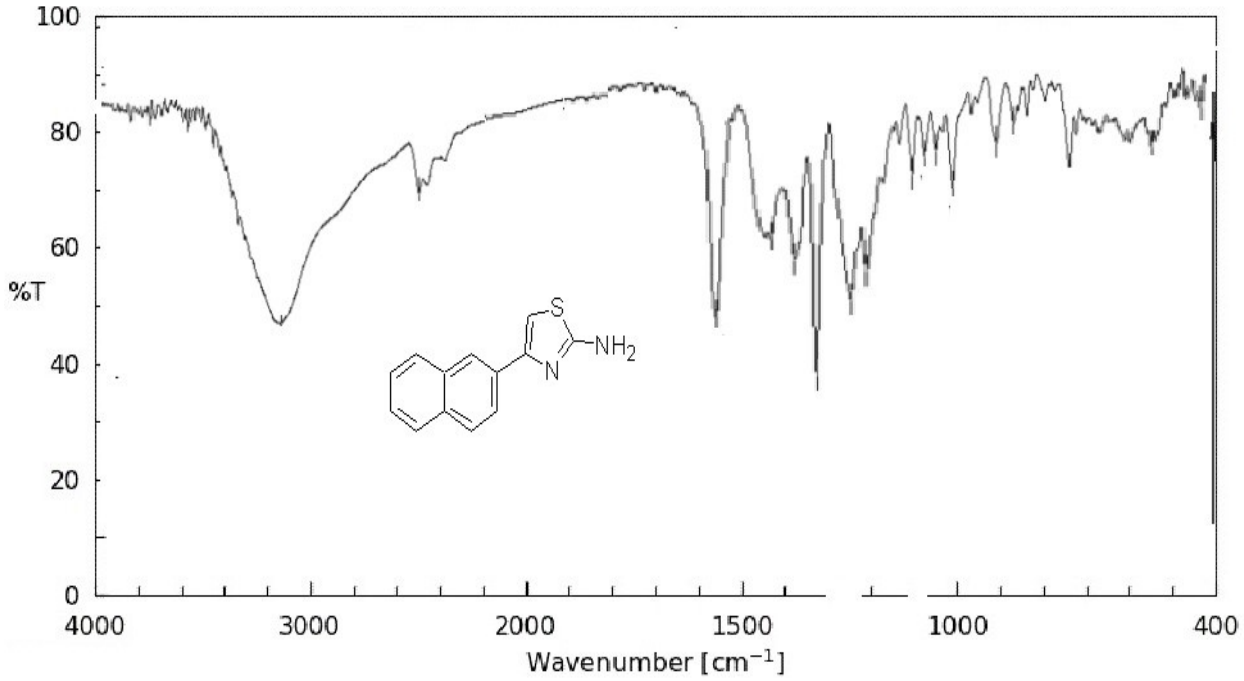

Fig. S5a. The recorded *FT-IR* spectrum of the compound NapTA

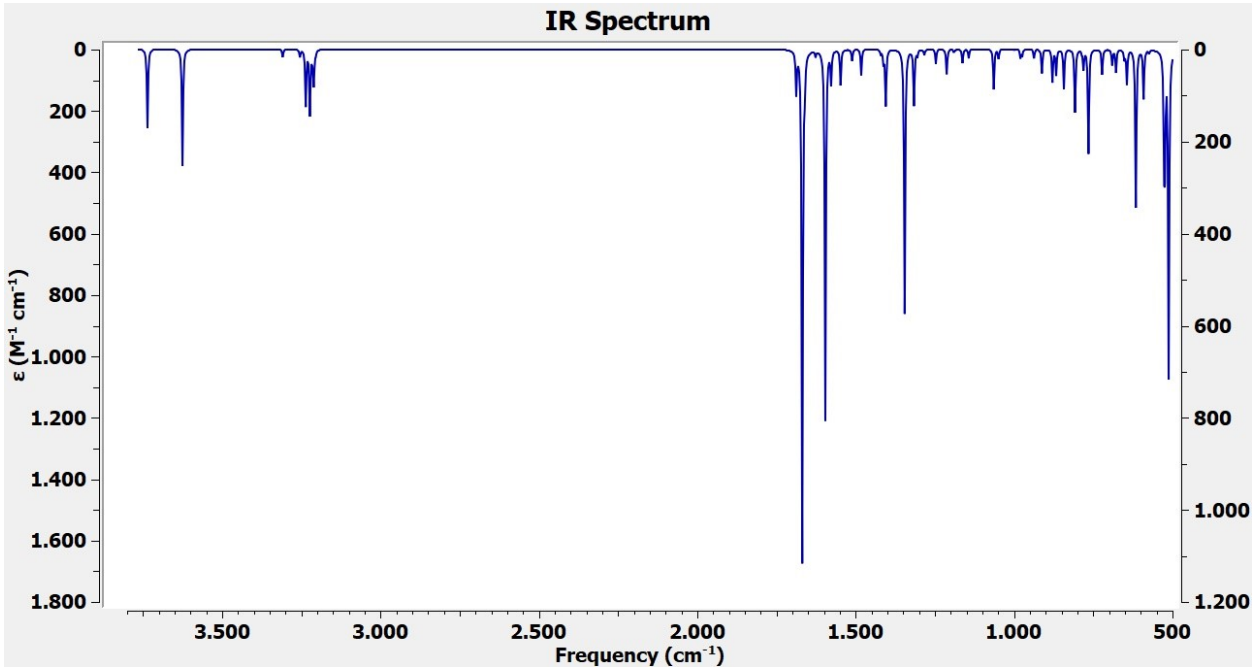

Fig. S5b. The calculated *FT-IR* spectrum of the compound NapTA

Table S2. The NMR chemical shifts

	PhTA (in $CDCl_3$)		BFTA (in DMSO)		FTA (in DMSO)		ThTA (in $CDCl_3$)		NapTA (in DMSO)	
Atom	***Exp.***	***Calc.***	***Exp.***	***Calc.***	***Exp.***	***Calc.***	***Exp.***	***Calc.***	***Exp.***	***Calc.***
^{13}C NMR										
1-C	127.5	134.1	101.1	80.2	167.6	179,8	166.6	177.8	167.2	179,6
2-C	129.3	135.6	---	---	141.2	149,3	137.5	152.4	148.8	158,4
3-C	126.9	134.0	102.1	80.2	105.0	113,8	102.2	111.0	101.5	115,3
4-C	128.3	135.1	146.2	147.9	---	---	---	---	---	---
5-C	124.4	131.1	118.4	127.9	---	---	---	---	---	---
6-C	135.5	142.8	128.5	133.2	---	---	---	---	---	---
7-C	---	---	145.4	142.3	---	---	---	---	---	---
8-C	---	---	107.3	123.7	---	---	---	---	---	---
9-C	---	---	148.1	149.1	---	---	---	---	---	---
10-C	---	---	---	---	151.6	159,6	143.3	153.9	125.8	132,6
11-C	---	---	---	---	101.5	112,7	122.5	126.7	127.5	135,3
12-C	168.4	178.1	---	---	----	---	---	---	128.1	140,6
13-C	152.1	157.9	---	---	112.6	119,2	123.4	133.1	131.3	141,2
14-C	101.6	114.0	---	---		---	---	---	123.1	130,7
15-C	---	---	---	---	140.8	149,4	127.5	137.2	132.1	140,8
17-C	---	---	167.1	179.3	---	---	---	---	---	---
18-C	---	---	148.5	157.8	---	---	---	---	---	---
19-C	---	---	104.9	114.3	---	---	---	---	126.8	135,0
20-C	---	---	---	---	---	---	---	---	127.9	135,4
22-C	---	---	---	---	---	---	---	---	126.4	133,4
23-C	---	---	---	---	---	---	---	---	124.8	133,0
^{1}H NMR										
5-H	---	---	---	---	6.73	6.92	6.58	6.87	7.48	7.25
7-H	7.75	8.44	---	---	---	---	---	---	---	---
8-H	7.35	7.67	---	---	6.51	4.68	5.53	4.41	7.10	4.70
9-H	7.28	7.49	---	---	6.51	4.96	5.53	4.81	7.10	5.03
10-H	7.35	7.61	6.11	5.35	---	---	---	---	---	---
11-H	7.75	8.02	6.94	5.38	---	---	---	---	---	---
12-H	---	---	6.11	5.34	---	---	---	---	---	---
13-H	---	---	6.85	5.37	---	---	---	---	---	---
14-H	---	---	7.02	7.56	7.10	6.96	7.30	7.58	---	---
15-H	---	---	7.33	8.25	---	---	---	---	---	---
16-H	6.85	7.03	7.33	7.90	6.73	6.73	7.01	7.17	7.87	8.22
17-H	---	---	---	---	7.62	7.69	7.20	7.37	7.97	8.53
18-H	---	---	---	---	---	---	---	---	7.97	8.28
19-H	5.48	4.45	---	---	---	---	---	---	---	---
20-H	5.59	4.88	---	---	---	---	---	---	---	---
21-H	---	---	7.02	7.06	---	---	---	---	8.35	8.59
24-H	---	---	3.43	4.65	---	---	---	---	7.97	8.28
25-H	---	---	3.43	4.97	---	---	---	---	7.87	7.83
26-H	---	---	---	---	---	---	---	---	7.52	7.80

