ESI for:

Highly Fluorescent Extended 2-(2'hydroxyphenyl)benzazole Dyes: Synthesis, Optical Properties and First-Principle Calculations

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S1 General information and equipments

All reactions were performed under a dry atmosphere of argon using standard Schlenck techniques. All chemicals were received from commercial sources (Aldrich, Alfa Aesar, Acros) and used without further purification. Dichloromethane were distilled over P_2O_5 under an argon atmosphere. Thin layer chromatography (TLC) was performed on silica gel coated with fluorescent indicator. Chromatographic purifications were conducted using 40-63 μm silica gel. All mixtures of solvents are given in v/v ratio.

^{1}H NMR (400.1 MHz) and ^{13}C NMR (100.5 MHz) spectra were recorded on a Bruker Advance 400 MHz spectrometer, ^{1}H NMR (300.1 MHz) and ^{13}C NMR (75.5 MHz) or a Bruker Advance 300 MHz spectrometer with perdeuterated solvents with residual protonated solvent signals as internal references.

Absorption spectra were recorded using a dual-beam grating Schimadzu UV-3000 absorption spectrometer with a 1 cm quartz cell. The steady-state fluorescence emission and excitation spectra were obtained by using a Horiba S2 Jobin Yvon Fluoromax 4. All fluorescence spectra were corrected. Solvents for spectroscopy were spectroscopic grade and were used as received. All fluorescence spectra were corrected.

The fluorescence quantum yield (Φ_{exp}) was calculated from eq (1).

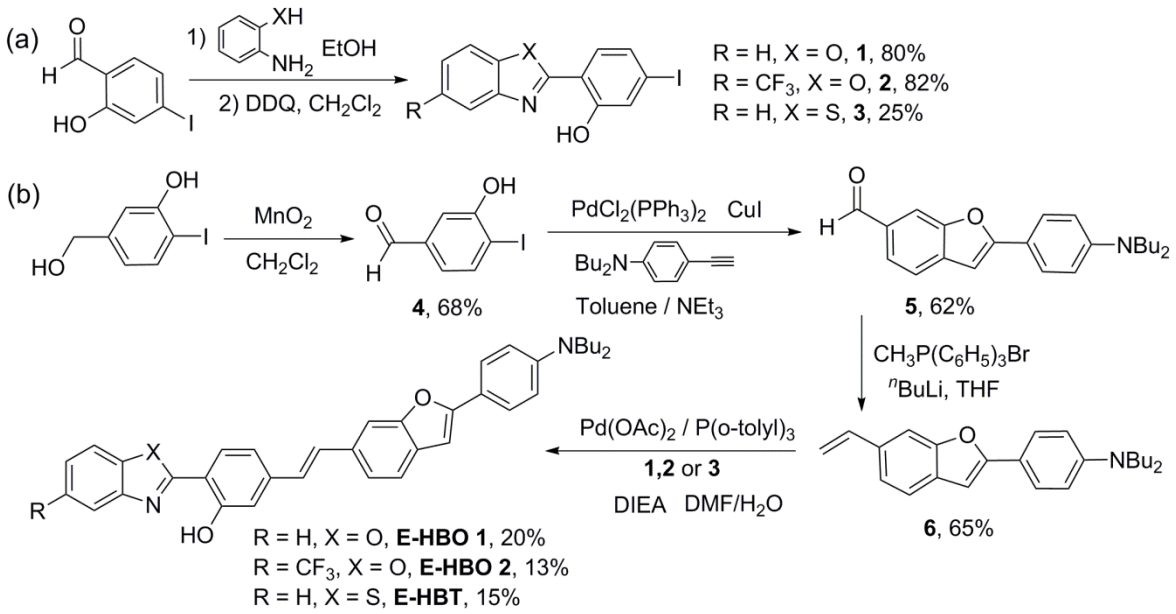
$$\Phi_{exp} = \Phi_{ref} \frac{I}{I_{ref}} \frac{OD_{ref}}{OD} \frac{\eta^2}{\eta^2_{ref}} \quad (eq\ 1)$$

I denotes the integral of the corrected emission spectrum, OD is the optical density at the excitation wavelength, and η is the refractive index of the medium. The reference systems used were: Quinine Φ= 55% in H_2SO_4 1N, λ_{exc} = 366 nm for dyes emitting below 480 nm, Rhodamine 6G, Φ= 88% in ethanol λ_{exc} = 488 nm for dyes emitting between 480 and 570 nm and cresyl violet, Φ= 55% λ_{exc} = 546 nm in ethanol for dyes emitting above 570 nm.

Luminescence lifetimes were measured on an Edinburgh Instruments spectrofluorimeter equipped with a R928 photomultiplier and a PicoQuant PDL 800-D pulsed diode connected to a GwInstect GFG- 8015G delay generator. No filter was used for the excitation. Emission wavelengths were selected by a monochromator. Lifetimes were deconvoluted with FS-900 software using a light-scattering solution (LUDOX) for instrument response. The excitation source was a laser diode (λ_{exc} = 320 nm).

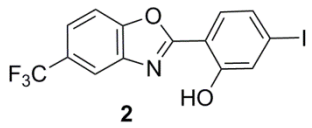
2-hydroxy-5-iodobenzaldehyde[1], p-(dibutylamino)phenyl acetylene[2] and HBO **1**[3] were synthesized according to reported procedures.

S2 Synthetic protocols



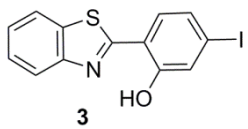
Scheme S1. Synthesis of **E-HBT**, **E-HBO 1** and **E-HBO 2**

General procedure for HBO and HBT 1-3:
A mixture of 2-hydroxy-5-iodobenzaldehyde and aminophenol (1 eqt) were refluxed in EtOH for 3 hours. An orange/red precipitate rapidly appeared that was filtered and further washed with EtOH before being redissolved in distilled CH_2Cl_2. 2,6-dichloro-3,5-dicyano-1,4-benzoquinone (DDQ) (1.2 eqt) was then added by portions and the resulting mixture stirred overnight at room temperature. The solvents were removed *in vacuo* and the crude mixture purified by column chromatography on SiO_2 (CH_2Cl_2/ Ether. Pet. 1:2) to avoid **1-3** as white powders.



2

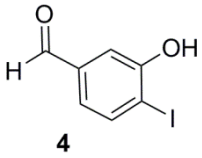
82%. ^{1}H NMR (400MHz, $CDCl_3$) δ (ppm): 11.14 (s, 1H, OH), 7.98 (s, 1H, CH Ar), 7.63-7.67 (m, 3H, CH Ar), 7.50 (s, 1H, CH Ar), 7.34 (dd, 1H, ^3J=10.8 Hz, ^4J=2.4 Hz, CH Ar). ^{13}C NMR (100.5Hz, $CDCl_3$) δ (ppm): 164.0, 158.8, 150.7, 140.0, 129.1, 127.9, 127.0, 122.9, 122.9, 117.0, 117.0, 111.2, 109.4, 100.8. ESI-HRMS: calcd for $C_{14}H_8F_3INO_2$ 405.9546 (M+H), found 405.9593 (M+H).



3

25%.^{1}H NMR (400MHz, $CDCl_3$) δ (ppm): 12.61 (s, 1H, OH), 7.98 (d, 1H, J=8.4Hz, CH Ar), 7.89 (d, 1H, J=8 Hz, CH Ar), 7.49-7.53 (m, 2H, CH Ar), 7.27-7.44 (m, 3H, CH Ar). ^{13}C NMR (75.5Hz, $CDCl_3$) δ (ppm): 168.6, 158.1, 151.7, 134.1, 132.4, 129.1, 128.7, 127.2, 126.9, 125.8, 122.2, 121.6, 116.4, 98.6. ESI-HRMS: calcd for $C_{13}H_9INOS$ 353.9444 (M+H), found 353.9410 (M+H).

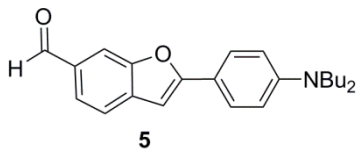
Compound 4[4]



4

5-(hydroxymethyl)-2-iodophénol (1 eqt) and MnO_2 (15 eqts) were stirred in CH_2Cl_2 at room temperature for three hours. The medium was then filtered on a pad of celite and washed several times with CH_2Cl_2. The filtrate is then evaporated *in vacuo* to lead to compound **4**[4]as a white powder (68% yield). ^{1}H NMR (400MHz, $CDCl_3$) δ (ppm): 9.92 (s, 1H, CHO), 7.87 (d, 1H, *J* = 8Hz, CH Ar), 7.44 (d, 1H, ^4J = 2Hz, CH Ar), 7.18 (dd, 1H, ^3J = 4Hz, ^4J = 2Hz, CH Ar), 5.79 (s, 1H, OH). ^{13}C NMR (75.5Hz, $CDCl_3$) δ (ppm): 191.3, 155.7, 139.3, 138.4, 123.0, 114.9, 93.7. ESI-HRMS: calcd for $C_7H_6IO_2$ 248.9407(M+H), found 248.9436 (M+H).

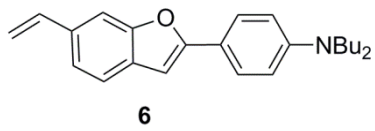
Compound 5



5

To a solution of compound **4** in toluene was added p-(dibutylamino)phenyl acetylene[2] (1.2 eqt), $PdCl_2(PPh_3)_2$ (5% mol.) and triethylamine (10 eqts). The resulting suspension was degassed with argon for 30 minutes before CuI (10% mol.) were added. The medium was stirred overnight at room temperature. After cooling down, the dark solution was taken up in dichloromethane, washed with water, dried ($MgSO_4$) and the solvents evaporated *in vacuo*. The crude residue was purified by silica gel chromatography eluting with CH_2Cl_2/Pet.Ether 1:1 leading to compound **5** as a beige oil (62% yield). ^{1}H NMR (400MHz, $CDCl_3$) δ (ppm): 10.00 (s, 1H, CHO), 7.93 (s, 1H, CH Ar), 7.70-7.72 (m, 3H, CH Ar), 7.55 (d, 1H, *J*=8 Hz, CH Ar), 6.77 (s, 1H, CH benzofuran), 6.68 (d, 2H, *J*=9.2Hz, CH Ar), 3.32 (t, 4H, *J*=8Hz, CH_2), 1.56-1.64 (m, 4H, CH_2), 1.33-1.43 (m, 4H, CH_2), 0.98 (t, 6H, *J*=7.4Hz, CH_3). ^{13}C NMR (75.5Hz, $CDCl_3$) δ (ppm): 191.6, 161.7, 154.2, 149.1, 136.4, 131.9, 127.0, 125.1, 120.0, 116.1, 111.8, 111.4, 97.7, 50.8, 29.5, 20.4, 14.0. ESI-HRMS: calcd for $C_{23}H_{27}NO_2$ 349.2036 (M), found 349.2046 (M).

Compound 6



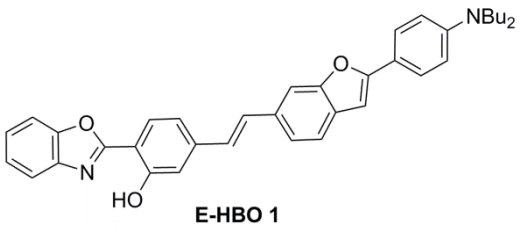
6

Methyltriphenylphosphine bromide (1.5 eqt) was dissolved in anhydrous THF and the resulting mixture was stirred for five minutes at -78 °C. *n*-BuLi 1.6M (1.5 eqt) was added dropwise at this temperature and the medium further stirred for one hour. A concentrated solution of compound **5** in THF was then added dropwise. After stirring one hour at -78 °C, the medium was allowed to stir at room temperature overnight. The crude solution was then extracted with dichloromethane, washed with water, dried ($MgSO_4$) and the solvents evaporated *in vacuo*. The crude oil was purified by silica gel chromatography eluting with CH_2Cl_2/Pet.Ether 2:1 leading to compound **6** as a yellow powder (65% yield). ^{1}H NMR (400MHz, $CDCl_3$) δ (ppm): 7.75 (d, 2H, *J*=8.8Hz, CH Ar), 7.59 (s, 1H, CH Ar), 7.48 (d, 1H, *J*=8Hz, CH Ar), 7.33 (dd, 1H, ^3J=8.2Hz, ^4J=1.2Hz CH Ar), 6.84-6.91 (m, 1H,CH Ar), 6.77 (s, 1H, CH benzofuran), 6.73 (d, 2H, *J*=8.8Hz, CH Ar), 5.83 (d, 1H, *J*=17.6Hz, CH=CH), 5.27 (d, 1H, *J*=10.8Hz, CH=CH), 3.36 (t, 4H, *J*=7.6Hz, CH_2), 1.61-1.69 (m, 4H, CH_2), 1.38-1.47 (m, 4H, CH_2), 1.03 (t, 6H, *J*=7.2Hz, CH_3). ^{13}C NMR (75.5Hz, $CDCl_3$) δ (ppm): 157.0, 154.0, 147.4, 136.3, 132.1, 128.9, 125.3, 120.4, 116.7, 116.3, 111.2, 110.5, 107.1, 96.6, 49.7, 28.4, 19.3, 13.0. ESI-HRMS: calcd for $C_{24}H_{30}NO$ 348.2322 (M+H), found 348.2349 (M+H).

General procedure for E-HBO 1, E-HBO 2, E-HBT

The appropriate compounds **1-3** (1 eqt) and compound **6** (1 eqt) were dissolved in a mixture of DMF, N,N-diisopropylethylamine and H_2O (10/0.3/0.3 v:v). P(^{o}-tolyl)$_3$ (20% mol) was then added in the medium which was degassed with Ar for 30 minutes. $Pd(oAc)_2$ (5% mol) was then added and the resulting mixture was stirred at 120 °C overnight. The crude medium was then extracted with dichloromethane, washed with water, dried ($MgSO_4$) and the solvents evaporated *in vacuo*. The crude oil was purified by silica gel chromatography eluting with CH_2Cl_2/Pet.Ether leading to **-HBO 1, E-HBO 2** or **E-HBT** as yellow to orange powders.

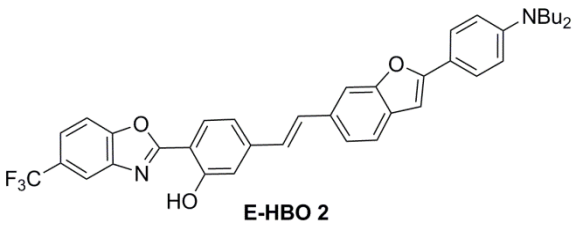
E-HBO 1



E-HBO 1

yellow powder. 20%. ^{1}H NMR (400MHz, $CDCl_3$) δ (ppm): 11.40 (s, 1H, OH), 7.99 (d, 1H, *J*=8.4Hz, CH Ar), 7.69-7.73 (m, 3H, CH Ar), 7.64 (s, 1H, CH Ar), 7.59-7.61 (m, 1H, CH Ar), 7.46-7.49 (m, 1H, CH Ar), 7.36-7.40 (m, 3H, CH Ar), 7.32 (d, 1H, *J*=16Hz, CH=CH), 7.26 (s, 1H, CH Ar), 7.19 (d, 1H, *J*=8.4Hz, CH Ar), 7.10 (d, 1H, *J*=16Hz, CH=CH), 6.75 (s, 1H, CH benzofuran), 6.69 (d, 2H, *J*=8.2Hz, CH Ar), 3.33 (t, 4H, *J*=7.7Hz, CH_2), 1.58-1.65 (m, 4H, CH_2), 1.34-1.44 (m, 4H, CH_2), 0.99 (t, 6H, *J*=7.7Hz, CH_3). ^{13}C NMR (75.5Hz, $CDCl_3$) δ (ppm): 162.9, 158.9, 155.1, 149.2, 148.6, 143.1, 140.2, 133.6, 132.2, 132.0, 130.6, 127.3, 126.5, 126.2, 125.2, 125.0, 122.3, 120.0, 119.1, 118.0, 117.2, 114.6, 111.5, 110.6, 109.3, 108.7, 97.8, 50.8, 29.5, 20.4, 14.0. ESI-HRMS: calcd for $C_{37}H_{37}N_2O_3$ 557.2799 (M+H), found 557.2792 (M+H).

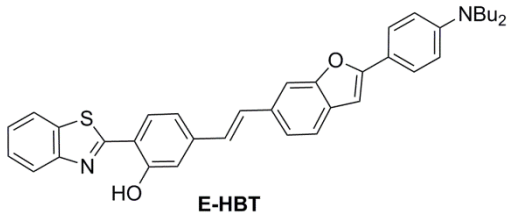
E-HBO 2



E-HBO 2

Orange powder. 13%. ^{1}H NMR (400MHz, $CDCl_3$) δ (ppm) : 11.10 (s, 1H, OH), 7.92 (d, 2H, *J* = 8.6 Hz, CH Ar), 7.57-7.64 (m, 5H, CH Ar), 7.40 (d, 1H, *J* = 8.5 Hz, CH Ar), 7.37 (d, 1H, *J* = 8.2 Hz, CH Ar), 7.29 (d, 1H, *J* = 8.2Hz, CH Ar), 7.24 (d, 1H, *J* = 16.1 Hz, CH=CH), 7.14 (d, 1H, *J* = 8.2 Hz, CH Ar), 7.02 (d, 1H, *J* = 16.1 Hz, CH=CH), 6.68 (s, 1H, CH benzofuran), 6.62 (d, 2H, *J* = 8.2 Hz, CH Ar), 3.26 (t, 4H, *J* = 7.7 Hz, CH_2), 1.50-1.58 (m, 4H, CH_2), 1.27-1.36 (m, 4H, CH_2), 0.91 (t, 6H, *J* = 7.7 Hz, CH_3). ^{13}C NMR (75.5Hz, $CDCl_3$) δ (ppm) : 164.6, 159.2, 158.6, 155.0, 150.8, 148.6, 143.9, 140.5, 132.5, 132.0, 130.7, 129.2, 128.0, 127.5, 127.1, 126.4, 125.9, 122.4, 120.0, 118.1, 117.1, 114.8, 111.5, 111.2, 111.0, 108.8, 108.5, 97.7, 50.8, 29.5, 20.4, 14.0. ESI-HRMS: calcd for $C_{38}H_{36}F_3N_2O_3$ 625.2673(M+H), found 625.2648(M+H).

E-HBT

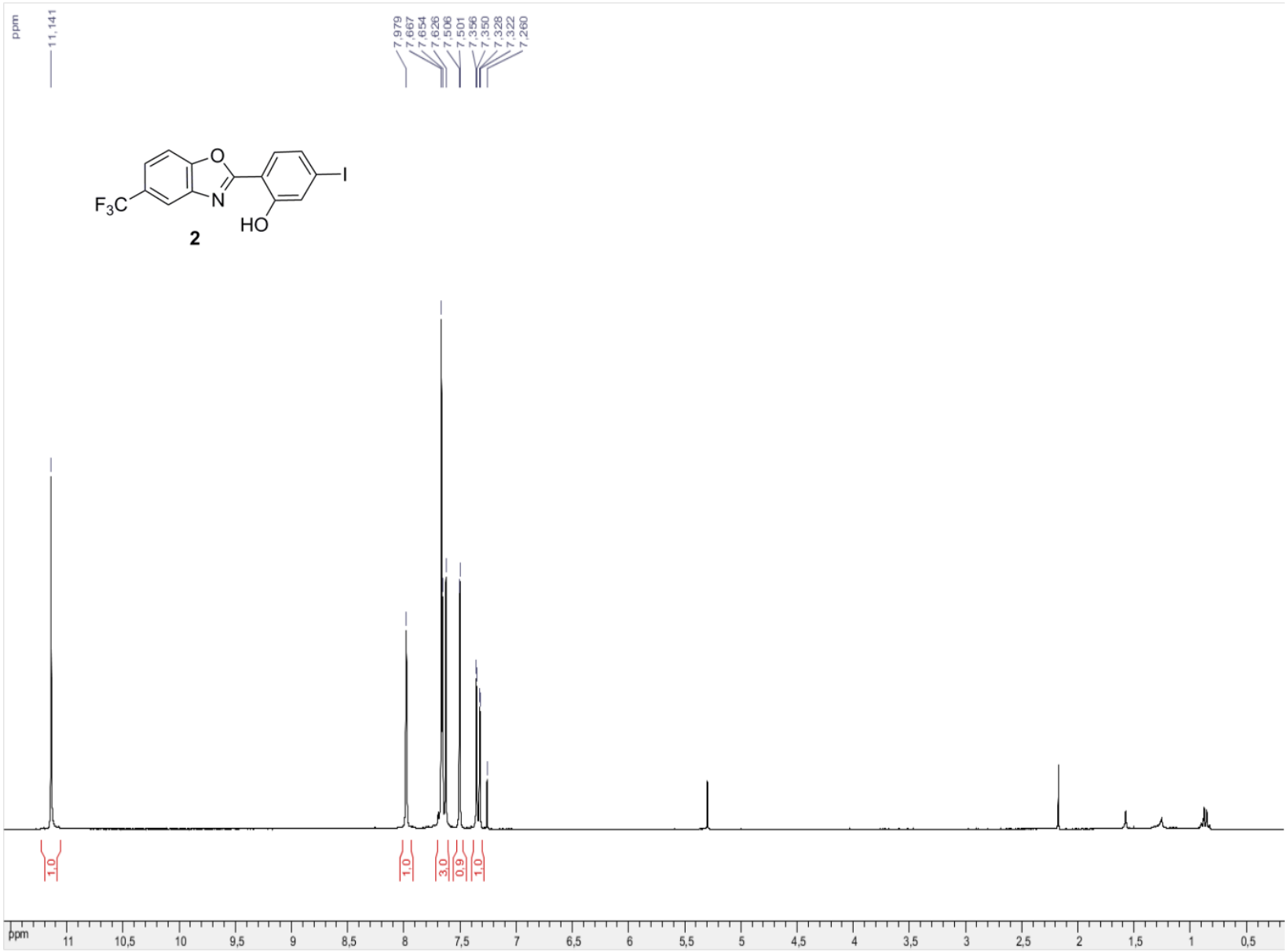


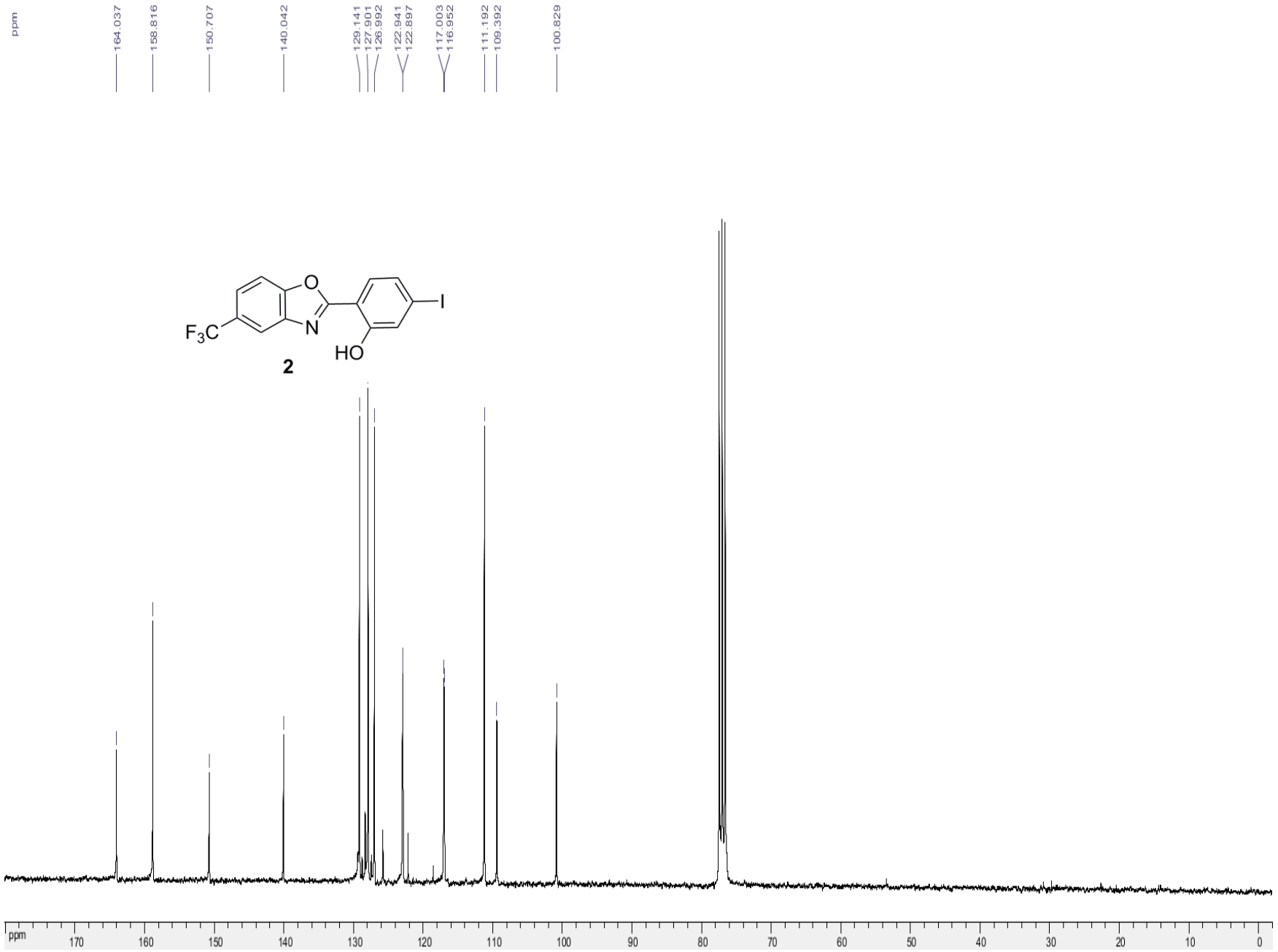
E-HBT

Orange powder. 15%. ^{1}H NMR (300MHz, $CDCl_3$) δ (ppm) : 12.53 (s, 1H, OH), 7.98 (d, 1H, *J* = 6 Hz, CH Ar), 7.89 (d, 1H, *J* = 5.7 Hz, CH Ar), 7.70 (d, 2H, *J* = 6.6 Hz, CH Ar), 7.65 (d, 2H, *J* = 6.3 Hz, CH Ar), 7.47-7.53 (m, 2H, CH Ar), 7.38-7.42 (m, 2H, CH Ar), 7.31 (d, 1H, *J* = 12 Hz, CH=CH), 7.25 (d, 1H, *J* = 6 Hz, CH Ar), 7.12 (d, 1H, *J* = 6 Hz, CH Ar), 7.08 (d, 1H, *J* = 12 Hz, CH=CH), 6.75 (s, 1H, CH benzofuran), 6.70 (d, 2H, *J* = 6.6 Hz, CH Ar), 3.33 (t, 4H, *J* = 5.7 Hz, CH_2), 1.56-1.65 (m, 4H, CH_2), 1.33-1.43 (m, 4H,

CH_2), 0.98 (t, 6H, J = 5.4 Hz, CH_3). ^{13}C NMR (75.5Hz, $CDCl_3$) δ (ppm) :169.1, 158.5, 158.2, 155.0, 152.0, 148.5, 142.3, 132.6, 132.2, 131.8, 130.5, 128.7, 126.7, 126.4, 126.1, 125.4, 122.3, 122.1, 121.5, 120.0, 118.0, 117.2, 115.8, 115.0, 111.5, 108.7, 97.7, 50.8, 29.5, 20.4, 14.0. ESI-HRMS: calcd for $C_{37}H_{37}N_2O_2S$ 573.2570 (M+H), found 573.2496 (M+H).

S3 ^{1}H and ^{13}C NMR Spectra

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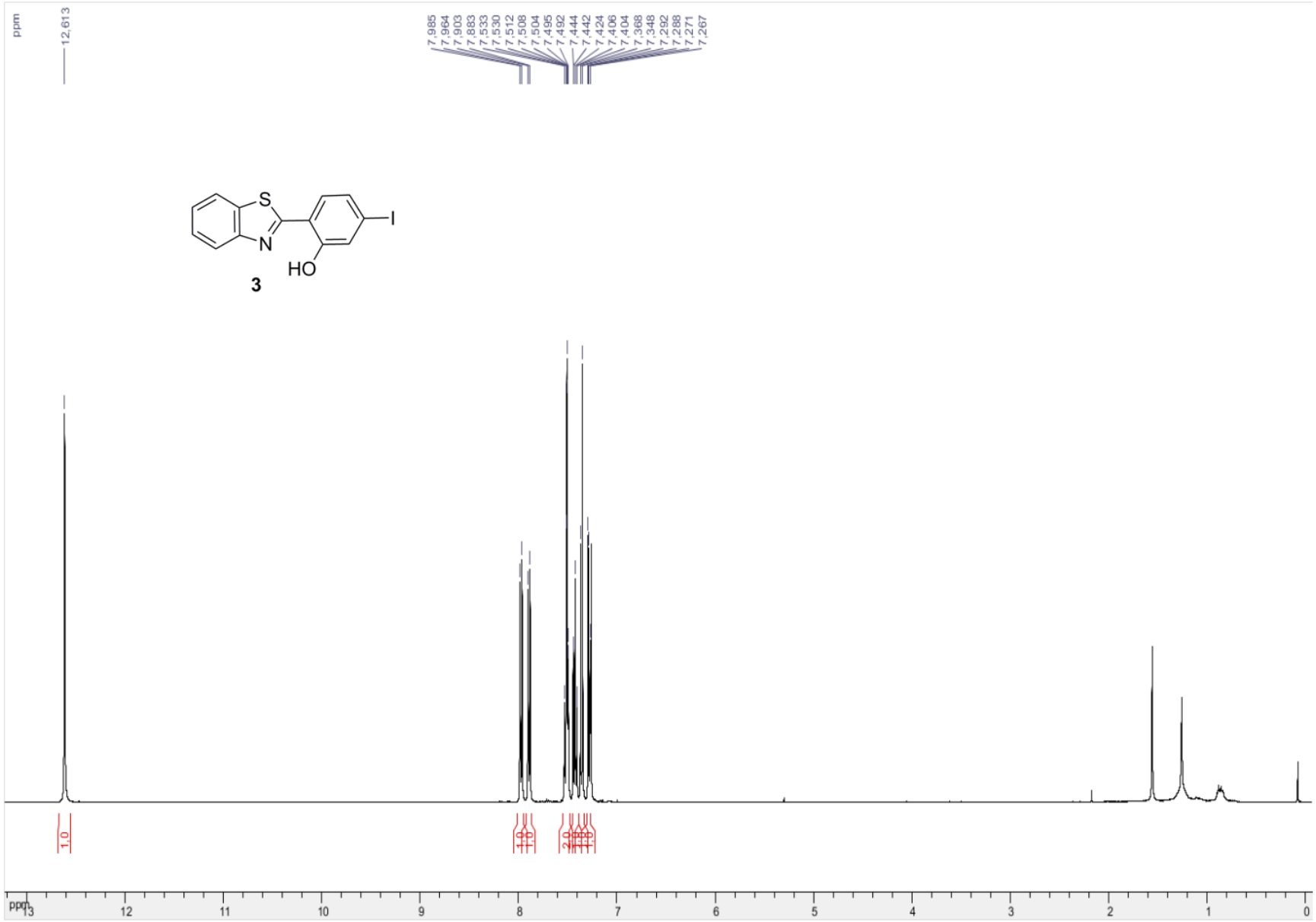
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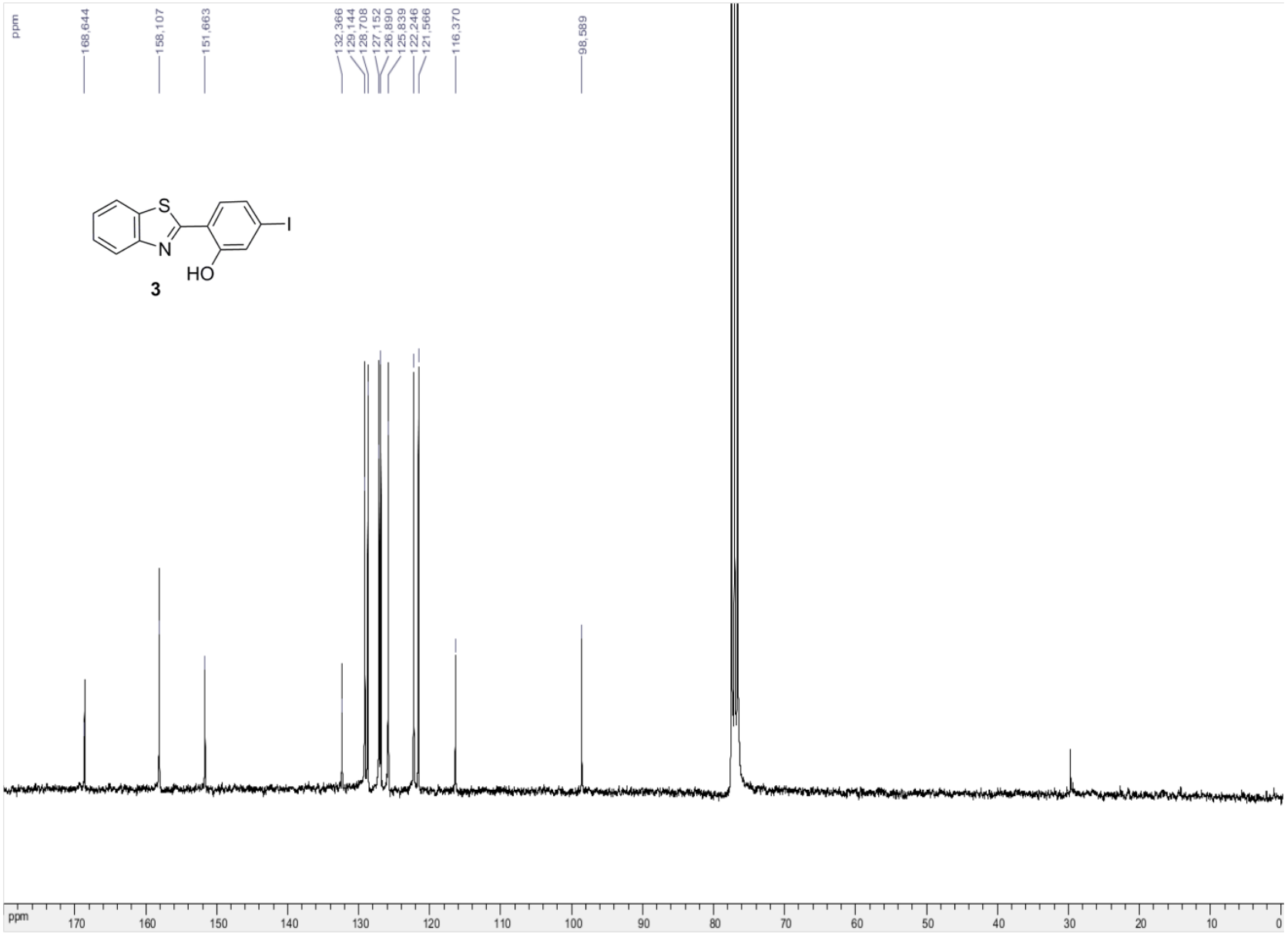
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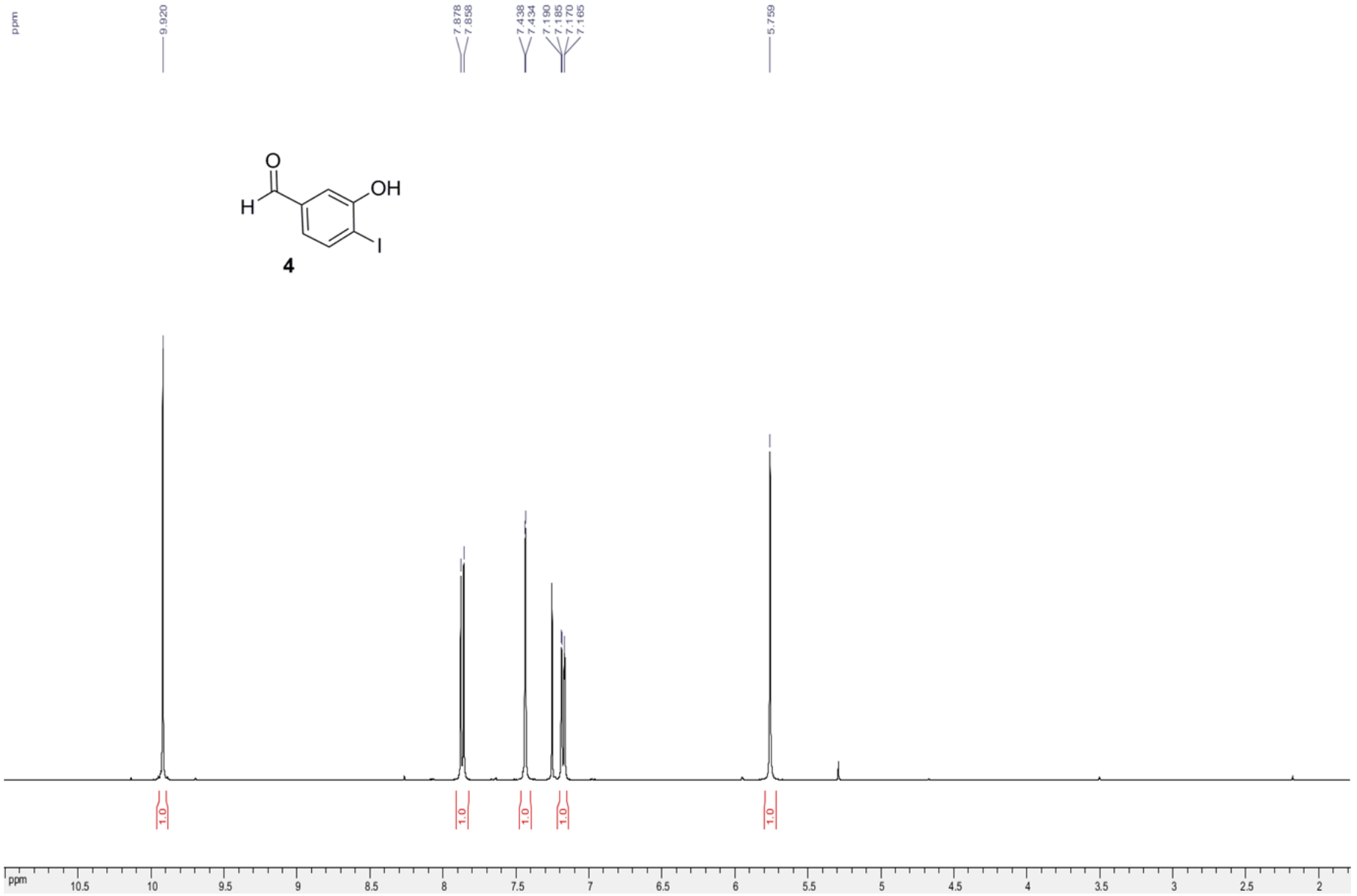
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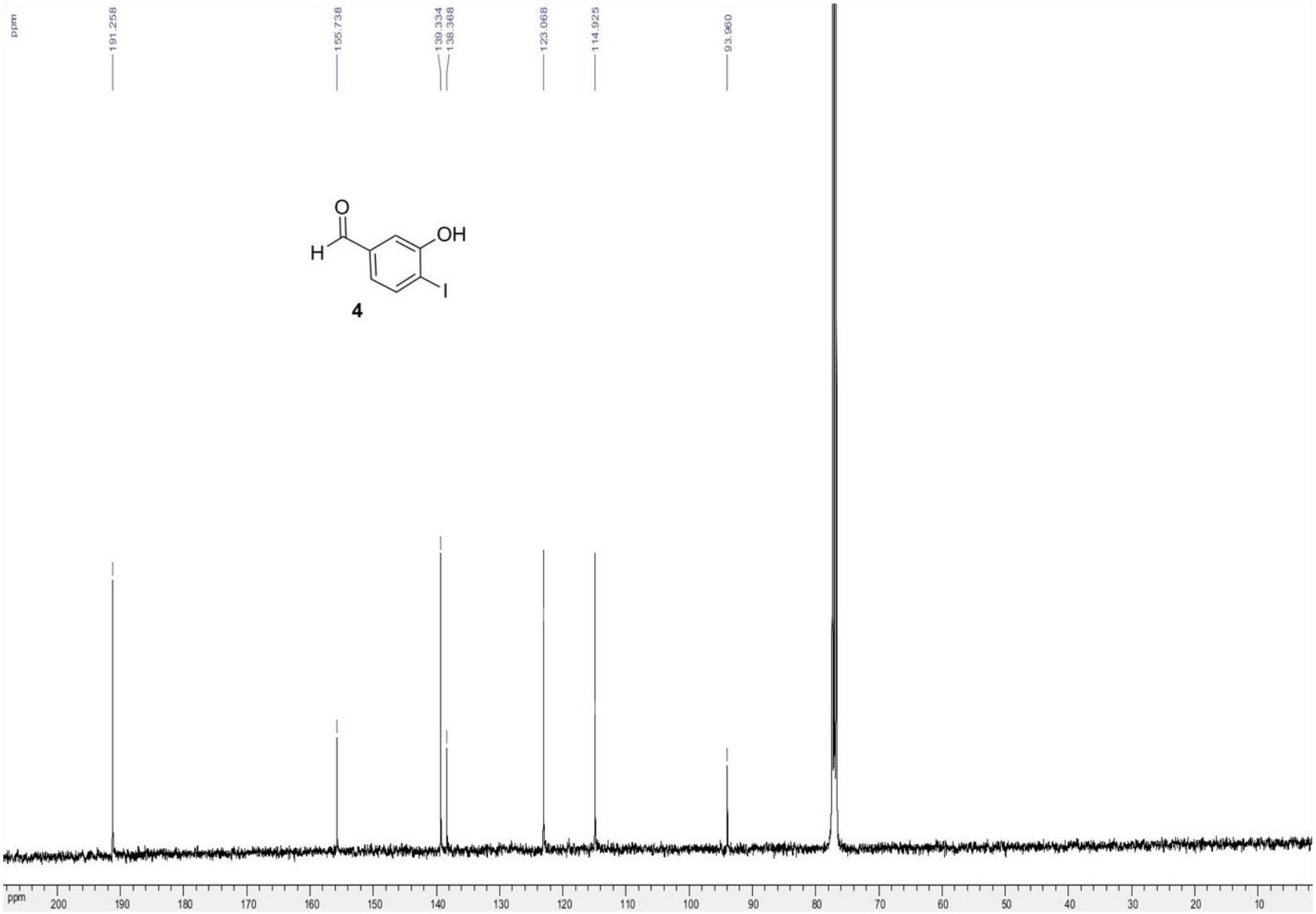
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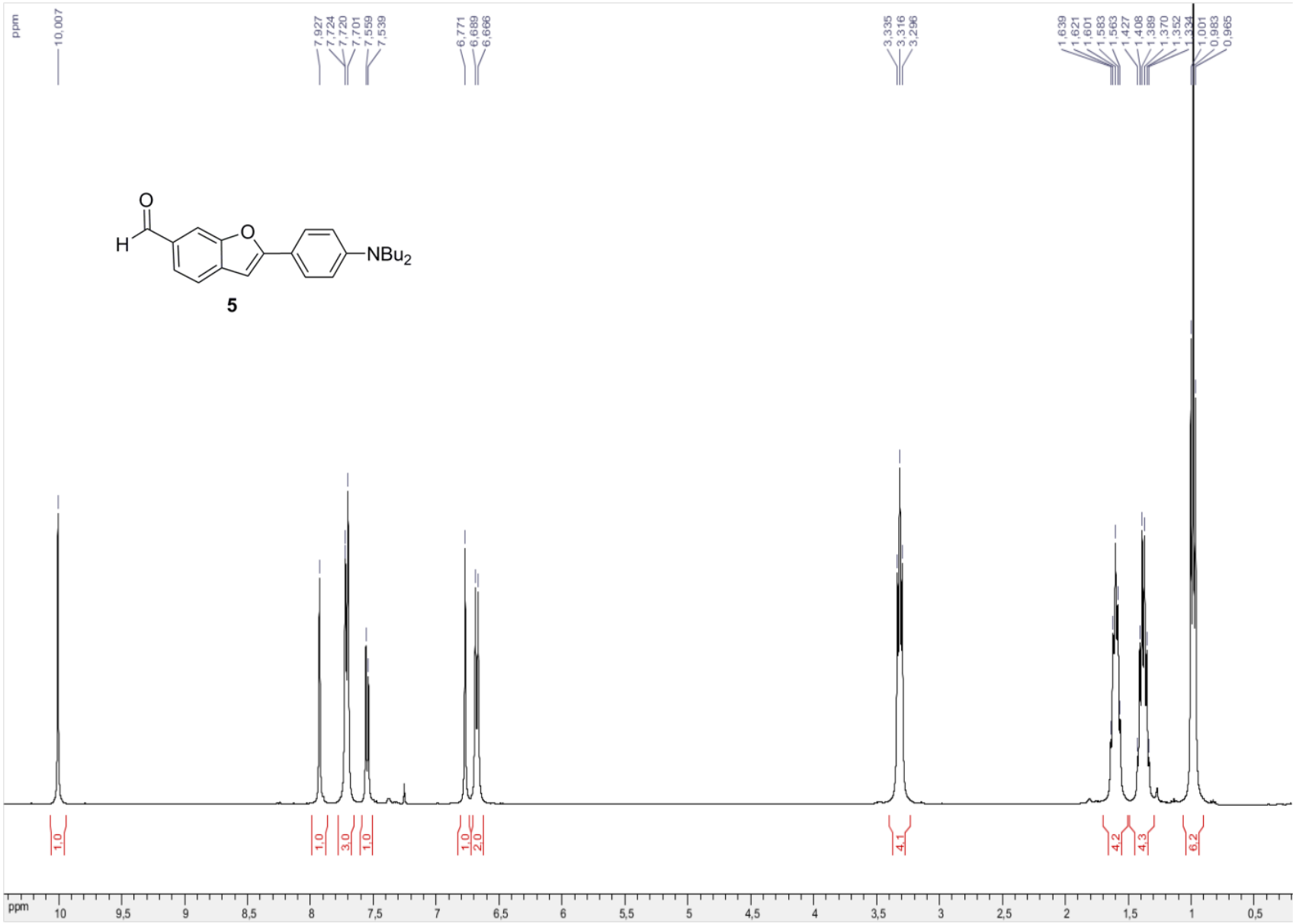
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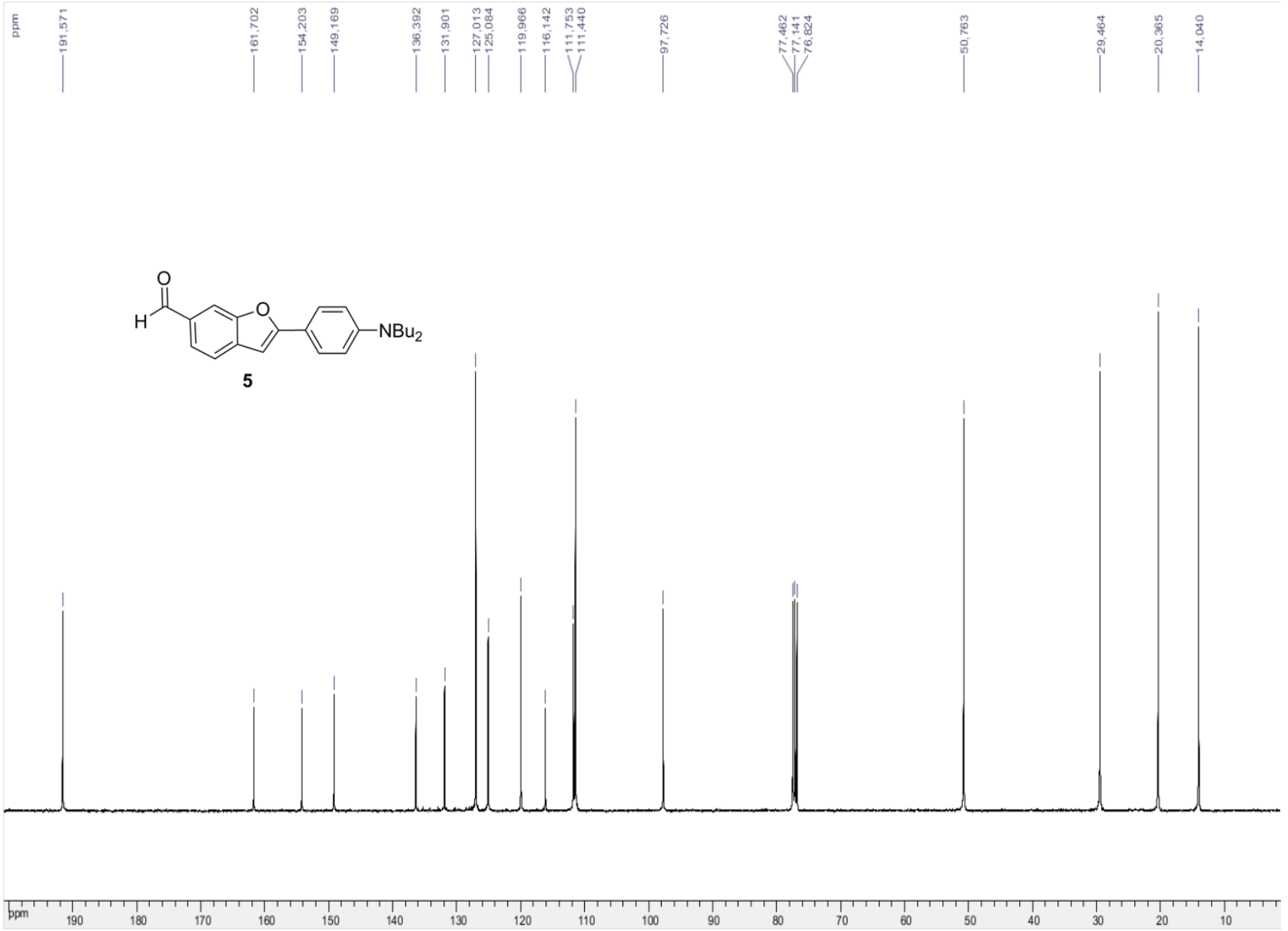
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20,365
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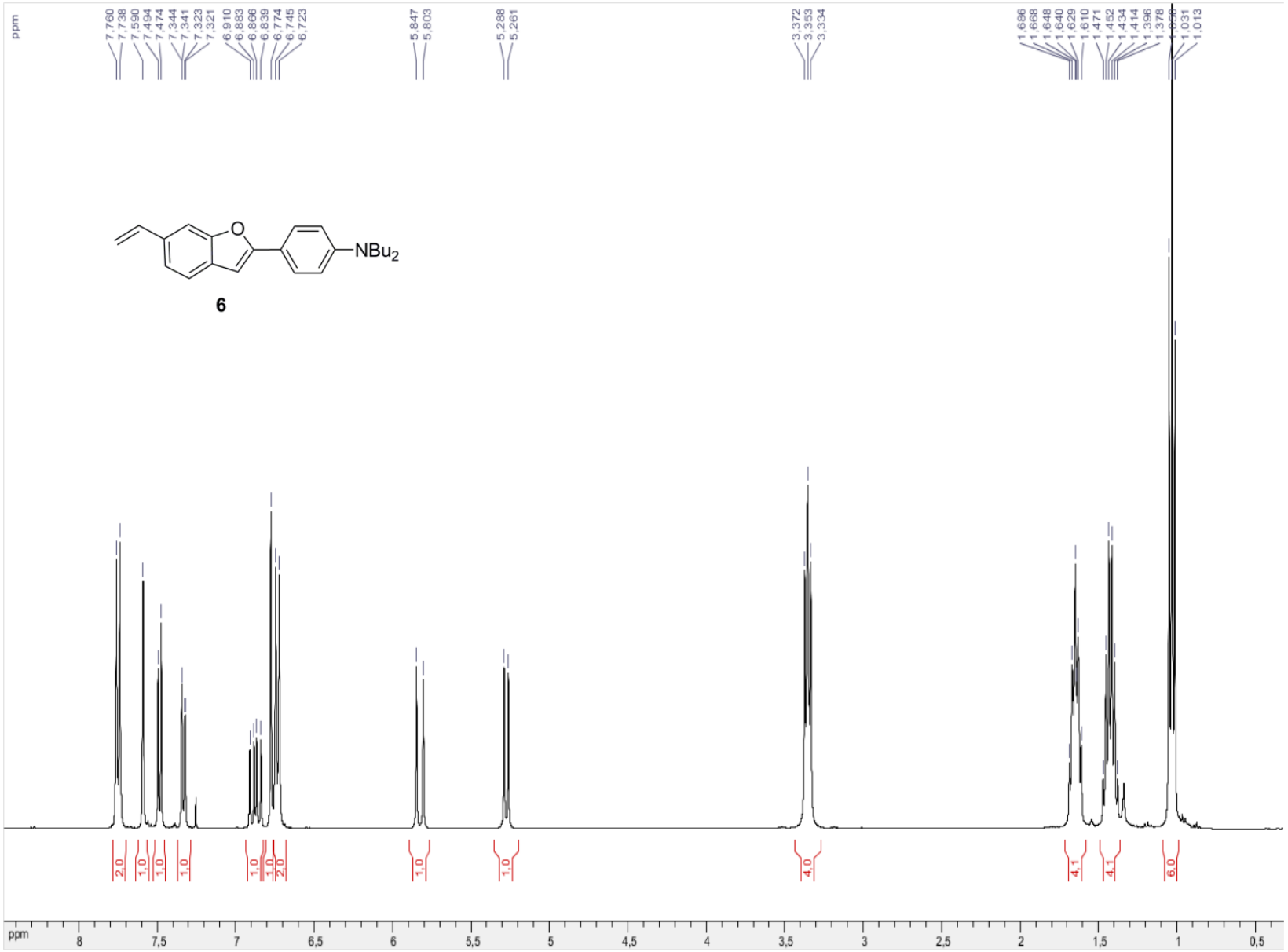
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6.774
6.745
6.723
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5.803
5.288
5.261
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3.334
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1.668
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1.640
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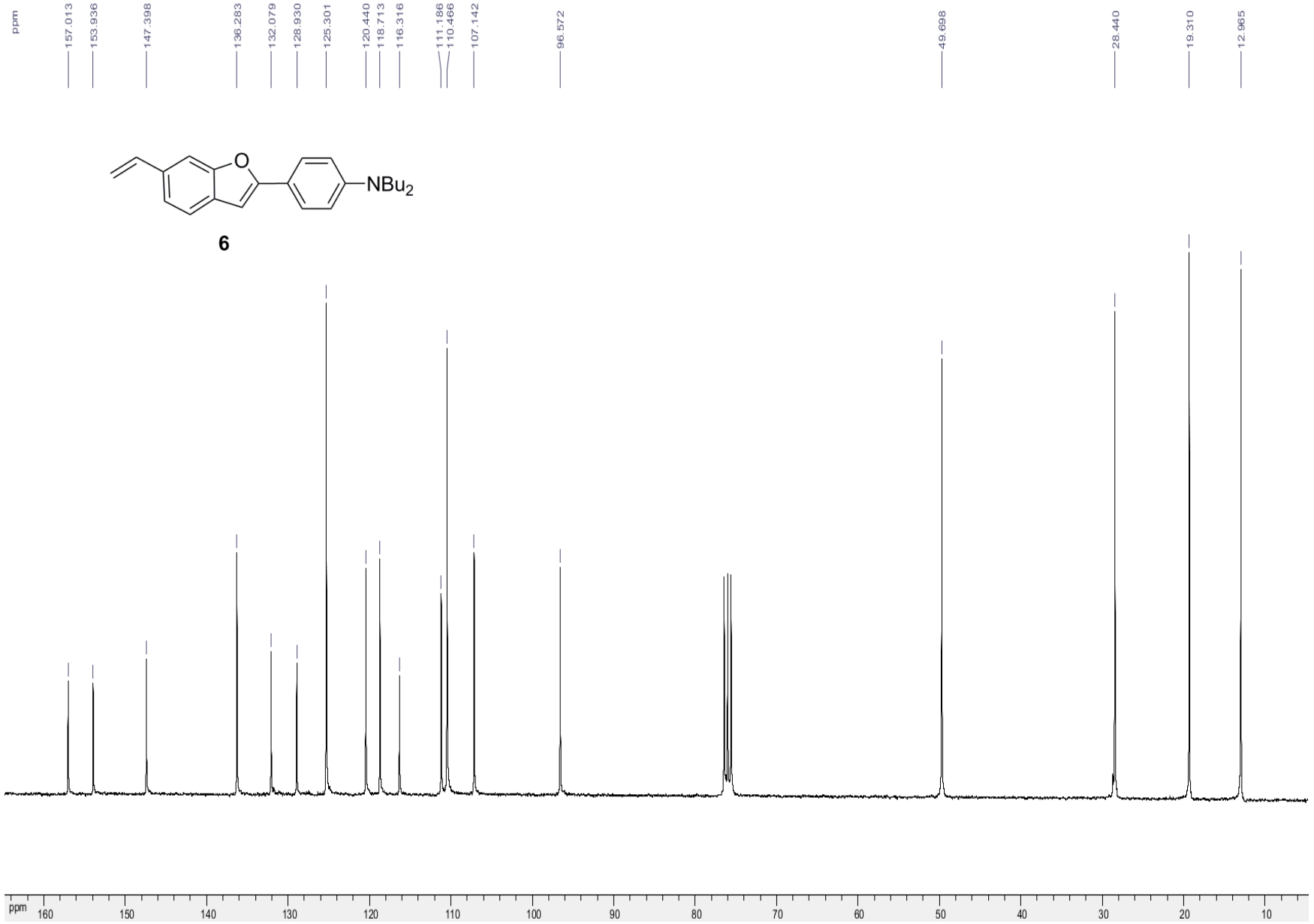
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28.440
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NBu2
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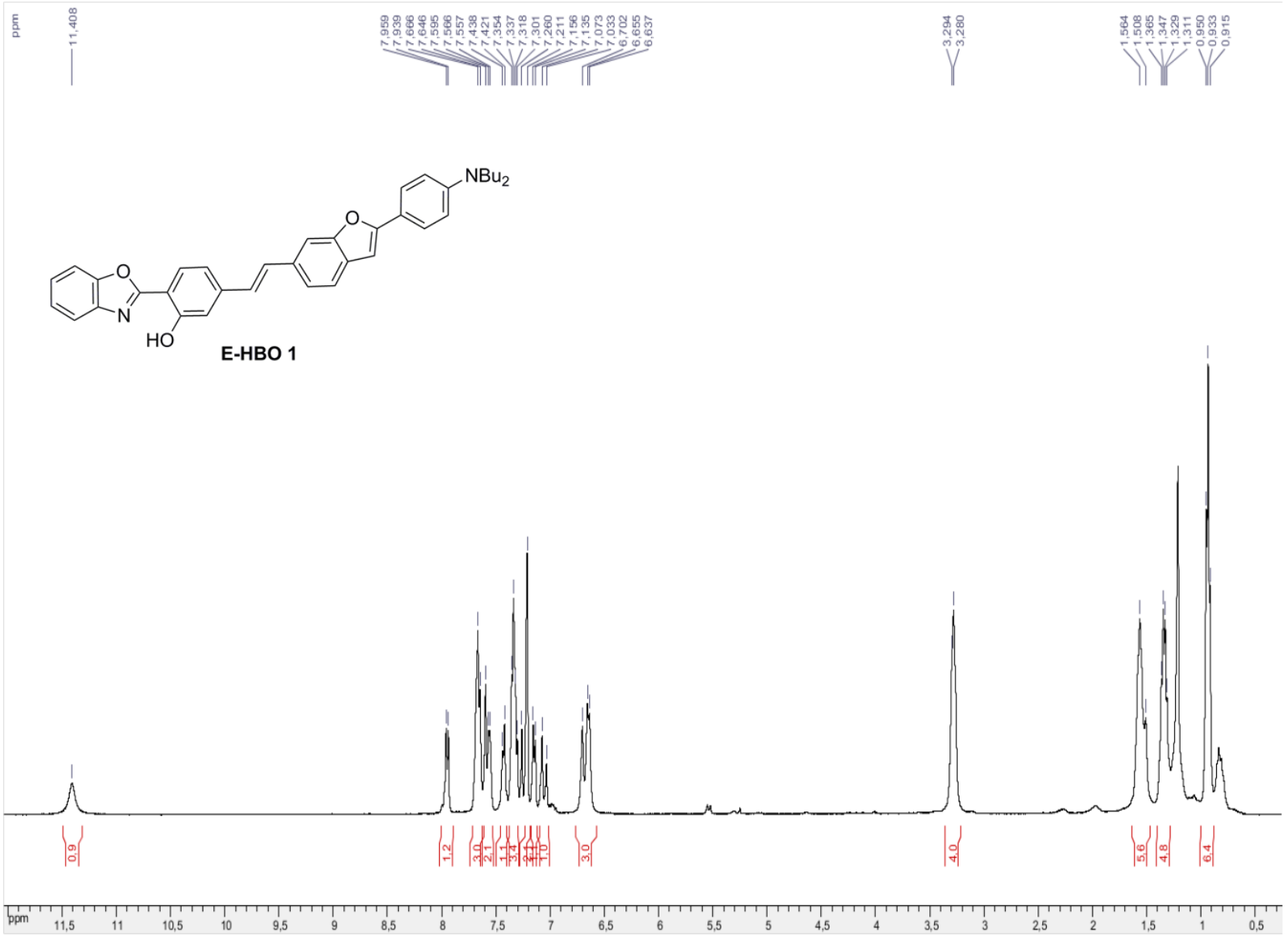
20
10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6,4
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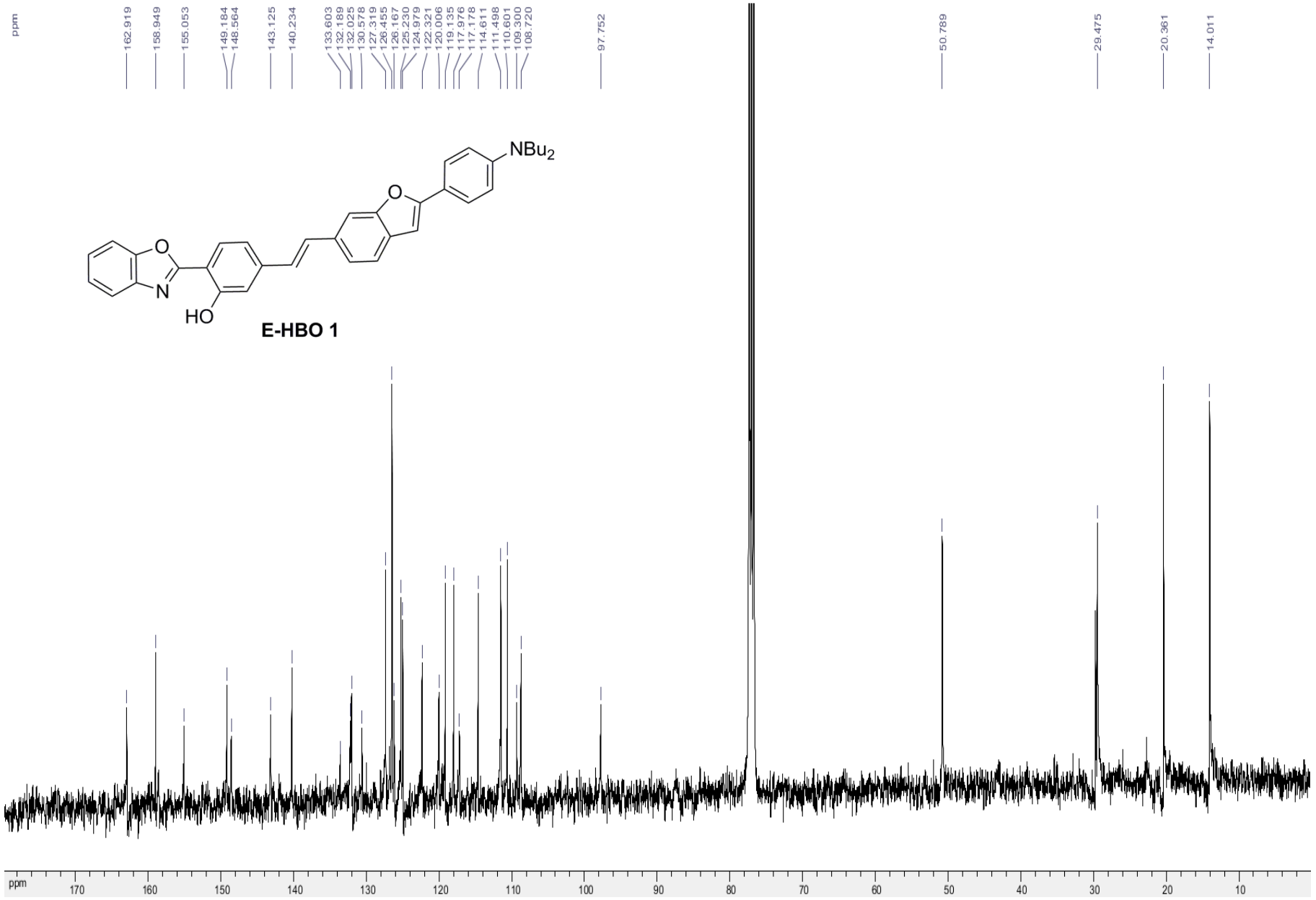
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126.167
125.230
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117.178
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N
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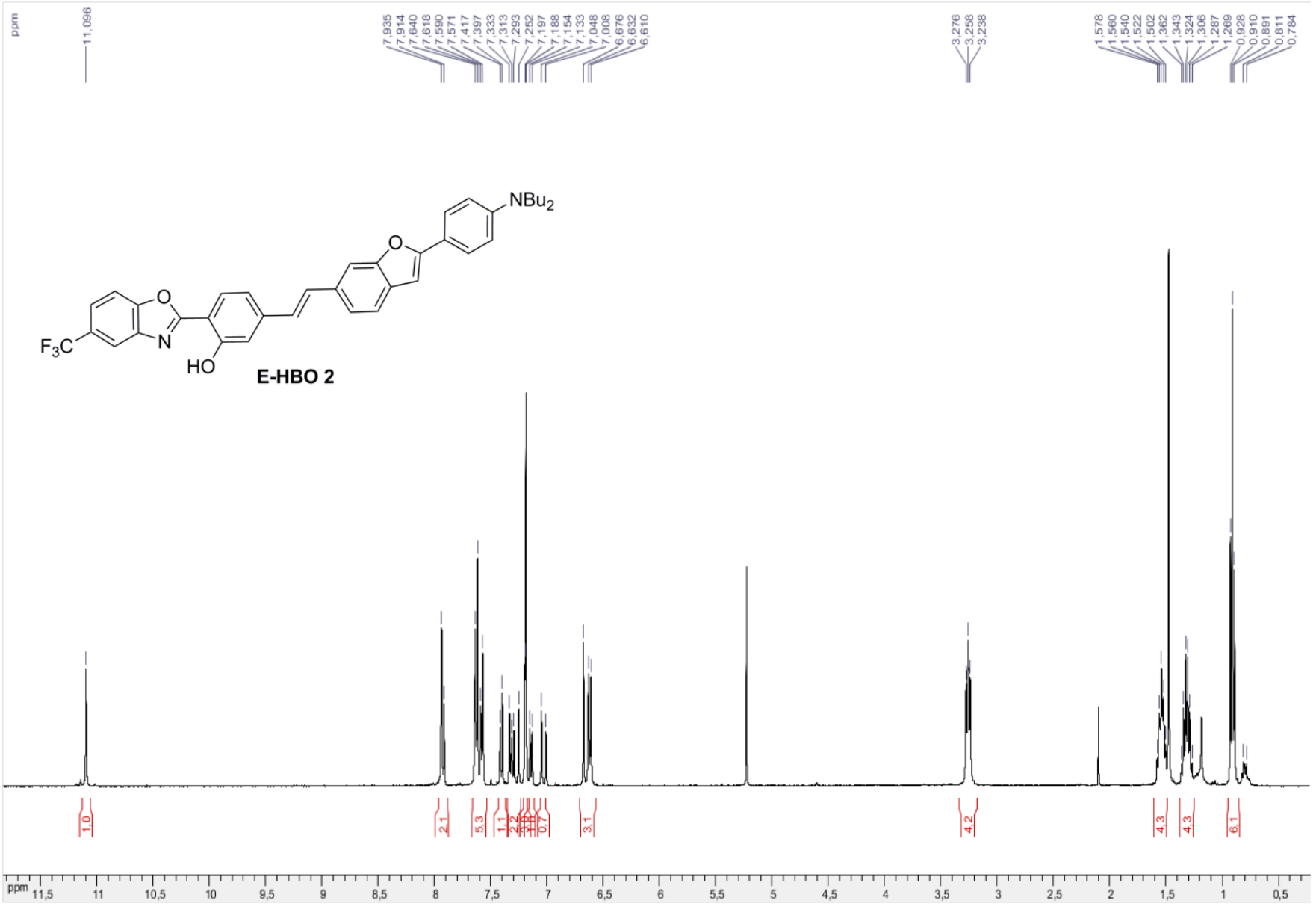
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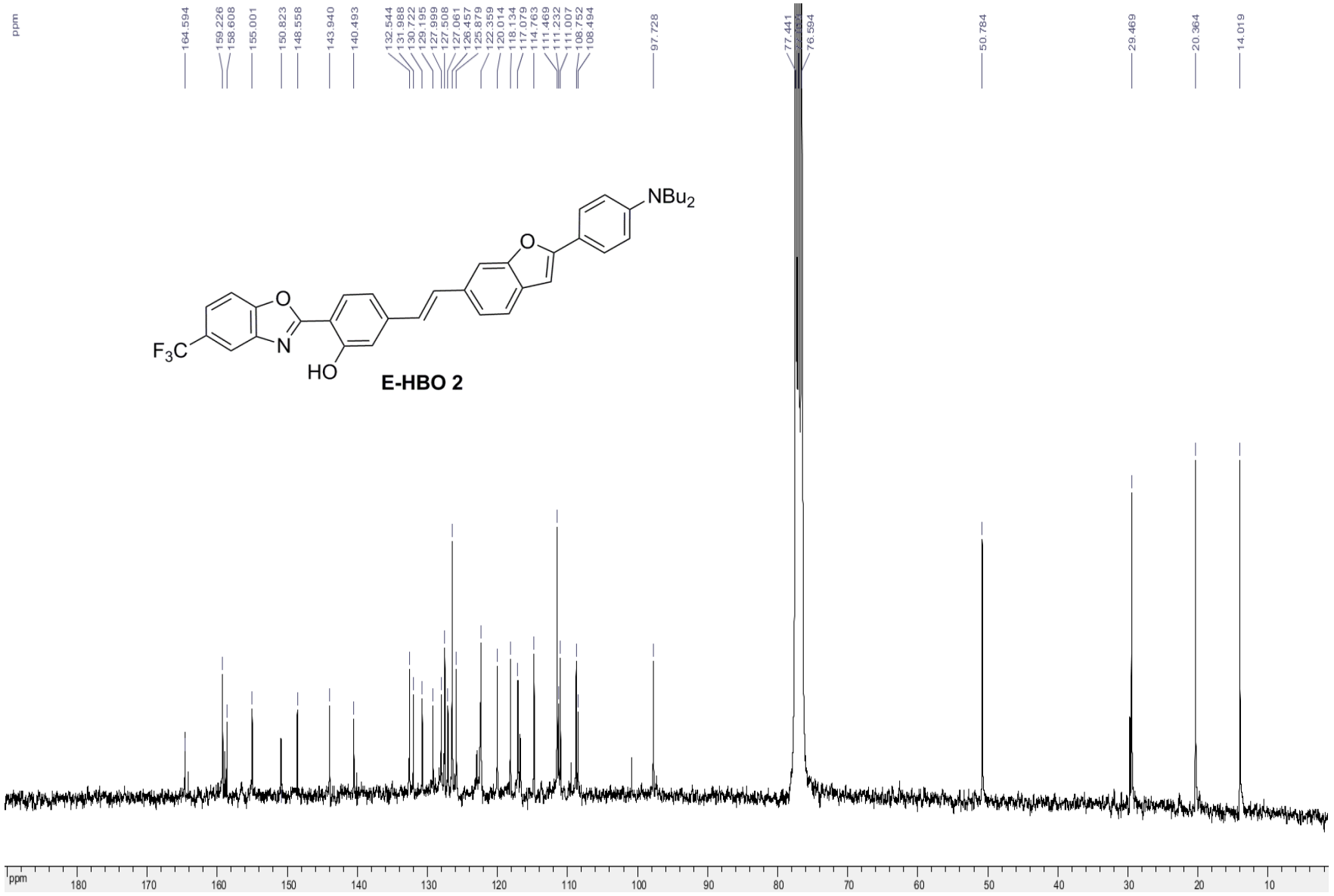
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126.457
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O
O
N
F3C
HO
E-HBO 2
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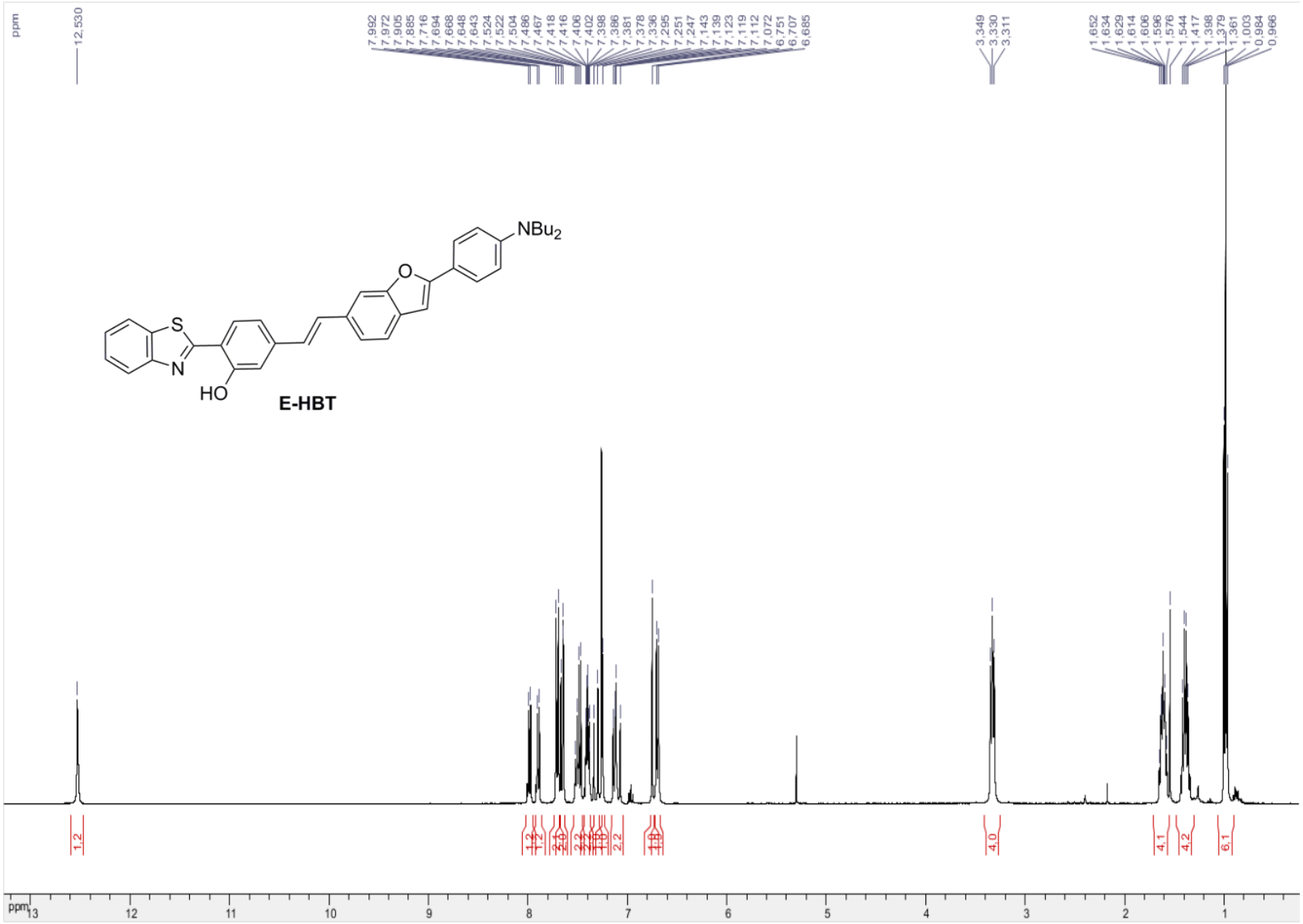
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7.247
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7.139
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7.119
7.112
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HO
E-HBT
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2.2
1.8
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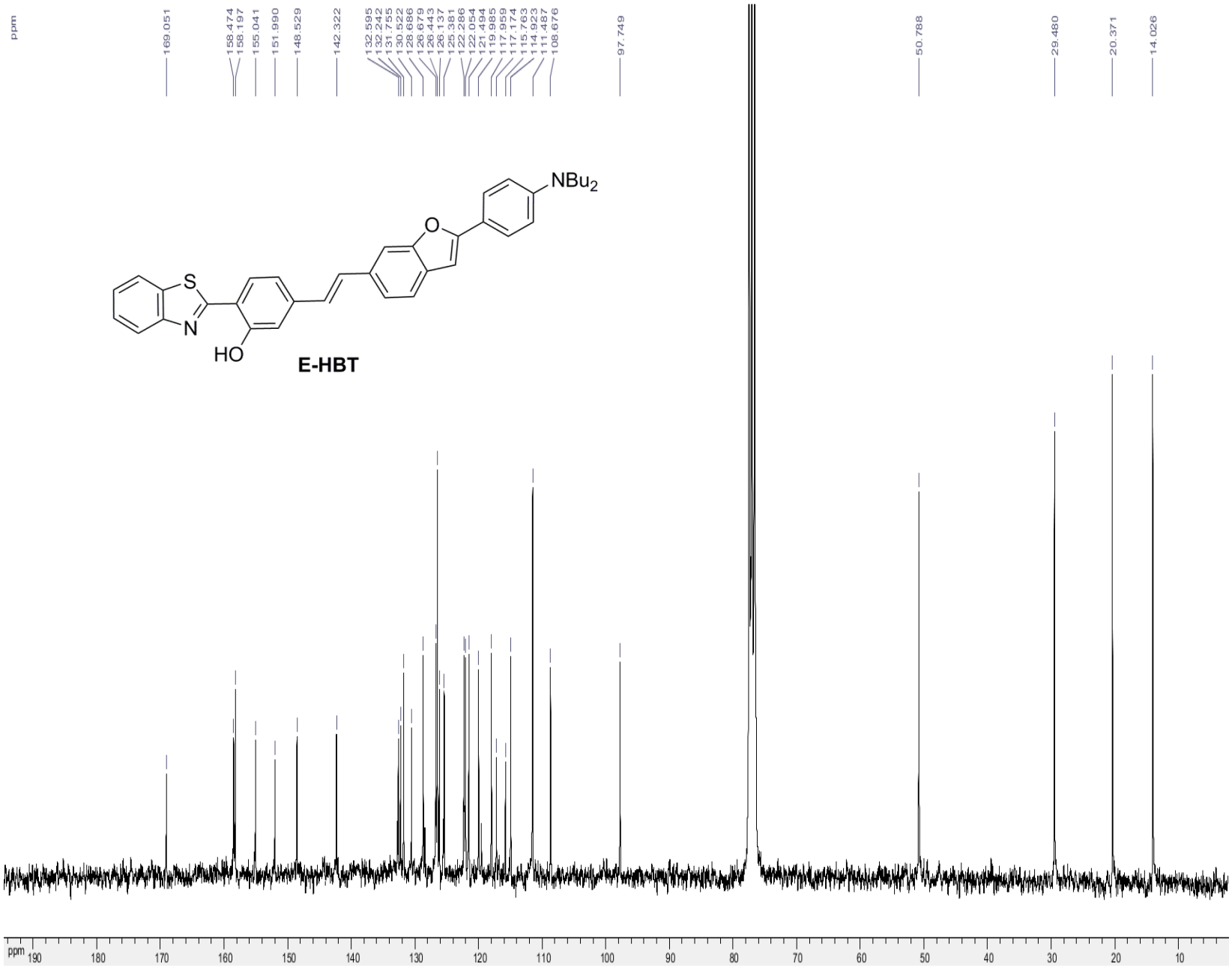
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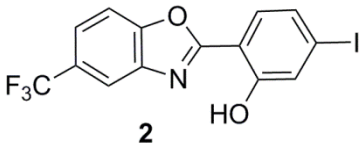
119.985
117.959
117.774
115.923
111.487
108.676
97.749
50.788
29.480
20.371
14.026
NBu2
O
S
N
HO
E-HBT
ppm 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

