

The Influence of the Alkylamino Group on the Solvatochromic Behavior of 5-(4-substituted-arylidene)-1,3-dimethylpyrimidine-2,4,6-triones. Synthesis, Spectroscopic and Computational Studies

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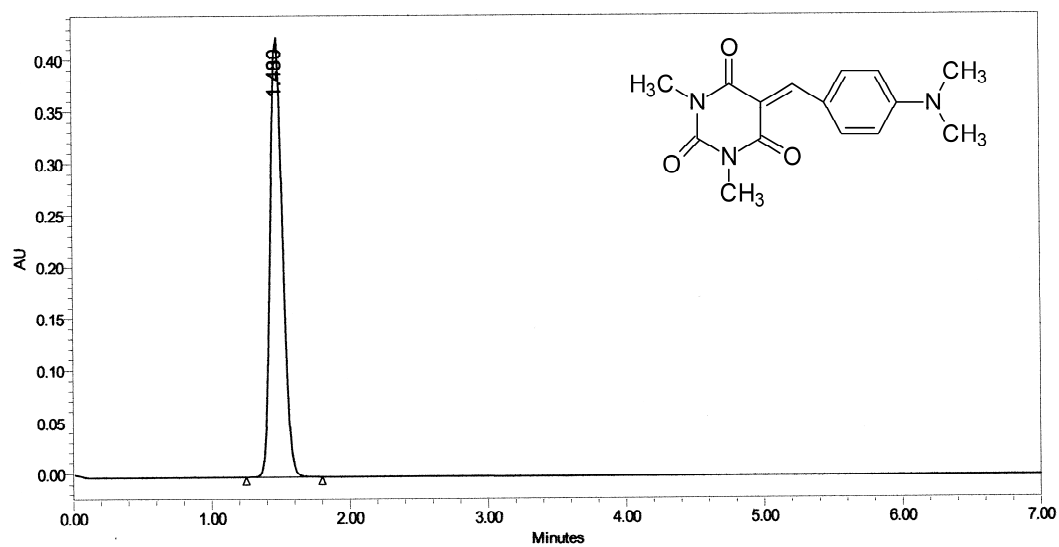
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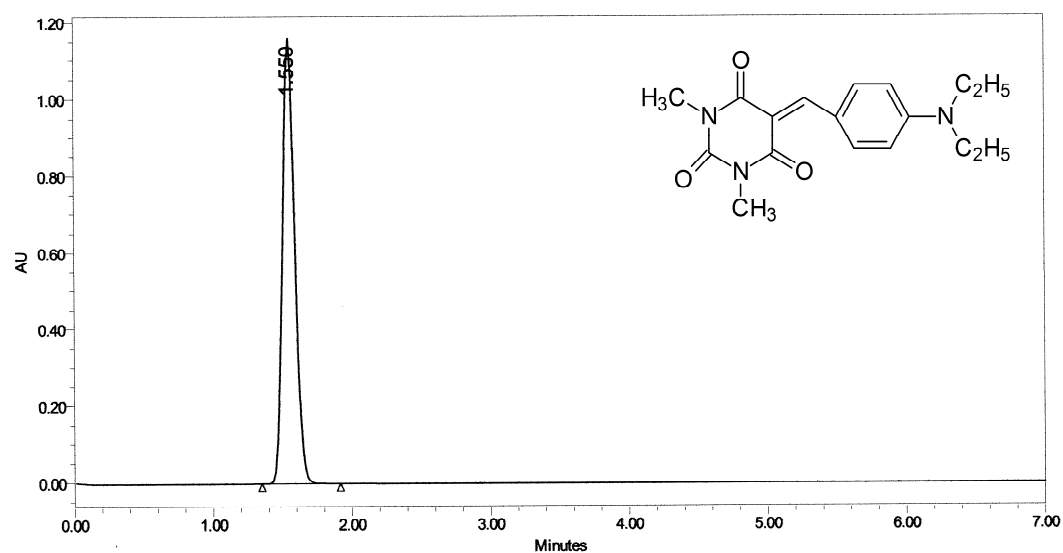
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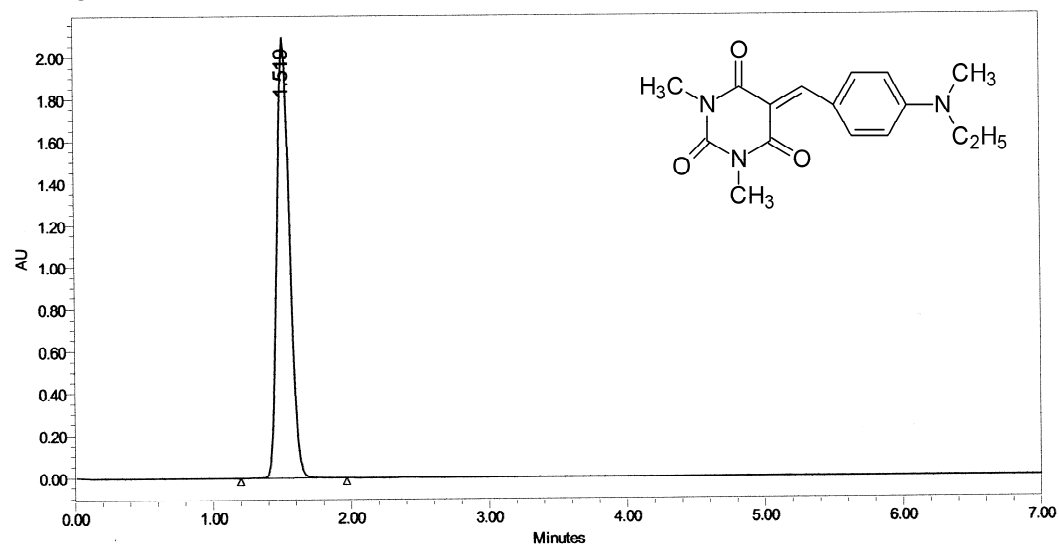
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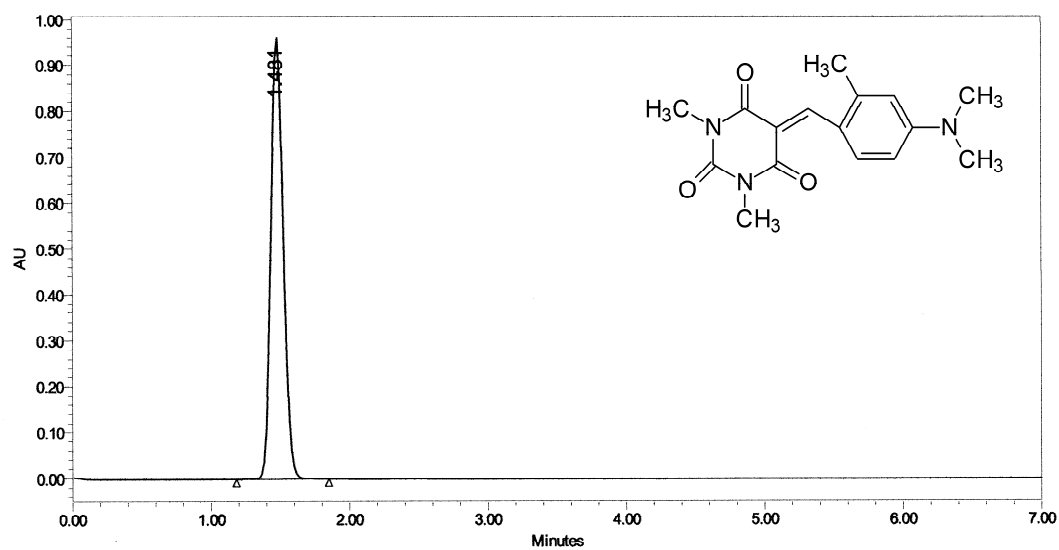
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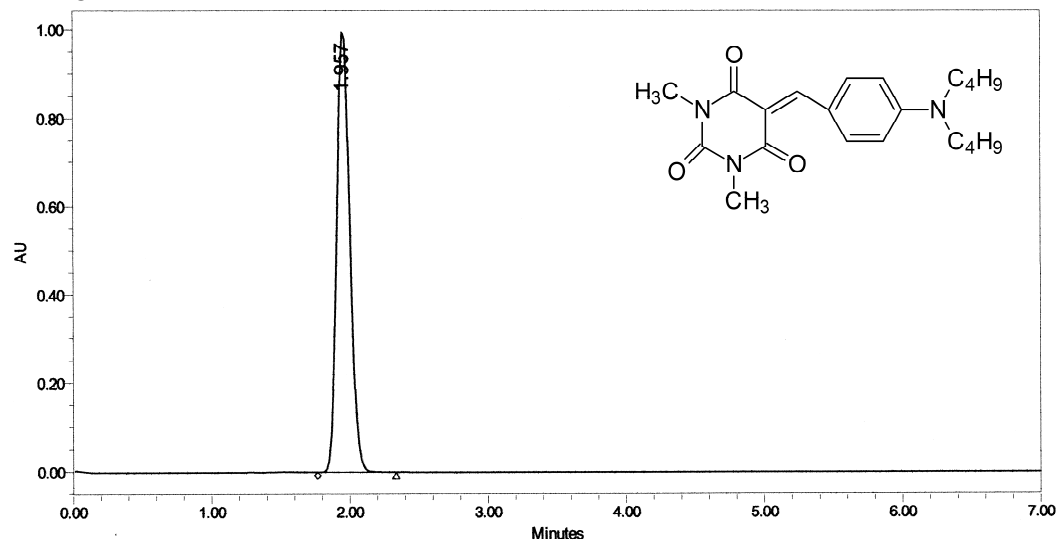
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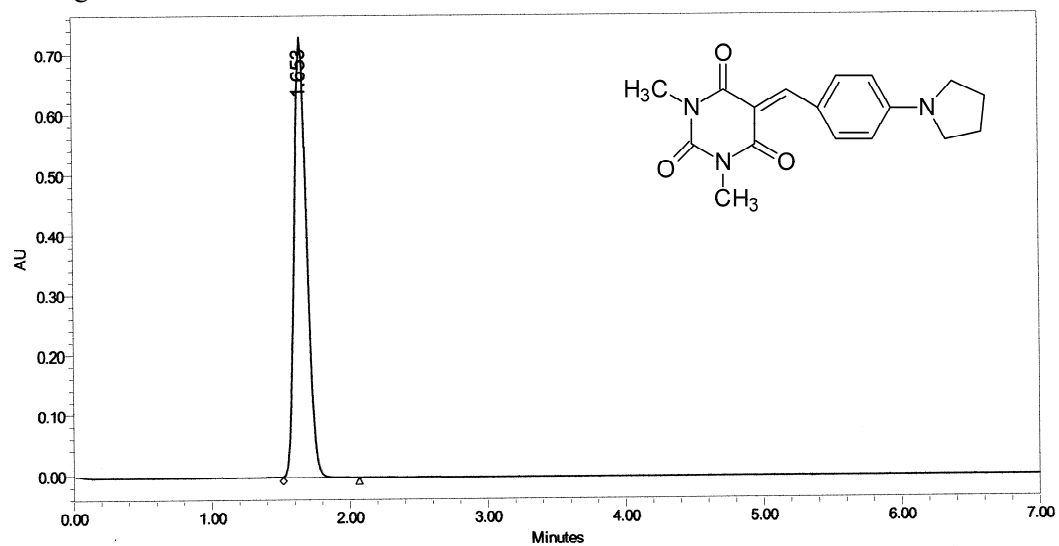
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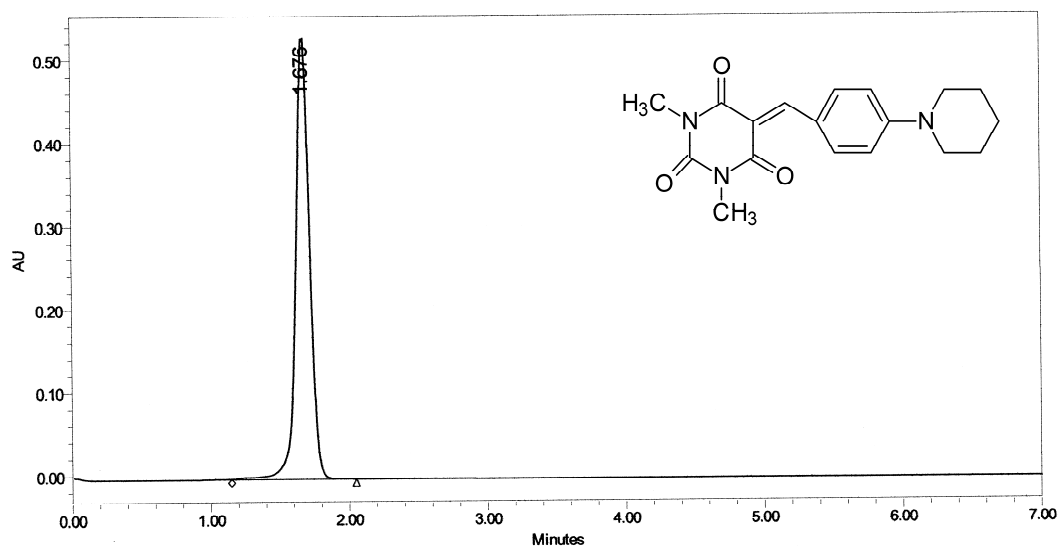
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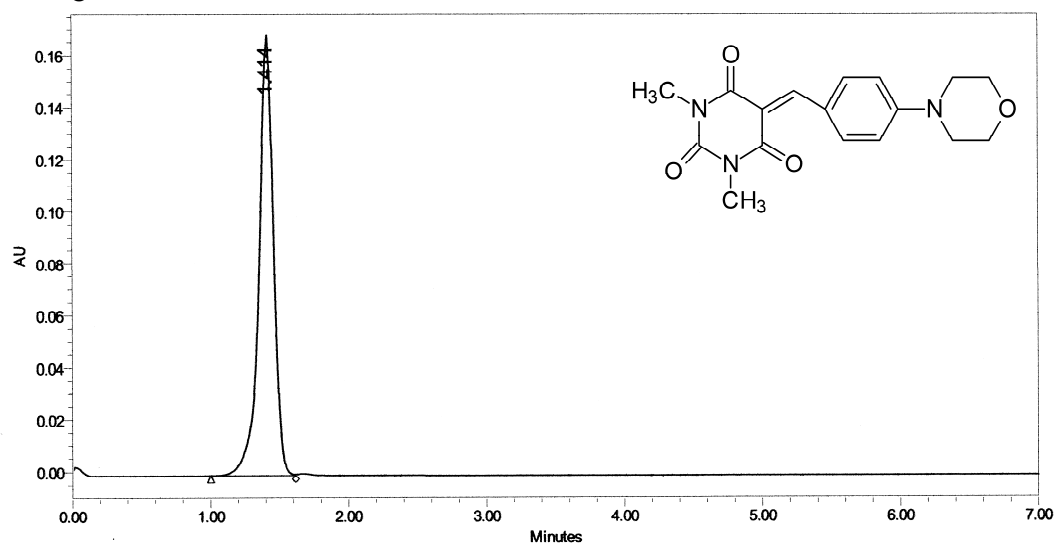
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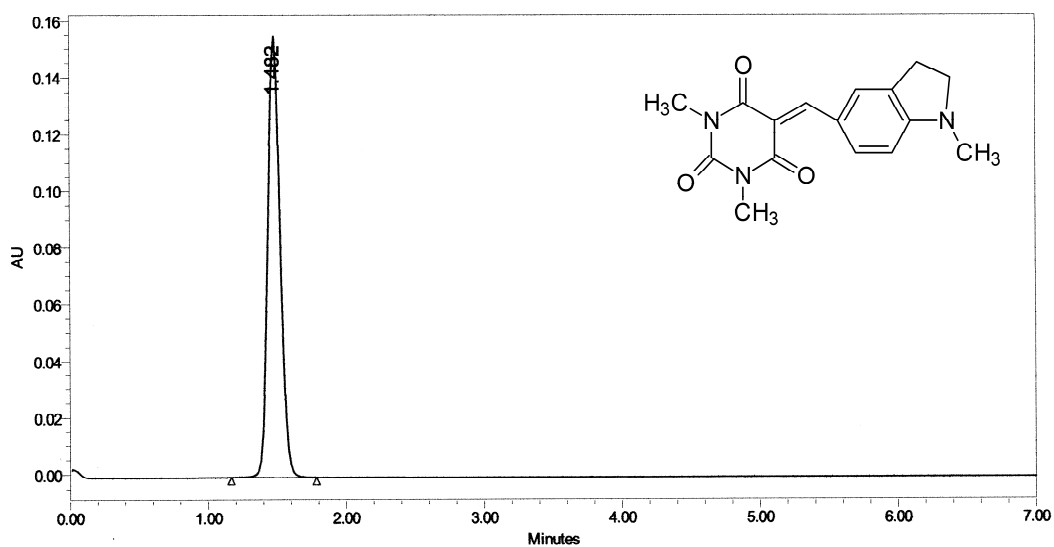
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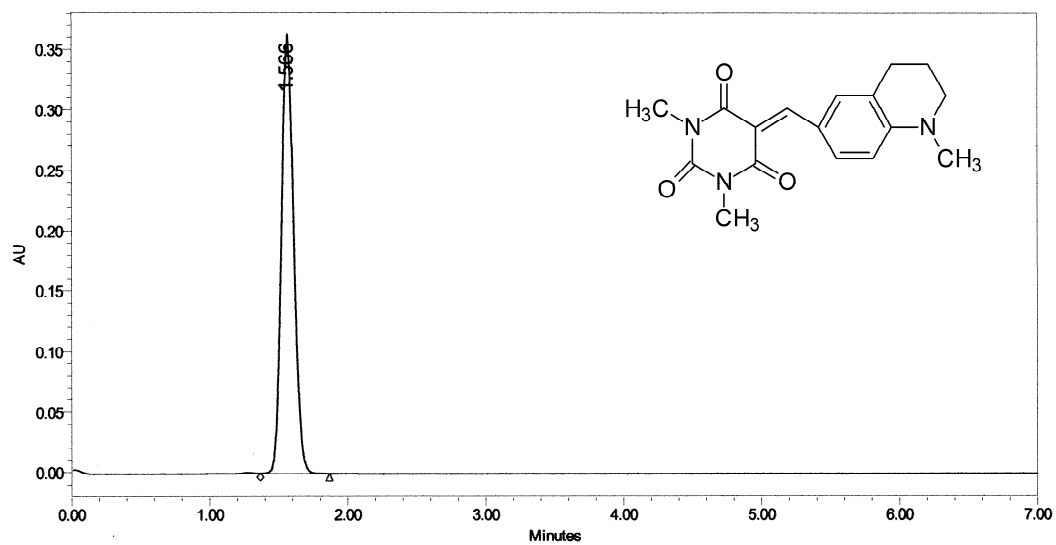
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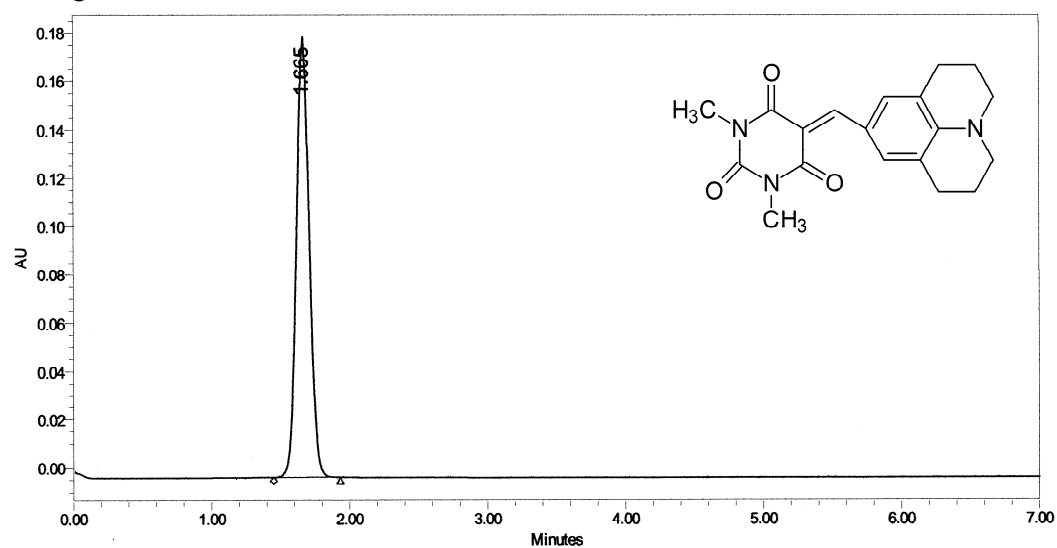
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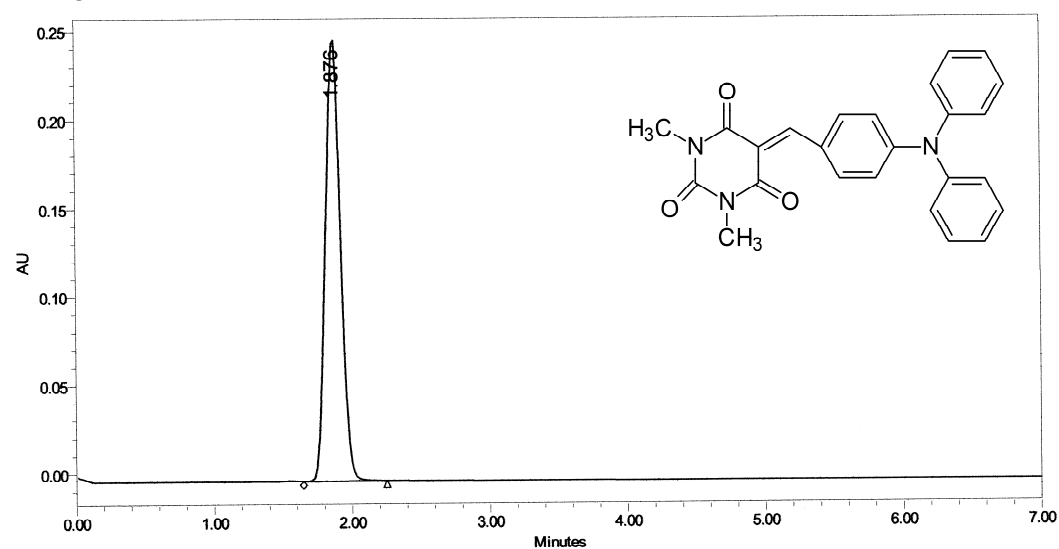
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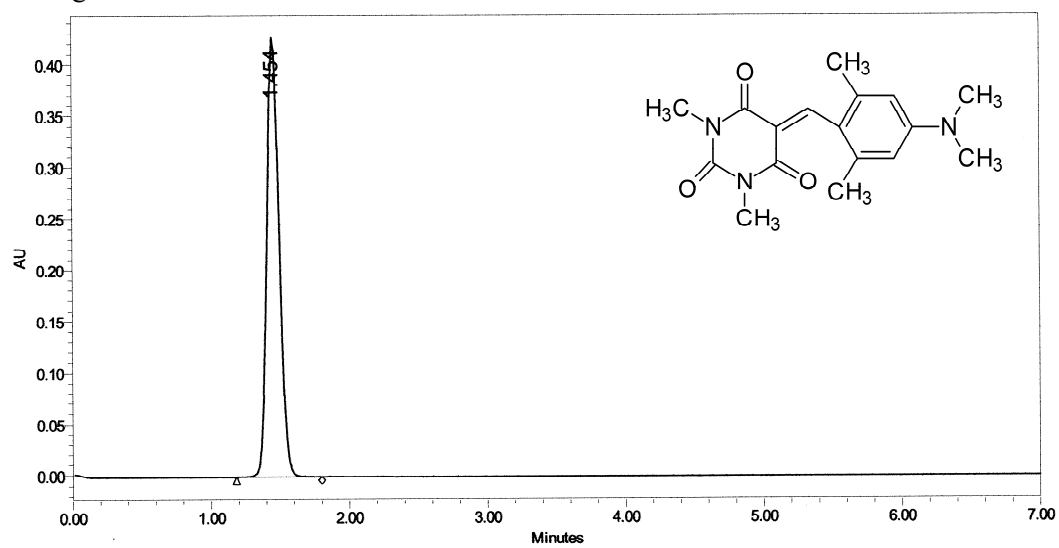
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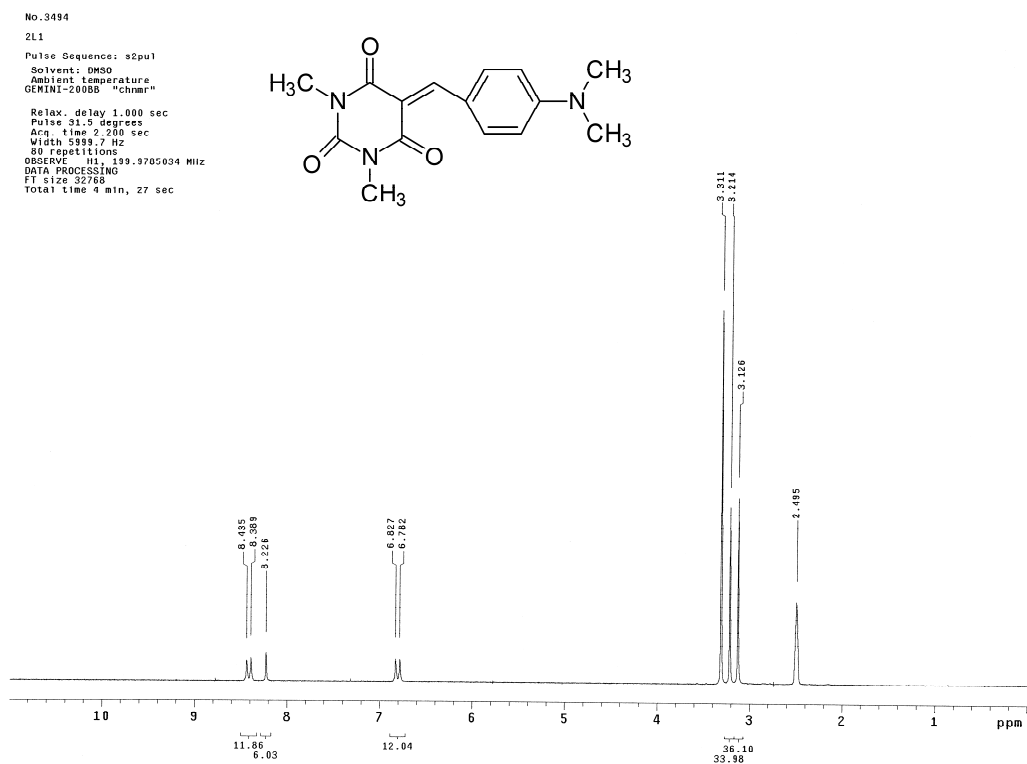
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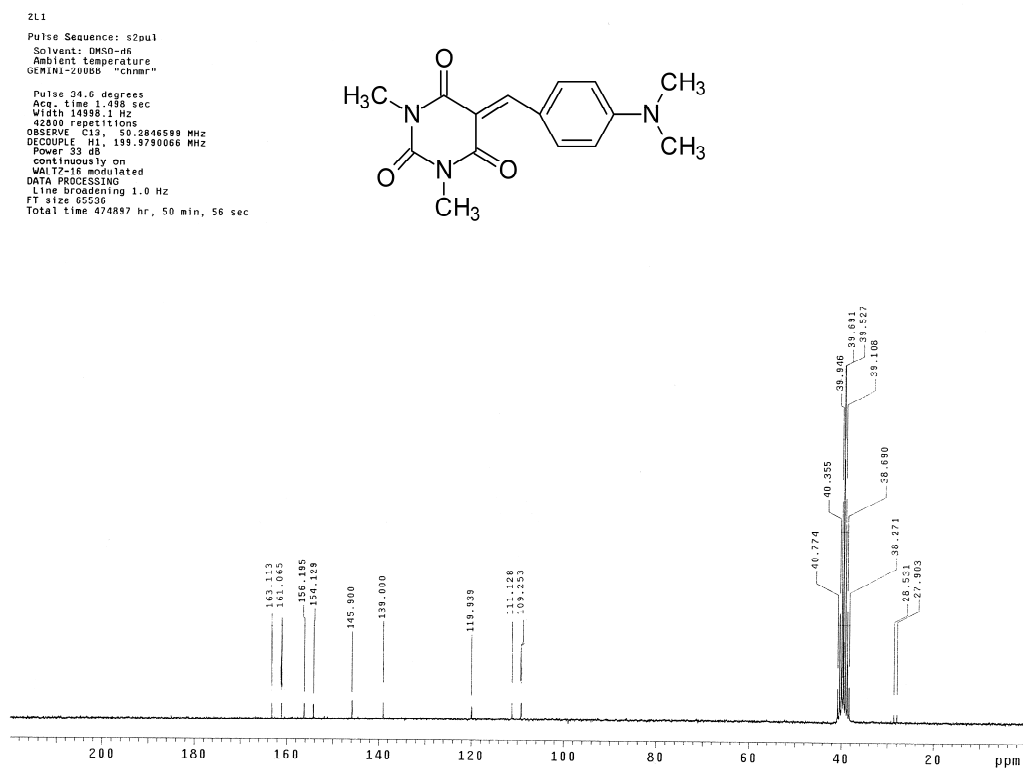
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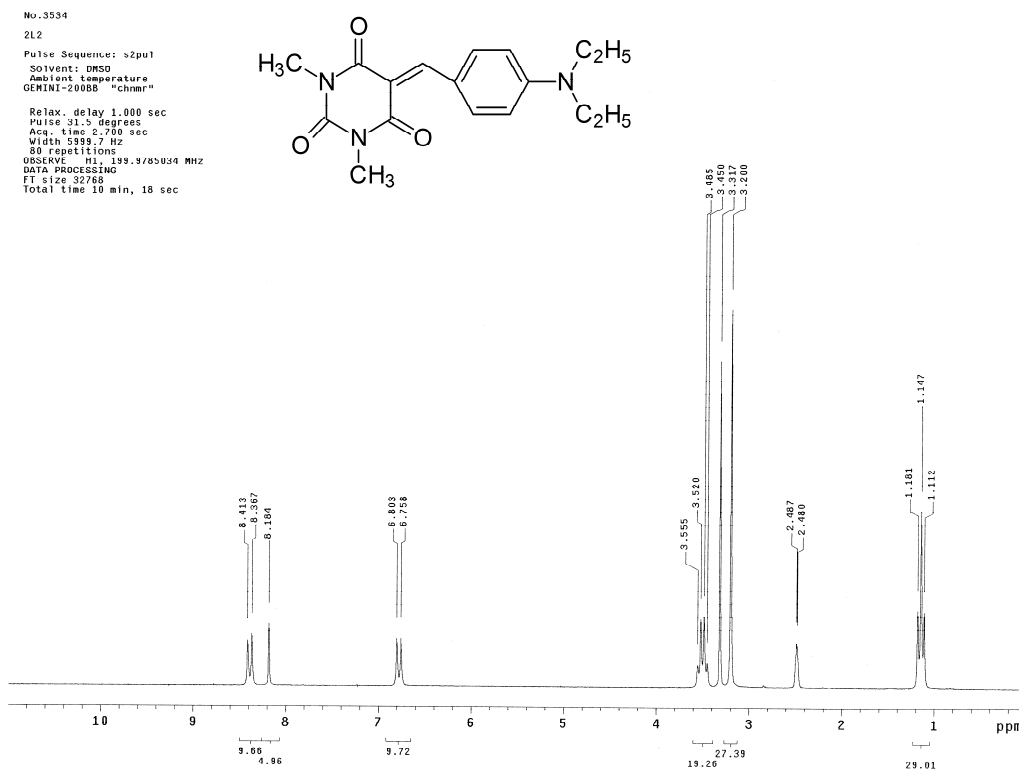
¹H NMR spectrum of **1**