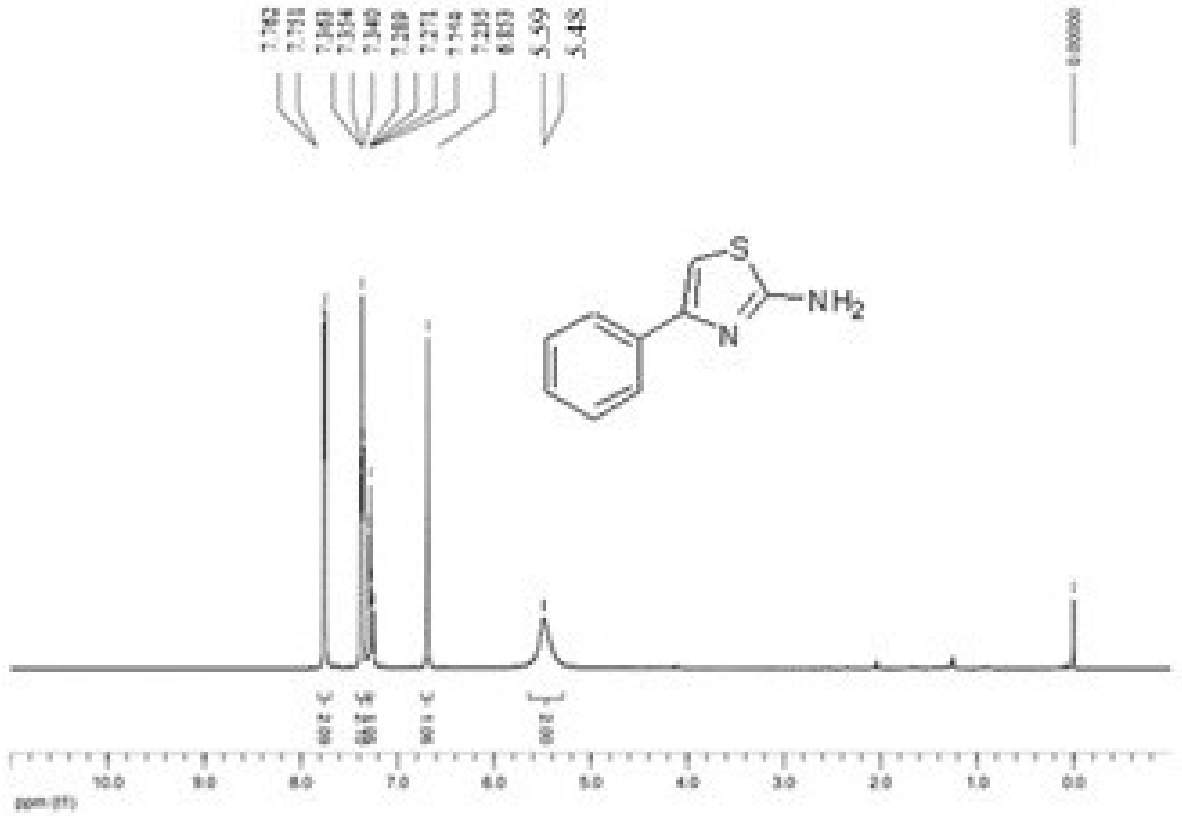

Fig. S6a. The recorded *^{1}H NMR* spectrum of the compound PhTA

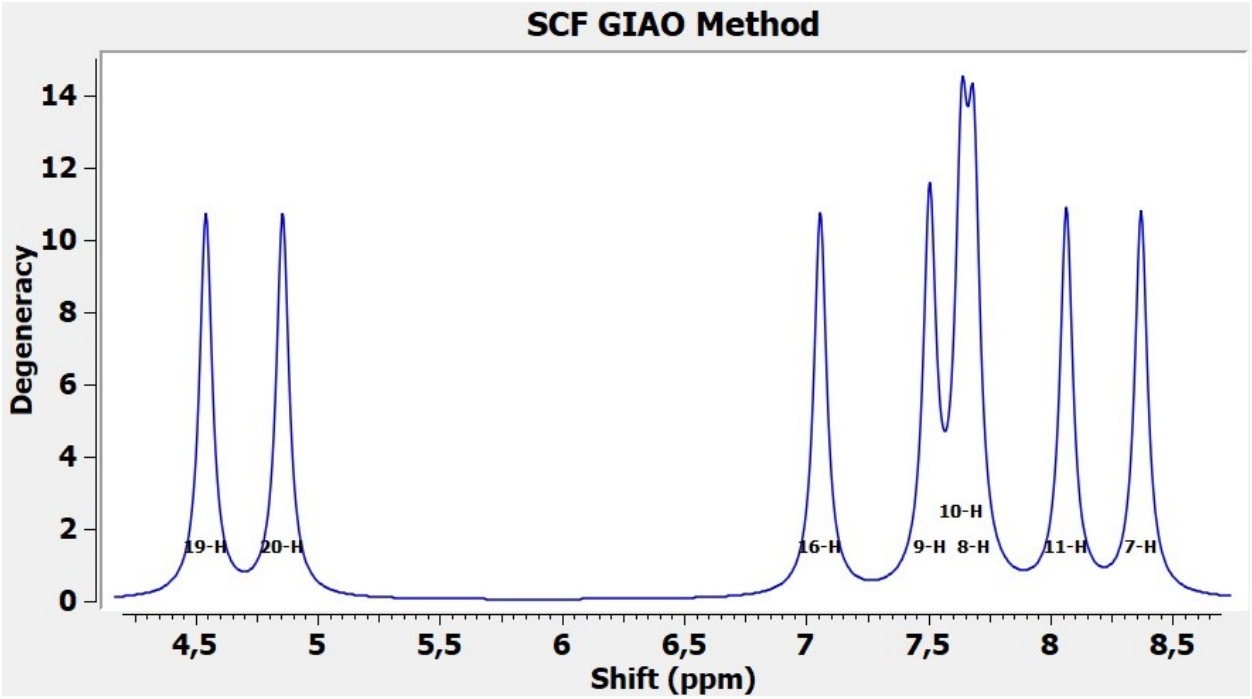

Fig. S6b. The calculated *^{1}H NMR* spectrum of the compound PhTA

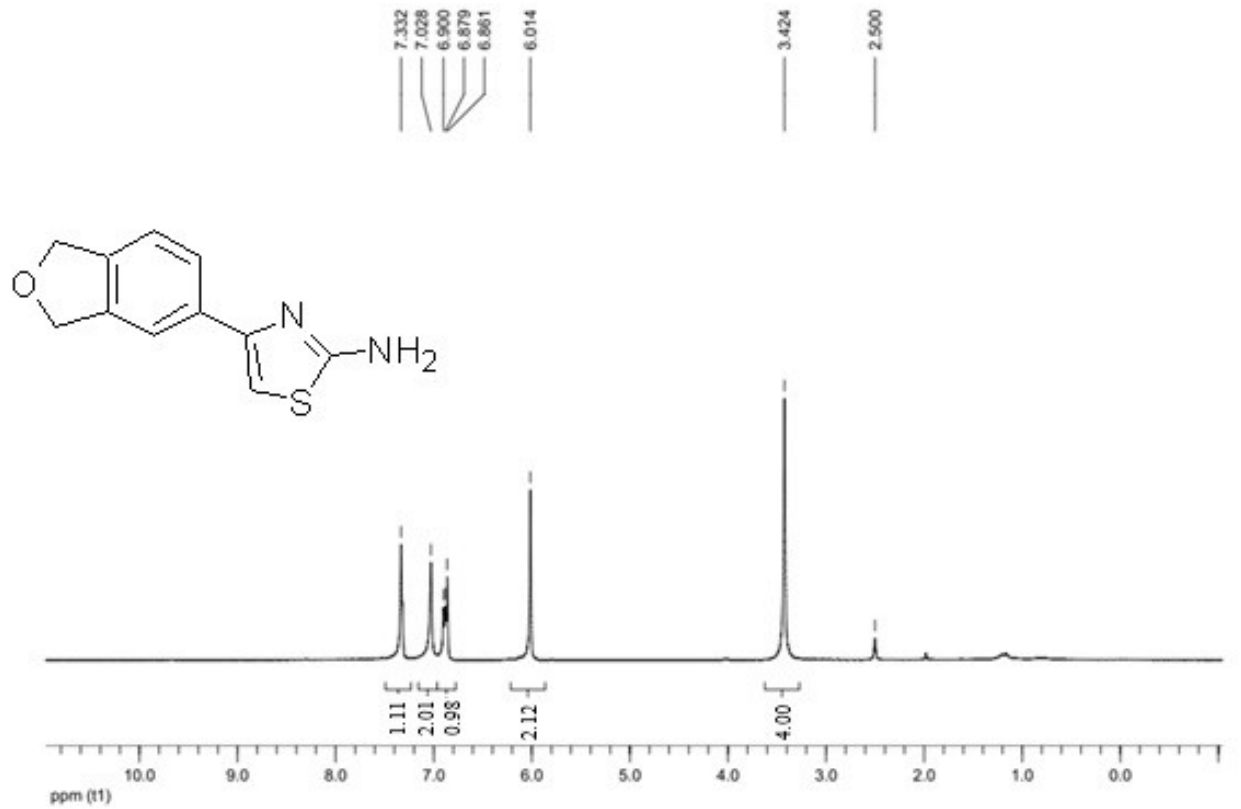

Fig. S7a The recorded *[1]H NMR* spectrum of the compound BFTA

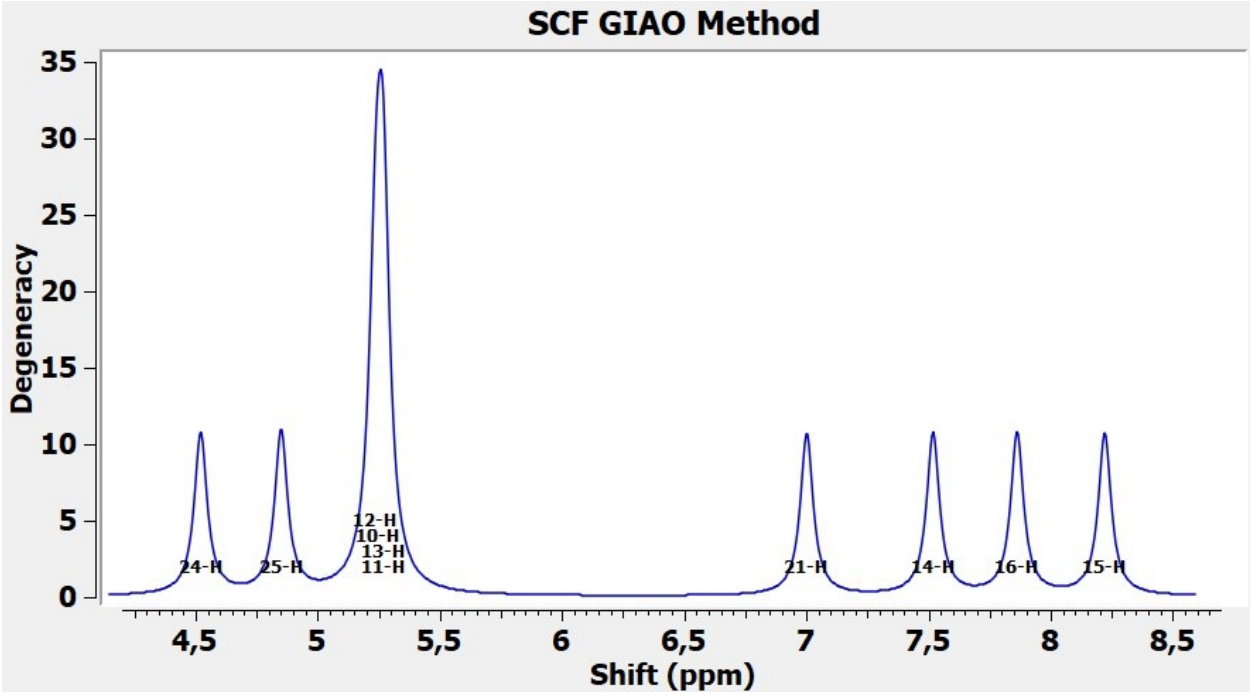

Fig. S7b. The calculated *[1]H NMR* spectrum of the compound BFTA

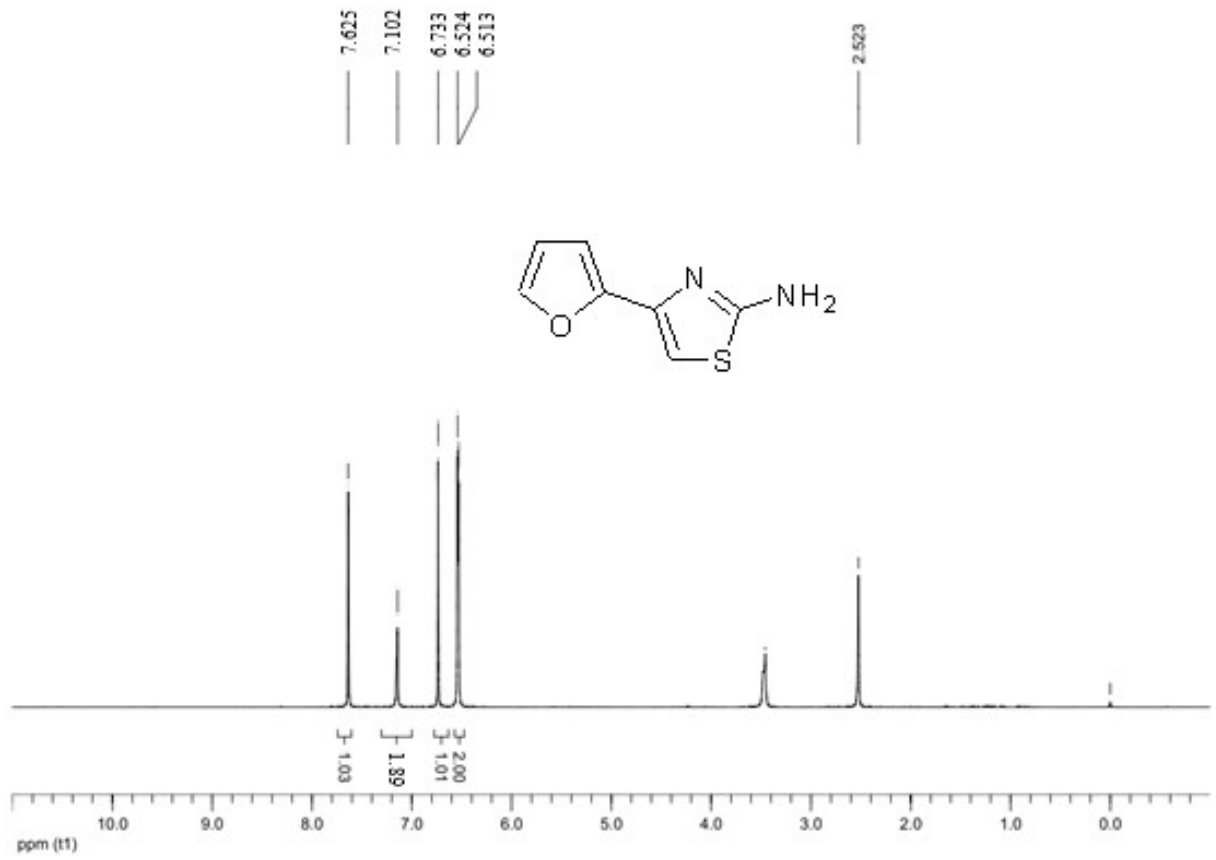

Fig. S8a. The recorded *[1]H NMR* spectrum of the compound FTA

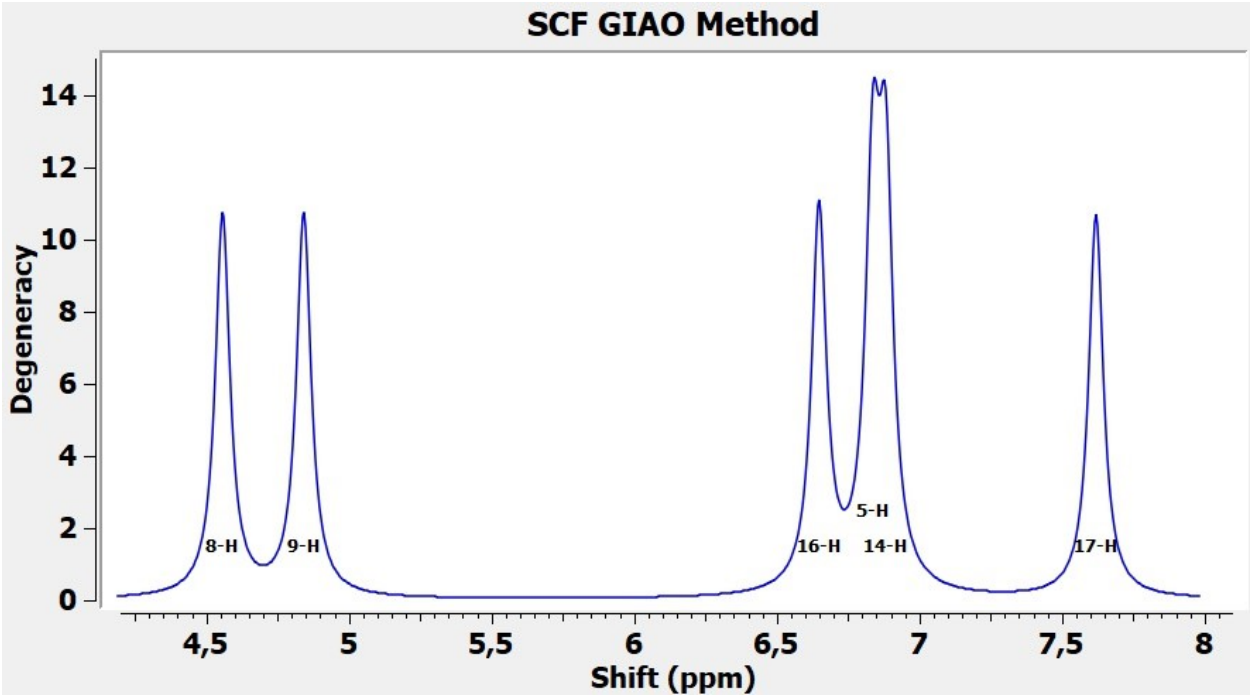

Fig. S8b. The calculated *[1]H NMR* spectrum of the compound FTA

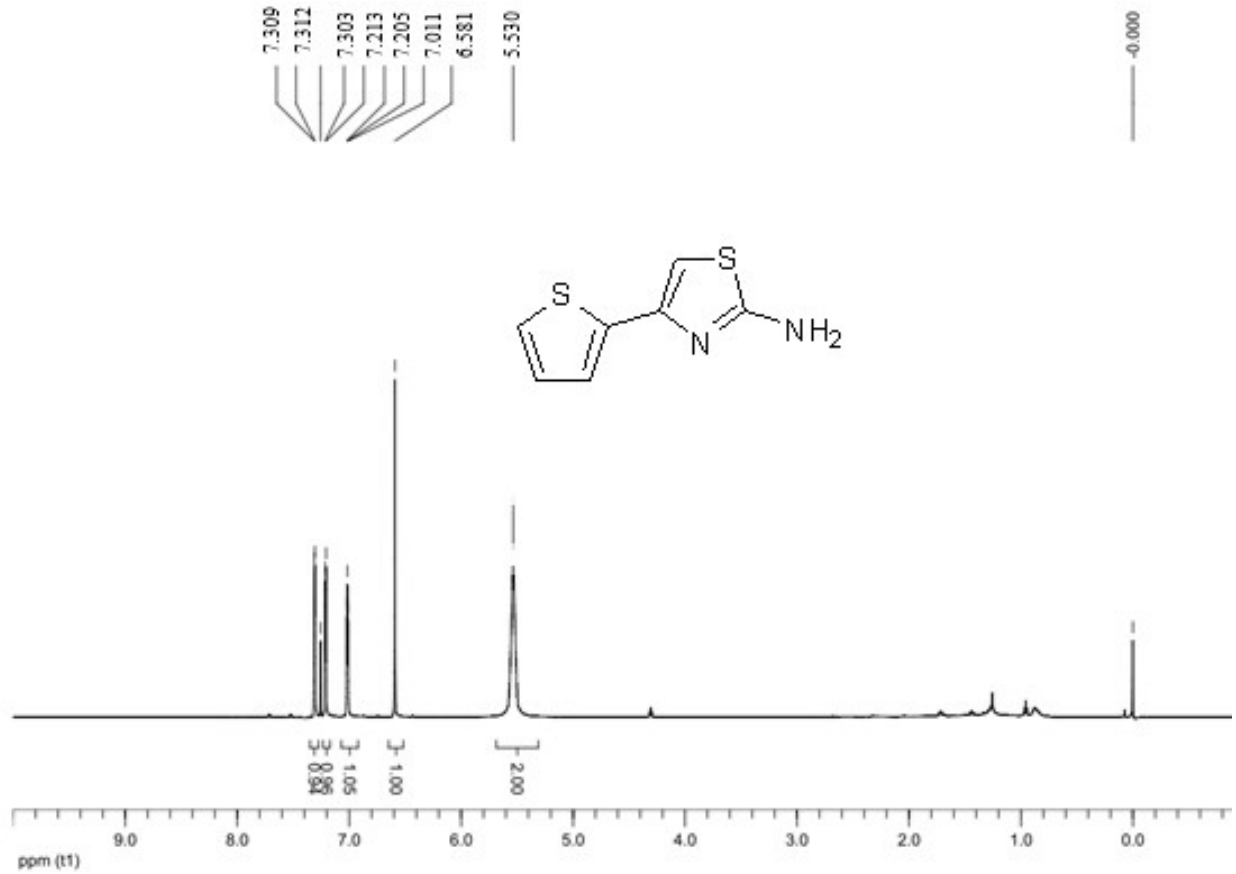

Fig. S9a. The recorded *[1]H NMR* spectrum of the compound THTA

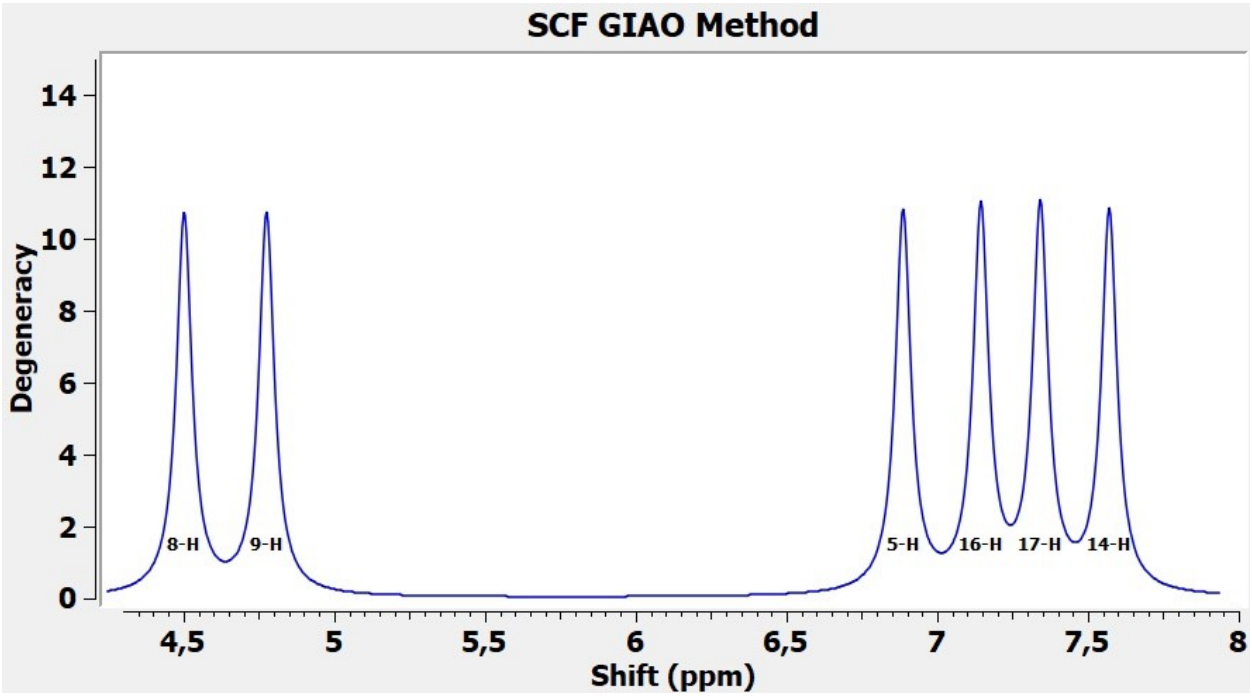

Fig. S9b. The calculated *[1]H NMR* spectrum of the compound THTA

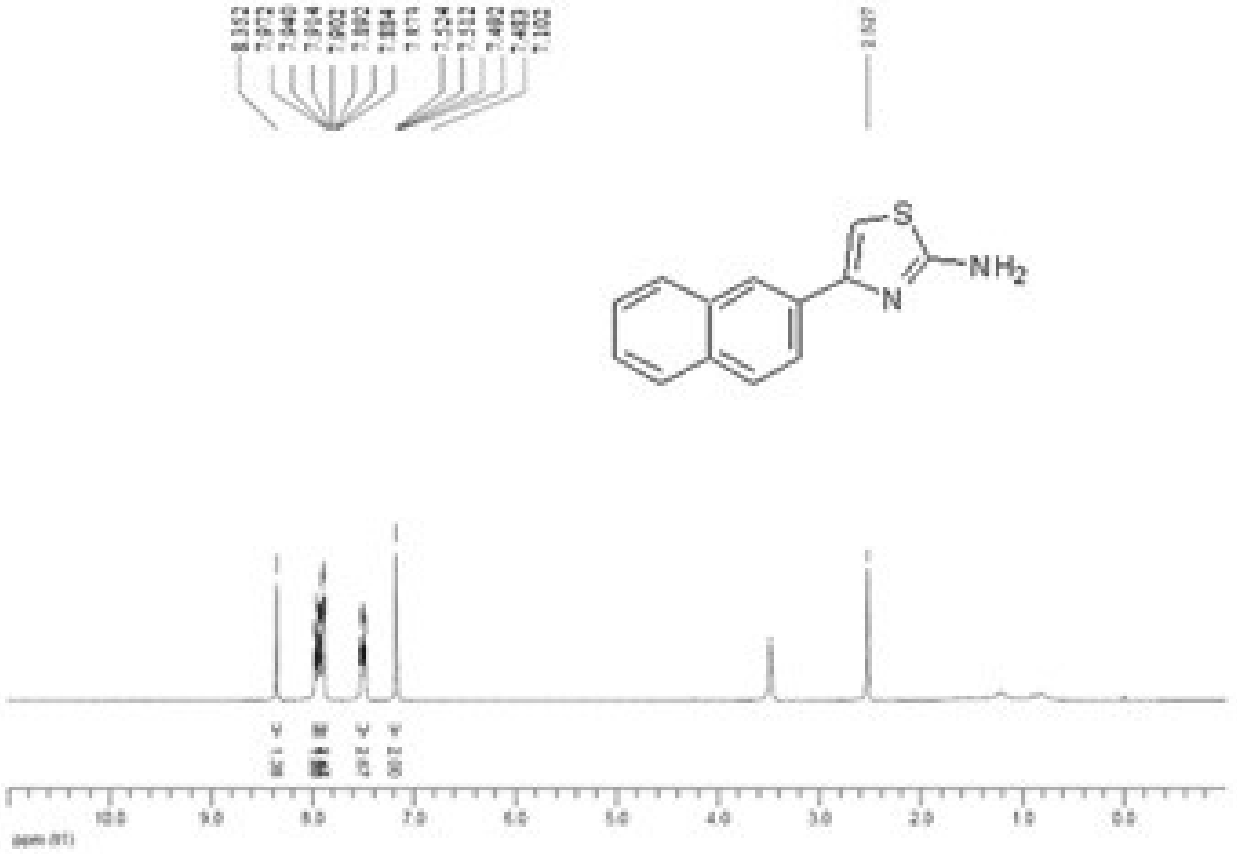

Fig S10a. The recorded *[1]H NMR* spectrum of the compound NapTA

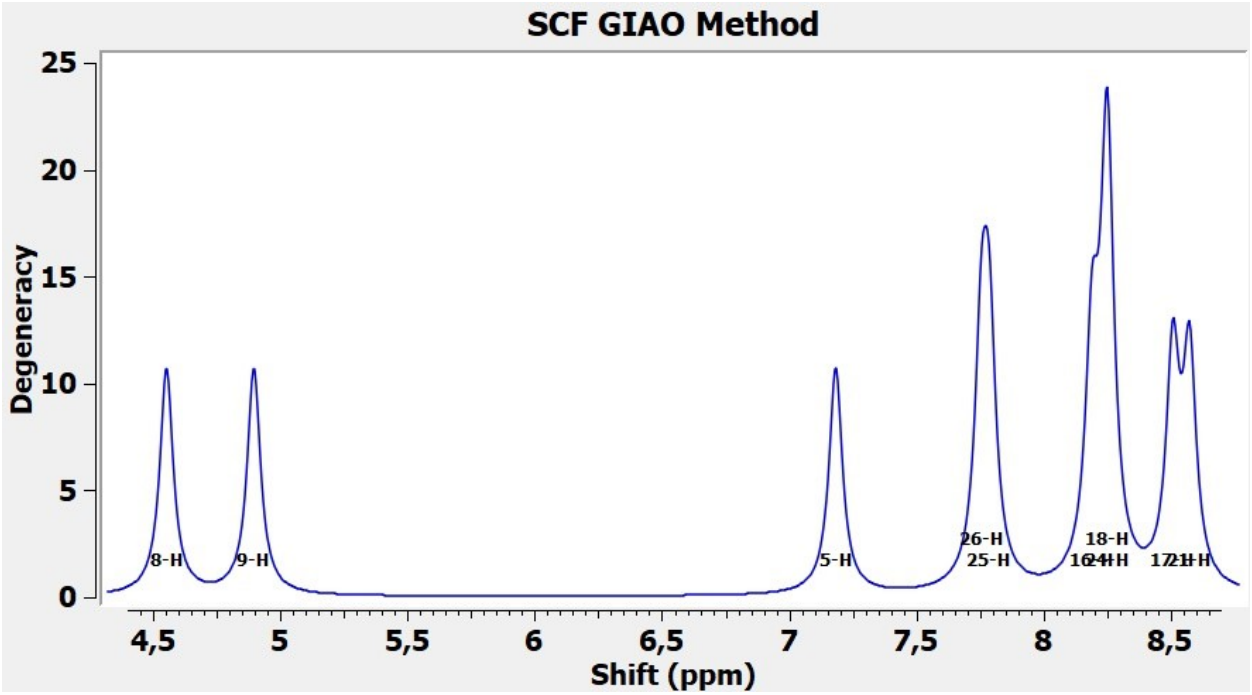

Fig S10b. The calculated *[1]H NMR* spectrum of the compound NapTA

