Functional Tuning of Phenothiazine-Based Dyes by Benzimidazole Auxiliary Chromophore: an Account on Optical and Photovoltaic Studies†

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Electronic Supplementary Information

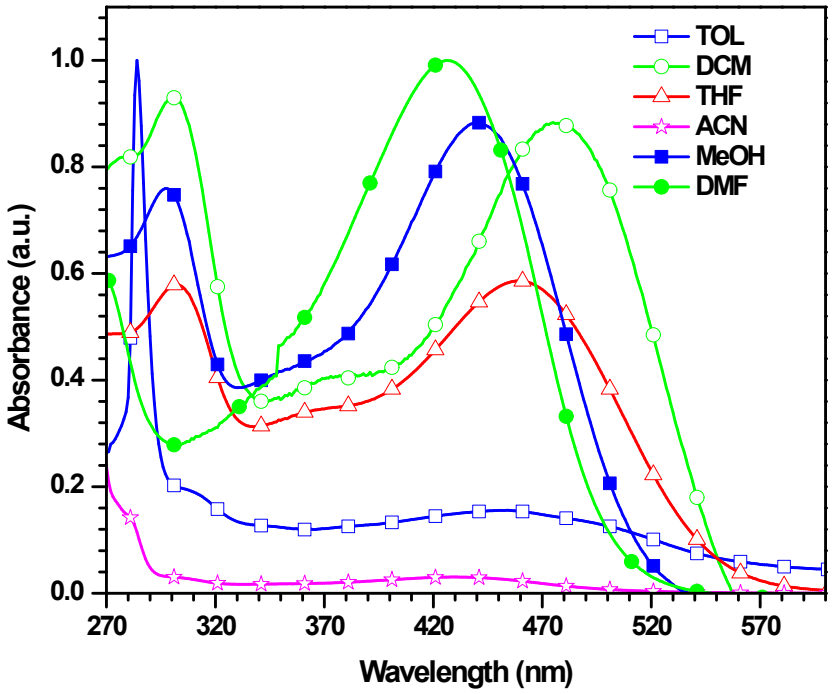

Fig. S1 Absorption spectra of **GJ2** recorded in different solvents.

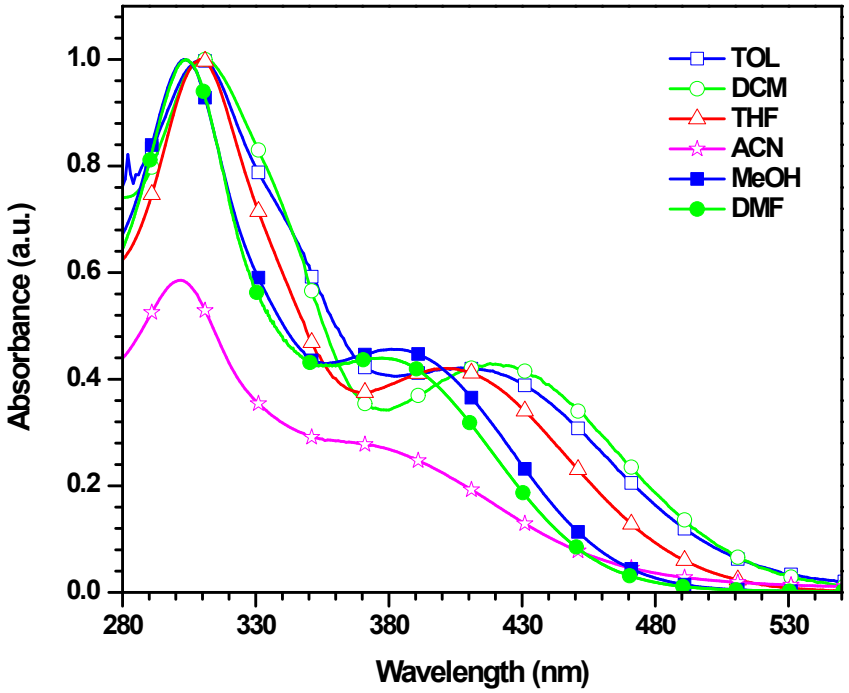

Fig. S2 Absorption spectra of **GJ3** recorded in different solvents.

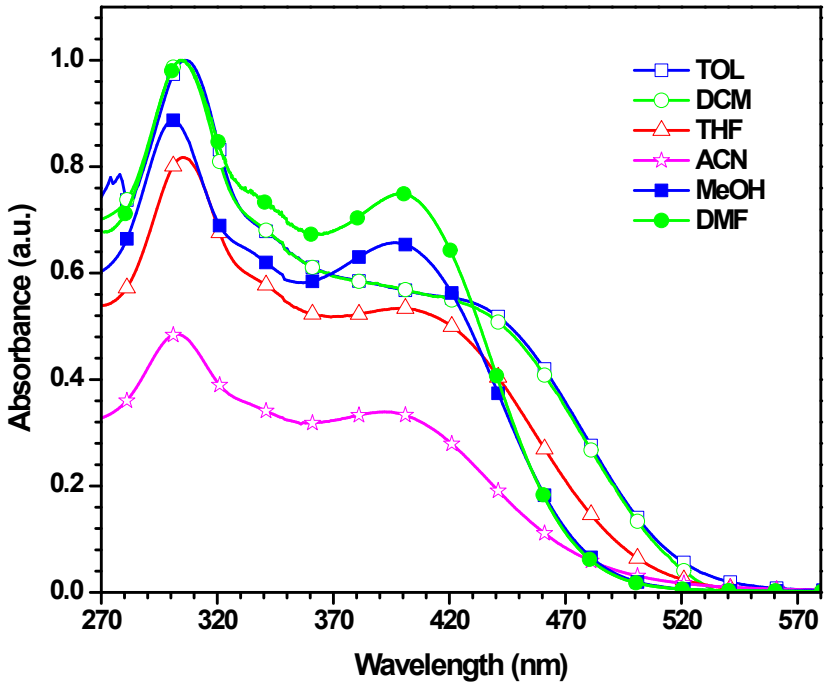

Fig. S3 Absorption spectra of **GJ4** recorded in different solvents.

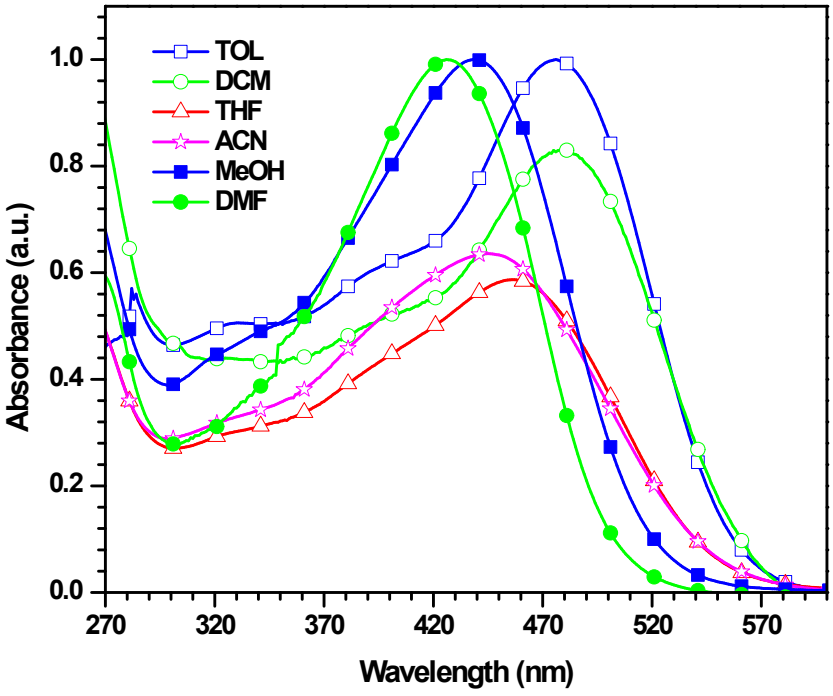

Fig. S4 Absorption spectra of **GJ5** recorded in different solvents.

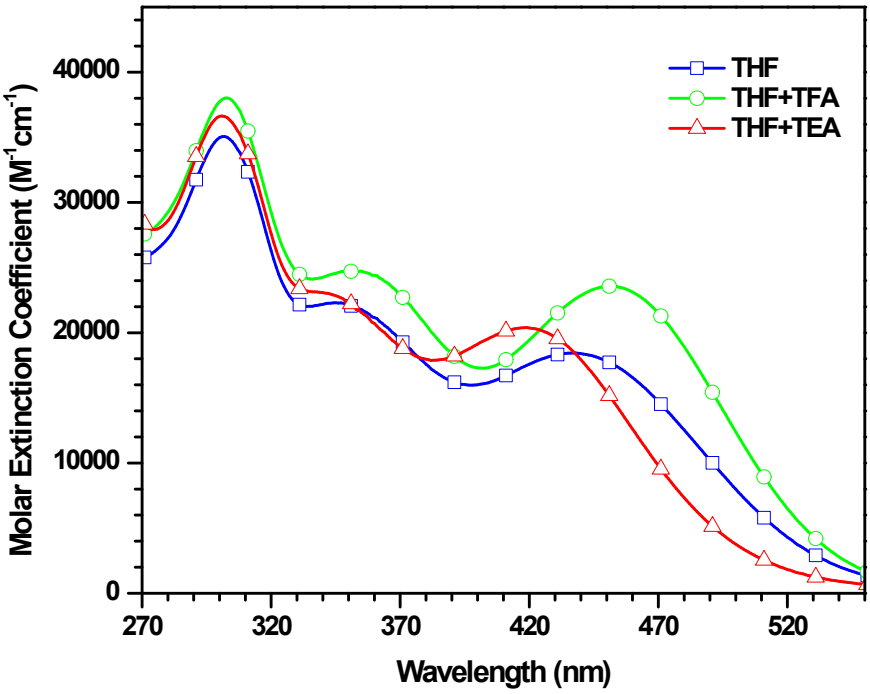

Fig. S5 Absorption spectra of **GJ1** recorded in THF before and after addition of TFA or TEA.

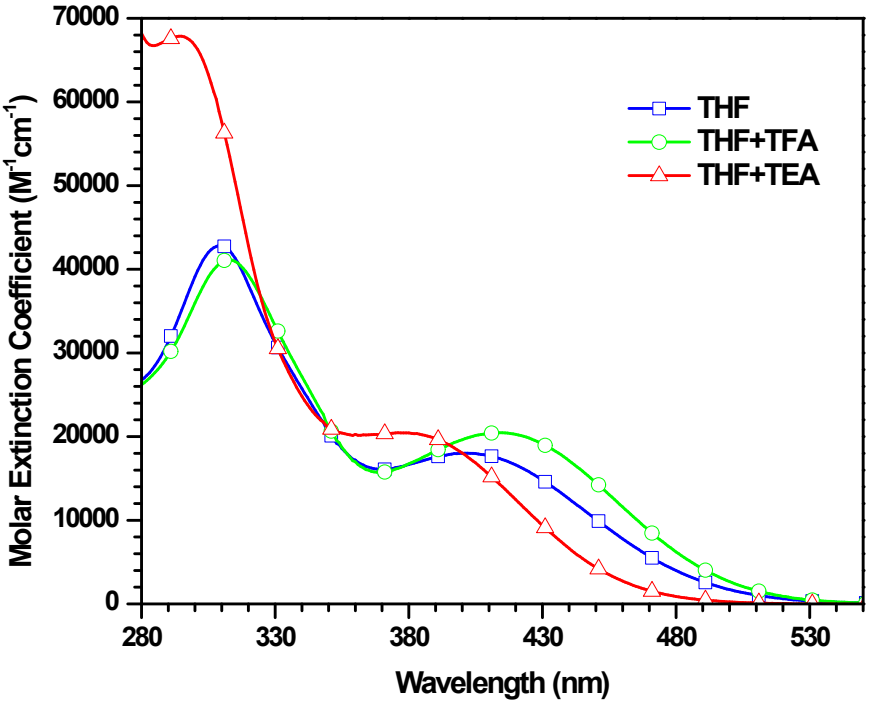

Fig. S6 Absorption spectra of **GJ3** recorded in THF before and after addition of TFA or TEA.

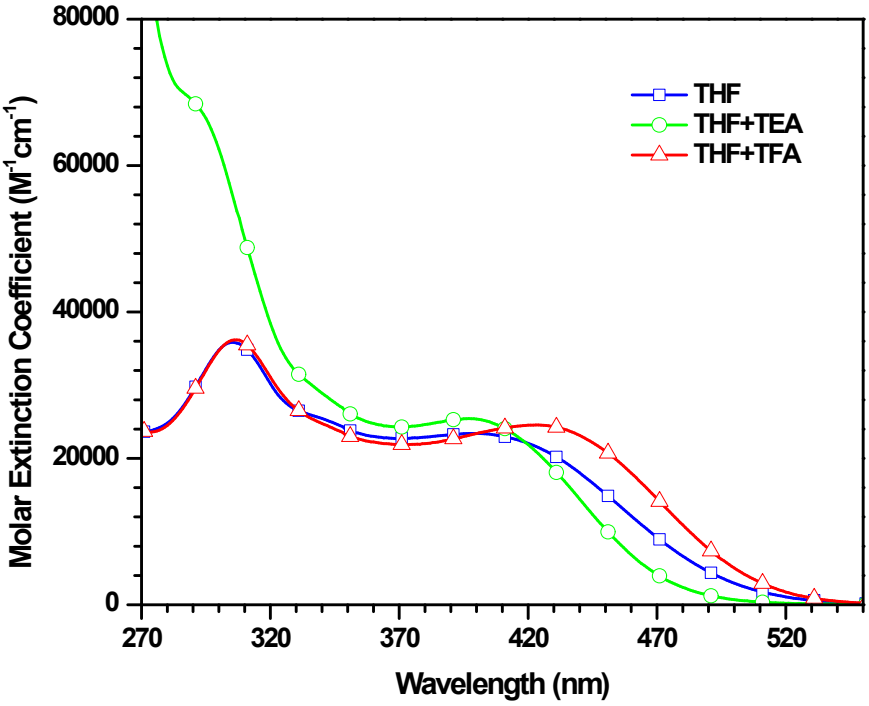

Fig. S7 Absorption spectra of the dye **GJ4** recorded in THF before and after addition of TFA or TEA.

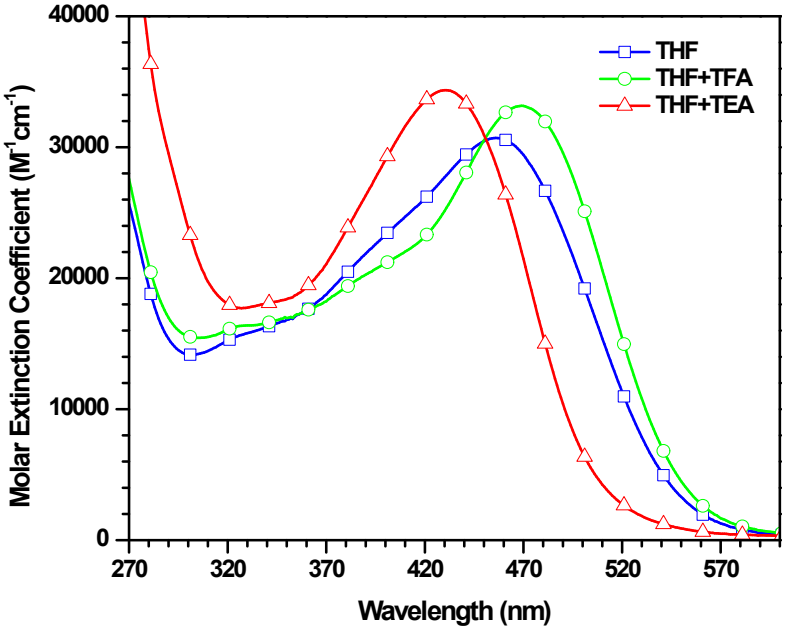

Fig. S8 Absorption spectra of the dye **GJ5** recorded in THF before and after addition of TFA or TEA.