S4 HRMS traces

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name	D:\Data\Service masse 2015\O37890SK.d
Method	esi low pos.m
Sample Name	MR10
Comment	



2

Acquisition Date	11/30/2015 10:44:54 AM
Operator	Administrator
Instrument	micrOTOF 66

Acquisition Parameter

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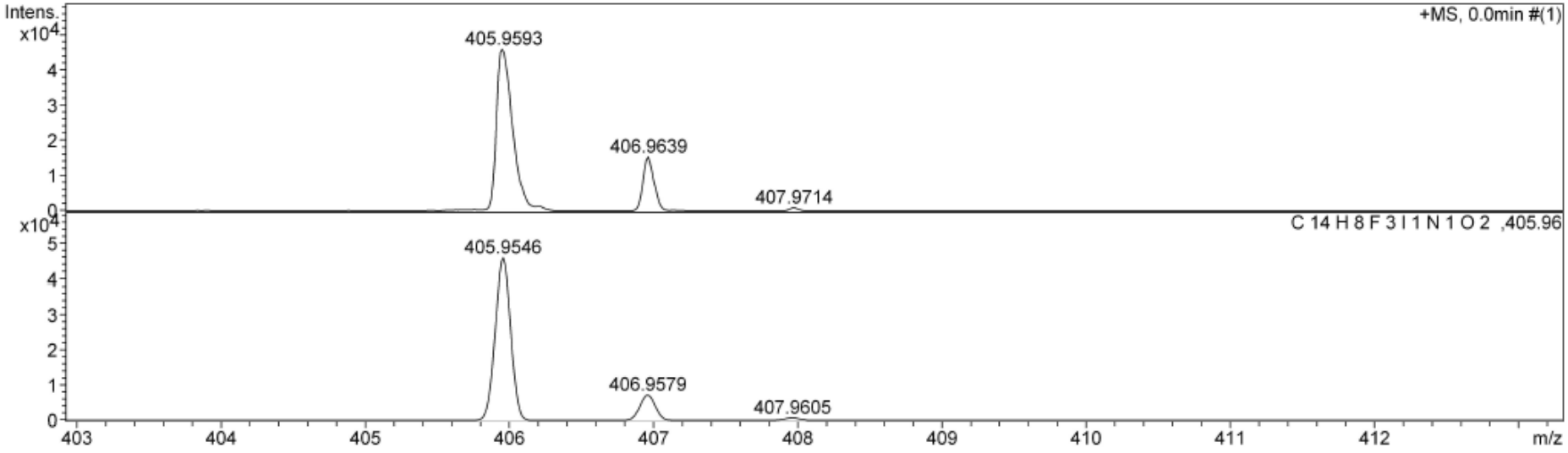
Scan Range	n/a	Capillary Exit	80.0 V	Set Pulsar Pull	817 V
Scan Begin	50 m/z	Hexapole RF	60.0 V	Set Pulsar Push	817 V
Scan End	3000 m/z	Skimmer 1	50.0 V	Set Reflector	1700 V
		Hexapole 1	24.3 V	Set Flight Tube	8600 V
				Set Detector TOF	2275 V



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e⁻
C 14 H 8 F 3 I 1 N 1 O 2	0.10	405.9546	-11.60	-12.49	9.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name	D:\Data\Service masse 2015\O37883SK.d	Acquisition Date	11/27/2015 4:08:18 PM
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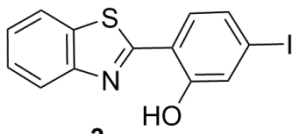
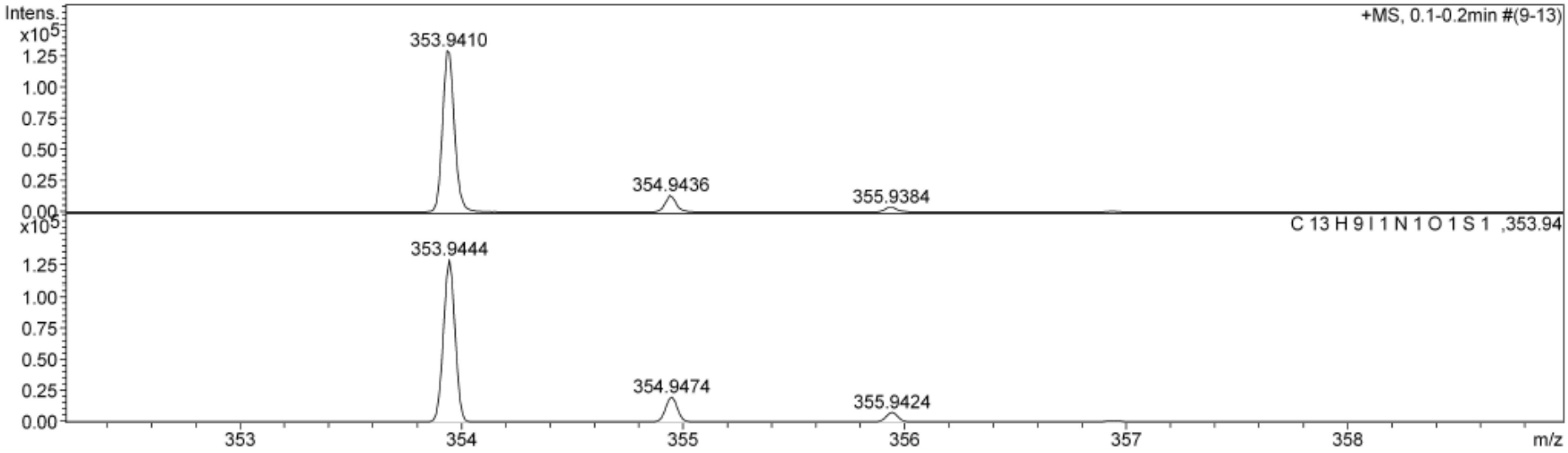
Sample Name	MR11	Operator	Administrator
Comment		Instrument	micrOTOF 66



3

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	74 V
Scan Range	n/a	Capillary Exit	80.0 V	Set Pulsar Pull	817 V
Scan Begin	50 m/z	Hexapole RF	60.0 V	Set Pulsar Push	810 V
Scan End	3000 m/z	Skimmer 1	50.0 V	Set Reflector	1700 V
		Hexapole 1	24.3 V	Set Flight Tube	8600 V
				Set Detector TOF	2275 V

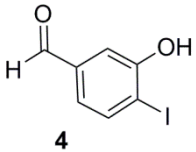


Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e⁻
C 13 H 9 I 1 N 1 O 1 S 1	0.03	353.9444	9.74	9.96	9.50	ok	even
C 13 H 8 I 1 N 1 O 1 S 1	0.76	352.9366	-3.84	-5.81	10.00	-	odd

Mass Spectrum Molecular Formula Report

Analysis Info

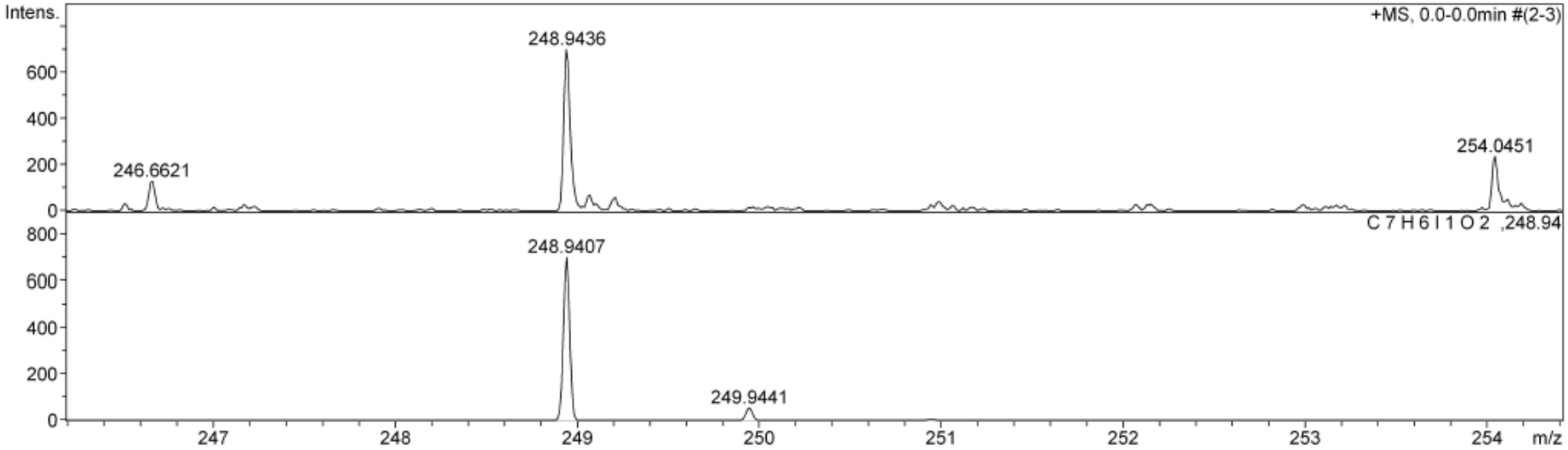
Analysis Name	D:\Data\Service masse 2015\O37984SK.d	Acquisition Date	12/3/2015 4:46:23 PM
Method	esi low pos.m		
Sample Name	AS669	Operator	Administrator
Comment		Instrument	micrOTOF 66



4

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	65 V
Scan Range	n/a	Capillary Exit	80.0 V	Set Pulsar Pull	817 V
Scan Begin	50 m/z	Hexapole RF	60.0 V	Set Pulsar Push	817 V
Scan End	3000 m/z	Skimmer 1	50.0 V	Set Reflector	1700 V
		Hexapole 1	24.3 V	Set Flight Tube	8600 V
				Set Detector TOF	2275 V

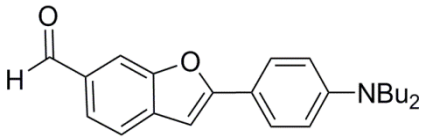


Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e⁻
C 7 H 6 I 1 O 2	0.05	248.9407	-11.69	-11.65	4.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

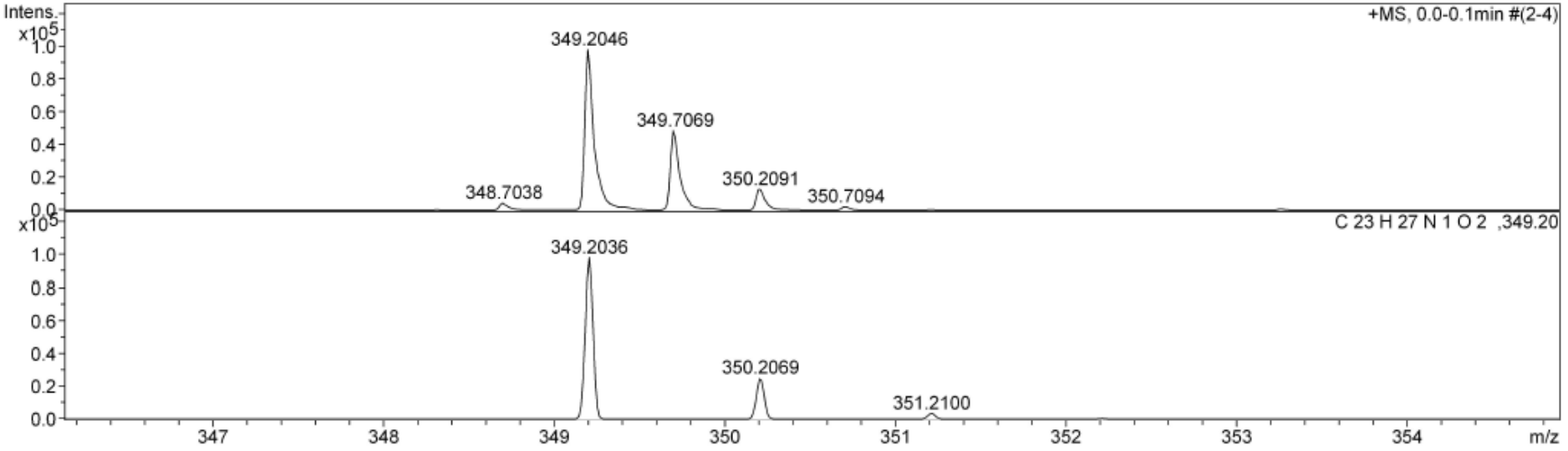
Analysis Name	D:\Data\Service masse	Acquisition Date	1/28/2016 2:34:49 PM
Method	esi low pos.m		
Sample Name	MR3F2	Operator	Administrator
Comment		Instrument	micrOTOF 66



5

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	65 V
Scan Range	n/a	Capillary Exit	80.0 V	Set Pulsar Pull	817 V
Scan Begin	50 m/z	Hexapole RF	60.0 V	Set Pulsar Push	817 V
Scan End	3000 m/z	Skimmer 1	50.0 V	Set Reflector	1700 V
		Hexapole 1	24.3 V	Set Flight Tube	8600 V
				Set Detector TOF	2275 V

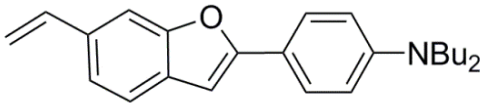


Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e⁻
C 23 H 27 N 1 O 2	0.08	349.2036	-2.86	-2.81	11.00	-	odd

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name
Method
Sample Name
Comment



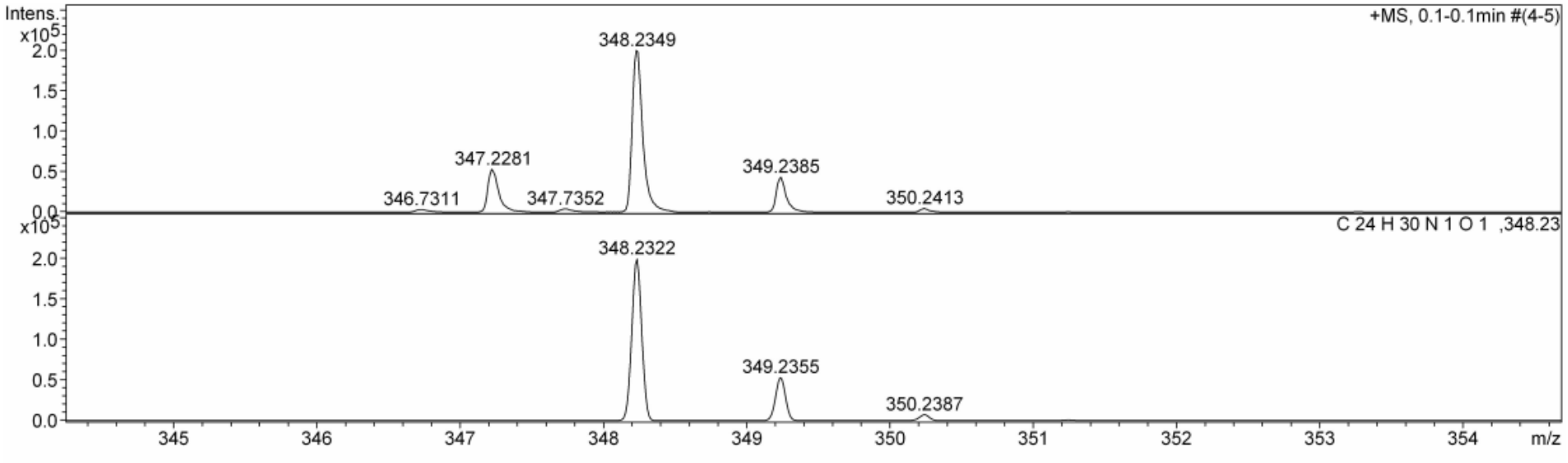
6

Acquisition Date 12/3/2015 9:21:30 AM

Operator Administrator
Instrument micrOTOF 66

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	65 V
Scan Range	n/a	Capillary Exit	80.0 V	Set Pulsar Pull	817 V
Scan Begin	50 m/z	Hexapole RF	60.0 V	Set Pulsar Push	817 V
Scan End	3000 m/z	Skimmer 1	50.0 V	Set Reflector	1700 V
		Hexapole 1	24.3 V	Set Flight Tube	8600 V
				Set Detector TOF	2275 V

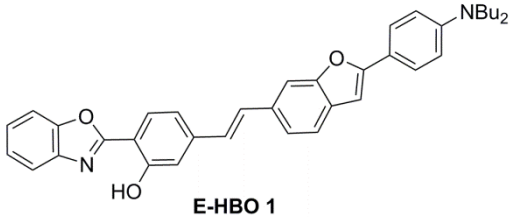


Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e⁻
C 24 H 30 N 1 O 1	0.03	348.2322	-7.92	-7.80	10.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name
Method
Sample Name
Comment



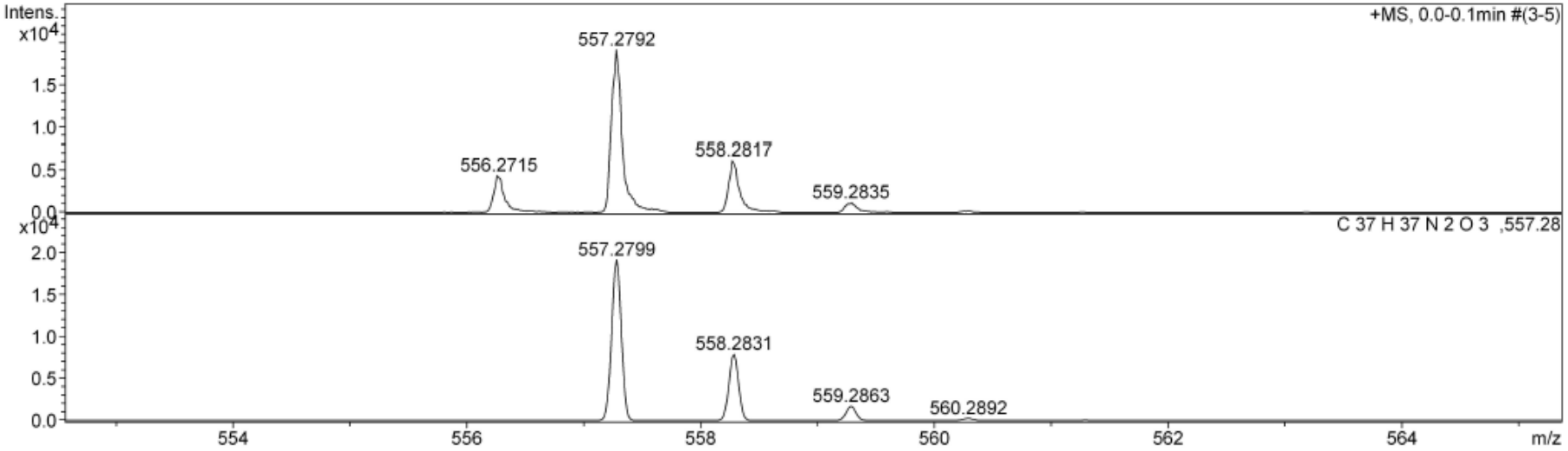
E-HBO 1

Acquisition Date 11/19/2015 9:09:07 AM

Operator Administrator
Instrument micrOTOF 66

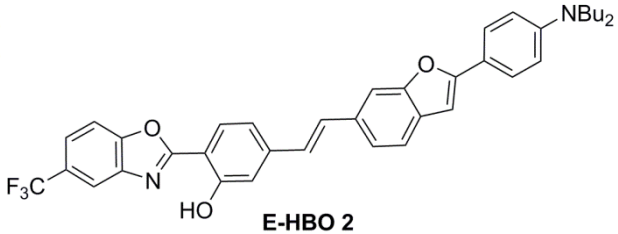
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	65 V
Scan Range	n/a	Capillary Exit	80.0 V	Set Pulsar Pull	817 V
Scan Begin	50 m/z	Hexapole RF	60.0 V	Set Pulsar Push	817 V
Scan End	3000 m/z	Skimmer 1	50.0 V	Set Reflector	1700 V
		Hexapole 1	24.3 V	Set Flight Tube	8600 V
				Set Detector TOF	2275 V



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e⁻
C 37 H 37 N 2 O 3	0.05	557.2799	1.27	2.14	20.50	ok	even
C 37 H 36 N 2 O 3	0.50	556.2720	-6.90	-5.37	21.00	-	odd

Mass Spectrum Molecular Formula Report

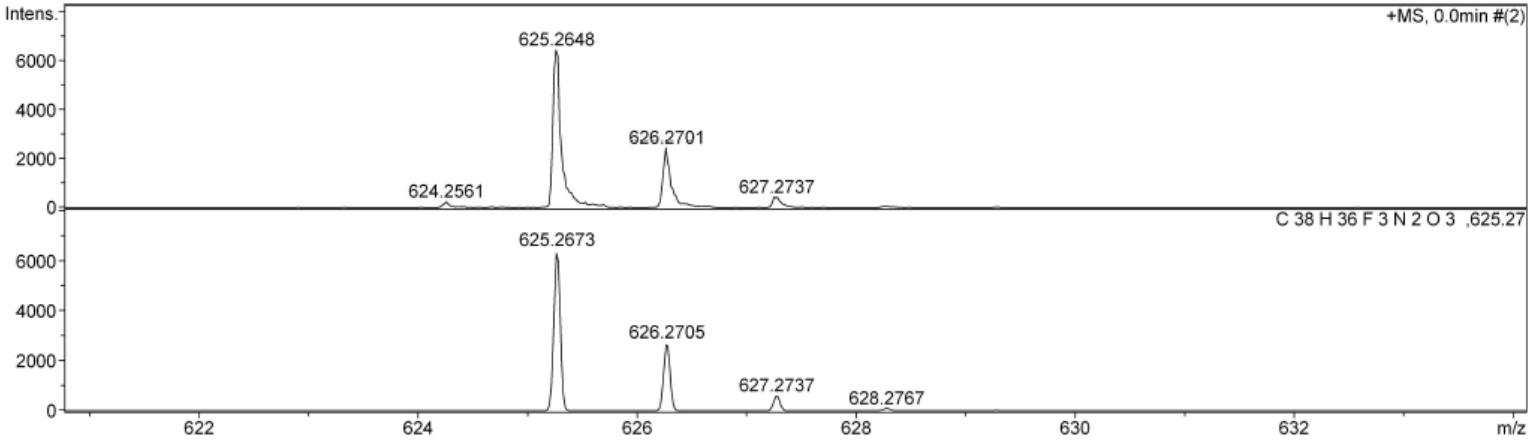


E-HBO 2

Acquisition Date	10/29/2015 11:05:30 AM
Operator	Administrator
Instrument	micrOTOF 66

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	65 V
Scan Range	n/a	Capillary Exit	80.0 V	Set Pulsar Pull	817 V
Scan Begin	50 m/z	Hexapole RF	60.0 V	Set Pulsar Push	817 V
Scan End	3000 m/z	Skimmer 1	50.0 V	Set Reflector	1700 V
		Hexapole 1	24.3 V	Set Flight Tube	8600 V
				Set Detector TOF	2275 V

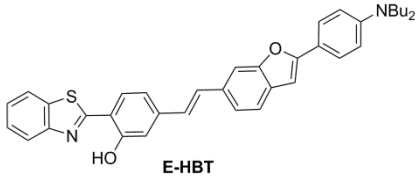


Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e⁻
C 38 H 36 F 3 N 2 O 3	0.03	625.2673	3.90	2.79	20.50	ok	even
C 38 H 35 F 3 N 2 O 3	0.58	624.2594	-3.38	-4.22	21.00	-	odd
C 38 H 34 F 3 N 2 O 3	0.73	623.2516	-10.90	-11.80	21.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

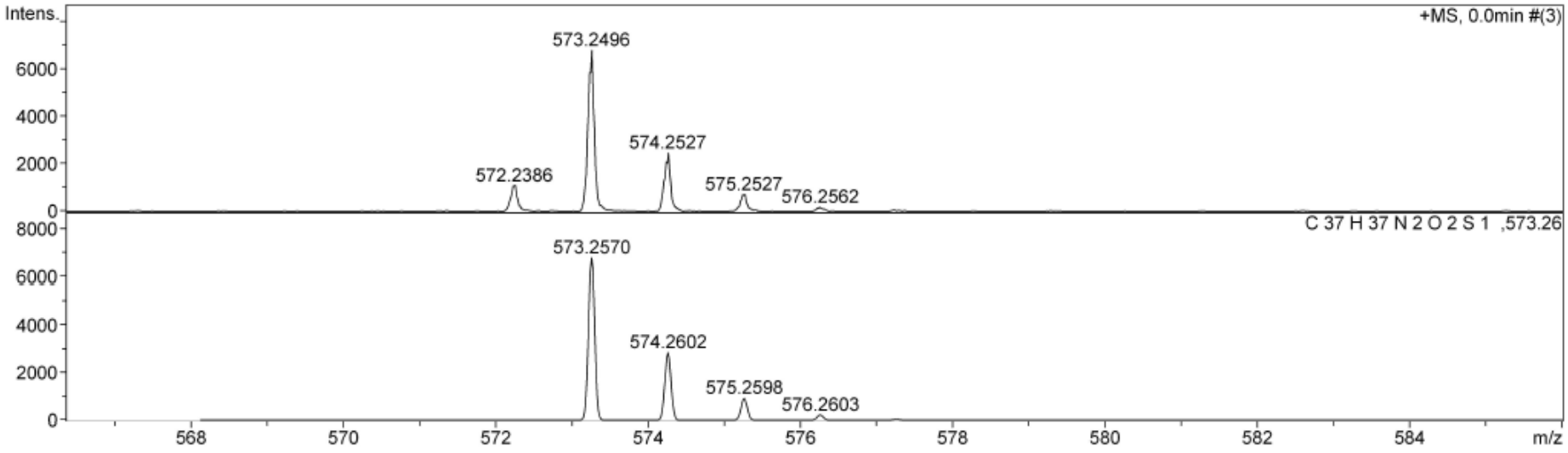
Analysis Name	D:\Data\Service masse 2015\O37884SK.d	Acquisition Date	11/27/2015 4:18:26 PM
Method	esi low pos.m	Operator	Administrator
Sample Name	MR14	Instrument	micrOTOF 66
Comment			



E-HBT

Acquisition Parameter

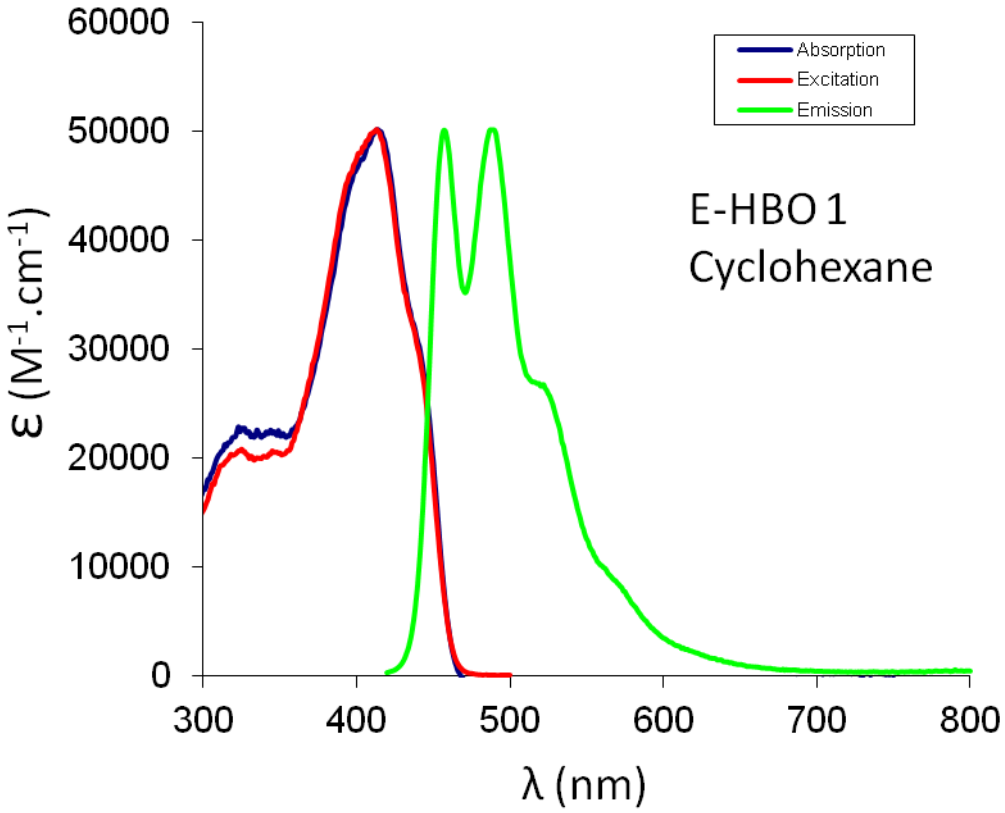
Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	74 V
Scan Range	n/a	Capillary Exit	80.0 V	Set Pulsar Pull	817 V
Scan Begin	50 m/z	Hexapole RF	60.0 V	Set Pulsar Push	810 V
Scan End	3000 m/z	Skimmer 1	50.0 V	Set Reflector	1700 V
		Hexapole 1	24.3 V	Set Flight Tube	8600 V
				Set Detector TOF	2275 V