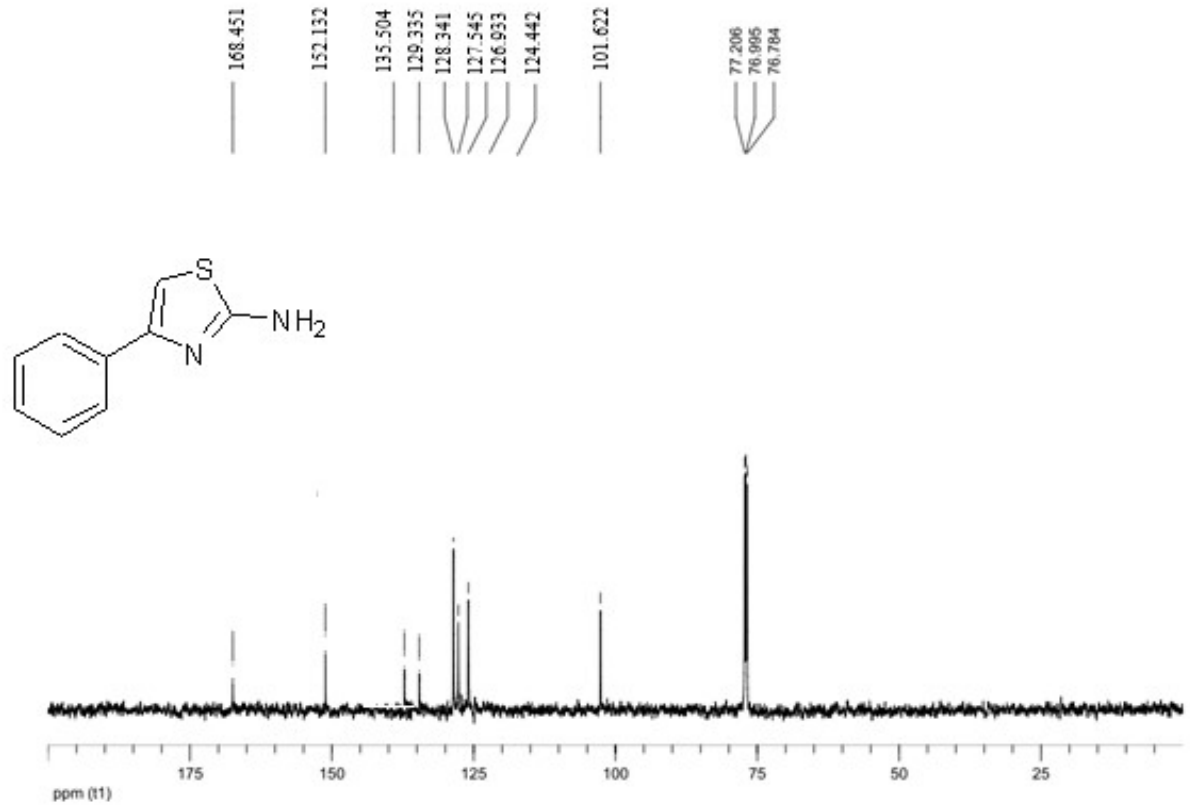

Fig. S11a. The recorded *^{13}C NMR* spectrum of the compound PhTA

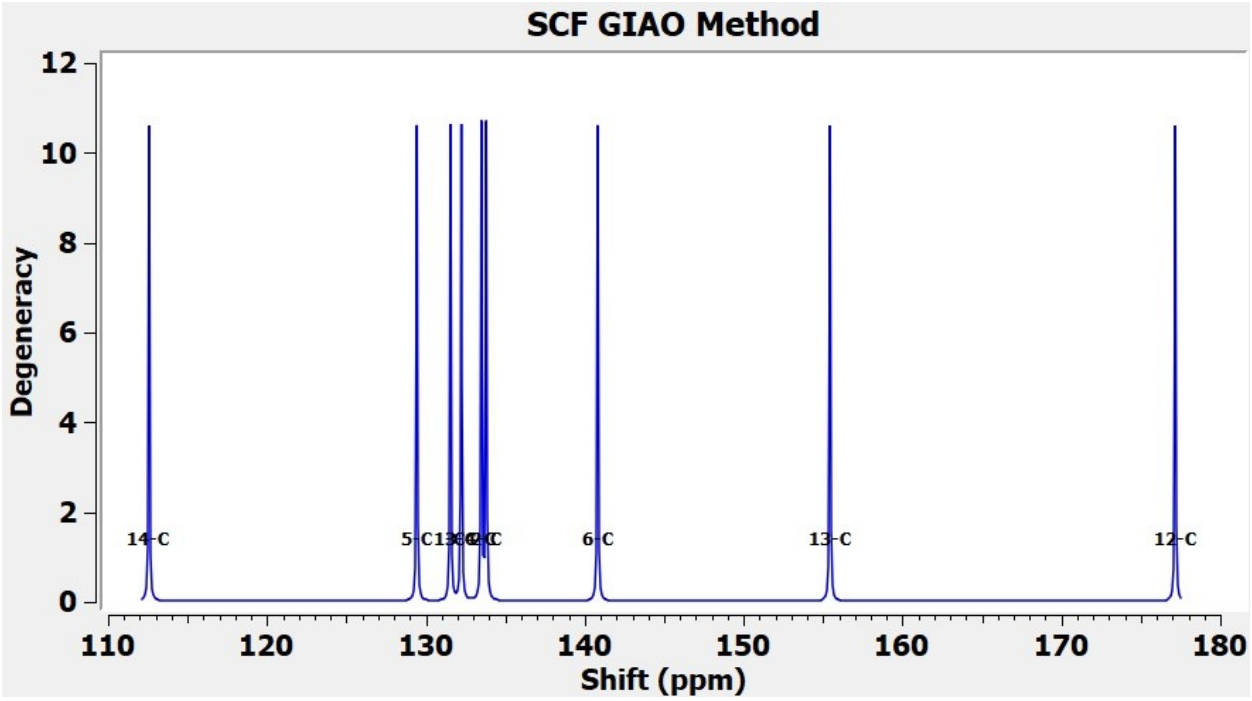

Fig. S11b. The calculated *^{13}C NMR* spectrum of the compound PhTA

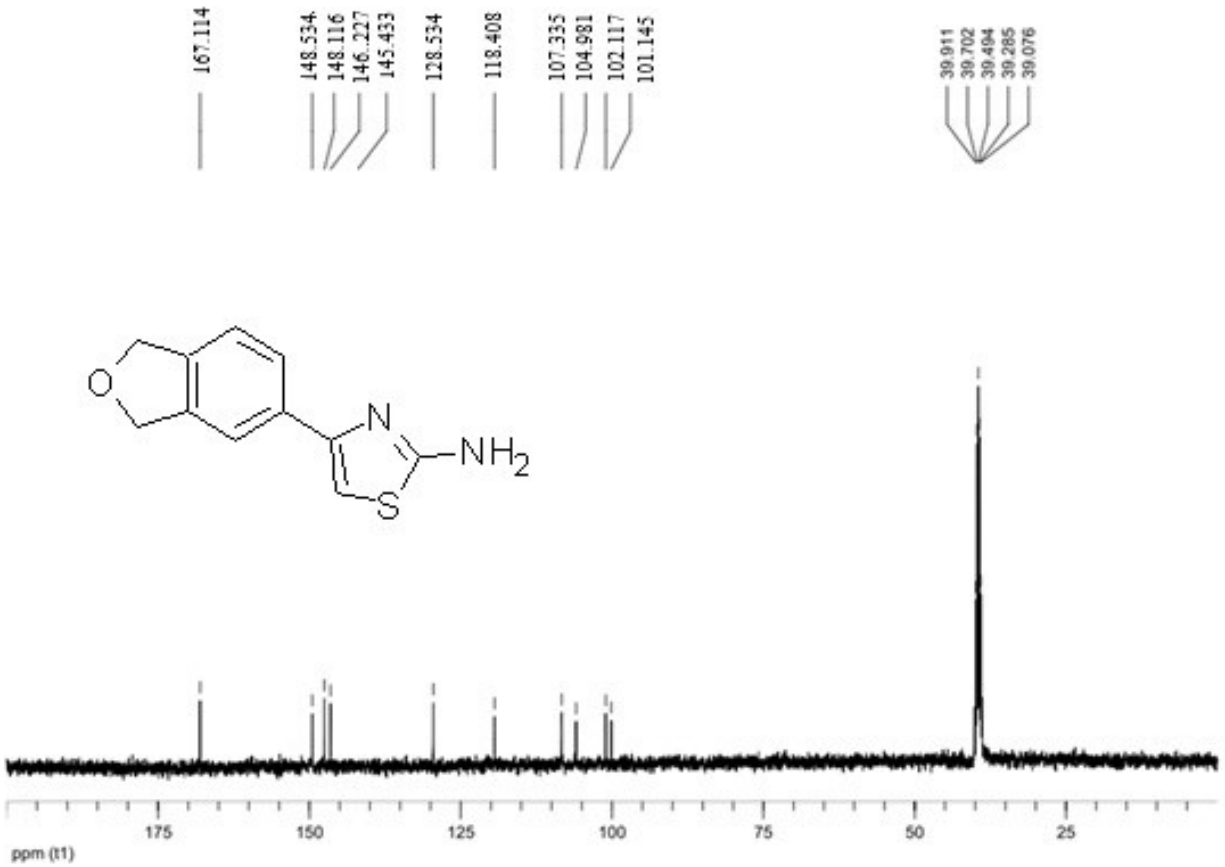

Fig. S12a. The recorded *[13]C NMR* spectrum of the compound BFTA

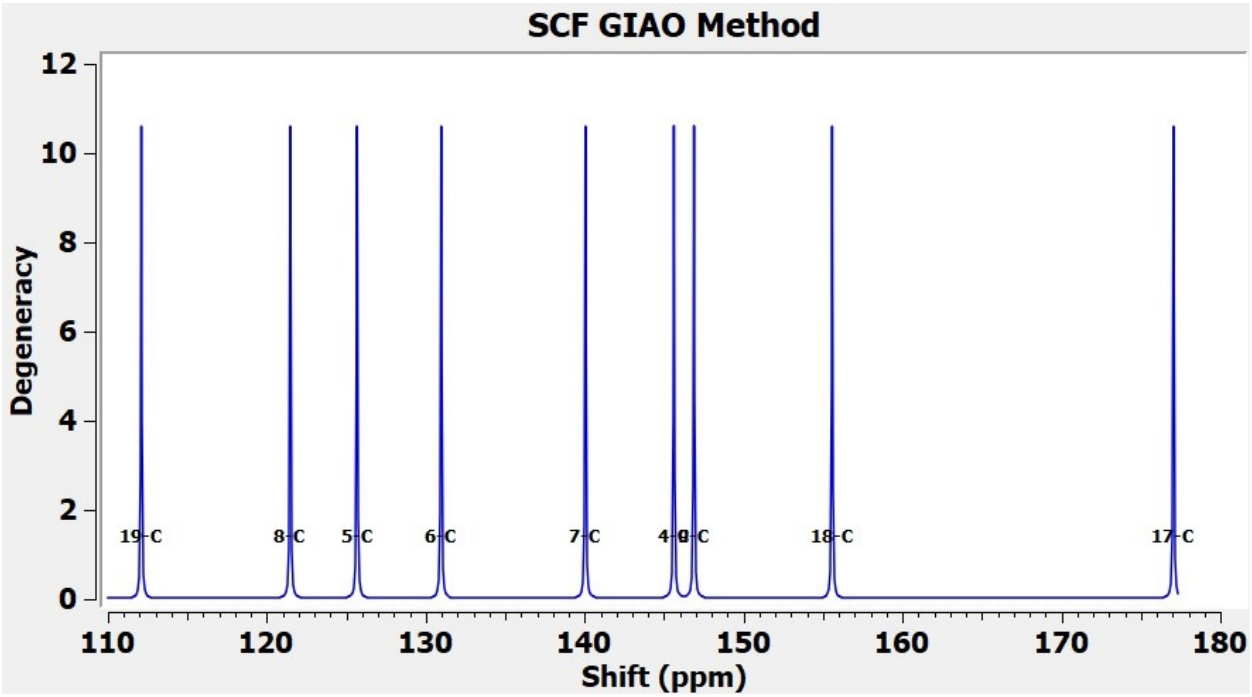

Fig. S12b. The calculated *[13]C NMR* spectrum of the compound BFTA

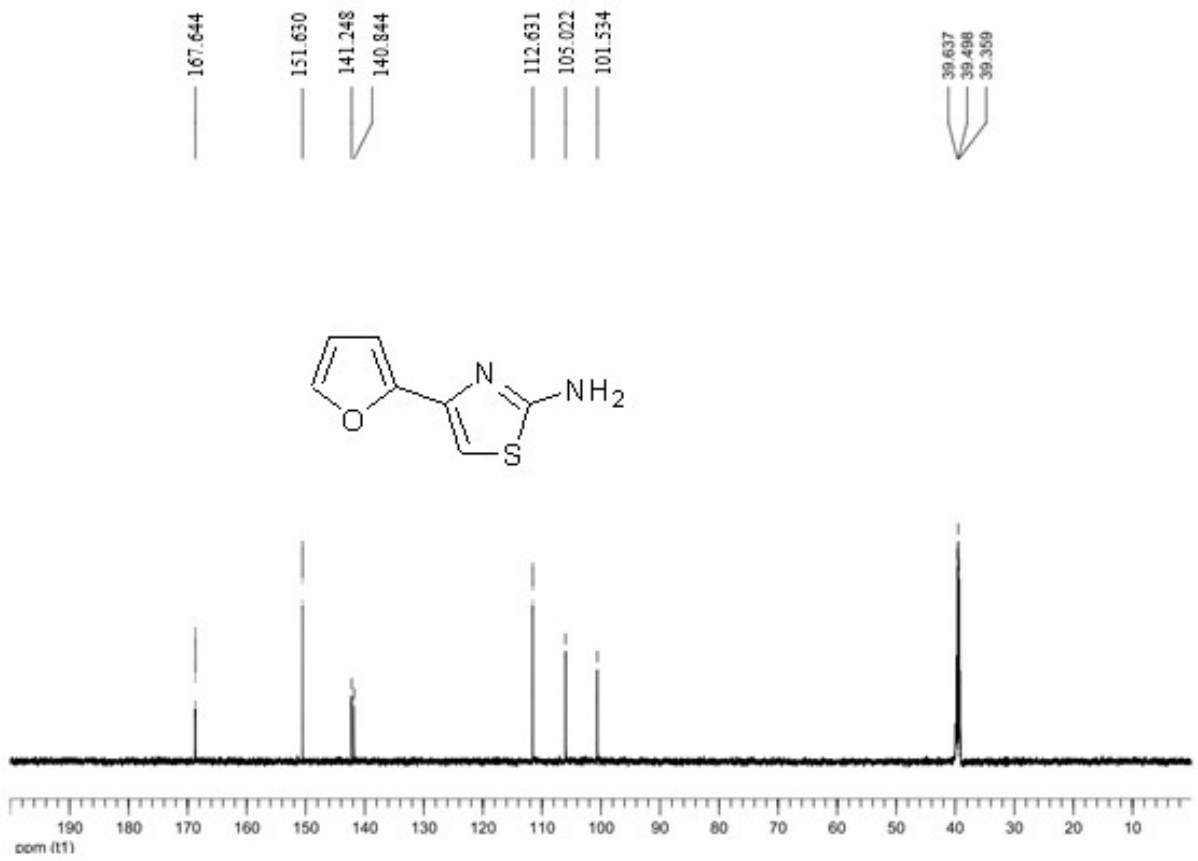

Fig. S13a. The recorded *[13]C NMR* spectrum of the compound FTA

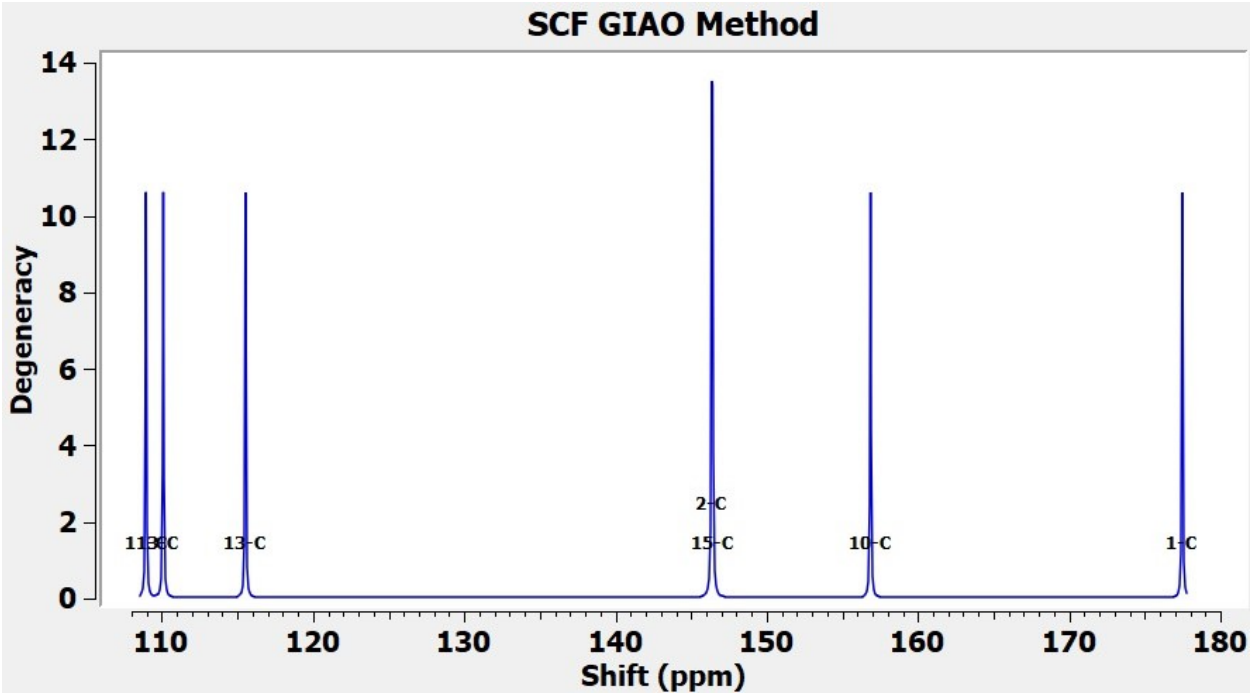

Fig. S13b. The calculated *[13]C NMR* spectrum of the compound FTA

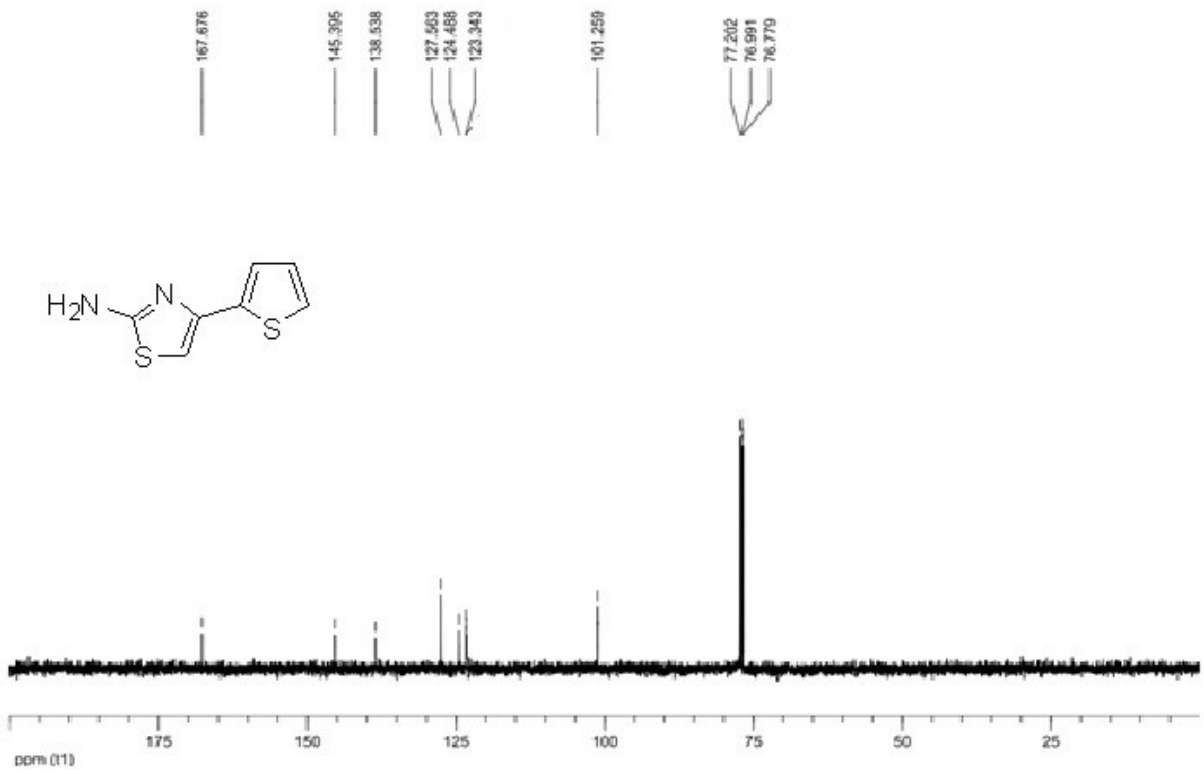

Fig. S14a. The recorded *[13]C NMR* spectrum of the compound ThTA

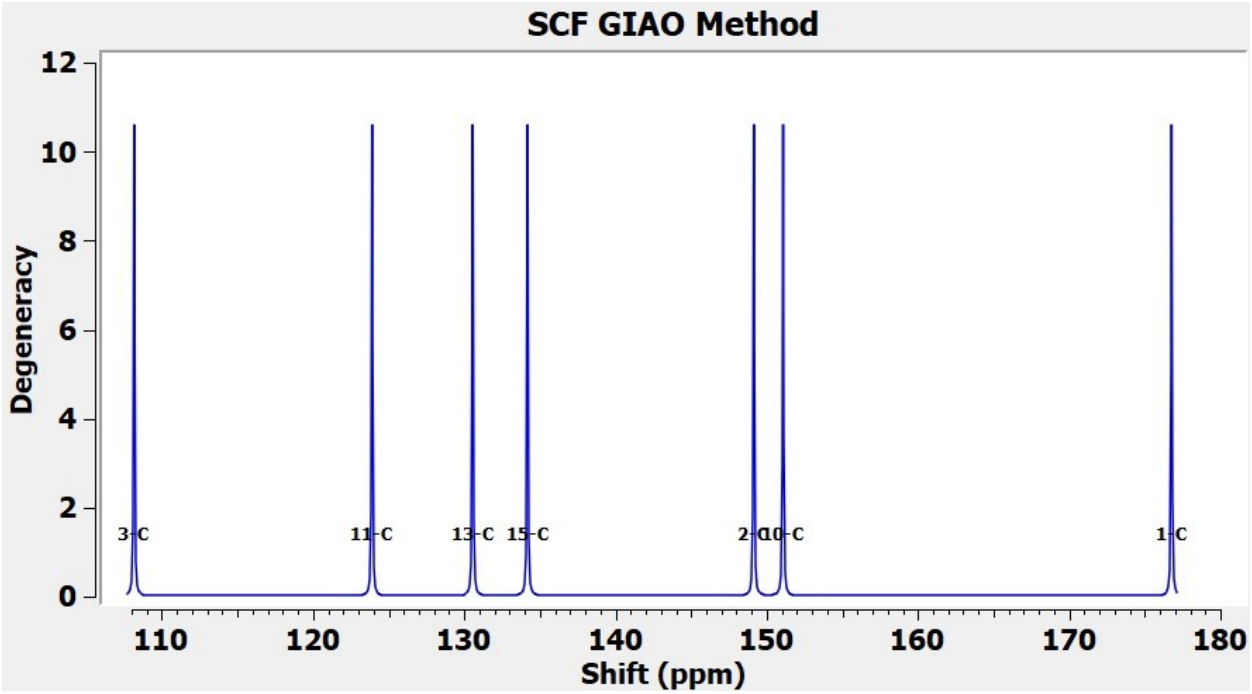

Fig. S14b. The calculated *[13]C NMR* spectrum of the compound ThTA

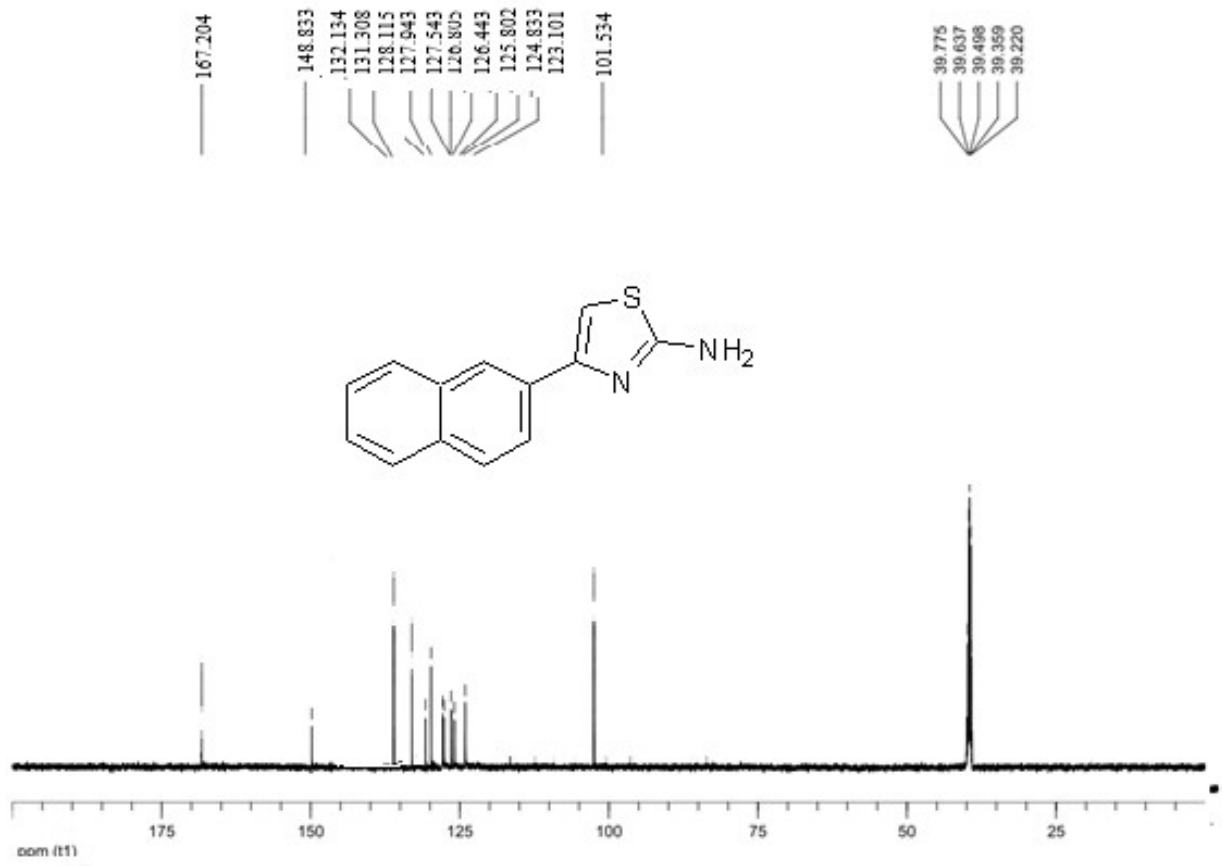

Fig. S15a. The recorded *^{13}C NMR* spectrum of the compound NapTA

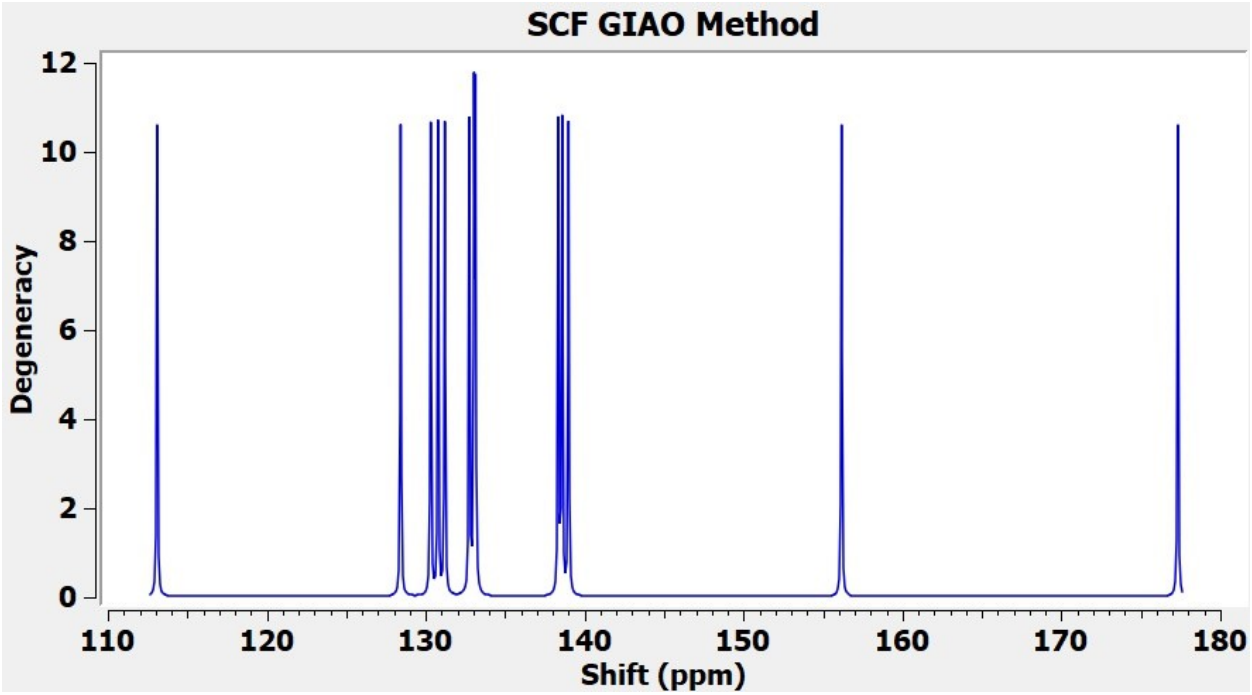

Fig. S15b. The calculated *^{13}C NMR* spectrum of the compound NapTA

