Electronic Supplementary Material (ESI) for New Journal of Chemistry
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Electronic Supplementary Information for paper titled:

The Amide Bridge in Donor-Acceptor Systems: Delocalization Depends on *Push-Pull* Stress

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1. Synthetic Procedures

Synthesis of 7-diethylaminocoumarin-3-carboxylic acid (1). 4-diethylamino-2-hydroxybenzaldehyde (1 mmol), Meldrum's acid (1.1 mmol), $ZrOCl_2 \cdot 8H_2O$ (0.5 mmol) were mixed in a flask and water (50mL) was added, followed by an hour of mixing in an ultrasound bath. The resulting orange solid (95% yield) was vacuum-filtered, dried and used without further purification.

General method for the synthesis of *push-pull* amides. Compound **1** (1mmol), EEDQ (1.25 mmol) and substituted aniline **2a-i** (1.25 mmol) were mixed in a dry flask, under nitrogen. CH_2Cl_2 was added dropwise until all the solids were dissolved. After 48 hours (or

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until no changes were observed in TLC), solvent was removed by evaporation and the resulting mixture was resuspended in acetone. The crude product was isolated by vacuum filtration and washed with 15 mL of cold acetone. Crystallization from CH_2Cl_2/acetone afforded the products **3a-i** as a yellow crystalline solid.

2. Single Crystal X-Ray Data for Compounds 3b, 3f, 3h and 31

Single crystal X-ray diffraction analyses of **3b** (T = 132 K), **3f** (T = 173 K), **3h** (T = 298 K) and **3i** (T = 298 K) were performed (λ MoKα= 0.71073 Å, graphite monochromator, K-CCD). All reflection data set were corrected for Lorentz and polarization effects. The crystals were mounted on conventional MicroLoops ™. The first structure solution was obtained using the SHELXS-971 or SIR20042 programs and then the SHELXL-971 program was applied for refinement and output data. All software manipulations were done under the WinGX3 environment program set. All heavier atoms were found by Fourier map difference and refined anisotropically. The hydrogen atoms were geometrically modeled and are not refined.

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Table S1. Crystallographic data of compounds **3b, 3f, 3h and 3i.**

Compound	**3b**	**3f**	**3h**	**3i**
Empirical formula	$C_{20}H_{19}F_1N_2O_3$	$C_{22}H_{22}N_2O_5$	$C_{21}H_{19}N_3O_3$	$C_{20}H_{19}N_3O_5$
Formula weight	354.37	394.42	361.39	379.40
Space Group	Pī	Pī	Pī	Pī
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
a (Å)	6.9499 (5)	8.4489 (4)	6.9026 (2)	4.9427 (2)
b (Å)	9.4914 (7)	8.9514 (4)	7.3751 (6)	12.5574 (4)
c (Å)	13.2856 (11)	12.9033 (7)	19.5370 (6)	14.6612 (5)
α (°)	104.262 (7)	92.365 (3)	81.881 (18)	98.169 (2)
β (°)	91.624 (6)	104.602 (2)	82.063 (18)	98.169 (2)
γ (°)	100.777 (6)	92.578 (3)	65.3173 (18)	92.6732 (19)
Volume (Å)³	831.83 (11)	942.00 (8)	891.18 (5)	886.65 (6)
Z	2	2	2	2
Crystal size (mm)	0.38 × 0.25 × 0.13	0.32 x 0.15 x 0.1	0.3 x 0.2 x 0.025	0.33 × 0.18 × 0.08
θ Range for data collection (°)	3.5 to 29.5	4.1 to 27.5	3.05 to 27.5	4.0 to 26.6
Index ranges	-9<=h=>9 -13<=k=>9 -18<=l=>18	-10<=h=>10 -11<=k=>11 -16<=l=>16	-8<=h=>8 -9<=k=>9 -24<=l=>25	-5<=h=>6 -15<=k=>15 -18<=l=>18
Reflections collected	3838	4202	4015	3543
Unique reflections (R_{int})	2363	3185	2854	2737
D (mg/m³)	1.415	1.391	1.347	1.429
Final *R* indices	R_1= 0.0896 WR_2= 0.132	R_1= 0.0702 WR_2= 0.1302	R_1= 0.0975 WR_2= 0.1789	R_1= 0.0658 WR_2= 0.1323
R indices (all data)	R_1= 0.0493 WR_2= 0.1178	R_1= 0.049 WR_2= 0.1162	R_1= 0.0685 WR_2= 0.1597	R_1= 0.0482 WR_2= 0.1198

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Table S2. Geometric parameters of hydrogen bonding **(**Å**, °)**

Compound	D-H···A	D-H	H···A	D···A	D-H···A
3b	N3-H1A···O3	0.90 (2)	1.89 (2)	2.683 (17)	145.9 (19)
3f	N1-H1A···O1	0.91 (2)	1.99 (2)	2.7518 (16)	140.3 (18)
3h	N2-H1A···O2	0.95 (3)	1.90 (3)	2.701 (2)	140.0 (2)
3i	N1-H1···O2	0.86 (2)	1.99 (2)	2.7222 (17)	141.8 (18)

Figure S1. Unit cells for compounds a) **3b**, b) **3f**, c) **3h** and d) **3i**.

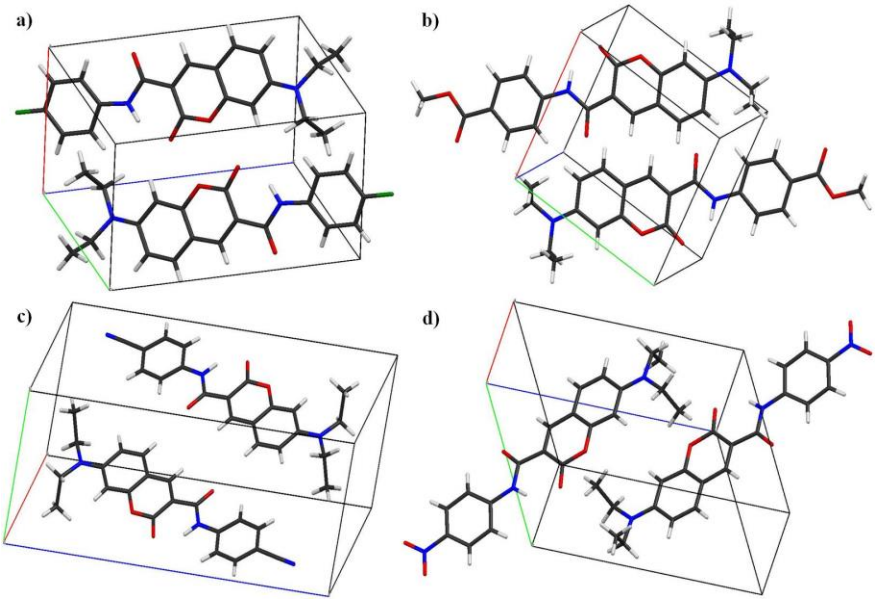

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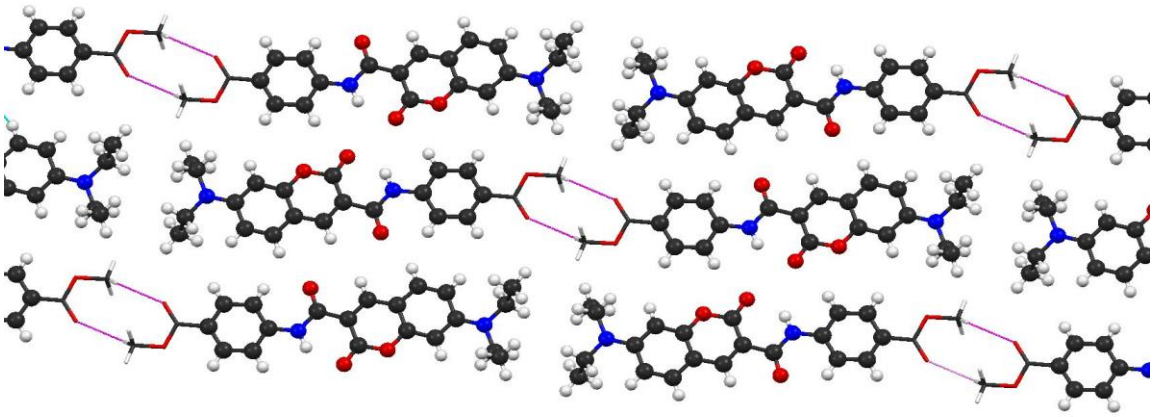
Figure S2. Hydrogen bond ring present in compound **3f**.



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3. DFT-Computed Structural Parameters for compounds 3a-i

Table S3. DFT-computed structural parameters of push-pull amides (*vacuum*). Bond distances are given in angstroms (Å).

Substitution		σ_{para}	Bond 1	Bond 2	Bond 3	Bond 4	Bond 5
Molecule	Group						
3a	H	0.000	1.507	1.360	1.406	1.018	1.873
3b	F	0.062	1.506	1.360	1.406	1.018	1.869
3c	CCH	0.230	1.505	1.363	1.402	1.018	1.868
3d	Cl	0.227	1.505	1.362	1.403	1.018	1.866
3e	Br	0.232	1.505	1.362	1.403	1.018	1.866
3f	CO_2Me	0.450	1.505	1.364	1.400	1.018	1.867
3g	CF_3	0.540	1.504	1.364	1.400	1.018	1.864
3h	CN	0.660	1.502	1.367	1.397	1.019	1.858
3i	NO_2	0.778	1.502	1.368	1.395	1.019	1.854

Table S4. DFT-computed structural parameters of push-pull amides (*MeCN*). Bond distances are given in angstroms (Å).

Substitution		σ_{para}	Bond 1	Bond 2	Bond 3	Bond 4	Bond 5
Molecule	Group						
3a	H	0.000	1.500	1.360	1.406	1.018	1.863
3b	F	0.062	1.499	1.360	1.406	1.019	1.861
3c	CCH	0.230	1.498	1.364	1.401	1.019	1.858
3d	Cl	0.227	1.498	1.363	1.402	1.019	1.859
3e	Br	0.232	1.498	1.363	1.402	1.019	1.859
3f	CO_2Me	0.450	1.497	1.366	1.398	1.019	1.855
3g	CF_3	0.540	1.497	1.365	1.399	1.019	1.856
3h	CN	0.660	1.495	1.368	1.395	1.020	1.851
3i	NO_2		1.495	1.370	1.392	1.020	1.848

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4. UV-Vis solvatochromic studies for compounds 3a-i

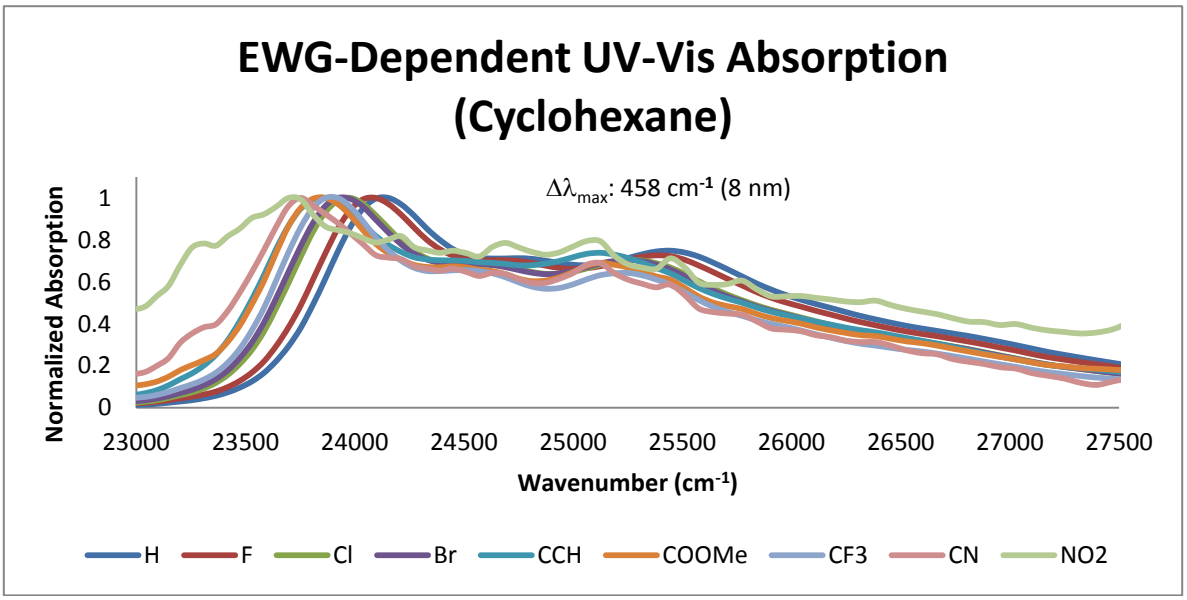

Figure S3. UV-Vis solvatochromic study of the family of compounds 3a-i in cyclohexane.

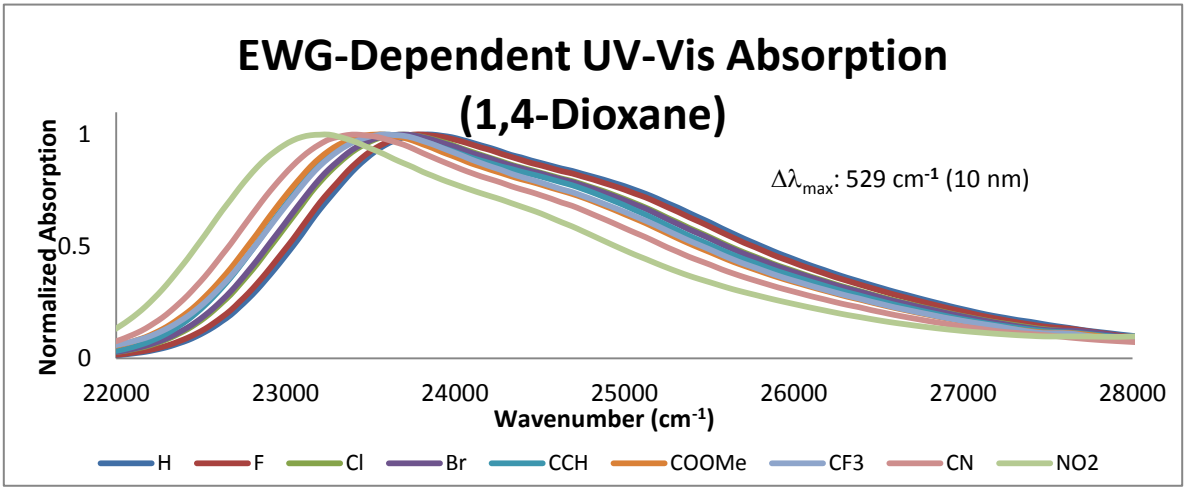

Figure S4. UV-Vis solvatochromic study of the family of compounds 3a-i in 1,4-dioxane.

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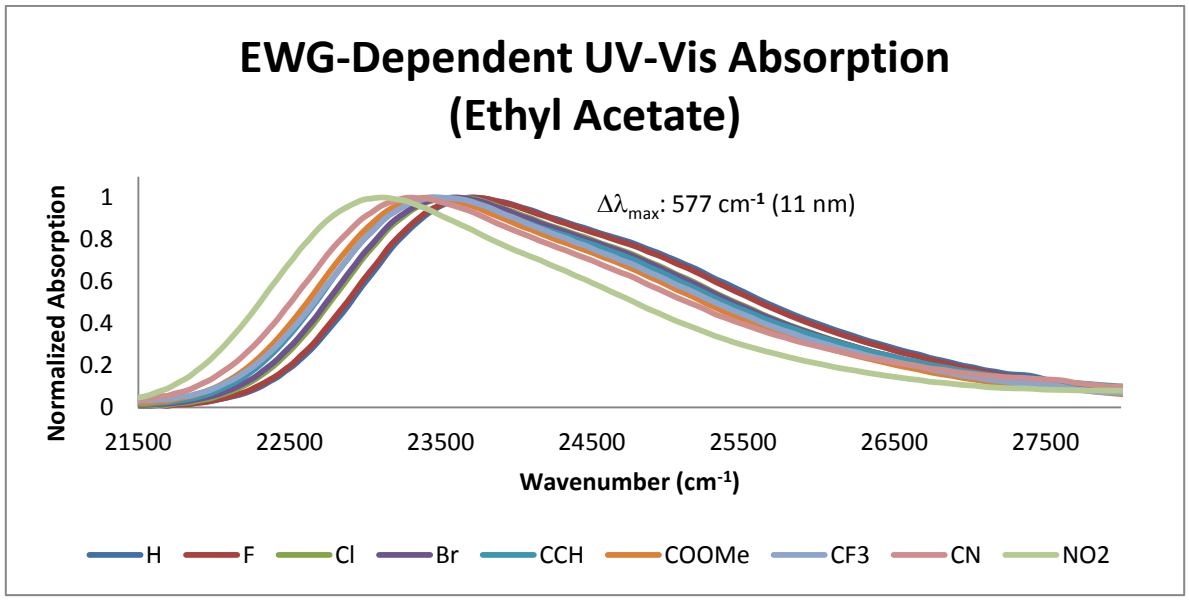

Figure S5. UV-Vis solvatochromic study of the family of compounds 3a-i in ethyl acetate.

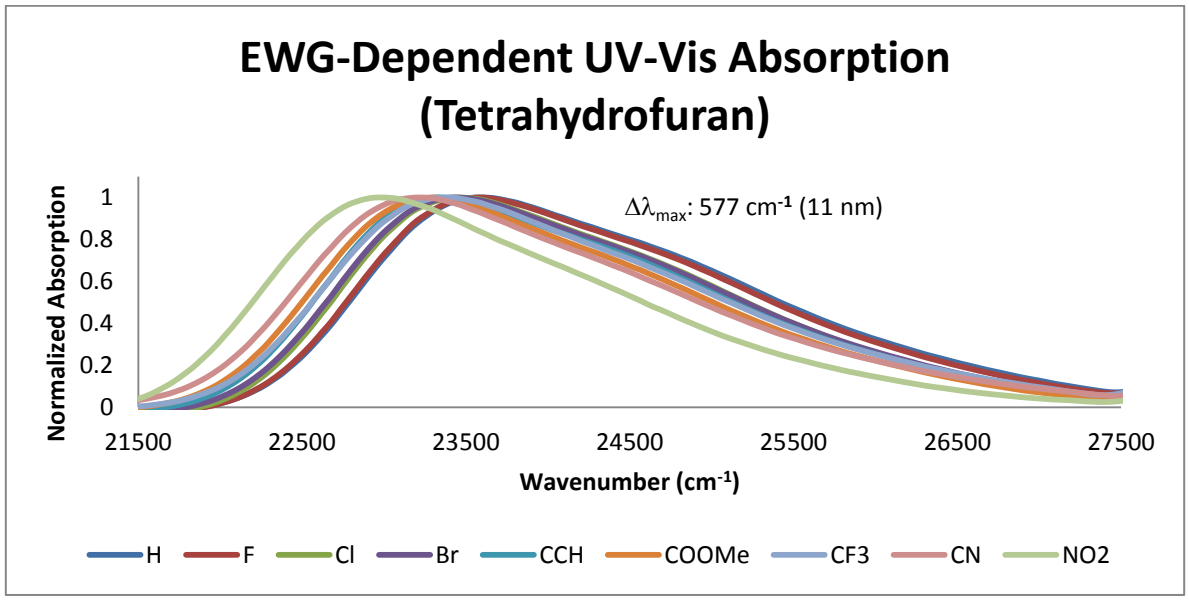

Figure S6. UV-Vis solvatochromic study of the family of compounds 3a-i in tetrahydrofuran.

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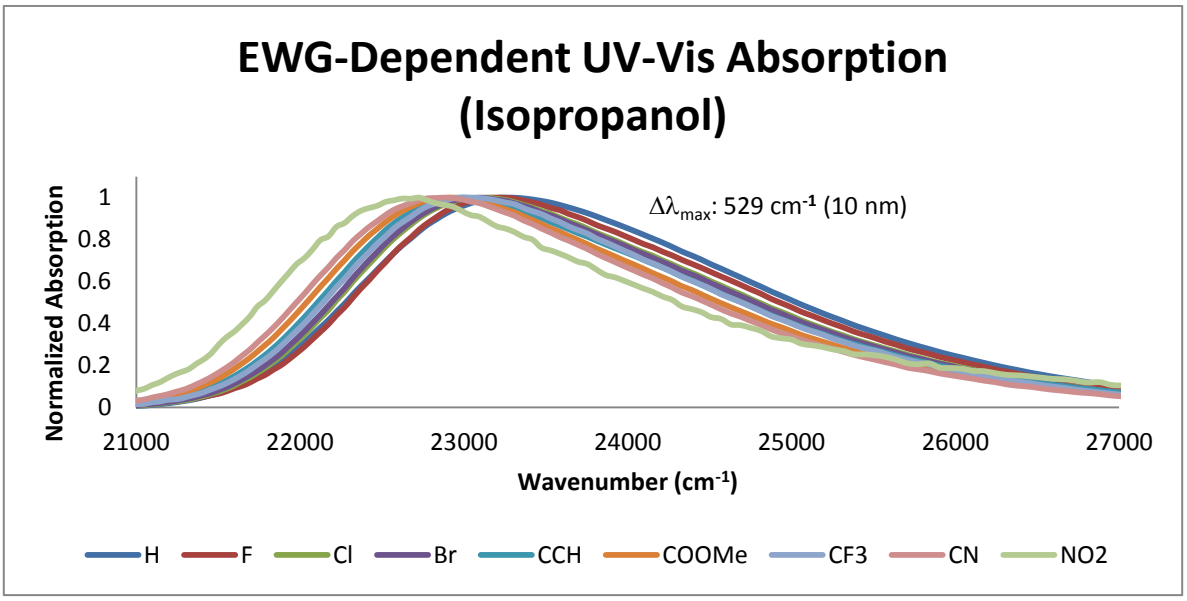

Figure S7. UV-Vis solvatochromic study of the family of compounds 3a-i in isopropanol.

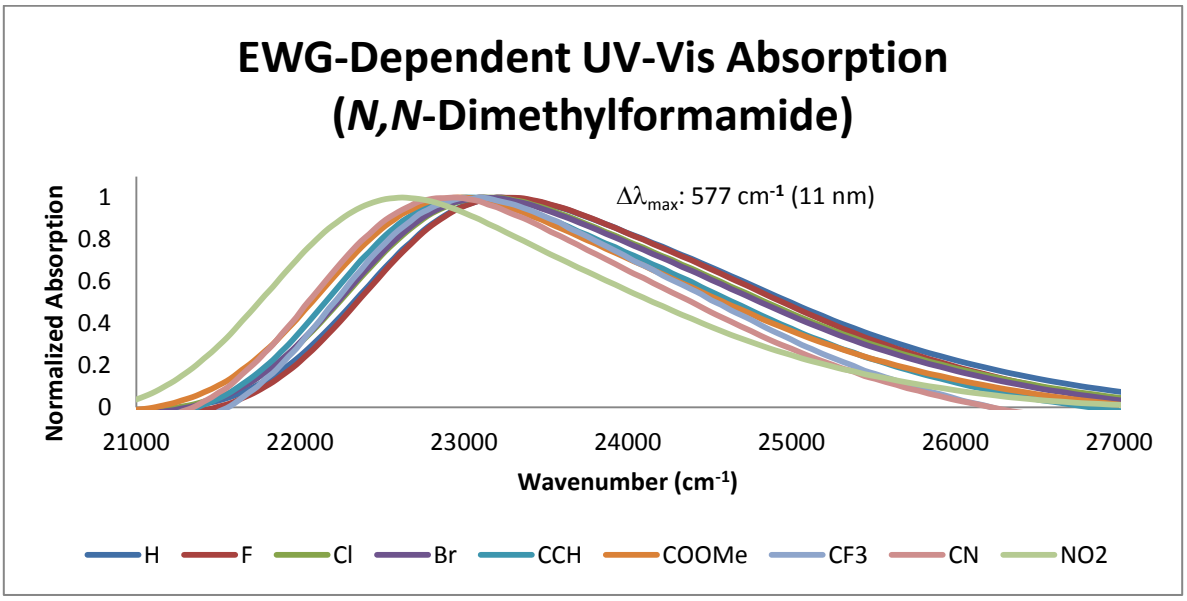

Figure S8. UV-Vis solvatochromic study of the family of compounds 3a-i in dimethylformamide.

