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N-Fluorobenzenesulfonimide as a Highly Effective Ag(I)-Catalyst Attenuator for Tryptamine-Derived Ynesulfonamide Cycloisomerization

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Part 1: Details of the DFT calculations

All of the DFT calculations were carried out using the GAUSSIAN 09 package.[1] DFT method B3LYP with a standard 6-31G (d) basis set (LANL2DZ basis set for Ag) was used for the geometry optimizations. The M11 functional, proposed by Truhlar et al., was used with a 6-311+G (d, p) basis set (LANL2DZ basis set for Ag) to calculate the single point energies. The solvent effects were taken into consideration using single point calculations based on the gas-phase stationary points with a SMD continuum solvation model.

B3LYP Geometries for All the Optimized Compounds and Transition States

the optimized state of **1-1** without NFSI

the number of imaginary frequencies: 1

the computed total energy: -1807.97494013 Hartrees

C	-1.04210	1.58869	-0.02544
C	-0.18216	0.97745	-0.71460
N	0.80443	0.54858	-1.45295
C	-2.09741	1.48871	0.96085
C	-2.89055	2.60846	1.27802
C	-2.34247	0.26391	1.61619
C	-3.90011	2.51254	2.23148
H	-2.72194	3.54713	0.75543
C	-3.35469	0.17680	2.56699
H	-1.73923	-0.60542	1.37899
C	-4.13247	1.29624	2.87848
H	-4.50635	3.38148	2.46670
H	-3.53583	-0.77112	3.06354
H	-4.91981	1.22068	3.62217
S	2.47931	0.98642	-0.92329
O	3.26322	0.96065	-2.15111
O	2.28198	2.24018	-0.16552

C	-2.44119	-2.80127	-0.66338
C	-1.06239	-2.48441	-0.82925
C	-0.17839	-2.73471	0.23696
C	-0.67779	-3.27464	1.41676
C	-2.04917	-3.57555	1.56002
C	-2.94751	-3.34488	0.52385
C	-2.16346	-2.00294	-2.73537
C	-0.90824	-1.96987	-2.16832
H	0.88290	-2.52422	0.13912
H	-0.00160	-3.47958	2.24137
H	-2.40626	-4.00767	2.48988
H	-3.99964	-3.58899	0.63203
N	-3.09138	-2.49214	-1.84195
C	-4.50530	-2.69831	-2.10391
H	-4.73321	-2.36160	-3.11612
H	-4.76702	-3.75819	-2.02119
H	-5.11892	-2.12685	-1.39993
Ag	0.15294	3.55843	-0.15868
H	-2.47243	-1.72672	-3.73504
C	0.35792	-1.52254	-2.84034
H	1.22185	-2.03114	-2.39787
H	0.34709	-1.81260	-3.89839
C	0.61027	-0.00418	-2.82736
H	1.50539	0.24874	-3.39799
H	-0.23882	0.53443	-3.25644
C	3.01898	-0.27607	0.19013
C	3.78374	-1.33020	-0.32353
C	2.67175	-0.20639	1.54314
C	4.20224	-2.33111	0.54710
H	4.06016	-1.35074	-1.37183

C	3.10434	-1.22130	2.39125
H	2.09403	0.62707	1.92551
C	3.87294	-2.29545	1.91284
H	4.80284	-3.15000	0.16241
H	2.84767	-1.17538	3.44538
C	4.36543	-3.36939	2.84783
H	4.39277	-4.34566	2.35630
H	5.38551	-3.14511	3.18263
H	3.73744	-3.44690	3.73871

the transition state from **1-1** to **1-2** without NFSI

the number of imaginary frequencies: 1

the computed total energy: -1807.95423869 Hartrees

C	1.13577	0.47493	0.12170
C	-0.13161	0.72715	0.15608
N	-1.25016	-0.01364	0.47916
C	2.44727	0.98175	-0.20205
C	3.20606	1.66418	0.77194
C	2.97790	0.83608	-1.50077
C	4.45113	2.19937	0.45042
H	2.79706	1.78586	1.77042
C	4.22507	1.36900	-1.81560
H	2.40171	0.30639	-2.25160
C	4.96324	2.04907	-0.84249
H	5.01851	2.74076	1.20144
H	4.62214	1.25671	-2.81954
H	5.93399	2.46651	-1.09221
S	-2.71449	0.82486	0.90982
O	-2.82208	0.86608	2.36780
O	-2.70926	2.08751	0.13626

C	3.66838	-2.03155	0.43938
C	2.46262	-2.22282	-0.27410
C	2.51241	-2.76896	-1.56435
C	3.75378	-3.09490	-2.10342
C	4.94136	-2.88337	-1.37828
C	4.91892	-2.34621	-0.09346
C	1.99801	-1.39618	1.79021
C	1.37877	-1.76818	0.58032
H	1.60385	-2.94162	-2.13368
H	3.80984	-3.52533	-3.09820
H	5.89328	-3.15014	-1.82611
H	5.83620	-2.18998	0.46432
N	3.34258	-1.51900	1.69994
C	4.31156	-1.17608	2.73207
H	3.78108	-0.83874	3.62318
H	4.91108	-2.05383	2.98902
H	4.97227	-0.37708	2.38446
Ag	-0.50003	2.80960	-0.54430
H	1.54367	-1.05421	2.70952
C	-0.06229	-2.18376	0.41754
H	-0.32377	-2.20508	-0.64540
H	-0.17641	-3.21181	0.78391
C	-1.07837	-1.31263	1.15924
H	-2.04763	-1.81632	1.15009
H	-0.79447	-1.16176	2.20765
C	-3.98240	-0.23097	0.24704
C	-4.86197	-0.85685	1.13251
C	-4.11636	-0.37053	-1.13921
C	-5.88674	-1.64619	0.61193
H	-4.74738	-0.71859	2.20191

C	-5.14447	-1.16402	-1.63365
H	-3.43477	0.13464	-1.81489
C	-6.04671	-1.81176	-0.77060
H	-6.57564	-2.13648	1.29336
H	-5.25653	-1.28001	-2.70791
C	-7.17539	-2.64125	-1.32814
H	-6.84765	-3.23704	-2.18519
H	5.83620	-2.18998	0.46432
N	3.34258	-1.51900	1.69994
C	4.31156	-1.17608	2.73207
H	3.78108	-0.83874	3.62318
H	4.91108	-2.05383	2.98902
H	4.97227	-0.37708	2.38446
Ag	-0.50003	2.80960	-0.54430
H	1.54367	-1.05421	2.70952
C	-0.06229	-2.18376	0.41754
H	-0.32377	-2.20508	-0.64540
H	-0.17641	-3.21181	0.78391
C	-1.07837	-1.31263	1.15924
H	-2.04763	-1.81632	1.15009
H	-0.79447	-1.16176	2.20765
C	-3.98240	-0.23097	0.24704
C	-4.86197	-0.85685	1.13251
C	-4.11636	-0.37053	-1.13921
C	-5.88674	-1.64619	0.61193
H	-4.74738	-0.71859	2.20191
C	-5.14447	-1.16402	-1.63365
H	-3.43477	0.13464	-1.81489
C	-6.04671	-1.81176	-0.77060
H	-6.57564	-2.13648	1.29336

H	-5.25653	-1.28001	-2.70791
C	-7.17539	-2.64125	-1.32814
H	-6.84765	-3.23704	-2.18519
H	-7.58757	-3.31779	-0.57574
H	-7.99128	-1.99615	-1.67553

the optimized state of **1-1** with NFSI

the number of imaginary frequencies: 1

the computed total energy: -3522.46787635 Hartrees

C	-1.28404	0.85906	-0.41506
C	-1.82519	-0.27330	-0.53717
N	-2.22796	-1.51113	-0.61461
C	-1.56995	2.26053	-0.15392
C	-0.55257	3.23023	-0.22118
C	-2.88088	2.66492	0.17254
C	-0.83708	4.56998	0.03323
H	0.45982	2.92998	-0.47508
C	-3.15620	4.00521	0.42570
H	-3.67497	1.92797	0.22469
C	-2.13786	4.96049	0.35785
H	-0.04367	5.30893	-0.02298
H	-4.17116	4.30112	0.67167
H	-2.35803	6.00523	0.55617
S	-1.84600	-2.56958	0.80312
O	-1.92053	-3.92630	0.26838
O	-0.60671	-2.00375	1.34082
C	-5.71759	1.39662	-2.06113
C	-5.39146	0.18036	-1.39546
C	-5.78020	0.01947	-0.05261
C	-6.46333	1.05087	0.58134

C	-6.77220	2.24890	-0.09739
C	-6.40504	2.43780	-1.42527
C	-4.65241	0.07496	-3.51991
C	-4.70546	-0.65241	-2.35206
H	-5.55818	-0.89901	0.48286
H	-6.77235	0.93277	1.61567
H	-7.31589	3.03195	0.42263
H	-6.65121	3.35687	-1.94797
N	-5.25085	1.30735	-3.35739
C	-5.39355	2.33042	-4.37676
H	-4.93378	1.97902	-5.30165
H	-6.44981	2.54356	-4.57210
H	-4.89737	3.25781	-4.07153
Ag	0.82981	0.06937	-0.33400
H	-4.24075	-0.19949	-4.48244
C	-4.17813	-2.04431	-2.14595
H	-4.71096	-2.53218	-1.32224
H	-4.37448	-2.65751	-3.03469
C	-2.66456	-2.14779	-1.89051
H	-2.35411	-3.19293	-1.84148
H	-2.10212	-1.65478	-2.68812
C	-3.16506	-2.30051	1.96005
C	-4.23941	-3.19552	1.97854
C	-3.10291	-1.20846	2.82972
C	-5.27032	-2.97967	2.88849
H	-4.25270	-4.04861	1.30931
C	-4.14867	-1.01299	3.72788
H	-2.25077	-0.53843	2.81335
C	-5.24377	-1.89014	3.77494
H	-6.10621	-3.67277	2.91660

H	-4.10991	-0.16882	4.41011
C	-6.35197	-1.69085	4.77771
H	-7.32184	-1.98270	4.36529
H	-6.17920	-2.30684	5.66856
H	-6.41510	-0.65032	5.10600
N	4.88062	-0.01711	-0.03175
S	3.80676	1.22200	0.77587
O	2.87175	1.77994	-0.22096
O	3.28835	0.50040	1.93252
S	3.97171	-1.10702	-1.17036
O	2.70450	-1.34954	-0.44297
O	3.97545	-0.53165	-2.50638
C	4.96446	-2.57148	-1.10010
C	4.83562	-3.42867	-0.00194
C	5.84516	-2.81992	-2.15663
C	5.62188	-4.57766	0.02676
H	4.13486	-3.20656	0.79512
C	6.62227	-3.97628	-2.10499
H	5.90662	-2.13386	-2.99377
C	6.51106	-4.84778	-1.01871
H	5.53818	-5.26361	0.86324
H	7.31031	-4.19637	-2.91451
H	7.11934	-5.74635	-0.98669
C	4.99940	2.44415	1.24397
C	5.66307	2.27839	2.46415
C	5.22673	3.53679	0.40091
C	6.58509	3.25015	2.84754
H	5.44999	1.42283	3.09511
C	6.15239	4.49590	0.80543
H	4.68647	3.63278	-0.53380

C	6.82834	4.35072	2.02081
H	7.10960	3.14966	3.79196
H	6.34514	5.35617	0.17297
H	7.54831	5.10319	2.32731
F	5.73404	0.71654	-0.88330

the transition state from **1-1** to **1-2** with NFSI

the number of imaginary frequencies: 1

the computed total energy: -3522.44910510 Hartrees

C	2.53729	-0.70352	-0.21575
C	1.78841	0.36056	-0.25056
N	2.07446	1.66403	-0.58606
C	2.49083	-2.13183	0.04191
C	2.02736	-3.02066	-0.94983
C	2.86868	-2.65331	1.29490
C	1.93145	-4.38627	-0.69005
H	1.71857	-2.62344	-1.91215
C	2.77657	-4.01967	1.54944
H	3.22715	-1.97643	2.06252
C	2.30994	-4.88802	0.55905
H	1.55079	-5.05701	-1.45450
H	3.06421	-4.40775	2.52167
H	2.23399	-5.95215	0.76160
S	0.84831	2.86080	-0.73506
O	0.97652	3.44878	-2.06880
O	-0.42176	2.24298	-0.31385
C	5.71561	-2.17202	-0.66324
C	5.47936	-1.03222	0.13771
C	6.05311	-0.96319	1.41415
C	6.82739	-2.03244	1.85631

C	7.03446	-3.16491	1.04693
C	6.48060	-3.25460	-0.22769
C	4.47320	-0.76035	-1.88132
C	4.62474	-0.13413	-0.62615
H	5.90102	-0.09460	2.04792
H	7.28389	-1.99344	2.84029
H	7.64267	-3.98255	1.42055
H	6.64600	-4.12762	-0.85010
N	5.07908	-1.97032	-1.89297
C	5.04333	-2.94143	-2.97746
H	4.53859	-2.49907	-3.83711
H	6.06159	-3.21403	-3.26822
H	4.50203	-3.83979	-2.66769
Ag	-0.27021	-0.24856	0.28831
H	3.95628	-0.40310	-2.76055
C	4.52120	1.34811	-0.36028
H	4.39877	1.52070	0.71413
H	5.46535	1.82703	-0.64840
C	3.39402	2.05836	-1.10958
H	3.50544	3.13582	-0.96652
H	3.44556	1.87103	-2.18836
C	1.30844	4.08929	0.47484
C	1.77536	5.32980	0.03868
C	1.17161	3.80305	1.83819
C	2.11894	6.29257	0.98841
H	1.85534	5.53540	-1.02309
C	1.52010	4.77710	2.76651
H	0.79331	2.84001	2.16449
C	1.99761	6.03592	2.36003
H	2.48262	7.26017	0.65488

H	1.41685	4.56231	3.82662
C	2.34525	7.08829	3.38306
H	1.43658	7.53551	3.80341
H	2.91029	6.66187	4.21764
H	2.93814	7.89478	2.94495
N	-4.10750	-0.71849	-0.22873
S	-3.35456	-1.72822	1.07031
O	-3.19158	-3.11789	0.66342
O	-2.18108	-0.90942	1.45129
S	-3.36668	-0.93116	-1.88483
O	-1.93234	-0.77953	-1.60439
O	-3.91003	-2.12573	-2.51079
C	-3.99618	0.52767	-2.67366
C	-3.32847	1.74257	-2.48481
C	-5.13680	0.40762	-3.47320
C	-3.83245	2.87206	-3.12690
H	-2.43829	1.80362	-1.86727
C	-5.62313	1.55193	-4.10312
H	-5.61562	-0.55612	-3.60409
C	-4.97382	2.77696	-3.92881
H	-3.32837	3.82508	-3.00394
H	-6.50459	1.48475	-4.73236
H	-5.35737	3.66328	-4.42492
C	-4.59179	-1.58010	2.33293
C	-4.70220	-0.38012	3.04258
C	-5.40831	-2.68513	2.58715
C	-5.66872	-0.29388	4.04188
H	-4.04672	0.45450	2.82136
C	-6.36642	-2.57789	3.59398
H	-5.28514	-3.59857	2.01654

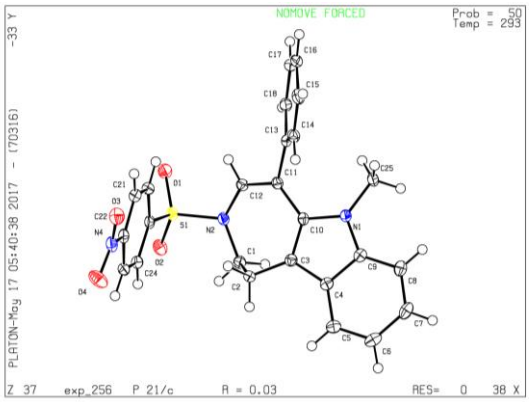
C	-6.49617	-1.38784	4.31444
O	-3.19158	-3.11789	0.66342
O	-2.18108	-0.90942	1.45129
S	-3.36668	-0.93116	-1.88483
O	-1.93234	-0.77953	-1.60439
O	-3.91003	-2.12573	-2.51079
C	-3.99618	0.52767	-2.67366
C	-3.32847	1.74257	-2.48481
C	-5.13680	0.40762	-3.47320
C	-3.83245	2.87206	-3.12690
H	-2.43829	1.80362	-1.86727
C	-5.62313	1.55193	-4.10312
H	-5.61562	-0.55612	-3.60409
C	-4.97382	2.77696	-3.92881
H	-3.32837	3.82508	-3.00394
H	-6.50459	1.48475	-4.73236
H	-5.35737	3.66328	-4.42492
C	-4.59179	-1.58010	2.33293
C	-4.70220	-0.38012	3.04258
C	-5.40831	-2.68513	2.58715
C	-5.66872	-0.29388	4.04188
H	-4.04672	0.45450	2.82136
C	-6.36642	-2.57789	3.59398
H	-5.28514	-3.59857	2.01654
C	-6.49617	-1.38784	4.31444
H	-5.77457	0.62503	4.60916
H	-7.00997	-3.42319	3.81433
H	-7.24631	-1.31188	5.09553
F	-5.40933	-1.25230	-0.37672

Part 2: References

[1] Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

Part 3: X-ray crystal information

CCDC 1550850 contains the supplementary crystallographic data for compound **2j**. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

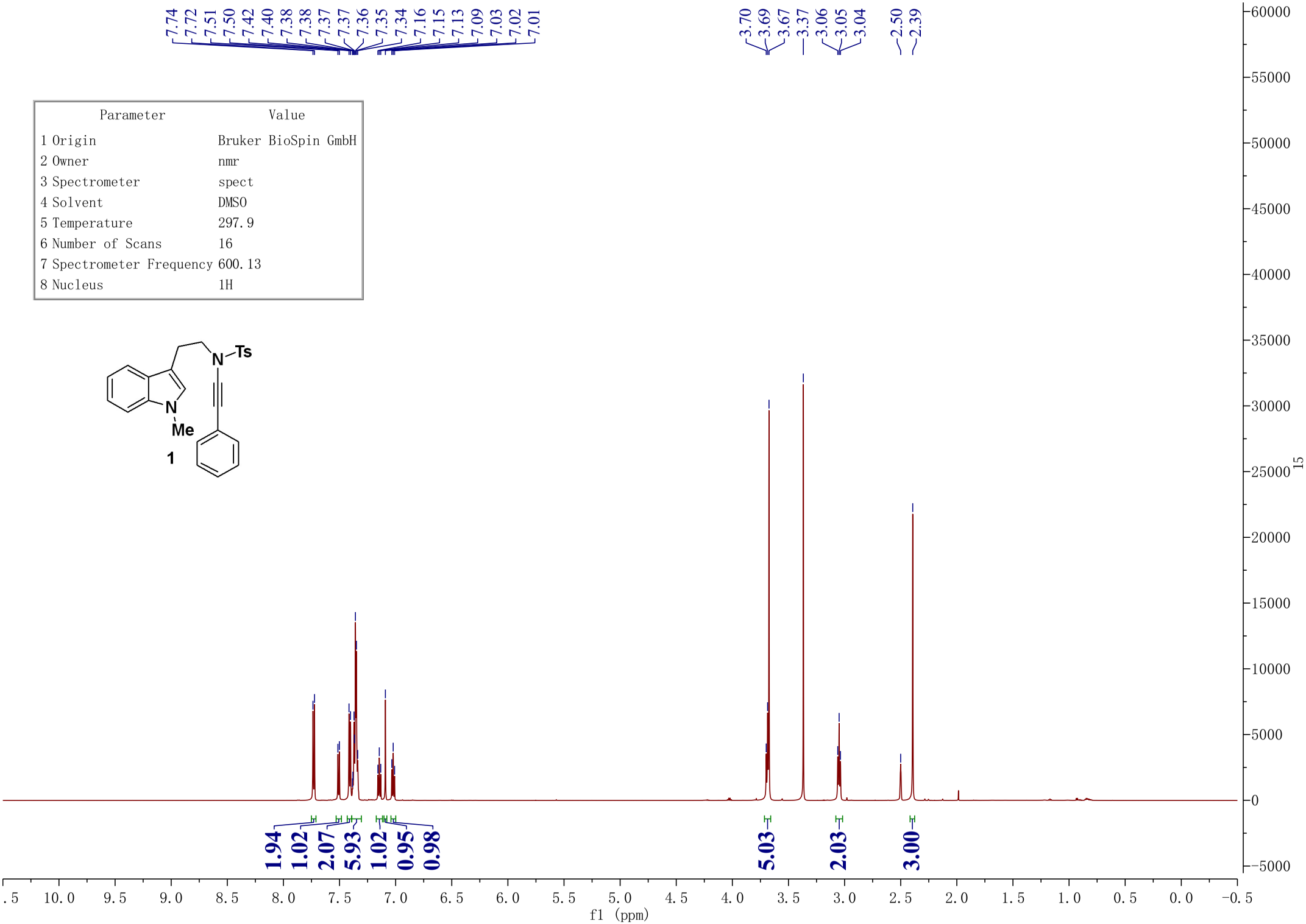


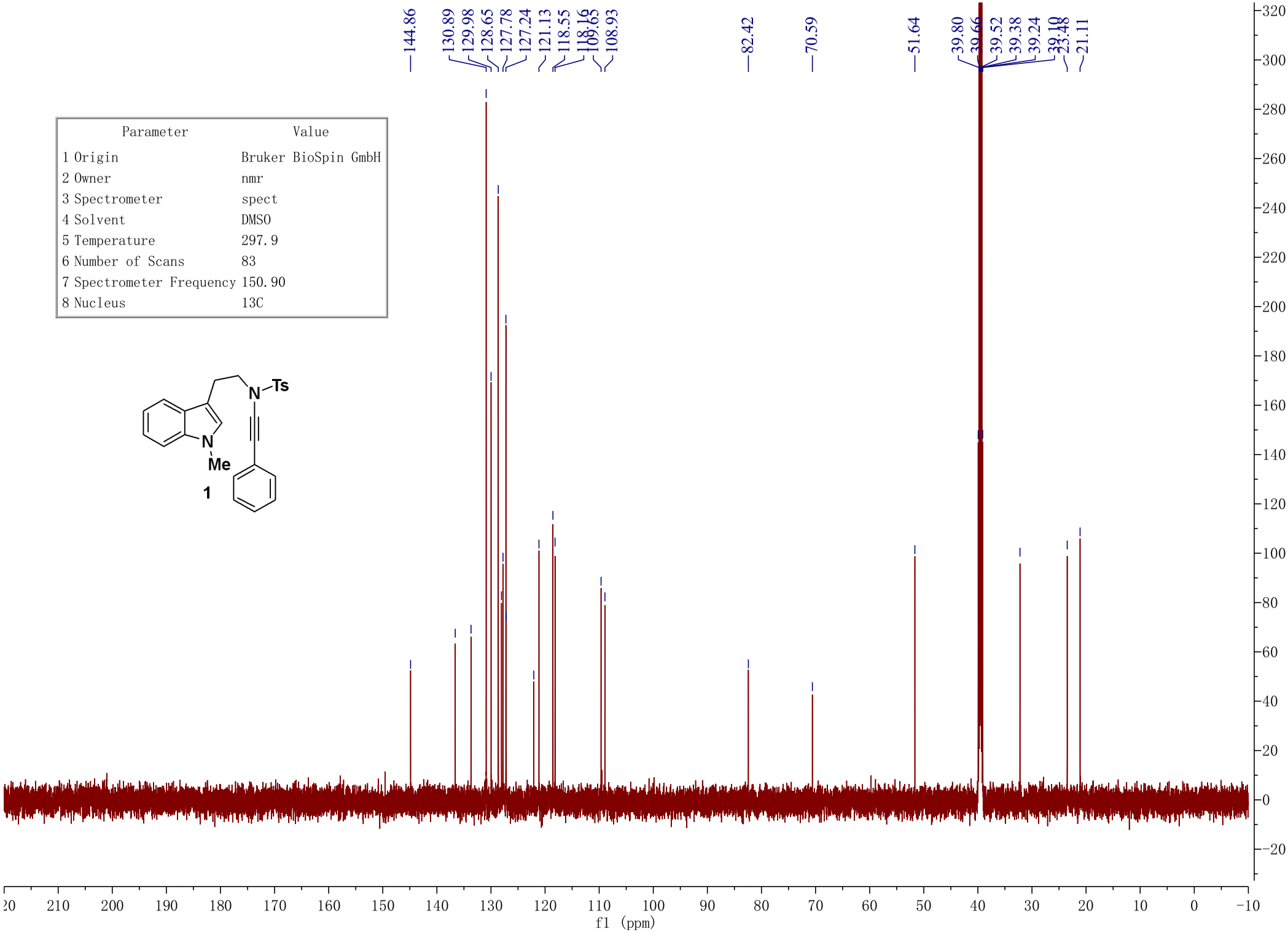
Single crystal X-ray diffraction of **2j**

Part 4: NMR spectra

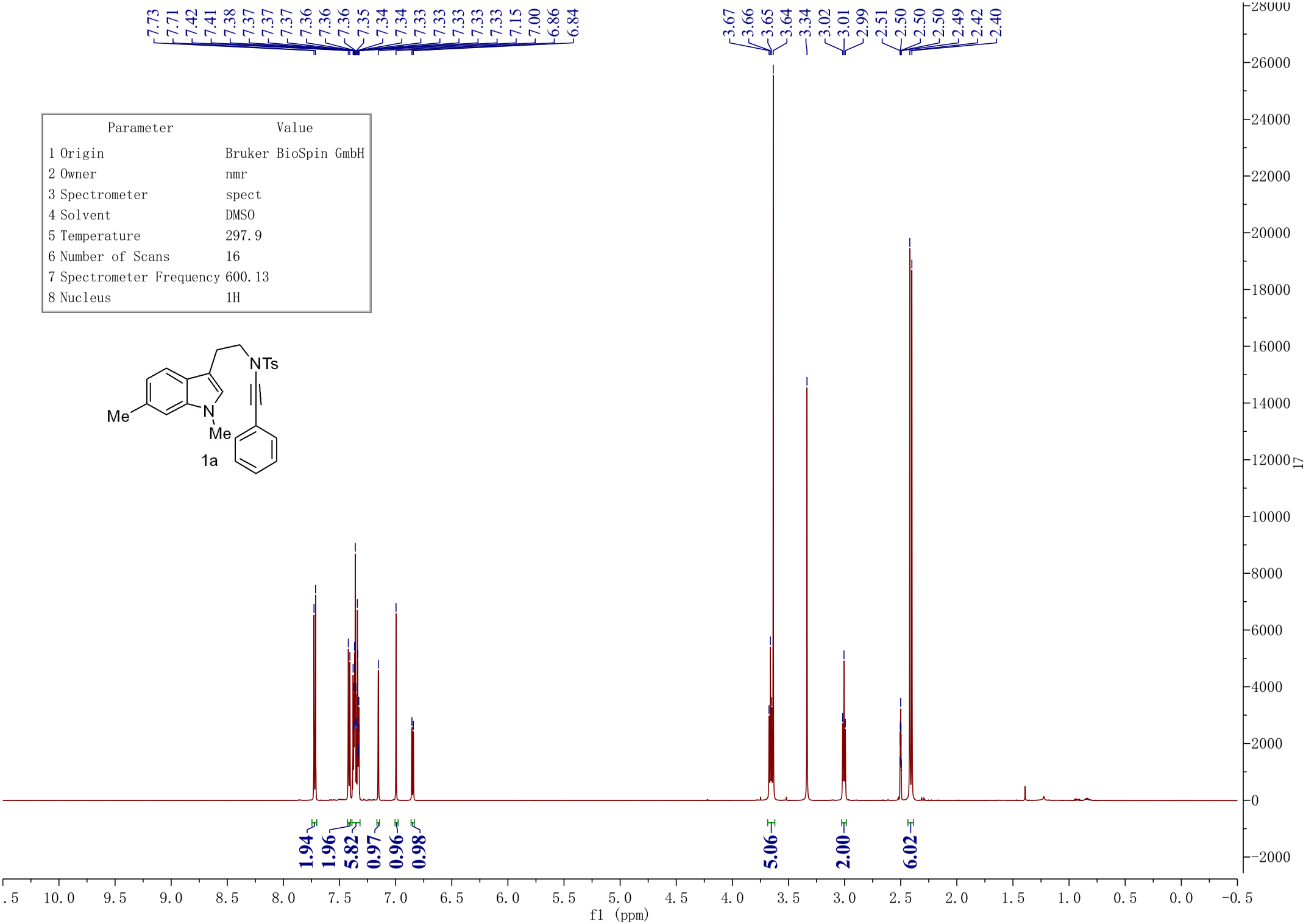
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

1

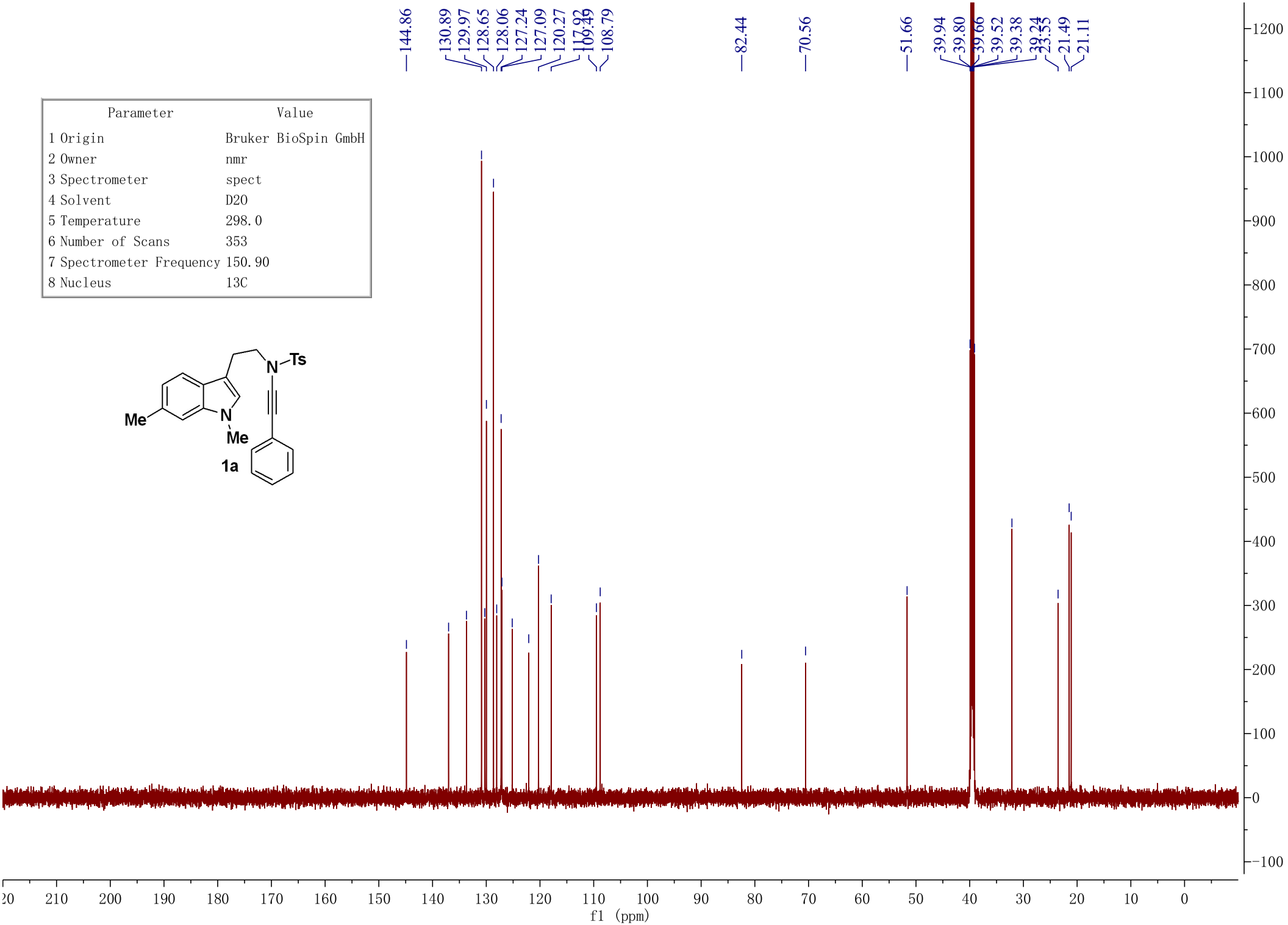


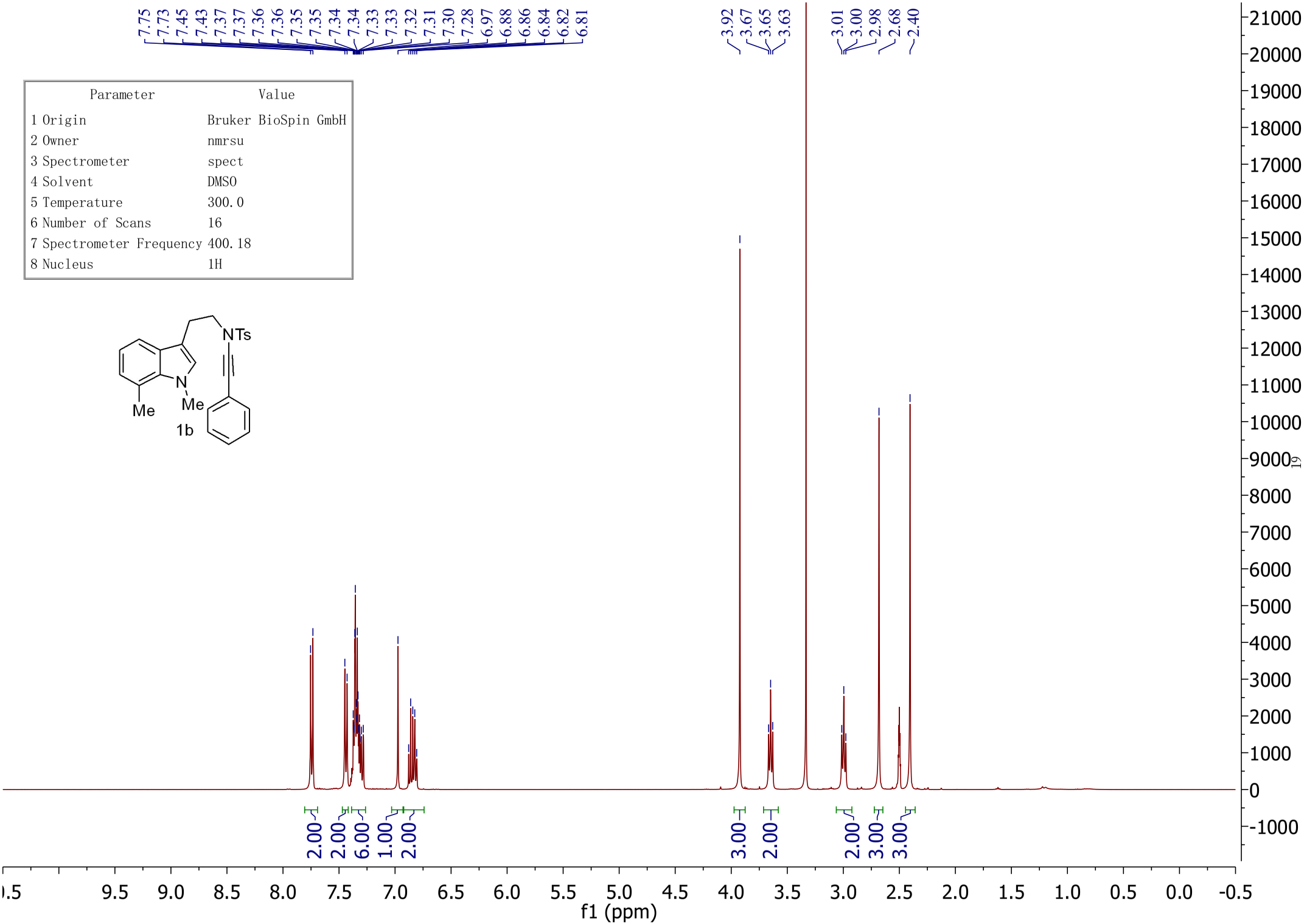


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	83
7 Spectrometer Frequency	150.90
8 Nucleus	13C



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H


144.86
130.89
129.97
128.65
128.06
127.24
127.09
120.27
117.92
109.49
108.79
82.44
70.56
51.66
39.94
39.80
39.66
39.52
39.38
39.24
23.55
21.49
21.11
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent D20
5 Temperature 298.0
6 Number of Scans 353
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
Ts
Me
N
Me
1a
f1 (ppm)


7.75
7.73
7.45
7.43
7.37
7.37
7.36
7.36
7.35
7.35
7.34
7.34
7.33
7.33
7.32
7.31
7.30
7.28
6.97
6.88
6.86
6.84
6.82
6.81
3.92
3.67
3.65
3.63
3.01
3.00
2.98
2.68
2.40
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 400.18
8 Nucleus 1H
NTs
N
Me
Me
1b
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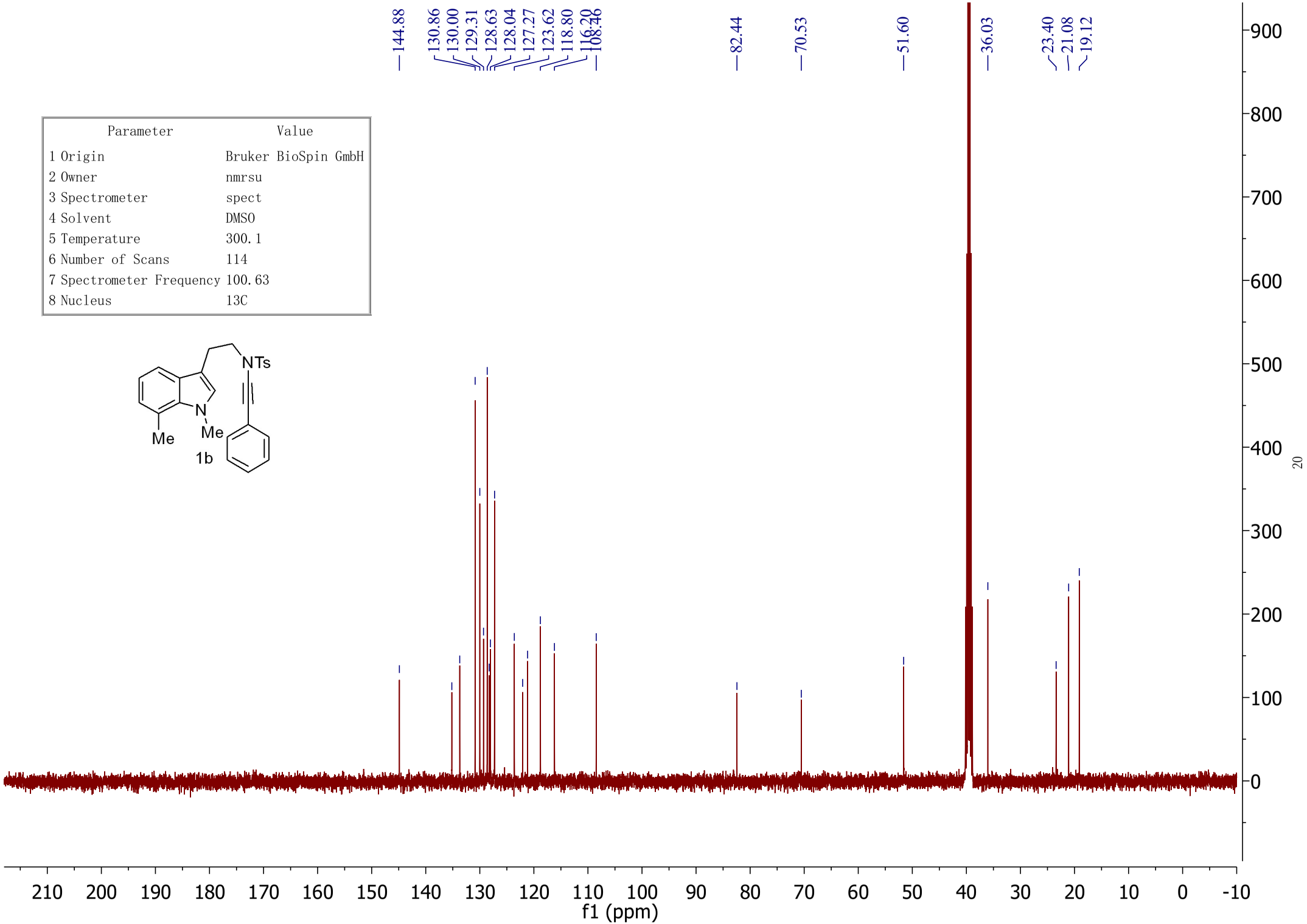
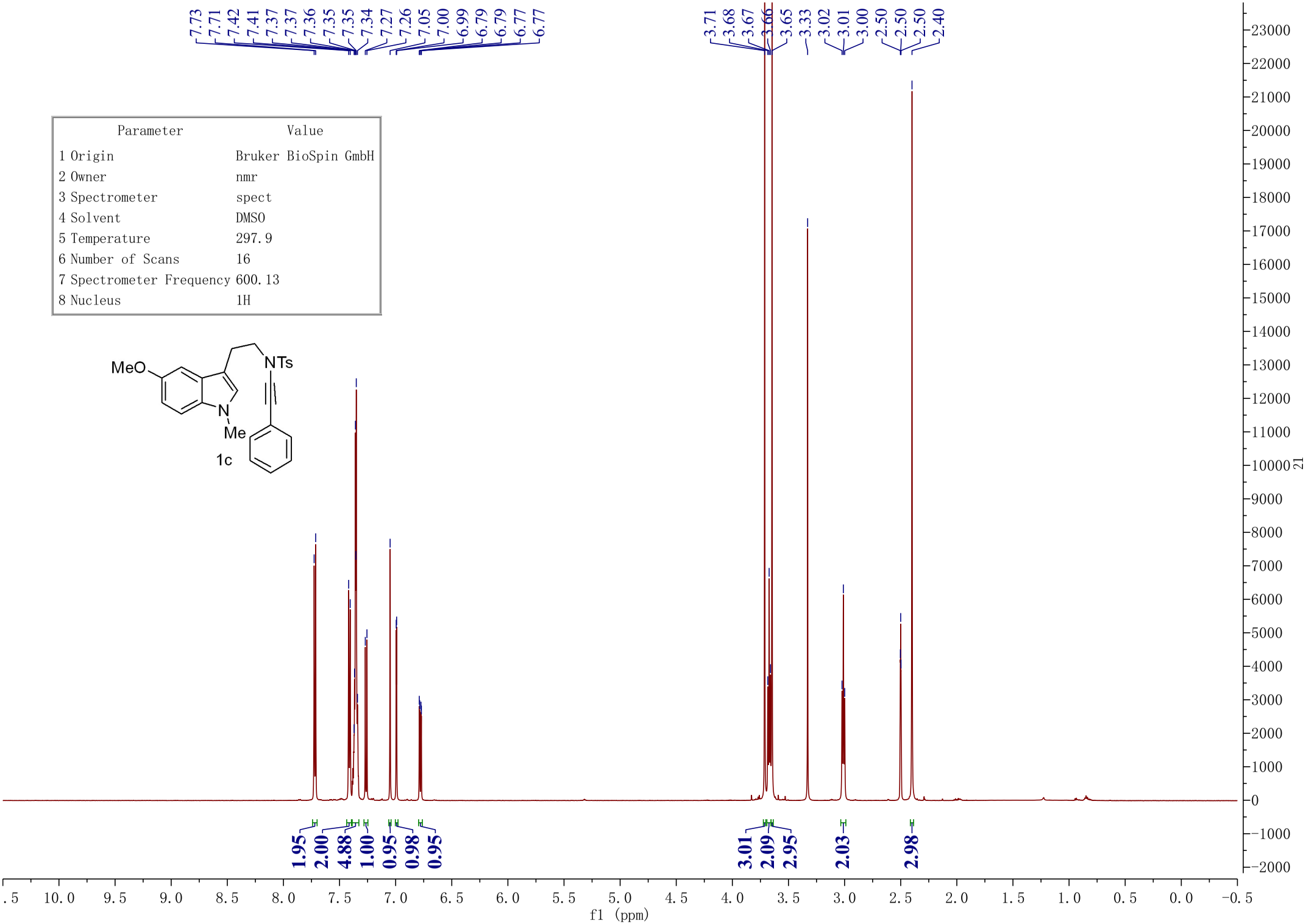
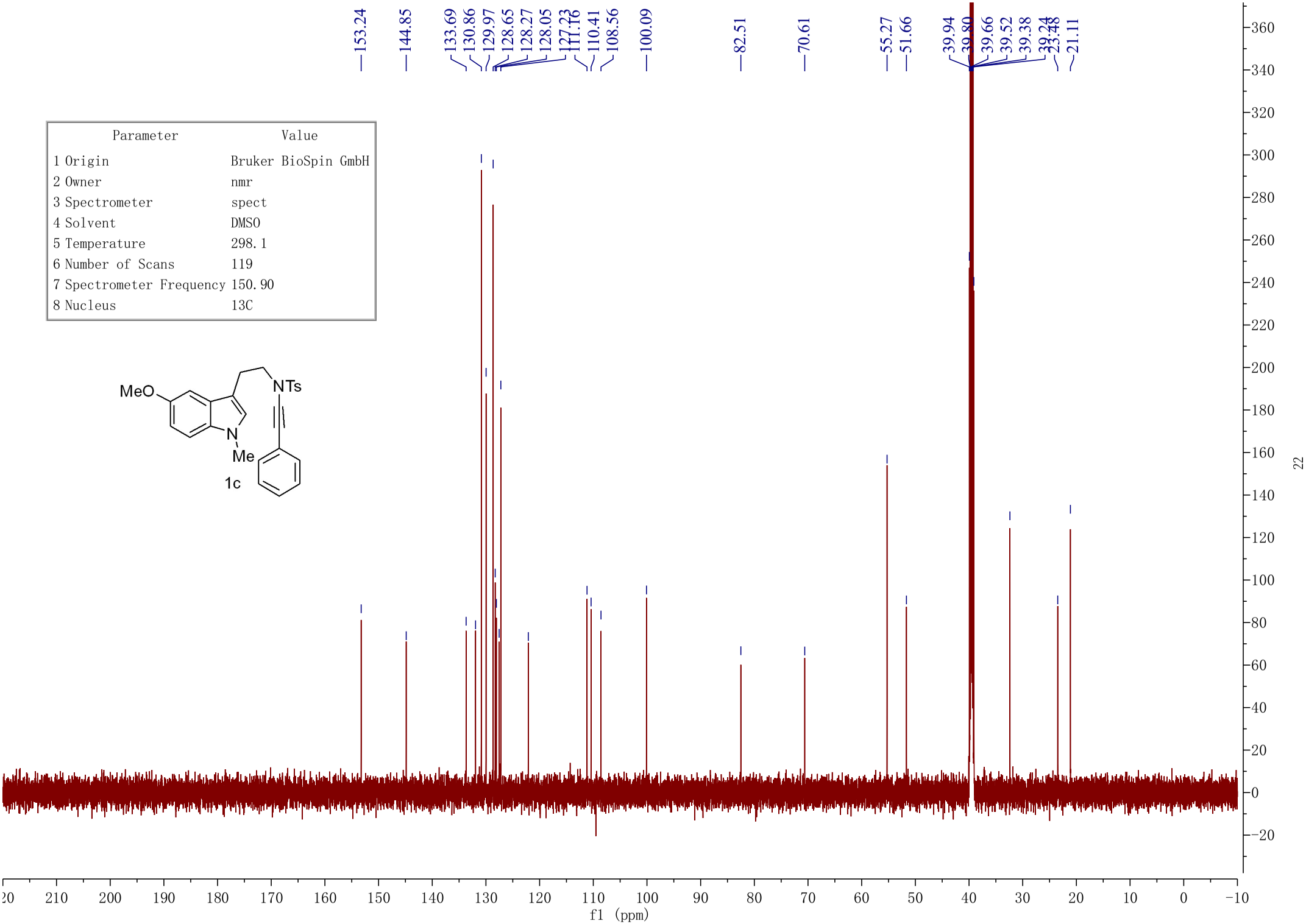
3.00
f1 (ppm)