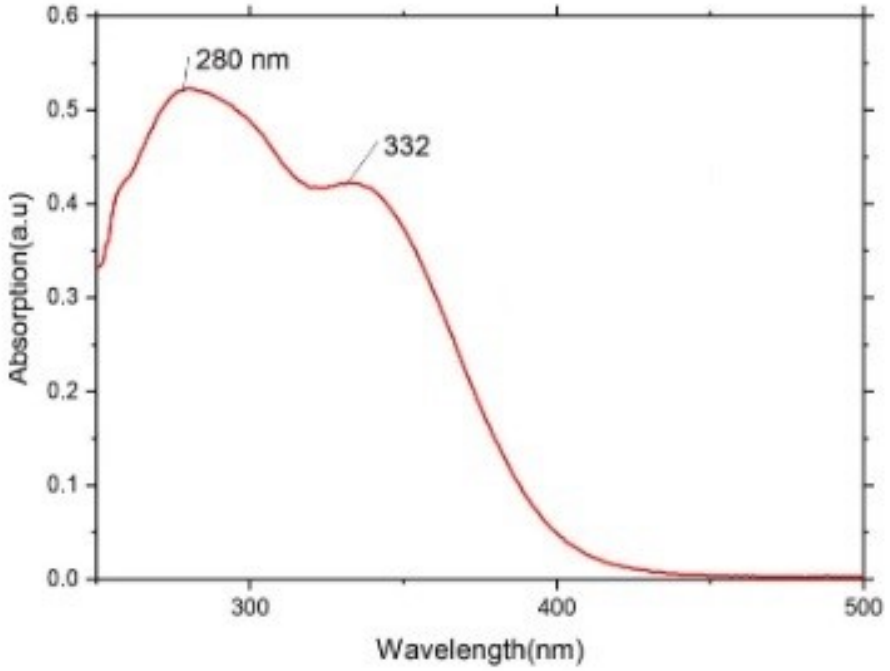

Fig. S16. The recorded UV-Vis spectrum of the compound PhTA

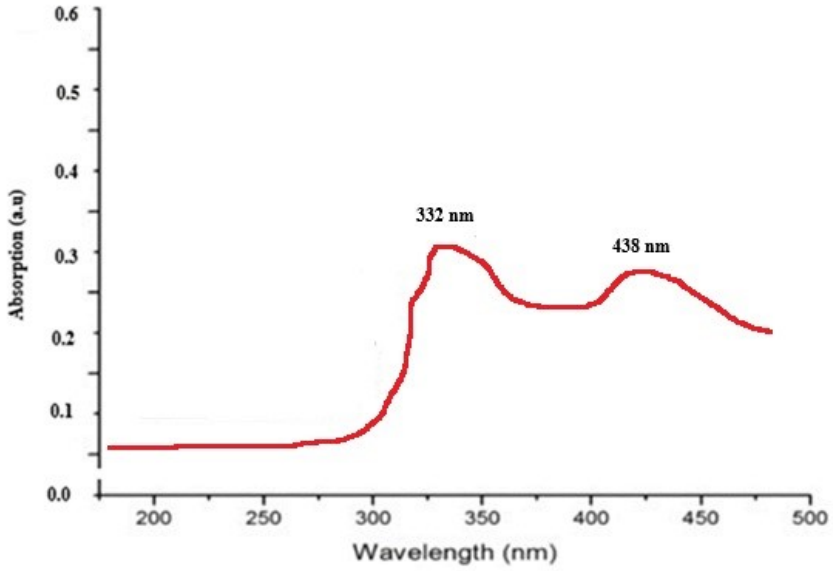

Fig. S17. The recorded UV-Vis spectrum of the compound BFTA

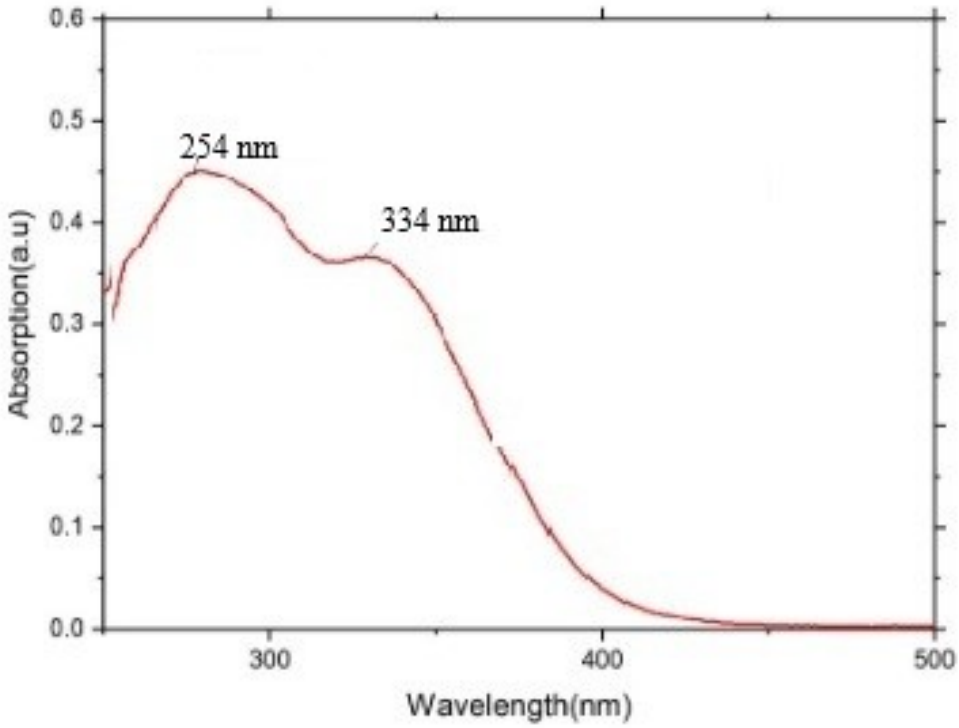

Fig. S18. The recorded UV-Vis spectrum of the compound FTA

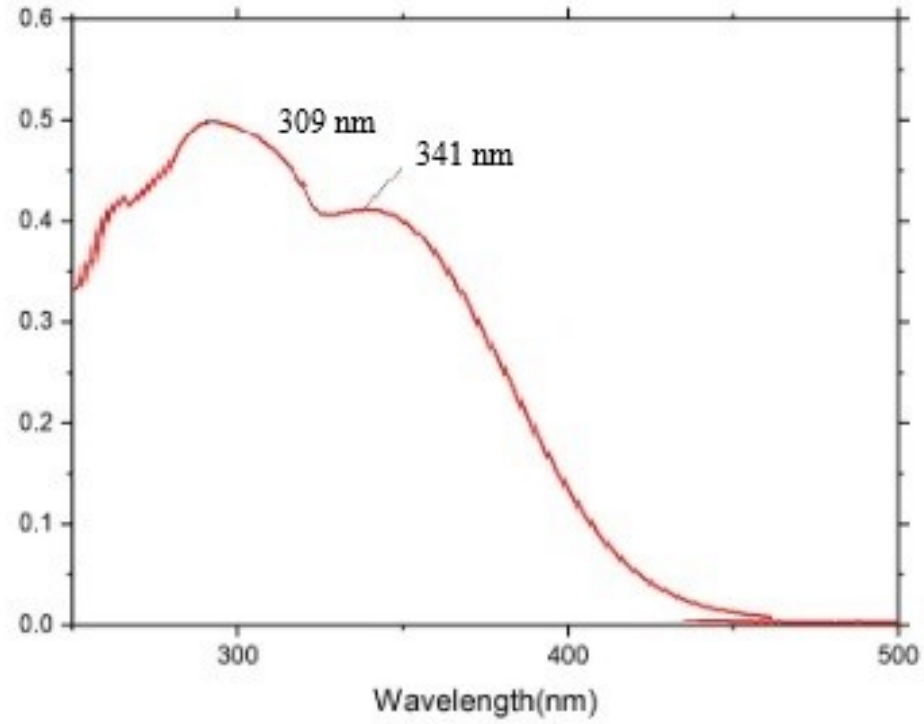

Fig. S19. The recorded UV-Vis spectrum of the compound ThTA

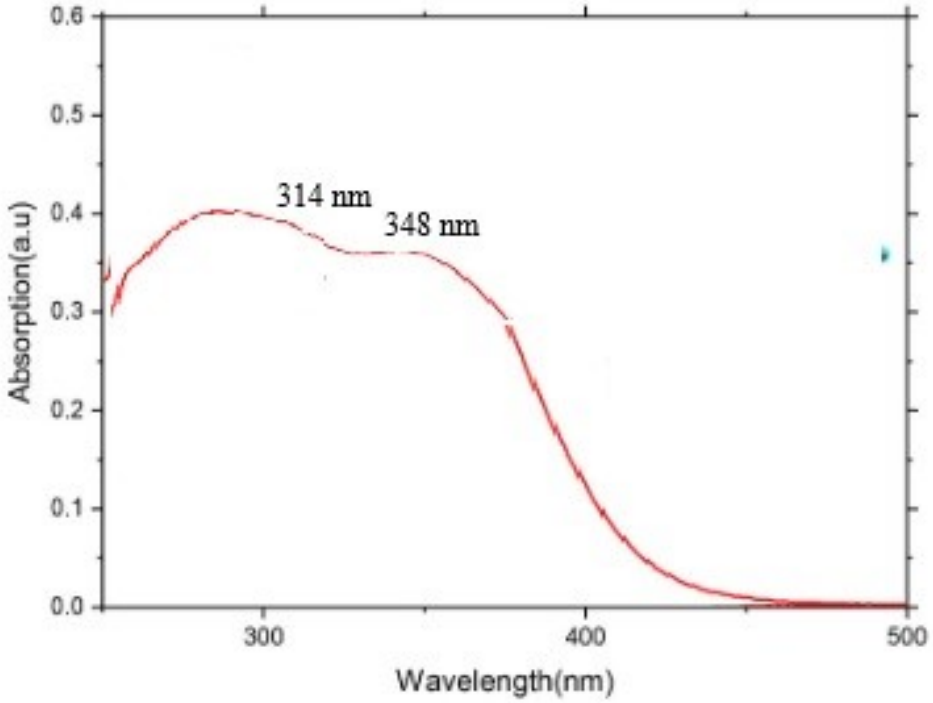

Fig. S20. The recorded UV-Vis spectrum of the compound NapTA

Table S3. The optimized parameters of PhTA

Bond lengths (Å)	
C1-C2	1.3925
C1-C6	1.4024
C1-H7	1.0821
C2-C3	1.3933
C2-H8	1.0845
C3-C4	1.3954
C3-H9	1.0842
C4-C5	1.3904
C4-H10	1.0844
C5-C6	1.4036
C5-H11	1.0839
C6-C13	1.4756
C12-S15	1.7667
C12-N17	1.2948
C12-N18	1.3763
C13-C14	1.366
C13-N17	1.3882
C14-S15	1.7439
C14-H16	1.0774
N18-H19	1.0086
N18-H20	1.0106
Bond Angles (°)	
C2-C1-C6	120.7015
C2-C1-H7	120.5557
C6-C1-H7	118.7428
C1-C2-C3	120.4088
C1-C2-H8	119.568
C3-C2-H8	120.0232

C2-C3-C4	119.3843
C2-C3-H9	120.3749
C4-C3-H9	120.2401
C3-C4-C5	120.2985
C3-C4-H10	120.0641