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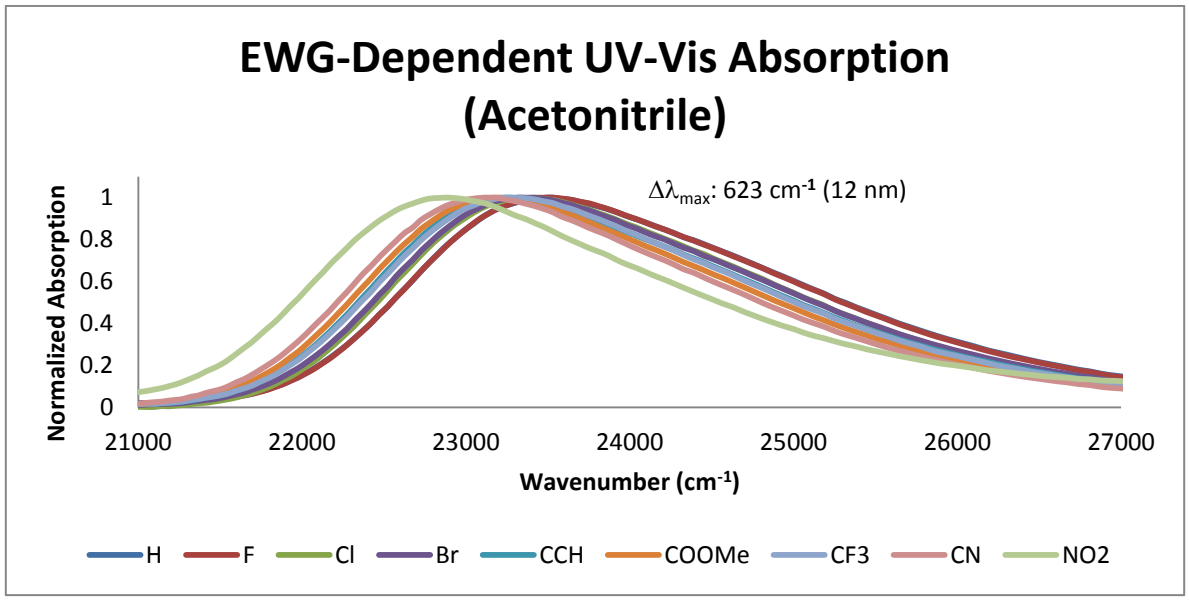

Figure S9. UV-Vis solvatochromic study of the family of compounds 3a-i in acetonitrile.

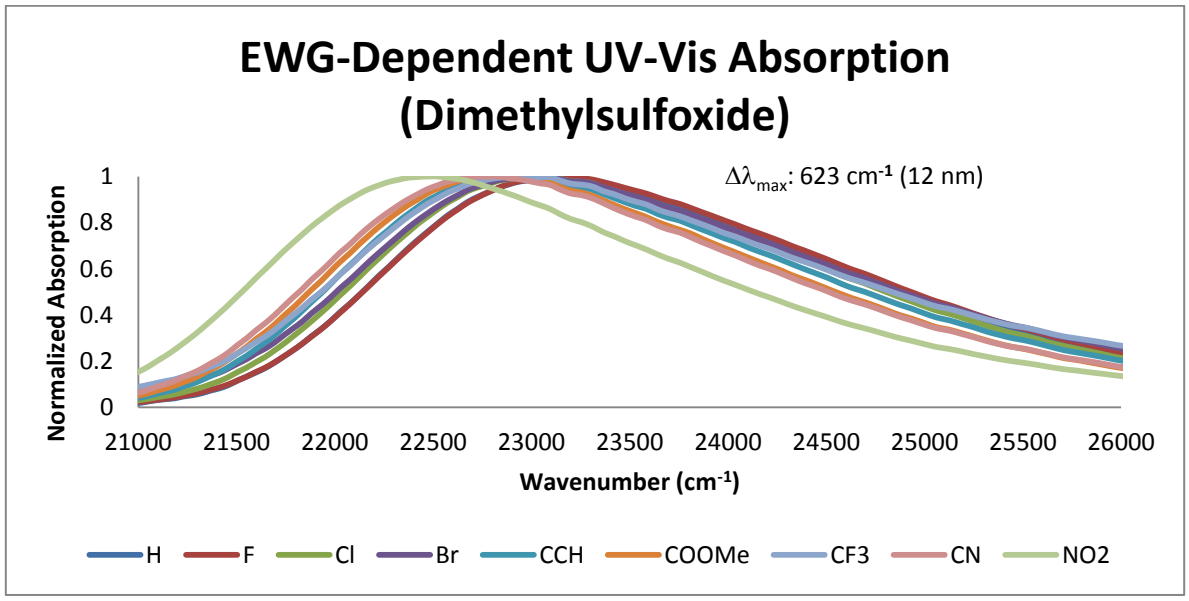

Figure S10. UV-Vis solvatochromic study of the family of compounds 3a-i in dimethylsulfoxide.

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5. Correlation between λ_{max} and σ_{para} for compounds 3a-i in different solvents

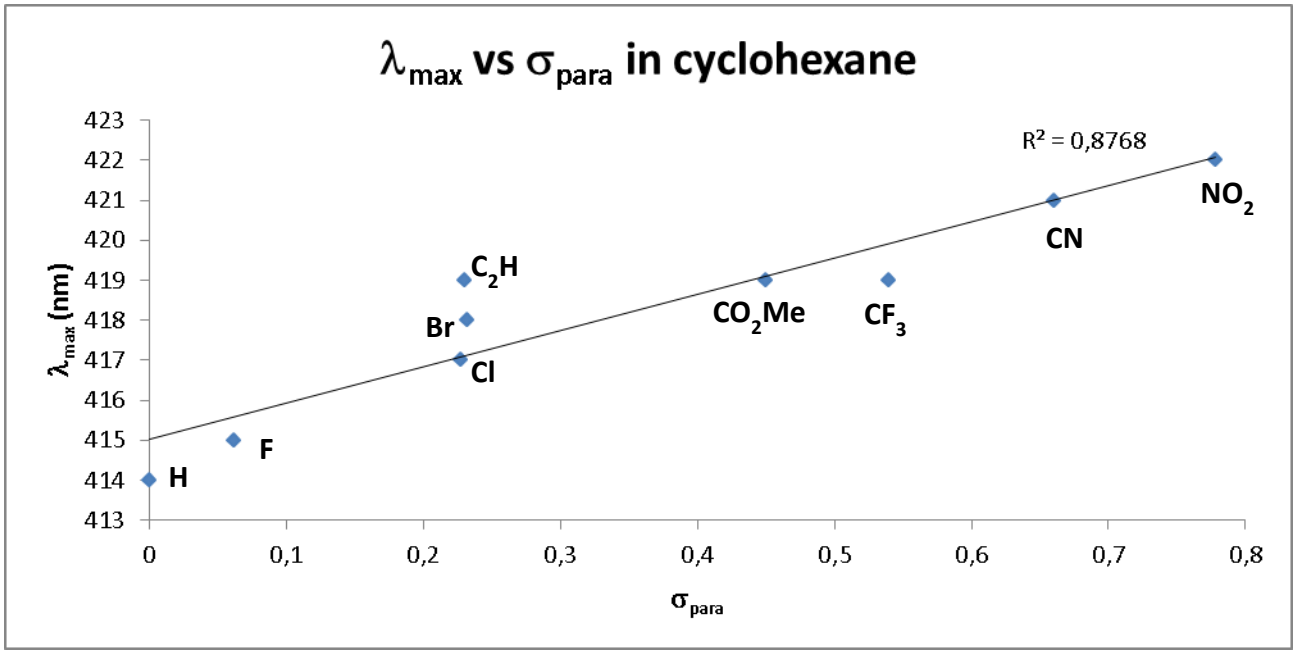

Figure S11. Correlation between λ_{max} and σ_{para} of compounds 3a-i in cyclohexane.

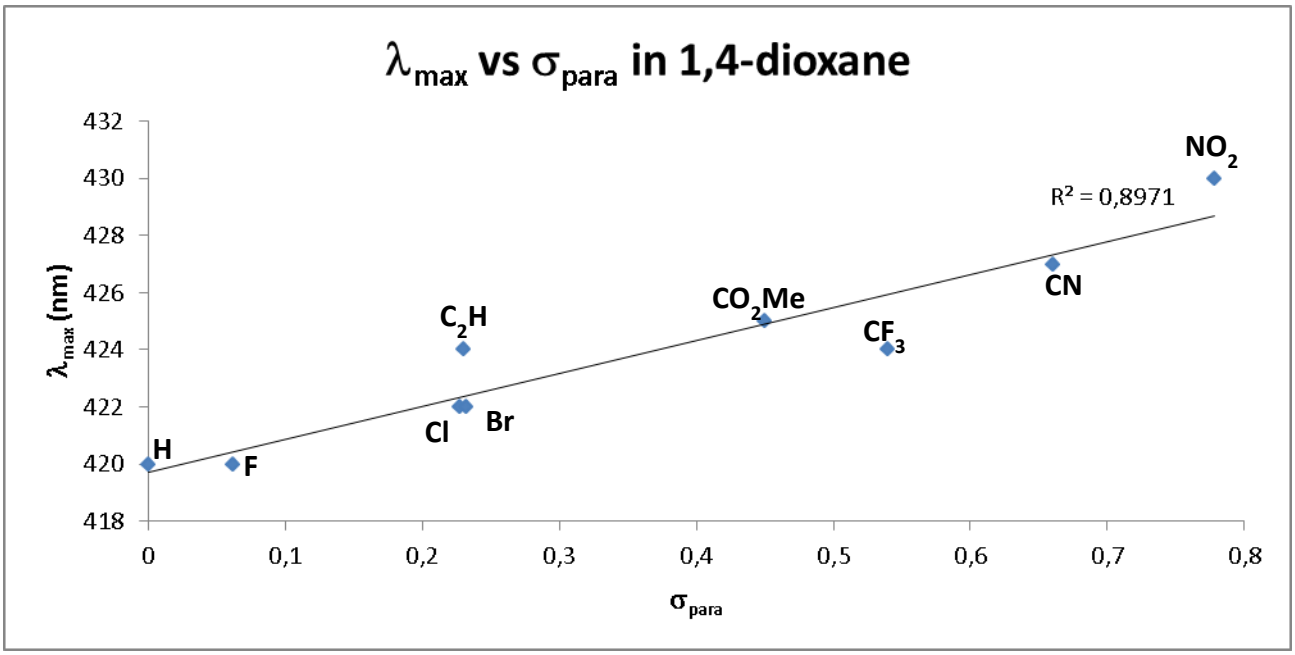

Figure S12. Correlation between λ_{max} and σ_{para} of compounds 3a-i in 1,4-dioxane.

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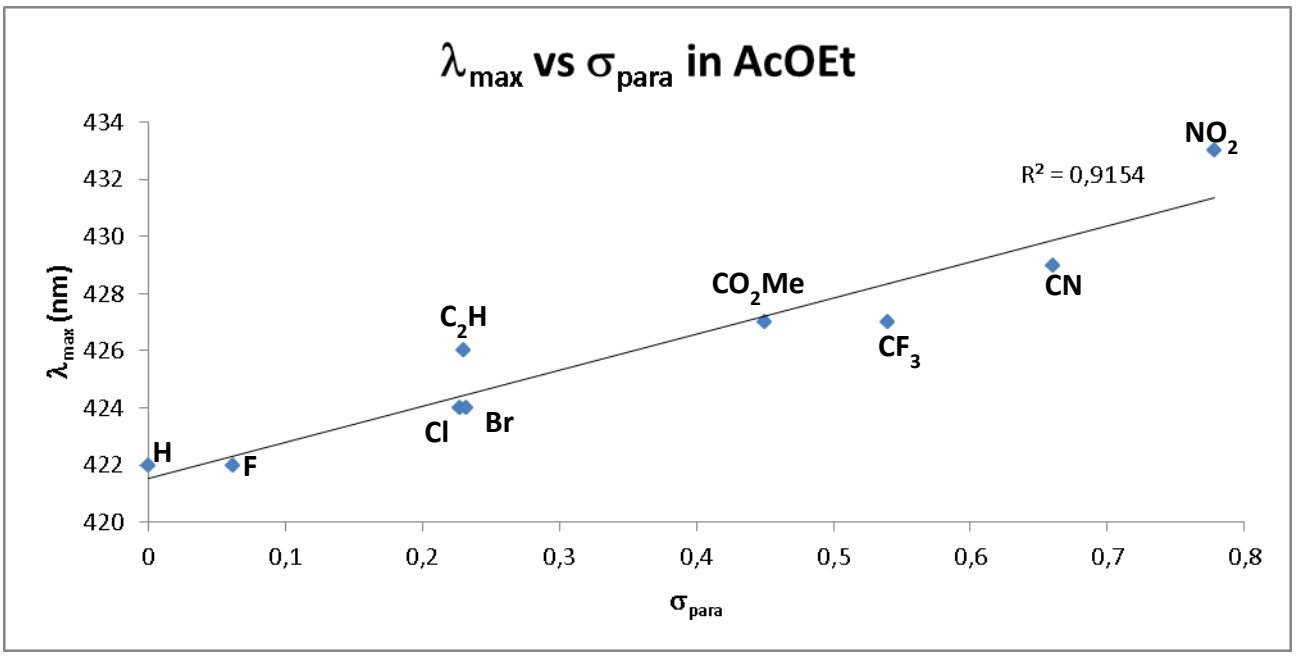

Figure S13. Correlation between λ_{max} and σ_{para} of compounds 3a-i in ethyl acetate.

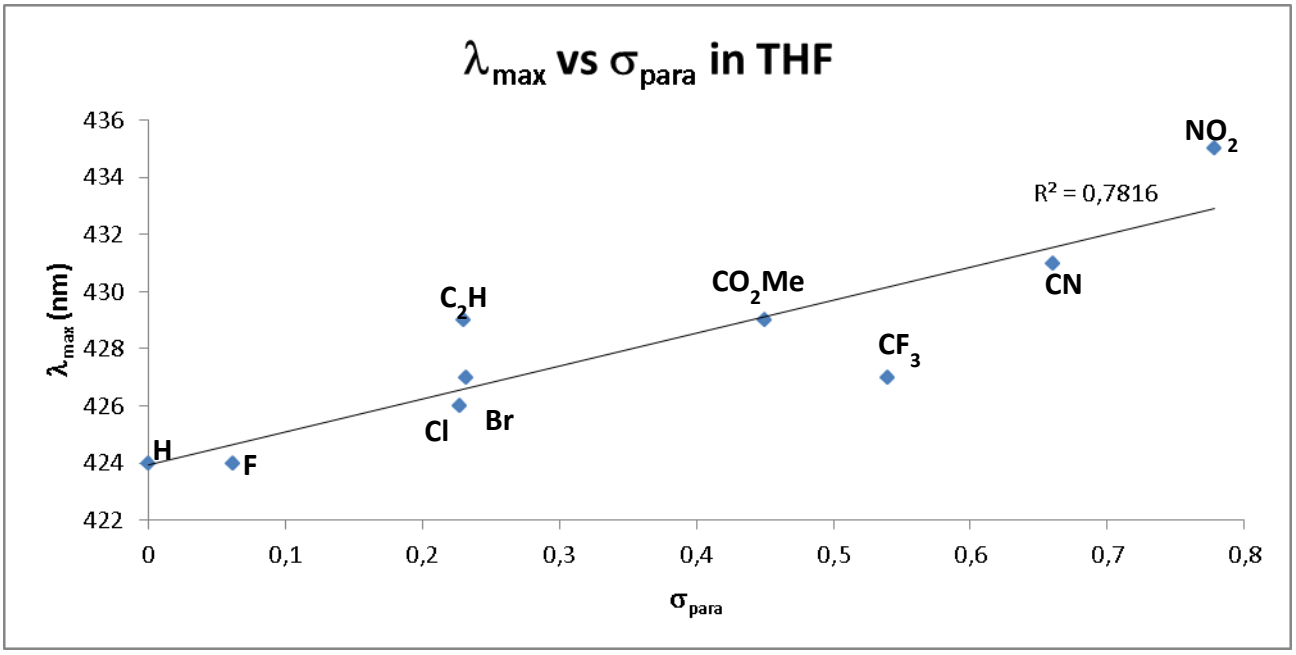

Figure S14. Correlation between λ_{max} and σ_{para} of compounds 3a-i in 1,4-THF.

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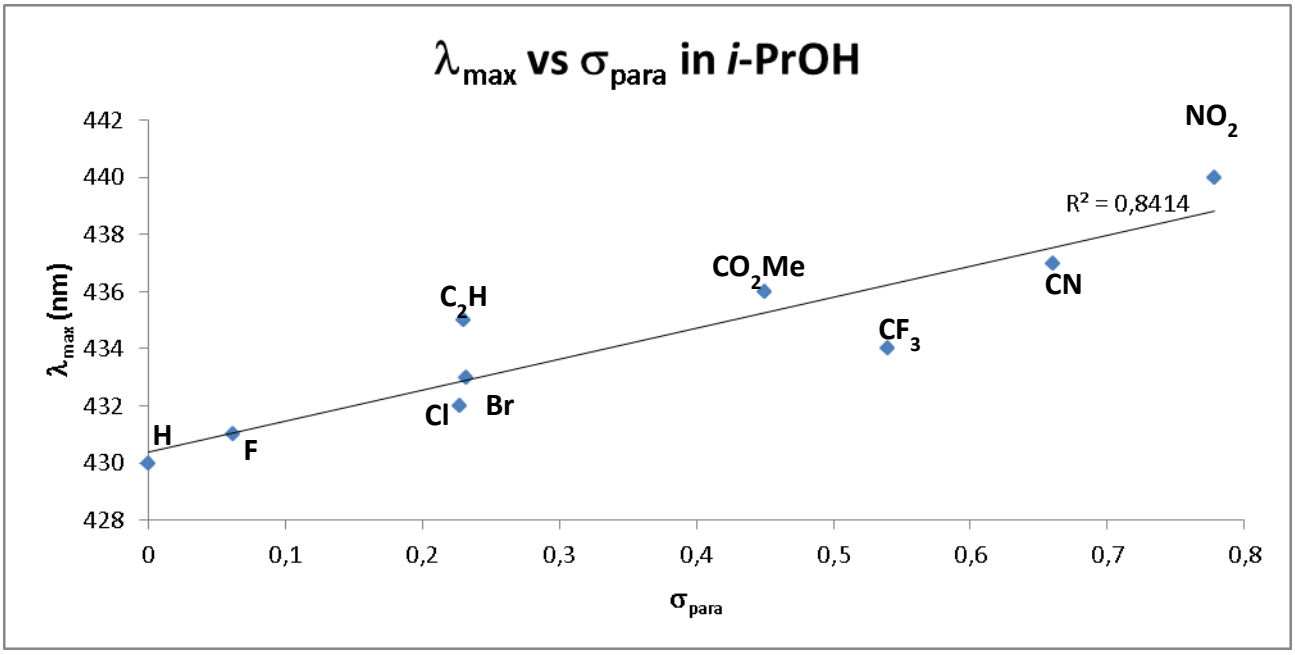

Figure S15. Correlation between λ_{max} and σ_{para} of compounds 3a-i in isopropanol.

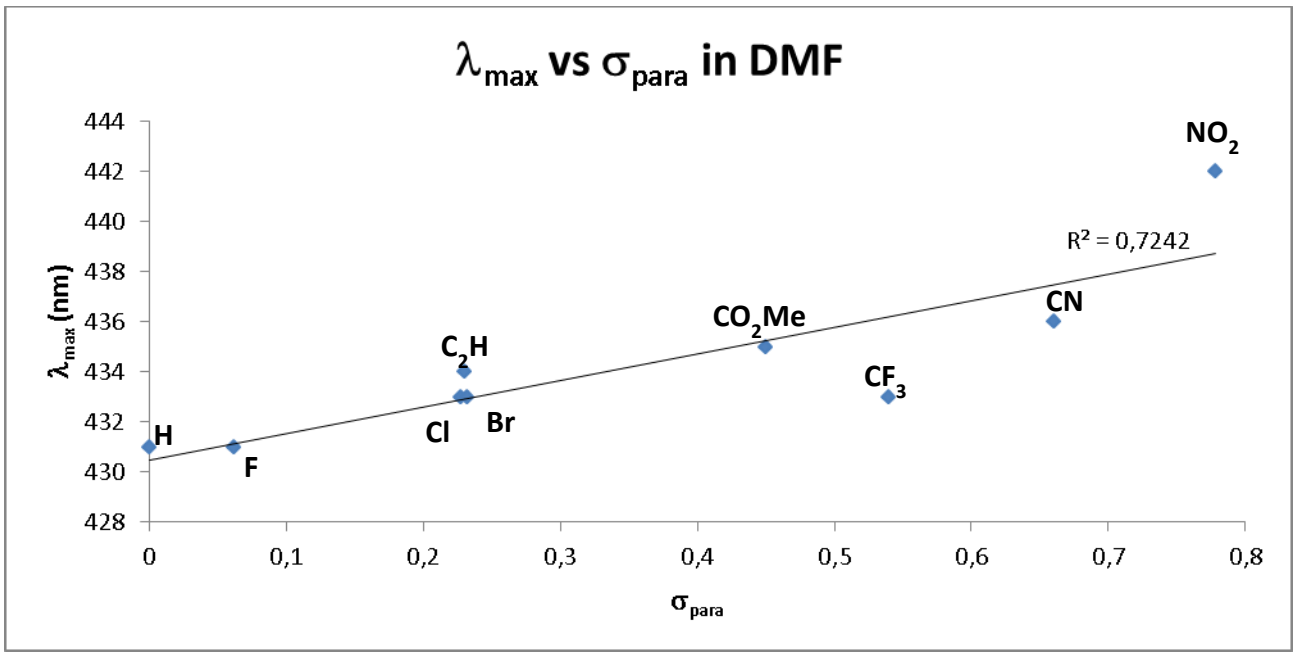

Figure S16. Correlation between λ_{max} and σ_{para} of compounds 3a-i in dimethylformamide.