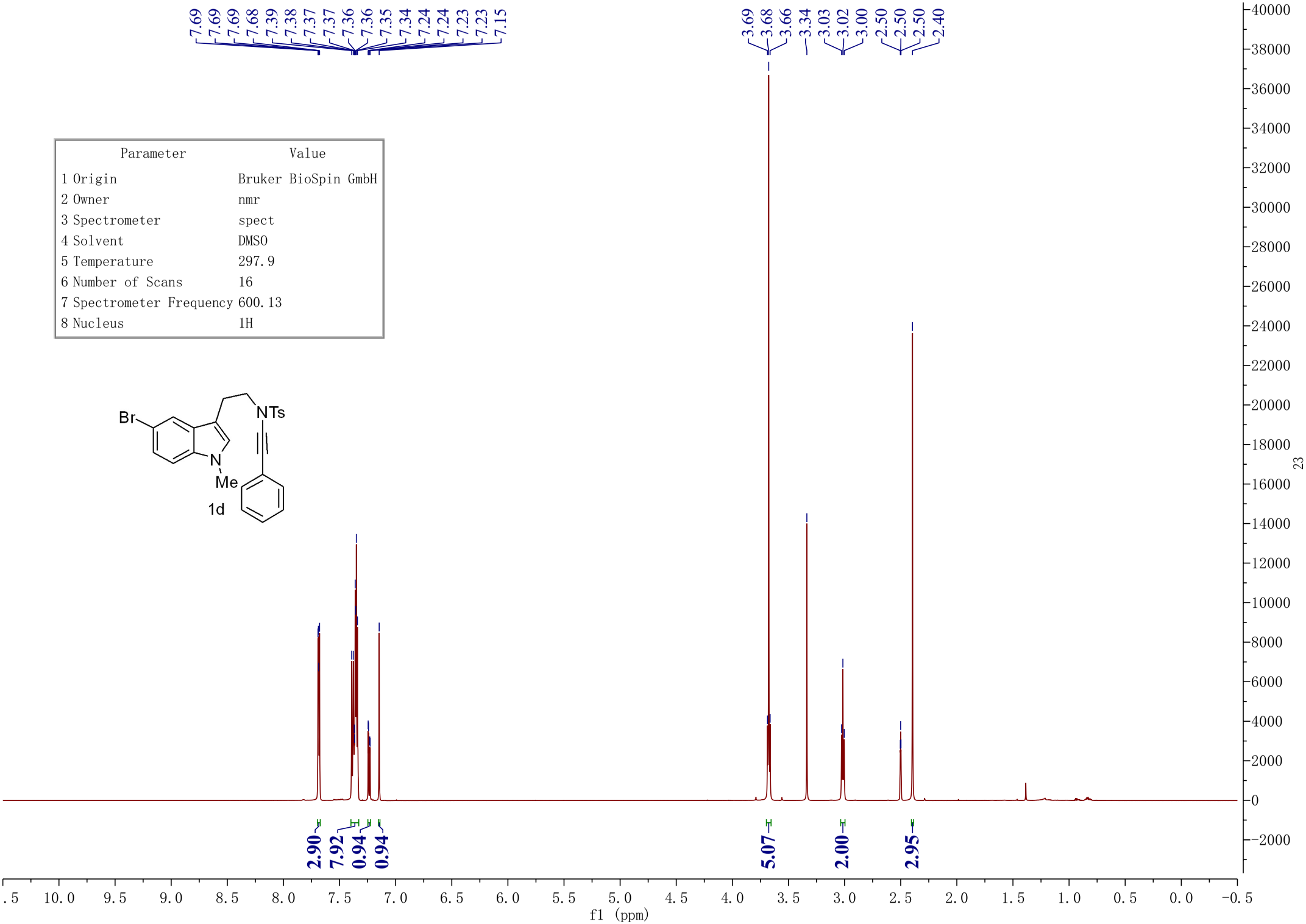
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.1
6 Number of Scans	114
7 Spectrometer Frequency	100.63
8 Nucleus	13C

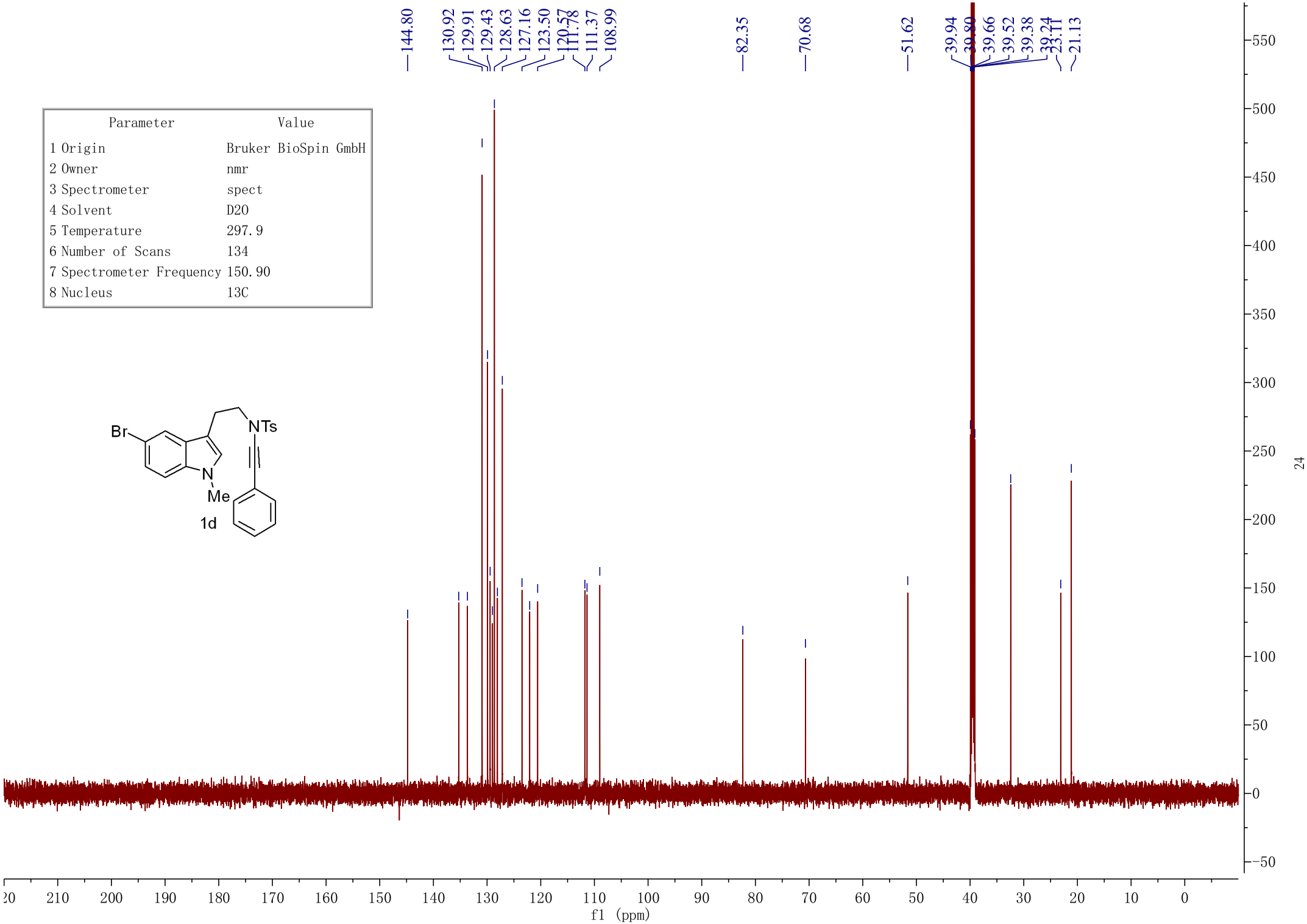


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

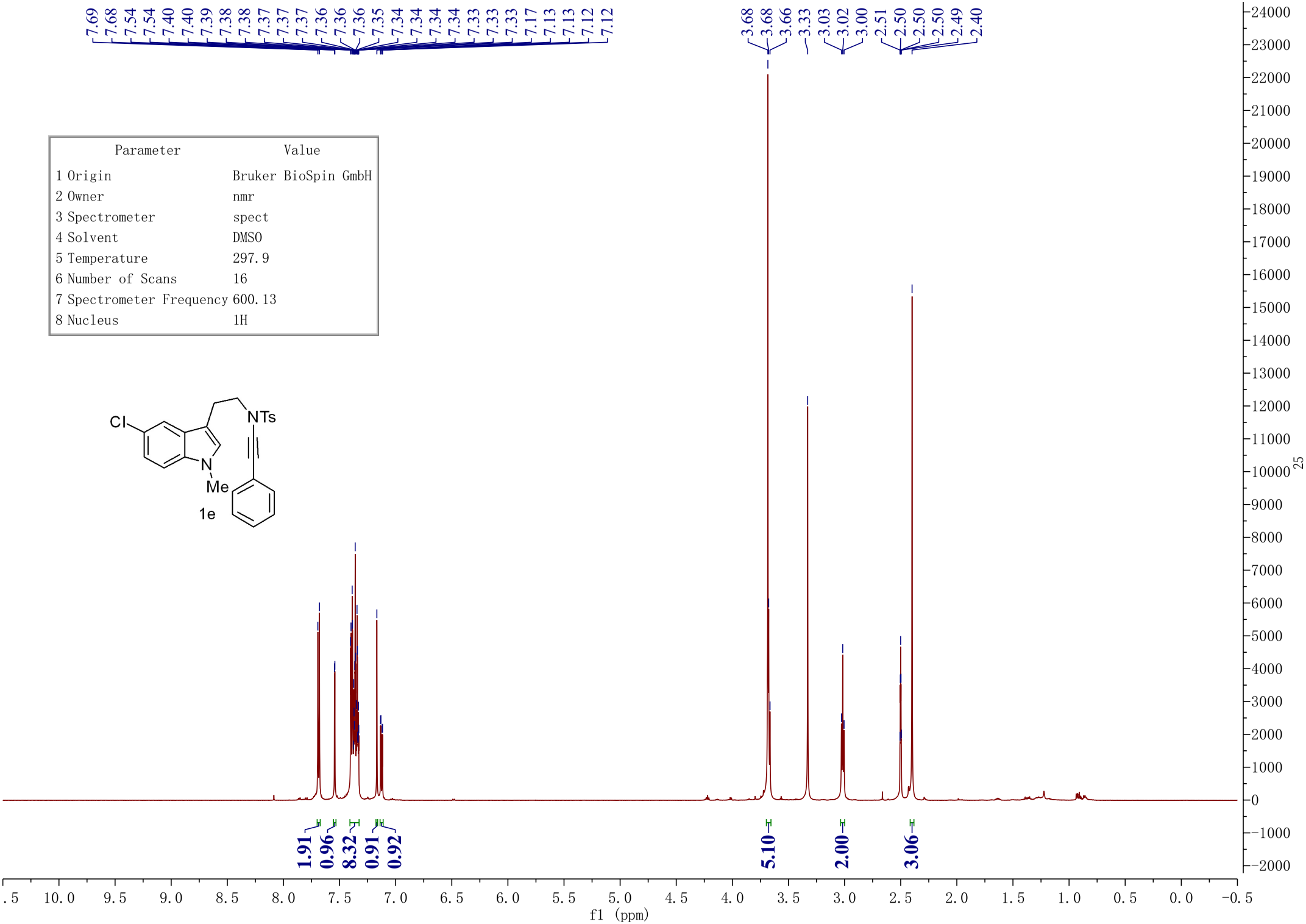


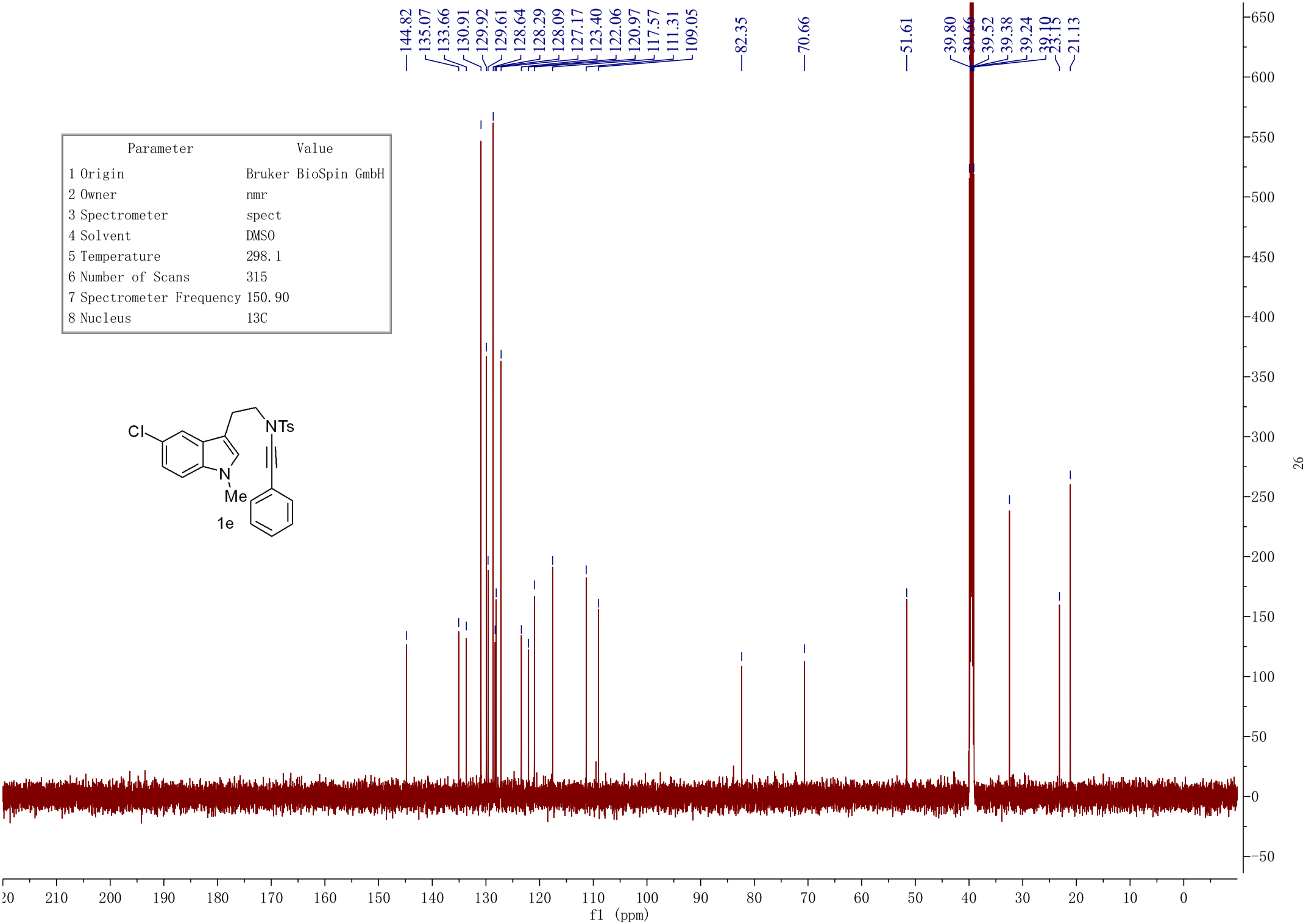
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.1
6 Number of Scans	119
7 Spectrometer Frequency	150.90
8 Nucleus	13C

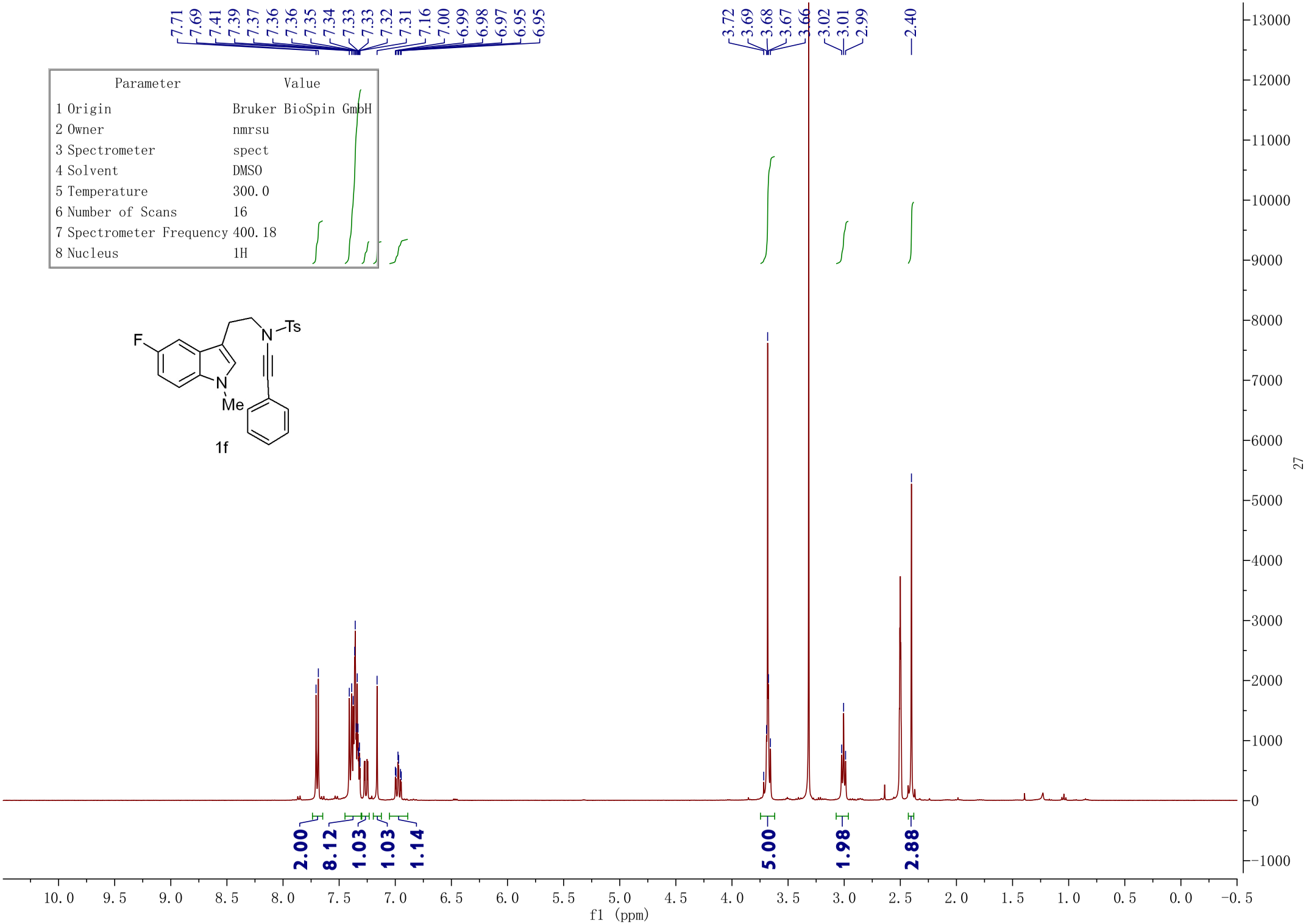

7.69 7.69 7.69 7.68 7.39 7.38 7.37 7.37 7.36 7.36 7.35 7.34 7.24 7.24 7.23 7.23 7.15
3.69 3.68 3.66 3.34 3.03 3.02 3.00 2.50 2.50 2.50 2.40
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Br
NTs
N
Me
1d
2.90
7.92
0.94
0.94
5.07
2.00
2.95
f1 (ppm)

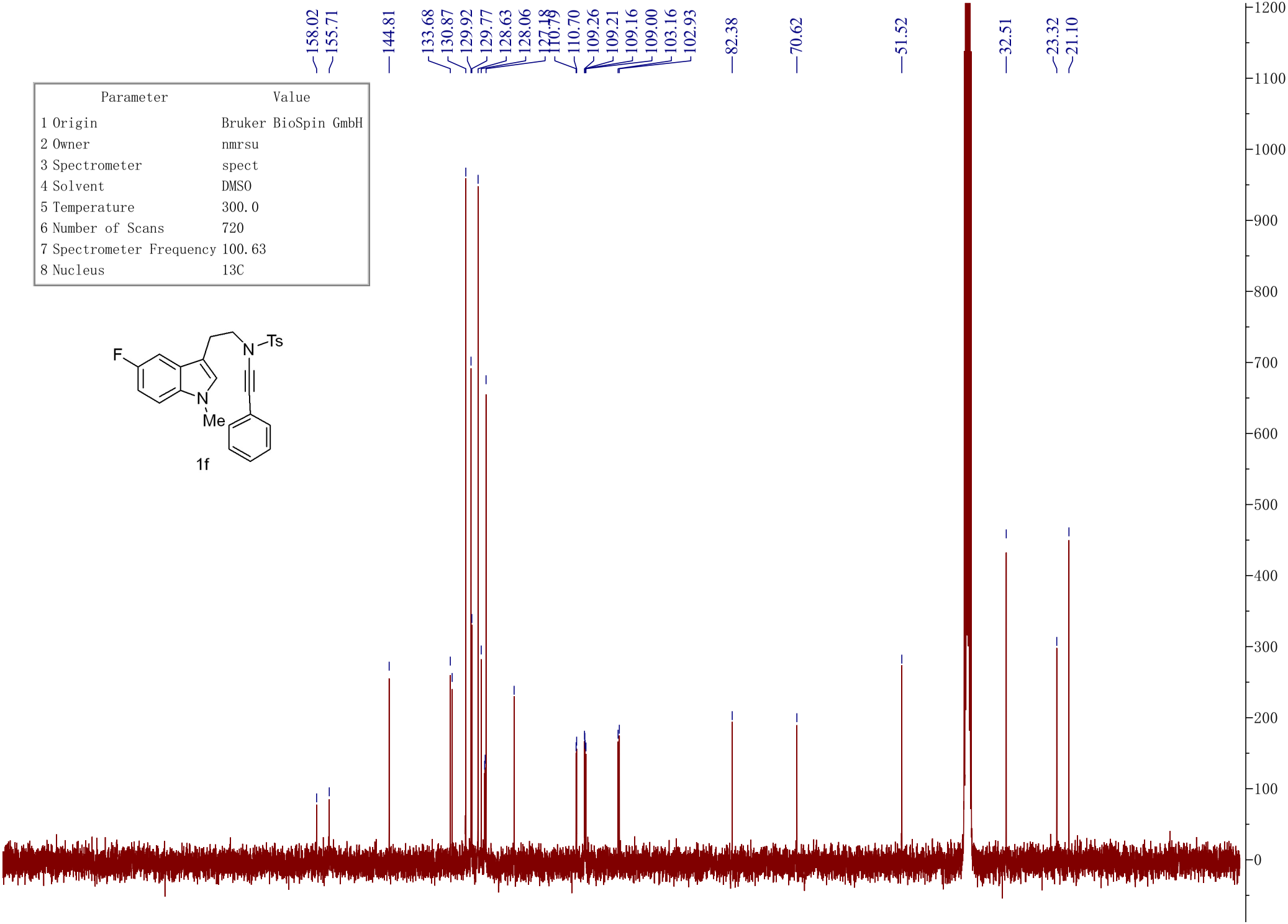


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	D20
5 Temperature	297.9
6 Number of Scans	134
7 Spectrometer Frequency	150.90
8 Nucleus	13C

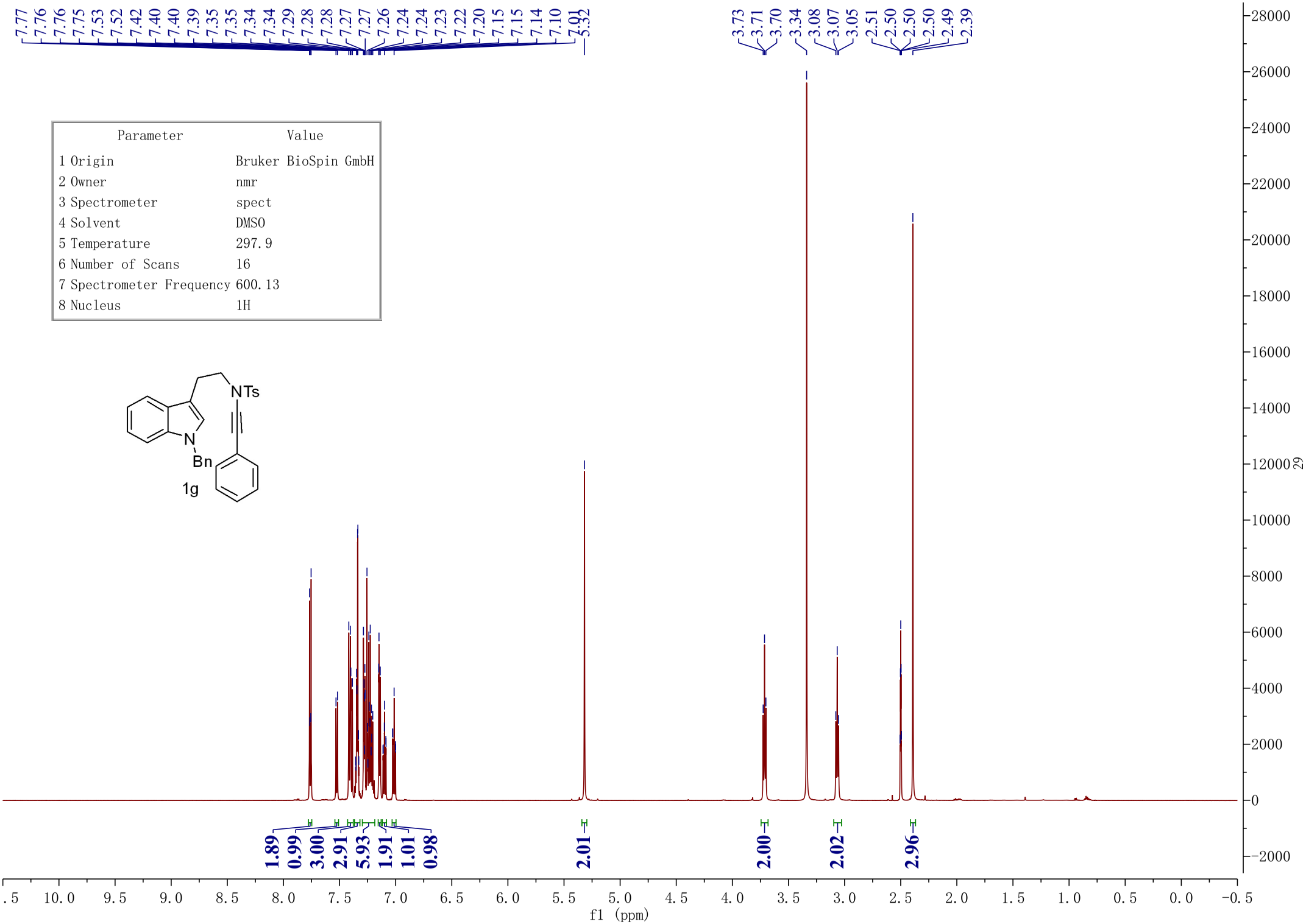

7.69 7.68 7.54 7.54 7.40 7.40 7.39 7.38 7.38 7.37 7.37 7.37 7.36 7.36 7.36 7.35 7.34 7.34 7.34 7.34 7.33 7.33 7.33 7.17 7.13 7.13 7.12 7.12
3.68 3.68 3.66 3.33 3.03 3.02 3.00 2.51 2.50 2.50 2.50 2.49 2.40
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Cl
NTs
N
Me
1e
1.91
0.96
8.32
0.91
0.92
5.10
2.00
3.06
f1 (ppm)

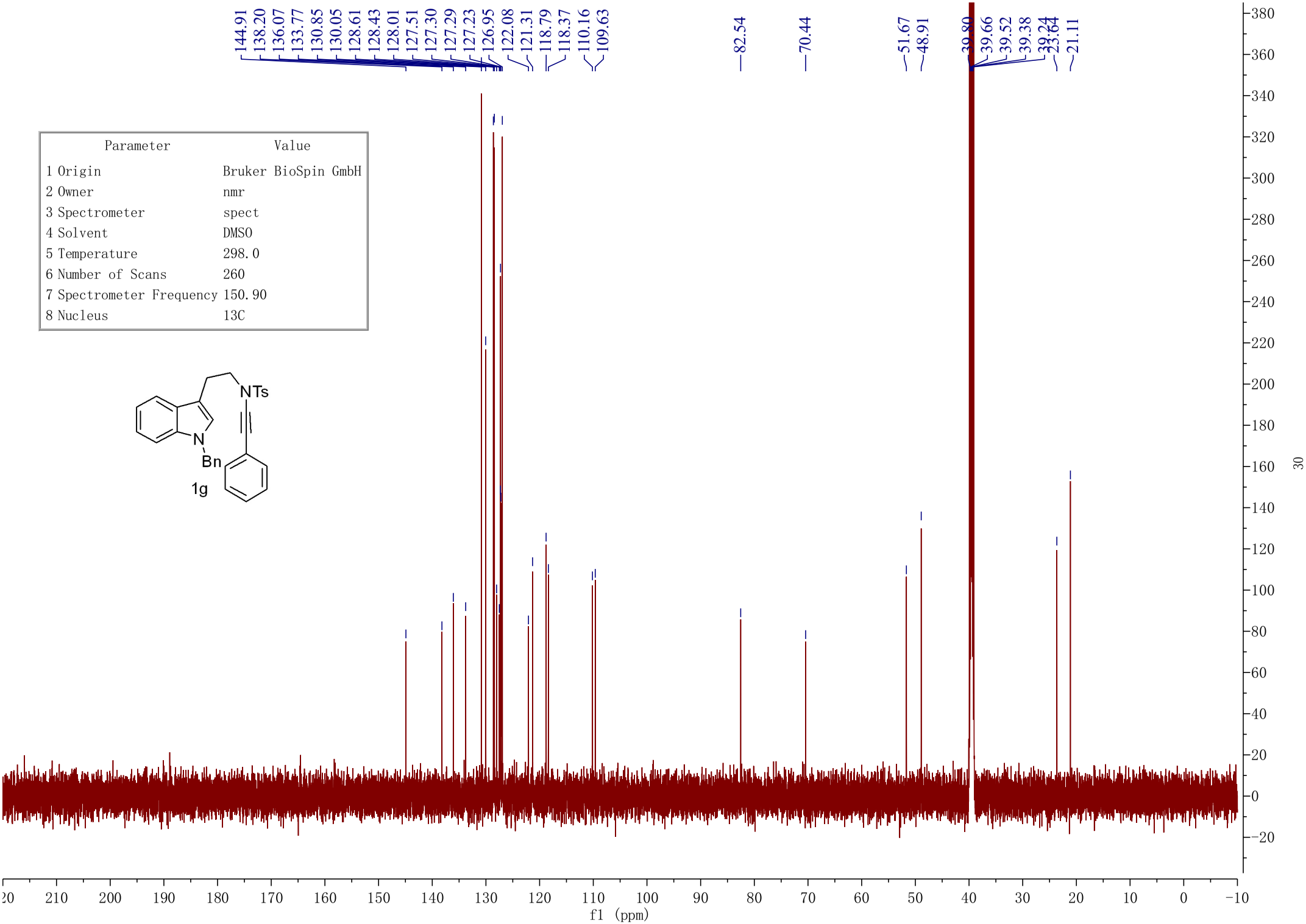

144.82
135.07
133.66
130.91
129.92
129.61
128.64
128.29
128.09
127.17
123.40
122.06
120.97
117.57
111.31
109.05
82.35
70.66
51.61
39.80
39.66
39.52
39.38
39.24
39.10
23.15
21.13
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.1
6 Number of Scans 315
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Cl
NTs
N
Me
1e
f1 (ppm)
26

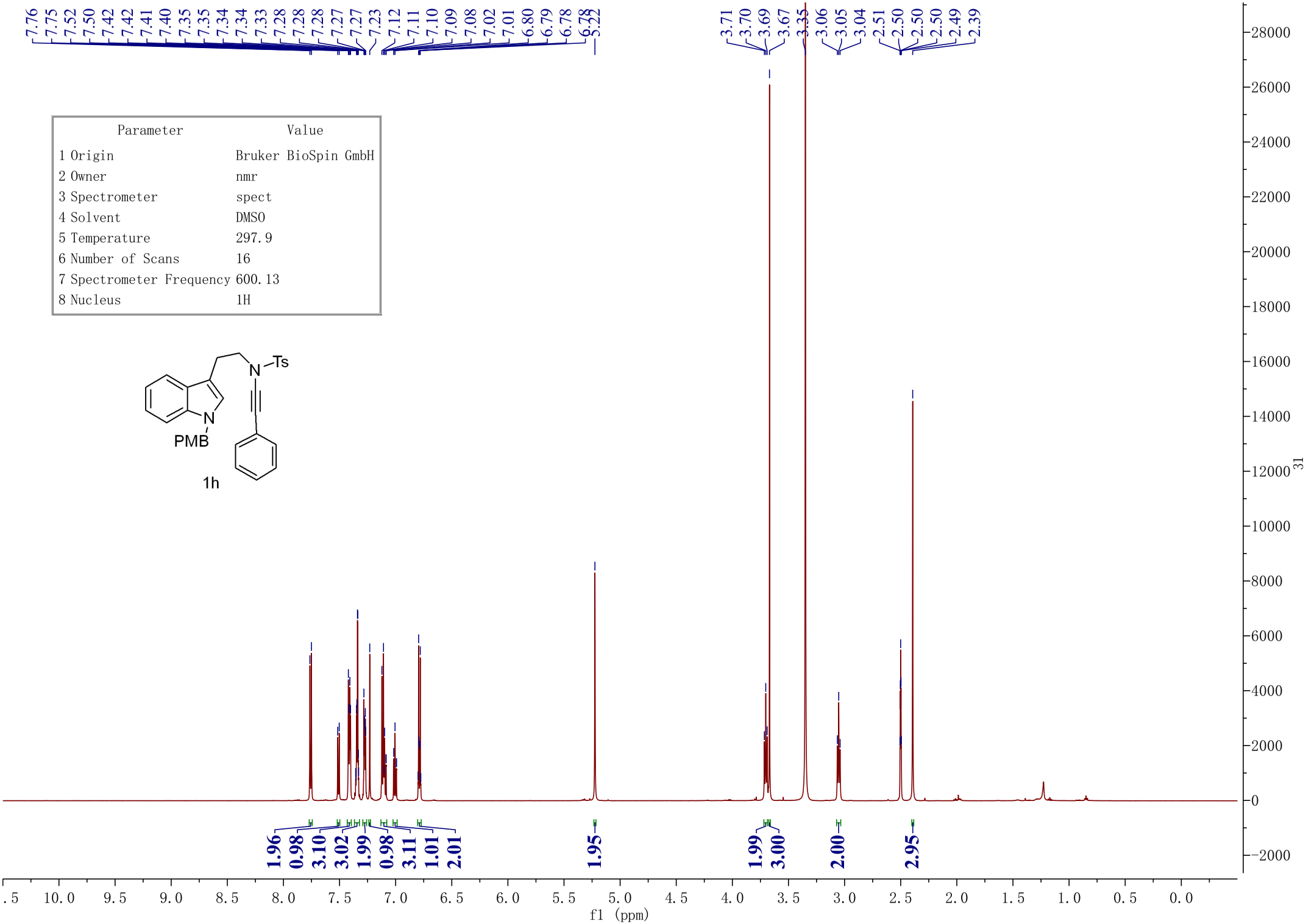

7.71
7.69
7.41
7.39
7.37
7.36
7.36
7.35
7.34
7.33
7.33
7.32
7.31
7.16
7.00
6.99
6.98
6.97
6.95
6.95
3.72
3.69
3.68
3.67
3.66
3.02
3.01
2.99
2.40
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 400.18
8 Nucleus 1H
F
N
Ts
N
Me
1f
2.00
8.12
1.03
1.03
1.14
5.00
1.98
2.88
f1 (ppm)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.0
6 Number of Scans	720
7 Spectrometer Frequency	100.63
8 Nucleus	13C

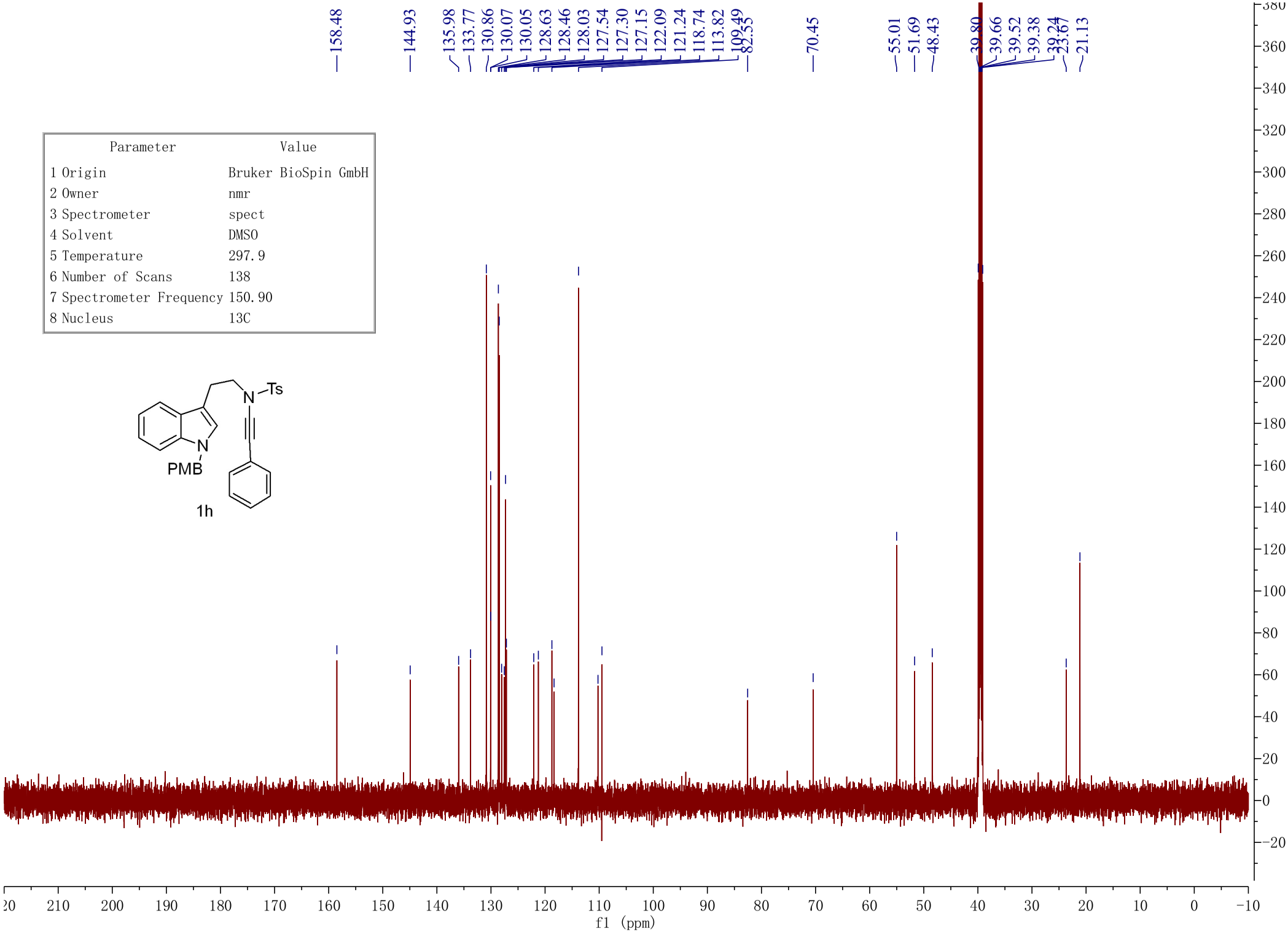

7.77 7.76 7.76 7.75 7.53 7.52 7.42 7.40 7.40 7.39 7.35 7.35 7.34 7.34 7.29 7.28 7.28 7.27 7.27 7.26 7.24 7.24 7.23 7.22 7.20 7.15 7.15 7.14 7.10 7.01 5.32
3.73 3.71 3.70 3.34 3.08 3.07 3.05 2.51 2.50 2.50 2.50 2.49 2.39
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
NTs
N
Bn
1g
1.89 0.99 3.00 2.91 5.93 1.91 1.01 0.98
2.01
2.00
2.02
2.96
f1 (ppm)

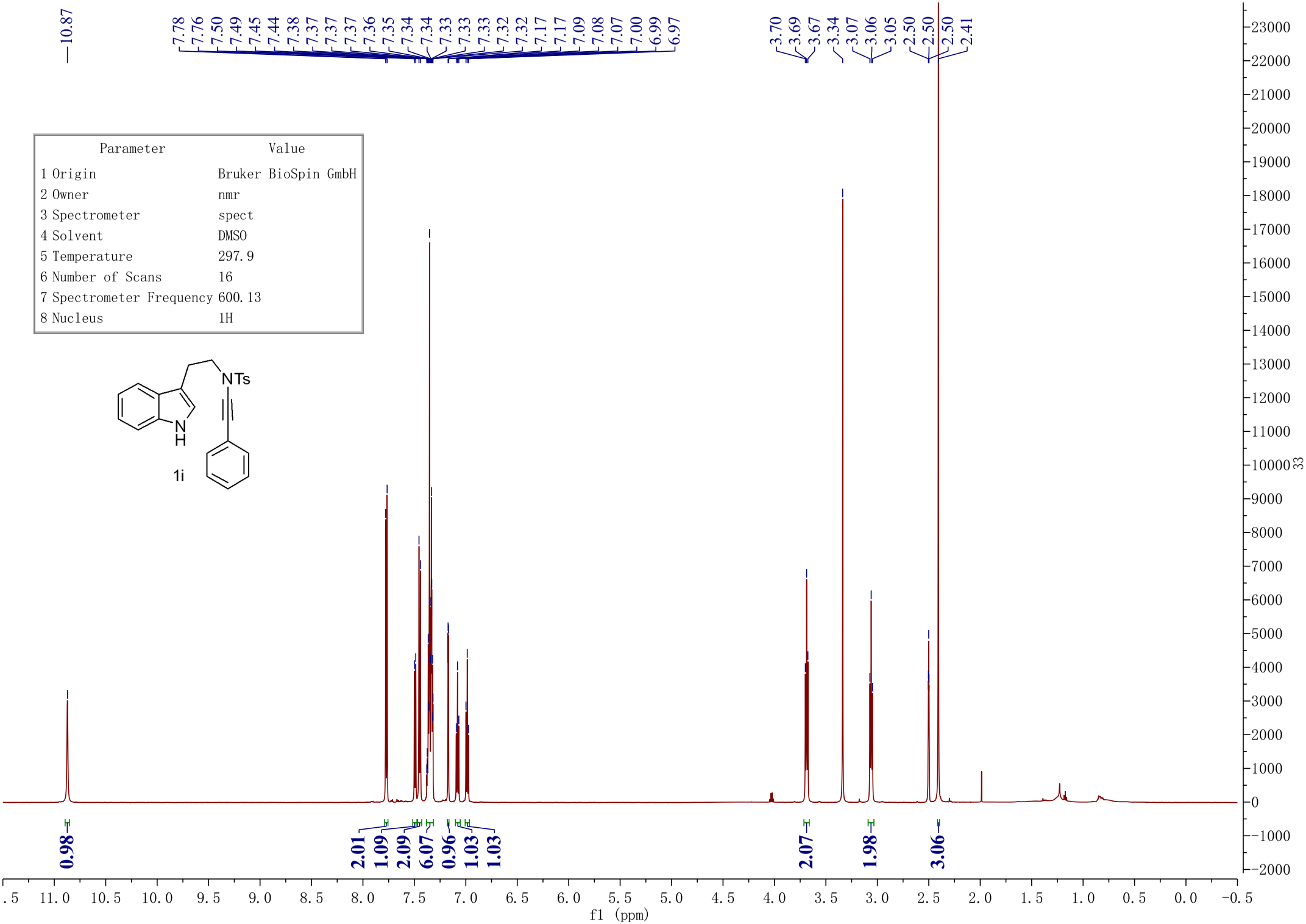

144.91
138.20
136.07
133.77
130.85
130.05
128.61
128.43
128.01
127.51
127.30
127.29
127.23
126.95
122.08
121.31
118.79
118.37
110.16
109.63
82.54
70.44
51.67
48.91
39.80
39.66
39.52
39.38
39.24
23.64
21.11
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 260
7 Spectrometer Frequency 150.90
8 Nucleus 13C
NTs
N
Bn
1g
f1 (ppm)
30



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

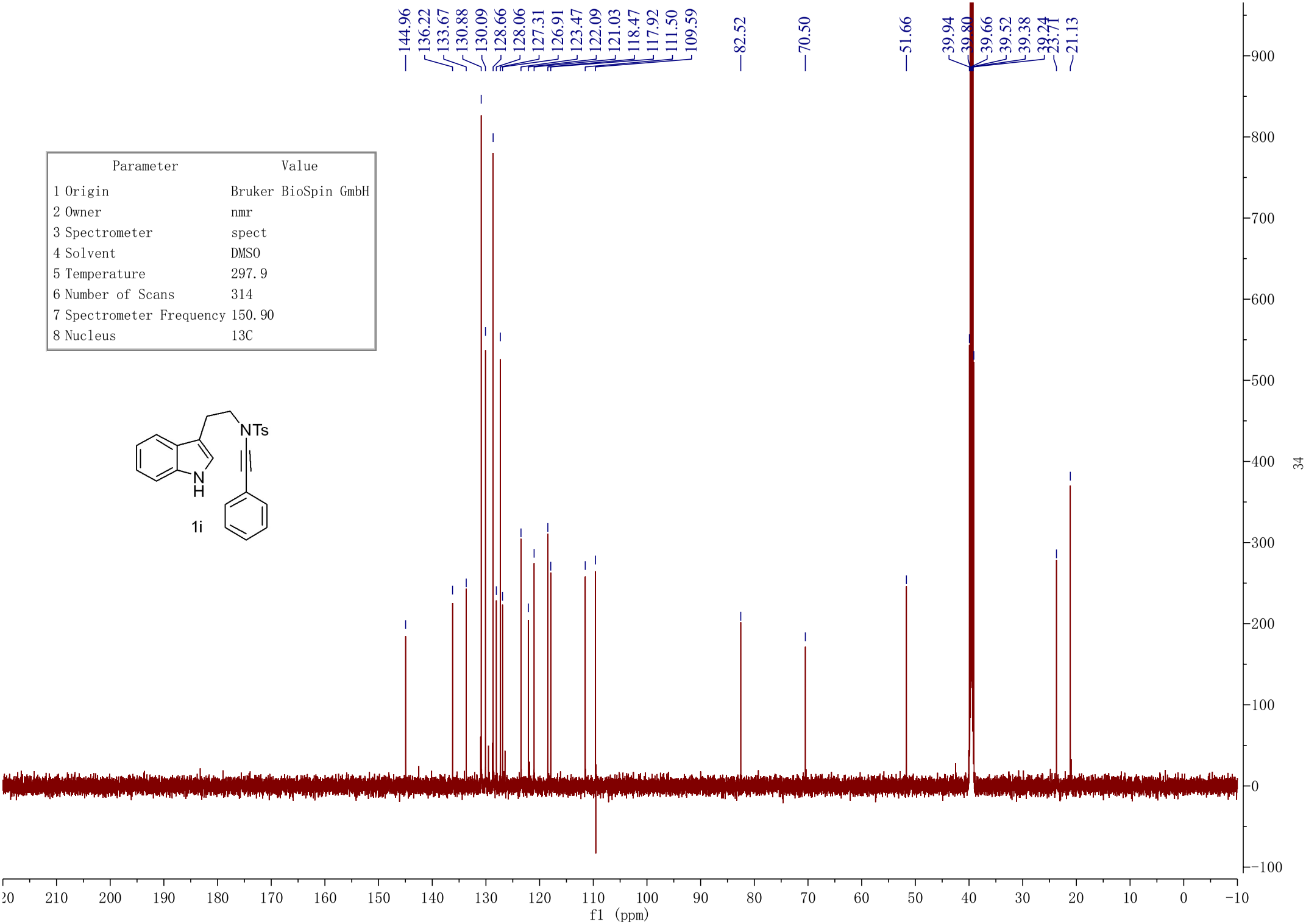
1h


158.48
144.93
135.98
133.77
130.86
130.07
130.05
128.63
128.46
128.03
127.54
127.30
127.15
122.09
121.24
118.74
113.82
109.49
82.55
70.45
55.01
51.69
48.43
39.80
39.66
39.52
39.38
39.24
23.67
21.13
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 138
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
Ts
N
PMB
1h
f1 (ppm)