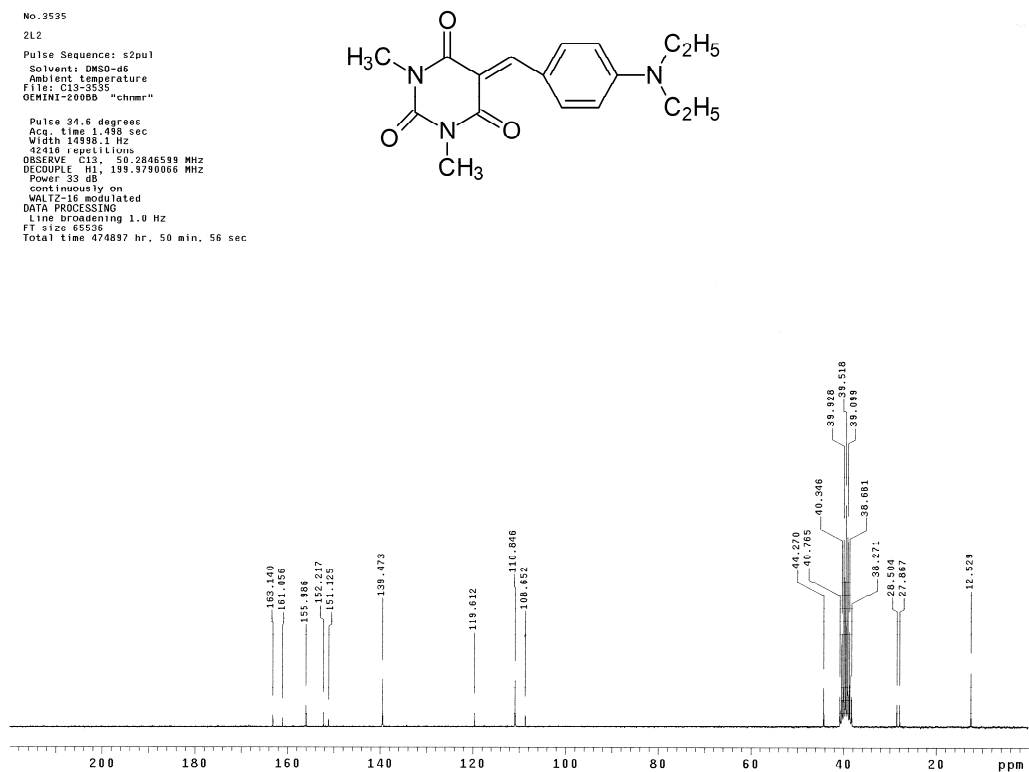
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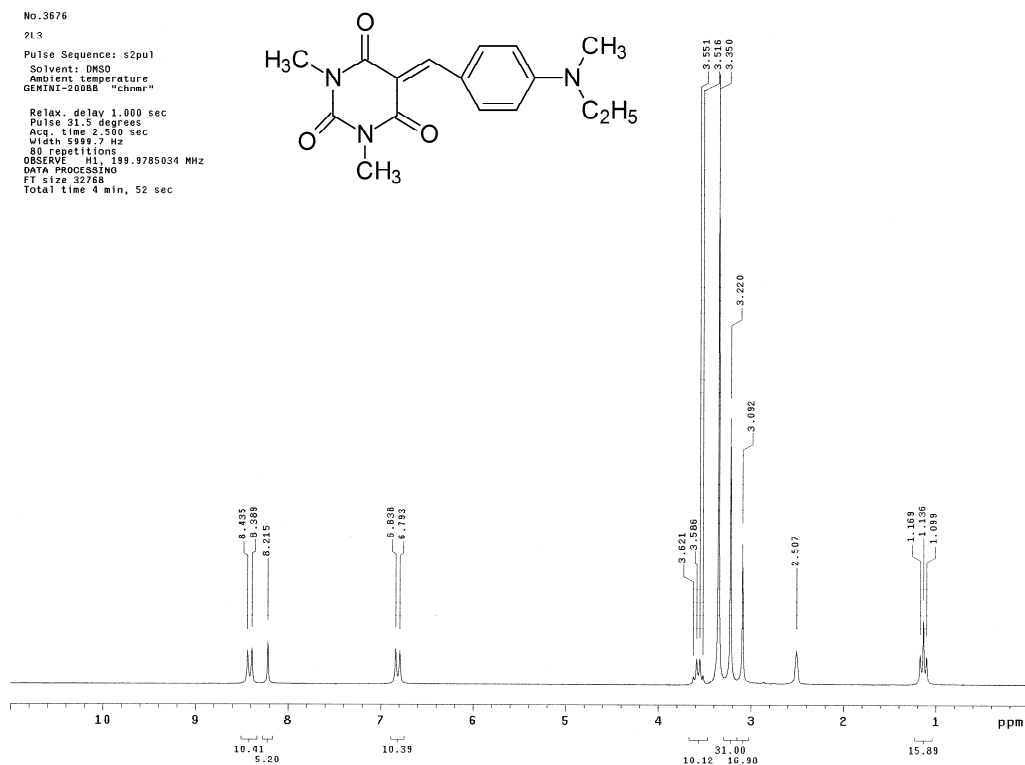
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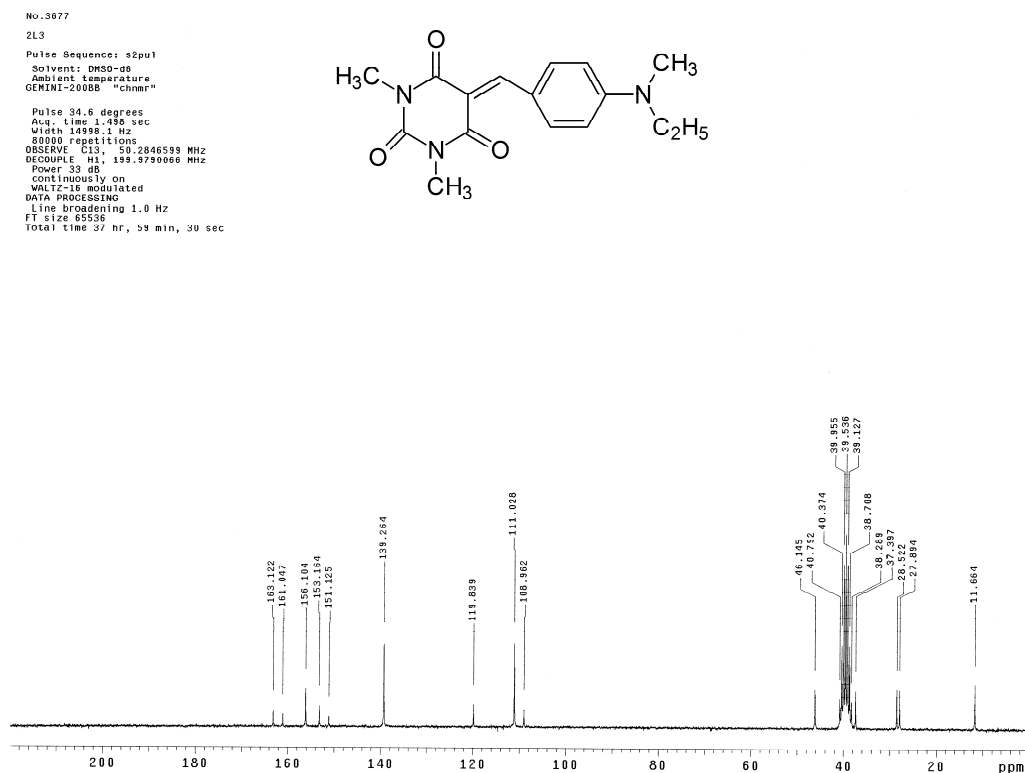
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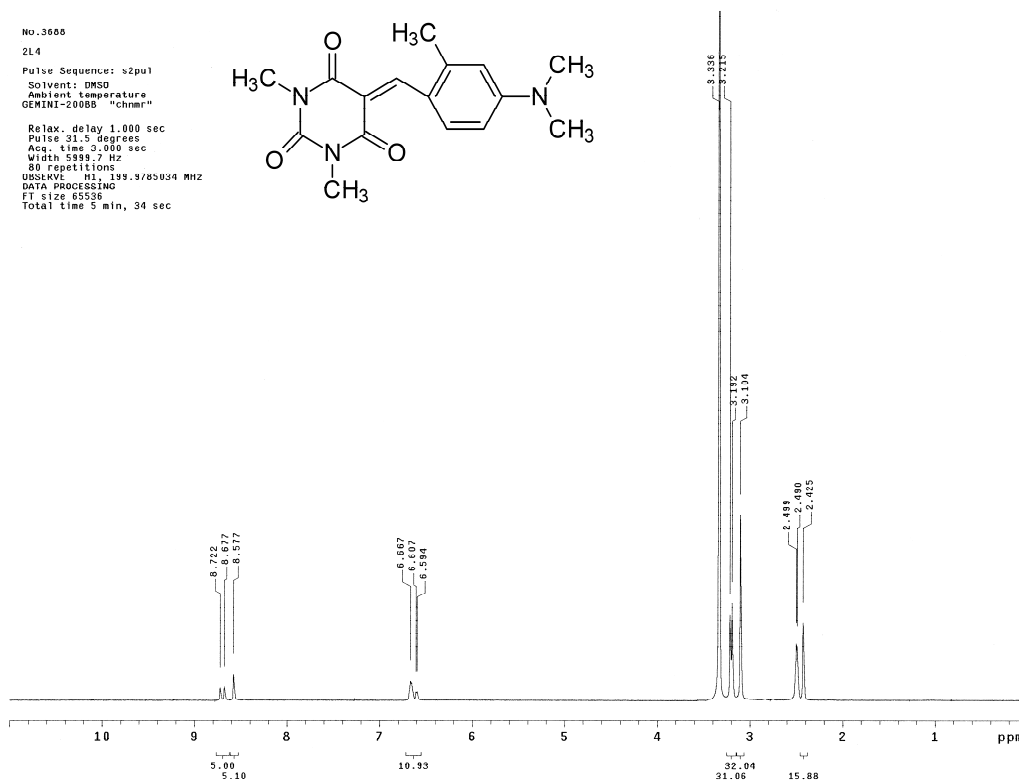
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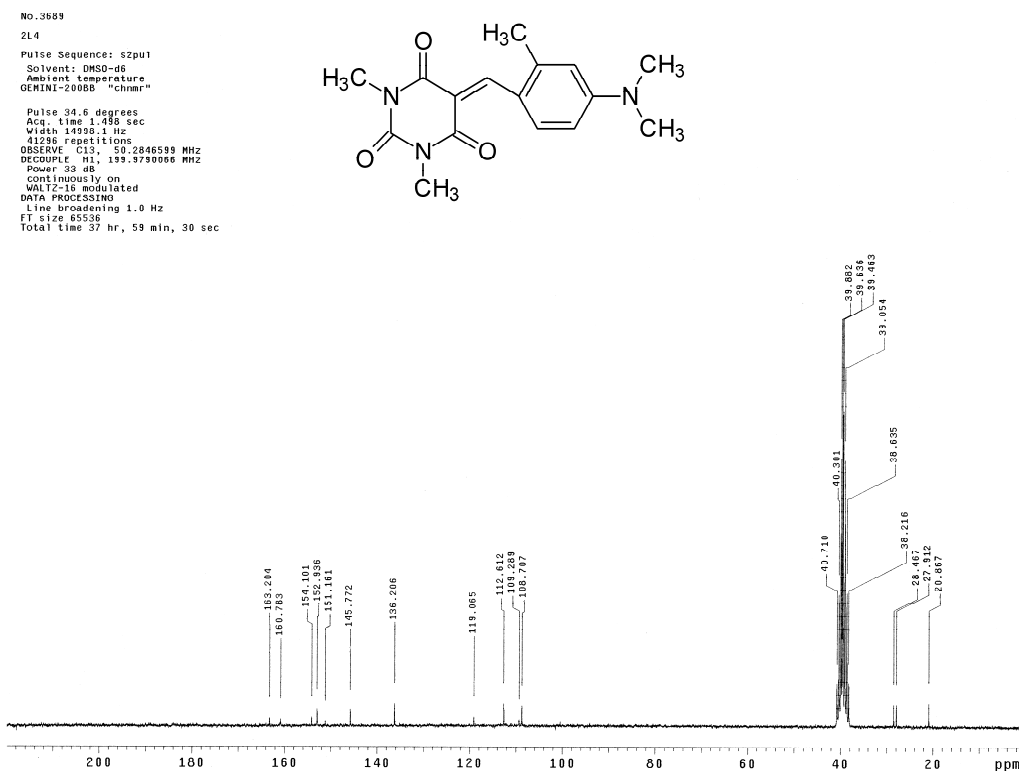
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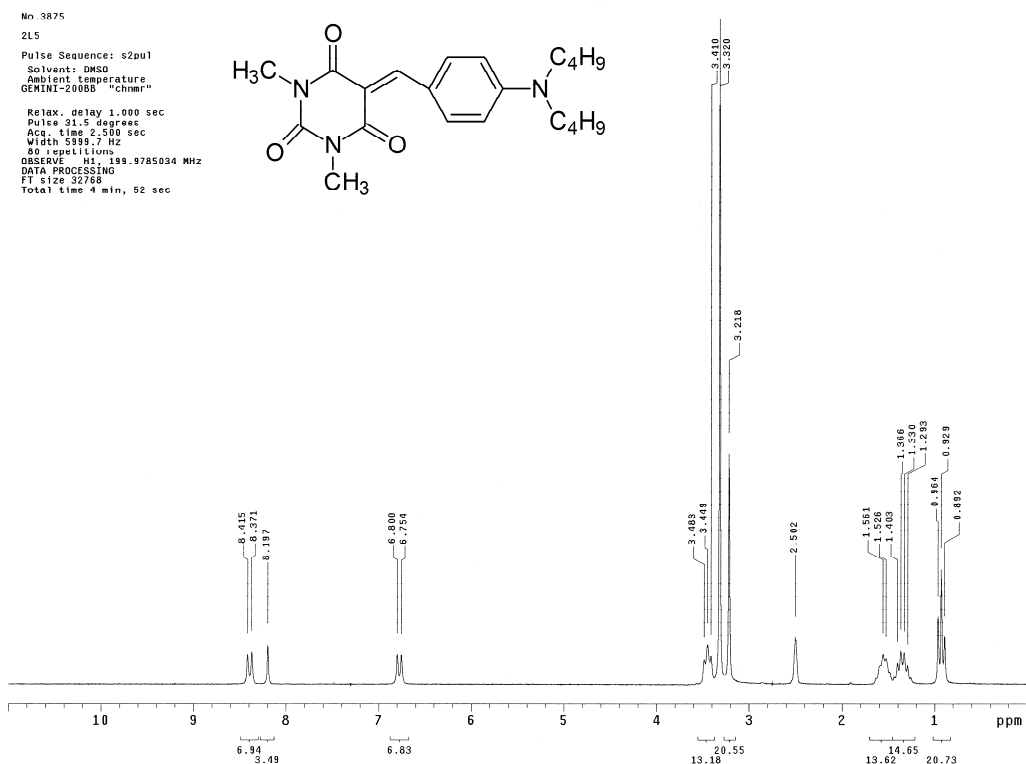
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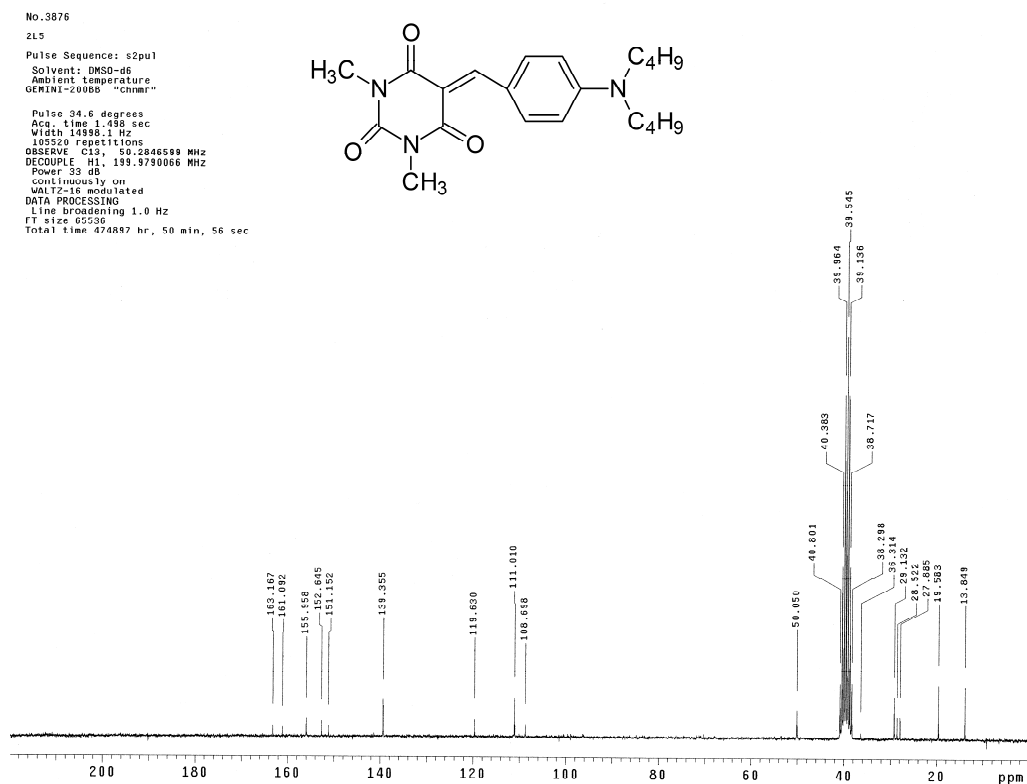
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¹H NMR spectrum of **5**