C5-C4-H10	119.6358
C4-C5-C6	120.8317
C4-C5-H11	119.1242
C6-C5-H11	120.0383
C1-C6-C5	118.3723
C1-C6-C13	119.9927
C5-C6-C13	121.6348
S15-C12-N17	114.6909
S15-C12-N18	121.0676
N17-C12-N18	124.1236
C6-C13-C14	126.1614
C6-C13-N17	119.0402
C14-C13-N17	114.7886
C13-C14-S15	110.6549
C13-C14-H16	129.3844
S15-C14-H16	119.9412
C12-S15-C14	88.1075
C12-N17-C13	111.7486
C12-N18-H19	117.3919
C12-N18-H20	113.687
H19-N18-H20	114.2241
Dihedral Angles (°)	
C6-C1-C2-C3	0.1598
C6-C1-C2-H8	-179.8965
H7-C1-C2-C3	-179.8239
H7-C1-C2-H8	0.1198
C2-C1-C6-C5	-0.5622
C2-C1-C6-C13	179.3013
H7-C1-C6-C5	179.4218
H7-C1-C6-C13	-0.7147
C1-C2-C3-C4	0.1979
C1-C2-C3-H9	179.8953
H8-C2-C3-C4	-179.7455
H8-C2-C3-H9	-0.0481
C2-C3-C4-C5	-0.1408
C2-C3-C4-H10	179.3951
H9-C3-C4-C5	-179.8386
H9-C3-C4-H10	-0.3027
C3-C4-C5-C6	-0.2749
C3-C4-C5-H11	178.8508
H10-C4-C5-C6	-179.8128
H10-C4-C5-H11	-0.6871
C4-C5-C6-C1	0.6201
C4-C5-C6-C13	-179.2411
H11-C5-C6-C1	-178.4976
H11-C5-C6-C13	1.6412
C1-C6-C13-C14	-168.1036
C1-C6-C13-N17	10.697
C5-C6-C13-C14	11.7554
C5-C6-C13-N17	-169.444
N17-C12-S15-C14	0.4489
N18-C12-S15-C14	176.6597