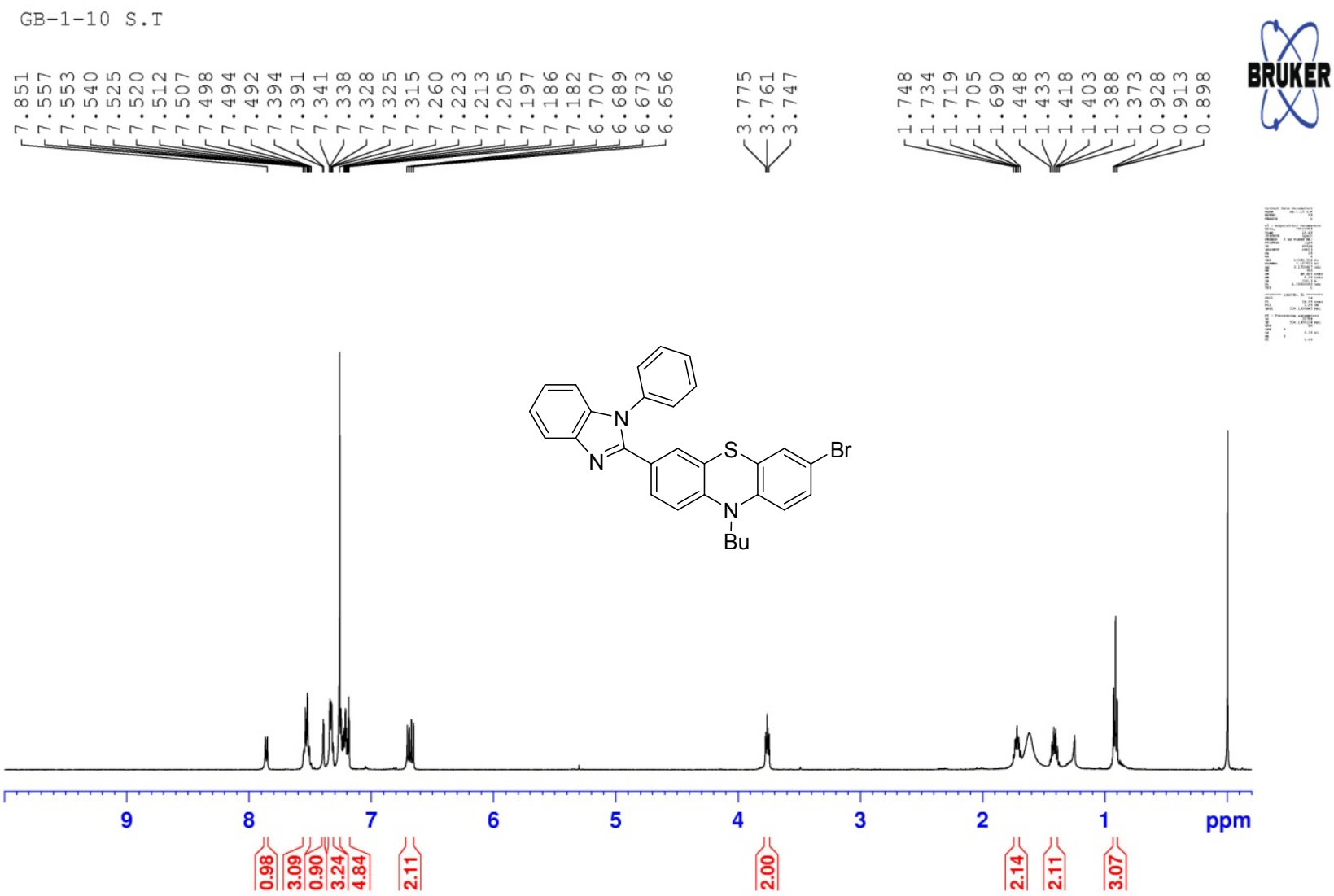

Fig. S9 ^{1}H NMR spectra of **2**.

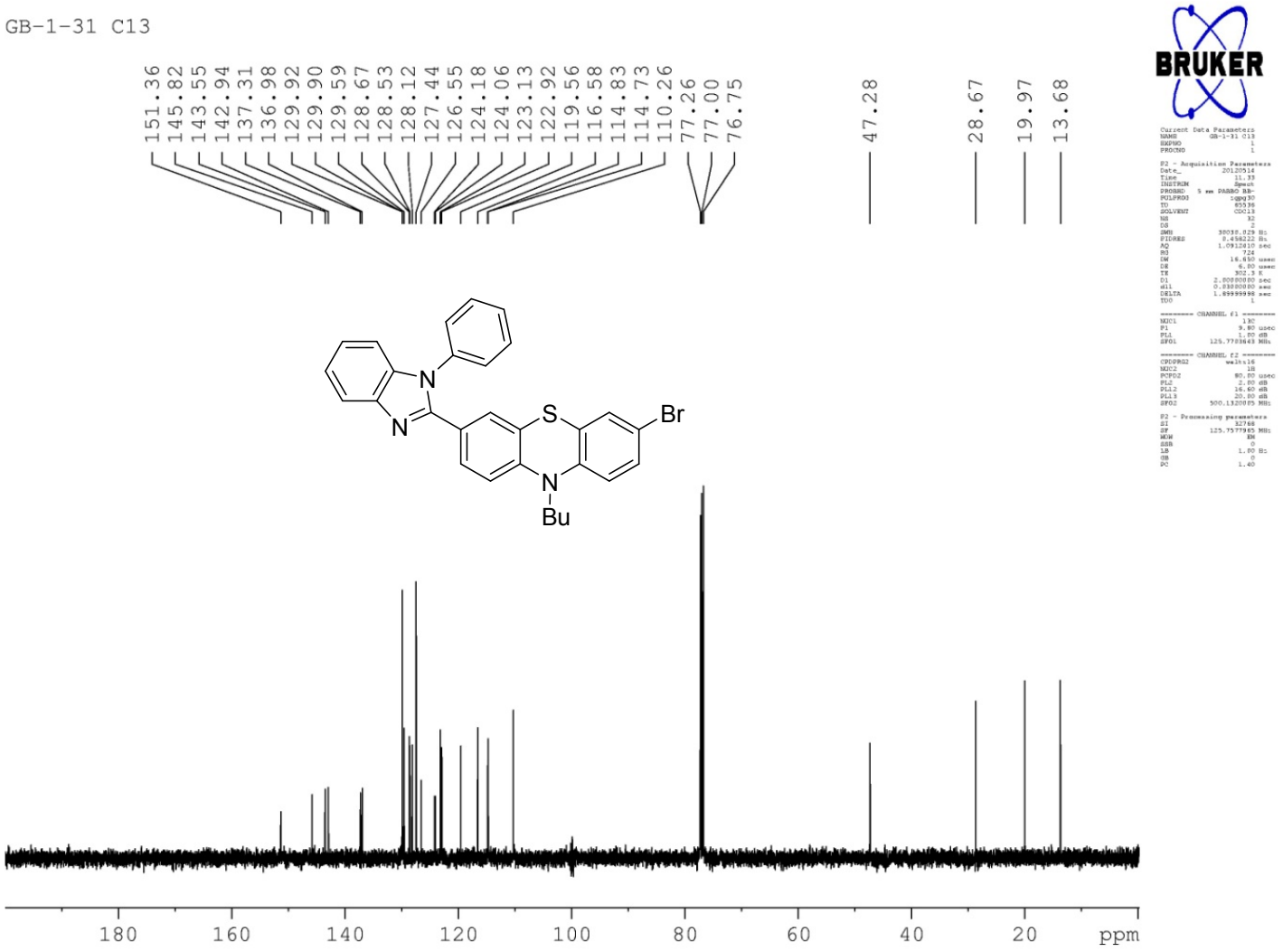

Fig. S10 ^{13}C NMR spectra of **2**.

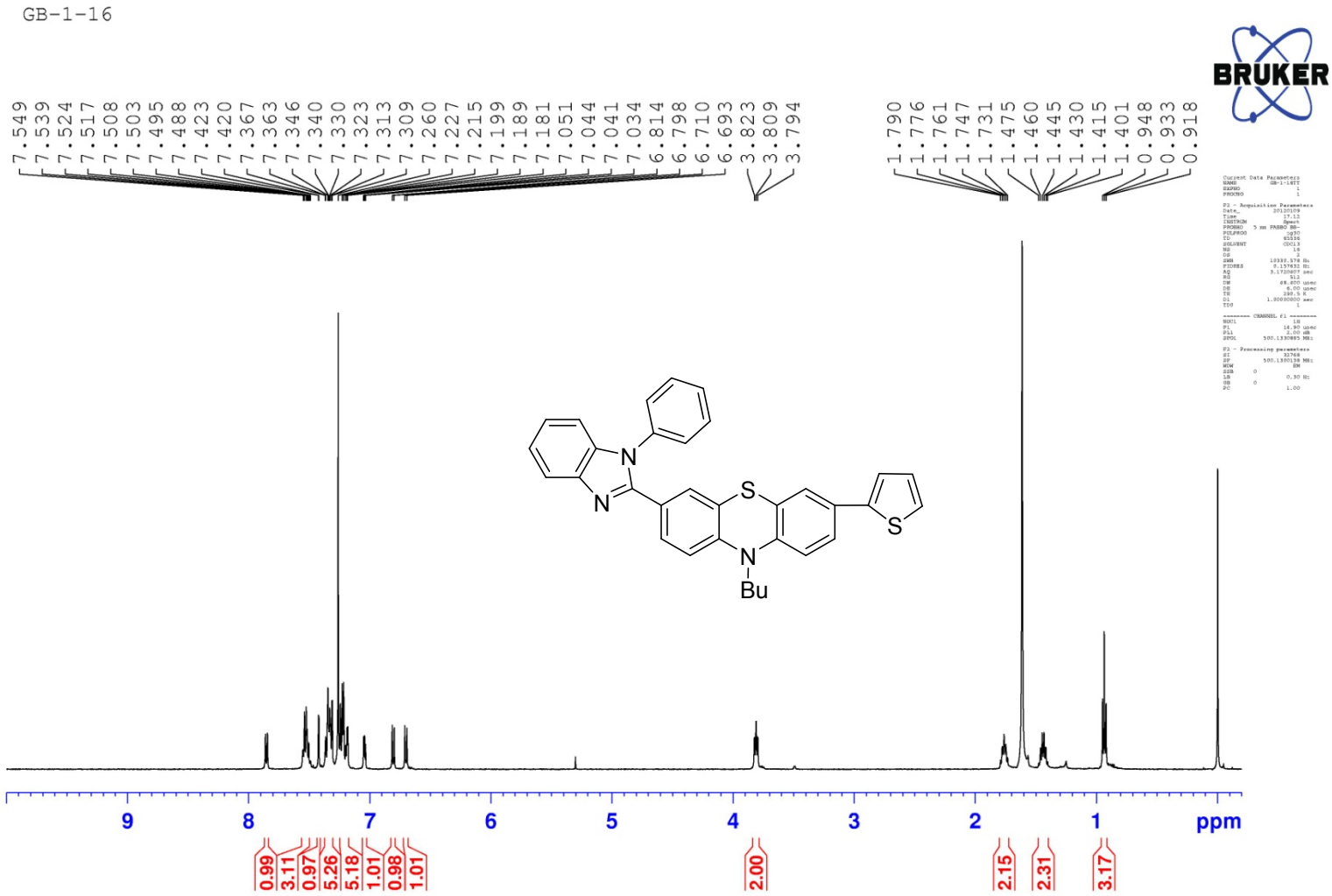

Fig. S11 ^{13}C NMR spectra of **6**.

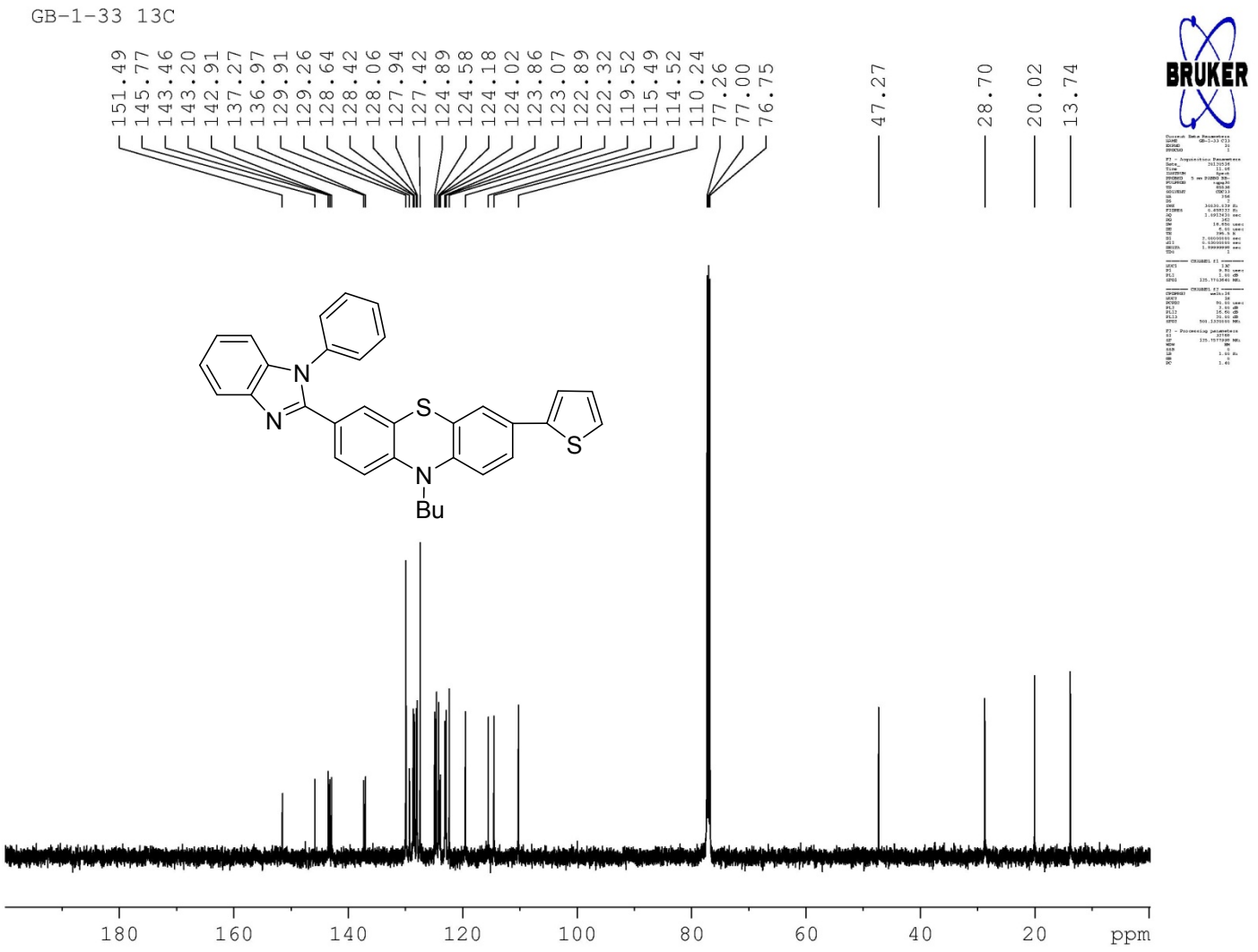

Fig. S12 ^{13}C NMR spectra of **6**.

