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Supporting Information

Design, Synthesis and Photophysical Studies of Styryl-Based Push-Pull Fluorophores with Remarkable Solvatofluorochromism

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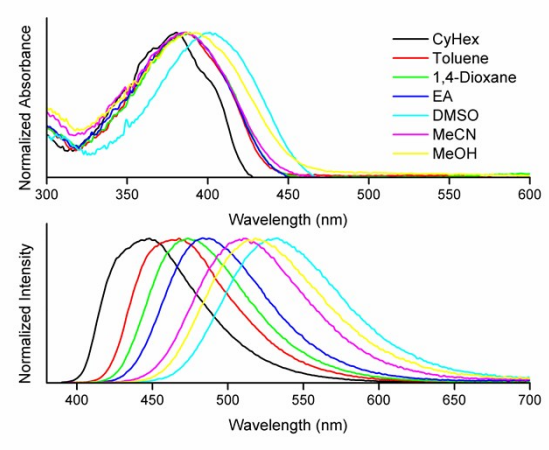
Summary

Photophysical characterization

Figures S1. Absorption and emission spectra of all push-pull dyes in different solvents.



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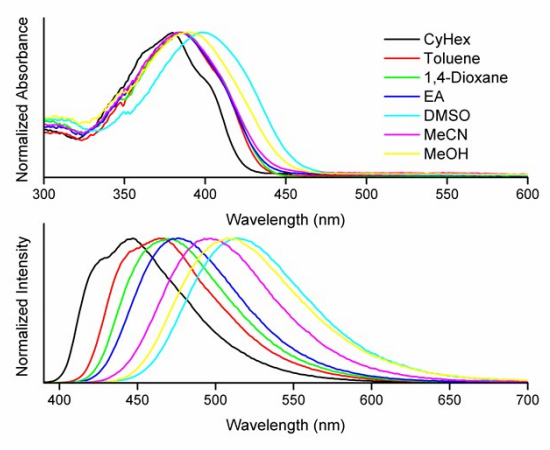

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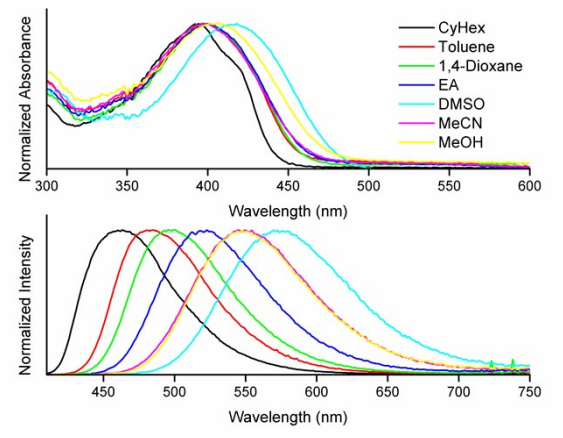

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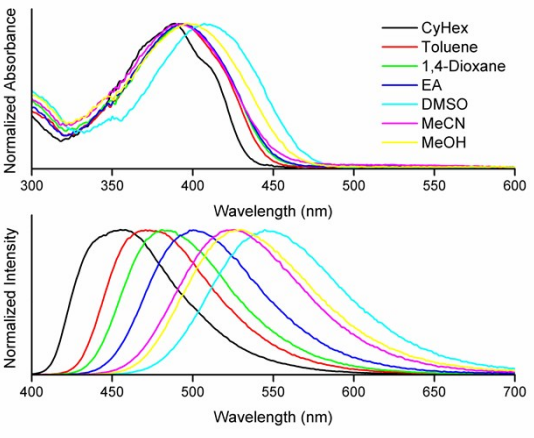

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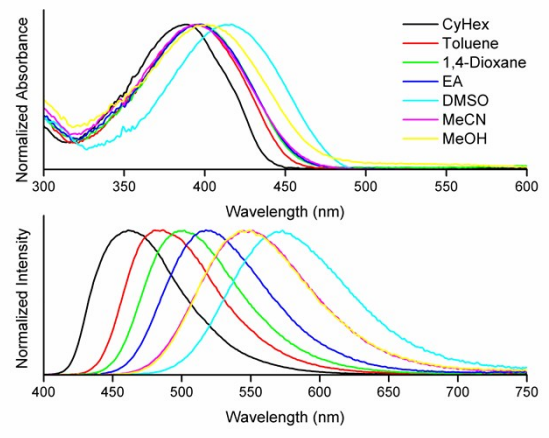

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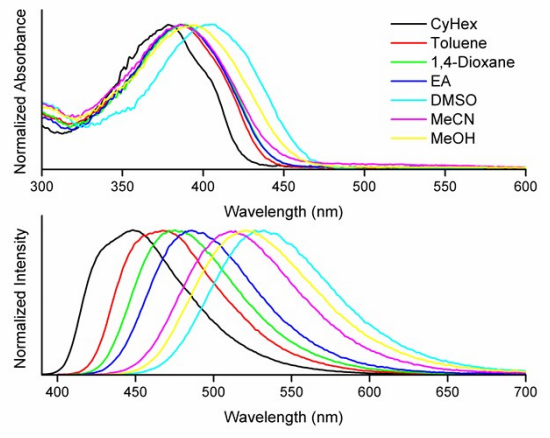

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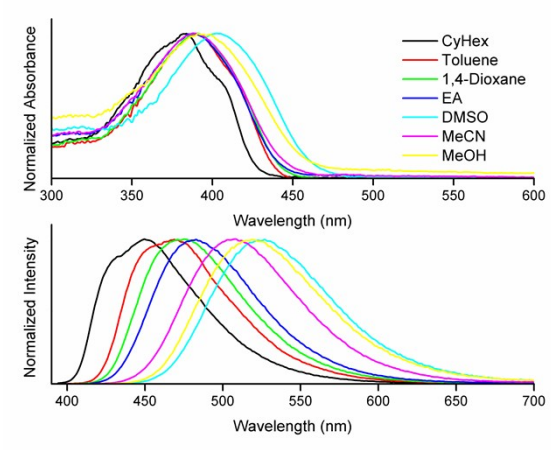

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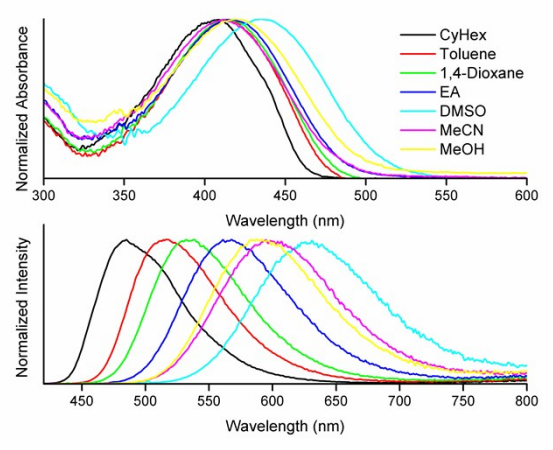

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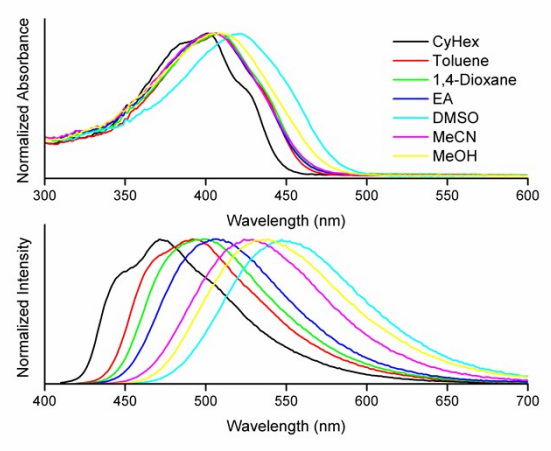

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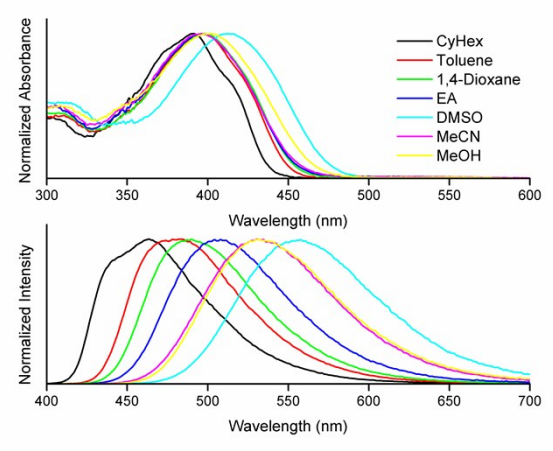

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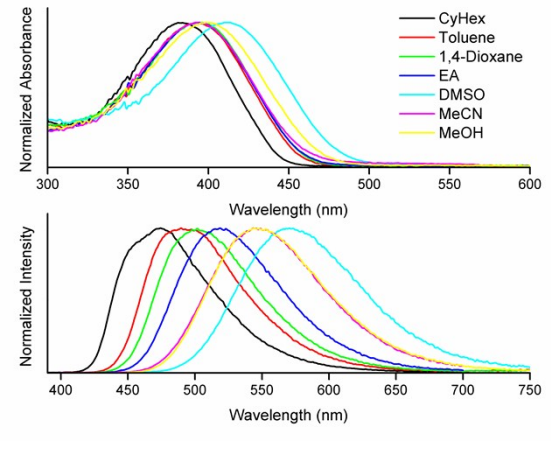

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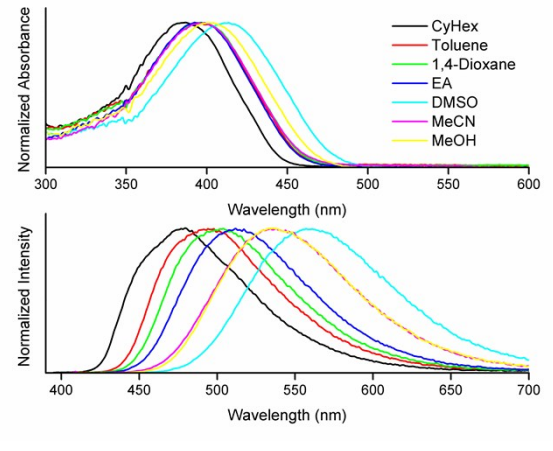

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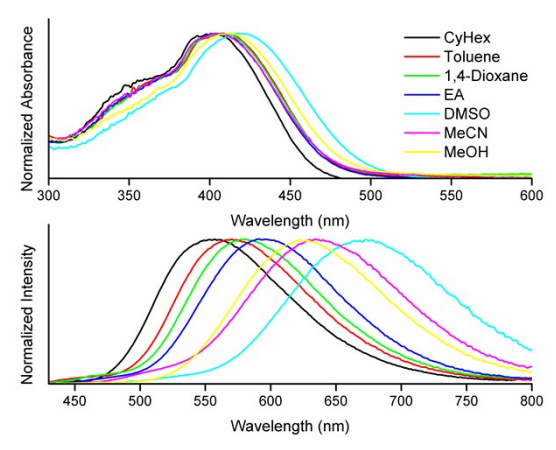

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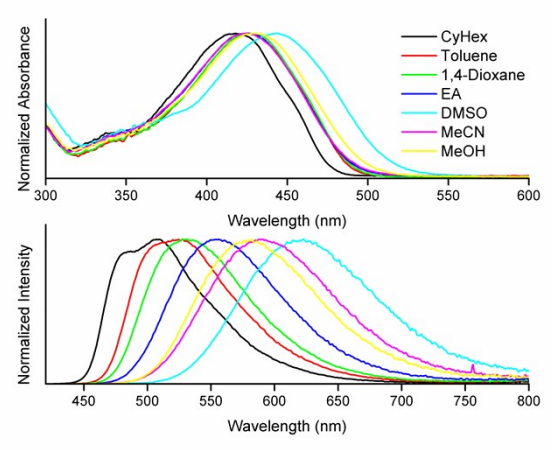

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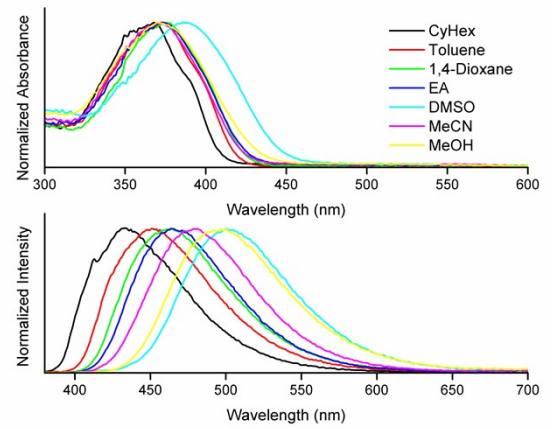

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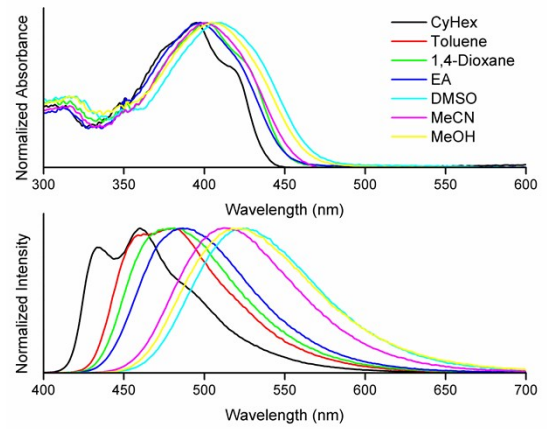

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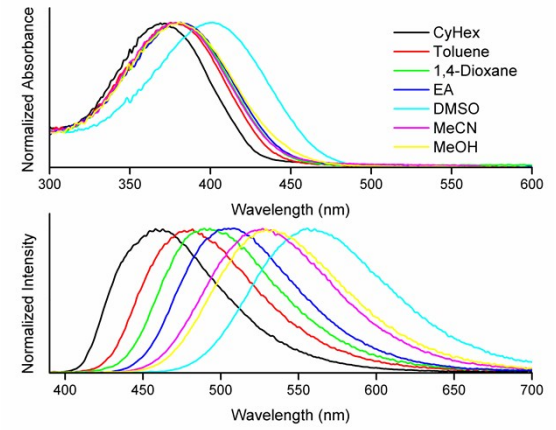

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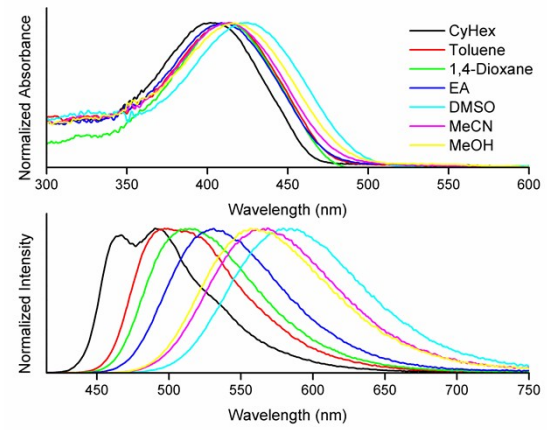

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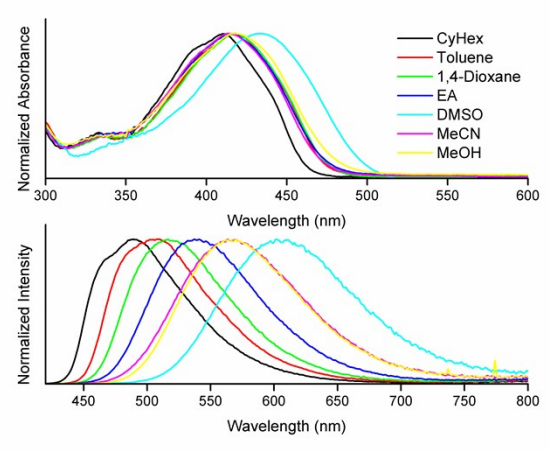

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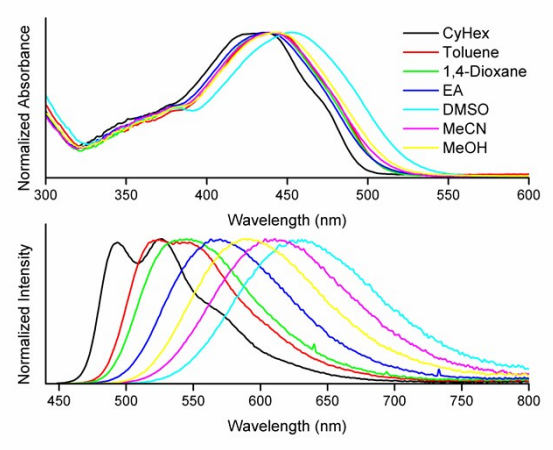


D14c

Transition dipole moment calculations

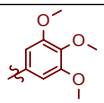
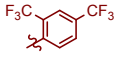
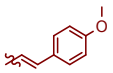
Stokes shift vs. orientation polarizability function (Δf) for **all dyes**. The linear plots shown were obtained with aprotic solvents according to the Lippert's equation.

Lippert's Equation $$\nu_{abs} - \nu_{em} = \frac{2}{hc}\Delta f \frac{(\mu_e - \mu_g)}{a^3}$$

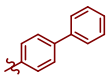
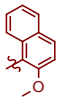
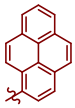
In this equation, h (= 6.6256 x 10^{-27} ergs) is the Planck's constant, c (= 2.9979 x 10^{10} cm/s) is the speed of light, and a is the radius of the Onsager's cavity. ν_{abs} and ν_{em} are the wavenumbers (cm^{-1}) of the absorption and emission, respectively, $\Delta\nu$ is the Stokes shift (cm^{-1}), Δf is the Lippert's parameter, and μ_e and μ_g are the dipole moments of the excited and ground states, respectively.

Table S1. Transition dipole moment (in Debye)

Varied phenyl/fixed amine (NHEt)

 **D1b**	 **D2b**	 **D3b**	 **D4b**	 **D5b**	 **D6b**	 **D7b**	 **D8b**	 **D9b**
10.3	9.9	11.7	11.4	12.2	10.5	11.0	13.4	10.9

Varied polycyclic aromatic/fixed amine (NHEt)

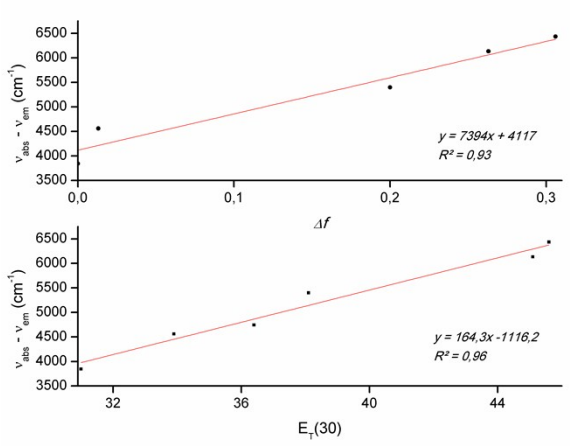
 **D10b**	 **D11b**	 **D12b**	 **D14b**

11.7	10.6	10.2	12.4

Fixed aryl/varied amine

D2a	D2c	D11a	D11c	D14a	D14c
9.2	11.6	10.0	14.8	11.7	14.2

Figures S2. Lippert-Mataga and Reichardt's $E_T(30)$ plots related to the Stokes shift of the solvatofluorochromic dyes



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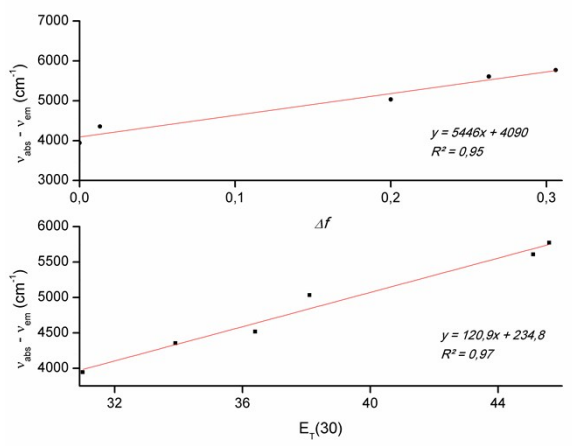

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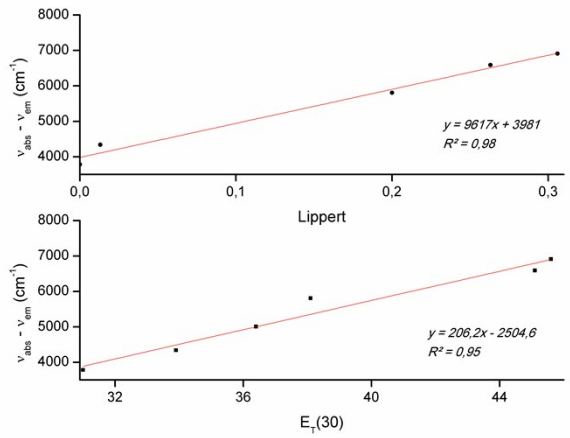

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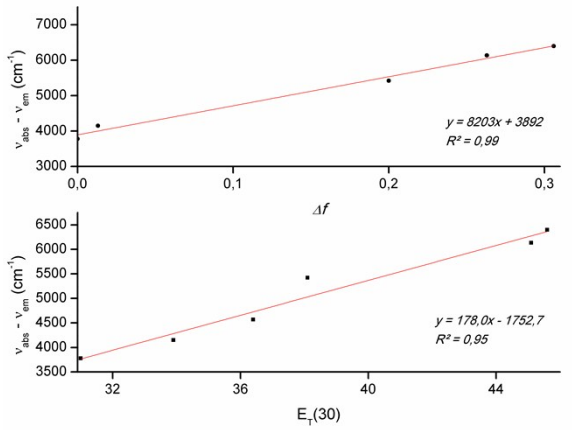

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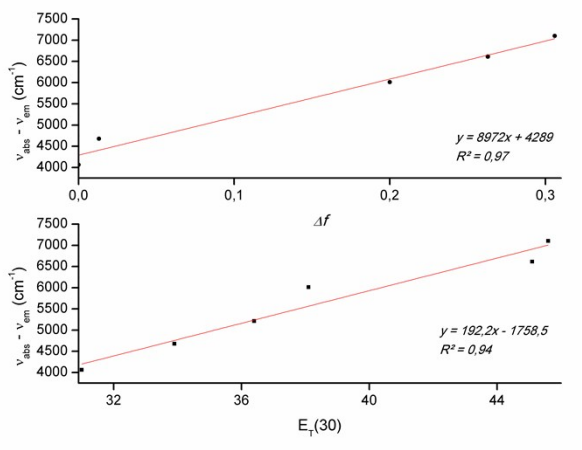

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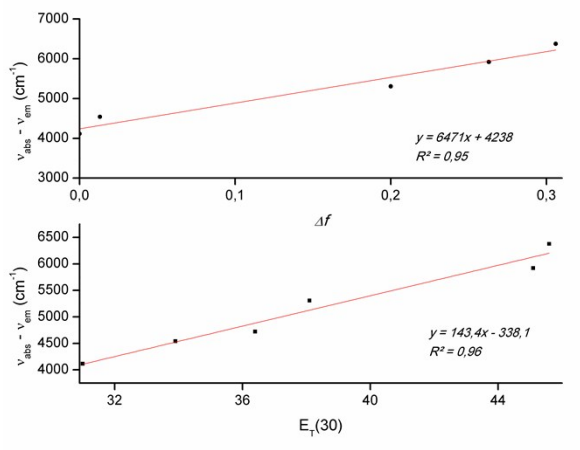

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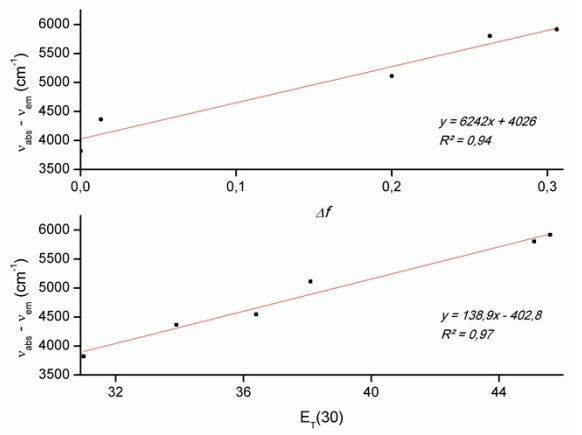

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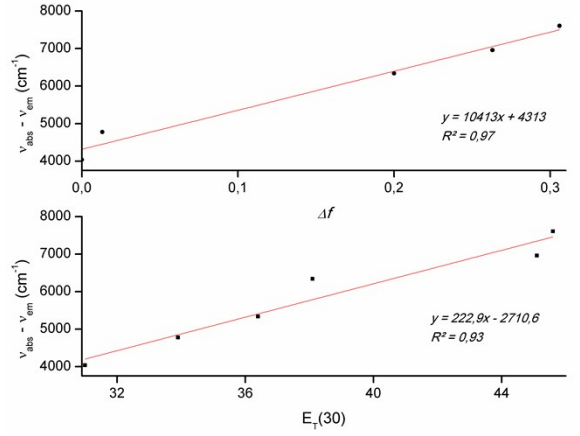

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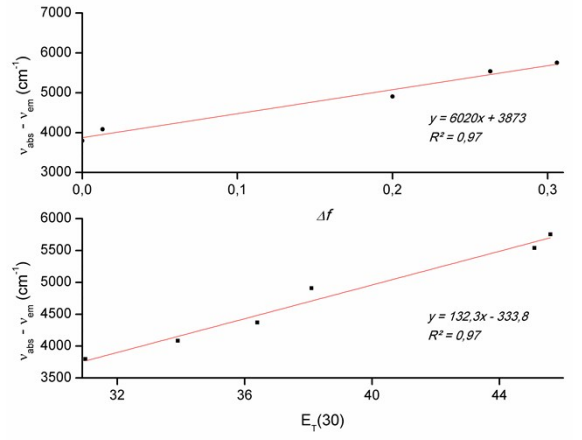

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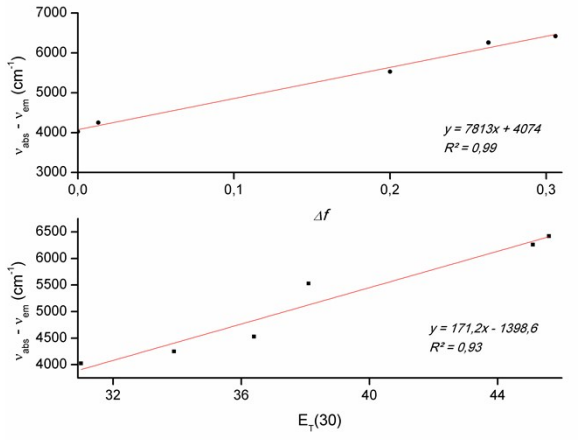

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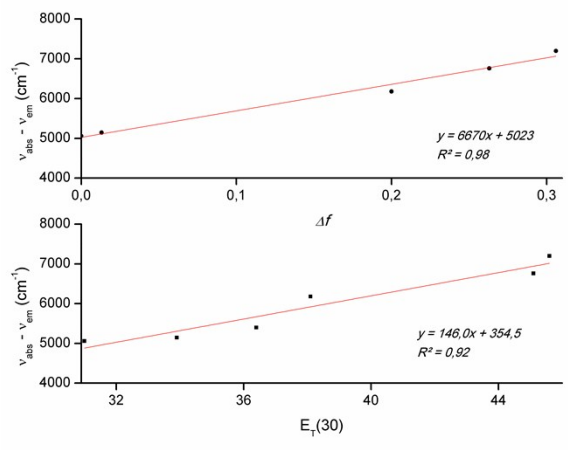

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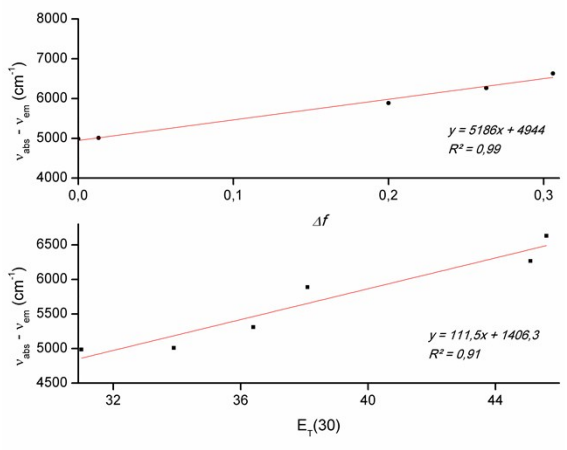

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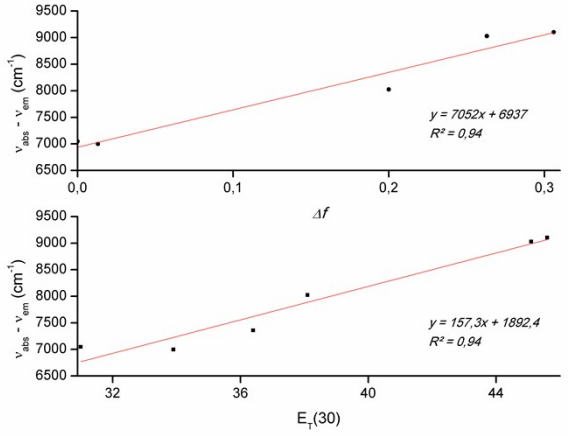

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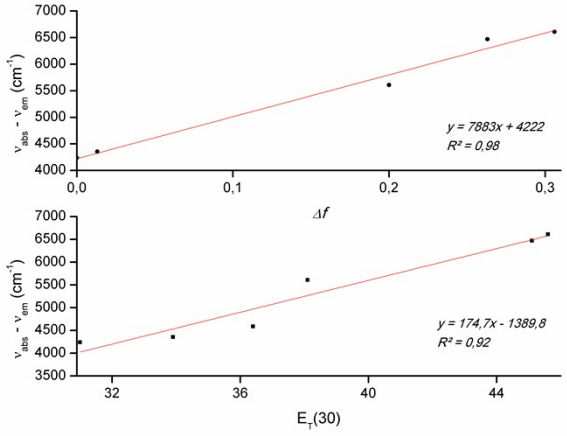

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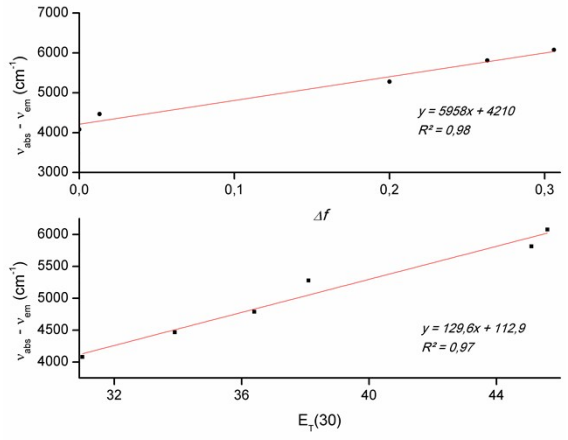

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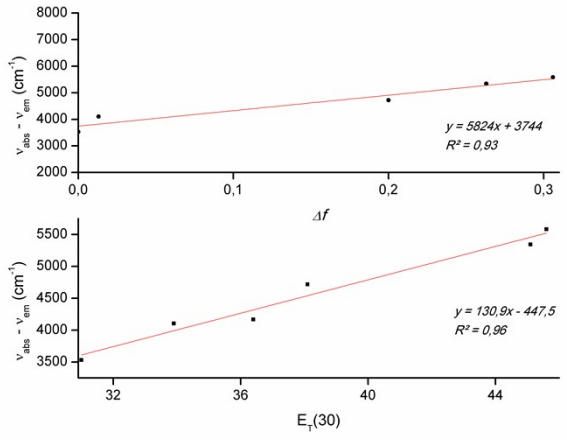

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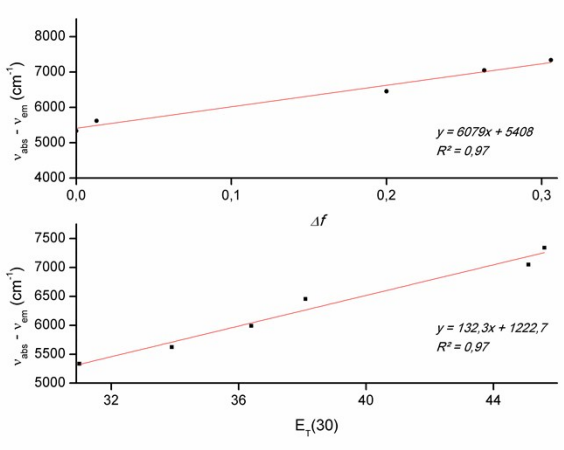

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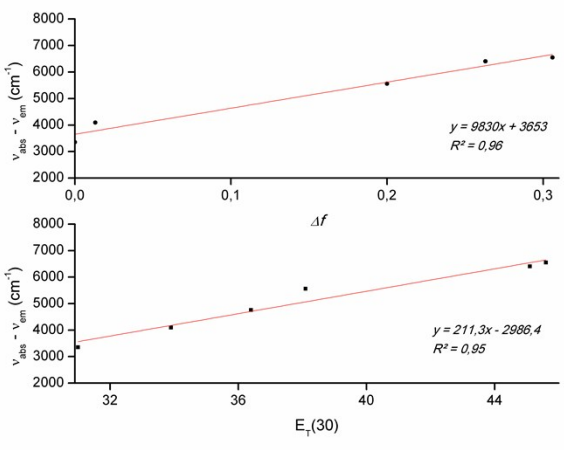

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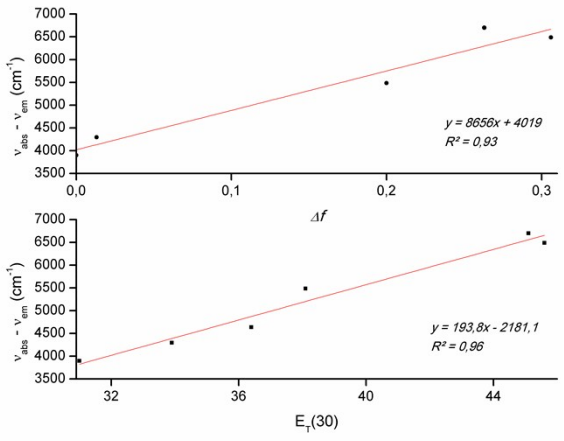

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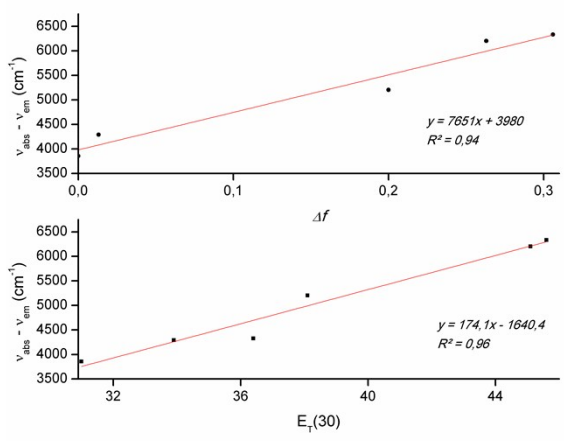


D14c

DFT calculations

(*Note: for all the reported (TD)DFT calculations, the the number of imaginary frequencies was 0.*)

Figure S3. Optimized ground state DFT structures for all dyes

D1b

D2b

D3b

D4b

D5b

D6b

D7b

D8b

D9b

D10b

D11b

D12b

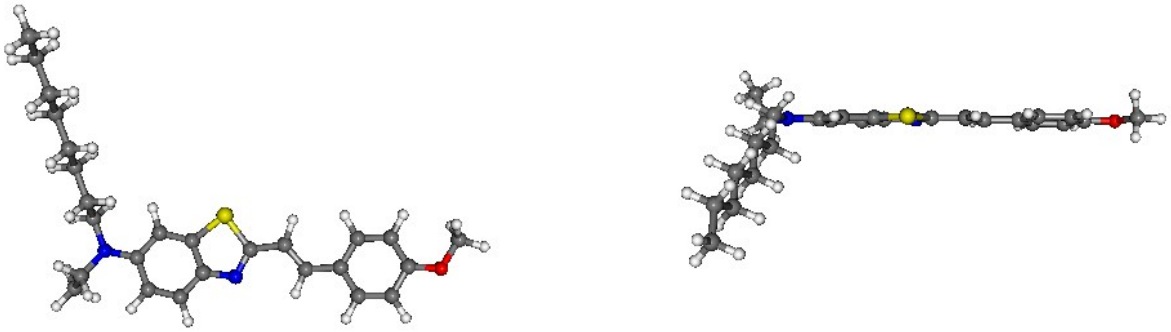
D13b

D14b

D2a

D11a

D14a



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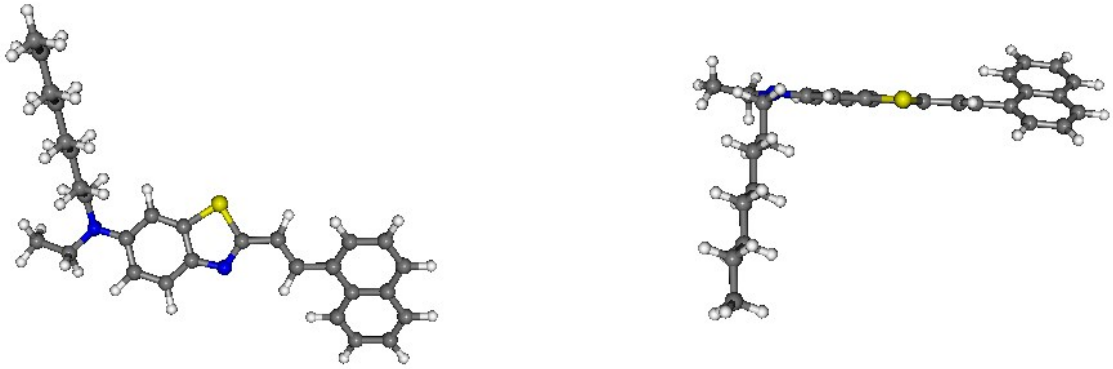

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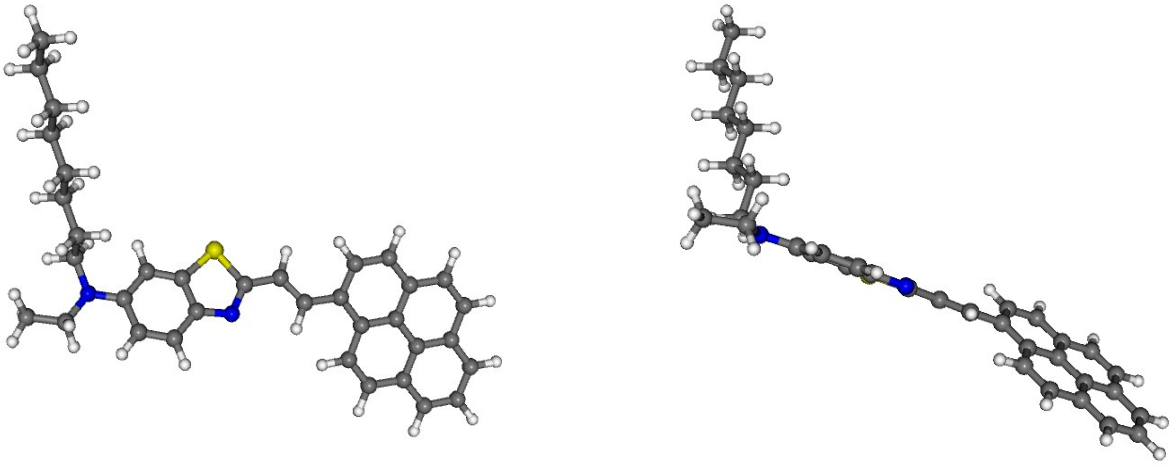


D14c

Table S2. Time-dependent TD-DFT calculations data

D1b

Solvent	λ_{abs}	λ_{abs} (calc.)	$S_0 \rightarrow S_1$ transition energy (eV)	f_{OS} (oscillator strentgh)
Cyclohexane	380	408	3.0367	1.0978
DMSO	400	418	2.9648	1.0802

D2b

Solvent	λ_{abs}	λ_{abs} (calc.)	$S_0 \rightarrow S_1$ transition energy (eV)	f_{OS} (oscillator strentgh)
Cyclohexane	380	406	3.0510	1.2858
DMSO	399	415	2.9864	1.2780

D3b

Solvent	λ_{abs}	λ_{abs} (calc.)	$S_0 \rightarrow S_1$ transition energy (eV)	f_{OS} (oscillator strentgh)
Cyclohexane	394	431	2.8731	1.0503
DMSO	417	441	2.8062	1.0375

D8b

Solvent	λ_{abs}	λ_{abs} (calc.)	$S_0 \rightarrow S_1$ transition energy (eV)	f_{OS} (oscillator strentgh)
Cyclohexane	407	450	2.7549	0.9642
DMSO	438	463	2.6767	0.9629

Total energy of optimized structures

D1b Cy	E(RmPW+HF-PW91)	=	-1165.18742125	A.U.
D1b DMSO	E(RmPW+HF-PW91)	=	-1165.20168224	A.U.
D1b gas	E(RmPW+HF-PW91)	=	-1165.18037351	A.U.
D2a gas	E(RmPW+HF-PW91)	=	-1201.08533457	A.U.
D2b Cy	E(RmPW+HF-PW91)	=	-1279.71515019	A.U.
D2b DMSO	E(RmPW+HF-PW91)	=	-1279.73038428	A.U.
D2b gas	E(RmPW+HF-PW91)	=	-1279.70755884	A.U.
D2c gas	E(RmPW+HF-PW91)	=	-1594.21353293	A.U.
D3b Cy	E(RmPW+HF-PW91)	=	-1502.25975566	A.U.
D3b DMSO	E(RmPW+HF-PW91)	=	-1502.27443001	A.U.
D3b gas	E(RmPW+HF-PW91)	=	-1502.25223554	A.U.
D4b gas	E(RmPW+HF-PW91)	=	-3738.88691143	A.U.
D5b gas	E(RmPW+HF-PW91)	=	-1502.24706149	A.U.
D6b gas	E(RmPW+HF-PW91)	=	-1394.22288895	A.U.
D7b gas	E(RmPW+HF-PW91)	=	-1508.74432782	A.U.
D8b Cy	E(RmPW+HF-PW91)	=	-1839.32417870	A.U.
D8b DMSO	E(RmPW+HF-PW91)	=	-1839.33813369	A.U.
D8b gas	E(RmPW+HF-PW91)	=	-1839.31722361	A.U.
D9b gas	E(RmPW+HF-PW91)	=	-1357.11386084	A.U.
D10b gas	E(RmPW+HF-PW91)	=	-1396.23659649	A.U.
D11a gas	E(RmPW+HF-PW91)	=	-1240.19704013	A.U.
D11b gas	E(RmPW+HF-PW91)	=	-1318.81943702	A.U.
D11c gas	E(RmPW+HF-PW91)	=	-1633.32221988	A.U.
D12b gas	E(RmPW+HF-PW91)	=	-1433.34278061	A.U.
D13b gas	E(RmPW+HF-PW91)	=	-1472.45050715	A.U.
D14a gas	E(RmPW+HF-PW91)	=	-1470.07581507	A.U.
D14b gas	E(RmPW+HF-PW91)	=	-1548.69812394	A.U.
D14c gas	E(RmPW+HF-PW91)	=	-1863.20100546	A.U.