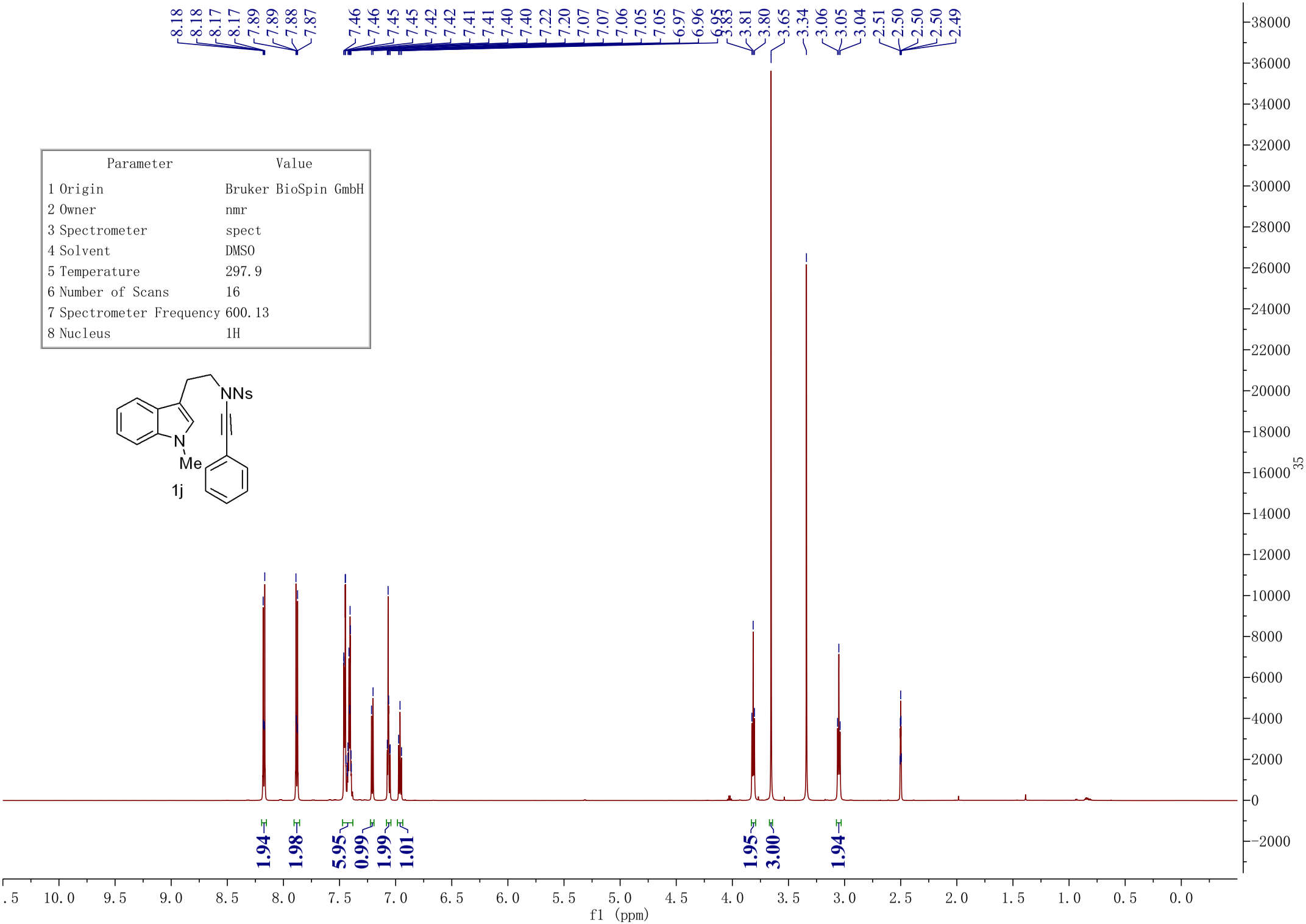


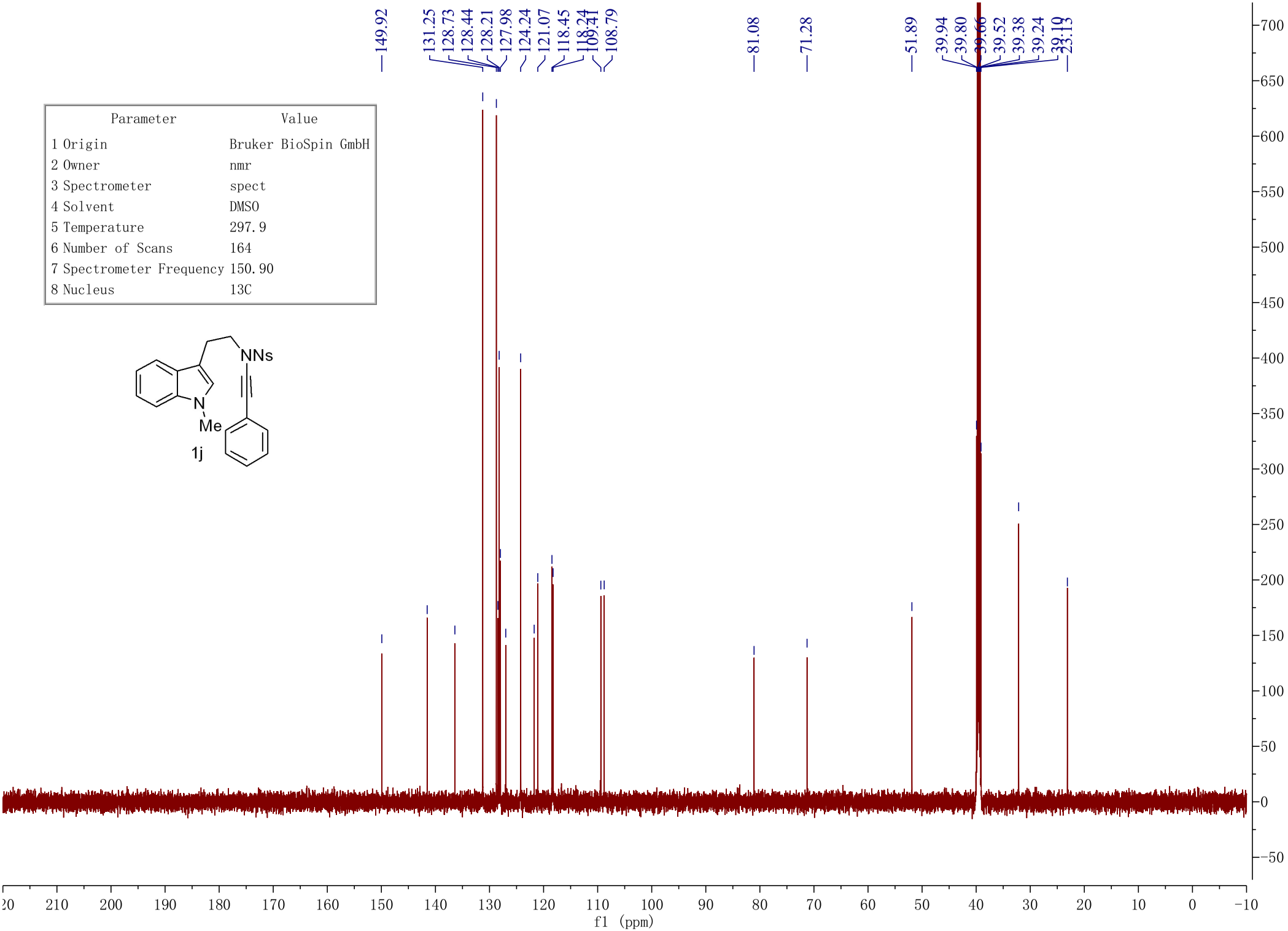
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

1i

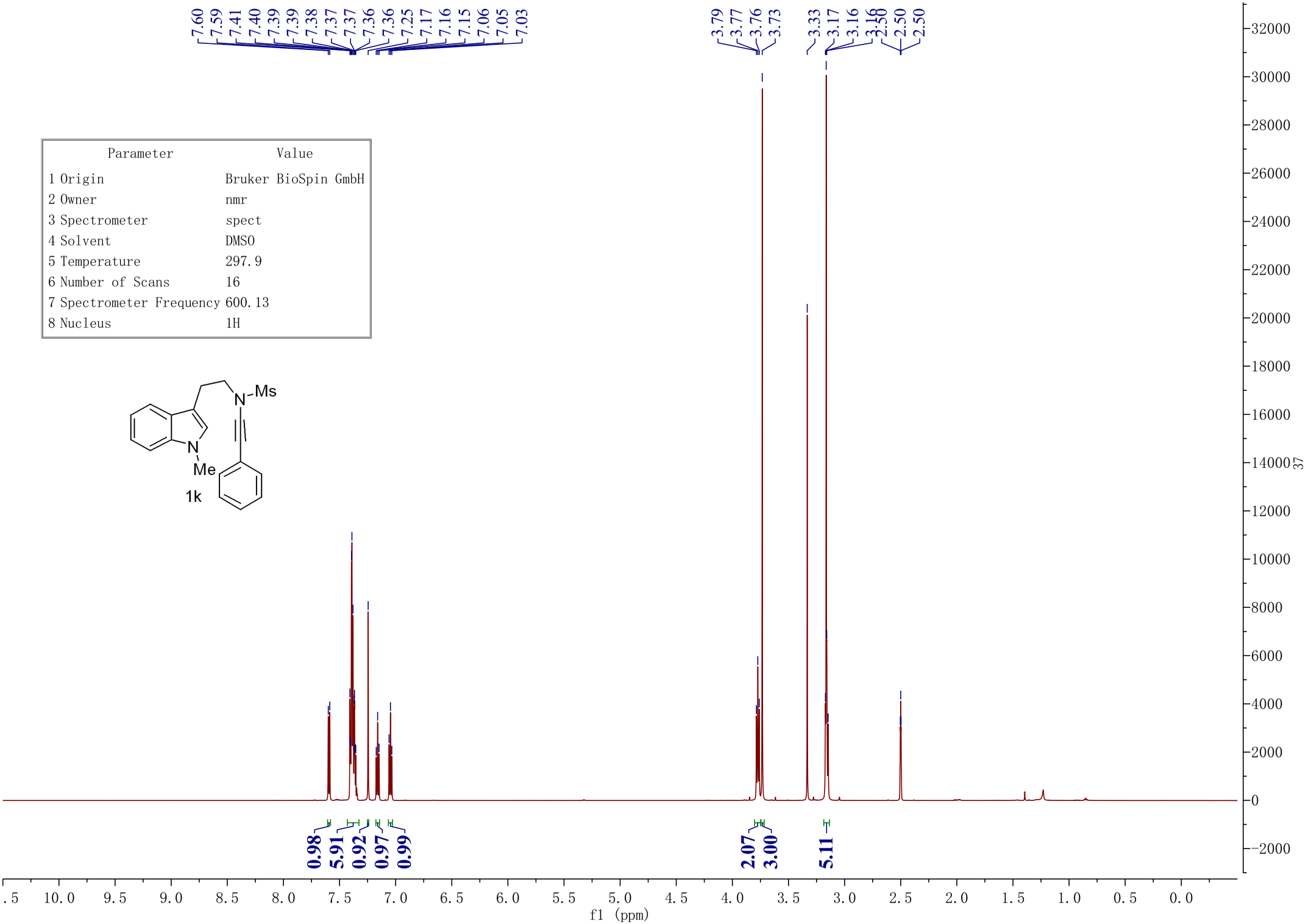


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	314
7 Spectrometer Frequency	150.90
8 Nucleus	13C

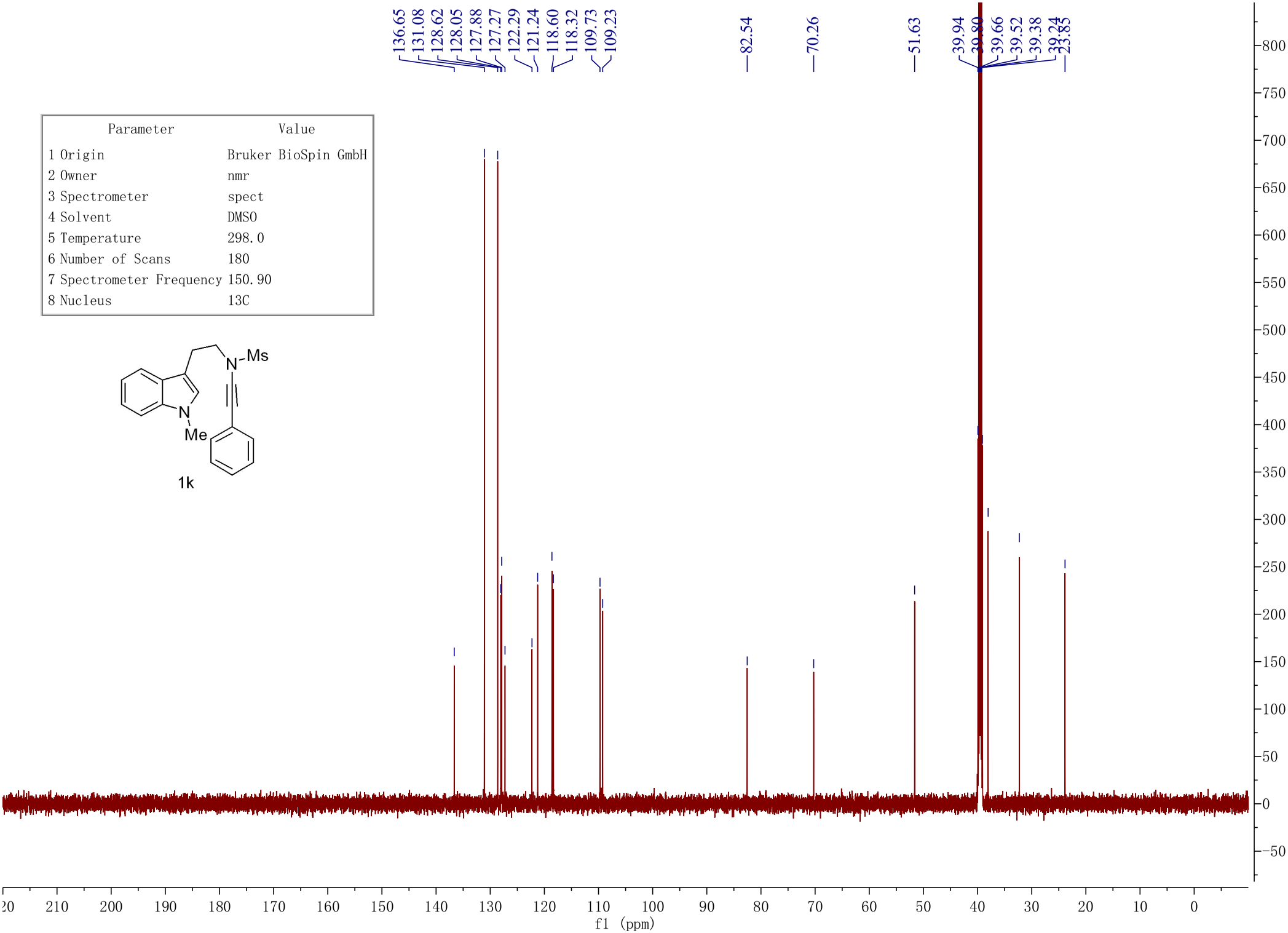

8.18 8.18 8.17 8.17 7.89 7.89 7.88 7.87 7.46 7.46 7.45 7.45 7.42 7.42 7.41 7.41 7.40 7.40 7.22 7.20 7.07 7.07 7.06 7.05 7.05 6.97 6.96 6.95 3.83 3.81 3.80 3.65 3.34 3.06 3.05 3.04 2.51 2.50 2.50 2.50 2.49
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
NNs
N
Me
1j
1.94 1.98 5.95 0.99 1.99 1.01 1.95 3.00 1.94
f1 (ppm)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	164
7 Spectrometer Frequency	150.90
8 Nucleus	13C

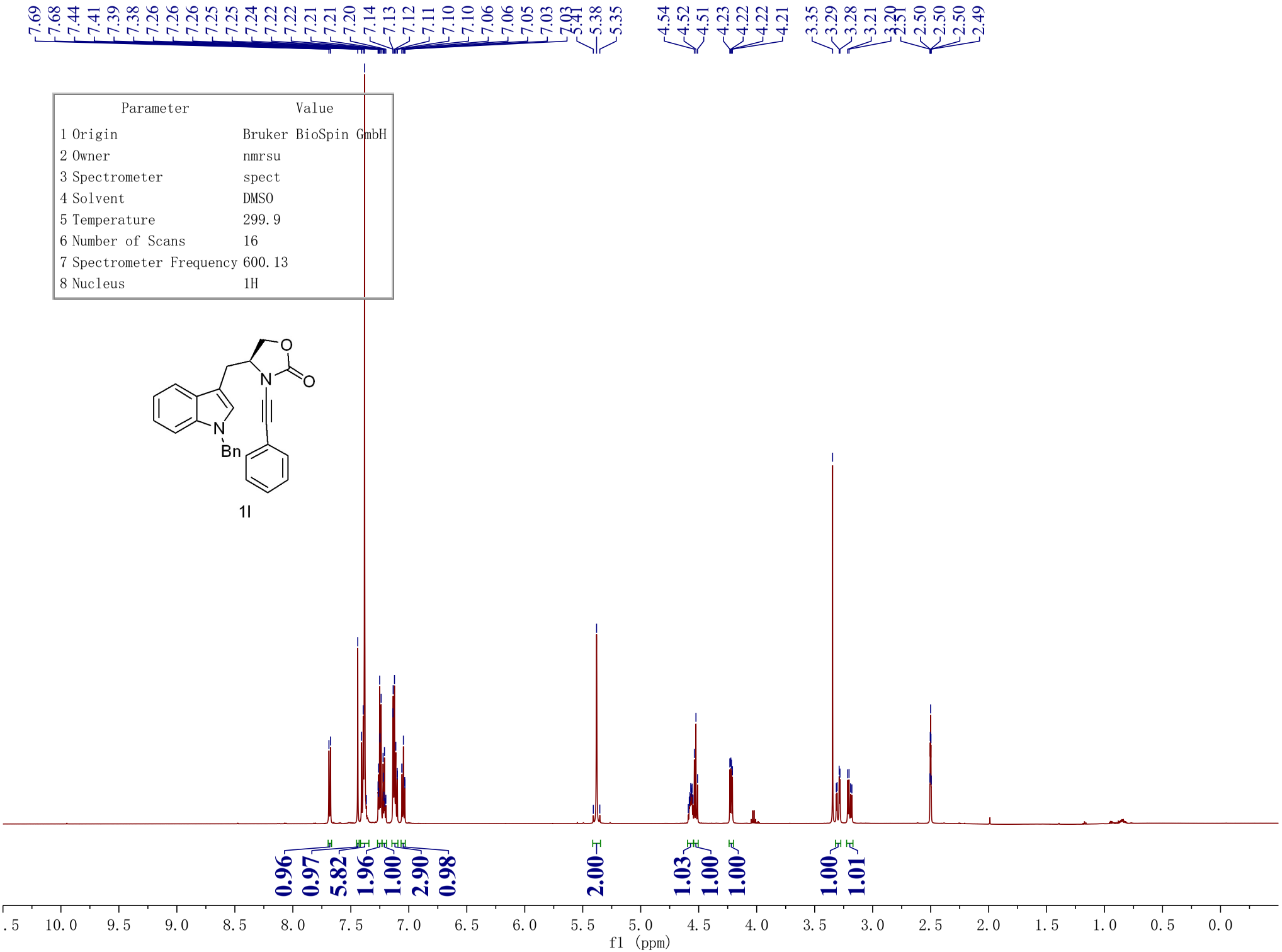


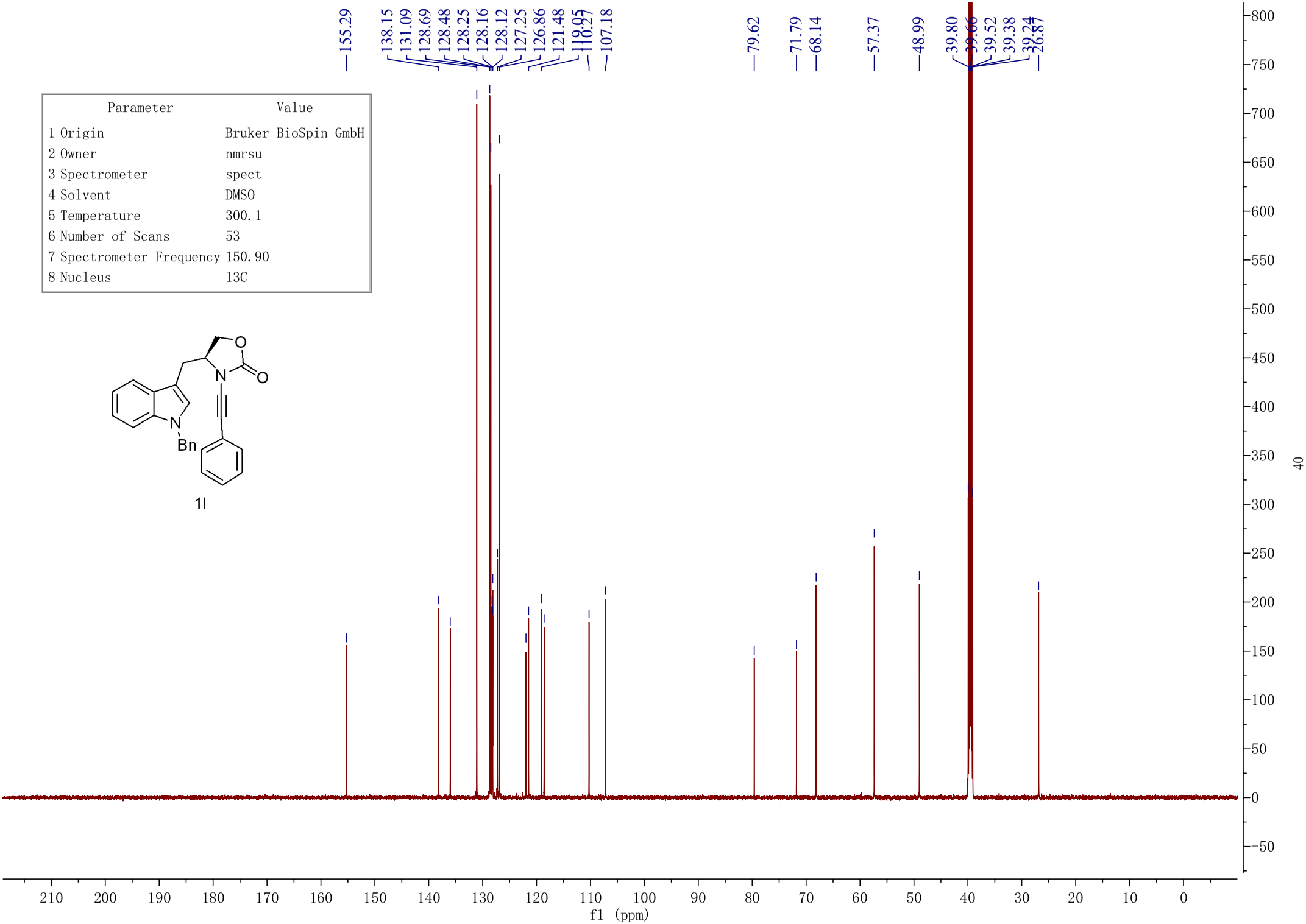
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

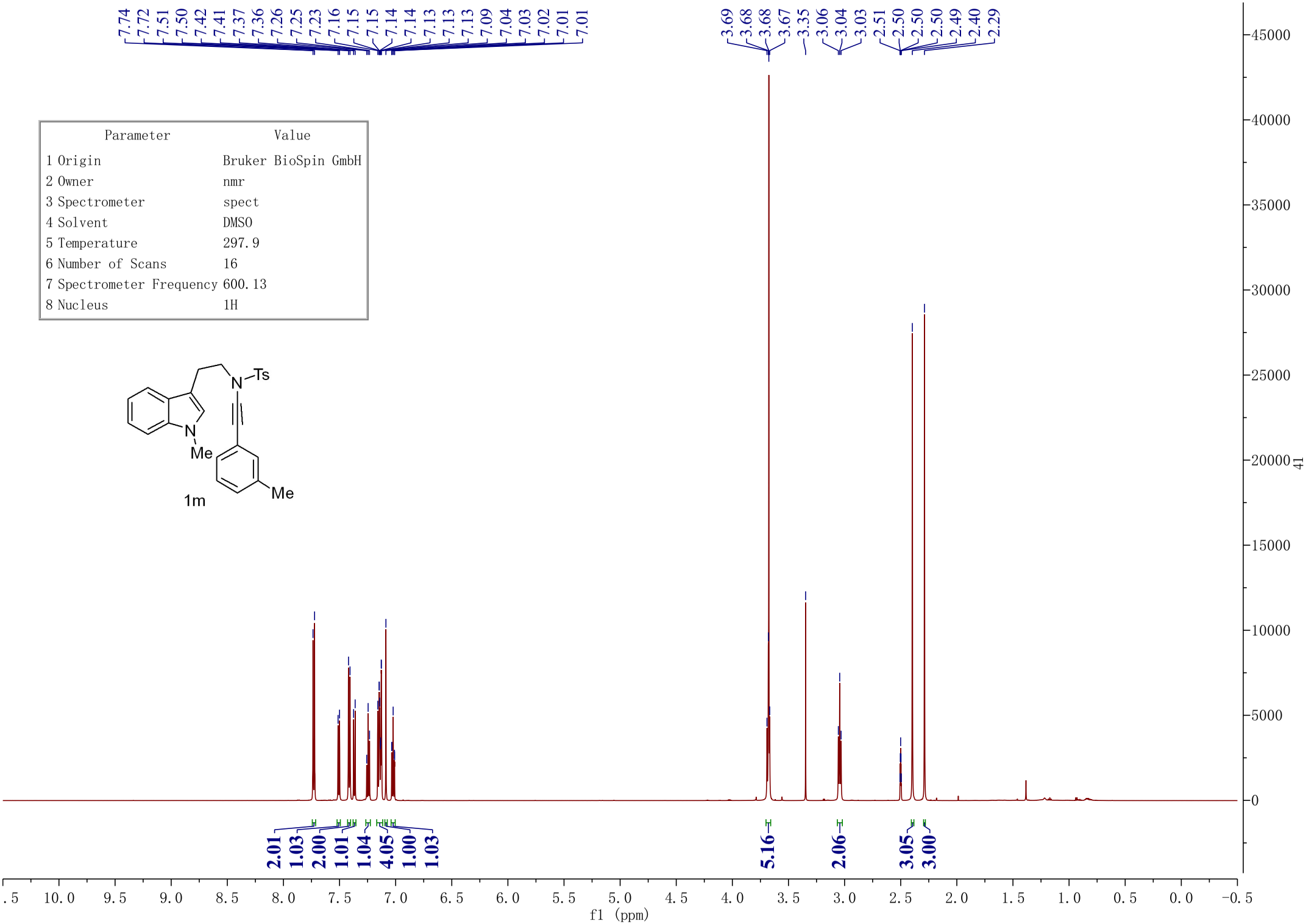


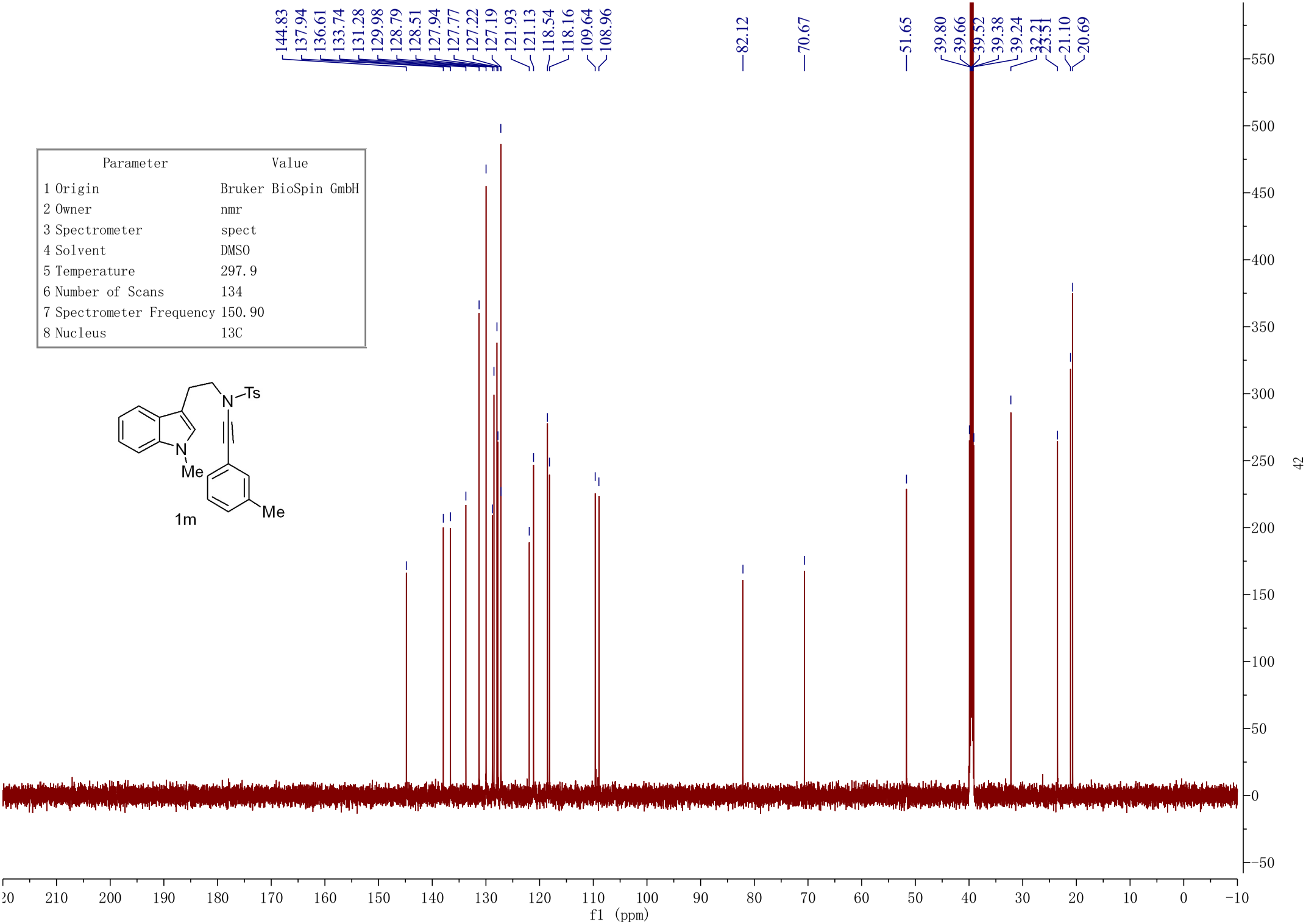
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.0
6 Number of Scans	180
7 Spectrometer Frequency	150.90
8 Nucleus	13C

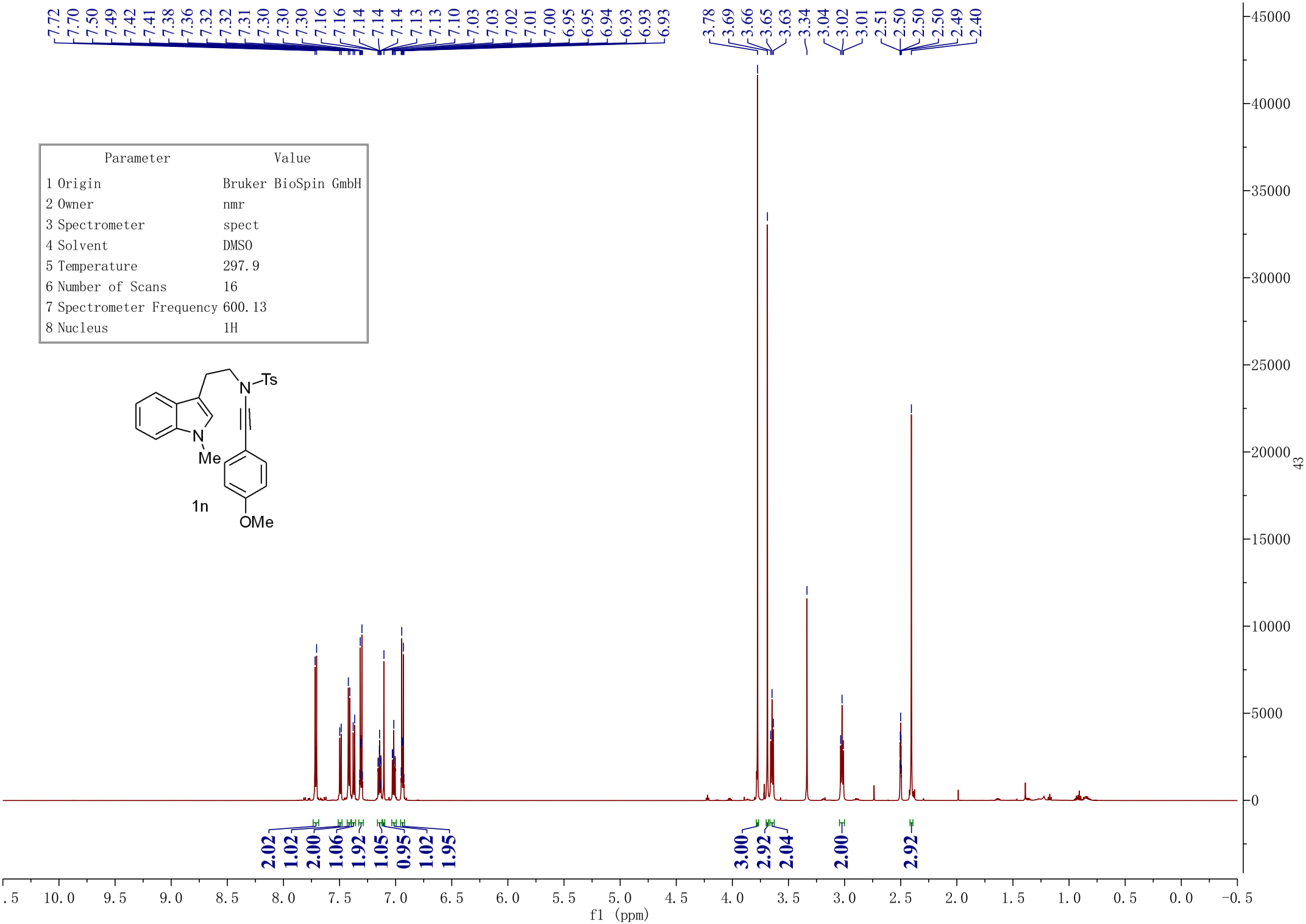
1k


7.69 7.68 7.44 7.41 7.39 7.38 7.26 7.26 7.26 7.25 7.25 7.24 7.22 7.22 7.21 7.21 7.20 7.14 7.13 7.12 7.11 7.10 7.10 7.06 7.06 7.05 7.03 7.03 5.41 5.38 5.35
4.54 4.52 4.51 4.23 4.22 4.22 4.21
3.35 3.29 3.28 3.21 3.20 2.51 2.50 2.50 2.50 2.49
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
O
N
Bn
1l
0.96 0.97 5.82 1.96 1.00 2.90 0.98
2.00
1.03 1.00 1.00
1.00 1.01
4500
4000
3500
3000
2500
2000
1500
1000
500
0
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


155.29
138.15
131.09
128.69
128.48
128.25
128.16
128.12
127.25
126.86
121.48
119.95
110.27
107.18
79.62
71.79
68.14
57.37
48.99
39.80
39.66
39.52
39.38
39.24
26.87
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.1
6 Number of Scans 53
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
O
N
Bn
1l
f1 (ppm)

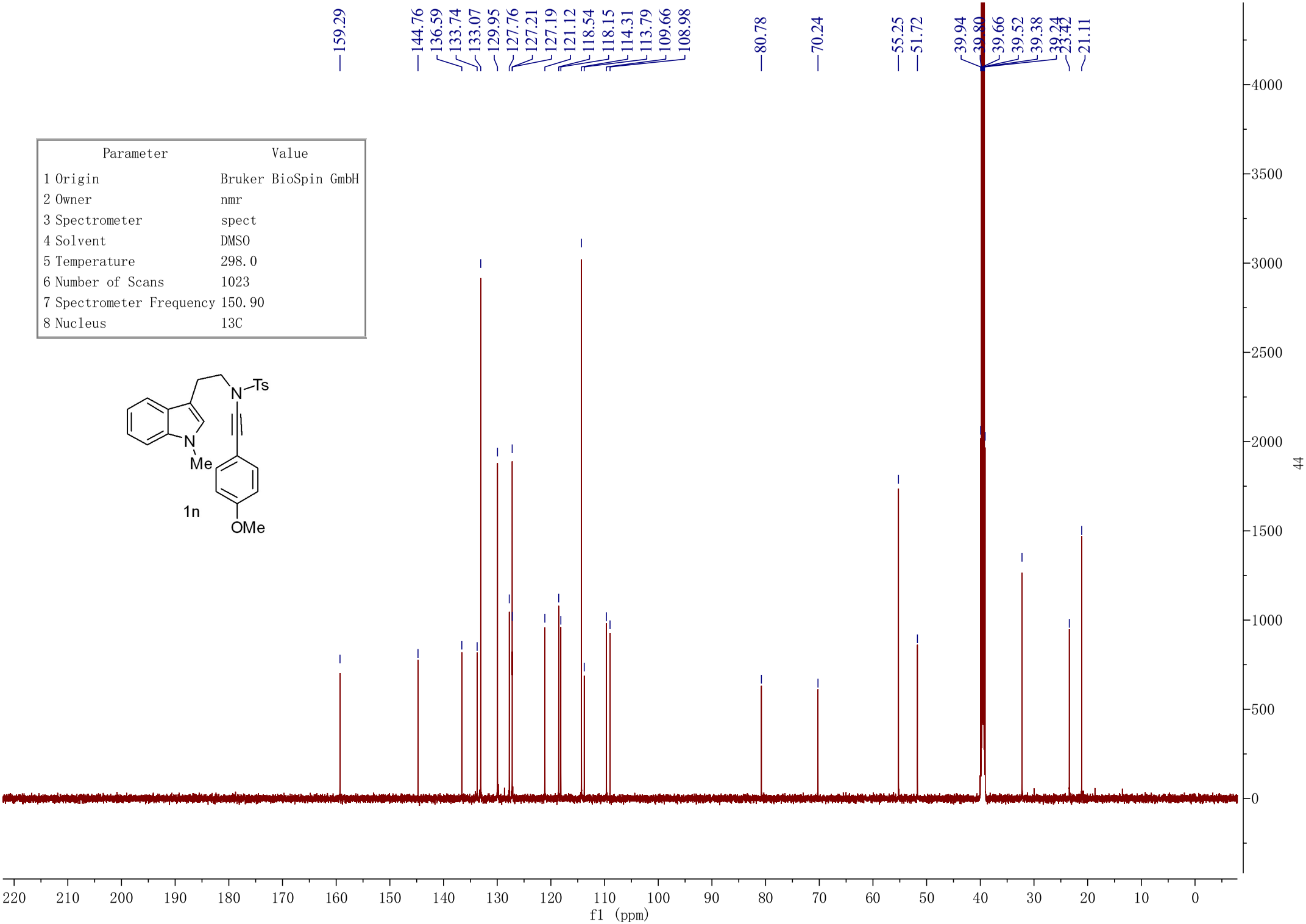

7.74 7.72 7.51 7.50 7.42 7.41 7.37 7.36 7.26 7.25 7.23 7.16 7.15 7.15 7.14 7.14 7.13 7.13 7.13 7.09 7.04 7.03 7.02 7.01 7.01
3.69 3.68 3.68 3.67 3.35 3.06 3.04 3.03 2.51 2.50 2.50 2.50 2.49 2.40 2.29
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
N
Ts
N
Me
Me
1m
2.01 1.03 2.00 1.01 1.04 4.05 1.00 1.03
5.16
2.06
3.05
3.00
f1 (ppm)

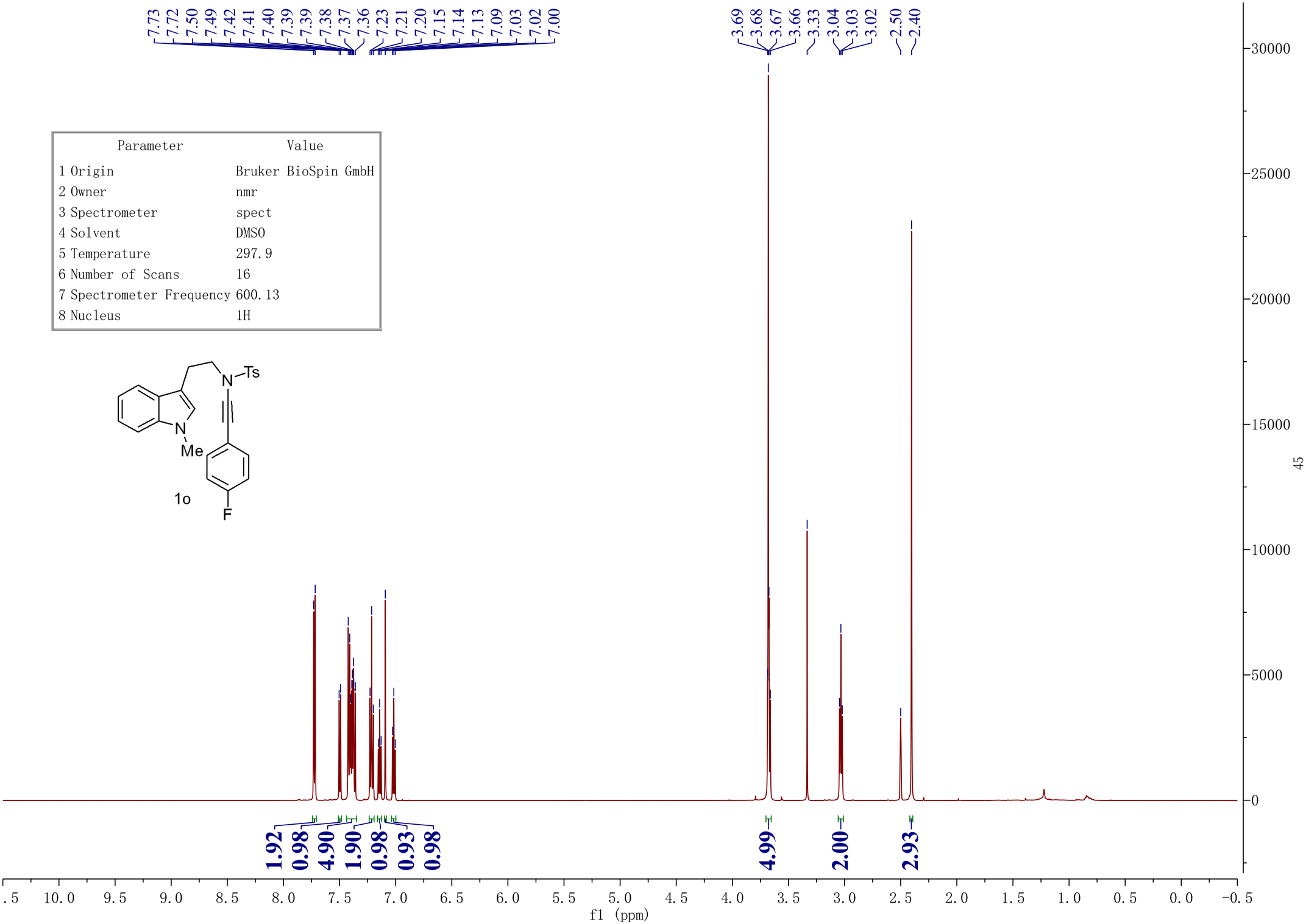

144.83
137.94
136.61
133.74
131.28
129.98
128.79
128.51
127.94
127.77
127.22
127.19
121.93
121.13
118.54
118.16
109.64
108.96
82.12
70.67
51.65
39.80
39.66
39.52
39.38
39.24
32.21
23.51
21.10
20.69
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 134
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
Ts
N
Me
Me
1m
f1 (ppm)



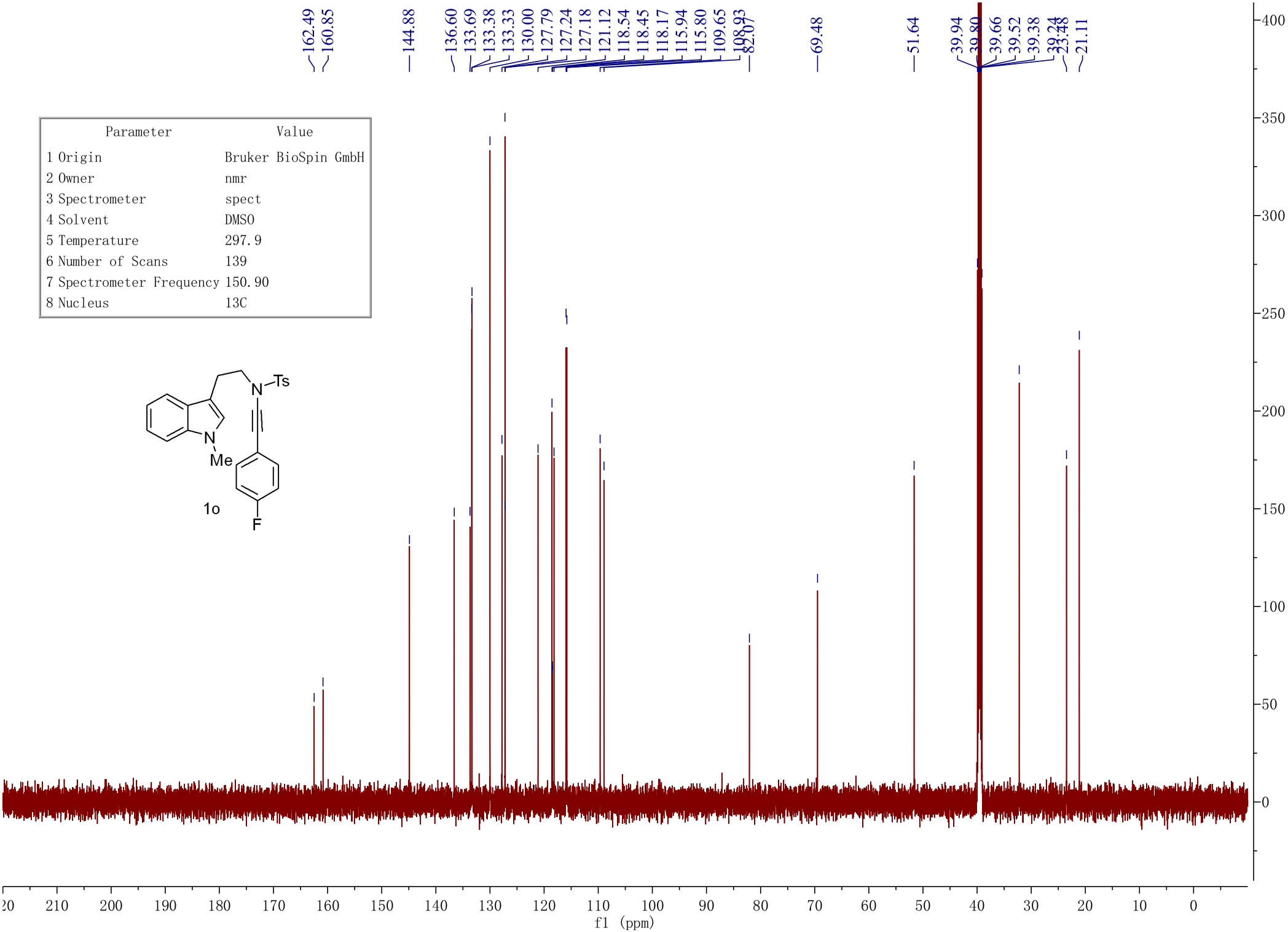
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