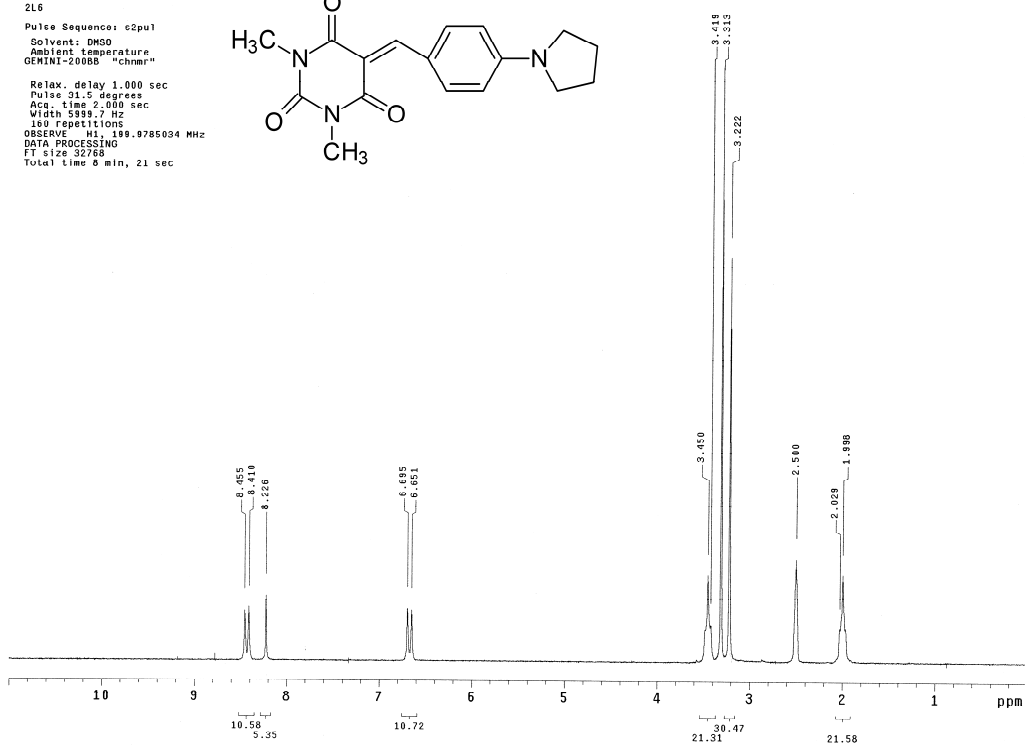
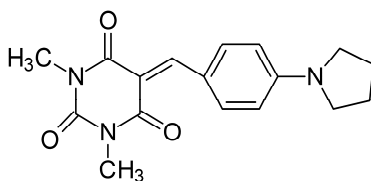


¹³C NMR spectrum of **5**



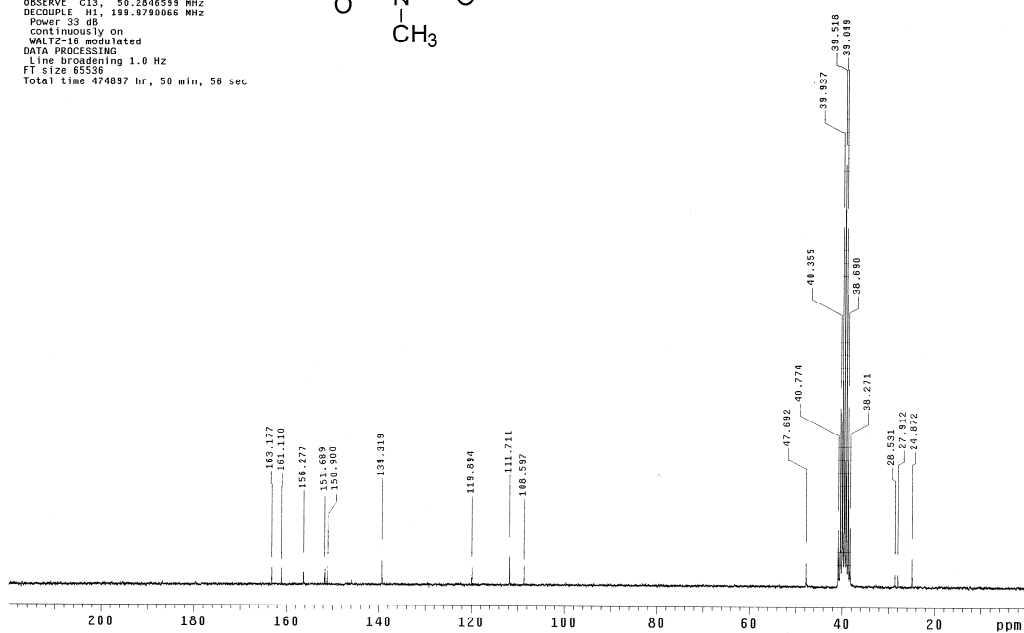
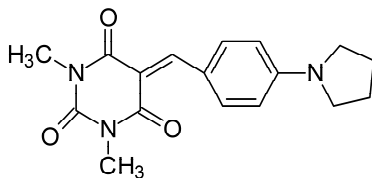
¹H NMR spectrum of 6

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Solvent: DMSO
Ambient temperature
GEMINI-200BS "chnmr"
Relax. delay 1.000 sec
Pulse 91.5 degrees
Acq. time 2.000 sec
Width 5999.7 Hz
100 repetitions
OBSERVE H1, 199.9785034 MHz
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Total time 8 min, 21 sec