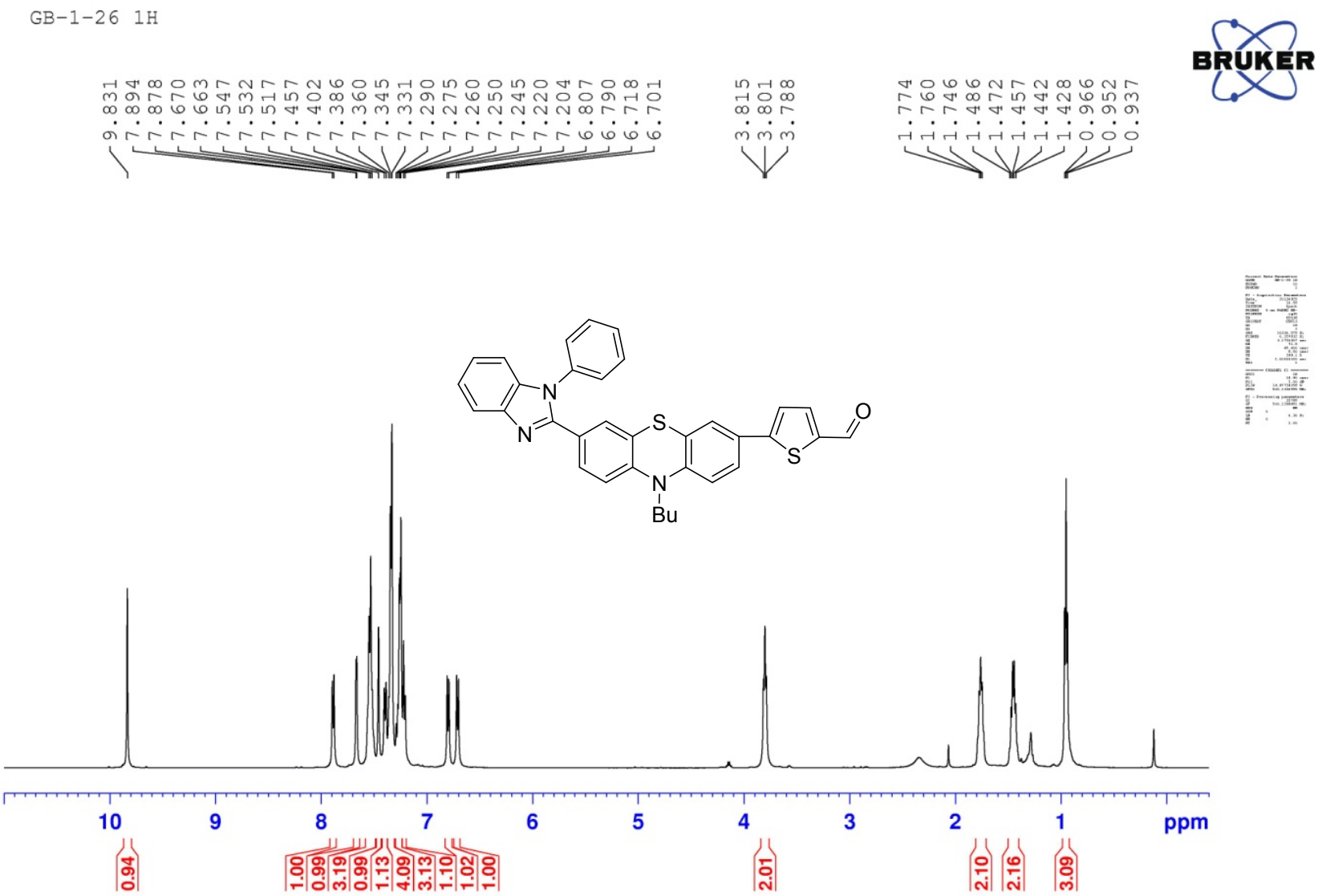

Fig. S13 ^{1}H NMR spectra of **3**.

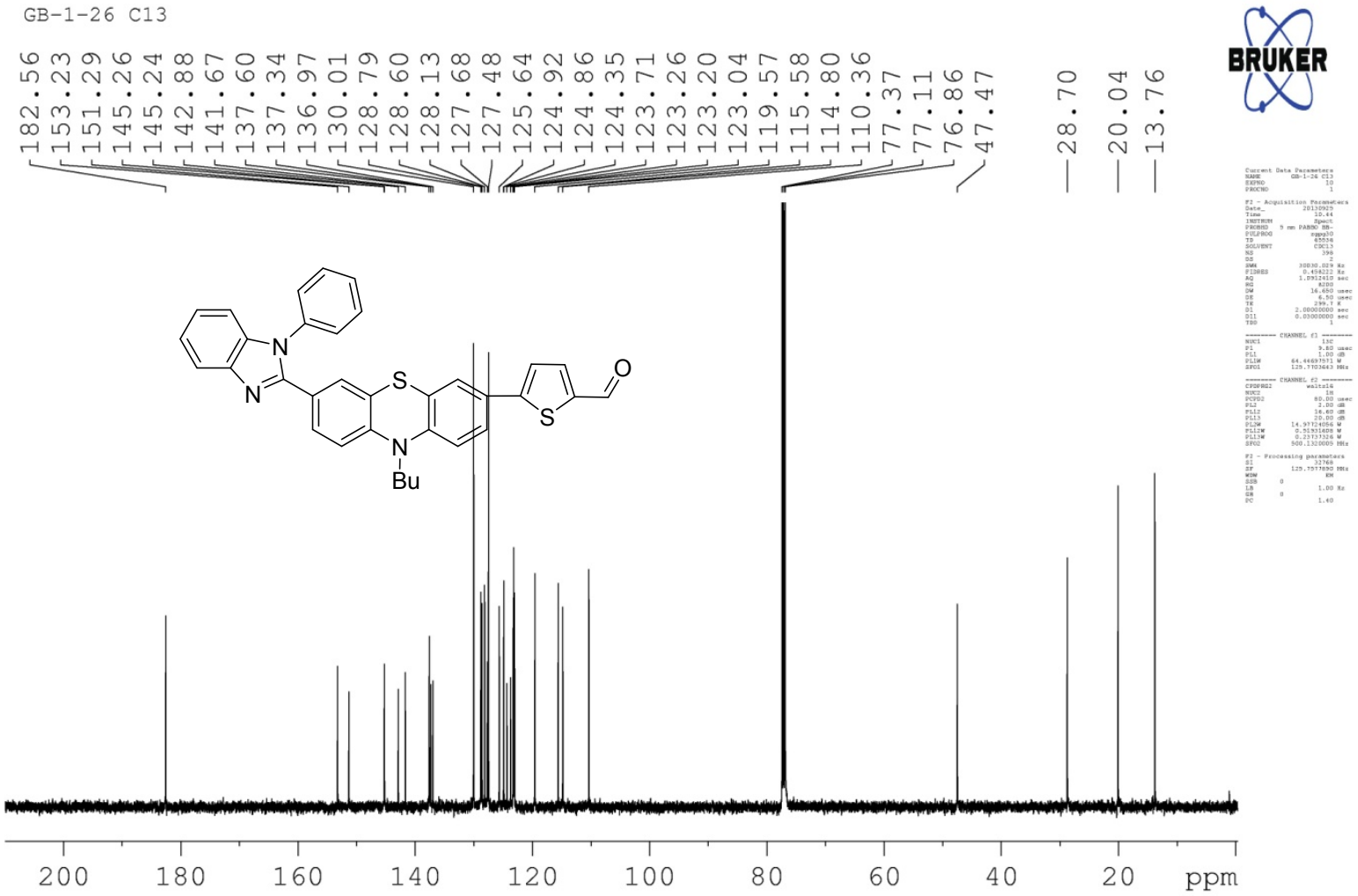

Fig. S14 ^{13}C NMR spectra of **3**.

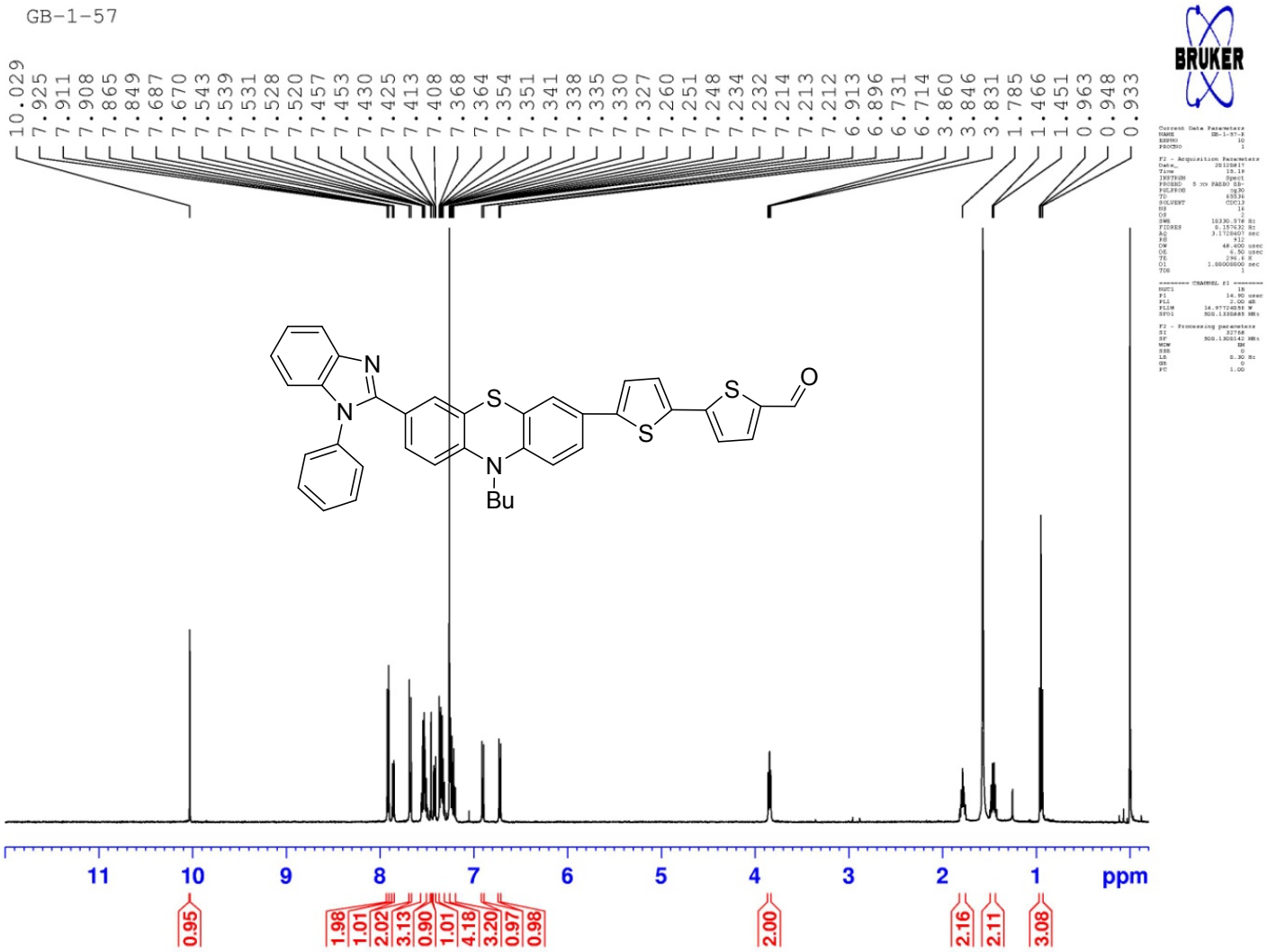

Fig. S15 ^{1}H NMR spectra of **4**.

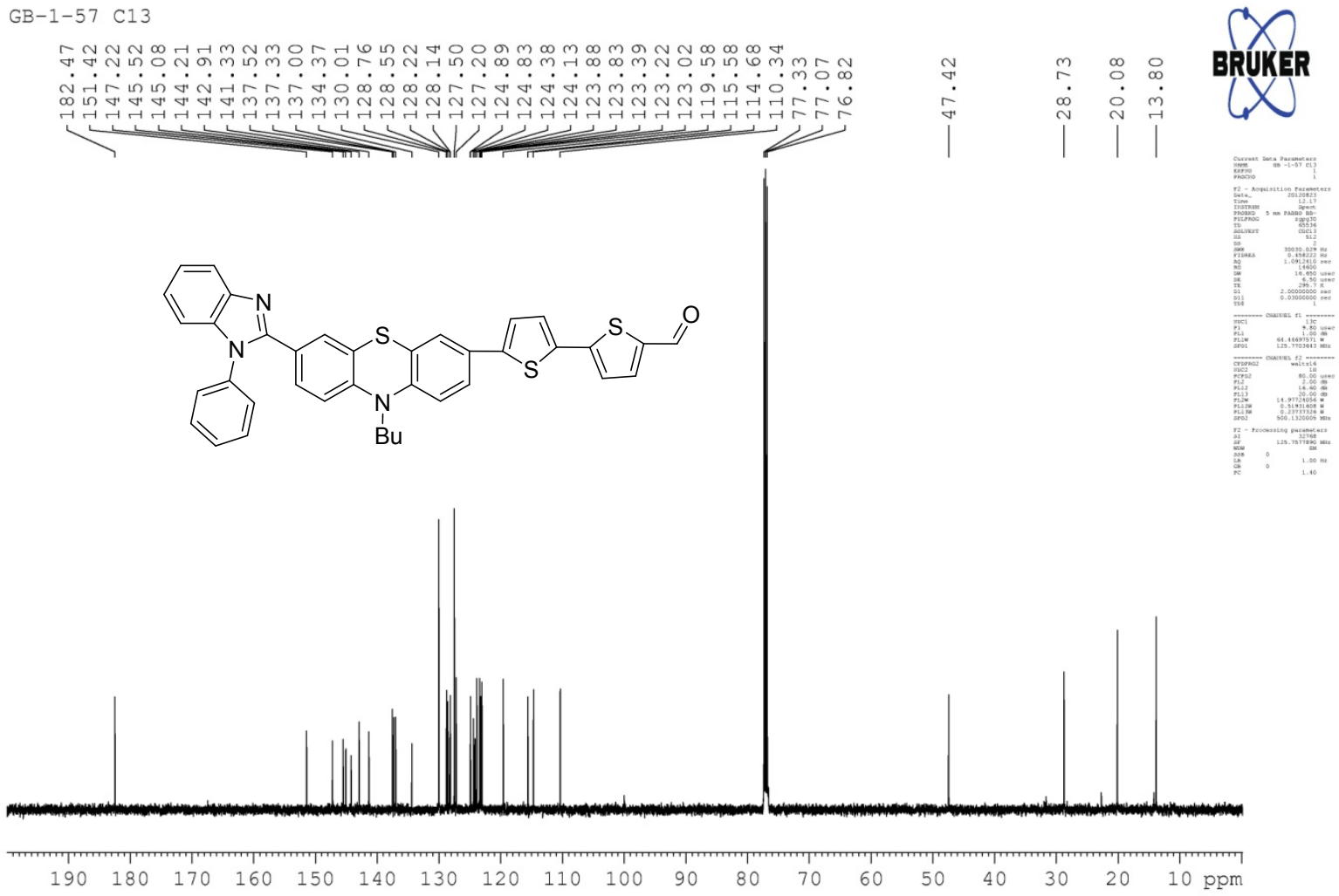

Fig. S16 ^{13}C NMR spectra of **4**.