Cartesian coordinates for the optimized structures

D1b (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.251789	-0.576066	-0.057055
2	6	0	-4.086717	0.542726	-0.055819
3	6	0	-3.510650	1.836045	-0.037797
4	6	0	-2.148882	2.022585	-0.023540
5	6	0	-1.296295	0.910627	-0.032112
6	6	0	-1.874645	-0.374000	-0.051151
7	16	0	-0.604120	-1.554909	-0.054179
8	6	0	0.583862	-0.238650	-0.029455
9	7	0	0.072367	0.950581	-0.020403
10	6	0	1.993442	-0.564202	-0.020065
11	6	0	2.957063	0.372457	0.004695
12	6	0	4.396797	0.151925	0.016272
13	6	0	5.244165	1.267217	0.048919
14	6	0	6.624147	1.122195	0.061719
15	6	0	7.190497	-0.145942	0.041768
16	6	0	6.363052	-1.266043	0.008874
17	6	0	4.986265	-1.120758	-0.003834
18	1	0	4.363065	-2.006620	-0.030200
19	1	0	6.797509	-2.258931	-0.007334
20	1	0	8.267543	-0.264220	0.051508
21	1	0	7.257879	2.001003	0.087190
22	1	0	4.806180	2.259328	0.064586
23	1	0	2.634301	1.409579	0.018210
24	1	0	2.239976	-1.620391	-0.033413
25	1	0	-1.722299	3.017862	-0.007663
26	1	0	-4.169955	2.697765	-0.041602
27	7	0	-5.461508	0.427503	-0.103042
28	6	0	-6.139829	-0.826658	0.134096
29	6	0	-7.644238	-0.631623	0.113758
30	1	0	-7.972459	-0.225895	-0.845539
31	1	0	-8.154187	-1.582617	0.274423
32	1	0	-7.965195	0.052425	0.904650
33	1	0	-5.831017	-1.270983	1.092550
34	1	0	-5.855306	-1.536120	-0.650205
35	1	0	-5.963040	1.245707	0.202006
36	1	0	-3.660544	-1.576927	-0.063835

D1b (cyclohexane)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-3.252285	-0.575076	-0.051390
2	6	0	-4.091900	0.541978	-0.051998
3	6	0	-3.518045	1.837753	-0.035988
4	6	0	-2.156620	2.028482	-0.023137
5	6	0	-1.300600	0.918397	-0.030564
6	6	0	-1.875969	-0.367497	-0.046747
7	16	0	-0.601352	-1.545246	-0.048404
8	6	0	0.584525	-0.227826	-0.027034
9	7	0	0.069175	0.961063	-0.019844
10	6	0	1.993813	-0.554949	-0.018178
11	6	0	2.961459	0.378468	0.004105
12	6	0	4.400507	0.151095	0.014590
13	6	0	5.251775	1.264002	0.048778
14	6	0	6.631692	1.113319	0.060816
15	6	0	7.192996	-0.157673	0.038270
16	6	0	6.361030	-1.275117	0.003536
17	6	0	4.984204	-1.124679	-0.008285
18	1	0	4.357930	-2.009366	-0.036475
19	1	0	6.792078	-2.270584	-0.014942
20	1	0	8.270665	-0.280331	0.047292
21	1	0	7.269534	1.990418	0.087653
22	1	0	4.817358	2.258830	0.066409
23	1	0	2.647759	1.419273	0.016515
24	1	0	2.236699	-1.612986	-0.029666
25	1	0	-1.734392	3.027103	-0.008854
26	1	0	-4.180710	2.698012	-0.039062
27	7	0	-5.464155	0.423921	-0.098534
28	6	0	-6.138600	-0.834378	0.135111
29	6	0	-7.644086	-0.651880	0.096105
30	1	0	-7.965282	-0.256705	-0.870111
31	1	0	-8.146294	-1.606831	0.258293
32	1	0	-7.979660	0.035671	0.877773
33	1	0	-5.837845	-1.271695	1.099284
34	1	0	-5.839247	-1.545302	-0.642433
35	1	0	-5.969664	1.245765	0.199218
36	1	0	-3.655814	-1.578755	-0.055722

D1b (DMSO)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.252178	-0.571360	-0.030985
2	6	0	-4.101558	0.541483	-0.038981
3	6	0	-3.533536	1.842917	-0.031760
4	6	0	-2.172935	2.043128	-0.026148
5	6	0	-1.309023	0.937181	-0.030291
6	6	0	-1.877512	-0.352086	-0.033233
7	16	0	-0.595479	-1.523629	-0.029572
8	6	0	0.584965	-0.203871	-0.024959
9	7	0	0.062622	0.985211	-0.026034
10	6	0	1.993891	-0.533170	-0.018898
11	6	0	2.969214	0.394054	0.003462

12	6	0	4.406626	0.150404	0.011159
13	6	0	5.268572	1.256254	0.053066
14	6	0	6.647921	1.090988	0.062193
15	6	0	7.196067	-0.186808	0.028922
16	6	0	6.352335	-1.296640	-0.013446
17	6	0	4.975794	-1.132887	-0.022575
18	1	0	4.340757	-2.013823	-0.057468
19	1	0	6.774057	-2.298279	-0.040363
20	1	0	8.274676	-0.320896	0.035523
21	1	0	7.296180	1.962980	0.094961
22	1	0	4.843292	2.257380	0.078765
23	1	0	2.673270	1.442544	0.019183
24	1	0	2.229929	-1.595526	-0.031994
25	1	0	-1.760843	3.049009	-0.018837
26	1	0	-4.205324	2.698826	-0.032945
27	7	0	-5.469904	0.418123	-0.085993
28	6	0	-6.132965	-0.848342	0.149809
29	6	0	-7.638915	-0.705522	0.037537
30	1	0	-7.926405	-0.353181	-0.955720
31	1	0	-8.121898	-1.668464	0.212098
32	1	0	-8.025836	0.001250	0.777047
33	1	0	-5.866635	-1.254213	1.137632
34	1	0	-5.782944	-1.572607	-0.593447
35	1	0	-5.981501	1.247368	0.207781
36	1	0	-3.642720	-1.581989	-0.024101

D2a (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.922269	-0.940906	-0.000043
2	6	0	5.839836	0.107990	-0.000010
3	6	0	5.373650	1.438325	-0.007218
4	6	0	4.026255	1.730110	-0.008381
5	6	0	3.091289	0.690261	-0.006677
6	6	0	3.566411	-0.638255	-0.004135
7	16	0	2.207026	-1.716389	-0.002300
8	6	0	1.125582	-0.308441	-0.003811
9	7	0	1.728412	0.836663	-0.006085
10	6	0	-0.303793	-0.526766	-0.002186
11	6	0	-1.194335	0.481317	-0.002304
12	6	0	-2.643935	0.377286	-0.000821
13	6	0	-3.338378	-0.836802	-0.005247
14	6	0	-4.723806	-0.885023	-0.003036
15	6	0	-5.460857	0.301139	0.003766
16	6	0	-4.789346	1.524661	0.007857
17	6	0	-3.409527	1.554551	0.005397
18	1	0	-2.900566	2.512313	0.008558
19	1	0	-5.372273	2.437172	0.012824
20	8	0	-6.811952	0.362784	0.006556
21	6	0	-7.538646	-0.846557	0.002078
22	1	0	-8.589462	-0.564827	0.005456

23	1	0	-7.327079	-1.437179	-0.894991
24	1	0	-7.323649	-1.445841	0.892569
25	1	0	-5.218909	-1.846706	-0.006985
26	1	0	-2.793453	-1.773365	-0.011159
27	1	0	-0.791048	1.490172	-0.003241
28	1	0	-0.629087	-1.561473	-0.000545
29	1	0	3.678388	2.755643	-0.011194
30	1	0	6.097259	2.246317	-0.016560
31	7	0	7.205918	-0.145427	-0.053042
32	1	0	7.494448	-1.051372	0.278165
33	1	0	7.795943	0.591732	0.296455
34	1	0	5.266363	-1.968622	-0.002484

D2b (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.110043	-0.614657	-0.057645
2	6	0	-4.980843	0.476254	-0.054491
3	6	0	-4.446881	1.786768	-0.036780
4	6	0	-3.091205	2.017099	-0.024608
5	6	0	-2.203102	0.933789	-0.035191
6	6	0	-2.740011	-0.368333	-0.053964
7	16	0	-1.431936	-1.508272	-0.059848
8	6	0	-0.285578	-0.153829	-0.036202
9	7	0	-0.835697	1.018050	-0.025713
10	6	0	1.132298	-0.436895	-0.028793
11	6	0	2.068225	0.528943	-0.004228
12	6	0	3.511666	0.358270	0.005701
13	6	0	4.149783	-0.886009	-0.022711
14	6	0	5.531487	-0.998329	-0.010273
15	6	0	6.322318	0.151879	0.031322
16	6	0	5.707698	1.404597	0.059103
17	6	0	4.330711	1.498296	0.045965
18	1	0	3.866608	2.478318	0.068087
19	1	0	6.331862	2.288890	0.090846
20	8	0	7.675068	0.150634	0.047047
21	6	0	8.344357	-1.090860	0.021925
22	1	0	9.407121	-0.859019	0.043152
23	1	0	8.091227	-1.699981	0.895637
24	1	0	8.116275	-1.650440	-0.890955
25	1	0	5.981337	-1.981753	-0.033877
26	1	0	3.562274	-1.795809	-0.056409
27	1	0	1.711546	1.555092	0.011148
28	1	0	1.410049	-1.485397	-0.042860
29	1	0	-2.697185	3.025746	-0.008983
30	1	0	-5.133419	2.627015	-0.039448
31	7	0	-6.352629	0.316639	-0.099799
32	6	0	-6.986898	-0.959360	0.142376
33	6	0	-8.497187	-0.815428	0.129611
34	1	0	-8.843602	-0.421617	-0.828260
35	1	0	-8.974047	-1.782952	0.293504

36	1	0	-8.837242	-0.141905	0.921609
37	1	0	-6.658433	-1.392827	1.099452
38	1	0	-6.682970	-1.659512	-0.642989
39	1	0	-6.877135	1.115665	0.217495
40	1	0	-4.486328	-1.628221	-0.064071

D2b (cyclohexane)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.108721	-0.614868	-0.059354
2	6	0	-4.986849	0.471800	-0.055110
3	6	0	-4.459152	1.786168	-0.037592
4	6	0	-3.104436	2.024172	-0.027339
5	6	0	-2.209990	0.945218	-0.038603
6	6	0	-2.740512	-0.359318	-0.056834
7	16	0	-1.425803	-1.492709	-0.064154
8	6	0	-0.285104	-0.134636	-0.040929
9	7	0	-0.841610	1.035635	-0.029888
10	6	0	1.132751	-0.417231	-0.033650
11	6	0	2.072954	0.545348	-0.007524
12	6	0	3.515599	0.365905	0.003636
13	6	0	4.146226	-0.882715	-0.028042
14	6	0	5.527452	-1.003044	-0.012632
15	6	0	6.324621	0.143175	0.035385
16	6	0	5.717117	1.399959	0.066143
17	6	0	4.340333	1.502021	0.050071
18	1	0	3.881933	2.485800	0.074969
19	1	0	6.345733	2.282426	0.103087
20	8	0	7.677011	0.133404	0.054833
21	6	0	8.339653	-1.114534	0.023831
22	1	0	9.403793	-0.889498	0.049270
23	1	0	8.078792	-1.726273	0.892930
24	1	0	8.109499	-1.665177	-0.893664
25	1	0	5.970123	-1.990146	-0.038405
26	1	0	3.554492	-1.790552	-0.066358
27	1	0	1.726214	1.575763	0.009380
28	1	0	1.407892	-1.467272	-0.048531
29	1	0	-2.717632	3.036996	-0.011724
30	1	0	-5.151187	2.622943	-0.037385
31	7	0	-6.355379	0.304781	-0.098666
32	6	0	-6.981176	-0.976416	0.147585
33	6	0	-8.492469	-0.845605	0.140825
34	1	0	-8.847365	-0.459010	-0.817089
35	1	0	-8.958302	-1.817653	0.309985
36	1	0	-8.834912	-0.172148	0.931734
37	1	0	-6.645077	-1.403738	1.104593
38	1	0	-6.674571	-1.676586	-0.636984
39	1	0	-6.886141	1.106781	0.209212
40	1	0	-4.477383	-1.631847	-0.066549

D2b (DMSO)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.106574	-0.615318	-0.047212
2	6	0	-4.997640	0.463825	-0.056335
3	6	0	-4.480707	1.785311	-0.057790
4	6	0	-3.127811	2.037262	-0.058470
5	6	0	-2.222124	0.965822	-0.058119
6	6	0	-2.741175	-0.343759	-0.053331
7	16	0	-1.415482	-1.466281	-0.046637
8	6	0	-0.284529	-0.102149	-0.050575
9	7	0	-0.851977	1.066272	-0.057219
10	6	0	1.133395	-0.384132	-0.041724
11	6	0	2.080725	0.572927	-0.007399
12	6	0	3.522030	0.377879	0.005302
13	6	0	4.140213	-0.877134	-0.064966
14	6	0	5.520764	-1.011030	-0.044472
15	6	0	6.327377	0.127035	0.047952
16	6	0	5.732259	1.389645	0.112778
17	6	0	4.355824	1.506166	0.090427
18	1	0	3.905866	2.495368	0.143968
19	1	0	6.367692	2.268566	0.181513
20	8	0	7.679666	0.104411	0.072600
21	6	0	8.334502	-1.151548	0.003193
22	1	0	9.400095	-0.935804	0.043691
23	1	0	8.060620	-1.787788	0.849672
24	1	0	8.104044	-1.667838	-0.933258
25	1	0	5.950811	-2.003925	-0.103271
26	1	0	3.541742	-1.781020	-0.139874
27	1	0	1.751103	1.611390	0.017225
28	1	0	1.403334	-1.438484	-0.060282
29	1	0	-2.754791	3.058354	-0.057104
30	1	0	-5.184255	2.615229	-0.059977
31	7	0	-6.362449	0.287262	-0.095516
32	6	0	-6.970012	-0.997735	0.187962
33	6	0	-8.482294	-0.906553	0.128260
34	1	0	-8.817046	-0.581744	-0.859603
35	1	0	-8.926858	-1.881262	0.336363
36	1	0	-8.865398	-0.199443	0.869444
37	1	0	-6.653935	-1.374452	1.172773
38	1	0	-6.622033	-1.724207	-0.554227
39	1	0	-6.895376	1.098119	0.209988
40	1	0	-4.459588	-1.639678	-0.035385

D3b (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.857153	-0.597491	-0.049086
2	6	0	-5.713204	0.505526	-0.038397

3	6	0	-5.161673	1.810746	-0.019851
4	6	0	-3.804693	2.023792	-0.014519
5	6	0	-2.930833	0.927719	-0.032587
6	6	0	-3.484519	-0.368496	-0.051697
7	16	0	-2.192208	-1.524383	-0.067305
8	6	0	-1.031189	-0.186433	-0.046448
9	7	0	-1.564408	0.993596	-0.030122
10	6	0	0.384744	-0.480870	-0.047226
11	6	0	1.329379	0.474946	-0.027969
12	6	0	2.771603	0.274729	-0.024796
13	6	0	3.378982	-0.989613	-0.051399
14	6	0	4.754723	-1.119260	-0.047626
15	6	0	5.563949	0.015109	-0.020494
16	6	0	4.984801	1.277897	0.006841
17	6	0	3.604802	1.400747	0.002400
18	1	0	3.156970	2.387769	0.019009
19	1	0	5.610020	2.161526	0.023708
20	6	0	7.052697	-0.134553	0.040028
21	9	0	7.492495	-0.252568	1.309589
22	9	0	7.691602	0.920139	-0.490202
23	9	0	7.477398	-1.228528	-0.613965
24	1	0	5.206767	-2.102718	-0.074287
25	1	0	2.771148	-1.885304	-0.078104
26	1	0	0.989610	1.506201	-0.011381
27	1	0	0.653022	-1.531790	-0.063287
28	1	0	-3.397242	3.026984	0.001684
29	1	0	-5.837793	2.659240	-0.015702
30	7	0	-7.083134	0.363948	-0.074767
31	6	0	-7.740428	-0.904330	0.145639
32	6	0	-9.247798	-0.733359	0.135123
33	1	0	-9.587627	-0.319790	-0.816765
34	1	0	-9.741004	-1.694933	0.284125
35	1	0	-9.576053	-0.066461	0.937473
36	1	0	-7.419807	-1.356472	1.096234
37	1	0	-7.447851	-1.597718	-0.650115
38	1	0	-7.603537	1.174285	0.218563
39	1	0	-5.247107	-1.605734	-0.056443

D3b (cyclohexane)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.856502	-0.597253	-0.045929
2	6	0	-5.719317	0.502210	-0.033970
3	6	0	-5.172694	1.810924	-0.016621
4	6	0	-3.816576	2.030826	-0.014201
5	6	0	-2.937127	0.938406	-0.033579
6	6	0	-3.485311	-0.360156	-0.051170
7	16	0	-2.186975	-1.510262	-0.068016
8	6	0	-1.030712	-0.169024	-0.049200
9	7	0	-1.569935	1.009600	-0.032924
10	6	0	0.385385	-0.462859	-0.050660

11	6	0	1.332999	0.490664	-0.030316
12	6	0	2.774637	0.283229	-0.026862
13	6	0	3.375478	-0.984591	-0.053574
14	6	0	4.750941	-1.120368	-0.048905
15	6	0	5.564446	0.011518	-0.021080
16	6	0	4.991783	1.277826	0.007184
17	6	0	3.612021	1.406564	0.001820
18	1	0	3.168592	2.396755	0.019273
19	1	0	5.619133	2.161285	0.026792
20	6	0	7.051043	-0.145010	0.040207
21	9	0	7.492639	-0.268419	1.311008
22	9	0	7.699231	0.906884	-0.485986
23	9	0	7.475124	-1.239695	-0.614680
24	1	0	5.196553	-2.108090	-0.073955
25	1	0	2.764499	-1.879261	-0.080553
26	1	0	1.001920	1.525701	-0.012573
27	1	0	0.651276	-1.515393	-0.067804
28	1	0	-3.415476	3.038052	0.001302
29	1	0	-5.853875	2.656509	-0.009753
30	7	0	-7.086621	0.355061	-0.067243
31	6	0	-7.735434	-0.919482	0.150635
32	6	0	-9.244401	-0.766462	0.125073
33	1	0	-9.580890	-0.363532	-0.832713
34	1	0	-9.725721	-1.733892	0.275825
35	1	0	-9.588049	-0.098165	0.919731
36	1	0	-7.418959	-1.364479	1.105966
37	1	0	-7.427541	-1.612621	-0.639648
38	1	0	-7.611764	1.166986	0.223009
39	1	0	-5.239106	-1.608995	-0.051665

D3b (DMSO)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.855828	-0.603515	-0.033184
2	6	0	-5.725834	0.493760	-0.021495
3	6	0	-5.183068	1.806757	0.001924
4	6	0	-3.827928	2.033240	0.006414
5	6	0	-2.942681	0.943571	-0.014704
6	6	0	-3.485461	-0.357369	-0.034662
7	16	0	-2.180074	-1.501746	-0.052061
8	6	0	-1.028336	-0.159211	-0.032387
9	7	0	-1.573918	1.019584	-0.014710
10	6	0	0.388341	-0.452129	-0.035830
11	6	0	1.337631	0.501385	-0.027453
12	6	0	2.779260	0.288356	-0.028281
13	6	0	3.374412	-0.982996	-0.036825
14	6	0	4.750310	-1.122647	-0.035285
15	6	0	5.565912	0.009154	-0.029215
16	6	0	4.998520	1.279332	-0.019886
17	6	0	3.618435	1.411726	-0.021172
18	1	0	3.177501	2.405720	-0.017410

19	1	0	5.626104	2.165675	-0.015093
20	6	0	7.050653	-0.150572	0.029178
21	9	0	7.500851	-0.250479	1.303010
22	9	0	7.704891	0.887373	-0.517799
23	9	0	7.475032	-1.258920	-0.603945
24	1	0	5.188959	-2.116521	-0.043310
25	1	0	2.761415	-1.879637	-0.045290
26	1	0	1.017529	1.541993	-0.018463
27	1	0	0.652394	-1.507642	-0.046112
28	1	0	-3.434817	3.046276	0.027193
29	1	0	-5.872011	2.648529	0.014985
30	7	0	-7.089640	0.349760	-0.064106
31	6	0	-7.744928	-0.923964	0.150006
32	6	0	-9.251560	-0.780540	0.041107
33	1	0	-9.538779	-0.412144	-0.946464
34	1	0	-9.733905	-1.746406	0.199625
35	1	0	-9.637884	-0.086278	0.792525
36	1	0	-7.477020	-1.343326	1.131626
37	1	0	-7.392656	-1.634858	-0.605105
38	1	0	-7.616065	1.173998	0.215604
39	1	0	-5.228726	-1.620669	-0.040514

D4b (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.936982	-0.598047	-0.052298
2	6	0	-5.792749	0.505045	-0.047797
3	6	0	-5.240821	1.809393	-0.031345
4	6	0	-3.883172	2.021690	-0.021915
5	6	0	-3.009779	0.925686	-0.033810
6	6	0	-3.564065	-0.369819	-0.051040
7	16	0	-2.271924	-1.526690	-0.059011
8	6	0	-1.109437	-0.188823	-0.038025
9	7	0	-1.642506	0.991070	-0.026902
10	6	0	0.306019	-0.486386	-0.033137
11	6	0	1.251887	0.468418	-0.011017
12	6	0	2.693983	0.271936	-0.003690
13	6	0	3.306058	-0.989496	-0.030383
14	6	0	4.683273	-1.121793	-0.021255
15	6	0	5.479195	0.018531	0.014761
16	6	0	4.908702	1.282539	0.041137
17	6	0	3.526534	1.397691	0.031473
18	1	0	3.079140	2.385228	0.052166
19	1	0	5.534362	2.164973	0.068768
20	35	0	7.365746	-0.161290	0.027643
21	1	0	5.139840	-2.102634	-0.042413
22	1	0	2.701939	-1.888082	-0.059662
23	1	0	0.910950	1.499495	0.004038
24	1	0	0.572444	-1.537814	-0.047201
25	1	0	-3.475446	3.024833	-0.007292
26	1	0	-5.916336	2.658436	-0.032318

27	7	0	-7.164064	0.363898	-0.089402
28	6	0	-7.819868	-0.903264	0.141700
29	6	0	-9.327496	-0.734624	0.126341
30	1	0	-9.665540	-0.329760	-0.829909
31	1	0	-9.819932	-1.695438	0.282928
32	1	0	-9.658486	-0.060893	0.921893
33	1	0	-7.500683	-1.347099	1.096854
34	1	0	-7.524908	-1.603199	-0.647346
35	1	0	-7.682290	1.173596	0.209959
36	1	0	-5.327076	-1.606298	-0.057849

D5b (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.172604	-0.584516	0.209340
2	6	0	4.896818	0.566042	-0.108576
3	6	0	4.204254	1.725103	-0.538371
4	6	0	2.835463	1.751489	-0.648892
5	6	0	2.092204	0.607872	-0.325202
6	6	0	2.785461	-0.542685	0.101965
7	16	0	1.632591	-1.796016	0.429366
8	6	0	0.332848	-0.682315	-0.029546
9	7	0	0.730463	0.495753	-0.388317
10	6	0	-1.040555	-1.135004	0.028690
11	6	0	-2.084640	-0.332592	-0.237176
12	6	0	-3.483860	-0.754237	-0.209059
13	6	0	-3.832574	-2.093125	-0.428593
14	6	0	-5.150219	-2.518114	-0.396933
15	6	0	-6.170183	-1.607329	-0.154649
16	6	0	-5.856298	-0.271551	0.051105
17	6	0	-4.534612	0.156992	0.022515
18	6	0	-4.247981	1.614011	0.265120
19	9	0	-3.681233	2.204556	-0.806047
20	9	0	-3.409937	1.802159	1.298745
21	9	0	-5.361231	2.311539	0.538545
22	1	0	-6.643187	0.446256	0.238932
23	1	0	-7.203861	-1.929440	-0.133827
24	1	0	-5.381897	-3.561369	-0.576517
25	1	0	-3.050660	-2.806277	-0.657980
26	1	0	-1.866093	0.701163	-0.475632
27	1	0	-1.194596	-2.166365	0.328341
28	1	0	2.318274	2.643662	-0.979297
29	1	0	4.778786	2.613753	-0.777772
30	7	0	6.268590	0.620510	0.012100
31	6	0	7.080833	-0.558131	0.210381
32	6	0	8.553738	-0.194831	0.222716
33	1	0	8.772629	0.522208	1.016766
34	1	0	9.163926	-1.083841	0.388509
35	1	0	8.861354	0.242967	-0.731214
36	1	0	6.885721	-1.310503	-0.568742
37	1	0	6.811880	-1.016305	1.168162

38	1	0	6.711383	1.366045	-0.499438
39	1	0	4.673305	-1.486308	0.533177

D6b (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.435767	0.526509	0.110676
2	6	0	-5.142085	-0.665112	-0.061479
3	6	0	-4.427851	-1.866394	-0.288283
4	6	0	-3.054577	-1.893858	-0.341375
5	6	0	-2.329574	-0.708245	-0.162120
6	6	0	-3.045157	0.484391	0.063488
7	16	0	-1.912693	1.785426	0.244810
8	6	0	-0.587509	0.630435	0.005420
9	7	0	-0.965511	-0.592280	-0.188327
10	6	0	0.776183	1.111784	0.045968
11	6	0	1.841218	0.306070	-0.108609
12	6	0	3.237192	0.720304	-0.085978
13	6	0	3.641869	2.060903	-0.167935
14	6	0	4.979407	2.408261	-0.125108
15	6	0	5.957565	1.423616	-0.024142
16	6	0	5.588231	0.088129	0.035786
17	6	0	4.233316	-0.265413	0.019021
18	8	0	3.881978	-1.584241	0.076222
19	6	0	3.928827	-2.146782	1.384587
20	1	0	3.649807	-3.194051	1.279124
21	1	0	4.934783	-2.072546	1.804532
22	1	0	3.213305	-1.645490	2.043469
23	8	0	6.553200	-0.870808	0.168354
24	6	0	6.766279	-1.663913	-0.994523
25	1	0	7.537192	-2.387864	-0.734641
26	1	0	5.853385	-2.186379	-1.288176
27	1	0	7.119142	-1.041496	-1.823008
28	1	0	7.011662	1.671408	0.004478
29	1	0	5.269655	3.450364	-0.184869
30	1	0	2.894505	2.836837	-0.278657
31	1	0	1.658567	-0.752545	-0.253699
32	1	0	0.900693	2.174693	0.224378
33	1	0	-2.521335	-2.819757	-0.517921
34	1	0	-4.987751	-2.786852	-0.416626
35	7	0	-6.519687	-0.715146	0.014053
36	6	0	-7.339063	0.475267	-0.013799
37	6	0	-8.811292	0.109002	-0.011239
38	1	0	-9.066896	-0.474854	0.875541
39	1	0	-9.428219	1.008821	-0.016876
40	1	0	-9.074561	-0.476794	-0.896694
41	1	0	-7.107835	1.097518	-0.891771
42	1	0	-7.114041	1.079877	0.871190
43	1	0	-6.935010	-1.526331	-0.414336
44	1	0	-4.952289	1.461268	0.278784

D7b (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.209960	-0.569714	-0.051939
2	6	0	-6.057456	0.539382	-0.070930
3	6	0	-5.495968	1.838901	-0.094112
4	6	0	-4.136243	2.040817	-0.099596
5	6	0	-3.271231	0.938584	-0.087367
6	6	0	-3.835175	-0.352366	-0.066310
7	16	0	-2.551533	-1.518978	-0.052060
8	6	0	-1.378197	-0.189373	-0.073324
9	7	0	-1.902986	0.994020	-0.090343
10	6	0	0.034653	-0.499292	-0.066596
11	6	0	0.988191	0.448005	-0.065392
12	6	0	2.429233	0.239923	-0.057196
13	6	0	3.262659	1.362864	-0.027679
14	6	0	4.644188	1.233363	-0.026137
15	6	0	5.229026	-0.035685	-0.060709
16	6	0	4.399899	-1.166986	-0.069843
17	6	0	3.023200	-1.028503	-0.071115
18	1	0	2.429986	-1.933645	-0.097041
19	8	0	4.943943	-2.416701	-0.155066
20	6	0	5.601023	-2.866548	1.024128
21	1	0	5.991440	-3.857529	0.797462
22	1	0	6.422758	-2.201324	1.296766
23	1	0	4.890565	-2.939015	1.853950
24	8	0	6.587023	-0.173974	-0.076104
25	6	0	7.142546	-0.218131	-1.388981
26	1	0	8.218474	-0.332291	-1.264811
27	1	0	6.745062	-1.070861	-1.945413
28	1	0	6.931683	0.710319	-1.926082
29	8	0	5.418368	2.356781	-0.067733
30	6	0	6.162228	2.619969	1.116533
31	1	0	6.727335	3.531027	0.925678
32	1	0	5.487843	2.783772	1.963179
33	1	0	6.848723	1.801550	1.342337
34	1	0	2.841955	2.361378	-0.017220
35	1	0	0.656573	1.482152	-0.068463
36	1	0	0.293574	-1.552617	-0.060236
37	1	0	-3.720869	3.040825	-0.115329
38	1	0	-6.165012	2.692862	-0.114118
39	7	0	-7.431467	0.407646	-0.098975
40	6	0	-8.092157	-0.847001	0.181197
41	6	0	-9.598845	-0.669496	0.176046
42	1	0	-9.944795	-0.295854	-0.790034
43	1	0	-10.095492	-1.621014	0.371569
44	1	0	-9.916968	0.033833	0.951018
45	1	0	-7.765498	-1.261605	1.147070
46	1	0	-7.809976	-1.574372	-0.587378
47	1	0	-7.938566	1.228130	0.190314
48	1	0	-5.607455	-1.574854	-0.027875

D8b (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.333660	-0.774279	-0.194687
2	6	0	-6.164194	0.304305	0.116865
3	6	0	-5.584225	1.534692	0.517724
4	6	0	-4.224315	1.698488	0.608081
5	6	0	-3.375257	0.627673	0.292389
6	6	0	-3.956800	-0.593455	-0.107650
7	16	0	-2.690826	-1.732144	-0.431373
8	6	0	-1.502996	-0.489505	-0.006283
9	7	0	-2.009837	0.650861	0.339130
10	6	0	-0.093550	-0.805874	-0.069633
11	6	0	0.871464	0.093107	0.189665
12	6	0	2.301454	-0.197766	0.150724
13	6	0	2.771989	-1.506876	0.327015
14	6	0	4.118273	-1.812508	0.281334
15	6	0	5.049094	-0.802342	0.065301
16	6	0	4.619966	0.506687	-0.094856
17	6	0	3.266310	0.810214	-0.052160
18	6	0	2.852990	2.244830	-0.251069
19	9	0	3.901118	3.041776	-0.500762
20	9	0	2.001258	2.386236	-1.279417
21	9	0	2.238579	2.745243	0.837612
22	1	0	5.341010	1.293652	-0.265384
23	6	0	6.513777	-1.120591	0.071575
24	9	0	7.008744	-1.158516	1.323975
25	9	0	7.232196	-0.212026	-0.602790
26	9	0	6.765656	-2.320275	-0.476641
27	1	0	4.447746	-2.834685	0.419537
28	1	0	2.062116	-2.298038	0.530801
29	1	0	0.558328	1.102309	0.426454
30	1	0	0.155814	-1.819132	-0.366816
31	1	0	-3.793934	2.642860	0.917046
32	1	0	-6.241430	2.365401	0.752080
33	7	0	-7.533571	0.217919	0.019167
34	6	0	-8.229358	-1.036182	-0.159596
35	6	0	-9.730698	-0.819178	-0.152203
36	1	0	-10.031013	-0.135443	-0.948993
37	1	0	-10.252519	-1.765490	-0.301039
38	1	0	-10.065557	-0.404458	0.802775
39	1	0	-7.949899	-1.757462	0.622855
40	1	0	-7.929538	-1.474770	-1.117479
41	1	0	-8.046615	0.933603	0.506713
42	1	0	-5.746969	-1.726081	-0.497676

D8b (cyclohexane)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.093977	-0.203655	0.087903
2	6	0	0.067832	-0.305756	1.481922
3	6	0	1.276142	-0.561045	2.181754
4	6	0	2.474631	-0.708593	1.528793
5	6	0	2.519725	-0.601448	0.130332
6	6	0	1.316455	-0.347149	-0.560621
7	16	0	1.657518	-0.268342	-2.258694
8	6	0	3.363447	-0.580218	-1.904075
9	7	0	3.638376	-0.726441	-0.645947
10	6	0	4.309206	-0.647339	-2.995688
11	6	0	5.629735	-0.823958	-2.815085
12	6	0	6.604146	-0.913129	-3.898592
13	6	0	6.211770	-1.316035	-5.183198
14	6	0	7.109987	-1.397113	-6.229651
15	6	0	8.448225	-1.083043	-6.017210
16	6	0	8.875600	-0.698557	-4.754841
17	6	0	7.969078	-0.614183	-3.706960
18	6	0	8.478097	-0.171851	-2.361654
19	9	0	9.780622	0.142531	-2.389754
20	9	0	7.826987	0.911759	-1.904998
21	9	0	8.335279	-1.132788	-1.427547
22	1	0	9.915714	-0.454114	-4.587333
23	6	0	9.433904	-1.223109	-7.136195
24	9	0	9.861443	-2.495598	-7.269369
25	9	0	10.525587	-0.466978	-6.951510
26	9	0	8.901943	-0.874997	-8.319690
27	1	0	6.770716	-1.711871	-7.209971
28	1	0	5.180440	-1.597120	-5.357597
29	1	0	5.988293	-0.888018	-1.795390
30	1	0	3.895708	-0.521531	-3.991802
31	1	0	3.388833	-0.904700	2.077639
32	1	0	1.241479	-0.635265	3.264400
33	7	0	-1.090129	-0.139388	2.200176
34	6	0	-2.396552	-0.087712	1.581977
35	6	0	-3.482378	0.050223	2.632060
36	1	0	-3.344120	0.959176	3.221626
37	1	0	-4.463683	0.097896	2.157763
38	1	0	-3.484670	-0.805553	3.312987
39	1	0	-2.577026	-0.984256	0.970329
40	1	0	-2.434406	0.771988	0.904001
41	1	0	-1.063337	-0.473393	3.152230
42	1	0	-0.809732	-0.016322	-0.476069

D8b (DMSO)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.336557	-0.785279	-0.173581
2	6	0	-6.182437	0.289626	0.127301

3	6	0	-5.612110	1.531893	0.520232
4	6	0	-4.254024	1.712711	0.605523
5	6	0	-3.391251	0.648166	0.295184
6	6	0	-3.962139	-0.583861	-0.089676
7	16	0	-2.683543	-1.713622	-0.401882
8	6	0	-1.505321	-0.459551	0.002779
9	7	0	-2.023312	0.684531	0.336558
10	6	0	-0.096752	-0.778892	-0.062181
11	6	0	0.878173	0.117392	0.175113
12	6	0	2.306158	-0.186760	0.136194
13	6	0	2.763026	-1.501998	0.302941
14	6	0	4.107917	-1.817517	0.262048
15	6	0	5.047784	-0.811801	0.059483
16	6	0	4.635113	0.504588	-0.092116
17	6	0	3.282153	0.814835	-0.055436
18	6	0	2.879598	2.249584	-0.248985
19	9	0	3.924819	3.048073	-0.500952
20	9	0	2.021492	2.403848	-1.276304
21	9	0	2.265875	2.757825	0.840853
22	1	0	5.366411	1.289398	-0.244029
23	6	0	6.506951	-1.143966	0.069123
24	9	0	7.009564	-1.166696	1.323875
25	9	0	7.241094	-0.255706	-0.618293
26	9	0	6.754904	-2.354520	-0.457766
27	1	0	4.421576	-2.849248	0.396357
28	1	0	2.049739	-2.298039	0.490999
29	1	0	0.578545	1.133741	0.398335
30	1	0	0.140862	-1.804771	-0.337414
31	1	0	-3.839422	2.670254	0.909709
32	1	0	-6.283286	2.354959	0.755971
33	7	0	-7.544416	0.196486	0.031072
34	6	0	-8.236684	-1.062155	-0.148598
35	6	0	-9.736255	-0.845909	-0.221016
36	1	0	-9.998798	-0.194552	-1.057792
37	1	0	-10.247681	-1.800160	-0.357460
38	1	0	-10.114323	-0.392363	0.699365
39	1	0	-7.996090	-1.760307	0.667039
40	1	0	-7.889979	-1.529333	-1.077053
41	1	0	-8.064844	0.939875	0.490299
42	1	0	-5.731724	-1.750682	-0.466323

D9b (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.253558	-0.550768	-0.046546
2	6	0	-6.022562	0.614267	-0.049310
3	6	0	-5.372713	1.871746	-0.043494
4	6	0	-4.002027	1.978913	-0.037497
5	6	0	-3.214729	0.819754	-0.042343
6	6	0	-3.867049	-0.429394	-0.049124
7	16	0	-2.667809	-1.682698	-0.050102

8	6	0	-1.403464	-0.437007	-0.040943
9	7	0	-1.846358	0.781092	-0.037896
10	6	0	-0.019644	-0.843118	-0.036835
11	6	0	1.011947	0.028106	-0.025152
12	6	0	2.390442	-0.362177	-0.020094
13	6	0	3.407590	0.525279	-0.004979
14	6	0	4.832326	0.242285	0.002534
15	6	0	5.739775	1.304572	0.028219
16	6	0	7.114673	1.103575	0.038305
17	6	0	7.617501	-0.194742	0.021780
18	6	0	6.727921	-1.274999	-0.005115
19	6	0	5.367944	-1.058217	-0.014421
20	1	0	4.706156	-1.915615	-0.035658
21	1	0	7.135781	-2.278196	-0.018367
22	8	0	8.932422	-0.512241	0.029573
23	6	0	9.873281	0.538305	0.060821
24	1	0	10.852556	0.064348	0.064120
25	1	0	9.786378	1.179756	-0.822072
26	1	0	9.763890	1.146117	0.964749
27	1	0	7.775486	1.959494	0.058884
28	1	0	5.360184	2.320783	0.041382
29	1	0	3.147421	1.581743	0.003830
30	1	0	2.596783	-1.429329	-0.028063
31	1	0	0.783599	1.090406	-0.018576
32	1	0	0.177204	-1.910848	-0.043049
33	1	0	-3.518505	2.947947	-0.031004
34	1	0	-5.980676	2.770428	-0.050526
35	7	0	-7.402811	0.578735	-0.089792
36	6	0	-8.151248	-0.631694	0.163428
37	6	0	-9.641873	-0.350117	0.144372
38	1	0	-9.948714	0.063069	-0.818787
39	1	0	-10.205812	-1.267893	0.317565
40	1	0	-9.920044	0.360598	0.927928
41	1	0	-7.866024	-1.082924	1.126090
42	1	0	-7.910413	-1.365024	-0.613502
43	1	0	-7.852758	1.426181	0.216170
44	1	0	-5.719941	-1.526156	-0.043876

D1ob (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.405363	-0.601433	-0.131045
2	6	0	-6.270413	0.484198	0.016352
3	6	0	-5.729908	1.778757	0.208407
4	6	0	-4.373756	1.998657	0.250764
5	6	0	-3.491078	0.921396	0.096021
6	6	0	-4.034190	-0.364694	-0.094579
7	16	0	-2.731991	-1.499776	-0.250902
8	6	0	-1.580180	-0.166278	-0.049899
9	7	0	-2.124124	0.997038	0.115562
10	6	0	-0.163016	-0.451912	-0.081477

11	6	0	0.776634	0.500696	0.053040
12	6	0	2.219174	0.316274	0.035435
13	6	0	3.045643	1.438248	0.178434
14	6	0	4.426074	1.325642	0.169054
15	6	0	5.044247	0.082049	0.017093
16	6	0	4.220634	-1.042580	-0.125878
17	6	0	2.843465	-0.930313	-0.117529
18	1	0	2.245930	-1.825547	-0.241786
19	1	0	4.673303	-2.016753	-0.271051
20	6	0	6.515134	-0.046228	0.008821
21	6	0	7.315727	0.902718	-0.635146
22	6	0	8.698480	0.781447	-0.641777
23	6	0	9.310612	-0.291334	-0.004058
24	6	0	8.527201	-1.241937	0.639889
25	6	0	7.144511	-1.120722	0.645902
26	1	0	6.544171	-1.853363	1.173072
27	1	0	8.994990	-2.077399	1.147898
28	1	0	10.390058	-0.385983	-0.009208
29	1	0	9.299771	1.522892	-1.155195
30	1	0	6.847106	1.728786	-1.157621
31	1	0	5.034517	2.211816	0.307902
32	1	0	2.589804	2.413796	0.308966
33	1	0	0.427703	1.520411	0.188468
34	1	0	0.111714	-1.491697	-0.222333
35	1	0	-3.974404	2.994186	0.399892
36	1	0	-6.412400	2.615143	0.317457
37	7	0	-7.641480	0.339414	-0.050308
38	6	0	-8.286193	-0.952945	0.003973
39	6	0	-9.795304	-0.797063	0.000280
40	1	0	-10.131384	-0.270858	-0.895660
41	1	0	-10.279404	-1.774505	0.023705
42	1	0	-10.137663	-0.238654	0.876295
43	1	0	-7.969281	-1.519806	0.892734
44	1	0	-7.979747	-1.537527	-0.870036
45	1	0	-8.165297	1.093545	0.363047
46	1	0	-5.787215	-1.603082	-0.271363