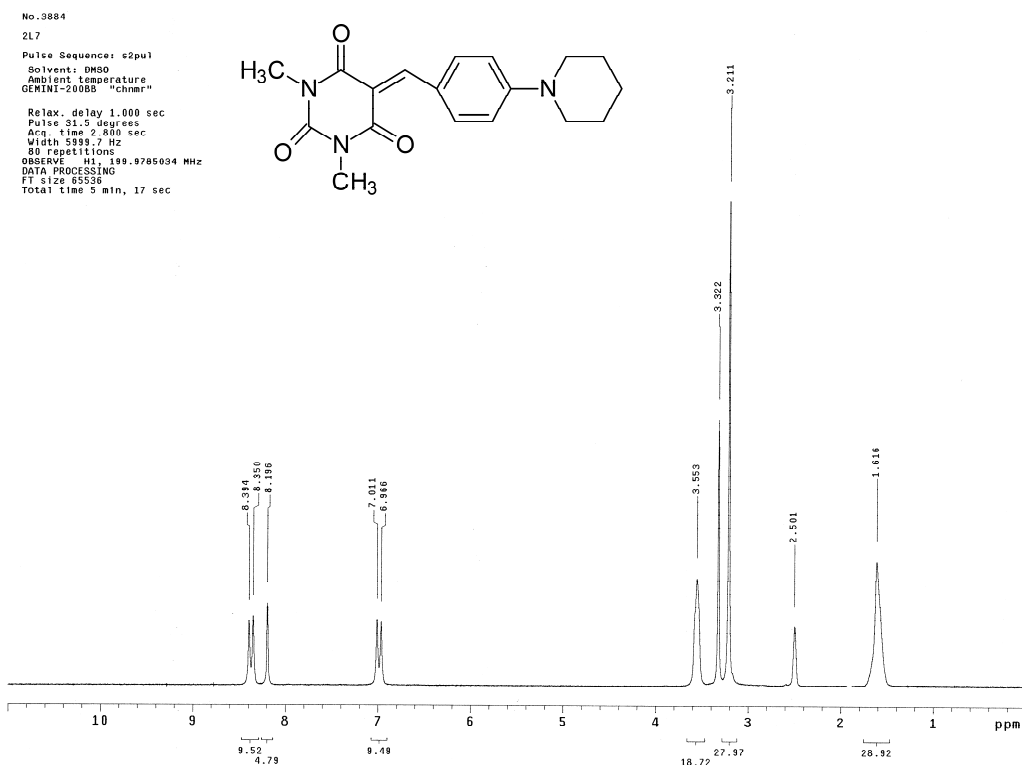


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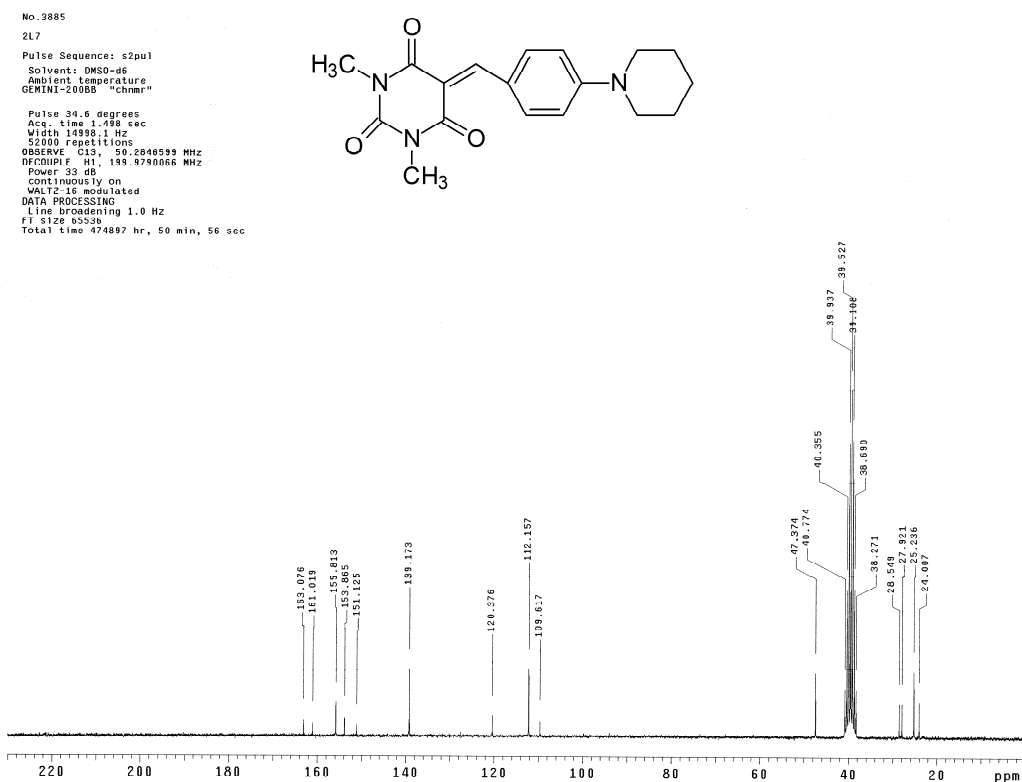
No. 9792
2L6
Pulse Sequence: s2pul
Solvent: DMSO-d6
Ambient temperature
GEMINI-200BS "chnmr"
Pulse 34.6 degrees
Acq. time 1.499 sec
Width 14998.1 Hz
99760 repetitions
OBSERVE C13, 99.2640599 MHz
DECOUPLE H1, 199.9780066 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 47:49:57 hr, 50 min, 58 sec



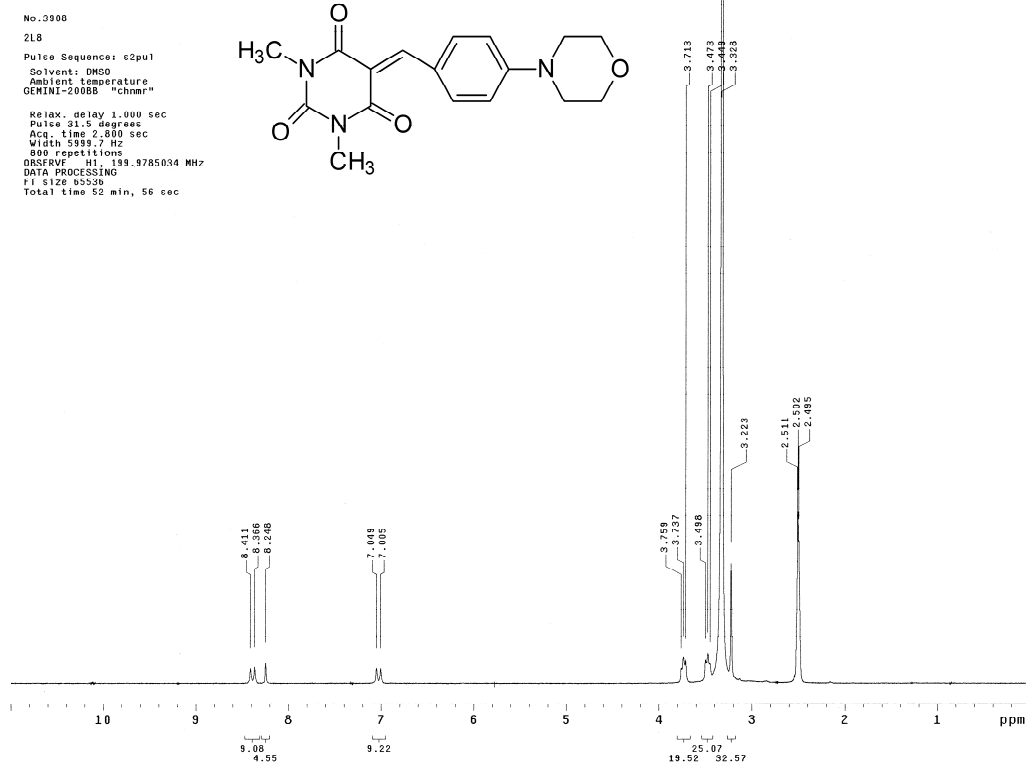
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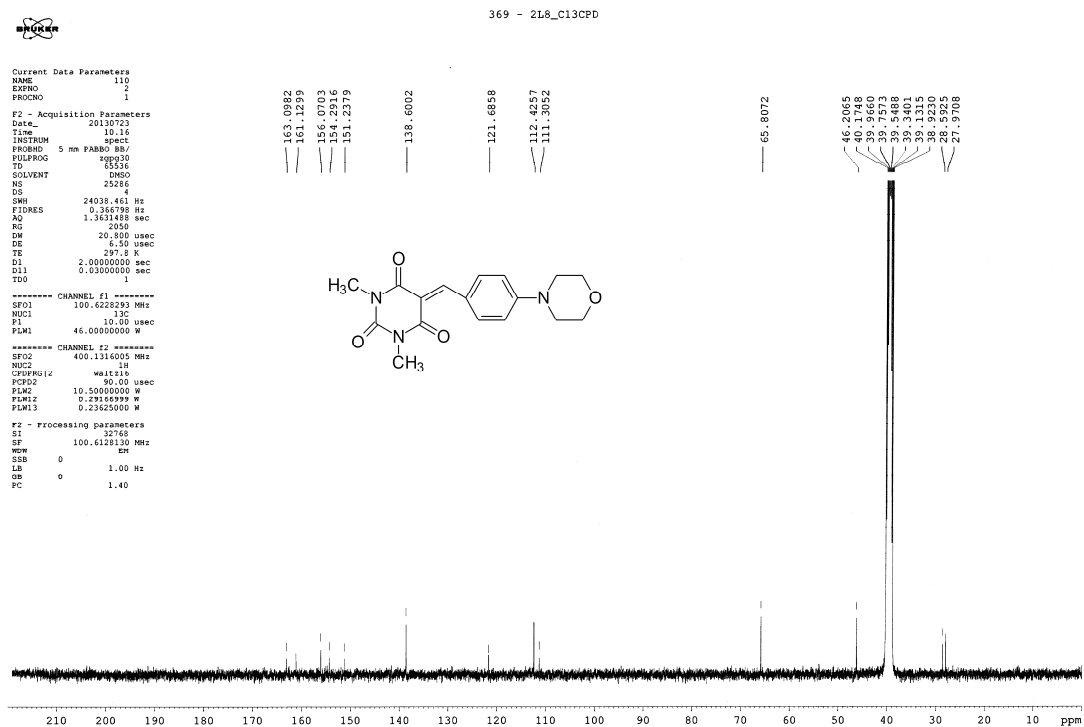
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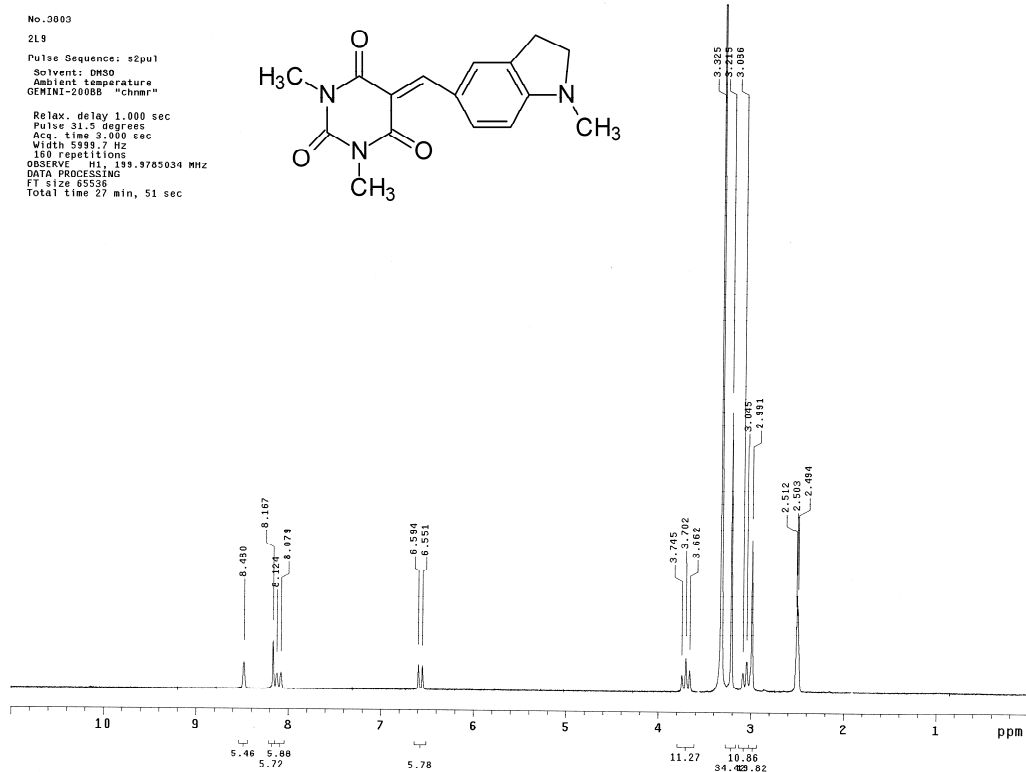
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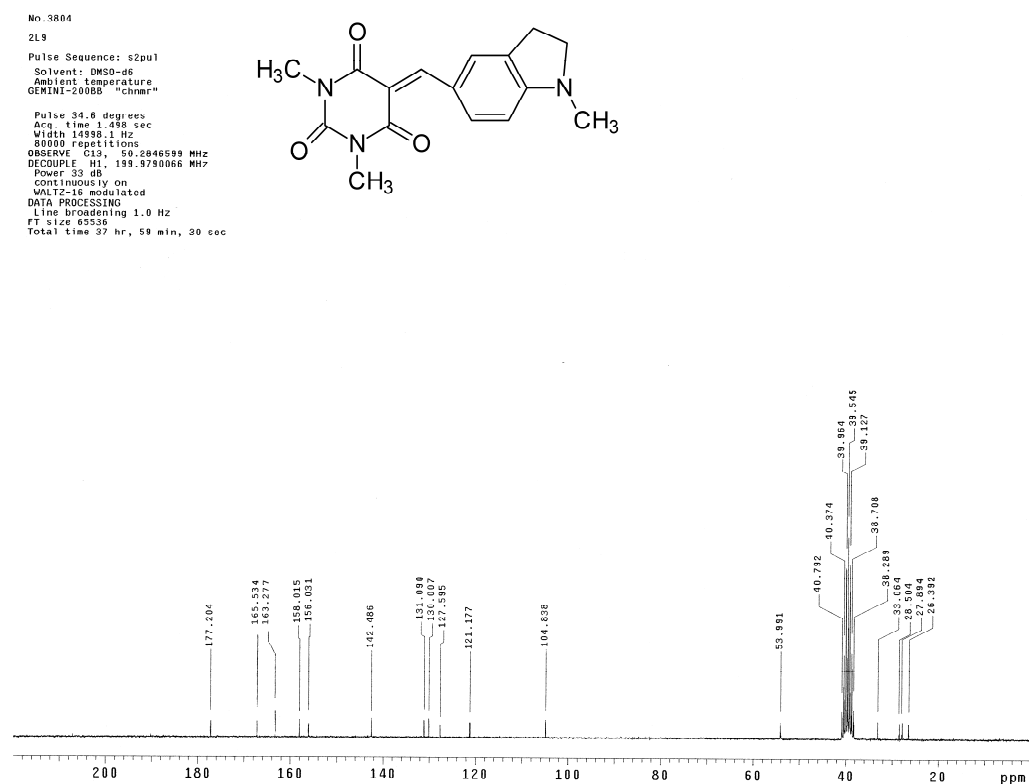
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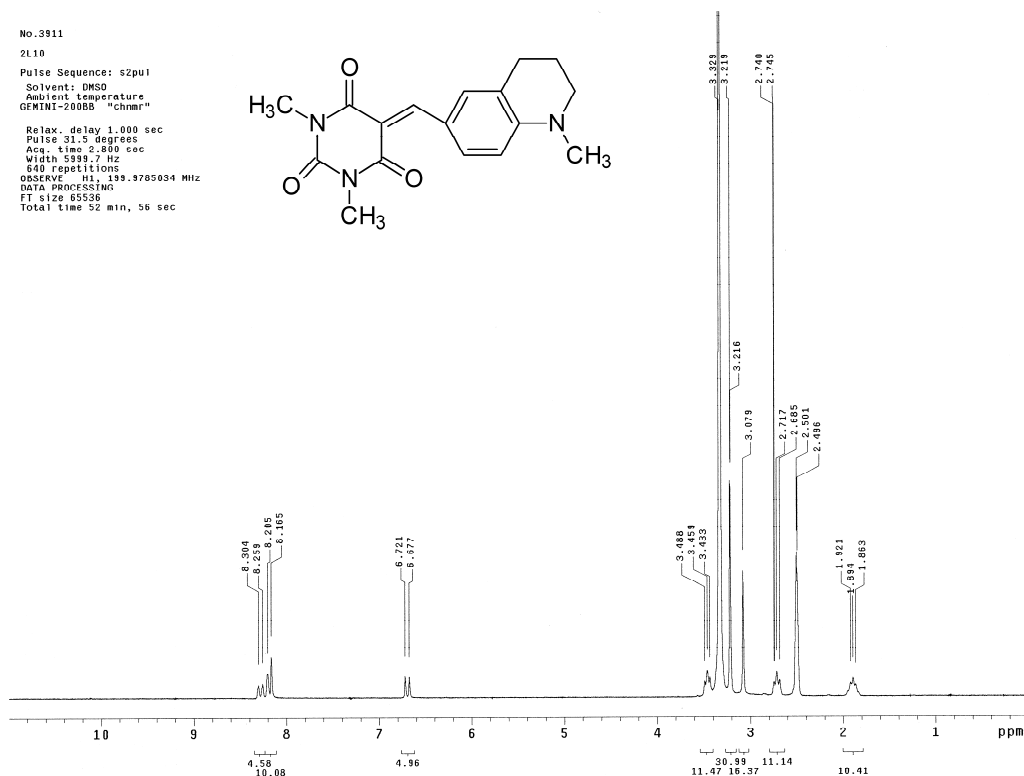
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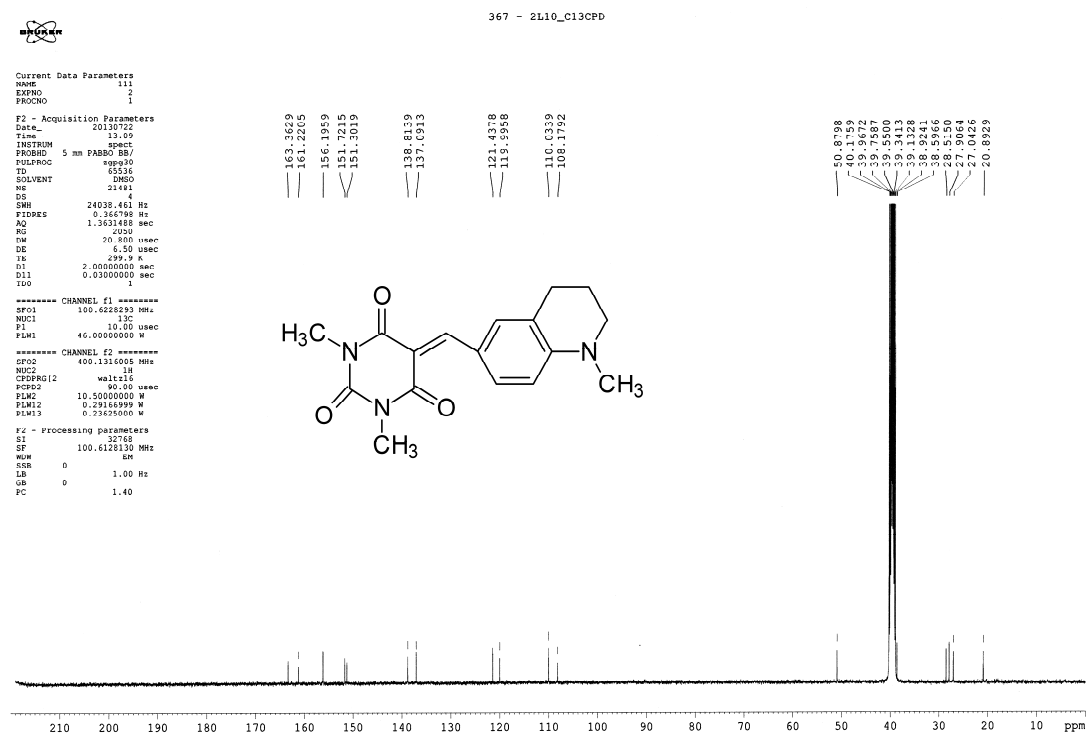
¹³C NMR spectrum of **9**