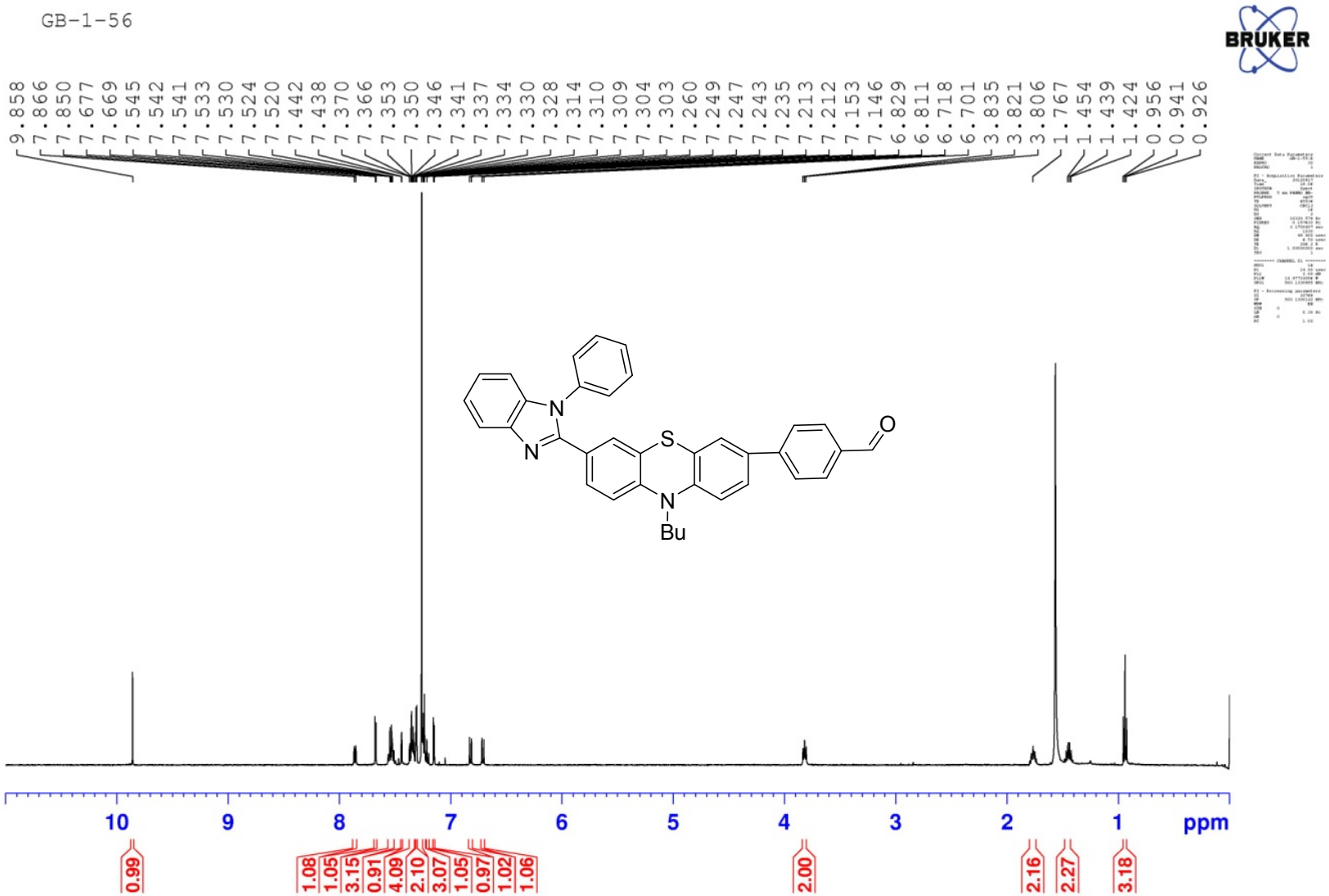

Fig. S17 ^{1}H NMR spectra of **5**.

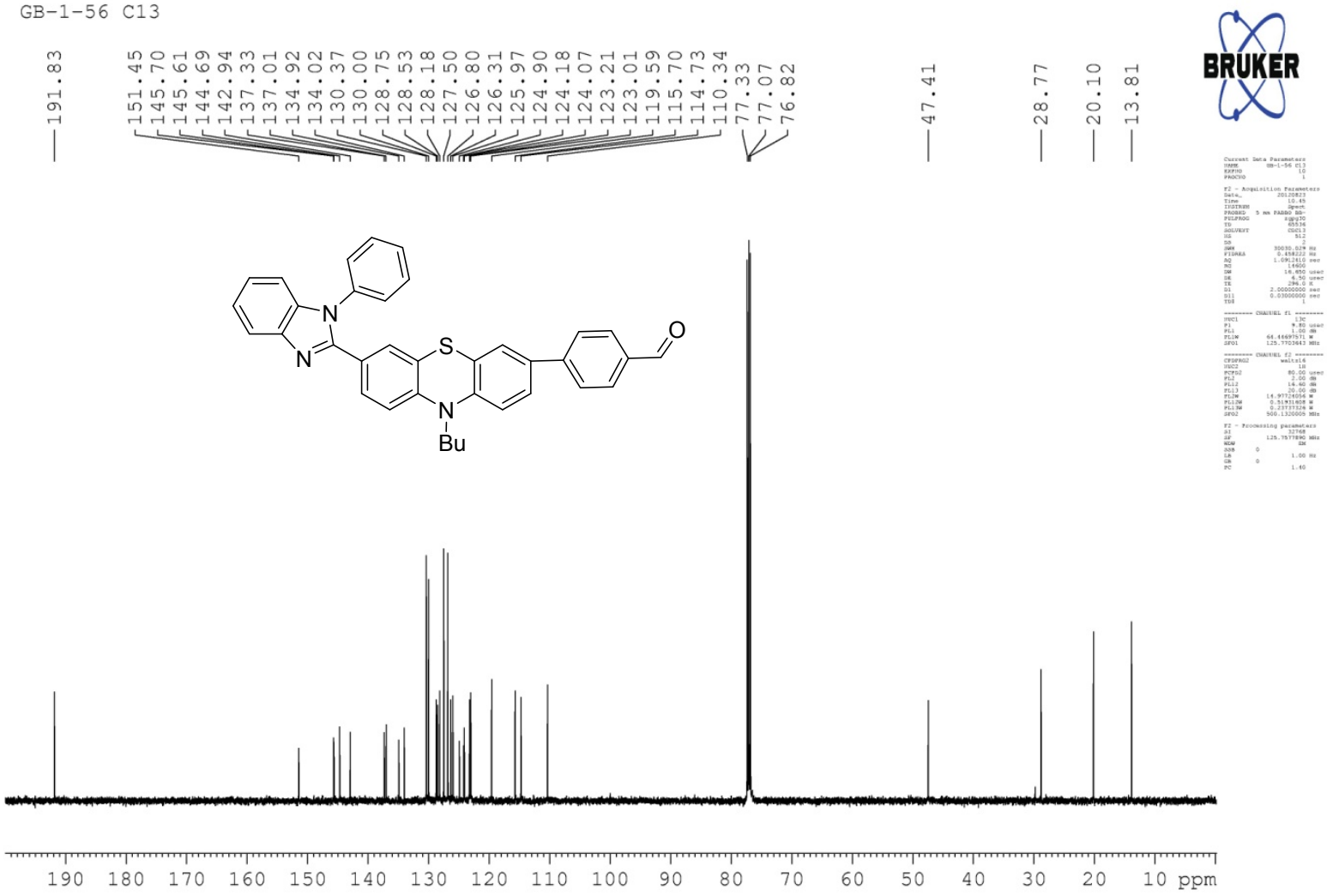

Fig. S18 ^{13}C NMR spectra of **5**.

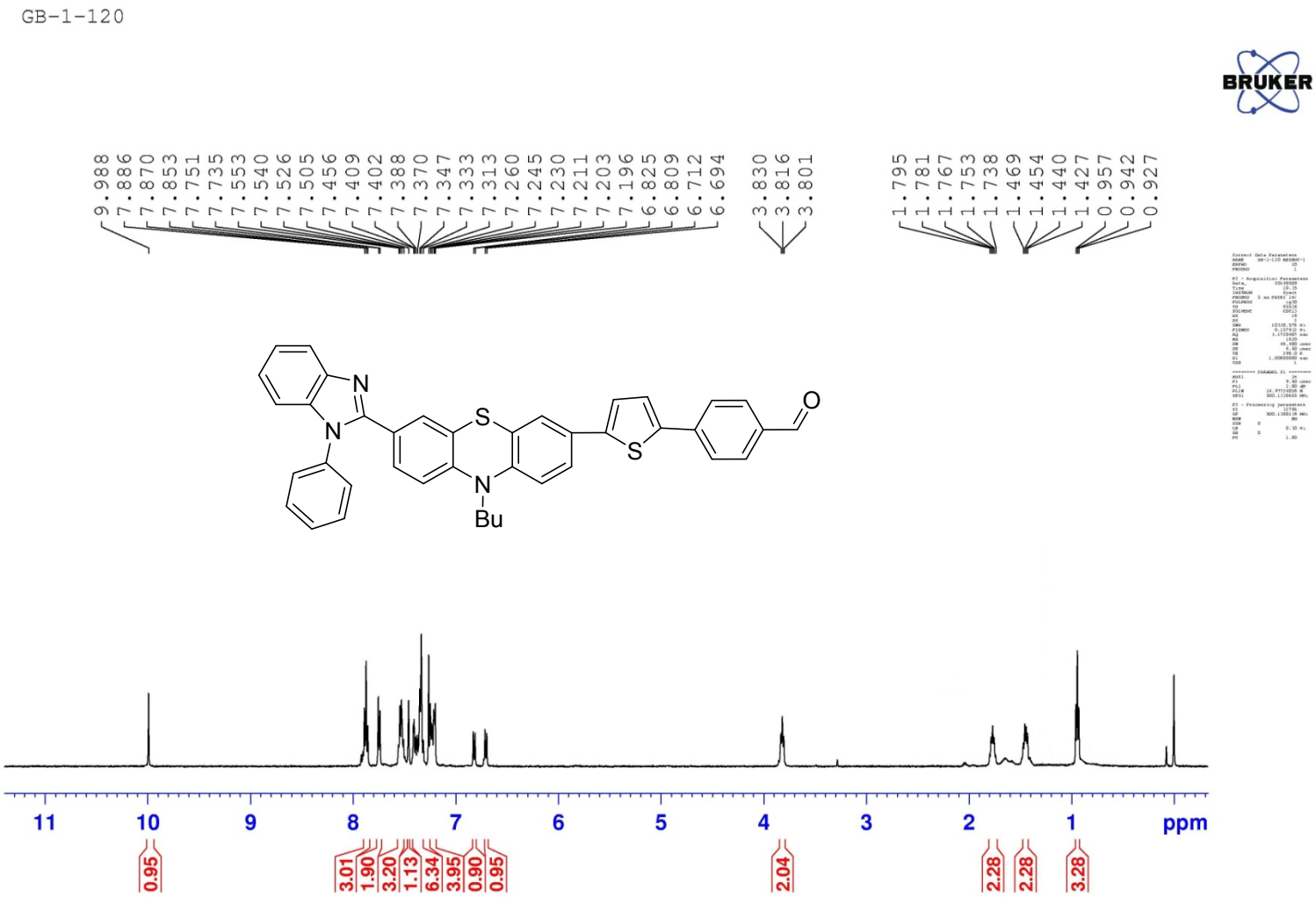

Fig. S19 ^{1}H NMR spectra of **8**.

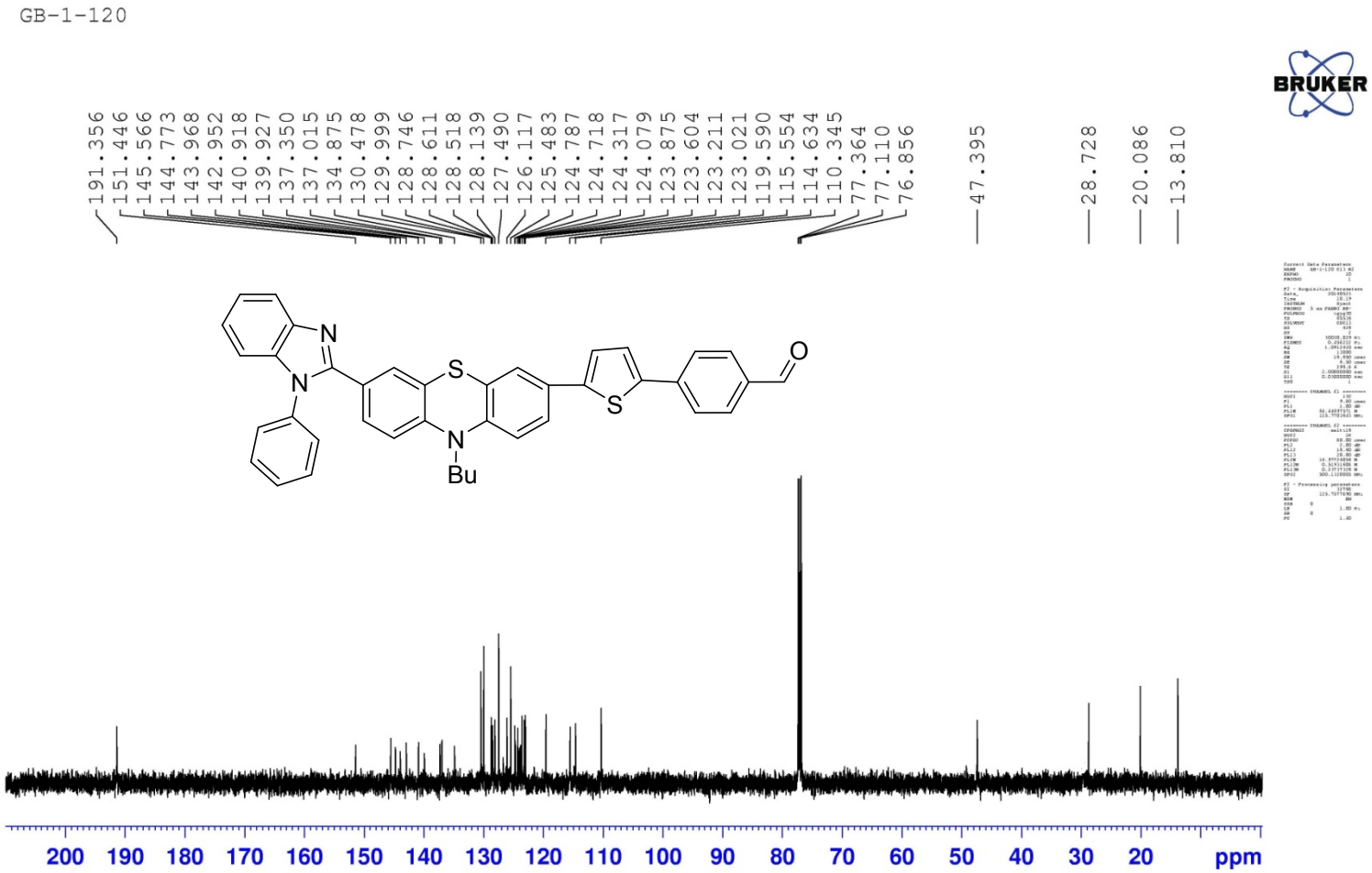

Fig. S20 ^{13}C NMR spectra of **8**.