D11a (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.073742	-0.589093	-0.374092
2	6	0	-5.829949	0.513738	0.018376
3	6	0	-5.181657	1.647536	0.550975
4	6	0	-3.811578	1.695538	0.689511
5	6	0	-3.036752	0.598358	0.299289
6	6	0	-3.693194	-0.533595	-0.228833
7	16	0	-2.504559	-1.733018	-0.625370
8	6	0	-1.240343	-0.627929	-0.055508
9	7	0	-1.671790	0.510843	0.381883
10	6	0	0.143212	-1.049551	-0.121713
11	6	0	1.165262	-0.259878	0.248711

12	6	0	2.572517	-0.646487	0.239003
13	6	0	2.944761	-1.956843	0.476779
14	6	0	4.292162	-2.351308	0.491886
15	6	0	5.283544	-1.428744	0.283600
16	6	0	4.962649	-0.072907	0.042808
17	6	0	3.595260	0.332673	0.012719
18	6	0	3.309011	1.690973	-0.266763
19	6	0	4.314208	2.600407	-0.476044
20	6	0	5.663655	2.199368	-0.428338
21	6	0	5.976517	0.889964	-0.178065
22	1	0	7.011857	0.567919	-0.148897
23	1	0	6.449307	2.926612	-0.596083
24	1	0	4.068478	3.634756	-0.686293
25	1	0	2.279674	2.019482	-0.328809
26	1	0	6.326846	-1.723806	0.305830
27	1	0	4.542000	-3.387272	0.688490
28	1	0	2.178565	-2.691511	0.694309
29	1	0	0.914450	0.741262	0.583065
30	1	0	0.329486	-2.044407	-0.512912
31	1	0	-3.323020	2.571322	1.098122
32	1	0	-5.782227	2.495711	0.861379
33	7	0	-7.216637	0.484030	-0.055104
34	1	0	-7.607703	-0.171667	-0.711263
35	1	0	-7.669763	1.382024	-0.095901
36	1	0	-5.559265	-1.469558	-0.778381

D11b (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.274444	-0.471027	-0.267553
2	6	0	-5.007384	0.650169	0.125398
3	6	0	-4.323887	1.778478	0.640117
4	6	0	-2.955067	1.803092	0.761657
5	6	0	-2.203349	0.689593	0.363424
6	6	0	-2.888146	-0.430514	-0.147907
7	16	0	-1.727161	-1.653872	-0.553241
8	6	0	-0.434535	-0.570977	-0.007101
9	7	0	-0.840059	0.578412	0.429152
10	6	0	0.940090	-1.017462	-0.088498
11	6	0	1.981746	-0.243219	0.259731
12	6	0	3.381307	-0.656277	0.235642
13	6	0	3.732859	-1.970752	0.482365
14	6	0	5.072960	-2.389710	0.484944
15	6	0	6.078541	-1.487767	0.255471
16	6	0	5.779321	-0.128833	0.004438
17	6	0	4.419160	0.301205	-0.013967
18	6	0	4.154116	1.661368	-0.305064
19	6	0	5.172881	2.550180	-0.536230
20	6	0	6.515385	2.125336	-0.499529
21	6	0	6.807602	0.813228	-0.238592
22	1	0	7.837276	0.472799	-0.218049

23	1	0	7.311975	2.836385	-0.684365
24	1	0	4.943263	3.586407	-0.755320
25	1	0	3.130058	2.007325	-0.358836
26	1	0	7.116501	-1.801676	0.268233
27	1	0	5.306225	-3.428135	0.688976
28	1	0	2.956162	-2.688918	0.717091
29	1	0	1.754160	0.765747	0.587039
30	1	0	1.103162	-2.019225	-0.472556
31	1	0	-2.445891	2.672150	1.159510
32	1	0	-4.904298	2.645264	0.938503
33	7	0	-6.380442	0.706528	-0.001867
34	6	0	-7.181348	-0.464360	-0.278626
35	6	0	-8.657216	-0.113104	-0.277622
36	1	0	-8.877246	0.650835	-1.026303
37	1	0	-9.259065	-0.994832	-0.502597
38	1	0	-8.974041	0.261505	0.699976
39	1	0	-6.984636	-1.263685	0.452073
40	1	0	-6.902835	-0.858410	-1.261752
41	1	0	-6.828540	1.402610	0.571412
42	1	0	-4.767709	-1.350660	-0.657159

D11c (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.631612	-1.385951	0.797961
2	6	0	2.114467	-2.512010	0.111044
3	6	0	1.230742	-3.163933	-0.789077
4	6	0	-0.069975	-2.745297	-0.977381
5	6	0	-0.557824	-1.637449	-0.282930
6	6	0	0.322202	-0.976322	0.598181
7	16	0	-0.515589	0.365685	1.315766
8	6	0	-1.957808	-0.070882	0.379157
9	7	0	-1.817219	-1.107425	-0.382686
10	6	0	-3.157112	0.726108	0.526116
11	6	0	-4.301413	0.455014	-0.124336
12	6	0	-5.521856	1.251072	-0.042722
13	6	0	-5.458576	2.617750	0.159597
14	6	0	-6.615631	3.410305	0.224370
15	6	0	-7.852131	2.840476	0.070376
16	6	0	-7.977961	1.449058	-0.147283
17	6	0	-6.807186	0.635428	-0.201092
18	6	0	-6.972837	-0.758677	-0.385828
19	6	0	-8.218641	-1.312538	-0.536163
20	6	0	-9.371070	-0.503366	-0.499371
21	6	0	-9.249164	0.846603	-0.304930
22	1	0	-10.130066	1.478194	-0.265088
23	1	0	-10.350067	-0.952365	-0.618856
24	1	0	-8.317934	-2.382349	-0.678099
25	1	0	-6.104292	-1.404258	-0.397538
26	1	0	-8.749655	3.448006	0.107383
27	1	0	-6.521604	4.478851	0.378500

28	1	0	-4.488839	3.095515	0.233766
29	1	0	-4.306846	-0.423787	-0.760402
30	1	0	-3.101173	1.562332	1.215474
31	1	0	-0.717870	-3.263373	-1.673869
32	1	0	1.573865	-4.011126	-1.363627
33	7	0	3.405191	-2.982666	0.317071
34	6	0	3.871083	-4.090035	-0.508488
35	6	0	5.190599	-4.701203	-0.068756
36	1	0	5.372935	-5.598616	-0.663565
37	1	0	5.163629	-4.997298	0.982348
38	1	0	6.041305	-4.034622	-0.221724
39	1	0	3.114993	-4.876661	-0.457728
40	1	0	3.943641	-3.792299	-1.566599
41	6	0	4.398960	-2.081693	0.876127
42	6	0	4.893354	-1.002091	-0.086169
43	6	0	5.899990	-0.057240	0.559654
44	6	0	6.393248	1.035180	-0.382225
45	6	0	7.396066	1.987459	0.259904
46	6	0	7.875865	3.087356	-0.679683
47	6	0	8.878304	4.042595	-0.040970
48	6	0	9.347700	5.140272	-0.986542
49	1	0	8.507566	5.748338	-1.333650
50	1	0	9.835981	4.719436	-1.870037
51	1	0	10.061992	5.809280	-0.500920
52	1	0	9.743189	3.471464	0.315823
53	1	0	8.427164	4.495082	0.849686
54	1	0	7.011256	3.659081	-1.039149
55	1	0	8.327651	2.632811	-1.570282
56	1	0	6.943647	2.443593	1.149229
57	1	0	8.260350	1.415788	0.620303
58	1	0	6.847954	0.572492	-1.266780
59	1	0	5.533548	1.608273	-0.749883
60	1	0	5.445948	0.407911	1.443775
61	1	0	6.758765	-0.631670	0.929555
62	1	0	5.346832	-1.482411	-0.961229
63	1	0	4.035760	-0.432840	-0.459413
64	1	0	5.241931	-2.679542	1.223207
65	1	0	3.993575	-1.622704	1.780879
66	1	0	2.258443	-0.836773	1.484324

D12b (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.534362	0.416827	-0.193618
2	6	0	5.267523	-0.739495	0.077510
3	6	0	4.580371	-1.935986	0.392342
4	6	0	3.207220	-1.992681	0.437257
5	6	0	2.455607	-0.843143	0.160584
6	6	0	3.144618	0.345026	-0.153082
7	16	0	1.982625	1.600207	-0.442146
8	6	0	0.681809	0.436799	-0.121771

9	7	0	1.088811	-0.758129	0.168792
10	6	0	-0.691311	0.886683	-0.203221
11	6	0	-1.719194	0.041567	0.017577
12	6	0	-3.149750	0.284910	0.000767
13	6	0	-3.709516	1.563838	0.086208
14	6	0	-5.103076	1.752643	0.167287
15	6	0	-5.951954	0.679898	0.150043
16	6	0	-5.457086	-0.634424	0.035397
17	6	0	-4.048098	-0.838340	-0.051430
18	6	0	-3.599595	-2.174994	-0.211246
19	6	0	-4.478694	-3.227221	-0.249376
20	6	0	-5.866292	-3.016461	-0.136854
21	6	0	-6.339811	-1.739882	-0.002533
22	1	0	-7.405482	-1.551360	0.072412
23	1	0	-6.548772	-3.857333	-0.166939
24	1	0	-4.097436	-4.233910	-0.376069
25	1	0	-2.545329	-2.383439	-0.327011
26	1	0	-7.022827	0.836647	0.216686
27	1	0	-5.509832	2.750966	0.247223
28	8	0	-2.855352	2.613793	0.106663
29	6	0	-3.357707	3.914917	0.326475
30	1	0	-2.486577	4.566521	0.357056
31	1	0	-4.015217	4.236087	-0.487034
32	1	0	-3.890241	3.983521	1.279639
33	1	0	-1.420773	-0.973116	0.251774
34	1	0	-0.853108	1.923660	-0.455416
35	1	0	2.695088	-2.915028	0.682054
36	1	0	5.160788	-2.829801	0.596238
37	7	0	6.648050	-0.761775	0.017058
38	6	0	7.436180	0.448727	-0.032255
39	6	0	8.917270	0.122446	0.010473
40	1	0	9.199423	-0.520811	-0.825718
41	1	0	9.511019	1.036044	-0.046042
42	1	0	9.183618	-0.386811	0.941211
43	1	0	7.176786	1.128053	0.794221
44	1	0	7.209042	0.980639	-0.962263
45	1	0	7.075364	-1.522781	0.519633
46	1	0	5.029984	1.348013	-0.430783

D13b (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.767969	0.336341	-0.471899
2	6	0	-5.614319	-0.461736	0.299668
3	6	0	-5.053113	-1.353512	1.245872
4	6	0	-3.694562	-1.458220	1.425794
5	6	0	-2.830434	-0.670229	0.653827
6	6	0	-3.393708	0.215376	-0.286056
7	16	0	-2.111419	1.062813	-1.089569
8	6	0	-0.940167	0.167155	-0.107072
9	7	0	-1.462720	-0.671851	0.728376

10	6	0	0.474926	0.412704	-0.301163
11	6	0	1.430870	-0.269845	0.349049
12	6	0	2.875045	-0.090716	0.178526
13	6	0	3.671648	-1.240829	-0.032744
14	6	0	5.086944	-1.107419	-0.223985
15	6	0	5.662265	0.160511	-0.211936
16	6	0	4.900632	1.302808	0.014945
17	6	0	3.484698	1.184507	0.236830
18	6	0	2.770438	2.376170	0.561533
19	6	0	3.390924	3.590984	0.600937
20	6	0	4.776255	3.707884	0.322098
21	6	0	5.507437	2.592002	0.048292
22	1	0	6.573243	2.662101	-0.140135
23	1	0	5.250712	4.681764	0.348227
24	1	0	2.822173	4.475890	0.861960
25	1	0	1.719166	2.306117	0.803651
26	1	0	6.730417	0.260252	-0.376239
27	6	0	5.874583	-2.274132	-0.440422
28	6	0	5.303657	-3.511138	-0.475704
29	6	0	3.902762	-3.647314	-0.308573
30	6	0	3.114840	-2.551090	-0.104462
31	1	0	2.044572	-2.679050	-0.007311
32	1	0	3.452699	-4.632136	-0.353902
33	1	0	5.913590	-4.391569	-0.640125
34	1	0	6.943582	-2.154599	-0.579481
35	1	0	1.100679	-1.050724	1.028418
36	1	0	0.742172	1.166687	-1.034176
37	1	0	-3.279337	-2.143000	2.154812
38	1	0	-5.721492	-1.971727	1.835972
39	7	0	-6.985406	-0.431658	0.147051
40	6	0	-7.658810	0.603847	-0.603625
41	6	0	-9.163484	0.427137	-0.523538
42	1	0	-9.516355	0.505243	0.508801
43	1	0	-9.669525	1.200389	-1.103408
44	1	0	-9.463801	-0.546276	-0.917009
45	1	0	-7.341505	0.544786	-1.650198
46	1	0	-7.378067	1.604696	-0.241811
47	1	0	-7.505146	-0.798059	0.927747
48	1	0	-5.166324	1.031301	-1.197816

D14a (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.588860	-0.411111	-0.325036
2	6	0	-7.266280	0.754225	0.029119
3	6	0	-6.537307	1.867601	0.496416
4	6	0	-5.164319	1.834753	0.607638
5	6	0	-4.467740	0.674230	0.254639
6	6	0	-5.204821	-0.436874	-0.207896
7	16	0	-4.101870	-1.725891	-0.569842
8	6	0	-2.758753	-0.678026	-0.075841

9	7	0	-3.109915	0.504943	0.315806
10	6	0	-1.407246	-1.188096	-0.144736
11	6	0	-0.333437	-0.443170	0.177157
12	6	0	1.050023	-0.892396	0.165781
13	6	0	1.354527	-2.255345	0.293443
14	6	0	2.653746	-2.715784	0.308204
15	6	0	3.730527	-1.828100	0.203420
16	6	0	3.461209	-0.439601	0.075184
17	6	0	2.117861	0.033673	0.053051
18	6	0	1.908774	1.441639	-0.109933
19	6	0	2.944948	2.310308	-0.212928
20	6	0	4.301213	1.863728	-0.174181
21	6	0	5.381542	2.745677	-0.277202
22	6	0	6.685871	2.274022	-0.242637
23	6	0	6.938571	0.916352	-0.108153
24	6	0	5.888039	-0.001169	-0.003469
25	6	0	4.547941	0.473042	-0.033230
26	6	0	6.119491	-1.405857	0.132909
27	6	0	5.086208	-2.278187	0.230824
28	1	0	5.272717	-3.341702	0.332531
29	1	0	7.143760	-1.761516	0.154916
30	1	0	7.959932	0.552631	-0.083750
31	1	0	7.512673	2.970010	-0.322700
32	1	0	5.187921	3.807158	-0.385423
33	1	0	2.753595	3.370863	-0.334850
34	1	0	0.898894	1.825076	-0.164612
35	1	0	2.851235	-3.776045	0.421647
36	1	0	0.544857	-2.963861	0.419669
37	1	0	-0.533643	0.579829	0.474503
38	1	0	-1.293545	-2.208809	-0.493726
39	1	0	-4.613483	2.695429	0.966077
40	1	0	-7.076903	2.765355	0.777977
41	7	0	-8.653376	0.809366	-0.017803
42	1	0	-9.098451	0.151370	-0.636160
43	1	0	-9.049983	1.731674	-0.091393
44	1	0	-7.136991	-1.276585	-0.678496

D14b (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.815052	-0.424918	0.166506
2	6	0	-6.488330	0.742367	-0.198429
3	6	0	-5.742374	1.863283	-0.636937
4	6	0	-4.370628	1.834259	-0.717069
5	6	0	-3.679440	0.668017	-0.362164
6	6	0	-4.426345	-0.444542	0.073655
7	16	0	-3.331006	-1.736303	0.448701
8	6	0	-1.977273	-0.686031	-0.007125
9	7	0	-2.321307	0.500624	-0.396078
10	6	0	-0.627152	-1.195477	0.084682
11	6	0	0.452149	-0.448393	-0.213601

12	6	0	1.835900	-0.895206	-0.179149
13	6	0	2.145933	-2.257598	-0.300324
14	6	0	3.446320	-2.714891	-0.294619
15	6	0	4.519451	-1.824630	-0.174992
16	6	0	4.244803	-0.436674	-0.052629
17	6	0	2.900106	0.033230	-0.050953
18	6	0	2.685364	1.440866	0.107541
19	6	0	3.717676	2.312279	0.224828
20	6	0	5.075468	1.869107	0.206059
21	6	0	6.152005	2.753925	0.323088
22	6	0	7.457874	2.285535	0.307753
23	6	0	7.715894	0.928321	0.178909
24	6	0	6.669260	0.007975	0.060493
25	6	0	5.327655	0.478816	0.070415
26	6	0	6.906145	-1.396340	-0.070486
27	6	0	5.876453	-2.271323	-0.181985
28	1	0	6.066998	-3.334537	-0.279499
29	1	0	7.931508	-1.749480	-0.077230
30	1	0	8.738401	0.567101	0.169634
31	1	0	8.281723	2.983733	0.398523
32	1	0	5.954176	3.815061	0.427018
33	1	0	3.521931	3.372454	0.343065
34	1	0	1.673888	1.821877	0.147107
35	1	0	3.647962	-3.774873	-0.403448
36	1	0	1.340118	-2.968395	-0.437845
37	1	0	0.255938	0.575617	-0.509872
38	1	0	-0.519654	-2.218138	0.430054
39	1	0	-3.813136	2.699611	-1.053511
40	1	0	-6.277222	2.763081	-0.922411
41	7	0	-7.865416	0.828997	-0.175392
42	6	0	-8.692931	-0.156962	0.481732
43	6	0	-10.154971	0.241696	0.410526
44	1	0	-10.482006	0.342223	-0.626527
45	1	0	-10.779431	-0.510959	0.894062
46	1	0	-10.330868	1.193192	0.920609
47	1	0	-8.391452	-0.294763	1.531325
48	1	0	-8.555268	-1.122324	-0.016751
49	1	0	-8.228683	1.768017	-0.159741
50	1	0	-6.355541	-1.295133	0.512177

D14c (gas)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.191273	-1.384658	0.781041
2	6	0	3.700965	-2.529845	0.146645
3	6	0	2.820439	-3.266353	-0.689599
4	6	0	1.498192	-2.913278	-0.859674
5	6	0	0.982825	-1.789041	-0.212335
6	6	0	1.860270	-1.041510	0.599784
7	16	0	0.989385	0.307155	1.262749
8	6	0	-0.461950	-0.243845	0.402871

9	7	0	-0.300458	-1.318612	-0.300776
10	6	0	-1.686825	0.510892	0.544357
11	6	0	-2.849477	0.134885	-0.020047
12	6	0	-4.101442	0.872750	0.056320
13	6	0	-4.091530	2.259764	0.262919
14	6	0	-5.254099	2.997830	0.328217
15	6	0	-6.502546	2.383448	0.181688
16	6	0	-6.552254	0.980596	-0.034400
17	6	0	-5.350039	0.219164	-0.097331
18	6	0	-5.464925	-1.196015	-0.288386
19	6	0	-6.669881	-1.801574	-0.431592
20	6	0	-7.889509	-1.058868	-0.388227
21	6	0	-9.140550	-1.666903	-0.532836
22	6	0	-10.304351	-0.913589	-0.477184
23	6	0	-10.244542	0.457767	-0.274303
24	6	0	-9.014798	1.106790	-0.123814
25	6	0	-7.816324	0.343831	-0.182988
26	6	0	-8.924106	2.518212	0.089027
27	6	0	-7.721502	3.126795	0.235234
28	1	0	-7.663779	4.197537	0.397872
29	1	0	-9.841713	3.094561	0.132775
30	1	0	-11.157267	1.041728	-0.229803
31	1	0	-11.266349	-1.399334	-0.591536
32	1	0	-9.191575	-2.738830	-0.688823
33	1	0	-6.723744	-2.875199	-0.575617
34	1	0	-4.569243	-1.802309	-0.307334
35	1	0	-5.206557	4.071042	0.476654
36	1	0	-3.139531	2.771095	0.338033
37	1	0	-2.836149	-0.794868	-0.577534
38	1	0	-1.632687	1.403666	1.158373
39	1	0	0.853375	-3.496784	-1.505443
40	1	0	3.182473	-4.130293	-1.226289
41	7	0	5.013011	-2.938604	0.342216
42	6	0	5.513300	-4.053719	-0.452822
43	6	0	6.866551	-4.590381	-0.018740
44	1	0	7.080064	-5.495758	-0.590670
45	1	0	6.870421	-4.856770	1.040614
46	1	0	7.683247	-3.890667	-0.205402
47	1	0	4.795418	-4.871795	-0.360966
48	1	0	5.552882	-3.789410	-1.521292
49	6	0	5.974205	-1.990517	0.877702
50	6	0	6.429516	-0.912983	-0.106572
51	6	0	7.404790	0.074947	0.522091
52	6	0	7.869241	1.164191	-0.438222
53	6	0	8.846513	2.151710	0.189510
54	6	0	9.302197	3.247869	-0.766546
55	6	0	10.281853	4.234786	-0.141138
56	6	0	10.728907	5.327921	-1.102761
57	1	0	9.876421	5.912080	-1.460660
58	1	0	11.228034	4.904368	-1.978880
59	1	0	11.427427	6.019858	-0.626410
60	1	0	11.158400	3.688439	0.225836
61	1	0	9.819141	4.690865	0.741716
62	1	0	8.425534	3.794539	-1.135643
63	1	0	9.765466	2.790217	-1.649633
64	1	0	8.381094	2.610988	1.070478

65	1	0	9.723528	1.607138	0.560954
66	1	0	8.336825	0.699023	-1.314730
67	1	0	6.995440	1.708817	-0.815731
68	1	0	6.934776	0.542739	1.396442
69	1	0	8.279119	-0.466655	0.904925
70	1	0	6.898304	-1.394101	-0.973062
71	1	0	5.553267	-0.379947	-0.489579
72	1	0	6.839291	-2.550035	1.234199
73	1	0	5.553569	-1.528544	1.774182
74	1	0	3.814739	-0.767802	1.410587

Hammet correlation

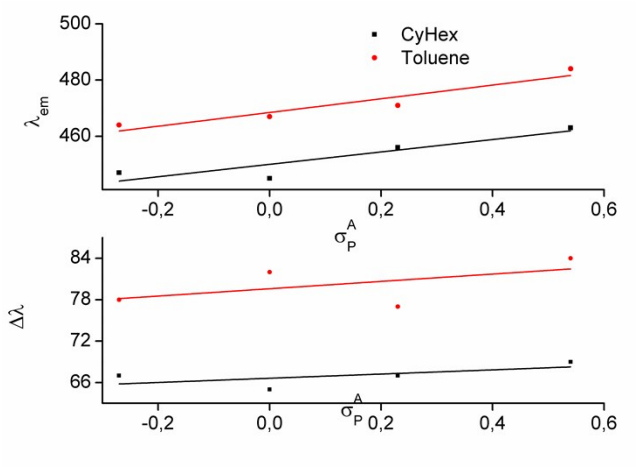


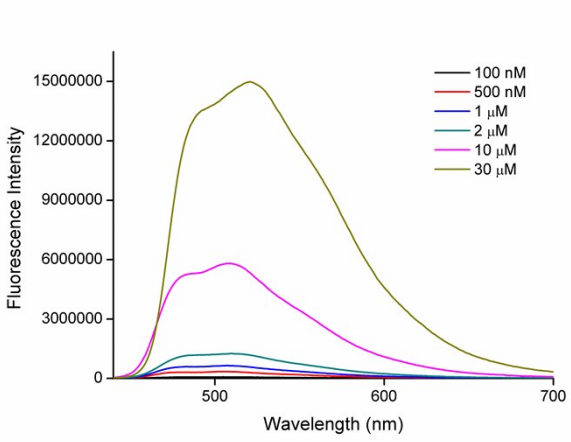
Figure S4. Dependence of the emission maxima (up) and Stokes shift (down) of **D1b**, **D2b**, **D3b** and **D4b** on the Hammett values (σ_p) in cyclohexane (black) and toluene (red). Correlation factors R^2 are, respectively, 0.74 and 0.86 for the emission maxima. No correlation was observed for the Stokes shift.

Table S3. Prediction study based on Hammett parameter model for dye **D1b**.

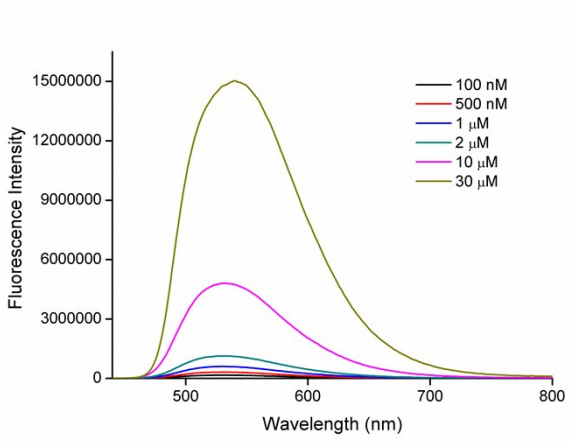
Solvent	***λ_{em} (experimentally/prediction)***	***$\Delta\lambda$ (experimentally/prediction)***
1,4-Dioxane	474/476	87/86
Ethyl acetate	486/489	101/101
Dimethyl sulfoxide	530/532	130/129
Acetonitrile	510/511	126/124
Methanol	519/520	130/127

Excimer studies

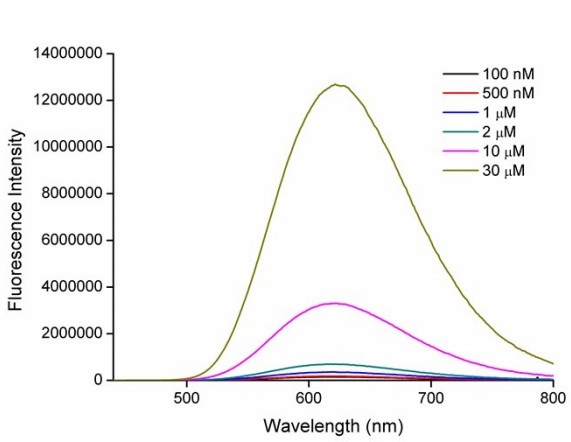
Figure S5. Excimer emission study of dye **D14b**.



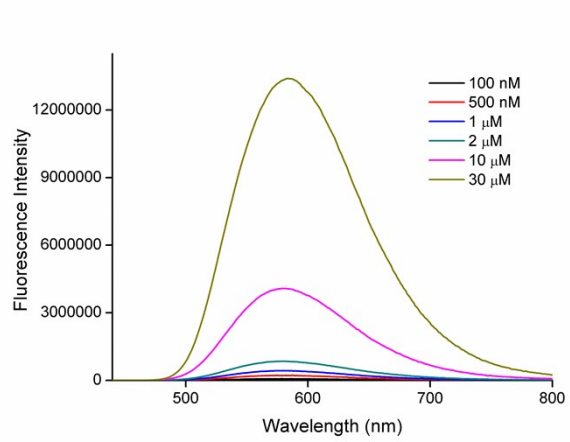
Cyclohexane



1,4-Dioxane

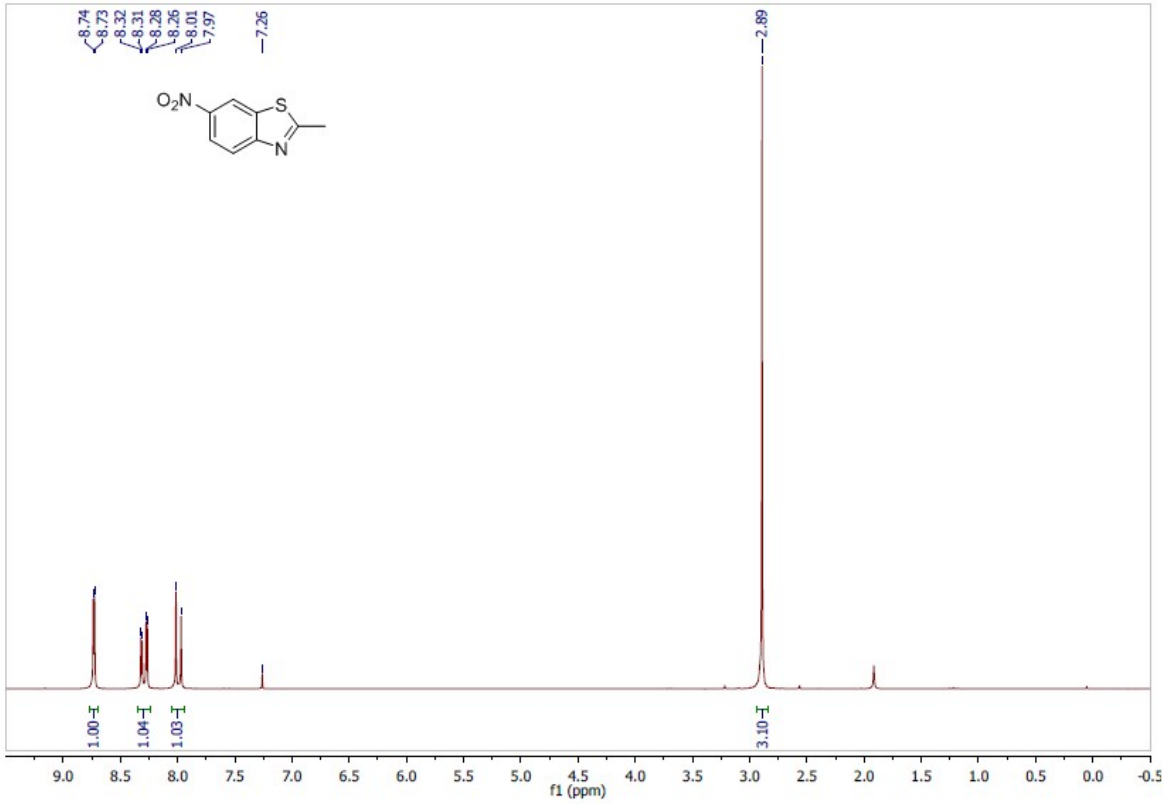


DMSO

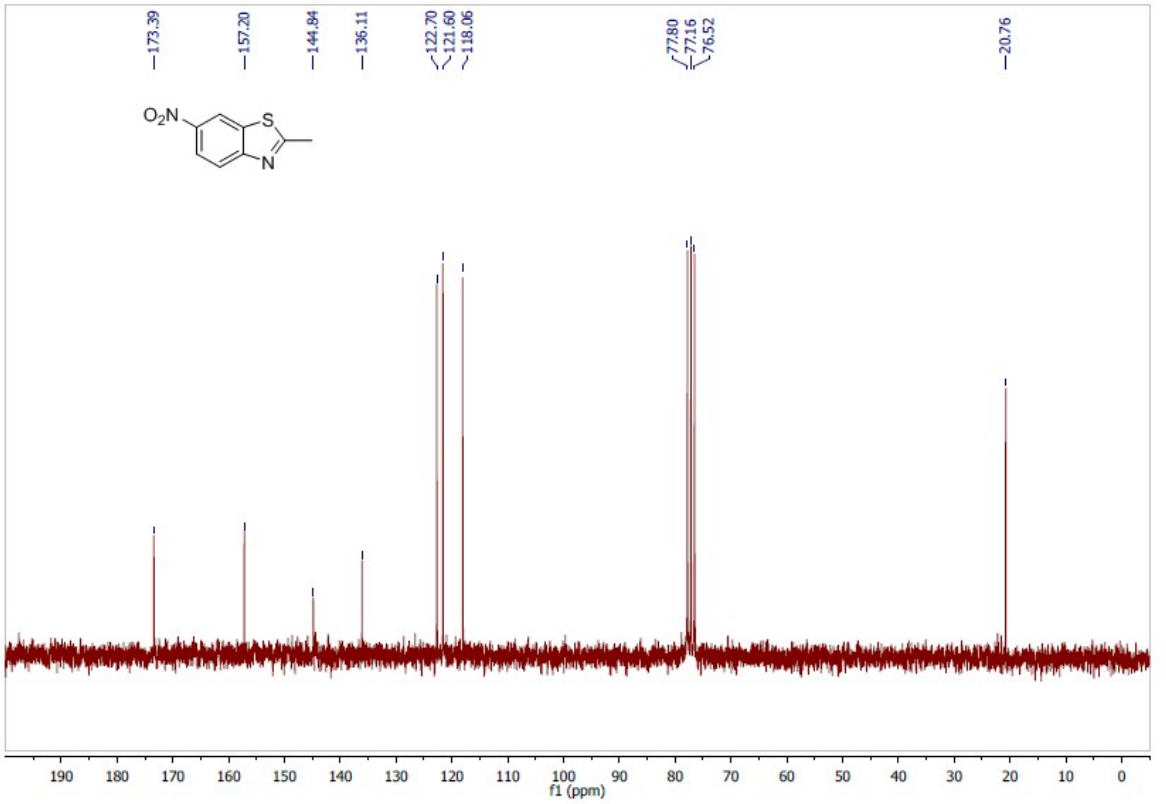


MeOH

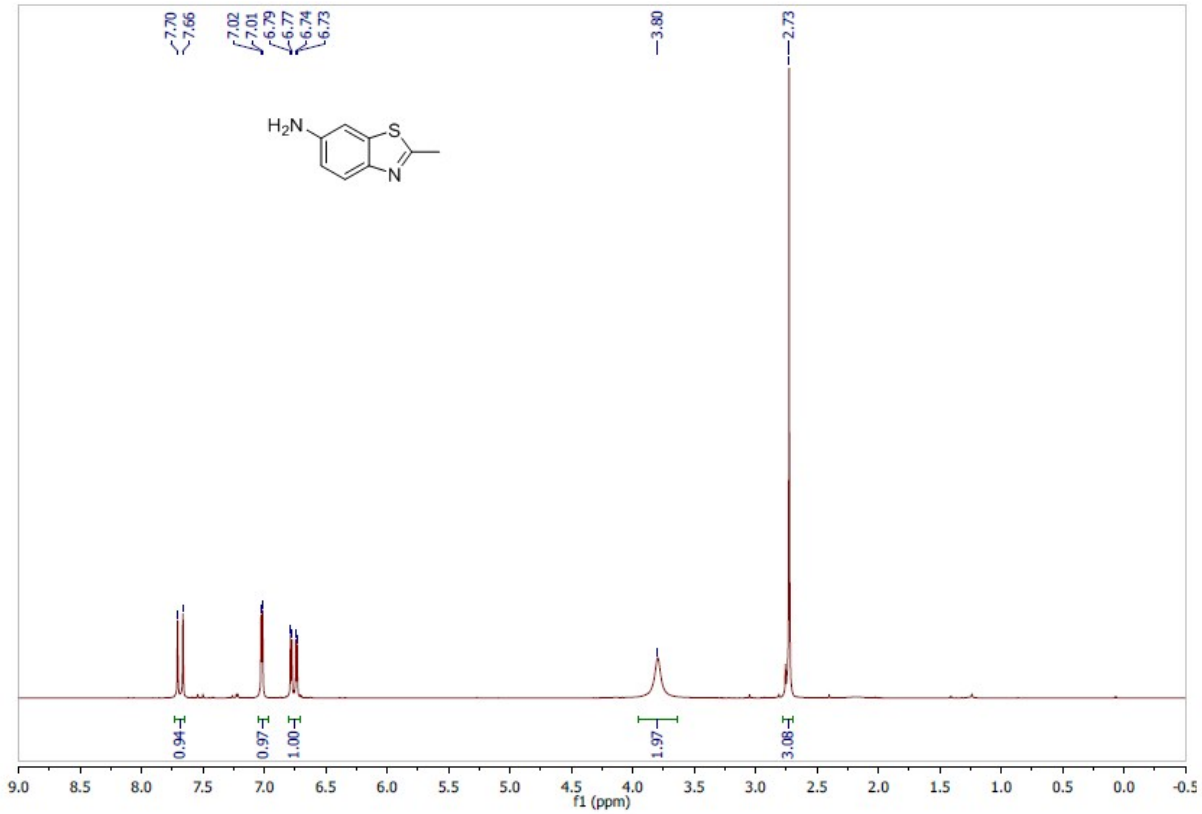
Copies of NMR ^{1}H, $^{13}C\{^{1}H\}$, $^{19}F\{^{1}H\}$ and HRMS spectra



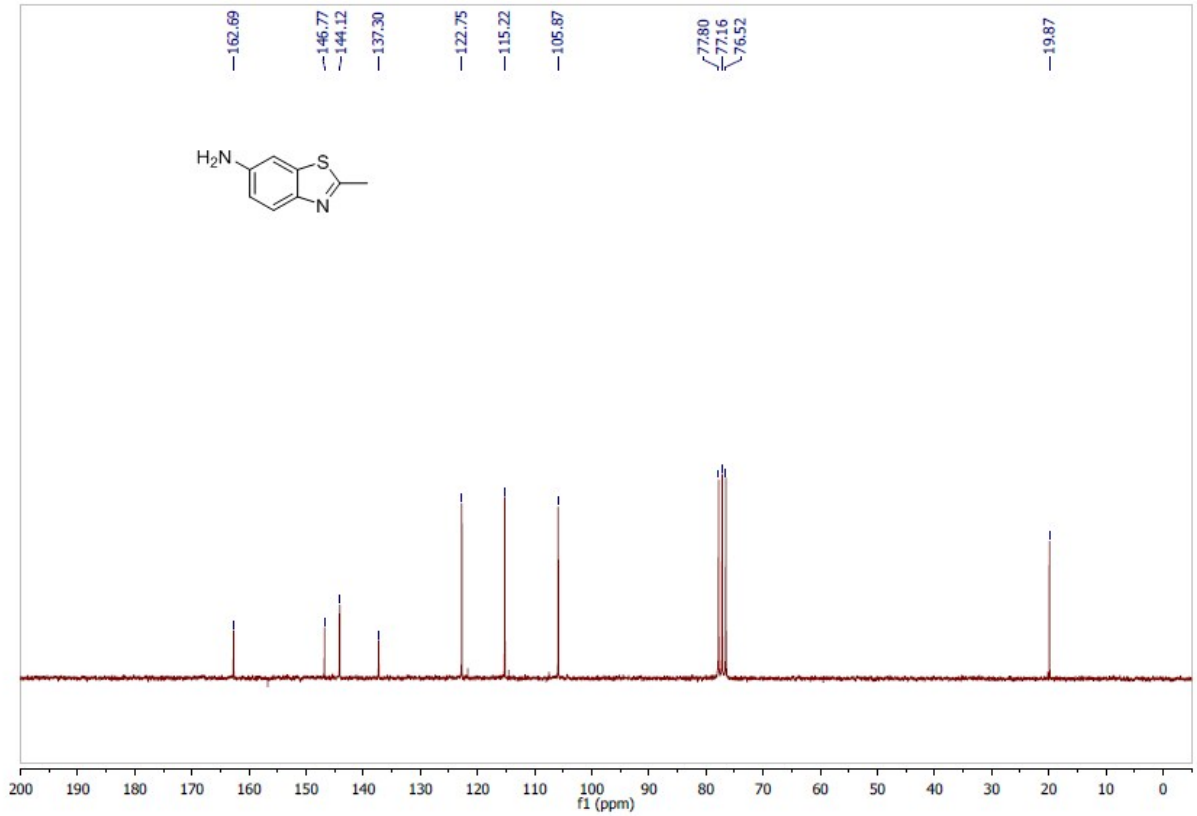
^{1}H NMR spectrum in $CDCl_3$ of compound **2**.



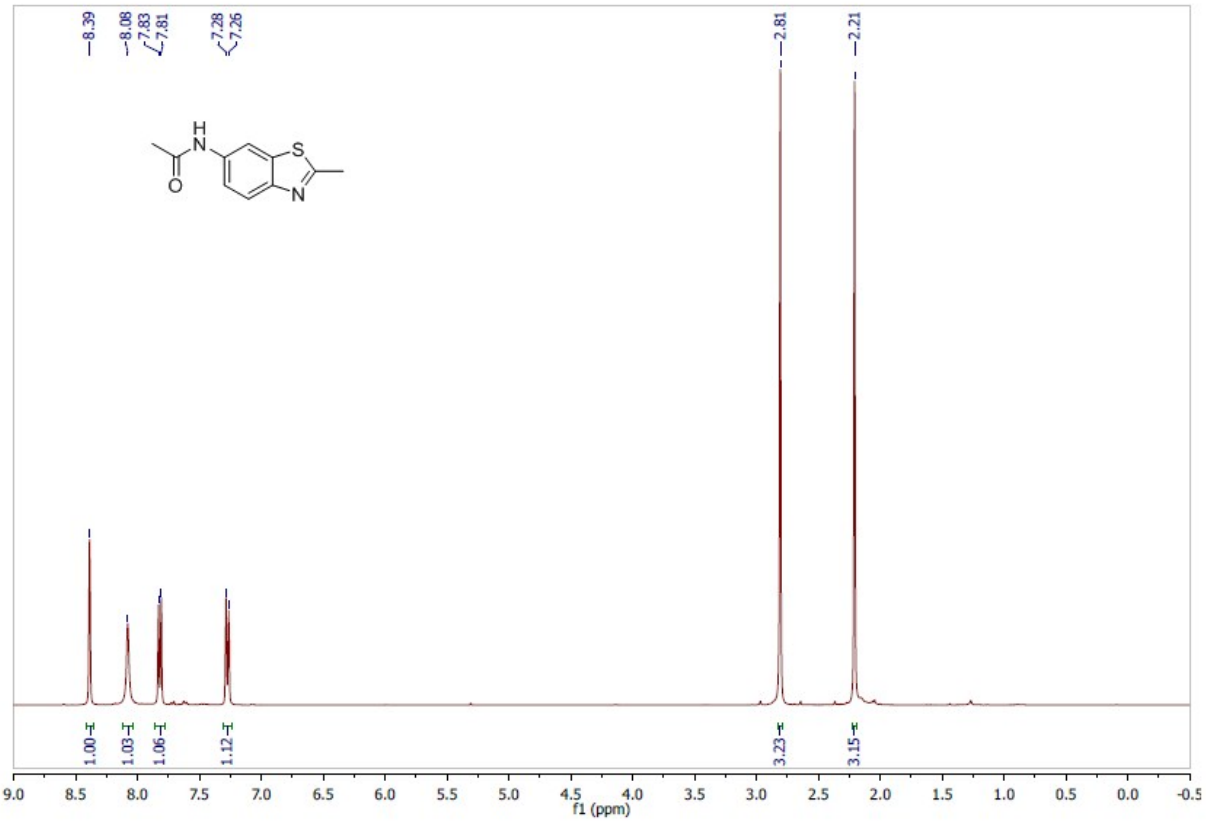
^{13}C NMR spectrum in $CDCl_3$ of compound **2**.