¹H NMR spectrum of 10

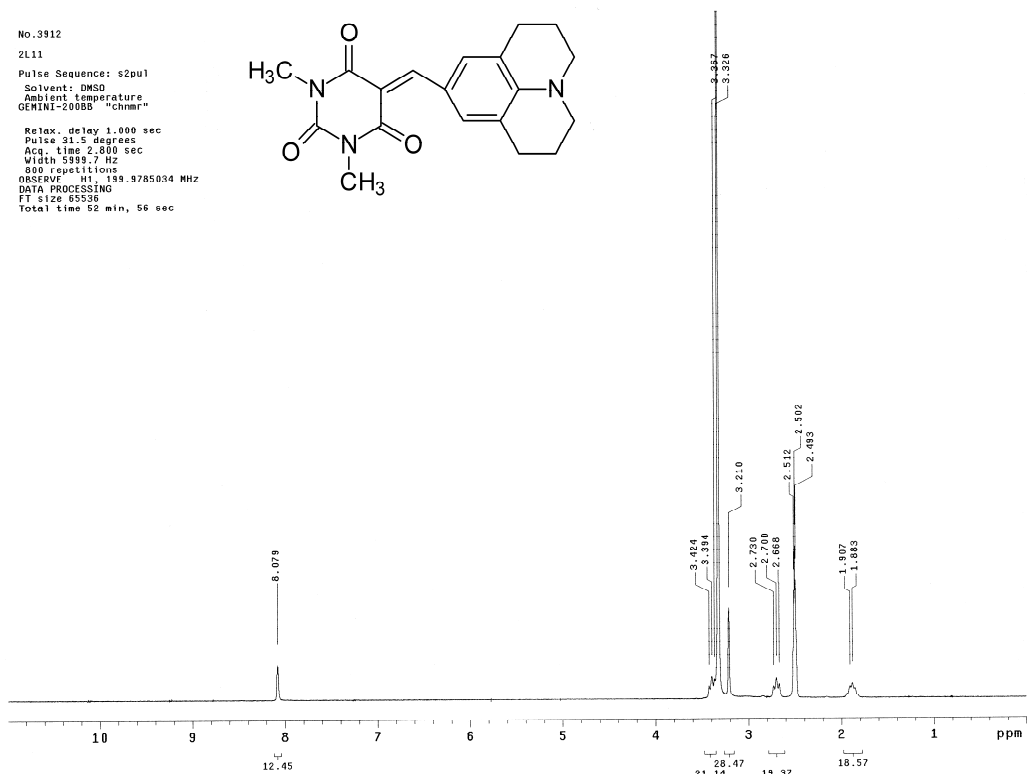
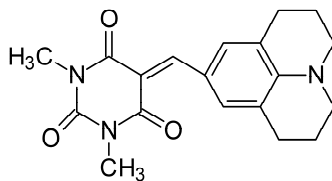


¹³C NMR spectrum of 10



¹H NMR spectrum of 11

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Solvent: DMSO
Ambient temperature
GEMINI-200BB "chmr"
Relax. delay 1.000 sec
Pulse 31.5 degrees
Acq. time 2.800 sec
Width 5999.7 Hz
800 repetitions
ORSERVF H1, 199.9785034 MHz
DATA PROCESSING
FT size 65536
Total time 52 min, 56 sec



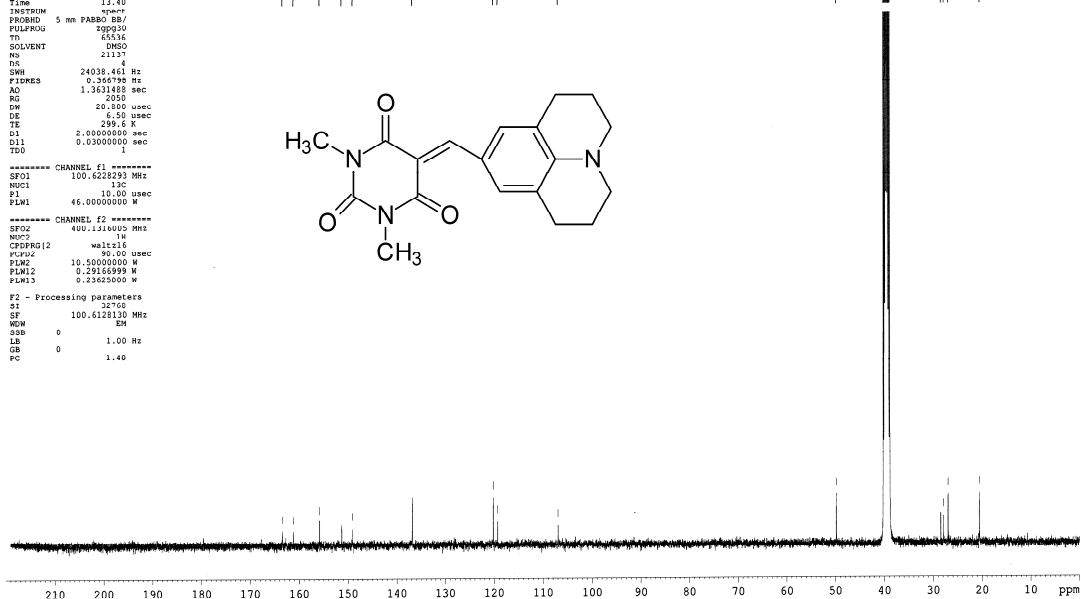
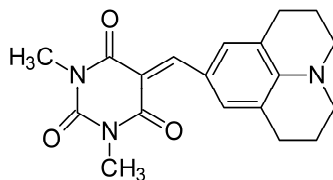
¹³C NMR spectrum of 11



380 - 2L11_C13CPD

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PROCNO 1
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INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
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DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 2050
DW 20.000 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
===== CHANNEL f1 =====
SFO1 100.628293 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W
===== CHANNEL f2 =====
SFO2 400.141800 MHz
NUC2 1H
CPCPG12 waltz16
PCPD2 90.00 usec
PLW2 10.50000000 W
PLW12 0.29166999 W
PLW13 0.23625000 W
F2 - Processing parameters
SI 32768
SF 100.6128130 MHz
WDW EM
SSB 0
LA 1.00 Hz
GB 0
PC 1.40

163.4571
161.2205
155.8661
151.3331
145.0658
136.8464
120.2230
117.3384
106.9651
19.8292
40.1768
39.7597
39.5509
39.3423
39.1229
38.9249
28.4801
27.8882
26.9755
20.5496



¹H NMR spectrum of 12

No. 2909

2L12

Pulse Sequence: s2pu1

Solvent: DMSO

Ambient temperature

GEVINI-20085 "chmr"

Relax. delay 1.000 sec

Pulse 31.5 degrees

Acq. time 2.500 sec

Width 5899.7 Hz

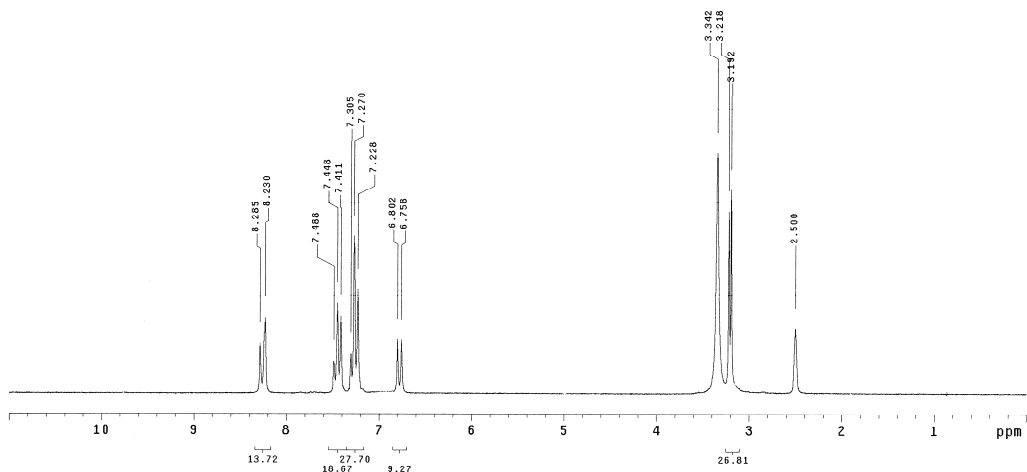
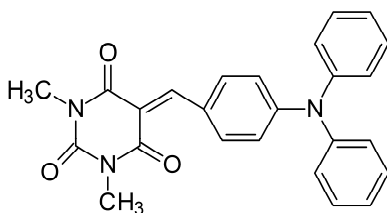
00 repetitions

OBSERVE H1, 199.9785034 MHz

DATA PROCESSING

FT size 32768

Total time 4 min, 52 sec



¹³C NMR spectrum of 12

No. 0910

2L12

Pulse Sequence: s2pu1

Solvent: DMSO-d6

Ambient temperature

GEVINI-20085 "chmr"

Pulse 34.6 degrees

Acq. time 1.490 sec

Width 14998.1 Hz

105800 repetitions

OBSERVE C13, 50.2846599 MHz

DECOUPLE H1, 199.9780066 MHz

Power 33 dB

continuously on

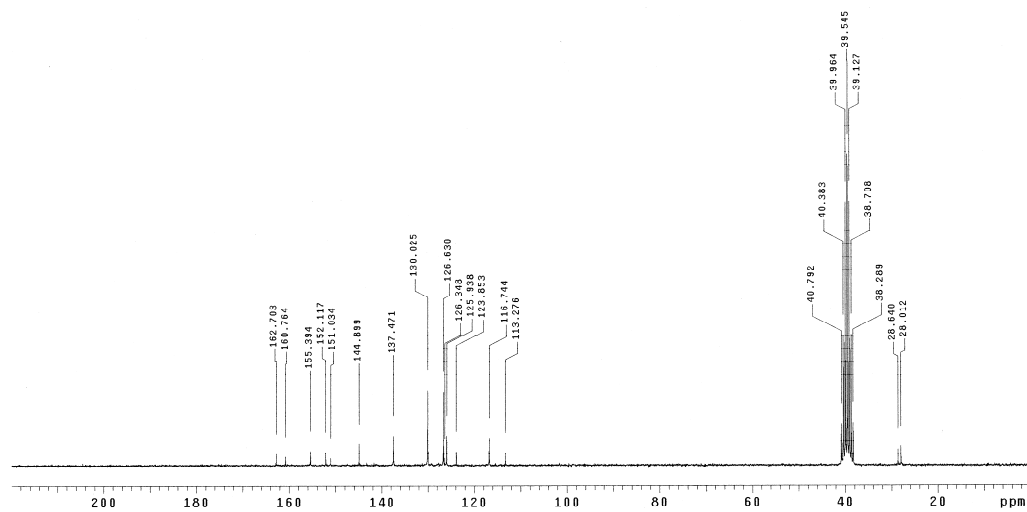
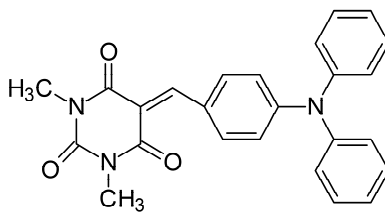
WALTZ-16 modulated

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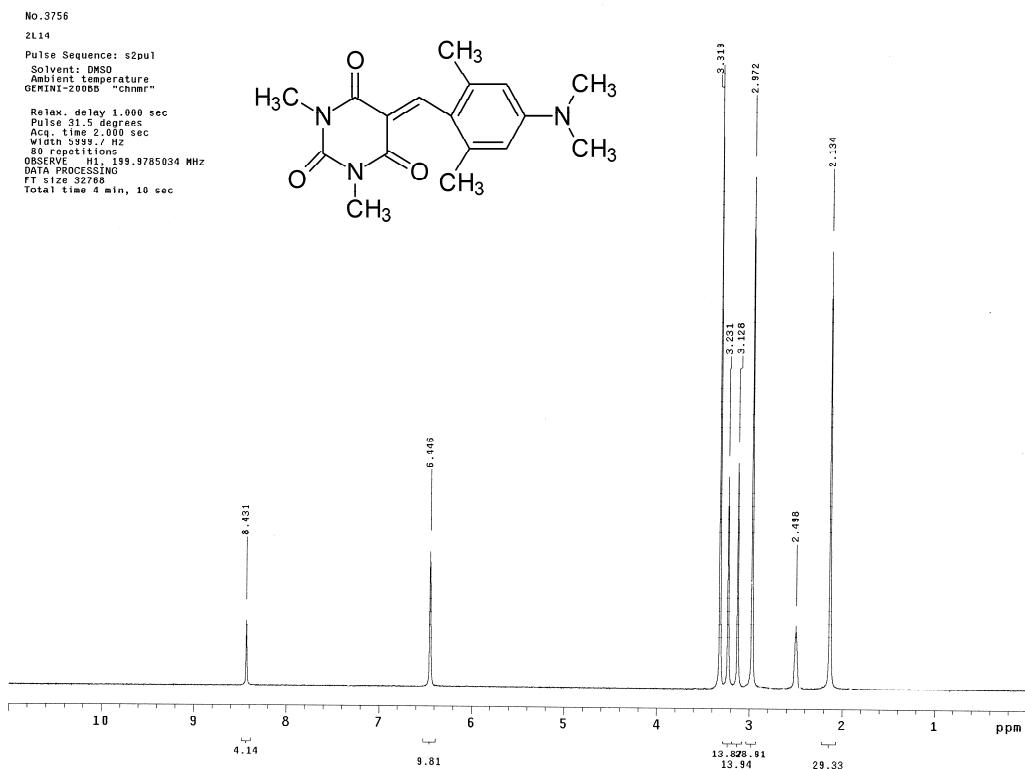
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FT size 65536

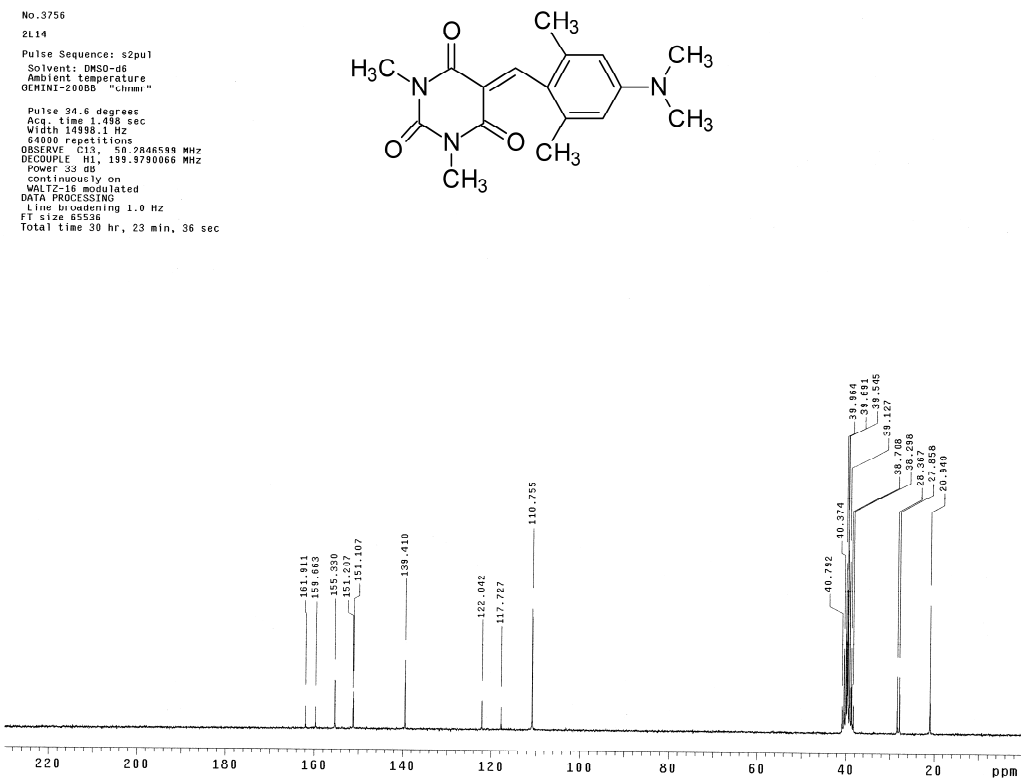
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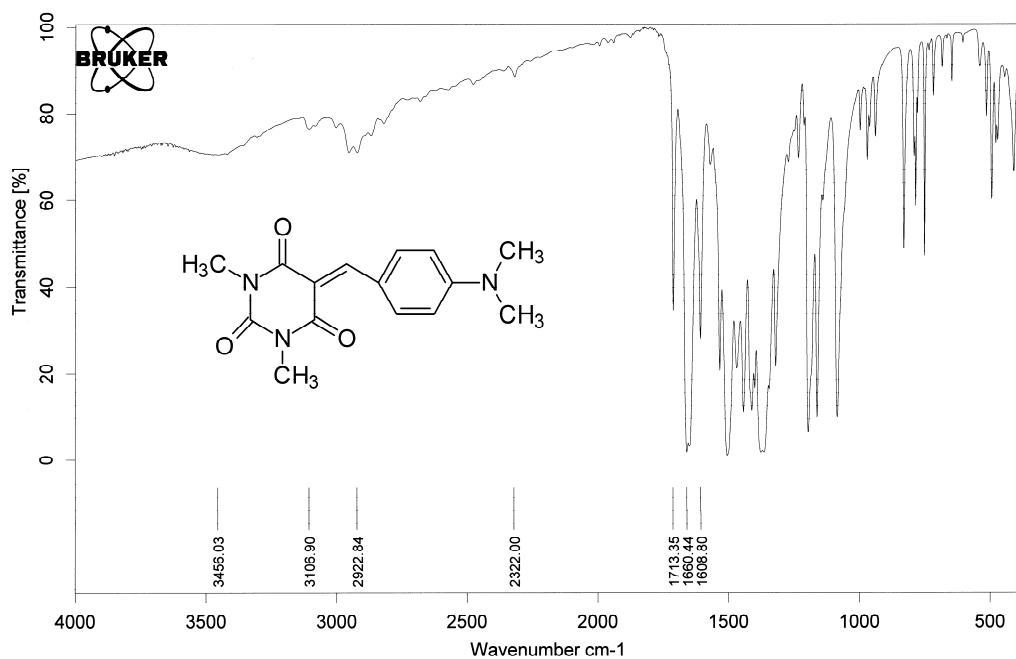
¹H NMR spectrum of 13



¹³C NMR spectrum of 13



IR spectrum of 1

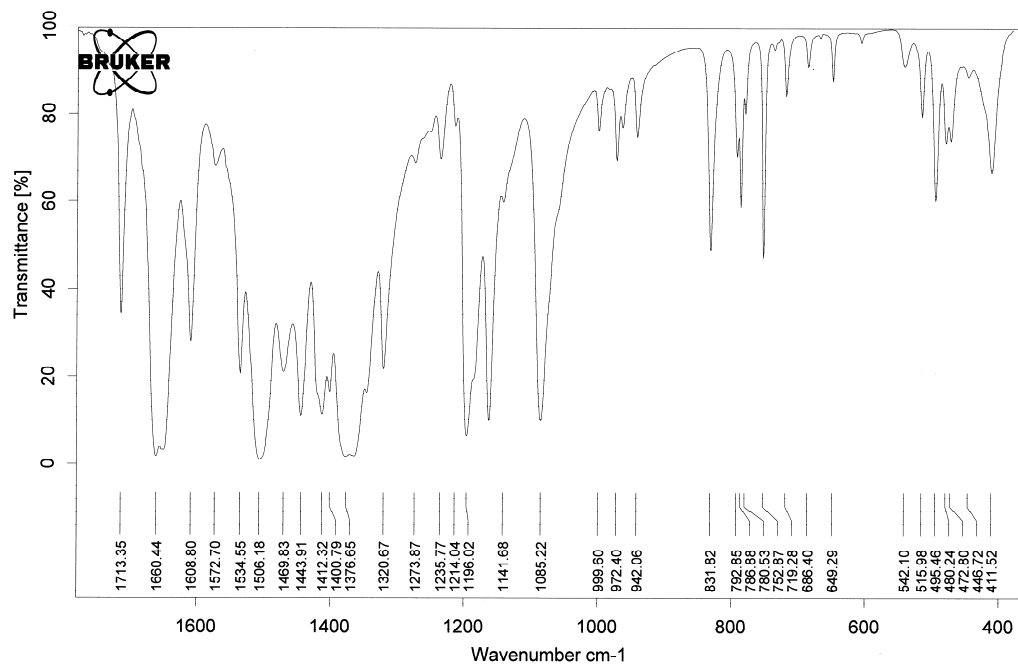


C:\Pomiary\bjed\bjed002.1 2L1 proszek w KBr

18/05/2012

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Enlarged spectrum in the range of 1600 - 400 cm⁻¹