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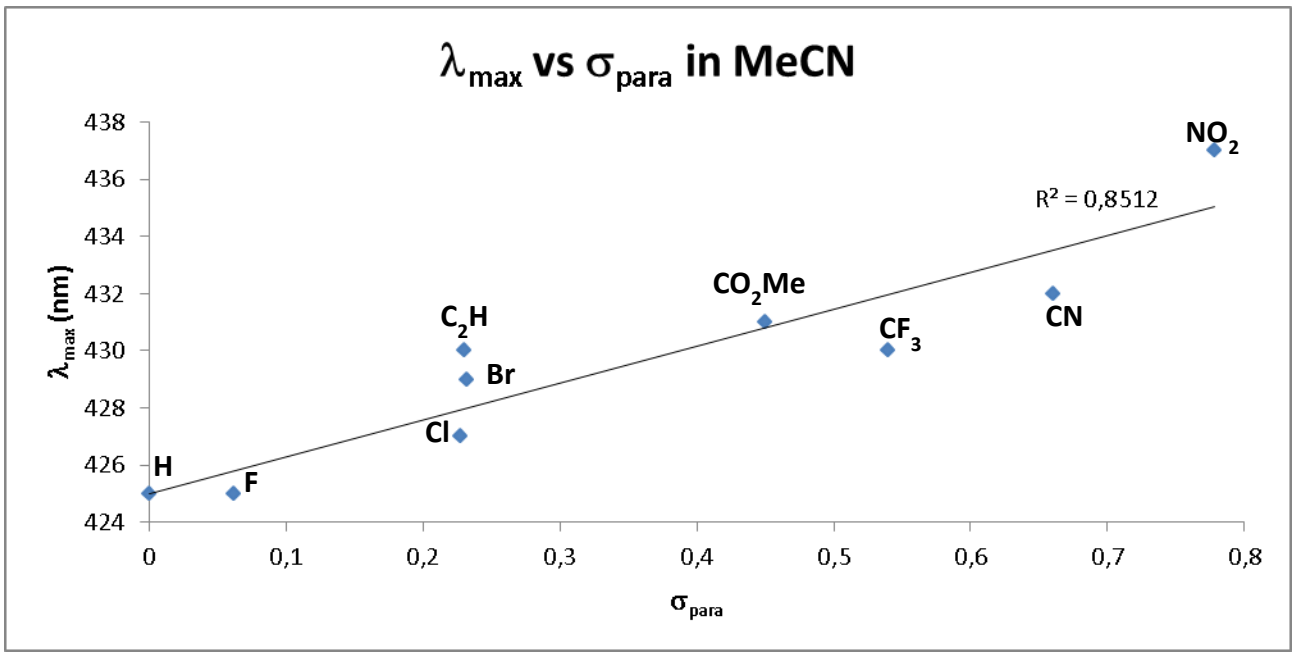

Figure S17. Correlation between λ_{max} and σ_{para} of compounds 3a-i in acetonitrile.

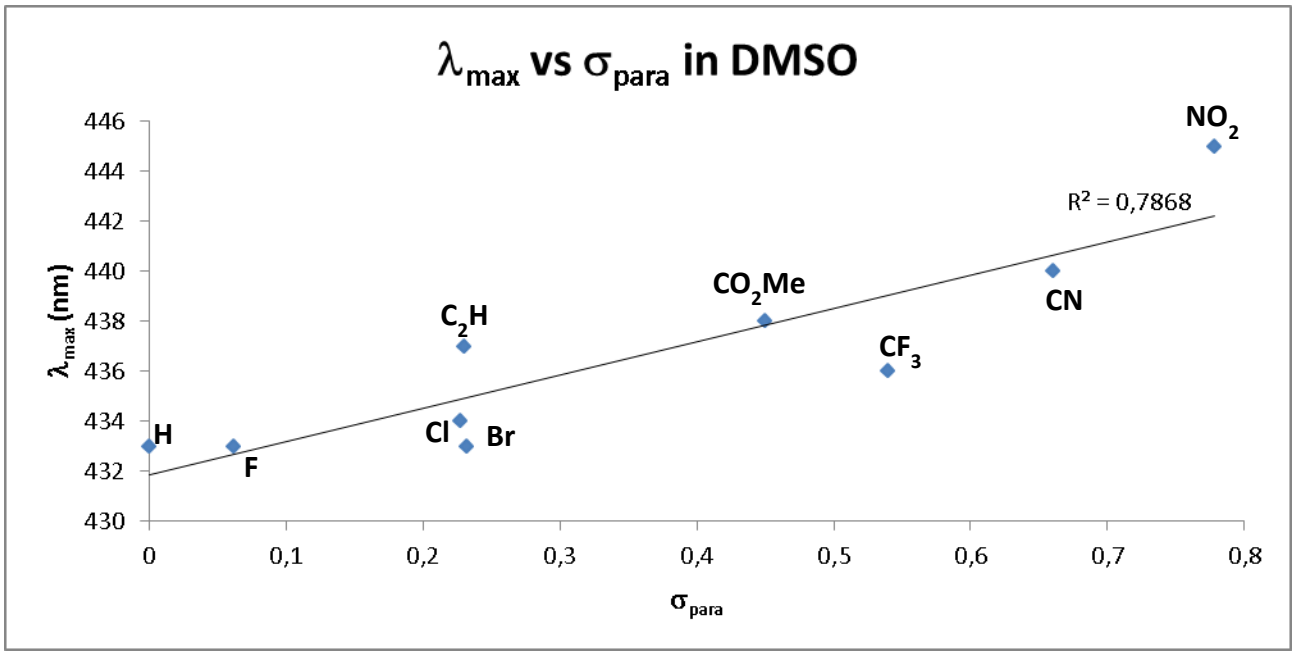

Figure S18. Correlation between λ_{max} and σ_{para} of compounds 3a-i in dimethylsulfoxide.

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6. Frontier Molecular Orbitals for compounds 3b-h

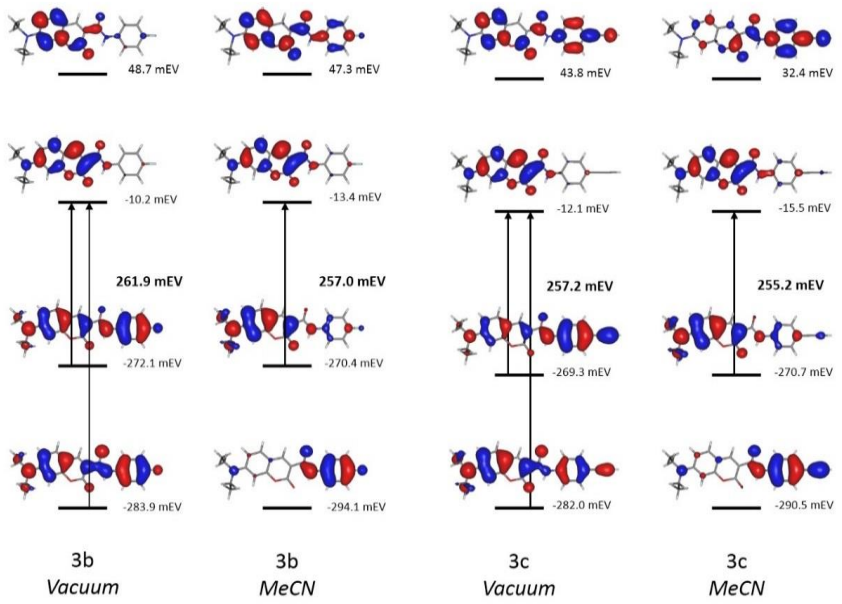

Figure S19. Frontier molecular orbitals for compounds **3b** and **3c**. Arrows represent the transitions involved in the first excited state, according to TDDFT computations. HOMO-LUMO gaps are also depicted.

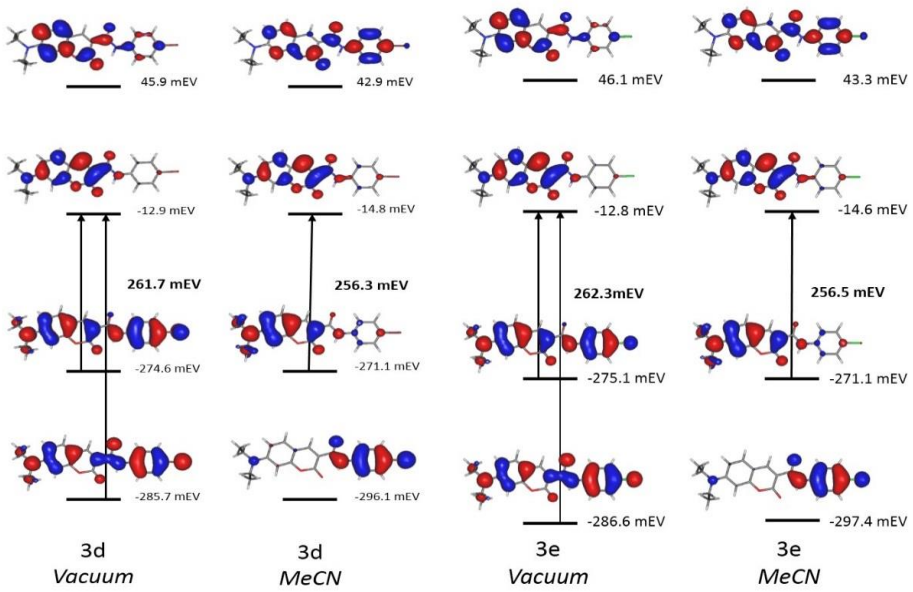

Figure S20. Frontier molecular orbitals for compounds **3d** and **3e**. Arrows represent the transitions involved in the first excited state, according to TDDFT computations. HOMO-LUMO gaps are also depicted.

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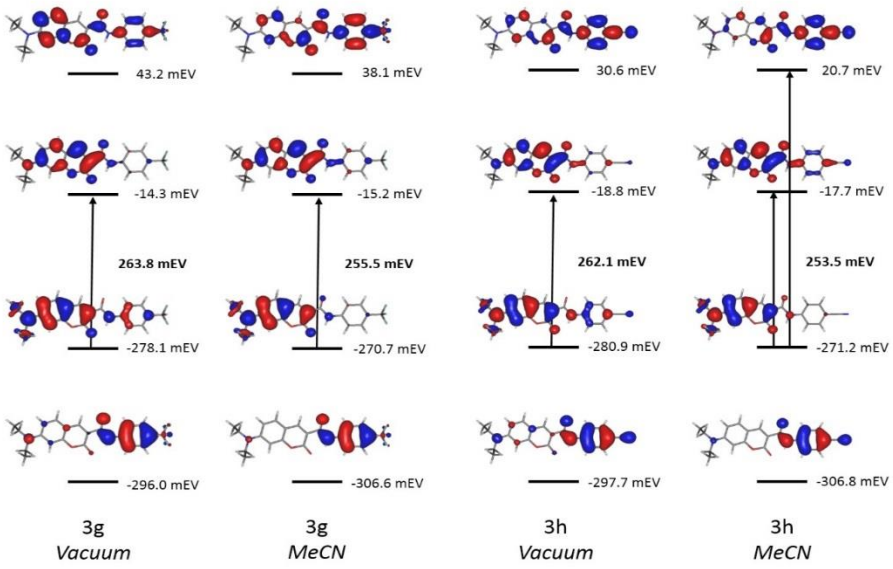

Figure S21. Frontier molecular orbitals for compounds **3g** and **3h**. Arrows represent the transitions involved in the first excited state, according to TDDFT computations. HOMO-LUMO gaps are also depicted.

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7. Molecular Geometries for compounds 3a-i

Molecule 3a (Vacuum)

H	-1.97900	-3.01280	-0.15099
C	-2.23492	-1.95796	-0.19692
C	-2.89675	0.74934	-0.30150
C	-1.19987	-1.00687	-0.18759
C	-3.55503	-1.58290	-0.25760
C	-3.92874	-0.20829	-0.32192
C	-1.57514	0.34102	-0.24172
H	-4.31091	-2.35672	-0.25710
H	-3.08680	1.81359	-0.32499
C	0.18854	-1.30587	-0.11765
H	0.53009	-2.33693	-0.07046
C	1.13230	-0.32796	-0.10562
C	0.71614	1.07057	-0.16512
O	-0.63274	1.31964	-0.22924
O	1.43952	2.04646	-0.16376
N	-5.24659	0.16396	-0.41887
C	2.57190	-0.76704	-0.02622
O	2.83682	-1.96165	0.02530
N	3.48807	0.23808	-0.01668
H	3.09529	1.17556	-0.06557
C	4.88841	0.14189	0.06047
C	7.68419	0.14012	0.21510
C	5.58260	-1.06947	0.14443
C	5.60253	1.34667	0.05301
C	6.98813	1.34330	0.12989
C	6.97246	-1.05465	0.22109
H	7.52417	2.28785	0.12328
H	7.50191	-2.00082	0.28760
C	-6.31551	-0.81999	-0.30102
H	-7.22175	-0.35935	-0.70392
H	-6.09844	-1.66918	-0.95806
C	-6.57876	-1.30315	1.12672
H	-6.90888	-0.47840	1.76469
H	-5.67754	-1.73303	1.57378
H	-7.36074	-2.06945	1.12782
C	-5.62095	1.57199	-0.43658
H	-6.61657	1.63870	-0.88490
H	-4.95271	2.10784	-1.11866
C	-5.62897	2.24367	0.93820
H	-6.39277	1.80366	1.58604
H	-5.84485	3.31203	0.83496
H	-4.66116	2.13657	1.43691
H	5.03372	-2.00035	0.14960
H	5.06454	2.28923	-0.01338
H	8.76807	0.13569	0.27714

Sum of electronic and zero-point Energies= -1108.663665

Sum of electronic and thermal Energies= -1108.641925

Sum of electronic and thermal Enthalpies= -1108.640981

Sum of electronic and thermal Free Energies= -1108.716456

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Molecule 3a (MeCN)

H	-1.99032	-3.02002	-0.13012
C	-2.24213	-1.96492	-0.18228
C	-2.89181	0.75244	-0.30249
C	-1.20145	-1.01343	-0.18157
C	-3.55792	-1.58516	-0.24169
C	-3.93017	-0.20553	-0.31466
C	-1.57607	0.33703	-0.24240
H	-4.31647	-2.35590	-0.23301
H	-3.08285	1.81632	-0.33169
C	0.17878	-1.31475	-0.11424
H	0.50716	-2.34922	-0.06382
C	1.13272	-0.33735	-0.10857
C	0.71930	1.05517	-0.17236
O	-0.62271	1.31078	-0.23676
O	1.44550	2.03690	-0.17500
N	-5.23865	0.16625	-0.40964
C	2.56626	-0.77189	-0.03124
O	2.84374	-1.96853	0.01992
N	3.48502	0.23137	-0.02105
H	3.09031	1.16899	-0.06921
C	4.88552	0.14044	0.05944
C	7.68515	0.15465	0.22120
C	5.59046	-1.06686	0.12737
C	5.59348	1.35033	0.07163
C	6.97964	1.35481	0.15186
C	6.98135	-1.04546	0.20783
H	7.50868	2.30303	0.16086
H	7.51654	-1.98913	0.26149
C	-6.31466	-0.81764	-0.30001
H	-7.21442	-0.35358	-0.71016
H	-6.09324	-1.66847	-0.95187
C	-6.58751	-1.29100	1.12798
H	-6.91646	-0.46069	1.75907
H	-5.69355	-1.72934	1.58191
H	-7.37530	-2.05068	1.12321
C	-5.61496	1.57734	-0.44443
H	-6.60800	1.63656	-0.89638
H	-4.94403	2.10732	-1.12739
C	-5.63037	2.25603	0.92575
H	-6.39502	1.81620	1.57224
H	-5.85212	3.32156	0.81011
H	-4.66314	2.16034	1.42854
H	5.05170	-2.00326	0.11818
H	5.05130	2.29091	0.01896
H	8.76870	0.15704	0.28594

Sum of electronic and zero-point Energies= -1108.679114

Sum of electronic and thermal Energies= -1108.657308

Sum of electronic and thermal Enthalpies= -1108.656364

Sum of electronic and thermal Free Energies= -1108.732177

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Molecule 3b (Vacuum)

H	-2.37184	-3.01312	-0.14667
C	-2.62624	-1.95792	-0.19268
C	-3.28405	0.75061	-0.29761
C	-1.58960	-1.00830	-0.18716
C	-3.94575	-1.58085	-0.24996
C	-4.31764	-0.20557	-0.31465
C	-1.96308	0.34025	-0.24119
H	-4.70285	-2.35346	-0.24673
H	-3.47255	1.81511	-0.32117
C	-0.20177	-1.30941	-0.12198
H	0.13821	-2.34102	-0.07565
C	0.74333	-0.33241	-0.11412
C	0.32907	1.06647	-0.17259
O	-1.01906	1.31758	-0.23206
O	1.05460	2.04114	-0.17358
N	-5.63485	0.16825	-0.40855
C	2.18217	-0.77146	-0.04142
O	2.44959	-1.96598	0.00970
N	3.09865	0.23296	-0.03754
H	2.70670	1.17106	-0.08423
C	4.49938	0.13076	0.02942
C	7.27010	0.11119	0.15928
C	5.18882	-1.08441	0.10418
C	5.22194	1.32999	0.02017
C	6.60818	1.32673	0.08495
C	6.57876	-1.08797	0.16930
H	7.17353	2.25202	0.07840
H	7.12684	-2.02201	0.22824
C	-6.70496	-0.81419	-0.28705
H	-7.61157	-0.35256	-0.68792
H	-6.49089	-1.66423	-0.94395
C	-6.96492	-1.29540	1.14188
H	-7.29198	-0.46942	1.77984
H	-6.06322	-1.72629	1.58700
H	-7.74810	-2.06045	1.14591
C	-6.00759	1.57681	-0.42952
H	-7.00380	1.64350	-0.87648
H	-5.33981	2.10991	-1.11414
C	-6.01257	2.25192	0.94352
H	-6.77566	1.81427	1.59378
H	-6.22769	3.32019	0.83793
H	-5.04401	2.14523	1.44089
H	4.63504	-2.01238	0.11109
H	4.69264	2.27740	-0.03876
F	8.61355	0.09941	0.22290

Sum of electronic and zero-point Energies= -1207.880284

Sum of electronic and thermal Energies= -1207.857704

Sum of electronic and thermal Enthalpies= -1207.856760

Sum of electronic and thermal Free Energies= -1207.934254

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Molecule 3b (MeCN)

H	-2.38259	-3.01899	-0.13391
C	-2.63306	-1.96344	-0.18317
C	-3.27911	0.75517	-0.29622
C	-1.59102	-1.01337	-0.18234
C	-3.94836	-1.58173	-0.23946
C	-4.31885	-0.20138	-0.30875
C	-1.96389	0.33781	-0.23959
H	-4.70791	-2.35150	-0.23130
H	-3.46869	1.81938	-0.32261
C	-0.21122	-1.31687	-0.11908
H	0.11583	-2.35191	-0.07165
C	0.74388	-0.34052	-0.11439
C	0.33248	1.05258	-0.17446
O	-1.00912	1.31033	-0.23399
O	1.06064	2.03297	-0.17775
N	-5.62687	0.17232	-0.40068
C	2.17670	-0.77603	-0.04368
O	2.45497	-1.97284	0.00638
N	3.09660	0.22570	-0.03863
H	2.70430	1.16454	-0.08459
C	4.49738	0.12682	0.02869
C	7.26876	0.11926	0.15947
C	5.19454	-1.08498	0.09840
C	5.21581	1.33012	0.02513
C	6.60233	1.33304	0.09037
C	6.58555	-1.08425	0.16414
H	7.16053	2.26267	0.08812
H	7.13556	-2.01746	0.21907
C	-6.70404	-0.81045	-0.29187
H	-7.60391	-0.34398	-0.69898
H	-6.48507	-1.65970	-0.94659
C	-6.97485	-1.28733	1.13531
H	-7.30159	-0.45828	1.76921
H	-6.08067	-1.72804	1.58651
H	-7.76360	-2.04601	1.12989
C	-6.00149	1.58394	-0.43316
H	-6.99468	1.64506	-0.88452
H	-5.33028	2.11418	-1.11562
C	-6.01541	2.26027	0.93817
H	-6.77997	1.81986	1.58437
H	-6.23643	3.32616	0.82454
H	-5.04791	2.16295	1.44015
H	4.64970	-2.01771	0.10145
H	4.68466	2.27615	-0.02901
F	8.61510	0.11344	0.22362

Sum of electronic and zero-point Energies= -1207.895484

Sum of electronic and thermal Energies= -1207.872810

Sum of electronic and thermal Enthalpies= -1207.871866

Sum of electronic and thermal Free Energies= -1207.949889

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Molecule 3c (Vacuum)

H	-2.61819	-3.01402	-0.14359
C	-2.87067	-1.95838	-0.18966
C	-3.52327	0.75163	-0.29457
C	-1.83201	-1.01072	-0.19040
C	-4.18954	-1.57868	-0.24087
C	-4.55894	-0.20256	-0.30542
C	-2.20305	0.33866	-0.24411
H	-4.94819	-2.34970	-0.23275
H	-3.70970	1.81647	-0.31832
C	-0.44491	-1.31460	-0.13132
H	-0.10731	-2.34699	-0.08532
C	0.50237	-0.33924	-0.12875
C	0.09078	1.06044	-0.18683
O	-1.25699	1.31406	-0.24060
O	0.81840	2.03347	-0.19228
N	-5.87549	0.17392	-0.39323
C	1.93988	-0.78129	-0.06107
O	2.20620	-1.97495	-0.01033
N	2.86007	0.22359	-0.06056
H	2.46807	1.16205	-0.10700
C	4.25669	0.12214	0.00423
C	7.06333	0.10804	0.13440
C	4.94877	-1.09205	0.07963
C	4.97820	1.32360	-0.00703
C	6.36047	1.31785	0.05716
C	6.33540	-1.08719	0.14382
H	4.39801	-2.02164	0.08801
H	4.44616	2.26955	-0.06664
H	6.90723	2.25511	0.04829
H	6.86791	-2.03098	0.20365
C	-6.94731	-0.80617	-0.26684
H	-7.85437	-0.34293	-0.66474
H	-6.73757	-1.65724	-0.92376
C	-6.24525	1.58338	-0.41415
H	-5.57939	2.11407	-1.10249
H	-7.24336	1.65171	-0.85652
C	-6.24217	2.25990	0.95816
H	-5.27156	2.15162	1.45119
H	-7.00318	1.82475	1.61252
H	-6.45536	3.32852	0.85238
C	-7.20283	-1.28525	1.16358
H	-7.52600	-0.45793	1.80177
H	-6.30033	-1.71733	1.60590
H	-7.98741	-2.04882	1.17138
C	8.49414	0.09676	0.20346
H	10.76454	0.07994	0.31636
C	9.69943	0.08884	0.26188

Sum of electronic and zero-point Energies= -1184.769576

Sum of electronic and thermal Energies= -1184.745673

Sum of electronic and thermal Enthalpies= -1184.744729

Sum of electronic and thermal Free Energies= -1184.825048

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Molecule 3c (MeCN)