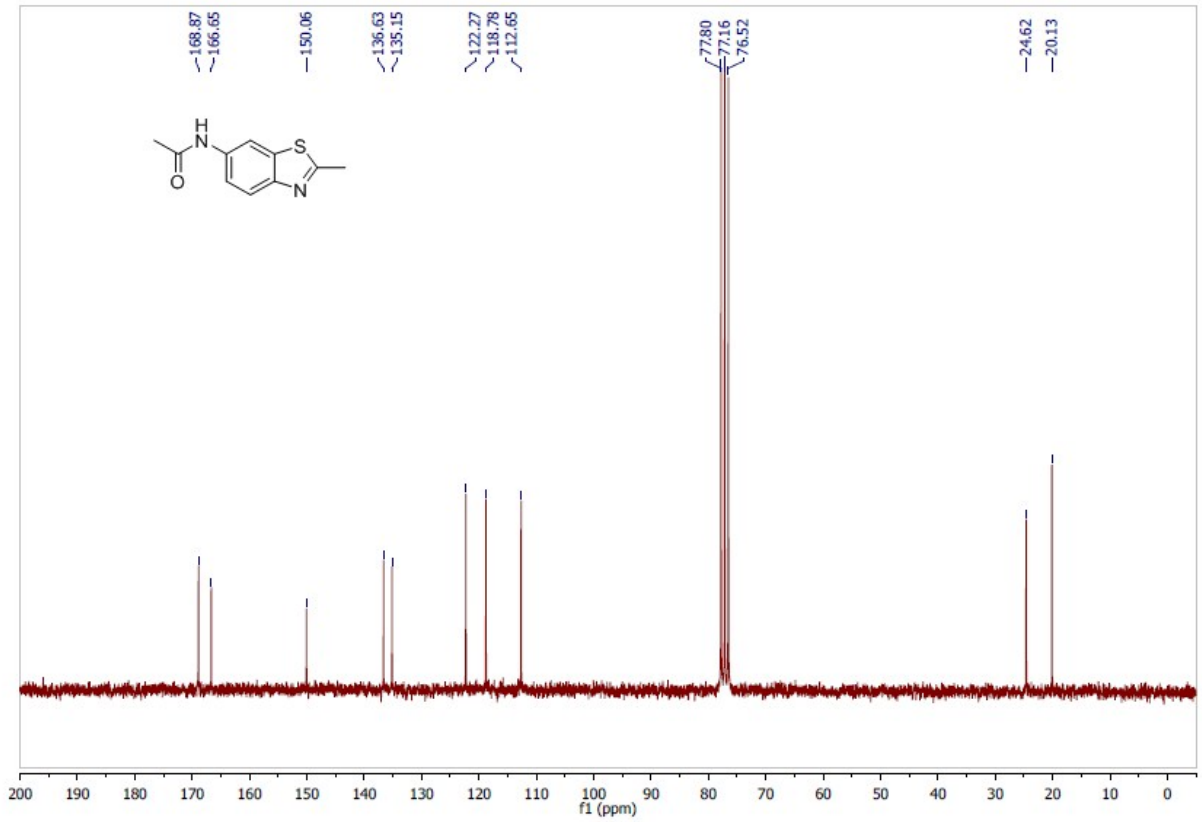
^{1}H NMR spectrum in $CDCl_3$ of compound **3**.



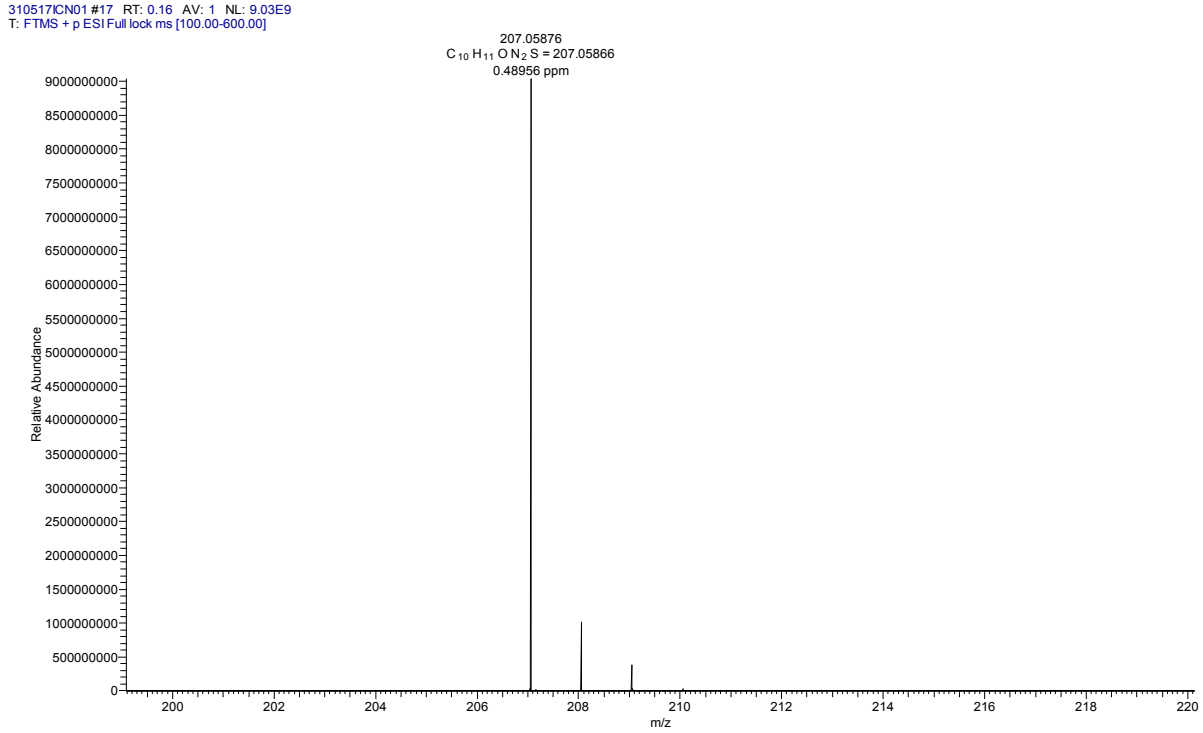
^{13}C NMR spectrum in $CDCl_3$ of compound **3**.



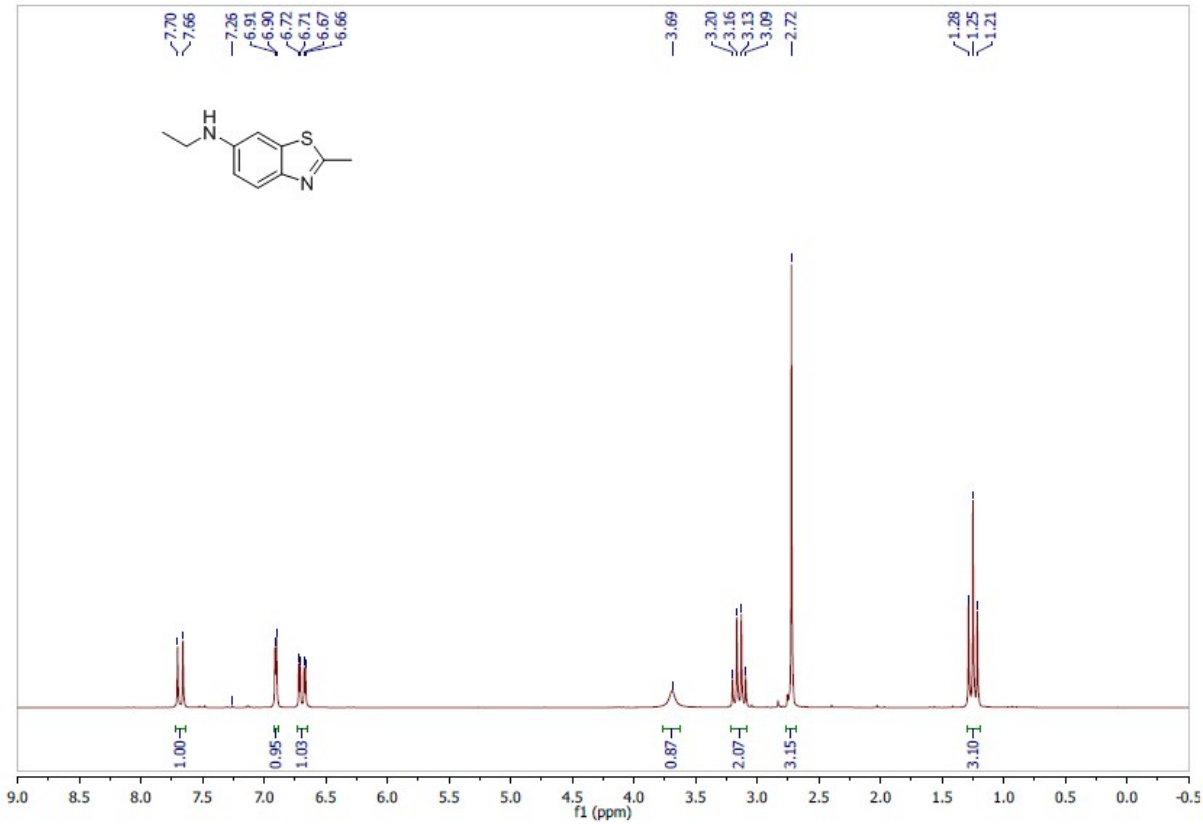
^{1}H NMR spectrum in $CDCl_3$ of compound **4**.



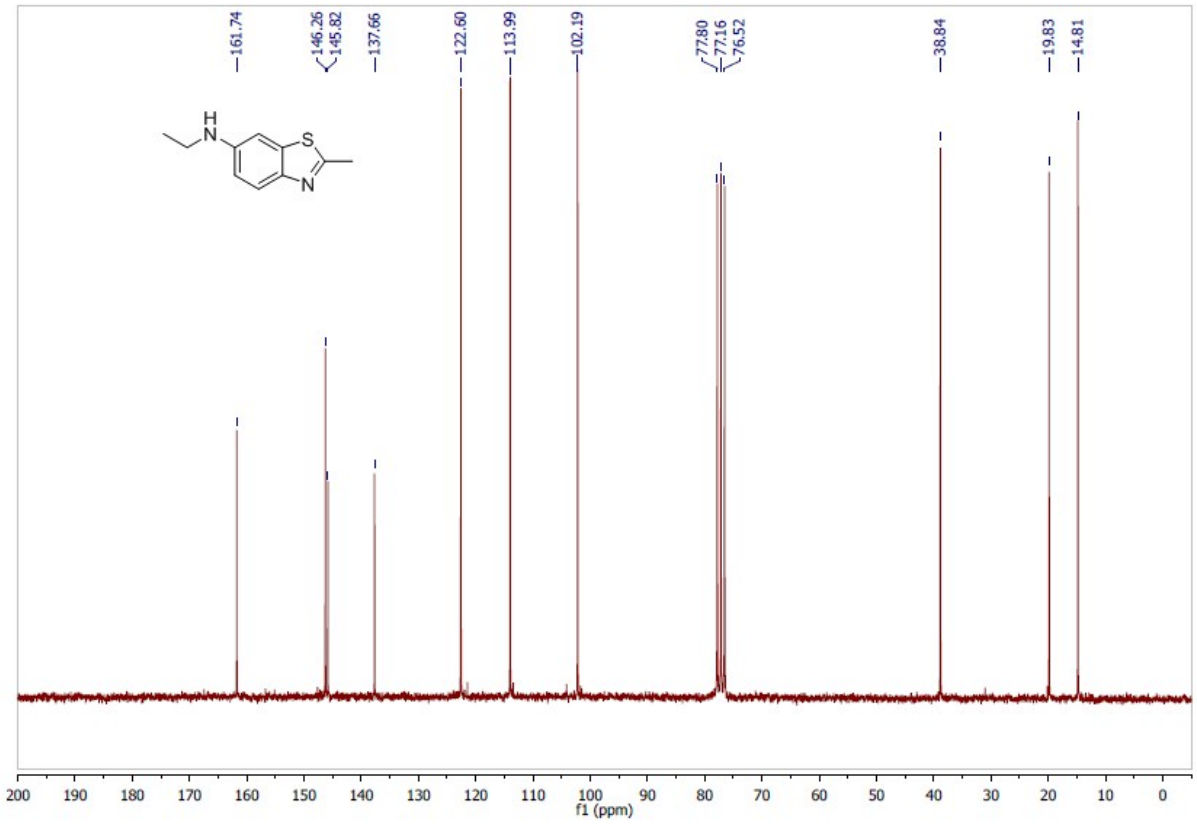
^{13}C NMR spectrum in $CDCl_3$ of compound **4**.



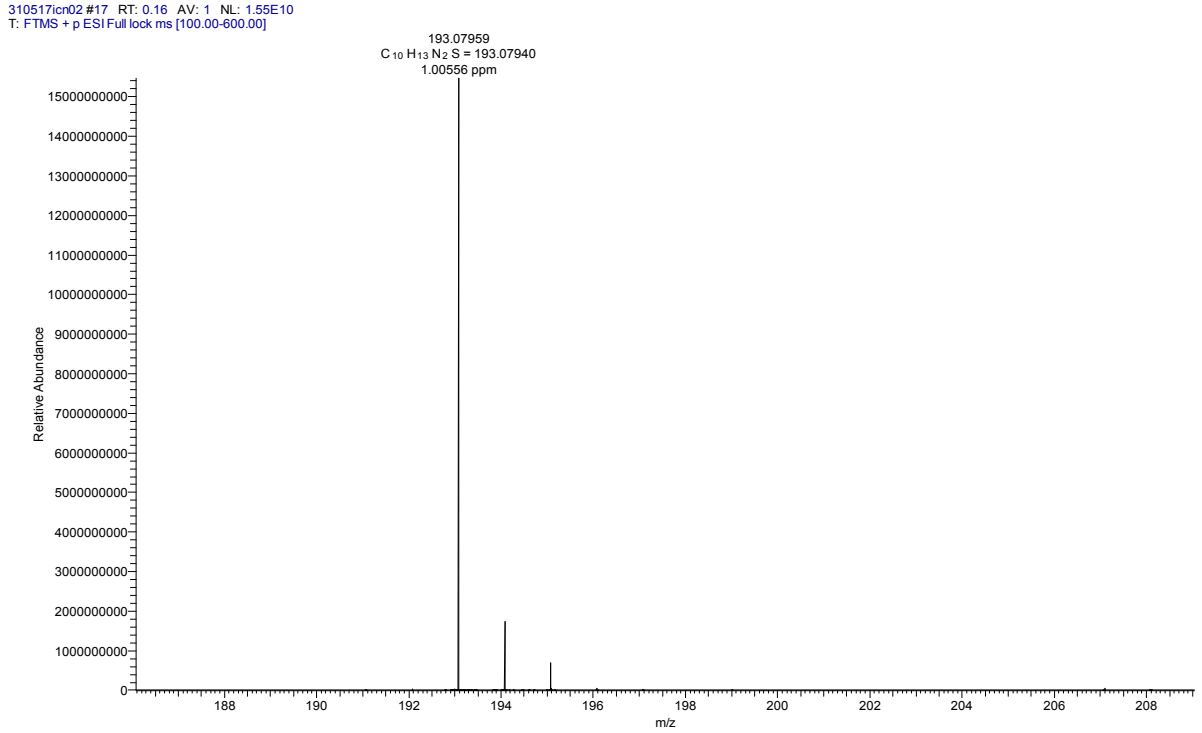
HRMS (ESI-MS) spectrum of compound **4**.



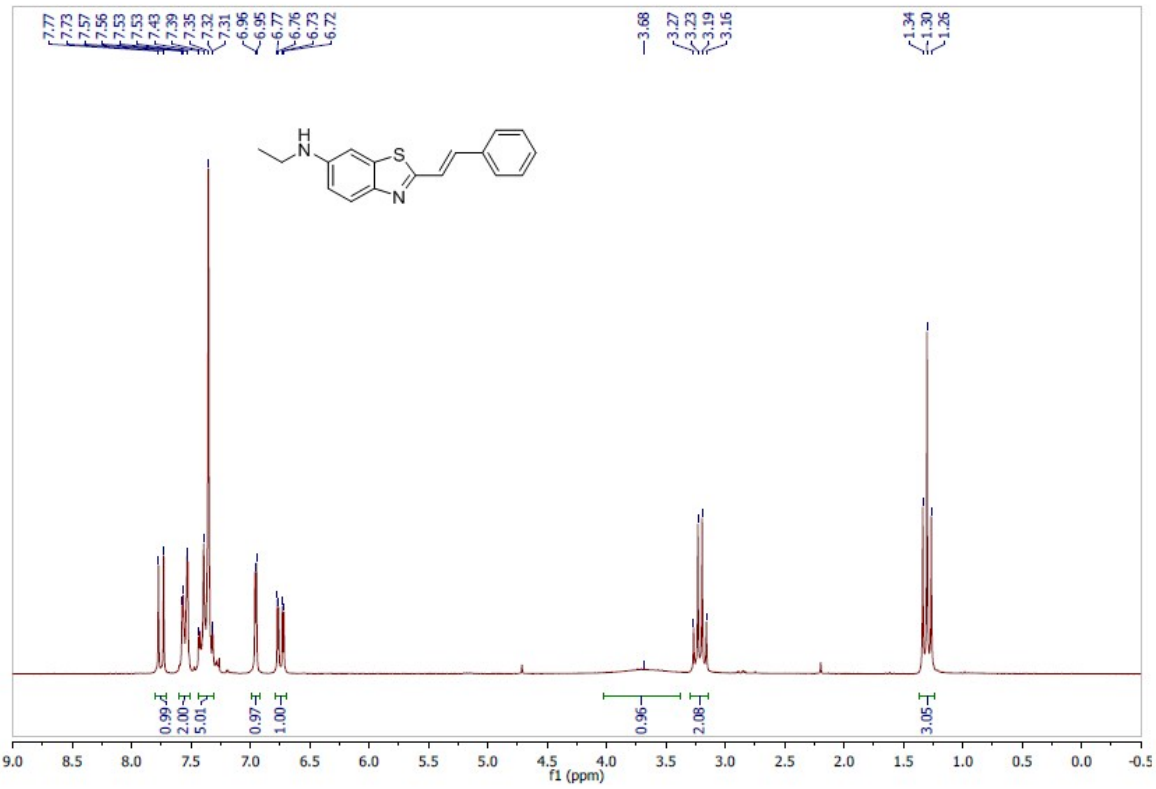
^{1}H NMR spectrum in $CDCl_3$ of compound **5**.



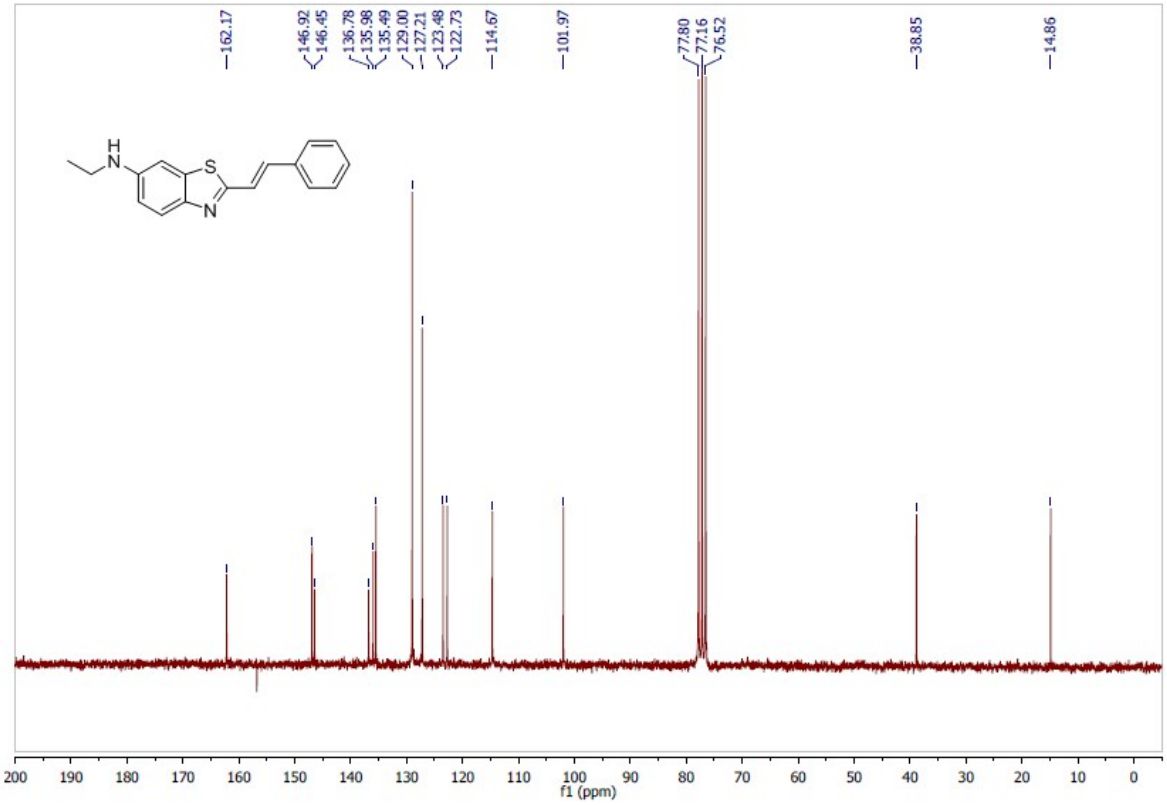
^{13}C NMR spectrum in $CDCl_3$ of compound **5**.



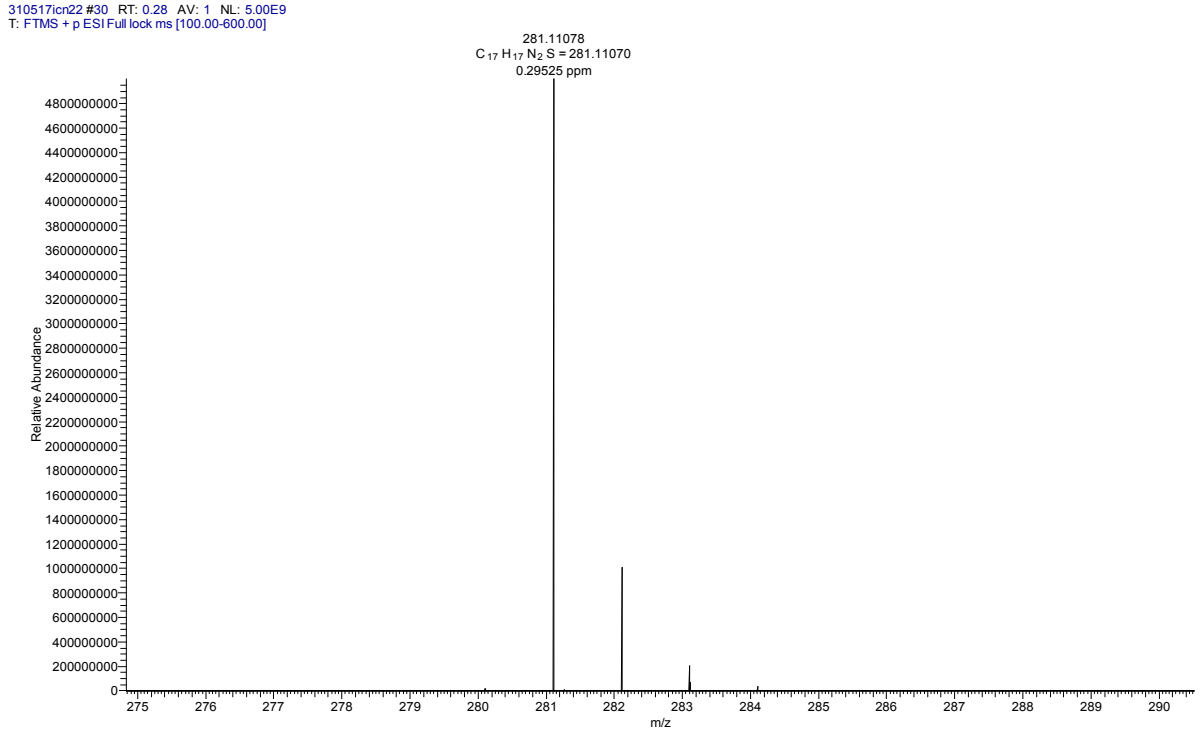
HRMS (ESI-MS) spectrum of compound **5**.



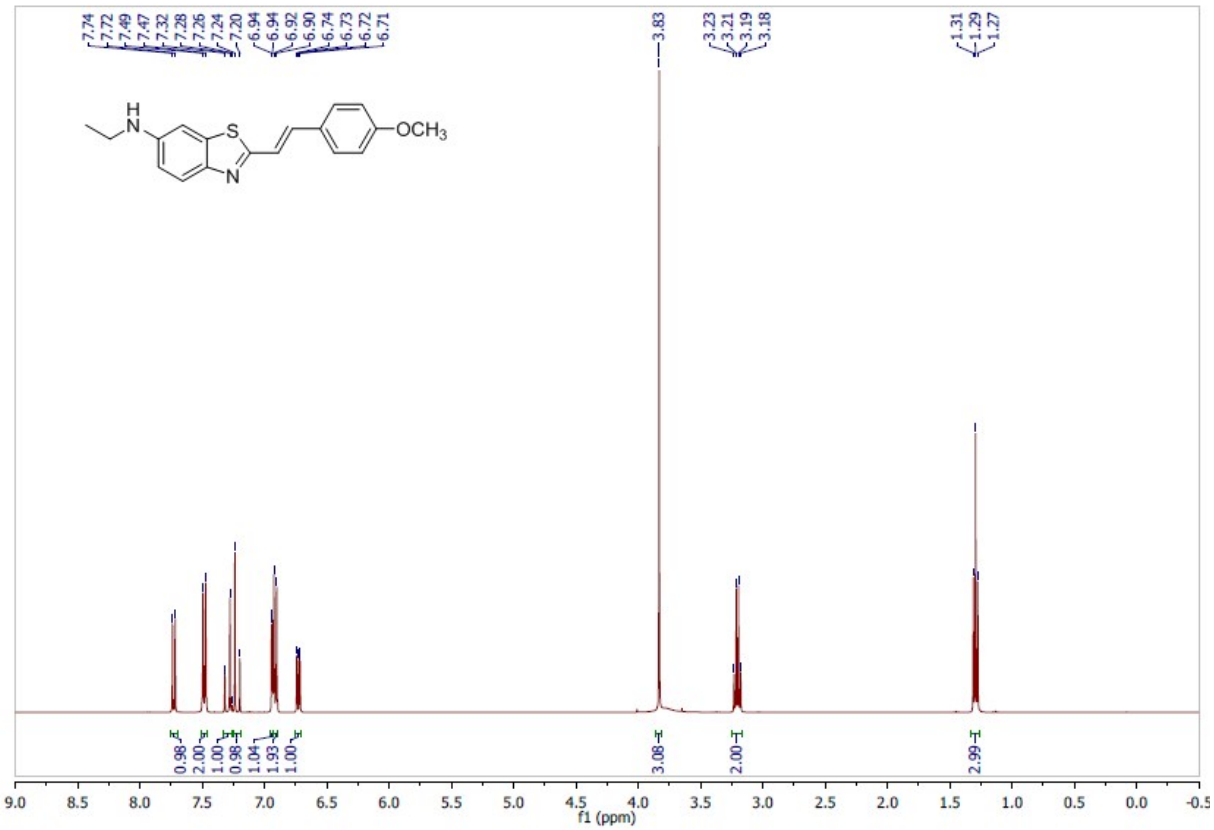
^{1}H NMR spectrum in $CDCl_3$ of compound **D1b**.



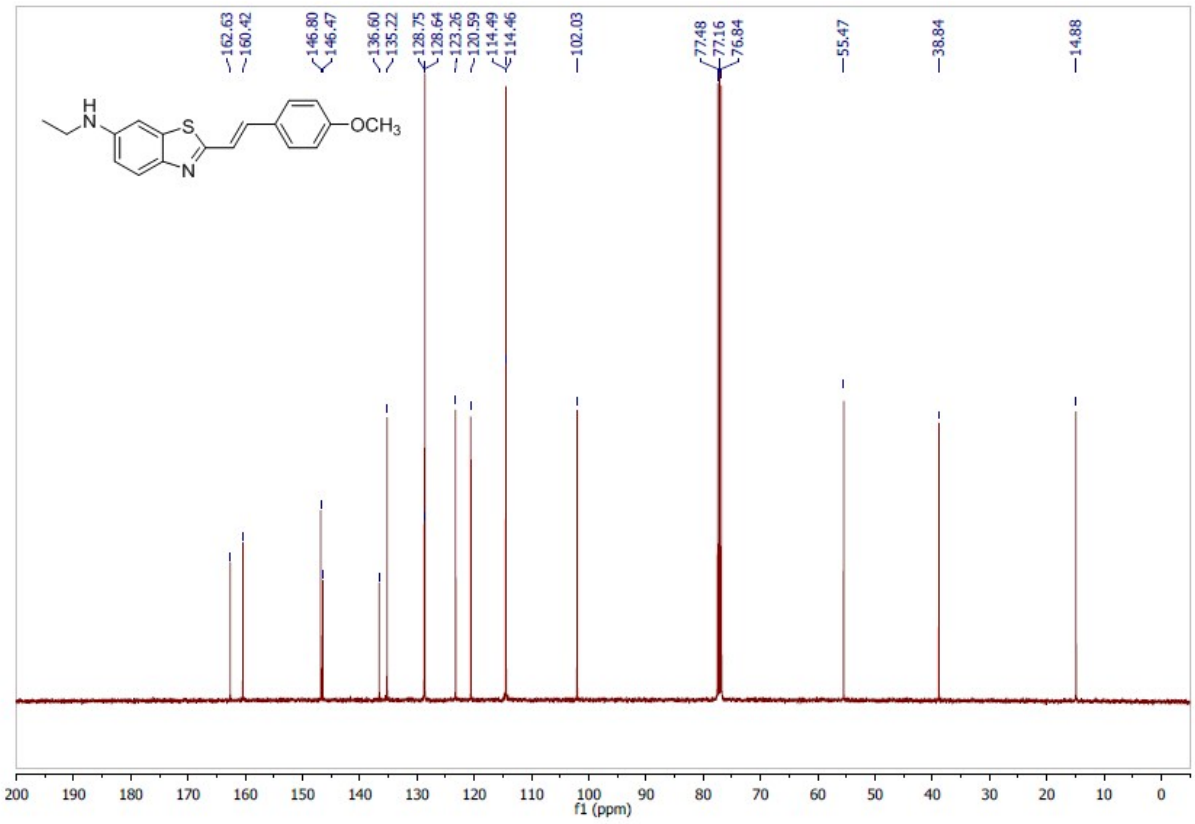
^{13}C NMR spectrum in $CDCl_3$ of compound **D1b**.



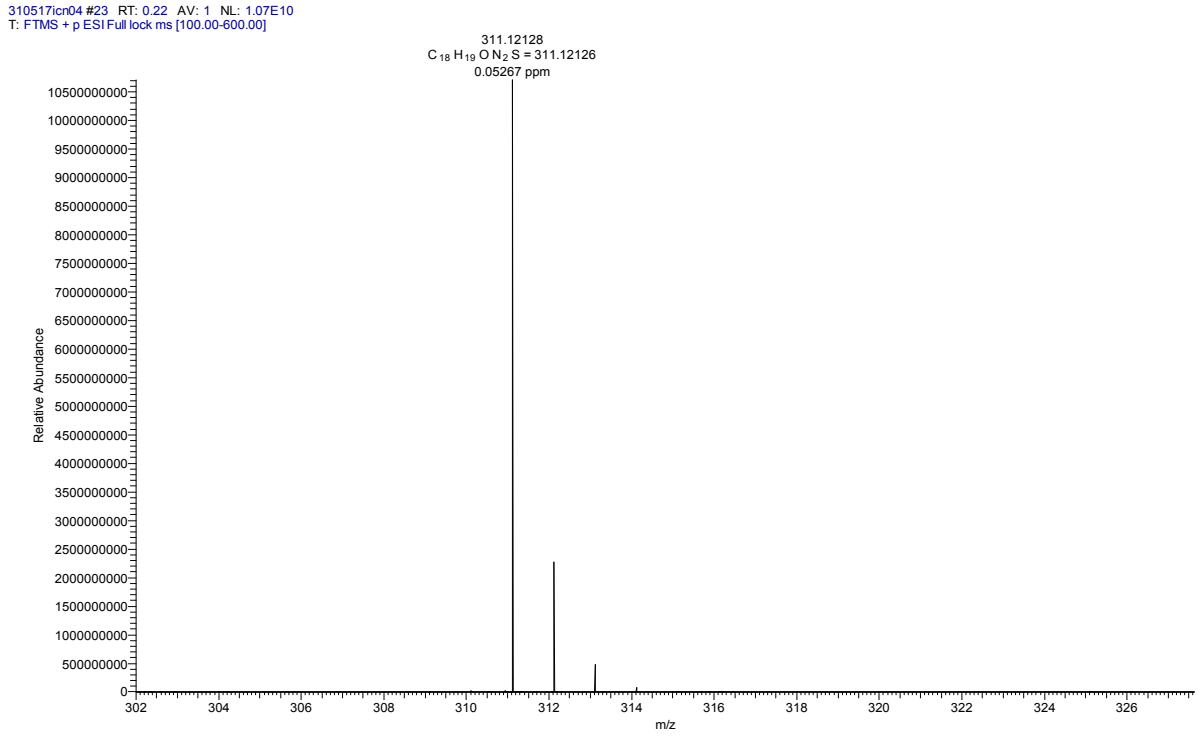
HRMS (ESI-MS) spectrum of dye **D1b**.



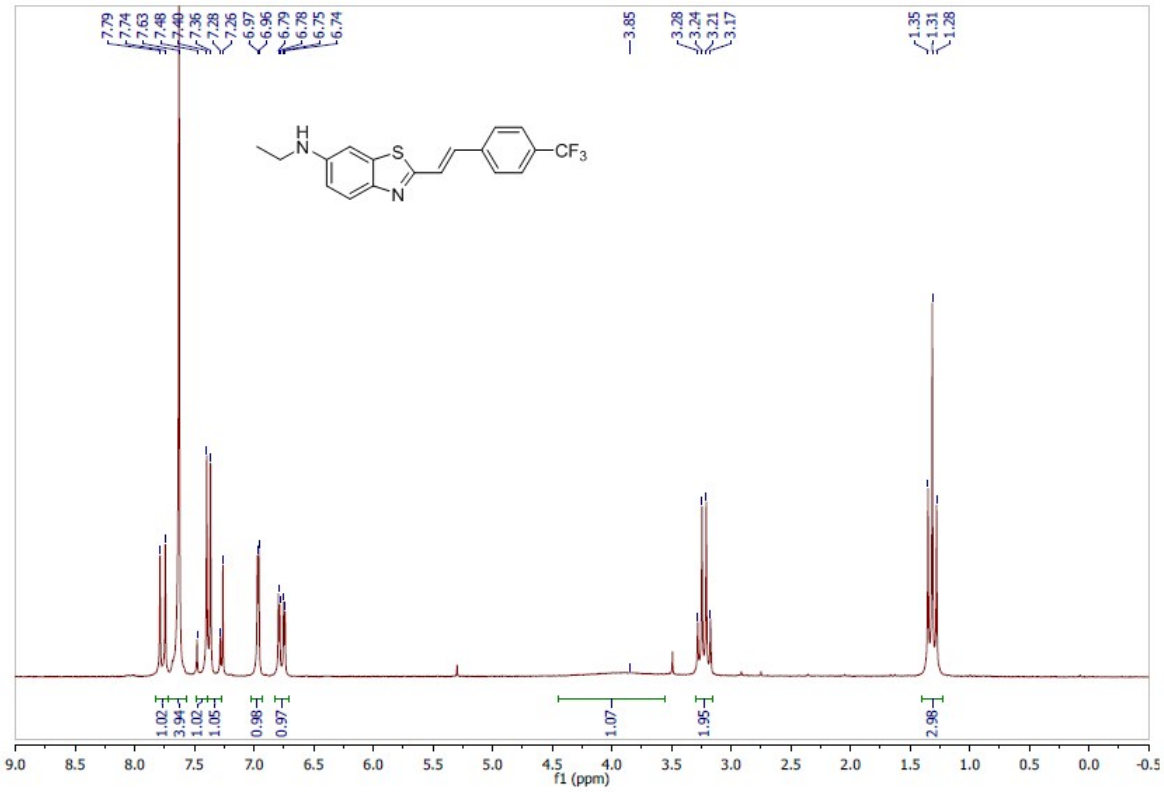
^{1}H NMR spectrum in $CDCl_3$ of compound D**2b**.



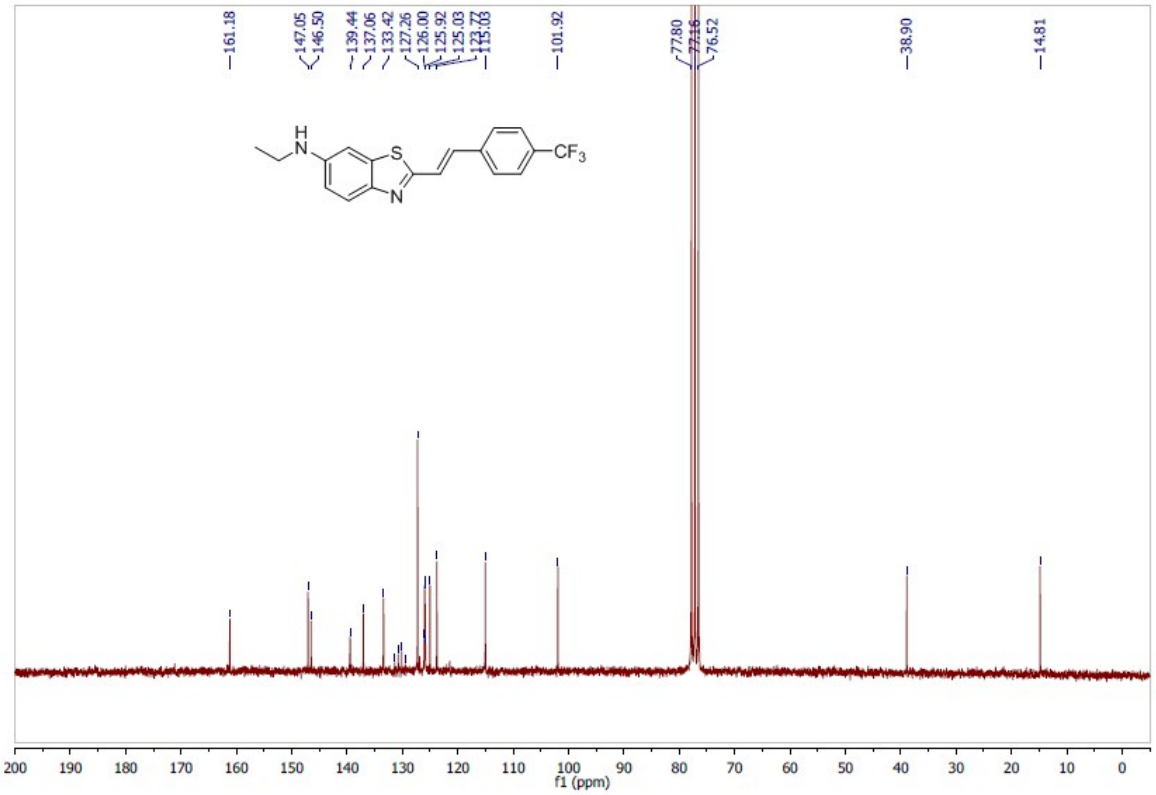
^{13}C NMR spectrum in $CDCl_3$ of compound **D2b**.