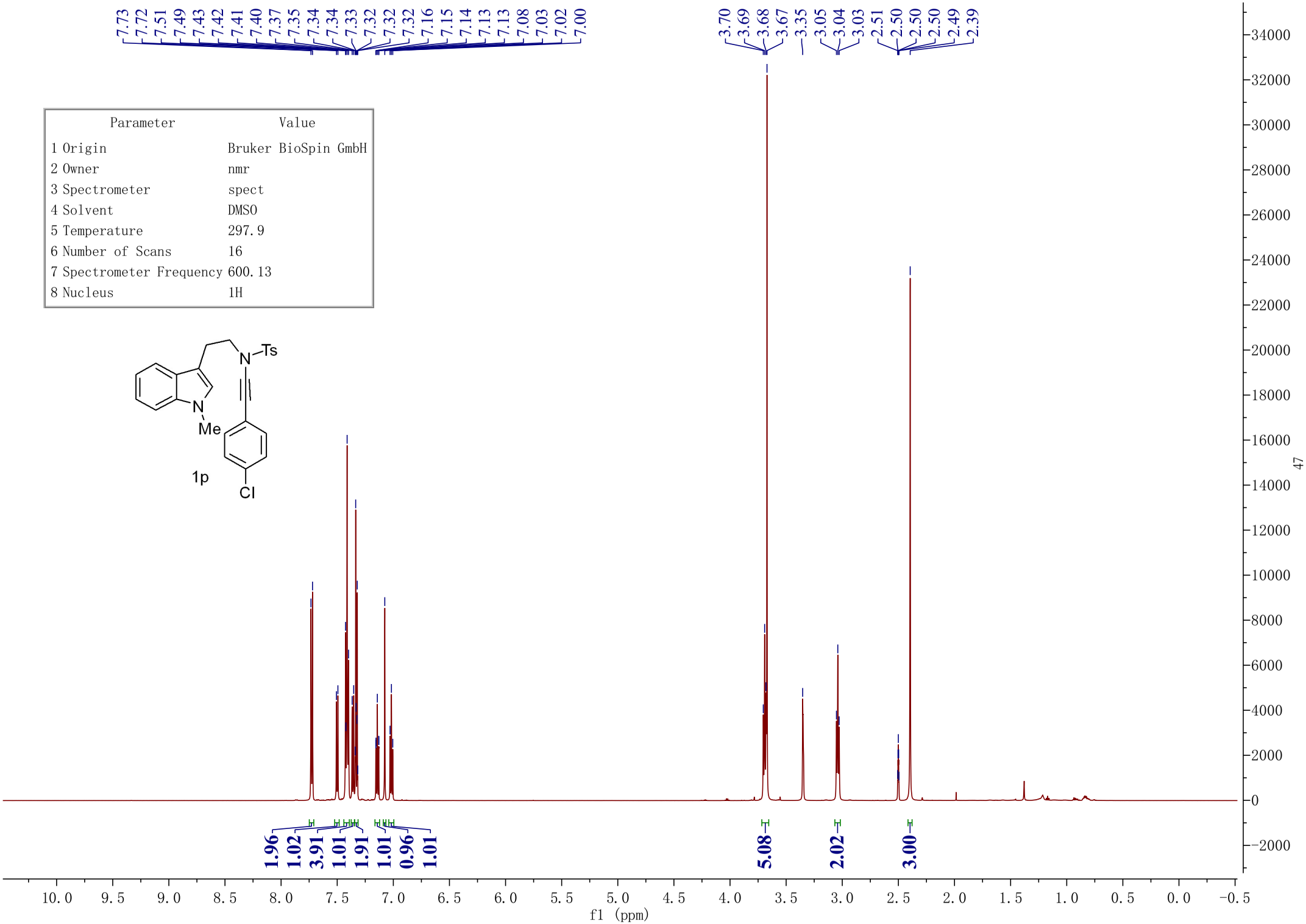
1n

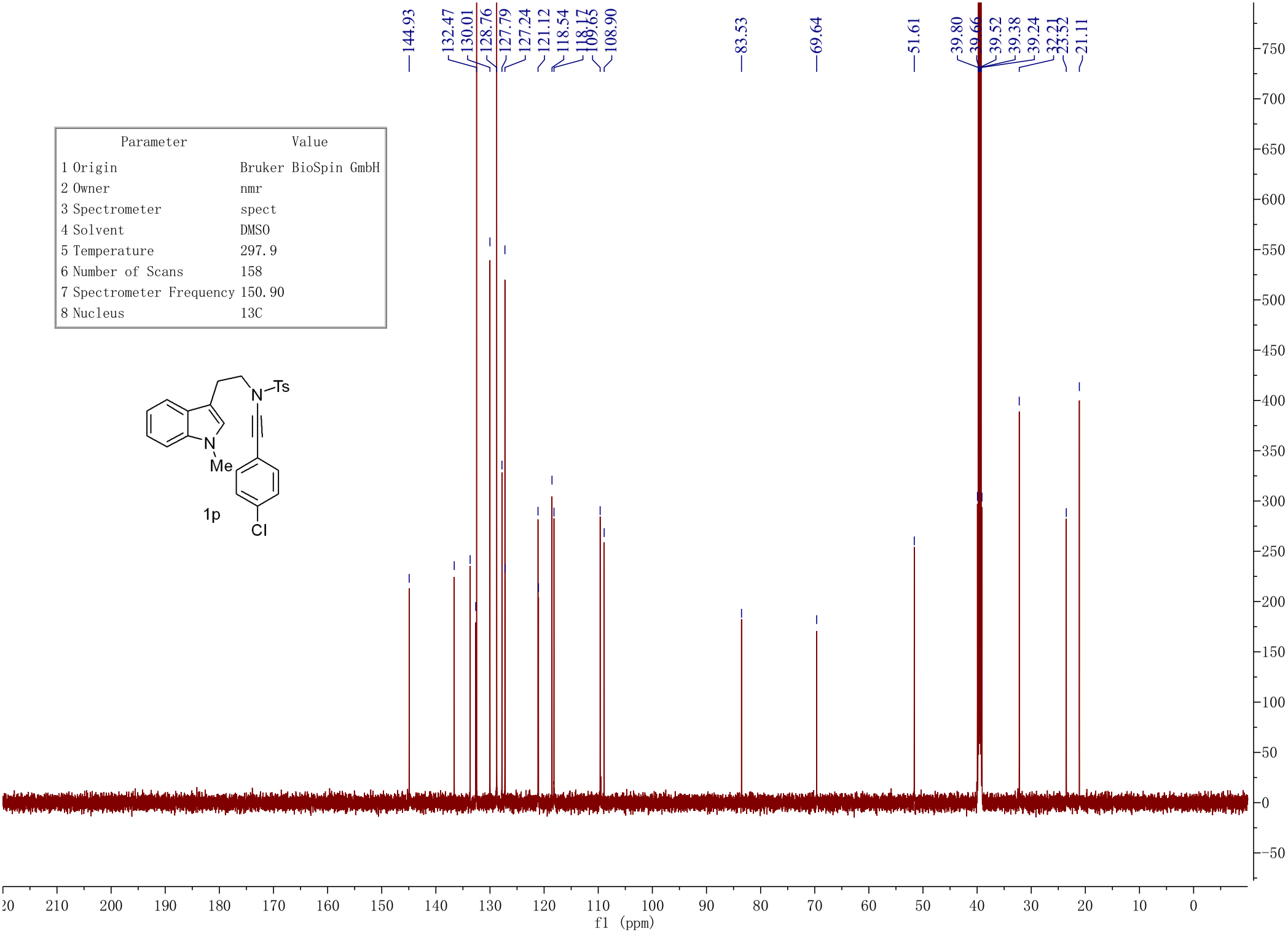

159.29
144.76
136.59
133.74
133.07
129.95
127.76
127.21
127.19
121.12
118.54
118.15
114.31
113.79
109.66
108.98
80.78
70.24
55.25
51.72
39.94
39.80
39.66
39.52
39.38
39.24
23.42
21.11
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 1023
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
Ts
N
Me
1n
OMe
f1 (ppm)

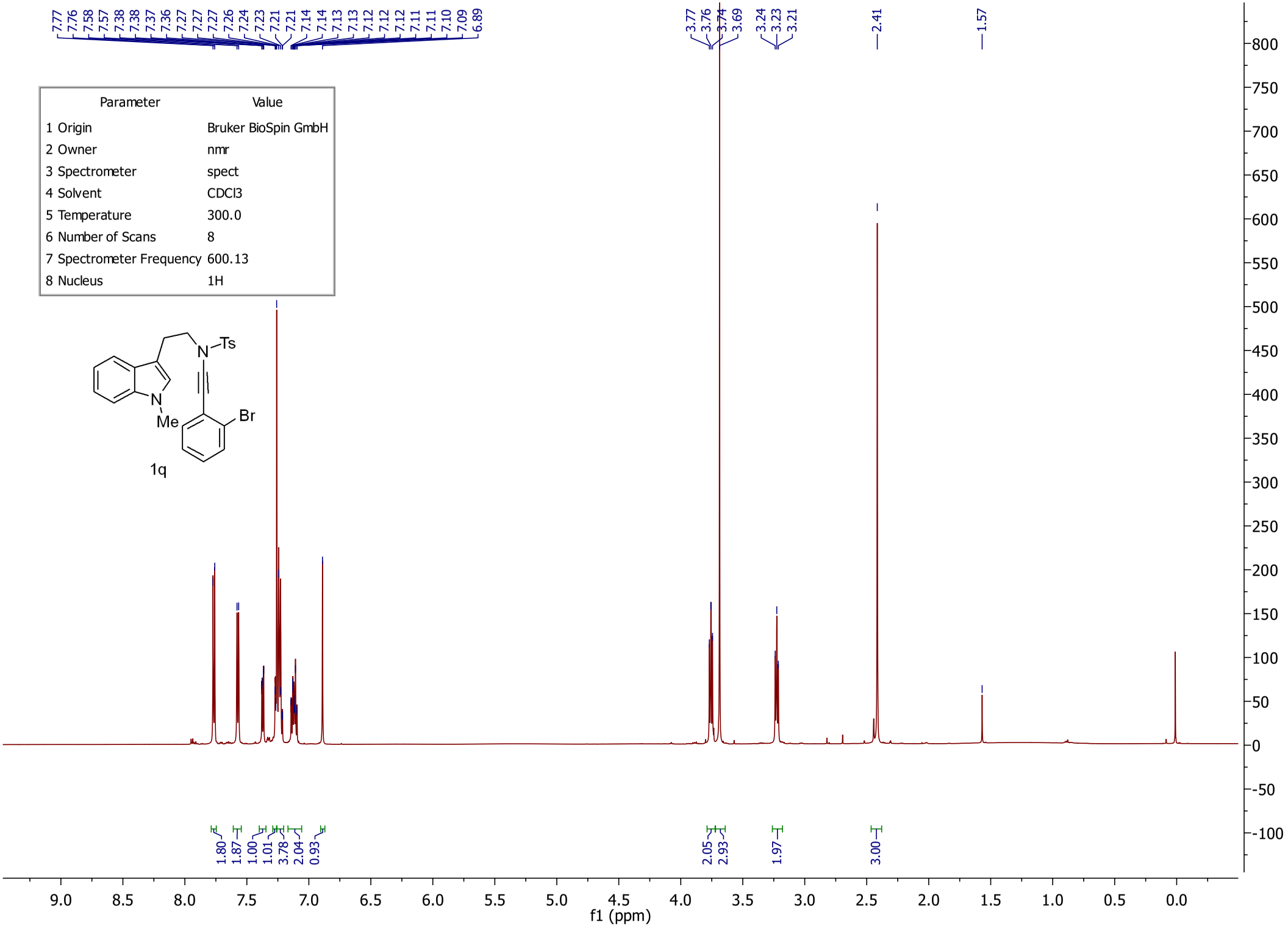


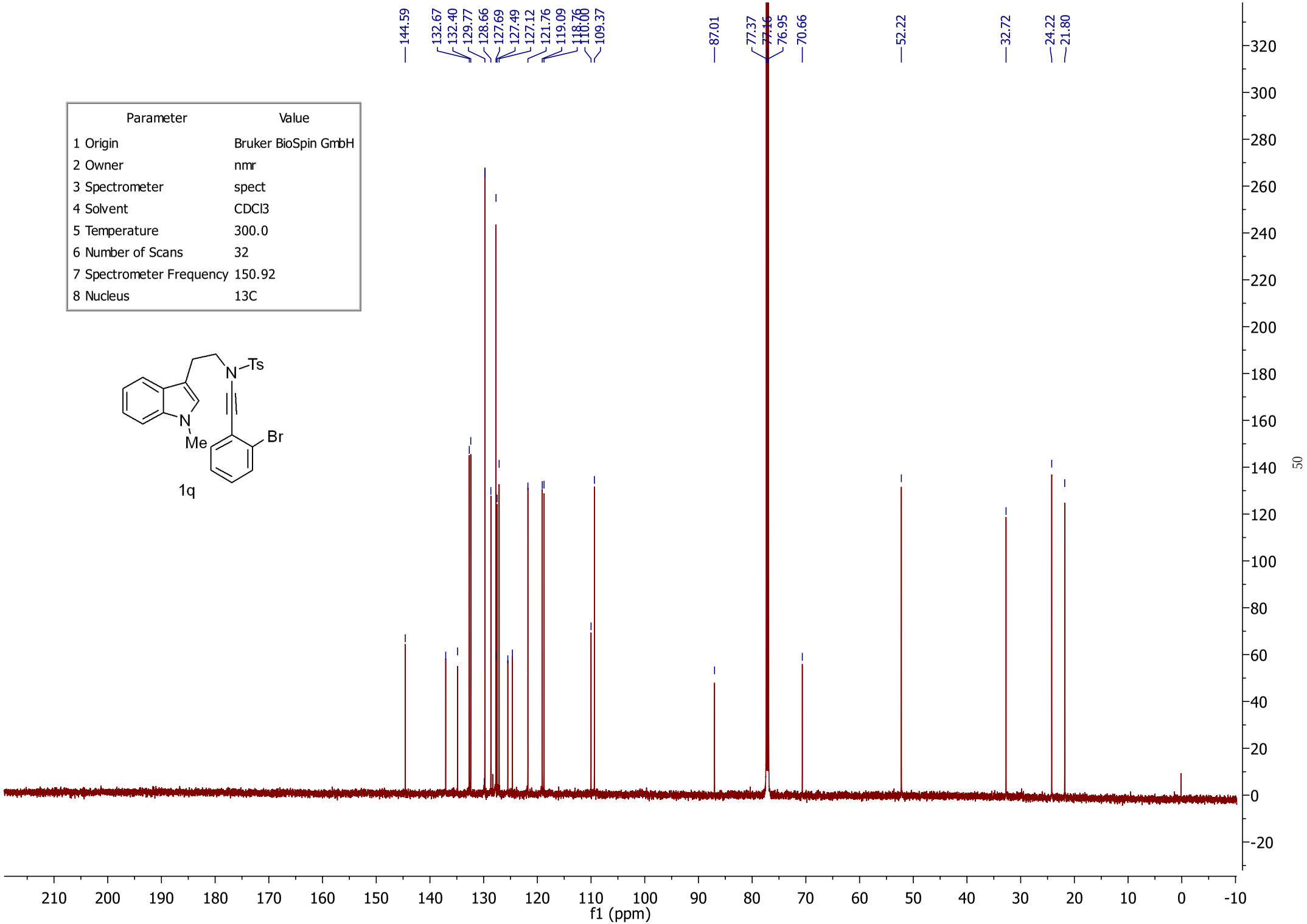
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

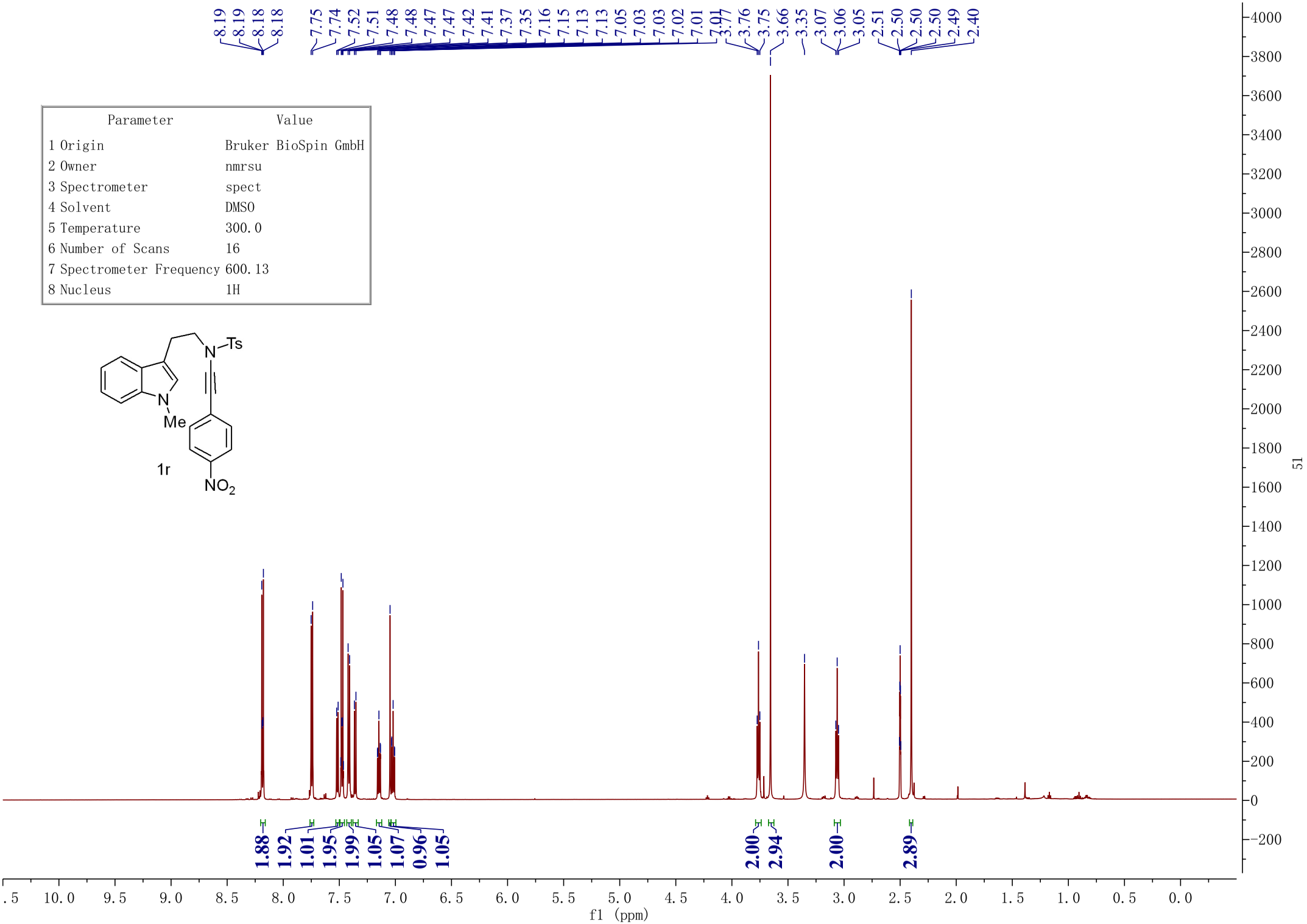

162.49
160.85
144.88
136.60
133.69
133.38
133.33
130.00
127.79
127.24
127.18
121.12
118.54
118.45
118.17
115.94
115.80
109.65
108.93
82.07
69.48
51.64
39.94
39.80
39.66
39.52
39.38
39.24
23.48
21.11
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 139
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
Ts
N
Me
1o
F
f1 (ppm)

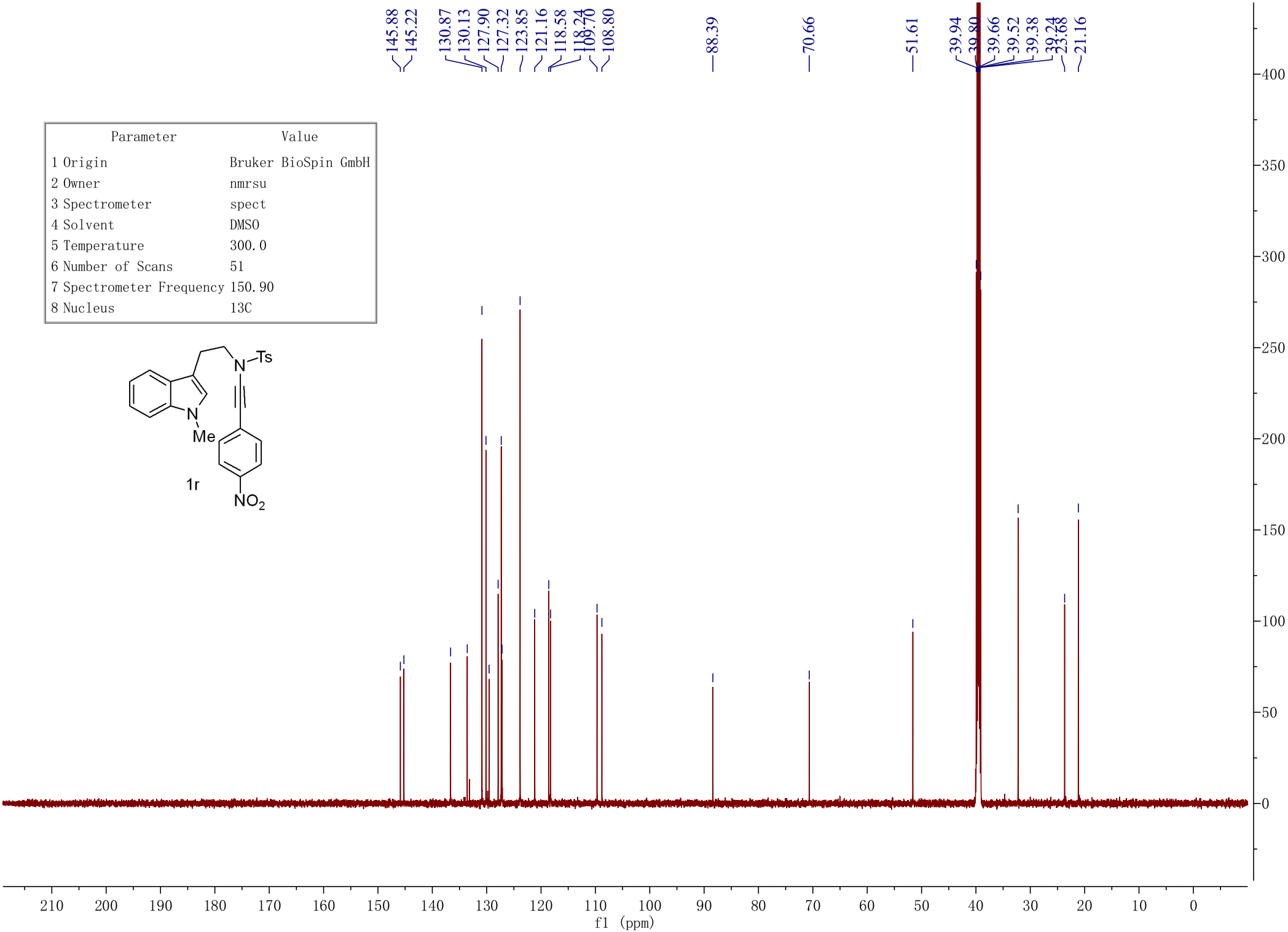

7.73 7.72 7.51 7.49 7.43 7.42 7.41 7.40 7.37 7.35 7.34 7.34 7.33 7.32 7.32 7.32 7.16 7.15 7.14 7.13 7.13 7.08 7.03 7.02 7.00
3.70 3.69 3.68 3.67 3.35 3.05 3.04 3.03 2.51 2.50 2.50 2.50 2.49 2.39
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
N
Ts
N
Me
1p
Cl
1.96 1.02 3.91 1.01 1.91 1.01 0.96 1.01
5.08
2.02
3.00
f1 (ppm)

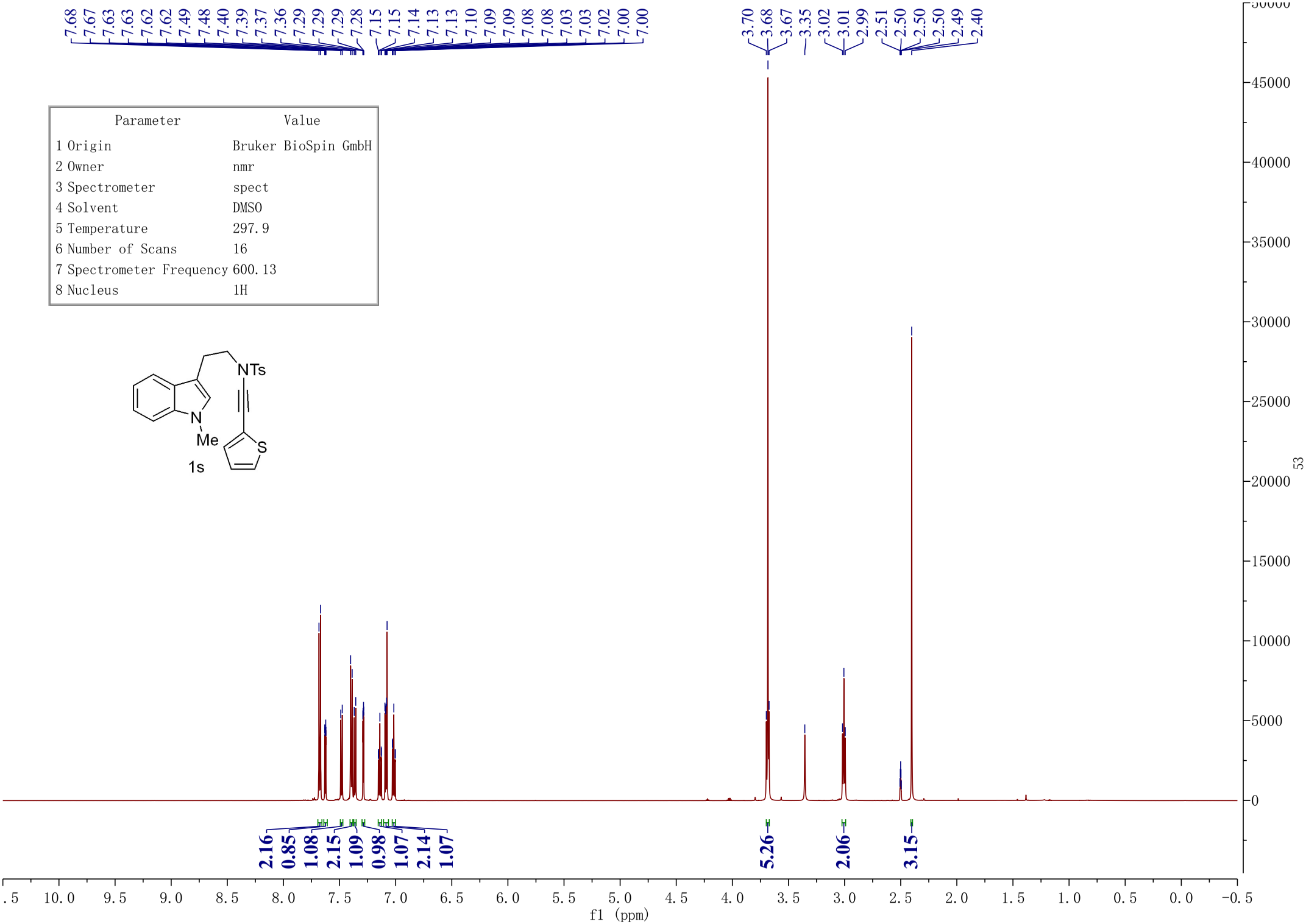

144.93
132.47
130.01
128.76
127.79
127.24
121.12
118.54
118.17
109.65
108.90
83.53
69.64
51.61
39.80
39.66
39.52
39.38
39.24
32.21
23.52
21.11
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 158
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
Ts
N
Me
1p
Cl
f1 (ppm)

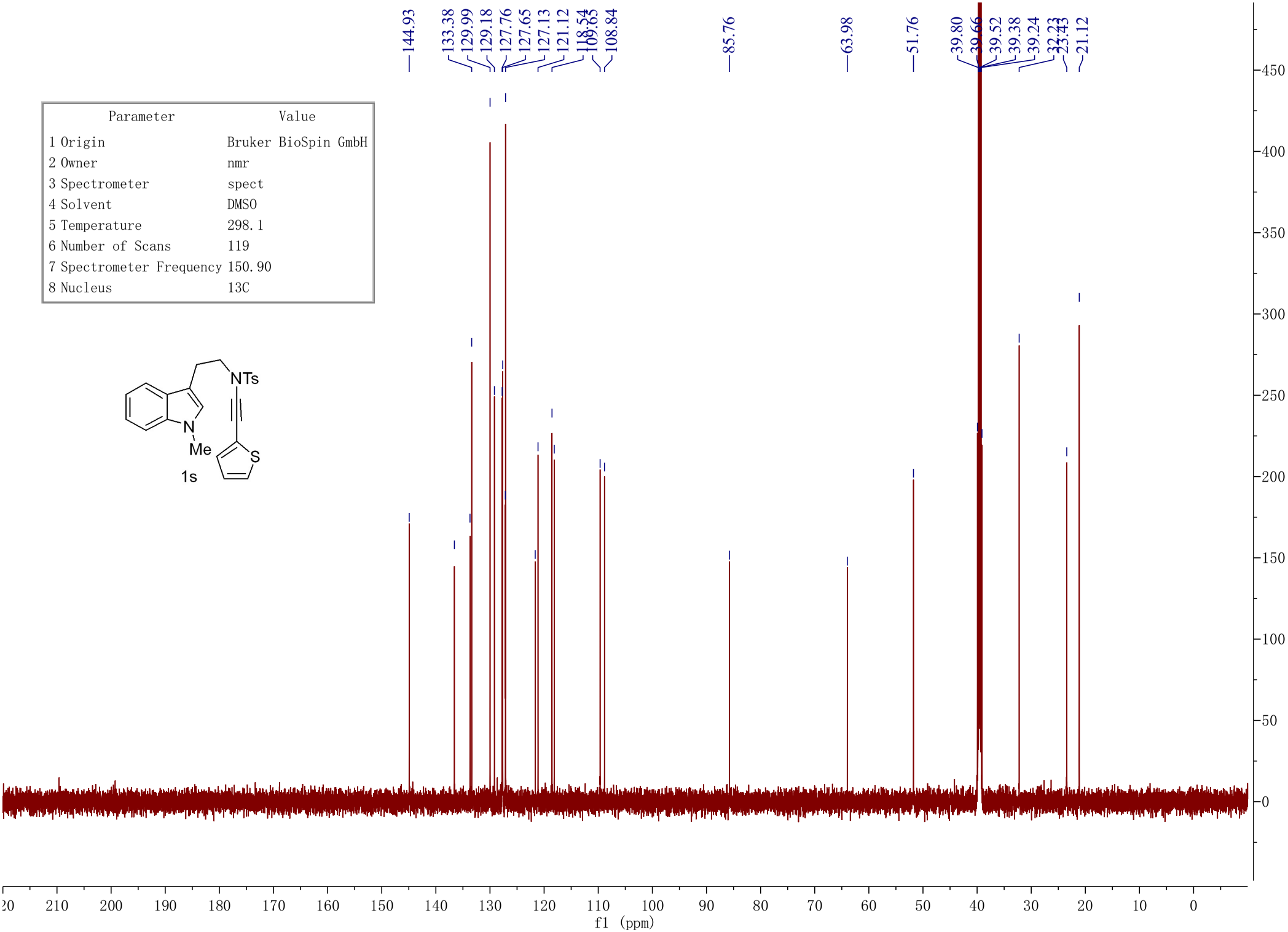

7.77 7.76 7.58 7.57 7.38 7.38 7.37 7.36 7.27 7.27 7.27 7.26 7.24 7.23 7.21 7.21 7.14 7.14 7.13 7.13 7.12 7.12 7.12 7.11 7.11 7.10 7.09 6.89
3.77 3.76 3.74 3.69 3.24 3.23 3.21 2.41 1.57
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 8
7 Spectrometer Frequency 600.13
8 Nucleus 1H
N
Ts
N
Me
Br
1q
1.80 1.87 1.00 1.01 3.78 2.04 0.93
2.05 2.93 1.97 3.00
f1 (ppm)


144.59
132.67
132.40
129.77
128.66
127.69
127.49
127.12
121.76
119.09
118.76
118.08
109.37
87.01
77.37
77.16
76.95
70.66
52.22
32.72
24.22
21.80
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 32
7 Spectrometer Frequency 150.92
8 Nucleus 13C
N
Ts
N
Me
Br
1q
f1 (ppm)

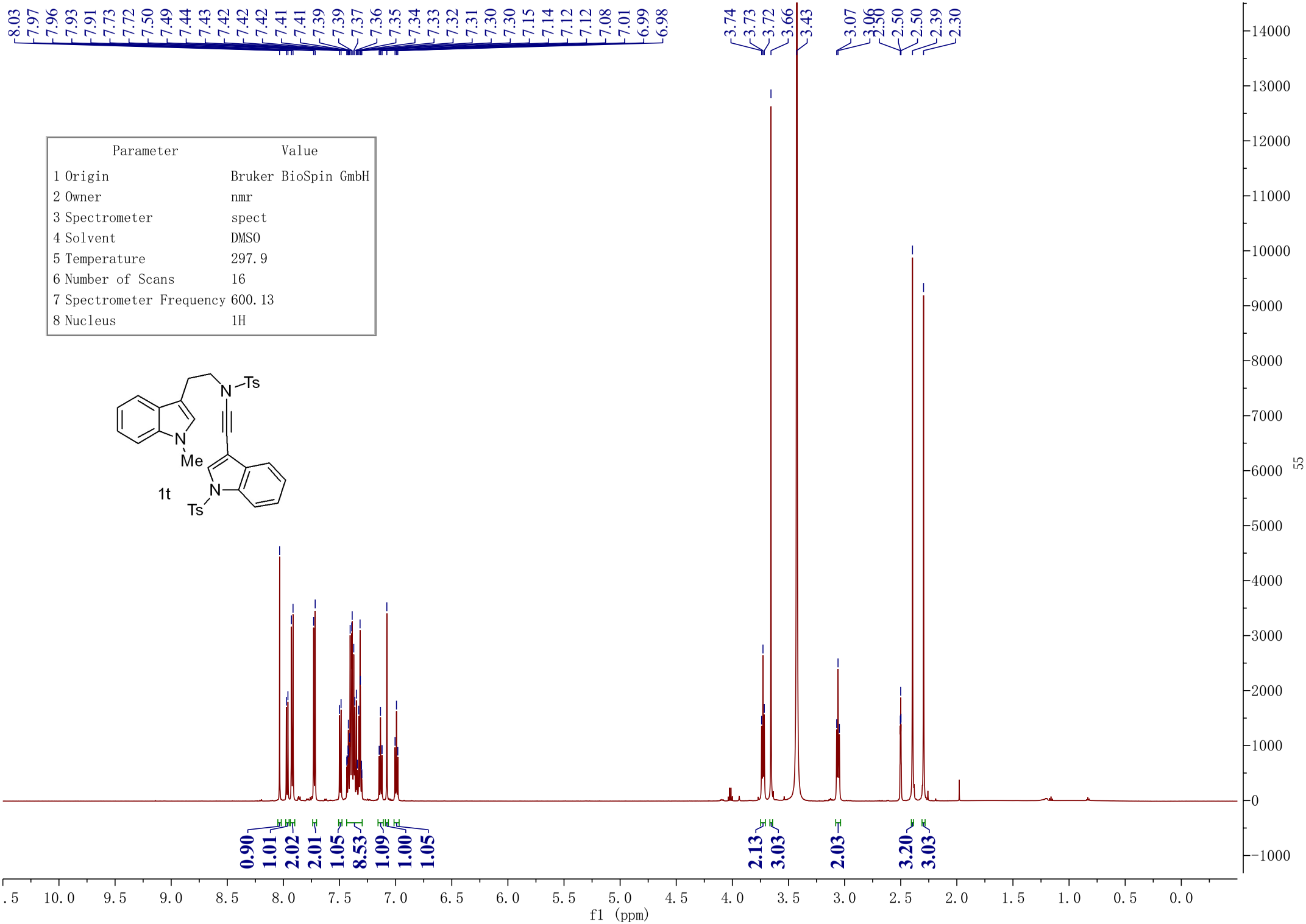

8.19 8.19 8.18 8.18 7.75 7.74 7.52 7.51 7.48 7.48 7.47 7.47 7.42 7.41 7.37 7.35 7.16 7.15 7.13 7.13 7.05 7.03 7.03 7.02 7.01 7.01 3.77 3.76 3.75 3.66 3.35 3.07 3.06 3.05 2.51 2.50 2.50 2.50 2.49 2.40
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
N
Ts
N
Me
1r
NO2
1.88 1.92 1.01 1.95 1.99 1.05 1.07 0.96 1.05 2.00 2.94 2.00 2.89
f1 (ppm)
51


145.88
145.22
130.87
130.13
127.90
127.32
123.85
121.16
118.58
118.24
109.70
108.80
88.39
70.66
51.61
39.94
39.80
39.66
39.52
39.38
39.24
23.68
21.16
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 51
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
Ts
N
Me
1r
NO2
f1 (ppm)

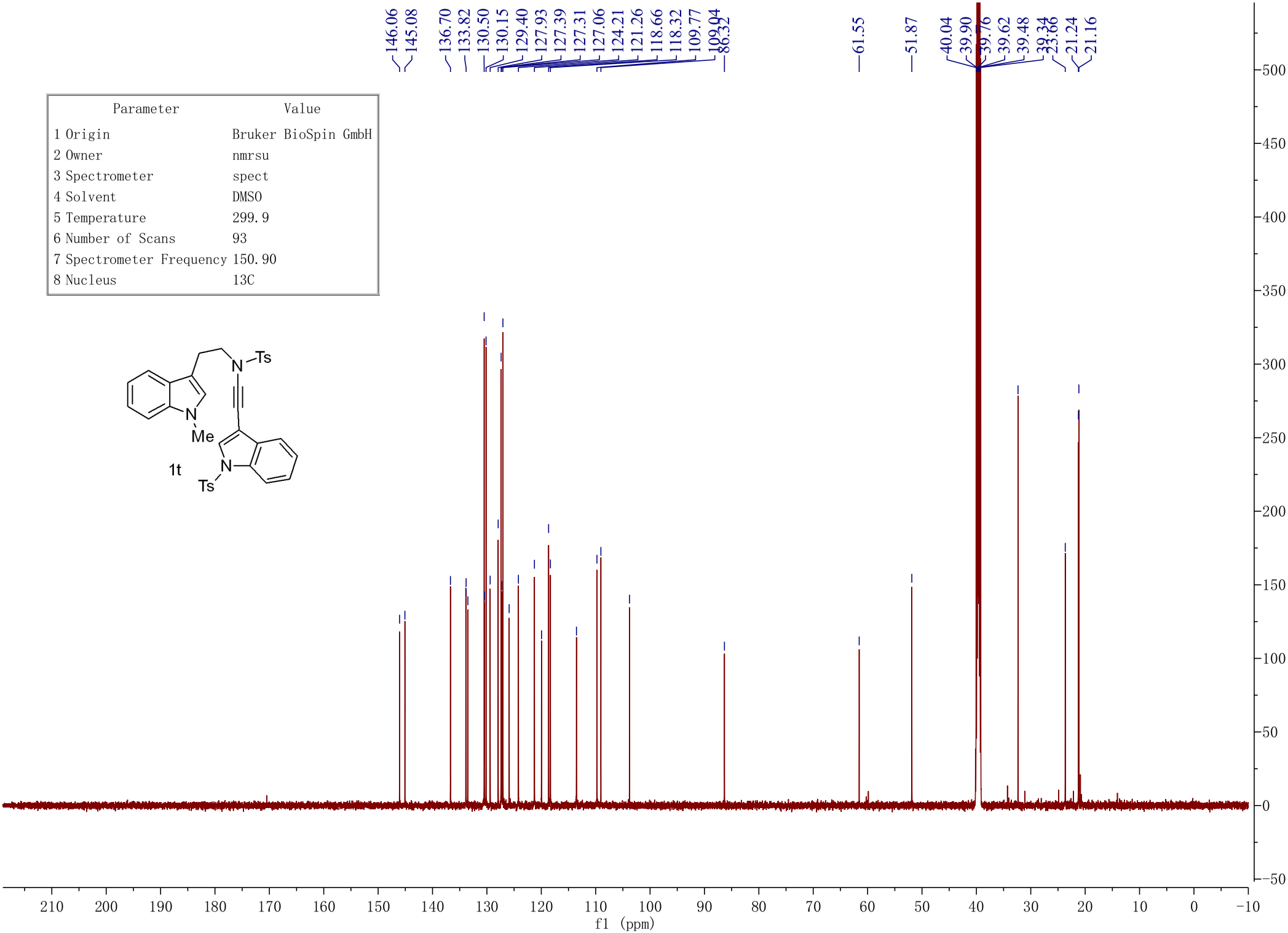

7.68 7.67 7.63 7.63 7.62 7.62 7.49 7.48 7.40 7.39 7.37 7.36 7.29 7.29 7.29 7.28 7.15 7.15 7.14 7.13 7.13 7.10 7.09 7.09 7.08 7.08 7.03 7.03 7.02 7.00 7.00
3.70 3.68 3.67 3.35 3.02 3.01 2.99 2.51 2.50 2.50 2.50 2.49 2.40
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
NTs
N
Me
S
1s
2.16 0.85 1.08 2.15 1.09 0.98 1.07 2.14 1.07
5.26
2.06
3.15
f1 (ppm)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.1
6 Number of Scans	119
7 Spectrometer Frequency	150.90
8 Nucleus	13C



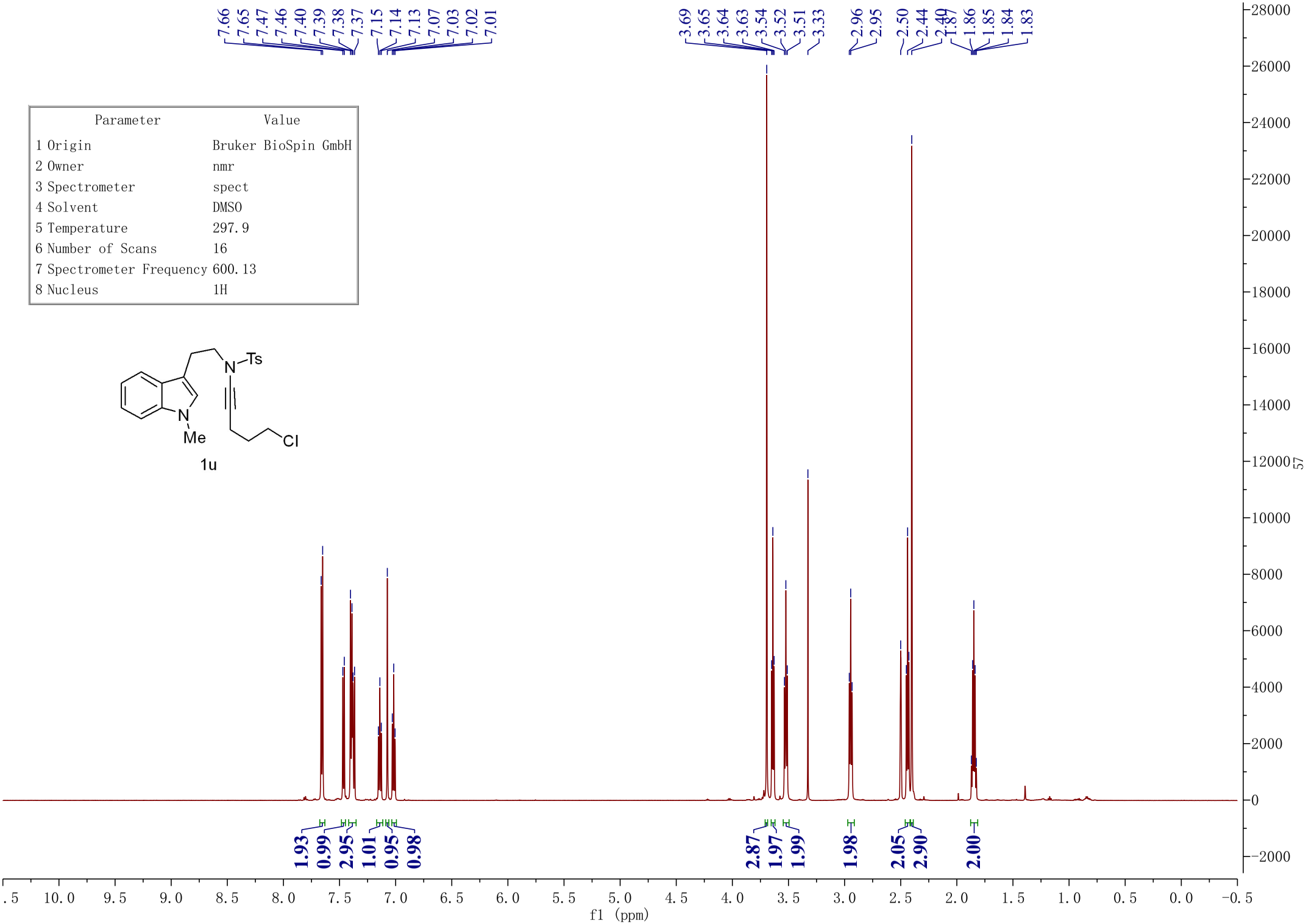
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

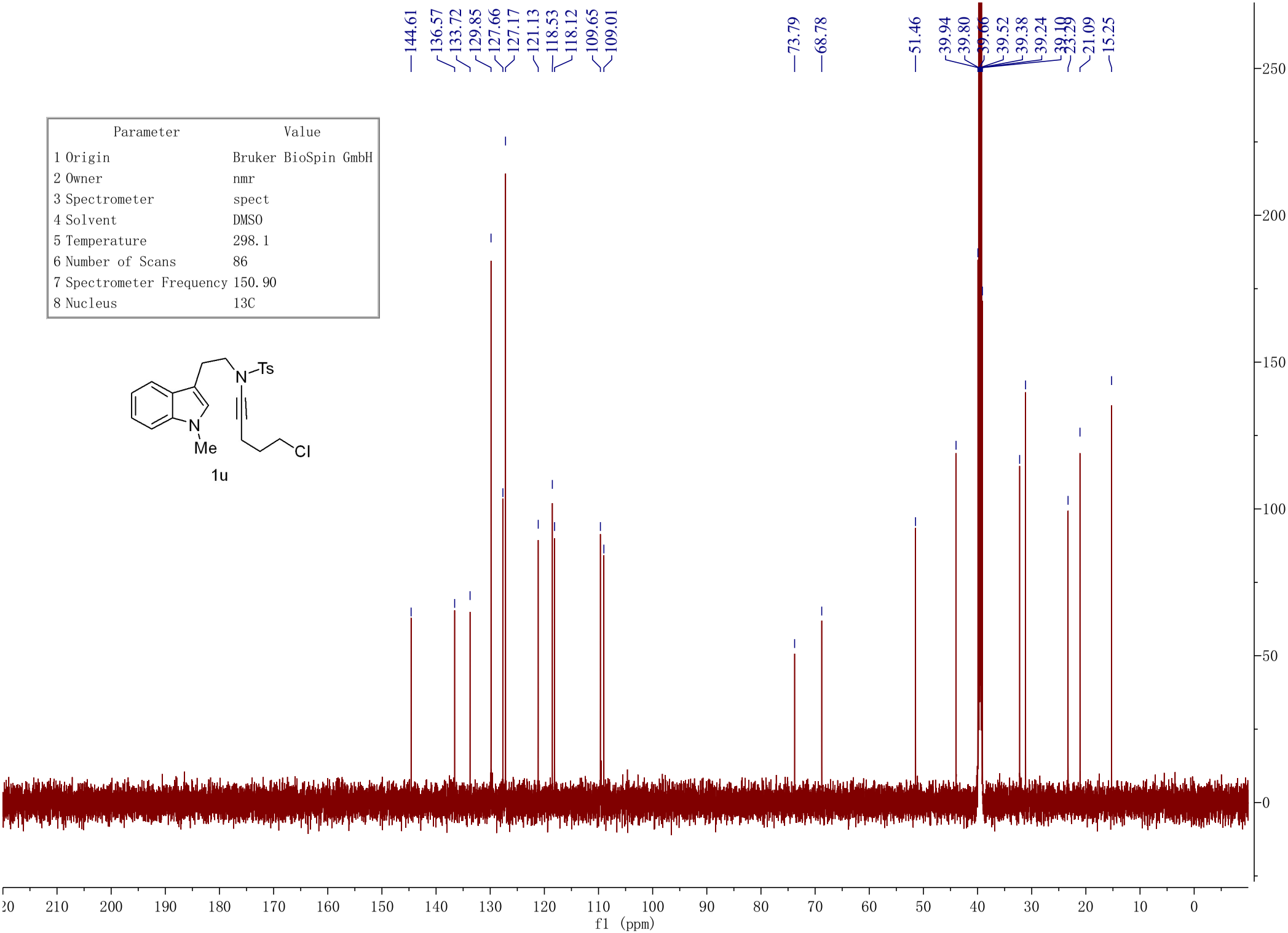


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	299.9
6 Number of Scans	93
7 Spectrometer Frequency	150.90
8 Nucleus	13C