H	-2.62938	-3.02000	-0.12909
C	-2.87784	-1.96405	-0.17943
C	-3.51811	0.75610	-0.29508
C	-1.83350	-1.01619	-0.18847
C	-4.19242	-1.57948	-0.22731
C	-4.56020	-0.19823	-0.29742
C	-2.20372	0.33597	-0.24671
H	-4.95369	-2.34740	-0.21144
H	-3.70548	1.82063	-0.32301
C	-0.45470	-1.32273	-0.13316
H	-0.13000	-2.35845	-0.08456
C	0.50288	-0.34800	-0.13703
C	0.09446	1.04584	-0.19863
O	-1.24676	1.30628	-0.25038
O	0.82493	2.02445	-0.20932
N	-5.86759	0.17837	-0.38040
C	1.93375	-0.78639	-0.07140
O	2.21199	-1.98178	-0.01956
N	2.85767	0.21653	-0.07189
H	2.46471	1.15555	-0.11885
C	4.25299	0.11808	-0.00222
C	7.06205	0.11363	0.14033
C	4.95241	-1.09349	0.06744
C	4.97167	1.32287	-0.00214
C	6.35395	1.32208	0.06810
C	6.33946	-1.08543	0.13800
H	4.40959	-2.02728	0.06735
H	4.43867	2.26791	-0.05651
H	6.89332	2.26367	0.06826
H	6.87212	-2.02954	0.19348
C	-6.94651	-0.80169	-0.26360
H	-7.84753	-0.33387	-0.66658
H	-6.73318	-1.65263	-0.91791
C	-6.23901	1.59098	-0.41233
H	-5.57186	2.11817	-1.10111
H	-7.23564	1.65380	-0.85574
C	-6.23984	2.26957	0.95790
H	-5.26852	2.17078	1.45217
H	-7.00016	1.83228	1.61120
H	-6.45914	3.33579	0.84415
C	-7.21018	-1.27504	1.16605
H	-7.53178	-0.44406	1.80004
H	-6.31434	-1.71654	1.61316
H	-8.00042	-2.03217	1.16659
C	8.49357	0.10741	0.21727
H	10.76619	0.09836	0.34469
C	9.69962	0.10302	0.28379

Sum of electronic and zero-point Energies= -1184.786415

Sum of electronic and thermal Energies= -1184.762466

Sum of electronic and thermal Enthalpies= -1184.761522

Sum of electronic and thermal Free Energies= -1184.842132

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Molecule 3d (Vacuum)

H	-2.76932	-3.01349	-0.14531
C	-3.02188	-1.95785	-0.19095
C	-3.67462	0.75228	-0.29462
C	-1.98326	-1.01006	-0.19098
C	-4.34069	-1.57824	-0.24227
C	-4.71028	-0.20204	-0.30612
C	-2.35445	0.33938	-0.24419
H	-5.09927	-2.34932	-0.23456
H	-3.86115	1.81710	-0.31811
C	-0.59630	-1.31382	-0.13174
H	-0.25859	-2.34618	-0.08594
C	0.35080	-0.33817	-0.12888
C	-0.06085	1.06134	-0.18681
O	-1.40839	1.31490	-0.24029
O	0.66703	2.03436	-0.19255
N	-6.02668	0.17437	-0.39381
C	1.78827	-0.77908	-0.06150
O	2.05626	-1.97268	-0.01001
N	2.70760	0.22573	-0.06222
H	2.31578	1.16424	-0.10884
C	4.10528	0.12137	0.00048
C	6.88748	0.09790	0.12387
C	4.79376	-1.09383	0.07760
C	4.83071	1.31895	-0.01496
C	6.21614	1.31265	0.04632
C	6.18330	-1.09833	0.13923
H	6.76955	2.24522	0.03409
H	6.71617	-2.04112	0.20012
C	-7.09856	-0.80621	-0.27124
H	-8.00491	-0.34253	-0.67023
H	-6.88718	-1.65601	-0.92923
C	-7.35679	-1.28774	1.15784
H	-7.68155	-0.46163	1.79678
H	-6.45504	-1.72029	1.60127
H	-8.14115	-2.05154	1.16275
C	-6.39671	1.58387	-0.41161
H	-7.39517	1.65283	-0.85305
H	-5.73151	2.11616	-1.09939
C	-6.39279	2.25742	0.96213
H	-7.15291	1.82034	1.61623
H	-6.60685	3.32610	0.85875
H	-5.42169	2.14885	1.45411
H	4.24094	-2.02229	0.08926
H	4.30425	2.26776	-0.07594
Cl	8.63661	0.07963	0.20310

Sum of electronic and zero-point Energies= -1568.255388

Sum of electronic and thermal Energies= -1568.232423

Sum of electronic and thermal Enthalpies= -1568.231479

Sum of electronic and thermal Free Energies= -1568.310184

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Molecule 3d (MeCN)

H	-2.77967	-3.01902	-0.13659
C	-3.02849	-1.96303	-0.18420
C	-3.66977	0.75713	-0.29295
C	-1.98459	-1.01472	-0.18787
C	-4.34315	-1.57890	-0.23409
C	-4.71142	-0.19764	-0.30080
C	-2.35526	0.33742	-0.24292
H	-5.10408	-2.34723	-0.22259
H	-3.85753	1.82167	-0.31790
C	-0.60568	-1.32086	-0.13072
H	-0.28053	-2.35654	-0.08454
C	0.35136	-0.34574	-0.13025
C	-0.05747	1.04806	-0.18888
O	-1.39871	1.30819	-0.24171
O	0.67279	2.02688	-0.19614
N	-6.01884	0.17854	-0.38580
C	1.78255	-0.78338	-0.06475
O	2.06132	-1.97909	-0.01414
N	2.70568	0.21887	-0.06482
H	2.31377	1.15825	-0.11082
C	4.10268	0.11694	-0.00116
C	6.88491	0.10243	0.12476
C	4.79750	-1.09579	0.07365
C	4.82534	1.31778	-0.01296
C	6.21104	1.31647	0.04959
C	6.18787	-1.09778	0.13672
H	6.75772	2.25298	0.04004
H	6.72084	-2.04066	0.19578
C	-7.09753	-0.80237	-0.27382
H	-7.99814	-0.33359	-0.67660
H	-6.88287	-1.65105	-0.93065
C	-7.36320	-1.28058	1.15383
H	-7.68616	-0.45187	1.79009
H	-6.46791	-1.72320	1.60092
H	-8.15312	-2.03805	1.15063
C	-6.39102	1.59101	-0.41491
H	-7.38637	1.65445	-0.86112
H	-5.72223	2.12062	-1.10021
C	-6.39641	2.26567	0.95724
H	-7.15831	1.82591	1.60701
H	-6.61618	3.33206	0.84596
H	-5.42644	2.16614	1.45402
H	4.25239	-2.02827	0.08296
H	4.29834	2.26573	-0.07150
Cl	8.63823	0.08995	0.20601

Sum of electronic and zero-point Energies= -1568.270817

Sum of electronic and thermal Energies= -1568.247756

Sum of electronic and thermal Enthalpies= -1568.246812

Sum of electronic and thermal Free Energies= -1568.326023

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Molecule 3e (Vacuum)

H	-3.53281	-3.01362	-0.14090
C	-3.78368	-1.95758	-0.18672
C	-4.43202	0.75362	-0.29077
C	-2.74335	-1.01166	-0.19355
C	-5.10204	-1.57563	-0.23174
C	-5.46942	-0.19885	-0.29580
C	-3.11237	0.33839	-0.24651
H	-5.86198	-2.34531	-0.21890
H	-4.61670	1.81874	-0.31462
C	-1.35667	-1.31790	-0.14148
H	-1.02066	-2.35085	-0.09637
C	-0.40782	-0.34394	-0.14489
C	-0.81721	1.05628	-0.20201
O	-2.16455	1.31221	-0.24868
O	-0.08758	2.02794	-0.21219
N	-6.78550	0.17983	-0.37768
C	1.02914	-0.78740	-0.08485
O	1.29536	-1.98135	-0.03408
N	1.95043	0.21585	-0.09132
H	1.56015	1.15512	-0.13627
C	3.34792	0.10887	-0.03558
C	6.13061	0.07990	0.07415
C	4.03420	-1.10801	0.03615
C	4.07541	1.30536	-0.05267
C	5.46107	1.29569	0.00189
C	5.42402	-1.11461	0.09092
H	6.01497	2.22789	-0.01138
H	5.95411	-2.05916	0.14759
C	-7.85851	-0.79871	-0.24895
H	-8.76583	-0.33412	-0.64467
H	-7.65150	-1.64990	-0.90656
C	-8.11127	-1.27759	1.18199
H	-8.43206	-0.44995	1.82098
H	-7.20825	-1.71073	1.62226
H	-8.89671	-2.04024	1.19153
C	-7.15295	1.58999	-0.39658
H	-8.15320	1.66013	-0.83377
H	-6.48963	2.11956	-1.08829
C	-7.14150	2.26620	0.97579
H	-7.89950	1.83188	1.63419
H	-7.35399	3.33508	0.87128
H	-6.16842	2.15676	1.46369
H	3.47983	-2.03555	0.04912
H	3.55048	2.25531	-0.10942
Br	8.02600	0.05641	0.15116

Sum of electronic and zero-point Energies= -3679.804813

Sum of electronic and thermal Energies= -3679.781627

Sum of electronic and thermal Enthalpies= -3679.780683

Sum of electronic and thermal Free Energies= -3679.860563

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Molecule 3e (MeCN)

H	-3.54380	-3.01890	-0.13257
C	-3.79081	-1.96248	-0.18021
C	-4.42721	0.75878	-0.28912
C	-2.74504	-1.01626	-0.19061
C	-5.10493	-1.57583	-0.22374
C	-5.47082	-0.19391	-0.29036
C	-3.11330	0.33657	-0.24543
H	-5.86728	-2.34266	-0.20725
H	-4.61293	1.82365	-0.31448
C	-1.36651	-1.32507	-0.14063
H	-1.04299	-2.36130	-0.09490
C	-0.40754	-0.35183	-0.14674
C	-0.81385	1.04275	-0.20466
O	-2.15487	1.30546	-0.25042
O	-0.08166	2.02004	-0.21687
N	-6.77788	0.18480	-0.36932
C	1.02298	-0.79239	-0.08862
O	1.29954	-1.98851	-0.03817
N	1.94844	0.20800	-0.09487
H	1.55841	1.14823	-0.13939
C	3.34518	0.10287	-0.03812
C	6.12862	0.08166	0.07436
C	4.03734	-1.11176	0.03259
C	4.07058	1.30219	-0.05286
C	5.45651	1.29679	0.00307
C	5.42796	-1.11628	0.08890
H	6.00409	2.23273	-0.00851
H	5.95770	-2.06113	0.14477
C	-7.85798	-0.79385	-0.25141
H	-8.75941	-0.32377	-0.65080
H	-7.64790	-1.64371	-0.90819
C	-8.11824	-1.26983	1.17796
H	-8.43713	-0.43979	1.81456
H	-7.22172	-1.71327	1.62177
H	-8.90936	-2.02604	1.17918
C	-7.14735	1.59800	-0.39848
H	-8.14474	1.66288	-0.83992
H	-6.48075	2.12521	-1.08777
C	-7.14446	2.27451	0.97274
H	-7.90401	1.83723	1.62695
H	-7.36262	3.34119	0.86112
H	-6.17225	2.17368	1.46487
H	3.49021	-2.04307	0.04406
H	3.54555	2.25146	-0.10835
Br	8.02760	0.06355	0.15361

Sum of electronic and zero-point Energies= -3679.820233

Sum of electronic and thermal Energies= -3679.796959

Sum of electronic and thermal Enthalpies= -3679.796015

Sum of electronic and thermal Free Energies= -3679.876336

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Molecule 3f (Vacuum)

H	-3.51305	-3.00416	-0.10884
C	-3.74431	-1.94421	-0.16556
C	-4.34234	0.77750	-0.29648
C	-2.68674	-1.01784	-0.18263
C	-5.05534	-1.53825	-0.21313
C	-5.39729	-0.15564	-0.29118
C	-3.03067	0.33836	-0.24844
H	-5.82892	-2.29398	-0.19063
H	-4.50754	1.84544	-0.33226
C	-1.30621	-1.34946	-0.12927
H	-0.98959	-2.38808	-0.07535
C	-0.33928	-0.39344	-0.14228
C	-0.72222	1.01366	-0.21067
O	-2.06472	1.29419	-0.26025
O	0.02553	1.97124	-0.22806
N	-6.70602	0.24690	-0.37579
C	1.08853	-0.86506	-0.07997
O	1.33065	-2.06276	-0.02213
N	2.03087	0.12143	-0.09243
H	1.65721	1.06738	-0.14249
C	3.42345	-0.00875	-0.03585
C	6.21980	-0.07826	0.07489
C	4.08982	-1.23890	0.03445
C	4.16805	1.18018	-0.05131
C	5.55013	1.14632	0.00375
C	5.47591	-1.25842	0.08872
H	3.51991	-2.15670	0.04625
H	3.65226	2.13526	-0.10697
H	6.11540	2.07134	-0.00779
H	6.00317	-2.20512	0.14415
C	-7.79672	-0.71193	-0.24761
H	-8.69300	-0.23584	-0.65472
H	-7.59864	-1.57201	-0.89615
C	-7.04766	1.66358	-0.39903
H	-6.38067	2.17775	-1.09894
H	-8.05005	1.74957	-0.82831
C	-7.01311	2.34661	0.96957
H	-6.03754	2.22564	1.44966
H	-7.77145	1.92729	1.63723
H	-7.21064	3.41796	0.86092
C	-8.06812	-1.17381	1.18548
H	-8.38394	-0.33613	1.81379
H	-7.17399	-1.61372	1.63709
H	-8.86302	-1.92660	1.19575
C	7.69919	-0.17711	0.13706
O	8.32030	-1.21560	0.19499
O	8.29569	1.03004	0.12286
C	9.71834	1.00524	0.18118
H	10.05934	0.50828	1.09289
H	10.03064	2.04959	0.17621
H	10.13131	0.47939	-0.68349

Sum of electronic and zero-point Energies= -1336.431962

Sum of electronic and thermal Energies= -1336.405686

Sum of electronic and thermal Enthalpies= -1336.404742

Sum of electronic and thermal Free Energies= -1336.491889

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Molecule 3f (MeCN)

H	-3.52683	-3.01012	-0.08999
C	-3.75296	-1.94984	-0.15217
C	-4.33581	0.78202	-0.29699
C	-2.68874	-1.02456	-0.17774
C	-5.05913	-1.53784	-0.19802
C	-5.39812	-0.14995	-0.28297
C	-3.03062	0.33459	-0.25001
H	-5.83577	-2.28977	-0.16807
H	-4.50045	1.84978	-0.33788
C	-1.31692	-1.35986	-0.12712
H	-1.01460	-2.40178	-0.06843
C	-0.33881	-0.40555	-0.14828
C	-0.71764	0.99591	-0.22280
O	-2.05318	1.28418	-0.27001
O	0.03371	1.95833	-0.24796
N	-6.69731	0.25366	-0.36371
C	1.08200	-0.87373	-0.08717
O	1.33631	-2.07312	-0.02427
N	2.02836	0.11063	-0.10486
H	1.65392	1.05717	-0.15705
C	3.41917	-0.01701	-0.04487
C	6.22021	-0.07913	0.07421
C	4.09237	-1.24506	0.02040
C	4.16256	1.17429	-0.05186
C	5.54459	1.14390	0.00732
C	5.47872	-1.26144	0.07898
H	3.52934	-2.16670	0.02558
H	3.64701	2.12902	-0.10325
H	6.10229	2.07347	0.00229
H	6.00215	-2.21049	0.13065
C	-7.79613	-0.70363	-0.24369
H	-8.68558	-0.22270	-0.65681
H	-7.59553	-1.56498	-0.88808
C	-7.03939	1.67377	-0.39978
H	-6.37088	2.18283	-1.10095
H	-8.04050	1.75460	-0.82988
C	-7.00765	2.36060	0.96595
H	-6.03096	2.24906	1.44674
H	-7.76527	1.94036	1.63345
H	-7.21084	3.42959	0.84833
C	-8.07646	-1.15705	1.18922
H	-8.38950	-0.31438	1.81200
H	-7.18993	-1.60690	1.64650
H	-8.87800	-1.90223	1.19303
C	7.70021	-0.16914	0.14113
O	8.32353	-1.21152	0.19320
O	8.28840	1.03375	0.13900
C	9.71627	1.03404	0.20162
H	10.06014	0.54510	1.11576
H	10.00822	2.08314	0.19978
H	10.13779	0.52083	-0.66558

Sum of electronic and zero-point Energies= -1336.450773

Sum of electronic and thermal Energies= -1336.424460

Sum of electronic and thermal Enthalpies= -1336.423516

Sum of electronic and thermal Free Energies= -1336.510412

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Molecule 3g (Vacuum)

H	-3.46326	-3.01438	-0.14204
C	-3.71261	-1.95803	-0.18855
C	-4.35687	0.75437	-0.29429
C	-2.67093	-1.01332	-0.19282
C	-5.03015	-1.57431	-0.23669
C	-5.39564	-0.19685	-0.30159
C	-3.03808	0.33741	-0.24681
H	-5.79117	-2.34294	-0.22551
H	-4.54011	1.81971	-0.31871
C	-1.28529	-1.32136	-0.13686
H	-0.95107	-2.35484	-0.09054
C	-0.33501	-0.34832	-0.13761
C	-0.74225	1.05233	-0.19621
O	-2.08889	1.30993	-0.24667
O	-0.01104	2.02291	-0.20449
N	-6.71069	0.18336	-0.38596
C	1.10055	-0.79335	-0.07270
O	1.36661	-1.98652	-0.02089
N	2.02403	0.21070	-0.07593
H	1.63322	1.14999	-0.12263
C	3.41877	0.10446	-0.01412
C	6.21086	0.07951	0.11395
C	4.10535	-1.11260	0.06322
C	4.14435	1.30404	-0.02711
C	5.52696	1.29141	0.03558
C	5.49319	-1.11202	0.12550
H	3.55082	-2.03972	0.07707
H	3.61575	2.25178	-0.08364
H	6.07525	2.22753	0.03104
H	6.01928	-2.05838	0.19171
C	-7.78529	-0.79415	-0.26084
H	-8.69086	-0.32843	-0.65914
H	-7.57714	-1.64526	-0.91812
C	-7.07672	1.59407	-0.40497
H	-6.41232	2.12320	-1.09595
H	-8.07645	1.66515	-0.84310
C	-7.06609	2.26966	0.96767
H	-6.09348	2.15975	1.45638
H	-7.82481	1.83539	1.62524
H	-7.27810	3.33864	0.86332
C	-8.04264	-1.27294	1.16927
H	-8.36466	-0.44512	1.80738
H	-7.14130	-1.70690	1.61214
H	-8.82873	-2.03492	1.17636
C	7.71093	0.06613	0.12482
F	8.22291	0.09118	-1.12151
F	8.20210	-1.03302	0.72330
F	8.21632	1.13450	0.76881

Sum of electronic and zero-point Energies= -1445.615193

Sum of electronic and thermal Energies= -1445.590745

Sum of electronic and thermal Enthalpies= -1445.589801

Sum of electronic and thermal Free Energies= -1445.671673

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Molecule 3g (MeCN)

H	-3.47527	-3.01985	-0.12962
C	-3.72033	-1.96309	-0.17919
C	-4.35163	0.75942	-0.29286
C	-2.67287	-1.01850	-0.18745
C	-5.03353	-1.57423	-0.22694
C	-5.39687	-0.19163	-0.29614
C	-3.03874	0.33505	-0.24468
H	-5.79719	-2.33976	-0.21160
H	-4.53548	1.82455	-0.32007
C	-1.29542	-1.32961	-0.13296
H	-0.97421	-2.36647	-0.08543
C	-0.33466	-0.35768	-0.13680
C	-0.73833	1.03747	-0.19712
O	-2.07863	1.30228	-0.24763
O	-0.00443	2.01354	-0.20766
N	-6.70282	0.18917	-0.37898
C	1.09428	-0.80046	-0.07379
O	1.37014	-1.99590	-0.02233
N	2.02216	0.20048	-0.07704
H	1.63185	1.14081	-0.12315
C	3.41599	0.09589	-0.01517
C	6.21028	0.07815	0.11225
C	4.10871	-1.11887	0.05726
C	4.13961	1.29842	-0.02392
C	5.52214	1.28964	0.03844
C	5.49738	-1.11642	0.11905
H	3.56140	-2.04976	0.06769
H	3.61073	2.24550	-0.07677
H	6.06379	2.22970	0.03528
H	6.02309	-2.06326	0.17931
C	-7.78490	-0.78787	-0.26527
H	-8.68390	-0.31688	-0.66898
H	-7.57301	-1.63848	-0.92043
C	-7.07003	1.60301	-0.40925
H	-6.40178	2.12902	-1.09787
H	-8.06673	1.66920	-0.85198
C	-7.06814	2.27989	0.96178
H	-6.09664	2.17850	1.45518
H	-7.82886	1.84342	1.61516
H	-7.28528	3.34670	0.84946
C	-8.05192	-1.26222	1.16340
H	-8.37257	-0.43120	1.79783
H	-7.15777	-1.70629	1.61135
H	-8.84390	-2.01752	1.16186
C	7.70886	0.07399	0.12549
F	8.22628	0.18317	-1.11674
F	8.21207	-1.05594	0.65327
F	8.20948	1.10312	0.83558

Sum of electronic and zero-point Energies= -1445.630730

Sum of electronic and thermal Energies= -1445.605250

Sum of electronic and thermal Enthalpies= -1445.604306

Sum of electronic and thermal Free Energies= -1445.690386

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Molecule 3h (Vacuum)

H	-2.61073	-3.01602	-0.14199
C	-2.86211	-1.96016	-0.18846
C	-3.51110	0.75165	-0.29453
C	-1.82211	-1.01304	-0.18876
C	-4.17988	-1.57905	-0.24059
C	-4.54807	-0.20191	-0.30571
C	-2.19197	0.33729	-0.24313
H	-4.93947	-2.34907	-0.23255
H	-3.69666	1.81659	-0.31873
C	-0.43684	-1.31827	-0.12870
H	-0.10102	-2.35122	-0.08206
C	0.51160	-0.34254	-0.12600
C	0.10172	1.05704	-0.18507
O	-1.24460	1.31177	-0.23943
O	0.83162	2.02898	-0.19059
N	-5.86290	0.17552	-0.39397
C	1.94678	-0.78292	-0.05757
O	2.21968	-1.97401	-0.00549
N	2.86833	0.22606	-0.05770
H	2.47268	1.16385	-0.10476
C	4.26025	0.12471	0.00689
C	7.05481	0.10847	0.13501
C	4.95064	-1.09232	0.08204
C	4.98203	1.32801	-0.00466
C	6.36315	1.32313	0.05860
C	6.33619	-1.09061	0.14558
H	4.39775	-2.02045	0.09045
H	4.44978	2.27332	-0.06396
H	6.91204	2.25876	0.04940
H	6.86936	-2.03369	0.20499
C	-6.93660	-0.80394	-0.27266
H	-7.84157	-0.33903	-0.67307
H	-6.72545	-1.65415	-0.93011
C	-6.23171	1.58572	-0.41595
H	-5.56476	2.11559	-1.10383
H	-7.22920	1.65434	-0.85940
C	-6.22975	2.26172	0.95644
H	-5.25950	2.15413	1.45033
H	-6.99102	1.82609	1.61012
H	-6.44355	3.33015	0.85050
C	-7.19708	-1.28376	1.15646
H	-7.52096	-0.45653	1.79436
H	-6.29680	-1.71787	1.60135
H	-7.98295	-2.04593	1.16097
C	8.48780	0.09605	0.20219
N	9.64628	0.08779	0.25646