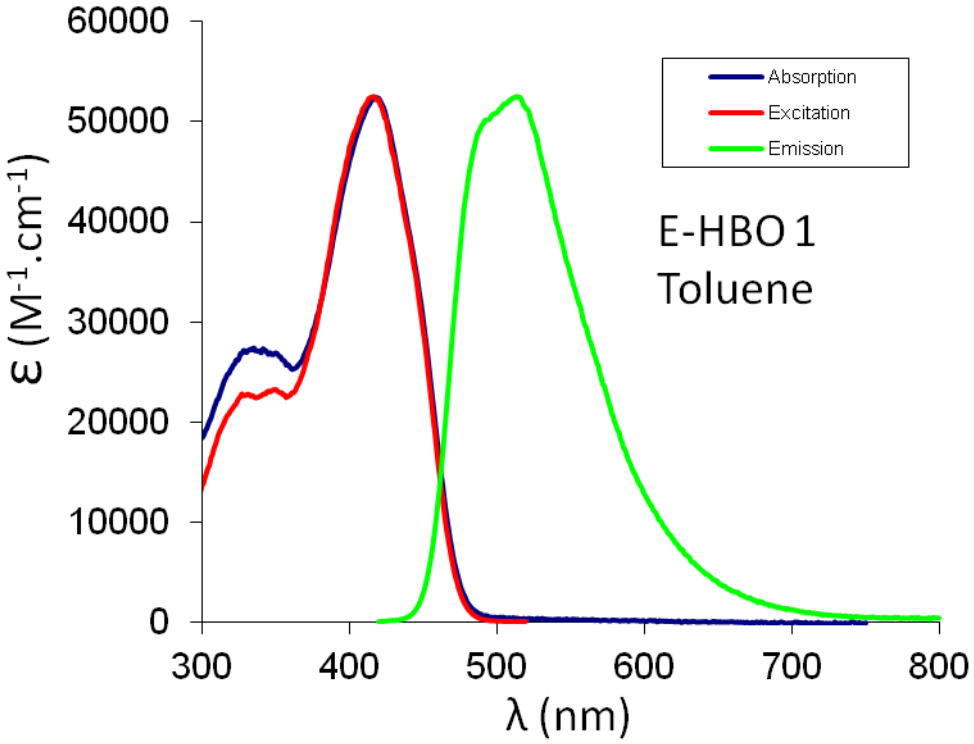


Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e⁻
C 37 H 37 N 2 O 2 S 1	0.03	573.2570	13.00	12.63	20.50	ok	even
C 37 H 36 N 2 O 2 S 1	0.52	572.2492	4.93	4.40	21.00	-	odd
C 37 H 35 N 2 O 2 S 1	0.69	571.2414	-9.43	-8.66	21.50	ok	even

Table S1. Photophysical data in solution at room temperature

Dye	λ_{abs} (nm)	ε ($M^{-1}.cm^{-1}$)	λ_{em} (nm)	Δ_{SS} (cm^{-1})	Φ_F [b]	τ (ns)	K_r ($10^8 s^{-1}$)	K_{nr} ($10^8 s^{-1}$)	Solvent
E-HBO1	414	49100	488	3600	0.85	1.2	7.08	1.25	cyclohexane
	418	51000	514	4400	0.75	1.3	5.77	1.92	toluene
	417	50000	592	6900	0.69	2.2	3.14	1.41	CH_2Cl_2
	386	60100	451	3700	0.56	0.9	6.22	4.89	$CH_2Cl_2 + HCl_g$
	412	58400	640	8400	0.41	2.1	1.95	2.81	Acetone
	412	41900	611	7700	0.40	1.5	2.67	4.00	EtOH
	416	55800	666	9000	0.20	1.6	1.25	5.00	CH_3CN
	426	41300	670	8600	0.18	1.5	1.20	5.47	DMSO
E-HBO2	423	31000	502	3700	0.91	1.3	7.00	0.69	cyclohexane
	423	38500	526	4900	0.80	1.5	5.33	1.33	toluene
	422	36000	619	7300	0.70	2.4	2.92	1.25	CH_2Cl_2
	387	50200	456	3700	0.52	0.9	6.56	4.56	$CH_2Cl_2 + HCl_g$
	418	37200	670	8900	0.16	2.4	0.67	3.5	Acetone
	416	25400	643	8300	0.18	1.0	1.80	8.20	EtOH
	426	36200	650	8100	0.12	0.6	2.00	14.7	DMSO
E-HBT	420	31800	496	3600	0.92	1.2	7.67	0.67	cyclohexane
	424	56000	521	4400	0.87	1.4	6.21	0.93	toluene
	423	63500	609	7100	0.67	2.4	2.79	1.38	CH_2Cl_2
	394	47200	461, 527	3500	0.16	1.0	1.07	5.60	$CH_2Cl_2 + HCl_g$
	418	40200	659	8700	0.26	1.6	1.63	4.63	Acetone
	416	28500	618	7800	0.12	1.4	0.86	6.29	EtOH
	416	53100	693	9400	0.09	0.9	1.00	10.01	CH_3CN


60000
50000
40000
30000
20000
10000
0
ε (M-1.cm-1)
300
400
500
600
700
800
λ (nm)
Absorption
Excitation
Emission
E-HBO 1
Cyclohexane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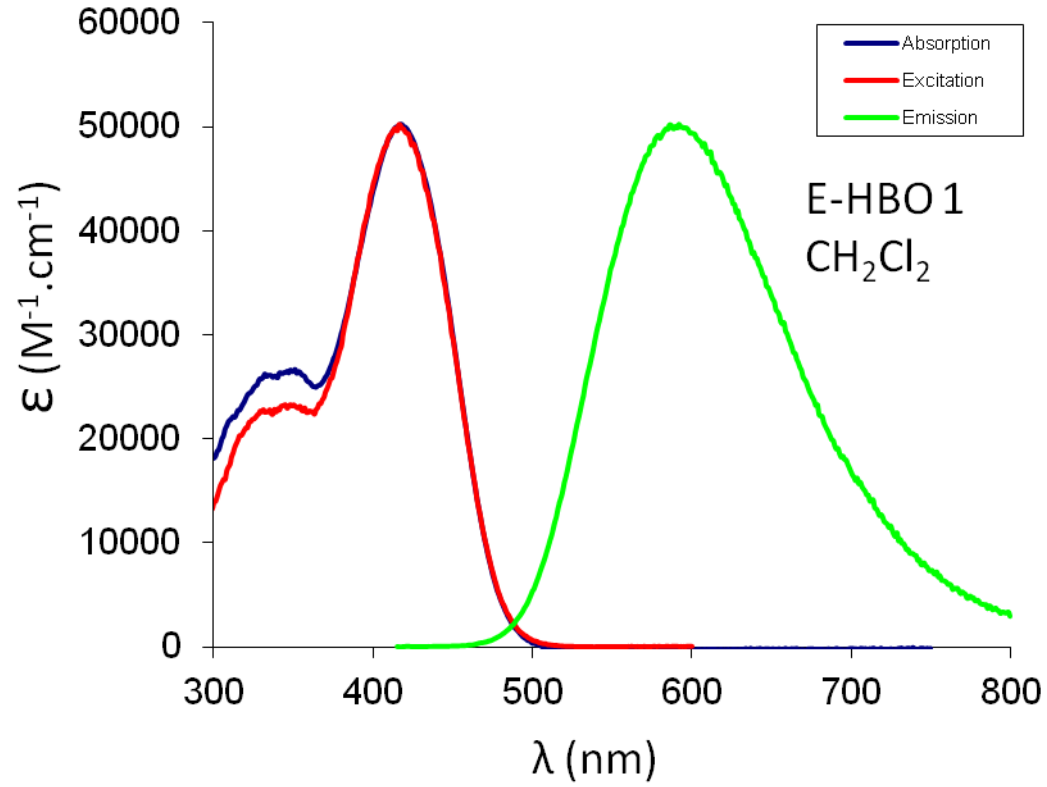
λ (nm)
Absorption
Excitation
Emission
E-HBO 1
Toluene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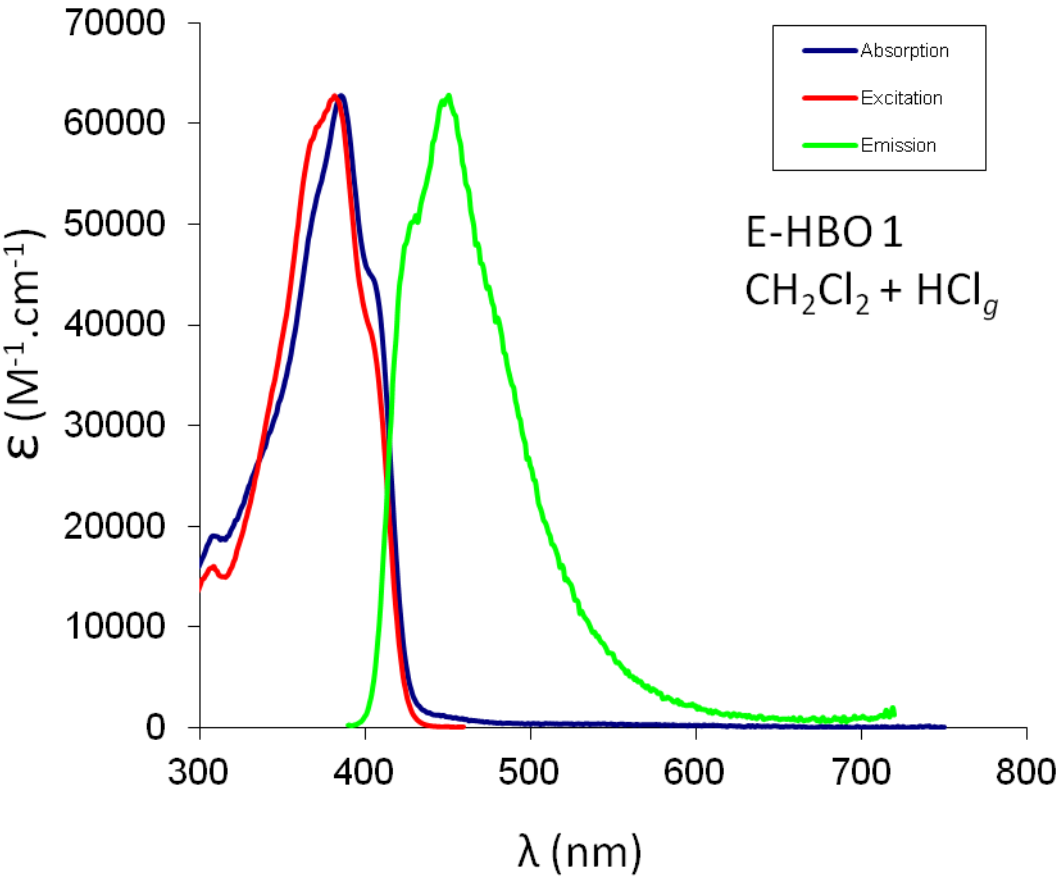
λ (nm)
Absorption
Excitation
Emission
E-HBO 1
CH2Cl2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ε (M-1.cm-1)
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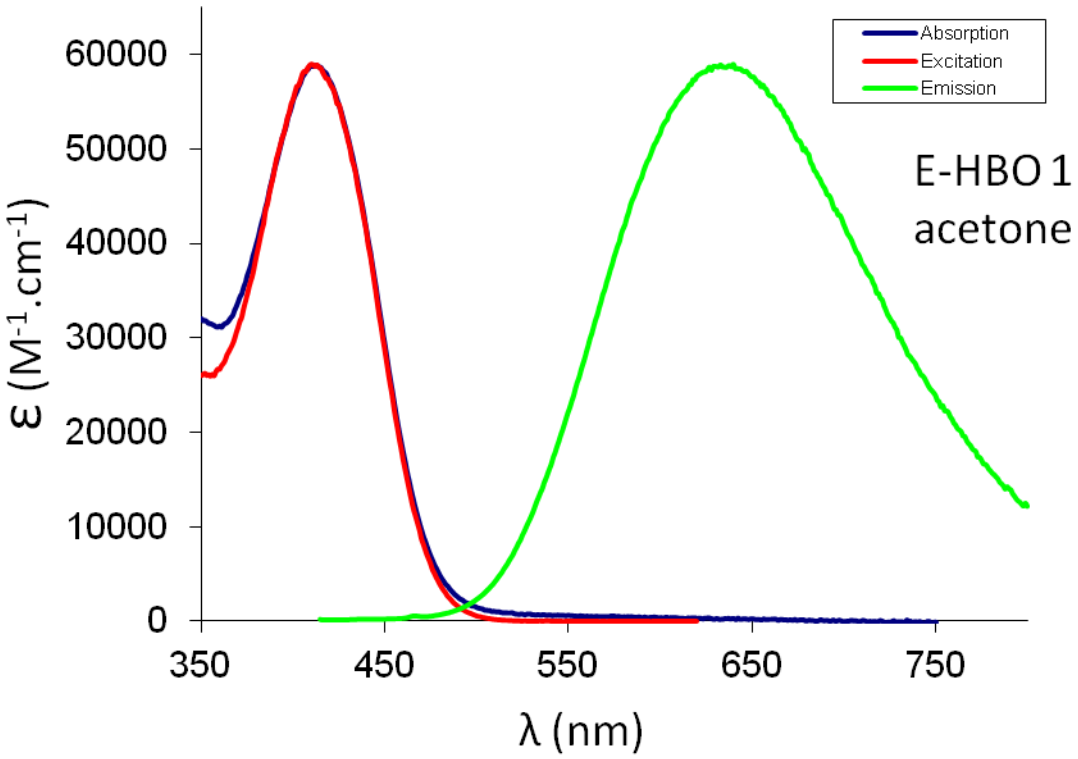
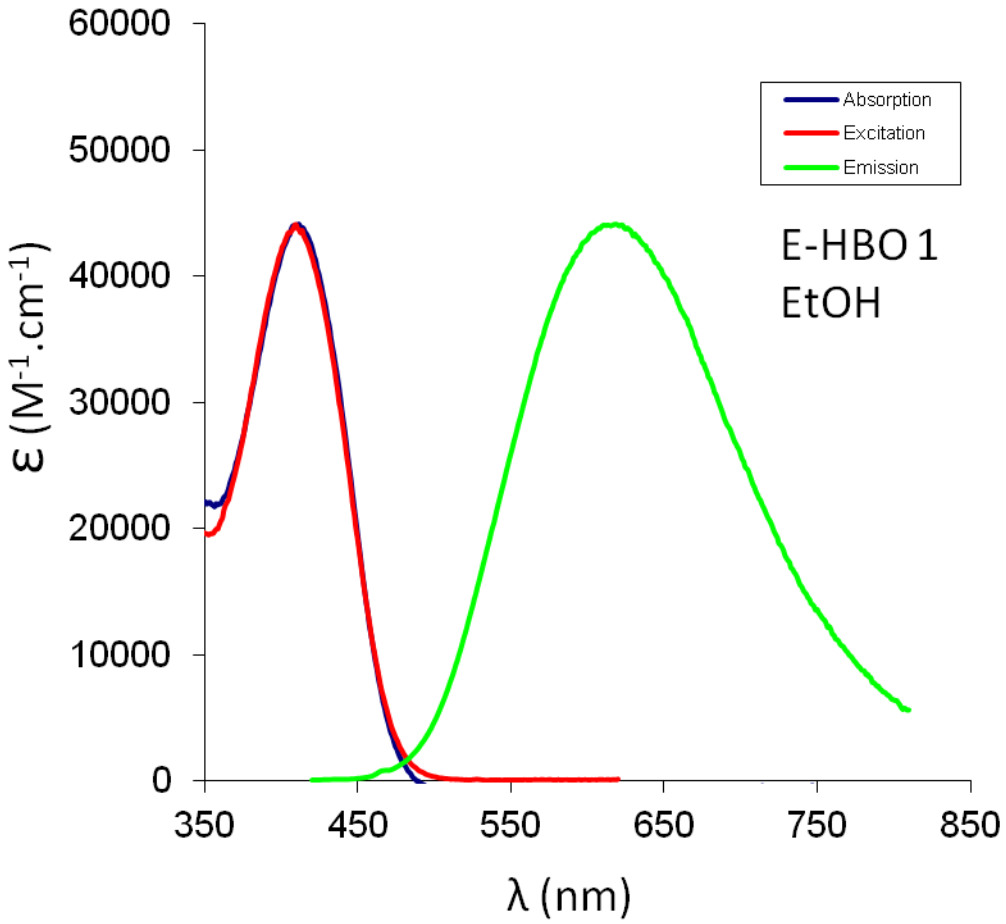
400
500
600
700
800
λ (nm)
Absorption
Excitation
Emission
E-HBO 1
CH2Cl2 + HClg


Absorption
Excitation
Emission
E-HBO 1
acetone
60000
50000
40000
30000
20000
10000
0
ε (M-1.cm-1)
350
450
550
650
750
λ (nm)


Absorption
Excitation
Emission
E-HBO 1
EtOH
60000
50000
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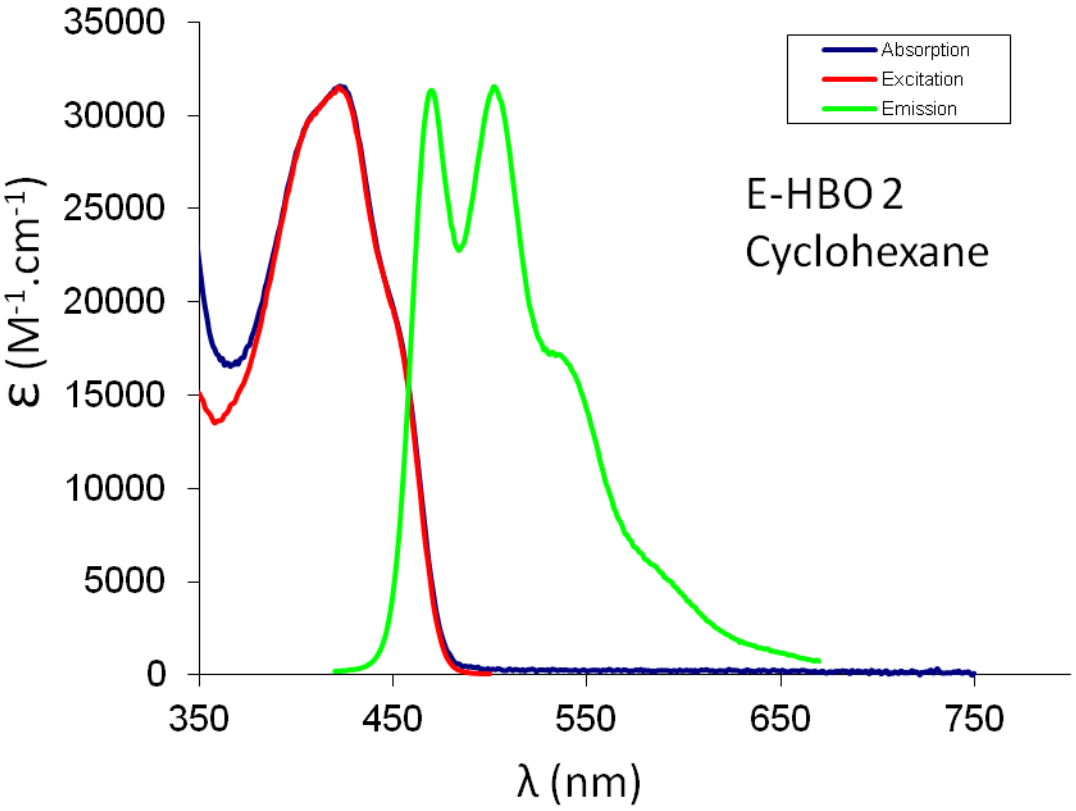
30000
20000
10000
0
ε (M-1.cm-1)
350
450
550
650
750
850
λ (nm)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30000
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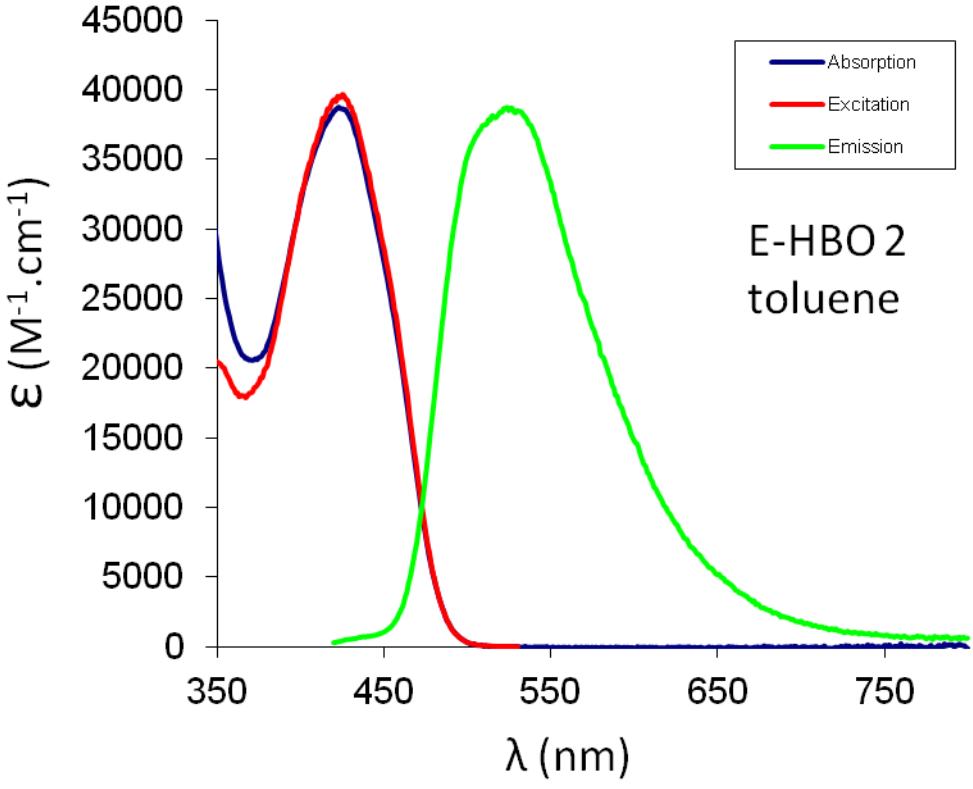
15000
10000
5000
0
ε (M-1.cm-1)
350
450
550
650
750
λ (nm)
Absorption
Excitation
Emission
E-HBO 2
Cyclohexane


45000
40000
35000
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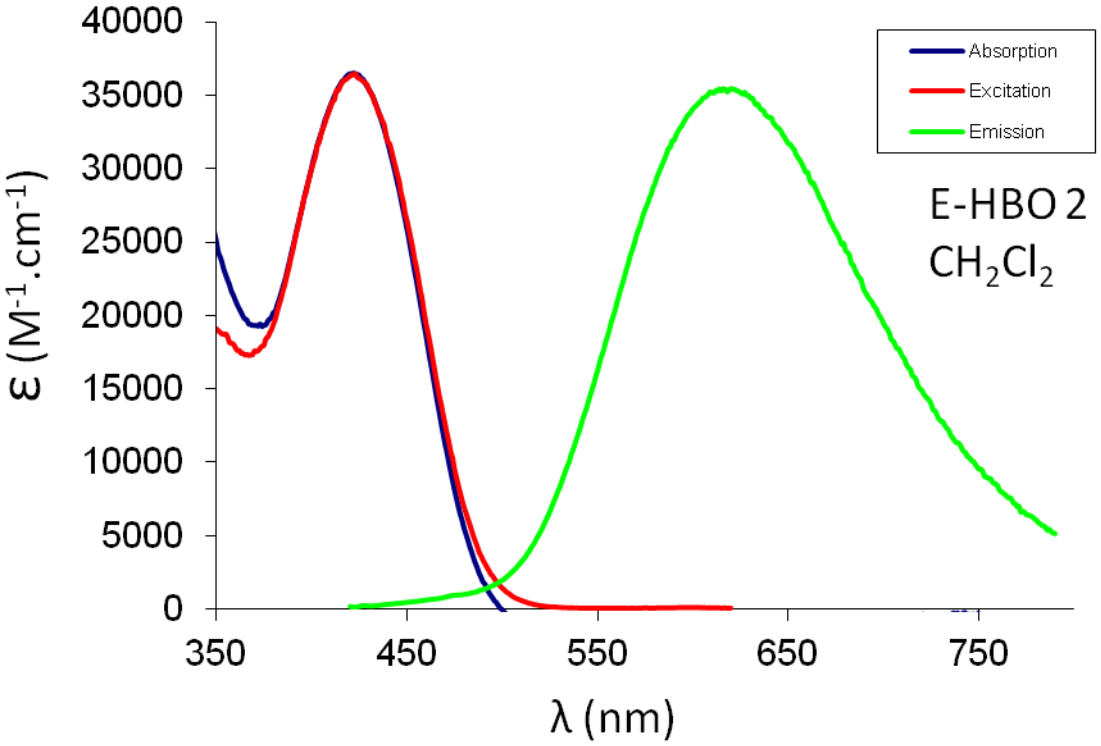
25000
20000
15000
10000
5000
0
ε (M-1.cm-1)
350
450
550
650
750
λ (nm)
Absorption
Excitation
Emission
E-HBO 2
toluene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35000
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20000
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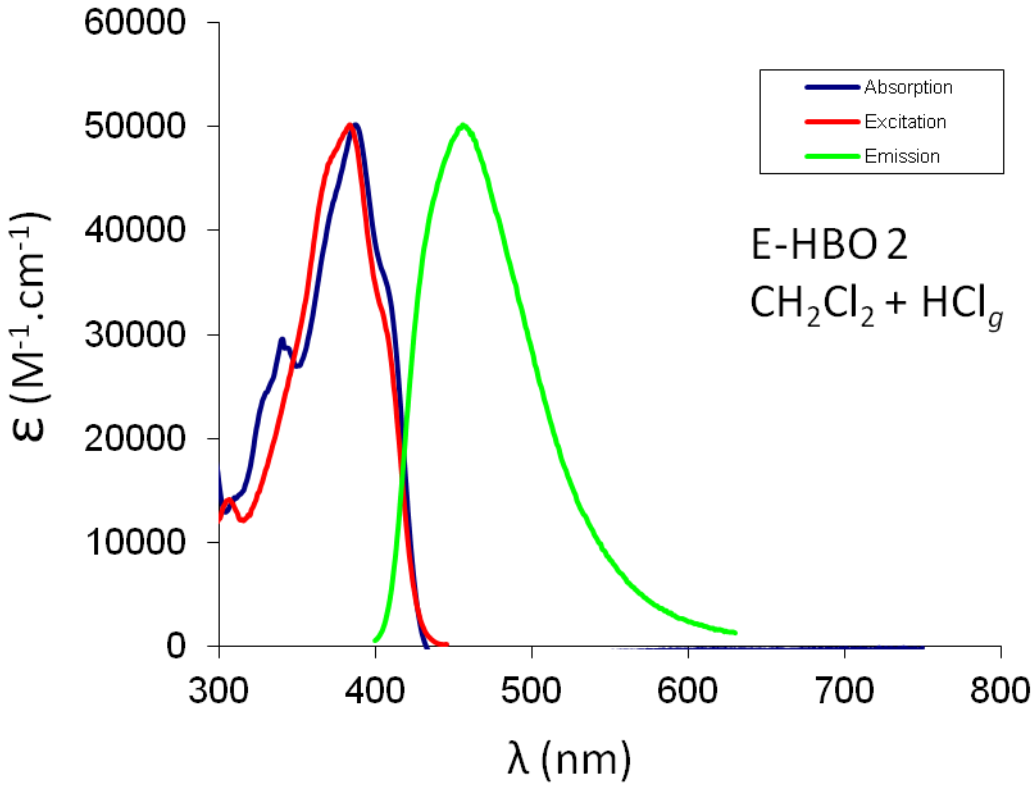
10000
5000
0
ε (M-1.cm-1)
350
450
550
650
750
λ (nm)
Absorption
Excitation
Emission
E-HBO 2
CH2Cl2


60000
50000
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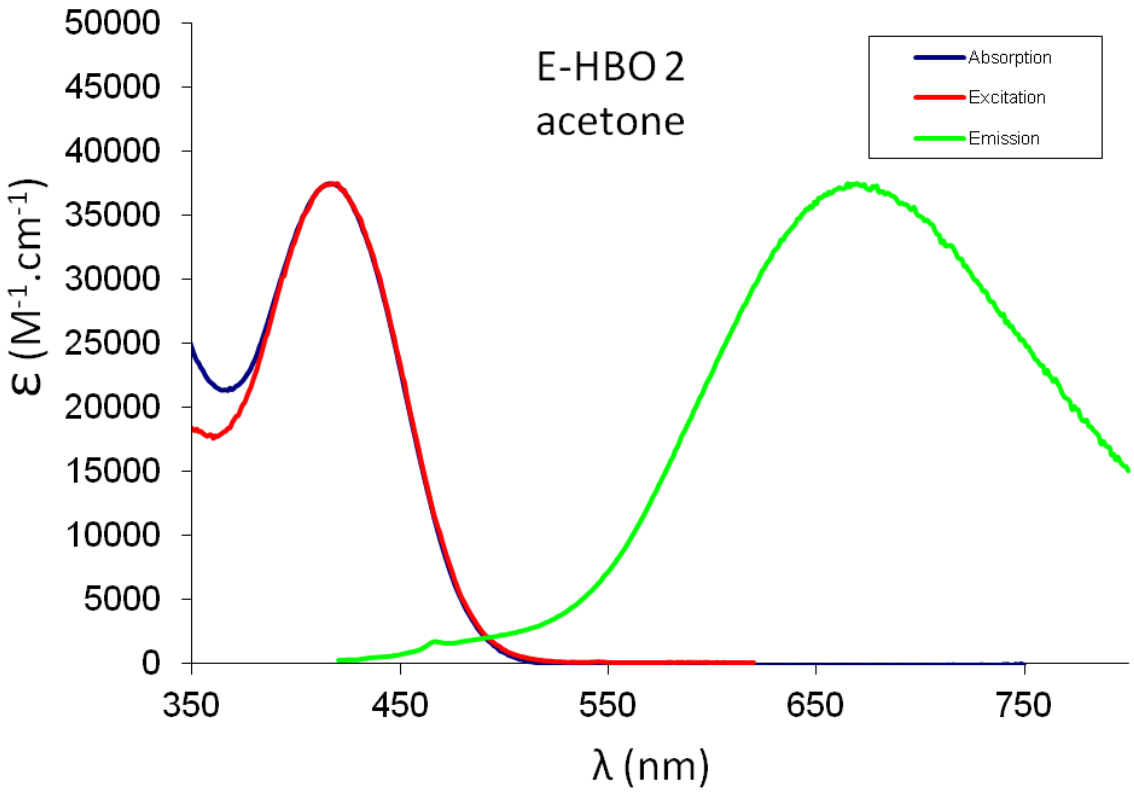
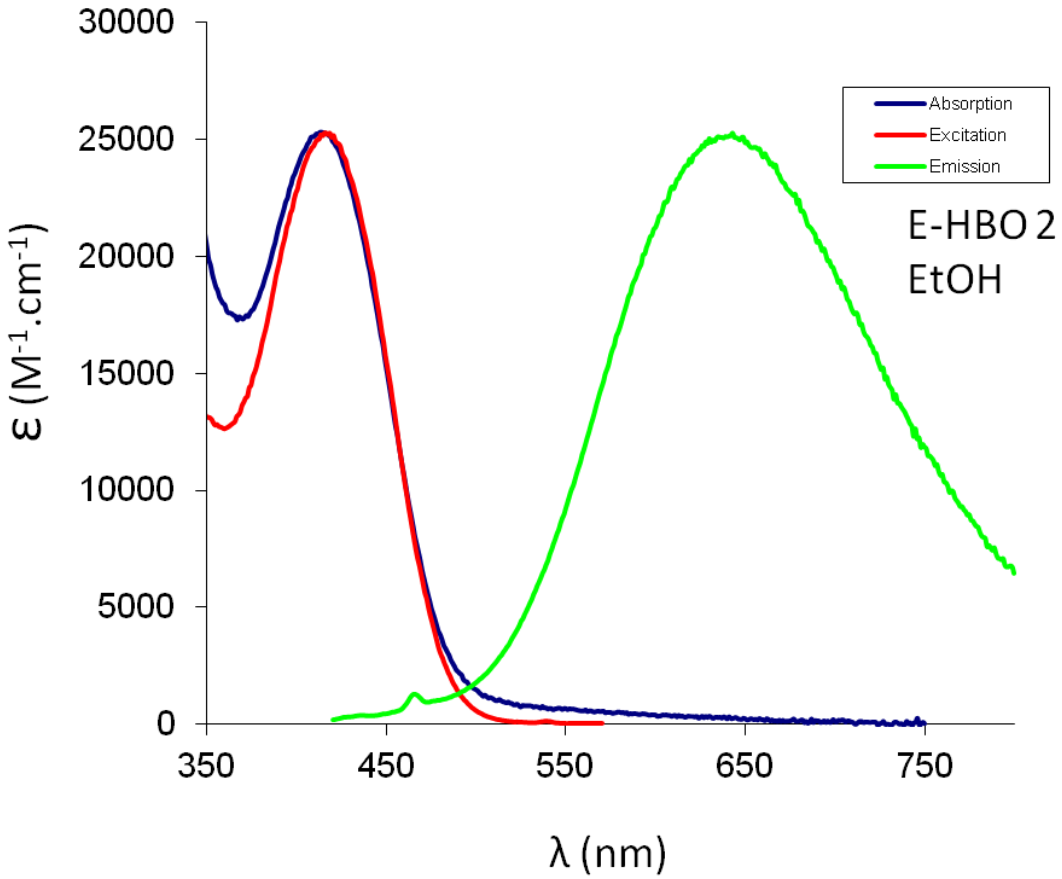
20000
10000
0
ε (M-1.cm-1)
300
400
500
600
700
800
λ (nm)
Absorption
Excitation
Emission
E-HBO 2
CH2Cl2 + HClg


E-HBO 2
acetone
Absorption
Excitation
Emission
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
ε (M-1.cm-1)
350
450
550
650
750
λ (nm)


E-HBO 2
EtOH
Absorption
Excitation
Emission
30000
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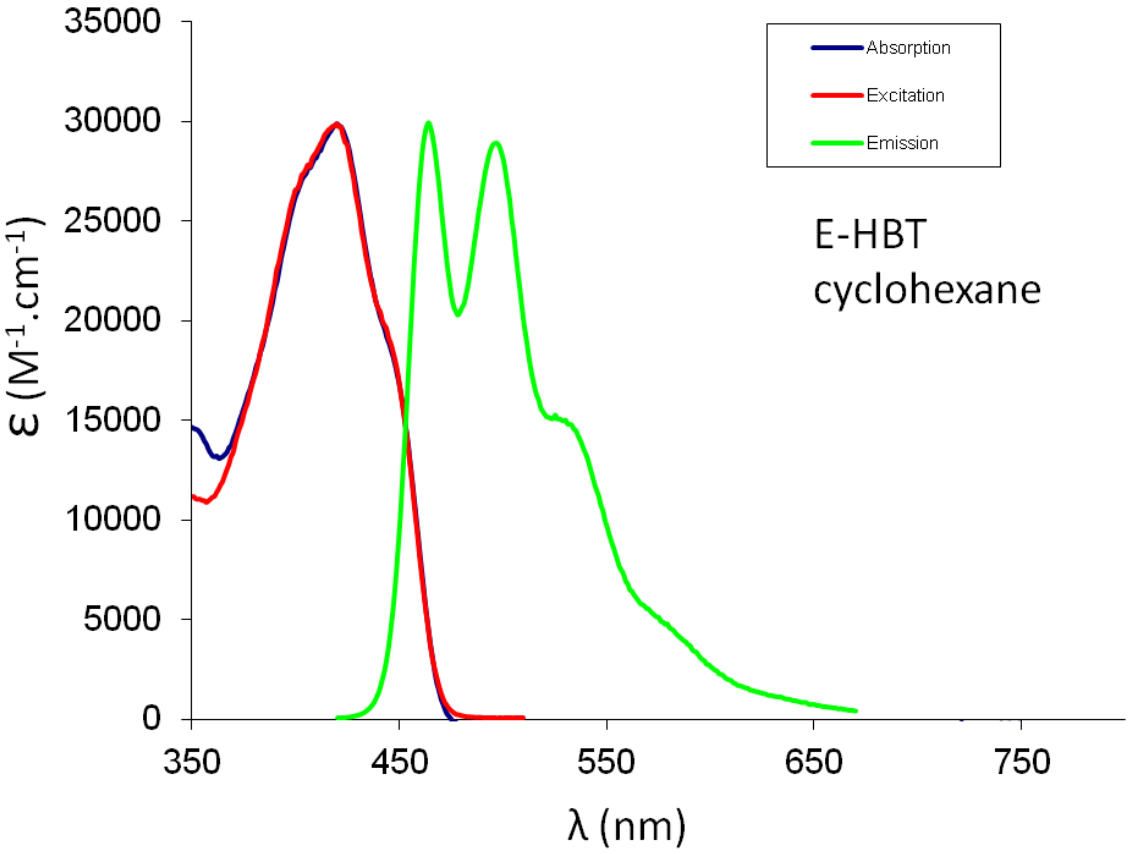
20000
15000
10000
5000
0
ε (M-1.cm-1)
350
450
550
650
750
λ (nm)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30000
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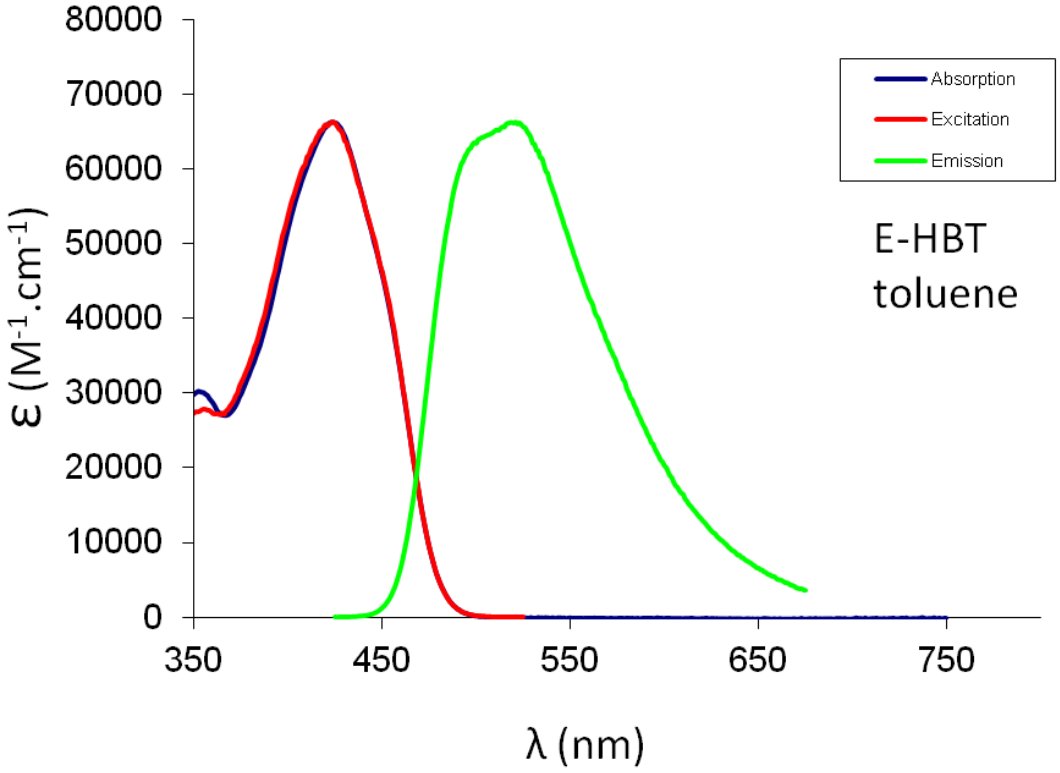
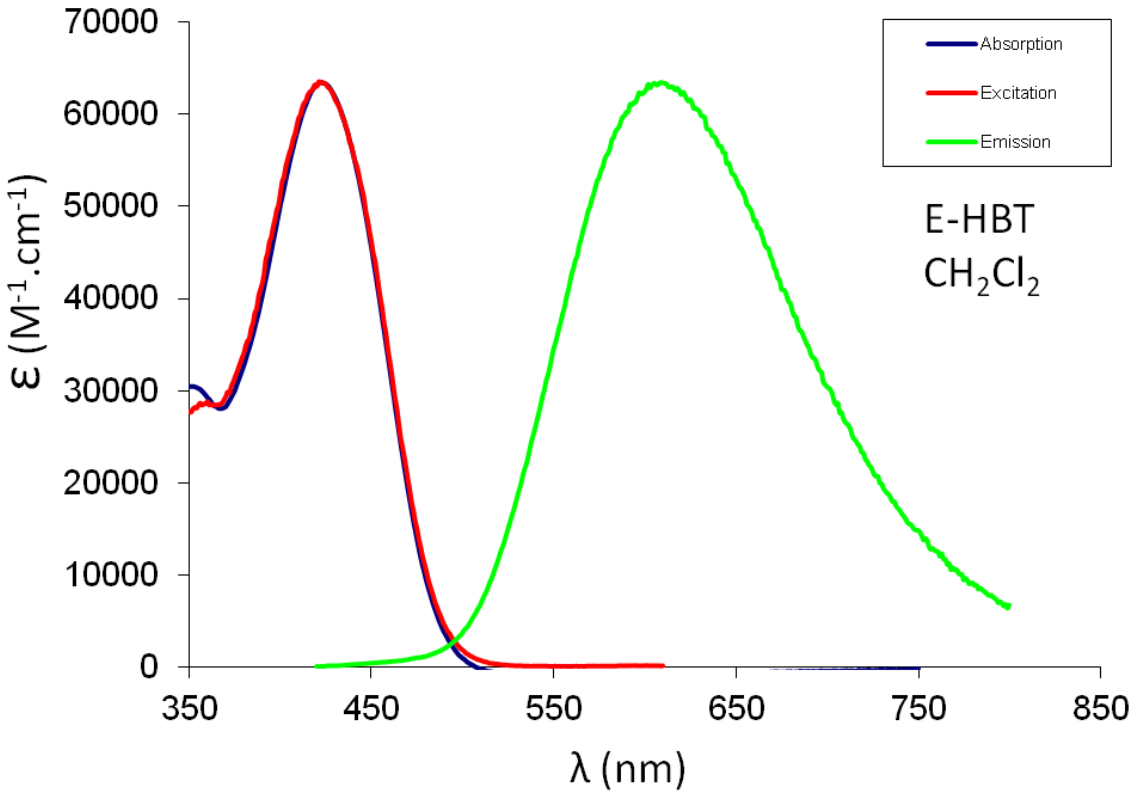
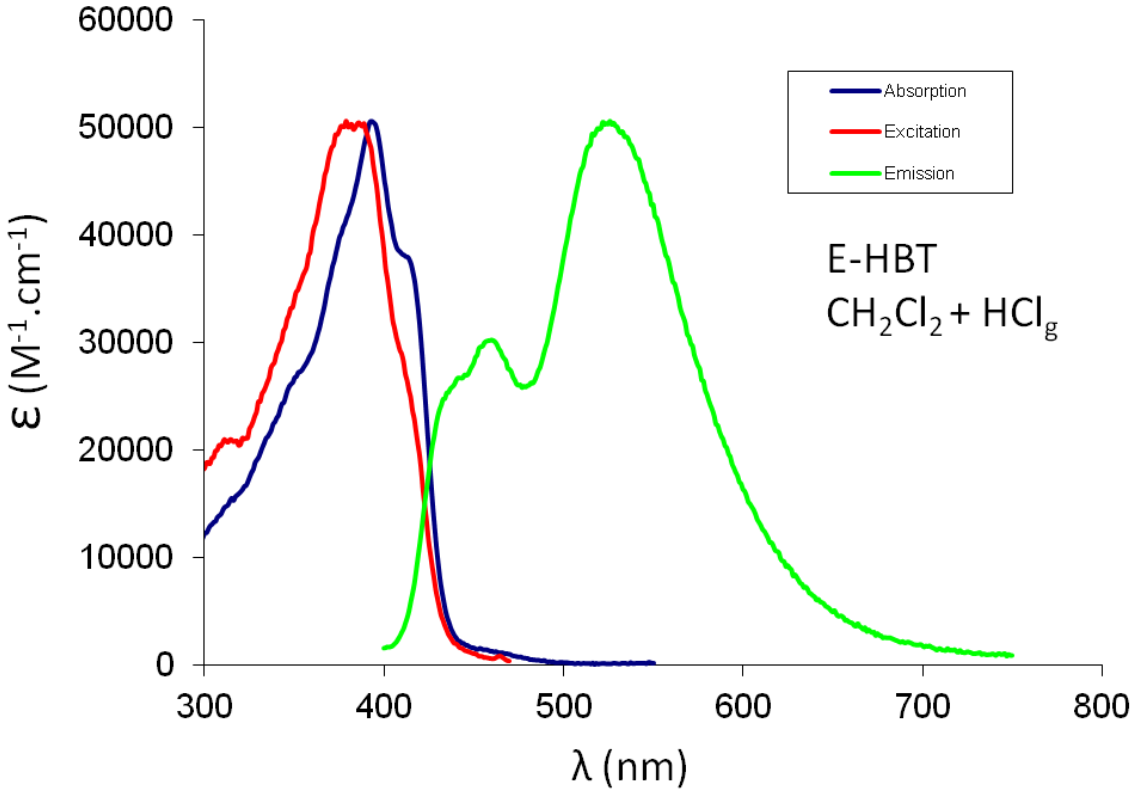
20000
15000
10000
5000
0
ε (M-1.cm-1)
350
450
550
650
750
λ (nm)
Absorption
Excitation
Emission
E-HBT
cyclohexane


80000
70000
60000
50000
40000
30000
20000
10000
0
ε (M-1.cm-1)
350
450
550
650
750
λ (nm)
Absorption
Excitation
Emission
E-HBT
toluene


70000
60000
50000
40000
30000
20000
10000
0
ε (M-1.cm-1)
350
450
550
650
750
850
λ (nm)
Absorption
Excitation
Emission
E-HBT
CH2Cl2


60000
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40000
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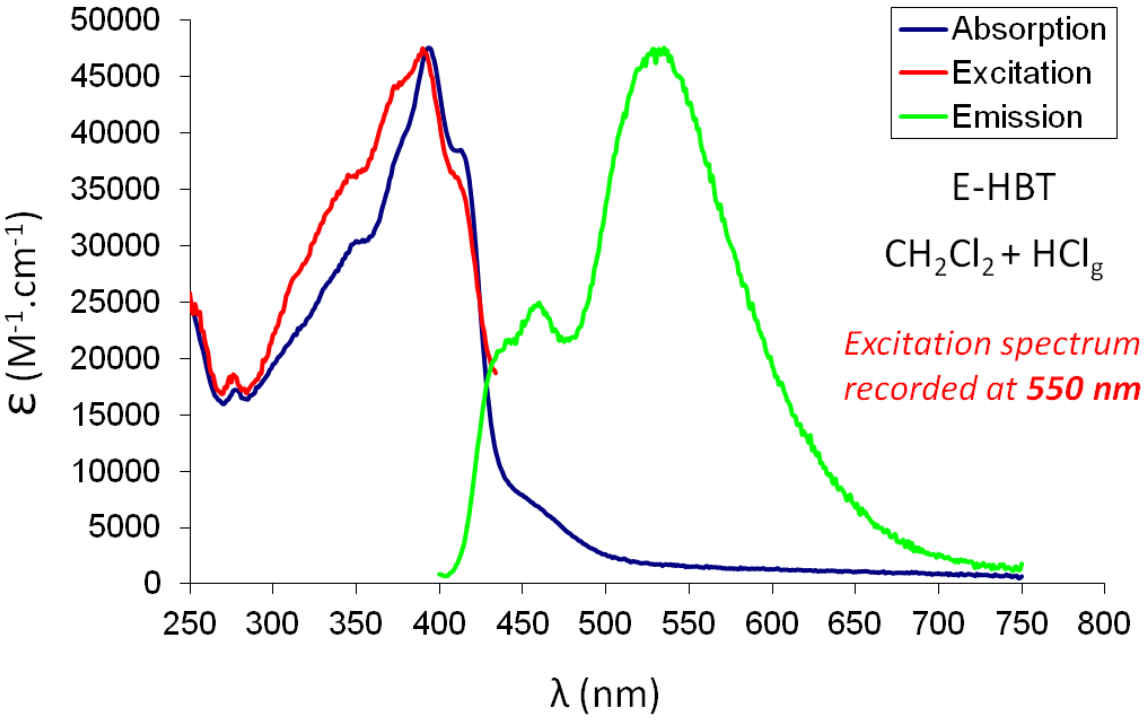
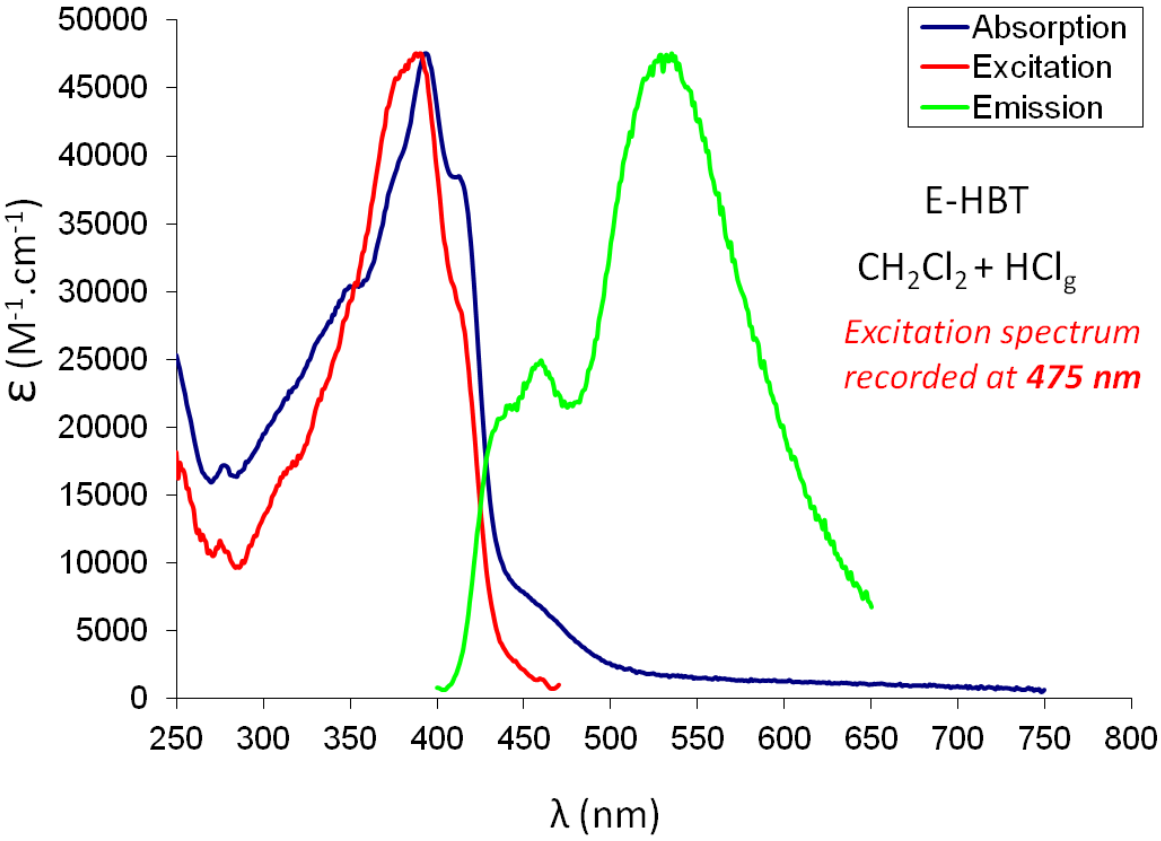
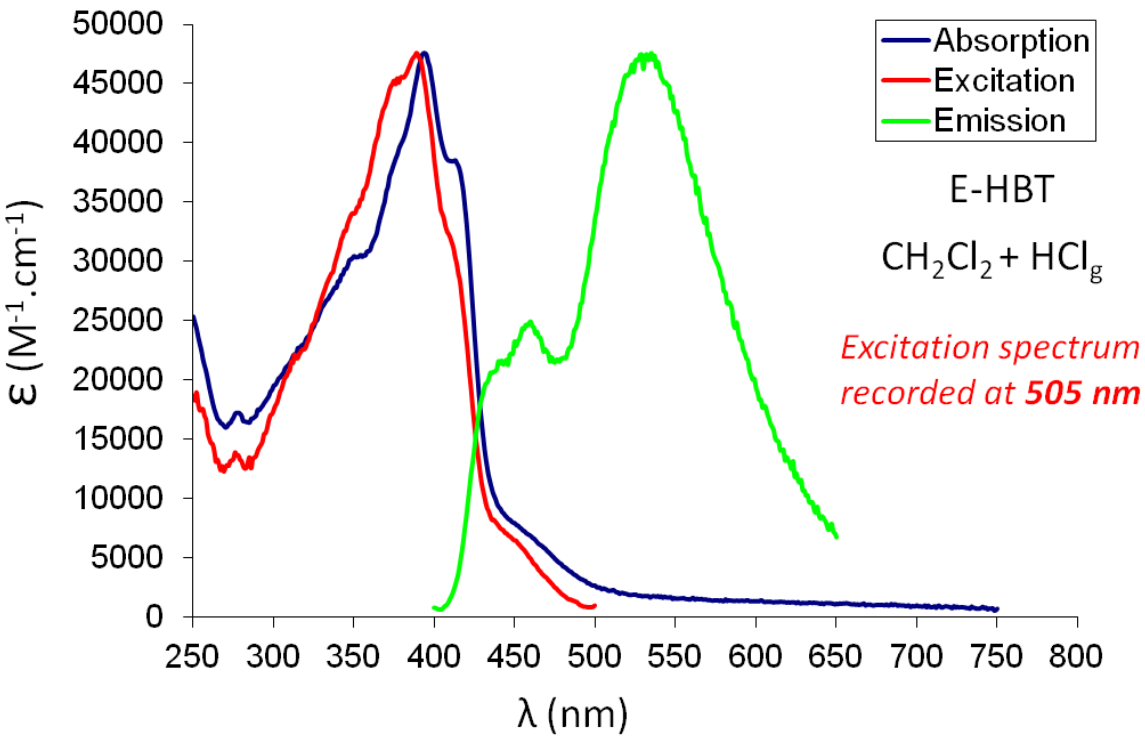
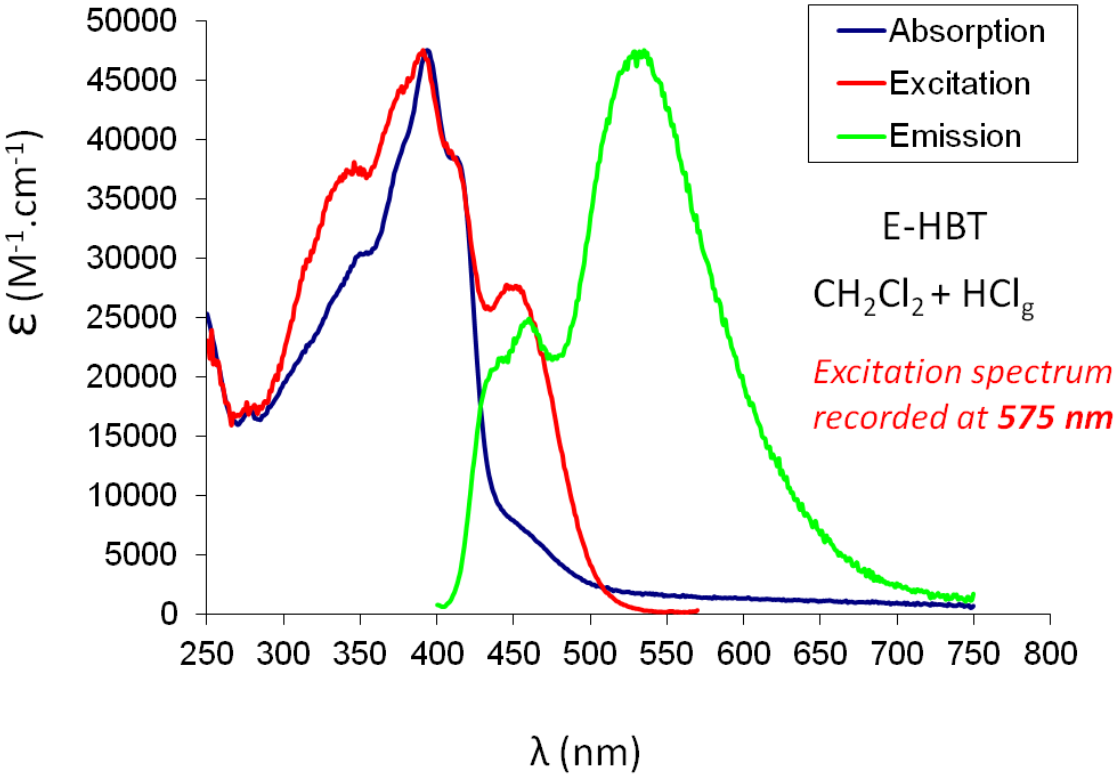
20000
10000
0
ε (M-1.cm-1)
300
400
500
600
700
800
λ (nm)
Absorption
Excitation
Emission
E-HBT
CH2Cl2 + HClg