S15-C12-N17-C13	0.0616

N18-C12-N17-C13	-176.0174
S15-C12-N18-H19	31.8198
S15-C12-N18-H20	168.8701
N17-C12-N18-H19	-152.3397
N17-C12-N18-H20	-15.2894
C6-C13-C14-S15	179.9169
C6-C13-C14-H16	1.5537
N17-C13-C14-S15	1.0719
N17-C13-C14-H16	-177.2913
C6-C13-N17-C12	-179.6777
C14-C13-N17-C12	-0.7443
C13-C14-S15-C12	-0.8287
H16-C14-S15-C12	177.7114

Table S4. The optimized parameters of BFTA

Bond lengths (Å)	
C1-O2	1.4348
C1-C9	1.5063
C1-H10	1.0945
C1-H11	1.0997
O2-C3	1.4354
C3-C4	1.5047
C3-H12	1.0946
C3-H13	1.0998
C4-C5	1.3897
C4-C9	1.3928
C5-C6	1.3938
C5-H14	1.085
C6-C7	1.4048
C6-H15	1.082
C7-C8	1.4053
C7-C18	1.4755
C8-C9	1.3863
C8-H16	1.0845
C17-S20	1.7664
C17-N22	1.295
C17-N23	1.376
C18-C19	1.3659
C18-N22	1.3881
C19-S20	1.7442
C19-H21	1.0774
N23-H24	1.0085
N23-H25	1.0106
Bond Angles (°)	
O2-C1-C9	105.0383
O2-C1-H10	108.2723
O2-C1-H11	110.0602
C9-C1-H10	113.4895
C9-C1-H11	111.7432
H10-C1-H11	108.1445
C1-O2-C3	110.4517
O2-C3-C4	105.0294
O2-C3-H12	108.3
O2-C3-H13	110.0335
C4-C3-H12	113.4813
C4-C3-H13	111.8123

H12-C3-H13	108.0916
C3-C4-C5	130.9967
C3-C4-C9	108.7637
C5-C4-C9	120.2262