Sum of electronic and zero-point Energies= -1200.876098

Sum of electronic and thermal Energies= -1200.852554

Sum of electronic and thermal Enthalpies= -1200.851610

Sum of electronic and thermal Free Energies= -1200.931367

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Molecule 3h (MeCN)

H	-2.61867	-3.02092	-0.12997
C	-2.86686	-1.96490	-0.17956
C	-3.50562	0.75623	-0.29355
C	-1.82209	-1.01693	-0.18322
C	-4.18077	-1.57999	-0.23185
C	-4.54803	-0.19819	-0.30138
C	-2.19185	0.33589	-0.24082
H	-4.94229	-2.34768	-0.22017
H	-3.69275	1.82080	-0.32052
C	-0.44465	-1.32404	-0.12408
H	-0.12082	-2.36008	-0.07647
C	0.51332	-0.34853	-0.12356
C	0.10585	1.04533	-0.18403
O	-1.23467	1.30603	-0.23942
O	0.83728	2.02342	-0.19087
N	-5.85447	0.17838	-0.38877
C	1.94209	-0.78598	-0.05658
O	2.22526	-1.97886	-0.00640
N	2.86773	0.22098	-0.05521
H	2.47214	1.15971	-0.10105
C	4.25772	0.12192	0.00819
C	7.05155	0.11315	0.13319
C	4.95395	-1.09378	0.07626
C	4.97690	1.32875	0.00265
C	6.35755	1.32858	0.06439
C	6.33939	-1.09072	0.13833
H	4.40797	-2.02536	0.08054
H	4.44392	2.27318	-0.05013
H	6.90029	2.26755	0.05976
H	6.87261	-2.03394	0.19175
C	-6.93417	-0.80193	-0.27820
H	-7.83338	-0.33313	-0.68392
H	-6.71825	-1.65159	-0.93326
C	-6.22630	1.59109	-0.42230
H	-5.55613	2.11871	-1.10770
H	-7.22071	1.65338	-0.87062
C	-6.23435	2.26876	0.94829
H	-5.26532	2.17061	1.44715
H	-6.99741	1.83035	1.59759
H	-6.45413	3.33480	0.83405
C	-7.20333	-1.27740	1.14964
H	-7.52710	-0.44733	1.78371
H	-6.30939	-1.71994	1.59949
H	-7.99380	-2.03424	1.14587
C	8.48309	0.10395	0.19819

Sum of electronic and zero-point Energies= -1200.895243

Sum of electronic and thermal Energies= -1200.871622

Sum of electronic and thermal Enthalpies= -1200.870678

Sum of electronic and thermal Free Energies= -1200.950757

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Molecule 3i (Vacuum)

O	-1.67006	1.30892	-0.23564
N	2.44022	0.21594	-0.06331
O	0.40785	2.02130	-0.18709
O	1.78836	-1.98346	-0.01502
N	-6.29073	0.18309	-0.39047
N	8.05837	0.08066	0.15493
O	8.61793	-1.00474	0.21861
O	8.63942	1.15700	0.13494
C	0.08223	-0.34941	-0.12757
C	-2.25275	-1.01484	-0.18940
C	-0.86845	-1.32332	-0.13133
H	-0.53511	-2.35721	-0.08752
C	-4.97696	-0.19726	-0.30362
C	-3.93772	0.75402	-0.29086
H	-4.12077	1.81941	-0.31284
C	-3.29498	-1.95970	-0.19045
H	-3.04602	-3.01621	-0.14616
C	-2.61969	0.33655	-0.24083
C	1.51604	-0.79258	-0.06319
C	-0.32455	1.05114	-0.18298
C	3.83045	0.11263	-0.00745
C	-4.61178	-1.57548	-0.24119
H	-5.37310	-2.34377	-0.23408
C	4.55304	1.31713	-0.02227
H	4.02071	2.26250	-0.07636
C	5.90544	-1.10870	0.11509
H	6.45445	-2.04066	0.16938
C	5.93416	1.31322	0.03058
H	6.50003	2.23628	0.01975
C	6.59908	0.09394	0.09909
C	4.51957	-1.10690	0.06168
H	3.96565	-2.03422	0.07282
C	-7.36642	-0.79478	-0.27289
H	-7.15590	-1.64360	-0.93229
H	-8.27009	-0.32731	-0.67320
C	-6.65697	1.59416	-0.40829
H	-7.65503	1.66563	-0.84992
H	-5.99031	2.12468	-1.09594
C	-6.65166	2.26651	0.96585
H	-7.41222	1.83006	1.61979
H	-6.86446	3.33543	0.86299
H	-5.68066	2.15667	1.45776
C	-7.62918	-1.27763	1.15474
H	-6.72994	-1.71382	1.59970
H	-8.41591	-2.03891	1.15648
H	-7.95294	-0.45158	1.79421
H	2.04513	1.15438	-0.10720

Sum of electronic and zero-point Energies= -1313.101892

Sum of electronic and thermal Energies= -1313.077677

Sum of electronic and thermal Enthalpies= -1313.076732

Sum of electronic and thermal Free Energies= -1313.158522

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Molecule 3i (MeCN)

O	-1.66041	1.30405	-0.23218
N	2.43953	0.21213	-0.06193
O	0.41318	2.01671	-0.18359
O	1.79405	-1.98713	-0.01458
N	-6.28225	0.18679	-0.38524
N	8.05010	0.08509	0.15226
O	8.62064	-0.99728	0.22187
O	8.63995	1.15918	0.12574
C	0.08384	-0.35464	-0.12550
C	-2.25267	-1.01809	-0.18704
C	-0.87636	-1.32852	-0.12987
H	-0.55507	-2.36555	-0.08729
C	-4.97687	-0.19295	-0.30051
C	-3.93236	0.75933	-0.28796
H	-4.11721	1.82440	-0.30921
C	-3.29958	-1.96397	-0.18809
H	-3.05359	-3.02074	-0.14404
C	-2.61967	0.33598	-0.23781
C	1.51082	-0.79486	-0.06233
C	-0.32059	1.04028	-0.17972
C	3.82670	0.11045	-0.00669
C	-4.61250	-1.57602	-0.23825
H	-5.37562	-2.34215	-0.23048
C	4.54888	1.31724	-0.02297
H	4.01758	2.26225	-0.07710
C	5.90595	-1.10891	0.11621
H	6.44973	-2.04369	0.17108
C	5.92901	1.31579	0.02870
H	6.48551	2.24427	0.01595
C	6.59796	0.09642	0.09825
C	4.52097	-1.10798	0.06343
H	3.97315	-2.03820	0.07603
C	-7.36411	-0.79187	-0.27970
H	-7.15046	-1.63802	-0.93999
H	-8.26256	-0.31872	-0.68200
C	-6.65129	1.60049	-0.41093
H	-7.64574	1.66720	-0.85852
H	-5.98037	2.13060	-1.09364
C	-6.65749	2.27036	0.96345
H	-7.42081	1.82938	1.61069
H	-6.87587	3.33732	0.85524
H	-5.68830	2.16811	1.46117
C	-7.63323	-1.27512	1.14549
H	-6.73984	-1.72176	1.59235
H	-8.42496	-2.03061	1.13769
H	-7.95532	-0.44824	1.78454
H	2.04433	1.15149	-0.10537

Sum of electronic and zero-point Energies= -1313.120558

Sum of electronic and thermal Energies= -1313.096220

Sum of electronic and thermal Enthalpies= -1313.095276

Sum of electronic and thermal Free Energies= -1313.177607

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Molecule 4a

C	-2.48967	0.65209	-0.20470
C	-4.02934	-1.64734	-0.27819
C	-1.84353	-0.59525	-0.19113
C	-3.86747	0.77229	-0.25561
C	-4.67931	-0.37787	-0.30852
C	-2.66069	-1.74032	-0.22621
H	-4.27696	1.77297	-0.24867
H	-2.19051	-2.71962	-0.20926
H	-4.60725	-2.56170	-0.29626
C	-0.42547	-0.61043	-0.13786
H	0.11527	-1.55320	-0.12756
C	0.28604	0.55043	-0.10001
O	-1.77982	1.80566	-0.16148
C	-0.39382	1.85333	-0.10462
O	0.12313	2.93517	-0.06600
N	1.68639	0.64189	-0.04688
N	2.28897	-0.45549	-0.07429
C	3.70365	-0.32444	-0.01628
C	6.45280	-0.28514	0.08282
C	4.41927	-1.52208	-0.04422
C	4.37619	0.90142	0.06216
C	5.75954	0.92207	0.11227
C	5.80608	-1.51093	0.00532
H	3.87056	-2.45571	-0.10599
H	3.80024	1.81941	0.08156
H	6.30856	1.85345	0.17323
H	6.38423	-2.42596	-0.01504
N	-6.04345	-0.28237	-0.40416
C	-6.88597	-1.47095	-0.35541
H	-7.85837	-1.19435	-0.77219
H	-6.47890	-2.22894	-1.03327
C	-6.70235	1.01785	-0.38648
H	-7.68809	0.88827	-0.84248
C	-7.07622	-2.05368	1.04640
H	-7.66506	-2.97550	0.99658
H	-7.60272	-1.34814	1.69544
H	-6.11464	-2.28591	1.51375
H	-6.15602	1.70011	-1.04599
C	-6.85649	1.63037	1.00682
H	-5.88785	1.73671	1.50389
H	-7.49462	1.00710	1.64009
H	-7.31467	2.62195	0.93336
N	7.91967	-0.26156	0.13467
O	8.50613	-1.33294	0.10108
O	8.46761	0.82752	0.20815

Sum of electronic and zero-point Energies= -1253.870897

Sum of electronic and thermal Energies= -1253.847332

Sum of electronic and thermal Enthalpies= -1253.846388

Sum of electronic and thermal Free Energies= -1253.927499

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Molecule 4b

C	-2.61539	0.41986	-0.18586
C	-4.41456	-1.66000	-0.41850
C	-2.11924	-0.88560	-0.26782
C	-3.96949	0.71028	-0.21867
C	-4.91134	-0.32664	-0.34954
C	-3.06461	-1.91840	-0.38334
H	-4.25393	1.75002	-0.13092
H	-2.71613	-2.94594	-0.44624
H	-5.09697	-2.49522	-0.50638
C	-0.70541	-1.06189	-0.22188
H	-0.30816	-2.07328	-0.28983
C	0.15740	-0.01463	-0.09930
O	-1.76699	1.47205	-0.06105
C	-0.39426	1.34777	-0.00835
O	0.23391	2.37124	0.10585
C	1.59688	-0.25442	-0.05951
H	1.85760	-1.30915	-0.14600
C	2.58274	0.65188	0.04565
H	2.32529	1.70452	0.08928
C	4.01418	0.32712	0.07119
C	6.74976	-0.18363	0.06700
C	4.93901	1.34583	-0.20594
C	4.50804	-0.95328	0.36981
C	5.86766	-1.21608	0.36478
C	6.30333	1.10070	-0.21554
H	4.57479	2.34519	-0.42510
H	3.82202	-1.75207	0.63214
H	6.25589	-2.20035	0.59558
H	7.01993	1.88194	-0.43647
N	-6.25844	-0.06537	-0.42970
C	-7.23618	-1.14429	-0.37884
H	-8.18752	-0.73045	-0.72467
H	-6.96523	-1.91507	-1.10919
C	-6.75524	1.30181	-0.36081
H	-7.73780	1.31621	-0.84215
C	-7.42366	-1.76640	1.00648
H	-8.15371	-2.58115	0.95936
H	-7.78698	-1.02342	1.72219
H	-6.48325	-2.17089	1.39248
H	-6.11371	1.94032	-0.97683
C	-6.86858	1.86776	1.05646
H	-5.91129	1.81013	1.58289
H	-7.60935	1.31439	1.64134
H	-7.17873	2.91727	1.02158
N	8.18815	-0.45629	0.06254
O	8.94244	0.46954	-0.19778
O	8.55226	-1.59508	0.31826

Sum of electronic and zero-point Energies= -1221.814684

Sum of electronic and thermal Energies= -1221.790927

Sum of electronic and thermal Enthalpies= -1221.789983

Sum of electronic and thermal Free Energies= -1221.870970

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Molecule 4c

C	-2.67708	0.50569	-0.21310
C	-4.39646	-1.65522	-0.31813
C	-2.13199	-0.78532	-0.22851
C	-4.04140	0.73847	-0.24773
C	-4.94400	-0.34011	-0.31427
C	-3.03750	-1.85810	-0.28043
H	-4.36637	1.76947	-0.21618
H	-2.64861	-2.87287	-0.28932
H	-5.04503	-2.52054	-0.35265
C	-0.71333	-0.91518	-0.18335
H	-0.26851	-1.90667	-0.19360
C	0.09097	0.18210	-0.12998
O	-1.87447	1.60081	-0.15643
C	-0.49650	1.53442	-0.11436
O	0.11498	2.56752	-0.06842
C	1.50751	0.08900	-0.08621
C	2.71430	0.00515	-0.04917
C	4.13757	-0.06608	-0.00378
C	6.89830	-0.19266	0.08654
C	4.78757	-1.30863	0.06204
C	4.90050	1.11291	-0.02352
C	6.28407	1.05222	0.02130
C	6.17076	-1.37629	0.10768
H	4.19815	-2.21888	0.07756
H	4.39506	2.07088	-0.07479
H	6.88944	1.94989	0.00688
H	6.69026	-2.32489	0.15984
N	-6.29941	-0.13393	-0.39279
C	-7.23400	-1.25006	-0.32850
H	-8.19403	-0.88606	-0.70513
H	-6.91639	-2.02870	-1.03095
C	-6.85146	1.21398	-0.35496
H	-7.84460	1.17052	-0.81166
C	-7.42520	-1.83960	1.07044
H	-8.12094	-2.68433	1.03264
H	-7.83343	-1.09234	1.75693
H	-6.47788	-2.19427	1.48724
H	-6.25318	1.85999	-1.00578
C	-6.95592	1.81857	1.04662
H	-5.98186	1.83775	1.54415
H	-7.64278	1.24061	1.67189
H	-7.33171	2.84526	0.98791
N	8.36233	-0.26049	0.13452
O	8.87779	-1.36686	0.19401
O	8.98067	0.79286	0.11225

Sum of electronic and zero-point Energies= -1220.580047

Sum of electronic and thermal Energies= -1220.556318

Sum of electronic and thermal Enthalpies= -1220.555374

Sum of electronic and thermal Free Energies= -1220.637092

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Molecule 4d

C	-2.55191	0.67680	-0.10911
C	-4.07999	-1.58932	-0.53343
C	-1.89945	-0.55531	-0.27255
C	-3.92970	0.80005	-0.15435
C	-4.73595	-0.33288	-0.37971
C	-2.71071	-1.68421	-0.48504
H	-4.34333	1.78764	-0.00383
H	-2.23647	-2.65353	-0.61165
H	-4.65251	-2.49297	-0.69406
C	-0.47956	-0.57234	-0.20536
H	0.06319	-1.50675	-0.32887
C	0.22606	0.57047	0.01428
O	-1.84686	1.81646	0.11071
C	-0.46853	1.84763	0.18724
O	0.05532	2.91496	0.38580
C	1.68487	0.59605	0.08673
H	2.13383	1.57554	0.28559
N	2.38152	-0.46592	-0.06209
C	3.77821	-0.36687	-0.03930
C	6.54481	-0.29287	0.02799
C	4.49582	-1.34736	0.65993
C	4.47612	0.63523	-0.72913
C	5.86195	0.67616	-0.69573
C	5.87857	-1.30781	0.70783
H	3.94594	-2.13092	1.16988
H	3.92745	1.36810	-1.31214
H	6.41676	1.44189	-1.22365
H	6.44807	-2.04912	1.25441
N	-6.10117	-0.23030	-0.46719
C	-6.93974	-1.41982	-0.55446
H	-7.92109	-1.09542	-0.91161
H	-6.54679	-2.08360	-1.33220
C	-6.76493	1.05252	-0.27063
H	-7.74876	0.98401	-0.74381
C	-7.09939	-2.17957	0.76397
H	-7.68882	-3.08885	0.60699
H	-7.61156	-1.56606	1.51043
H	-6.12800	-2.46865	1.17610
H	-6.21949	1.82181	-0.82710
C	-6.92523	1.46545	1.19392
H	-5.95939	1.49241	1.70676
H	-7.57253	0.76570	1.73044
H	-7.37565	2.46118	1.25897
N	8.00707	-0.25310	0.06532
O	8.58389	-1.11806	0.70859
O	8.56883	0.64299	-0.54780

Sum of electronic and zero-point Energies= -1237.864318

Sum of electronic and thermal Energies= -1237.840673

Sum of electronic and thermal Enthalpies= -1237.839729

Sum of electronic and thermal Free Energies= -1237.920653

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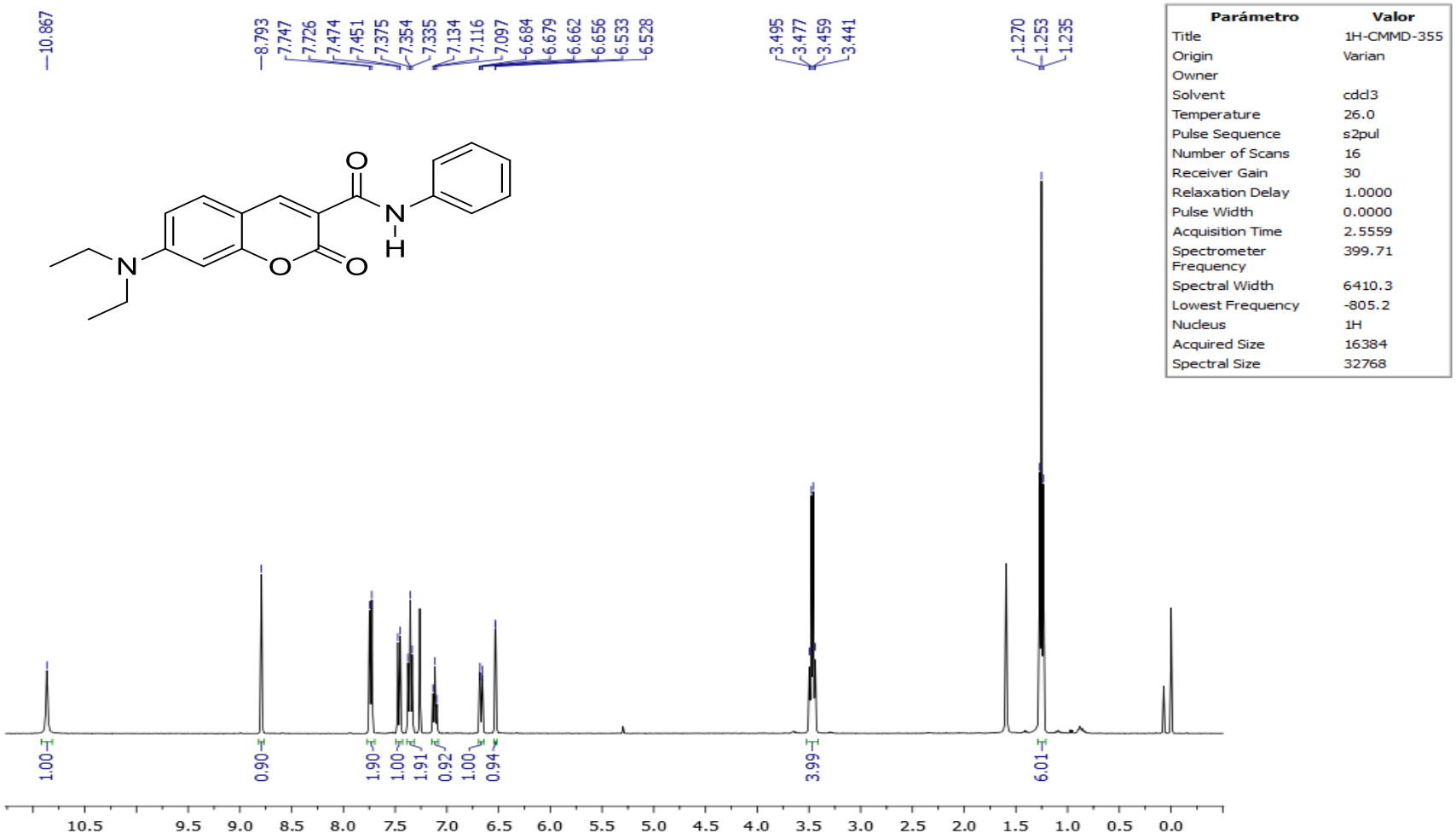
8. ^{1}H and ^{13}C NMR Spectra for Compounds 3a-i



^{1}H-NMR Spectra for 7-(diethylamino)-2-oxo-*N*-phenyl-*2H*--chromene-3-carboxamide **(3a)**