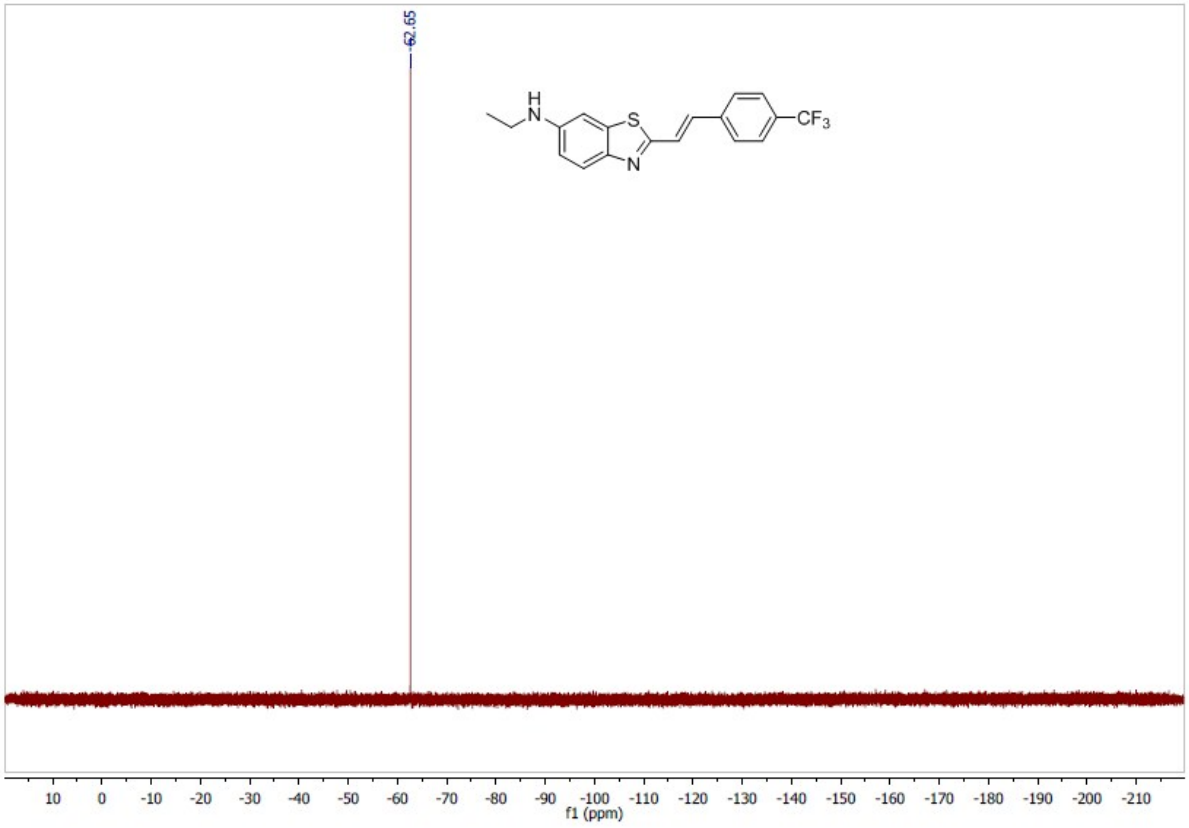
HRMS (ESI-MS) spectrum of dye **D2b**.



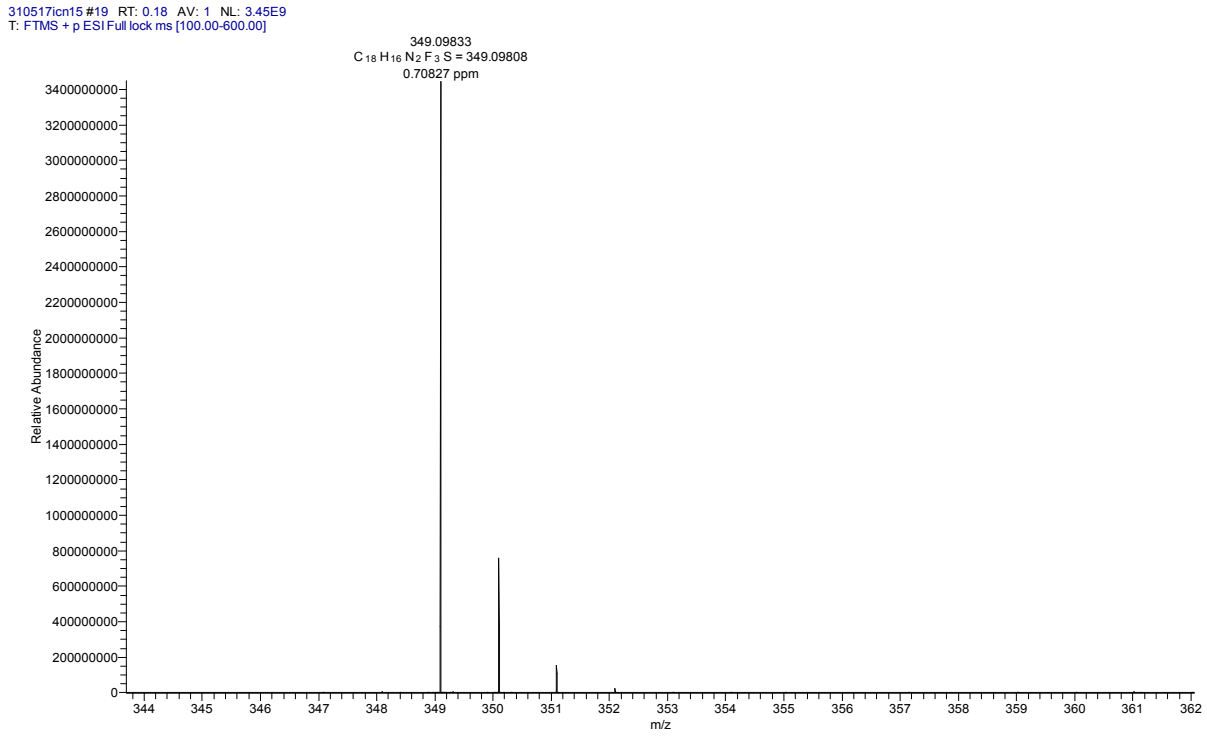
^{1}H NMR spectrum in $CDCl_3$ of compound **D3b**.



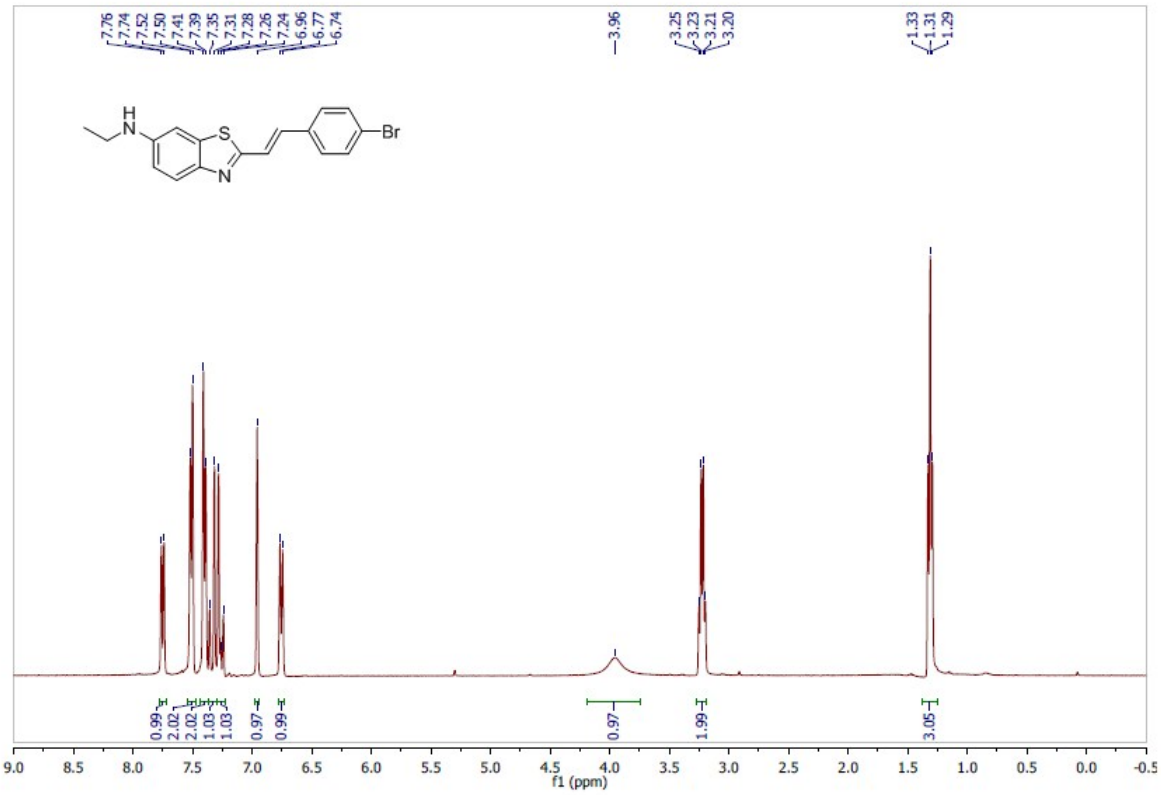
^{13}C NMR spectrum in $CDCl_3$ of compound **D3b**.



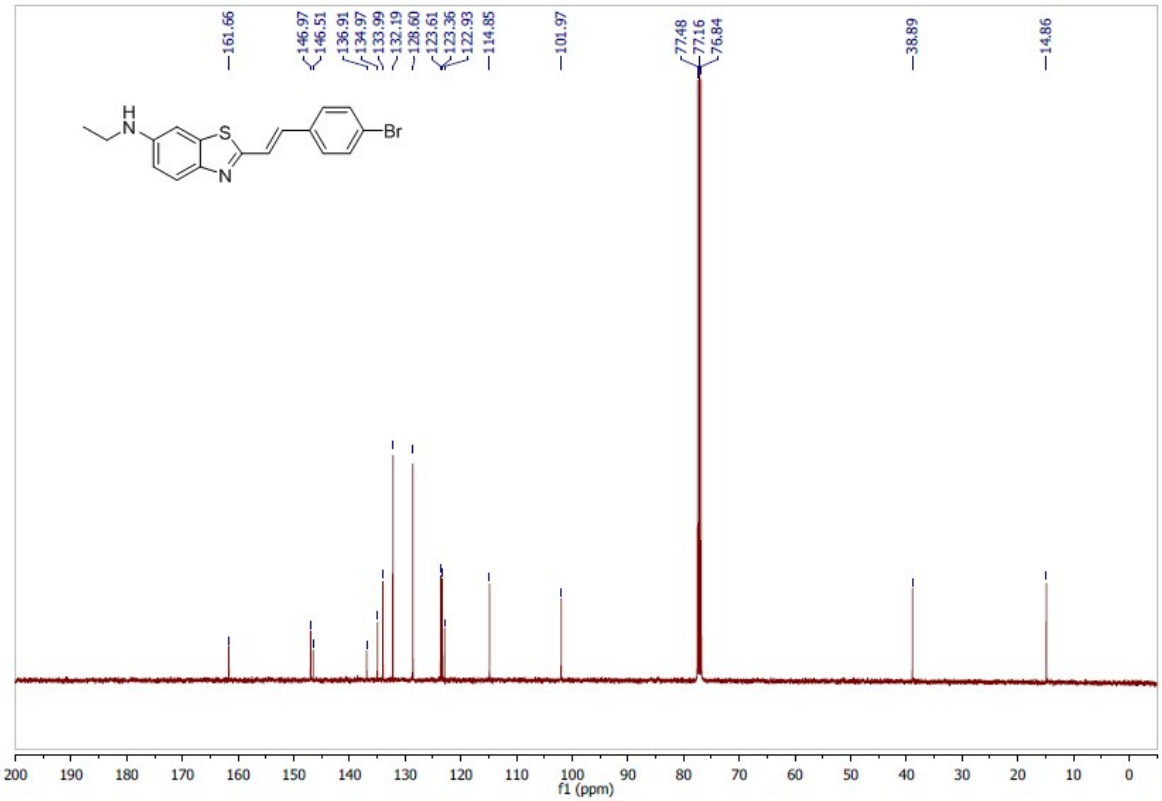
^{19}F NMR spectrum in $CDCl_3$ of compound **D3b**.



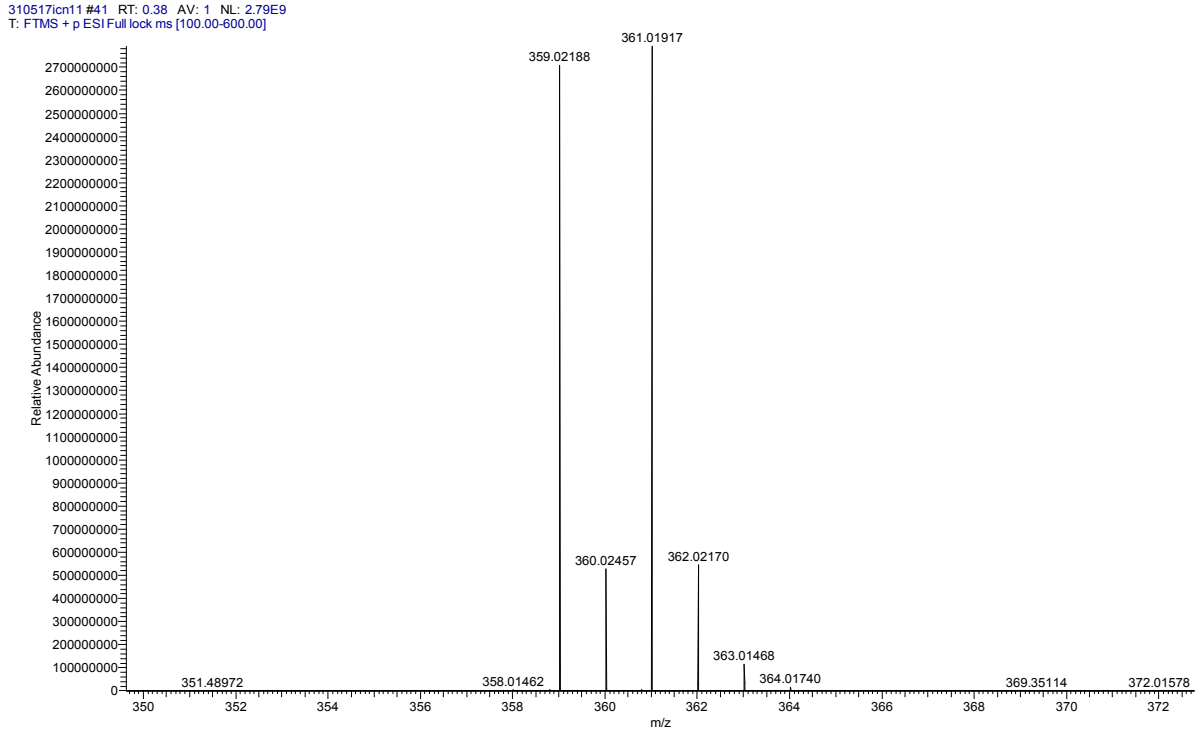
HRMS (ESI-MS) spectrum of dye **D3b**.



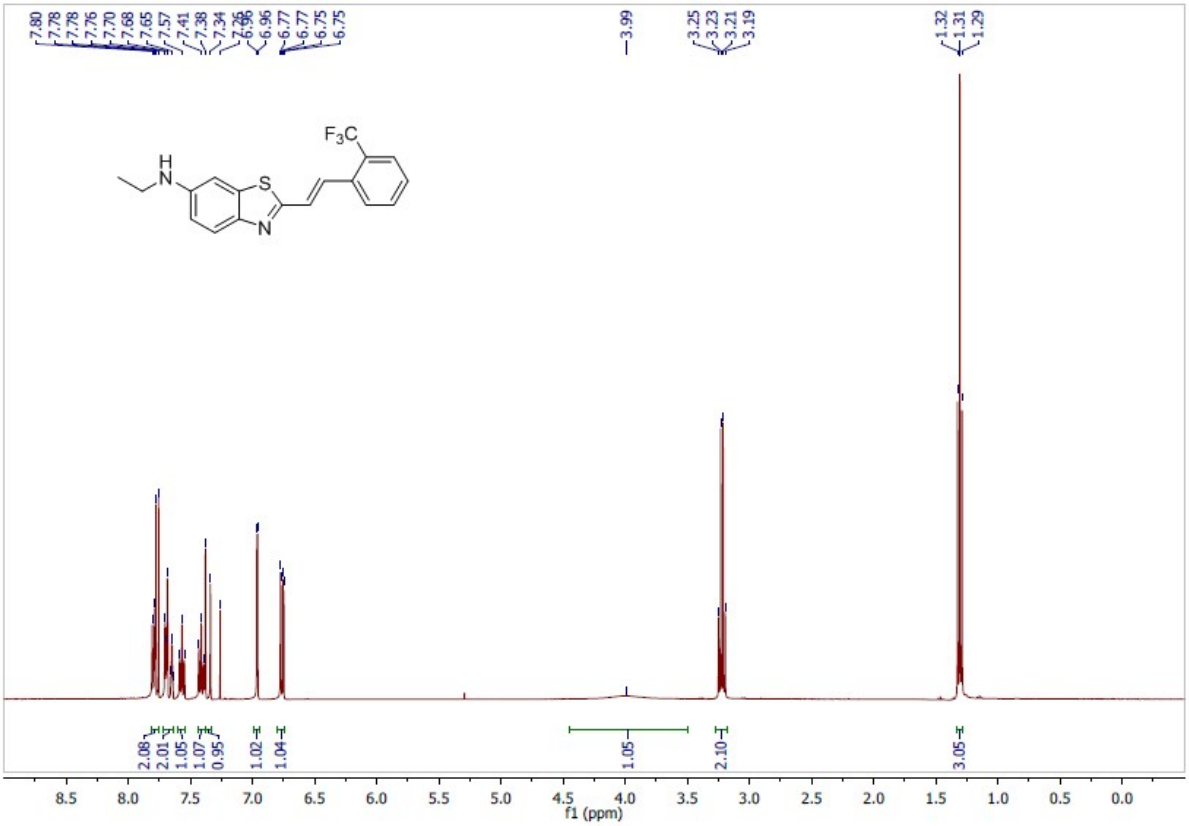
^{1}H NMR spectrum in $CDCl_3$ of compound **D4b**.



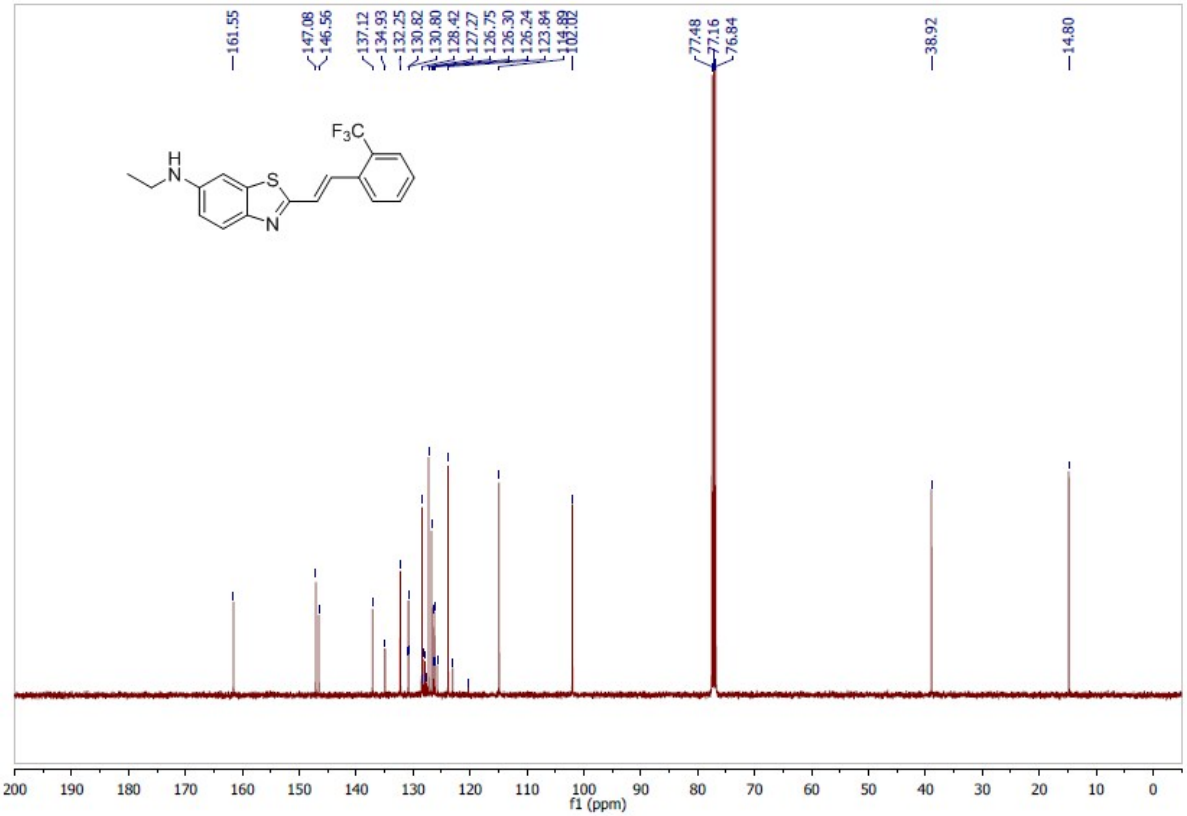
^{13}C NMR spectrum in $CDCl_3$ of compound **D4b**.



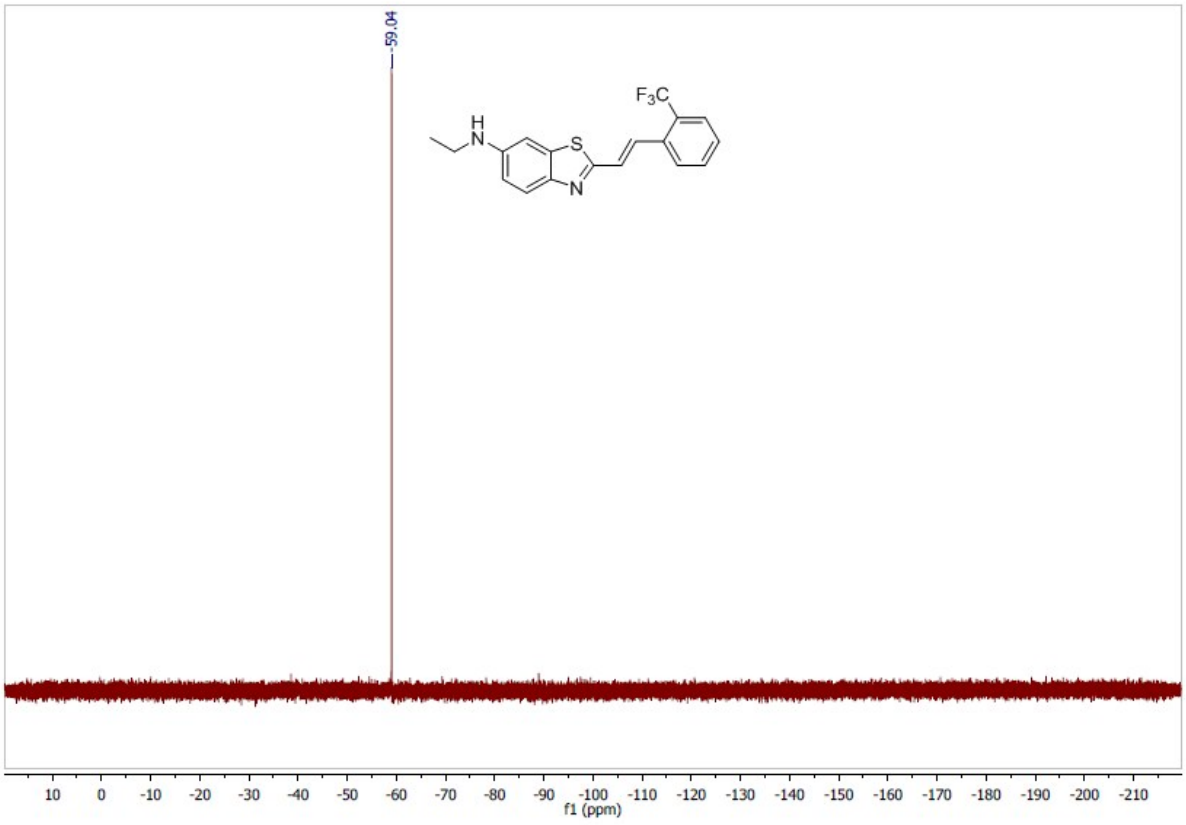
HRMS (ESI-MS) spectrum of dye **D4b**.



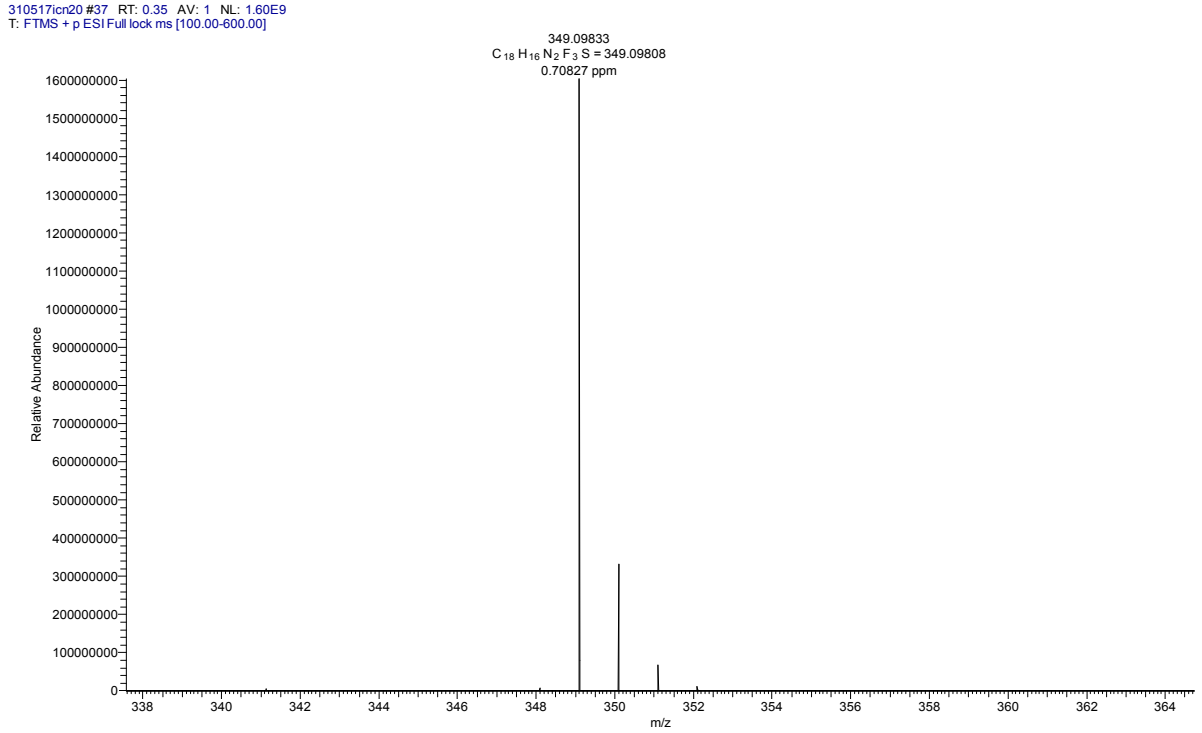
^{1}H NMR spectrum in $CDCl_3$ of compound **D5b**.



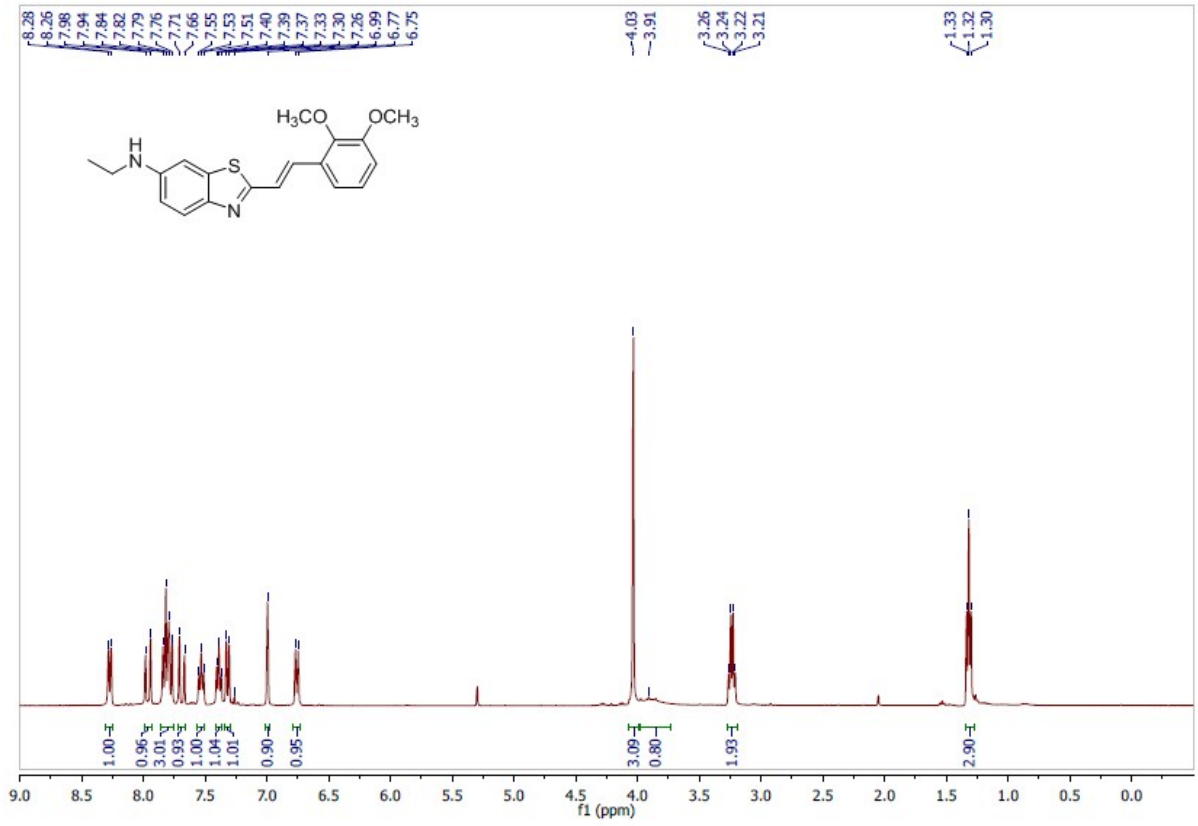
^{13}C NMR spectrum in $CDCl_3$ of compound **D5b**.



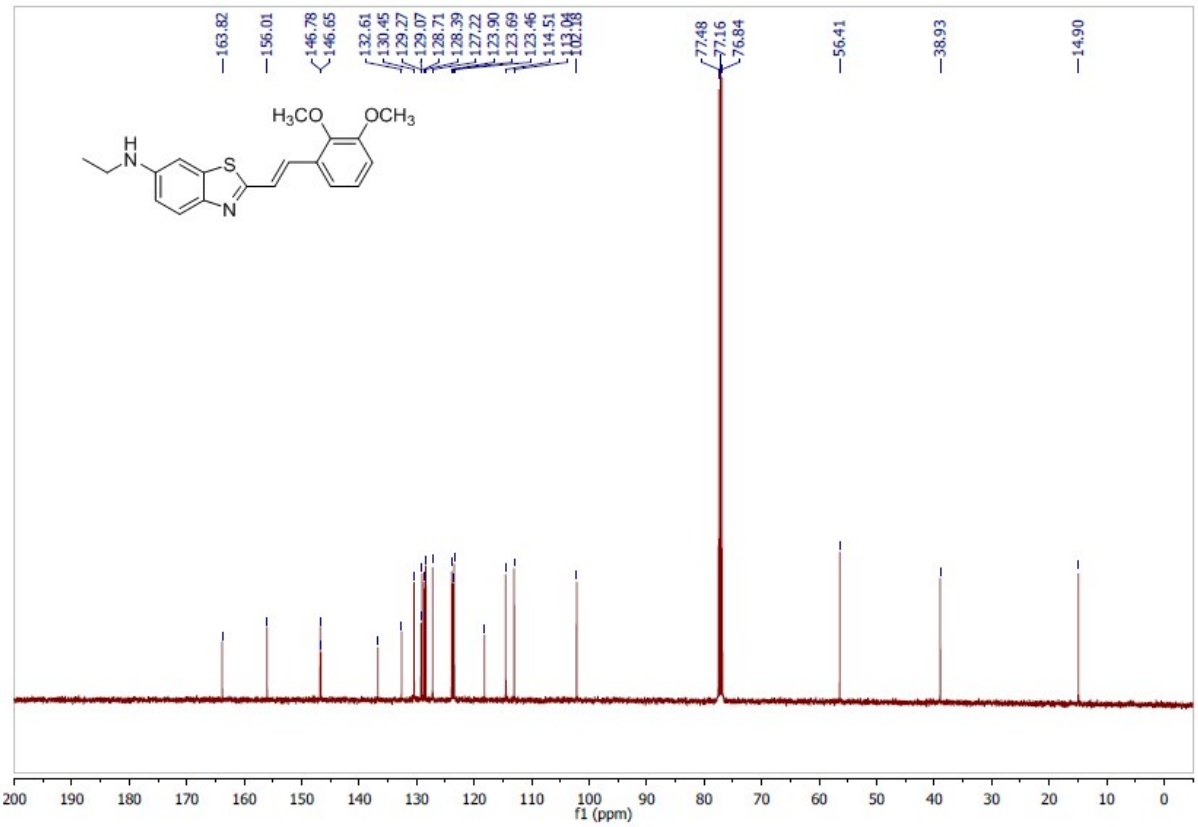
^{19}F NMR spectrum in $CDCl_3$ of compound **D5b**.



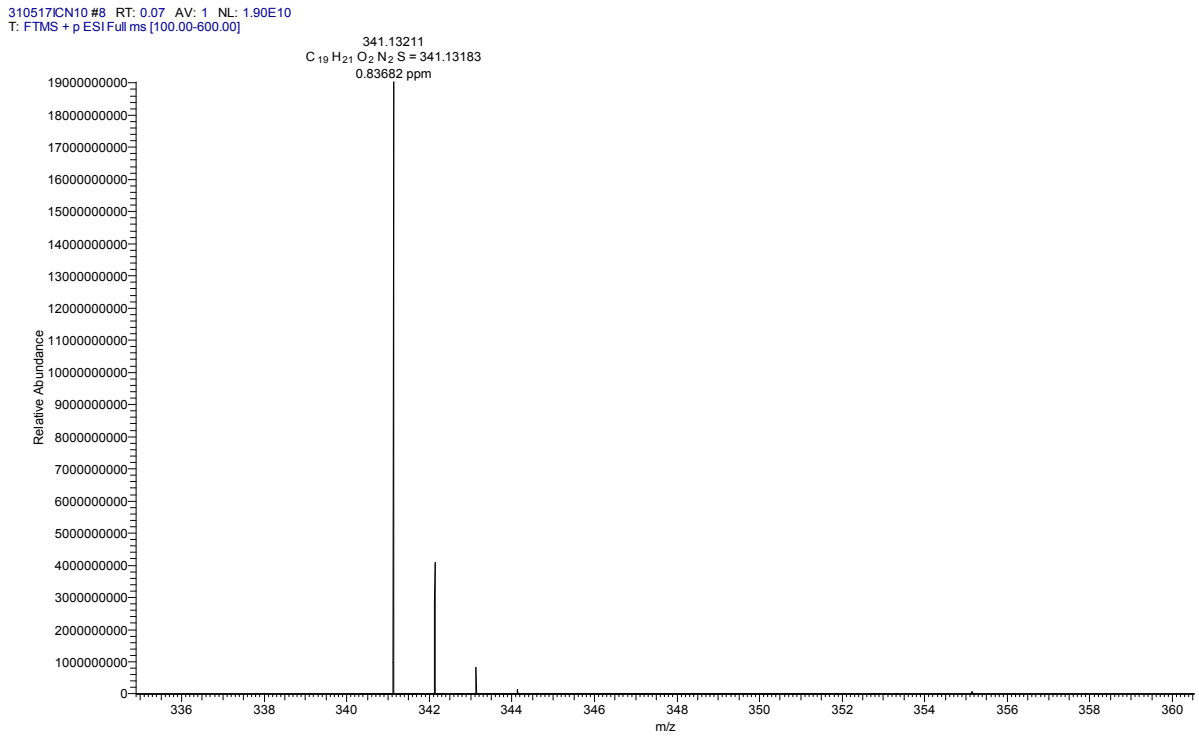
HRMS (ESI-MS) spectrum of dye **D5b**.



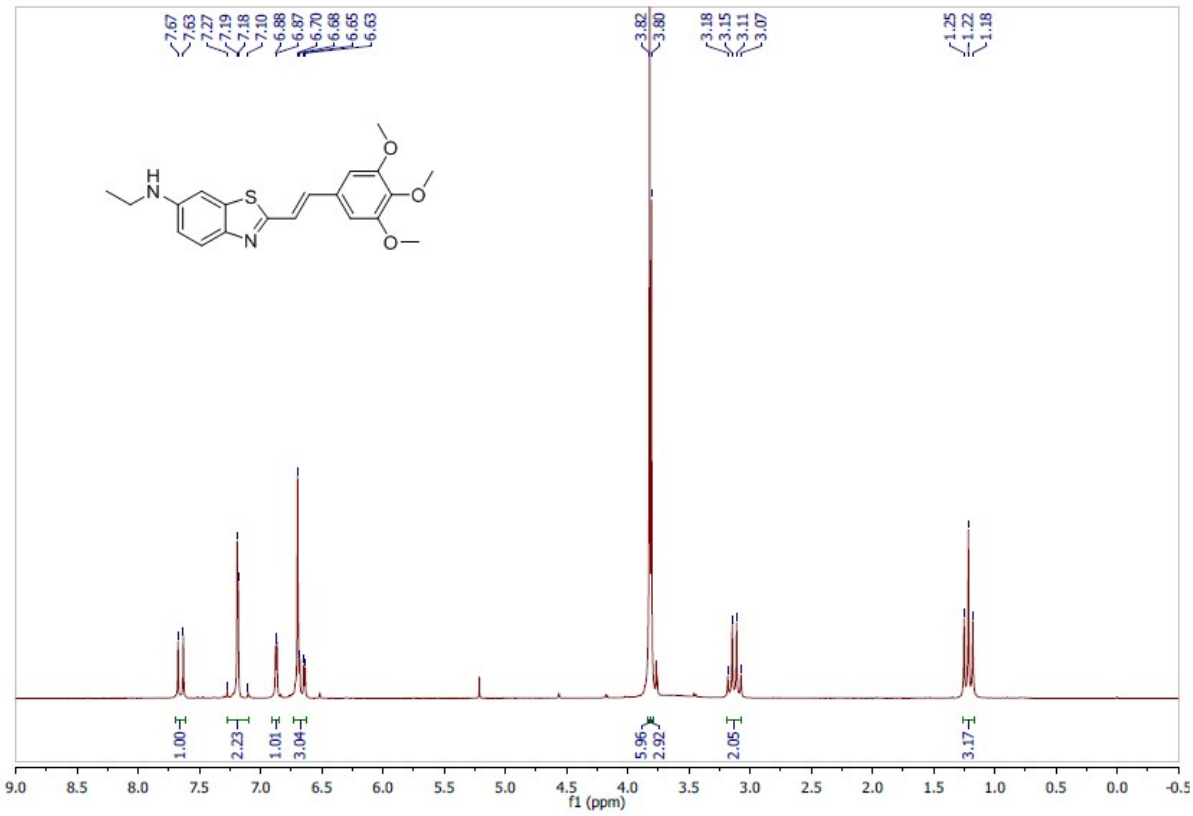
^{1}H NMR spectrum of compound **D6b**.



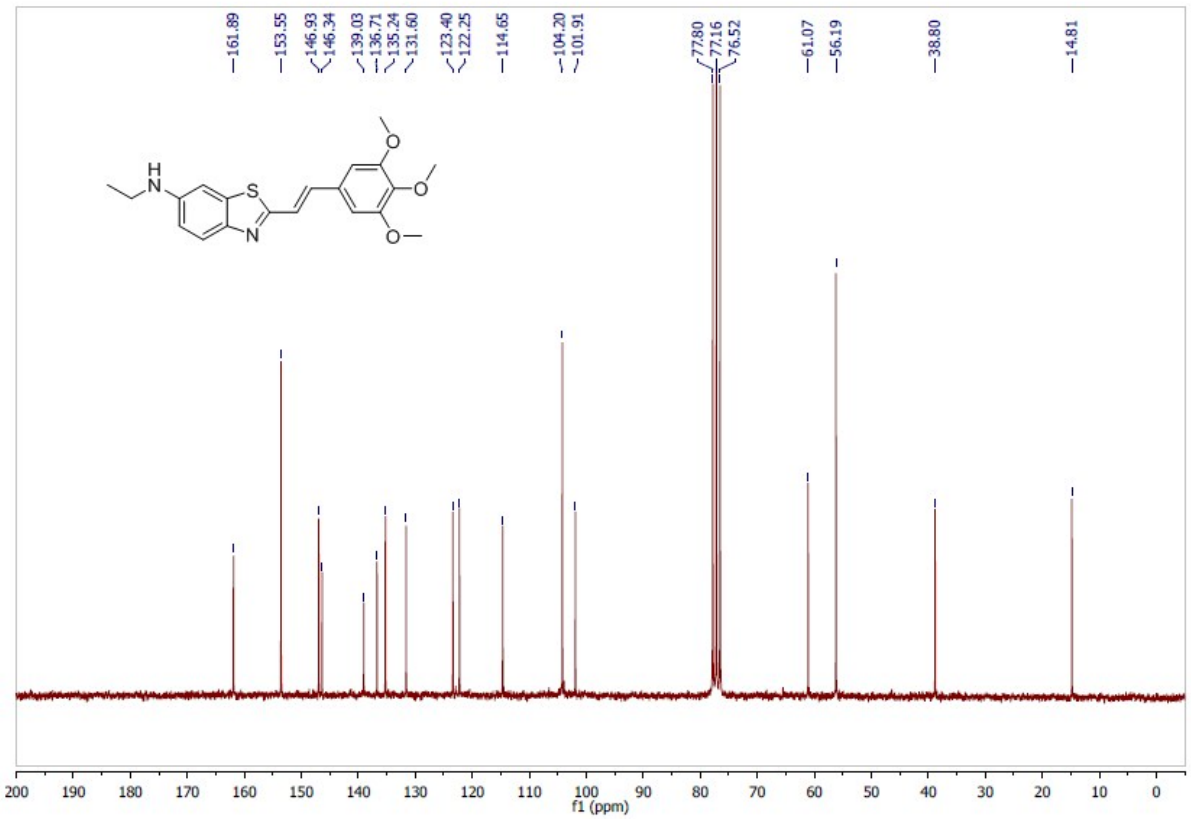
^{13}C NMR spectrum in $CDCl_3$ of compound **D6b**.