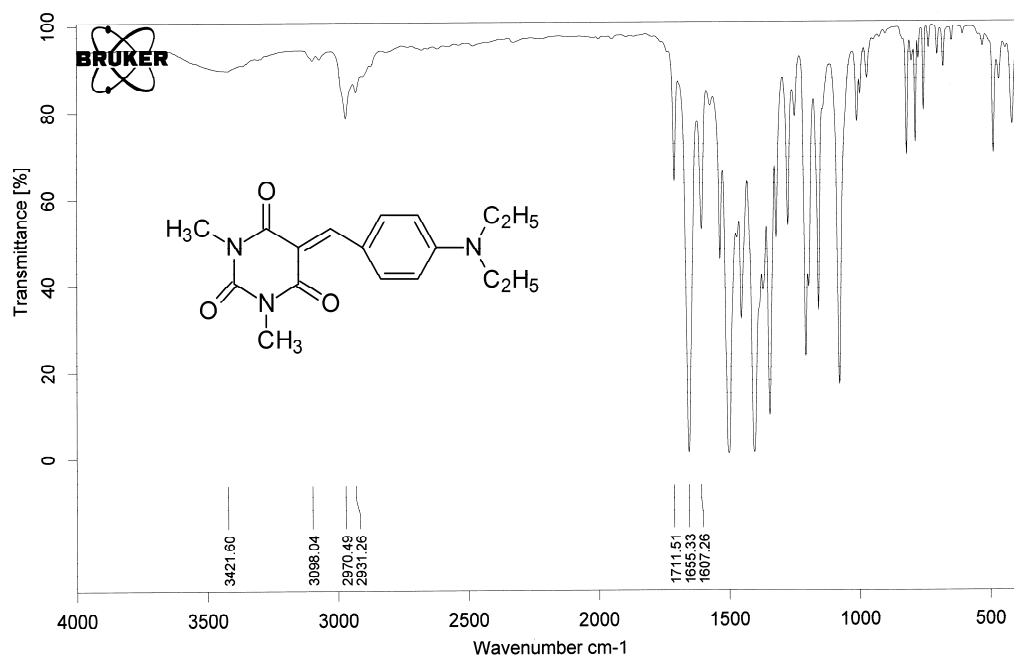


C:\Pomiary\bjed\bjed002.1 2L1 proszek w KBr

18/05/2012

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IR spectrum of 2

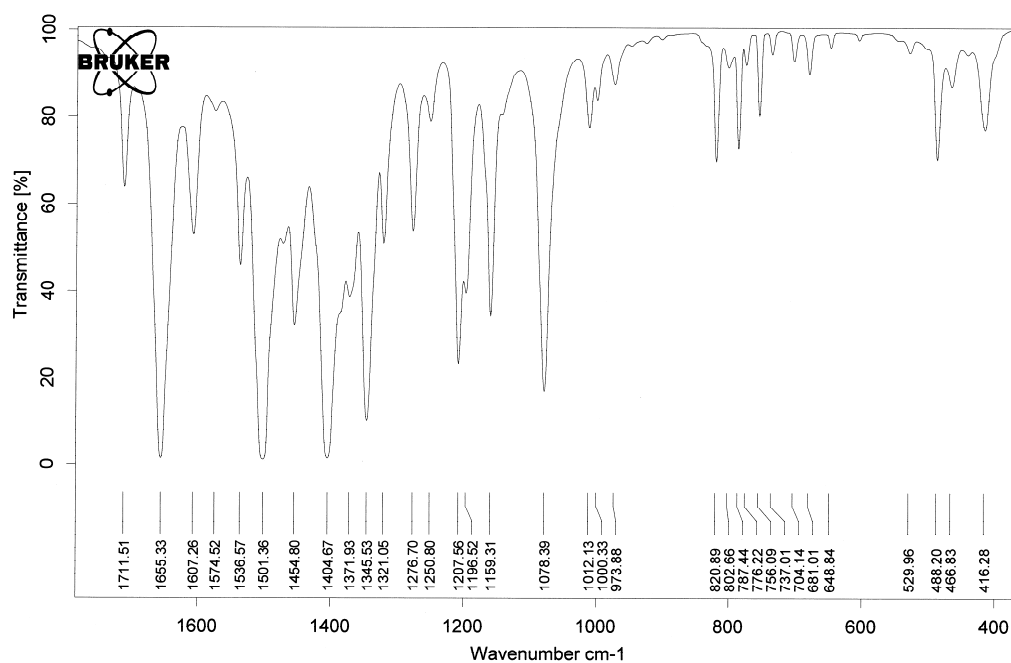


C:\Pomiary\bjed\bjed011.1 2L2 | Av. of 2 proszek w KBr

01/06/2012

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Enlarged spectrum in the range of 1600 - 400 cm^{-1}

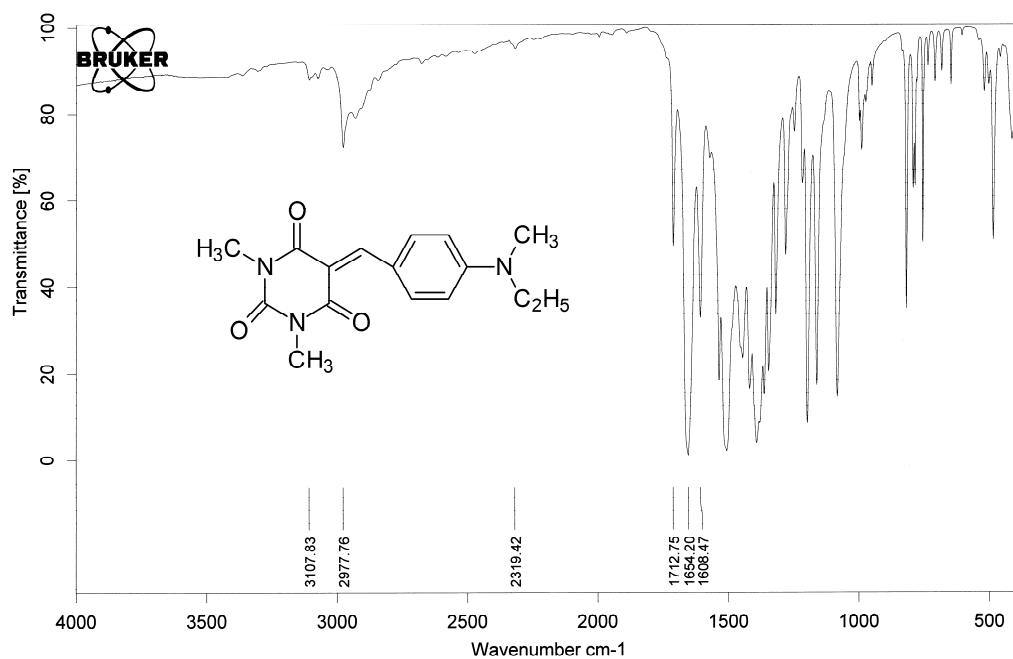


C:\Pomiary\bjed\bjed011.1 2L2 | Av. of 2 proszek w KBr

01/06/2012

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IR spectrum of 3

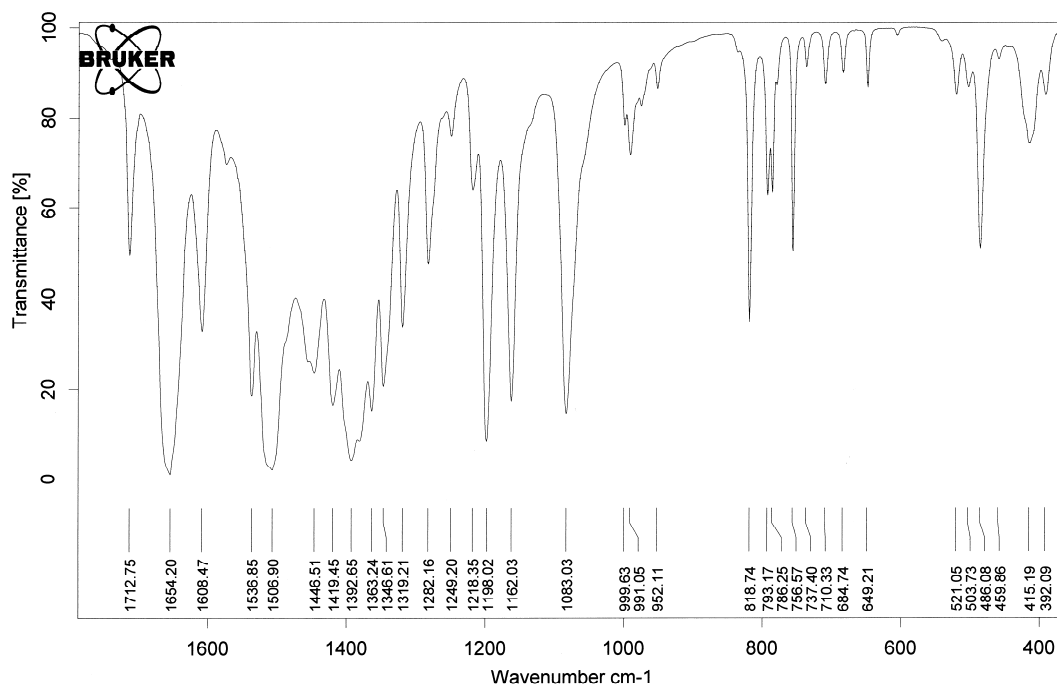


C:\Pomiary\bjed\bjed012.1 2L3 proszek w KBr

01/06/2012

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Enlarged spectrum in the range of 1600 - 400 cm⁻¹

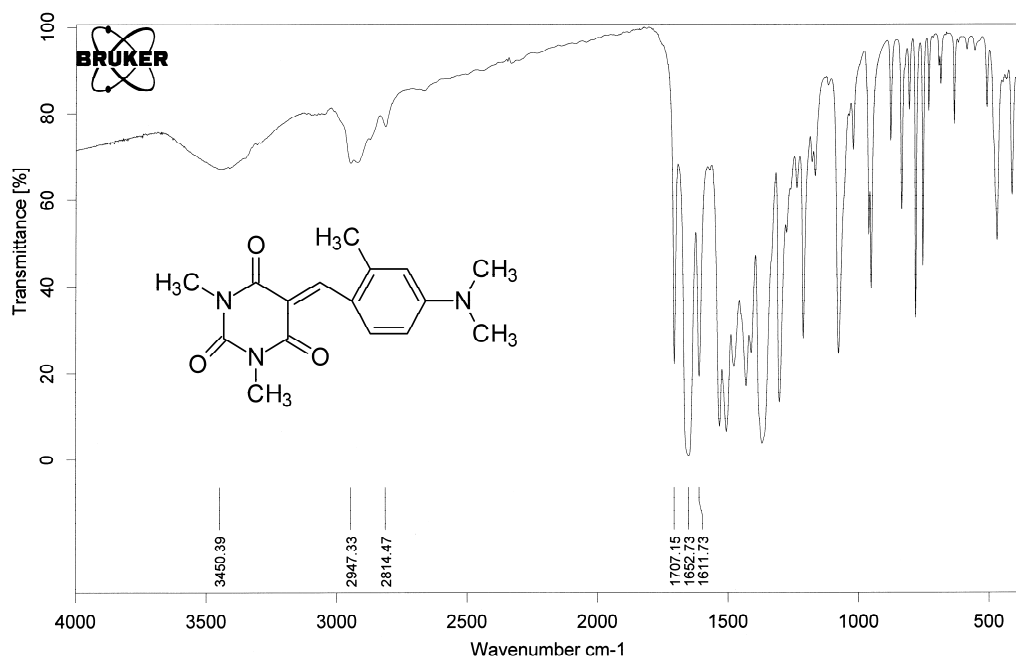


C:\Pomiary\bjed\bjed012.1 2L3 proszek w KBr

01/06/2012

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IR spectrum of 4

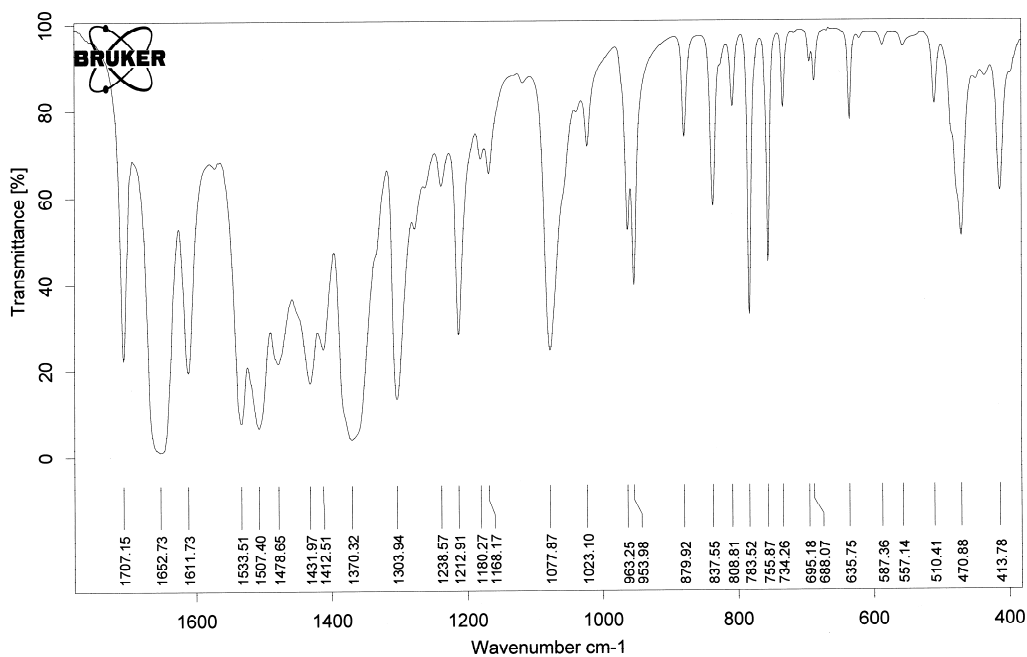


C:\Pomiary\bjed\bjed013.1 2L4 proszek w KBr

01/06/2012

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Enlarged spectrum in the range of 1600 - 400 cm⁻¹

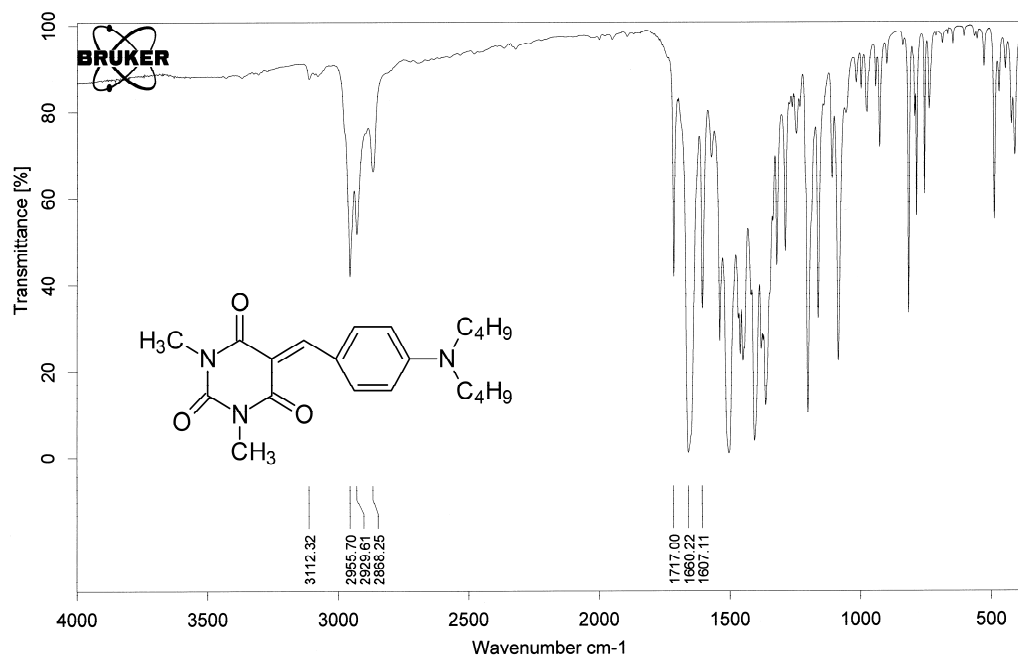


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01/06/2012

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IR spectrum of 5

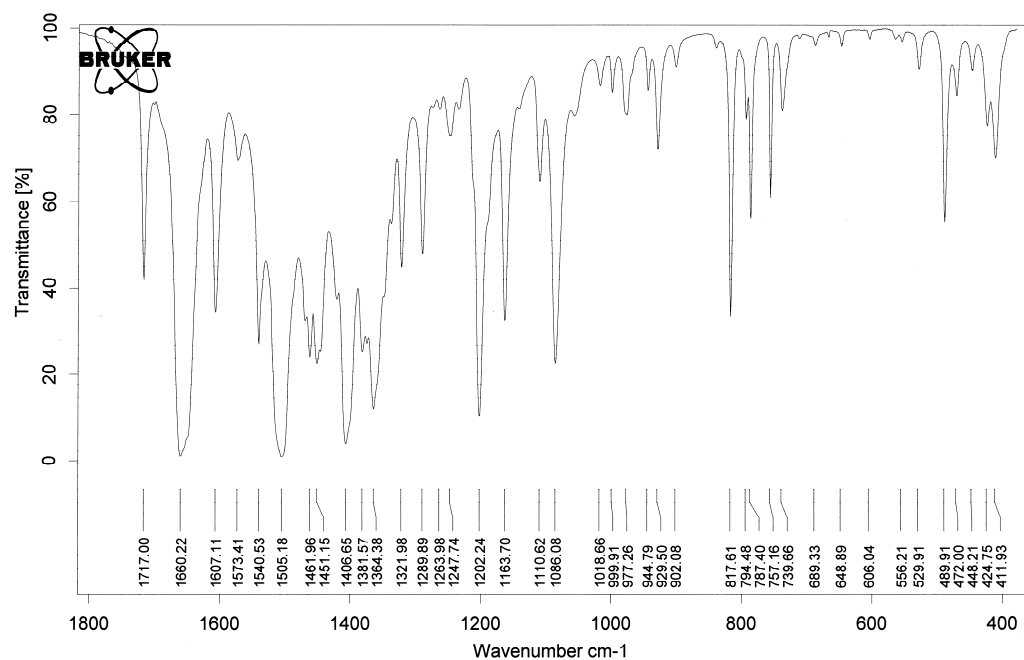


C:\Pomiary\bjed\bjed006.1 215 proszek w KBr

21/05/2012

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Enlarged spectrum in the range of 1600 - 400 cm⁻¹