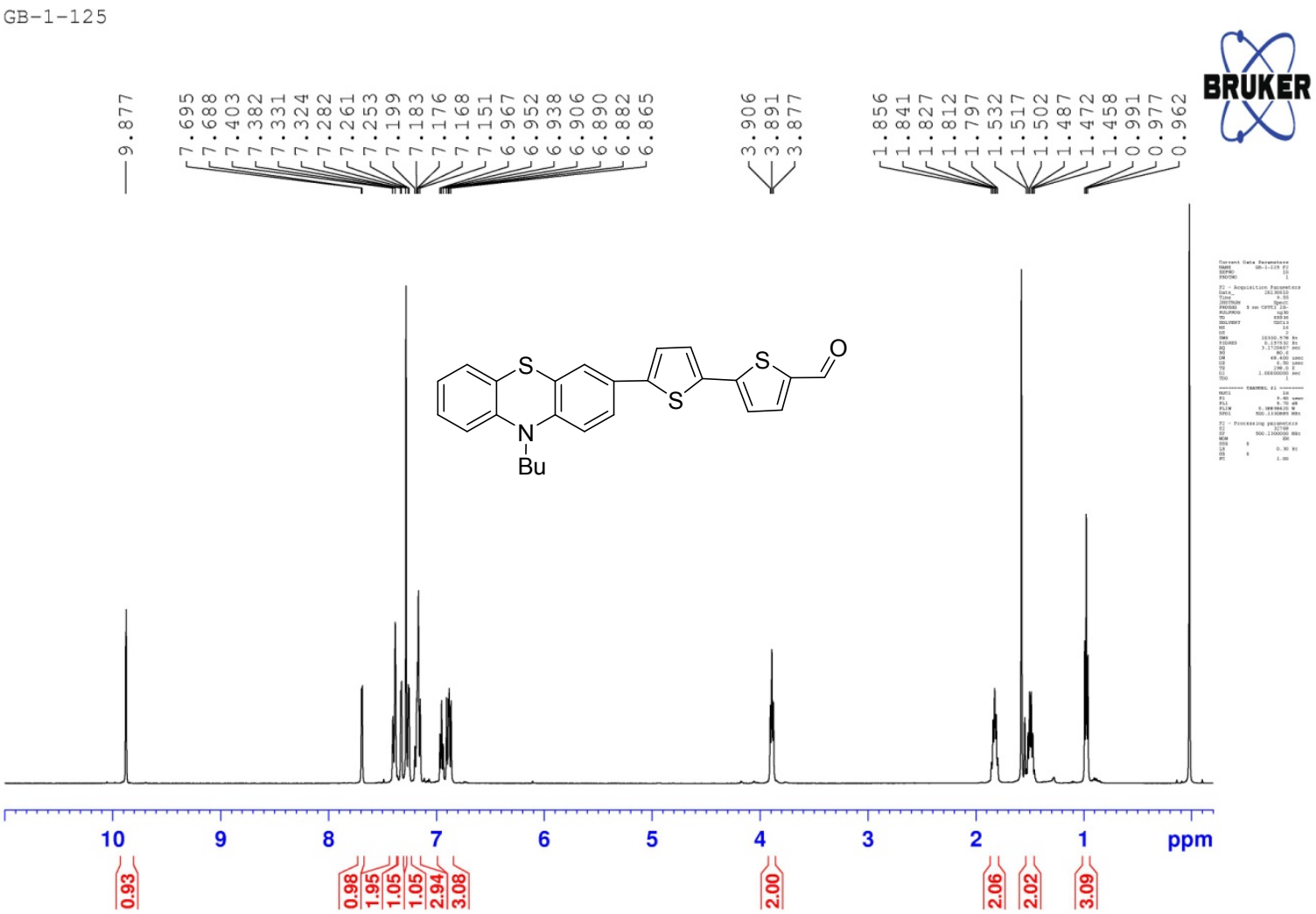

Fig. S21 ^{1}H NMR spectra of **10**.

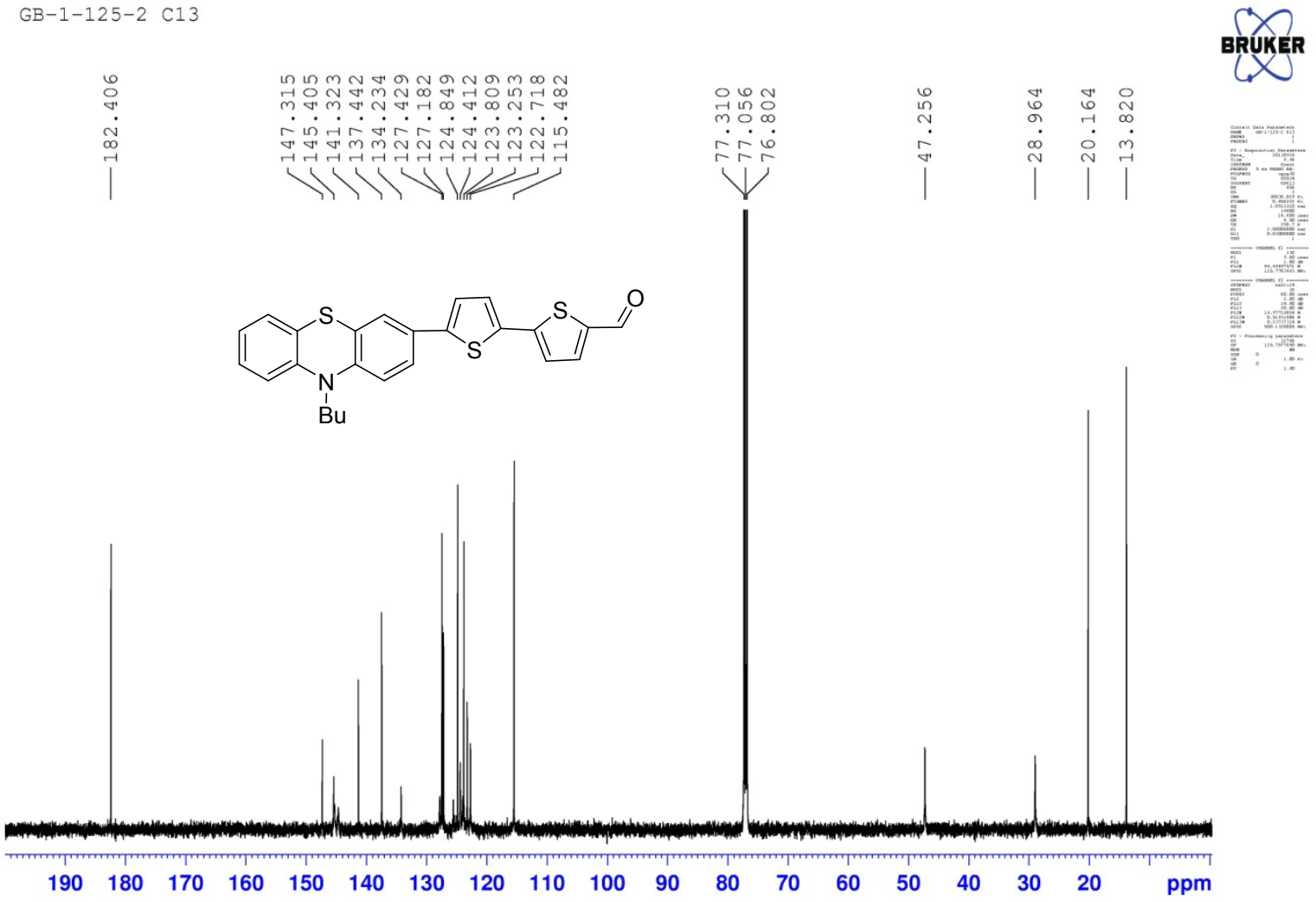

Fig. S22 ^{13}C NMR spectra of **10**.

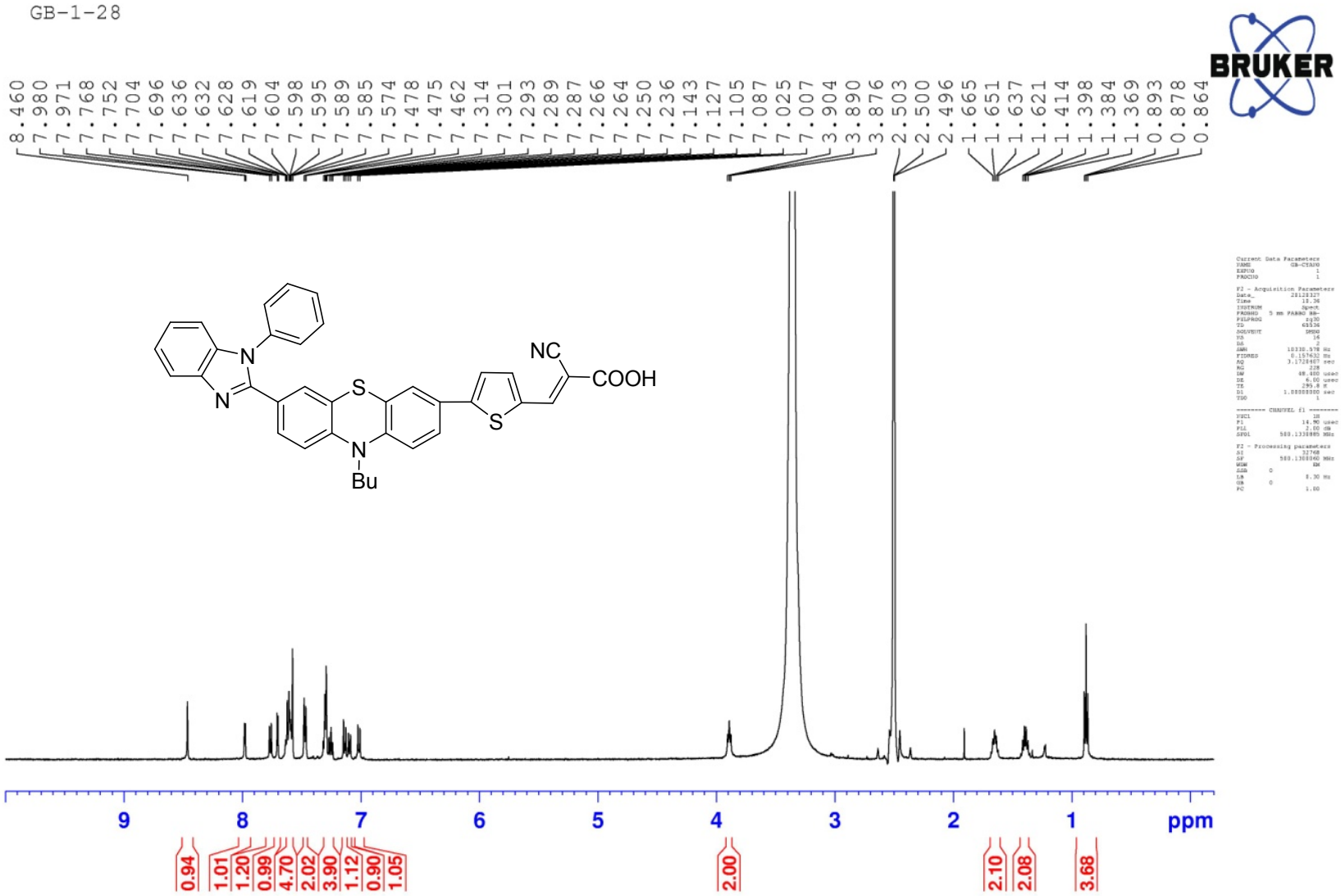

Fig. S23 ^{1}H NMR spectra of **GJ1**.

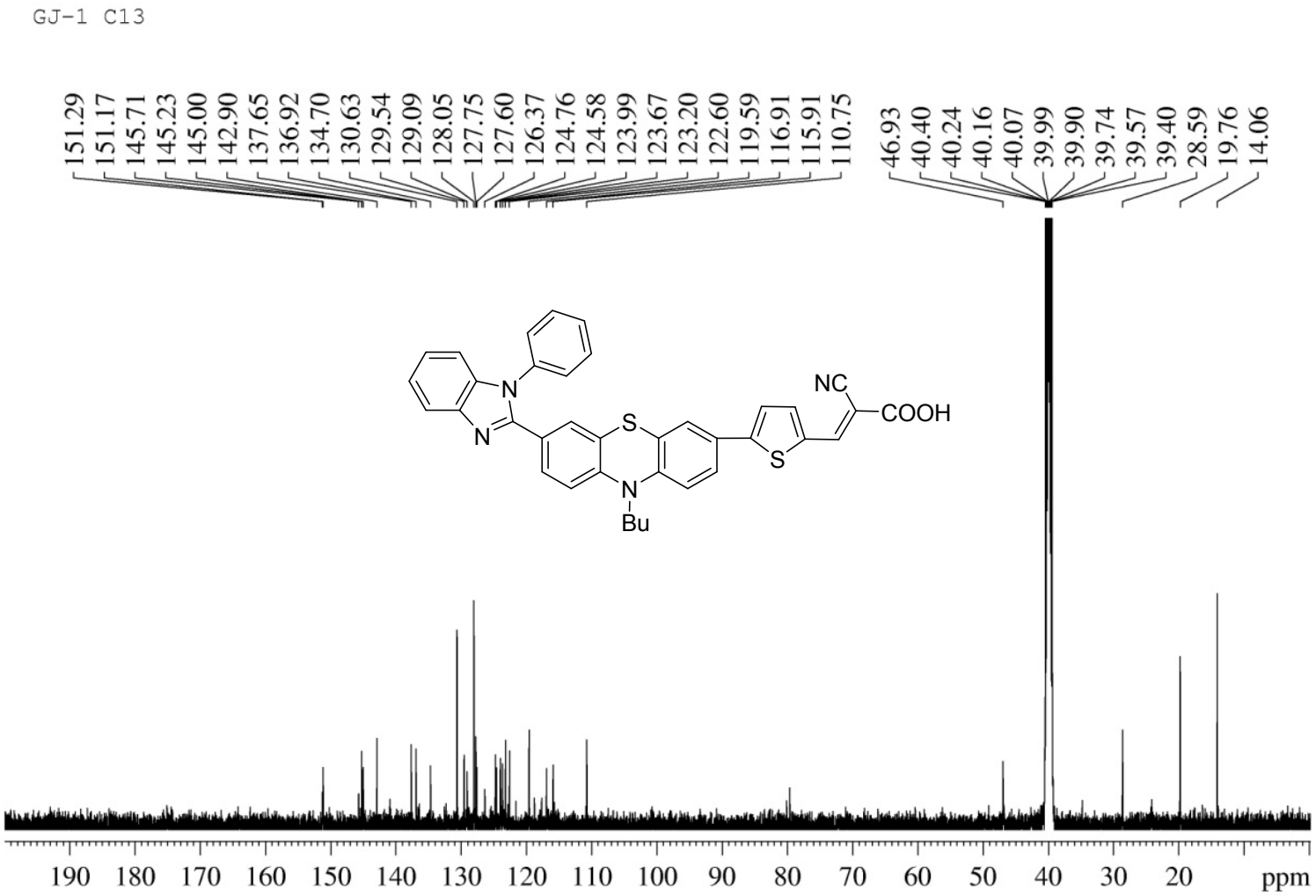

Fig. S24 ^{13}C NMR spectra of **GJ1**.