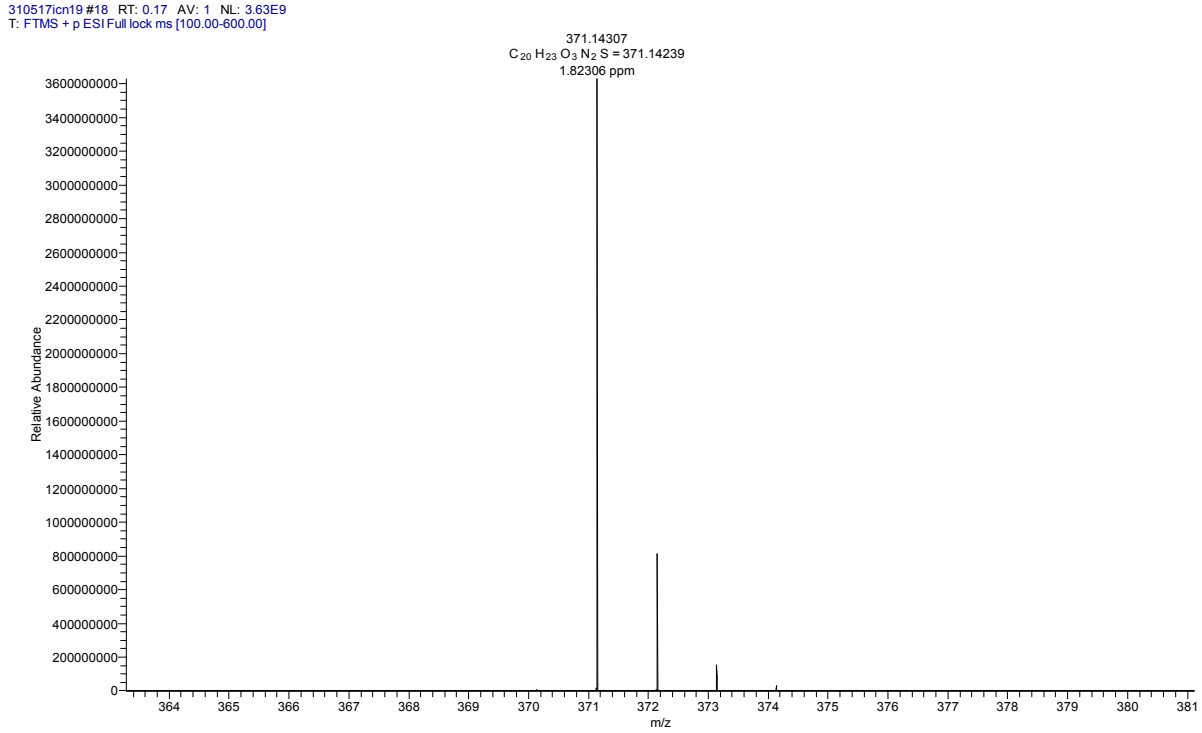
HRMS (ESI-MS) spectrum of dye **D6b**.



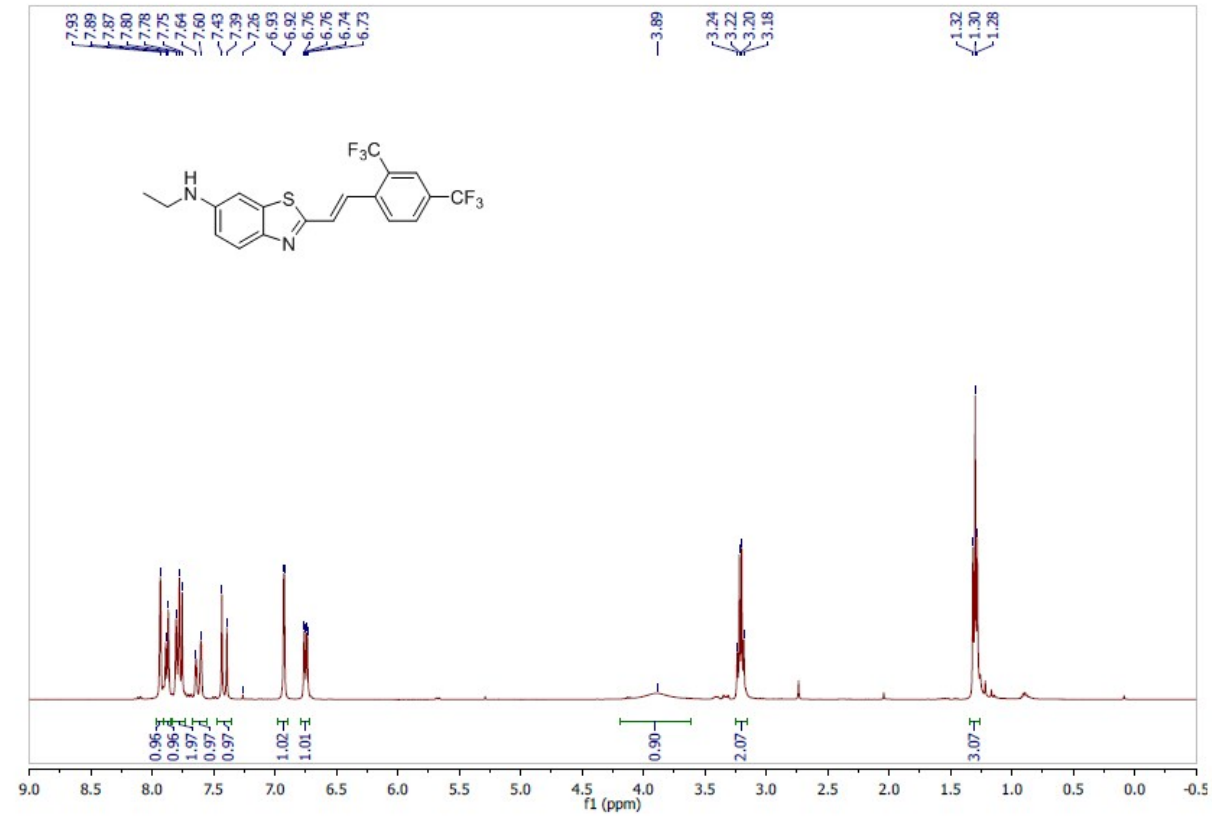
^{1}H NMR spectrum in $CDCl_3$ of compound **D7b**.



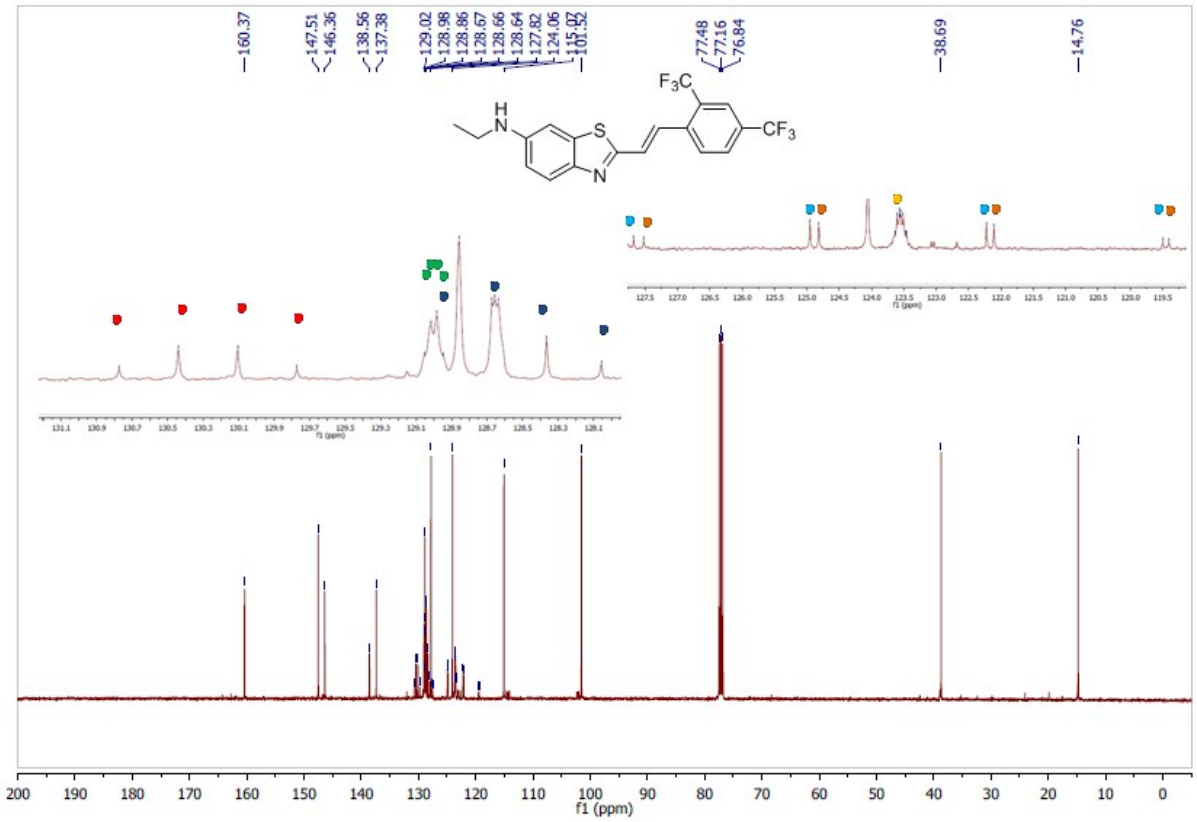
^{13}C NMR spectrum in $CDCl_3$ of compound **D7b**.



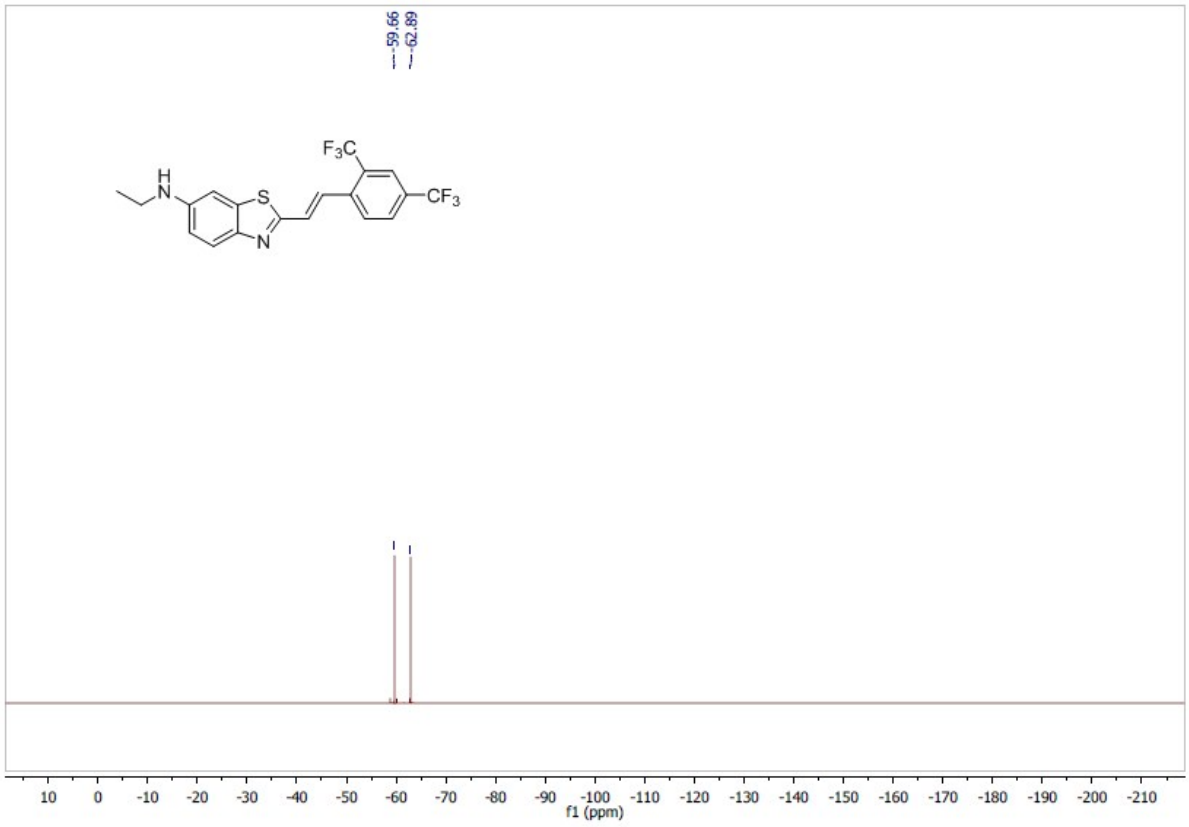
HRMS (ESI-MS) spectrum of dye **D7b**.



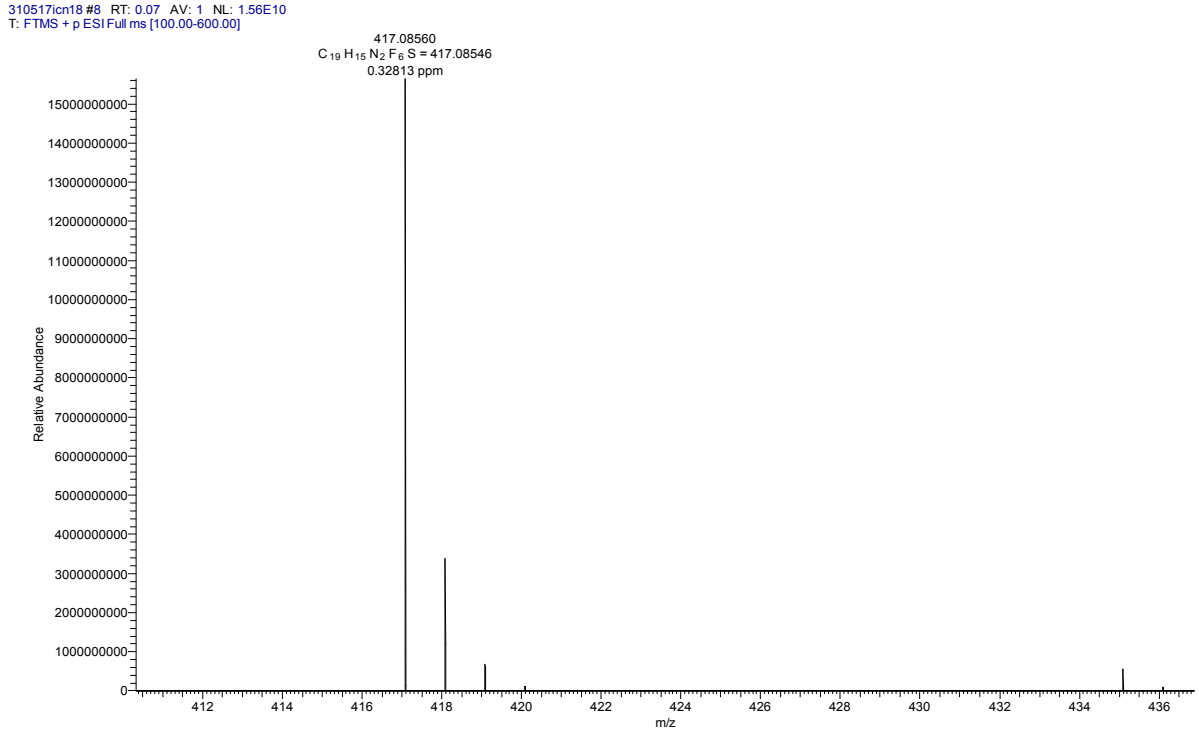
^{1}H NMR spectrum in $CDCl_3$ of compound **D8b**.



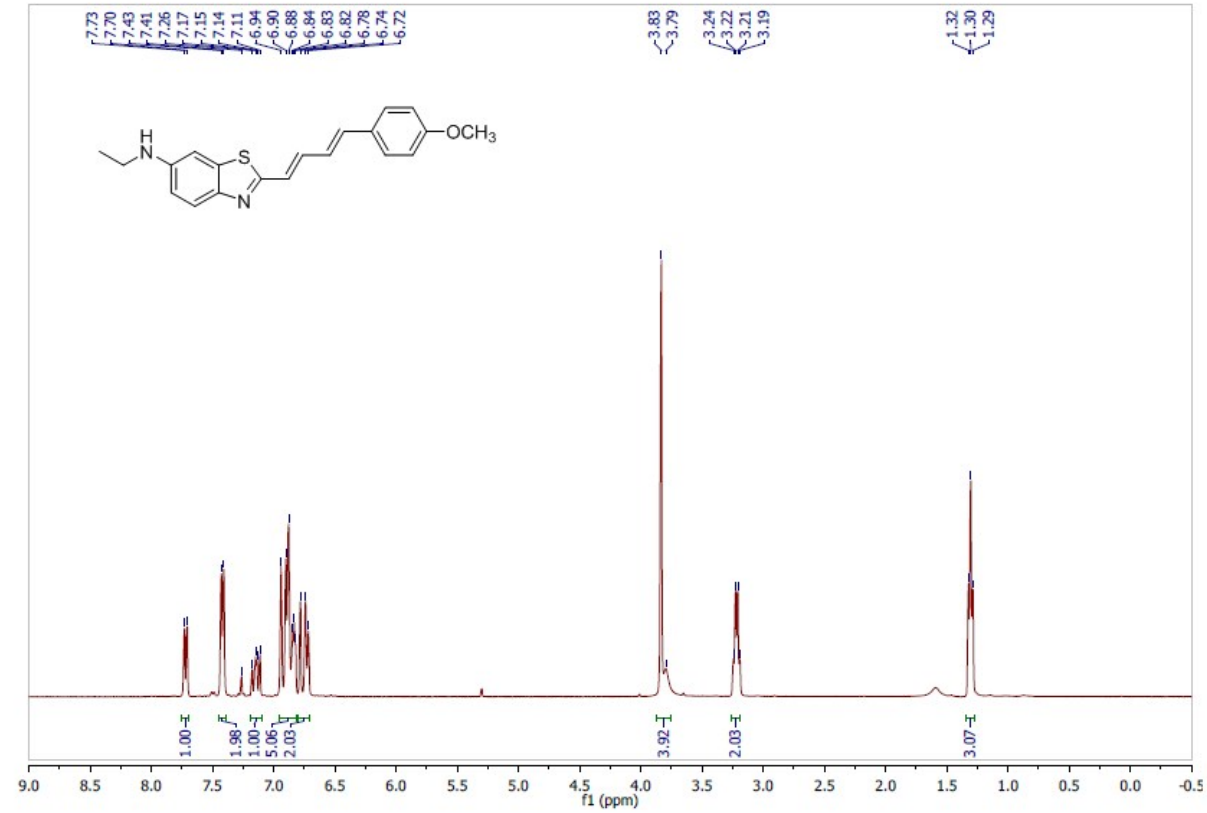
^{13}C NMR spectrum in $CDCl_3$ of compound **D8b**.



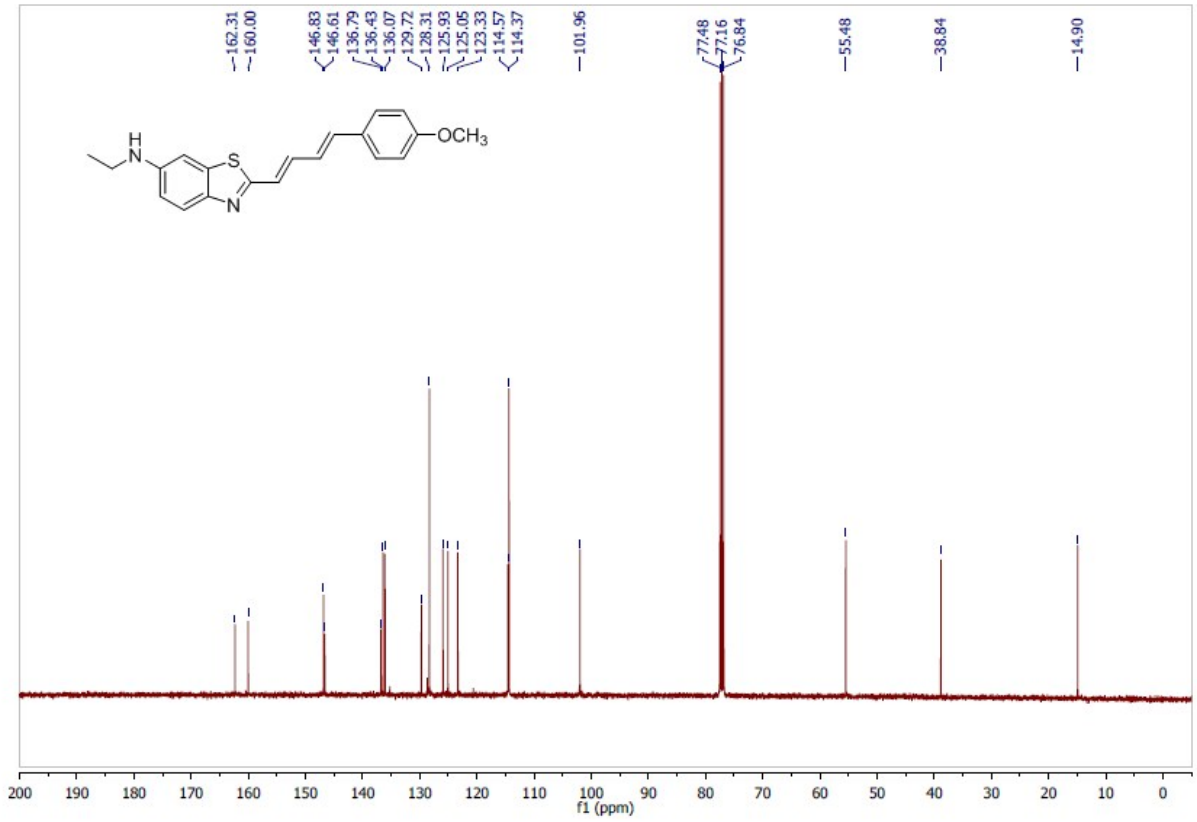
^{19}F NMR spectrum in $CDCl_3$ of compound **D8b**.



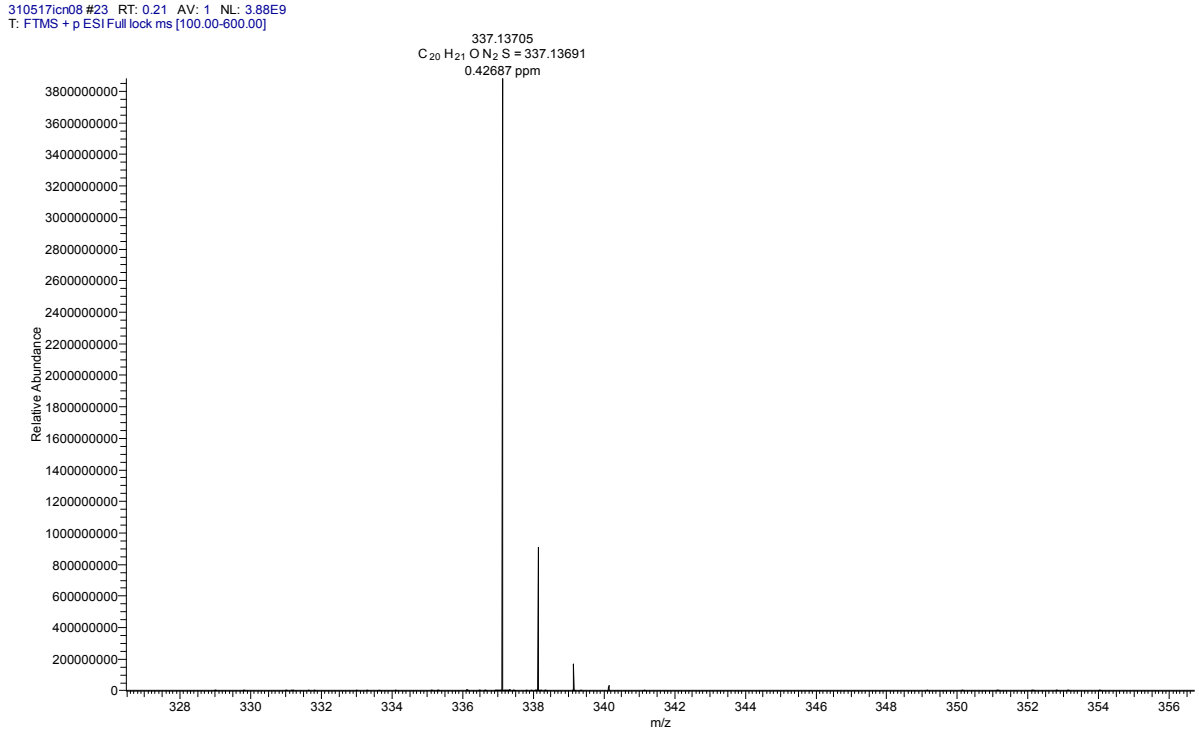
HRMS (ESI-MS) spectrum of dye **D8b**.



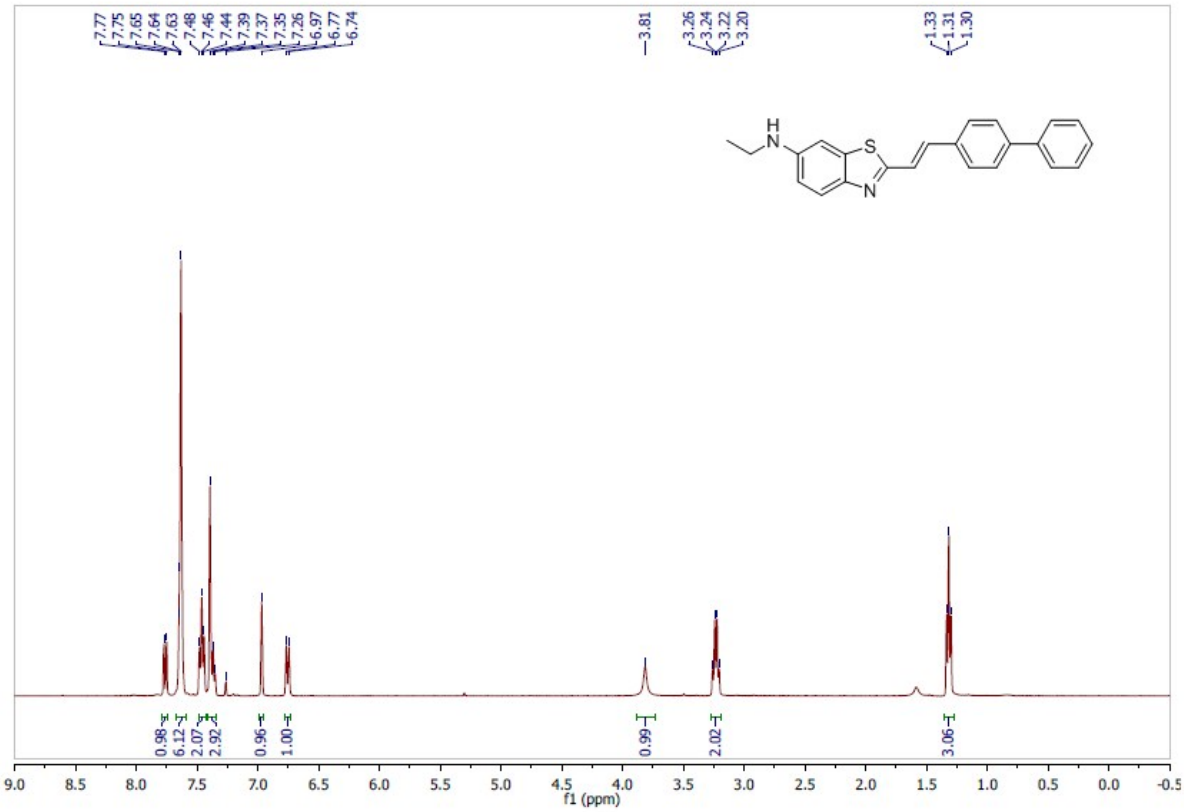
^{1}H NMR spectrum in $CDCl_3$ of compound **D9b**.



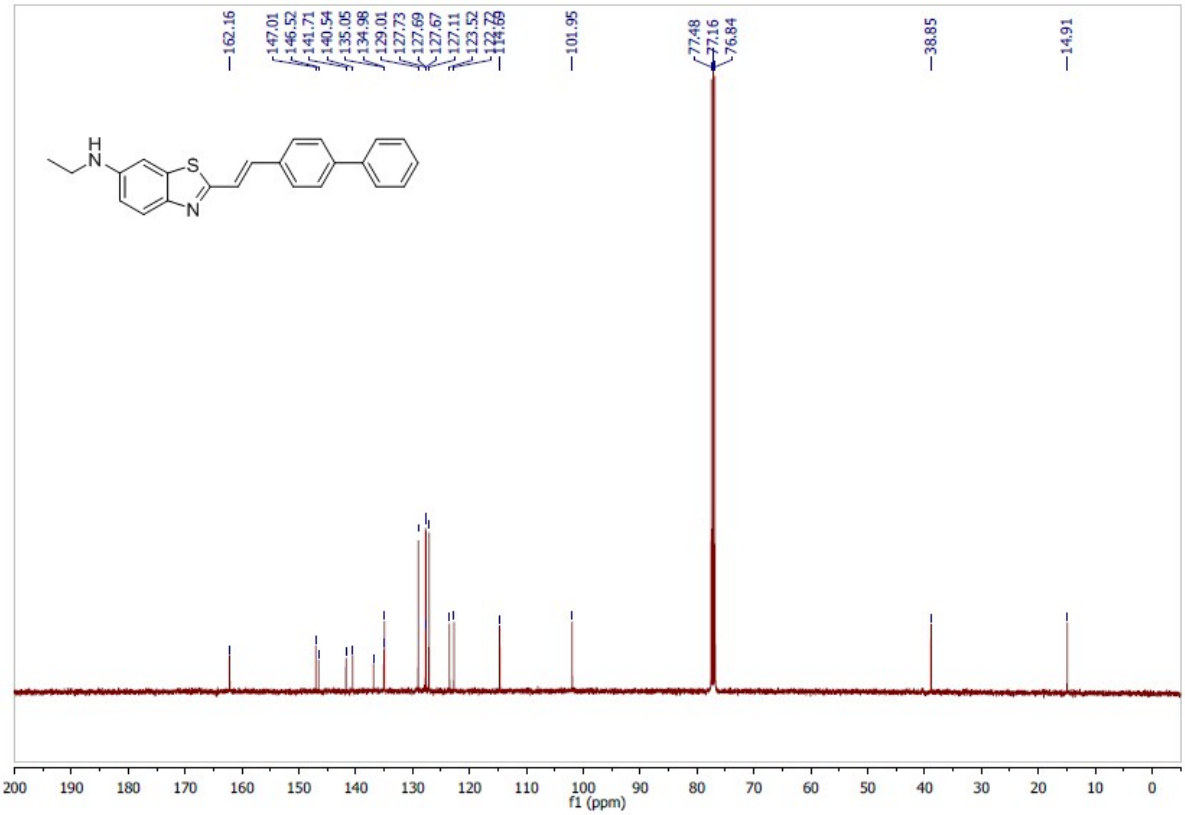
^{13}C NMR spectrum in $CDCl_3$ of compound **D9b**.



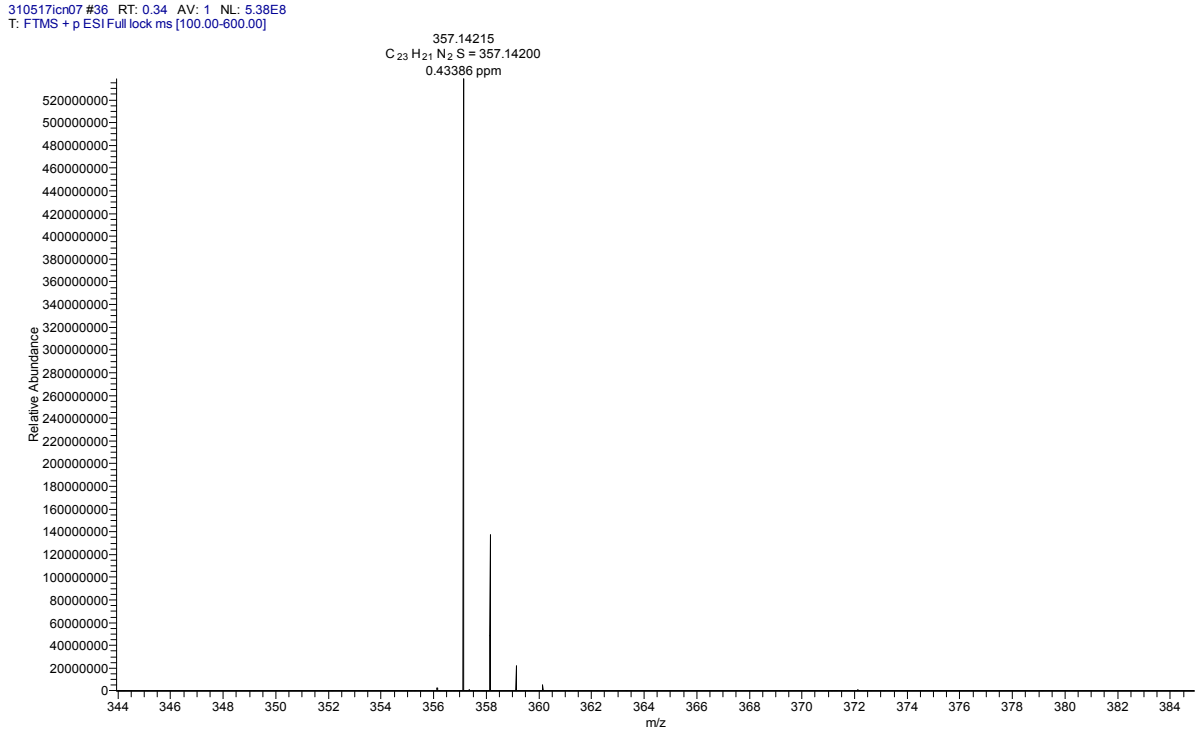
HRMS (ESI-MS) spectrum of dye **D9b**.



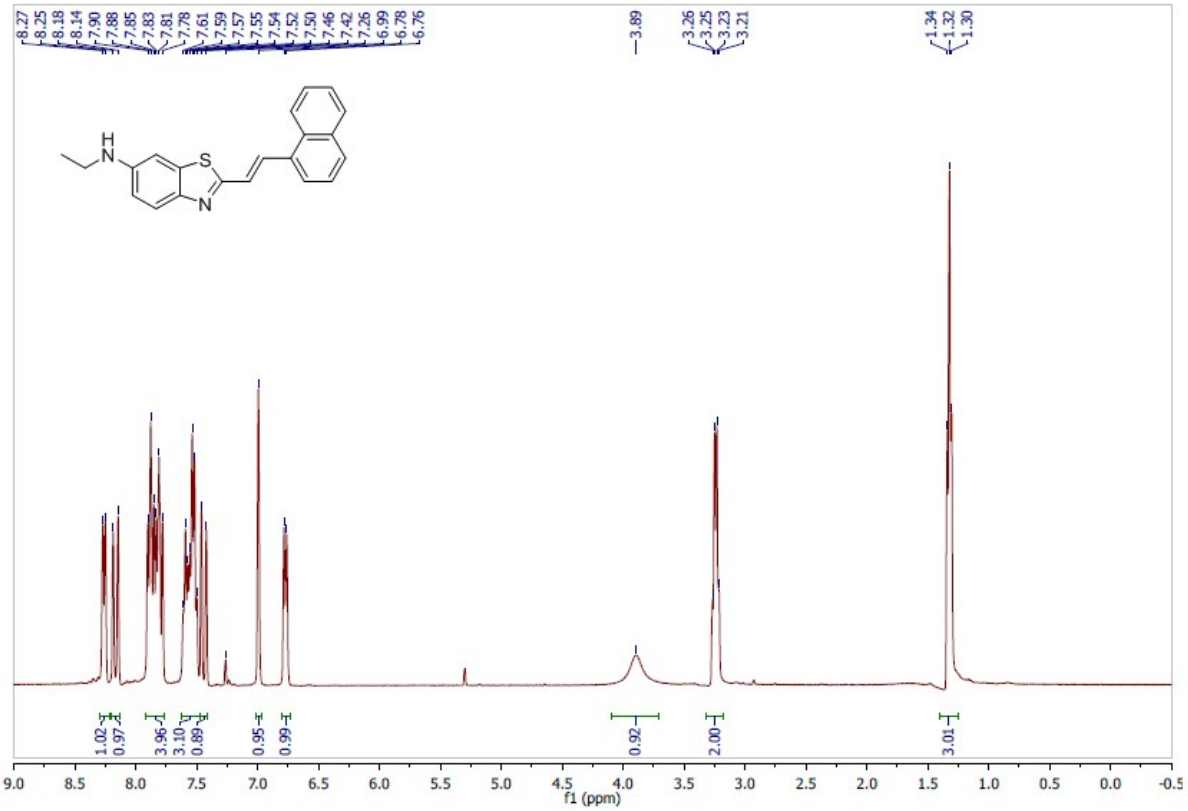
^{1}H NMR spectrum in $CDCl_3$ of compound **D10b**.



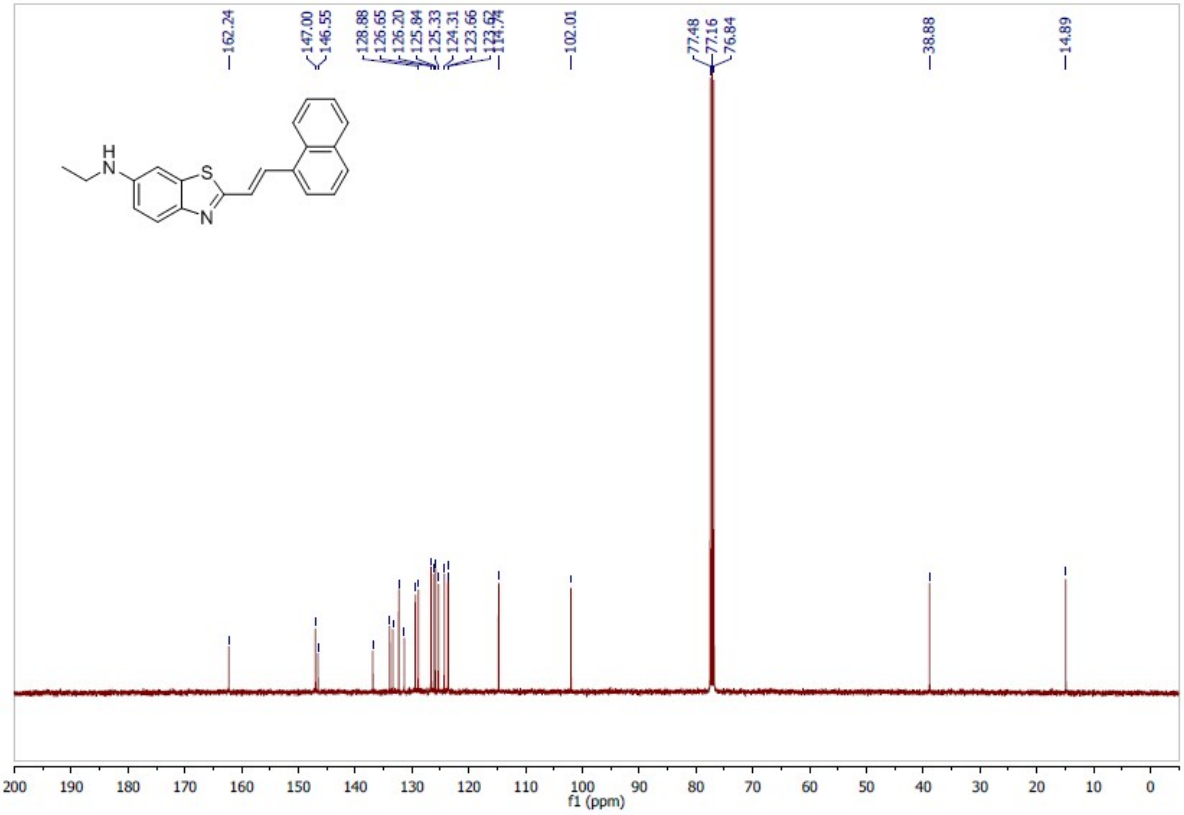
^{13}C NMR spectrum in $CDCl_3$ of compound **D10b**.



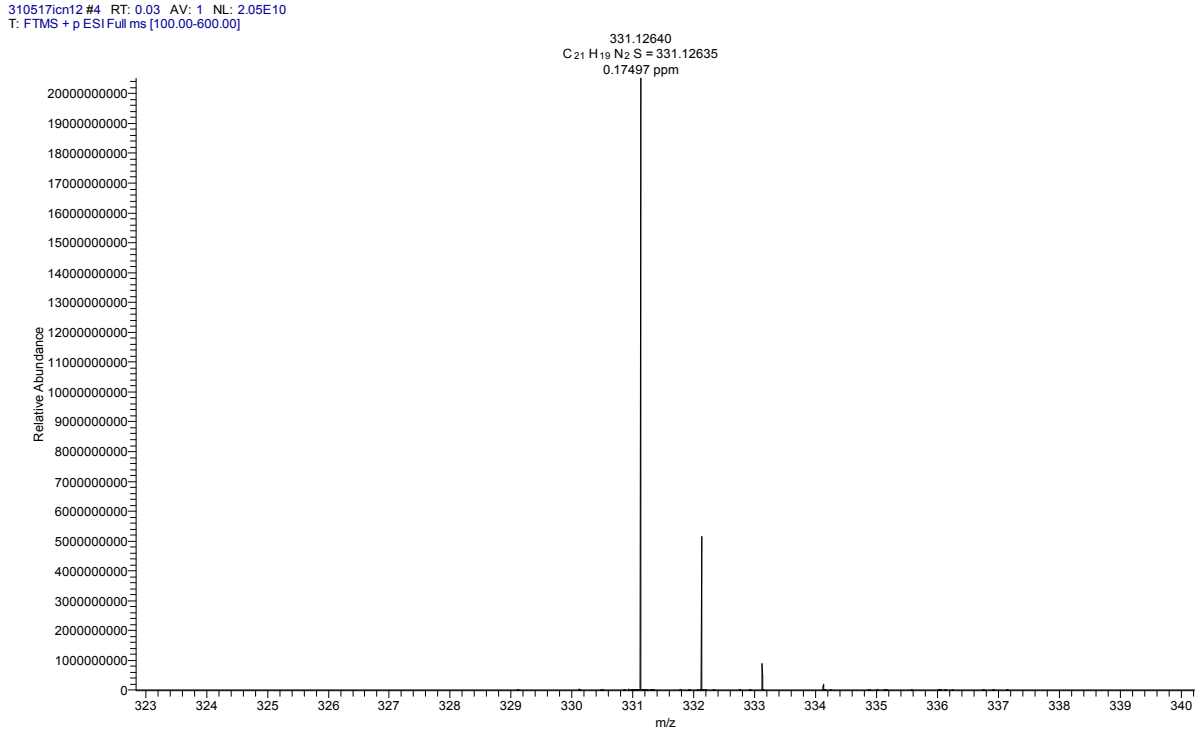
HRMS (ESI-MS) spectrum of dye **D10b**.