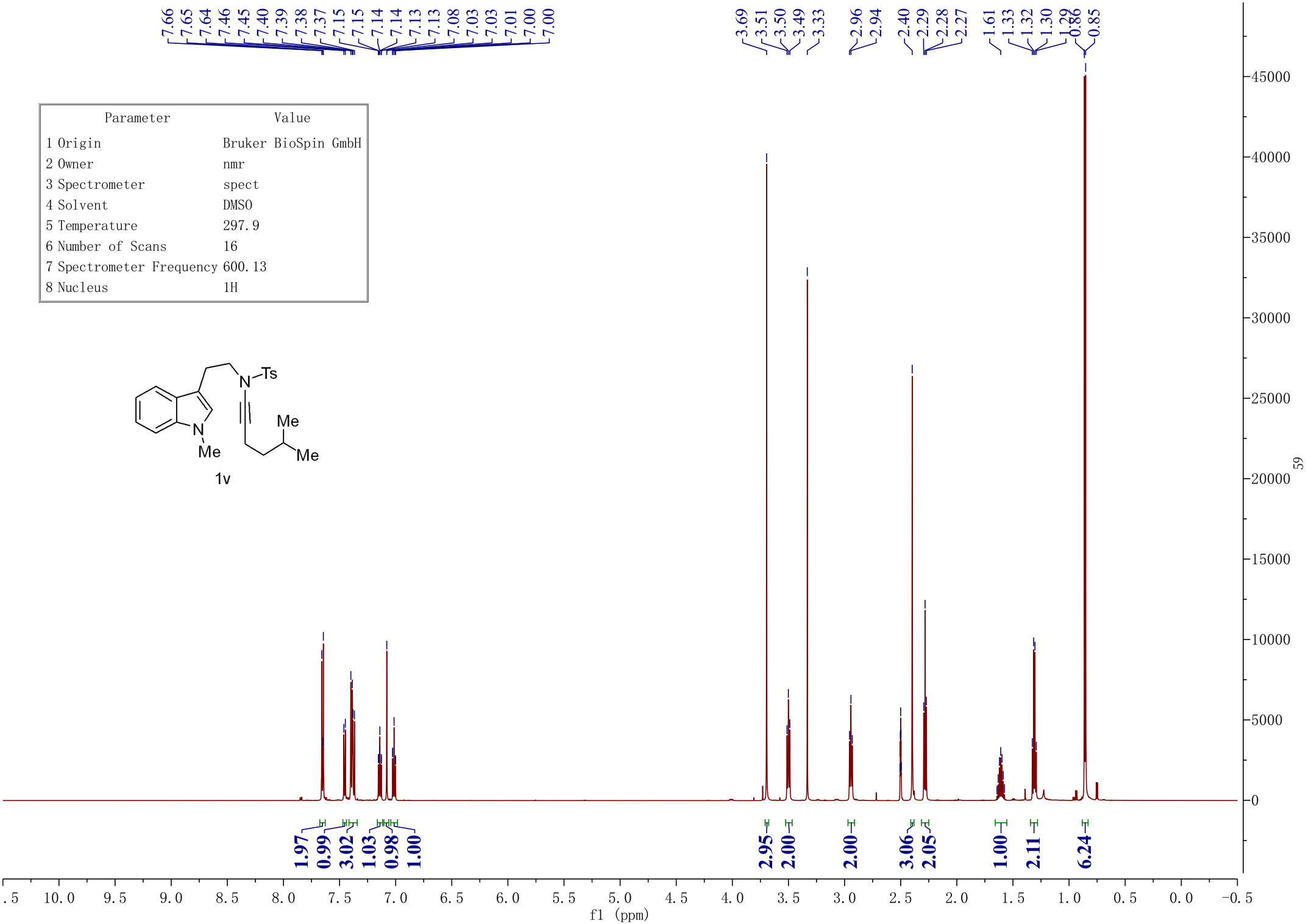
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

1u





Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.1
6 Number of Scans	86
7 Spectrometer Frequency	150.90
8 Nucleus	13C

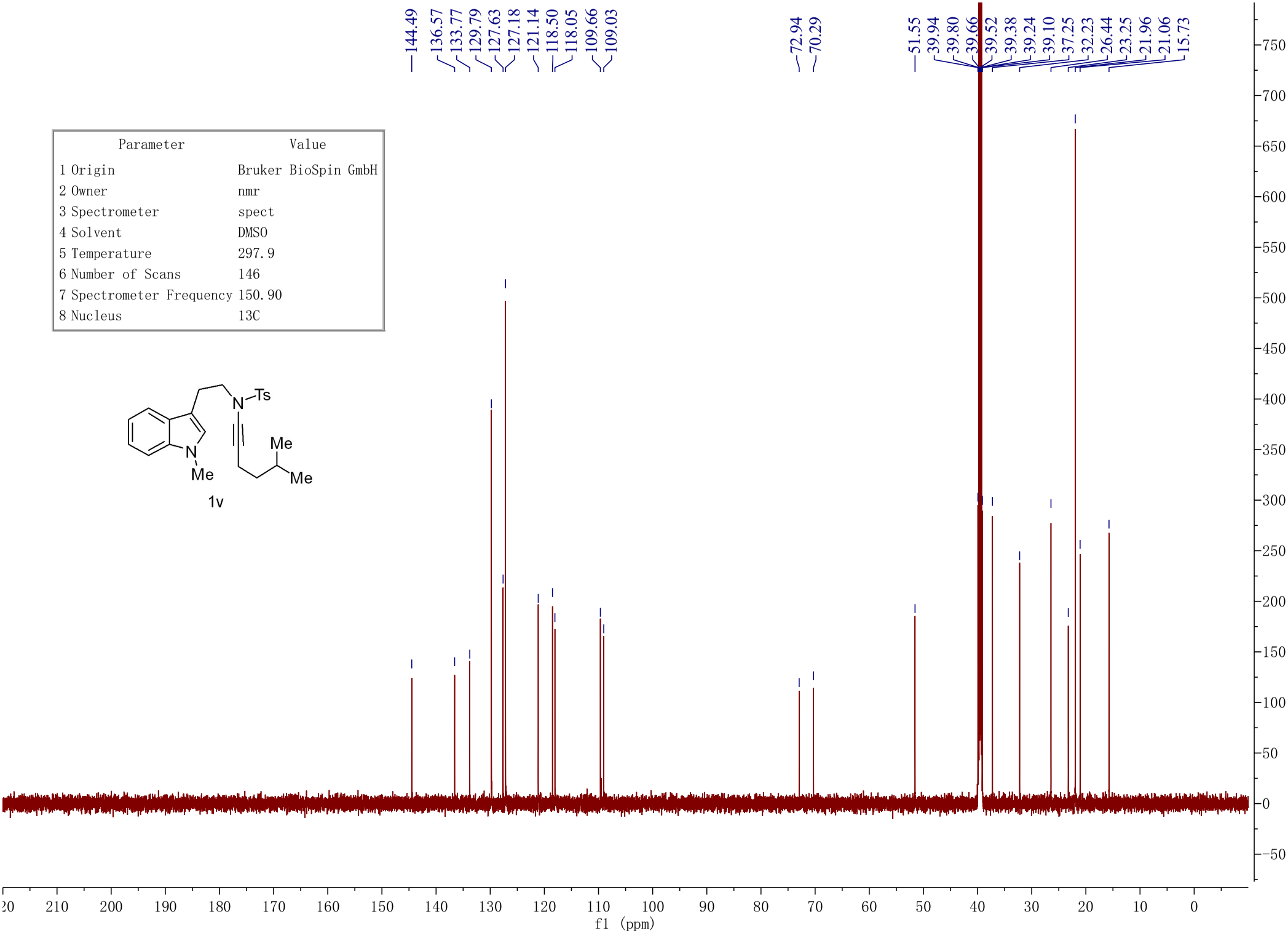


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

1v

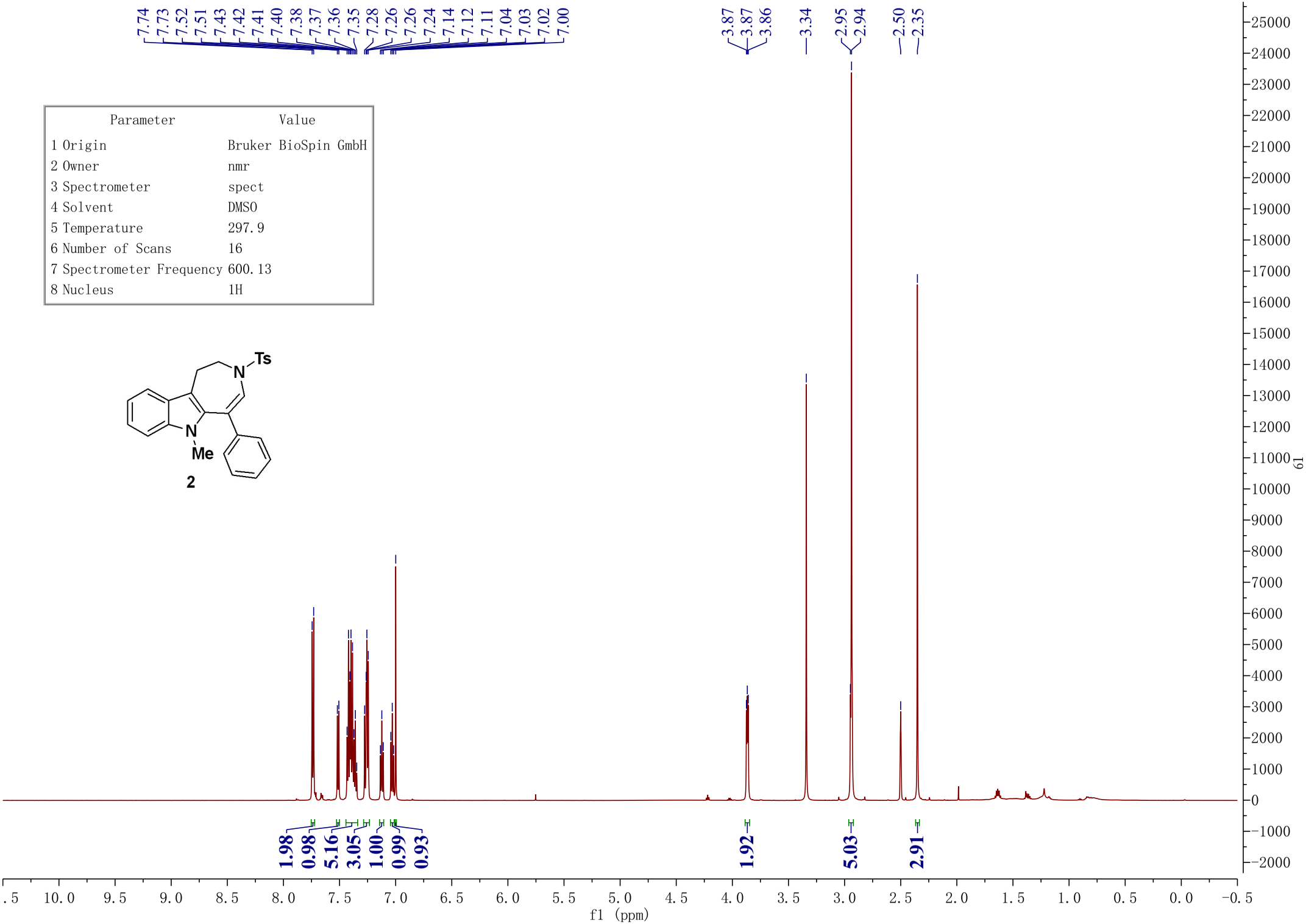
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	146
7 Spectrometer Frequency	150.90
8 Nucleus	13C

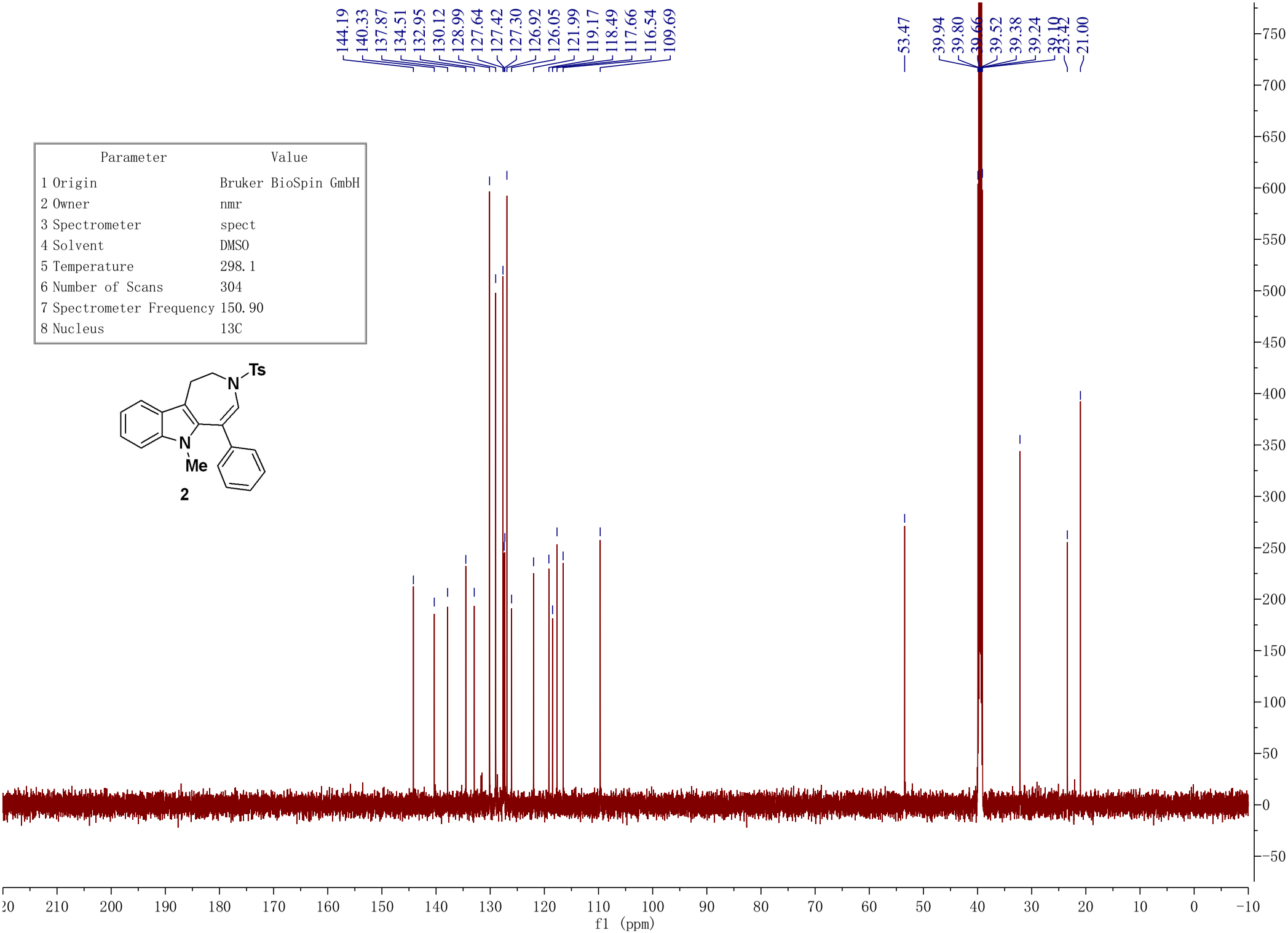
1v



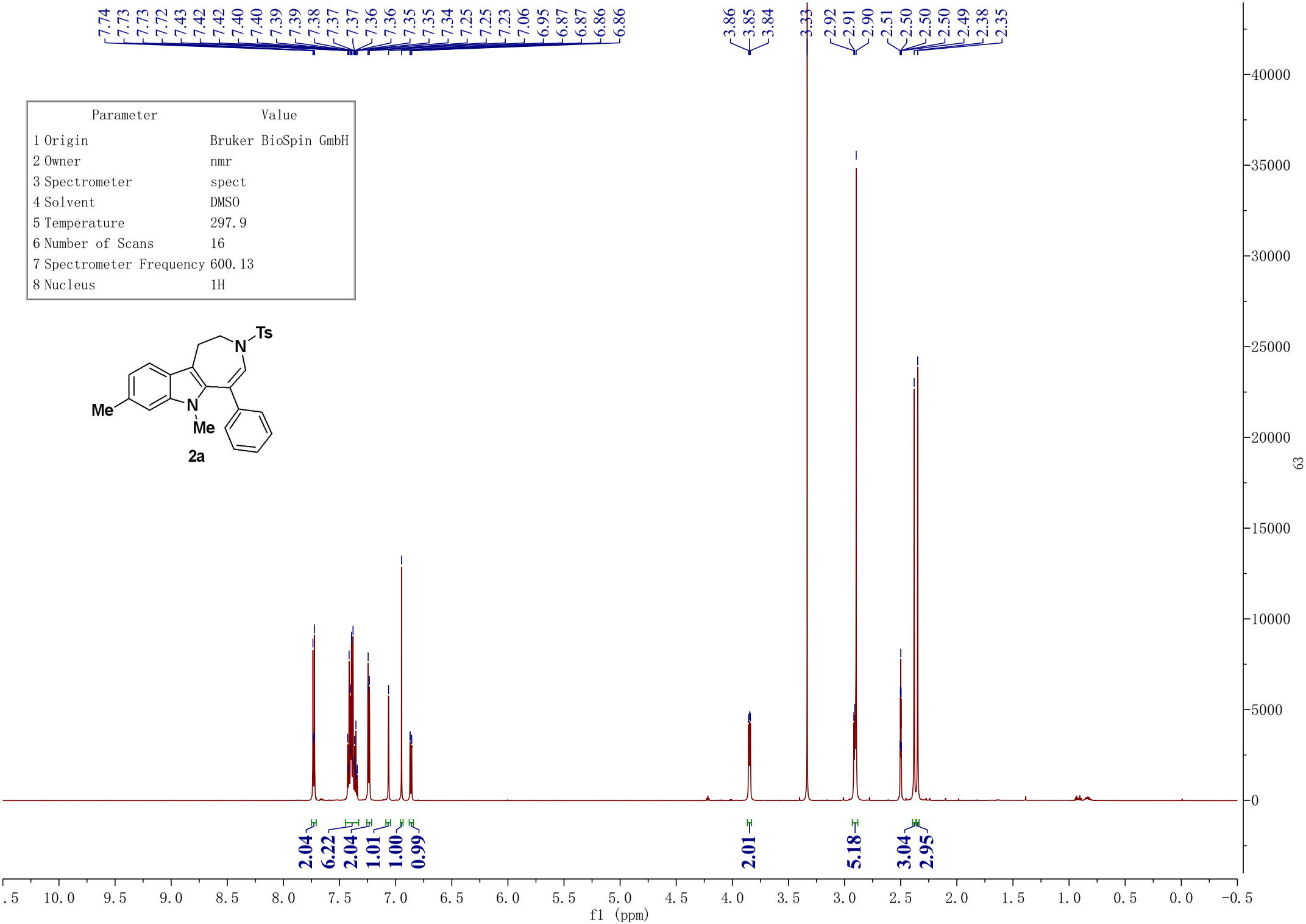
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

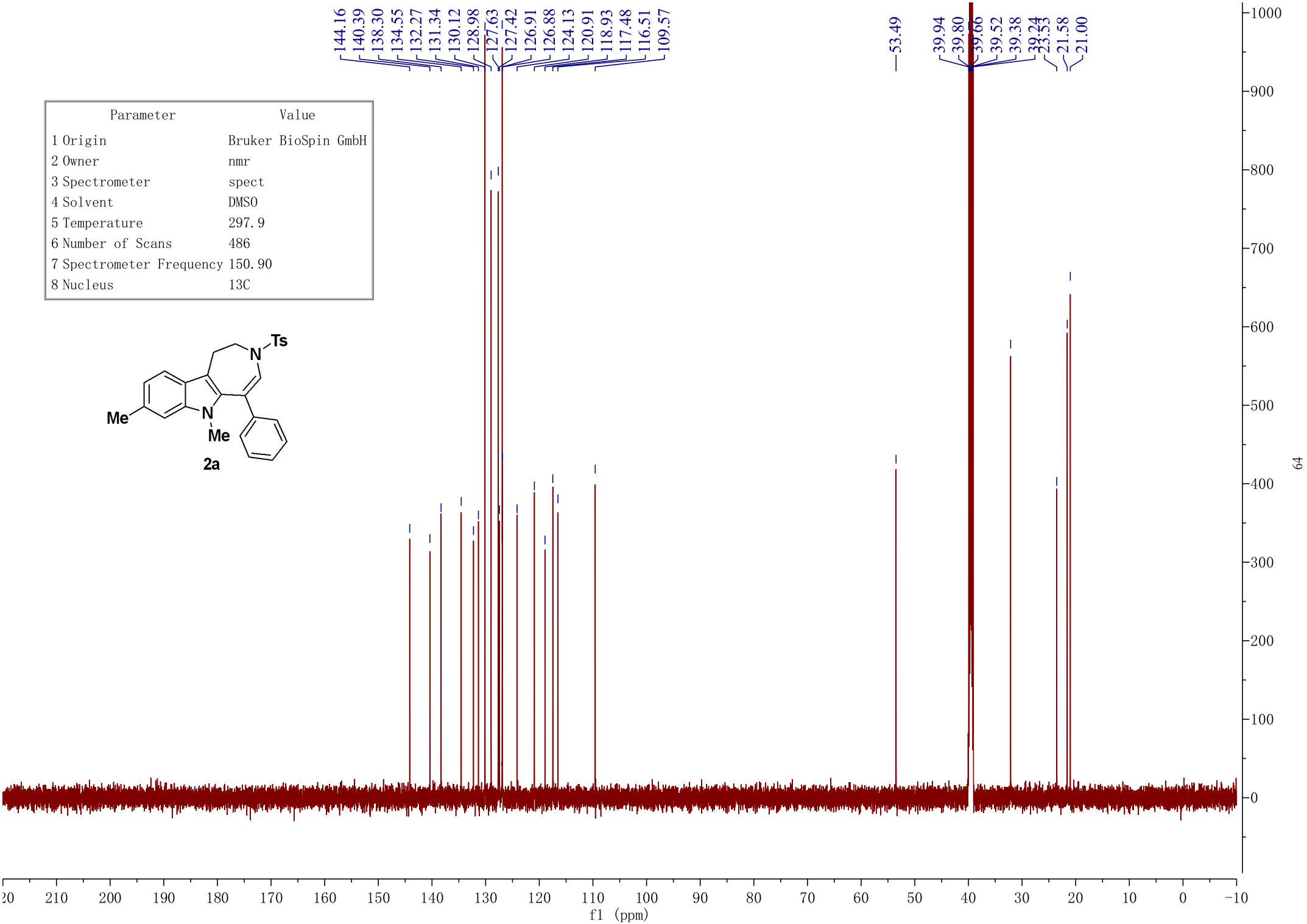
2



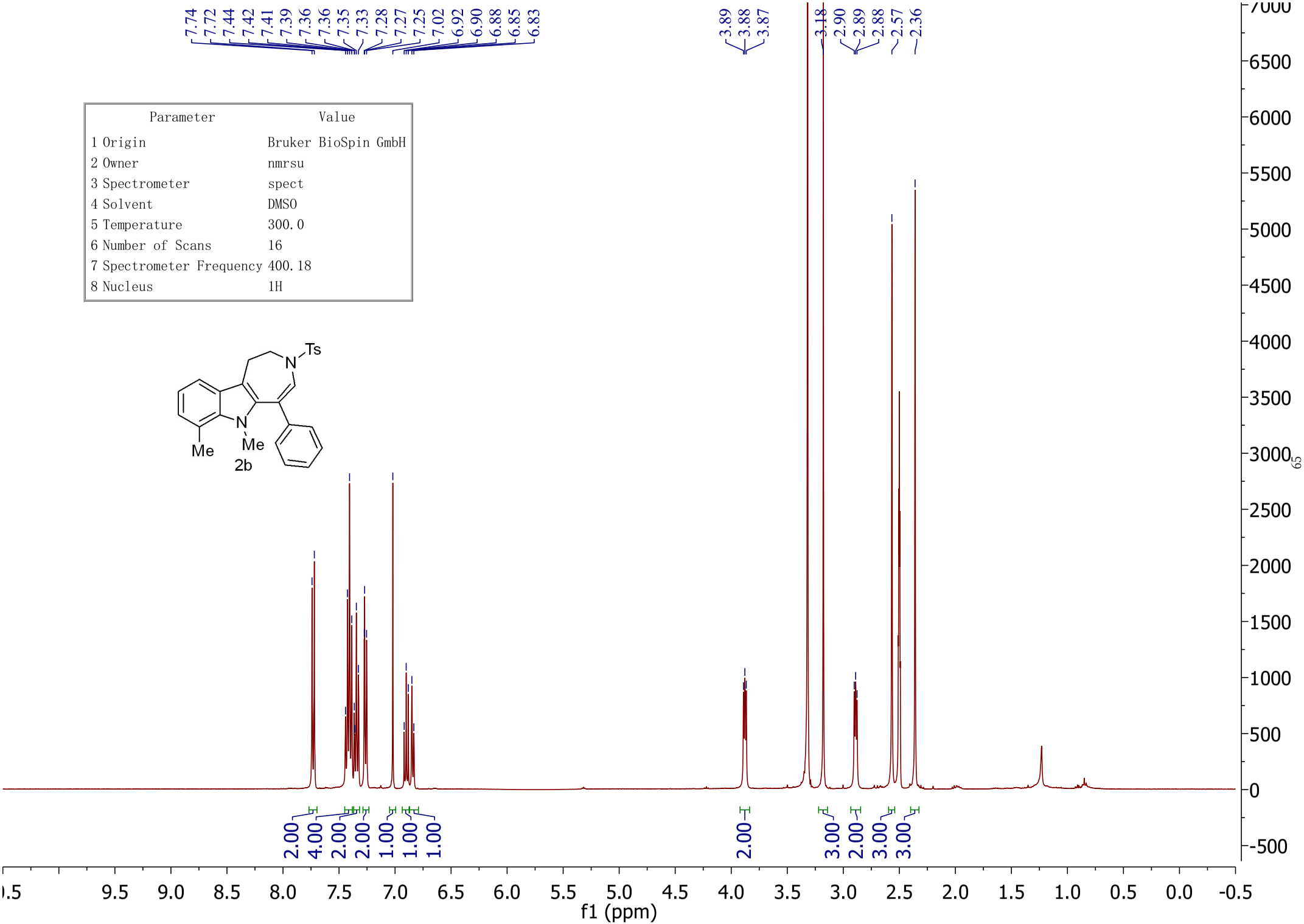


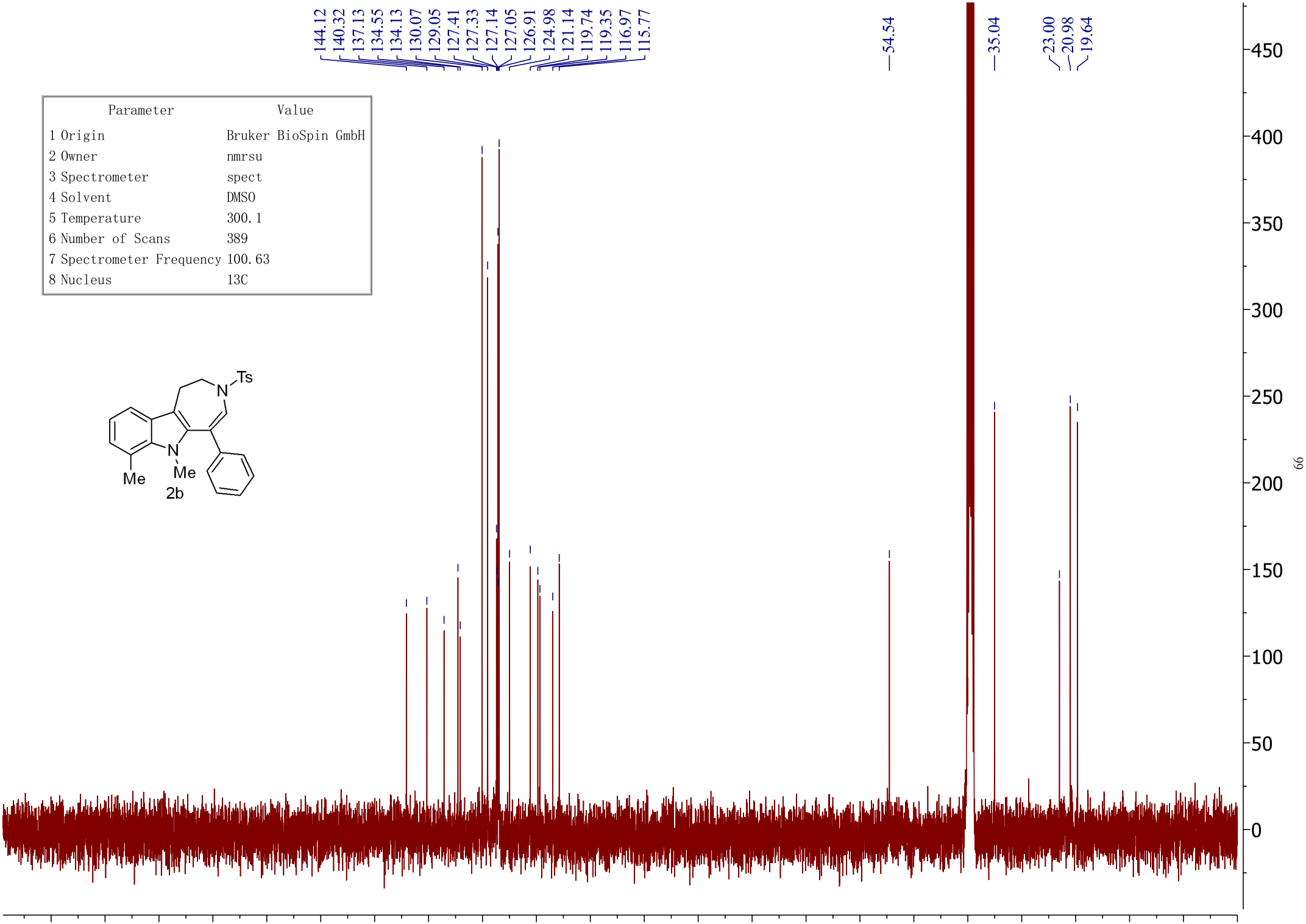
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.1
6 Number of Scans	304
7 Spectrometer Frequency	150.90
8 Nucleus	13C


7.74 7.73 7.73 7.72 7.43 7.42 7.42 7.40 7.40 7.39 7.39 7.38 7.37 7.37 7.36 7.36 7.35 7.35 7.34 7.25 7.25 7.23 7.06 6.95 6.87 6.87 6.86 6.86
3.86 3.85 3.84 3.33 2.92 2.91 2.90 2.51 2.50 2.50 2.50 2.49 2.38 2.35
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Ts
N
Me
N
Me
2a
2.04 6.22 2.04 1.01 1.00 0.99 2.01 5.18 3.04 2.95
f1 (ppm)

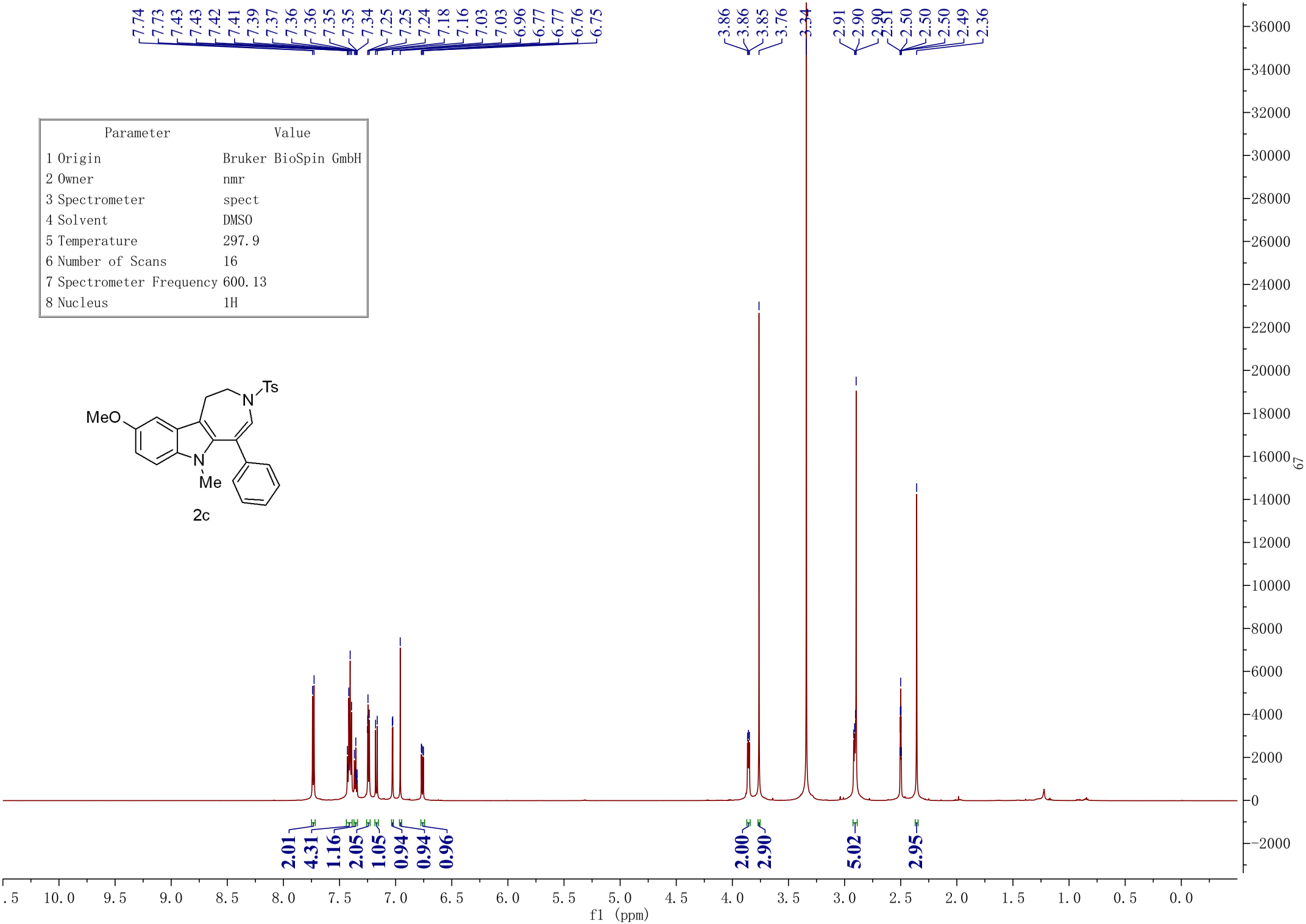


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	486
7 Spectrometer Frequency	150.90
8 Nucleus	13C

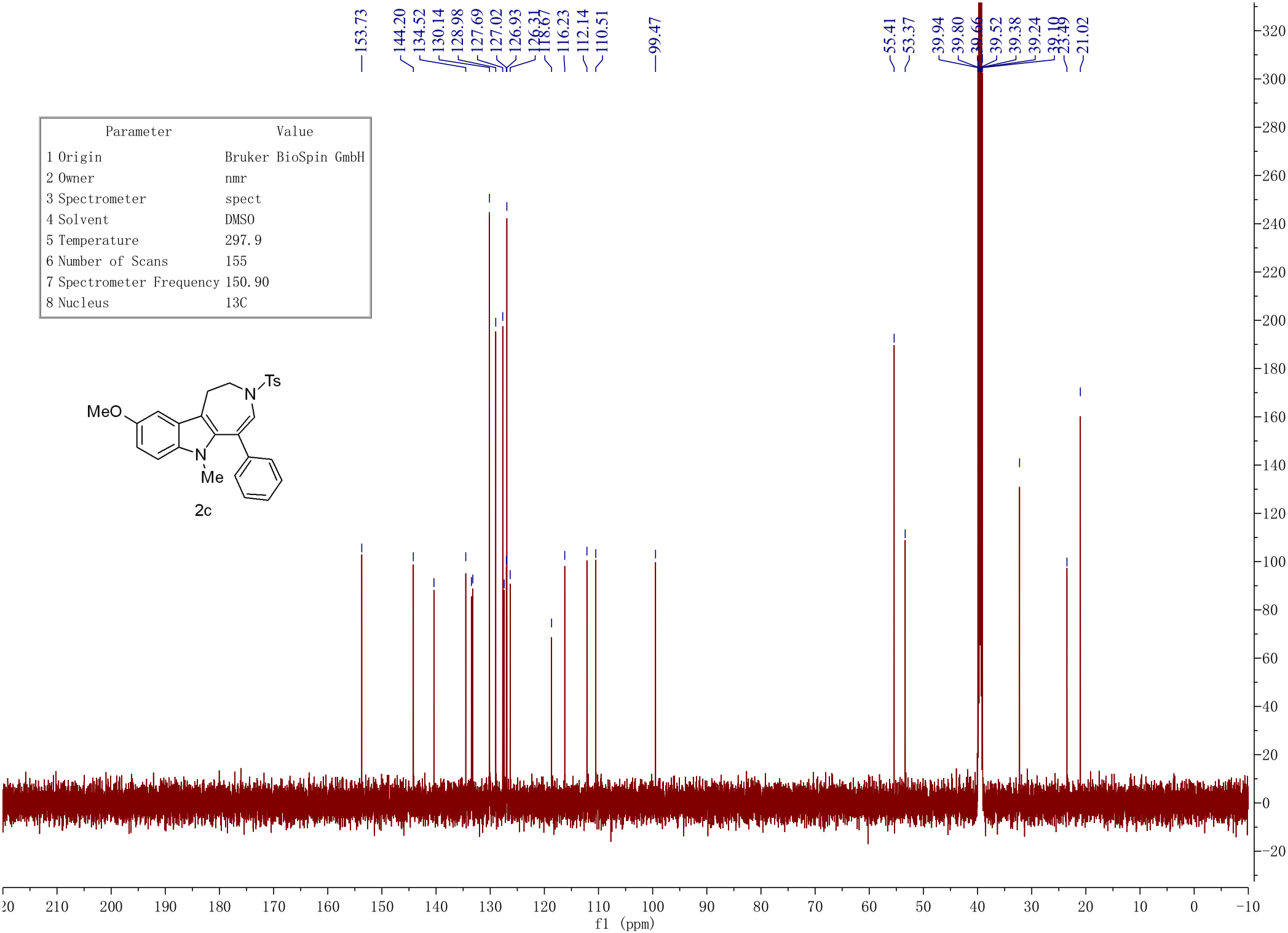

7.74
7.72
7.44
7.42
7.41
7.39
7.36
7.36
7.35
7.33
7.28
7.27
7.25
7.02
6.92
6.90
6.88
6.85
6.83
3.89
3.88
3.87
3.18
2.90
2.89
2.88
2.57
2.36
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 400.18
8 Nucleus 1H
Ts
N
N
Me
Me
2b
2.00
4.00
2.00
2.00
1.00
1.00
1.00
2.00
3.00
2.00
3.00
3.00
f1 (ppm)



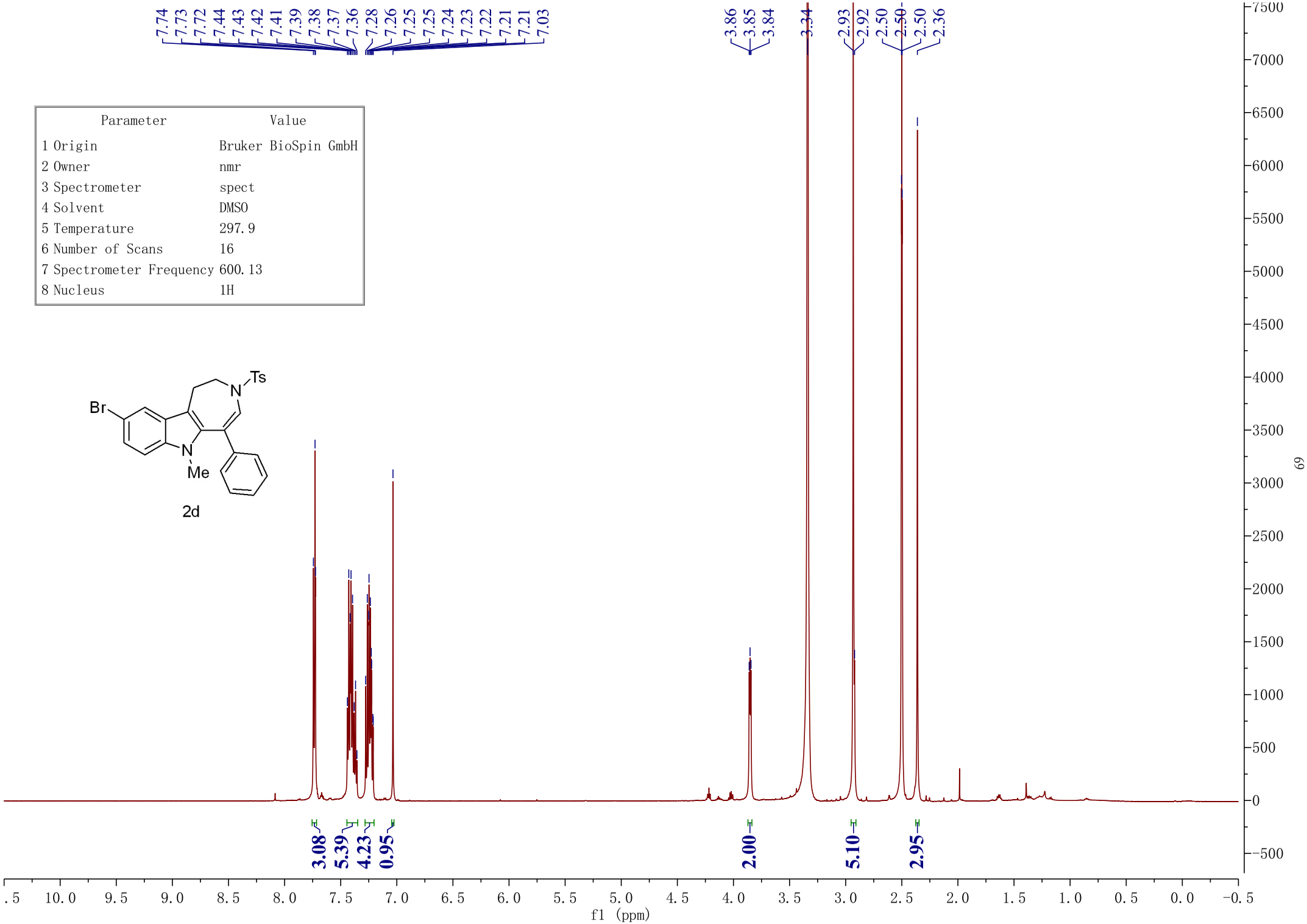
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.1
6 Number of Scans	389
7 Spectrometer Frequency	100.63
8 Nucleus	13C