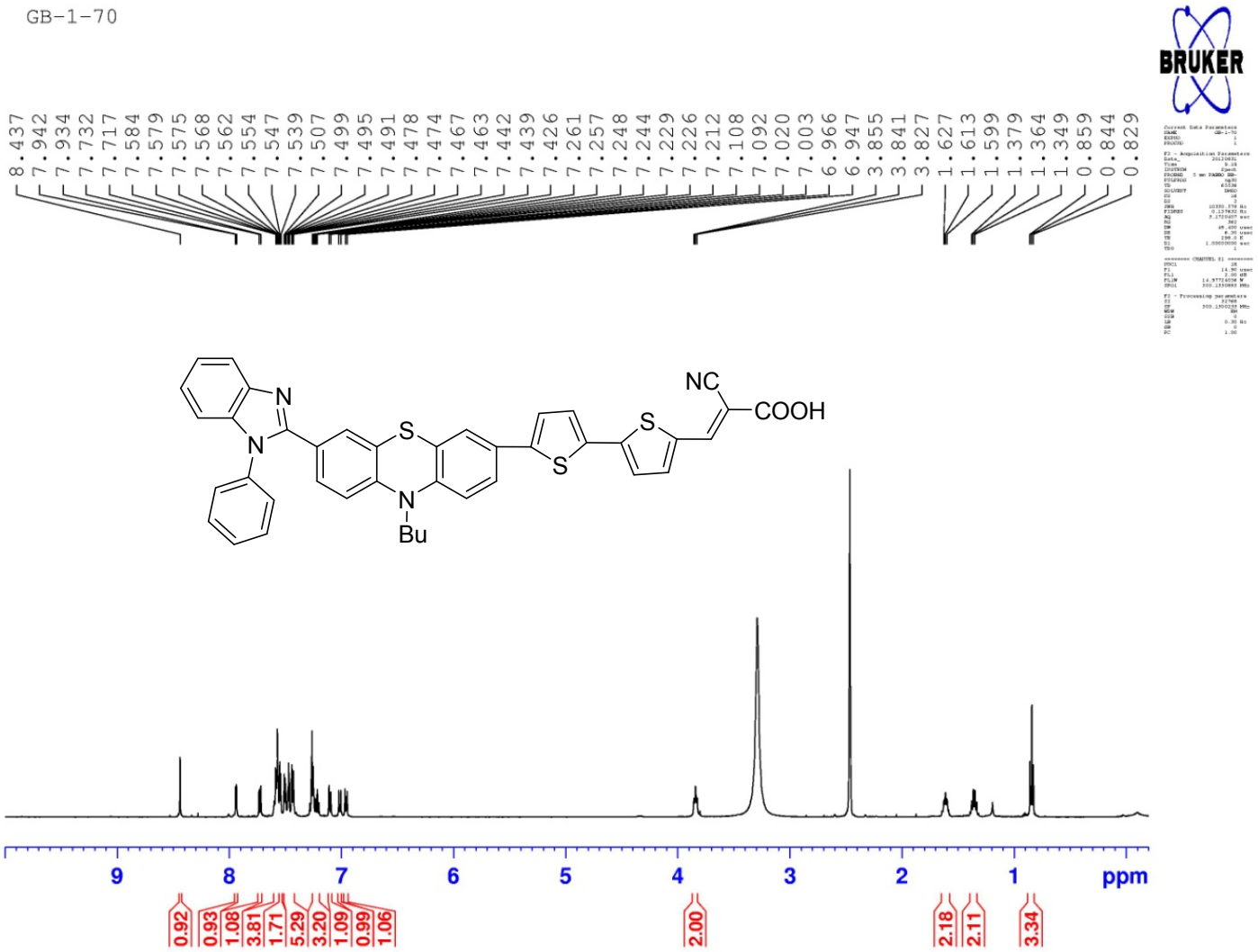

Fig. S25 ^{1}H NMR spectra of **GJ2**.

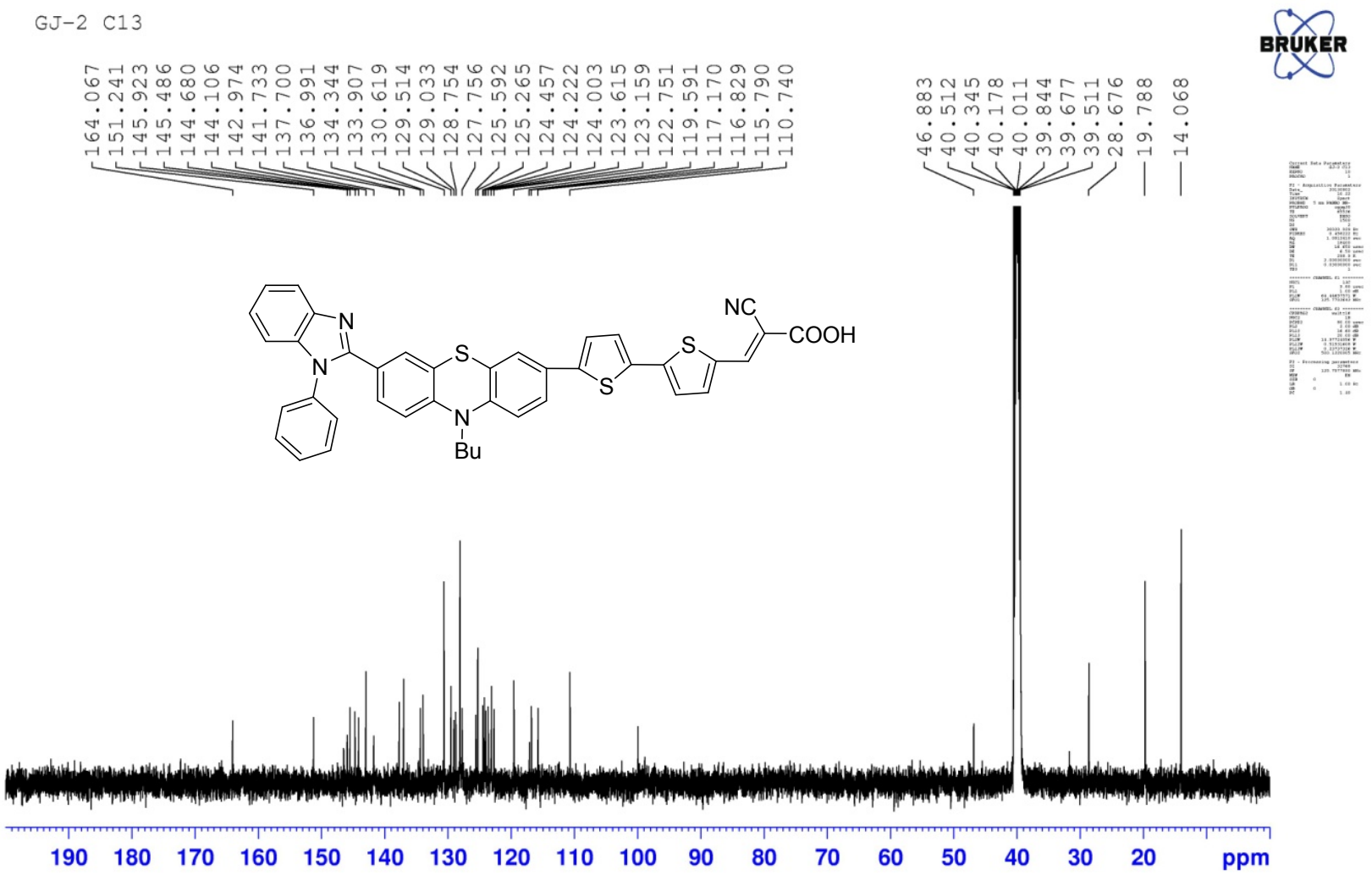

Fig. S26 ^{13}C NMR spectra of **GJ2**.

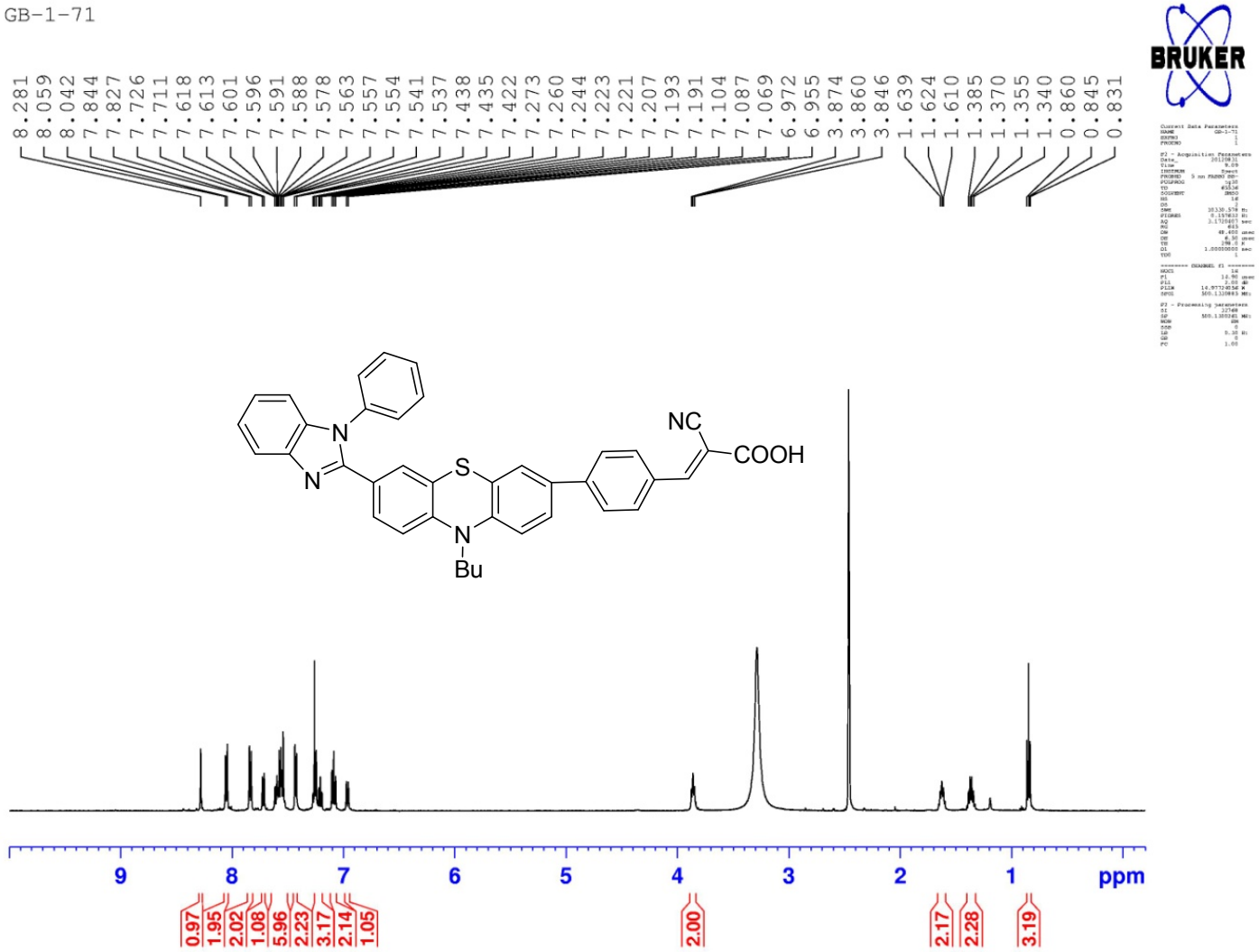

Fig. S27 ^{1}H NMR spectra of **GJ3**.

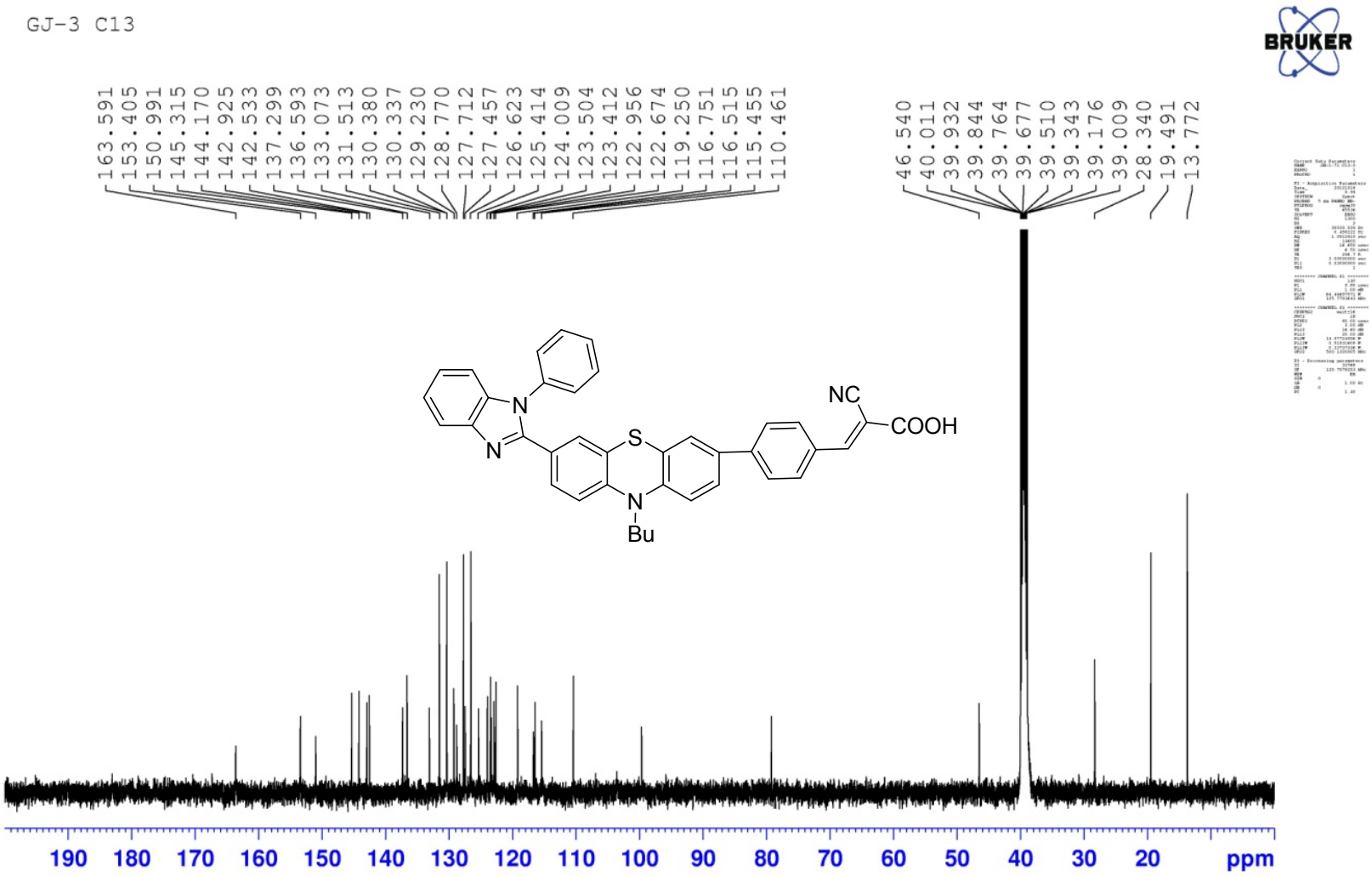

Fig. S28 ^{13}C NMR spectra of **GJ3**.