Absorption
Excitation
Emission
E-HBT
$CH_2Cl_2 + HCl_g$
*Excitation spectrum recorded at **550 nm***
ε ($M^{-1}.cm^{-1}$)
λ (nm)


Absorption
Excitation
Emission
E-HBT
$CH_2Cl_2 + HCl_g$
*Excitation spectrum recorded at **475 nm***
ε ($M^{-1}.cm^{-1}$)
λ (nm)


50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
ε (M-1.cm-1)
250 300 350 400 450 500 550 600 650 700 750 800
λ (nm)
Absorption
Excitation
Emission
E-HBT
CH2Cl2 + HClg
Excitation spectrum
recorded at 505 nm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40000
35000
30000
25000
20000
15000
10000
5000
0
ε (M-1.cm-1)
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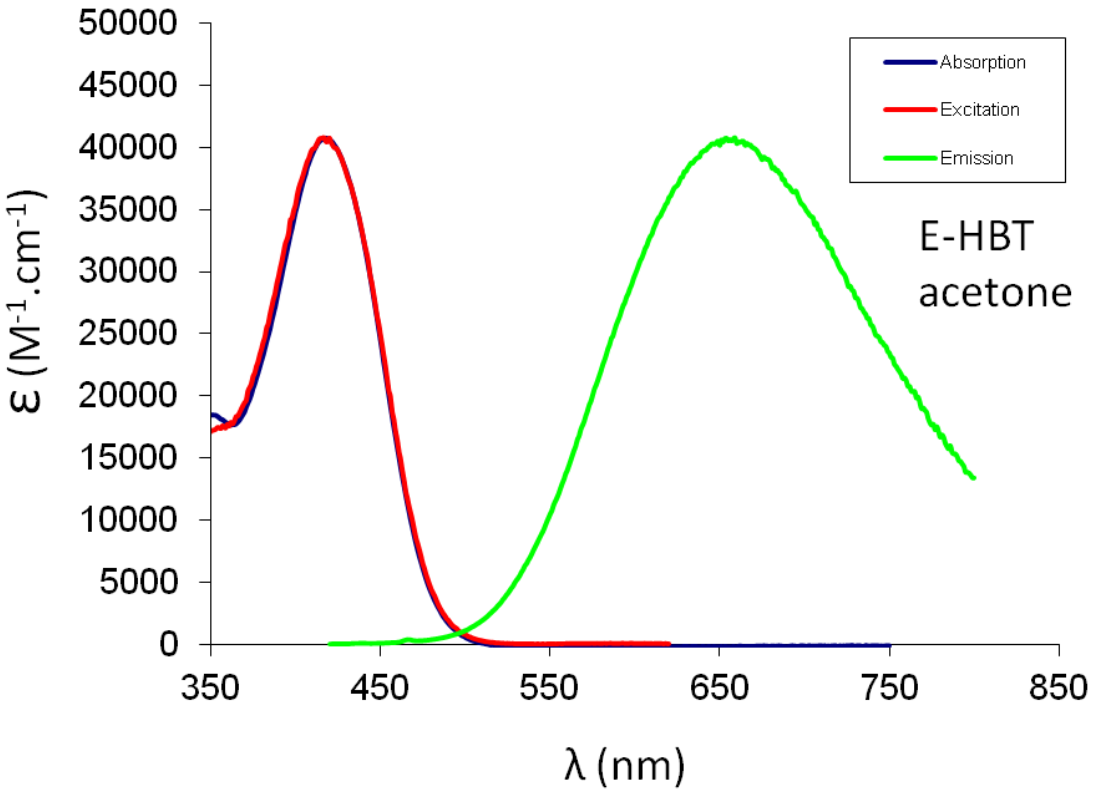
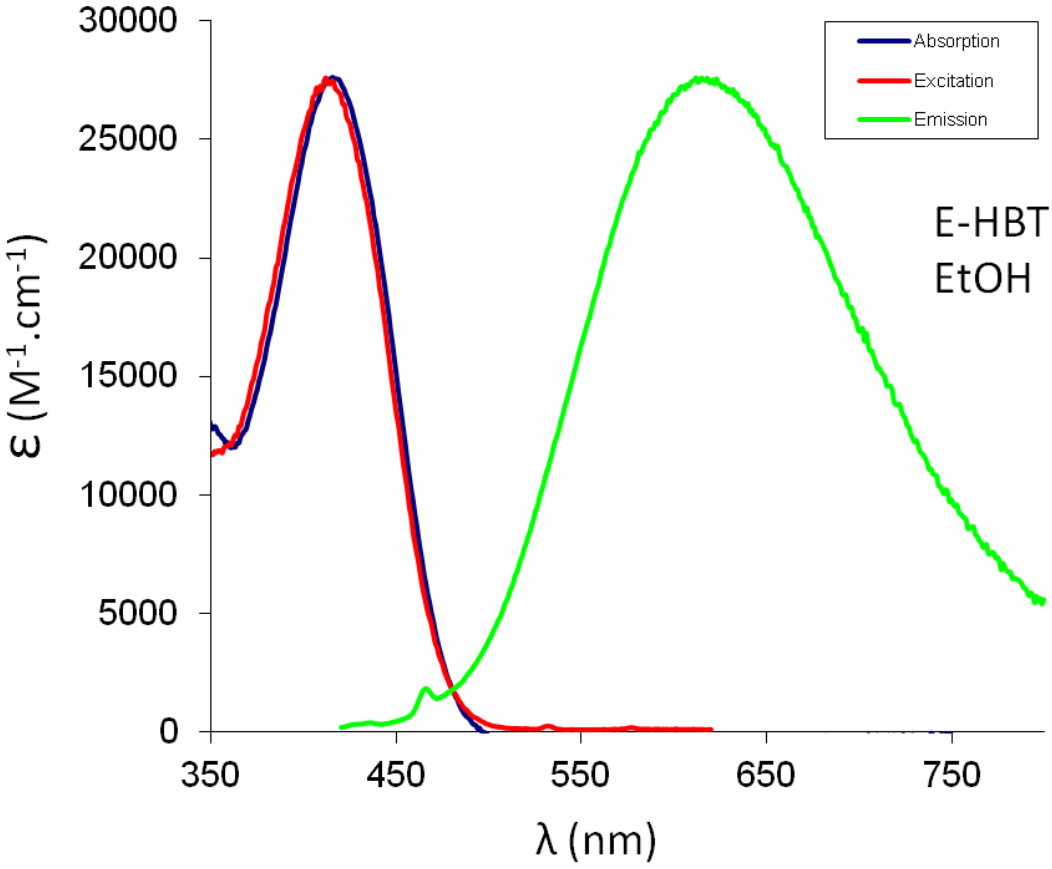
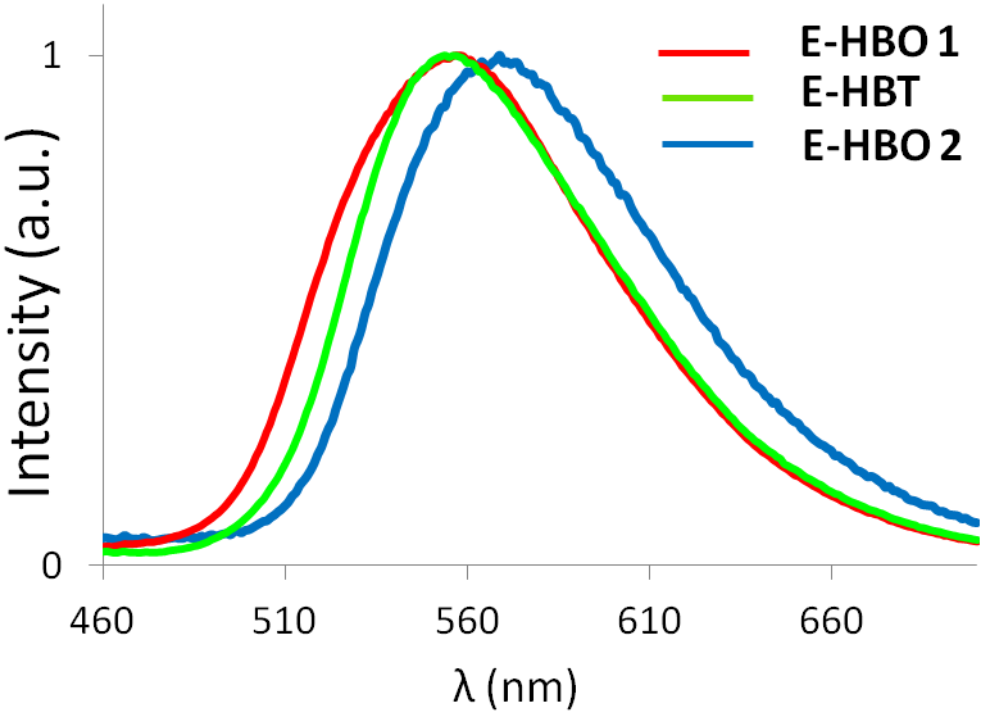
λ (nm)
Absorption
Excitation
Emission
E-HBT
CH2Cl2 + HClg
Excitation spectrum
recorded at 575 nm





S6 Solid-state spectroscopic data


E-HBO 1
E-HBT
E-HBO 2
Intensity (a.u.)
1
0
460
510
560
610
660
λ (nm)

S7 Lippert-Mataga plot

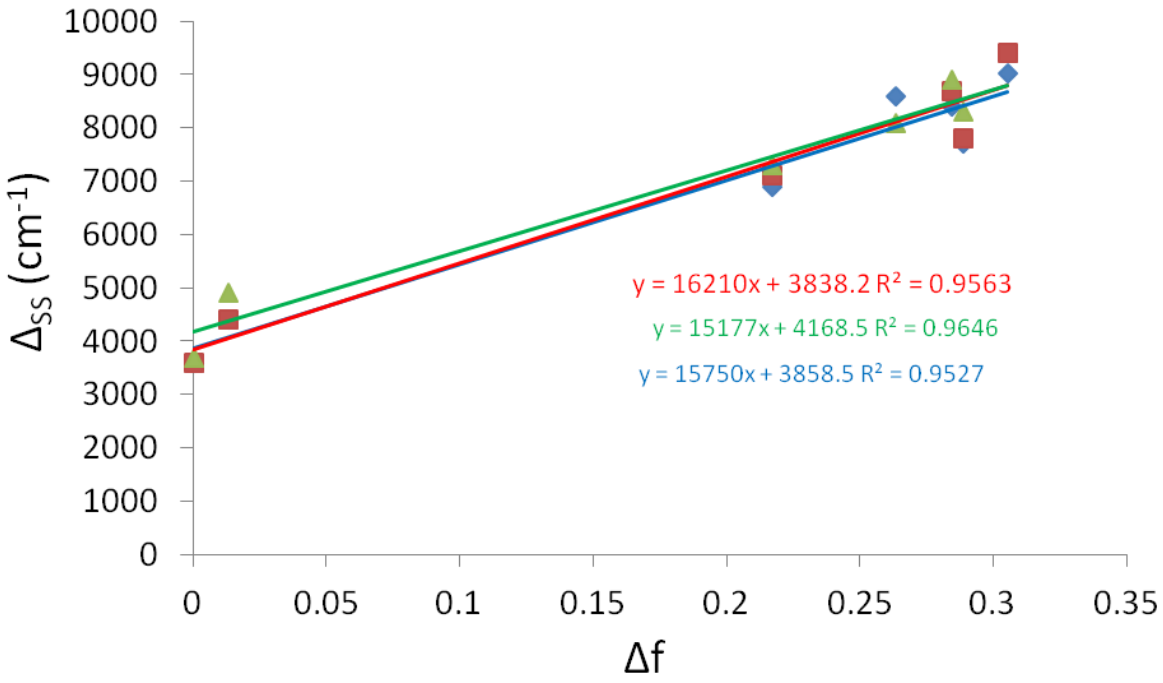


Figure S1. Lippert-Mataga plot for **E-HBO 1**(blue), **E-HBO 2** (green) and **E-HBT** (red)

The Stokes shift Δ_{SS} (cm^{-1}) was plotted against the orientation polarizability Δf for the different solvents listed in Table S1.
Δf is obtained for each solvent using the following equation:

$$\Delta f = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1}$$

where ε is the dielectric constant and n is the refractive index of the solvent.[5]

The Lippert-Mataga equation[6] can be used to correlate the energy difference between absorption ($h\nu_{abs}$) and emission ($h\nu_{em}$), also known as Stokes' shift (Δ_{SS}), with solvent polarity represented by Δf. The Lippert-Mataga relation is based on the assumption that the energy difference is only proportional to the solvent orientation polarizability (known as the general solvent effect).
The Lippert-Mataga equation is as follow:

$$\Delta_{SS} = \nu_{abs} - \nu_{em} = \frac{2\,\Delta\mu^2}{hc\,a^3}\left(\frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1}\right) + \text{constant}$$

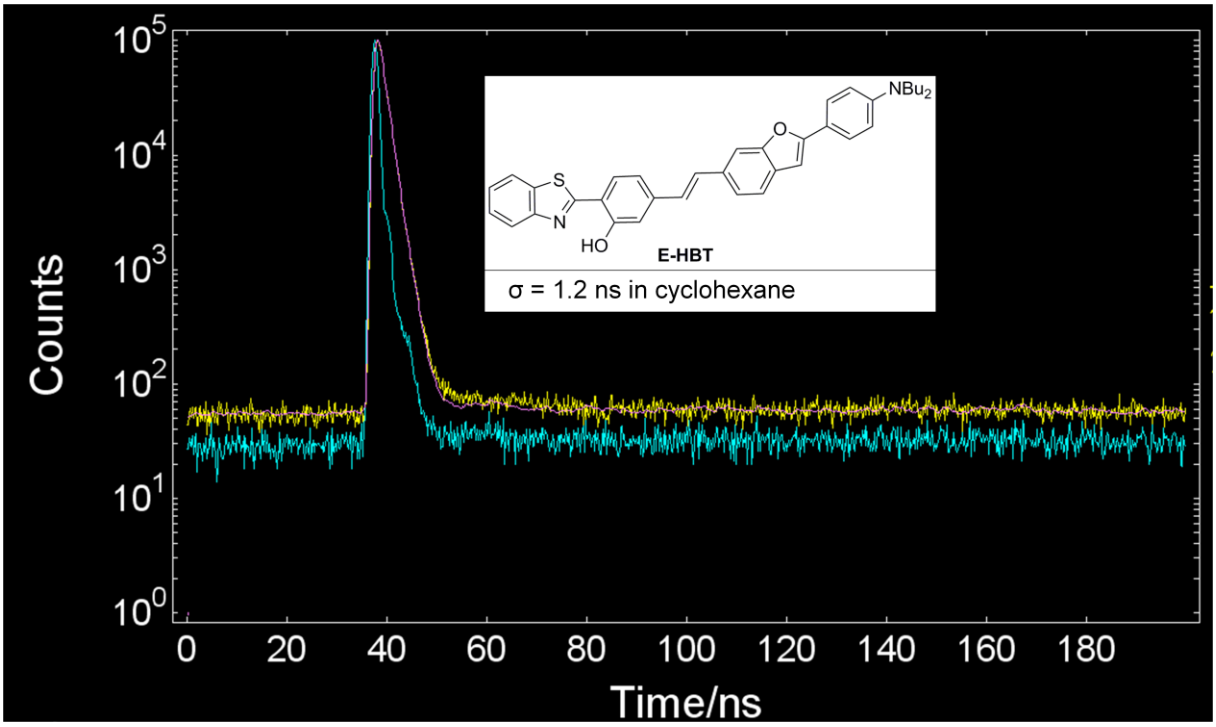
where ν_{abs} and ν_{em} are the wavenumbers (cm^{-1}) corresponding to the absorption and the emission, respectively, h is Planck's constant, c is the speed of light, and a is the Onsager radius of the solvent cavity in which the fluorophore resides.
From this equation, it can be deducted:

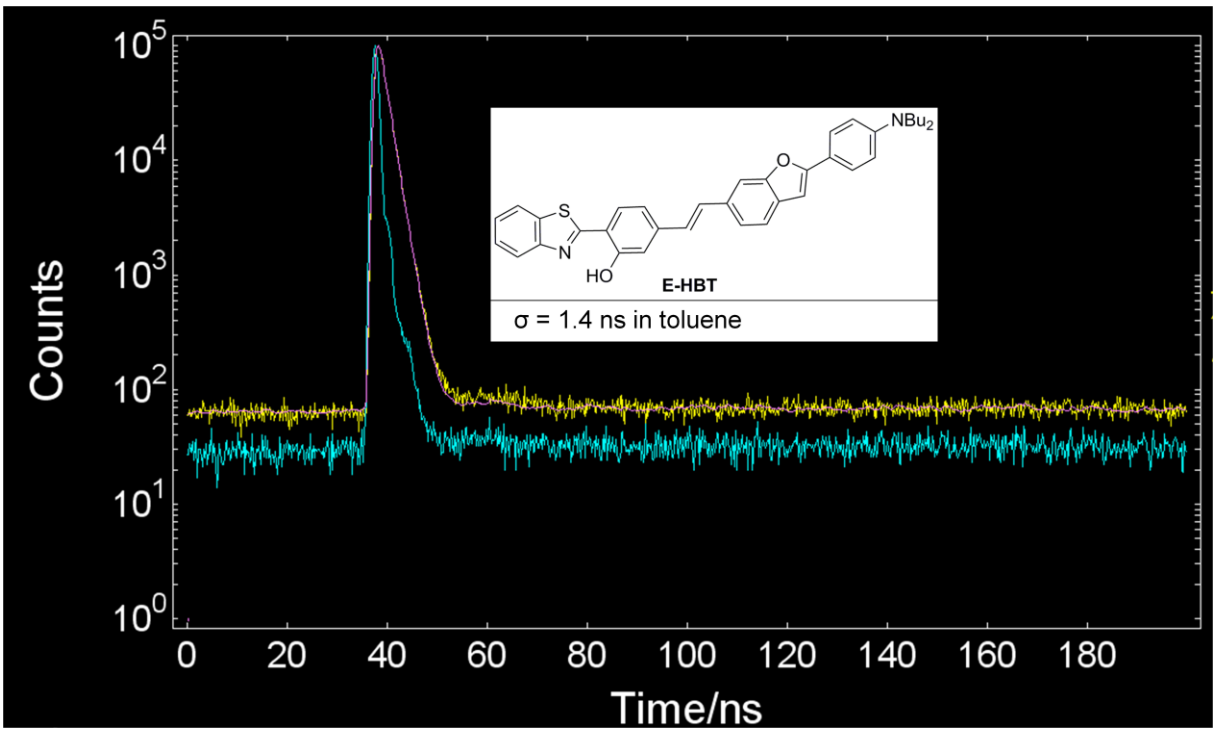
$$\text{Slope} = \frac{2\,\Delta\mu^2}{hc\,a^3}$$

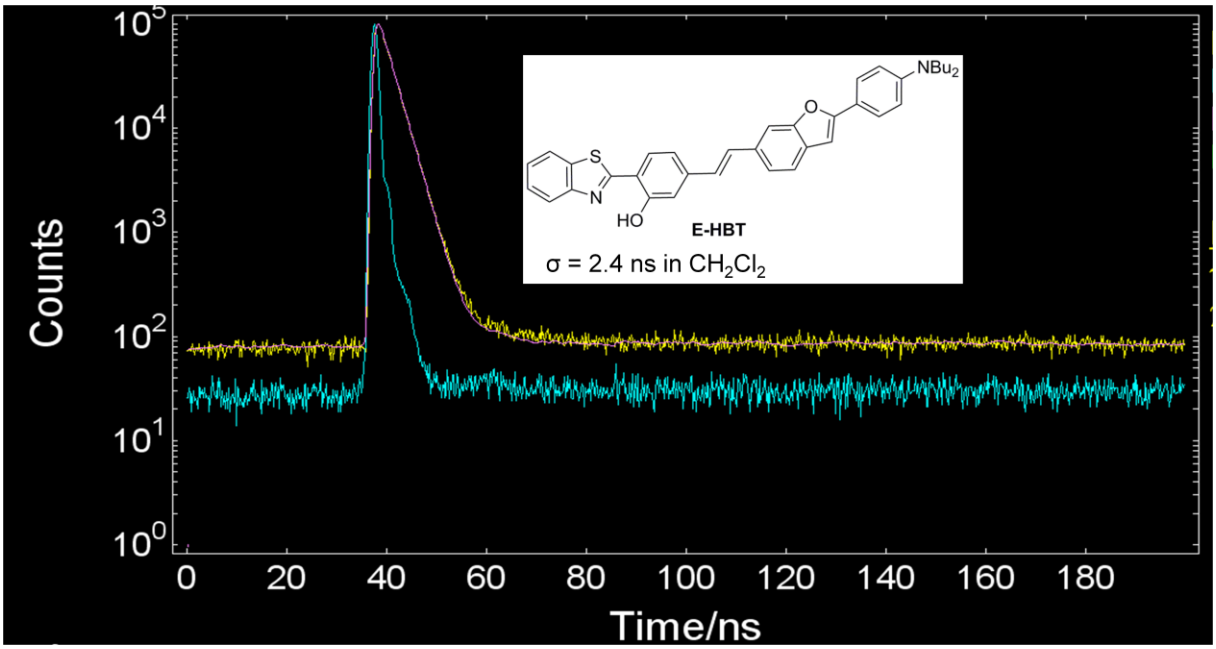
where $\Delta\mu$ is the dipole moment difference between the ground and excited states.
Based on the assumption that the Onsager cavity radius a equals 5.3 Å, which is half of the optimized distance between the two farthest atoms of the molecule in the direction of charge separation (10.61 Å)[7] and on the slopes determined on Fig.S1, $\Delta\mu$ can be estimated for each probe; 15.3 D for **E-HBO1**, 14.9 D for **E-HBO2** and 15.5 D for **E-HBT**, which is in the range of values reported for similar solvatochromic structures (3-20D).[8]

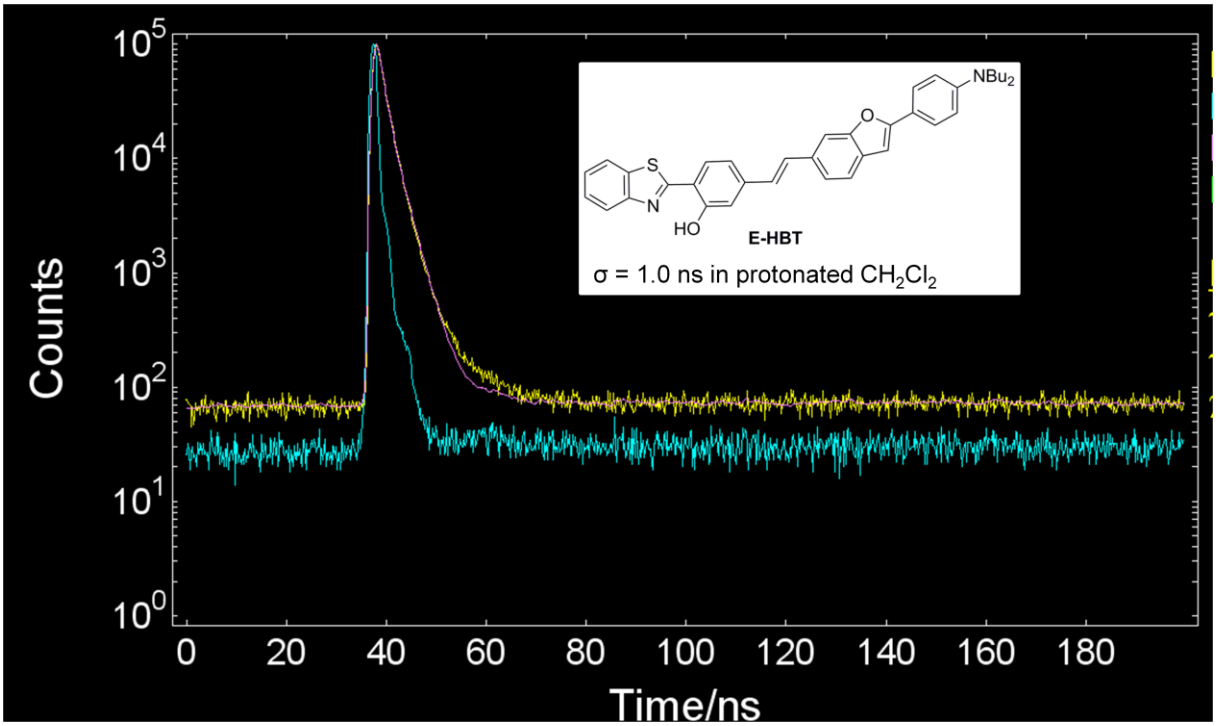
S8.Fluorescence decay curves

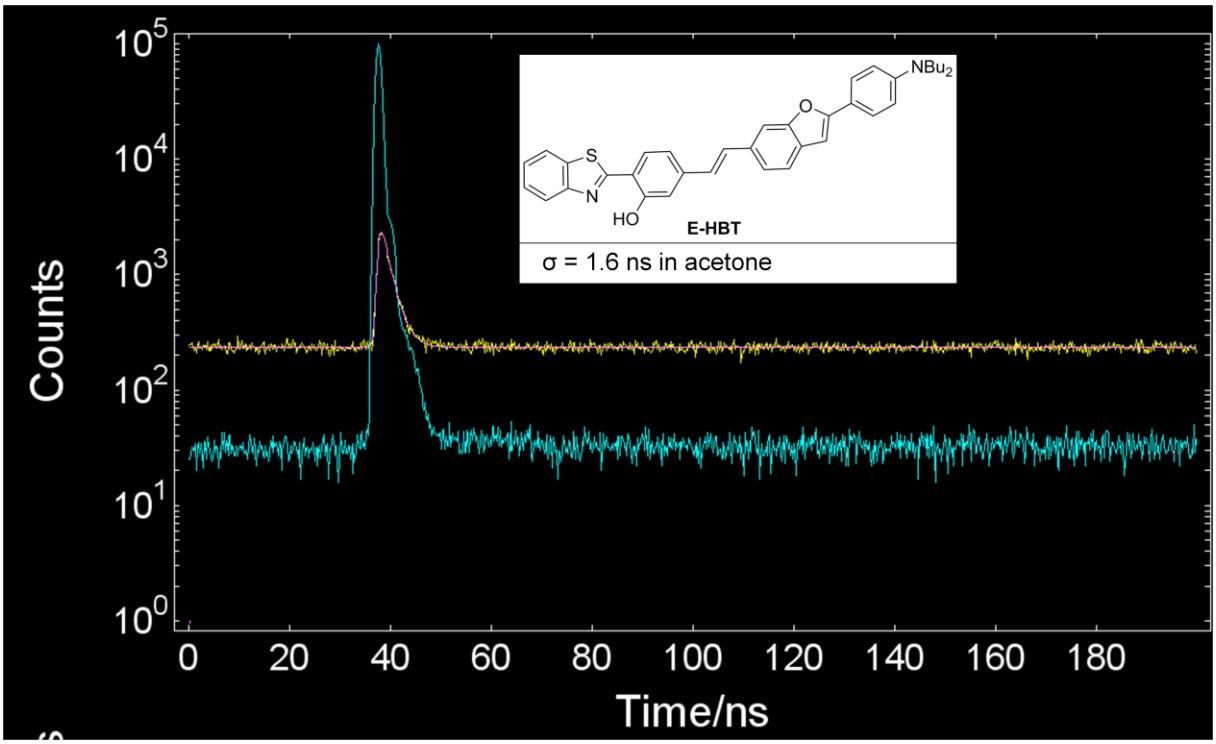
Fluorescence decay curves of **E-HBT**, **E-HBO 1** and **2** are presented below (reference in blue, decay in yellow and fit in purple)