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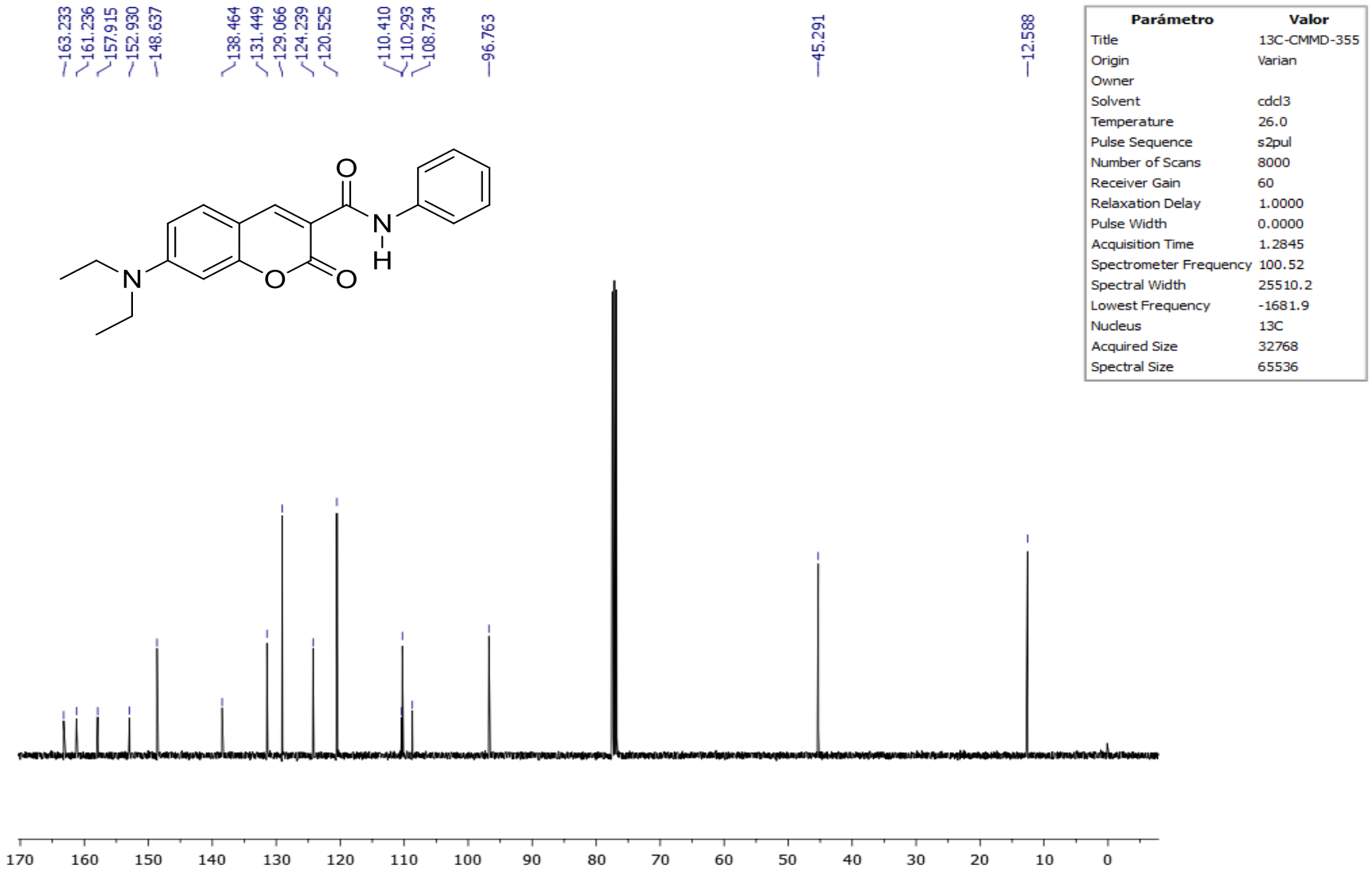

Parámetro	Valor
Title	13C-CMMD-355
Origin	Varian
Owner	
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	8000
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Spectrometer Frequency	100.52
Spectral Width	25510.2
Lowest Frequency	-1681.9
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

^{13}C-NMR Spectra for 7-(diethylamino)-2-oxo-*N*-phenyl-*2H*--chromene-3-carboxamide **(3a)**

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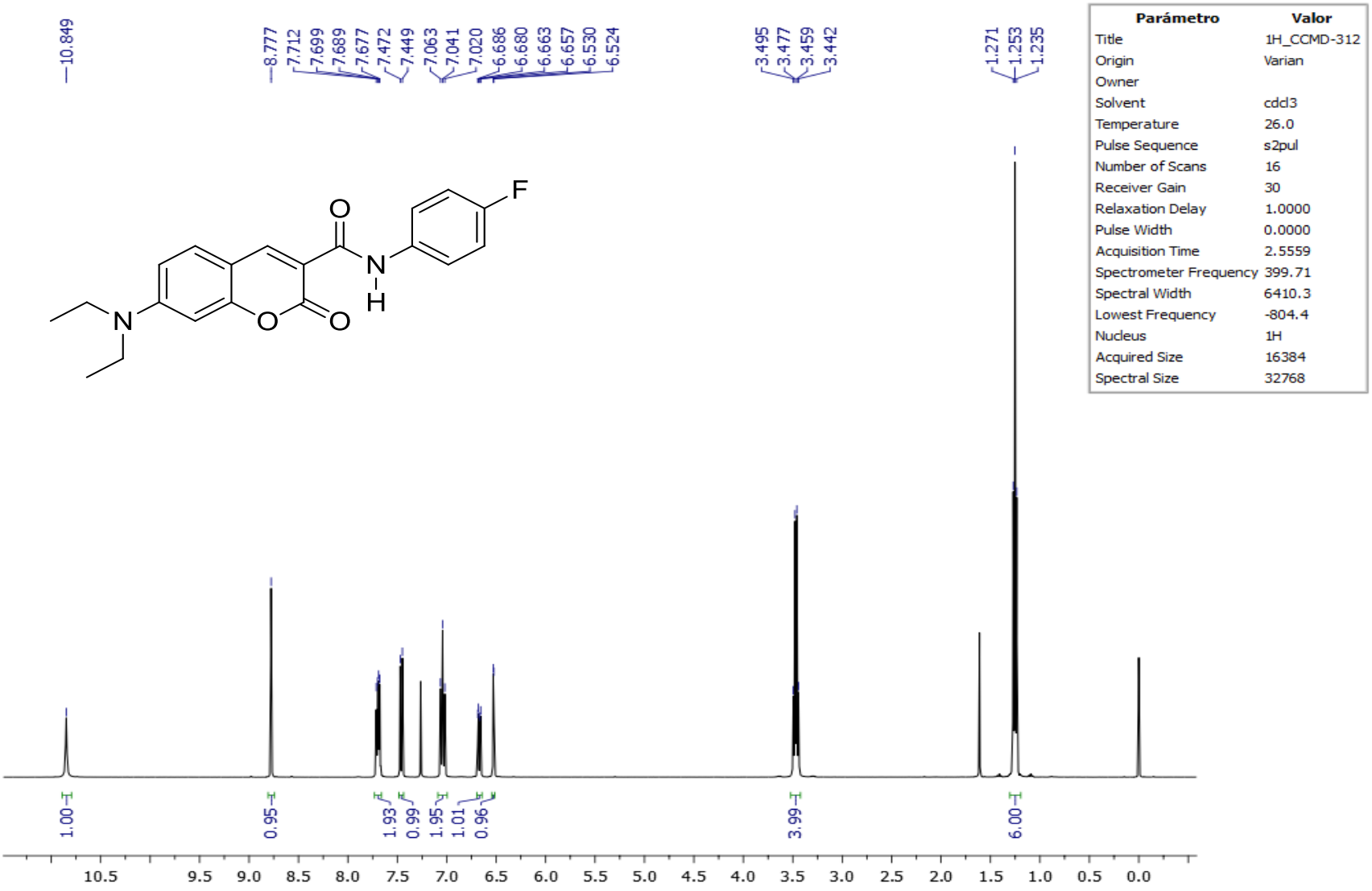

Parámetro	Valor
Title	1H_CCMD-312
Origin	Varian
Owner	
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	16
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.5559
Spectrometer Frequency	399.71
Spectral Width	6410.3
Lowest Frequency	-804.4
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

^{1}H-NMR Spectra for 7-(diethylamino)-*N*-(4-fluorophenyl)-2-oxo-*2H*--chromene-3-carboxamide **(3b)**

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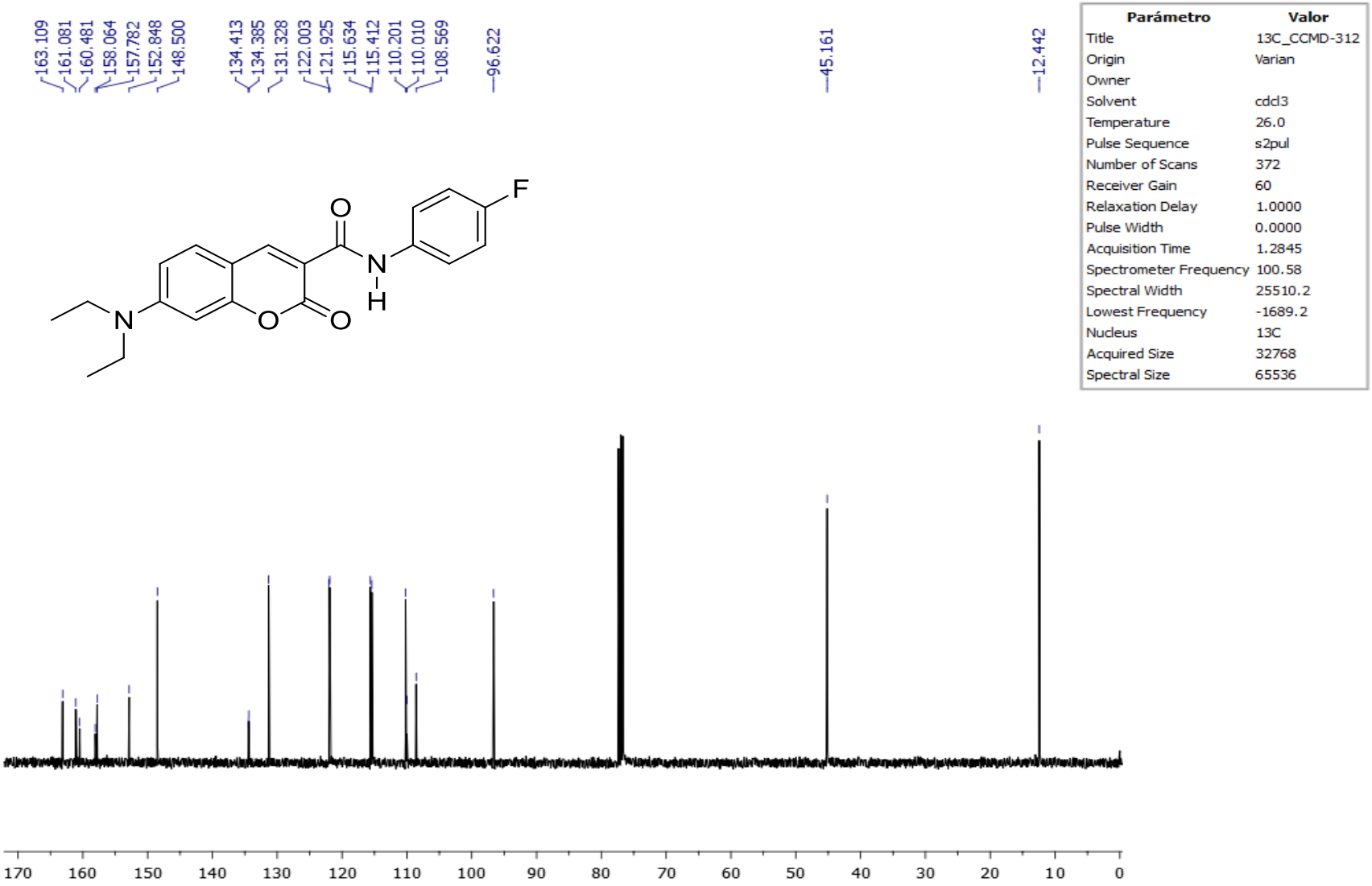

Parámetro	Valor
Title	13C_CCMD-312
Origin	Varian
Owner	
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	372
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Spectrometer Frequency	100.58
Spectral Width	25510.2
Lowest Frequency	-1689.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

^{13}C-NMR Spectra for 7-(diethylamino)-*N*-(4-fluorophenyl)-2-oxo-*2H*--chromene-3-carboxamide **(3b)**

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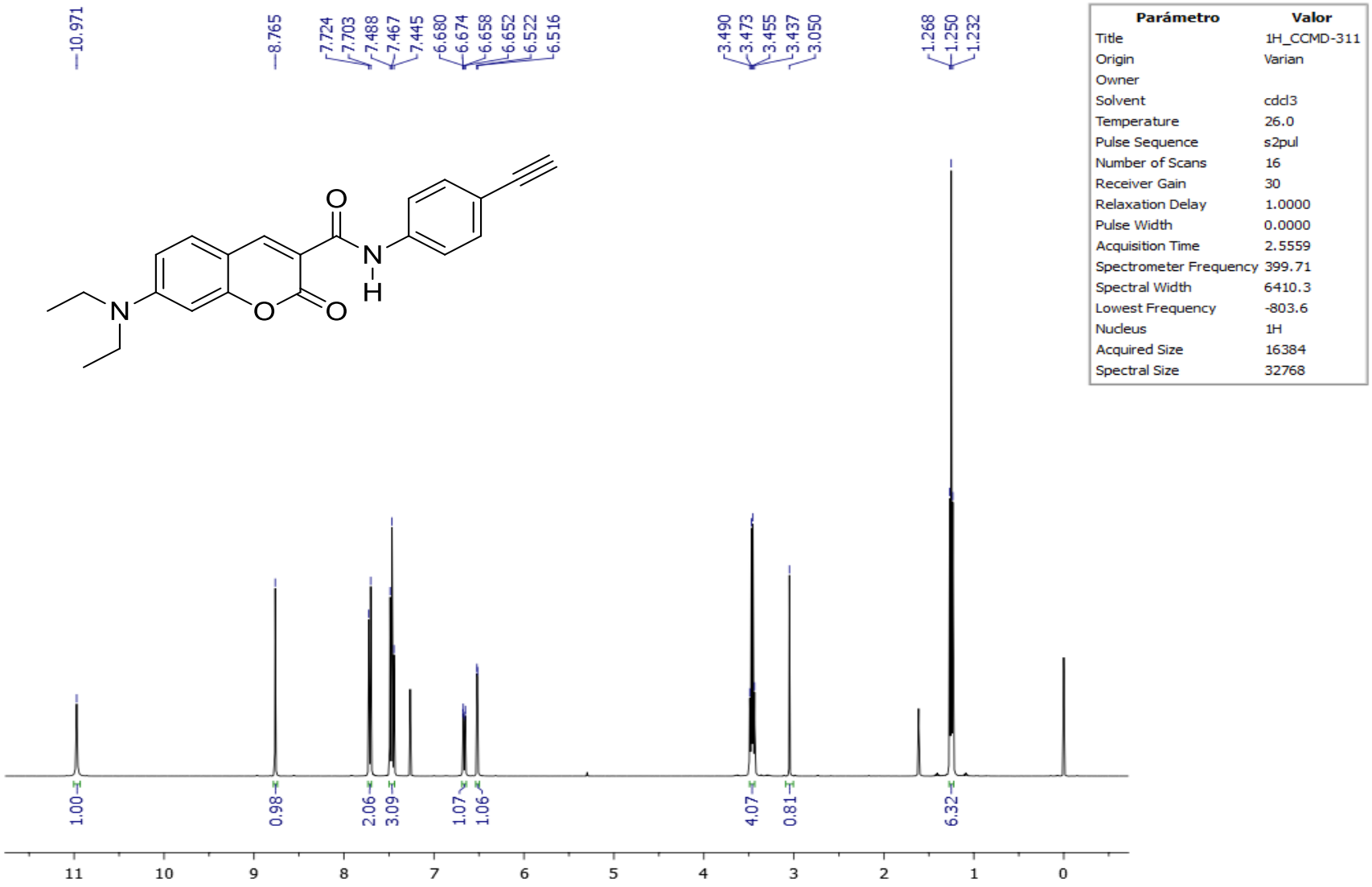

Parámetro	Valor
Title	1H_CCMD-311
Origin	Varian
Owner	
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	16
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.5559
Spectrometer Frequency	399.71
Spectral Width	6410.3
Lowest Frequency	-803.6
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

^{1}H-NMR Spectra for 7-(diethylamino)-*N*-(4-ethynylphenyl)-2-oxo-*2H*--chromene-3-carboxamide **(3c)**

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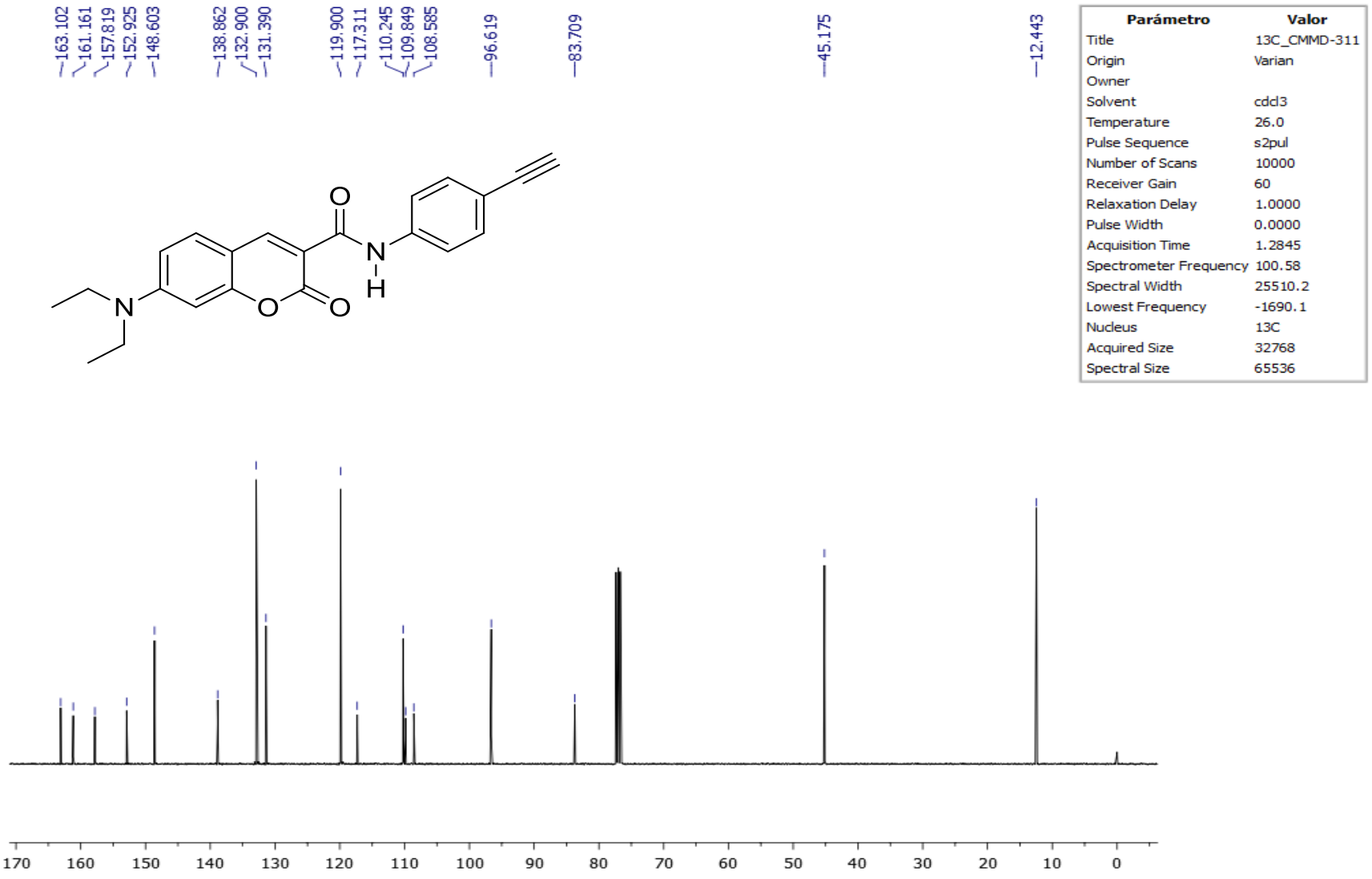

Parámetro	Valor
Title	13C_CMMD-311
Origin	Varian
Owner	
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	10000
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Spectrometer Frequency	100.58
Spectral Width	25510.2
Lowest Frequency	-1690.1
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

^{13}C-NMR Spectra for 7-(diethylamino)-*N*-(4-ethynylphenyl)-2-oxo-*2H*--chromene-3-carboxamide **(3c)**

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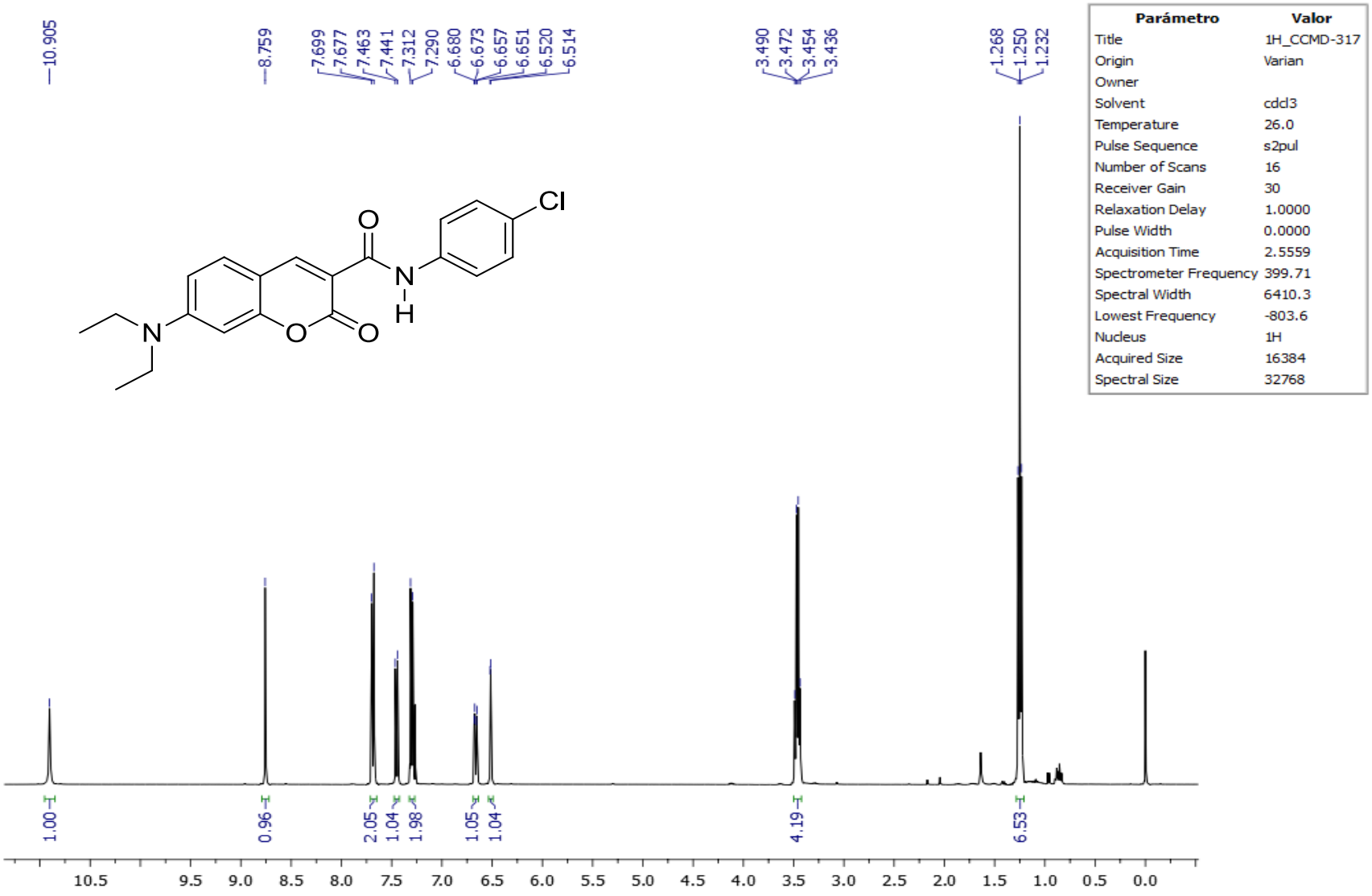

Parámetro	Valor
Title	1H_CCMD-317
Origin	Varian
Owner	
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	16
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.5559
Spectrometer Frequency	399.71
Spectral Width	6410.3
Lowest Frequency	-803.6
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