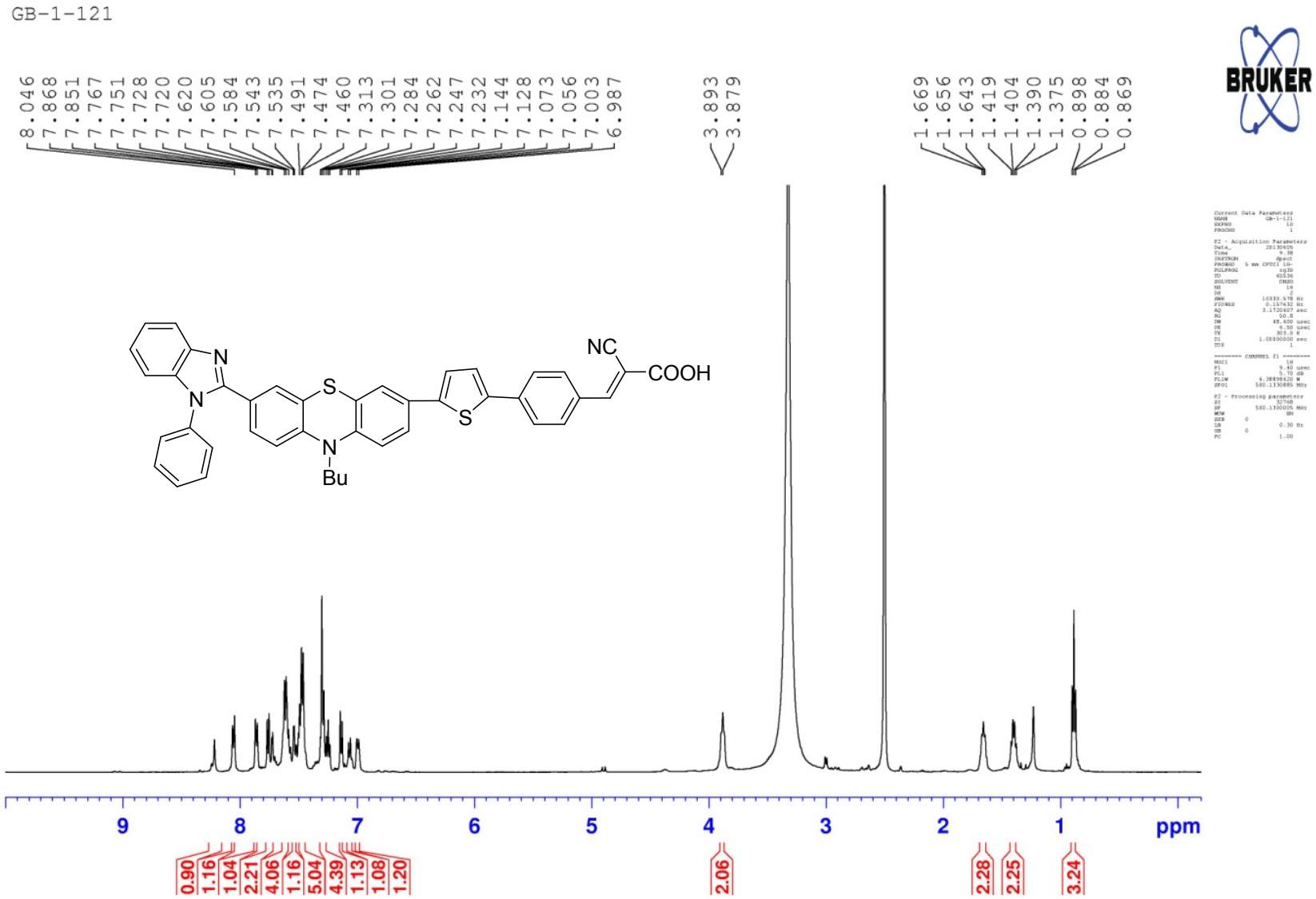

Fig. S29 ^{1}H NMR spectra of **GJ4**.

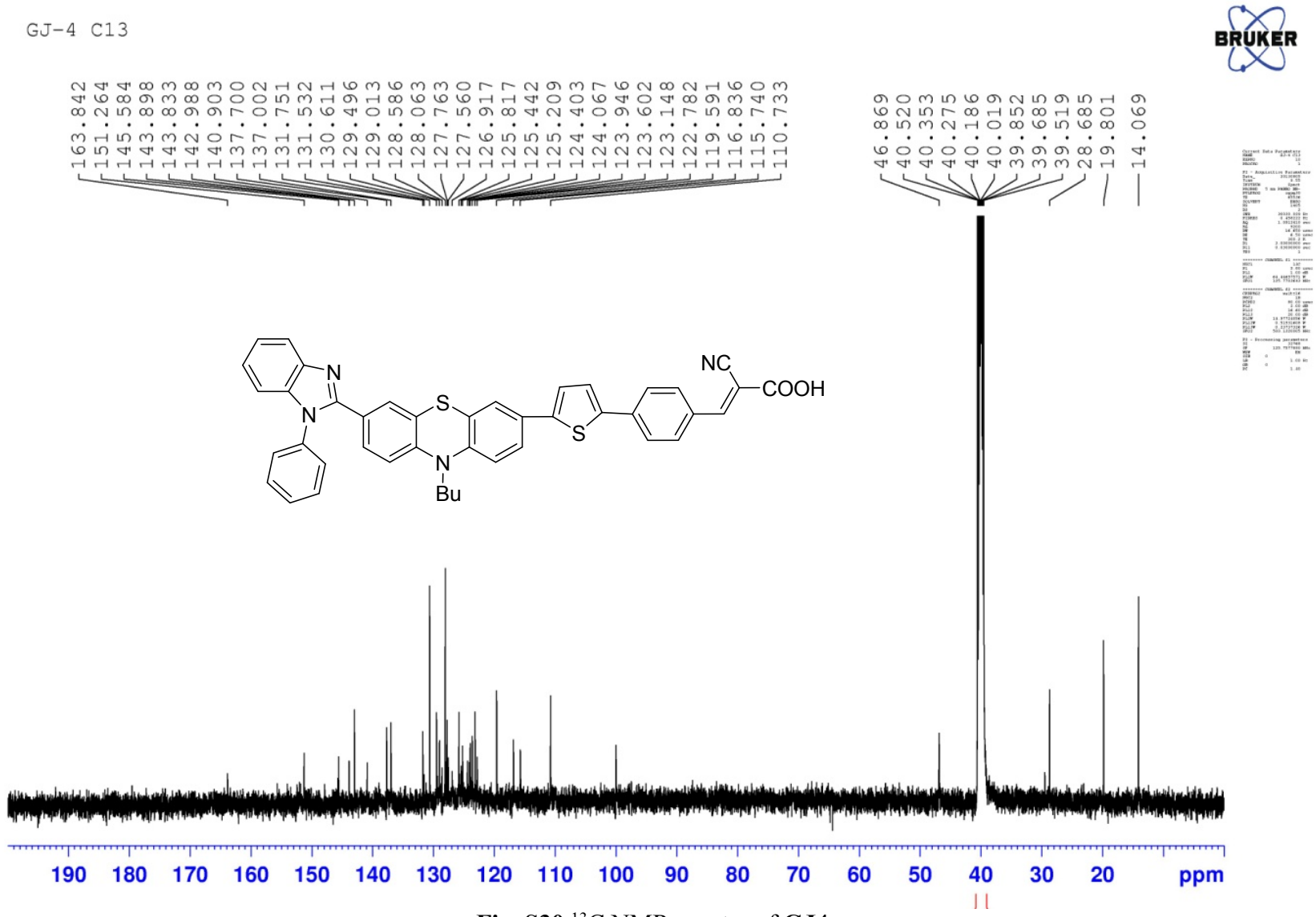

Fig. S30 ^{13}C NMR spectra of **GJ4**.

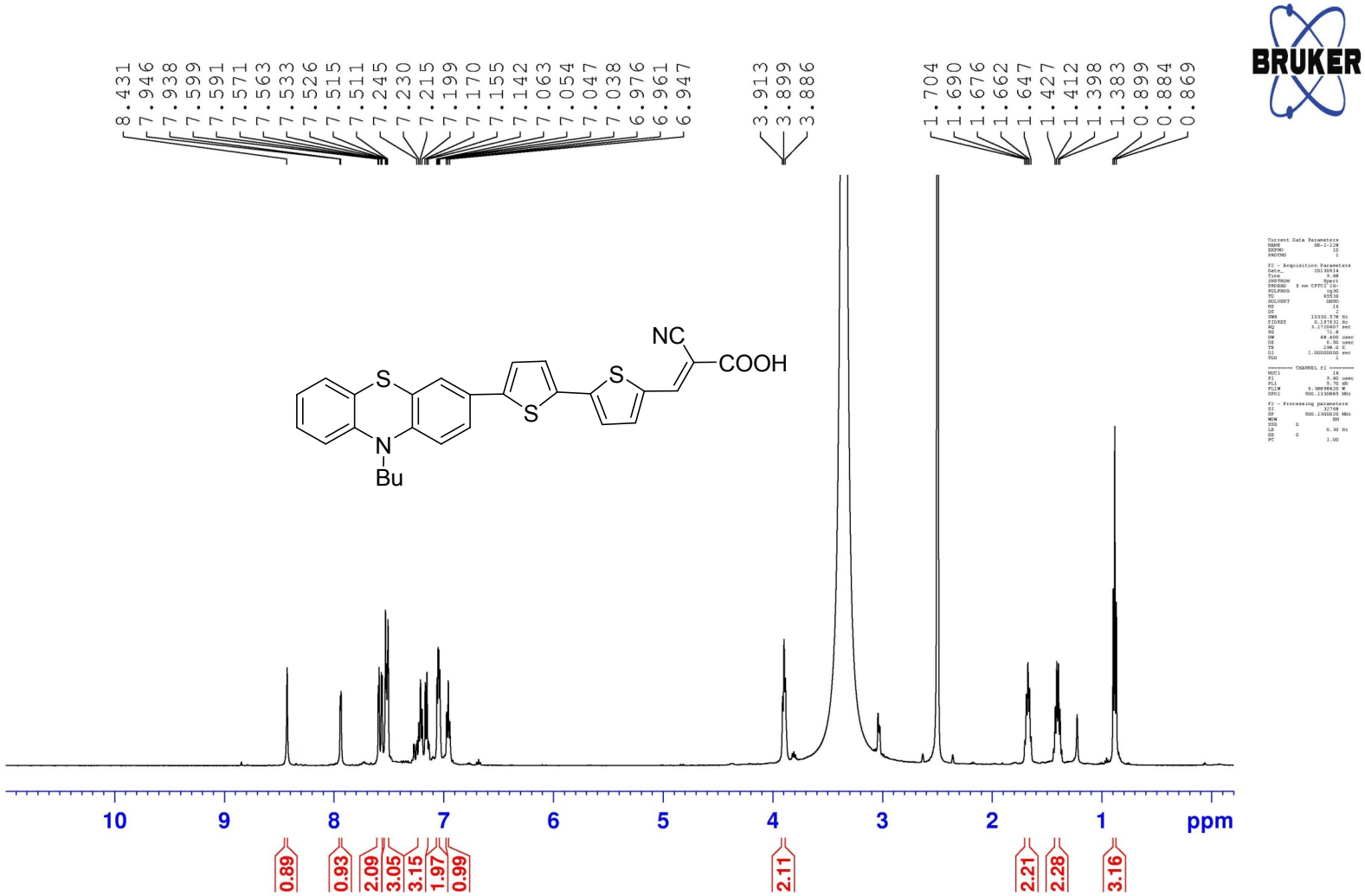

Fig. S31 ^{1}H NMR spectra of **GJ5**.

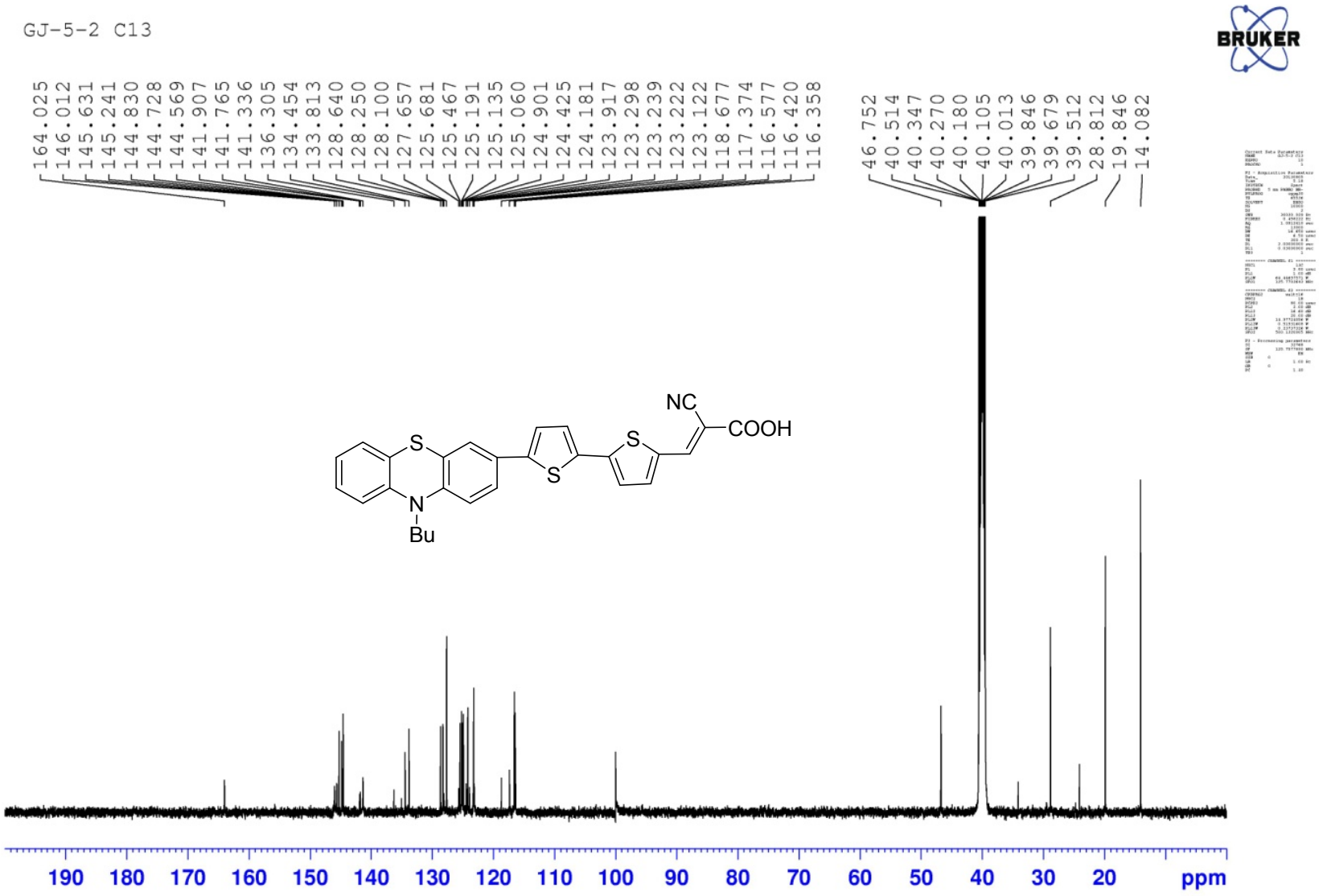

Fig. S32 ^{13}C NMR spectra of **GJ5**.

Table S1 Cartesian coordinates for the optimized structure of **GJ1**.