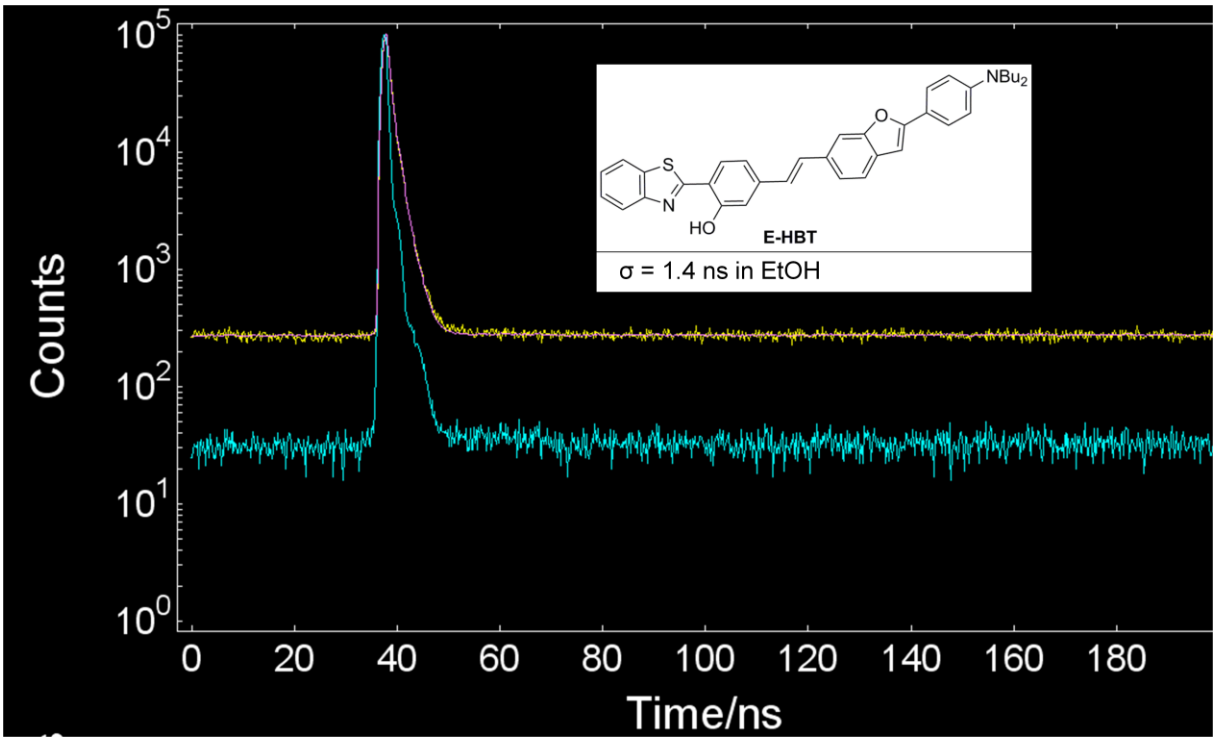


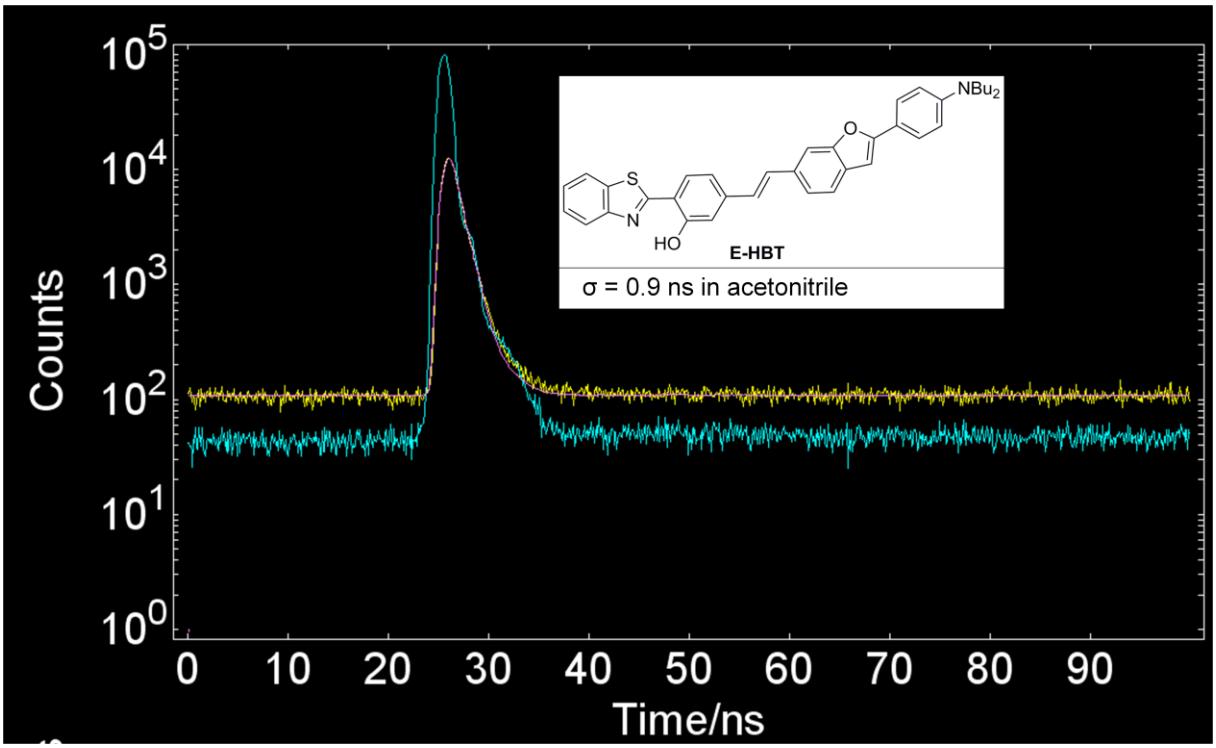


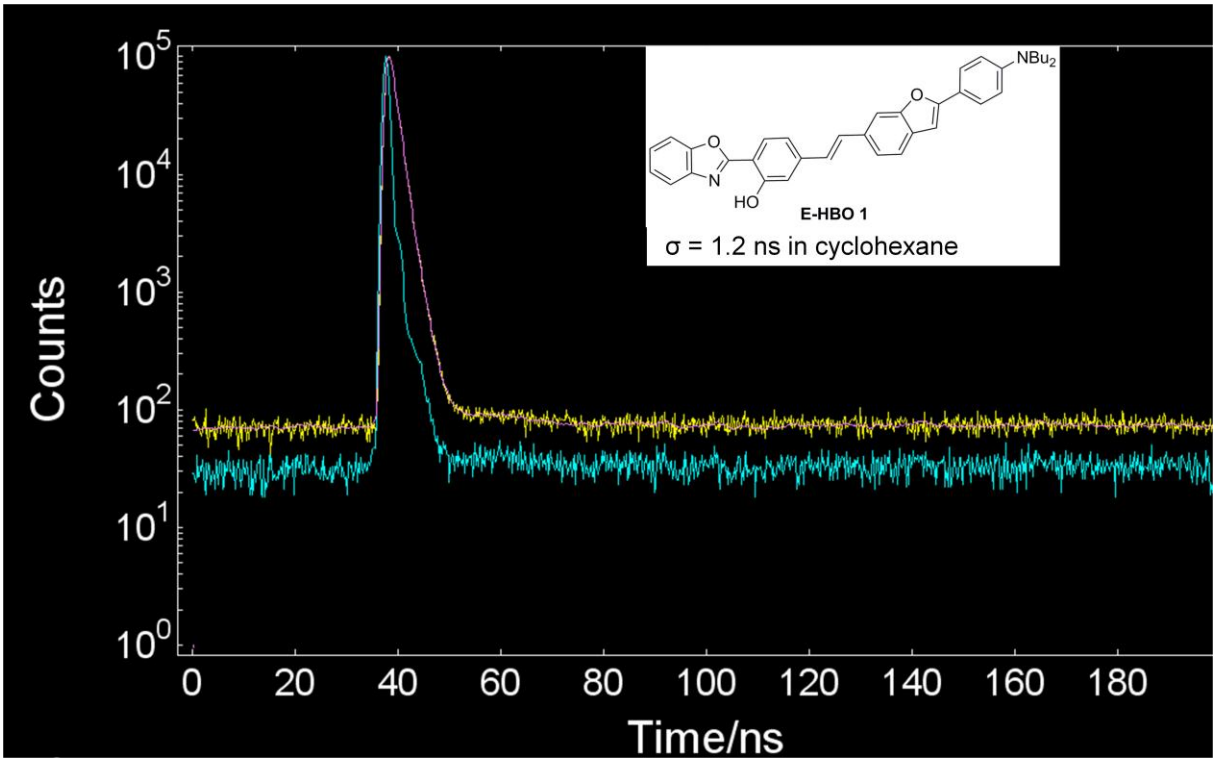

Counts
Time/ns
E-HBT
σ = 2.4 ns in CH_2Cl_2

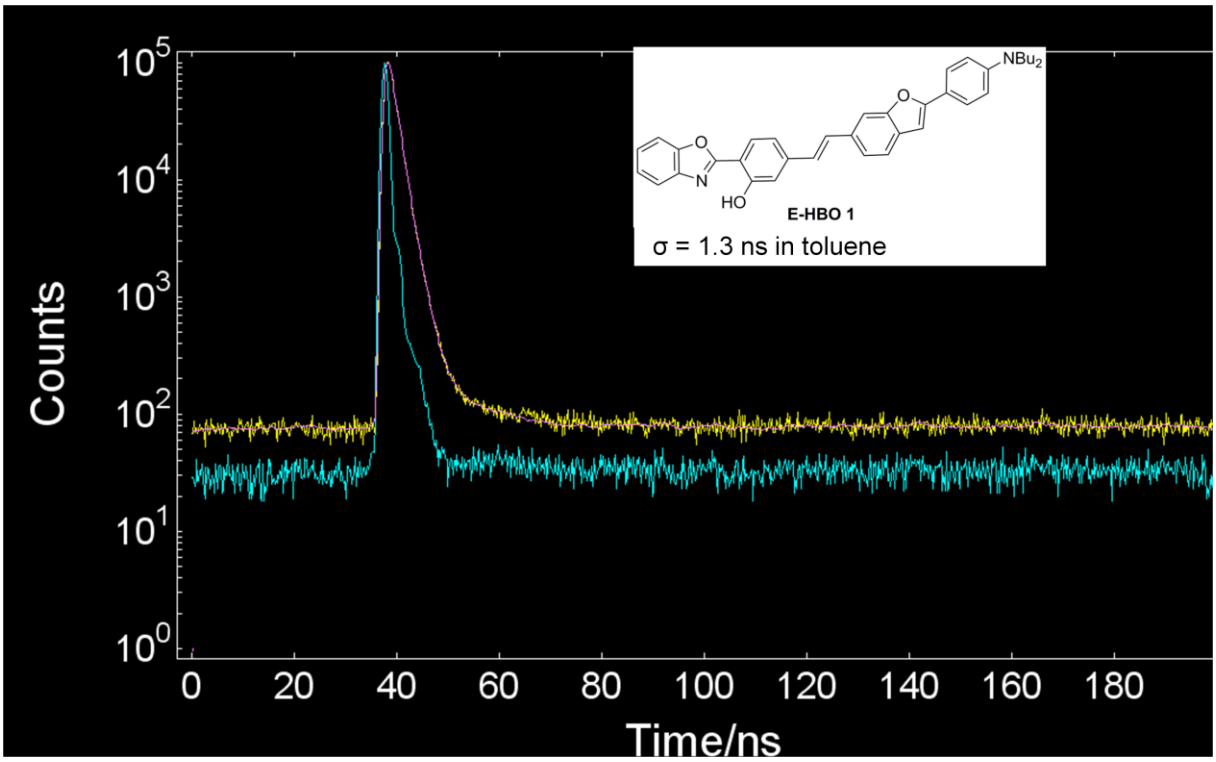

Counts
Time/ns
E-HBT
σ = 1.0 ns in protonated CH_2Cl_2

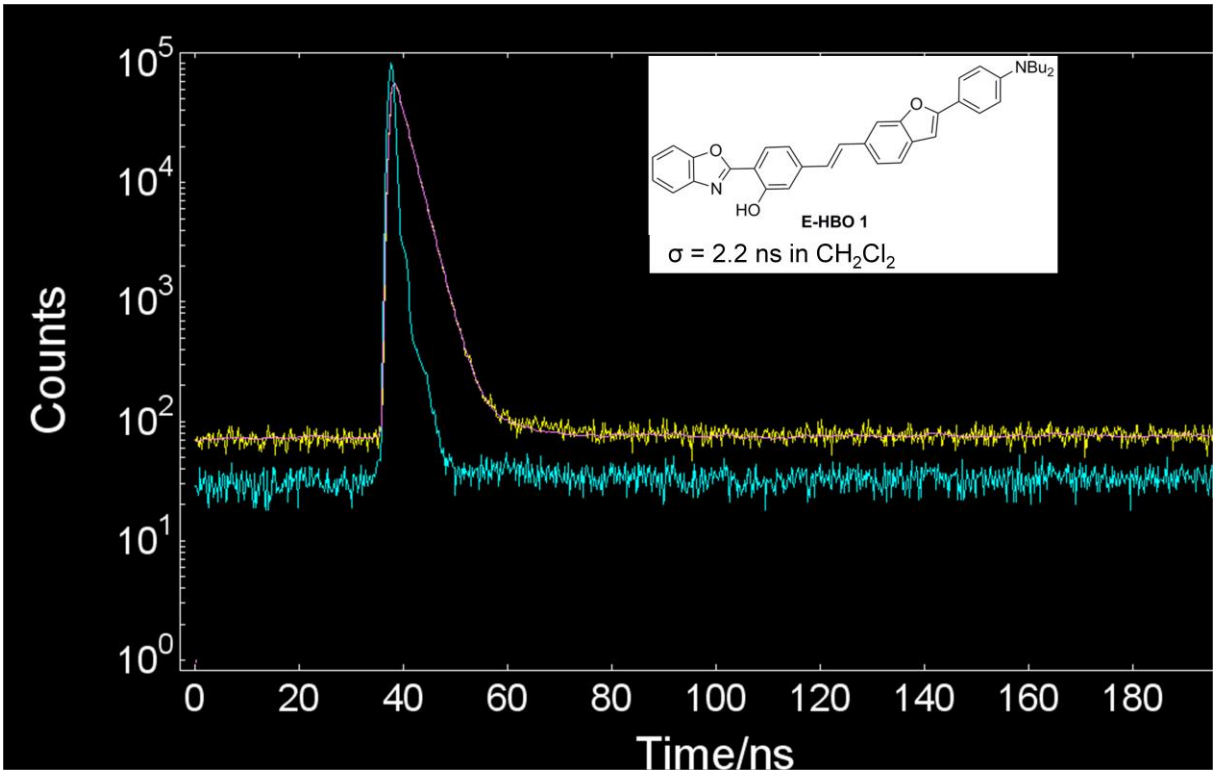

Counts
Time/ns
E-HBT
σ = 1.6 ns in acetone

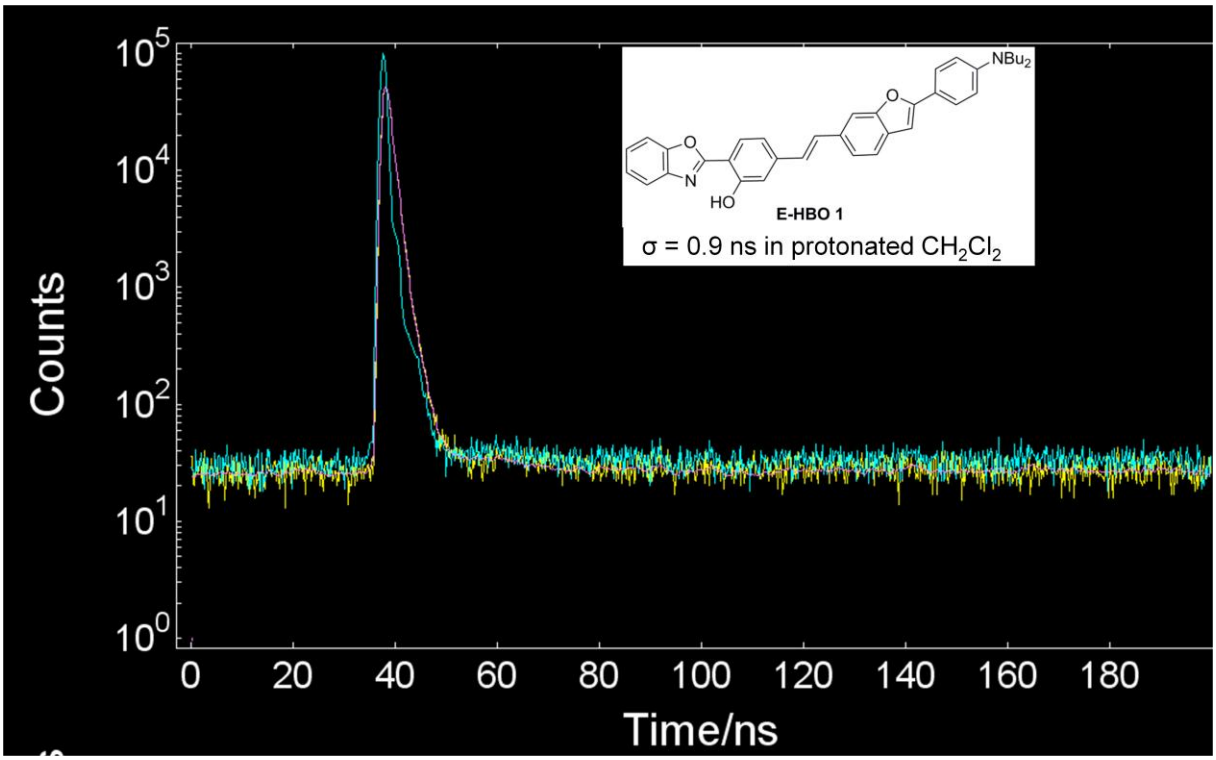

Counts
Time/ns
E-HBT
σ = 1.4 ns in EtOH

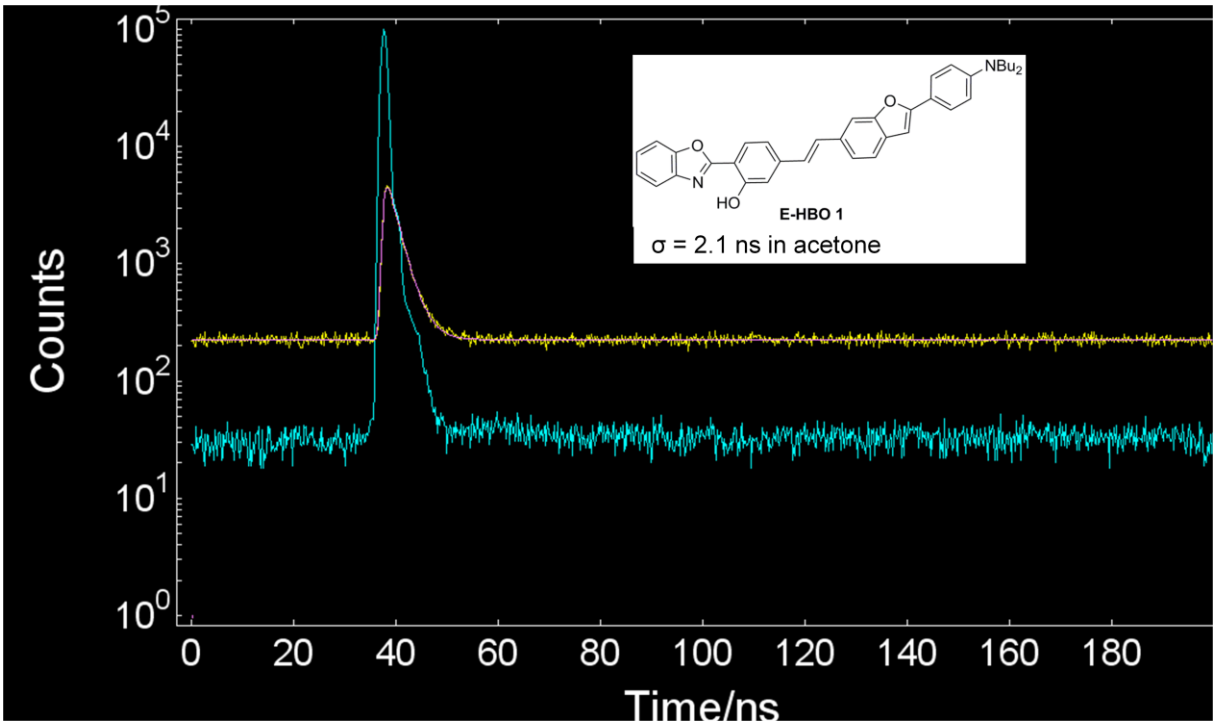

Counts
Time/ns
NBu2
S
N
O
HO
E-HBT
σ = 0.9 ns in acetonitrile

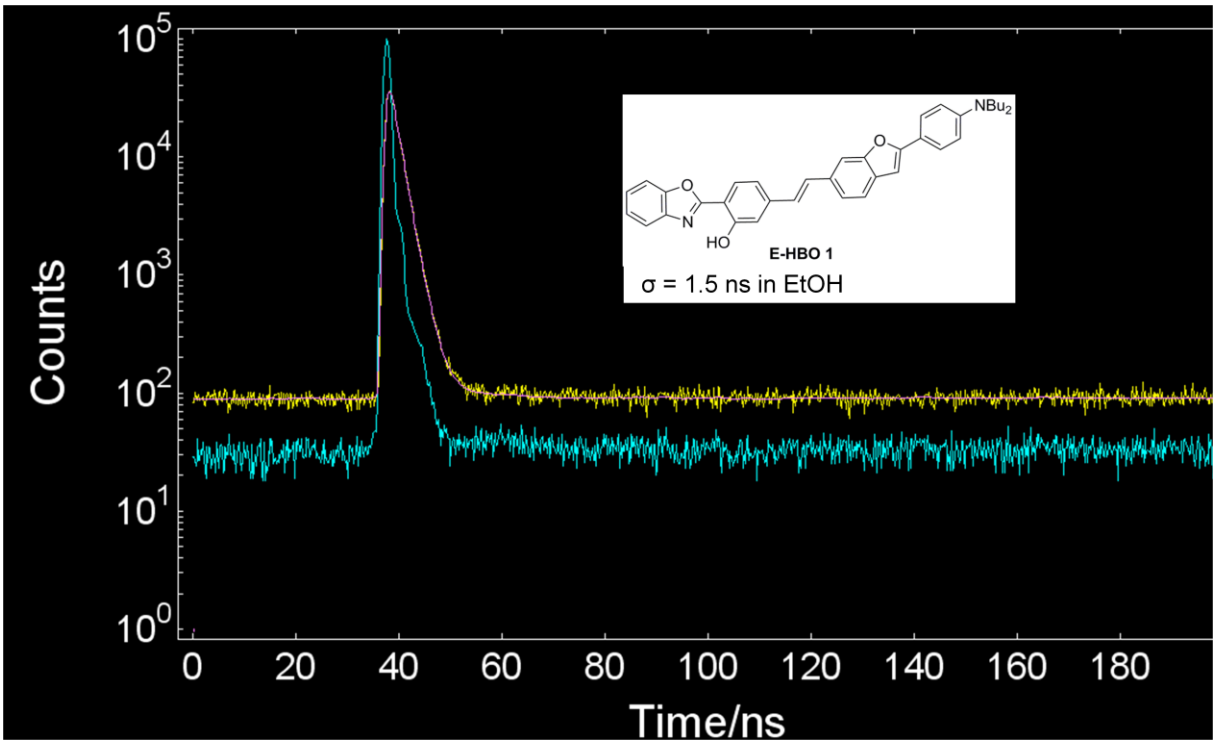

Counts
Time/ns
NBu2
O
N
O
HO
E-HBO 1
σ = 1.2 ns in cyclohexane

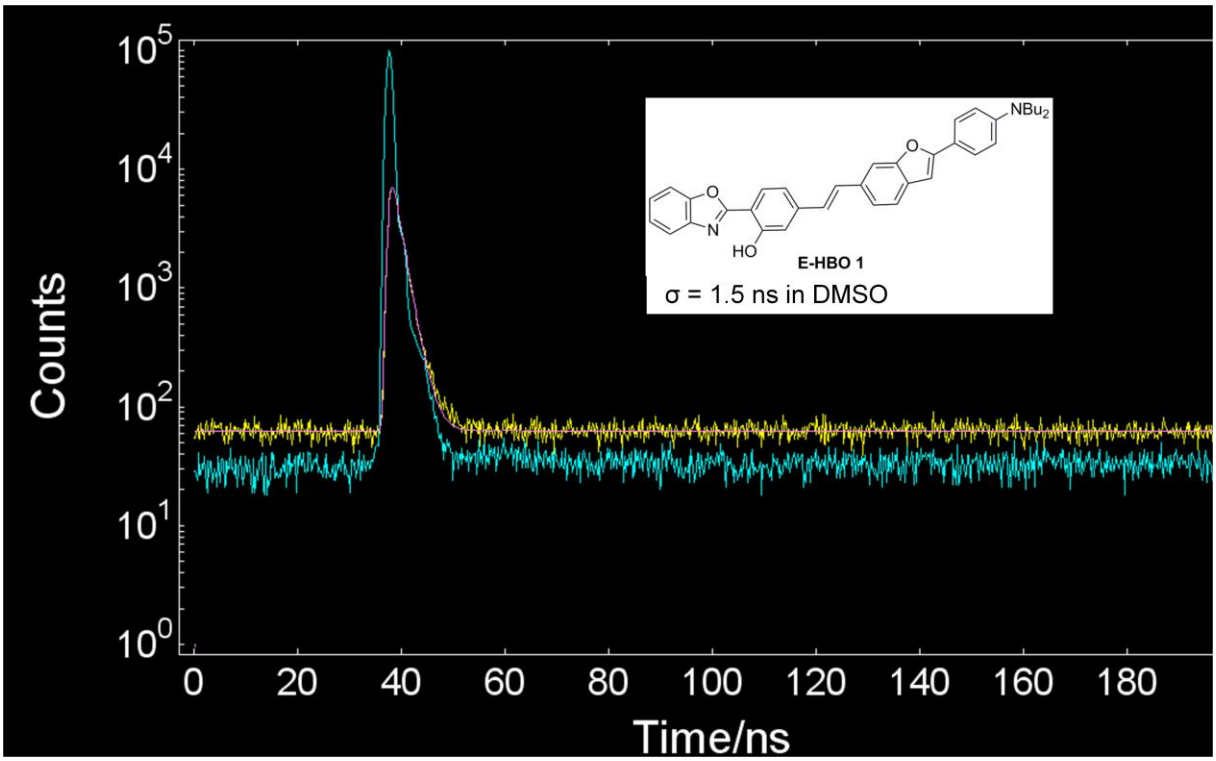

Counts
Time/ns
E-HBO 1
σ = 1.3 ns in toluene

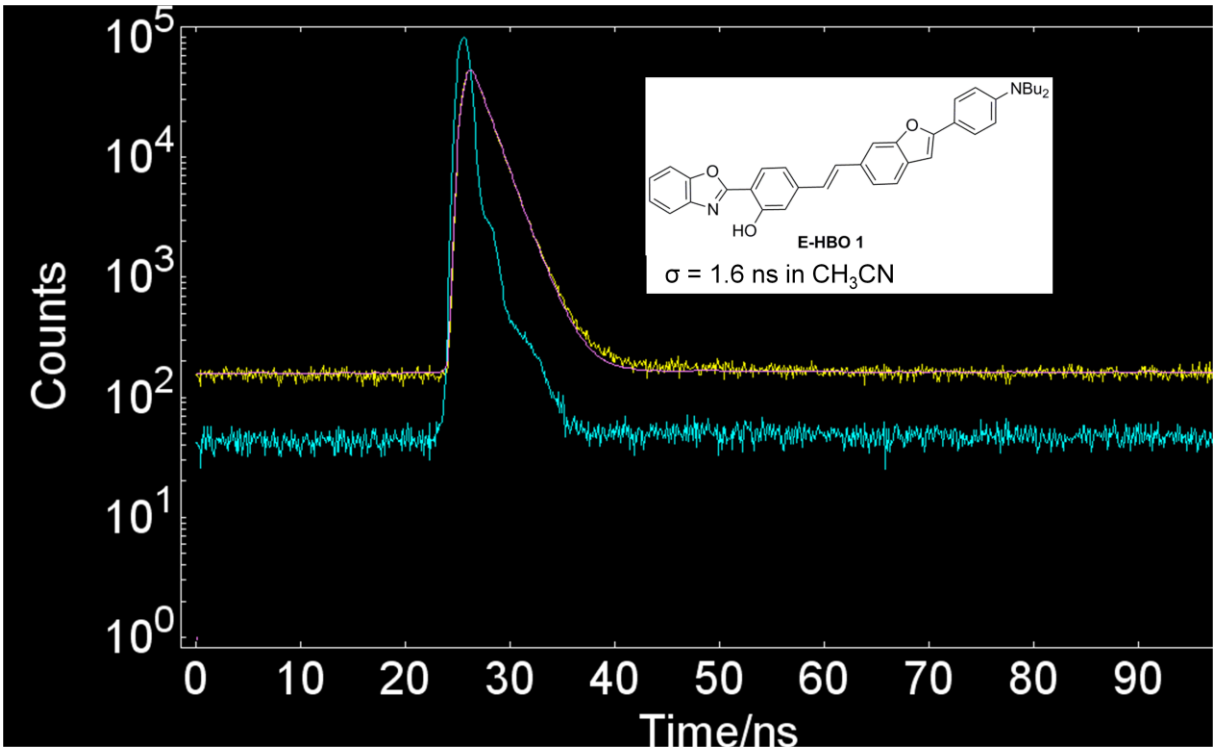

Counts
Time/ns
E-HBO 1
σ = 2.2 ns in CH2Cl2

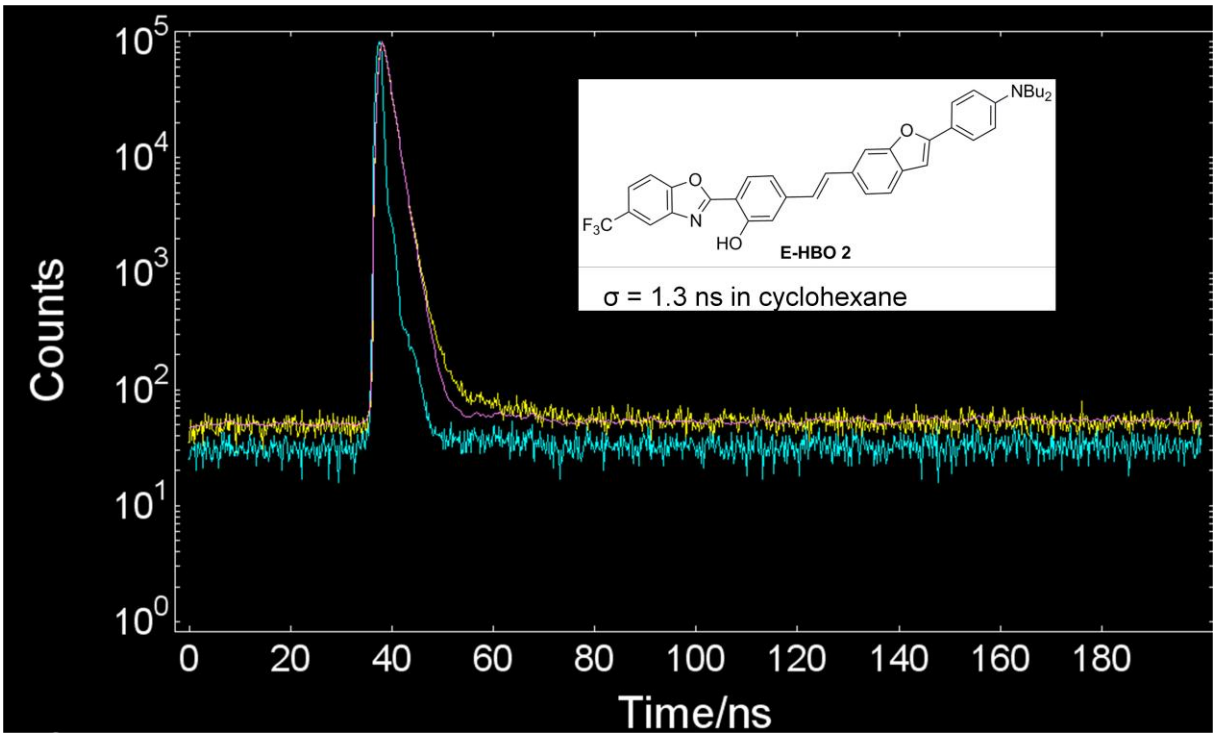

Counts
Time/ns
E-HBO 1
σ = 0.9 ns in protonated CH_2Cl_2

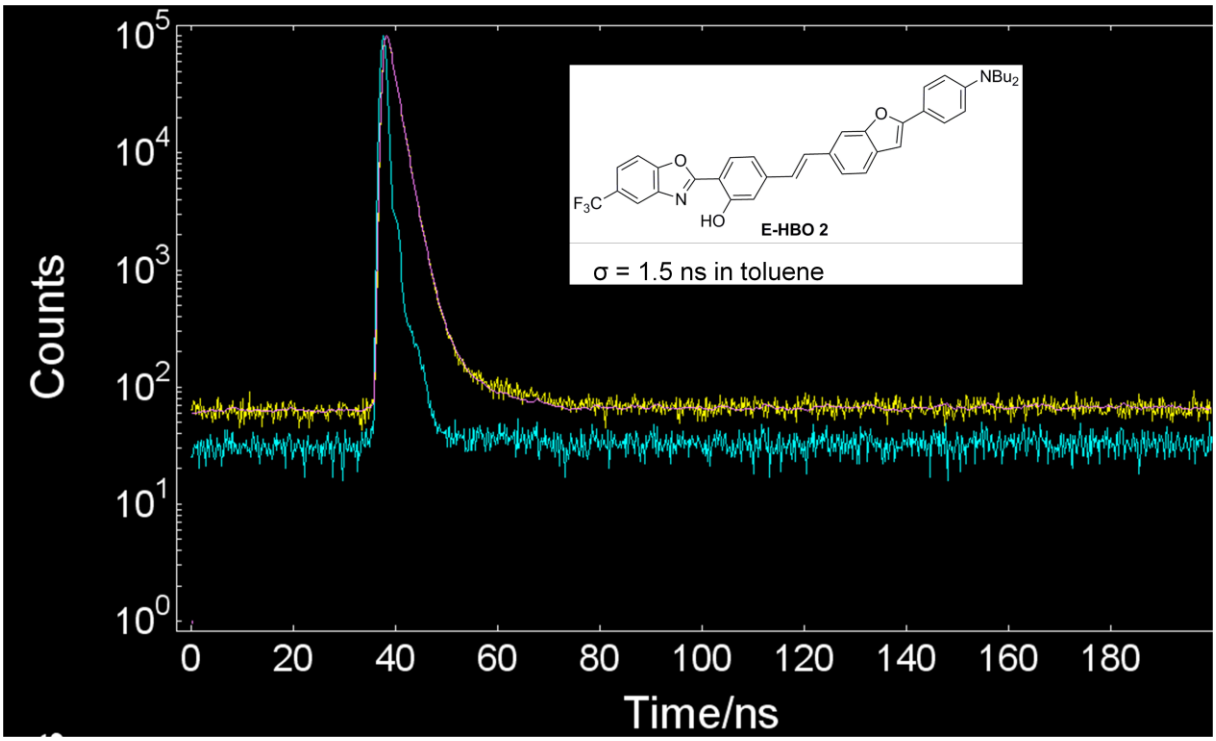

Counts
Time/ns
E-HBO 1
σ = 2.1 ns in acetone

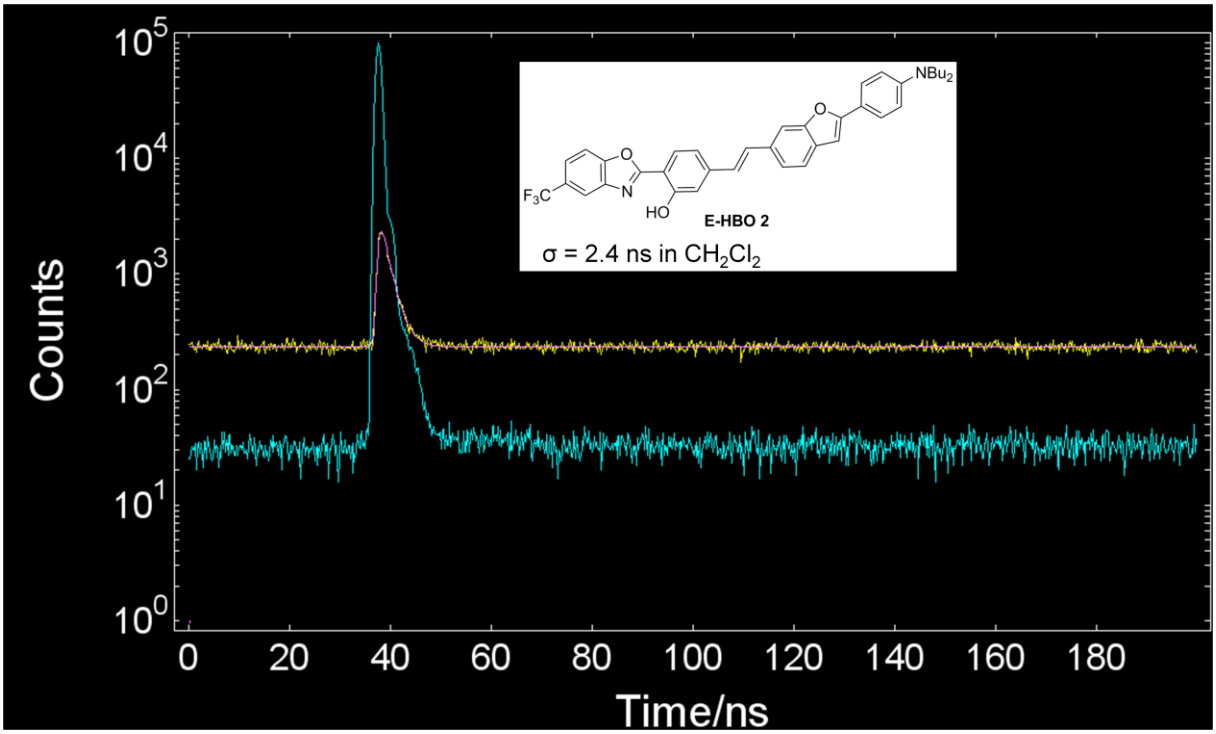

Counts
Time/ns
E-HBO 1
σ = 1.5 ns in EtOH

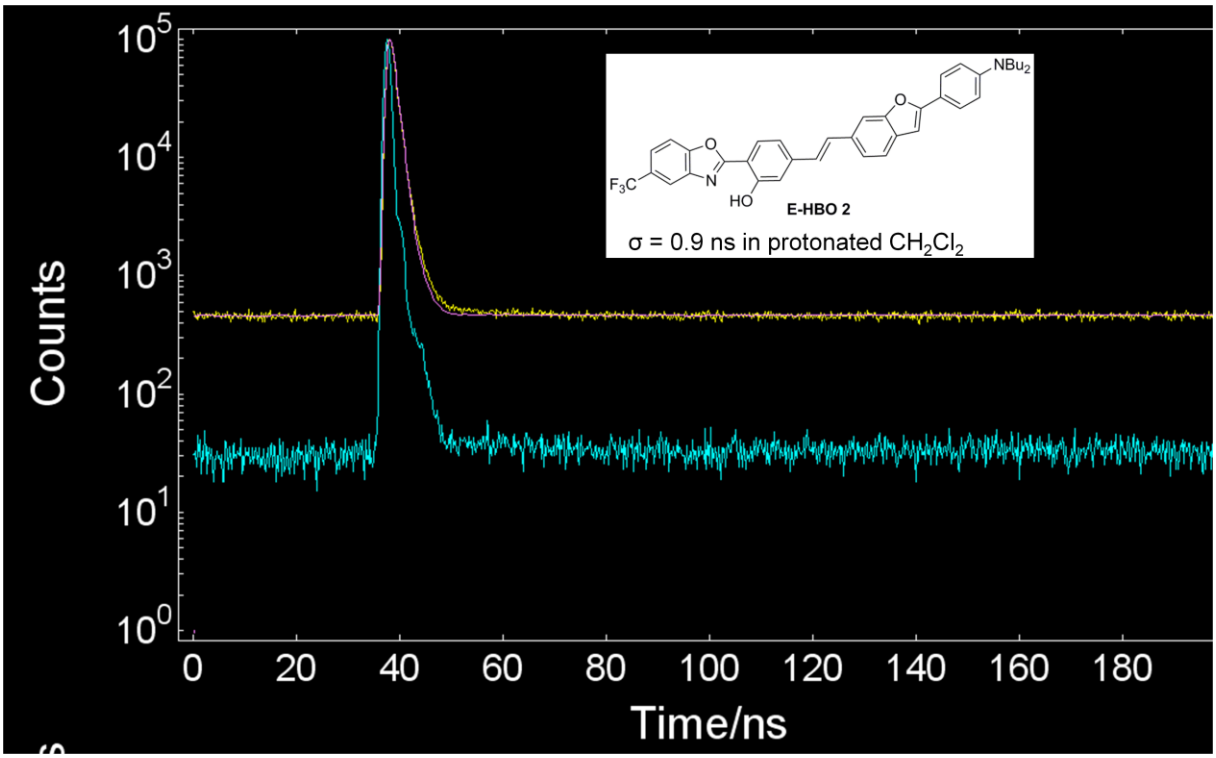

Counts
Time/ns
E-HBO 1
σ = 1.5 ns in DMSO

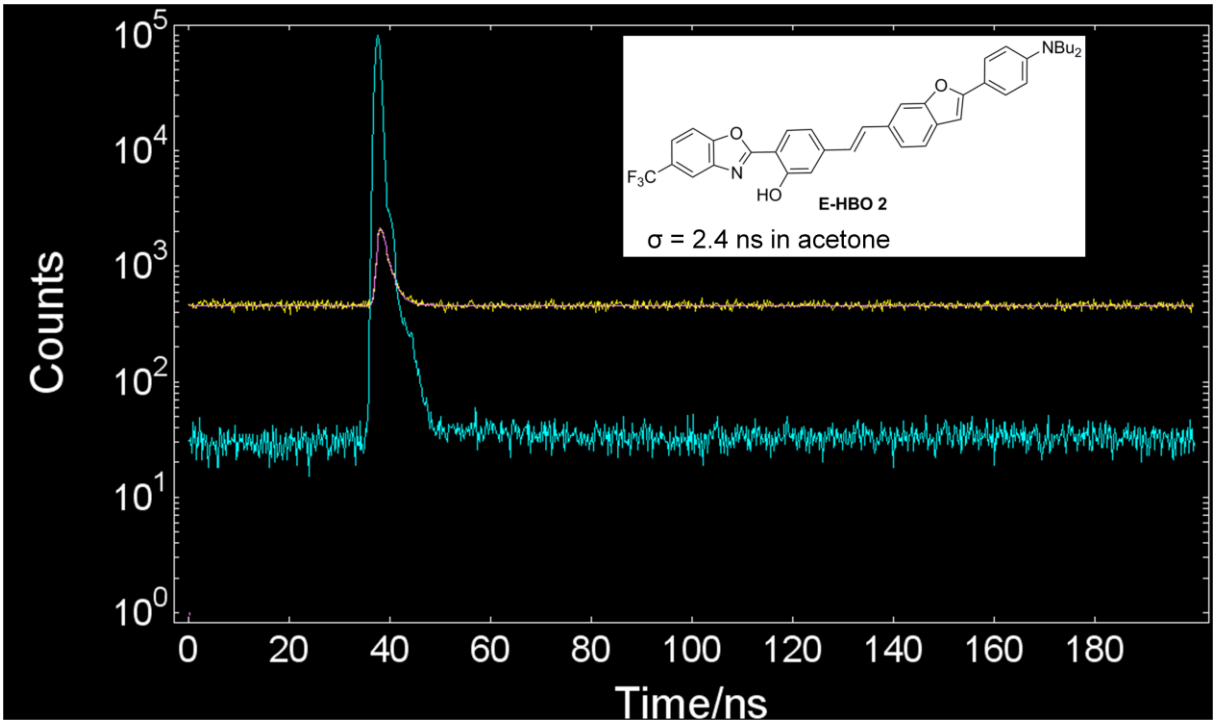

Counts
Time/ns
E-HBO 1
σ = 1.6 ns in CH3CN

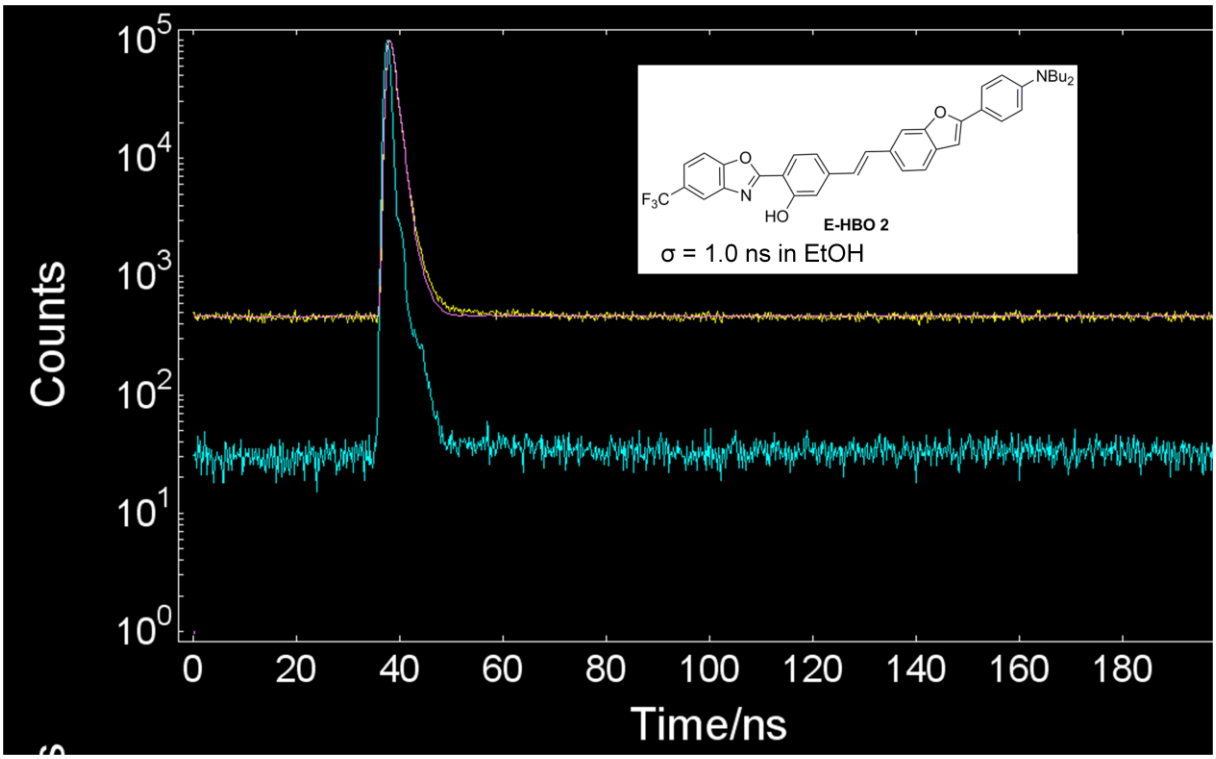

Counts
Time/ns
E-HBO 2
σ = 1.3 ns in cyclohexane

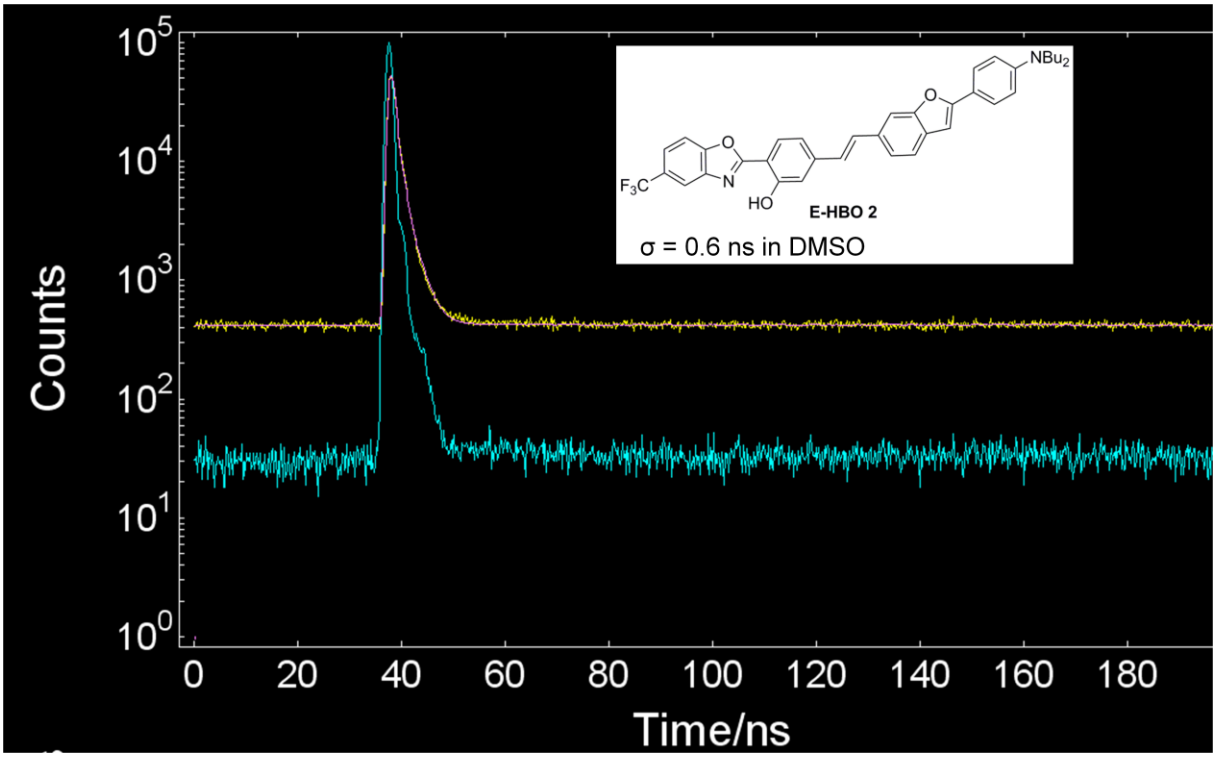

Counts
Time/ns
E-HBO 2
σ = 1.5 ns in toluene


Counts
Time/ns
E-HBO 2
σ = 2.4 ns in CH2Cl2


Counts
Time/ns
E-HBO 2
σ = 0.9 ns in protonated CH_2Cl_2


Counts
Time/ns
E-HBO 2
σ = 2.4 ns in acetone


Counts
Time/ns
E-HBO 2
σ = 1.0 ns in EtOH


Counts
Time/ns
E-HBO 2
σ = 0.6 ns in DMSO

S9 Theoretical calculations

Computational details

The structures and vibrational frequencies of all molecules have been obtained with (TD-) DFT and the total and transition energies with ADC(2) whereas the solvent effects were determined with the Polarizable Continuum Model (PCM).[9] The different properties (*P*), except when noted below, were obtained as,

$$P = P(\text{Gas, ADC}) + P(\text{PCM, TD}) - P(\text{Gaz,TD})$$

For all (TD-)DFT calculations, we have used the Gaussian09.D01 program,[10] applying default thresholds and algorithms, except for the following: we have tightened both the self-consistent field (10^{-10} a.u.) and geometry optimization (10^{-5} a.u.) convergence thresholds, as well as used a (99,590) pruned integration grid (so-called *ultrafine* grid). These (TD-)DFT calculations were made with Zhao and Truhlar's M06-2X meta-GGA hybrid exchange-correlation functional,[11] a choice justified by previous works showing that M06-2X is suited for both optical spectra and ESIPT.[11-18] Following Ref. 12, we determine the geometrical and vibrational parameters with the 6-31G(d) atomic basis set, whereas the total and transition energies are computed with 6-311+G(2d,p), so that all energies present in the main text are corrected for basis-set effects. For each molecule, both the ground state (GS) and first excited state (ES) have been fully optimized using DFT/TD-DFT analytical gradients and considering both the *enol* and *keto* forms of each compound. The nature of all structures was confirmed by analytical (GS) or numerical (ES) Hessian calculations that returned 0 (minima) imaginary vibrational modes.

Environmental effects (here: cyclohexane, dichloromethane and acetone) have been accounted for using the well-known PCM,[9] as implemented in Gaussian09.[10] While geometry optimizations and Hessian calculations have been performed with the popular linear-response (LR) PCM approach for both GS and ES, all transitions energies have been determined with the more accurate corrected-LR (cLR) approach.[19] cLR is indeed necessary to obtain valuable emission energies. Of course, although we applied the *equilibrium* limit for optimization and vibrational whereas both absorption and fluorescence wavelengths were corrected for *nonequilibrium* effects.

The gas phase ADC(2) total and transition energies determined on the (TD-)DFT structures have been obtained with the Turbomole code.[20] These ADC(2) calculations relied on the so-called ADC(2)-s formalism[21] and were obtained with the resolution of identity technique.[22,23] For all ADC(2) calculations, we have used the a*ug*-cc-pVDZ atomic basis set.

Vibrationally resolved spectra have been obtained using the FCclasses program.[24] The Franck-Condon approximation has been applied as we obviously consider only strongly dipole-allowed ES.[25,26] The reported spectra have been simulated by using convoluting Gaussian functions that represent a half width at half-maximum (HWHM) that has been applied to allow accurate comparisons with experimental results. A maximum number of 25 overtones for each mode and 20 combination bands on each pair of modes were included in

the calculation. The number of integrals (10^{12}) to be computed for each class was set to allow convergence of the FC factor (> 0.9). Note that the experimental absorption and emission bands have been renormalized to obtain band shapes and allow direct theory-experiment comparisons. We redirect the reader to Ref. 27 for more details about the procedure.

The density variation plots have been obtained through the difference in total densities of the first ES and GS. To quantify charge transfer (CT) in the dyes, we used Le Bahers' model,[28,29] which determines the distance between the barycenters of density gain/depletion. This model provides a CT distance expressed in Angstrom, and we applied a home-made code for it.[30]

The charges have been computed using the Merz-Kollman[31] approach at the M06-2X/6-311+G(2d,p) level.

All compounds have been modeled by replacing the NBu_2 by NMe_2 groups for the sake of computational efficiency.

Assessment of the most stable isomer in the ground-state (performed at the TD-DFT level - no ADC correction)

We first assessed the most stable rotamer, considering the **E-HBO 1** molecule. The *enol* GS energies of the four possible *trans* rotamers (see figure S2) have been computed and we found that they differ by 0.02-0.03 eV only, the most stable being the 0-0 form of figure S2. For this rotamer, we computed the corresponding *cis* isomer and found that, the formation of the latter is clearly impossible in the GS (the energy difference between both reaching 0.19 eV). Considering the *trans* isomer, we also assessed the possible GS formation of the *keto* (K) and the *enol'* (E') forms (see Scheme S3). One clearly notices that starting with the most stable E isomer, both K and E' forms cannot be reached thermally as the barriers for attaining these structures are 0.54 and 0.56 eV, respectively. The only existing form in the GS is therefore canonical *trans* enol and the photophysical processes start with absorption of light by this form, as one could expect. We note that all the *trans* rotamers absorbs at the same energy (3.23 ± 0.02 eV) and all the following calculations have been performed on the 0-0 form.

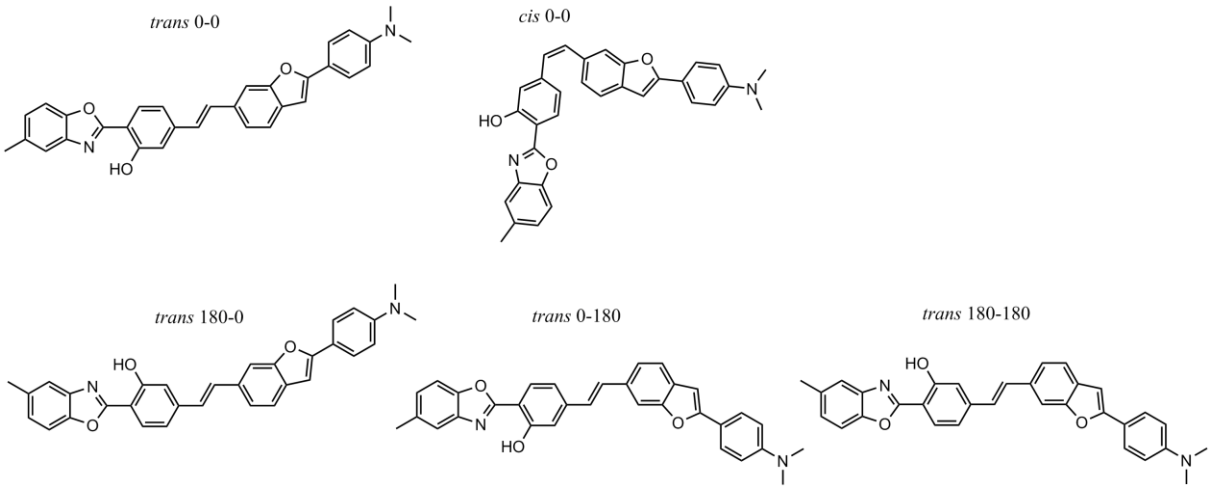


Figure S2. Possible rotamers of **E-HBO 1**

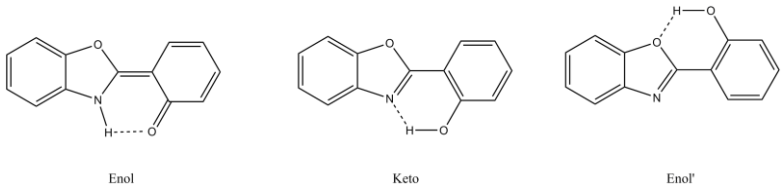


Figure S3. Possible isomers of a typical ESIPT dye.

Cartesian coodinates of the enol and keto structures considered in this paper

The Cartesian coordinates (Å) of all the structures [at the PCM-M06-2X/6-31G(d)] in both the ground and excited state in different solvent conditions are reported below for the enol (**E-**) and keto (**K-**) forms of the **HBO 1**, **HBO 2** and **HBT** species. For all compounds, we report the DFT or TD-DFT *G* energies at the same level of theory. Note that the values within text are further corrected with ADC(2) energy differences.

*Coordinates for **HBO 1**:*

Enol-HBO 1 ground-state structure in cyclohexane *G* -1529.905536 au

6	-5.284954	1.509918	0.005222
6	-5.602453	0.135336	0.003794
6	-6.989799	-0.278912	0.003314
6	-8.641734	-1.672139	0.001993
6	-9.451373	-2.794231	0.000983
6	-10.821814	-2.545213	0.001130
6	-11.333387	-1.237301	0.002229
6	-10.498591	-0.125242	0.003233
6	-9.124834	-0.362295	0.003104
1	-9.041476	-3.797354	0.000142
1	-11.510403	-3.383557	0.000375
1	-10.889763	0.885986	0.004079
8	-7.274533	-1.609102	0.002129
7	-8.032888	0.500411	0.003928
8	-6.212446	2.480235	0.006073
6	-4.561015	-0.808041	0.003106
6	-3.942458	1.895480	0.005813
6	-3.240695	-0.414228	0.003692
1	-4.816737	-1.862680	0.002300
1	-3.724237	2.959063	0.006858
1	-7.109213	2.073142	0.005537
1	-2.462550	-1.168674	0.003731
6	-1.528501	1.450204	0.005307
1	-1.435697	2.534222	0.010685
6	-0.420124	0.691827	-0.001011
1	-0.523342	-0.392049	-0.007700
6	-2.910177	0.957981	0.004860
6	0.967710	1.163650	-0.000651
6	1.987677	0.205084	-0.012271
6	1.308561	2.538142	0.011006
6	3.294244	0.660045	-0.011931
1	1.764585	-0.857100	-0.021416
6	2.621633	2.971223	0.011093
1	0.517043	3.279948	0.020564
6	3.649934	2.015895	-0.000589
1	2.850844	4.032018	0.020296
1	-12.408845	-1.093756	0.002293
8	4.411020	-0.117034	-0.022150
6	5.489445	0.732630	-0.017445
6	5.085320	2.034987	-0.004717
1	5.726376	2.904129	-0.000100
6	6.803267	0.106768	-0.027204
6	6.947014	-1.285264	-0.049835
6	7.968727	0.883038	-0.008675
6	8.197435	-1.880847	-0.058168
1	6.060809	-1.911279	-0.057291
6	9.224135	0.302728	-0.017048
1	7.895018	1.966631	0.017531
6	9.374632	-1.102056	-0.051387

1	8.256931	-2.962131	-0.069257
1	10.094684	0.946502	0.004842
7	10.620733	-1.686421	-0.081495
6	11.796092	-0.862177	0.112522
1	11.785750	-0.341783	1.080815
1	12.683599	-1.493524	0.069252
1	11.882084	-0.110162	-0.679478
6	10.732893	-3.122948	0.068179
1	10.221494	-3.642604	-0.749478
1	11.785840	-3.402517	0.033551
1	10.309112	-3.477453	1.018549

Keto-HBO 1 ground-state structure in cyclohexane *G* -1529.883855 au

6	5.3096800	-1.4660180	0.1940590
6	5.5708390	-0.0510580	-0.0167520
6	6.9071320	0.3528810	0.0034640
6	8.6962760	1.6154000	-0.0859840
6	9.5583810	2.6854060	-0.2034930
6	10.9162920	2.3888360	-0.0689360
6	11.3599390	1.0833620	0.1699090
6	10.4727940	0.0135200	0.2858940
6	9.1234540	0.3097600	0.1520020
1	9.1959890	3.6894930	-0.3884700
1	11.6416780	3.1906000	-0.1519710
1	10.8159160	-0.9976480	0.4705310
8	7.3201210	1.6229210	-0.1751610
7	7.9620200	-0.4489070	0.2003430
8	6.2237300	-2.3126340	0.3892620
6	4.5124270	0.8743320	-0.2372550
6	3.9176690	-1.8348330	0.1642550
6	3.2159280	0.4598070	-0.2528380
1	4.7592960	1.9203060	-0.3968850
1	3.6952230	-2.8865550	0.3208720
1	2.4237120	1.1763160	-0.4331520
6	1.5224040	-1.4184250	-0.0446910
1	1.4269450	-2.4968480	0.0649570
6	0.4153000	-0.6648590	-0.1474460
1	0.5166200	0.4160090	-0.2254760
6	2.9049060	-0.9273020	-0.0436120
6	-0.9714900	-1.1419420	-0.1477610
6	-1.9961770	-0.1892700	-0.1113030
6	-1.3055030	-2.5175620	-0.1858540
6	-3.3003720	-0.6514120	-0.1022140
1	-1.7784320	0.8737820	-0.0857910
6	-2.6163480	-2.9578820	-0.1772030
1	-0.5095700	-3.2531360	-0.2347230
6	-3.6492070	-2.0086810	-0.1319840
1	-2.8401870	-4.0193930	-0.2103250
1	12.4238180	0.8962240	0.2678060
8	-4.4210810	0.1196100	-0.0653870
6	-5.4951260	-0.7356490	-0.0715070
6	-5.0847270	-2.0352070	-0.1119160
1	-5.7215190	-2.9074010	-0.1269960
6	-6.8120000	-0.1166630	-0.0352470
6	-6.9625280	1.2745700	-0.0122160
6	-7.9733410	-0.8989490	-0.0164570
6	-8.2156440	1.8636740	0.0241060
1	-6.0794590	1.9050090	-0.0188760
6	-9.2313330	-0.3250040	0.0193980
1	-7.8941890	-1.9824520	-0.0247270

6	-9.3888340	1.0792030	0.0315220
1	-8.2800990	2.9444760	0.0477500
1	-10.0982490	-0.9737380	0.0397920
7	-10.6384820	1.6582430	0.0455130
6	-11.8041010	0.8225690	0.2495040
1	-11.7653550	0.2767970	1.2031100
1	-12.6955440	1.4499110	0.2464080
1	-11.9077300	0.0913420	-0.5595550
6	-10.7524610	3.0877600	0.2509330
1	-10.2590910	3.6391160	-0.5568730
1	-11.8068450	3.3641530	0.2468440
1	-10.3111370	3.4089750	1.2052650
1	7.7359060	-1.4520520	0.3475130

Enol-HBO 1 excited-state structure in cyclohexane *G* -1529.794583 au

6	5.269350	-1.534870	-0.000026
6	5.608182	-0.144347	-0.000006
6	6.973931	0.257943	-0.000003
6	8.637661	1.649962	0.000015
6	9.451446	2.766513	0.000030
6	10.824977	2.516631	0.000025
6	11.331005	1.207946	0.000005
6	10.492865	0.097145	-0.000010
6	9.116082	0.332140	-0.000005
1	9.043487	3.770689	0.000045
1	11.514917	3.353988	0.000036
1	10.882889	-0.914667	-0.000026
8	7.272953	1.595696	0.000016
7	8.033487	-0.524551	-0.000016
8	6.211071	-2.497948	-0.000042
6	4.556890	0.807141	0.000012
6	3.943670	-1.913322	-0.000028
6	3.243532	0.423890	0.000009
1	4.818249	1.860520	0.000029
1	3.718930	-2.975762	-0.000044
1	7.102206	-2.077472	-0.000038
1	2.471060	1.184601	0.000028
6	1.544136	-1.417367	-0.000015
1	1.420850	-2.497976	-0.000023
6	0.403319	-0.619598	-0.000013
1	0.530195	0.460334	-0.000025
6	2.885634	-0.963773	-0.000012
6	-0.936695	-1.070728	-0.000001
6	-1.994982	-0.107922	-0.000014
6	-1.289737	-2.471083	0.000026
6	-3.278052	-0.573025	-0.000001
1	-1.777235	0.954661	-0.000033
6	-2.584946	-2.908061	0.000038
1	-0.493169	-3.206256	0.000041
6	-3.634865	-1.949786	0.000024
1	-2.812641	-3.968983	0.000059
1	12.406293	1.060365	0.000001
8	-4.410303	0.192678	-0.000010
6	-5.479117	-0.666550	0.000009
6	-5.036927	-1.987152	0.000028
1	-5.669124	-2.863417	0.000044
6	-6.782501	-0.092140	0.000005
6	-6.966351	1.308999	-0.000013
6	-7.939335	-0.904555	0.000019
6	-8.224573	1.866825	-0.000018

1	-6.094760	1.954610	-0.000022
6	-9.201022	-0.358390	0.000014
1	-7.836733	-1.985565	0.000034
6	-9.386599	1.050778	-0.000006
1	-8.317289	2.945727	-0.000029
1	-10.057641	-1.020660	0.000026
7	-10.634551	1.597726	-0.000012
6	-11.805754	0.740865	0.000007
1	-11.831470	0.100265	0.889662
1	-12.700289	1.362060	-0.000006
1	-11.831470	0.100229	-0.889621
6	-10.796019	3.039987	-0.000024
1	-10.341121	3.491909	-0.889535
1	-11.858562	3.278668	-0.000030
1	-10.341126	3.491926	0.889482

Keto-HBO 1 excited-state structure in cyclohexane *G* -1529.774607 au

6	5.297778	-1.481580	-0.000001
6	5.570952	-0.033288	0.000008
6	6.905114	0.356019	0.000005
6	8.716286	1.593116	-0.000001
6	9.599291	2.651511	-0.000002
6	10.957962	2.317380	-0.000011
6	11.380443	0.984309	-0.000017
6	10.474919	-0.077407	-0.000016
6	9.123883	0.252518	-0.000007
1	9.252167	3.677937	0.000003
1	11.696756	3.111353	-0.000012
1	10.803594	-1.109983	-0.000021
8	7.342649	1.642024	0.000007
7	7.960437	-0.484465	-0.000002
8	6.243392	-2.334346	-0.000010
6	4.509413	0.919209	0.000017
6	3.931076	-1.835181	-0.000001
6	3.210361	0.511930	0.000018
1	4.757445	1.976935	0.000022
1	3.701728	-2.897073	-0.000010
1	2.419489	1.253241	0.000023
6	1.536570	-1.346942	0.000006
1	1.418609	-2.428516	-0.000001
6	0.391995	-0.561797	0.000011
1	0.504410	0.519588	0.000015
6	2.883864	-0.895059	0.000009
6	-0.946455	-1.029459	0.000012
6	-2.012726	-0.078855	0.000007
6	-1.284218	-2.431745	0.000014
6	-3.292397	-0.556997	0.000004
1	-1.806257	0.986025	0.000007
6	-2.575692	-2.882513	0.000011
1	-0.480447	-3.158969	0.000018
6	-3.634623	-1.935963	0.000004
1	-2.791710	-3.945893	0.000012
1	12.443439	0.766969	-0.000024
8	-4.431788	0.197407	0.000000
6	-5.491974	-0.672517	-0.000004
6	-5.038215	-1.987101	0.000000
1	-5.661608	-2.869606	-0.000001
6	-6.802186	-0.108776	-0.000007
6	-6.998317	1.289747	0.000000
6	-7.950949	-0.931007	-0.000018

6	-8.261997	1.836690	0.000000
1	-6.132603	1.943263	0.000006
6	-9.218088	-0.396021	-0.000019
1	-7.838778	-2.011104	-0.000028
6	-9.416263	1.010797	-0.000007
1	-8.364156	2.914768	0.000003
1	-10.068617	-1.066156	-0.000031
7	-10.669926	1.546890	-0.000005
6	-11.832733	0.679295	-0.000010
1	-11.852784	0.038160	0.889520
1	-12.733180	1.291984	0.000007
1	-11.852799	0.038189	-0.889562
6	-10.843792	2.987329	0.000011
1	-10.392875	3.443643	-0.889405
1	-11.908405	3.216967	0.000024
1	-10.392859	3.443623	0.889429
1	7.676146	-1.498859	-0.000009

Enol-HBO 1 ground-state structure in dichloromethane *G* -1529.912473 au

6	5.2847610	-1.5083650	0.0065800
6	5.6027680	-0.1340330	0.0033600
6	6.9909510	0.2800720	0.0027650
6	8.6445730	1.6710340	0.0000000
6	9.4546810	2.7931480	-0.0023340
6	10.8250480	2.5423640	-0.0014230
6	11.3359350	1.2335560	0.0016520
6	10.5004200	0.1217010	0.0039700
6	9.1266090	0.3608030	0.0031000
1	9.0462510	3.7968360	-0.0046920
1	11.5142460	3.3801040	-0.0031360
1	10.8919720	-0.8894350	0.0063420
8	7.2766420	1.6086590	-0.0002000
7	8.0328920	-0.5008900	0.0048070
8	6.2152220	-2.4786280	0.0091470
6	4.5614090	0.8092870	0.0008570
6	3.9430190	-1.8952630	0.0071480
6	3.2404130	0.4151410	0.0014110
1	4.8154390	1.8643090	-0.0014640
1	3.7228610	-2.9585990	0.0096250
1	7.1114500	-2.0683420	0.0083790
1	2.4630850	1.1704260	-0.0003050
6	1.5283540	-1.4499790	0.0049770
1	1.4355080	-2.5339960	0.0099840
6	0.4210010	-0.6892170	-0.0006640
1	0.5241570	0.3945990	-0.0063900
6	2.9101360	-0.9570210	0.0044670
6	-0.9670720	-1.1615400	-0.0005290
6	-1.9868110	-0.2017060	-0.0096480
6	-1.3077720	-2.5365200	0.0082530
6	-3.2933090	-0.6574690	-0.0097100
1	-1.7625330	0.8603070	-0.0165300
6	-2.6213820	-2.9697520	0.0079710
1	-0.5168940	-3.2791040	0.0156400
6	-3.6494570	-2.0135570	-0.0012620
1	-2.8510220	-4.0304070	0.0148700
1	12.4112170	1.0892730	0.0022360
8	-4.4109630	0.1194360	-0.0178110
6	-5.4900520	-0.7311900	-0.0146380
6	-5.0850980	-2.0338000	-0.0048870
1	-5.7249610	-2.9039860	-0.0013620

6	-6.8038090	-0.1056760	-0.0225260
6	-6.9495080	1.2871470	-0.0366450
6	-7.9692700	-0.8840310	-0.0111600
6	-8.2003300	1.8819880	-0.0432650
1	-6.0651150	1.9160690	-0.0390940
6	-9.2253260	-0.3052510	-0.0178960
1	-7.8952480	-1.9677960	0.0072510
6	-9.3782090	1.1011780	-0.0425680
1	-8.2610290	2.9632720	-0.0480620
1	-10.0951770	-0.9501550	-0.0023190
7	-10.6215510	1.6825890	-0.0689910
6	-11.8015710	0.8548270	0.0887980
1	-11.8026450	0.3133580	1.0447580
1	-12.6869800	1.4886750	0.0502130
1	-11.8778540	0.1205560	-0.7207000
6	-10.7388170	3.1218930	0.0612950
1	-10.2316050	3.6336970	-0.7639860
1	-11.7927320	3.3963260	0.0287110
1	-10.3126910	3.4877580	1.0055620

Keto-HBO 1 ground-state structure in dichloromethane *G* -1529.893473 au

6	5.3158600	-1.4908410	0.1267590
6	5.5753010	-0.0692350	-0.0097650
6	6.9151060	0.3405640	0.0036710
6	8.6876490	1.6270940	-0.0551980
6	9.5342080	2.7138420	-0.1326100
6	10.8971420	2.4251100	-0.0437350
6	11.3607780	1.1129190	0.1137240
6	10.4891480	0.0273110	0.1898030
6	9.1343090	0.3167260	0.1011160
1	9.1578420	3.7223310	-0.2544260
1	11.6121560	3.2384730	-0.0981780
1	10.8460140	-0.9884640	0.3115060
8	7.3087980	1.6204280	-0.1134230
7	7.9802000	-0.4569770	0.1324710
8	6.2335560	-2.3501170	0.2541380
6	4.5164740	0.8684230	-0.1514890
6	3.9232110	-1.8544820	0.1071050
6	3.2158400	0.4596240	-0.1615210
1	4.7624270	1.9217860	-0.2532960
1	3.6979480	-2.9128540	0.2076400
1	2.4237030	1.1898430	-0.2750920
6	1.5233090	-1.4267680	-0.0273170
1	1.4294310	-2.5078630	0.0542010
6	0.4157190	-0.6701100	-0.1054250
1	0.5162460	0.4118300	-0.1674940
6	2.9061330	-0.9348260	-0.0273270
6	-0.9715250	-1.1469620	-0.1037850
6	-1.9950600	-0.1914670	-0.0839810
6	-1.3072270	-2.5230460	-0.1218910
6	-3.2998290	-0.6524750	-0.0739860
1	-1.7750430	0.8714310	-0.0731240
6	-2.6191880	-2.9616530	-0.1125660
1	-0.5131920	-3.2617270	-0.1516400
6	-3.6508340	-2.0098020	-0.0860020
1	-2.8446820	-4.0231280	-0.1290070
1	12.4285380	0.9342960	0.1784370
8	-4.4204340	0.1201600	-0.0521150
6	-5.4963000	-0.7346650	-0.0499590
6	-5.0865780	-2.0354760	-0.0704780

1	-5.7232510	-2.9080170	-0.0747800
6	-6.8123890	-0.1140960	-0.0271580
6	-6.9632820	1.2781700	-0.0184490
6	-7.9747440	-0.8968520	-0.0078550
6	-8.2162210	1.8682890	0.0045870
1	-6.0812750	1.9103900	-0.0263270
6	-9.2328410	-0.3227500	0.0149380
1	-7.8965490	-1.9804860	-0.0062520
6	-9.3911010	1.0832070	0.0134040
1	-8.2807710	2.9492940	0.0168100
1	-10.0999650	-0.9711870	0.0357750
7	-10.6370530	1.6604710	0.0161160
6	-11.8105230	0.8261780	0.1879490
1	-11.7905670	0.2735020	1.1373320
1	-12.6989170	1.4569080	0.1742560
1	-11.9002050	0.1012050	-0.6284550
6	-10.7565070	3.0966960	0.1754210
1	-10.2637740	3.6253010	-0.6479690
1	-11.8116180	3.3682830	0.1640530
1	-10.3167560	3.4464550	1.1196150
1	7.7886460	-1.4677190	0.2296200