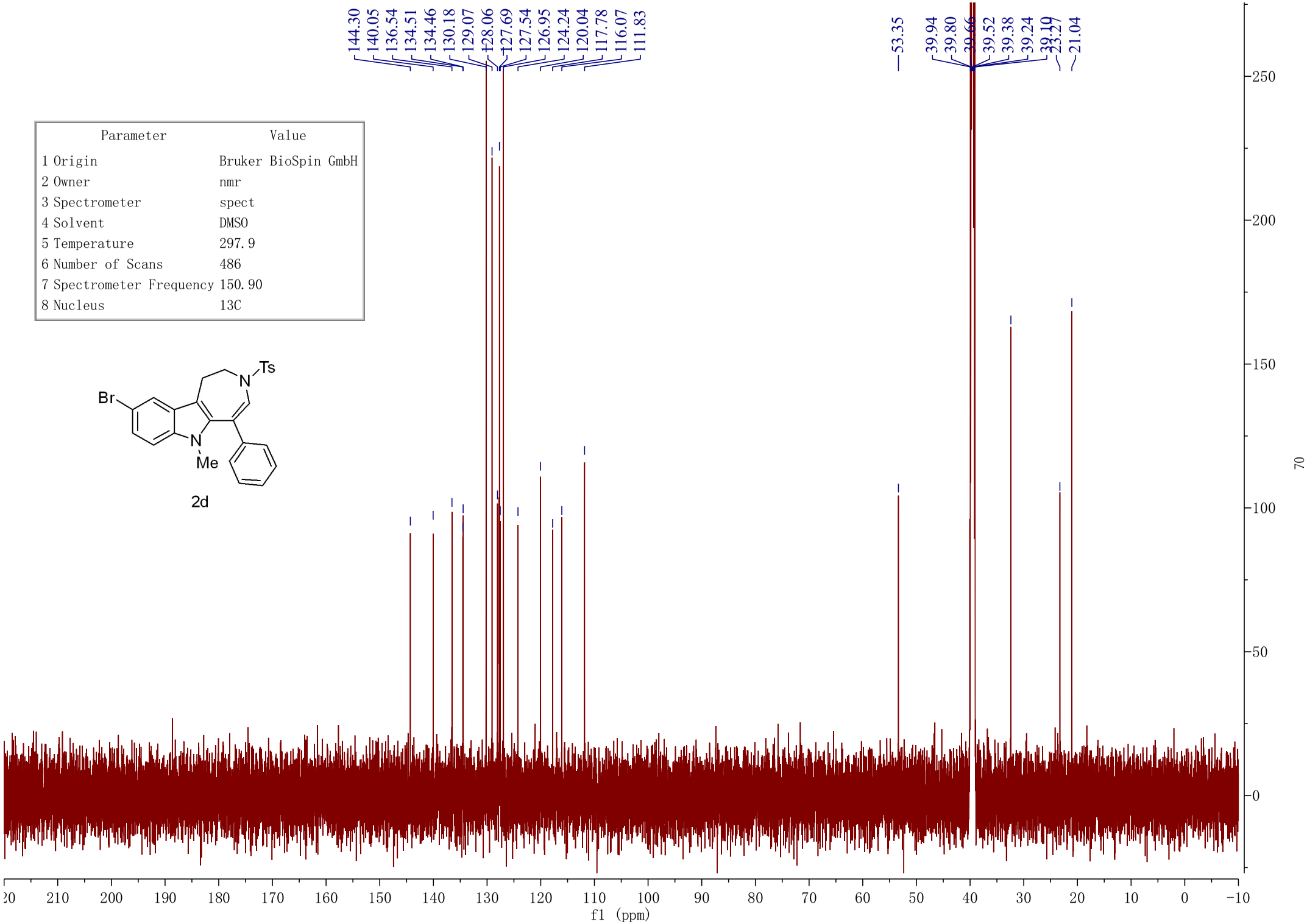


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H



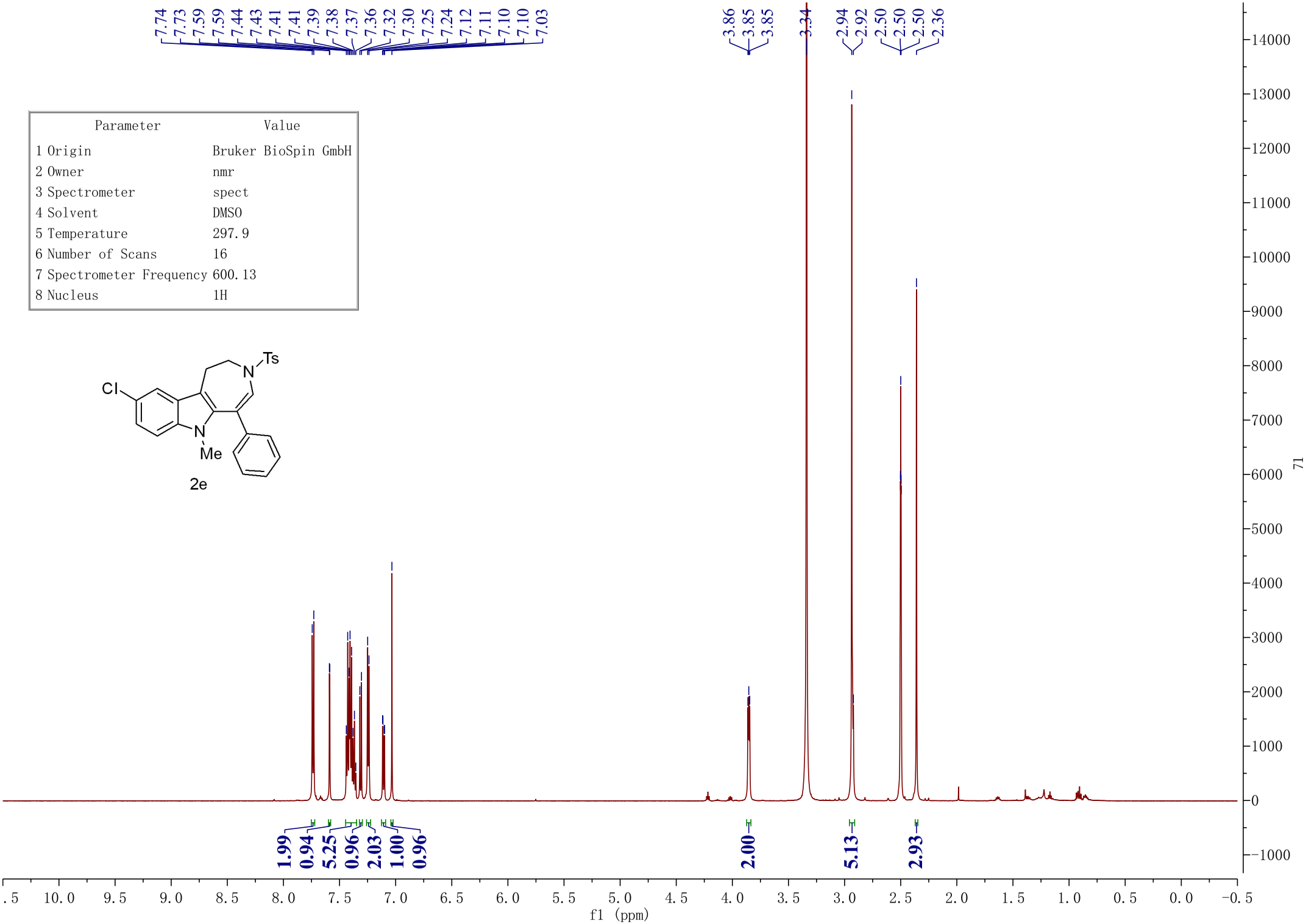
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	155
7 Spectrometer Frequency	150.90
8 Nucleus	13C

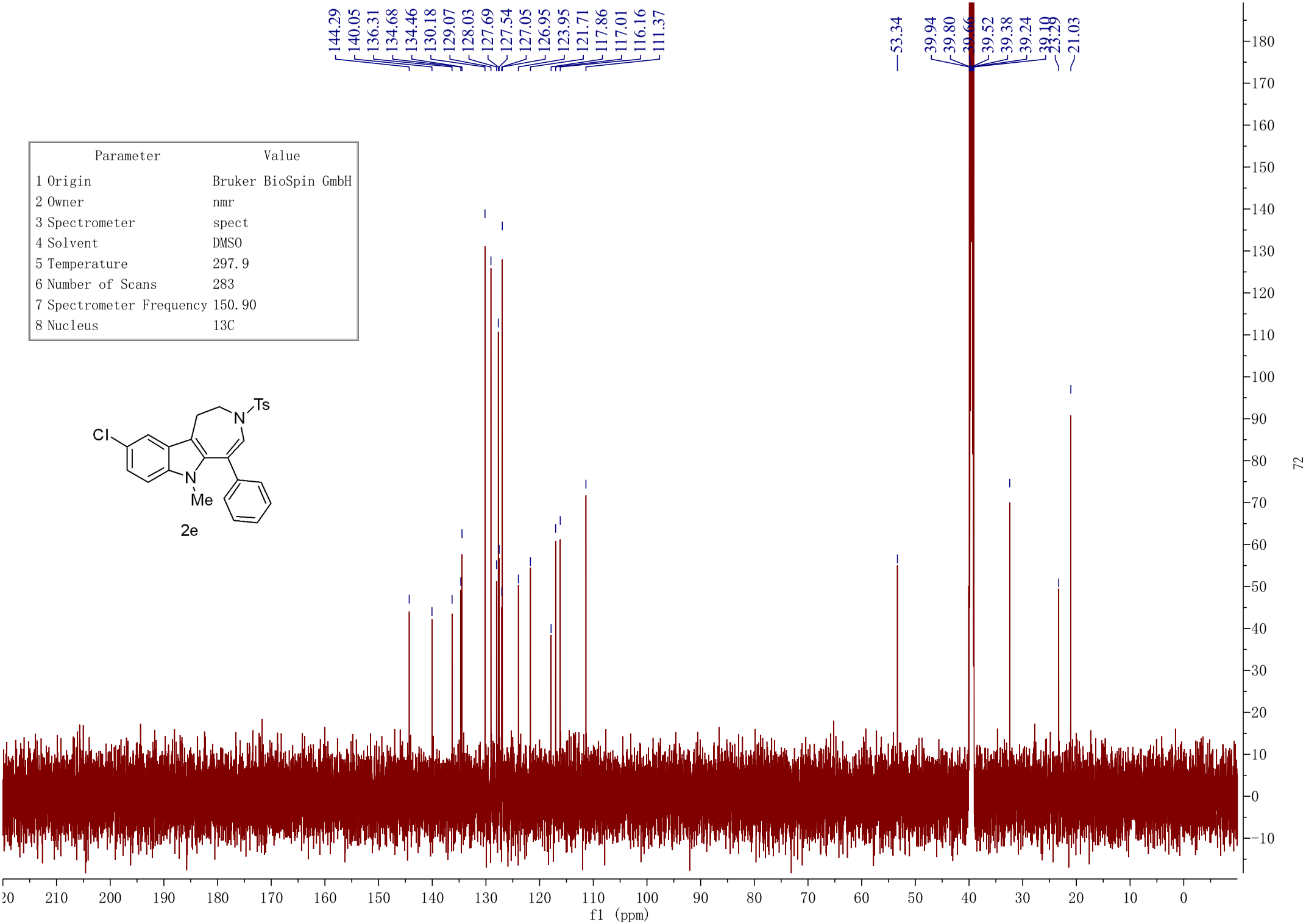

7.74
7.73
7.72
7.44
7.43
7.42
7.41
7.39
7.38
7.37
7.36
7.28
7.26
7.25
7.25
7.24
7.23
7.22
7.21
7.21
7.03
3.86
3.85
3.84
3.34
2.93
2.92
2.50
2.50
2.50
2.36
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Br
N
Ts
N
Me
2d
3.08
5.39
4.23
0.95
2.00
5.10
2.95
f1 (ppm)

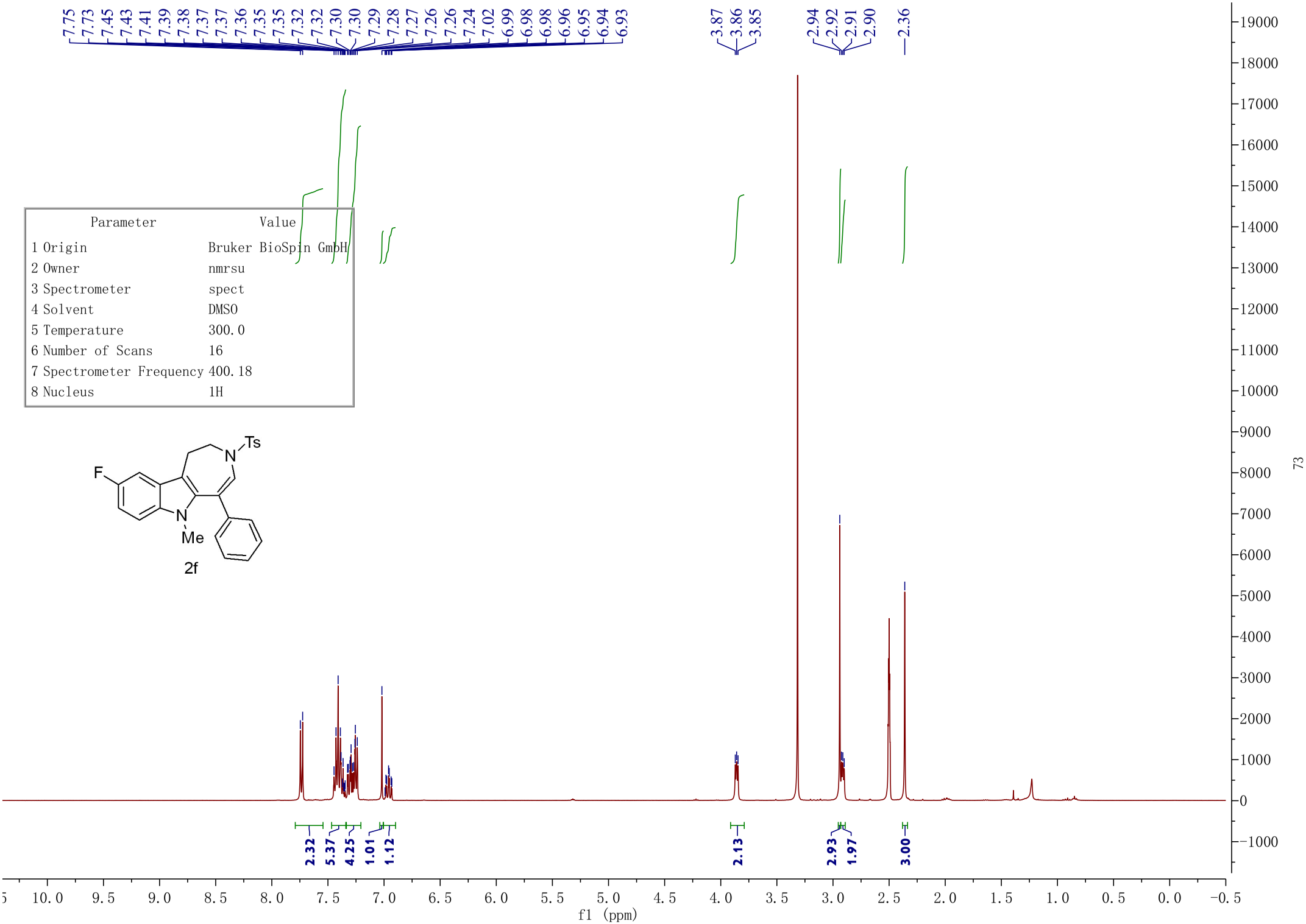

144.30
140.05
136.54
134.51
134.46
130.18
129.07
128.06
127.69
127.54
126.95
124.24
120.04
117.78
116.07
111.83
53.35
39.94
39.80
39.66
39.52
39.38
39.24
39.10
23.27
21.04
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 486
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Br
N
Ts
N
Me
2d
f1 (ppm)

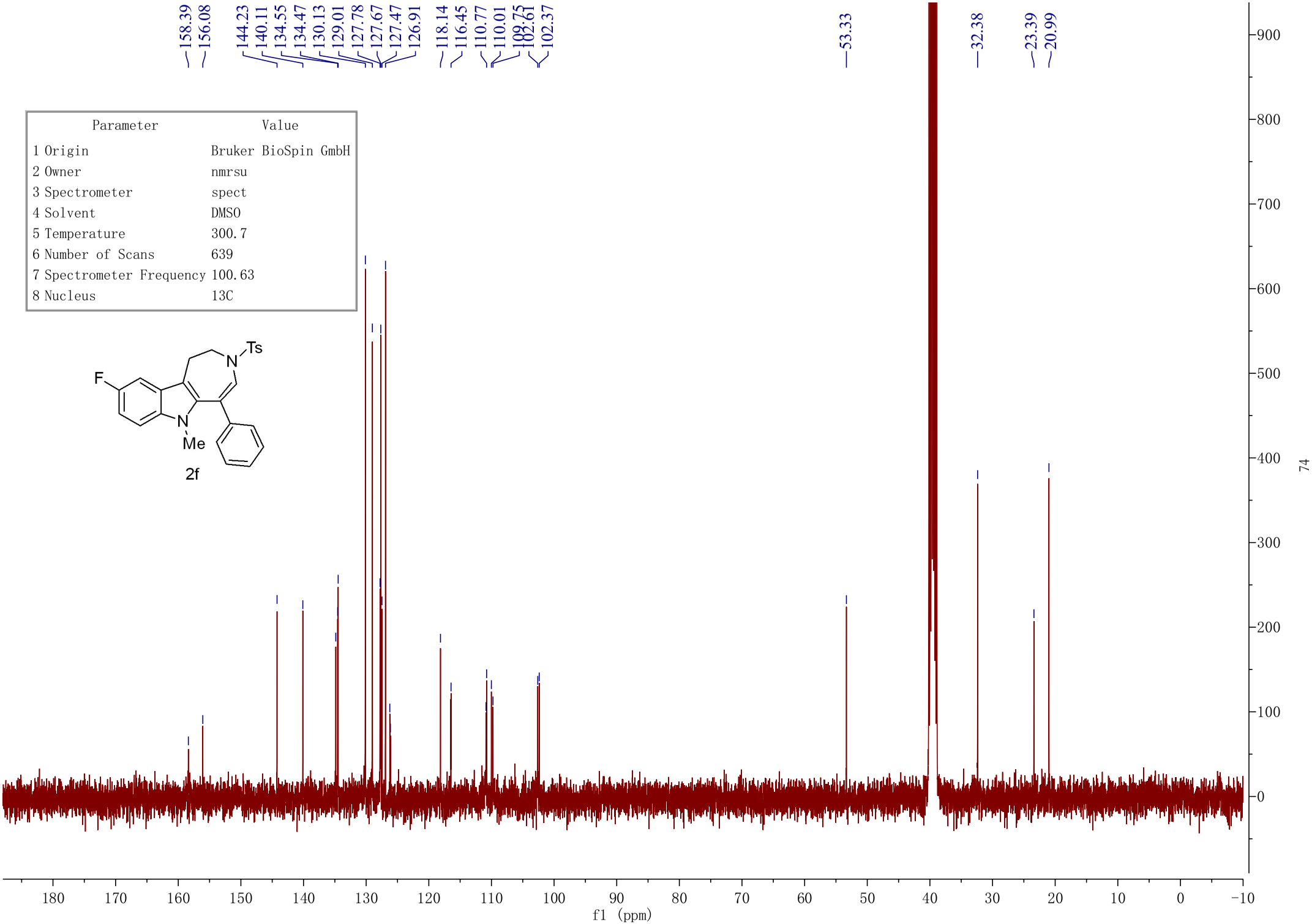
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

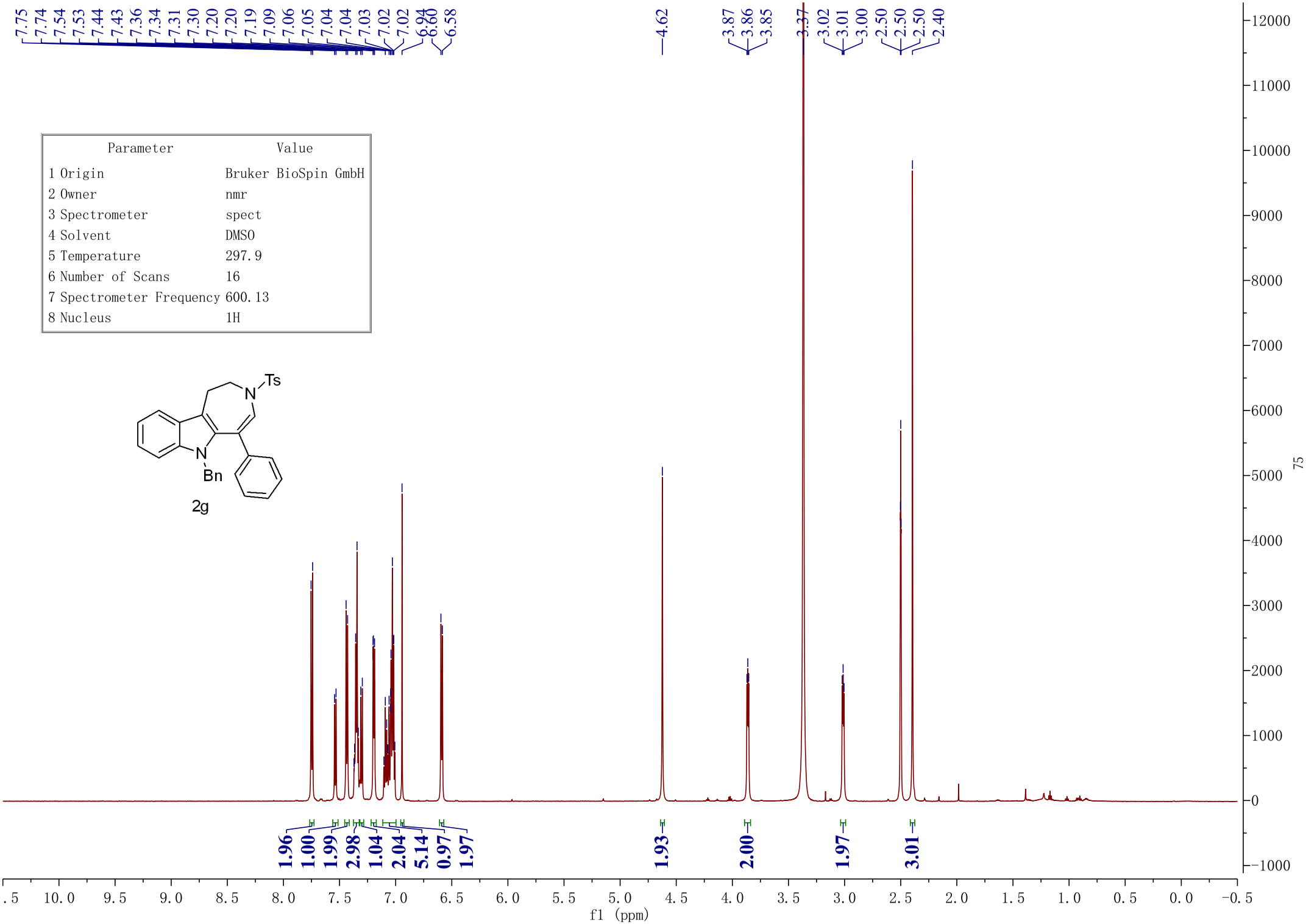
2e




144.29
140.05
136.31
134.68
134.46
130.18
129.07
128.03
127.69
127.54
127.05
126.95
123.95
121.71
117.86
117.01
116.16
111.37
53.34
39.94
39.80
39.66
39.52
39.38
39.24
39.10
23.29
21.03
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 283
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Cl
N
Ts
N
Me
2e
f1 (ppm)
72

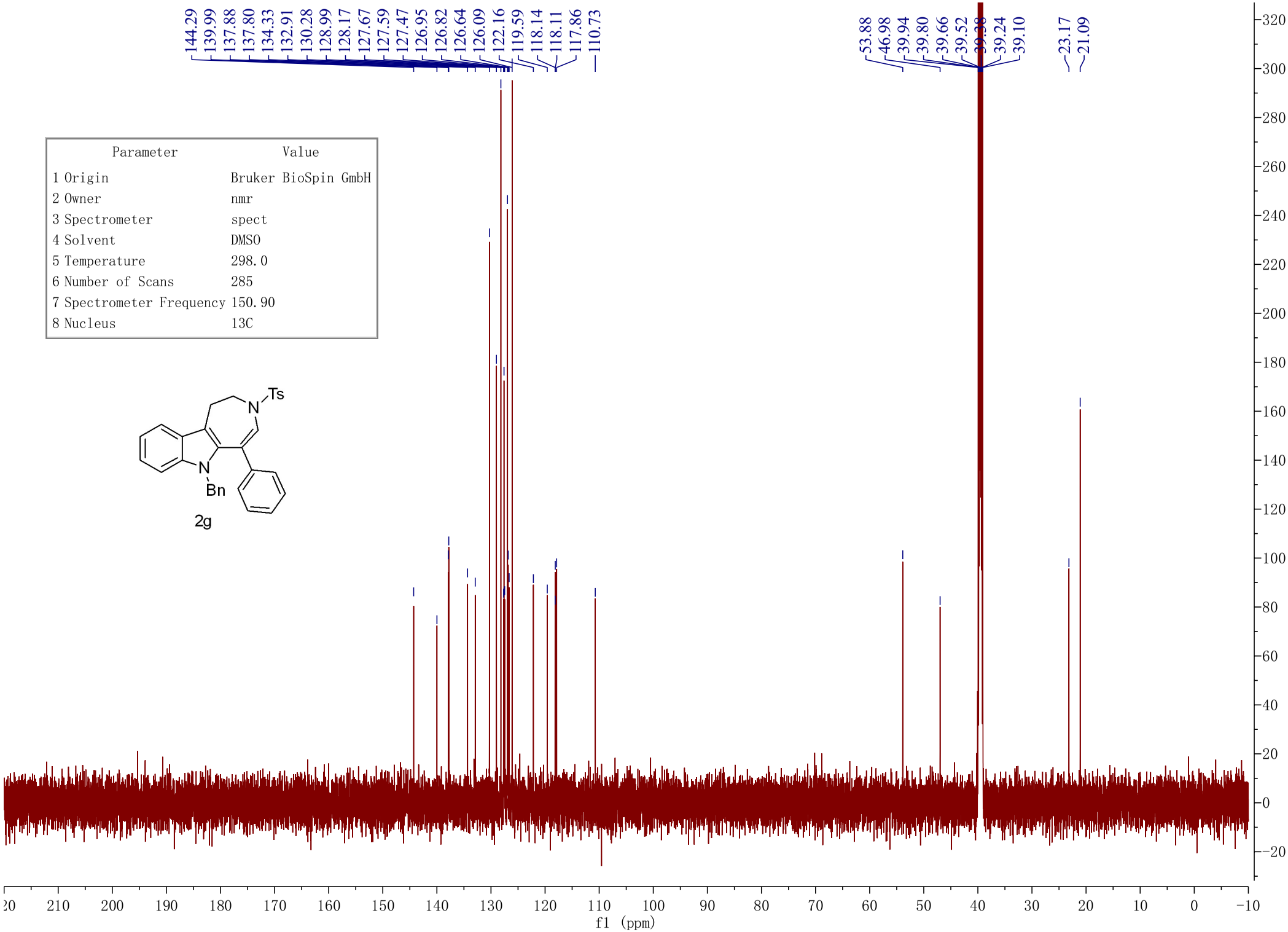

7.75 7.73 7.45 7.43 7.41 7.39 7.38 7.37 7.37 7.36 7.35 7.35 7.32 7.32 7.30 7.30 7.29 7.28 7.27 7.26 7.26 7.24 7.02 6.99 6.98 6.98 6.96 6.95 6.94 6.93
3.87 3.86 3.85
2.94 2.92 2.91 2.90
2.36
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 400.18
8 Nucleus 1H
F
N
Ts
N
Me
2f
2.32
5.37
4.25
1.01
1.12
2.13
2.93
1.97
3.00
f1 (ppm)


158.39
156.08
144.23
140.11
134.55
134.47
130.13
129.01
127.78
127.67
127.47
126.91
118.14
116.45
110.77
110.01
109.75
102.61
102.37
53.33
32.38
23.39
20.99
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.7
6 Number of Scans 639
7 Spectrometer Frequency 100.63
8 Nucleus 13C
F
N
Ts
N
Me
2f
f1 (ppm)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

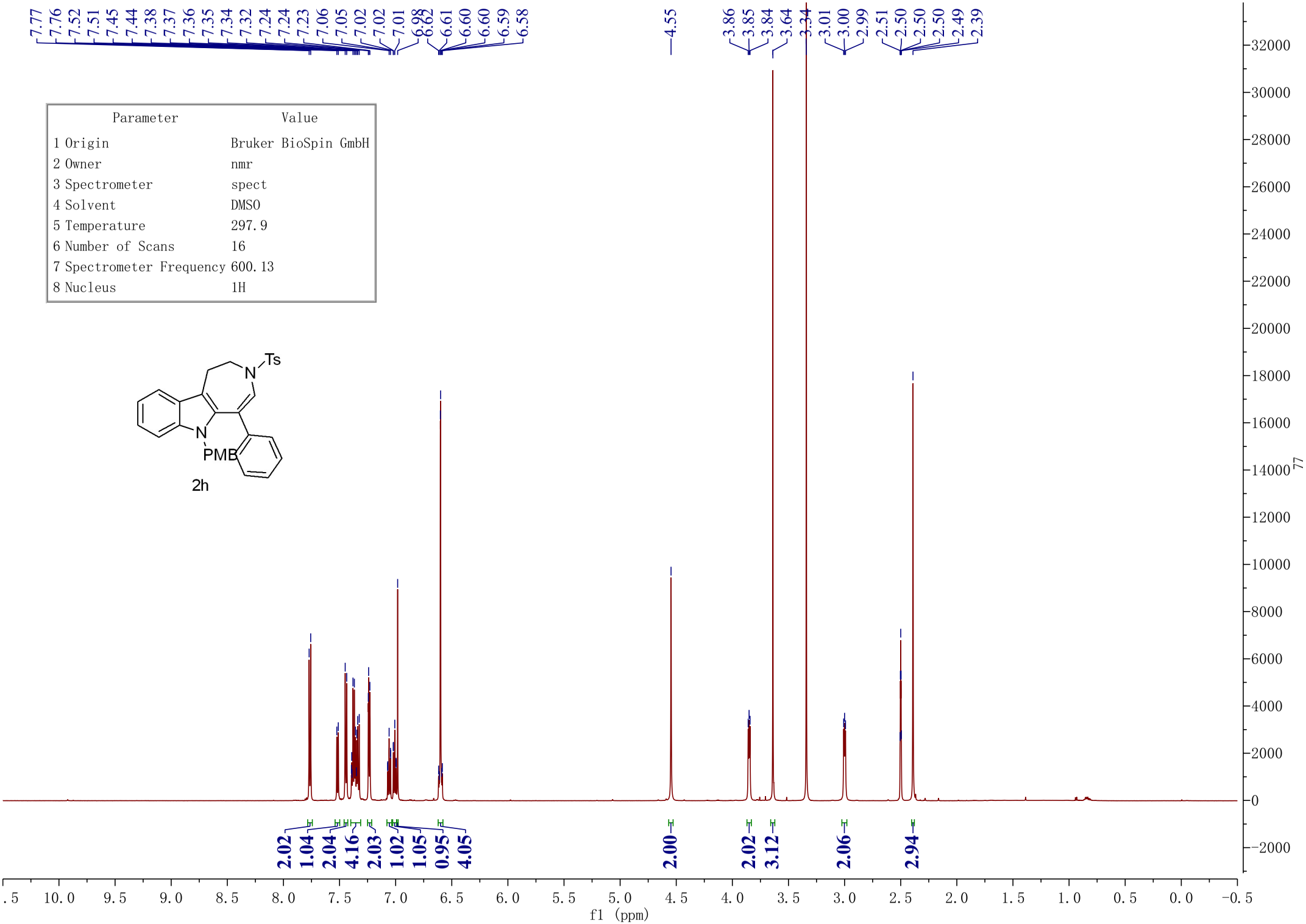
2g

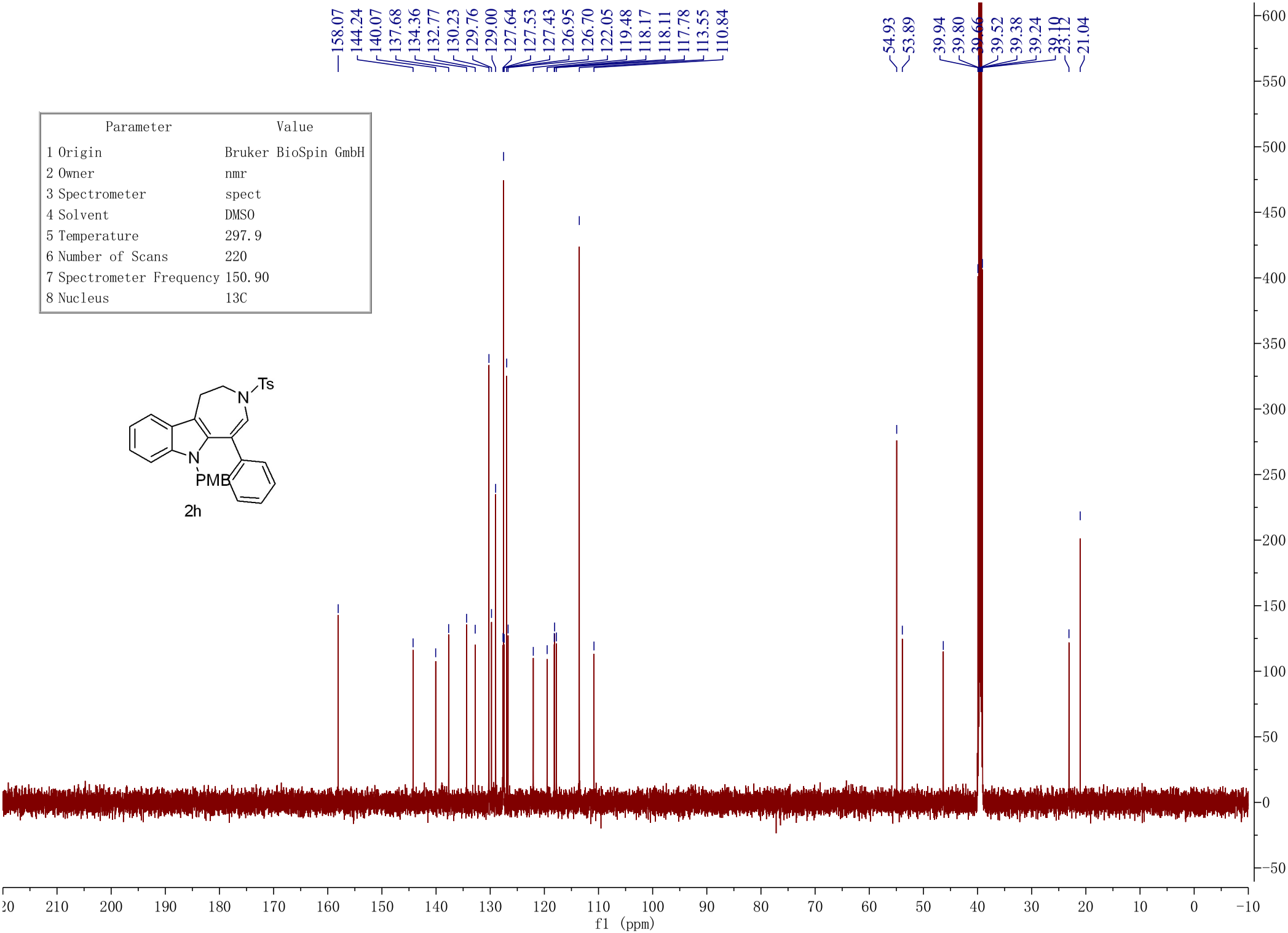


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.0
6 Number of Scans	285
7 Spectrometer Frequency	150.90
8 Nucleus	13C

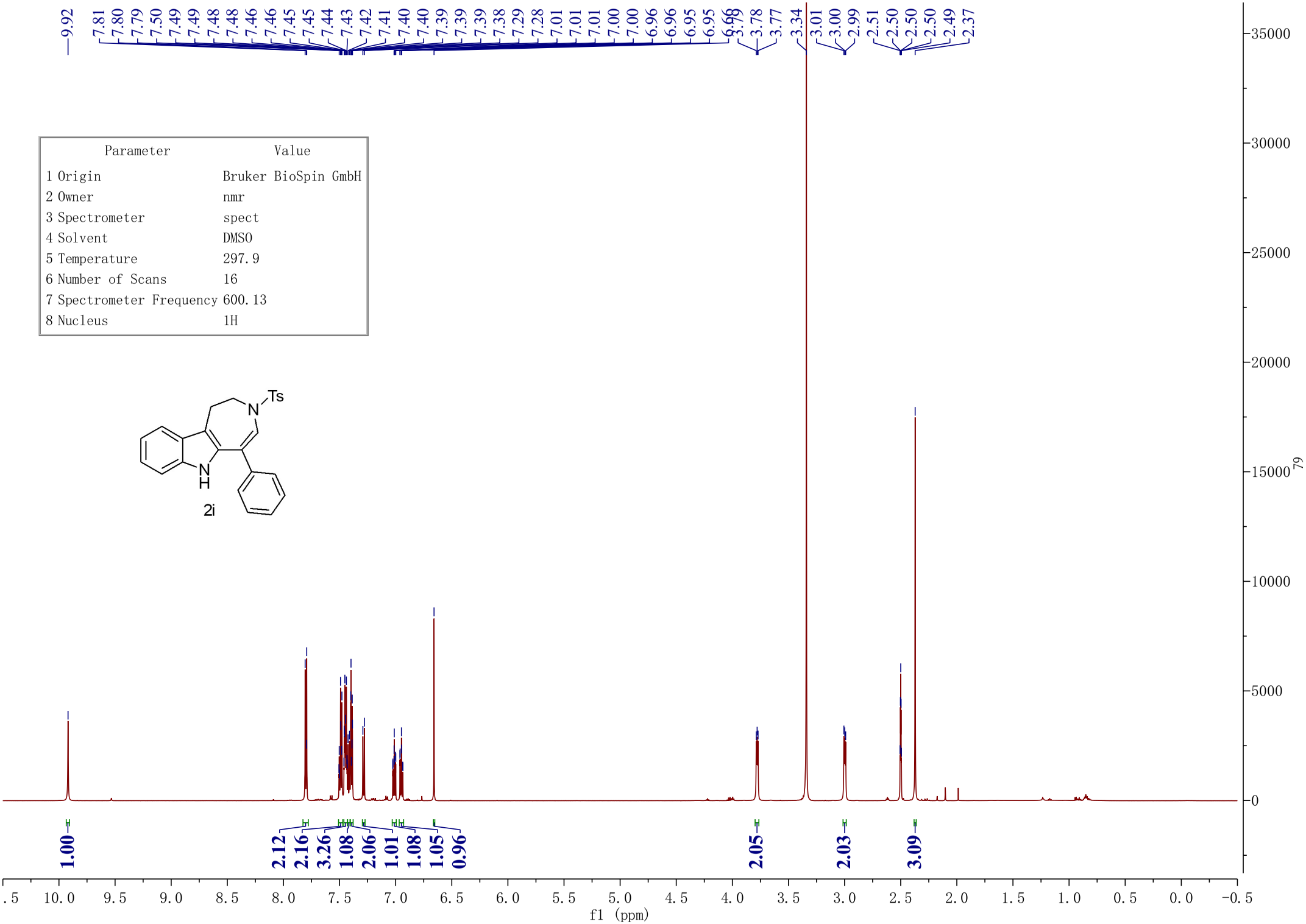
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

2h

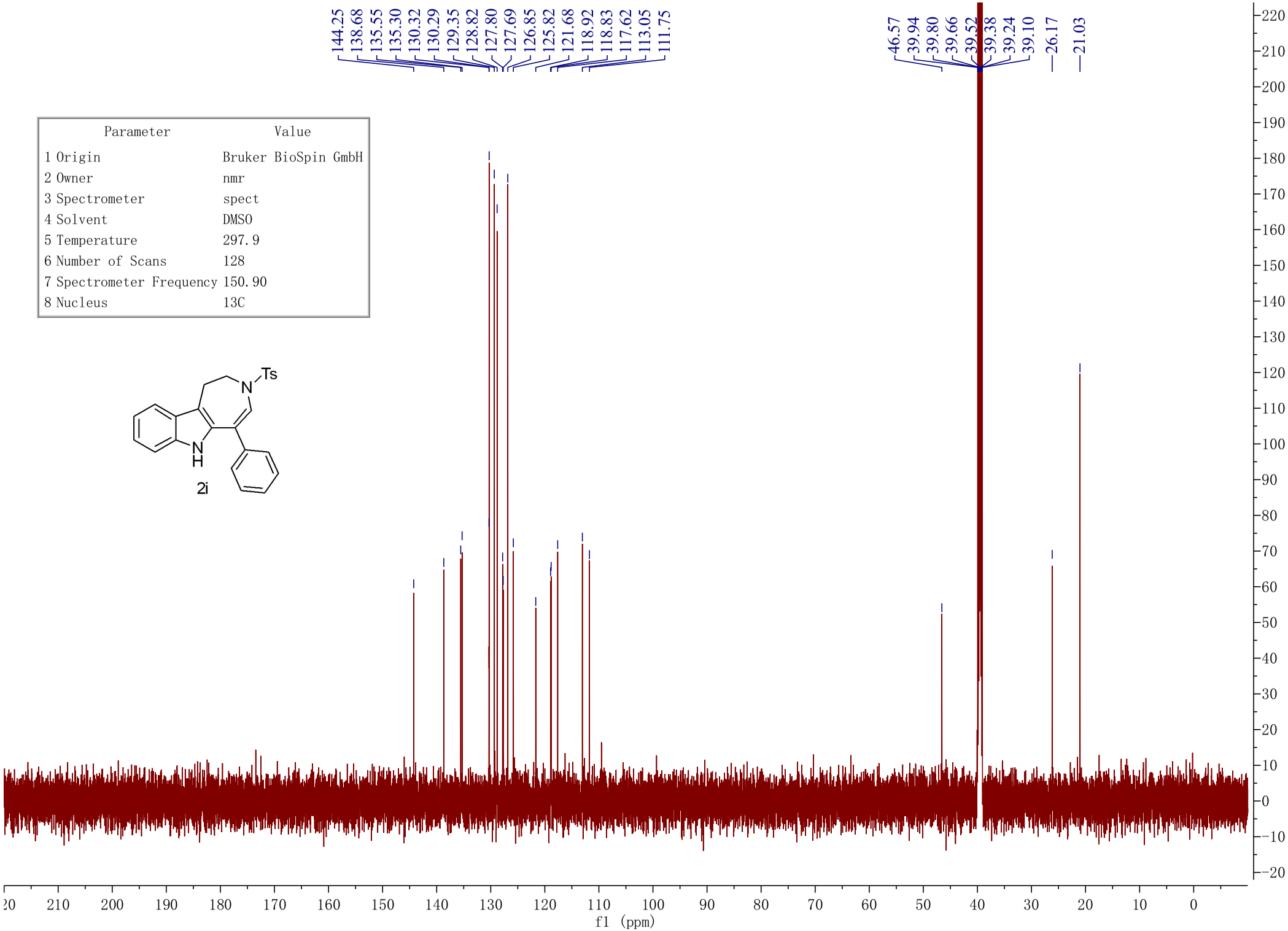


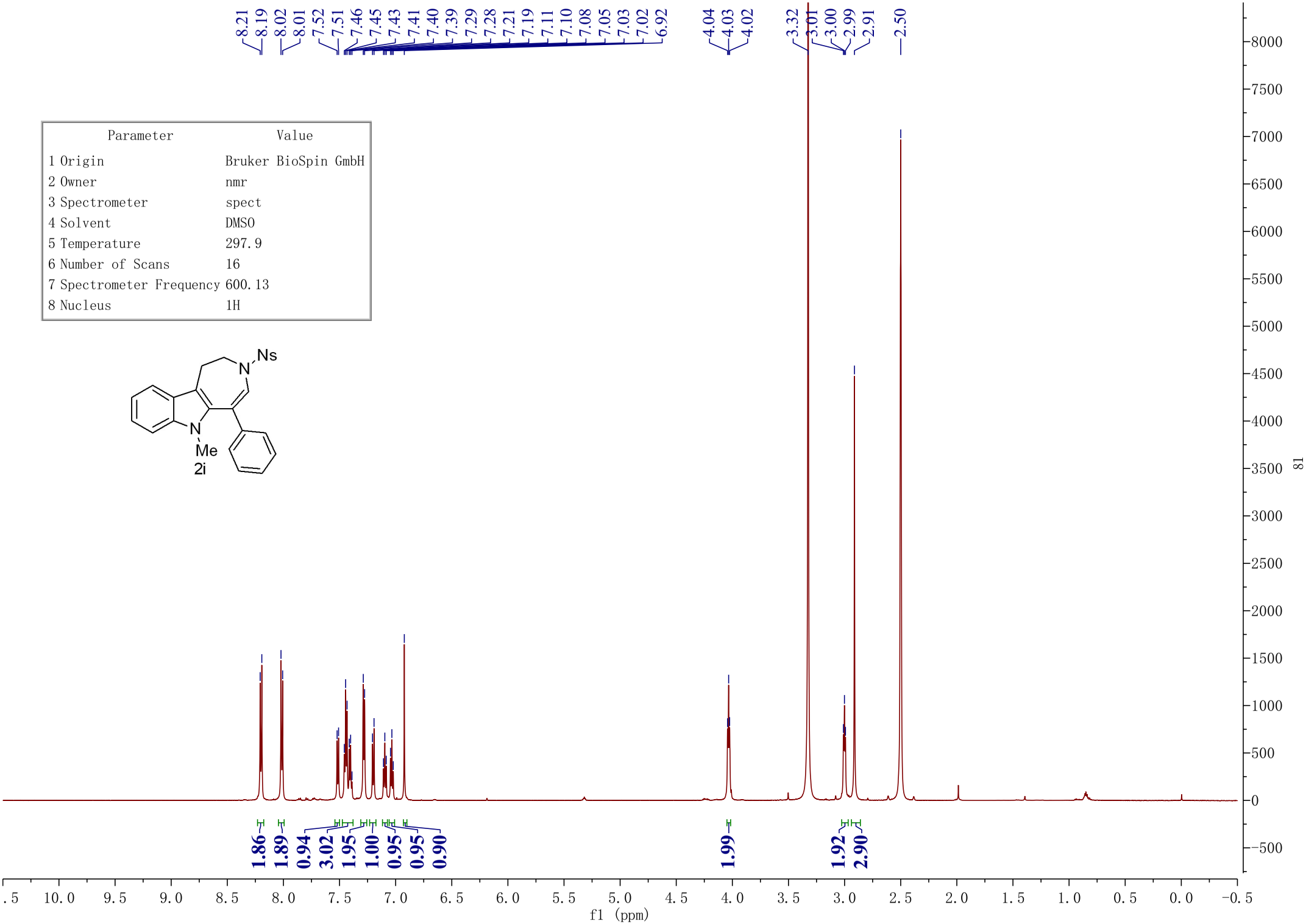


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	220
7 Spectrometer Frequency	150.90
8 Nucleus	13C

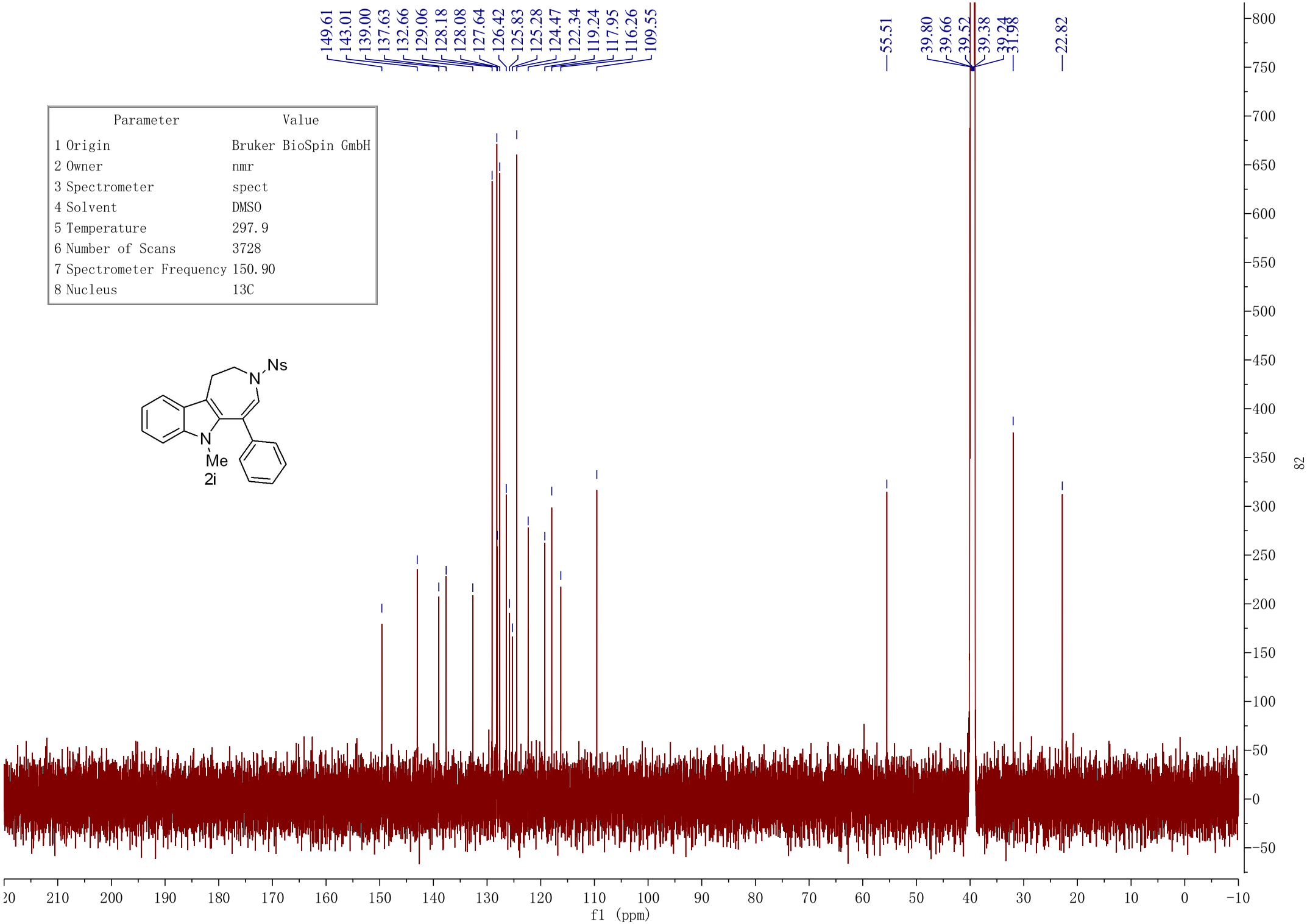


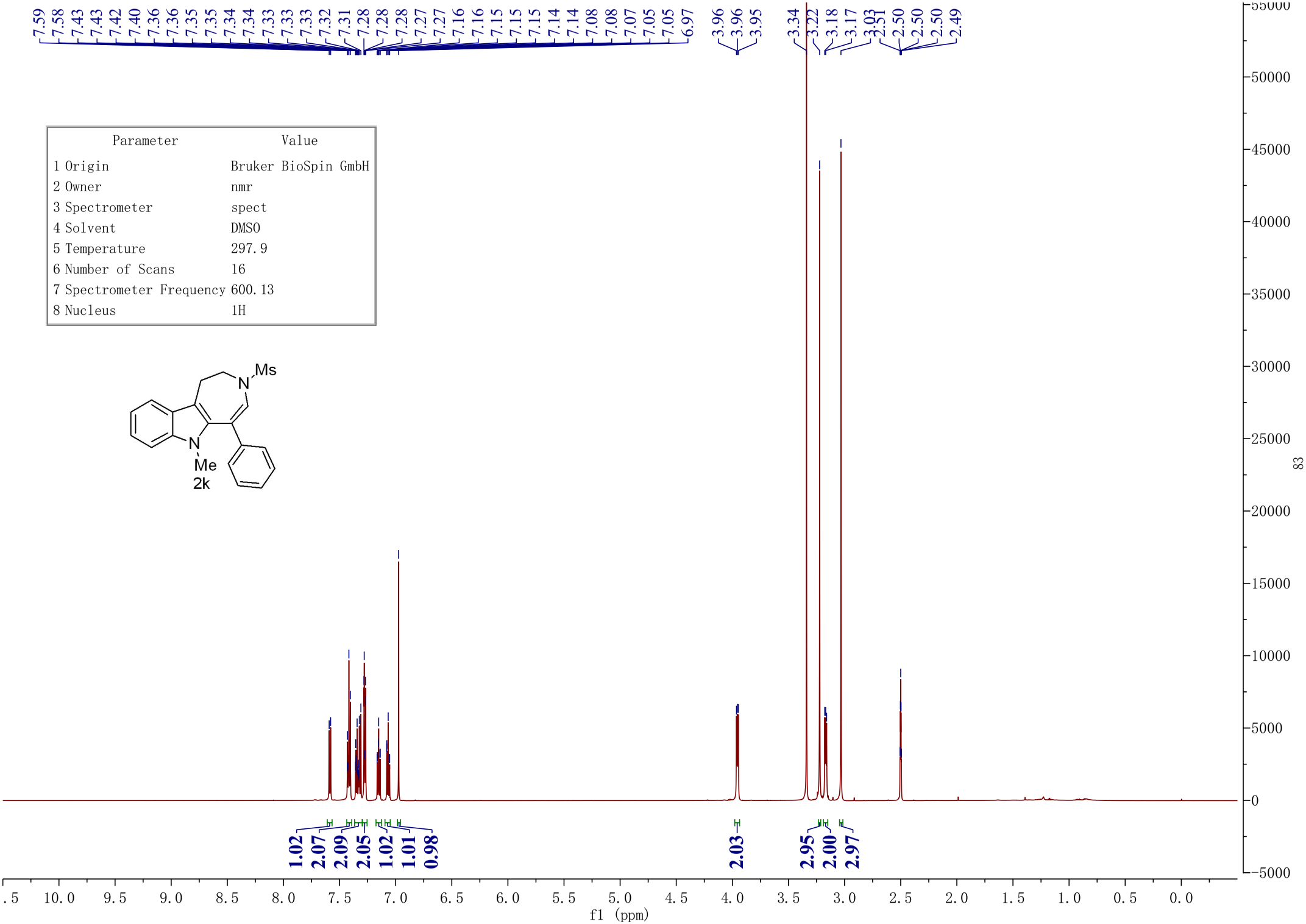
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H