C4-C5-C6	119.0349
C4-C5-H14	121.1031
C6-C5-H14	119.8619
C5-C6-C7	121.2354
C5-C6-H15	120.3111
C7-C6-H15	118.4531
C6-C7-C8	118.95
C6-C7-C18	119.7051
C8-C7-C18	121.3441
C7-C8-C9	119.4684
C7-C8-H16	120.2432
C9-C8-H16	120.2831
C1-C9-C4	108.6122
C1-C9-C8	130.2929
C4-C9-C8	121.0781
S20-C17-N22	114.7158
S20-C17-N23	121.1163
N22-C17-N23	124.0879
C7-C18-C19	126.0888
C7-C18-N22	119.0648
C19-C18-N22	114.8452
C18-C19-S20	110.6195
C18-C19-H21	129.4014
S20-C19-H21	119.9612
C17-S20-C19	88.113
C17-N22-C18	111.705
C17-N23-H24	117.4293
C17-N23-H25	113.7415
H24-N23-H25	114.2558
Dihedral Angles (°)	
C9-C1-O2-C3	14.4908
H10-C1-O2-C3	136.0473
H11-C1-O2-C3	-105.9378
O2-C1-C9-C4	-8.8335
O2-C1-C9-C8	172.6808
H10-C1-C9-C4	-126.9162
H10-C1-C9-C8	54.598
H11-C1-C9-C4	110.476
H11-C1-C9-C8	-68.0098
C1-O2-C3-C4	-14.3373
C1-O2-C3-H12	-135.8937
C1-O2-C3-H13	106.1542
O2-C3-C4-C5	-172.9577
O2-C3-C4-C9	8.4057
H12-C3-C4-C5	-54.8514
H12-C3-C4-C9	126.512
H13-C3-C4-C5	67.7336
H13-C3-C4-C9	-110.903
C3-C4-C5-C6	-178.912
C3-C4-C5-H14	1.2343
C9-C4-C5-C6	-0.4062
C9-C4-C5-H14	179.7402
C3-C4-C9-C1	0.2619
C3-C4-C9-C8	178.9133