Enol-HBO 1 excited-state structure in dichloromethane *G* -1529.807042 au

6	-5.268894	-1.535668	-0.000001
6	-5.608374	-0.145469	-0.000001
6	-6.973721	0.257445	0.000000
6	-8.638229	1.650012	0.000001
6	-9.450587	2.767904	0.000002
6	-10.824516	2.518753	0.000003
6	-11.331798	1.210277	0.000002
6	-10.494123	0.098336	0.000002
6	-9.117415	0.333098	0.000001
1	-9.042620	3.772069	0.000002
1	-11.513563	3.356698	0.000003
1	-10.886510	-0.912675	0.000001
8	-7.272309	1.594222	0.000001
7	-8.033543	-0.525027	0.000000
8	-6.215917	-2.498298	-0.000001
6	-4.554013	0.804028	-0.000001
6	-3.945484	-1.917620	-0.000002
6	-3.241102	0.420060	-0.000001
1	-4.811823	1.858455	-0.000001
1	-3.720768	-2.980312	-0.000002
1	-7.105295	-2.072547	-0.000001
1	-2.469413	1.181516	-0.000002
6	-1.545134	-1.425050	-0.000002
1	-1.421700	-2.505573	-0.000003
6	-0.399831	-0.623933	-0.000001
1	-0.528509	0.455967	0.000001
6	-2.881491	-0.969351	-0.000002
6	0.935384	-1.071296	-0.000002
6	1.994934	-0.103545	0.000000
6	1.292689	-2.473208	-0.000006
6	3.276425	-0.566235	-0.000001
1	1.773849	0.958473	0.000003
6	2.587636	-2.906883	-0.000007
1	0.498347	-3.210934	-0.000008
6	3.637343	-1.944396	-0.000005
1	2.819106	-3.966850	-0.000010
1	-12.407055	1.063320	0.000003

8	4.408701	0.200383	0.000000
6	5.479061	-0.657502	-0.000002
6	5.035360	-1.981912	-0.000005
1	5.667649	-2.858145	-0.000007
6	6.779792	-0.086566	0.000000
6	6.967417	1.316148	0.000004
6	7.936087	-0.903687	-0.000002
6	8.225560	1.870803	0.000006
1	6.098384	1.965345	0.000005
6	9.197846	-0.361260	0.000000
1	7.831287	-1.984362	-0.000005
6	9.387581	1.049997	0.000004
1	8.321463	2.949303	0.000008
1	10.052894	-1.025277	-0.000002
7	10.632333	1.591481	0.000007
6	11.804342	0.731649	0.000002
1	11.827126	0.092149	-0.889737
1	12.698472	1.352510	0.000008
1	11.827124	0.092138	0.889734
6	10.800364	3.035271	0.000007
1	10.346931	3.486956	0.889639
1	11.863701	3.267997	0.000010
1	10.346935	3.486957	-0.889626

Keto-HBO 1 excited-state structure in dichloromethane *G* -1529.788234 au

6	-5.301958	-1.522735	0.000003
6	-5.575010	-0.077000	0.000001
6	-6.904168	0.326284	0.000000
6	-8.687428	1.609430	-0.000002
6	-9.541034	2.692005	-0.000004
6	-10.907585	2.393216	-0.000004
6	-11.365619	1.071350	-0.000003
6	-10.488195	-0.014182	-0.000001
6	-9.130292	0.282350	-0.000001
1	-9.167634	3.709136	-0.000005
1	-11.625091	3.206356	-0.000006
1	-10.843585	-1.037807	0.000000
8	-7.311482	1.620582	-0.000001
7	-7.982604	-0.484992	0.000001
8	-6.248293	-2.376869	0.000001
6	-4.510269	0.875467	0.000001
6	-3.934838	-1.874645	0.000003
6	-3.211114	0.472680	0.000002
1	-4.758170	1.933342	0.000000
1	-3.701537	-2.936380	0.000003
1	-2.423007	1.216841	0.000001
6	-1.538784	-1.387272	0.000003
1	-1.417291	-2.468471	0.000004
6	-0.391481	-0.594588	0.000003
1	-0.510589	0.486215	0.000002
6	-2.881069	-0.934828	0.000003
6	0.943311	-1.051789	0.000003
6	2.006944	-0.090597	0.000002
6	1.292295	-2.454594	0.000004
6	3.286748	-0.560071	0.000002
1	1.791847	0.972672	0.000001
6	2.585304	-2.895765	0.000004
1	0.493985	-3.188002	0.000004
6	3.639979	-1.939495	0.000003
1	2.810527	-3.957079	0.000004

1	-12.433804	0.882120	-0.000003
8	4.422647	0.200757	0.000001
6	5.488684	-0.662709	0.000001
6	5.038656	-1.984227	0.000002
1	5.666388	-2.863703	0.000002
6	6.792588	-0.097416	0.000000
6	6.986441	1.304199	-0.000001
6	7.945024	-0.919542	-0.000001
6	8.247216	1.853335	-0.000002
1	6.120340	1.957310	0.000000
6	9.209392	-0.382680	-0.000002
1	7.835423	-1.999757	0.000000
6	9.405437	1.027523	-0.000003
1	8.347888	2.931412	-0.000002
1	10.061437	-1.050576	-0.000003
7	10.652906	1.563601	-0.000004
6	11.820848	0.698482	-0.000005
1	11.840805	0.058770	-0.889702
1	12.717863	1.315193	-0.000007
1	11.840807	0.058772	0.889694
6	10.827197	3.006520	-0.000004
1	10.375739	3.460338	0.889591
1	11.891548	3.234682	-0.000005
1	10.375737	3.460339	-0.889598
1	-7.768035	-1.499967	0.000002

Enol-HBO 1 ground-state structure in dichloromethane + HCl *G* -1530.326043 au

6	5.2792540	1.4586110	0.3397540
6	5.6075020	0.1330740	-0.0143320
6	6.9908840	-0.2972280	0.0286280
6	8.6479910	-1.6679610	-0.1779400
6	9.4652830	-2.7613690	-0.4065650
6	10.8225550	-2.5534880	-0.1718000
6	11.3146100	-1.3127480	0.2672730
6	10.4724740	-0.2286500	0.4895970
6	9.1115470	-0.4252590	0.2576190
1	9.0717340	-3.7124810	-0.7452490
1	11.5165790	-3.3715710	-0.3325040
1	10.8492180	0.7300100	0.8283190
8	7.2890950	-1.5755870	-0.3214390
7	8.0158210	0.4255800	0.3772950
8	6.1929530	2.3654260	0.7250610
6	4.5846070	-0.7447760	-0.4092490
6	3.9431450	1.8631340	0.2924980
6	3.2687380	-0.3341980	-0.4509610
1	4.8488560	-1.7591130	-0.6900260
1	3.7137860	2.8874410	0.5703670
1	7.0870790	1.9503020	0.7144360
1	2.5051390	-1.0300830	-0.7790650
6	1.5470190	1.4831500	-0.0994290
1	1.4476550	2.5573160	0.0433380
6	0.4459250	0.7265130	-0.2342660
1	0.5519440	-0.3531990	-0.3228220
6	2.9282290	0.9858870	-0.0892600
6	-0.9412180	1.2053750	-0.2433070
6	-1.9642270	0.2557890	-0.1668610
6	-1.2689220	2.5829430	-0.3284300
6	-3.2677280	0.7259390	-0.1616650
1	-1.7488600	-0.8060660	-0.1066700
6	-2.5762990	3.0294520	-0.3238870

1	-0.4700270	3.3116130	-0.4145160
6	-3.6097690	2.0824400	-0.2357530
1	-2.7989140	4.0890490	-0.3938950
1	12.3803240	-1.2003600	0.4364020
8	-4.3906390	-0.0383580	-0.0866230
6	-5.4562870	0.8244670	-0.1126390
6	-5.0453490	2.1187920	-0.2027410
1	-5.6755990	2.9955980	-0.2372320
6	-6.7787110	0.2131230	-0.0334680
6	-6.9089180	-1.1760640	0.0971680
6	-7.9307730	1.0074650	-0.0833220
6	-8.1635360	-1.7638960	0.1822900
1	-6.0220550	-1.7974910	0.1345380
6	-9.1892420	0.4285350	0.0013910
1	-7.8506090	2.0838350	-0.1890980
6	-9.2877970	-0.9498640	0.1360900
1	-8.2454660	-2.8410650	0.2854450
1	-10.0783740	1.0513750	-0.0378600
7	-10.6316440	-1.5573510	0.2296730
1	-11.3052100	-0.7842500	0.2049970
6	-10.9405080	-2.4414460	-0.9447560
1	-10.2663370	-3.2962750	-0.9151970
1	-11.9754720	-2.7710700	-0.8613450
1	-10.7863220	-1.8649070	-1.8550660
6	-10.8473090	-2.2744700	1.5315140
1	-10.6256750	-1.5829540	2.3422640
1	-11.8851620	-2.6023550	1.5708980
1	-10.1777590	-3.1324020	1.5656170

Keto-HBO 1 ground-state structure in dichloromethane +HCl *G* -1530.307653 au

6	5.3345580	1.4700000	0.2773970
6	5.6172710	0.0810060	-0.0331380
6	6.9597560	-0.3225190	0.0050720
6	8.7465040	-1.5835500	-0.1218340
6	9.6082240	-2.6472330	-0.2951740
6	10.9600990	-2.3686770	-0.0873220
6	11.3990960	-1.0883550	0.2733560
6	10.5126020	-0.0259590	0.4437370
6	9.1685710	-0.3053100	0.2365630
1	9.2510340	-3.6310440	-0.5745920
1	11.6862530	-3.1647270	-0.2088120
1	10.8506910	0.9649900	0.7222620
8	7.3732540	-1.5729660	-0.2603730
7	8.0056570	0.4532990	0.3039220
8	6.2322990	2.3073480	0.5746350
6	4.5813000	-0.8321190	-0.3670740
6	3.9406350	1.8284140	0.2228110
6	3.2782080	-0.4308490	-0.3992210
1	4.8462530	-1.8592650	-0.6019320
1	3.6970550	2.8623030	0.4523010
1	2.5034070	-1.1372910	-0.6717440
6	1.5569420	1.4073420	-0.0994530
1	1.4453860	2.4800130	0.0467710
6	0.4632890	0.6403670	-0.2381860
1	0.5783660	-0.4369030	-0.3398430
6	2.9457020	0.9295850	-0.0917610
6	-0.9293460	1.1044060	-0.2370290
6	-1.9413820	0.1420700	-0.1764590
6	-1.2740860	2.4792950	-0.2960060
6	-3.2503730	0.5963790	-0.1601950

1	-1.7134780	-0.9181130	-0.1359800
6	-2.5867630	2.9100540	-0.2810990
1	-0.4841520	3.2190780	-0.3686010
6	-3.6090600	1.9496370	-0.2082130
1	-2.8218180	3.9681420	-0.3305790
1	12.4592010	-0.9167930	0.4246820
8	-4.3636350	-0.1829090	-0.0959810
6	-5.4398920	0.6670630	-0.1020530
6	-5.0450930	1.9677880	-0.1697820
1	-5.6863490	2.8371590	-0.1865510
6	-6.7534550	0.0367210	-0.0278480
6	-6.8650580	-1.3551060	0.0624160
6	-7.9175230	0.8187130	-0.0407040
6	-8.1153040	-1.9562660	0.1446880
1	-5.9718750	-1.9684350	0.0712560
6	-9.1687760	0.2277280	0.0415670
1	-7.8488890	1.8985960	-0.1141100
6	-9.2484270	-1.1578690	0.1354850
1	-8.1949410	-3.0371100	0.2161730
1	-10.0574640	0.8505250	0.0329570
7	-10.5710250	-1.8083640	0.2405530
1	-10.3964130	-2.8177860	0.2984480
6	-11.2923690	-1.4211830	1.4997350
1	-11.5231660	-0.3581950	1.4504210
1	-12.2086000	-2.0065430	1.5612910
1	-10.6371650	-1.6312170	2.3433070
6	-11.4203660	-1.5875050	-0.9780260
1	-10.8515430	-1.9052390	-1.8500480
1	-12.3303580	-2.1763840	-0.8697930
1	-11.6607760	-0.5275670	-1.0431750
1	7.7986610	1.4410550	0.5248040

Enol-HBO 1 excited-state structure in dichloromethane +HCl *G* -1530.217207 au

6	5.306829	1.540540	0.039990
6	5.647613	0.148158	0.019414
6	7.015503	-0.250321	0.011921
6	8.685293	-1.629707	-0.018443
6	9.505549	-2.742579	-0.043204
6	10.875503	-2.480972	-0.041171
6	11.375708	-1.167405	-0.015435
6	10.533051	-0.062408	0.009187
6	9.156793	-0.309123	0.007218
1	9.105638	-3.749552	-0.063051
1	11.571535	-3.312830	-0.060096
1	10.917281	0.951313	0.028856
8	7.320504	-1.582632	-0.014848
7	8.068797	0.539503	0.026190
8	6.246505	2.503356	0.057394
6	4.602102	-0.810320	0.003511
6	3.981786	1.915301	0.041043
6	3.287991	-0.432952	0.006365
1	4.867846	-1.862133	-0.011911
1	3.748911	2.975621	0.055594
1	7.140508	2.086537	0.052765
1	2.519084	-1.196305	-0.007682
6	1.591744	1.406047	0.020465
1	1.458899	2.484841	0.024965
6	0.451163	0.591270	0.013828
1	0.588990	-0.486919	0.023656
6	2.926560	0.958091	0.023613

6	-0.883506	1.031712	-0.002436
6	-1.933467	0.054399	0.005815
6	-1.246145	2.432158	-0.029841
6	-3.218595	0.510630	-0.013824
1	-1.704084	-1.005364	0.028005
6	-2.544376	2.856194	-0.051441
1	-0.457066	3.174964	-0.035943
6	-3.582732	1.885259	-0.045041
1	-2.784177	3.913765	-0.073427
1	12.450026	-1.015291	-0.014954
8	-4.346071	-0.259387	-0.007713
6	-5.414669	0.598117	-0.035898
6	-4.987446	1.915318	-0.060053
1	-5.621278	2.790220	-0.081609
6	-6.725174	0.007585	-0.025730
6	-6.880023	-1.390845	0.042266
6	-7.877254	0.820381	-0.078814
6	-8.145279	-1.956624	0.066136
1	-6.004030	-2.027420	0.080477
6	-9.140312	0.258660	-0.057367
1	-7.781513	1.899000	-0.137629
6	-9.260052	-1.128302	0.019877
1	-8.256424	-3.036005	0.122839
1	-10.013620	0.901672	-0.100510
7	-10.602044	-1.742010	0.054661
1	-10.458855	-2.754785	0.137636
6	-11.395004	-1.315798	1.257045
1	-11.594782	-0.248501	1.175244
1	-12.328709	-1.876439	1.266665
1	-10.804195	-1.525921	2.146577
6	-11.369454	-1.514437	-1.216823
1	-10.758039	-1.856815	-2.049729
1	-12.300837	-2.076334	-1.158862
1	-11.574078	-0.448629	-1.305520

Keto-HBO 1 excited-state structure in dichloromethane + HCl *G* -1530.202560 au

6	5.342103	1.582678	0.066156
6	5.642248	0.120944	0.007052
6	6.986474	-0.290631	0.009137
6	8.719644	-1.637310	-0.026456
6	9.534440	-2.750695	-0.065653
6	10.908342	-2.498145	-0.033411
6	11.415484	-1.192176	0.034367
6	10.583173	-0.076047	0.073333
6	9.212574	-0.326160	0.041239
1	9.125712	-3.752459	-0.117903
1	11.598183	-3.334283	-0.061650
1	10.973949	0.933035	0.125355
8	7.350263	-1.595387	-0.045046
7	8.097715	0.476861	0.061381
8	6.295037	2.404766	0.118826
6	4.593145	-0.809166	-0.050368
6	3.975510	1.949549	0.058703
6	3.274413	-0.377138	-0.052974
1	4.816123	-1.870171	-0.093636
1	3.756653	3.012503	0.101352
1	2.491160	-1.125387	-0.100104
6	1.559857	1.445222	-0.004657
1	1.430691	2.525815	0.026190
6	0.447176	0.655668	-0.039314

1	0.563315	-0.425728	-0.059955
6	2.929509	1.014201	0.001059
6	-0.927405	1.110022	-0.045279
6	-1.950976	0.143967	-0.047568
6	-1.286493	2.491339	-0.048638
6	-3.256796	0.594216	-0.049367
1	-1.722119	-0.916719	-0.044840
6	-2.597531	2.915342	-0.052633
1	-0.501576	3.239570	-0.050787
6	-3.622824	1.950287	-0.052790
1	-2.834761	3.974280	-0.056032
1	12.489976	-1.045779	0.057172
8	-4.370665	-0.189520	-0.046312
6	-5.450785	0.658086	-0.047570
6	-5.053421	1.963727	-0.052529
1	-5.697013	2.831804	-0.051367
6	-6.761231	0.027997	-0.031515
6	-6.875934	-1.367662	0.015795
6	-7.927980	0.809107	-0.056457
6	-8.127027	-1.970418	0.046331
1	-5.982788	-1.980858	0.032822
6	-9.179573	0.215597	-0.026584
1	-7.859061	1.890685	-0.098382
6	-9.261164	-1.172707	0.028073
1	-8.207897	-3.052961	0.086095
1	-10.068417	0.838189	-0.044717
7	-10.585432	-1.826228	0.077139
1	-10.410936	-2.836331	0.124287
6	-11.352251	-1.460099	1.315422
1	-11.573273	-0.394553	1.279187
1	-12.274903	-2.038201	1.329130
1	-10.733163	-1.692296	2.180111
6	-11.393731	-1.585771	-1.165484
1	-10.792156	-1.878026	-2.024317
1	-12.301002	-2.185486	-1.102819
1	-11.641702	-0.526659	-1.214428
1	7.978118	1.493767	0.105339

Enol-HBO 1 ground-state structure in acetone *G* -1529.914292 au

6	5.2847450	-1.5081640	0.0067930
6	5.6027260	-0.1338460	0.0037380
6	6.9910490	0.2803650	0.0025720
6	8.6448450	1.6710240	-0.0009420
6	9.4549350	2.7932350	-0.0036550
6	10.8253220	2.5422400	-0.0034700
6	11.3362250	1.2332970	-0.0007130
6	10.5006770	0.1213850	0.0019990
6	9.1268160	0.3607550	0.0018520
1	9.0466880	3.7969870	-0.0057700
1	11.5145390	3.3799350	-0.0055170
1	10.8924560	-0.8896770	0.0041250
8	7.2767880	1.6086210	-0.0004600
7	8.0328310	-0.5008550	0.0040650
8	6.2158820	-2.4783590	0.0088230
6	4.5613040	0.8093820	0.0018300
6	3.9431900	-1.8954840	0.0077220
6	3.2401870	0.4150510	0.0027570
1	4.8148420	1.8645160	-0.0003700
1	3.7227280	-2.9587940	0.0100100
1	7.1119830	-2.0673900	0.0078030

1	2.4630110	1.1704990	0.0014380
6	1.5283220	-1.4503690	0.0062370
1	1.4355070	-2.5343880	0.0105800
6	0.4212090	-0.6890550	0.0013440
1	0.5243710	0.3947300	-0.0036750
6	2.9101050	-0.9571450	0.0055830
6	-0.9669300	-1.1614860	0.0012880
6	-1.9865850	-0.2013240	-0.0072400
6	-1.3076250	-2.5365900	0.0091120
6	-3.2930770	-0.6572750	-0.0078250
1	-1.7620240	0.8606560	-0.0133450
6	-2.6213670	-2.9698380	0.0083080
1	-0.5169250	-3.2793910	0.0161130
6	-3.6493620	-2.0134100	-0.0005070
1	-2.8511310	-4.0304520	0.0144240
1	12.4114830	1.0889780	-0.0007020
8	-4.4109140	0.1196110	-0.0156300
6	-5.4901670	-0.7312230	-0.0134530
6	-5.0850780	-2.0339010	-0.0045220
1	-5.7246250	-2.9043630	-0.0015240
6	-6.8038300	-0.1055880	-0.0213450
6	-6.9496480	1.2874830	-0.0303030
6	-7.9694860	-0.8841800	-0.0153640
6	-8.2004210	1.8824760	-0.0369160
1	-6.0655180	1.9168480	-0.0287100
6	-9.2255440	-0.3054150	-0.0221880
1	-7.8957030	-1.9680300	-0.0015080
6	-9.3786300	1.1014680	-0.0413530
1	-8.2610940	2.9637800	-0.0376810
1	-10.0953820	-0.9504250	-0.0111090
7	-10.6212380	1.6825000	-0.0674010
6	-11.8025920	0.8537660	0.0777160
1	-11.8078630	0.3046500	1.0291180
1	-12.6873910	1.4883850	0.0407020
1	-11.8753860	0.1259940	-0.7379700
6	-10.7396160	3.1221170	0.0616110
1	-10.2318190	3.6339650	-0.7633100
1	-11.7936430	3.3956750	0.0283260
1	-10.3145000	3.4882980	1.0060460

Keto-HBO 1 ground-state structure in acetone *G* -1529.895457 au

6	5.3158250	-1.4938680	0.1294140
6	5.5761520	-0.0732350	-0.0091840
6	6.9168910	0.3376030	0.0037130
6	8.6866310	1.6274760	-0.0578550
6	9.5308130	2.7160790	-0.1376460
6	10.8941620	2.4299000	-0.0482350
6	11.3605520	1.1187260	0.1120040
6	10.4913210	0.0314720	0.1904180
6	9.1359510	0.3185470	0.1011400
1	9.1526290	3.7236040	-0.2615930
1	11.6076380	3.2444710	-0.1044350
1	10.8499360	-0.9833870	0.3143200
8	7.3076120	1.6173690	-0.1159240
7	7.9829550	-0.4573210	0.1341050
8	6.2332830	-2.3540550	0.2583520
6	4.5184820	0.8648330	-0.1528220
6	3.9231210	-1.8564270	0.1098700
6	3.2168590	0.4573890	-0.1627680
1	4.7651930	1.9178330	-0.2563840

1	3.6962820	-2.9144250	0.2118320
1	2.4257330	1.1884290	-0.2782470
6	1.5231150	-1.4277170	-0.0263680
1	1.4287380	-2.5088650	0.0541170
6	0.4159510	-0.6701200	-0.1033590
1	0.5168150	0.4118740	-0.1638450
6	2.9062150	-0.9361140	-0.0264240
6	-0.9714530	-1.1468080	-0.1023810
6	-1.9947890	-0.1908920	-0.0806520
6	-1.3073190	-2.5229240	-0.1232790
6	-3.2996050	-0.6519450	-0.0717160
1	-1.7743820	0.8719230	-0.0677940
6	-2.6194610	-2.9614190	-0.1149640
1	-0.5135670	-3.2618810	-0.1545160
6	-3.6509050	-2.0092640	-0.0866050
1	-2.8452220	-4.0227790	-0.1336340
1	12.4286680	0.9425220	0.1770310
8	-4.4203020	0.1207210	-0.0486030
6	-5.4964380	-0.7341930	-0.0486300
6	-5.0866980	-2.0350800	-0.0715360
1	-5.7231320	-2.9078210	-0.0774490
6	-6.8123760	-0.1134670	-0.0253940
6	-6.9632490	1.2789540	-0.0087310
6	-7.9750540	-0.8963890	-0.0141140
6	-8.2161200	1.8692270	0.0144750
1	-6.0814040	1.9115220	-0.0105550
6	-9.2331410	-0.3223260	0.0087150
1	-7.8972120	-1.9800370	-0.0194640
6	-9.3914560	1.0840240	0.0156080
1	-8.2805900	2.9501560	0.0328910
1	-10.1003810	-0.9707810	0.0228230
7	-10.6365560	1.6608730	0.0190780
6	-11.8119870	0.8254270	0.1736210
1	-11.7976160	0.2618620	1.1164830
1	-12.6996050	1.4571140	0.1626030
1	-11.8973700	0.1098910	-0.6515740
6	-10.7574290	3.0972820	0.1781260
1	-10.2639390	3.6267070	-0.6443410
1	-11.8126930	3.3678490	0.1660560
1	-10.3190000	3.4466120	1.1229080
1	7.7975800	-1.4680530	0.2332530

Enol-HBO 1 excited-state structure in acetone *G* -1529.809848 au

6	-5.268890	-1.535950	-0.000002
6	-5.608364	-0.145793	-0.000002
6	-6.973663	0.257379	0.000000
6	-8.638186	1.650176	0.000002
6	-9.450106	2.768469	0.000003
6	-10.824141	2.519608	0.000005
6	-11.331850	1.211225	0.000006
6	-10.494402	0.098936	0.000004
6	-9.117679	0.333517	0.000002
1	-9.042032	3.772582	0.000003
1	-11.512900	3.357748	0.000006
1	-10.887477	-0.911830	0.000005
8	-7.271997	1.593903	0.000000
7	-8.033554	-0.525042	0.000001
8	-6.217078	-2.498404	-0.000001
6	-4.553247	0.803170	-0.000003
6	-3.945975	-1.918854	-0.000003

6	-3.240448	0.418901	-0.000004
1	-4.810128	1.857862	-0.000004
1	-3.721456	-2.981652	-0.000002
1	-7.106091	-2.071528	0.000000
1	-2.468907	1.180510	-0.000005
6	-1.545357	-1.427225	-0.000004
1	-1.421911	-2.507734	-0.000004
6	-0.399053	-0.625300	-0.000004
1	-0.528199	0.454570	-0.000003
6	-2.880594	-0.970966	-0.000004
6	0.935114	-1.071742	-0.000004
6	1.994905	-0.102762	-0.000002
6	1.293487	-2.474018	-0.000007
6	3.276055	-0.564844	-0.000003
1	1.772980	0.959121	-0.000001
6	2.588387	-2.906869	-0.000007
1	0.499701	-3.212398	-0.000009
6	3.638007	-1.943335	-0.000005
1	2.820795	-3.966597	-0.000009
1	-12.407110	1.064527	0.000007
8	4.408305	0.202046	-0.000001
6	5.479050	-0.655489	-0.000002
6	5.035066	-1.980836	-0.000004
1	5.667412	-2.857035	-0.000005
6	6.779109	-0.085279	0.000000
6	6.967472	1.317838	0.000003
6	7.935357	-0.903403	-0.000001
6	8.225547	1.871871	0.000005
1	6.098941	1.967742	0.000004
6	9.197073	-0.361710	0.000001
1	7.830132	-1.984003	-0.000003
6	9.387615	1.050040	0.000005
1	8.322091	2.950289	0.000007
1	10.051799	-1.026081	0.000000
7	10.631658	1.590364	0.000008
6	11.803808	0.729856	0.000004
1	11.825881	0.090581	-0.889741
1	12.697874	1.350604	0.000010
1	11.825878	0.090571	0.889743
6	10.801146	3.034466	0.000008
1	10.348016	3.486095	0.889658
1	11.864663	3.265881	0.000011
1	10.348021	3.486095	-0.889646

Keto-HBO 1 excited-state structure in acetone *G* -1529.791507 au

6	5.302473	-1.528642	-0.000002
6	5.575939	-0.083572	0.000002
6	6.904693	0.321711	0.000001
6	8.683595	1.611572	0.000000
6	9.532786	2.697730	0.000001
6	10.900350	2.403981	-0.000002
6	11.363593	1.083740	-0.000004
6	10.490364	-0.005211	-0.000004
6	9.131566	0.286646	-0.000002
1	9.155700	3.713488	0.000002
1	11.614733	3.219834	-0.000001
1	10.849487	-1.027529	-0.000006
8	7.307235	1.616988	0.000002
7	7.986112	-0.485256	-0.000002
8	6.249170	-2.383405	-0.000009

6	4.510739	0.868808	0.000005
6	3.935578	-1.880413	-0.000002
6	3.211347	0.466948	0.000006
1	4.758538	1.926728	0.000008
1	3.701416	-2.942132	-0.000006
1	2.423966	1.211882	0.000008
6	1.539108	-1.393187	0.000001
1	1.416993	-2.474329	-0.000002
6	0.391046	-0.599044	0.000004
1	0.511345	0.481656	0.000006
6	2.880285	-0.940584	0.000001
6	-0.942833	-1.054422	0.000002
6	-2.006271	-0.091331	0.000004
6	-1.293727	-2.457474	-0.000001
6	-3.285920	-0.559466	0.000002
1	-1.789722	0.971679	0.000007
6	-2.586874	-2.897098	-0.000003
1	-0.496367	-3.191974	-0.000002
6	-3.640996	-1.939129	-0.000001
1	-2.813682	-3.958037	-0.000005
1	12.432467	0.898670	-0.000006
8	-4.421392	0.202255	0.000003
6	-5.488310	-0.660266	0.000000
6	-5.038561	-1.983122	-0.000003
1	-5.666830	-2.862225	-0.000006
6	-6.791099	-0.095245	0.000000
6	-6.985112	1.306962	0.000003
6	-7.943918	-0.917955	-0.000003
6	-8.245514	1.855967	0.000003
1	-6.119226	1.960386	0.000005
6	-9.207933	-0.381311	-0.000003
1	-7.834333	-1.998132	-0.000005
6	-9.404182	1.029550	0.000000
1	-8.346400	2.933995	0.000006
1	-10.059956	-1.049166	-0.000005
7	-10.650591	1.564949	0.000001
6	-11.819130	0.699689	-0.000002
1	-11.838634	0.060253	0.889715
1	-12.715766	1.316731	0.000000
1	-11.838634	0.060258	-0.889723
6	-10.825802	3.008289	0.000003
1	-10.374466	3.461813	-0.889623
1	-11.890235	3.235519	0.000003
1	-10.374467	3.461810	0.889632
1	7.781638	-1.500444	-0.000003

*Coordinates for **HBO 2**:*

Enol-HBO 2 ground-state structure in cyclohexane *G* -1866.844341 au

6	3.7167220	-1.7062440	0.2346380
6	4.0765710	-0.3848200	-0.1061900
6	5.4690940	0.0044620	-0.0887400
6	7.1527060	1.3400740	-0.3127490
6	7.9912440	2.4176700	-0.5449060
6	9.3457260	2.1758150	-0.3527520
6	9.8095470	0.9123610	0.0511910
6	8.9543110	-0.1581060	0.2799540
6	7.5949310	0.0779000	0.0884410
1	7.6135360	3.3833460	-0.8583260

1	10.0634450	2.9721950	-0.5203130
1	9.3242490	-1.1284120	0.5887030
7	6.4861900	-0.7482740	0.2204500
8	4.6071340	-2.6472250	0.5843280
6	3.0705530	0.5295020	-0.4646930
6	2.3679260	-2.0685910	0.2118770
6	1.7443670	0.1585480	-0.4833150
1	3.3592840	1.5397730	-0.7359900
1	2.1164390	-3.0899130	0.4807520
1	5.5137840	-2.2666240	0.5618380
1	0.9942660	0.8805190	-0.7848640
6	-0.0232260	-1.6122710	-0.1207670
1	-0.1524290	-2.6838640	0.0166130
6	-1.1046870	-0.8232340	-0.2308200
1	-0.9638070	0.2531990	-0.3160170
6	1.3709000	-1.1573710	-0.1333500
6	-2.5062590	-1.2514250	-0.2211520
6	-3.4962840	-0.2641540	-0.1554170
6	-2.8870470	-2.6139450	-0.2781850
6	-4.8149170	-0.6816320	-0.1348920
1	-3.2416660	0.7902080	-0.1156130
6	-4.2121090	-3.0092080	-0.2577040
1	-2.1172480	-3.3747430	-0.3545220
6	-5.2107670	-2.0257810	-0.1813480
1	-4.4730520	-4.0615320	-0.3066100
8	-5.9072340	0.1264410	-0.0697380
6	-7.0103430	-0.6909150	-0.0741500
6	-6.6456870	-2.0033040	-0.1413690
1	-7.3126740	-2.8524980	-0.1617660
6	-8.3032190	-0.0261530	-0.0090250
6	-8.4015550	1.3693750	0.0347580
6	-9.4921910	-0.7655670	0.0176160
6	-9.6308790	2.0039170	0.0982850
1	-7.4958570	1.9667000	0.0225320
6	-10.7271970	-0.1460920	0.0806060
1	-9.4533270	-1.8510540	-0.0060400
6	-10.8322130	1.2629650	0.1139450
1	-9.6549770	3.0859280	0.1369230
1	-11.6174030	-0.7622700	0.1059160
7	-12.0583530	1.8868390	0.1560270
6	-13.2530340	1.0919790	0.3548390
1	-13.2247830	0.5251830	1.2962910
1	-14.1197540	1.7526200	0.3755060
1	-13.3930780	0.3823970	-0.4680450
6	-12.1177320	3.3184160	0.3698860
1	-11.6193210	3.8566280	-0.4438270
1	-13.1614130	3.6321930	0.3866810
1	-11.6483100	3.6178990	1.3176910
8	5.7941070	1.2849590	-0.4236140
6	11.2876990	0.7528370	0.2625850
9	11.9865630	1.2103880	-0.7888170
9	11.6382120	-0.5254570	0.4542180
9	11.7107220	1.4469240	1.3320160

Keto-HBO 2 ground-state structure in cyclohexane *G* -1866.822127 au

6	3.7711520	-1.6261760	0.1224840
6	4.0532250	-0.2148700	-0.0991080
6	5.3920000	0.1650200	-0.0925220
6	7.1989350	1.4002880	-0.2022610
6	8.0760950	2.4561380	-0.3375180

6	9.4292310	2.1431590	-0.2154370
6	9.8471000	0.8309730	0.0286770
6	8.9511230	-0.2294380	0.1619570
6	7.6075260	0.0881010	0.0404660
1	7.7290950	3.4637780	-0.5305310
1	10.1726840	2.9258900	-0.3177820
1	9.2908980	-1.2417240	0.3439660
7	6.4387770	-0.6526440	0.1003170
8	4.6738240	-2.4837710	0.3139320
6	3.0053540	0.7265420	-0.3155460
6	2.3732670	-1.9742820	0.1079100
6	1.7046860	0.3302010	-0.3162380
1	3.2657310	1.7677760	-0.4837840
1	2.1366090	-3.0214610	0.2730380
1	0.9212040	1.0568550	-0.4935560
6	-0.0163120	-1.5201730	-0.0802560
1	-0.1290040	-2.5962100	0.0352850
6	-1.1111250	-0.7473920	-0.1748560
1	-0.9916270	0.3311170	-0.2595710
6	1.3735680	-1.0525250	-0.0954540
6	-2.5059420	-1.1989000	-0.1579430
6	-3.5121960	-0.2265610	-0.1242830
6	-2.8656160	-2.5683960	-0.1763970
6	-4.8245120	-0.6638920	-0.0989430
1	-3.2743780	0.8324200	-0.1133430
6	-4.1843440	-2.9837660	-0.1516940
1	-2.0841190	-3.3194820	-0.2220020
6	-5.1988430	-2.0147290	-0.1093690
1	-4.4283350	-4.0411560	-0.1696600
8	-5.9301250	0.1283230	-0.0619150
6	-7.0199850	-0.7065840	-0.0484260
6	-6.6342170	-2.0141530	-0.0767720
1	-7.2873860	-2.8742780	-0.0767410
6	-8.3243780	-0.0622660	-0.0084250
6	-8.4480580	1.3318520	-0.0111340
6	-9.5000260	-0.8216040	0.0399690
6	-9.6890260	1.9456980	0.0282060
1	-7.5532870	1.9448480	-0.0408670
6	-10.7462580	-0.2229140	0.0792030
1	-9.4415570	-1.9063760	0.0530660
6	-10.8768190	1.1841790	0.0652940
1	-9.7326440	3.0278020	0.0309120
1	-11.6251280	-0.8541430	0.1231420
7	-12.1145470	1.7870870	0.0830340
6	-13.2944790	0.9778600	0.3098820
1	-13.2578480	0.4466890	1.2716930
1	-14.1734730	1.6224640	0.3045650
1	-13.4194620	0.2359970	-0.4864590
6	-12.1996480	3.2229020	0.2557460
1	-11.7076910	3.7461360	-0.5714830
1	-13.2487450	3.5186160	0.2598600
1	-11.7391350	3.5578400	1.1961020
1	6.1990940	-1.6518740	0.2559690
8	5.8271940	1.4298570	-0.2817390
6	11.3176850	0.5733440	0.2058800
9	11.6271730	-0.7139680	0.0015680
9	12.0521460	1.3087050	-0.6409990
9	11.7258790	0.8859610	1.4454250

Enol-HBO 2 excited-state structure in cyclohaxane *G* -1866.736499 au

6	-3.718535	1.735135	0.003679
6	-4.089643	0.352395	-0.022544
6	-5.461355	-0.018178	-0.022557
6	-7.151914	-1.378134	-0.041361
6	-7.986887	-2.479508	-0.064220
6	-9.353252	-2.207131	-0.050365
6	-9.825267	-0.886463	-0.014878
6	-8.973372	0.213287	0.007393
6	-7.603018	-0.050122	-0.007338
1	-7.599669	-3.490942	-0.094427
1	-10.066502	-3.024318	-0.072661
1	-9.353628	1.227457	0.031070
7	-6.507579	0.784503	0.002973
8	-4.636805	2.720356	0.028446
6	-3.059447	-0.623409	-0.048082
6	-2.384788	2.082595	0.003773
6	-1.738408	-0.269765	-0.046789
1	-3.344154	-1.670473	-0.068834
1	-2.135677	3.139338	0.024521
1	-5.537910	2.324408	0.027053
1	-0.983490	-1.047626	-0.067688
6	0.002712	1.531812	-0.015717
1	0.150230	2.609262	0.000735
6	1.124609	0.709232	-0.026278
1	0.974479	-0.367608	-0.035448
6	-1.349190	1.109002	-0.020059
6	2.474936	1.131643	-0.021977
6	3.510401	0.145491	-0.021916
6	2.858378	2.523651	-0.017012
6	4.803737	0.581736	-0.015143
1	3.268781	-0.911877	-0.025516
6	4.162997	2.931658	-0.011154
1	2.078456	3.276368	-0.019325
6	5.190923	1.949961	-0.009482
1	4.414374	3.987125	-0.007947
8	5.918308	-0.209038	-0.011870
6	7.005537	0.625568	-0.003964
6	6.593339	1.956185	-0.002721
1	7.245063	2.817990	0.003187
6	8.295624	0.022767	0.002650
6	8.448499	-1.382225	0.003348
6	9.469660	0.810273	0.009773
6	9.693801	-1.967333	0.011282
1	7.563007	-2.008569	-0.002099
6	10.718808	0.237064	0.017541
1	9.390410	1.893199	0.009126
6	10.873607	-1.176304	0.018876
1	9.762883	-3.047931	0.011870
1	11.589559	0.880463	0.022828
7	12.108379	-1.749690	0.027239
6	13.298550	-0.918525	0.034975
1	13.332121	-0.278838	0.924867
1	14.179032	-1.559333	0.040809
1	13.343758	-0.279184	-0.854629
6	12.239188	-3.195532	0.029921
1	11.780608	-3.638269	-0.862132
1	13.296342	-3.456552	0.037081
1	11.769066	-3.636015	0.917088
8	-5.790814	-1.352008	-0.050915
6	-11.310246	-0.680415	0.045776

9	-11.956358	-1.461556	-0.836454
9	-11.660210	0.587871	-0.210480
9	-11.806562	-0.987948	1.257059

Enol-HBO 2 ground-state structure in dichloromethane *G* -1866.853311 au

6	-3.7261450	1.7154700	0.1610580
6	-4.0793080	0.3700220	-0.0751810
6	-5.4733590	-0.0171220	-0.0629200
6	-7.1535430	-1.3658520	-0.2160880
6	-7.9872400	-2.4607280	-0.3745480
6	-9.3455780	-2.2026780	-0.2402670
6	-9.8169640	-0.9078140	0.0380620
6	-8.9668420	0.1795100	0.1941770
6	-7.6033840	-0.0733330	0.0603830
1	-7.6040070	-3.4507050	-0.5897190
1	-10.0590130	-3.0124950	-0.3535860
1	-9.3422740	1.1730510	0.4076270
7	-6.4959270	0.7609200	0.1506960
8	-4.6269100	2.6828220	0.4036620
6	-3.0653580	-0.5713170	-0.3239660
6	-2.3771310	2.0761600	0.1456540
6	-1.7377320	-0.2026540	-0.3371600
1	-3.3466550	-1.6022870	-0.5123510
1	-2.1296390	3.1168270	0.3320010
1	-5.5329980	2.2983760	0.3870880
1	-0.9823440	-0.9509150	-0.5472560
6	0.0213440	1.5983320	-0.0842720
1	0.1442180	2.6752600	0.0097400
6	1.1065660	0.8095510	-0.1584770
1	0.9722800	-0.2693510	-0.2162820
6	-1.3717780	1.1390690	-0.0938950
6	2.5068700	1.2434440	-0.1512500
6	3.4995970	0.2568100	-0.1046190
6	2.8845350	2.6080030	-0.1916850
6	4.8175520	0.6775150	-0.0908070
1	3.2465130	-0.7983510	-0.0767960
6	4.2093680	3.0059140	-0.1776490
1	2.1139140	3.3698720	-0.2451920
6	5.2106820	2.0230490	-0.1240440
1	4.4679010	4.0593350	-0.2123300
8	5.9129900	-0.1288700	-0.0458950
6	7.0149950	0.6917850	-0.0504650
6	6.6462250	2.0043760	-0.0970970
1	7.3100880	2.8563030	-0.1112940
6	8.3099240	0.0296290	-0.0073840
6	8.4136480	-1.3663780	0.0360310
6	9.4978580	0.7731880	-0.0037260
6	9.6456110	-1.9977780	0.0776090
1	7.5107880	-1.9684200	0.0408560
6	10.7356840	0.1576090	0.0372830
1	9.4562580	1.8585520	-0.0299270
6	10.8463500	-1.2526490	0.0709520
1	9.6735980	-3.0797050	0.1165460
1	11.6242800	0.7765910	0.0443350
7	12.0717690	-1.8710030	0.0922190
6	13.2729550	-1.0727040	0.2422200
1	13.2704560	-0.4927520	1.1752940
1	14.1392920	-1.7334440	0.2489900
1	13.3884960	-0.3748190	-0.5943740
6	12.1428750	-3.3070160	0.2798740

1	11.6349840	-3.8351530	-0.5346290
1	13.1883110	-3.6138800	0.2777080
1	11.6889890	-3.6229800	1.2292010
8	-5.7920010	-1.3204270	-0.2932150
6	-11.3005210	-0.7309710	0.1815620
9	-11.9586640	-1.1858590	-0.8978820
9	-11.6482880	0.5513190	0.3511890
9	-11.7801050	-1.4164810	1.2335080

Keto-HBO 2 ground-state structure in dichloromethane *G* -1866.831500 au

6	-3.7731210	1.6656680	0.0789580
6	-4.0558650	0.2501450	-0.0892970
6	-5.3979170	-0.1360140	-0.0817560
6	-7.1880340	-1.3962980	-0.1607730
6	-8.0497100	-2.4693210	-0.2624290
6	-9.4065530	-2.1674080	-0.1649910
6	-9.8427340	-0.8506880	0.0237590
6	-8.9627650	0.2257940	0.1234520
6	-7.6148020	-0.0821240	0.0259820
1	-7.6896700	-3.4796260	-0.4119420
1	-10.1383220	-2.9639730	-0.2424540
1	-9.3134740	1.2407600	0.2641550
7	-6.4536200	0.6745780	0.0675470
8	-4.6768720	2.5343350	0.2257170
6	-3.0105030	-0.7018130	-0.2541860
6	-2.3744040	2.0080500	0.0675240
6	-1.7056900	-0.3119590	-0.2551200
1	-3.2724480	-1.7484090	-0.3815080
1	-2.1326410	3.0599490	0.1930750
1	-0.9246020	-1.0504100	-0.3891670
6	0.0177430	1.5422720	-0.0725670
1	0.1311700	2.6207450	0.0174450
6	1.1111280	0.7642510	-0.1438490
1	0.9900130	-0.3152070	-0.2118760
6	-1.3732160	1.0755360	-0.0870100
6	2.5073940	1.2125660	-0.1253270
6	3.5103460	0.2354770	-0.1047850
6	2.8717660	2.5813990	-0.1276750
6	4.8241980	0.6687450	-0.0788390
1	3.2679070	-0.8225650	-0.1055240
6	4.1925300	2.9921030	-0.1024240
1	2.0937030	3.3368940	-0.1573200
6	5.2037310	2.0184580	-0.0750270
1	4.4403720	4.0486730	-0.1067550
8	5.9278750	-0.1275460	-0.0536260
6	7.0214540	0.7041840	-0.0333020
6	6.6394520	2.0136240	-0.0458160
1	7.2946010	2.8723640	-0.0371320
6	8.3234530	0.0550270	-0.0037360
6	8.4437370	-1.3401680	-0.0214300
6	9.5021340	0.8113460	0.0490040
6	9.6828550	-1.9583480	0.0076920
1	7.5483560	-1.9523590	-0.0554490
6	10.7468440	0.2090900	0.0783590
1	9.4474960	1.8961720	0.0727670
6	10.8743560	-1.1997950	0.0502400
1	9.7235300	-3.0405500	-0.0016390
1	11.6275610	0.8374850	0.1257160
7	12.1070650	-1.8042890	0.0599520
6	13.2960660	-0.9996240	0.2632980

1	13.2747880	-0.4644730	1.2225970
1	14.1705310	-1.6495050	0.2499040
1	13.4130940	-0.2616870	-0.5379340
6	12.1930150	-3.2460160	0.1881130
1	11.7027300	-3.7450890	-0.6549820
1	13.2420590	-3.5403500	0.1877440
1	11.7301870	-3.6070970	1.1168390
1	-6.2495030	1.6804990	0.1871930
8	-5.8146300	-1.4094480	-0.2251870
6	-11.3182900	-0.6081530	0.1735980
9	-11.6412220	0.6742290	-0.0410590
9	-12.0311540	-1.3549000	-0.6826700
9	-11.7469720	-0.9214440	1.4071390

Enol-HBO 2 excited-state structure in dichloromethane *G* -1866.748842 au

6	-3.7182950	1.7377560	0.0071010
6	-4.0895280	0.3551900	-0.0291850
6	-5.4603500	-0.0167280	-0.0278480
6	-7.1506610	-1.3778330	-0.0520870
6	-7.9835900	-2.4806510	-0.0811860
6	-9.3503230	-2.2099490	-0.0599070
6	-9.8234870	-0.8900250	-0.0116130
6	-8.9729160	0.2113200	0.0168680
6	-7.6029910	-0.0510910	-0.0051760
1	-7.5962460	-3.4916160	-0.1213230
1	-10.0610540	-3.0291400	-0.0862190
1	-9.3543310	1.2248960	0.0508710
7	-6.5070840	0.7853440	0.0081970
8	-4.6423130	2.7218090	0.0427280
6	-3.0558790	-0.6181090	-0.0659430
6	-2.3870780	2.0893310	0.0061310
6	-1.7355790	-0.2632590	-0.0653650
1	-3.3368920	-1.6661450	-0.0946810
1	-2.1382420	3.1461760	0.0349210
1	-5.5416010	2.3200920	0.0411430
1	-0.9811910	-1.0412830	-0.0950500
6	0.0011650	1.5427540	-0.0229080
1	0.1489190	2.6199290	0.0008980
6	1.1278800	0.7164240	-0.0390100
1	0.9755580	-0.3602250	-0.0530070
6	-1.3449050	1.1174840	-0.0282220
6	2.4728820	1.1345160	-0.0327990
6	3.5094240	0.1429010	-0.0347640
6	2.8612600	2.5279290	-0.0230940
6	4.8010800	0.5762580	-0.0242100
1	3.2640780	-0.9137140	-0.0418850
6	4.1656630	2.9320330	-0.0141860
1	2.0839470	3.2835150	-0.0245630
6	5.1929830	1.9457330	-0.0135690
1	4.4211930	3.9863580	-0.0075980
8	5.9154170	-0.2158020	-0.0206330
6	7.0044250	0.6170350	-0.0073620
6	6.5912850	1.9516160	-0.0035140
1	7.2432960	2.8132130	0.0066350
6	8.2916890	0.0170090	0.0020380
6	8.4475550	-1.3896570	0.0009030
6	9.4657090	0.8083910	0.0146880
6	9.6925610	-1.9723670	0.0126680
1	7.5642530	-2.0191860	-0.0088190
6	10.7147160	0.2380610	0.0261950

1	9.3849900	1.8910890	0.0154200
6	10.8727950	-1.1774100	0.0261900
1	9.7641190	-3.0526980	0.0118530
1	11.5842960	0.8827210	0.0356940
7	12.1044080	-1.7461750	0.0388380
6	13.2956750	-0.9127340	0.0524500
1	13.3231890	-0.2752100	0.9433700
1	14.1755010	-1.5535810	0.0608340
1	13.3418290	-0.2731190	-0.8361640
6	12.2405900	-3.1936320	0.0408320
1	11.7869370	-3.6351550	-0.8536380
1	13.2984380	-3.4496300	0.0523100
1	11.7677600	-3.6344370	0.9256980
8	-5.7888370	-1.3493640	-0.0663310
6	-11.3076870	-0.6843140	0.0583890
9	-11.9615890	-1.4707830	-0.8133930
9	-11.6610880	0.5822650	-0.2032330
9	-11.7962760	-0.9830480	1.2758380

Keto-HBO 2 excited-state structure in dichloromethane *G* -1866.727909 au

6	3.7590050	-1.6515240	-0.0141490
6	4.0578350	-0.2102760	-0.0029180
6	5.3909400	0.1648490	-0.0074970
6	7.2007850	1.4100150	-0.0063980
6	8.0769410	2.4737610	-0.0074960
6	9.4364990	2.1503240	-0.0226190
6	9.8569350	0.8184670	-0.0375990
6	8.9621320	-0.2546370	-0.0379010
6	7.6140380	0.0712330	-0.0207360
1	7.7273520	3.4988220	-0.0012110
1	10.1752540	2.9435930	-0.0297260
1	9.3041040	-1.2822970	-0.0565390
7	6.4540600	-0.6705580	-0.0217630
8	4.6901820	-2.5228200	-0.0265740
6	3.0081510	0.7615300	0.0114490
6	2.3864690	-1.9792760	-0.0103870
6	1.7034680	0.3807500	0.0140100
1	3.2741800	1.8149210	0.0201550
1	2.1343400	-3.0365800	-0.0190240
1	0.9279590	1.1379980	0.0253740
6	0.0002670	-1.4521170	0.0036250
1	-0.1375560	-2.5312560	-0.0033230
6	-1.1350230	-0.6425030	0.0101790
1	-1.0006060	0.4364690	0.0138730
6	1.3493370	-1.0208600	0.0026480
6	-2.4758000	-1.0817260	0.0102290
6	-3.5257070	-0.1056860	0.0113240
6	-2.8435050	-2.4799890	0.0086070
6	-4.8115880	-0.5574910	0.0095610
1	-3.2956510	0.9543900	0.0125600
6	-4.1420710	-2.9033640	0.0074410
1	-2.0553670	-3.2241940	0.0088390
6	-5.1834570	-1.9322610	0.0075560
1	-4.3821410	-3.9613410	0.0064130
8	-5.9370890	0.2184720	0.0088820
6	-7.0141200	-0.6301160	0.0062580
6	-6.5817360	-1.9585210	0.0056740
1	-7.2211750	-2.8295040	0.0036440
6	-8.3100120	-0.0490810	0.0037830
6	-8.4866090	1.3552040	0.0028720

6	-9.4723390	-0.8578280	0.0014440
6	-9.7401590	1.9193200	-0.0005940
1	-7.6125760	1.9976150	0.0047100
6	-10.7296840	-0.3060850	-0.0019160
1	-9.3755110	-1.9391990	0.0022780
6	-10.9085700	1.1069210	-0.0033090
1	-9.8279490	2.9984620	-0.0013630
1	-11.5897550	-0.9634810	-0.0036530
7	-12.1484980	1.6574920	-0.0071770
6	-13.3274470	0.8066620	-0.0099270
1	-13.3574220	0.1682650	0.8802710
1	-14.2165890	1.4345600	-0.0128820
1	-13.3523900	0.1669620	-0.8993540
6	-12.3060260	3.1027630	-0.0094010
1	-11.8467220	3.5496130	-0.8983490
1	-13.3676030	3.3430950	-0.0127660
1	-11.8518870	3.5518200	0.8810770
1	6.2123740	-1.6816590	-0.0286250
8	5.8305060	1.4526290	0.0015880
6	11.3287230	0.5246910	0.0092570
9	11.6236450	-0.6469530	-0.5737060
9	12.0498300	1.4739100	-0.6055480
9	11.7822570	0.4529600	1.2726540

Enol-HBO 2 ground-state structure in dichloromethane + HCl *G* -1867.266000 au

6	-3.7430710	1.6693830	-0.2666400
6	-4.1236180	0.3757980	0.1488300
6	-5.5207060	-0.0026690	0.1193910
6	-7.2242700	-1.3034730	0.3828210
6	-8.0802670	-2.3569020	0.6603130
6	-9.4249370	-2.1169990	0.4081050
6	-9.8625340	-0.8792540	-0.0953080
6	-8.9907600	0.1671350	-0.3671660
6	-7.6407230	-0.0676840	-0.1155590
1	-7.7233220	-3.3031620	1.0481330
1	-10.1541260	-2.8968380	0.6025020
1	-9.3398630	1.1166510	-0.7546410
7	-6.5187450	0.7375230	-0.2698790
8	-4.6174030	2.5931560	-0.6986060
6	-3.1369030	-0.5225020	0.5896140
6	-2.3920230	2.0224530	-0.2335270
6	-1.8065160	-0.1625700	0.6161460
1	-3.4414530	-1.5108280	0.9181240
1	-2.1217580	3.0221730	-0.5597160
1	-5.5279200	2.2191430	-0.6759570
1	-1.0711550	-0.8703310	0.9812440
6	-0.0134810	1.5644800	0.1791360
1	0.1296750	2.6285470	0.0025130
6	1.0557950	0.7656040	0.3263090
1	0.9053670	-0.3061310	0.4440200
6	-1.4136860	1.1243680	0.1917590
6	2.4615030	1.1864440	0.3069980
6	3.4431260	0.1945590	0.2264240
6	2.8464000	2.5503810	0.3664360
6	4.7642230	0.6108400	0.1887660
1	3.1833690	-0.8582470	0.1861510
6	4.1706320	2.9427840	0.3302300
1	2.0795680	3.3120730	0.4582290
6	5.1626640	1.9531020	0.2349020
1	4.4374840	3.9931970	0.3807650