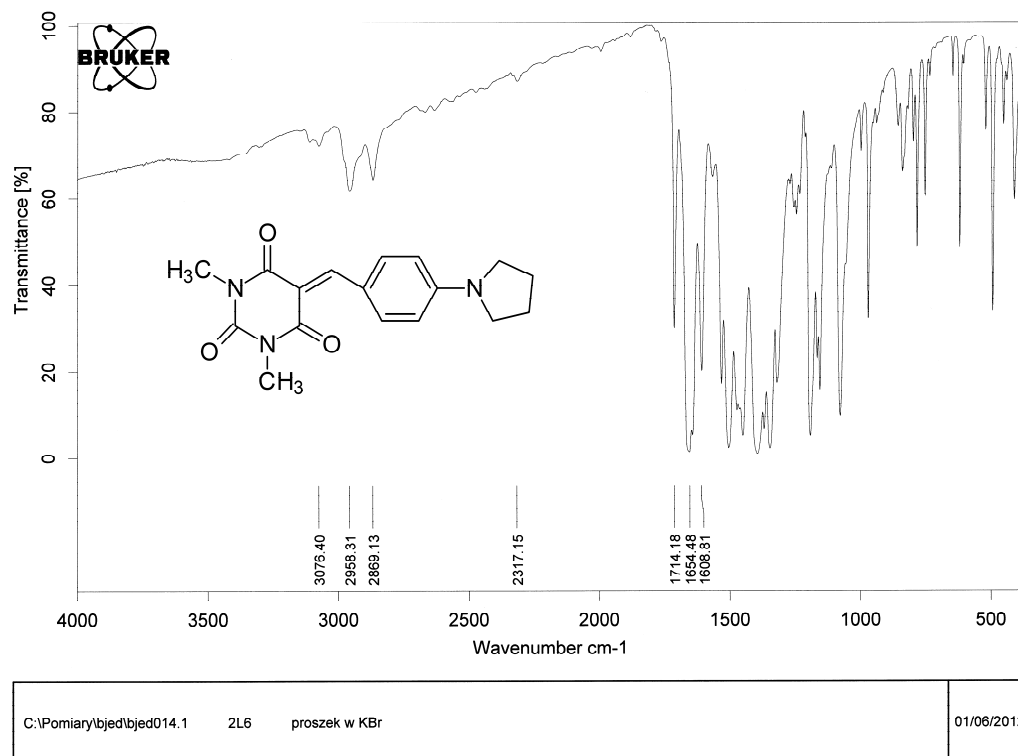


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21/05/2012

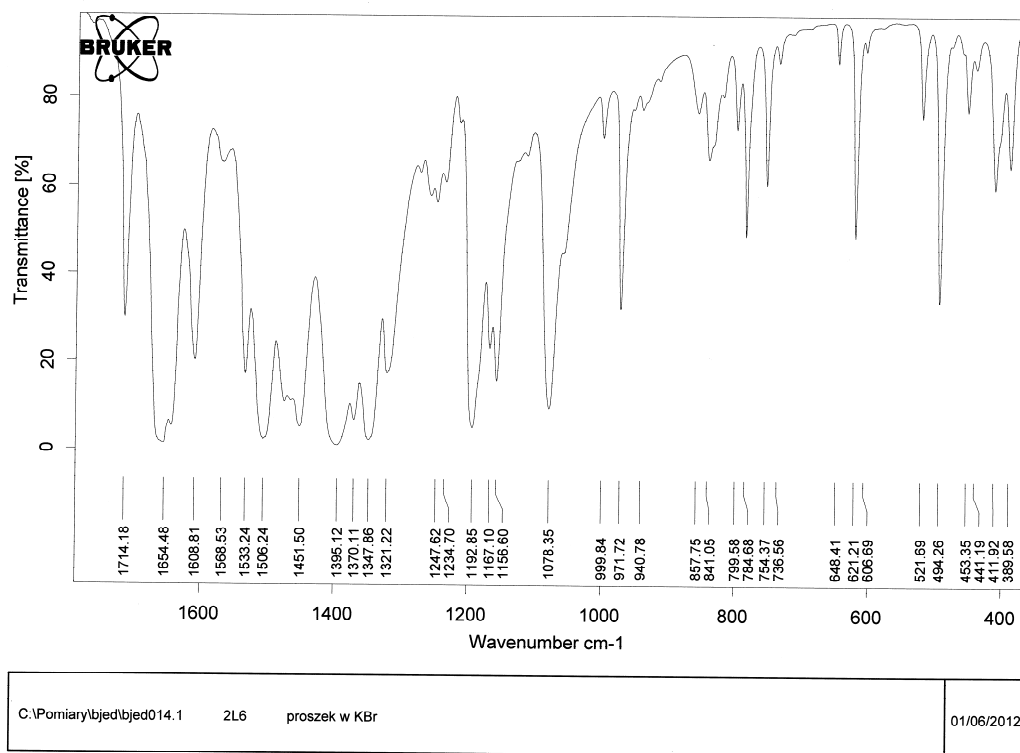
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IR spectrum of 6



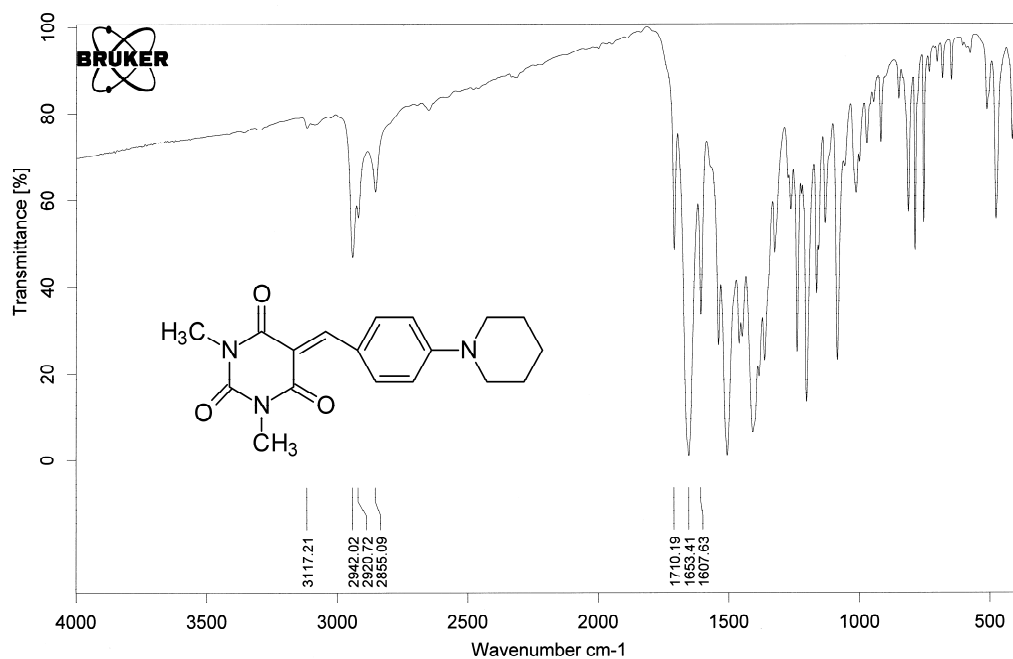
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Enlarged spectrum in the range of 1600 - 400 cm⁻¹



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IR spectrum of 7



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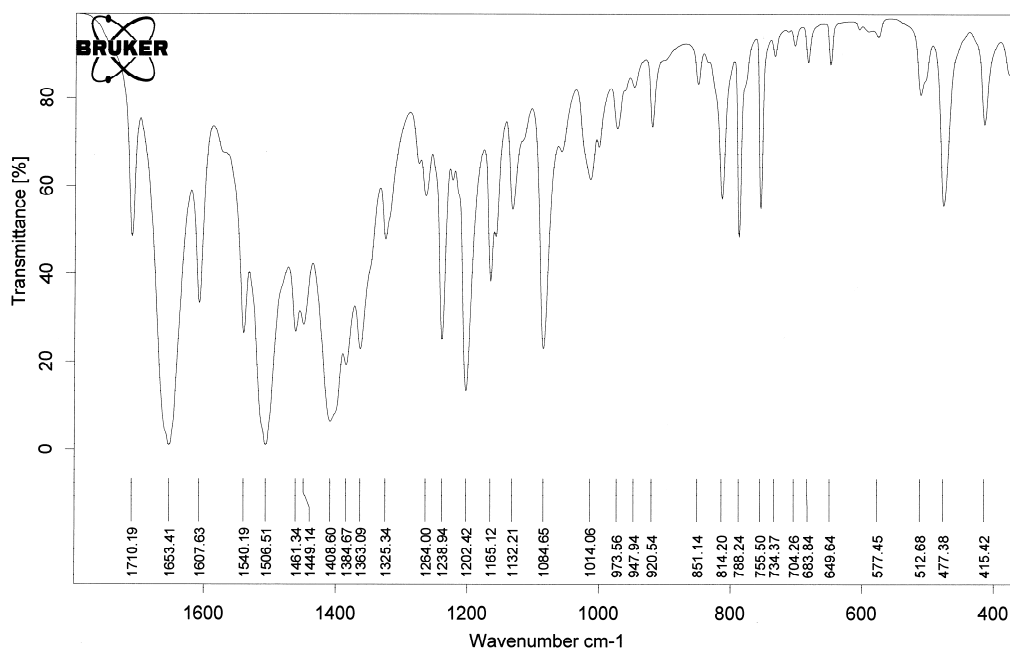
217

proszek w KBr

21/05/2012

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Enlarged spectrum in the range of 1600 - 400 cm⁻¹



C:\Pomiary\bjed\bjed007.1

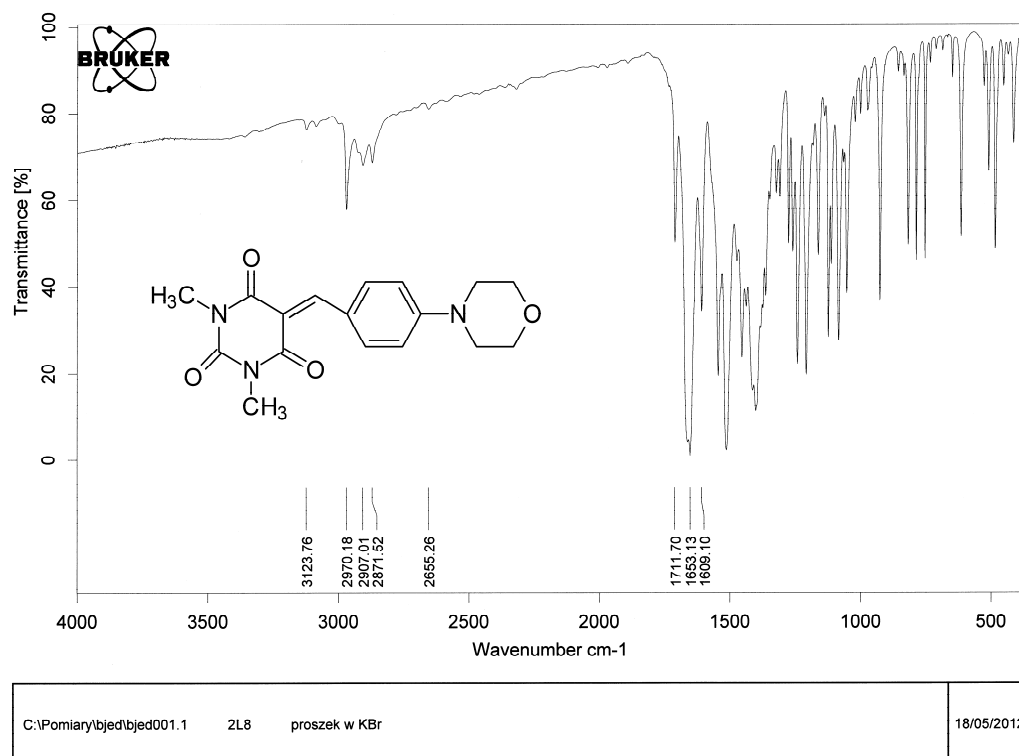
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proszek w KBr

21/05/2012

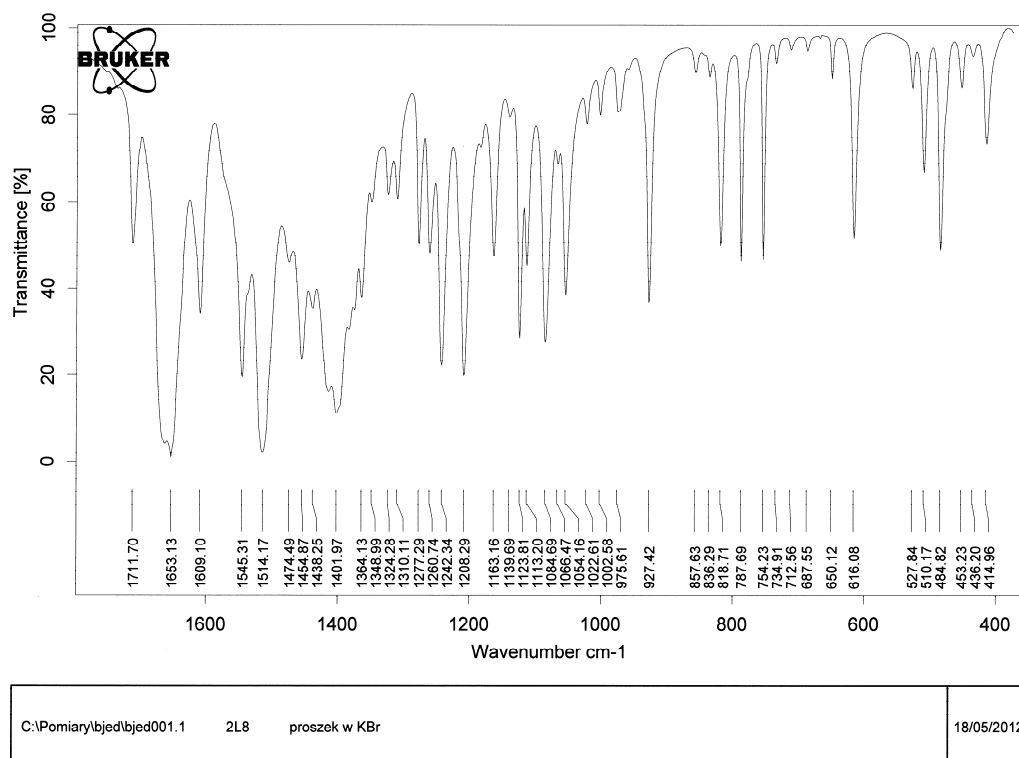
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IR spectrum of 8



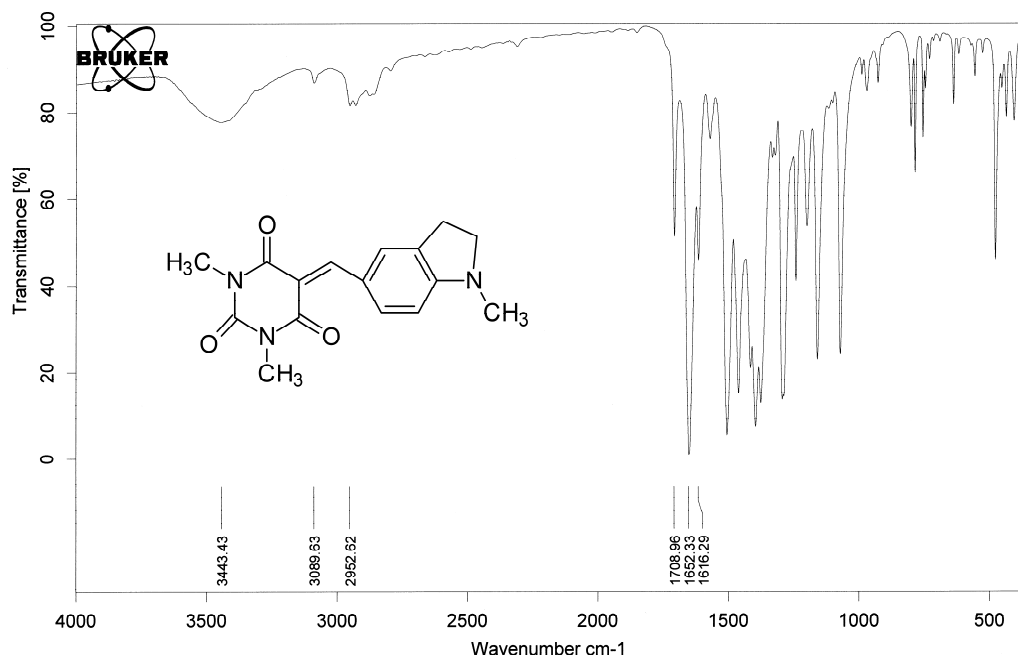
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Enlarged spectrum in the range of 1600 - 400 cm⁻¹



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IR spectrum of 9

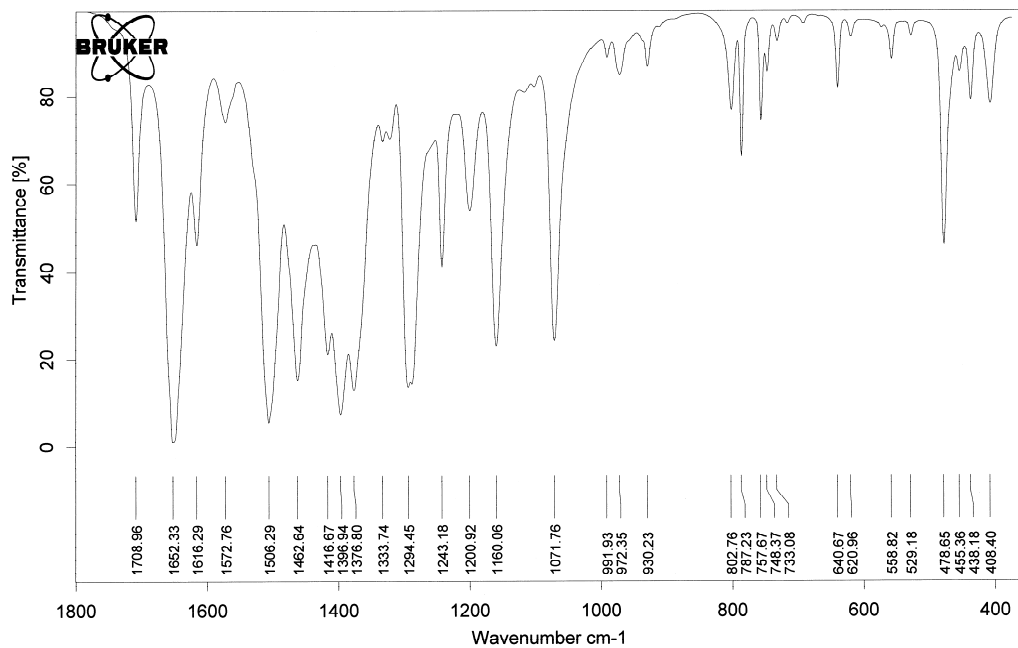


C:\Pomiary\bjed\bjed015.1 2L9 | Av. of 2 proszek w KBr

01/06/2012

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Enlarged spectrum in the range of 1600 - 400 cm⁻¹