C5-C4-C9-C1	-178.5472
C5-C4-C9-C8	0.1043
C4-C5-C6-C7	-0.0005
C4-C5-C6-H15	-179.7866
H14-C5-C6-C7	179.855
H14-C5-C6-15	0.0689
C5-C6-C7-C8	0.6994
C5-C6-C7-C18	-178.9857
H15-C6-C7-C8	-179.5105
H15-C6-C7-C18	0.8043
C6-C7-C8-C9	-0.9911
C6-C7-C8-H16	178.1708
C18-C7-C8-C9	178.6887
C18-C7-C8-H16	-2.1494
C6-C7-C18-C19	164.1333
C6-C7-C18-N22	-15.4417
C8-C7-C18-C19	-15.5441
C8-C7-C18-N22	164.8809
C7-C8-C9-C1	178.9289
C7-C8-C9-C4	0.6045
H16-C8-C9-C1	-0.2326
H16-C8-C9-C4	-178.557
N22-C17-S20-C19	0.3814
N23-C17-S20-C19	177.2557
S20-C17-N22-C18	-0.3535
N23-C17-N22-C18	-177.1223
S20-C17-N23-H24	30.0411
S20-C17-N23-H25	167.2562
N22-C17-N23-H24	-153.3876
N22-C17-N23-H25	-16.1726
C7-C18-C19-S20	-179.4169
C7-C18-C19-H21	-0.9842
N22-C18-C19-S20	0.1737
N22-C18-C19-H21	178.6064
C7-C18-2N2-C17	179.7357
C19-C18-N22-C17	0.1142
C18-C19-S20-C17	-0.2943
H21-C19-S20-C17	-178.8965

Table S5. The optimized parameters of FTA

Bond lengths (Å)	
C1-S4	1.7686
C1-N6	1.2952
C1-N7	1.3759
C2-C3	1.3668
C2-N6	1.3845
C2-C10	1.4541
C3-S4	1.7431
C3-H5	1.0777
N7-H8	1.0086
N7-H9	1.0108
C10-C11	1.3691
C10-O12	1.366
C11-C13	1.4288
C11-H14	1.0783
O12-C15	1.3597
C13-C15	1.3602

C13-H16	1.0784
C15-H17	1.0767
Bond Angles (°)	
S4-C1-N6	114.8481
S4-C1-N7	121.0624
N6-C1-N7	123.962
C3-C2-N6	115.5818
C3-C2-C10	124.6058
N6-C2-C10	119.8124
C2-C3-S4	110.1413
C2-C3-H5	129.0788
S4-C3-H5	120.7544
C1-S4-C3	88.1899
C1-N6-C2	111.2177
C1-N7-H8	117.4063
C1-N7-H9	113.4727
H8-N7-H9	114.2562
C2-C10-C11	132.8015
C2-C10-O12	117.7027
C11-C10-O12	109.4944
C10-C11-C13	106.5817
C10-C11-H14	126.2678
C13-C11-H14	127.136
C10-O12-C15	107.378
C11-C13-C15	106.0848
C11-C13-H16	127.4237
C15-C13-H16	126.4879
O12-C15-C13	110.4599
O12-C15-H17	115.8513
C13-C15-H17	133.6877
Dihedral Angles (°)	
N6-C1-S4-C3	0.8952
N7-C1-S4-C3	176.947
S4-C1-N6-C2	-0.2128
N7-C1-N6-C2	-176.135
S4-C1-N7-H8	32.7346
S4-C1-N7-H9	169.5921
N6-C1-N7-H8	-151.5856
N6-C1-N7-H9	-14.728
N6-C2-C3-S4	1.5281
N6-C2-C3-H5	-176.6151
C10-C2-C3-S4	-178.4775
C10-C2-C3-H5	3.3793
C3-C2-N6-C1	-0.8703
C10-C2-N6-C1	179.1351
C3-C2-C10-C11	17.9036
C3-C2-C10-O12	-161.6149
N6-C2-C10-C11	-162.1023
N6-C2-C10-O12	18.3792
C2-C3-S4-C1	-1.3014
H5-C3-S4-C1	177.0214
C2-C10-C11-C13	-179.2123
C2-C10-C11-H14	2.0908
O12-C10-C11-C13	0.3354
O12-C10-C11-H14	-178.3615
C2-C10-O12-C15	179.3747
C11-C10-O12-C15	-0.2505

C10-C11-C13-C15	-0.2911
C10-C11-C13-H16	-179.6304
H14-C11-C13-C15	178.391
H14-C11-C13-H16	-0.9483
C10-O12-C15-C13	0.0587
C10-O12-C15-H17	179.7306
C11-C13-C15-O12	0.1447
C11-C13-C15-H17	-179.447
H16-C13-C15-O12	179.492
H16-C13-C15-H17	-0.0996

Table S6. The optimized parameters of ThTA

Bond lengths (Å	
C1-S4	1.7667
C1-N6	1.2954
C1-N7	1.375
C2-C3	1.3665
C2-N6	1.3871
C2-C10	1.457
C3-S4	1.7445
C3-H5	1.0775
N7-H8	1.0084
N7-H9	1.0106
C10-C11	1.3754
C10-S12	1.7478
C11-C13	1.421
C11-H14	1.0822
S12-C15	1.7305
C13-C15	1.3679
C13-H16	1.0821
C15-H17	1.0793
Bond Angles (°	
S4-C1-N6	114.6704
S4-C1-N7	121.1691
N6-C1-N7	124.0568
C3-C2-N6	115.1899
C3-C2-C10	126.2364
N6-C2-C10	118.5715
C2-C3-S4	110.299
C2-C3-H5	129.2776
S4-C3-H5	120.4212
C1-S4-C3	88.269
C1-N6-C2	111.5656
C1-N7-H8	117.5097
C1-N7-H9	113.7668
H8-N7-H9	114.3755
C2-C10-C11	129.5433
C2-C10-S12	119.8855
C11-C10-S12	110.5711
C10-C11-C13	113.3569
C10-C11-H14	123.1939
C13-C11-H14	123.4489
C10-S12-C15	91.5741
C11-C13-C15	112.6514
C11-C13-H16	123.856
C15-C13-H16	123.4925

S12-C15-C13	111.8465
S12-C15-H17	119.8607
C13-C15-H17	128.2926
Dihedral Angles (°	
N6-C1-S4-C3	0.4967
N7-C1-S4-C3	176.9385
S4-C1-N6-C2	-0.1359
N7-C1-N6-C2	-176.4609
S4-C1-N7-H8	31.2161
S4-C1-N7-H9	168.7588
N6-C1-N7-H8	-152.6872
N6-C1-N7-H9	-15.1445
N6-C2-C3-S4	0.8146
N6-C2-C3-H5	-178.6458
C10-C2-C3-S4	-179.7357
C10-C2-C3-H5	0.804
C3-C2-N6-C1	-0.4493
C10-C2-N6-C1	-179.944
C3-C2-C10-C11	2.0332
C3-C2-C10-S12	-177.8161
N6-C2-C10-C11	-178.5338
N6-C2-C10-S12	1.617
C2-C3-S4-C1	-0.7077
H5-C3-S4-C1	178.8078
C2-C10-C11-C13	-179.8145
C2-C10-C11-H14	0.3928
S12-C10-C11-C13	0.046
S12-C10-C11-H14	-179.7467
C2-C10-S12-C15	179.8272
C11-C10-S12-C15	-0.0487
C10-C11-C13-C15	-0.0166
C10-C11-C13-H16	-179.9109
H14-C11-C13-C15	179.7755
H14-C11-C13-H16	-0.1188
C10-S12-C15-C13	0.0399
C10-S12-C15-H17	179.8815
C11-C13-C15-S12	-0.0212
C11-C13-C15-H17	-179.8461
H16-C13-C15-S12	179.8735
H16-C13-C15-H17	0.0486

Table S7. The optimized parameters of NapTA

Bond lengths (Å	
C1-S4	1.7663
C1-N6	1.2953
C1-N7	1.3765
C2-C3	1.3659
C2-N6	1.388
C2-C15	1.4749
C3-S4	1.7438
C3-H5	1.0775
N7-H8	1.0085
N7-H9	1.0106
C10-C11	1.3715
C10-C15	1.4236
C10-H17	1.0822

C11-C12	1.4194
C11-H18	1.0853
C12-C13	1.4307
C12-C19	1.4186
C13-C14	1.4158
C13-C20	1.4212
C14-C15	1.3824
C14-H21	1.0849
H16-C19	1.0852
C19-C23	1.3749
C20-C22	1.3741
C20-H24	1.0853
C22-C23	1.4155
C22-H25	1.0843
C23-H26	1.0842
Bond Angles (°	
S4-C1-N6	114.6977
S4-C1-N7	121.141
N6-C1-N7	124.0809
C3-C2-N6	114.9235
C3-C2-C15	126.0292
N6-C2-C15	119.0459
C2-C3-S4	110.5562
C2-C3-H5	129.2615
S4-C3-H5	120.1587
C1-S4-C3	88.1612
C1-N6-C2	111.6593
C1-N7-H8	117.3551
C1-N7-H9	113.6579
H8-N7-H9	114.186
C11-C10-C15	120.9037
C11-C10-H17	120.7181
C15-C10-H17	118.3782
C10-C11-C12	121.2193
C10-C11-H18	119.9744
C12-C11-H18	118.8063
C11-C12-C13	118.3511
C11-C12-C19	122.662
C13-C12-C19	118.9857
C12-C13-C14	119.0929
C12-C13-C20	118.7539
C14-C13-C20	122.1524
C13-C14-C15	121.6763
C13-C14-H21	118.1284
C15-C14-H21	120.1854
C2-C15-C10	119.3874
C2-C15-C14	121.8648
C10-C15-C14	118.7475
C12-C19-H16	118.7953
C12-C19-C23	120.8392
H16-C19-2C3	120.3655
C13-C20-C22	120.85
C13-C20-H24	118.8187
C22-C20-H24	120.3313
C20-C22-C23	120.3285
C20-C22-H25	120.0787
C23-C22-H25	119.5928
C19-C23-C22	120.2422

C19-C23-H26	120.1357
C22-C23-H26	119.6221
Dihedral Angles (°	
N6-C1-S4-C3	0.3857
N7-C1-S4-C3	177.253
S4-C1-N6-C2	-0.511
N7-C1-N6-C2	-177.2736
S4-C1-N7-H8	30.1861
S4-C1-N7-H9	167.094
N6-C1-N7-H8	-153.2506
N6-C1-N7-H9	-16.3427
N6-C2-C3-S4	-0.104
N6-C2-C3-H5	178.1001
C15-C2-C3-S4	-179.6685
C15-C2-C3-H5	-1.4644
C3-C2-N6-C1	0.3988
C15-C2-N6-C1	179.9959
C3-C2-C15-C10	159.4599
C3-C2-C15-C14	-20.3405
N6-C2-C15-C10	-20.0883
N6-C2-C15-C14	160.1113
C2-C3-S4-C1	-0.1423
H5-C3-S4-C1	-178.5342
C15-C10-C11-C12	-0.3363
C15-C10-C11-H18	179.6922
H17-C10-C11-C12	179.7345
H17-C10-C11-H18	-0.237
C11-C10-C15-C2	-178.771
C11-C10-C15-C14	1.0356
H17-C10-C15-C2	1.1599
H17-C10-C15-C14	-179.0335
C10-C11-C12-C13	-0.3325
C10-C11-C12-C19	-179.9415
H18-C11-C12-C13	179.6393
H18-C11-C12-C19	0.0303
C11-C12-C13-C14	0.3009
C11-C12-C13-C20	-179.394
C19-C12-C13-C14	179.9246
C19-C12-C13-C20	0.2297
C11-C12-C19-H16	-0.4249
C11-C12-C19-C23	179.5667
C13-C12-C19-H16	179.9684
C13-C12-C19-C23	-0.0399
C12-C13-C14-C15	0.4113
C12-C13-C14-H21	-178.4505
C20-C13-C14-C15	-179.9046
C20-C13-C14-H21	1.2336
C12-C13-C20-C22	-0.2657
C12-C13-C20-H24	179.831
C14-C13-C20-C22	-179.9508
C14-C13-C20-H24	0.1458
C13-C14-C15-C2	178.732
C13-C14-C15-C10	-1.0695
H21-C14-C15-C2	-2.4292
H21-C14-C15-C10	177.7692
C12-C19-C23-C22	-0.1214
C12-C19-C23-H26	179.9769
H16-C19-C23-C22	179.8701

H16-C19-C23-H26	-0.0316
C13-C20-C22-C23	0.108
C13-C20-C22-H25	-179.8882
H24-C20-C22-C23	-179.9901
H24-C20-C22-H25	0.0138
C20-C22-C23-C19	0.089
C20-C22-C23-H26	179.9911
H25-C22-C23-C19	-179.9149
H25-C22-C23-H26	-0.0127