8	5.8530480	-0.1999330	0.1018620
6	6.9531340	0.6186090	0.0910510
6	6.5976140	1.9299620	0.1705160
1	7.2642560	2.7801600	0.1795220
6	8.2470050	-0.0481140	-0.0083500
6	8.3195530	-1.4428340	-0.0928980
6	9.4310140	0.7029920	-0.0255900
6	9.5515550	-2.0776270	-0.1979570
1	7.4105740	-2.0324420	-0.0791030
6	10.6640250	0.0785390	-0.1309990
1	9.3920500	1.7847560	0.0415050
6	10.7051170	-1.3091740	-0.2178370
1	9.6012820	-3.1605400	-0.2644330
1	11.5688200	0.6774470	-0.1465090
7	12.0088850	-1.9934090	-0.3425860
6	12.7253530	-1.6191200	-1.6085300
1	12.9812590	-0.5619570	-1.5584210
1	13.6271850	-2.2252100	-1.6819210
1	12.0565430	-1.8109660	-2.4456980
6	12.8776710	-1.7986560	0.8670120
1	12.3093610	-2.1004730	1.7450080
1	13.7688360	-2.4137990	0.7485680
1	13.1496260	-0.7462060	0.9305750
8	-5.8684430	-1.2526790	0.5298230
6	-11.3340100	-0.7185820	-0.3448230
9	-11.7786800	-1.6006280	-1.2559080
9	-11.6457160	0.5053710	-0.7900640
9	-12.0506810	-0.9336390	0.7711640
1	11.8081780	-2.9977460	-0.4020000

Keto-HBO 2 ground-state structure in dichloromethane + HCl *G* -1867.244875 au

6	3.8022410	1.6379680	0.1759520
6	4.1013710	0.2413730	-0.0891780
6	5.4474150	-0.1351050	-0.0747940
6	7.2496790	-1.3724760	-0.2072020
6	8.1225830	-2.4306760	-0.3611300
6	9.4730790	-2.1276320	-0.2053090
6	9.8934880	-0.8243520	0.0880480
6	9.0029370	0.2359480	0.2420270
6	7.6603180	-0.0732690	0.0860780
1	7.7744750	-3.4312910	-0.5853450
1	10.2127200	-2.9143050	-0.3078270
1	9.3408090	1.2386700	0.4722700
7	6.4911570	0.6691870	0.1606660
8	4.6927740	2.4994480	0.4135690
6	3.0709720	-0.7023150	-0.3577120
6	2.4006220	1.9711370	0.1483790
6	1.7627560	-0.3225840	-0.3686020
1	3.3465460	-1.7336610	-0.5590170
1	2.1458010	3.0088910	0.3452740
1	0.9927530	-1.0519510	-0.5887730
6	0.0183780	1.4997660	-0.0967980
1	-0.1075120	2.5724270	0.0362880
6	-1.0648500	0.7143890	-0.2139080
1	-0.9345910	-0.3615860	-0.3102420
6	1.4144150	1.0451300	-0.1049970
6	-2.4647250	1.1554620	-0.2016280
6	-3.4599310	0.1750220	-0.1532600
6	-2.8331590	2.5249390	-0.2391710
6	-4.7765740	0.6062080	-0.1301230

1	-3.2136370	-0.8815140	-0.1286030
6	-4.1530440	2.9325240	-0.2171230
1	-2.0566780	3.2798520	-0.2990780
6	-5.1585890	1.9535780	-0.1582800
1	-4.4062740	3.9870250	-0.2497370
8	-5.8761000	-0.1930870	-0.0774070
6	-6.9668360	0.6380810	-0.0710800
6	-6.5946600	1.9463700	-0.1194780
1	-7.2510640	2.8045180	-0.1245800
6	-8.2694050	-0.0158820	-0.0076830
6	-8.3575790	-1.4111900	0.0482010
6	-9.4461140	0.7468730	0.0035390
6	-9.5973670	-2.0349950	0.1210640
1	-7.4543940	-2.0096810	0.0378700
6	-10.6869800	0.1332780	0.0763900
1	-9.3955060	1.8292860	-0.0422970
6	-10.7434040	-1.2553070	0.1373020
1	-9.6589510	-3.1184150	0.1661680
1	-11.5858300	0.7412310	0.0875500
7	-12.0552300	-1.9289740	0.2319120
6	-12.7889210	-1.5629590	1.4901930
1	-13.0333830	-0.5027290	1.4491520
1	-13.6979710	-2.1602770	1.5404230
1	-12.1364420	-1.7722910	2.3360280
6	-12.9028920	-1.7129900	-0.9889000
1	-12.3240050	-2.0114400	-1.8611030
1	-13.8018190	-2.3204390	-0.8907620
1	-13.1632200	-0.6572050	-1.0452370
1	6.2767060	1.6622590	0.3484140
8	5.8779530	-1.3907290	-0.3027520
6	11.3710510	-0.5722780	0.1981420
9	11.6403850	0.6156500	0.7548970
9	11.9761430	-1.5135910	0.9381150
9	11.9645400	-0.5901020	-1.0062460
1	-11.8642960	-2.9357340	0.2831650

Enol-HBO 2 excited-state structure in dichloromethane + HCl *G* -1867.158045 au

6	-3.7596090	1.7424460	0.0473260
6	-4.1254420	0.3571480	-0.0141090
6	-5.4981690	-0.0175560	-0.0156500
6	-7.1866900	-1.3734210	-0.0654330
6	-8.0221580	-2.4749220	-0.1169210
6	-9.3859530	-2.1994370	-0.0872430
6	-9.8582880	-0.8780330	-0.0092390
6	-9.0080700	0.2196630	0.0415380
6	-7.6377150	-0.0473850	0.0112320
1	-7.6377590	-3.4857040	-0.1795700
1	-10.0993180	-3.0157940	-0.1299920
1	-9.3861500	1.2333370	0.0983800
7	-6.5411240	0.7855480	0.0404520
8	-4.6808410	2.7213540	0.1075750
6	-3.0968870	-0.6188380	-0.0748280
6	-2.4284430	2.0937060	0.0445440
6	-1.7768870	-0.2643670	-0.0748370
1	-3.3808620	-1.6648980	-0.1219410
1	-2.1767310	3.1487010	0.0917460
1	-5.5825890	2.3243480	0.1027880
1	-1.0221600	-1.0402880	-0.1238970
6	-0.0479730	1.5423560	-0.0142350
1	0.1061950	2.6176960	0.0223640

6	1.0760760	0.7053000	-0.0480380
1	0.9163490	-0.3696020	-0.0663320
6	-1.3906190	1.1190350	-0.0152370
6	2.4195340	1.1178010	-0.0521820
6	3.4461770	0.1165330	-0.0616510
6	2.8139560	2.5099570	-0.0457660
6	4.7412500	0.5434970	-0.0594670
1	3.1924240	-0.9378850	-0.0654640
6	4.1218930	2.9040810	-0.0476280
1	2.0420610	3.2706440	-0.0420550
6	5.1375820	1.9093070	-0.0538060
1	4.3858330	3.9559910	-0.0438140
8	5.8497150	-0.2528200	-0.0589880
6	6.9378100	0.5785580	-0.0519800
6	6.5432450	1.9059710	-0.0508220
1	7.1984400	2.7652660	-0.0431890
6	8.2324470	-0.0482740	-0.0333550
6	8.3431200	-1.4515360	-0.0004800
6	9.4084290	0.7302260	-0.0390350
6	9.5898130	-2.0559860	0.0367960
1	7.4480340	-2.0620670	0.0008030
6	10.6538520	0.1297210	-0.0030710
1	9.3463550	1.8125200	-0.0700560
6	10.7297130	-1.2618150	0.0391380
1	9.6669480	-3.1391780	0.0658540
1	11.5459710	0.7479110	-0.0059050
7	12.0494880	-1.9207060	0.0981380
6	12.8707770	-1.6819420	-1.1368380
1	13.1200400	-0.6230350	-1.1839700
1	13.7769350	-2.2825100	-1.0647970
1	12.2770780	-1.9745010	-2.0010280
6	12.8073050	-1.5614310	1.3444810
1	12.1791580	-1.7942680	2.2024460
1	13.7274160	-2.1433990	1.3643130
1	13.0330780	-0.4967430	1.3135540
8	-5.8257550	-1.3461160	-0.0817810
6	-11.3438620	-0.6748130	0.0594140
9	-11.9873330	-1.4081470	-0.8640540
9	-11.6923630	0.6049590	-0.1305110
9	-11.8412110	-1.0460210	1.2520840
1	11.8706110	-2.9301980	0.1418020

Keto-HBO 2 excited-state structure in dichloromethane + HCl *G* -1867.139264 au

6	-3.7863820	1.7546330	-0.0976770
6	-4.1211850	0.3048430	0.0220350
6	-5.4759890	-0.0737720	0.0154810
6	-7.2398750	-1.3770500	0.0843840
6	-8.0802150	-2.4695870	0.1581020
6	-9.4461620	-2.1923860	0.0840000
6	-9.9124700	-0.8792860	-0.0570480
6	-9.0603250	0.2211150	-0.1321960
6	-7.6993980	-0.0589870	-0.0565480
1	-7.6973800	-3.4770630	0.2624770
1	-10.1599320	-3.0072450	0.1296480
1	-9.4339120	1.2310580	-0.2472360
6	-6.5679710	0.7158600	-0.0958320
8	-4.7197020	2.5942060	-0.2018170
6	-3.0967360	-0.6424900	0.1387330
6	-2.4118500	2.0915340	-0.0857860
6	-1.7648320	-0.2389130	0.1414100

1	-3.3425510	-1.6955670	0.2275820
1	-2.1689160	3.1464570	-0.1728690
1	-1.0008000	-1.0023380	0.2370810
6	-0.0068290	1.5411390	0.0318380
1	0.1433760	2.6173330	-0.0350730
6	1.0866280	0.7324370	0.0977810
1	0.9497190	-0.3458510	0.1442740
6	-1.3881140	1.1364980	0.0282090
6	2.4727820	1.1612330	0.0984460
6	3.4754490	0.1759320	0.0957180
6	2.8566670	2.5343800	0.1005060
6	4.7905540	0.6010000	0.0869180
1	3.2260190	-0.8800910	0.0944840
6	4.1761120	2.9335640	0.0942210
1	2.0860470	3.2972240	0.1130070
6	5.1818410	1.9491590	0.0854960
1	4.4333810	3.9877450	0.0972240
8	5.8887190	-0.2040720	0.0745070
6	6.9845600	0.6224810	0.0639200
6	6.6135030	1.9350310	0.0716200
1	7.2737190	2.7904470	0.0634600
6	8.2830700	-0.0335480	0.0331960
6	8.3700950	-1.4311260	-0.0028240
6	9.4640010	0.7255080	0.0304890
6	9.6088980	-2.0582170	-0.0505720
1	7.4653580	-2.0273320	0.0019260
6	10.7034240	0.1079030	-0.0170980
1	9.4163000	1.8085660	0.0629320
6	10.7577940	-1.2819200	-0.0612360
1	9.6684640	-3.1423740	-0.0813620
1	11.6039950	0.7134550	-0.0221770
6	12.0690460	-1.9593390	-0.1328710
6	12.8185370	-1.6075550	-1.3857940
1	13.0600300	-0.5463090	-1.3544240
1	13.7296910	-2.2028600	-1.4168840
1	12.1779090	-1.8286470	-2.2376460
6	12.9040190	-1.7328610	1.0946450
1	12.3140590	-2.0173950	1.9640550
1	13.8008430	-2.3461300	1.0142900
1	13.1691280	-0.6777330	1.1406240
1	-6.4229920	1.7273210	-0.1845800
8	-5.8745020	-1.3665770	0.1261820
6	-11.3976550	-0.6473400	-0.0705030
9	-11.7185890	0.5008870	-0.6824930
9	-12.0489400	-1.6373530	-0.6974480
9	-11.8981360	-0.5813980	1.1739620
1	11.8762910	-2.9661230	-0.1762390

Enol-HBO 2 ground-state structure in acetone *G* -1866.854224 au

6	-3.7282330	1.7168650	0.1390460
6	-4.0799830	0.3656840	-0.0638370
6	-5.4744680	-0.0206870	-0.0534060
6	-7.1541900	-1.3717710	-0.1870260
6	-7.9871270	-2.4700650	-0.3249260
6	-9.3463350	-2.2080380	-0.2084280
6	-9.8191150	-0.9062450	0.0334490
6	-8.9698180	0.1844340	0.1692270
6	-7.6054720	-0.0724980	0.0530800
1	-7.6029390	-3.4653870	-0.5117510
1	-10.0590840	-3.0204270	-0.3067920

1	-9.3462830	1.1831510	0.3548810
7	-6.4981010	0.7632080	0.1318900
8	-4.6311930	2.6906230	0.3477750
6	-3.0643020	-0.5823340	-0.2776450
6	-2.3791210	2.0770040	0.1253700
6	-1.7362620	-0.2144330	-0.2892490
1	-3.3440410	-1.6182200	-0.4394450
1	-2.1324030	3.1222920	0.2852050
1	-5.5371810	2.3053280	0.3341260
1	-0.9797310	-0.9691950	-0.4699020
6	0.0209420	1.5938210	-0.0725780
1	0.1422640	2.6721250	0.0061010
6	1.1071110	0.8051220	-0.1343520
1	0.9745120	-0.2744410	-0.1817260
6	-1.3719420	1.1335120	-0.0805040
6	2.5070410	1.2406510	-0.1287910
6	3.5006380	0.2544160	-0.0877070
6	2.8836370	2.6057750	-0.1652690
6	4.8183470	0.6762310	-0.0767870
1	3.2481620	-0.8009780	-0.0626900
6	4.2083130	3.0046400	-0.1540010
1	2.1126590	3.3677260	-0.2119410
6	5.2104890	2.0221670	-0.1070560
1	4.4660290	4.0583570	-0.1851160
8	5.9147400	-0.1294350	-0.0379360
6	7.0162650	0.6922840	-0.0435280
6	6.6461960	2.0047970	-0.0846600
1	7.3089890	2.8576130	-0.0980420
6	8.3118000	0.0309370	-0.0073100
6	8.4169760	-1.3652350	0.0342290
6	9.4993660	0.7755960	-0.0091360
6	9.6496050	-1.9958380	0.0687690
1	7.5148980	-1.9684770	0.0430760
6	10.7378880	0.1609850	0.0248130
1	9.4570570	1.8609510	-0.0344650
6	10.8500490	-1.2495700	0.0567460
1	9.6786150	-3.0777950	0.1063920
1	11.6259830	0.7807150	0.0275720
7	12.0753770	-1.8664890	0.0713720
6	13.2778770	-1.0673300	0.2086850
1	13.2825170	-0.4847420	1.1399350
1	14.1442110	-1.7279440	0.2107390
1	13.3863340	-0.3717300	-0.6307760
6	12.1494910	-3.3037170	0.2505040
1	11.6387840	-3.8283140	-0.5645530
1	13.1953330	-3.6087810	0.2426610
1	11.7000130	-3.6250990	1.1999480
8	-5.7919600	-1.3288640	-0.2534900
6	-11.3038780	-0.7248970	0.1557790
9	-11.9486010	-1.1798740	-0.9319220
9	-11.6508600	0.5586280	0.3178790
9	-11.8004330	-1.4071910	1.2020330

Keto-HBO 2 ground-state structure in acetone *G* -1866.833598 au

6	-3.7730870	1.6720480	0.0782120
6	-4.0563990	0.2569450	-0.0867580
6	-5.3994190	-0.1303180	-0.0799920
6	-7.1863340	-1.3945680	-0.1588800
6	-8.0452460	-2.4700490	-0.2595470
6	-9.4026690	-2.1706660	-0.1644410

6	-9.8420060	-0.8542690	0.0211810
6	-8.9648840	0.2244570	0.1198900
6	-7.6162370	-0.0812230	0.0246800
1	-7.6830010	-3.4798880	-0.4066040
1	-10.1323400	-2.9692160	-0.2412020
1	-9.3173120	1.2390950	0.2584820
7	-6.4563620	0.6780670	0.0662440
8	-4.6767550	2.5421990	0.2217930
6	-3.0120280	-0.6960790	-0.2479000
6	-2.3742690	2.0132520	0.0674550
6	-1.7062010	-0.3077060	-0.2483950
1	-3.2746050	-1.7428020	-0.3727390
1	-2.1310940	3.0652270	0.1904390
1	-0.9260110	-1.0476740	-0.3794620
6	0.0181770	1.5459500	-0.0691160
1	0.1320110	2.6246390	0.0180060
6	1.1110850	0.7668580	-0.1377230
1	0.9894650	-0.3126660	-0.2033310
6	-1.3730610	1.0794670	-0.0836360
6	2.5076490	1.2146100	-0.1196880
6	3.5100000	0.2366710	-0.0992790
6	2.8727930	2.5833550	-0.1225740
6	4.8241070	0.6694070	-0.0744120
1	3.2667200	-0.8212000	-0.0996670
6	4.1939380	2.9933580	-0.0984350
1	2.0953430	3.3395390	-0.1515560
6	5.2045500	2.0189440	-0.0715410
1	4.4424820	4.0497460	-0.1031770
8	5.9275180	-0.1274670	-0.0497850
6	7.0217780	0.7038280	-0.0308820
6	6.6403680	2.0135550	-0.0435020
1	7.2956660	2.8722230	-0.0351520
6	8.3232970	0.0537350	-0.0025450
6	8.4424770	-1.3418620	-0.0113010
6	9.5030230	0.8095800	0.0396070
6	9.6811480	-1.9610320	0.0164860
1	7.5467190	-1.9539730	-0.0371860
6	10.7473580	0.2064910	0.0675210
1	9.4496840	1.8946200	0.0554130
6	10.8737940	-1.2030370	0.0486980
1	9.7208570	-3.0433140	0.0142720
1	11.6287780	0.8344980	0.1061320
7	12.1053180	-1.8080200	0.0574020
6	13.2971550	-1.0027270	0.2431600
1	13.2828580	-0.4572190	1.1965610
1	14.1704040	-1.6540980	0.2313090
1	13.4096260	-0.2736040	-0.5667680
6	12.1916660	-3.2498330	0.1875600
1	11.6981950	-3.7505740	-0.6527090
1	13.2406300	-3.5440980	0.1844650
1	11.7319940	-3.6086730	1.1185530
1	-6.2589470	1.6845420	0.1841270
8	-5.8127050	-1.4042460	-0.2213270
6	-11.3182060	-0.6148000	0.1683350
9	-11.6440550	0.6666530	-0.0477580
9	-12.0284550	-1.3636360	-0.6884490
9	-11.7487300	-0.9280620	1.4014740

Enol-HBO 2 excited-state structure in acetone *G* -1866.751492 au

6	-3.7183960	1.7387650	0.0082400

6	-4.0894010	0.3562490	-0.0319430
6	-5.4600530	-0.0162420	-0.0300520
6	-7.1500240	-1.3778300	-0.0560900
6	-7.9823100	-2.4810850	-0.0873510
6	-9.3491590	-2.2110430	-0.0632570
6	-9.8228200	-0.8914610	-0.0103290
6	-8.9727130	0.2103530	0.0202690
6	-7.6028570	-0.0515400	-0.0045080
1	-7.5947840	-3.4918080	-0.1311190
1	-10.0591900	-3.0307620	-0.0909750
1	-9.3546160	1.2236480	0.0579240
7	-6.5069250	0.7854970	0.0098530
8	-4.6437520	2.7223380	0.0480140
6	-3.0548760	-0.6162470	-0.0730330
6	-2.3877460	2.0915440	0.0069410
6	-1.7347700	-0.2608870	-0.0726800
1	-3.3348620	-1.6645030	-0.1049080
1	-2.1392270	3.1484440	0.0388100
1	-5.5426310	2.3192910	0.0462720
1	-0.9804540	-1.0388350	-0.1057960
6	0.0008040	1.5462620	-0.0255730
1	0.1485700	2.6233470	0.0010620
6	1.1285960	0.7190640	-0.0436770
1	0.9757240	-0.3574970	-0.0594230
6	-1.3439940	1.1203080	-0.0313980
6	2.4724570	1.1360550	-0.0367560
6	3.5091120	0.1430160	-0.0394580
6	2.8621630	2.5297590	-0.0253290
6	4.8004380	0.5755570	-0.0274940
1	3.2627530	-0.9133980	-0.0479090
6	4.1665620	2.9327970	-0.0152780
1	2.0855480	3.2861230	-0.0265420
6	5.1936150	1.9452730	-0.0150130
1	4.4232360	3.9868160	-0.0074670
8	5.9146190	-0.2169590	-0.0237950
6	7.0041310	0.6153250	-0.0085300
6	6.5909570	1.9508940	-0.0037270
1	7.2431100	2.8123740	0.0079690
6	8.2906190	0.0156840	0.0018890
6	8.4468040	-1.3914250	-0.0000900
6	9.4648350	0.8076600	0.0167120
6	9.6915840	-1.9739150	0.0130480
1	7.5638230	-2.0214110	-0.0115050
6	10.7136490	0.2376380	0.0295870
1	9.3840660	1.8903190	0.0180780
6	10.8720840	-1.1783470	0.0289260
1	9.7634440	-3.0542010	0.0115550
1	11.5831120	0.8823800	0.0407380
7	12.1028800	-1.7463870	0.0431730
6	13.2944780	-0.9126400	0.0592820
1	13.3199630	-0.2758120	0.9505960
1	14.1740690	-1.5536040	0.0687950
1	13.3416300	-0.2727060	-0.8288870
6	12.2399710	-3.1942030	0.0445240
1	11.7879890	-3.6350060	-0.8509940
1	13.2979170	-3.4493240	0.0576720
1	11.7657550	-3.6353520	0.9283250
8	-5.7880410	-1.3485370	-0.0721510
6	-11.3068310	-0.6859600	0.0633060
9	-11.9633960	-1.4751820	-0.8038910

9	-11.6613810	0.5797800	-0.2012880
9	-11.7919680	-0.9805180	1.2832950

Keto-HBO 2 excited-state structure in acetone *G* -1866.731086 au

6	3.7590810	-1.6680710	-0.0162240
6	4.0581900	-0.2273390	0.0028970
6	5.3905800	0.1507350	-0.0025790
6	7.1941800	1.4057460	0.0012150
6	8.0640680	2.4747250	0.0041860
6	9.4251450	2.1588530	-0.0166840
6	9.8530190	0.8293010	-0.0408980
6	8.9644080	-0.2488530	-0.0450560
6	7.6148640	0.0699120	-0.0222450
1	7.7090140	3.4978160	0.0176630
1	10.1592170	2.9564880	-0.0209270
1	9.3115200	-1.2746320	-0.0705710
7	6.4582960	-0.6784620	-0.0245320
8	4.6907950	-2.5392540	-0.0357280
6	3.0080870	0.7442600	0.0254150
6	2.3867010	-1.9957800	-0.0116960
6	1.7032770	0.3642140	0.0281160
1	3.2739390	1.7976360	0.0401720
1	2.1337990	-3.0529950	-0.0263460
1	0.9285540	1.1221230	0.0459600
6	-0.0000440	-1.4681530	0.0089110
1	-0.1393800	-2.5470710	-0.0030700
6	-1.1353710	-0.6559940	0.0189690
1	-0.9985800	0.4226700	0.0257710
6	1.3480630	-1.0374610	0.0088130
6	-2.4757400	-1.0915200	0.0176080
6	-3.5238950	-0.1119350	0.0193700
6	-2.8475760	-2.4893770	0.0135100
6	-4.8103070	-0.5603340	0.0151580
1	-3.2907280	0.9474990	0.0224520
6	-4.1469800	-2.9091000	0.0102820
1	-2.0615690	-3.2359150	0.0138230
6	-5.1862530	-1.9346730	0.0104850
1	-4.3903010	-3.9663020	0.0075340
8	-5.9340660	0.2183730	0.0138540
6	-7.0133690	-0.6274670	0.0080890
6	-6.5835380	-1.9578530	0.0063670
1	-7.2249360	-2.8274020	0.0018990
6	-8.3071730	-0.0442780	0.0036420
6	-8.4812680	1.3608860	0.0032650
6	-9.4713920	-0.8513210	-0.0016670
6	-9.7333950	1.9272880	-0.0027160
1	-7.6062540	2.0019770	0.0073990
6	-10.7273680	-0.2973630	-0.0074830
1	-9.3766690	-1.9328420	-0.0011940
6	-10.9037650	1.1165800	-0.0086220
1	-9.8192890	3.0065560	-0.0030750
1	-11.5886560	-0.9530900	-0.0114550
7	-12.1416770	1.6688900	-0.0152390
6	-13.3227550	0.8201560	-0.0211780
1	-13.3556000	0.1816650	0.8686740
1	-14.2103570	1.4500140	-0.0259470
1	-13.3463590	0.1811220	-0.9109490
6	-12.2972700	3.1148550	-0.0175940
1	-11.8349770	3.5607040	-0.9053310
1	-13.3584600	3.3563740	-0.0235910

1	-11.8446210	3.5626300	0.8741210
1	6.2306640	-1.6900620	-0.0369740
8	5.8234750	1.4401870	0.0131040
6	11.3266140	0.5440480	-0.0006190
9	11.6262680	-0.6251660	-0.5861190
9	12.0396540	1.4981200	-0.6173310
9	11.7862030	0.4736540	1.2608160

*Coordinates for **HBT**:*

Enol-HBT ground-state structure in cyclohexane *G* -1852.873129 au

6	4.9924880	-1.4605140	0.0048750
6	5.3121550	-0.0829920	0.0036040
6	6.7038730	0.3465950	0.0029850
6	8.8311180	1.5844130	0.0016690
6	9.9692050	2.3899910	0.0008670
6	11.2088010	1.7654490	0.0010320
6	11.3141790	0.3657050	0.0019740
6	10.1831590	-0.4340240	0.0027750
6	8.9258970	0.1803980	0.0026240
1	9.8884510	3.4717720	0.0001350
1	12.1092840	2.3708050	0.0004180
1	10.2483210	-1.5168550	0.0035040
7	7.7107220	-0.4792420	0.0033470
8	5.9173440	-2.4310600	0.0054740
6	4.2550900	0.8449110	0.0031880
6	3.6506570	-1.8527550	0.0055770
6	2.9362450	0.4484480	0.0038680
1	4.4846920	1.9076230	0.0024980
1	3.4415630	-2.9182680	0.0064950
1	6.8114440	-2.0122140	0.0048450
1	2.1563490	1.2010310	0.0040950
6	1.2330580	-1.4246930	0.0054050
1	1.1464870	-2.5092290	0.0105450
6	0.1205270	-0.6723710	-0.0006020
1	0.2179250	0.4120730	-0.0070730
6	2.6115850	-0.9248670	0.0048830
6	-1.2646440	-1.1519240	-0.0001970
6	-2.2902030	-0.1993340	-0.0117180
6	-1.5975640	-2.5283890	0.0113780
6	-3.5941120	-0.6619320	-0.0114170
1	-2.0733590	0.8641480	-0.0207970
6	-2.9080720	-2.9691310	0.0114460
1	-0.8017450	-3.2655750	0.0208880
6	-3.9419260	-2.0198240	-0.0001840
1	-3.1310690	-4.0312570	0.0205820
1	12.2964330	-0.0951950	0.0020740
8	-4.7154110	0.1086490	-0.0216290
6	-5.7888690	-0.7472780	-0.0170540
6	-5.3771810	-2.0472500	-0.0043670
1	-6.0131510	-2.9201190	0.0002110
6	-7.1063580	-0.1291450	-0.0269650
6	-7.2583550	1.2620210	-0.0487200
6	-8.2672100	-0.9123290	-0.0095500
6	-8.5123120	1.8501500	-0.0573180
1	-6.3758720	1.8932920	-0.0552690
6	-9.5260510	-0.3394910	-0.0181870
1	-8.1870810	-1.9954830	0.0159230
6	-9.6848570	1.0643780	-0.0517350

1	-8.5782570	2.9310690	-0.0677020
1	-10.3927740	-0.9884410	0.0028300
7	-10.9344180	1.6413870	-0.0822810
6	-12.1049200	0.8100940	0.1110070
1	-12.0920180	0.2895900	1.0792180
1	-12.9961670	1.4361270	0.0673180
1	-12.1859680	0.0577290	-0.6811720
6	-11.0551270	3.0770720	0.0687910
1	-10.5462090	3.6005440	-0.7479730
1	-12.1096780	3.3504770	0.0336500
1	-10.6341350	3.4331270	1.0198300
16	7.1528310	2.0555750	0.0016930

Keto-HBT ground-state structure in cyclohexane *G* -1852.855175 au

6	5.0159940	-1.4104500	0.2044190
6	5.2855380	-0.0031000	-0.0482410
6	6.6254770	0.4215650	-0.0282480
6	8.8651550	1.5139030	-0.0694570
6	10.0344710	2.2646510	-0.1267910
6	11.2431390	1.6121600	0.0920910
6	11.2802490	0.2389890	0.3622310
6	10.1150610	-0.5139800	0.4202940
6	8.9032300	0.1391990	0.2010550
1	10.0034710	3.3284770	-0.3363800
1	12.1678770	2.1774610	0.0520150
1	10.1341090	-1.5781270	0.6286640
7	7.6379090	-0.4188750	0.2131200
8	5.9276330	-2.2559050	0.4389320
6	4.2162440	0.8979910	-0.3098730
6	3.6293310	-1.7899530	0.1721080
6	2.9201790	0.4805900	-0.3268710
1	4.4446800	1.9443070	-0.5051730
1	3.4145680	-2.8378480	0.3613590
1	2.1291210	1.1883270	-0.5433830
6	1.2319190	-1.3957530	-0.0742300
1	1.1403180	-2.4728120	0.0509730
6	0.1222210	-0.6475300	-0.1886130
1	0.2196350	0.4331360	-0.2751920
6	2.6114550	-0.8980280	-0.0751860
6	-1.2621820	-1.1309630	-0.1874910
6	-2.2916300	-0.1840810	-0.1361940
6	-1.5887740	-2.5078790	-0.2391340
6	-3.5931430	-0.6535260	-0.1243950
1	-2.0794780	0.8798150	-0.1006430
6	-2.8971540	-2.9554730	-0.2279720
1	-0.7888930	-3.2380720	-0.3027880
6	-3.9347630	-2.0123940	-0.1665190
1	-3.1154870	-4.0177110	-0.2723760
1	12.2350850	-0.2478730	0.5293610
8	-4.7177840	0.1108490	-0.0731090
6	-5.7871640	-0.7501860	-0.0822050
6	-5.3699370	-2.0469890	-0.1387330
1	-6.0020150	-2.9224940	-0.1587690
6	-7.1070760	-0.1388700	-0.0310050
6	-7.2647020	1.2509880	0.0156270
6	-8.2642320	-0.9275170	-0.0204780
6	-8.5206630	1.8327690	0.0675140
1	-6.3849170	1.8860510	0.0154400
6	-9.5249900	-0.3609170	0.0307210
1	-8.1794960	-2.0102760	-0.0479220

6	-9.6897050	1.0420480	0.0675290
1	-8.5906870	2.9126650	0.1094190
1	-10.3884610	-1.0144150	0.0436030
7	-10.9422070	1.6140860	0.0978170
6	-12.1023840	0.7688990	0.2936670
1	-12.0548800	0.2061890	1.2369640
1	-12.9969330	1.3916380	0.3075590
1	-12.2074810	0.0519040	-0.5278580
6	-11.0625740	3.0394550	0.3271020
1	-10.5769070	3.6065380	-0.4744670
1	-12.1184070	3.3101820	0.3336670
1	-10.6173300	3.3474400	1.2839600
1	7.3100700	-1.4098160	0.3805470
16	7.2076370	2.0515990	-0.3005040

Enol-HBT excited-state structure in cyclohexane *G* -1852.764416 au

6	4.976560	-1.488404	-0.000009
6	5.317607	-0.091683	-0.000002
6	6.682813	0.323998	0.000000
6	8.822689	1.564677	0.000006
6	9.959334	2.367543	0.000008
6	11.203833	1.746761	0.000004
6	11.307107	0.347138	-0.000003
6	10.177453	-0.454277	-0.000005
6	8.911610	0.153089	-0.000001
1	9.876701	3.449586	0.000014
1	12.103431	2.353495	0.000007
1	10.246152	-1.537011	-0.000011
7	7.711219	-0.505313	-0.000004
8	5.918105	-2.447707	-0.000014
6	4.248600	0.844355	0.000004
6	3.652670	-1.873209	-0.000010
6	2.937946	0.456188	0.000002
1	4.483614	1.905889	0.000010
1	3.436431	-2.937461	-0.000016
1	6.806466	-2.011903	-0.000012
1	2.162485	1.213815	0.000009
6	1.249360	-1.393493	-0.000007
1	1.132282	-2.474829	-0.000009
6	0.104470	-0.603270	-0.000010
1	0.224139	0.477490	-0.000021
6	2.587673	-0.932965	-0.000005
6	-1.233466	-1.063761	-0.000003
6	-2.295517	-0.107293	-0.000013
6	-1.577672	-2.465167	0.000014
6	-3.576628	-0.579532	-0.000005
1	-2.083692	0.956512	-0.000026
6	-2.871128	-2.909292	0.000021
1	-0.777244	-3.196111	0.000023
6	-3.925177	-1.957187	0.000011
1	-3.092861	-3.971452	0.000034
1	12.289542	-0.114497	-0.000006
8	-4.712662	0.179566	-0.000011
6	-5.776061	-0.685160	0.000002
6	-5.328716	-2.001960	0.000014
1	-5.956188	-2.881521	0.000024
6	-7.083912	-0.115314	0.000001
6	-7.273176	1.283889	-0.000004
6	-8.235919	-0.932481	0.000004
6	-8.534148	1.836757	-0.000005

1	-6.404500	1.933469	-0.000005
6	-9.500585	-0.391899	0.000003
1	-8.128658	-2.013072	0.000008
6	-9.692242	1.015971	-0.000003
1	-8.631302	2.915248	-0.000006
1	-10.354138	-1.058095	0.000006
7	-10.942788	1.557588	-0.000006
6	-12.109986	0.695438	0.000004
1	-12.133015	0.054670	0.889629
1	-13.007365	1.312550	-0.000003
1	-12.133015	0.054652	-0.889608
6	-11.110218	2.999080	-0.000003
1	-10.657327	3.453105	-0.889485
1	-12.173768	3.233367	-0.000010
1	-10.657338	3.453101	0.889487
16	7.144723	2.042311	0.000012

Keto-HBT excited-state structure in cyclohexane *G* -1852.750818 au

6	5.009489	-1.453760	-0.000013
6	5.286305	0.002596	-0.000009
6	6.623064	0.425079	-0.000007
6	8.865897	1.511325	0.000008
6	10.035592	2.261130	0.000018
6	11.253387	1.585545	0.000012
6	11.294820	0.184907	-0.000003
6	10.132741	-0.572211	-0.000013
6	8.904934	0.100937	-0.000007
1	9.999549	3.345520	0.000029
1	12.178191	2.152222	0.000020
1	10.158742	-1.656446	-0.000026
7	7.654923	-0.450814	-0.000017
8	5.962276	-2.300619	-0.000019
6	4.208895	0.931357	-0.000008
6	3.650620	-1.822772	-0.000010
6	2.909748	0.509667	-0.000006
1	4.428683	1.997054	-0.000011
1	3.436468	-2.887568	-0.000011
1	2.114259	1.246066	-0.000008
6	1.245663	-1.354494	0.000000
1	1.134156	-2.436933	-0.000003
6	0.102553	-0.579120	0.000006
1	0.206376	0.503286	0.000008
6	2.593727	-0.896157	-0.000005
6	-1.241044	-1.055088	0.000009
6	-2.302614	-0.108646	0.000007
6	-1.573351	-2.453122	0.000014
6	-3.585572	-0.588343	0.000008
1	-2.098245	0.956815	0.000003
6	-2.867494	-2.906122	0.000015
1	-0.769141	-3.180079	0.000019
6	-3.923938	-1.963219	0.000012
1	-3.080965	-3.970069	0.000019
1	12.255264	-0.320191	-0.000007
8	-4.723787	0.164977	0.000005
6	-5.782817	-0.705467	0.000007
6	-5.335141	-2.014042	0.000011
1	-5.958253	-2.896562	0.000013
6	-7.098066	-0.132715	0.000004
6	-7.287885	1.262747	0.000001
6	-8.246092	-0.949409	0.000003

6	-8.551346	1.815752	-0.000003
1	-6.420352	1.914028	0.000002
6	-9.513657	-0.409984	0.000000
1	-8.137812	-2.030050	0.000006
6	-9.707056	0.995465	-0.000004
1	-8.648623	2.894310	-0.000005
1	-10.365885	-1.078019	-0.000001
7	-10.960979	1.536826	-0.000009
6	-12.125193	0.672594	-0.000010
1	-12.148015	0.030899	0.889330
1	-13.024387	1.287433	-0.000014
1	-12.148010	0.030894	-0.889346
6	-11.128213	2.977144	-0.000013
1	-10.675585	3.432705	-0.889233
1	-12.191901	3.211819	-0.000017
1	-10.675590	3.432709	0.889208
1	7.296972	-1.459465	-0.000019
16	7.205054	2.083327	0.000012

Enol-HBT ground-state structure in dichloromethane *G* -1852.880667 au

6	4.9926430	-1.4578880	0.0054790
6	5.3120830	-0.0804070	0.0033090
6	6.7046280	0.3498480	0.0023830
6	8.8334030	1.5827630	0.0001030
6	9.9724030	2.3878210	-0.0013420
6	11.2111430	1.7609090	-0.0008290
6	11.3151030	0.3604530	0.0010870
6	10.1831300	-0.4384400	0.0025370
6	8.9266520	0.1785380	0.0020390
1	9.8930440	3.4695970	-0.0028260
1	12.1123470	2.3650500	-0.0019360
1	10.2481010	-1.5213470	0.0040220
7	7.7096230	-0.4788490	0.0032890
8	5.9210460	-2.4279680	0.0067790
6	4.2548010	0.8471040	0.0021610
6	3.6517270	-1.8520490	0.0063270
6	2.9354470	0.4495150	0.0029730
1	4.4825620	1.9100790	0.0006720
1	3.4411110	-2.9174310	0.0079530
1	6.8146900	-2.0050910	0.0058940
1	2.1560560	1.2026260	0.0023460
6	1.2330970	-1.4248780	0.0055490
1	1.1466780	-2.5094500	0.0099570
6	0.1214350	-0.6703740	0.0005330
1	0.2187100	0.4140070	-0.0047510
6	2.6116030	-0.9238330	0.0049340
6	-1.2639640	-1.1504640	0.0006850
6	-2.2892790	-0.1965790	-0.0085270
6	-1.5967890	-2.5273960	0.0095270
6	-3.5931280	-0.6599250	-0.0087140
1	-2.0712310	0.8667360	-0.0154410
6	-2.9078630	-2.9682460	0.0091370
1	-0.8016090	-3.2653750	0.0170830
6	-3.9414670	-2.0180380	-0.0002680
1	-3.1313360	-4.0302230	0.0160900
1	12.2968590	-0.1013440	0.0014370
8	-4.7152500	0.1105420	-0.0170050
6	-5.7894280	-0.7462850	-0.0139860
6	-5.3769840	-2.0465270	-0.0040940
1	-6.0118220	-2.9203800	-0.0005880

6	-7.1067810	-0.1283550	-0.0222210
6	-7.2605150	1.2636110	-0.0356470
6	-8.2677430	-0.9134350	-0.0119860
6	-8.5147640	1.8512010	-0.0427040
1	-6.3797520	1.8976160	-0.0372050
6	-9.5271330	-0.3419290	-0.0191620
1	-8.1874690	-1.9967660	0.0058200
6	-9.6881050	1.0635970	-0.0431900
1	-8.5817550	2.9321190	-0.0469580
1	-10.3932680	-0.9918420	-0.0044630
7	-10.9347640	1.6378680	-0.0701550
6	-12.1101170	0.8032440	0.0862380
1	-12.1088880	0.2612790	1.0419190
1	-12.9991260	1.4320080	0.0472160
1	-12.1814770	0.0689650	-0.7237010
6	-11.0603930	3.0763860	0.0609030
1	-10.5556720	3.5916060	-0.7637830
1	-12.1158560	3.3447540	0.0278770
1	-10.6369290	3.4441540	1.0056310
16	7.1554120	2.0565800	-0.0001140

Keto-HBT ground-state structure in dichloromethane *G* -1852.864767 au

6	5.0210080	-1.4326760	0.1640810
6	5.2891100	-0.0194680	-0.0419460
6	6.6315860	0.4126740	-0.0240300
6	8.8592700	1.5269090	-0.0557890
6	10.0202750	2.2926950	-0.1018550
6	11.2370220	1.6443250	0.0804530
6	11.2916700	0.2623920	0.3036410
6	10.1353910	-0.5048180	0.3501990
6	8.9155290	0.1450390	0.1672330
1	9.9765680	3.3624680	-0.2746310
1	12.1556190	2.2199530	0.0486790
1	10.1679070	-1.5749300	0.5225260
7	7.6535140	-0.4246390	0.1752150
8	5.9342790	-2.2897490	0.3581320
6	4.2188880	0.8910770	-0.2571460
6	3.6336390	-1.8079980	0.1351200
6	2.9194580	0.4779710	-0.2730270
1	4.4454770	1.9437080	-0.4161010
1	3.4164740	-2.8616090	0.2888150
1	2.1288250	1.1970610	-0.4502670
6	1.2322280	-1.4057440	-0.0672640
1	1.1423440	-2.4854710	0.0344810
6	0.1220370	-0.6543490	-0.1596380
1	0.2187890	0.4274640	-0.2305390
6	2.6118840	-0.9066750	-0.0680910
6	-1.2629040	-1.1373490	-0.1566600
6	-2.2910440	-0.1874120	-0.1164100
6	-1.5914900	-2.5147270	-0.1940060
6	-3.5932280	-0.6554850	-0.1034980
1	-2.0764600	0.8763640	-0.0914410
6	-2.9010780	-2.9603750	-0.1817790
1	-0.7936090	-3.2482030	-0.2440020
6	-3.9373030	-2.0143960	-0.1329760
1	-3.1212780	-4.0225920	-0.2141430
1	12.2534610	-0.2193120	0.4428380
8	-4.7176170	0.1108080	-0.0623100
6	-5.7889930	-0.7496050	-0.0651390
6	-5.3727300	-2.0478090	-0.1077090

1	-6.0049040	-2.9235320	-0.1197040
6	-7.1079820	-0.1363020	-0.0232170
6	-7.2655460	1.2547320	0.0149790
6	-8.2663860	-0.9250940	-0.0142000
6	-8.5211630	1.8379920	0.0573320
1	-6.3866100	1.8912760	0.0152590
6	-9.5270980	-0.3578670	0.0275800
1	-8.1829070	-2.0081070	-0.0363310
6	-9.6921380	1.0470180	0.0567050
1	-8.5909710	2.9181710	0.0922480
1	-10.3909740	-1.0108620	0.0391620
7	-10.9407670	1.6178990	0.0793310
6	-12.1092310	0.7743150	0.2395130
1	-12.0803470	0.2000990	1.1757750
1	-13.0005700	1.4009760	0.2462980
1	-12.2010910	0.0678320	-0.5927310
6	-11.0661730	3.0499030	0.2691180
1	-10.5820430	3.5980020	-0.5466190
1	-12.1226610	3.3162940	0.2710050
1	-10.6212620	3.3822010	1.2171790
1	7.3576580	-1.4208430	0.3134220
16	7.1939370	2.0536840	-0.2480630

Enol-HBT excited-state structure in dichloromethane *G* -1852.776914 au

6	4.9760310	-1.4900620	0.0000010
6	5.3172610	-0.0934520	0.0000000
6	6.6814110	0.3231830	-0.0000010
6	8.8217470	1.5651660	-0.0000030
6	9.9572370	2.3703710	-0.0000040
6	11.2026100	1.7504610	-0.0000050
6	11.3076810	0.3508380	-0.0000050
6	10.1782200	-0.4522680	-0.0000040
6	8.9122890	0.1543210	-0.0000030
1	9.8734160	3.4522190	-0.0000040
1	12.1013470	2.3582680	-0.0000060
1	10.2497540	-1.5349400	-0.0000040
7	7.7105680	-0.5057470	-0.0000020
8	5.9236170	-2.4485850	0.0000000
6	4.2450890	0.8407320	0.0000010
6	3.6547840	-1.8785750	0.0000020
6	2.9352100	0.4516380	0.0000020
1	4.4769120	1.9030900	0.0000010
1	3.4384960	-2.9430690	0.0000020
1	6.8100960	-2.0069130	-0.0000010
1	2.1603810	1.2098250	0.0000030
6	1.2507730	-1.4021440	0.0000030
1	1.1331720	-2.4833320	0.0000030
6	0.1012490	-0.6079530	0.0000020
1	0.2230380	0.4726980	0.0000010
6	2.5833650	-0.9396230	0.0000020
6	-1.2316120	-1.0644700	0.0000030
6	-2.2949390	-0.1029030	0.0000020
6	-1.5801140	-2.4676240	0.0000050
6	-3.5744090	-0.5727560	0.0000020
1	-2.0796560	0.9603160	0.0000000
6	-2.8733180	-2.9083140	0.0000050
1	-0.7818730	-3.2010760	0.0000060
6	-3.9270360	-1.9518910	0.0000040
1	-3.0989820	-3.9695050	0.0000060
1	12.2904670	-0.1097780	-0.0000060

8	-4.7105350	0.1872420	0.0000010
6	-5.7753230	-0.6762070	0.0000020
6	-5.3265520	-1.9967400	0.0000030
1	-5.9541480	-2.8762430	0.0000040
6	-7.0806010	-0.1097520	0.0000010
6	-7.2735160	1.2909740	-0.0000010
6	-8.2320620	-0.9314940	0.0000010
6	-8.5344190	1.8407780	-0.0000020
1	-6.4073340	1.9440250	-0.0000010
6	-9.4968000	-0.3945060	0.0000000
1	-8.1226940	-2.0117550	0.0000020
6	-9.6925060	1.0153830	-0.0000020
1	-8.6346380	2.9188730	-0.0000020
1	-10.3488140	-1.0624050	0.0000010
7	-10.9399450	1.5517260	-0.0000040
6	-12.1079120	0.6866800	0.0000000
1	-12.1280980	0.0469660	0.8896920
1	-13.0048950	1.3034670	-0.0000040
1	-12.1280960	0.0469570	-0.8896870
6	-11.1137600	2.9946820	-0.0000020
1	-10.6622780	3.4484990	-0.8895850
1	-12.1780590	3.2231690	-0.0000050
1	-10.6622830	3.4484960	0.8895860
16	7.1422050	2.0415120	-0.0000020

Keto-HBT excited-state structure in dichloromethane *G* -1852.763352 au

6	-5.0097940	-1.4770830	0.0000020
6	-5.2890830	-0.0251090	0.0000030
6	-6.6205880	0.4030320	0.0000020
6	-8.8548180	1.5175250	0.0000010
6	-10.0142790	2.2837770	0.0000010
6	-11.2405660	1.6234310	-0.0000020
6	-11.3004150	0.2236720	-0.0000050
6	-10.1469460	-0.5484970	-0.0000060
6	-8.9129080	0.1100820	-0.0000020
1	-9.9642440	3.3674600	0.0000030
1	-12.1577280	2.2022520	-0.0000020
1	-10.1877700	-1.6322160	-0.0000080
7	-7.6656840	-0.4579120	-0.0000020
8	-5.9591320	-2.3326840	0.0000020
6	-4.2094470	0.9090190	0.0000040
6	-3.6499830	-1.8384670	0.0000000
6	-2.9106050	0.4983920	0.0000030
1	-4.4338400	1.9738460	0.0000050
1	-3.4270790	-2.9022170	-0.0000020
1	-2.1197430	1.2396660	0.0000040
6	-1.2476950	-1.3661740	-0.0000010
1	-1.1322200	-2.4481190	-0.0000030
6	-0.0989070	-0.5824720	-0.0000010
1	-0.2089730	0.4992890	0.0000000
6	-2.5883400	-0.9081270	0.0000000
6	1.2367420	-1.0513520	-0.0000020
6	2.3012670	-0.0978740	-0.0000010
6	1.5752920	-2.4531590	-0.0000020
6	3.5810130	-0.5746610	-0.0000010
1	2.0924130	0.9667190	-0.0000010
6	2.8680890	-2.9017230	-0.0000030
1	0.7734360	-3.1826940	-0.0000030
6	3.9248750	-1.9528020	-0.0000020
1	3.0867670	-3.9644110	-0.0000030

1	-12.2669440	-0.2693850	-0.0000080
8	4.7198170	0.1797250	-0.0000010
6	5.7802200	-0.6891230	-0.0000010
6	5.3288840	-2.0038500	-0.0000020
1	5.9522280	-2.8862810	-0.0000020
6	7.0909380	-0.1233180	0.0000000
6	7.2865440	1.2748490	0.0000010
6	8.2385480	-0.9468180	0.0000000
6	8.5498800	1.8225300	0.0000010
1	6.4221760	1.9304090	0.0000010
6	9.5059490	-0.4127170	0.0000000
1	8.1267250	-2.0269240	0.0000000
6	9.7051570	0.9954250	0.0000010
1	8.6520280	2.9004850	0.0000020
1	10.3559940	-1.0832060	0.0000010
7	10.9554610	1.5294180	0.0000010
6	12.1202200	0.6611070	0.0000010
1	12.1391910	0.0208180	-0.8895170
1	13.0193370	1.2749790	0.0000010
1	12.1391910	0.0208170	0.8895190
6	11.1317120	2.9714400	0.0000020
1	10.6811980	3.4269620	0.8894230
1	12.1964820	3.1983000	0.0000020
1	10.6811980	3.4269630	-0.8894180
1	-7.3506640	-1.4643340	-0.0000050
16	-7.1855520	2.0680140	0.0000040

Enol-HBT ground-state structure in dichloromethane ¨+ HCl *G* -1853.294437 au

6	5.0151210	1.4914000	-0.0362450
6	5.3589160	0.0913710	-0.0190100
6	6.7247490	-0.3207970	-0.0102470
6	8.8692840	-1.5423790	0.0187730
6	10.0121110	-2.3385410	0.0379860
6	11.2497550	-1.7064110	0.0316100
6	11.3453400	-0.3039840	0.0062040
6	10.2122280	0.4898750	-0.0129130
6	8.9504200	-0.1293240	-0.0063840
1	9.9383650	-3.4207120	0.0576250
1	12.1539870	-2.3057090	0.0465860
1	10.2737610	1.5727970	-0.0324950
7	7.7462440	0.5186900	-0.0220640
8	5.9557390	2.4492730	-0.0497700
6	4.2936600	-0.8511440	-0.0081260
6	3.6925100	1.8731210	-0.0379050
6	2.9833280	-0.4675220	-0.0115150
1	4.5320230	-1.9112660	0.0036880
1	3.4688320	2.9355090	-0.0495590
1	6.8467930	2.0149160	-0.0447980
1	2.2107780	-1.2272030	-0.0015180
6	1.2976740	1.3803660	-0.0213510
1	1.1709980	2.4599660	-0.0235500
6	0.1536900	0.5734130	-0.0163260
1	0.2839680	-0.5057480	-0.0261350
6	2.6292890	0.9259990	-0.0246420
6	-1.1805830	1.0230680	-0.0007410
6	-2.2334720	0.0529370	-0.0083960
6	-1.5340630	2.4240010	0.0254360
6	-3.5178340	0.5165870	0.0110220
1	-2.0104070	-1.0082530	-0.0296020
6	-2.8311100	2.8554940	0.0466930

1	-0.7410680	3.1626430	0.0306510
6	-3.8730570	1.8912460	0.0412390
1	-3.0646770	3.9145200	0.0677140
1	12.3252580	0.1621700	0.0016120
8	-4.6488270	-0.2473460	0.0057890
6	-5.7122040	0.6160210	0.0336960
6	-5.2809290	1.9284200	0.0566340
1	-5.9100440	2.8066760	0.0775900
6	-7.0281270	0.0296520	0.0243870
6	-7.1885910	-1.3664050	-0.0459900
6	-8.1745170	0.8476970	0.0807850
6	-8.4569530	-1.9270280	-0.0690360
1	-6.3154720	-2.0067780	-0.0868080
6	-9.4408720	0.2921870	0.0602370
1	-8.0732540	1.9256880	0.1416040
6	-9.5669110	-1.0934440	-0.0195820
1	-8.5731320	-3.0057390	-0.1277060
1	-10.3111030	0.9390350	0.1060980
7	-10.9124680	-1.6998650	-0.0527730
6	-11.6733580	-1.4733820	1.2228150
1	-11.8693010	-0.4064990	1.3178970
1	-12.6092580	-2.0276600	1.1652110
1	-11.0615820	-1.8249700	2.0516250
6	-11.7069610	-1.2632100	-1.2502960
1	-11.1197800	-1.4713710	-2.1427300
1	-12.6431770	-1.8196220	-1.2600920
1	-11.9017210	-0.1954810	-1.1620660
16	7.1969900	-2.0316720	0.0214580
1	-10.7755590	-2.7130410	-0.1413330

Keto-HBT ground-state structure in dichloromethane + HCl *G* -1853.278678 au

6	-5.0483270	1.4242570	0.2270580
6	-5.3330100	0.0295910	-0.0628490
6	-6.6786180	-0.3958670	-0.0321900
6	-8.9126860	-1.4953500	-0.0706710
6	-10.0793300	-2.2515130	-0.1329580
6	-11.2859570	-1.6107570	0.1260400
6	-11.3254950	-0.2458470	0.4398600
6	-10.1636830	0.5115630	0.5026390
6	-8.9538530	-0.1307940	0.2429880
1	-10.0473050	-3.3079080	-0.3761240
1	-12.2088330	-2.1787630	0.0833870
1	-10.1843700	1.5684240	0.7443020
7	-7.6880620	0.4312700	0.2513290
8	-5.9475900	2.2719670	0.5053030
6	-4.2785190	-0.8711050	-0.3724930
6	-3.6585540	1.7923720	0.1798990
6	-2.9763350	-0.4662310	-0.4010320
1	-4.5190400	-1.9085710	-0.5971130
1	-3.4278030	2.8319610	0.3962990
1	-2.1977130	-1.1747220	-0.6566760
6	-1.2673890	1.3854960	-0.1168030
1	-1.1637410	2.4605350	0.0170660
6	-0.1684060	0.6235050	-0.2409720
1	-0.2769650	-0.4554510	-0.3315440
6	-2.6524080	0.8987260	-0.1122820
6	1.2215470	1.0949740	-0.2387290
6	2.2384590	0.1381960	-0.1710600
6	1.5592320	2.4713440	-0.3040530
6	3.5450350	0.5993530	-0.1552010