^{1}H-NMR Spectra for *N*-(4-chlorophenyl)-7-(diethylamino)-2-oxo-*2H*--chromene-3-carboxamide **(3d)**

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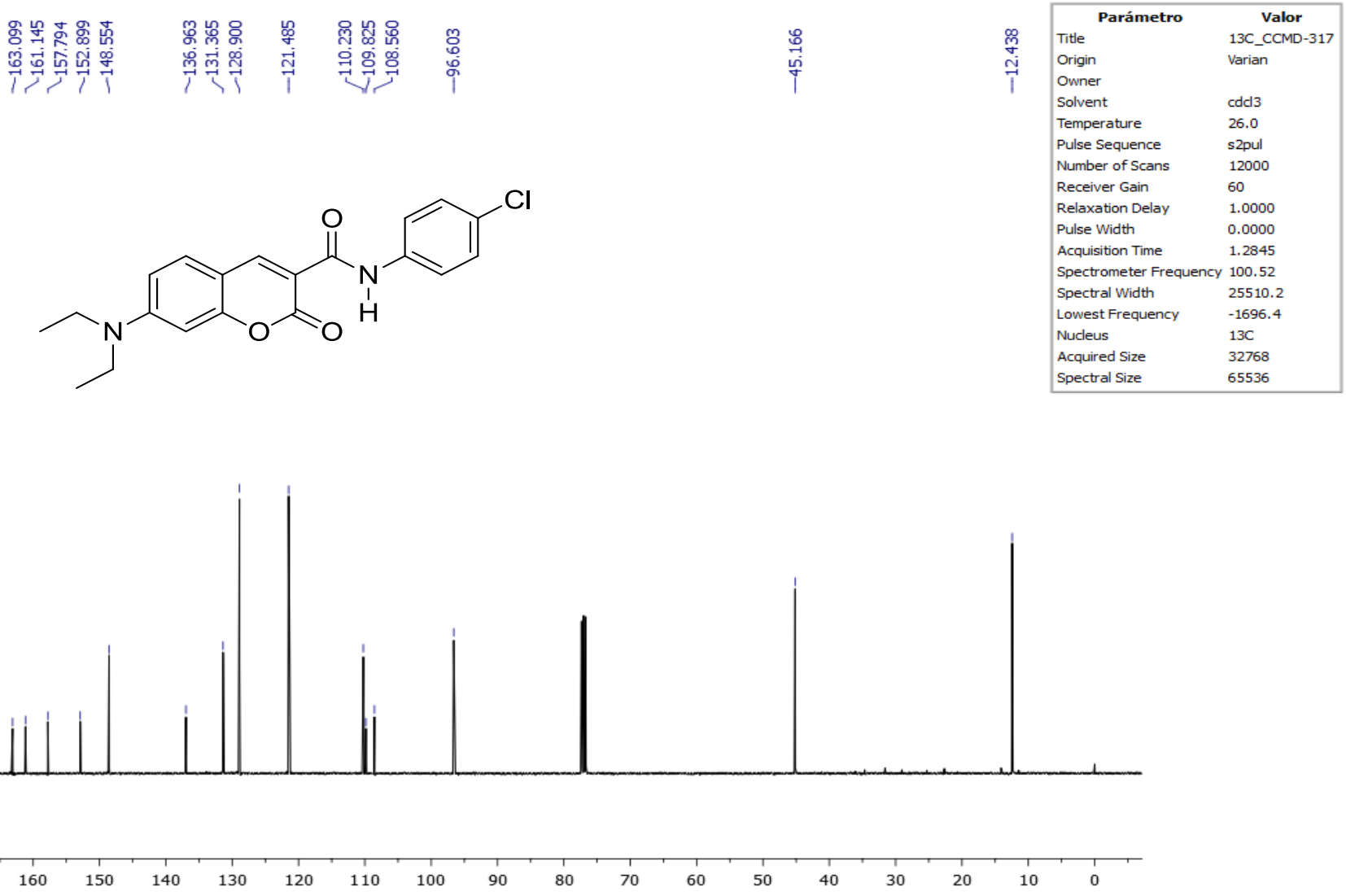

Parámetro	Valor
Title	13C_CCMD-317
Origin	Varian
Owner	
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	12000
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Spectrometer Frequency	100.52
Spectral Width	25510.2
Lowest Frequency	-1696.4
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

^{13}C-NMR Spectra for *N*-(4-chlorophenyl)-7-(diethylamino)-2-oxo-*2H*--chromene-3-carboxamide **(3d)**

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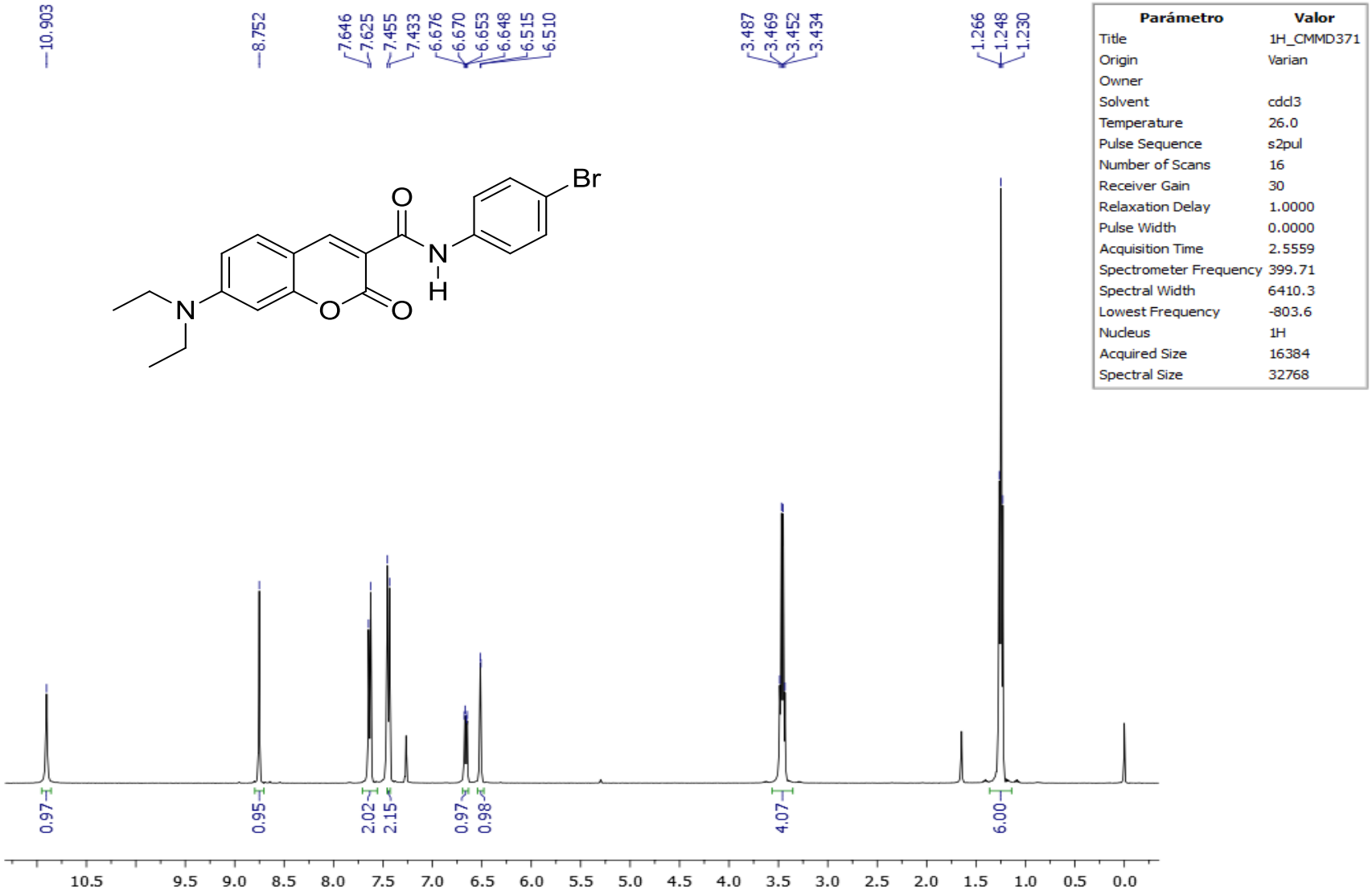

Parámetro	Valor
Title	1H_CMMD371
Origin	Varian
Owner	
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	16
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.5559
Spectrometer Frequency	399.71
Spectral Width	6410.3
Lowest Frequency	-803.6
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

^{1}H-NMR Spectra for *N*-(4-bromophenyl)-7-(diethylamino)-2-oxo-*2H*--chromene-3-carboxamide **(3e)**

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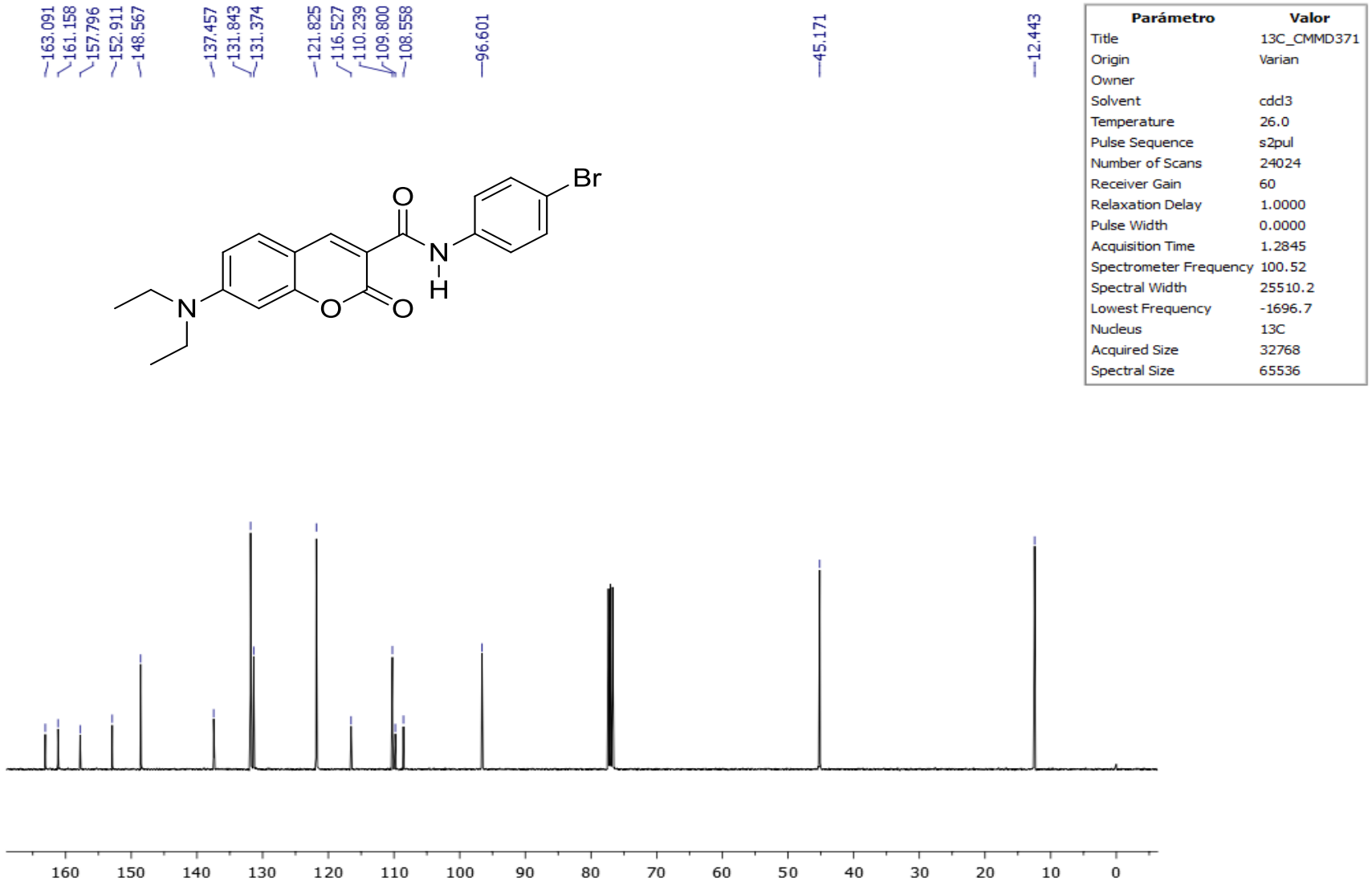

Parámetro	Valor
Title	13C_CMMD371
Origin	Varian
Owner	
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	24024
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Spectrometer Frequency	100.52
Spectral Width	25510.2
Lowest Frequency	-1696.7
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

^{13}C-NMR Spectra for *N*-(4-bromophenyl)-7-(diethylamino)-2-oxo-*2H*--chromene-3-carboxamide **(3e)**

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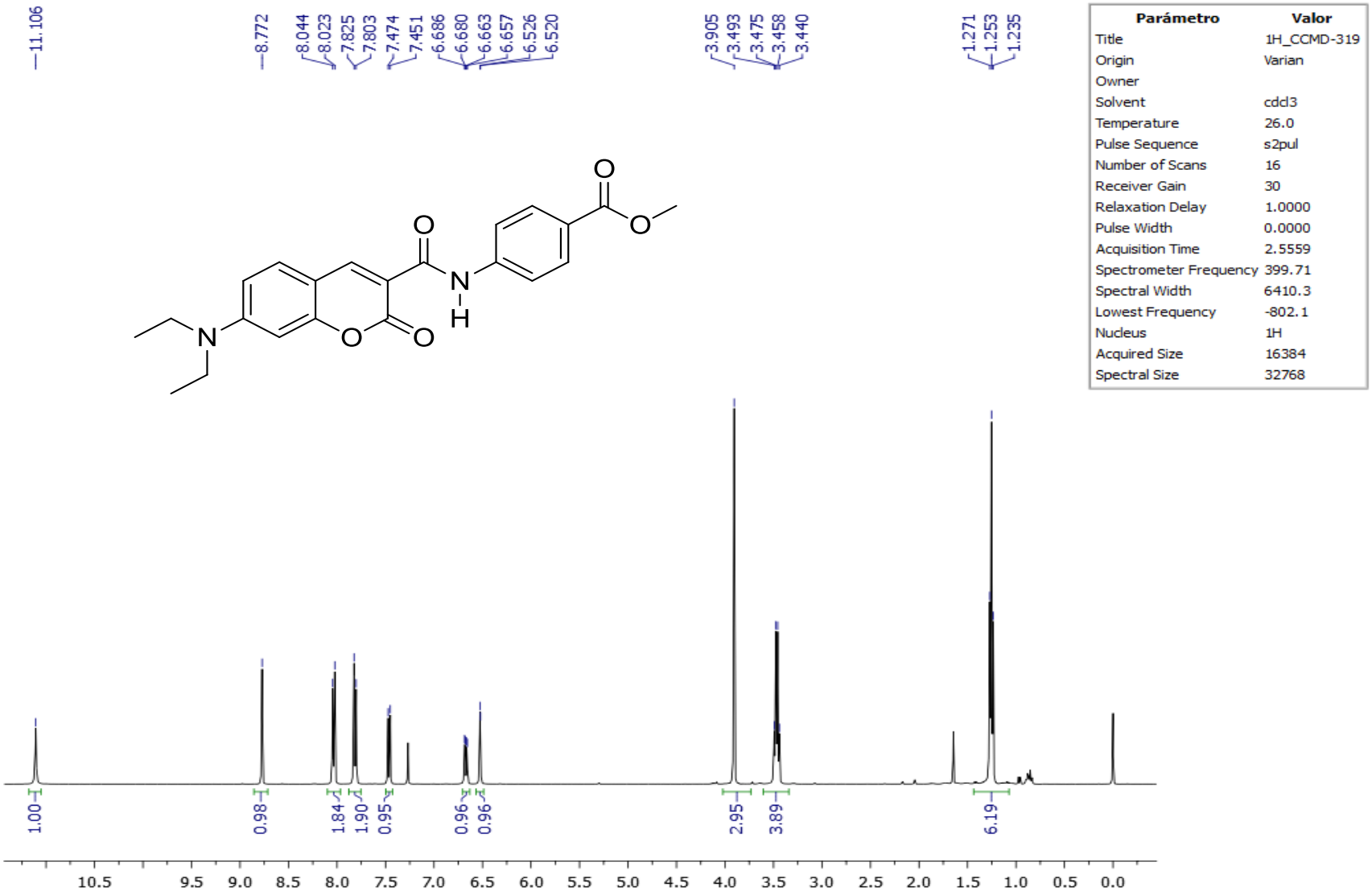

Parámetro	Valor
Title	1H_CCMD-319
Origin	Varian
Owner	
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	16
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.5559
Spectrometer Frequency	399.71
Spectral Width	6410.3
Lowest Frequency	-802.1
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

^{1}H-NMR Spectra for methyl-4-(7-(diethylamino)-2-oxo-*2H*--chromene-3-carboxamide)benzoate **(3f)**

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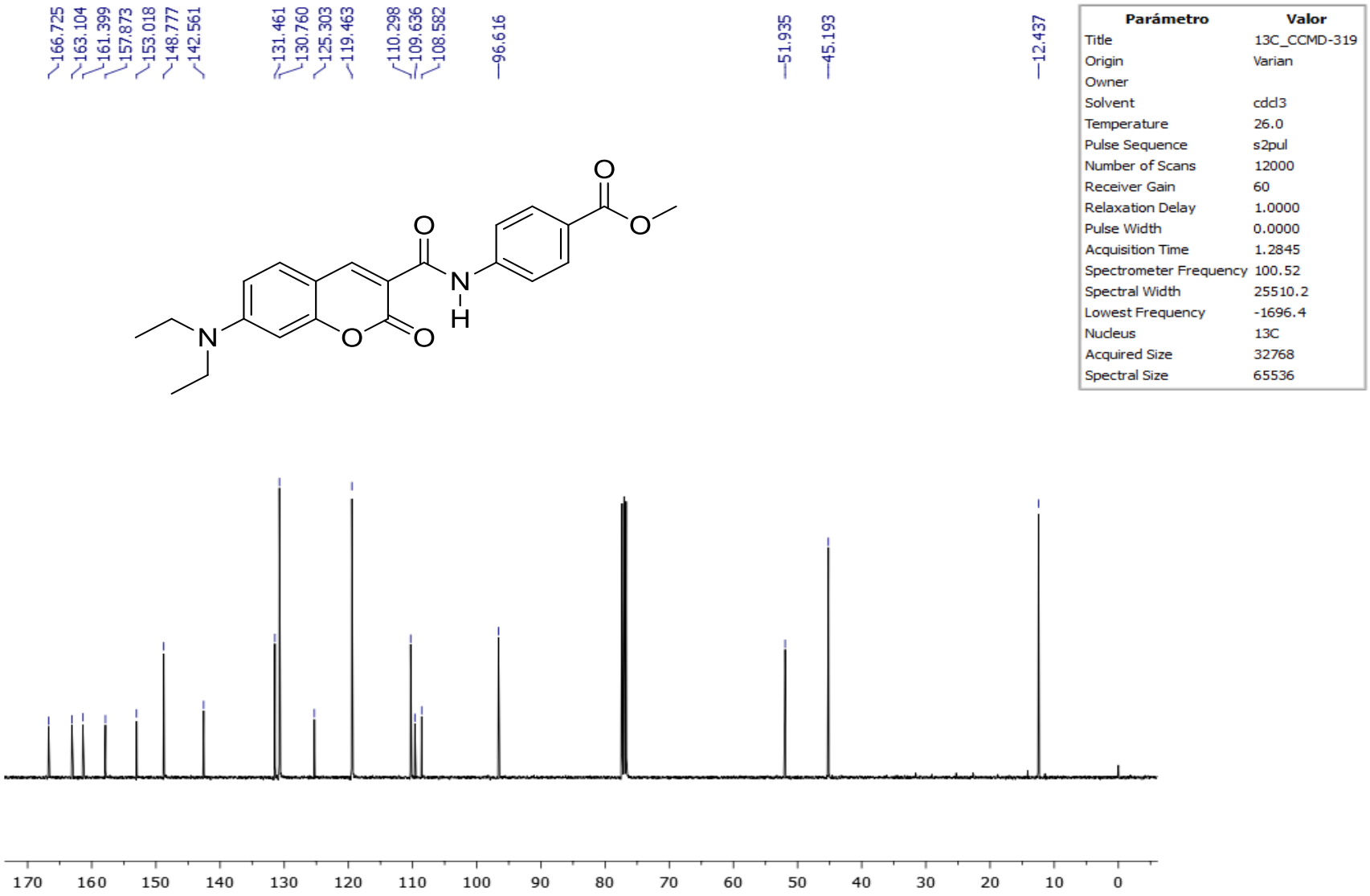

Parámetro	Valor
Title	13C_CCMD-319
Origin	Varian
Owner	
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	12000
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Spectrometer Frequency	100.52
Spectral Width	25510.2
Lowest Frequency	-1696.4
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

^{13}C-NMR Spectra for methyl-4-(7-(diethylamino)-2-oxo-*2H*--chromene-3-carboxamide)benzoate **(3f)**

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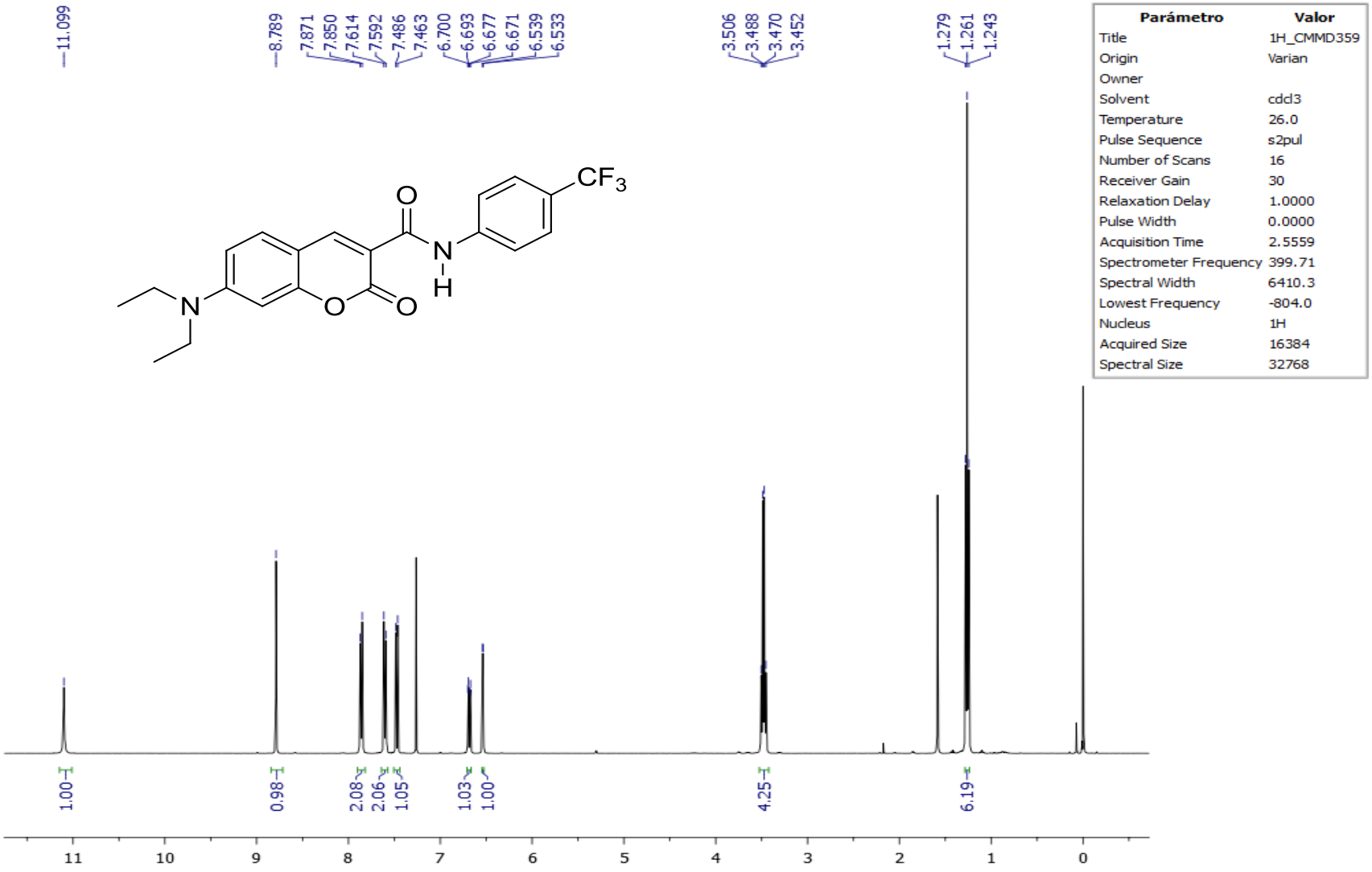