144.25
138.68
135.55
135.30
130.32
130.29
129.35
128.82
127.80
127.69
126.85
125.82
121.68
118.92
118.83
117.62
113.05
111.75
46.57
39.94
39.80
39.66
39.52
39.38
39.24
39.10
26.17
21.03
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 128
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Ts
N
N
H
2i
f1 (ppm)



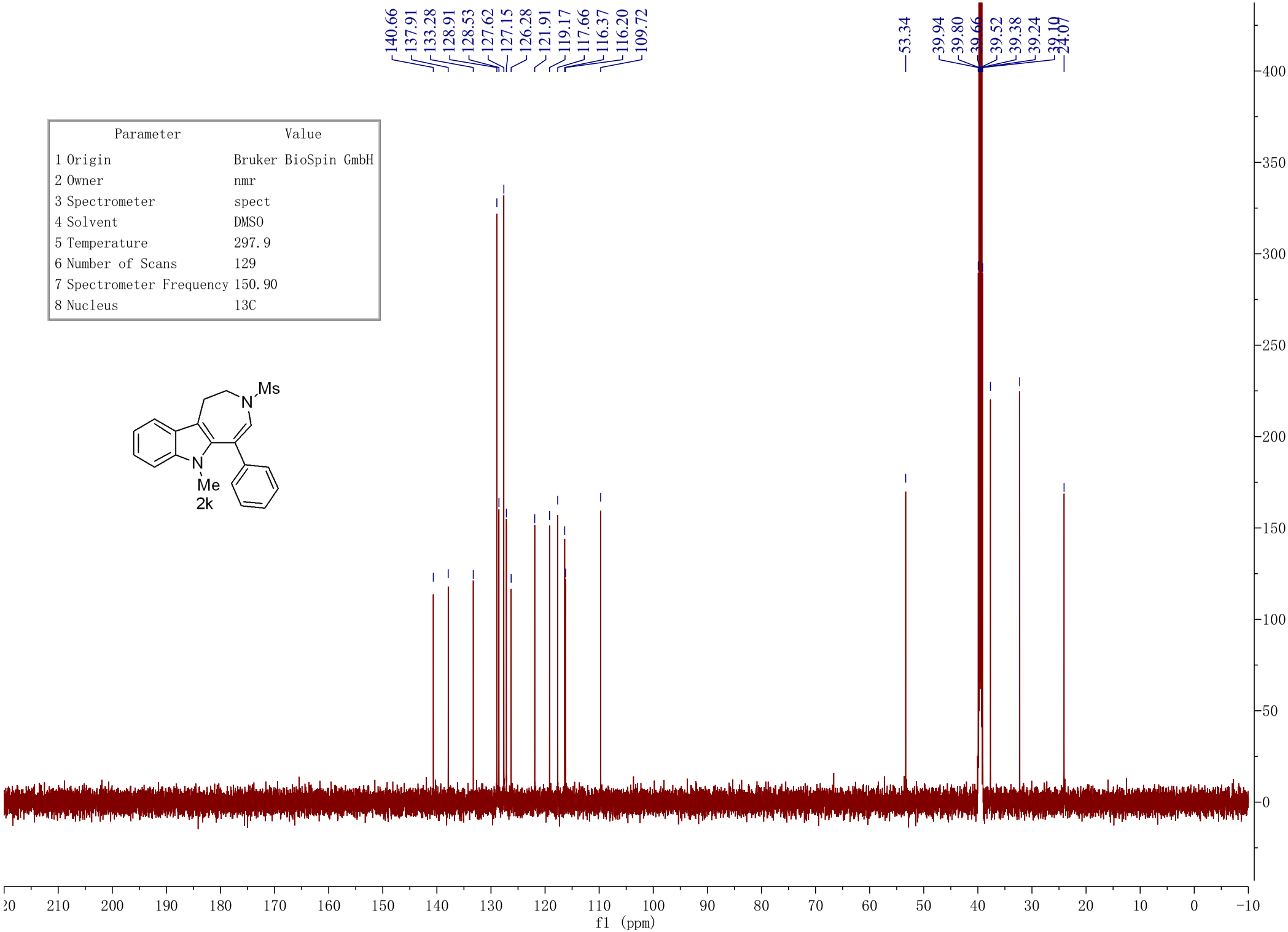
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H


149.61
143.01
139.00
137.63
132.66
129.06
128.18
128.08
127.64
126.42
125.83
125.28
124.47
122.34
119.24
117.95
116.26
109.55
55.51
39.80
39.66
39.52
39.38
39.24
31.98
22.82
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 3728
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Ns
N
N
Me
2i
f1 (ppm)

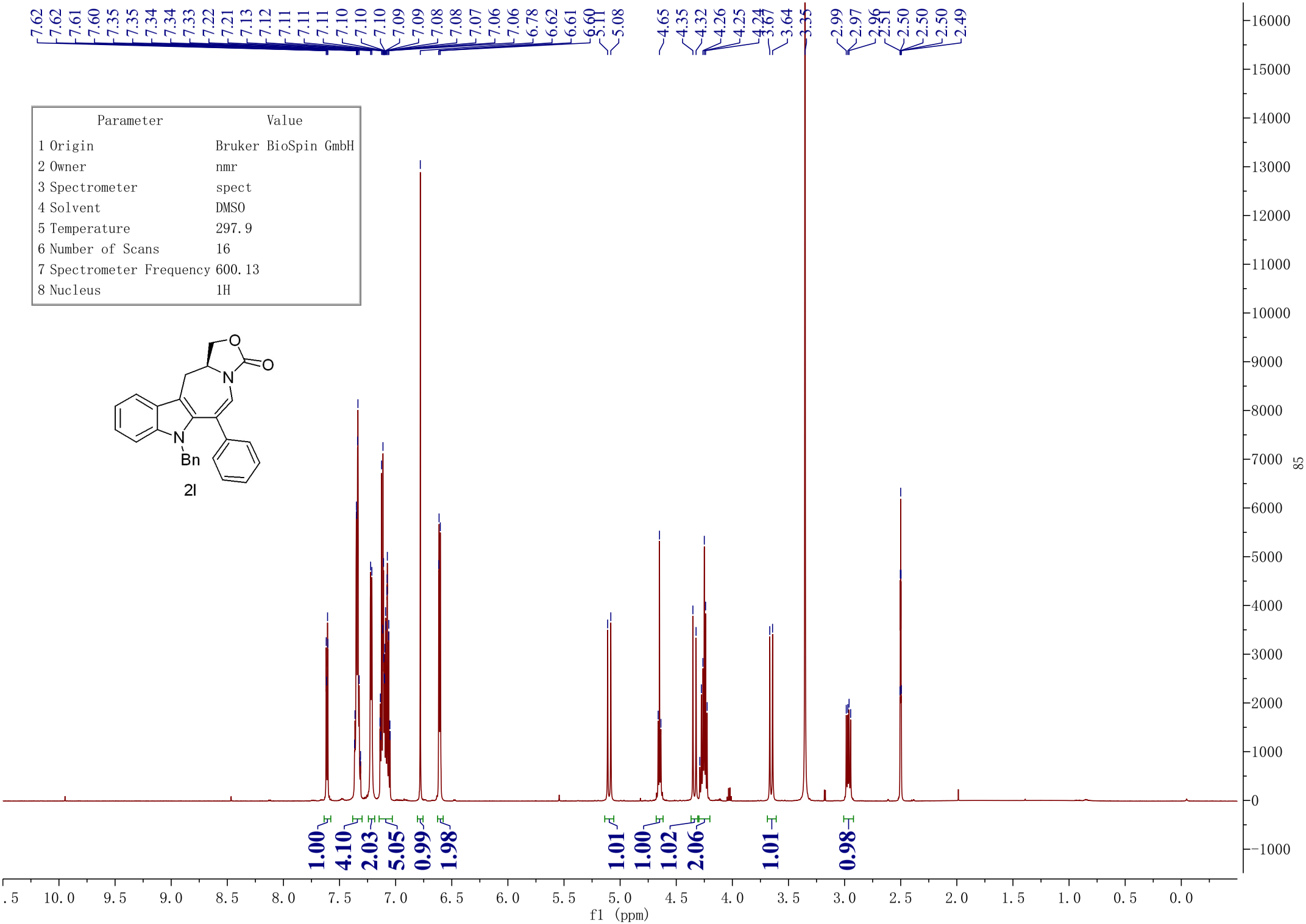


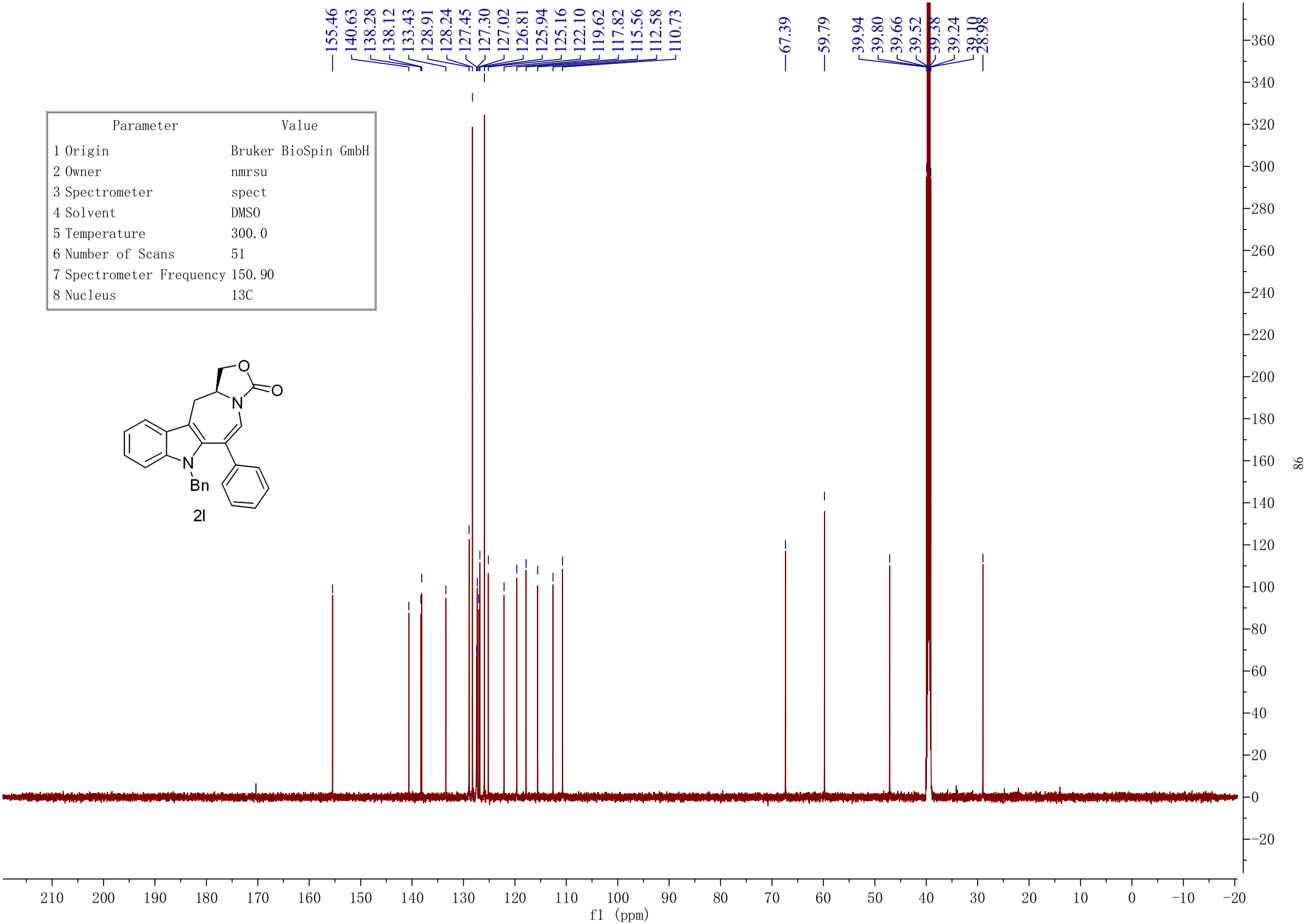
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

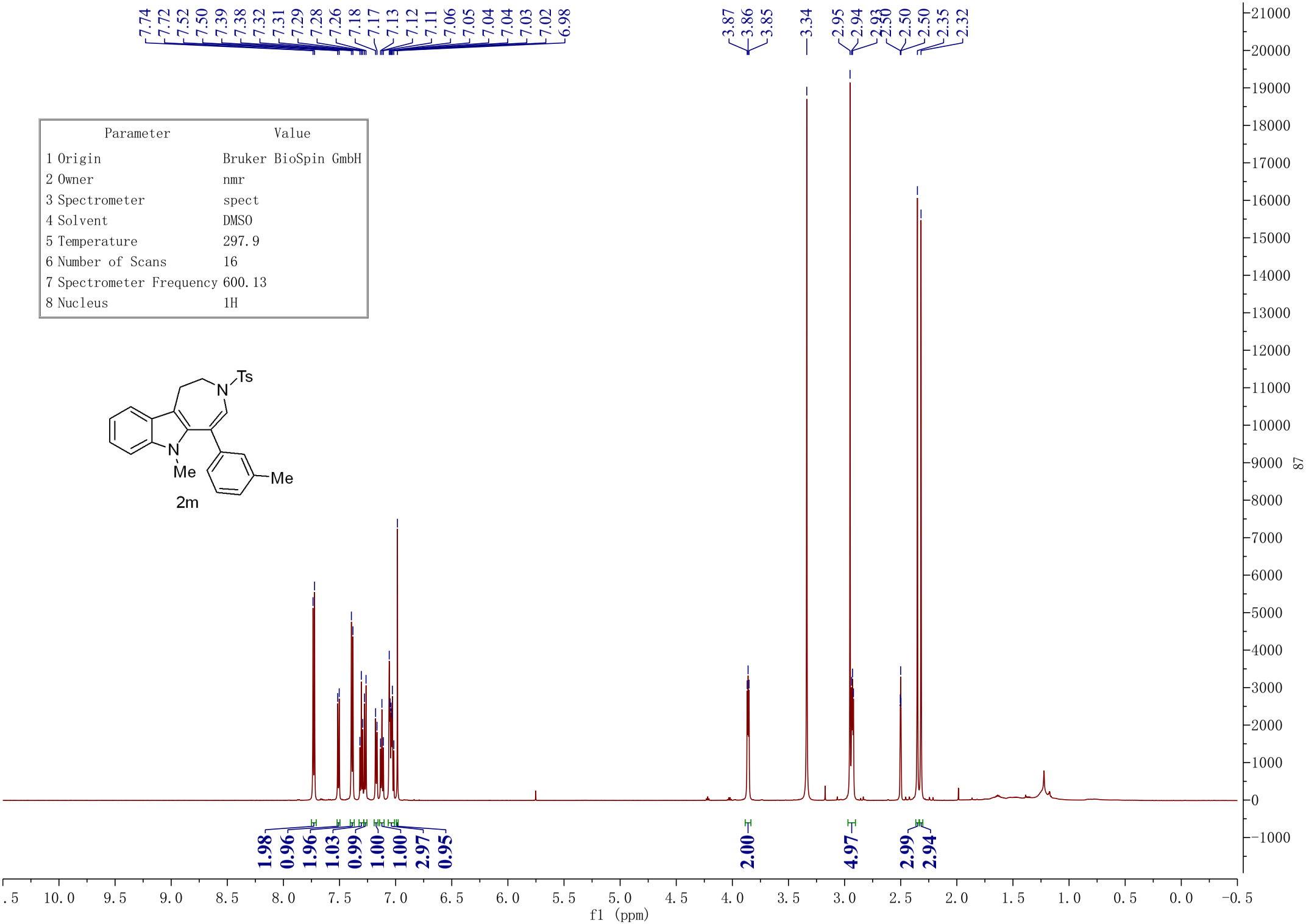
2k



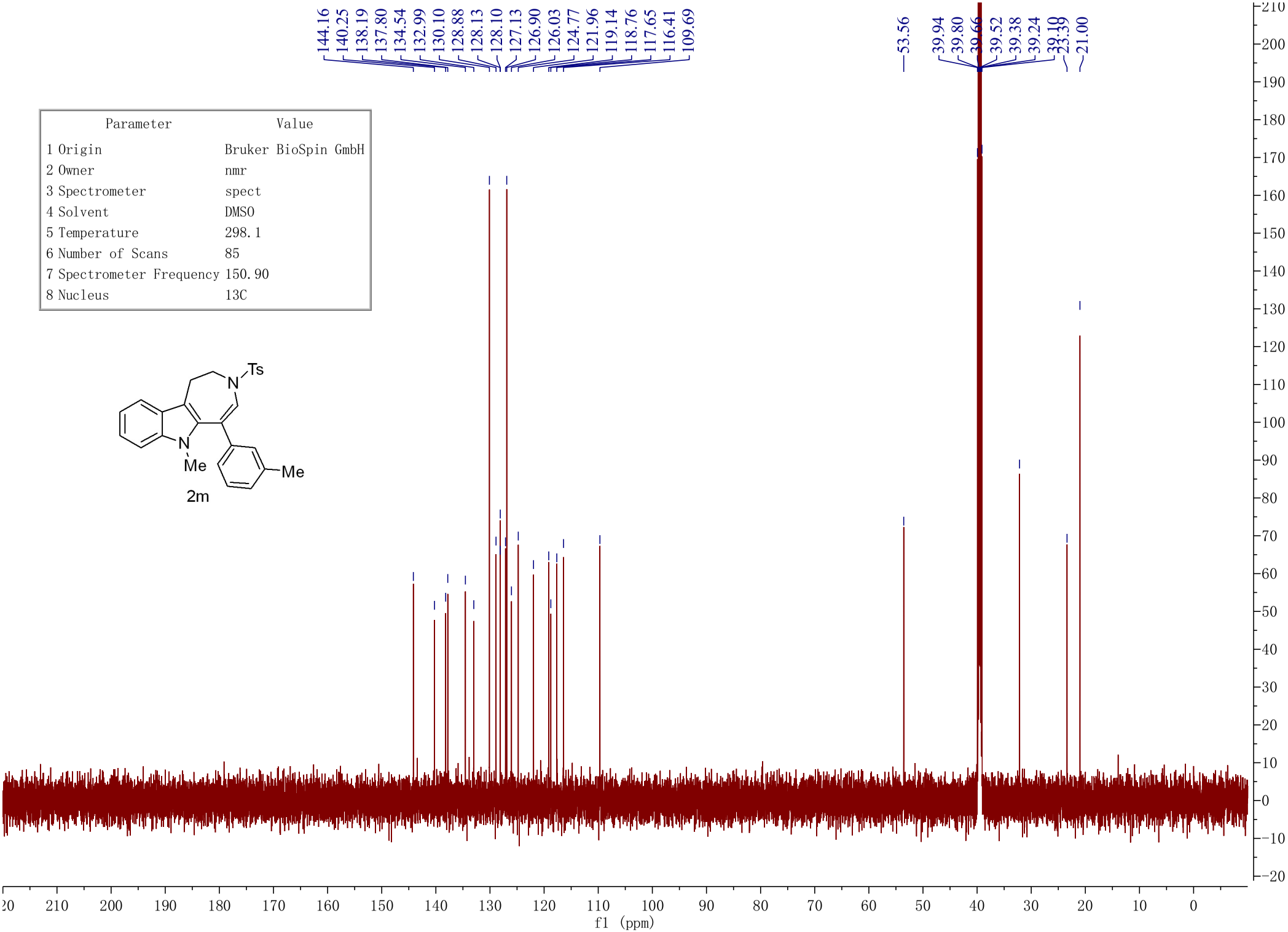
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	129
7 Spectrometer Frequency	150.90
8 Nucleus	13C


7.62 7.62 7.61 7.60 7.35 7.35 7.34 7.34 7.33 7.22 7.21 7.13 7.12 7.11 7.11 7.11 7.10 7.10 7.10 7.09 7.09 7.08 7.08 7.07 7.06 7.06 6.78 6.62 6.61 6.60 5.11 5.08
4.65 4.35 4.32 4.26 4.25 4.24 3.67 3.64 3.35
2.99 2.97 2.96 2.51 2.50 2.50 2.50 2.49
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
O
N
N
Bn
2l
1.00 4.10 2.03 5.05 0.99 1.98 1.01 1.00 1.02 2.06 1.01 0.98
f1 (ppm)

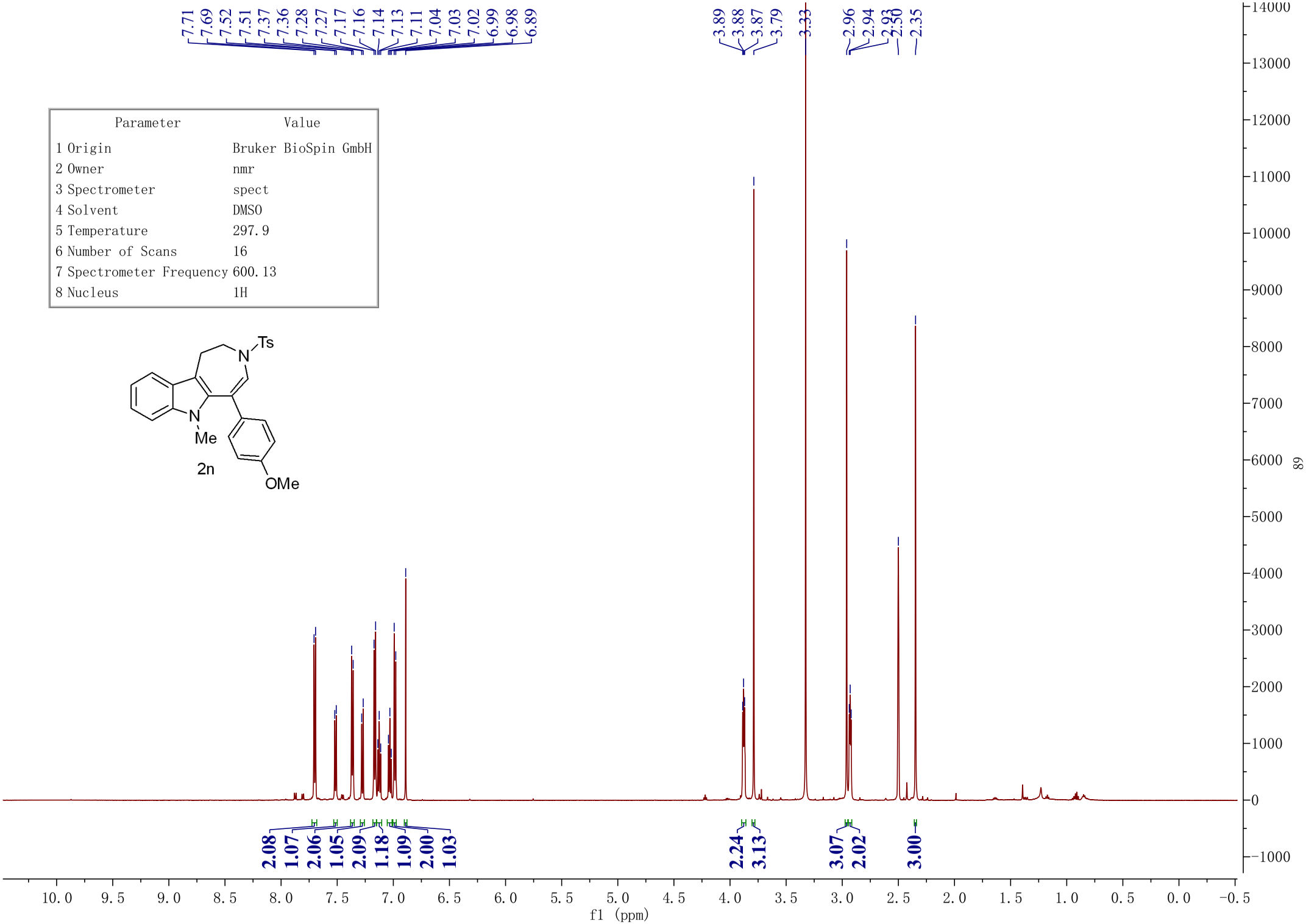

155.46
140.63
138.28
138.12
133.43
128.91
128.24
127.45
127.30
127.02
126.81
125.94
125.16
122.10
119.62
117.82
115.56
112.58
110.73
67.39
59.79
39.94
39.80
39.66
39.52
39.38
39.24
39.10
28.98
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 51
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
O
N
N
Bn
2l
f1 (ppm)



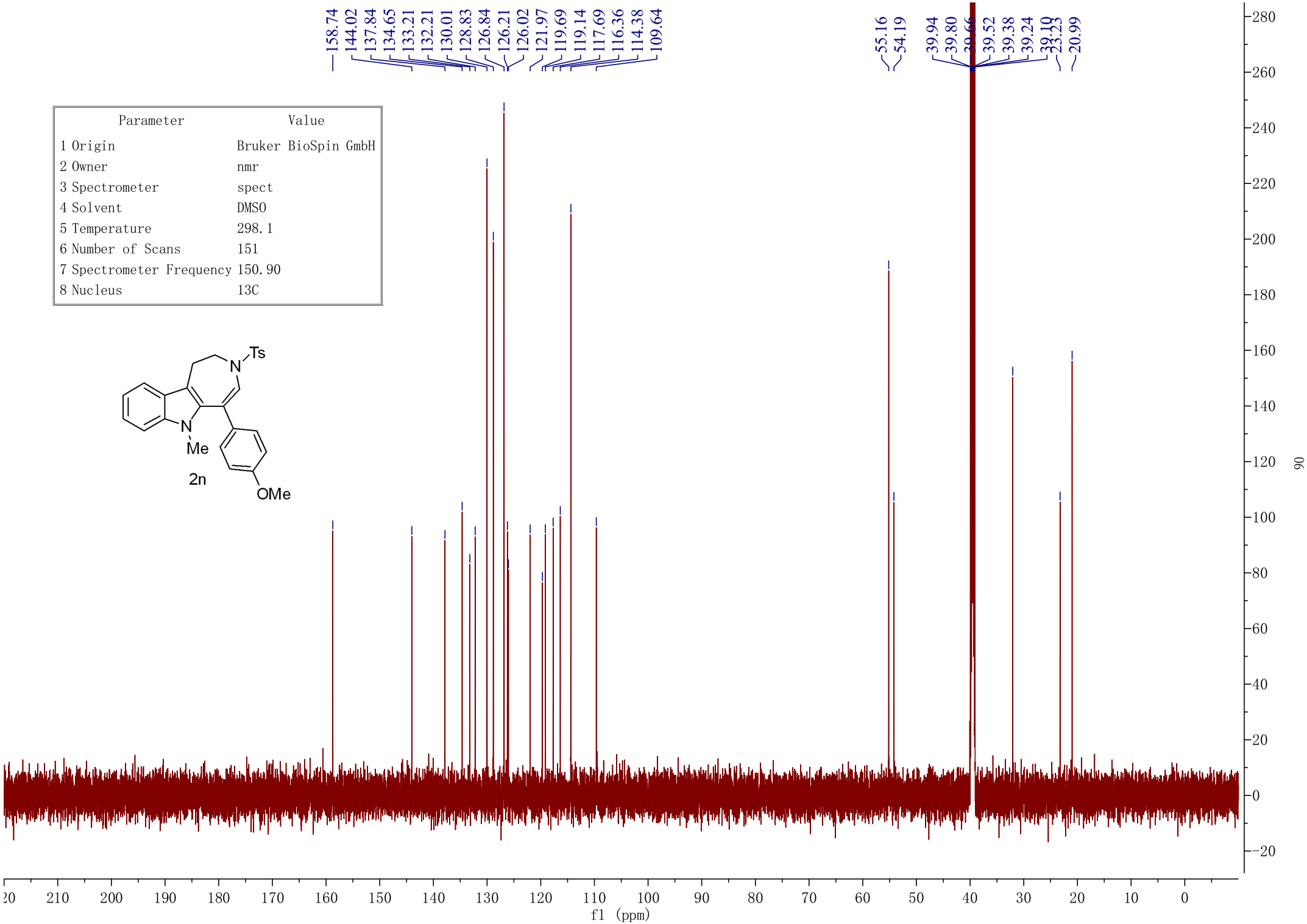
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.1
6 Number of Scans	85
7 Spectrometer Frequency	150.90
8 Nucleus	13C

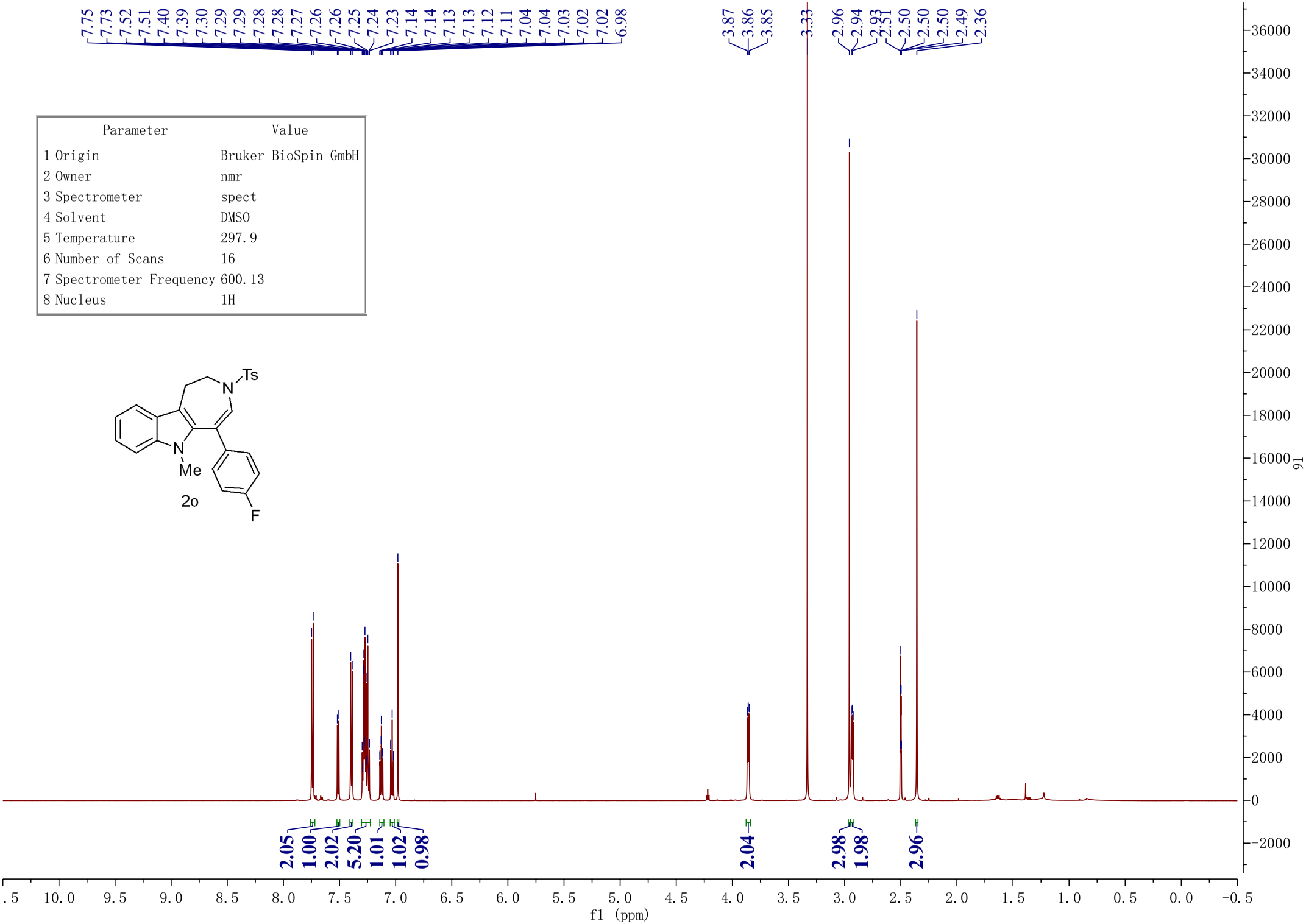


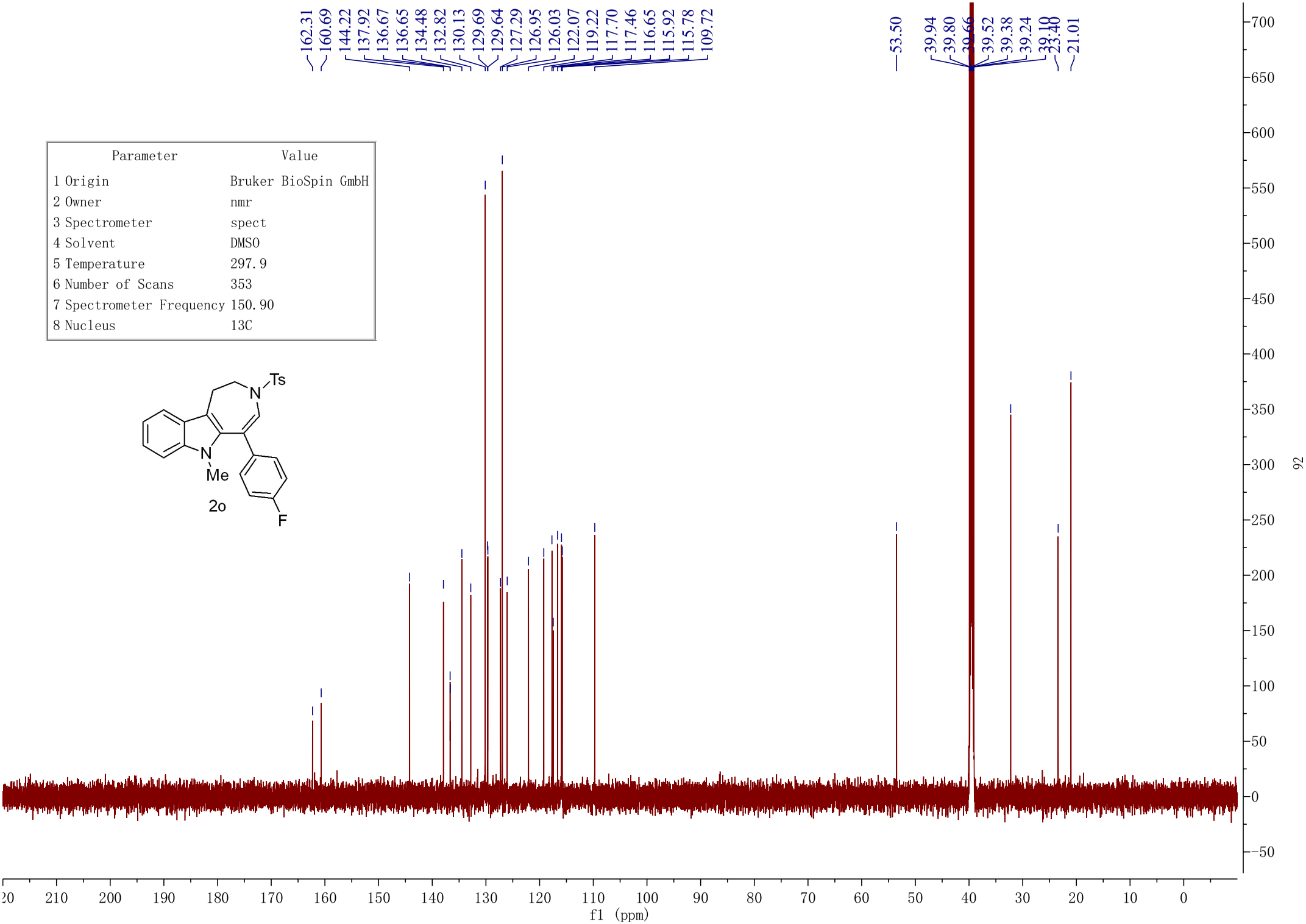
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

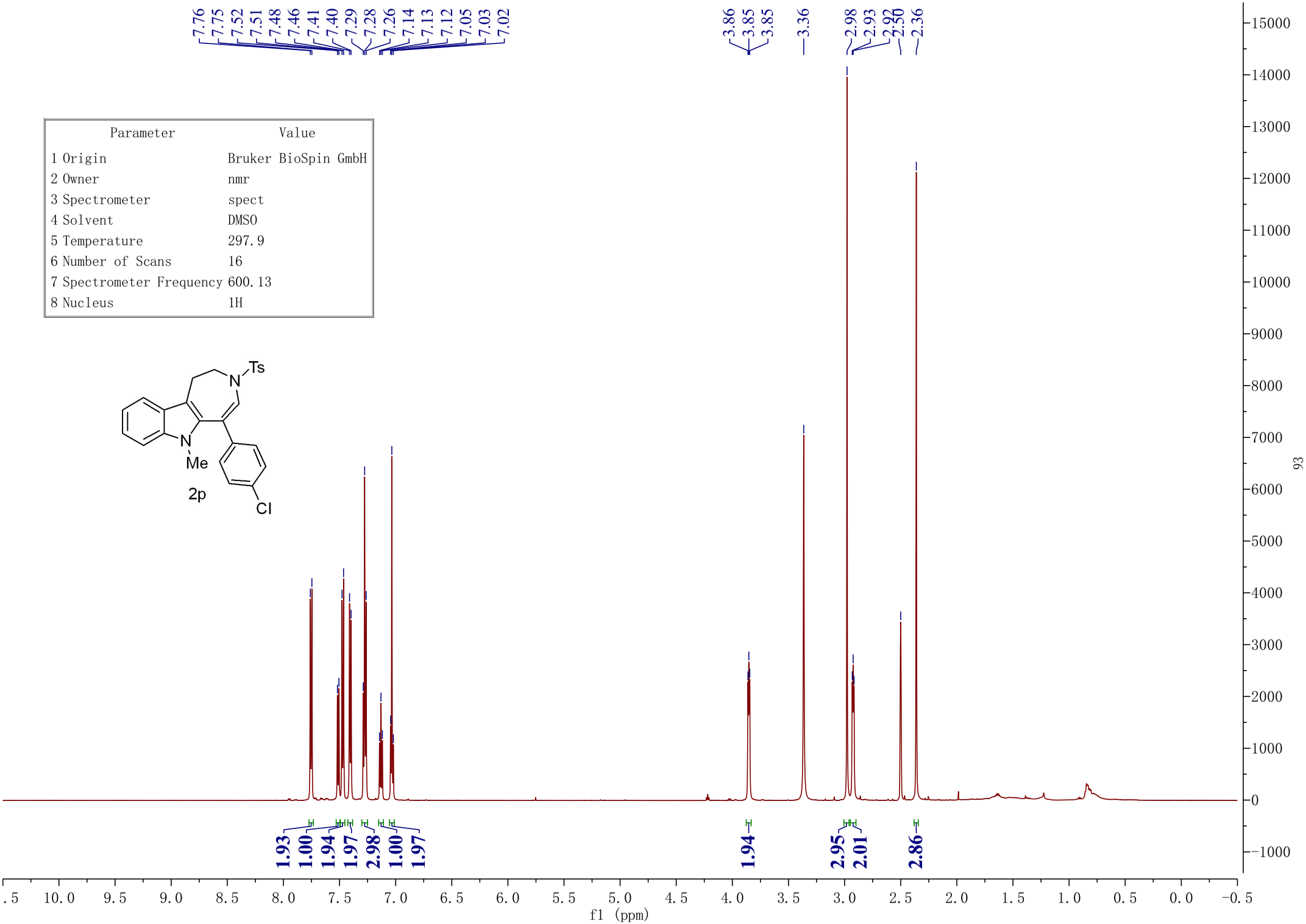

158.74
144.02
137.84
134.65
133.21
132.21
130.01
128.83
126.84
126.21
126.02
121.97
119.69
119.14
117.69
116.36
114.38
109.64
55.16
54.19
39.94
39.80
39.66
39.52
39.38
39.24
39.10
23.23
20.99
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.1
6 Number of Scans 151
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Ts
N
N
Me
2n
OMe
f1 (ppm)

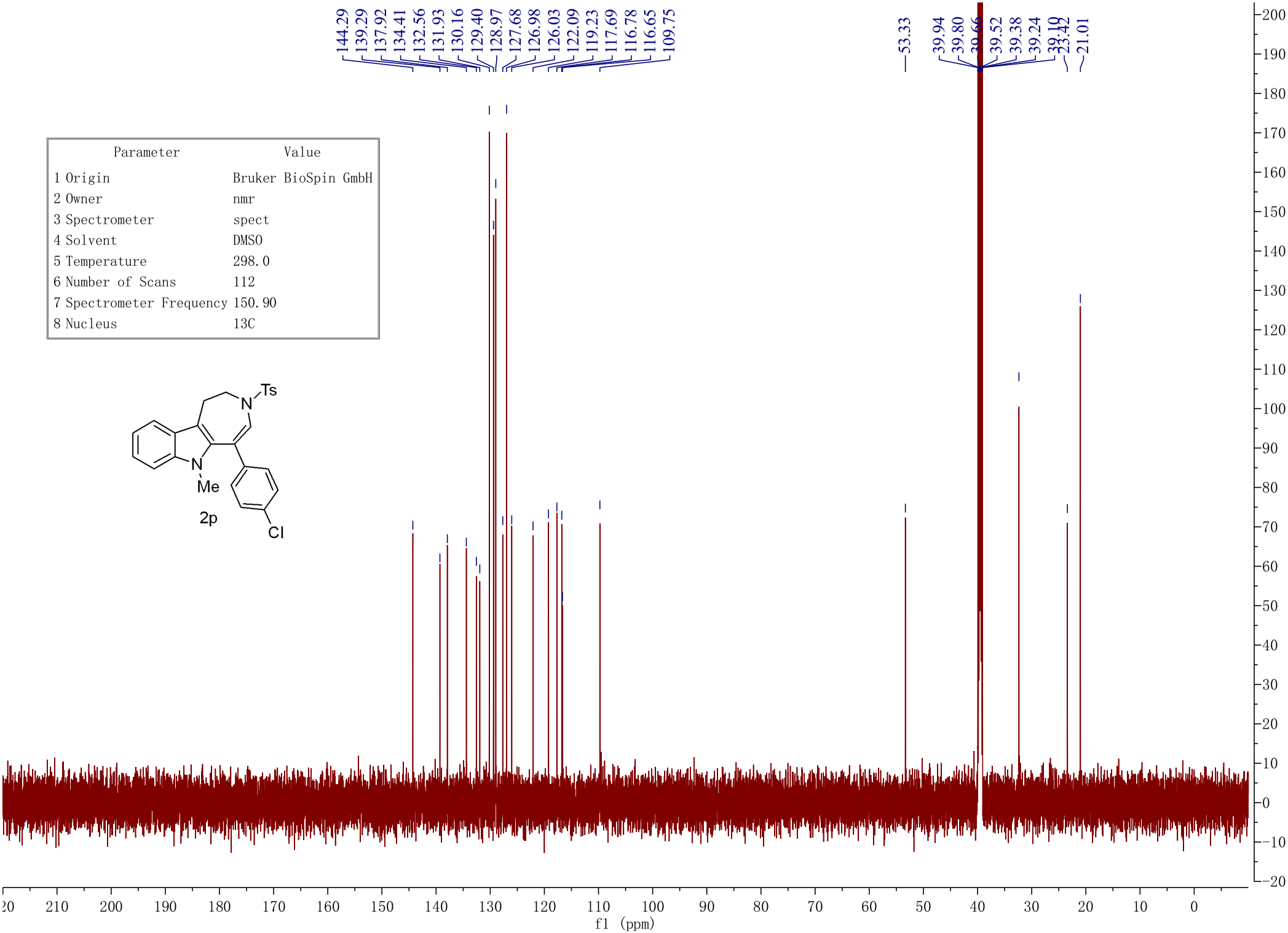
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