1	2.0160210	-0.9229400	-0.1254610
6	2.8696080	2.9089530	-0.2892620
1	0.7656590	3.2067330	-0.3812990
6	3.8967450	1.9541990	-0.2099560
1	3.0992880	3.9679790	-0.3436700
1	-12.2799000	0.2299830	0.6375980
8	4.6622470	-0.1737910	-0.0855210
6	5.7340530	0.6817270	-0.0950180
6	5.3325710	1.9800180	-0.1699510
1	5.9692500	2.8526520	-0.1904340
6	7.0509200	0.0587820	-0.0168970
6	7.1699640	-1.3316680	0.0843980
6	8.2108310	0.8467670	-0.0376200
6	8.4235080	-1.9255830	0.1691570
1	6.2800160	-1.9495620	0.0995910
6	9.4653190	0.2630490	0.0470580
1	8.1364250	1.9256410	-0.1196640
6	9.5524170	-1.1213700	0.1511660
1	8.5089570	-3.0054180	0.2491540
1	10.3507110	0.8904110	0.0319390
7	10.8785920	-1.7641590	0.2582810
6	11.7274840	-1.5410420	-0.9601700
1	11.9612800	-0.4798120	-1.0279150
1	12.6411090	-2.1238110	-0.8496450
1	11.1614090	-1.8646530	-1.8318220
6	11.5967800	-1.3703320	1.5172300
1	10.9416430	-1.5813710	2.3605960
1	12.5157300	-1.9511830	1.5813620
1	11.8224080	-0.3063500	1.4654190
1	-7.3840900	1.4148030	0.4455510
16	-7.2570090	-2.0157390	-0.3442750
1	10.7096260	-2.7744510	0.3180390

Enol-HBT excited-state structure in dichloromethane + HCl *G* -1853.187198 au

6	-5.015121	1.491400	0.036245
6	-5.358916	0.091371	0.019010
6	-6.724749	-0.320797	0.010247
6	-8.869284	-1.542379	-0.018773
6	-10.012111	-2.338541	-0.037986
6	-11.249755	-1.706411	-0.031610
6	-11.345340	-0.303984	-0.006204
6	-10.212228	0.489875	0.012913
6	-8.950420	-0.129324	0.006384
1	-9.938365	-3.420712	-0.057625
1	-12.153987	-2.305709	-0.046586
1	-10.273761	1.572797	0.032495
7	-7.746244	0.518690	0.022064
8	-5.955739	2.449273	0.049770
6	-4.293660	-0.851144	0.008126
6	-3.692510	1.873121	0.037905
6	-2.983328	-0.467522	0.011515
1	-4.532023	-1.911266	-0.003688
1	-3.468832	2.935509	0.049559
1	-6.846793	2.014916	0.044798
1	-2.210778	-1.227203	0.001518
6	-1.297674	1.380366	0.021351
1	-1.170998	2.459966	0.023550
6	-0.153690	0.573413	0.016326
1	-0.283968	-0.505748	0.026135
6	-2.629289	0.925999	0.024642

6	1.180583	1.023068	0.000741
6	2.233472	0.052937	0.008396
6	1.534063	2.424001	-0.025436
6	3.517834	0.516587	-0.011022
1	2.010407	-1.008253	0.029602
6	2.831110	2.855494	-0.046693
1	0.741068	3.162643	-0.030651
6	3.873057	1.891246	-0.041239
1	3.064677	3.914520	-0.067714
1	-12.325258	0.162170	-0.001612
8	4.648827	-0.247346	-0.005789
6	5.712204	0.616021	-0.033696
6	5.280929	1.928420	-0.056634
1	5.910044	2.806676	-0.077590
6	7.028127	0.029652	-0.024387
6	7.188591	-1.366405	0.045990
6	8.174517	0.847697	-0.080785
6	8.456953	-1.927028	0.069036
1	6.315472	-2.006778	0.086808
6	9.440872	0.292187	-0.060237
1	8.073254	1.925688	-0.141604
6	9.566911	-1.093444	0.019582
1	8.573132	-3.005739	0.127706
1	10.311103	0.939035	-0.106098
7	10.912468	-1.699865	0.052773
6	11.673358	-1.473382	-1.222815
1	11.869301	-0.406499	-1.317897
1	12.609258	-2.027660	-1.165211
1	11.061582	-1.824970	-2.051625
6	11.706961	-1.263210	1.250296
1	11.119780	-1.471371	2.142730
1	12.643177	-1.819622	1.260092
1	11.901721	-0.195481	1.162066
16	-7.196990	-2.031672	-0.021458
1	10.775559	-2.713041	0.141333

Keto-HBT excited-state structure in dichloromethane + HCl *G* -1853.179104 au

6	-5.051082	1.530504	0.060736
6	-5.358306	0.067612	-0.006809
6	-6.705313	-0.368447	-0.002130
6	-8.899575	-1.547611	-0.019536
6	-10.034295	-2.352046	-0.039580
6	-11.278382	-1.732056	0.016838
6	-11.384537	-0.333852	0.092588
6	-10.261653	0.477378	0.113227
6	-9.005230	-0.142013	0.055460
1	-9.948713	-3.431688	-0.097782
1	-12.177139	-2.338644	0.002226
1	-10.337644	1.557413	0.172514
7	-7.780728	0.460193	0.061888
8	-5.990290	2.369326	0.121510
6	-4.292211	-0.845031	-0.074496
6	-3.682266	1.899630	0.052507
6	-2.973992	-0.414629	-0.077500
1	-4.494762	-1.911634	-0.126511
1	-3.470430	2.963844	0.102266
1	-2.190585	-1.162271	-0.132821
6	-1.263727	1.418979	-0.016518
1	-1.145262	2.500576	0.020884
6	-0.150404	0.640275	-0.054920

1	-0.259089	-0.441964	-0.081800
6	-2.635122	0.972756	-0.013346
6	1.226265	1.104600	-0.056781
6	2.251264	0.144080	-0.057121
6	1.575402	2.486098	-0.057748
6	3.556178	0.601004	-0.054357
1	2.027605	-0.917737	-0.056313
6	2.885095	2.917506	-0.057268
1	0.786114	3.229743	-0.061961
6	3.914023	1.957917	-0.055228
1	3.116820	3.977621	-0.059009
1	-12.367508	0.123127	0.136065
8	4.673439	-0.177081	-0.048800
6	5.748678	0.675838	-0.046027
6	5.346444	1.978631	-0.050734
1	5.985541	2.849923	-0.046547
6	7.063250	0.050631	-0.026938
6	7.183294	-1.343742	0.024018
6	8.225646	0.836993	-0.052764
6	8.437131	-1.941220	0.057238
1	6.292751	-1.960699	0.041792
6	9.480136	0.249133	-0.020339
1	8.151820	1.918112	-0.097690
6	9.567412	-1.138419	0.037925
1	8.522658	-3.023273	0.099889
1	10.366259	0.875539	-0.039536
7	10.894458	-1.786178	0.089285
6	11.701315	-1.546198	-1.154415
1	11.943737	-0.486011	-1.207331
1	12.611667	-2.140953	-1.089518
1	11.101150	-1.844809	-2.012061
6	11.659943	-1.412721	1.326250
1	11.040964	-1.641820	2.191823
1	12.583480	-1.989313	1.342956
1	11.879310	-0.347010	1.285179
1	-7.559119	1.466966	0.107600
16	-7.219838	-2.039607	-0.076711
1	10.724202	-2.796859	0.139763

Enol-HBT ground-state structure in acetone *G* -1852.882467 au

6	4.9926120	-1.4571070	0.0057500
6	5.3120720	-0.0796370	0.0036460
6	6.7048420	0.3506450	0.0022580
6	8.8340360	1.5822170	-0.0008760
6	9.9733510	2.3870380	-0.0028060
6	11.2118380	1.7594590	-0.0027450
6	11.3153460	0.3588280	-0.0007930
6	10.1830700	-0.4397590	0.0011440
6	8.9268180	0.1779180	0.0010970
1	9.8944520	3.4688280	-0.0043190
1	12.1132580	2.3632400	-0.0042420
1	10.2478890	-1.5226910	0.0026620
7	7.7093340	-0.4788520	0.0028370
8	5.9216610	-2.4271820	0.0066850
6	4.2547880	0.8478710	0.0029210
6	3.6518670	-1.8516200	0.0068800
6	2.9352910	0.4500980	0.0040310
1	4.4821560	1.9109050	0.0014970
1	3.4408840	-2.9169700	0.0084020
1	6.8152770	-2.0035760	0.0056150

1	2.1560750	1.2034040	0.0036630
6	1.2330570	-1.4245420	0.0066000
1	1.1466580	-2.5091190	0.0103960
6	0.1216100	-0.6695140	0.0022820
1	0.2188520	0.4148450	-0.0023400
6	2.6115740	-0.9232550	0.0058670
6	-1.2638230	-1.1498180	0.0022720
6	-2.2891560	-0.1957120	-0.0063690
6	-1.5965070	-2.5269090	0.0102320
6	-3.5929530	-0.6593810	-0.0070030
1	-2.0709330	0.8675920	-0.0125640
6	-2.9076640	-2.9679130	0.0093950
1	-0.8014280	-3.2650220	0.0174090
6	-3.9412850	-2.0175800	0.0004100
1	-3.1311520	-4.0298720	0.0156300
1	12.2969490	-0.1032530	-0.0008020
8	-4.7153430	0.1109440	-0.0149800
6	-5.7895900	-0.7462130	-0.0128360
6	-5.3768680	-2.0464750	-0.0037280
1	-6.0113010	-2.9206650	-0.0006990
6	-7.1069290	-0.1283380	-0.0210070
6	-7.2609900	1.2638470	-0.0298760
6	-8.2679650	-0.9138240	-0.0154710
6	-8.5152800	1.8514030	-0.0368600
1	-6.3805830	1.8984160	-0.0279390
6	-9.5274410	-0.3425260	-0.0226650
1	-8.1877550	-1.9972200	-0.0017110
6	-9.6888310	1.0634210	-0.0417780
1	-8.5824080	2.9323290	-0.0375770
1	-10.3934650	-0.9926600	-0.0119300
7	-10.9348390	1.6371060	-0.0682500
6	-12.1113720	0.8013840	0.0758340
1	-12.1140340	0.2519500	1.0270620
1	-12.9998660	1.4307990	0.0384370
1	-12.1793350	0.0734410	-0.7401220
6	-11.0617950	3.0759980	0.0605340
1	-10.5568830	3.5907770	-0.7643440
1	-12.1174250	3.3432760	0.0270170
1	-10.6390640	3.4448200	1.0050110
16	7.1561770	2.0567830	-0.0005000

Keto-HBT ground-state structure in acetone *G* -1852.866785 au

6	5.0227200	-1.4371280	0.1460140
6	5.2903040	-0.0211500	-0.0368300
6	6.6338490	0.4117080	-0.0213990
6	8.8594170	1.5290350	-0.0503480
6	10.0190260	2.2975650	-0.0916910
6	11.2377260	1.6477100	0.0709080
6	11.2959920	0.2620690	0.2703170
6	10.1412840	-0.5077280	0.3120330
6	8.9194040	0.1437620	0.1486280
1	9.9727190	3.3700190	-0.2459050
1	12.1552890	2.2251310	0.0424270
1	10.1766740	-1.5804890	0.4661430
7	7.6577340	-0.4275000	0.1557820
8	5.9368880	-2.2988850	0.3178890
6	4.2194530	0.8937590	-0.2269750
6	3.6350310	-1.8106760	0.1207990
6	2.9189410	0.4823130	-0.2405880
1	4.4454300	1.9490840	-0.3675020

1	3.4174860	-2.8667280	0.2568660
1	2.1280460	1.2060370	-0.3966200
6	1.2322310	-1.4045940	-0.0579590
1	1.1430580	-2.4851840	0.0349150
6	0.1216450	-0.6526980	-0.1428260
1	0.2177520	0.4294870	-0.2083660
6	2.6118970	-0.9052140	-0.0590880
6	-1.2631810	-1.1363180	-0.1401410
6	-2.2915660	-0.1862160	-0.1041330
6	-1.5914610	-2.5140120	-0.1734950
6	-3.5936760	-0.6546920	-0.0922790
1	-2.0770040	0.8776460	-0.0821280
6	-2.9010850	-2.9599160	-0.1622760
1	-0.7936520	-3.2478920	-0.2185880
6	-3.9375420	-2.0138050	-0.1183980
1	-3.1211170	-4.0222440	-0.1912470
1	12.2594600	-0.2203160	0.3946000
8	-4.7184890	0.1114180	-0.0554800
6	-5.7898330	-0.7494540	-0.0578570
6	-5.3730310	-2.0477620	-0.0956780
1	-6.0046580	-2.9239340	-0.1062000
6	-7.1089900	-0.1363520	-0.0208300
6	-7.2672740	1.2549140	0.0141360
6	-8.2673380	-0.9257420	-0.0140170
6	-8.5231680	1.8379640	0.0511660
1	-6.3888240	1.8922000	0.0158770
6	-9.5283760	-0.3589340	0.0224380
1	-8.1836330	-2.0087810	-0.0340200
6	-9.6942110	1.0463380	0.0484660
1	-8.5934770	2.9182000	0.0835210
1	-10.3920540	-1.0122120	0.0322300
7	-10.9422870	1.6162600	0.0663360
6	-12.1125680	0.7724370	0.2141550
1	-12.0903230	0.1948550	1.1483190
1	-13.0034700	1.3995590	0.2173380
1	-12.1985900	0.0689070	-0.6212680
6	-11.0701260	3.0499400	0.2433880
1	-10.5850680	3.5921140	-0.5758210
1	-12.1269340	3.3146560	0.2416570
1	-10.6273380	3.3902350	1.1894110
1	7.3676700	-1.4259840	0.2787290
16	7.1921410	2.0563320	-0.2213940

Enol-HBT excited-state structure in acetone *G* -1852.779697 au

6	4.9758970	-1.4901160	0.0000000
6	5.3172200	-0.0935410	0.0000000
6	6.6812700	0.3231990	-0.0000010
6	8.8218600	1.5650090	-0.0000030
6	9.9572600	2.3705520	-0.0000030
6	11.2027090	1.7505860	-0.0000040
6	11.3079560	0.3509370	-0.0000050
6	10.1783950	-0.4523540	-0.0000040
6	8.9125580	0.1543180	-0.0000030
1	9.8733980	3.4523720	-0.0000030
1	12.1013560	2.3584720	-0.0000050
1	10.2503840	-1.5350260	-0.0000040
7	7.7103890	-0.5059240	-0.0000020
8	5.9246830	-2.4485280	0.0000000
6	4.2443810	0.8402730	0.0000010
6	3.6551850	-1.8794600	0.0000010

6	2.9346250	0.4509880	0.0000010
1	4.4754800	1.9028160	0.0000000
1	3.4389500	-2.9440310	0.0000010
1	6.8108320	-2.0056760	-0.0000010
1	2.1599990	1.2093840	0.0000020
6	1.2510210	-1.4037290	0.0000020
1	1.1333040	-2.4848860	0.0000030
6	0.1004530	-0.6086070	0.0000020
1	0.2227420	0.4720030	0.0000010
6	2.5823880	-0.9407620	0.0000020
6	-1.2312670	-1.0642720	0.0000030
6	-2.2949460	-0.1015660	0.0000020
6	-1.5806880	-2.4678730	0.0000050
6	-3.5740100	-0.5709700	0.0000020
1	-2.0789220	0.9615390	0.0000000
6	-2.8737910	-2.9078590	0.0000050
1	-0.7829180	-3.2018820	0.0000060
6	-3.9275010	-1.9504900	0.0000040
1	-3.1003000	-3.9688330	0.0000070
1	12.2907460	-0.1095970	-0.0000050
8	-4.7102200	0.1891580	0.0000010
6	-5.7752460	-0.6740820	0.0000020
6	-5.3260580	-1.9954790	0.0000040
1	-5.9536150	-2.8750160	0.0000050
6	-7.0799520	-0.1085170	0.0000010
6	-7.2737800	1.2925700	0.0000000
6	-8.2312380	-0.9314040	0.0000020
6	-8.5346980	1.8415910	-0.0000020
1	-6.4081790	1.9464290	-0.0000010
6	-9.4960140	-0.3953050	0.0000000
1	-8.1213040	-2.0115740	0.0000030
6	-9.6927110	1.0150320	-0.0000020
1	-8.6356870	2.9195910	-0.0000020
1	-10.3476150	-1.0636750	0.0000010
7	-10.9395370	1.5500710	-0.0000040
6	-12.1075160	0.6841970	0.0000000
1	-12.1269210	0.0446940	0.8896930
1	-13.0045250	1.3007480	-0.0000040
1	-12.1269190	0.0446860	-0.8896880
6	-11.1149840	2.9933000	-0.0000020
1	-10.6638630	3.4471350	-0.8896000
1	-12.1794870	3.2203460	-0.0000050
1	-10.6638680	3.4471330	0.8896000
16	7.1420360	2.0413620	-0.0000020

Keto-HBT excited-state structure in acetone *G* -1852.766388 au

6	-5.0101550	-1.4831780	0.0000020
6	-5.2895710	-0.0318330	0.0000000
6	-6.6200520	0.3983310	0.0000000
6	-8.8512560	1.5204960	0.0000010
6	-10.0078920	2.2912390	0.0000010
6	-11.2364630	1.6351090	0.0000020
6	-11.3014160	0.2355740	0.0000010
6	-10.1504880	-0.5407750	0.0000010
6	-8.9145700	0.1137340	0.0000000
1	-9.9539900	3.3746960	0.0000010
1	-12.1515010	2.2172430	0.0000020
1	-10.1953970	-1.6243080	0.0000000
7	-7.6683780	-0.4587210	-0.0000010
8	-5.9595930	-2.3398030	0.0000050

6	-4.2090930	0.9024550	-0.0000020
6	-3.6505210	-1.8441200	0.0000000
6	-2.9103080	0.4930570	-0.0000030
1	-4.4334700	1.9672920	-0.0000040
1	-3.4265570	-2.9078260	0.0000010
1	-2.1201690	1.2350920	-0.0000050
6	-1.2480680	-1.3719940	-0.0000030
1	-1.1318690	-2.4538610	-0.0000020
6	-0.0982000	-0.5865340	-0.0000030
1	-0.2096490	0.4950790	-0.0000040
6	-2.5871570	-0.9136810	-0.0000020
6	1.2361020	-1.0535150	-0.0000030
6	2.3006650	-0.0980350	-0.0000030
6	1.5765900	-2.4558390	-0.0000040
6	3.5800480	-0.5735680	-0.0000020
1	2.0903320	0.9662860	-0.0000030
6	2.8693960	-2.9028410	-0.0000030
1	0.7756060	-3.1863650	-0.0000050
6	3.9257420	-1.9521430	-0.0000020
1	3.0897090	-3.9651430	-0.0000030
1	-12.2696510	-0.2540490	0.0000020
8	4.7185470	0.1816160	-0.0000010
6	5.7796870	-0.6863470	-0.0000010
6	5.3283870	-2.0025490	-0.0000010
1	5.9522210	-2.8846460	-0.0000010
6	7.0891940	-0.1211060	0.0000000
6	7.2850810	1.2777230	0.0000010
6	8.2371870	-0.9453160	0.0000000
6	8.5480440	1.8251440	0.0000030
1	6.4209570	1.9336290	0.0000020
6	9.5042300	-0.4115110	0.0000010
1	8.1253040	-2.0253740	0.0000000
6	9.7037390	0.9973180	0.0000030
1	8.6504920	2.9030410	0.0000040
1	10.3542210	-1.0820010	0.0000010
7	10.9529740	1.5305490	0.0000040
6	12.1183240	0.6620540	0.0000030
1	12.1368120	0.0220490	-0.8895360
1	13.0170760	1.2762370	0.0000040
1	12.1368110	0.0220470	0.8895410
6	11.1302570	2.9730020	0.0000050
1	10.6798940	3.4282500	0.8894580
1	12.1951220	3.1988460	0.0000060
1	10.6798950	3.4282520	-0.8894470
1	-7.3627510	-1.4651620	-0.0000020
16	-7.1798780	2.0650800	0.0000000

Frontier molecular orbitals

In Figures S4, S5 and S6, we report the frontier molecular orbitals involved in the lowest energy transition in different solvent for **E-HBO 1**, **E-HBO 2** and **E-HBT**, respectively. This transition presents a major HOMO -> LUMO contribution and minor HOMO-1 -> LUMO and HOMO -> LUMO+1 contributions for the non-protonated dyes, whereas the transition of the protonated species shows a major HOMO -> LUMO contribution and a minor HOMO-1 -> LUMO+1 contribution.

Qualitatively, when going from cyclohexane to dichloromethane to acetonitrile, the orbitals of the neutral species present the same topology.

Interestingly, one observes a change in the orbitals' topology (particularly on the HOMO and LUMO orbitals) when protonating the terminal dimethylamino group. Indeed, one can clearly see a charge-transfer character of the HOMO-LUMO transition for the neutral species, *i.e.*, the HOMO is centered on the π-extention with no density on the ESIPT system (hydroxyphenylbenzazole) whereas the LUMO is localized over the whole molecule except on the terminal dimethylaminophenyl. In contrast, when considering protonated compounds, one observes that the frontier orbitals are located all along the molecule except on the terminal $-NHMe_2^+$. This is consistent with the density difference plots given in the main text.

In Figures S7, S8 and S9, we report the frontier orbitals for the keto form of the **HBO-1**, **HBT** and **HBO-2** species. As observed for the enol form, the orbitals present similar general topology irrespective of the considered compound. Nevertheless, when comparing the three derivatives, one can notice that the density on the heteroatom is larger for **HBT** orbitals than for **HBO** ones.

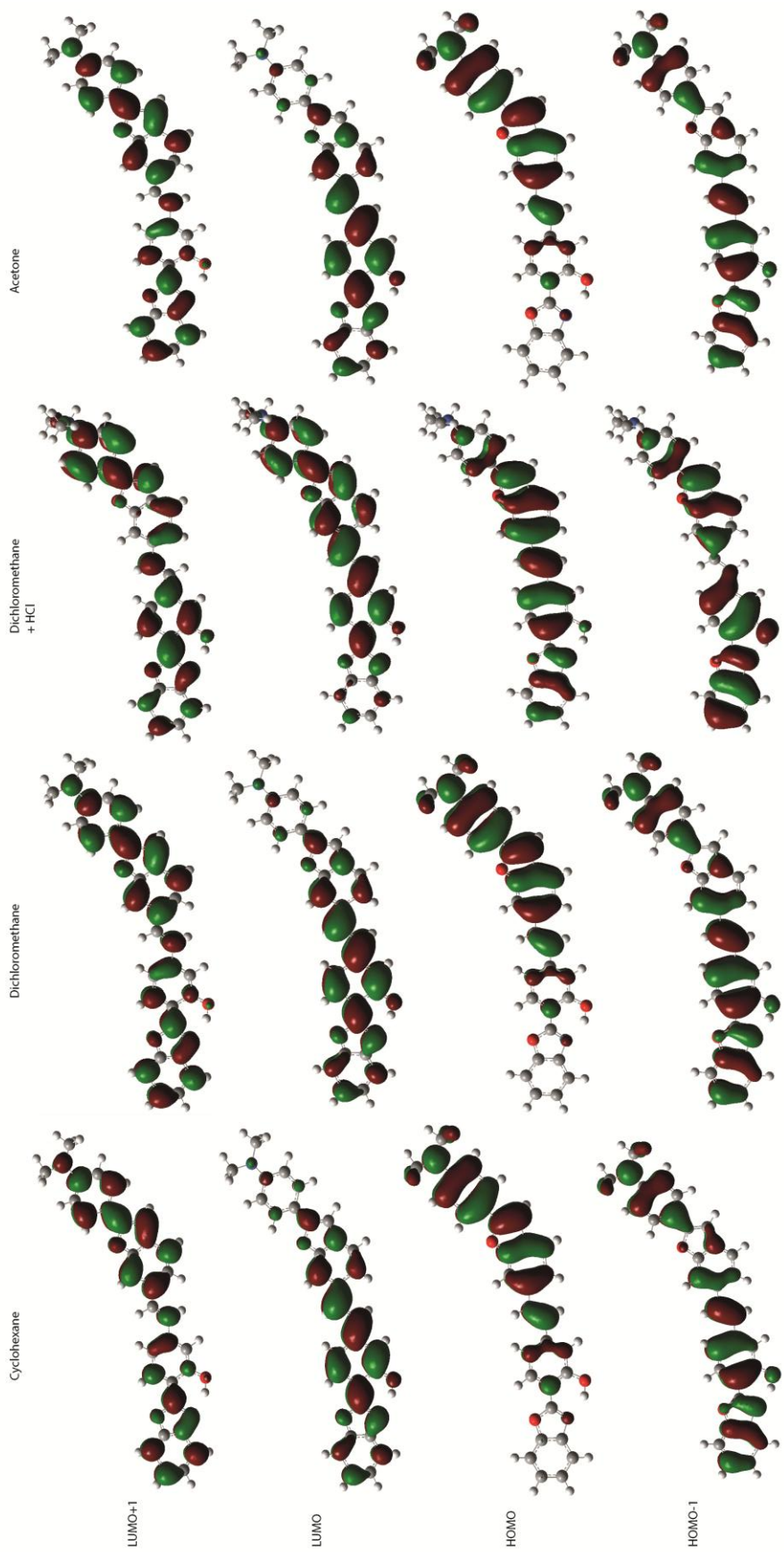


Figure S4. Representation of the frontier orbitals (isovalue=0.02 a.u.) in different solvents for the **E-HBO 1** molecule.

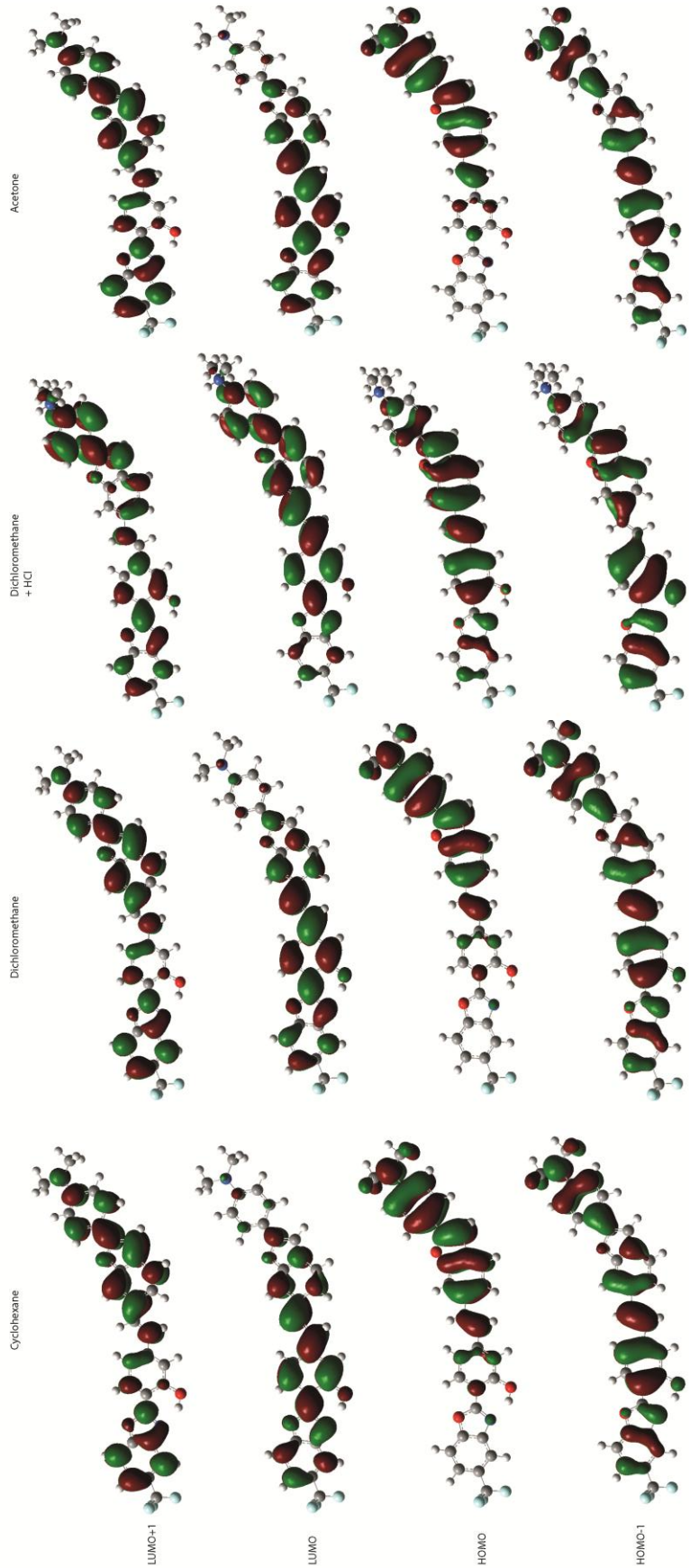


Figure S5. Representation of the frontier orbitals (isovalue=0.02 a.u.) in different solvents for the **E-HBO 2** molecule.

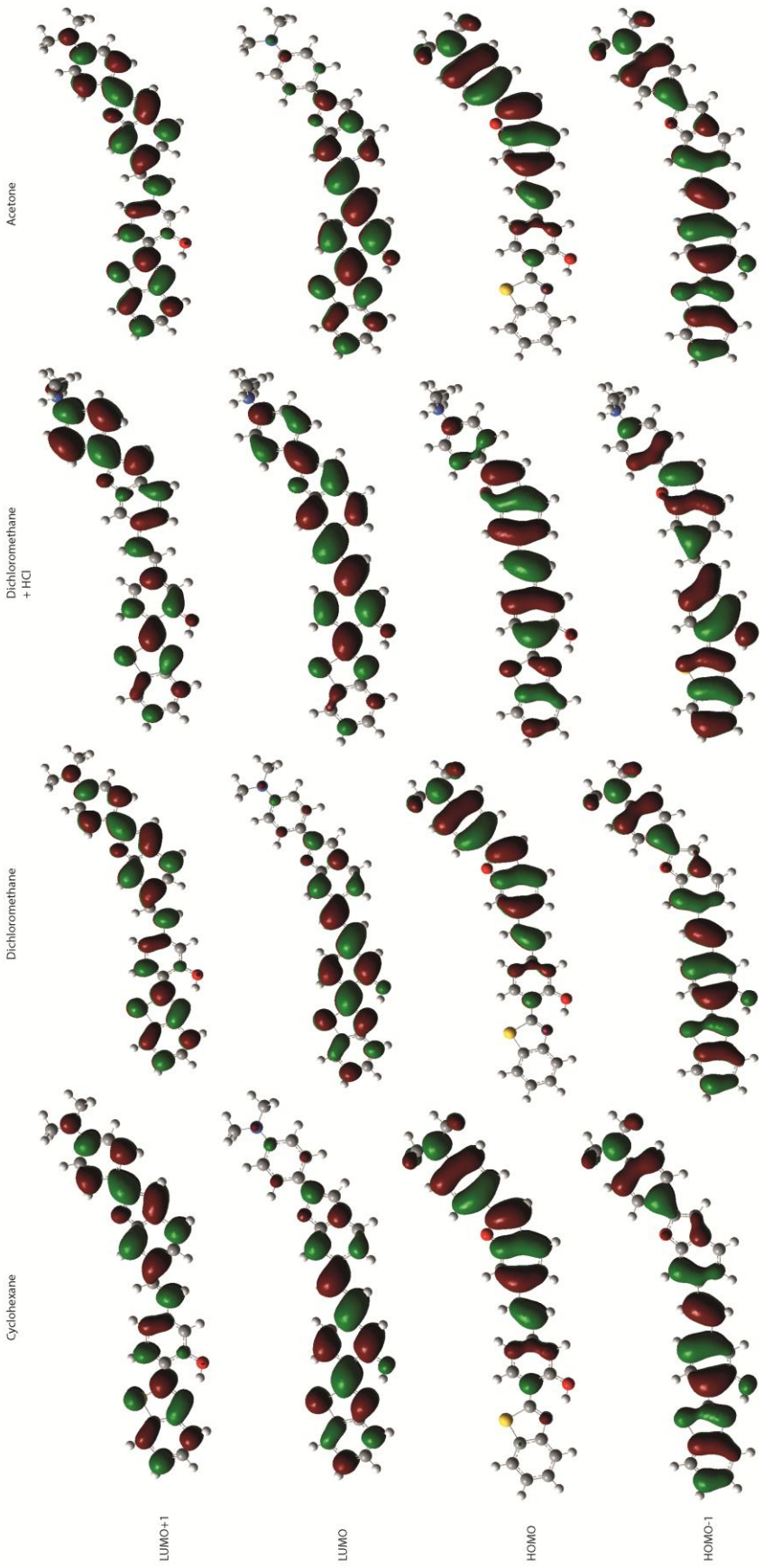


Figure S6. Representation of the frontier orbitals (isovalue=0.02 a.u.) in different solvents for the **E-HBT** molecule.

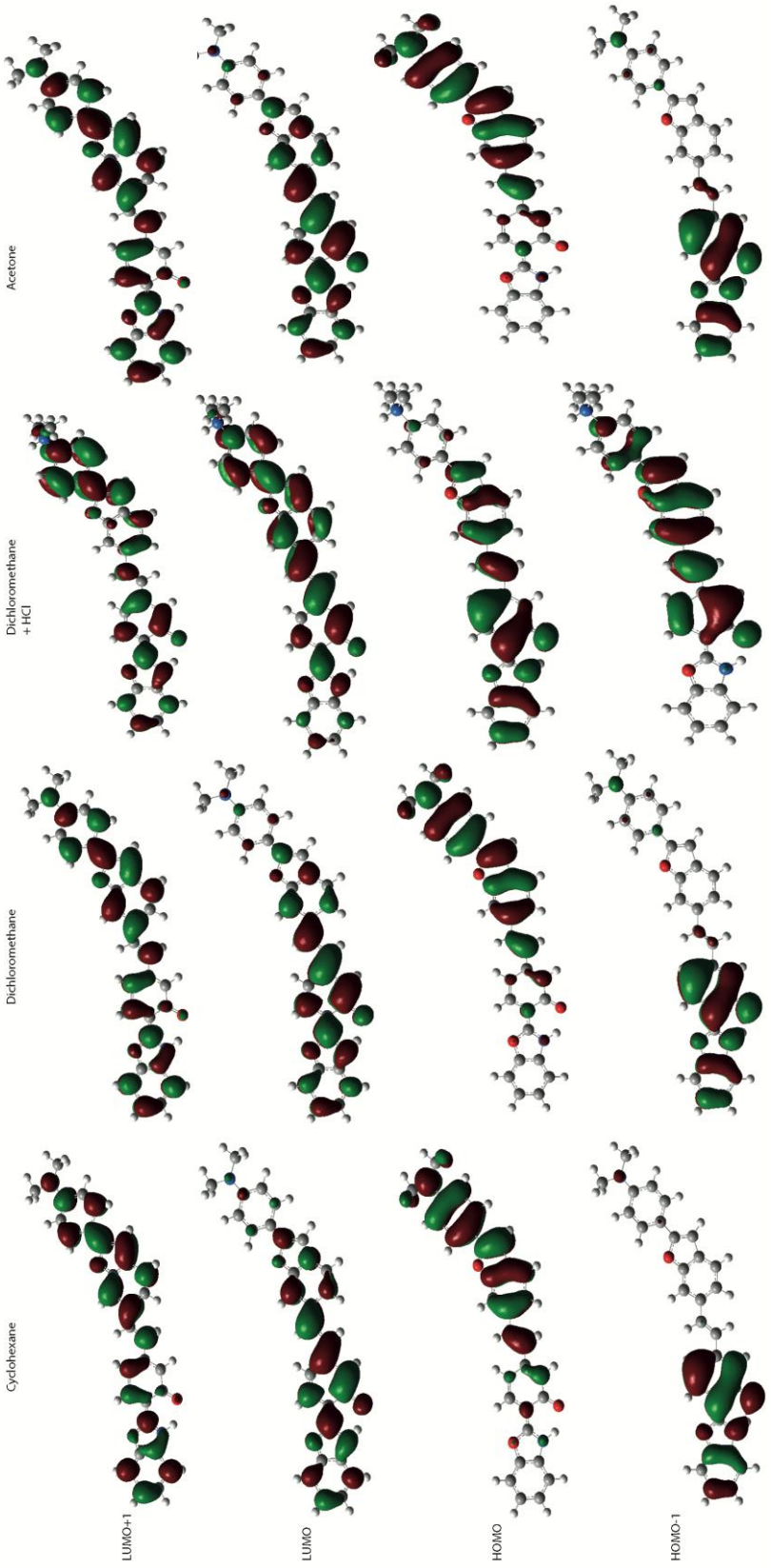


Figure S7. Representation of the frontier orbitals (isovalue=0.02 a.u.) in different solvents for the **K-HBO 1**

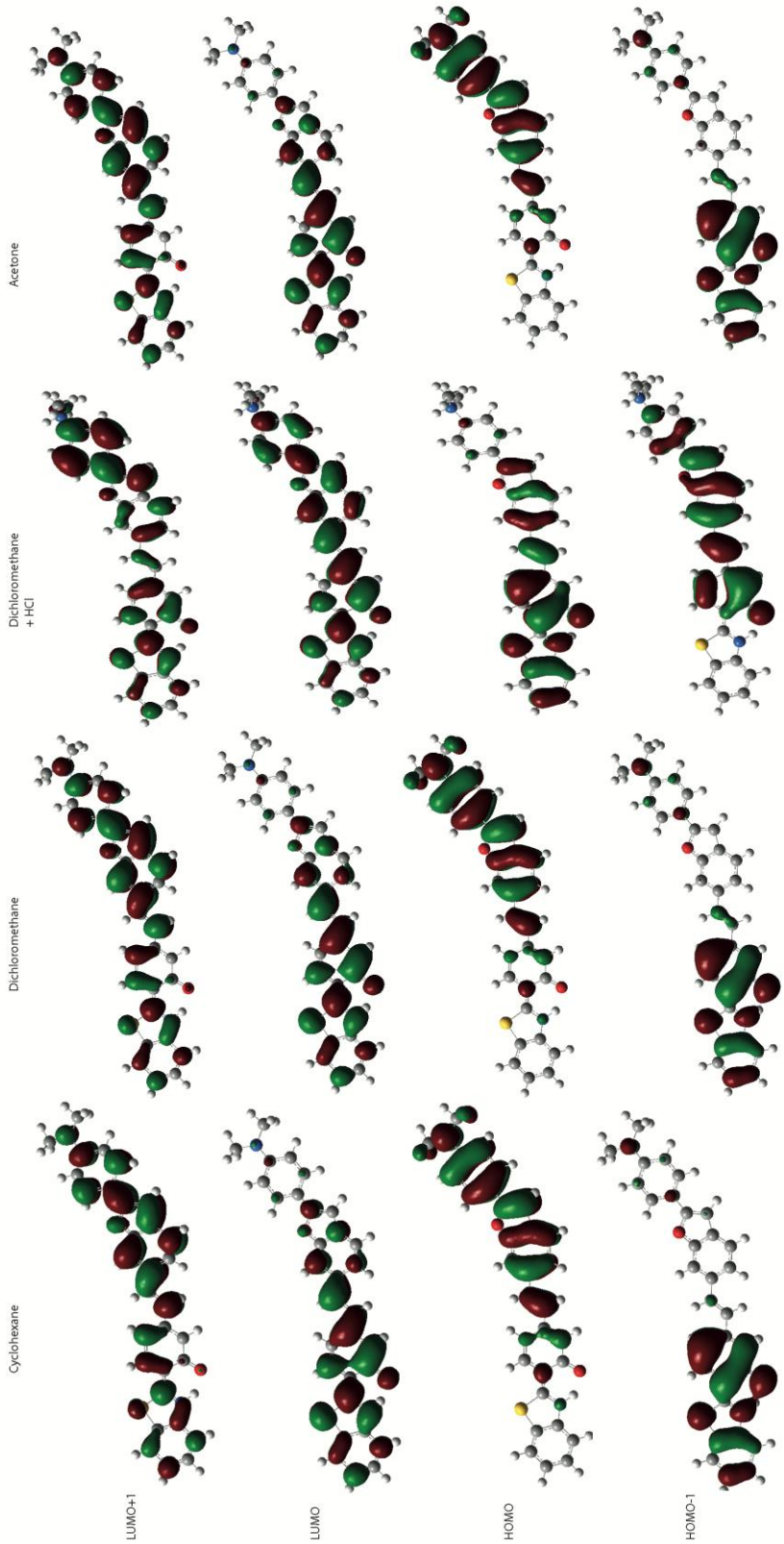


Figure S8. Representation of the frontier orbitals (isovalue=0.02 a.u.) in different solvents for the **K-HBT**

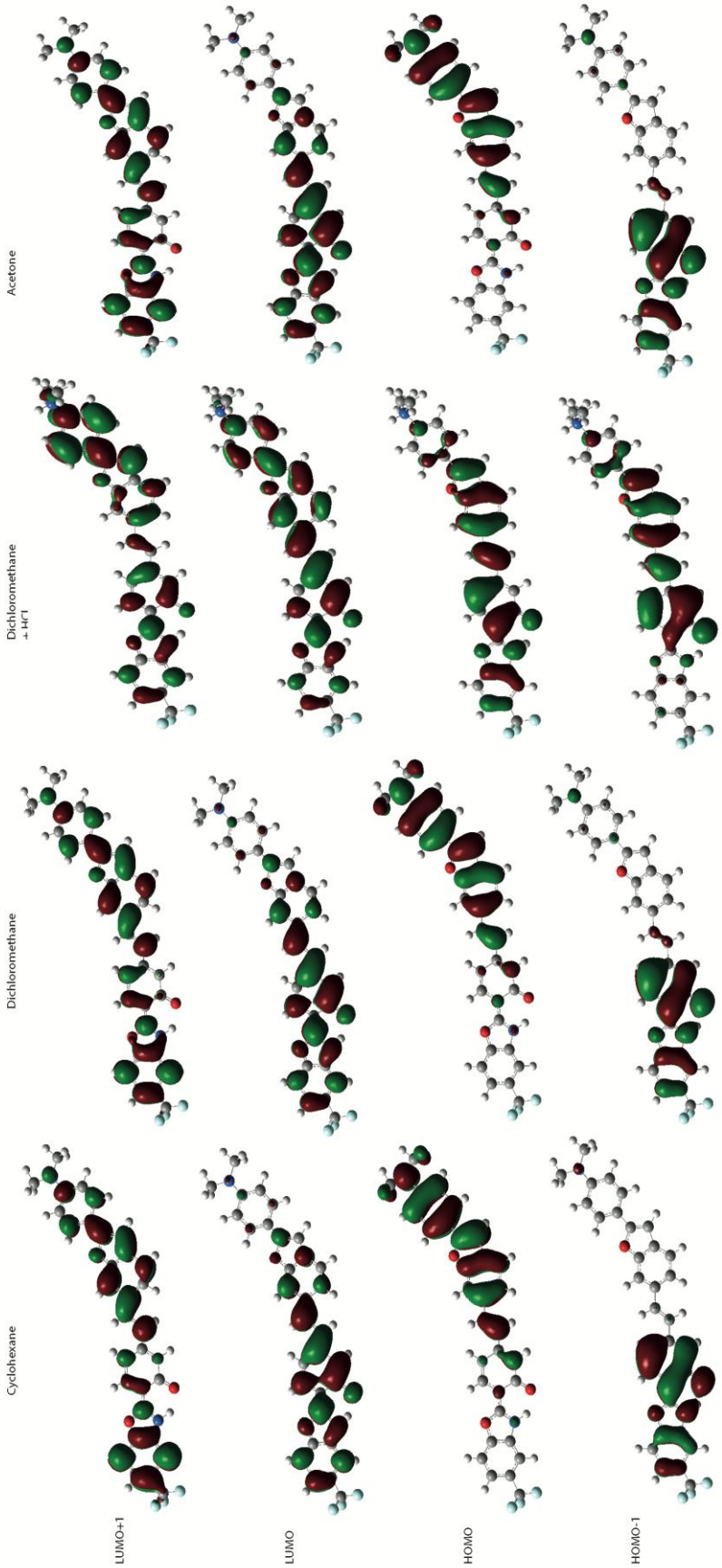


Figure S9. Representation of the frontier orbitals (isovalue=0.02 a.u.) in different solvents for the **K-HBO-2**

Density difference plots

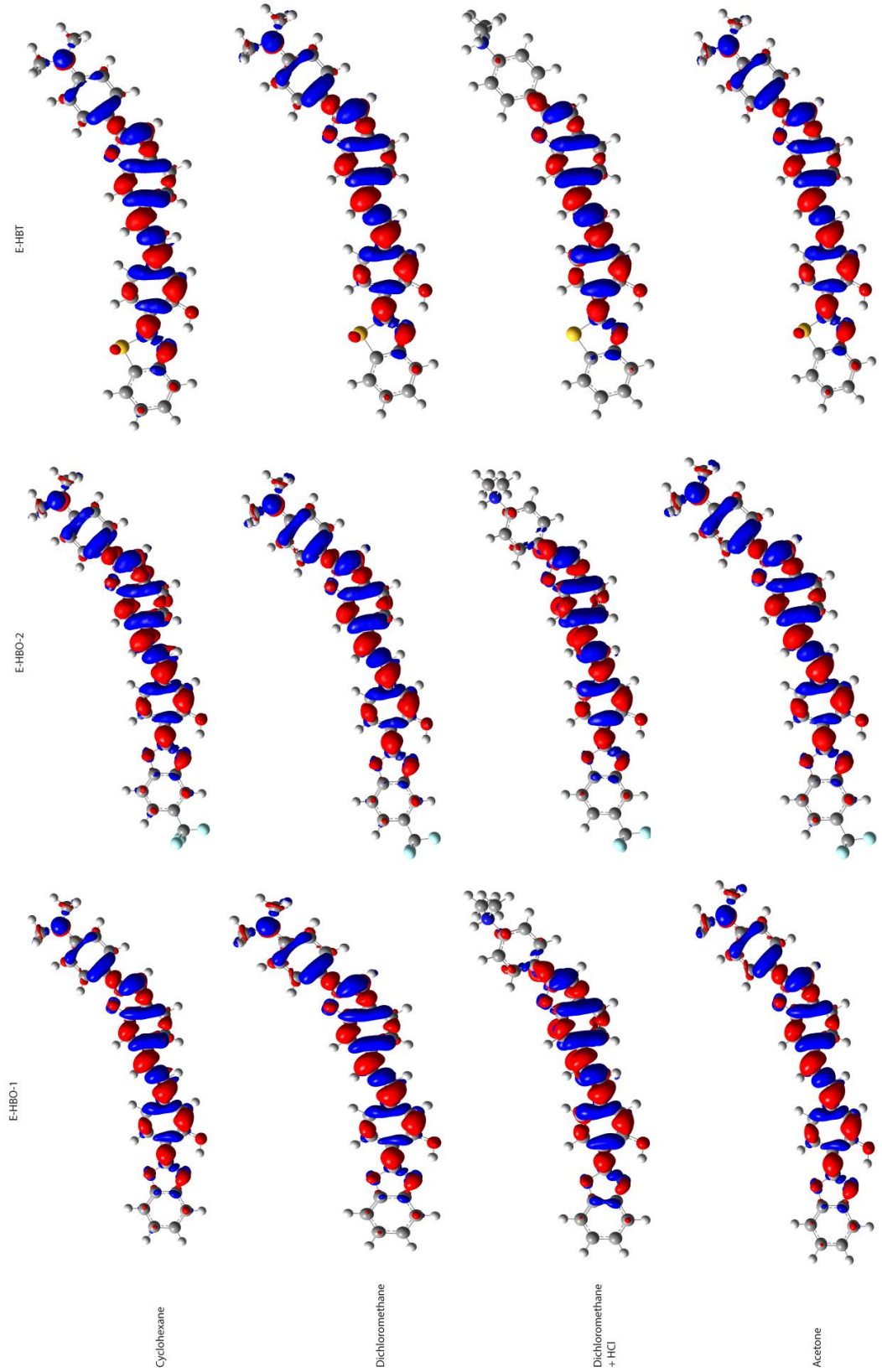


Figure S10. Density difference plots (isovalue=0.0008 a.u.) for **E-HBO 1**, **E-HBO 2** and **E-HBT** in different solvents. The blue (red) regions indicate a decrease (increase) of electron density upon absorption of light.

In Figure S10, we report the density difference plots corresponding to the S_0 -> S_1 transition for the three compounds in different solvents. Qualitatively, no striking changes can be observed for the neutral species when changing the solvent, the nature of the heteroatom (X=O or S) or the R group (from H to CF_3).

CC2 additional calculations

Table S2: Free energy differences corrected with ADC(2) or CC2 approach with the aug-cc-pVDZ basis set for the **E-HBT** series.

HBT- aug-cc-pVDZ in eV	ΔG^{ES}(adc2)	ΔG^{ES}(cc2)	$\Delta\Delta G^{ES}$(cc2-adc2)
Cyclohexane	0.231	0.207	0.024
Dichloromethane	0.245	0.203	0.041
Dichloromethane + HCl	0.091	0.124	-0.032
Acetone	0.238	0.194	0.044

MK Charges

Table S3: Merz-kollman charges (in *e*) for **E-HBO 1**-**2** and **E-HBT** on the N, O and H aoms involved in the ESIPT process.

E-HBO 1	**GS N**	**GS O**	**GS H**	**ES N**	**ES O**	**ES H**	**ΔN**	**ΔO**	**ΔH**
Cyclohexane	-0.605	-0.595	0.421	-0.641	-0.609	0.424	-0.036	-0.04	0.002
CH_2Cl_2	-0.607	-0.612	0.424	-0.646	-0.627	0.426	-0.038	-0.015	0.002
CH_2Cl_2 + HCl_g	-0572	-0.586	0.396	-0.584	-0.583	0.395	-0.012	0.003	-0.001
Acetone	-0.609	-0.616	0.425	-0.647	-.630	0.427	-0.039	-0.014	0.002
E-HBO 2	**GS N**	**GS O**	**GS H**	**ES N**	**ES O**	**ES H**	**ΔN**	**ΔO**	**ΔH**
Cyclohexane	-0.536	-0.567	0.394	-0.569	-0.581	0.396	-0.033	-0.014	0.002
CH_2Cl_2	-0.549	-0.592	0.406	-0.583	-0.606	0.407	-0.034	-0.014	0.001
CH_2Cl_2 + HCl_g	-0.576	-0.591	0.405	-0.593	-0.590	0.405	-0.017	0.001	0.000
Acetone	-0.569	-0.601	0.416	-0.605	-0.615	0.417	-0.036	-0.013	0.001
E-HBT	**GS N**	**GS O**	**GS H**	**ES N**	**ES O**	**ES H**	**ΔN**	**ΔO**	**ΔH**
Cyclohexane	-0.371	-0.579	0.375	-0.421	-0.588	0.379	-0.050	-0.009	0.003
CH_2Cl_2	-0.366	-0.598	0.380	-0.417	-0.608	0.383	-0.051	-0.011	0.002
CH_2Cl_2 + HCl_g	-0.371	-0.599	0.388	-0.404	-0.601	0.390	-0.033	-0.003	0.002
Acetone	-0.365	-0.602	0.381	-0.416	-0.612	0.383	-0.051	-0.011	0.002

Vibrationally resolved spectra

In Figure S11, we compare the theoretical and experimental band shapes for a typical case (**E-HBO 1** in cyclohexane). It is rather clear that there is a very good match between the experimental and theoretical band topologies. For the emission, the second band (at ca. 454 nm) is mainly provoked by a vibronic coupling with a vibrational mode corresponding to the elongation of single/contraction of double bonds, i.e., to the so-called ECC (effective conjugation coordinate) mode. This finding is consistent with the density difference plots appearing in the main text. Similar effects are found for absorption.

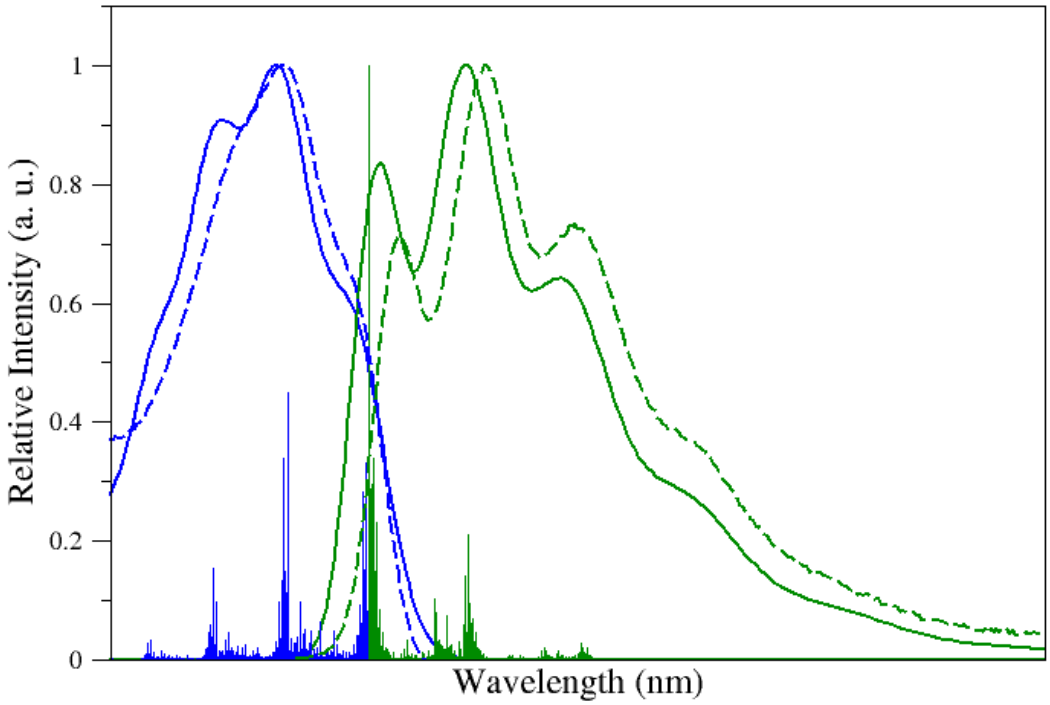


Figure S11. Vibrationally resolved absorption (HWHM=0.08 eV) and emission (HWHM=0.065 eV) for **E-HBO 1** in cyclohexane (full lines + stick contributions) as compared to the experimental spectrum (broken lines).. For the sake of clarity, the 0-0 energies have been set to the same value in both experiment and theory. Note that the experimental spectra have been renormalised to obtain lineshapes directly comparable to theoretical values (see above).

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