Parámetro	Valor
Title	1H_CMMD359
Origin	Varian
Owner	
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	16
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.5559
Spectrometer Frequency	399.71
Spectral Width	6410.3
Lowest Frequency	-804.0
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

^{1}H-NMR Spectra for 7-(diethylamino)-2-oxo-*N*-(4-(trifluoromethyl)phenyl)-*2H*--chromene-3-carboxamide **(3g)**

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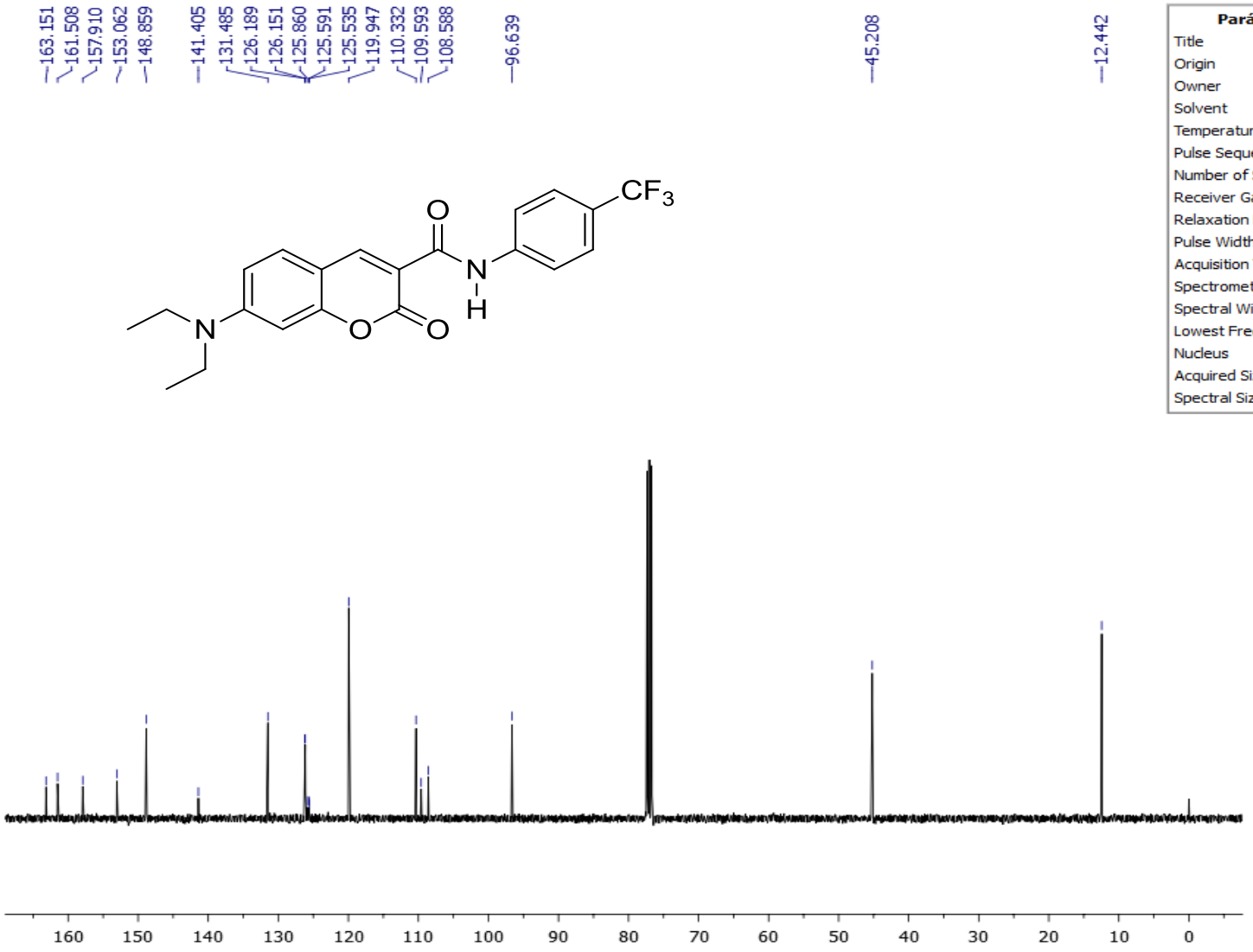

Parámetro	Valor
Title	13C_CMMD359
Origin	Varian
Owner	
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	944
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Spectrometer Frequency	100.58
Spectral Width	25510.2
Lowest Frequency	-1689.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

^{13}C-NMR Spectra for 7-(diethylamino)-2-oxo-*N*-(4-(trifluoromethyl)phenyl)-*2H*--chromene-3-carboxamide **(3g)**

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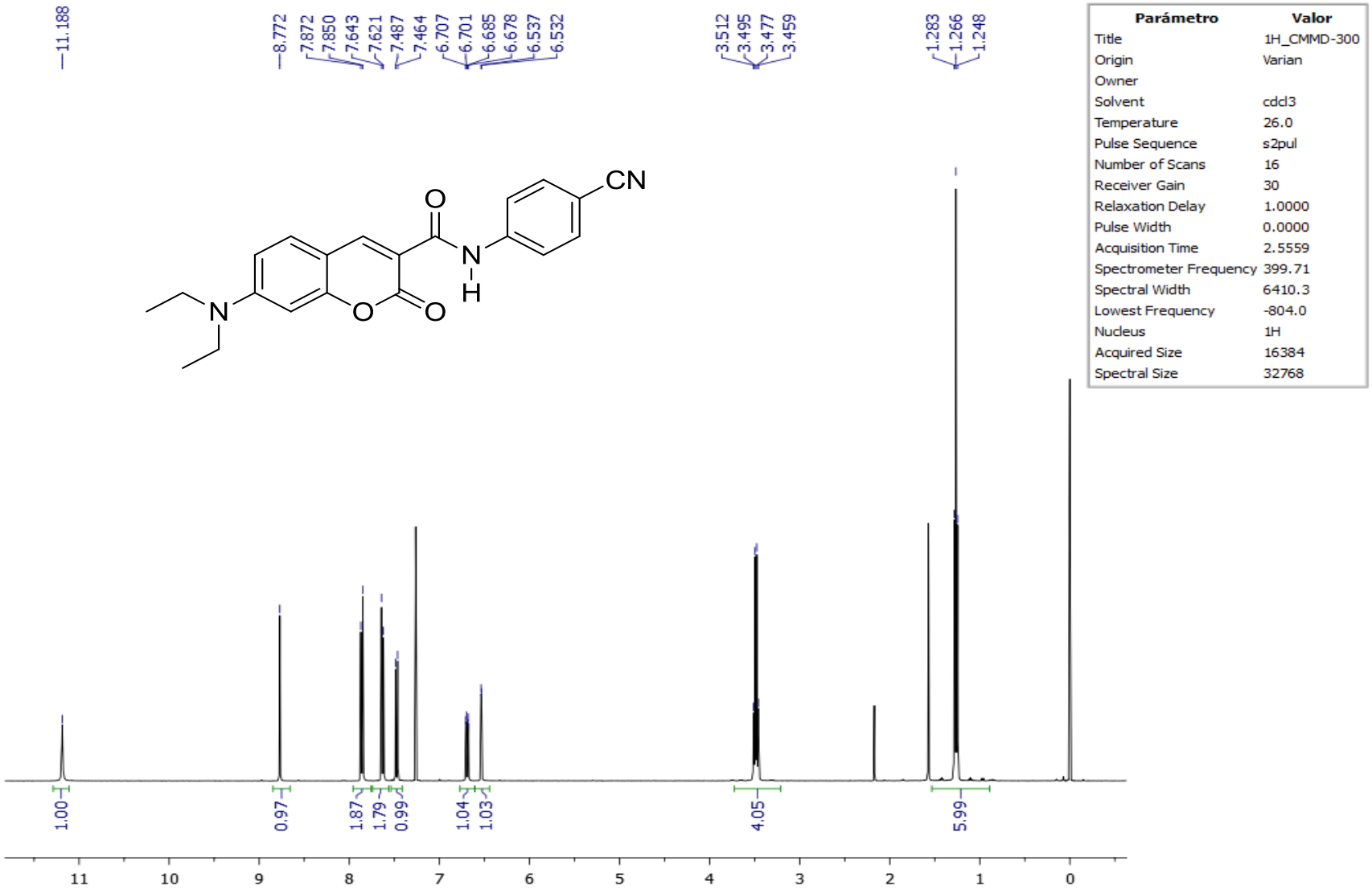

Parámetro	Valor
Title	1H_CMMD-300
Origin	Varian
Owner	
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	16
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.5559
Spectrometer Frequency	399.71
Spectral Width	6410.3
Lowest Frequency	-804.0
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

^{1}H-NMR Spectra for *N*-(4-cyanophenyl)-7-(diethylamino)-2-oxo-*2H*--chromene-3-carboxamide **(3h)**

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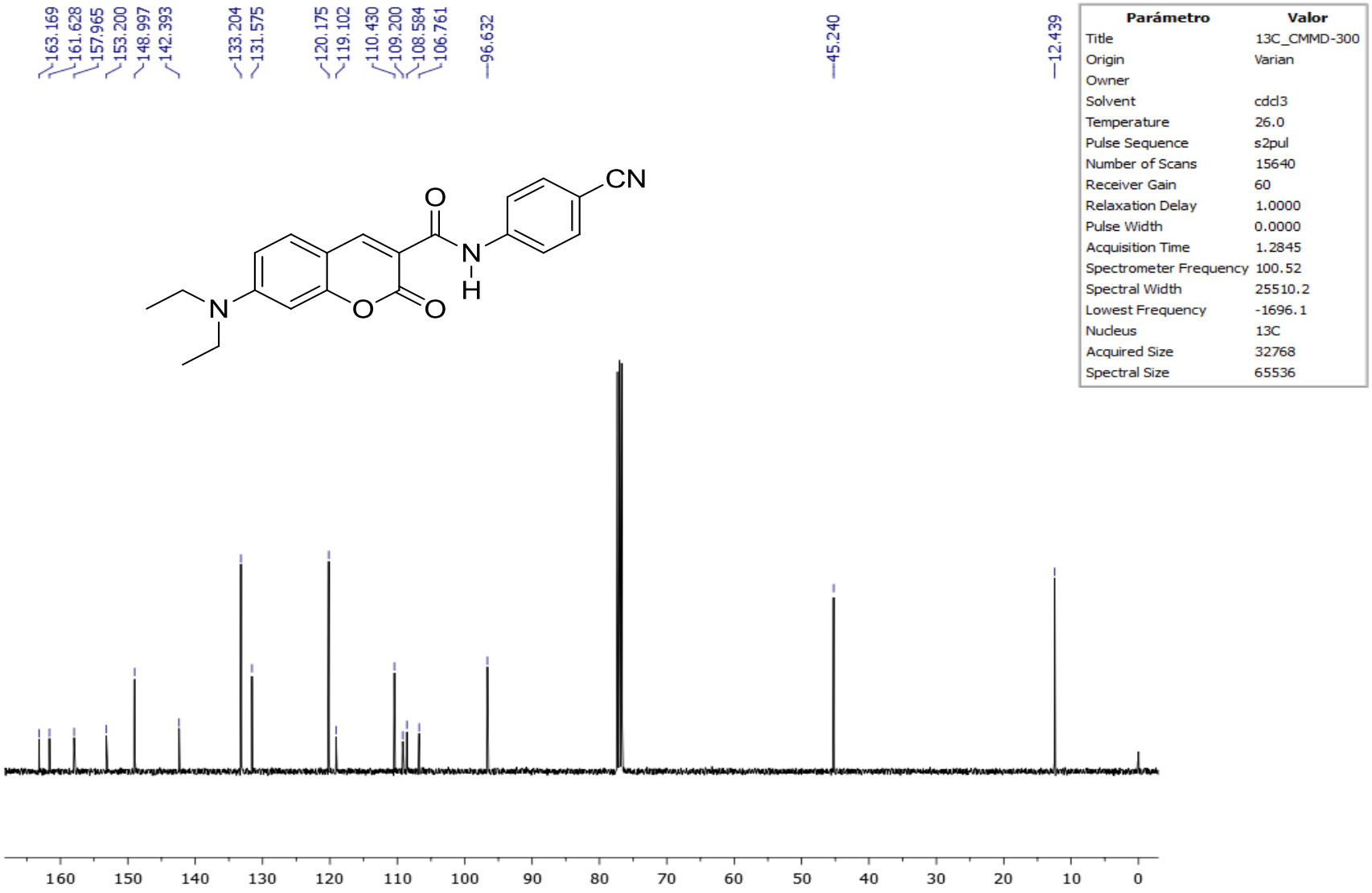

Parámetro	Valor
Title	13C_CMMD-300
Origin	Varian
Owner	
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	15640
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Spectrometer Frequency	100.52
Spectral Width	25510.2
Lowest Frequency	-1696.1
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

^{13}C-NMR Spectra for *N*-(4-cyanophenyl)-7-(diethylamino)-2-oxo-*2H*--chromene-3-carboxamide **(3h)**

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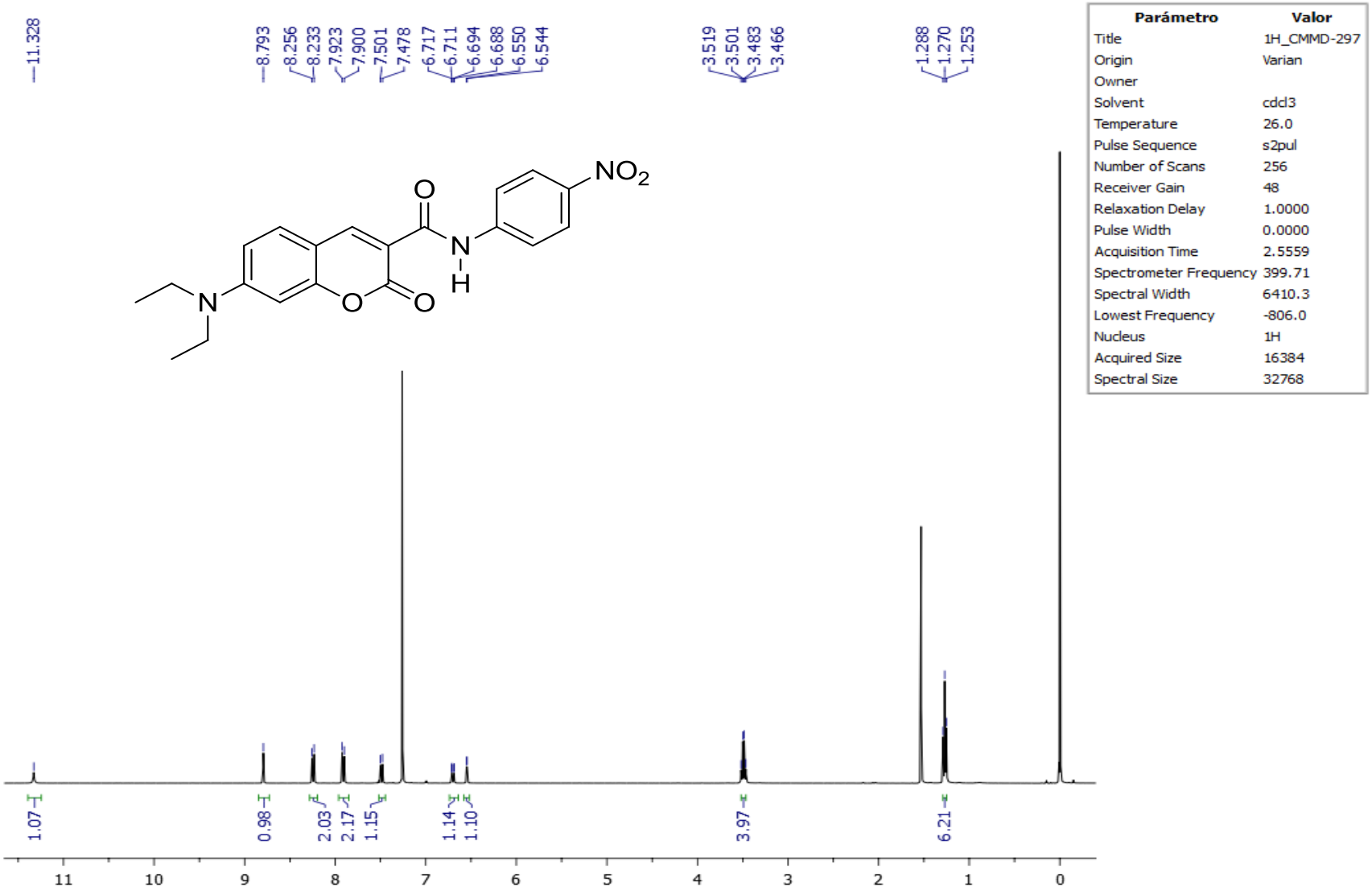

Parámetro	Valor
Title	1H_CMMD-297
Origin	Varian
Owner	
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	256
Receiver Gain	48
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.5559
Spectrometer Frequency	399.71
Spectral Width	6410.3
Lowest Frequency	-806.0
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

^{1}H-NMR Spectra for **7**-(diethylamino)-*N*-(4-nitrophenyl)-2-oxo-*2H*--chromene-3-carboxamide **(3i)**

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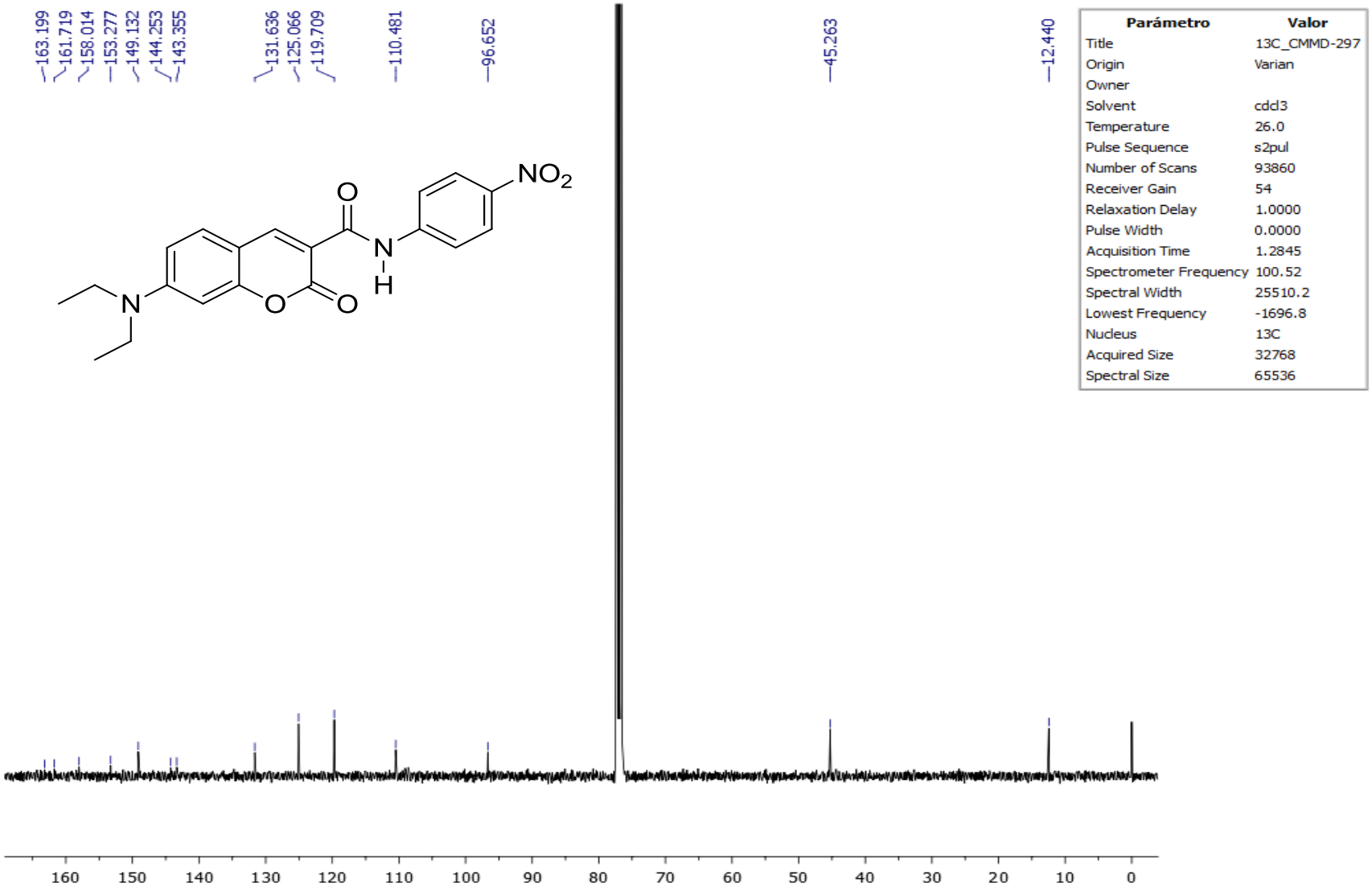

Parámetro	Valor
Title	13C_CMMD-297
Origin	Varian
Owner	
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	93860
Receiver Gain	54
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Spectrometer Frequency	100.52
Spectral Width	25510.2
Lowest Frequency	-1696.8
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

^{13}C-NMR Spectra for **7**-(diethylamino)-*N*-(4-nitrophenyl)-2-oxo-*2H*--chromene-3-carboxamide **(3i)**