At. No.	X	Y	Z
6	-3.556108	-0.107283	0.167558
6	-2.450337	-0.602089	0.885706
6	-1.226231	0.053696	0.867482
6	-1.040989	1.225870	0.102061
6	-2.134849	1.698078	-0.643014
6	-3.367134	1.056840	-0.596366
6	1.380298	1.069012	0.047495
6	1.454942	-0.116973	0.804942
6	2.579763	-0.929924	0.752471
1	2.612616	-1.854536	1.318401
6	3.695643	-0.571241	-0.024178
6	3.620233	0.603683	-0.785554
6	2.477545	1.400085	-0.760154
1	-2.554805	-1.491284	1.499345
1	-2.022375	2.562984	-1.286862
1	-4.181052	1.447675	-1.200137
1	4.438825	0.892657	-1.433949
1	2.442920	2.284450	-1.386385
16	0.106778	-0.523517	1.899717
7	0.213283	1.868162	0.100123
6	4.840527	-1.493715	-0.040189
7	4.711285	-2.782167	0.199374
7	6.160720	-1.135647	-0.339099
6	5.974654	-3.322013	0.064700
6	6.904924	-2.313770	-0.273891
6	6.736044	0.164165	-0.480793
6	6.404293	-4.647460	0.215239
6	8.264860	-2.576779	-0.448969
6	7.376192	0.507947	-1.676346
6	6.691030	1.074287	0.580674
1	5.692238	-5.425826	0.471572
6	7.755289	-4.920736	0.032489
6	8.671794	-3.899766	-0.291849
1	8.973243	-1.791501	-0.693426
1	7.399940	-0.207504	-2.492820
6	7.967246	1.765338	-1.808532
6	7.272085	2.333515	0.435461
1	6.203757	0.789682	1.507828
1	8.116336	-5.939446	0.143372
1	9.721205	-4.149316	-0.422027
1	8.464554	2.029588	-2.737554
6	7.912782	2.681094	-0.756137
1	7.233230	3.039931	1.259909
1	8.369925	3.660773	-0.862734

6	0.300232	3.292875	-0.243181
1	0.591591	3.437904	-1.295273
6	1.232756	4.078382	0.689836
6	1.273208	5.571024	0.335667
1	2.247594	3.665986	0.652856
1	0.880151	3.945404	1.720689
6	2.183763	6.377427	1.267186
1	1.613939	5.691956	-0.702651
1	0.255335	5.984433	0.372168
1	1.847480	6.306395	2.308451
1	3.216539	6.010478	1.226746
1	-0.704662	3.705823	-0.138911
6	-4.838926	-0.805234	0.212660
6	-5.078867	-2.132014	0.543301
16	-6.329717	0.018998	-0.172350
6	-6.436417	-2.483494	0.476562
1	-4.289763	-2.831843	0.792476
6	-7.275174	-1.440422	0.093331
1	-6.815498	-3.478706	0.686301
6	-8.687040	-1.573518	-0.049455
6	-9.640908	-0.666065	-0.429176
1	-9.058679	-2.567682	0.184490
6	-9.335340	0.684356	-0.775414
6	-11.074884	-1.029990	-0.510357
7	-9.058069	1.780729	-1.053439
8	-11.962021	-0.272084	-0.842135
8	-11.312789	-2.326500	-0.169962
1	-12.276024	-2.443872	-0.260871
1	2.195006	7.437726	0.991613

Table S2 Cartesian coordinates for the optimized structure of **GJ2**.

At. No.	X	Y	Z
6	-1.891064	0.831038	-0.052995
6	-0.896368	0.158027	0.681824
6	0.416557	0.612712	0.703656
6	0.802722	1.753897	-0.031208
6	-0.181099	2.399450	-0.797571
6	-1.500041	1.957998	-0.793977
6	3.174192	1.234287	-0.024492
6	3.043891	0.034488	0.703960
6	4.035925	-0.936919	0.666050
1	3.910862	-1.867091	1.209655
6	5.220360	-0.732433	-0.063489
6	5.347708	0.455426	-0.797349
6	4.335727	1.412719	-0.789745
1	-1.157434	-0.711495	1.276888
1	0.084430	3.244159	-1.423392
1	-2.226344	2.476827	-1.413181
1	6.223694	0.631190	-1.410447
1	4.454763	2.303986	-1.395739
16	1.616790	-0.186564	1.751055
7	2.140904	2.199206	0.018730
6	6.219121	-1.811534	-0.061871
7	5.896504	-3.073514	0.130783
7	7.589560	-1.639304	-0.292846
6	7.075361	-3.785797	0.033634
6	8.154591	-2.913385	-0.232295
6	8.349644	-0.432247	-0.363357
6	7.305025	-5.162538	0.160966
6	9.470129	-3.363848	-0.355312
6	9.098895	-0.154936	-1.511859
6	8.373436	0.449739	0.722304
1	6.478299	-5.837025	0.361416
6	8.610755	-5.621875	0.029051
6	9.677422	-4.735026	-0.222094
1	10.293896	-2.682280	-0.542839
1	9.068424	-0.847017	-2.348004
6	9.867603	1.008434	-1.573087
6	9.133010	1.616638	0.647542
1	7.798859	0.215771	1.612879
1	8.817653	-6.684260	0.123690
1	10.685921	-5.128808	-0.313456
1	10.449411	1.220718	-2.465676
6	9.882596	1.897838	-0.497141
1	9.147249	2.301579	1.490704
1	10.478587	2.804638	-0.548590

6	2.448594	3.600834	-0.287357
1	2.781065	3.724915	-1.330126
6	3.467584	4.218631	0.680571
6	3.720551	5.701474	0.376738
1	4.415371	3.669978	0.639721
1	3.084989	4.103623	1.702813
6	4.728673	6.340956	1.336899
1	4.082268	5.807699	-0.656116
1	2.770518	6.252446	0.424853
1	4.380499	6.279278	2.374862
1	5.701284	5.836966	1.283315
1	1.513964	4.156747	-0.191191
6	-3.271007	0.347438	-0.042482
6	-3.737412	-0.926638	0.219104
16	-4.613978	1.424413	-0.370971
6	-5.142928	-1.048652	0.144442
1	-3.079150	-1.762910	0.425482
6	-5.788218	0.131866	-0.176335
1	-5.669609	-1.984494	0.300475
1	4.887389	7.398864	1.100151
6	-7.197067	0.376692	-0.344342
6	-7.821880	1.530225	-0.806970
16	-8.373158	-0.854965	0.056671
6	-9.218945	1.422980	-0.844549
1	-7.275660	2.414233	-1.116736
6	-9.708748	0.191631	-0.415208
1	-9.877863	2.216976	-1.181055
6	-11.093798	-0.136148	-0.374140
6	-11.733611	-1.285791	0.011504
1	-11.744122	0.668758	-0.706317
6	-11.039062	-2.442895	0.474823
6	-13.209283	-1.407298	-0.026990
7	-10.445837	-3.372677	0.849075
8	-13.829970	-2.396734	0.300753
8	-13.822833	-0.277403	-0.475498
1	-14.776414	-0.477744	-0.455471

Table S3 Cartesian coordinates for the optimized structure of **GJ3**.

At. No.	X	Y	Z
6	-3.516112	1.165307	-0.158737
6	-2.552480	0.475165	0.597401
6	-1.225481	0.890368	0.631971
6	-0.792113	1.997664	-0.126664
6	-1.744380	2.656336	-0.921512
6	-3.079062	2.262552	-0.917023
6	1.558992	1.393695	-0.078857
6	1.378236	0.220365	0.681255
6	2.334101	-0.787178	0.680548
1	2.169538	-1.696632	1.248087
6	3.532106	-0.647006	-0.042233
6	3.709856	0.514481	-0.807041
6	2.733645	1.508036	-0.836228
1	-2.846686	-0.373745	1.207103
1	-1.442306	3.472400	-1.568583
1	-3.780567	2.788288	-1.557895
1	4.597270	0.641643	-1.415645
1	2.891916	2.377466	-1.464546
16	-0.066982	0.080309	1.717199
7	0.561024	2.396659	-0.072787
6	4.488766	-1.762819	-0.000110
7	4.115901	-3.004260	0.231098
7	5.866348	-1.652106	-0.227001
6	5.266226	-3.764833	0.165883
6	6.380589	-2.944604	-0.120418
6	6.673397	-0.478569	-0.333489
6	5.440347	-5.144414	0.340607
6	7.678172	-3.450333	-0.217881
6	7.433615	-0.266348	-1.488606
6	6.730320	0.435406	0.724068
1	4.586263	-5.778717	0.556879
6	6.727786	-5.658829	0.234558
6	7.830233	-4.823360	-0.037397
1	8.529532	-2.808305	-0.421096
1	7.377262	-0.982580	-2.302751
6	8.245937	0.864544	-1.584763
6	7.533879	1.569633	0.614439
1	6.146154	0.251555	1.620142
1	6.891957	-6.724724	0.366221
1	8.823029	-5.259193	-0.107463
1	8.835978	1.026467	-2.482500
6	8.294163	1.786166	-0.537235
1	7.573508	2.279601	1.435803

1	8.924150	2.667651	-0.616209
6	0.923683	3.774602	-0.422294
1	1.275345	3.849550	-1.463464
6	1.951099	4.387802	0.539733
6	2.290943	5.837522	0.168858
1	2.868718	3.788752	0.551348
1	1.539098	4.345226	1.556136
6	3.299152	6.475781	1.129776
1	2.691856	5.868945	-0.854450
1	1.370378	6.438352	0.153585
1	2.911846	6.493406	2.155494
1	4.242834	5.917072	1.141808
1	0.009346	4.367698	-0.360352
1	3.525797	7.507988	0.840590
6	-4.931962	0.740493	-0.164364
6	-5.971897	1.681871	-0.281449
6	-5.290101	-0.618298	-0.055068
6	-7.298496	1.279766	-0.289631
1	-5.734661	2.739917	-0.336708
6	-6.615628	-1.025891	-0.060360
1	-4.511275	-1.372244	0.005942
6	-7.659341	-0.081279	-0.178820
1	-8.082587	2.028666	-0.371400
1	-6.838996	-2.082407	0.017338
6	-9.077545	-0.388361	-0.196304
6	-9.756065	-1.570392	-0.118413
1	-9.718117	0.484420	-0.289219
6	-9.138254	-2.853956	0.007342
6	-11.242899	-1.615142	-0.160101
7	-8.623404	-3.892664	0.109715
8	-11.899497	-2.632203	-0.095944
8	-11.810787	-0.385885	-0.279138
1	-12.772229	-0.545806	-0.294559

Table S4 Cartesian coordinates for the optimized structure of **GJ4**.

At. No.	X	Y	Z
6	-1.824137	0.436139	0.087079
6	-0.773788	-0.165598	0.805300
6	0.505975	0.376128	0.802076
6	0.801665	1.537738	0.057806
6	-0.237585	2.115424	-0.688823
6	-1.524045	1.586210	-0.660240
6	3.200497	1.169038	0.012800
6	3.163136	-0.033695	0.747136
6	4.213081	-0.941062	0.687773
1	4.159857	-1.874847	1.236951
6	5.364374	-0.666083	-0.071140
6	5.399251	0.524302	-0.811139
6	4.329945	1.416565	-0.780849
1	-0.965503	-1.049314	1.405914
1	-0.040985	2.975229	-1.319532
1	-2.295735	2.054015	-1.264979
1	6.247031	0.751988	-1.446368
1	4.378568	2.311194	-1.391580
16	1.776696	-0.339659	1.826759
7	2.110408	2.067603	0.078735
6	6.429025	-1.679945	-0.090260
7	6.192556	-2.958354	0.119048
7	7.779173	-1.423464	-0.359687
6	7.411081	-3.595488	-0.006214
6	8.425160	-2.658788	-0.307592
6	8.460329	-0.172137	-0.459930
6	7.731193	-4.953829	0.123531
6	9.762703	-3.025919	-0.464886
6	9.156294	0.141722	-1.632318
6	8.463068	0.717613	0.619634
1	6.954890	-5.677735	0.351345
6	9.059427	-5.330502	-0.041789
6	10.060264	-4.380066	-0.328701
1	10.535656	-2.294897	-0.680228
1	9.142741	-0.557162	-2.463256
6	9.850970	1.348846	-1.723406
6	9.148162	1.927627	0.515376
1	7.931100	0.455792	1.528744
1	9.336071	-6.376819	0.053854
1	11.088768	-4.710135	-0.445903
1	10.391561	1.589477	-2.634519
6	9.844753	2.245119	-0.653058
1	9.146347	2.618332	1.353945
1	10.383067	3.185774	-0.727435

6	2.323281	3.484226	-0.237937
1	2.626786	3.624354	-1.287647
6	3.321328	4.167825	0.707370
6	3.483548	5.660237	0.389445
1	4.298408	3.674256	0.653281
1	2.964136	4.038714	1.737096
6	4.470125	6.363565	1.327105
1	3.820494	5.778979	-0.650398
1	2.504667	6.156814	0.450819
1	4.144007	6.290744	2.371500
1	5.468782	5.915156	1.259945
1	1.358002	3.981539	-0.124762
6	-3.166625	-0.145326	0.118241
6	-3.533290	-1.452265	0.369332
16	-4.592100	0.832585	-0.162646
6	-4.930204	-1.672118	0.326602
1	-2.811519	-2.242720	0.542450
6	-5.668208	-0.540570	0.039451
1	-5.378763	-2.649471	0.465864
1	4.564332	7.426840	1.080086
6	-7.114061	-0.409433	-0.094382
6	-7.706642	0.692835	-0.743538
6	-7.976091	-1.398686	0.430048
6	-9.082755	0.792307	-0.861391
1	-7.079493	1.467804	-1.174617
6	-9.351319	-1.305166	0.305572
1	-7.556046	-2.246184	0.961941
6	-9.946399	-0.200478	-0.346874
1	-9.511251	1.652012	-1.370679
1	-9.967745	-2.089101	0.726976
6	-11.368910	0.003603	-0.531974
6	-12.452898	-0.746173	-0.172126
1	-11.620302	0.922448	-1.054591
6	-12.380860	-1.994231	0.521650
6	-13.838480	-0.306915	-0.487281
7	-12.306573	-3.009258	1.086451
8	-14.837575	-0.929624	-0.197036
8	-13.885175	0.882174	-1.144773
1	-14.832437	1.058441	-1.292254

Table S5 Cartesian coordinates for the optimized structure of **GJ5**

At. No.	X	Y	Z
6	2.623414	0.024282	-0.005498
6	2.223150	-1.232581	0.411073
16	1.218636	0.991044	-0.431167
6	0.822792	-1.415273	0.404335
1	2.922758	-1.997388	0.732294
6	0.114093	-0.305731	-0.016884
1	0.341928	-2.329390	0.733583
6	-1.332050	-0.144385	-0.144383
6	-2.165144	-1.269935	-0.290523
6	-1.955198	1.111430	-0.128644
6	-3.542197	-1.147114	-0.422144
1	-1.726409	-2.260936	-0.354457
6	-3.337136	1.237582	-0.222796
1	-1.360386	2.011621	-0.002012
6	-4.176257	0.116013	-0.361492
16	-4.476587	-2.598320	-0.847856
1	-3.758690	2.232305	-0.173731
7	-5.573933	0.239728	-0.462844
6	-6.037426	-2.155334	-0.119656
6	-6.446528	-0.806284	-0.070198
6	-6.145388	1.561804	-0.750656
6	-6.887938	-3.179897	0.295687
6	-7.756531	-0.545373	0.367825
6	-6.365214	2.508488	0.446659
1	-7.097503	1.394674	-1.265151
1	-5.487498	2.043955	-1.481836
1	-6.528809	-4.204746	0.261310
6	-8.187454	-2.901562	0.718924
6	-8.617434	-1.578519	0.741374
1	-8.121020	0.471494	0.422862
6	-6.953713	3.853715	-0.000552
1	-7.031421	2.041764	1.181539
1	-5.419538	2.677648	0.974738
1	-8.847638	-3.708271	1.022409
1	-9.625064	-1.332899	1.064620
6	-7.185867	4.822589	1.163243
1	-6.281553	4.319336	-0.735629
1	-7.902905	3.679027	-0.527172
1	-7.606140	5.771433	0.812107
1	-7.882177	4.400813	1.898066
1	-6.248304	5.046104	1.686324
6	3.955130	0.559047	-0.115015
6	4.339408	1.858520	-0.430664
16	5.352661	-0.458654	0.155596

6	5.729862	2.033142	-0.449022
1	3.628653	2.652333	-0.631867
6	6.454253	0.881406	-0.149714
1	6.218191	2.976777	-0.670296
6	7.876325	0.831544	-0.107115
6	8.731098	-0.203909	0.171497
1	8.354631	1.780304	-0.335624
6	8.279465	-1.518557	0.493292
6	10.201292	-0.026117	0.158188
7	7.882372	-2.582206	0.753118
8	11.005805	-0.902416	0.396317
8	10.578989	1.244503	-0.153931
1	11.553268	1.235612	-0.131086