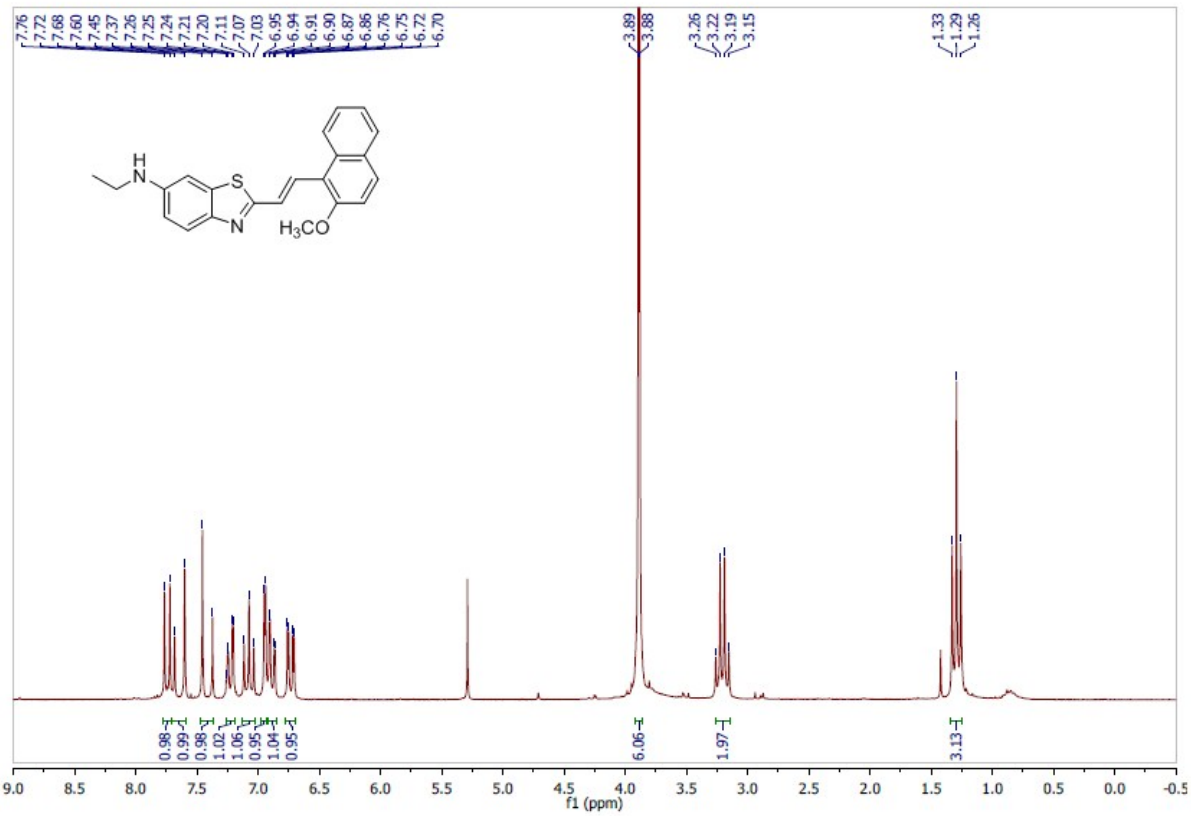
^{1}H NMR spectrum in $CDCl_3$ of compound **D11b**.



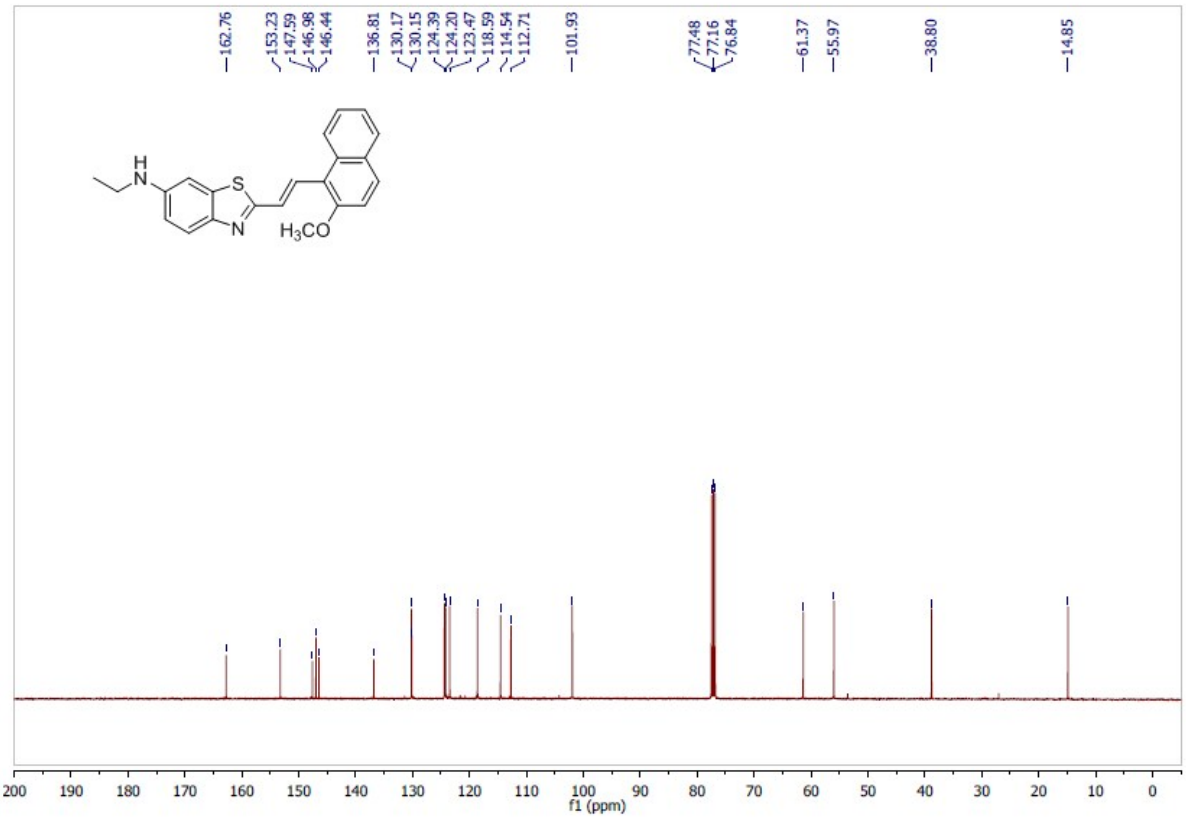
^{13}C NMR spectrum in $CDCl_3$ of compound **D11b**.



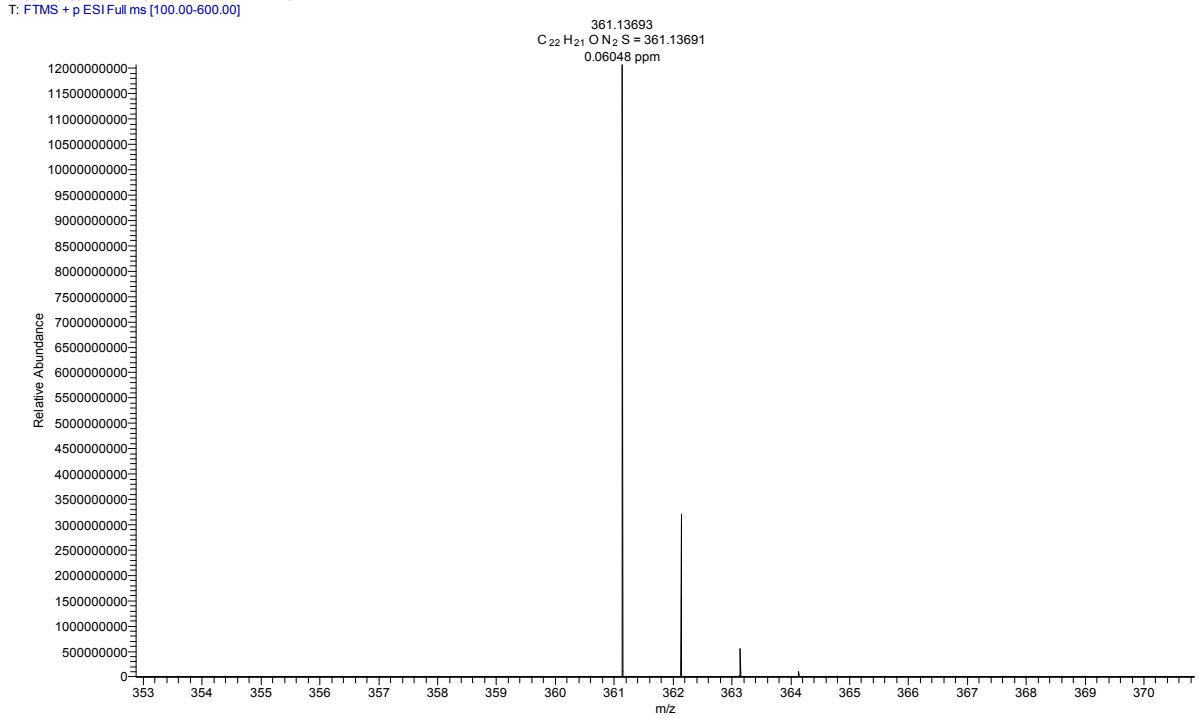
HRMS (ESI-MS) spectrum of dye **D11b**.



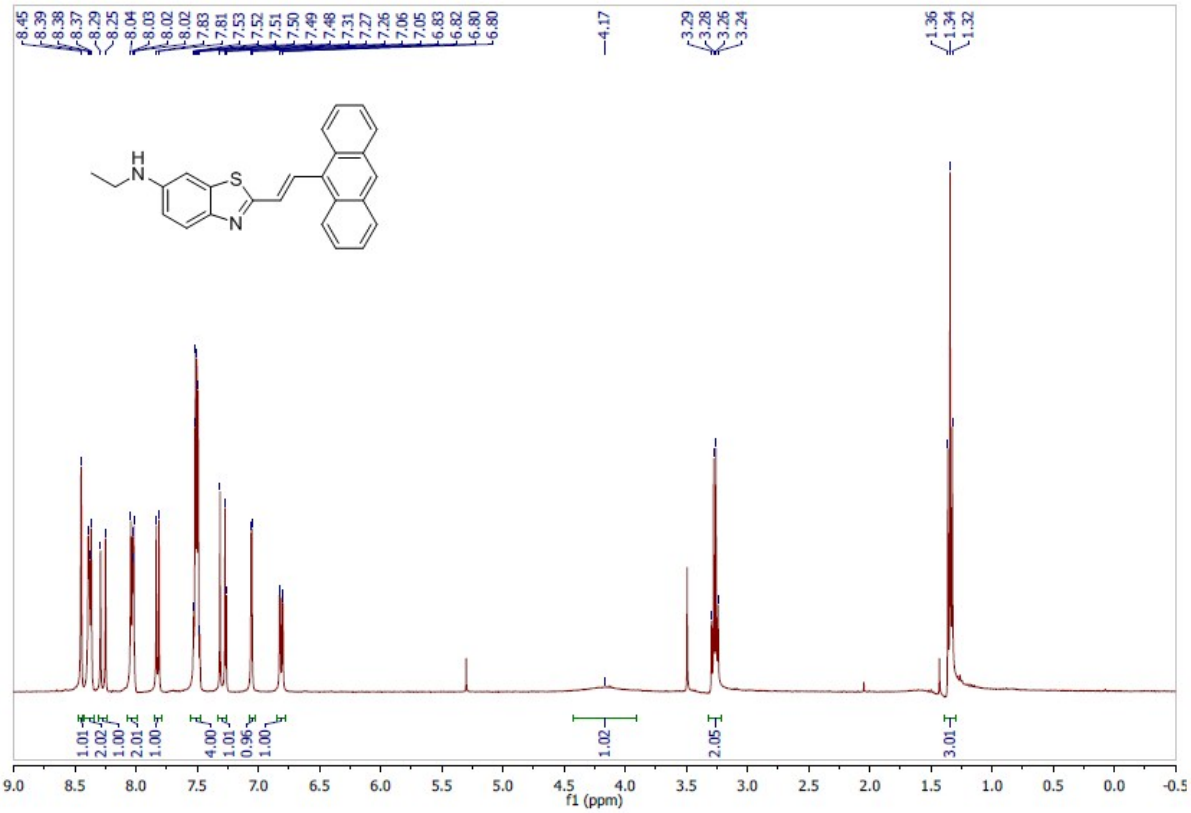
^{1}H NMR spectrum in $CDCl_3$ of compound **D12b**.



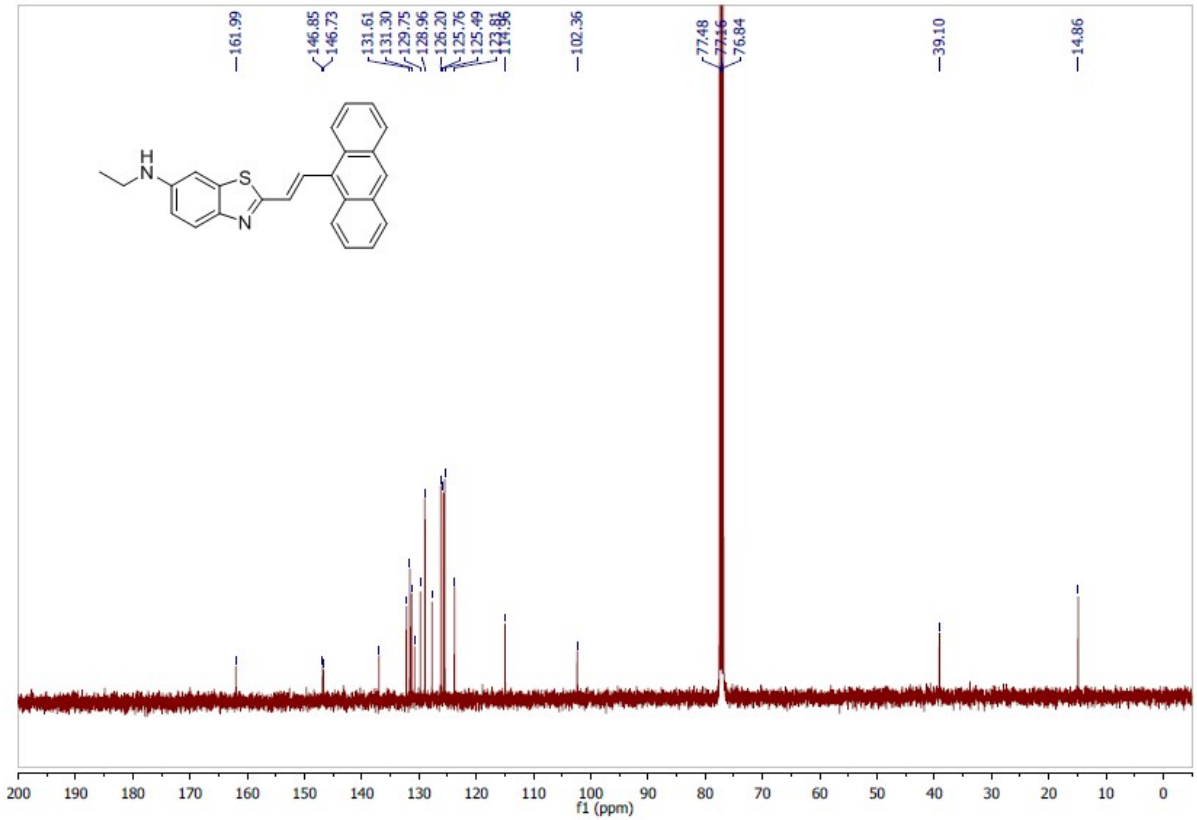
^{13}C NMR spectrum in $CDCl_3$ of compound **D12b**.



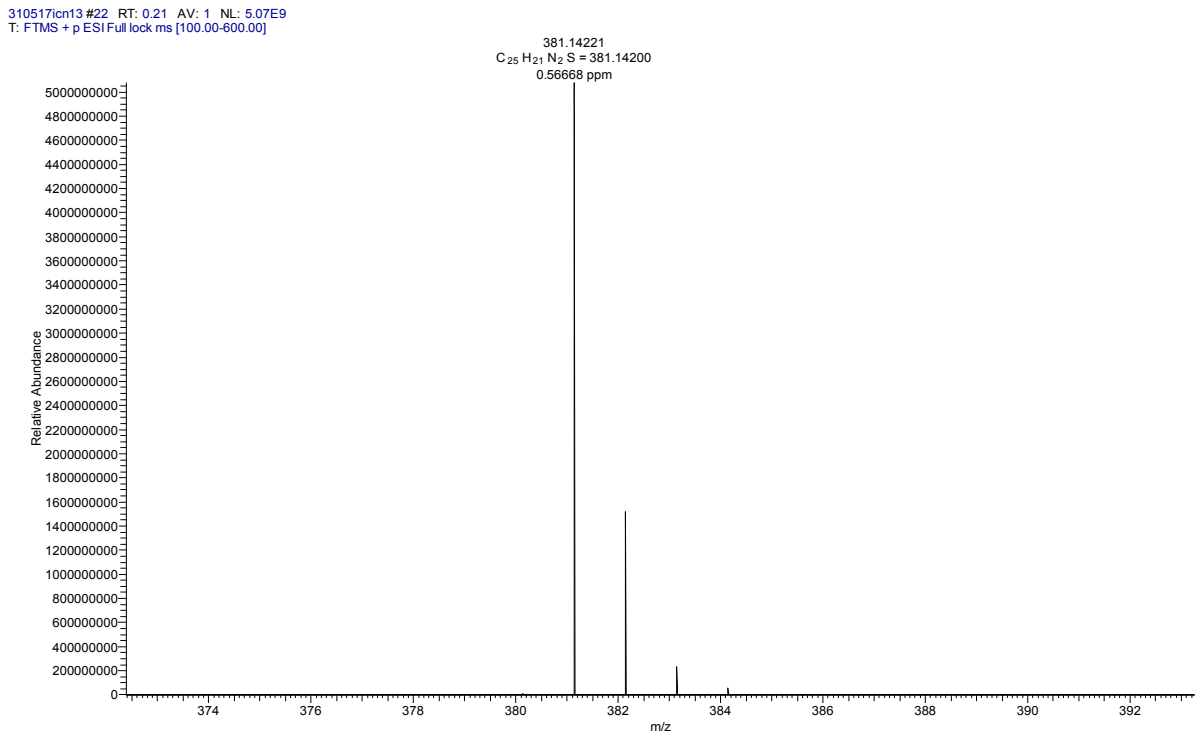
HRMS (ESI-MS) spectrum of dye **D12b**.



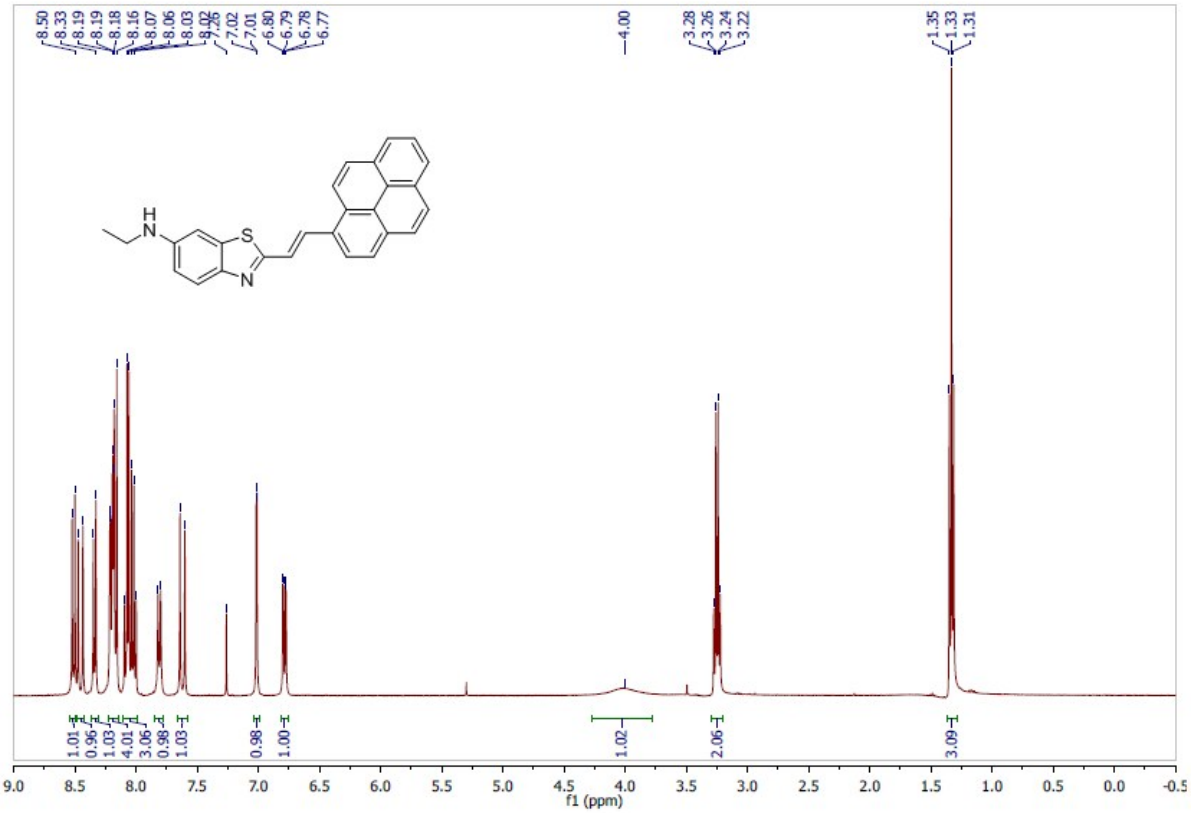
^{1}H NMR spectrum in $CDCl_3$ of compound **D13b**.



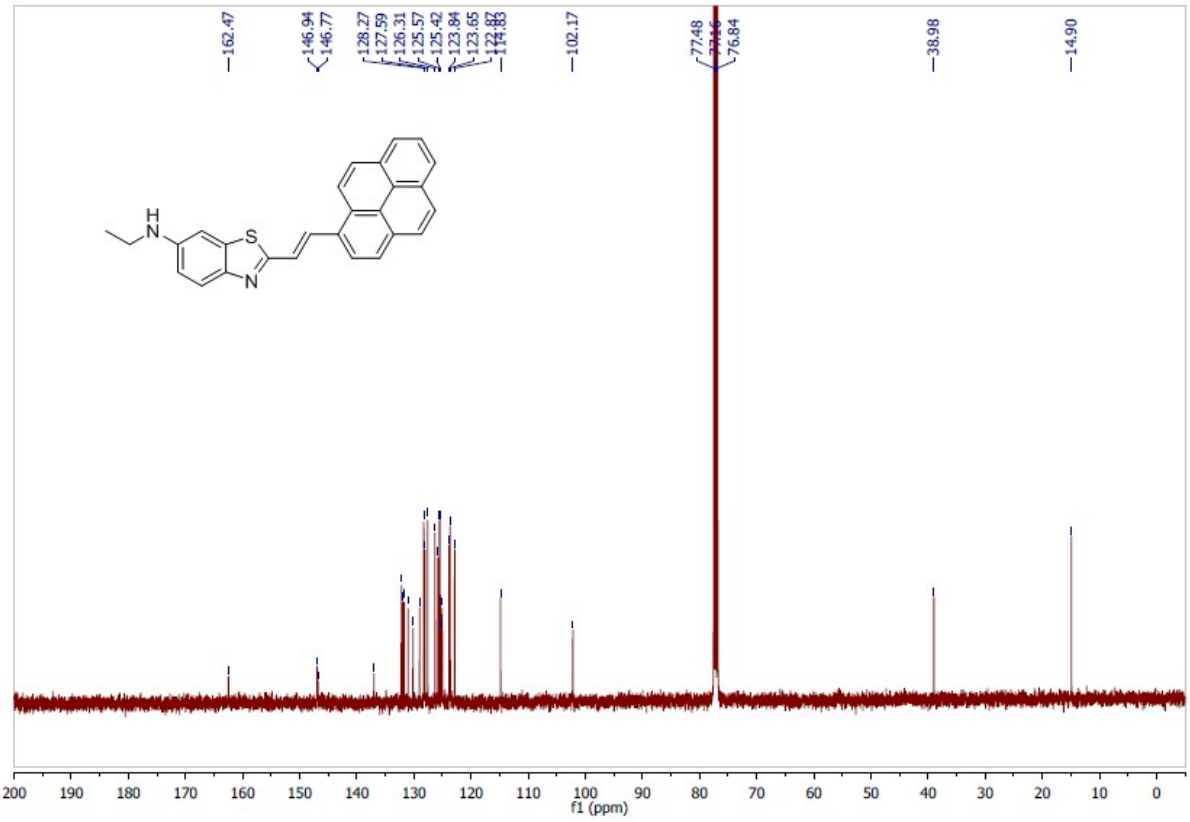
^{13}C NMR spectrum in $CDCl_3$ of compound **D13b**.



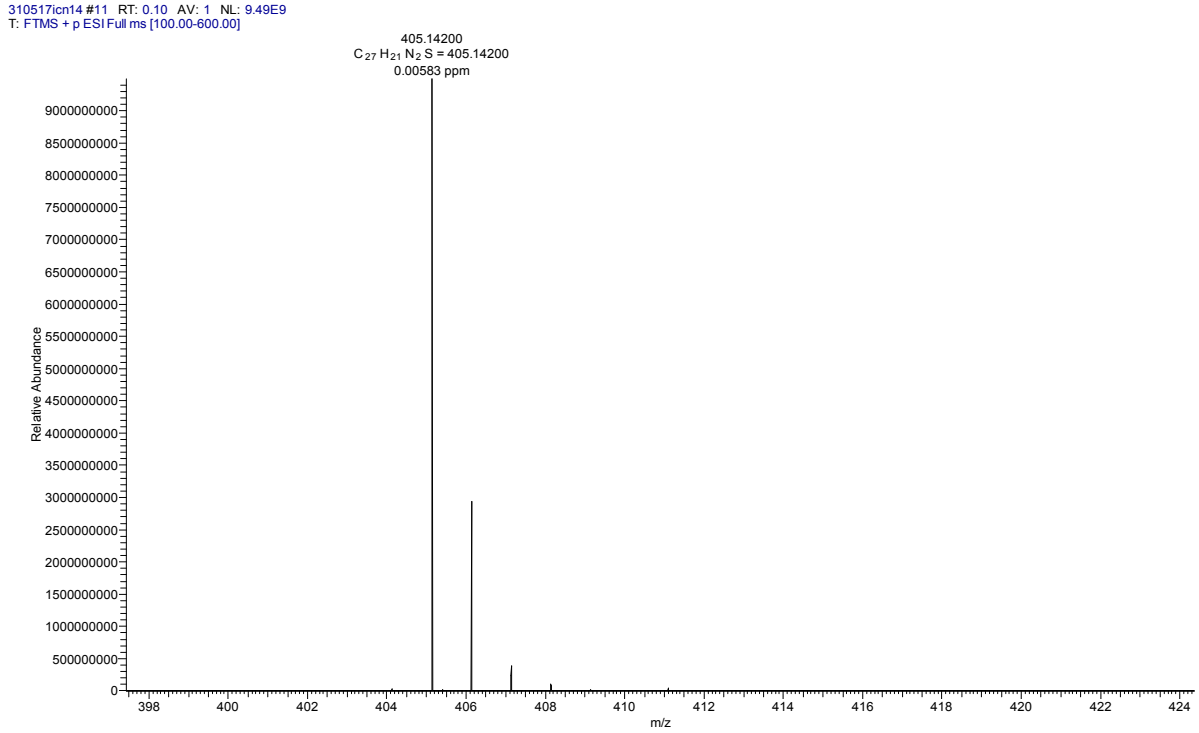
HRMS (ESI-MS) spectrum of dye **D13b**.



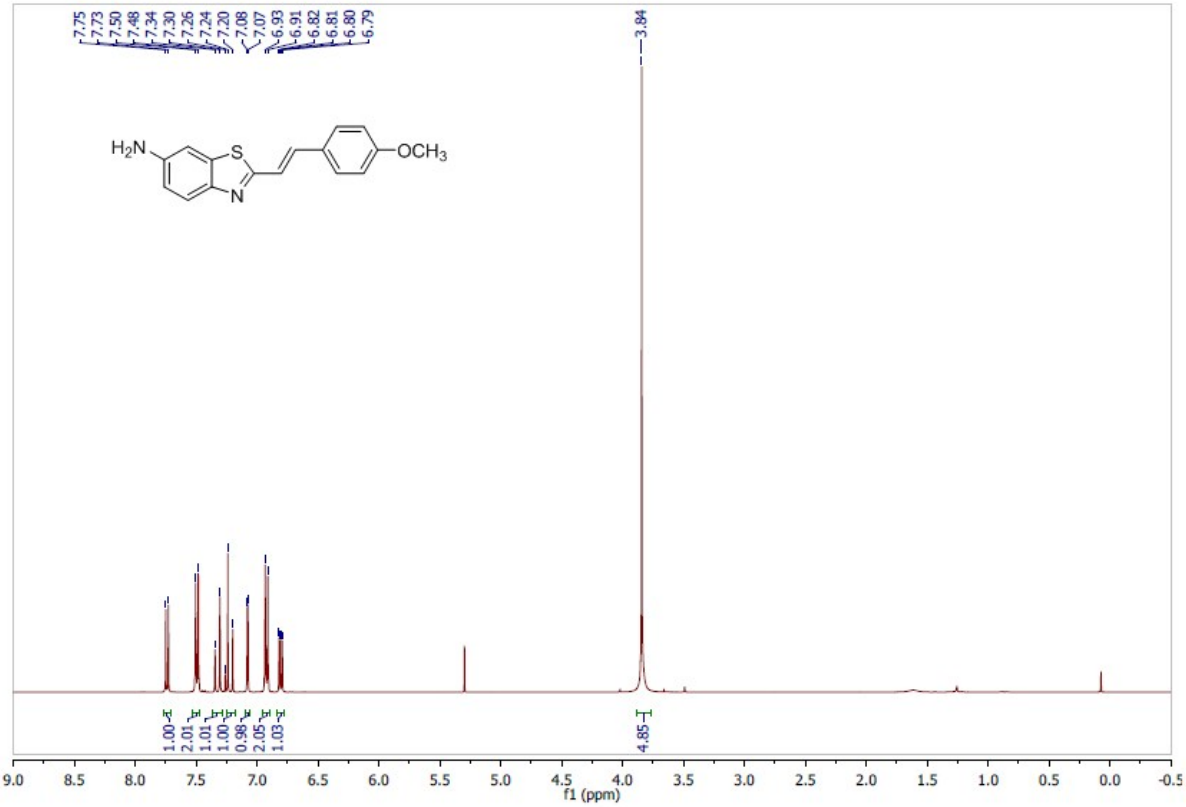
^{1}H NMR spectrum in $CDCl_3$ of compound **D14b**.



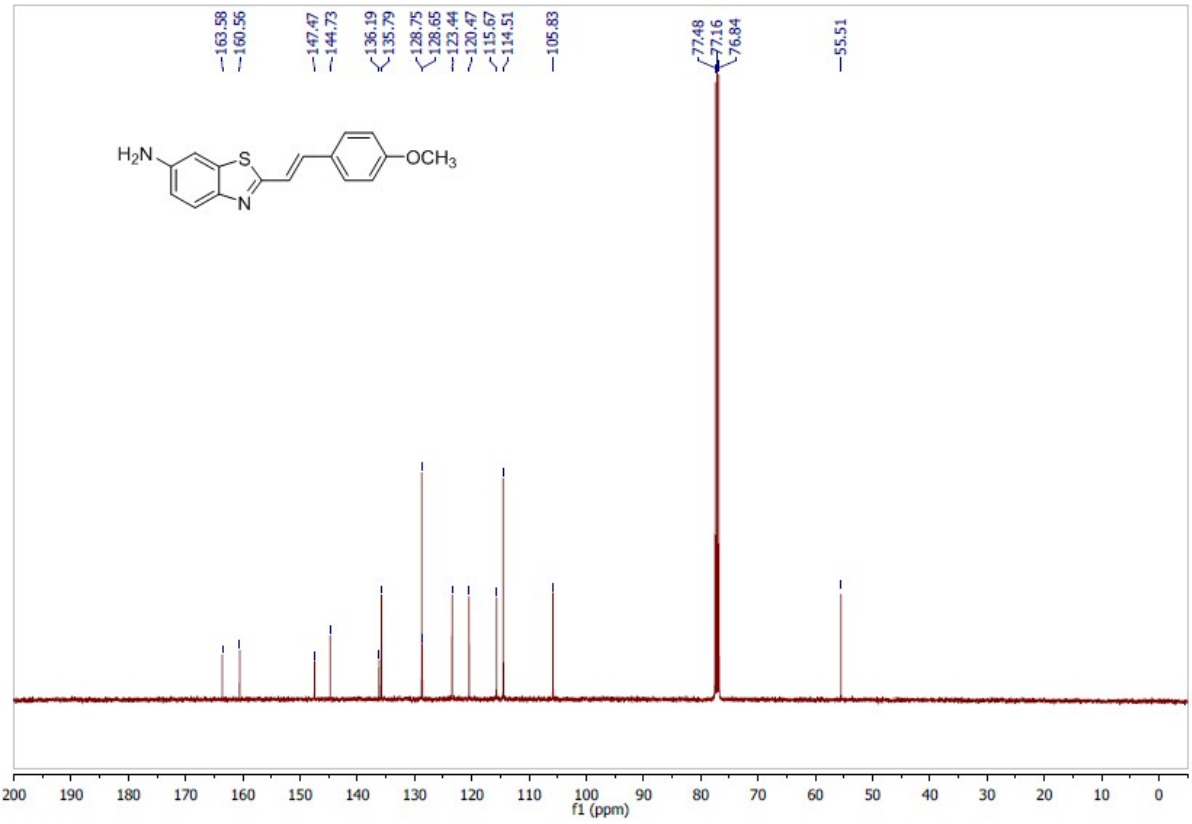
^{13}C NMR spectrum in $CDCl_3$ of compound **D14b**.



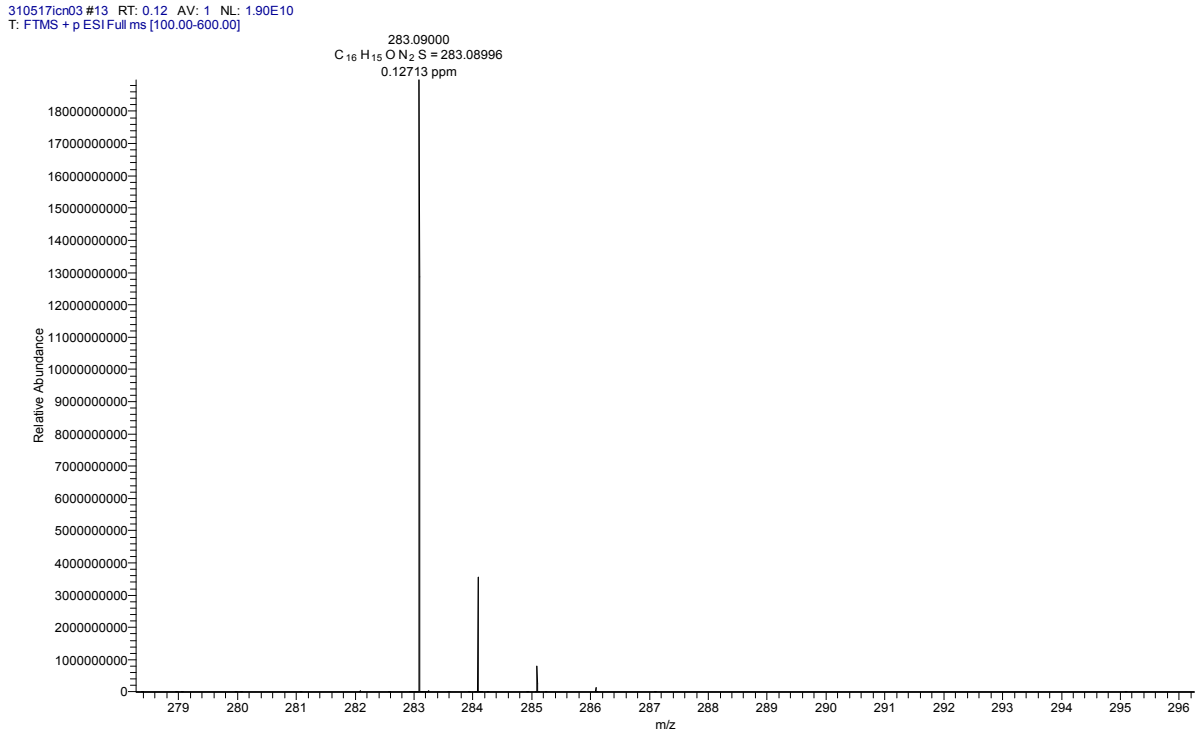
HRMS (ESI-MS) spectrum of dye **D14b**.



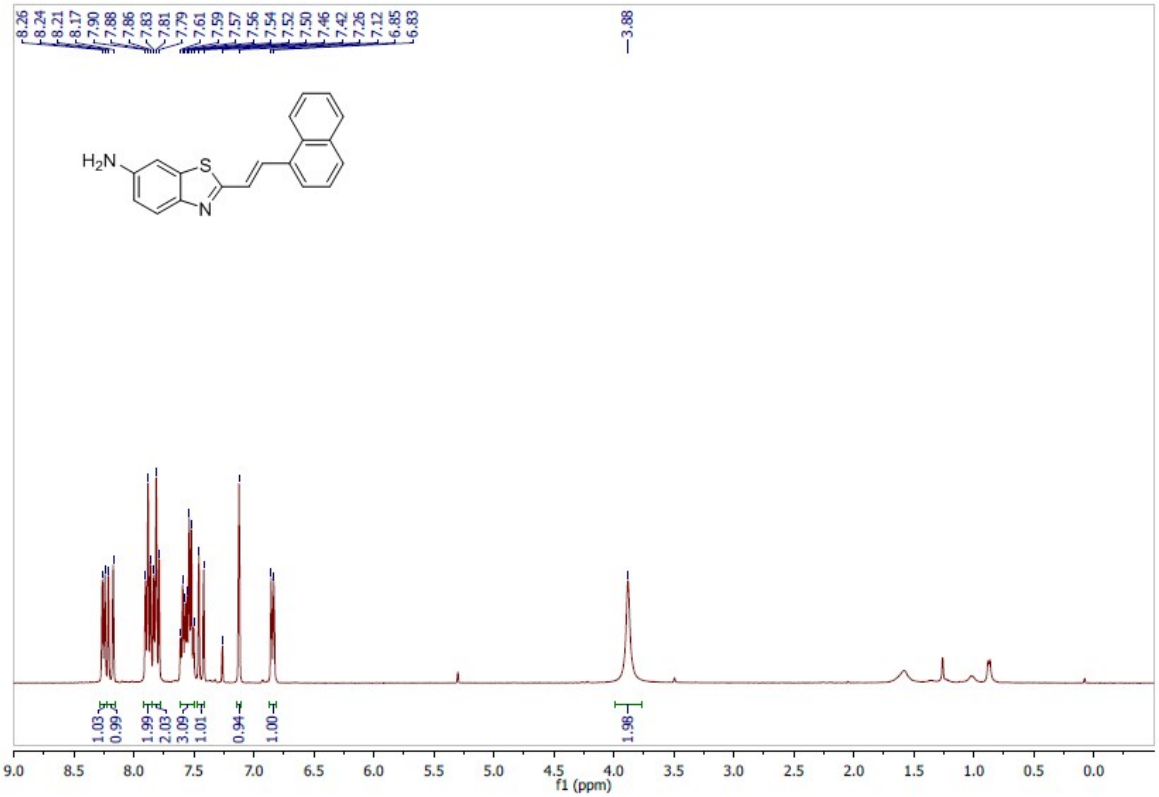
^{1}H NMR spectrum in $CDCl_3$ of compound **D2a**.