2o

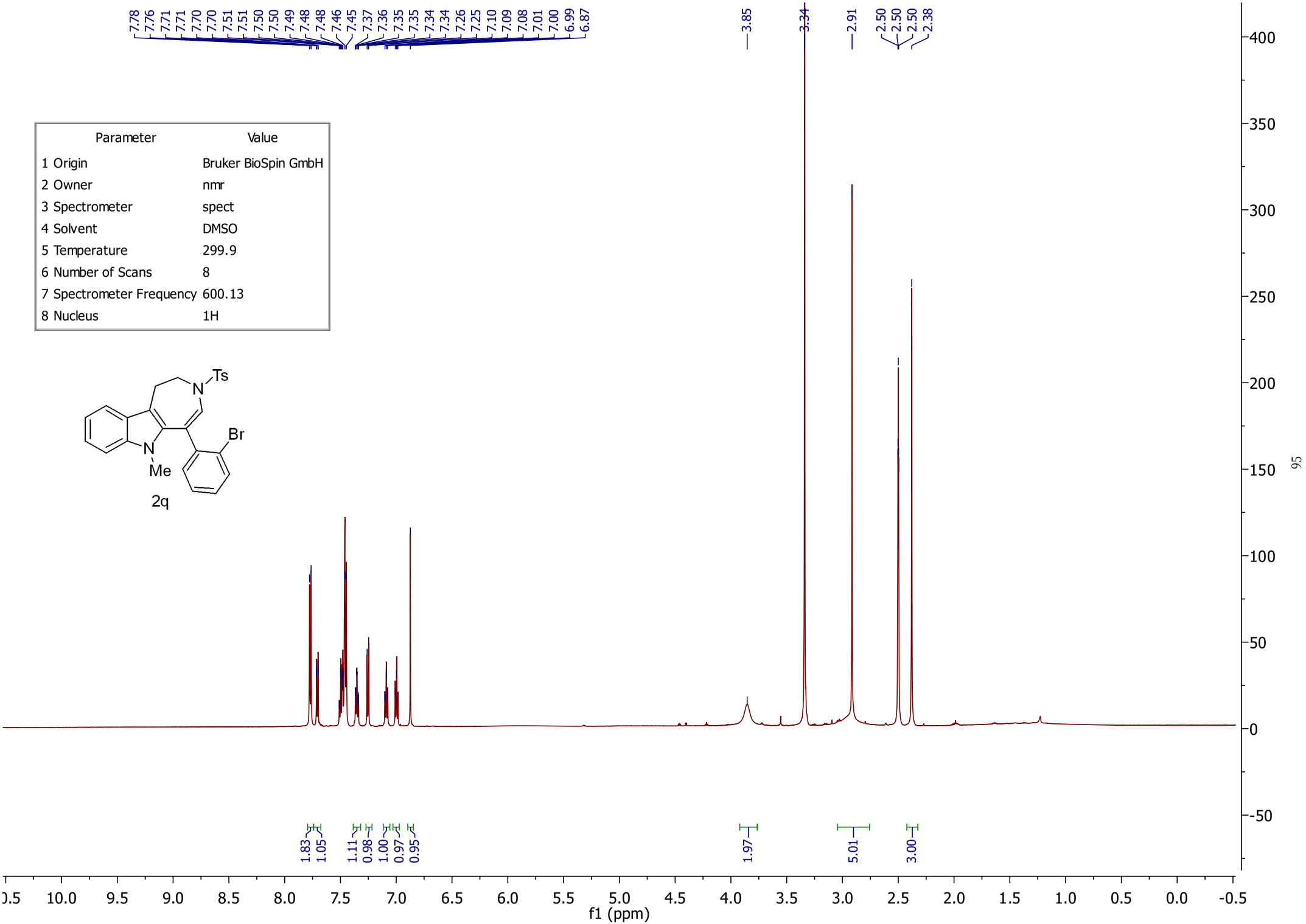



162.31
160.69
144.22
137.92
136.67
136.65
134.48
132.82
130.13
129.69
129.64
127.29
126.95
126.03
122.07
119.22
117.70
117.46
116.65
115.92
115.78
109.72
53.50
39.94
39.80
39.66
39.52
39.38
39.24
39.10
23.40
21.01
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 353
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Ts
N
N
Me
2o
F
f1 (ppm)


7.76
7.75
7.52
7.51
7.48
7.46
7.41
7.40
7.29
7.28
7.26
7.14
7.13
7.12
7.05
7.03
7.02
3.86
3.85
3.85
3.36
2.98
2.93
2.92
2.50
2.36
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Ts
N
N
Me
2p
Cl
1.93
1.00
1.94
1.97
2.98
1.00
1.97
1.94
2.95
2.01
2.86
f1 (ppm)

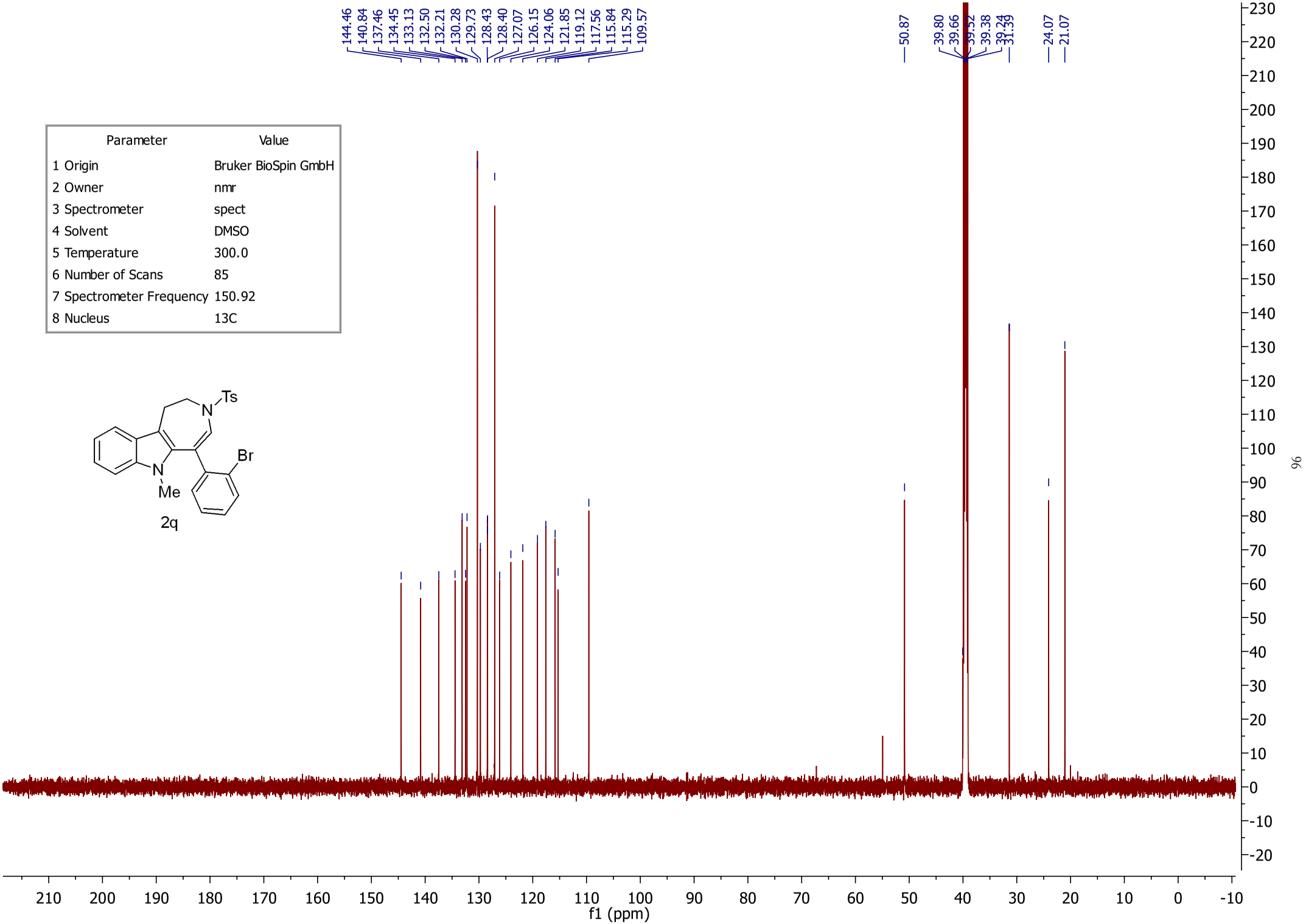


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.0
6 Number of Scans	112
7 Spectrometer Frequency	150.90
8 Nucleus	13C

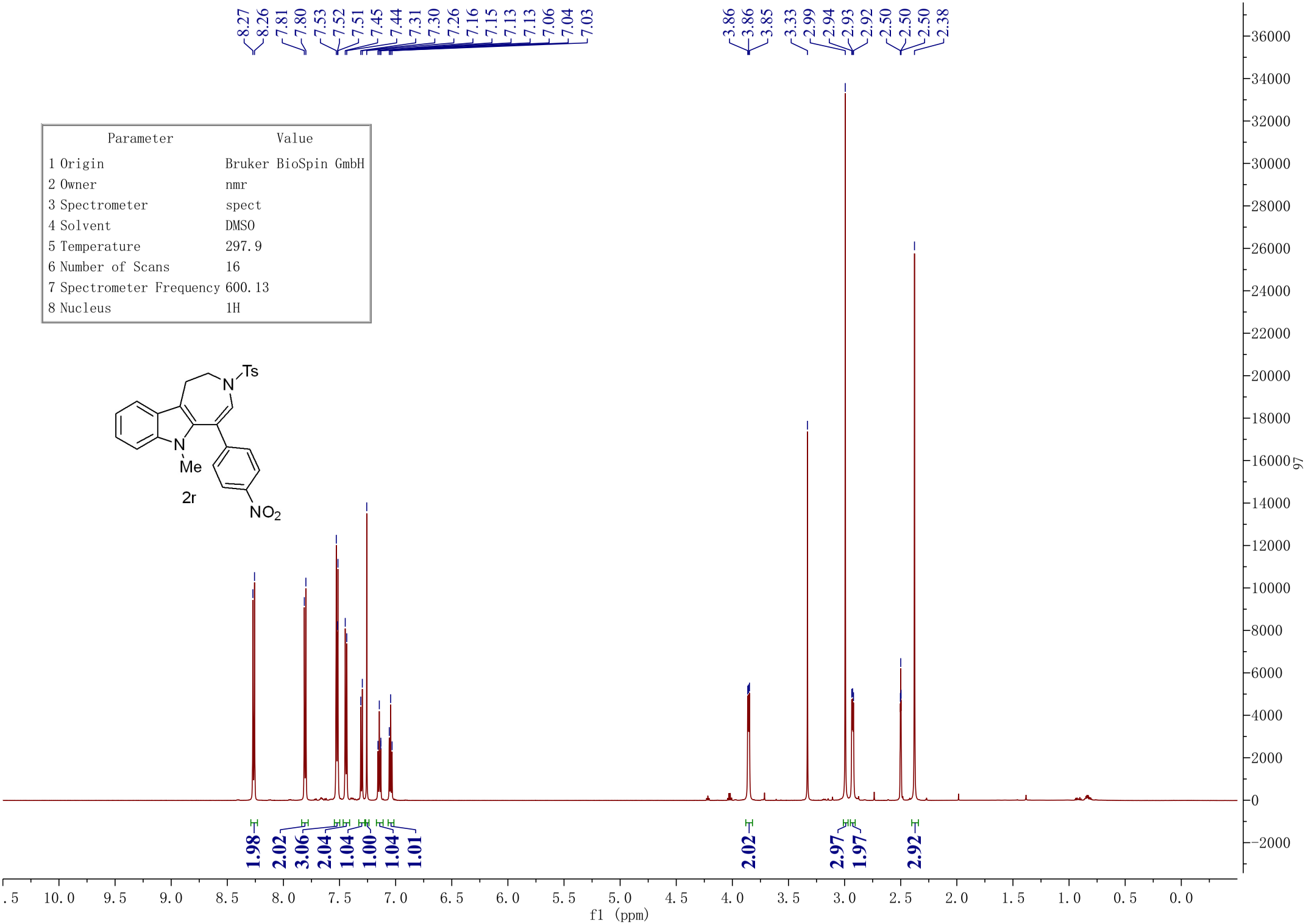


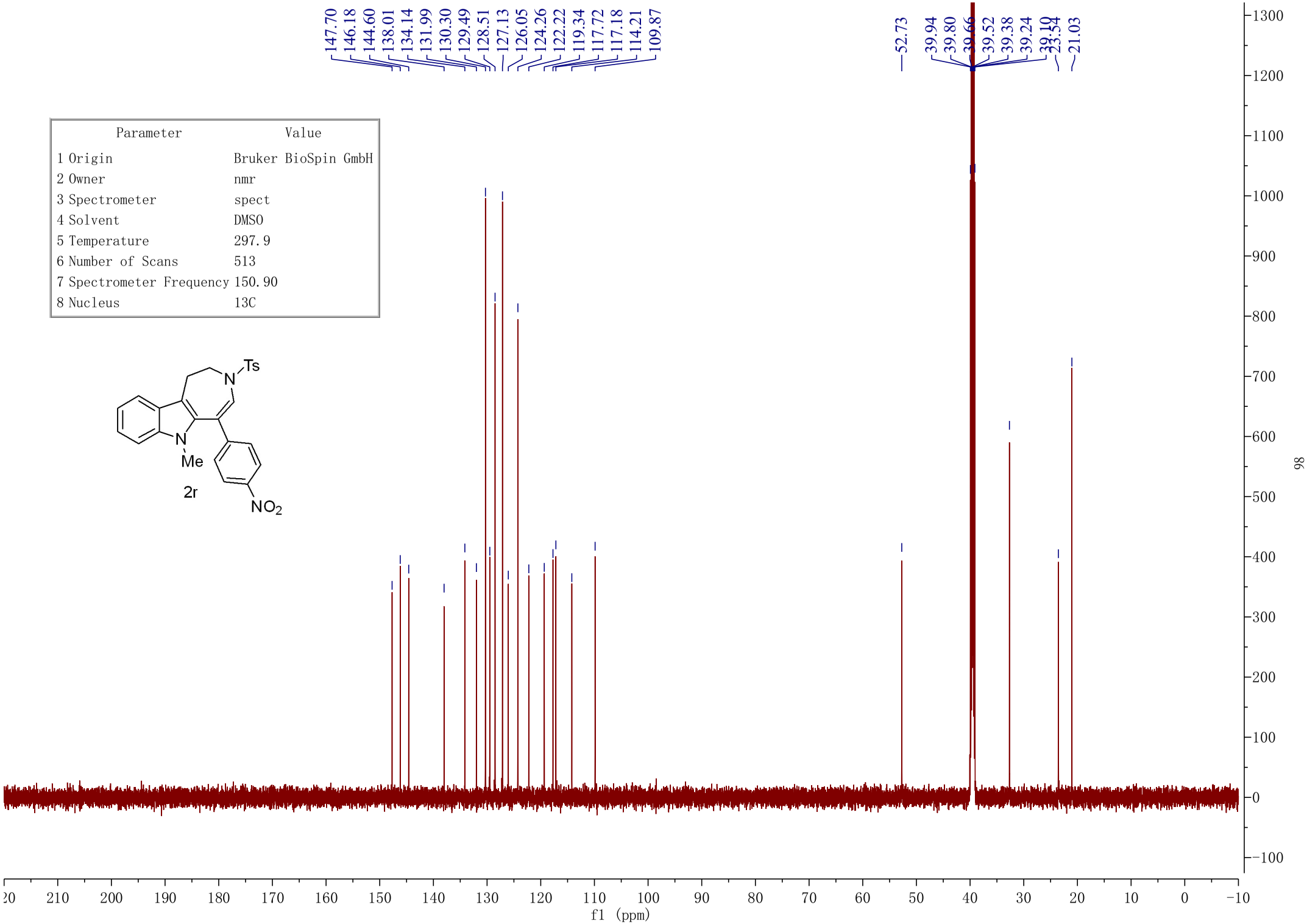
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	299.9
6 Number of Scans	8
7 Spectrometer Frequency	600.13
8 Nucleus	1H

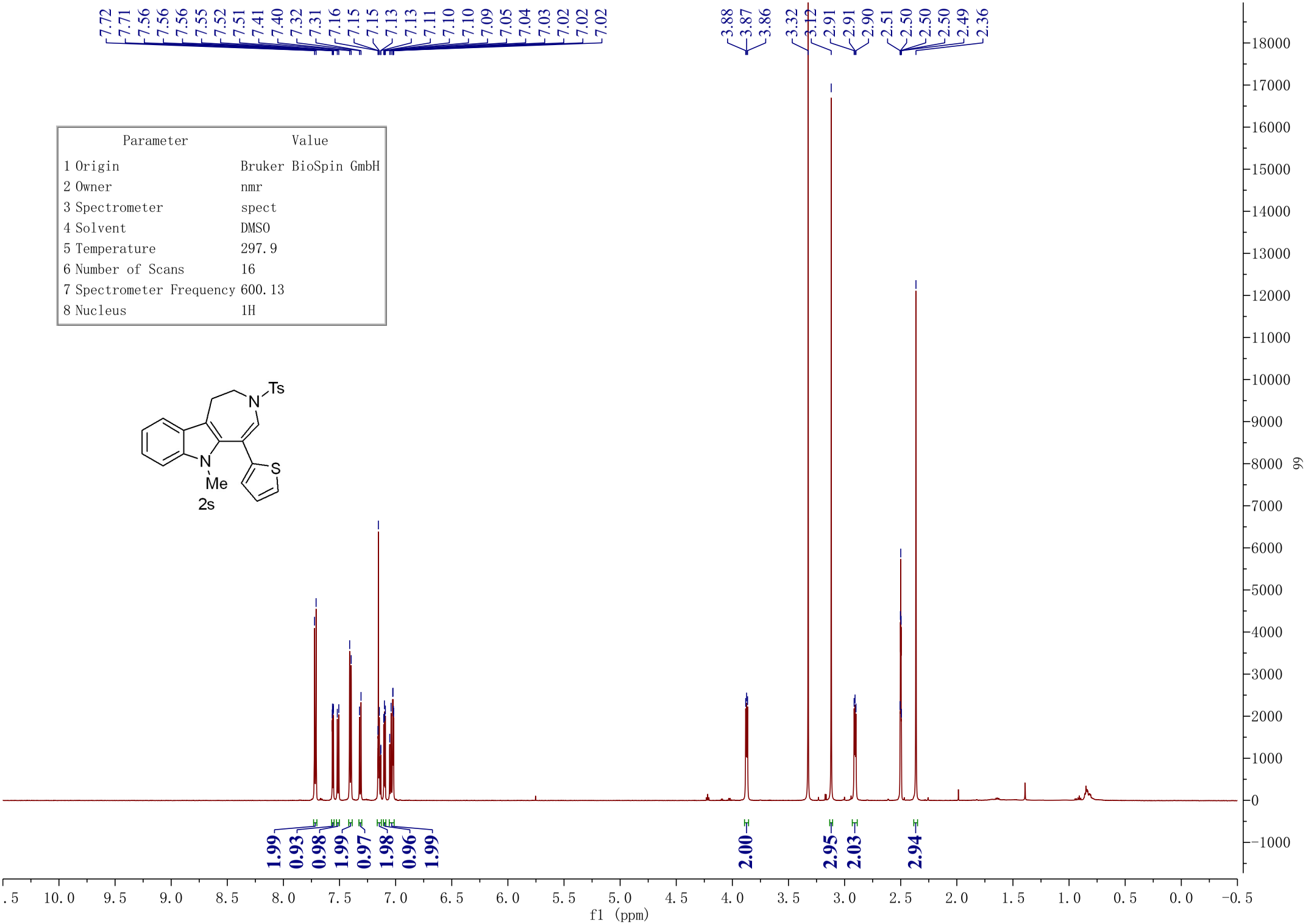
2q

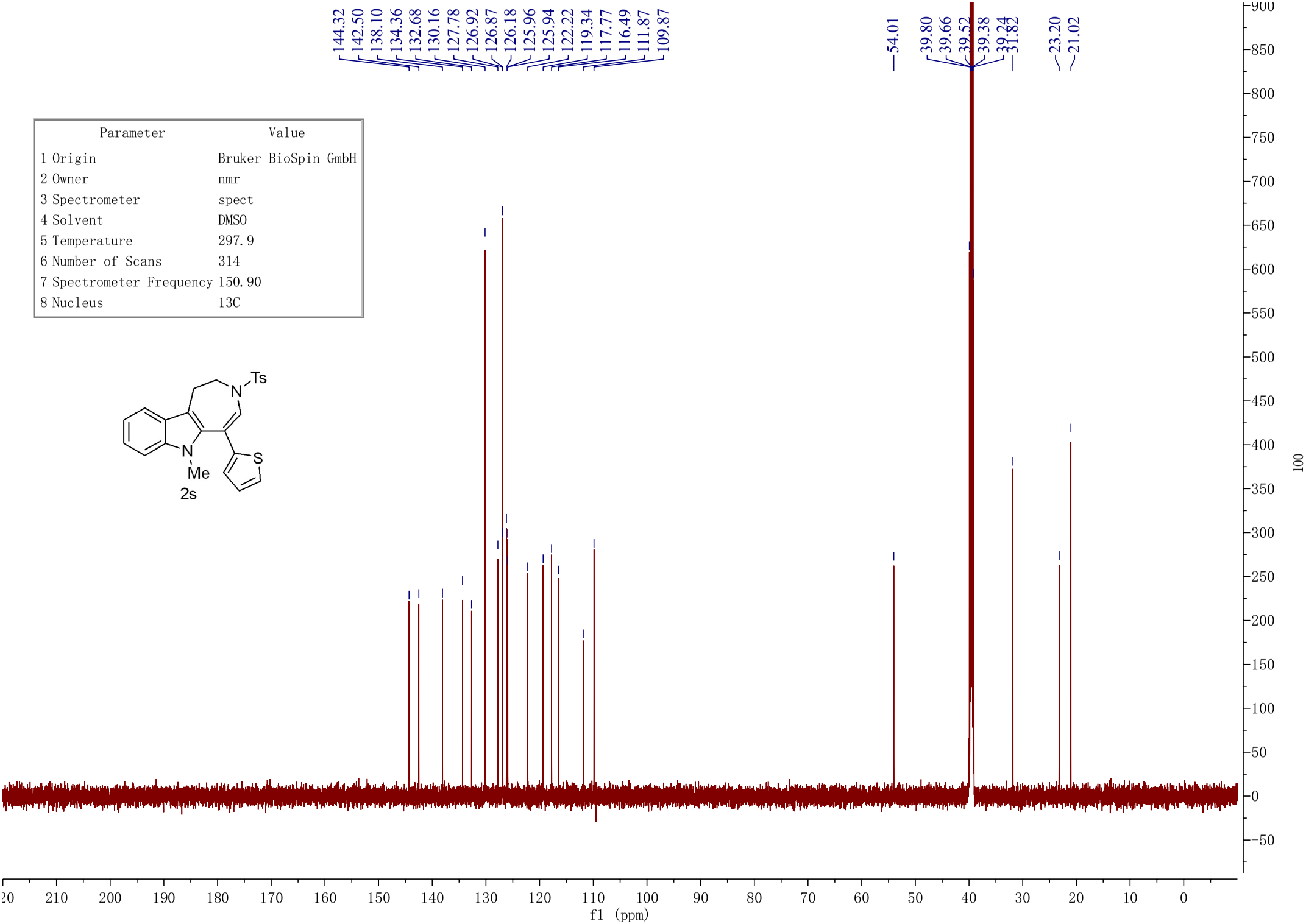


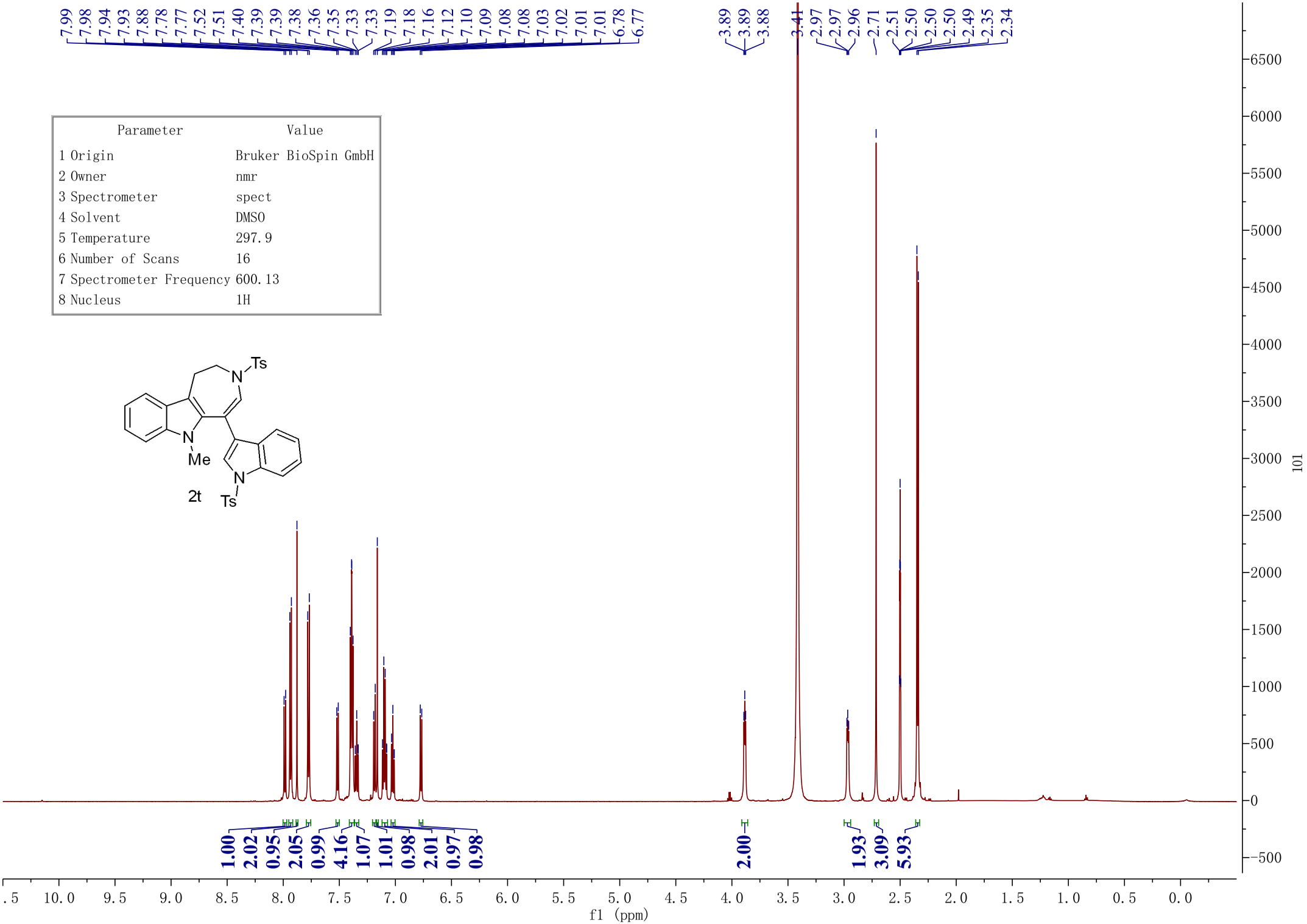
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.0
6 Number of Scans	85
7 Spectrometer Frequency	150.92
8 Nucleus	13C

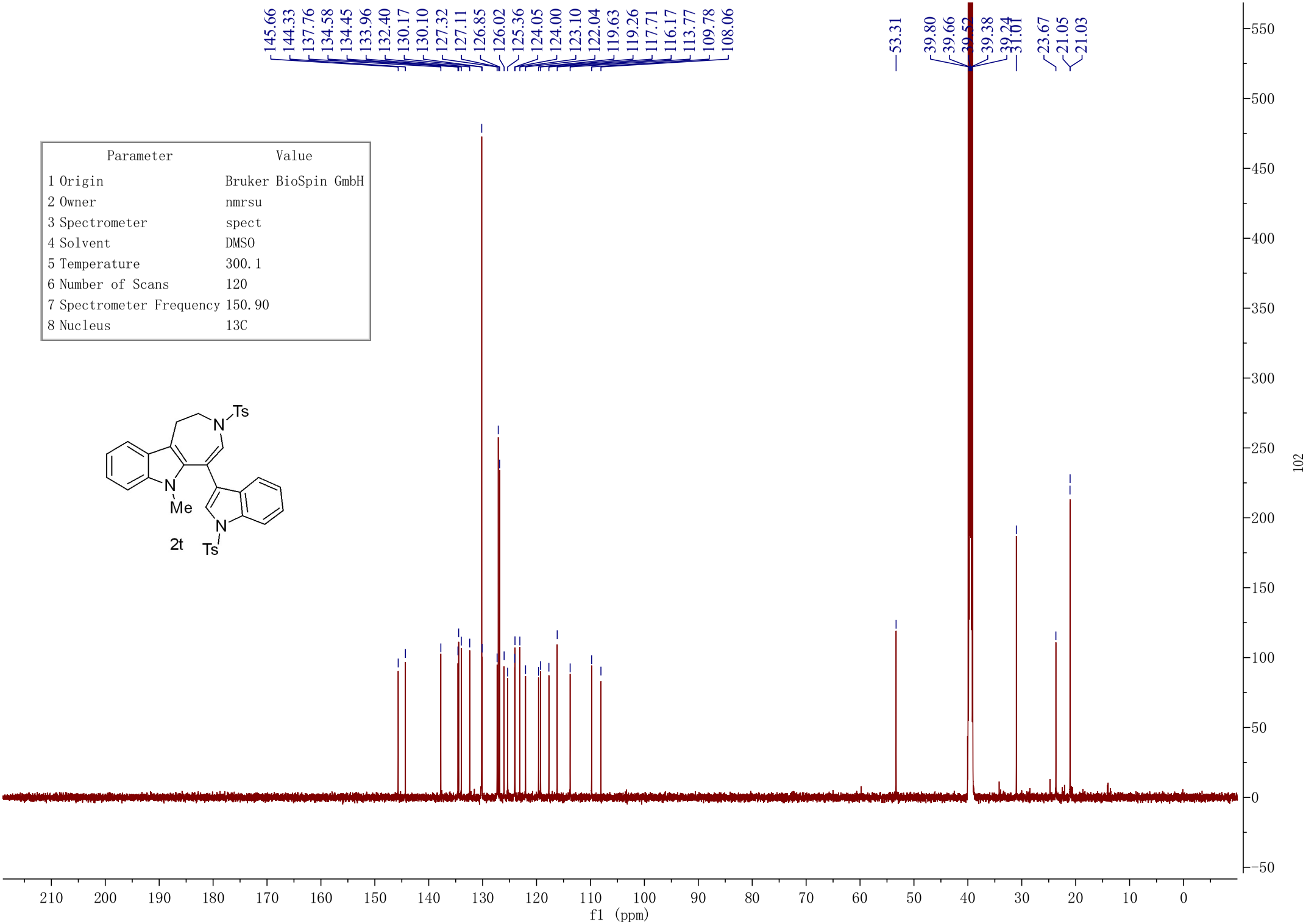

8.27
8.26
7.81
7.80
7.53
7.52
7.51
7.45
7.44
7.31
7.30
7.26
7.16
7.15
7.13
7.13
7.06
7.04
7.03
3.86
3.86
3.85
3.33
2.99
2.94
2.93
2.92
2.50
2.50
2.50
2.38
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Ts
N
N
Me
2r
NO2
1.98
2.02
3.06
2.04
1.04
1.00
1.04
1.01
2.02
2.97
1.97
2.92
f1 (ppm)

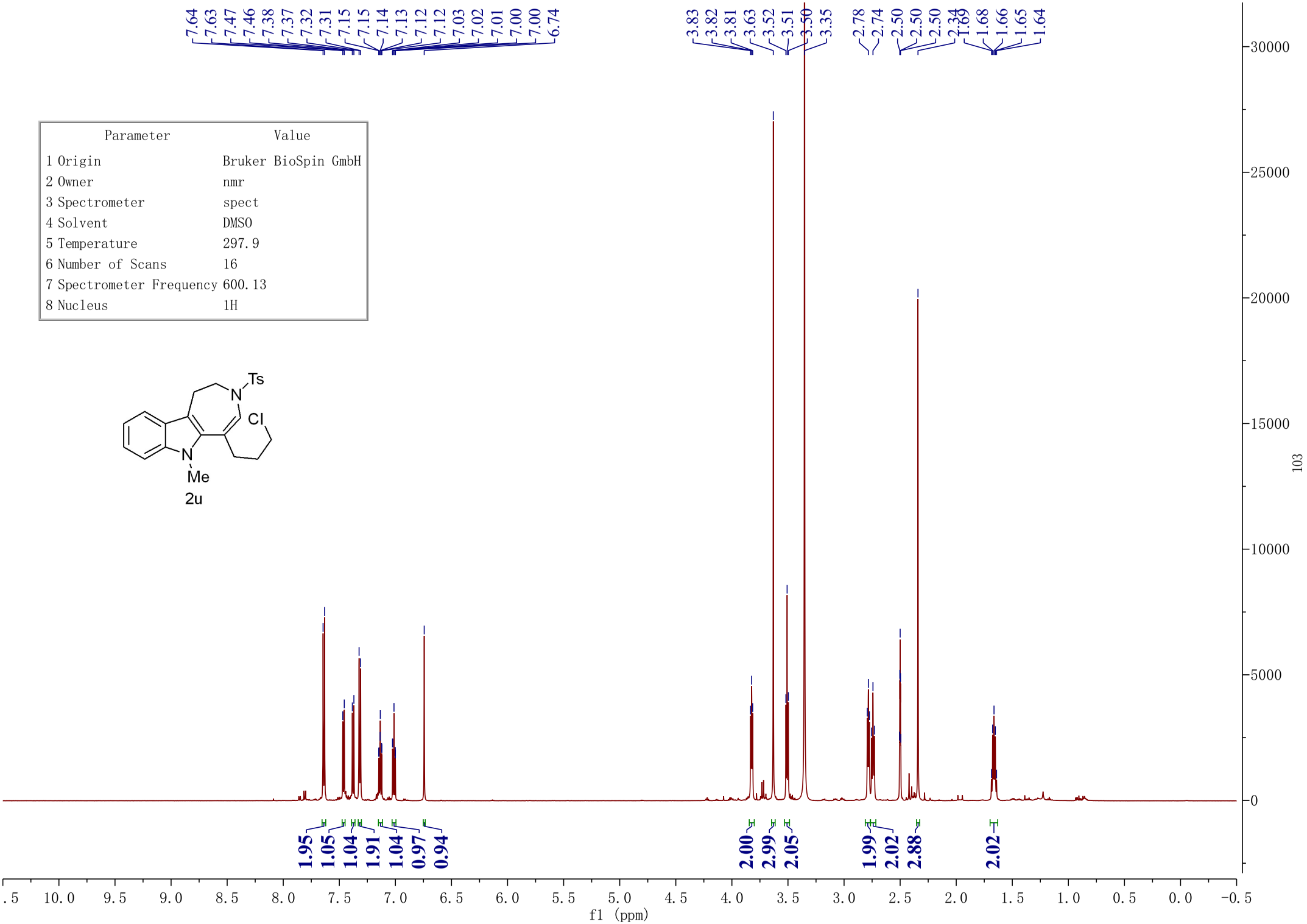

147.70
146.18
144.60
138.01
134.14
131.99
130.30
129.49
128.51
127.13
126.05
124.26
122.22
119.34
117.72
117.18
114.21
109.87
52.73
39.94
39.80
39.66
39.52
39.38
39.24
39.10
23.54
21.03
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 513
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Ts
N
N
Me
2r
NO2
f1 (ppm)


7.72 7.71 7.56 7.56 7.56 7.55 7.52 7.51 7.41 7.40 7.32 7.31 7.16 7.15 7.15 7.13 7.13 7.11 7.10 7.10 7.09 7.05 7.04 7.03 7.02 7.02 7.02
3.88 3.87 3.86 3.32 3.12 2.91 2.91 2.90 2.51 2.50 2.50 2.50 2.49 2.36
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Ts
N
N
Me
S
2s
1.99 0.93 0.98 1.99 0.97 1.98 0.96 1.99
2.00 2.95 2.03 2.94
f1 (ppm)


144.32
142.50
138.10
134.36
132.68
130.16
127.78
126.92
126.87
126.18
125.96
125.94
122.22
119.34
117.77
116.49
111.87
109.87
54.01
39.80
39.66
39.52
39.38
39.24
31.82
23.20
21.02
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 314
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Ts
N
N
Me
S
2s
f1 (ppm)
100

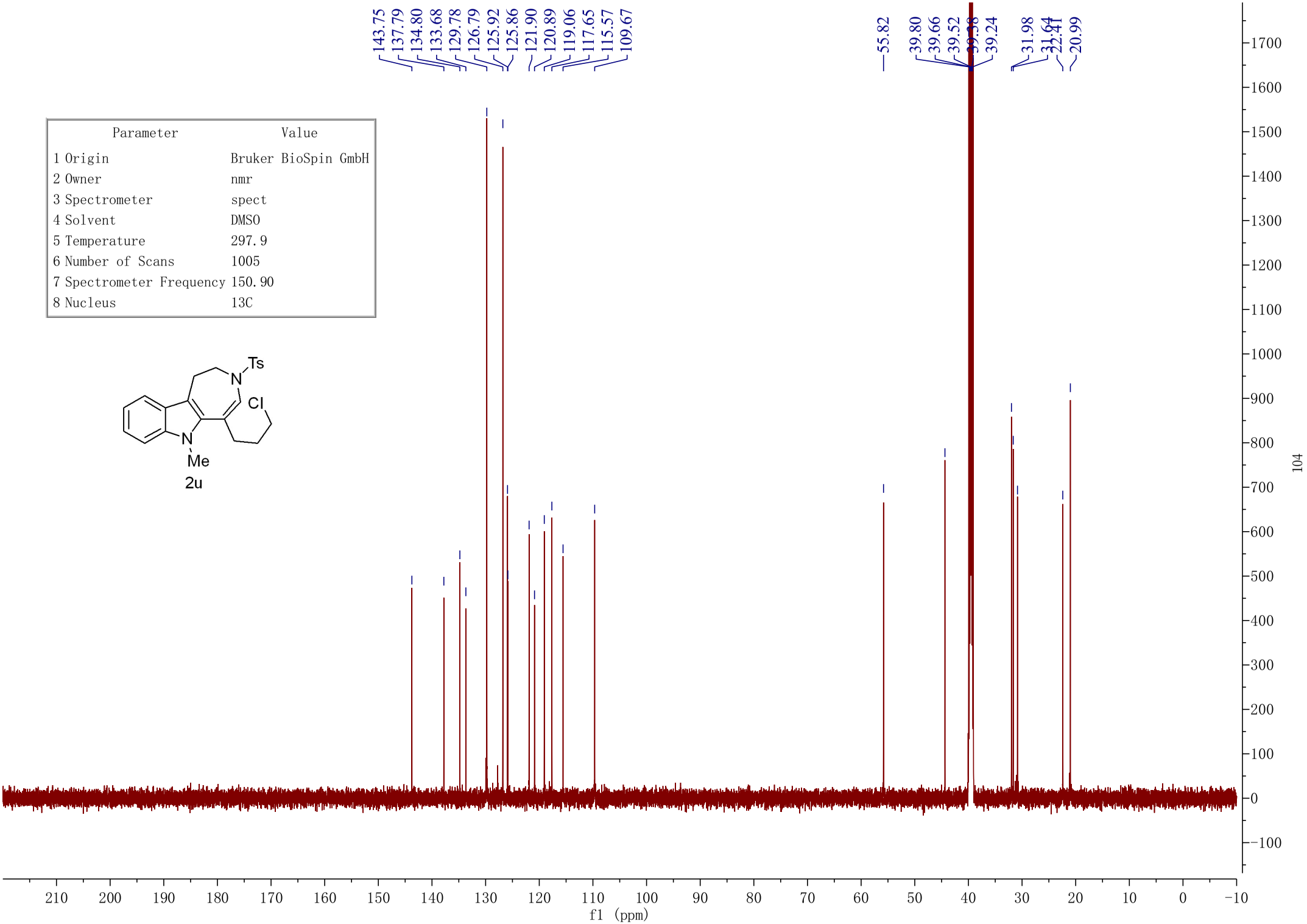

7.99 7.98 7.94 7.93 7.88 7.78 7.77 7.52 7.51 7.40 7.39 7.39 7.38 7.36 7.35 7.33 7.33 7.19 7.18 7.16 7.12 7.10 7.09 7.08 7.08 7.03 7.02 7.01 7.01 6.78 6.77
3.89 3.89 3.88 3.41 2.97 2.97 2.96 2.71 2.51 2.50 2.50 2.50 2.49 2.35 2.34
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmr
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 297.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Ts
N
N
Me
N
Ts
2t
1.00 2.02 0.95 2.05 0.99 4.16 1.07 1.01 0.98 2.01 0.97 0.98
2.00
1.93 3.09 5.93
f1 (ppm)
101


145.66
144.33
137.76
134.58
134.45
133.96
132.40
130.17
130.10
127.32
127.11
126.85
126.02
125.36
124.05
124.00
123.10
122.04
119.63
119.26
117.71
116.17
113.77
109.78
108.06
53.31
39.80
39.66
39.38
39.24
31.01
23.67
21.05
21.03
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.1
6 Number of Scans 120
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Ts
N
N
Me
N
Ts
2t
f1 (ppm)
102

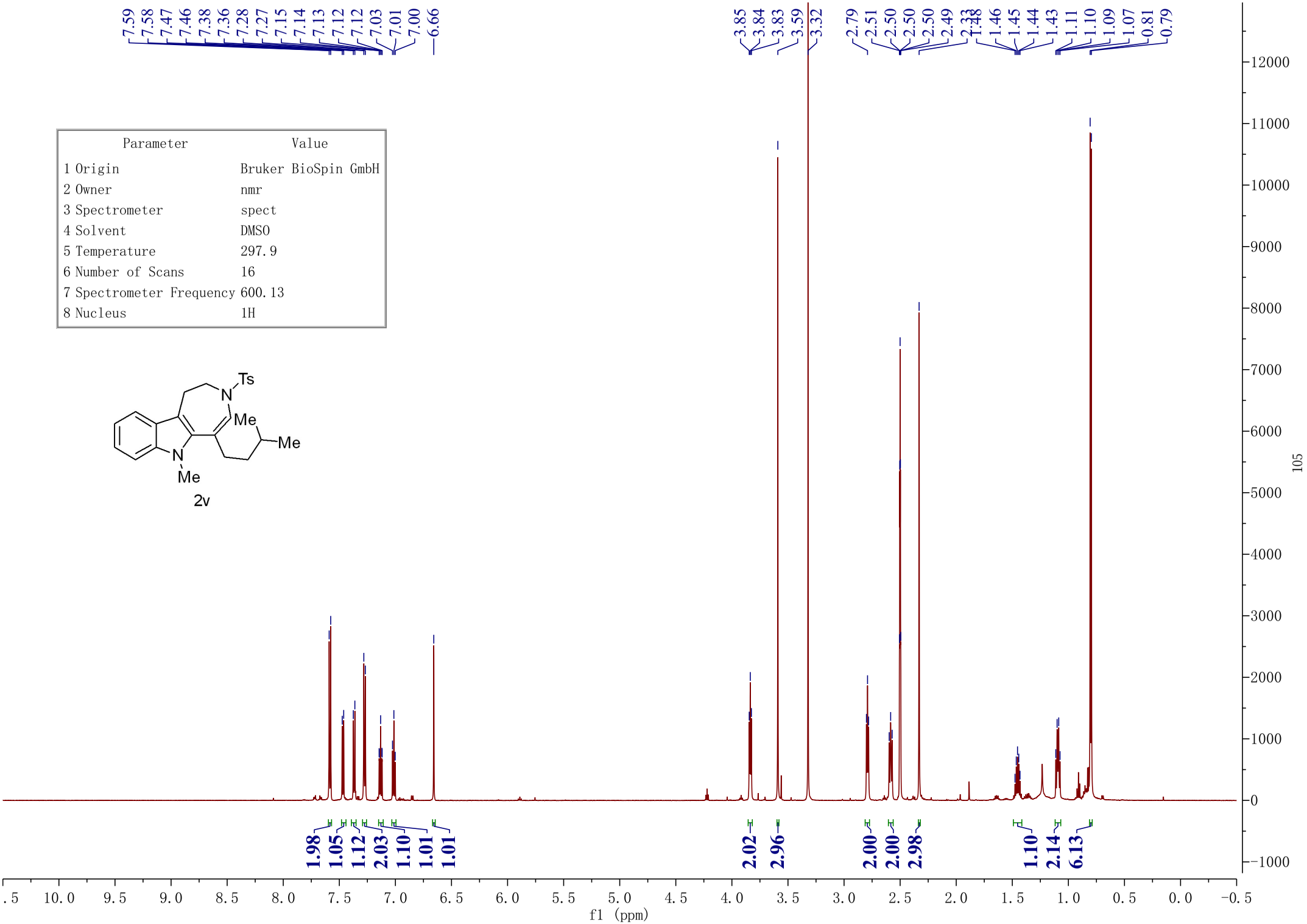


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

2u

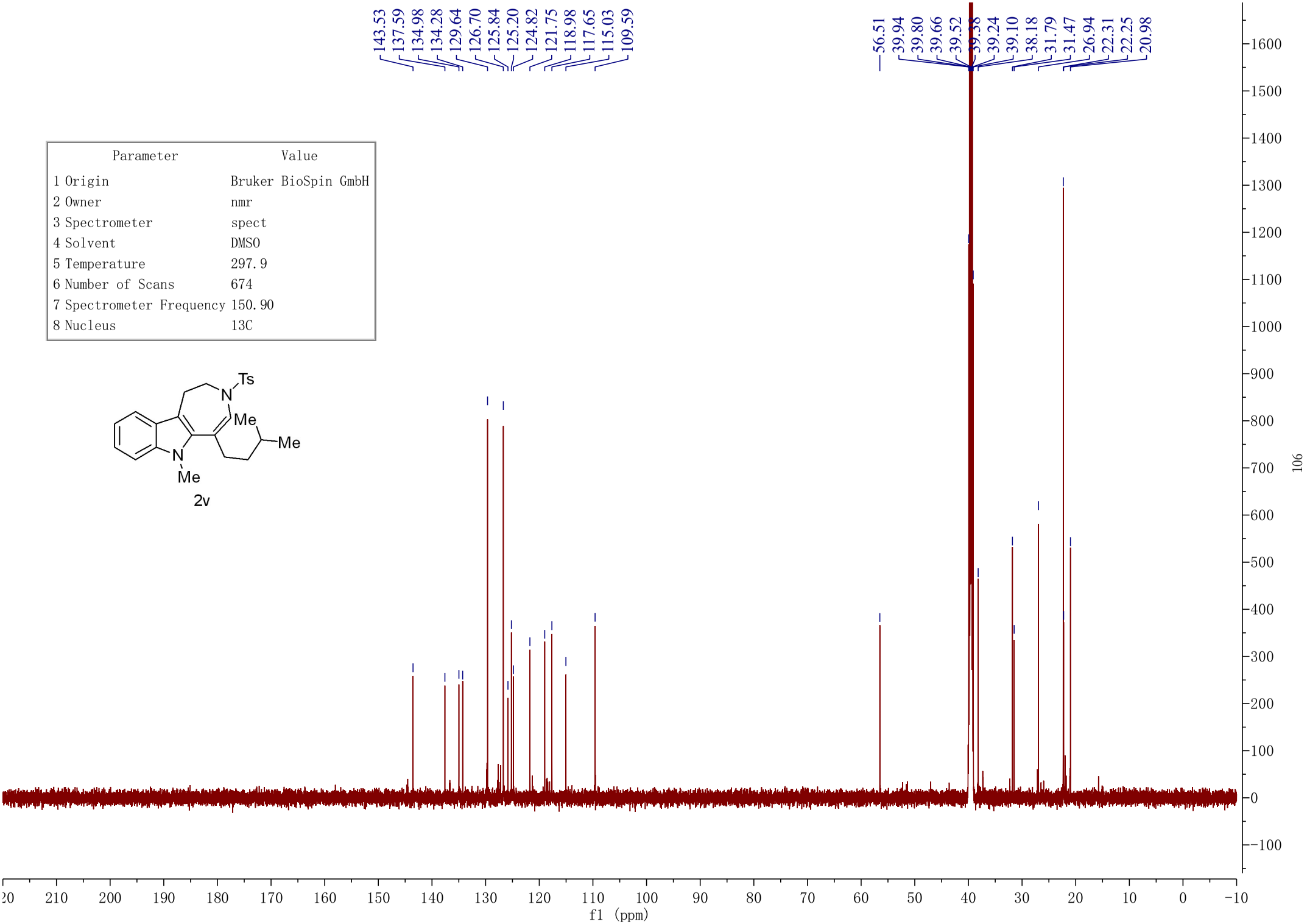


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	1005
7 Spectrometer Frequency	150.90
8 Nucleus	13C



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

2v



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmr
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	297.9
6 Number of Scans	674
7 Spectrometer Frequency	150.90
8 Nucleus	13C