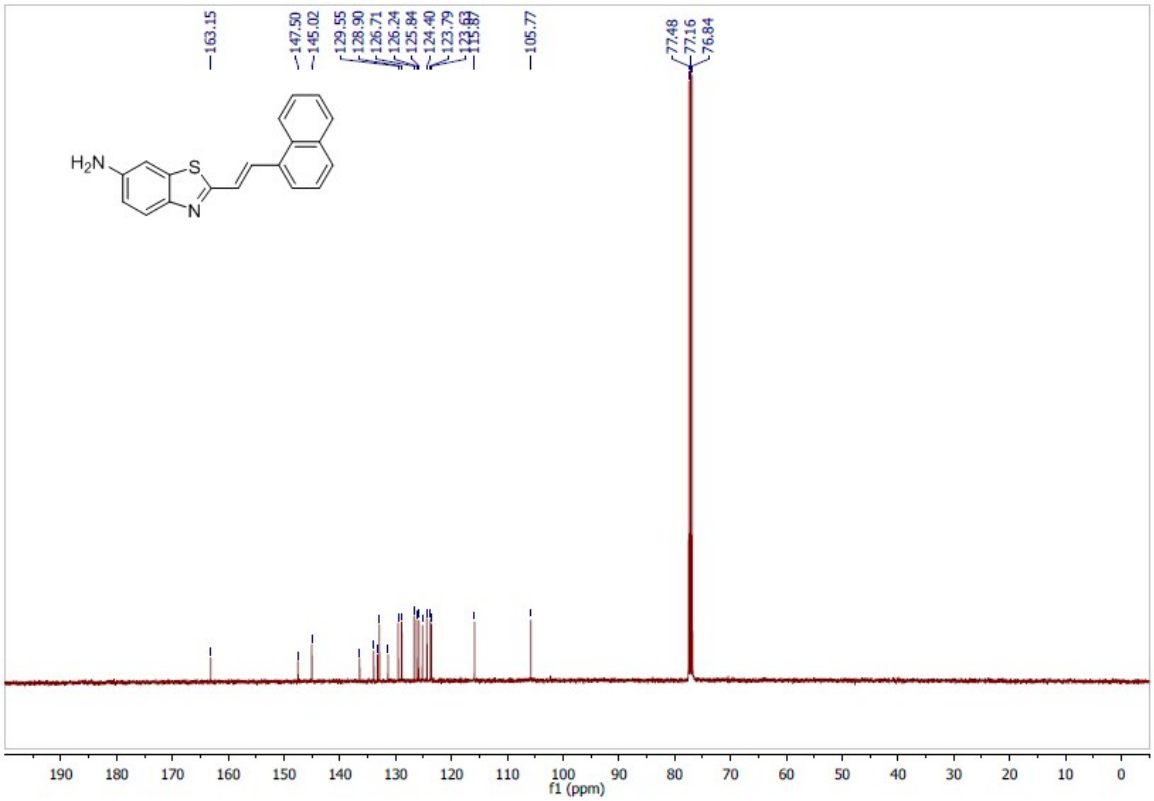
^{13}C NMR spectrum in $CDCl_3$ of compound **D2a**.



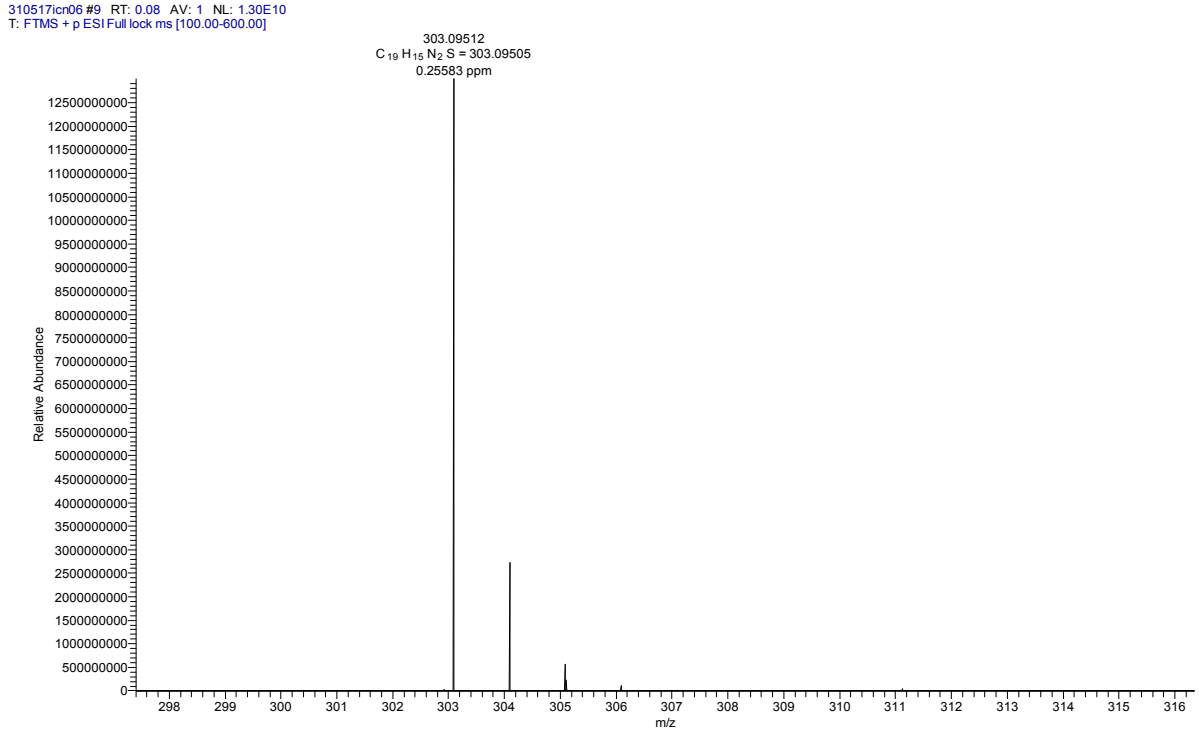
HRMS (ESI-MS) spectrum of dye **D2a**.



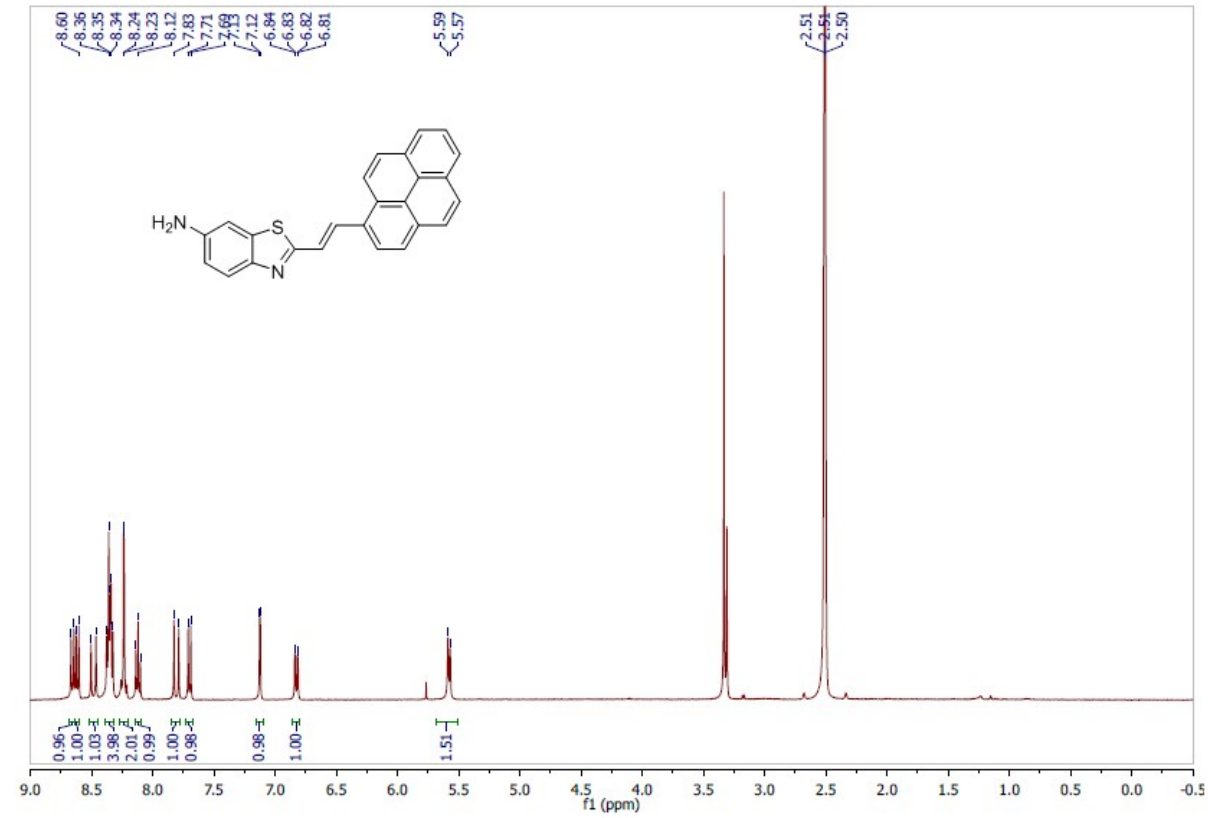
^{1}H NMR spectrum in $CDCl_3$ of compound **D11a**.



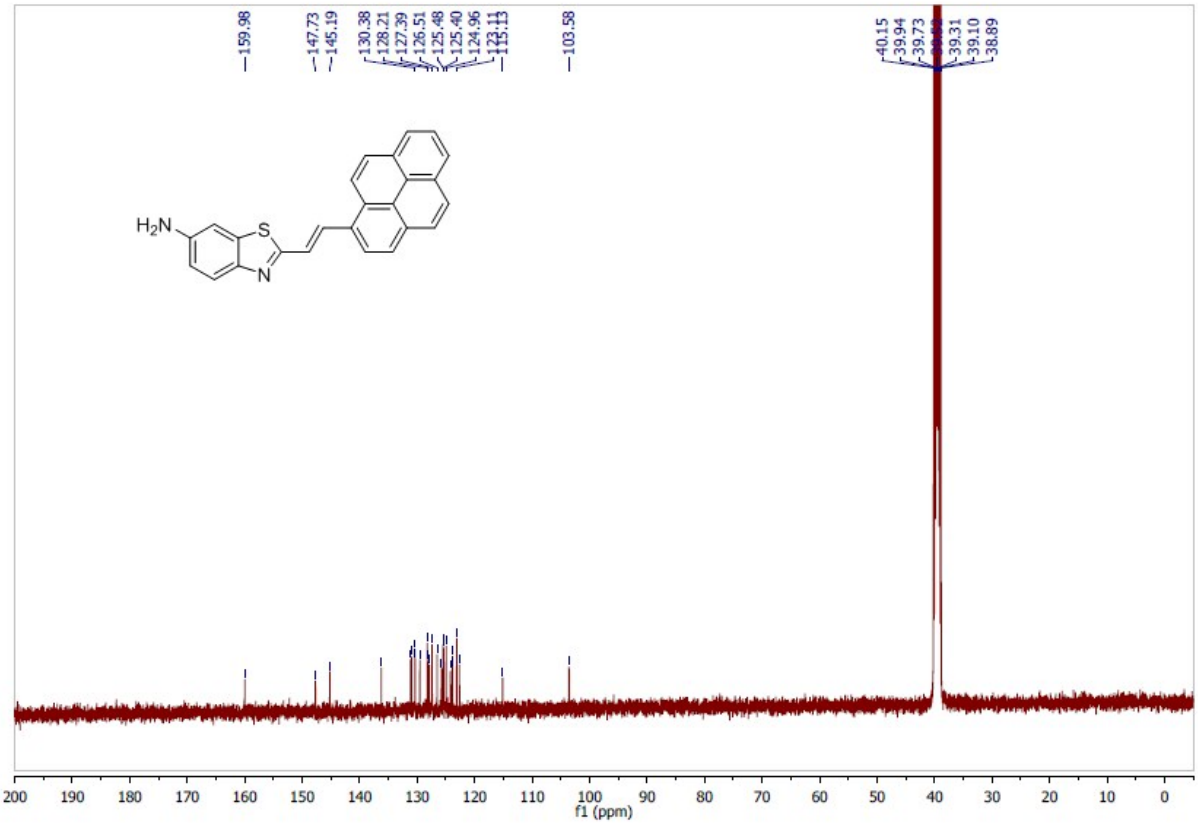
^{13}C NMR spectrum in $CDCl_3$ of compound **D11a**.



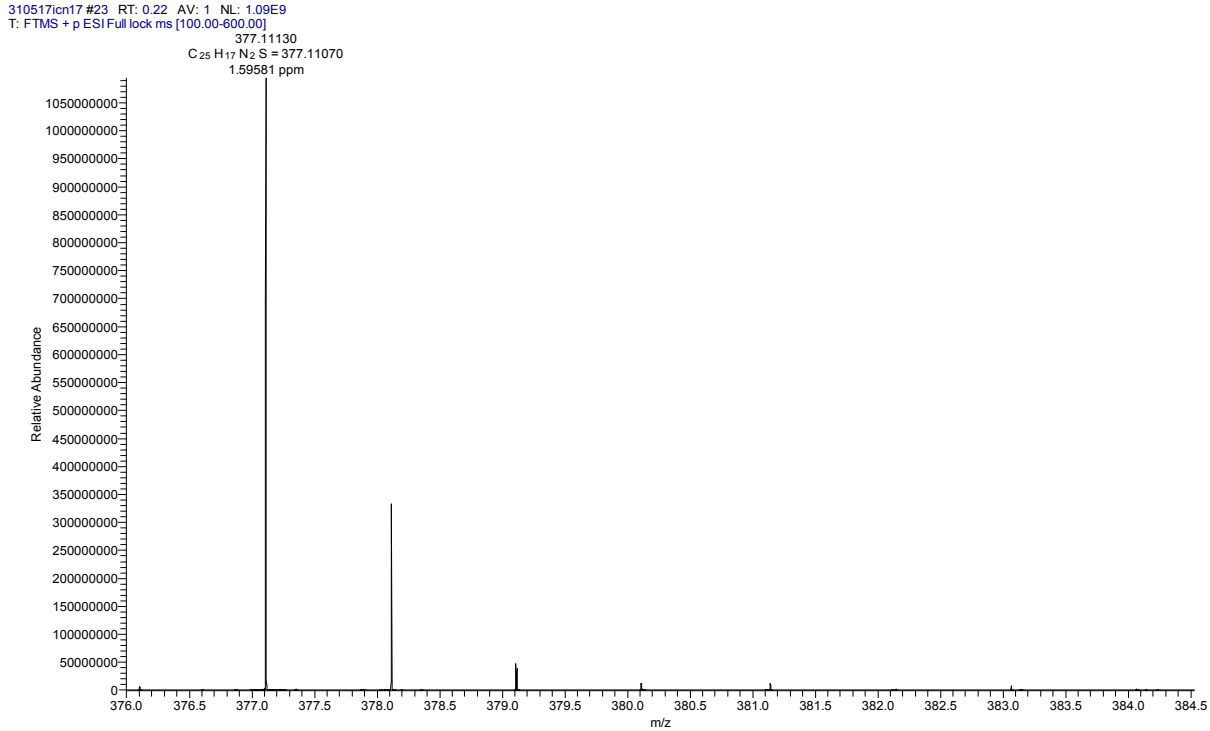
HRMS (ESI-MS) spectrum of dye **D11a**.



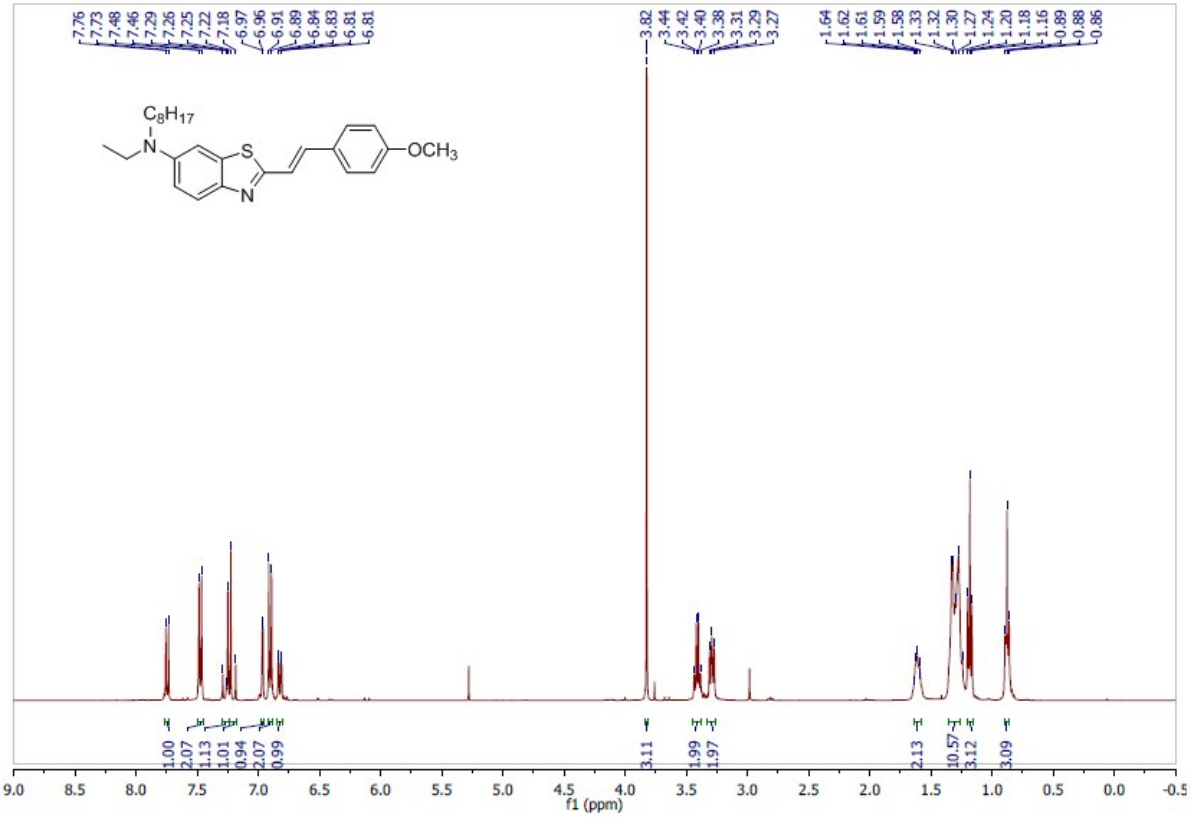
^{1}H NMR spectrum in DMSO-d_6 of compound **D14a**.



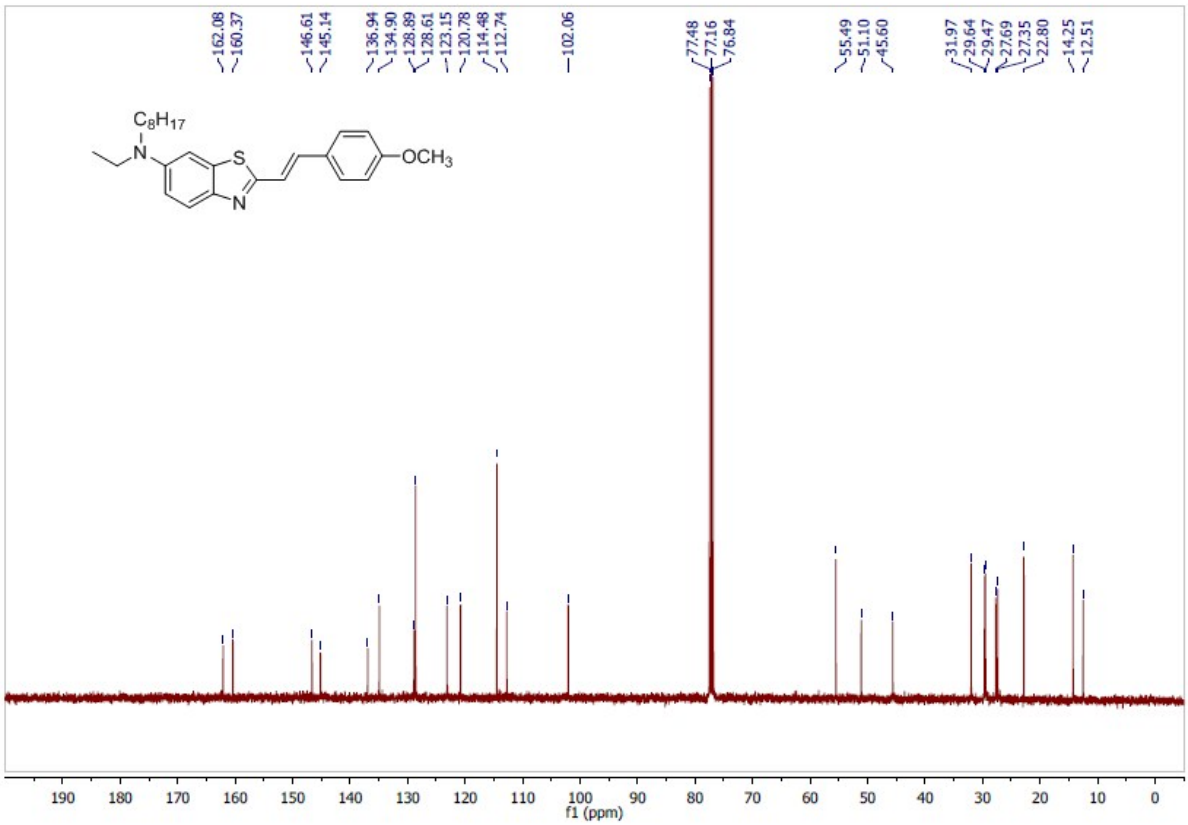
^{13}C NMR spectrum in DMSO-d_6 of compound **D14a**.



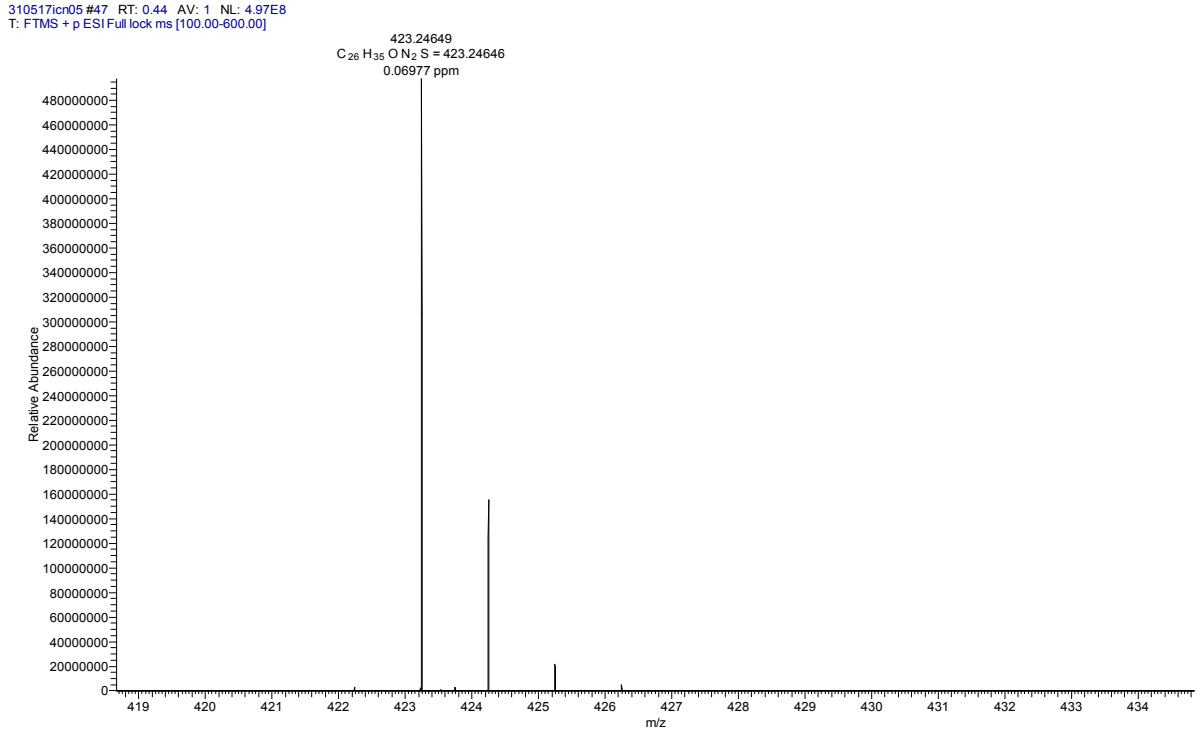
HRMS (ESI-MS) spectrum of dye **D14a**.



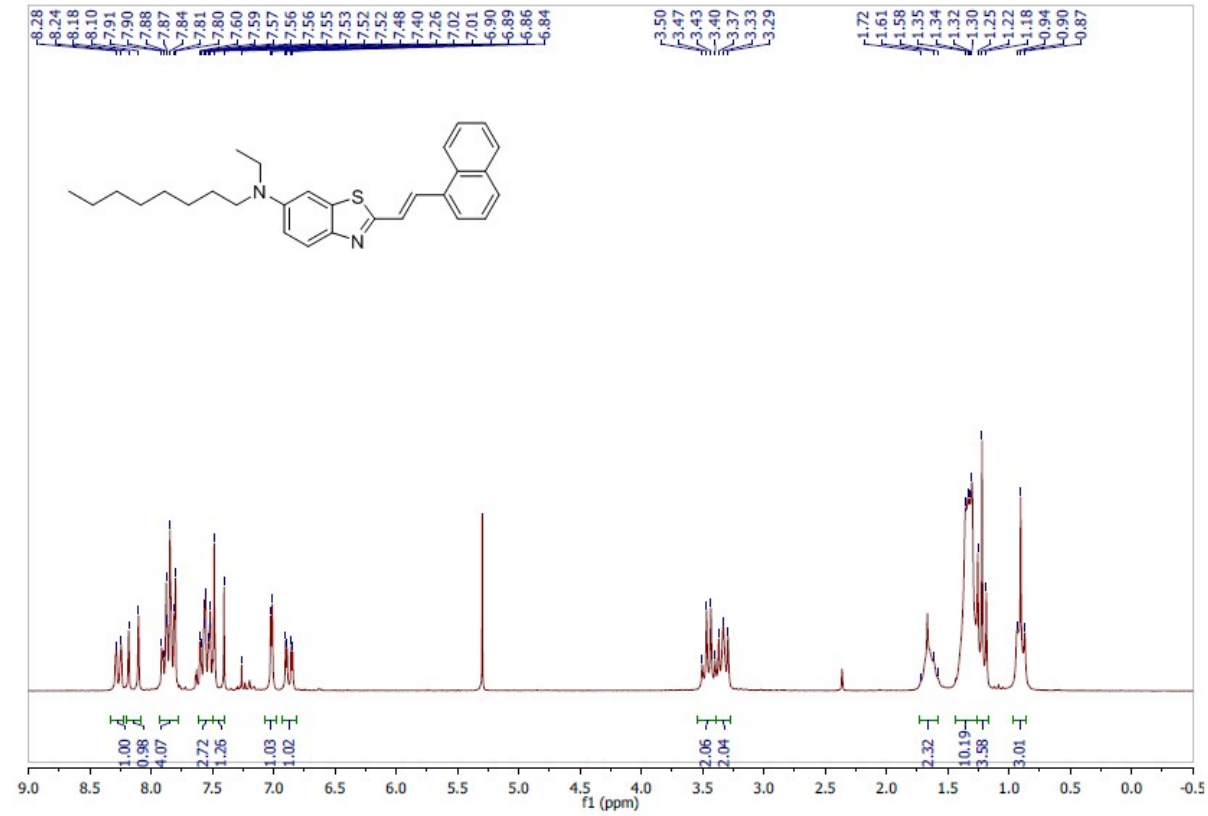
^{1}H NMR spectrum in $CDCl_3$ of compound **D2c**.



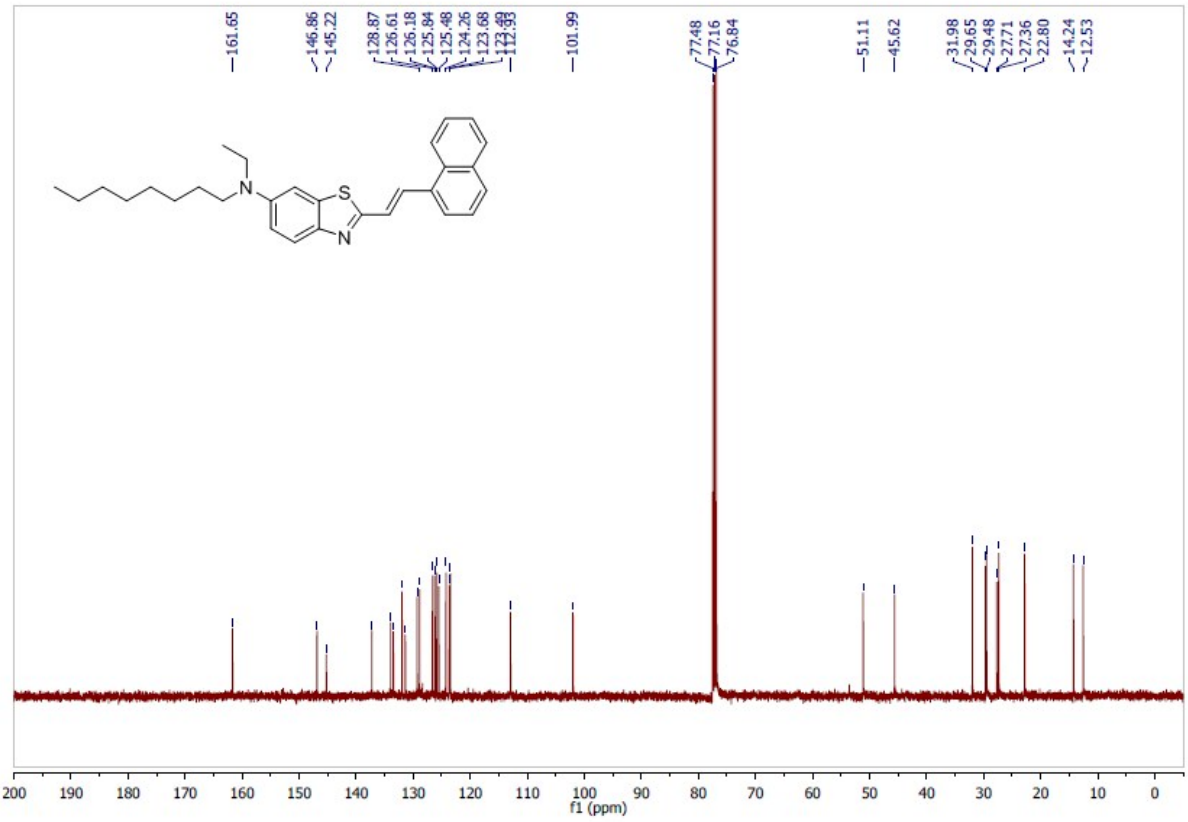
^{13}C NMR spectrum in $CDCl_3$ of compound **D2c**.



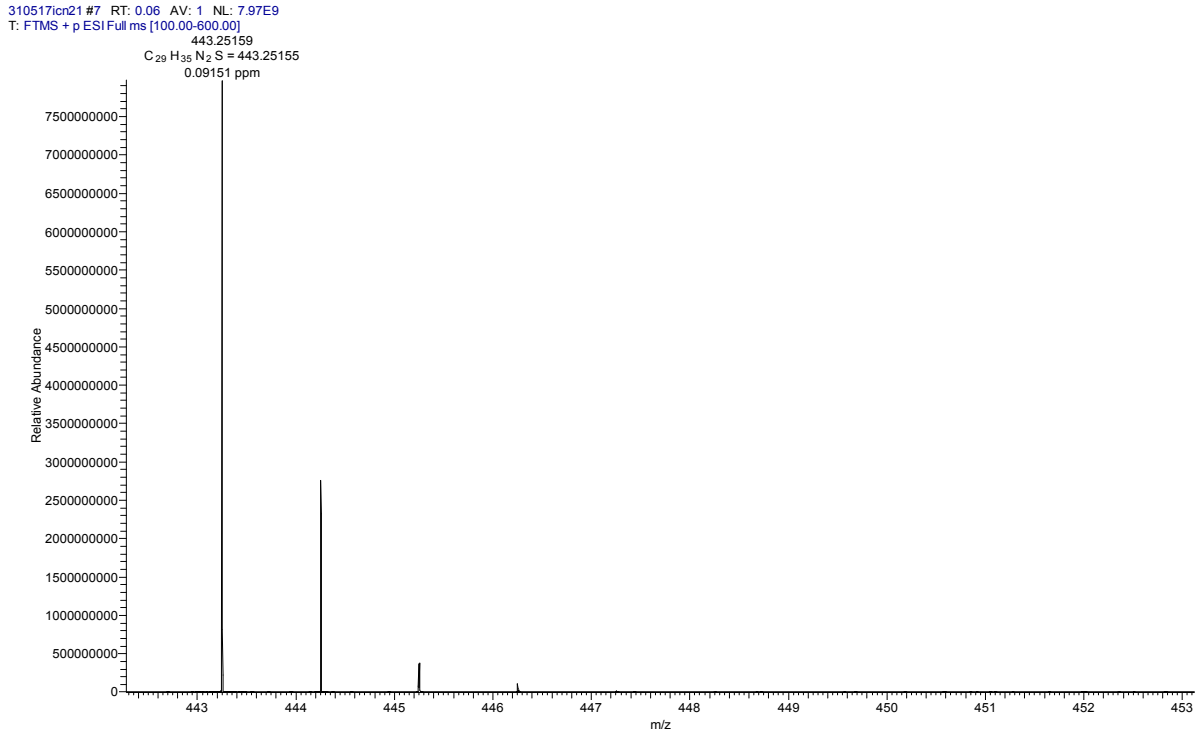
HRMS (ESI-MS) spectrum of dye **D2c**.



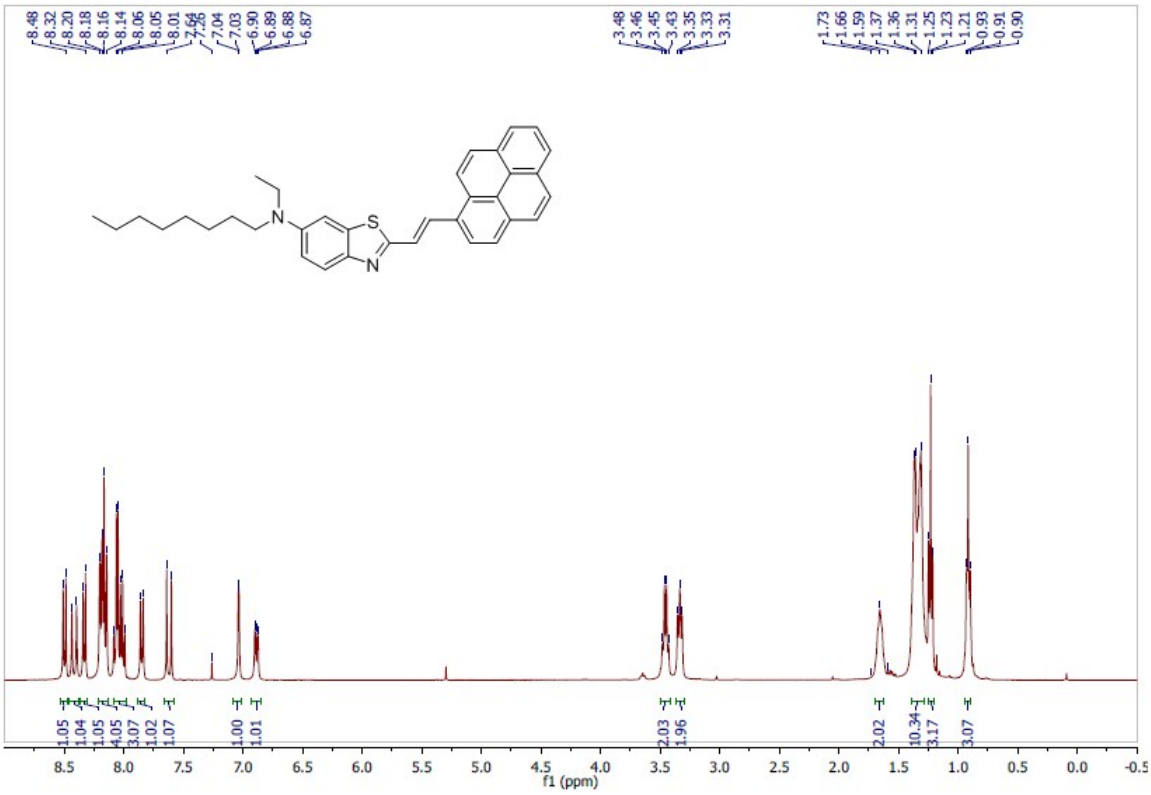
^{1}H NMR spectrum in $CDCl_3$ of compound **D11c**.



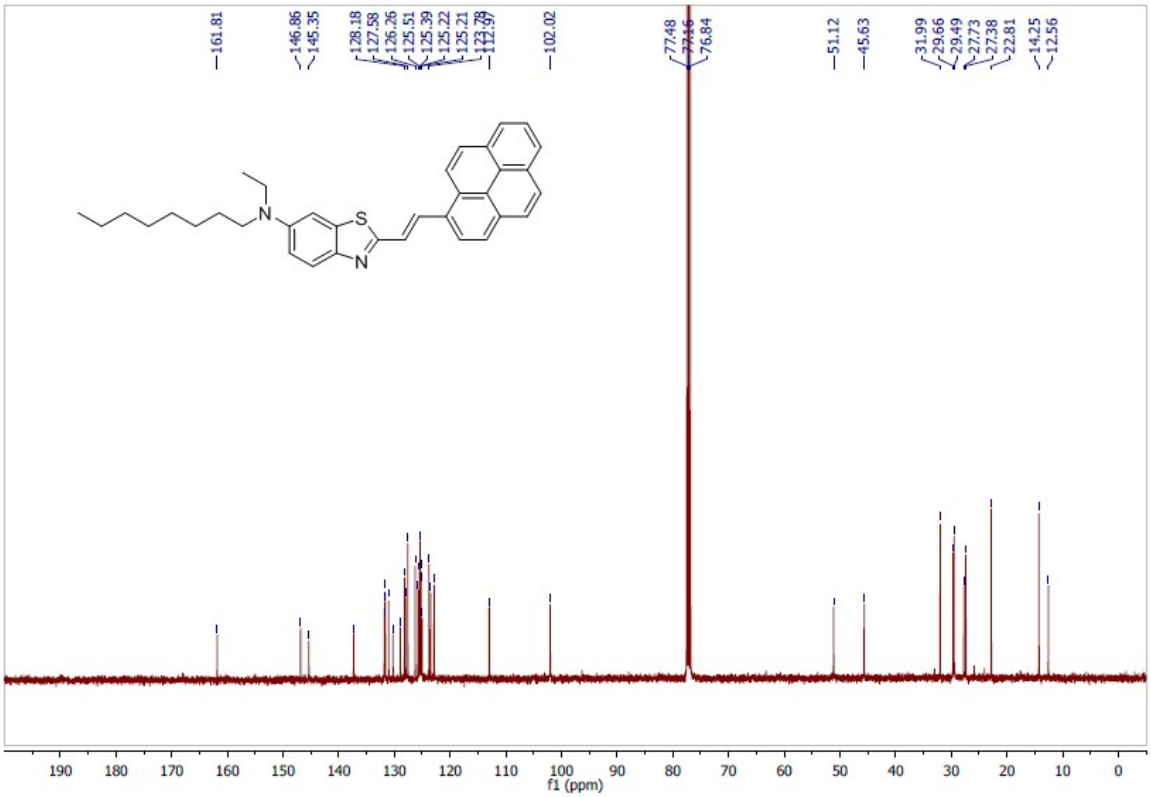
^{13}C NMR spectrum in $CDCl_3$ of compound **D11c**.



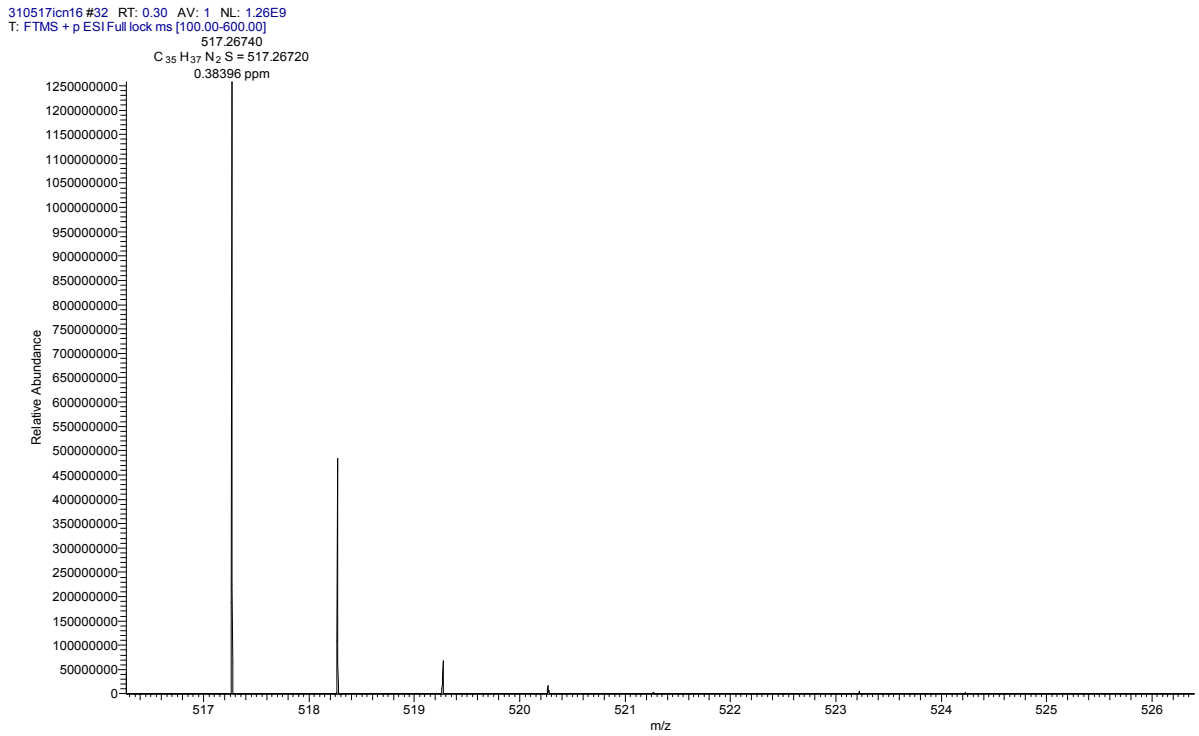
HRMS (ESI-MS) spectrum of dye **D11c**.



^{1}H NMR spectrum in $CDCl_3$ of compound **D14c**.



^{13}C NMR spectrum in $CDCl_3$ of compound **D14c**.



HRMS (ESI-MS) spectrum of dye **D14c**.