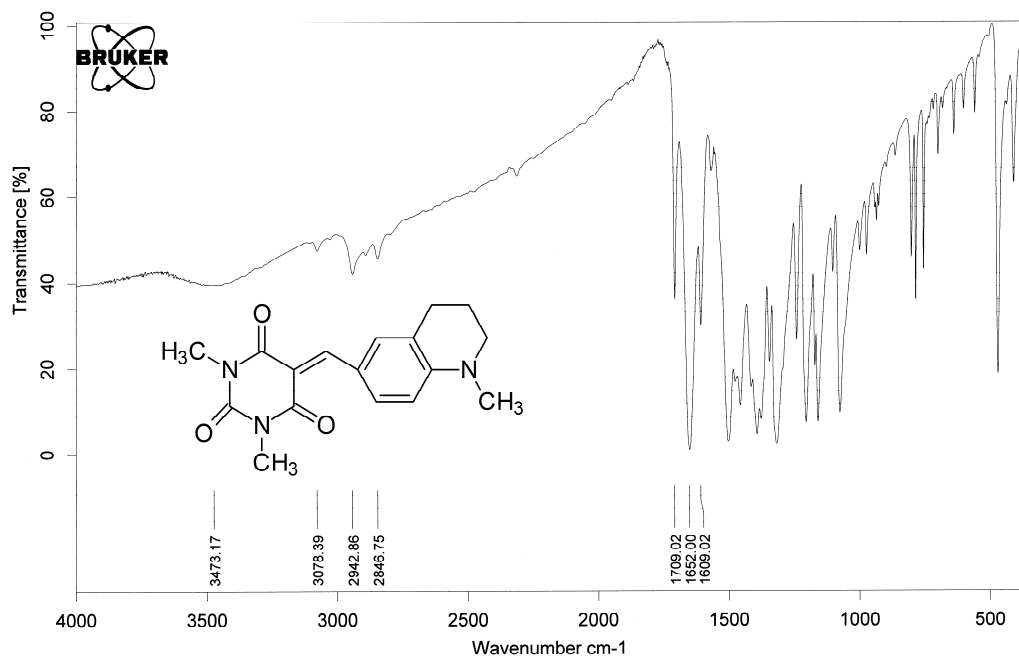


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IR spectrum of 10

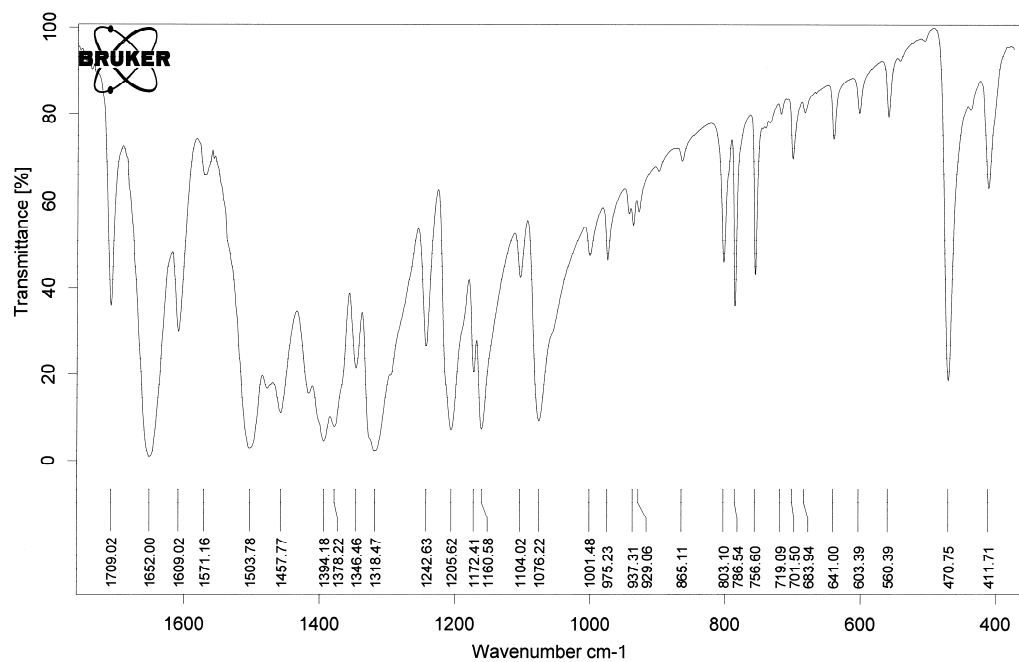


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Enlarged spectrum in the range of 1600 - 400 cm⁻¹

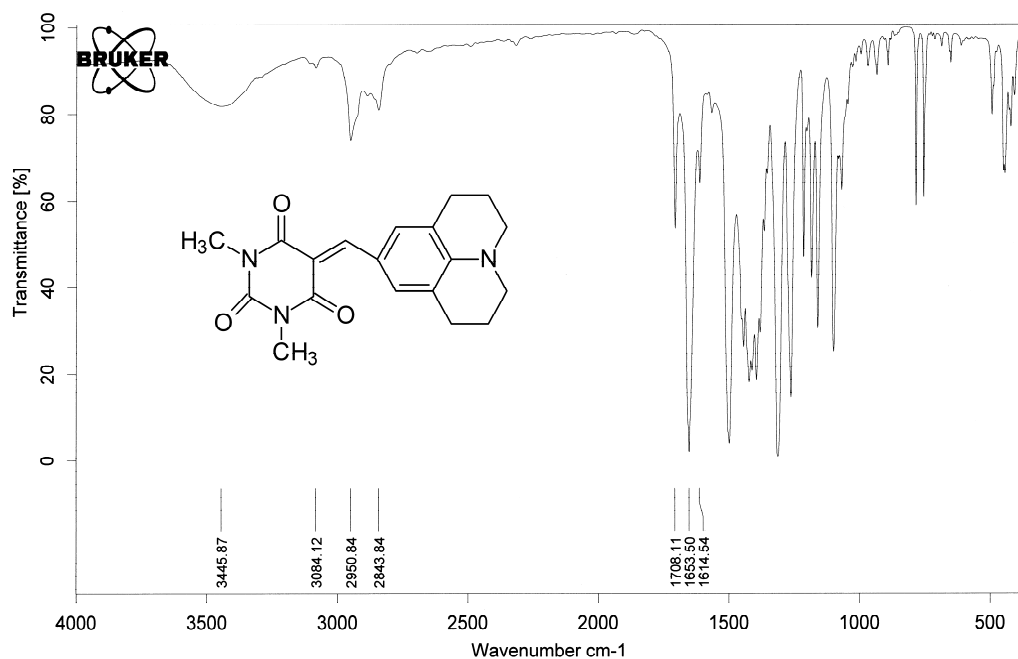


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IR spectrum of 11

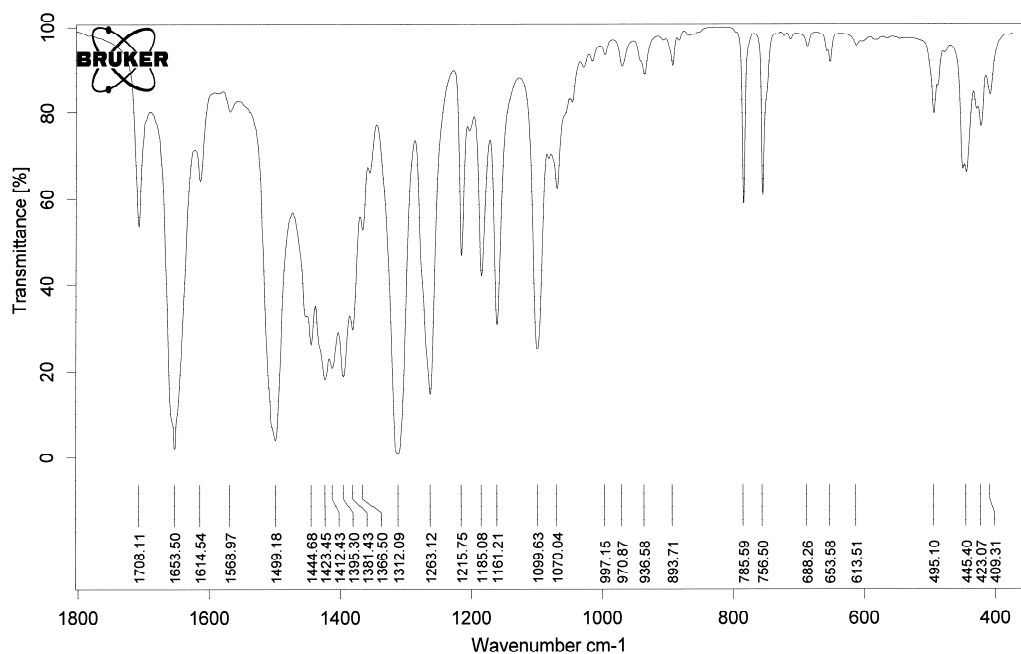


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Enlarged spectrum in the range of 1600 - 400 cm⁻¹

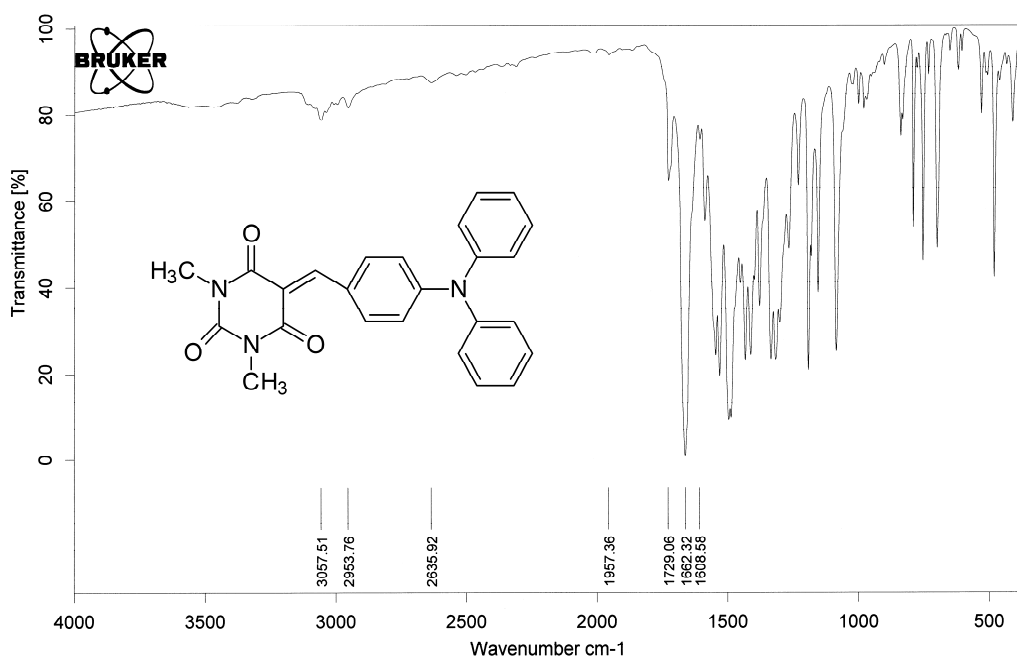


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IR spectrum of 12

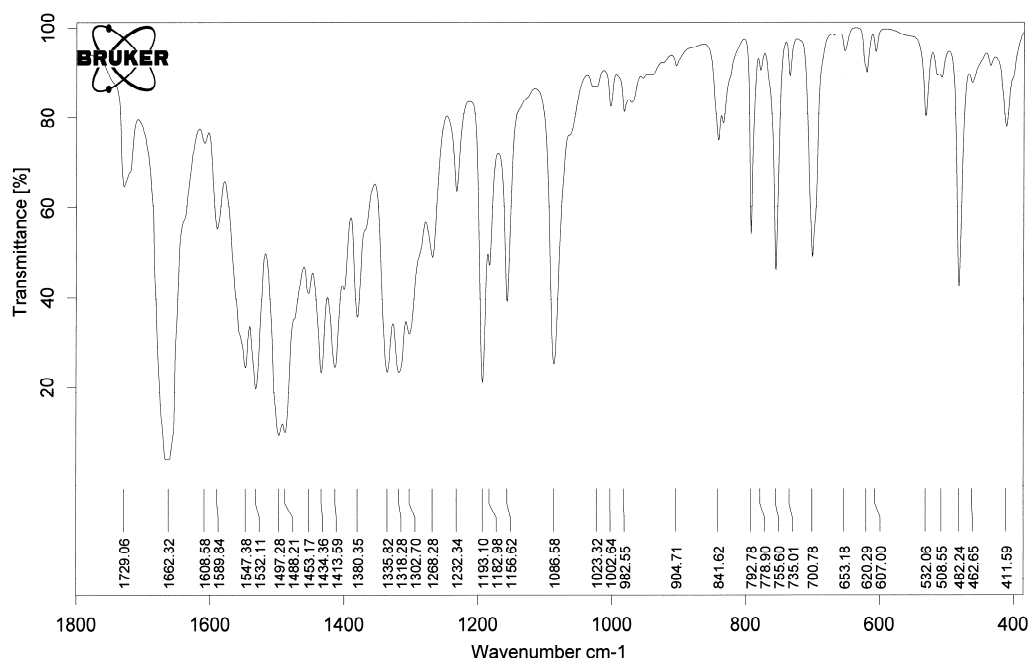


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Enlarged spectrum in the range of 1600 - 400 cm⁻¹

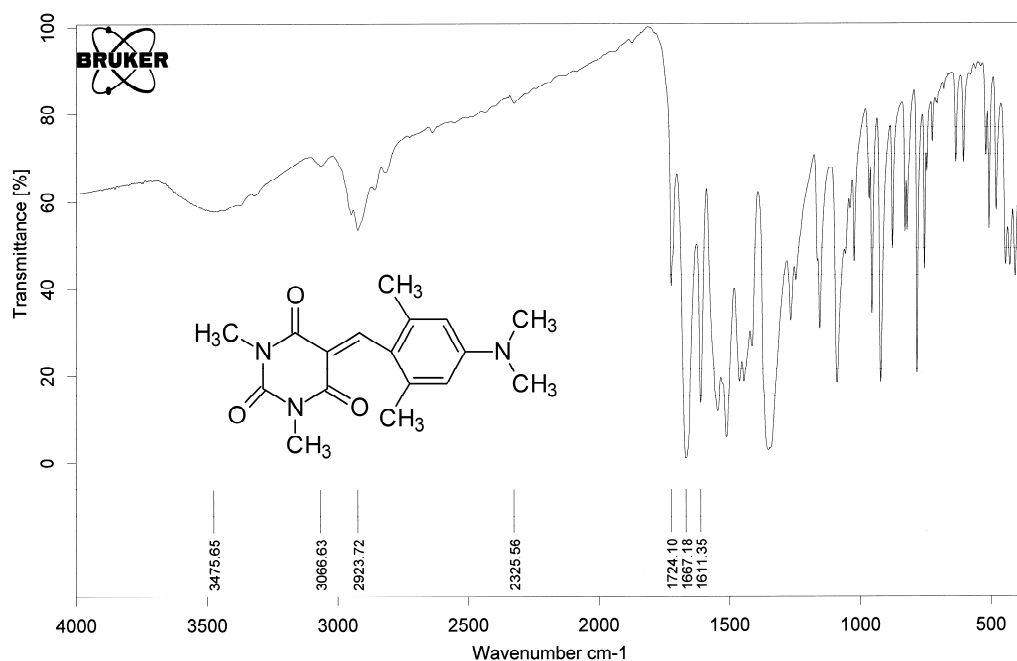


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IR spectrum of 13

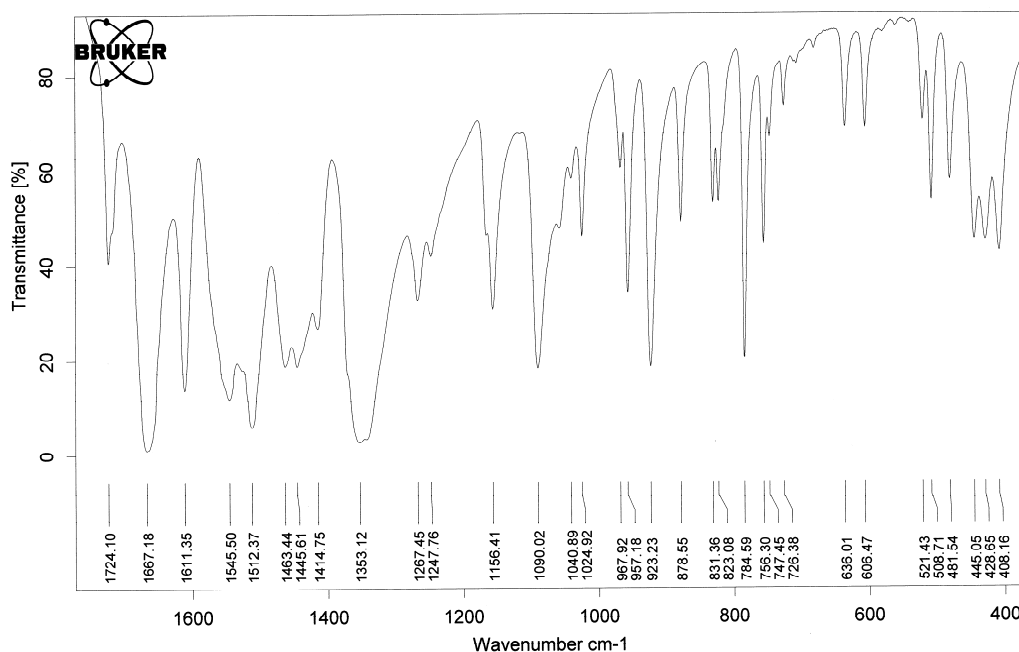


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Enlarged spectrum in the range of 1600 - 400 cm⁻¹



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Table S1. Photophysical Data^a for Compounds **1-13**

| Solvent | λ_{\max}^{ab} | ε_{\max} | FWHM ^{ab} | f_{os} | δ_{IPA} | λ_{\max}^{fl} | $\Delta\nu$ | λ_{\max}^{ab} | ε_{\max} | FWHM ^{ab} | f_{os} | δ_{IPA} | λ_{\max}^{fl} | $\Delta\nu$ |
|-------------------|-----------------------|----------------------|--------------------|----------|----------------|-----------------------|-------------|-----------------------|----------------------|--------------------|----------|----------------|-----------------------|-------------|
| | Compound 1 | | | | | | | Compound 2 | | | | | | |
| 1,4-Dx | 450 | 7.03 | 2287 | 0.825 | 2.69 | 515 | 2805 | 455 | 7.20 | 2079 | 0.759 | 2.73 | 516 | 2598 |
| Toluene | 452 | 7.03 | 2091 | 0.738 | 2.69 | 516 | 2744 | 457 | 9.03 | 1916 | 0.951 | 3.45 | 517 | 2539 |
| Et ₂ O | 446 | 6.67 | 2200 | 0.742 | 2.55 | 511 | 2852 | 451.5 | 9.10 | 1991 | 0.910 | 3.48 | 515 | 2731 |
| EtOAc | 452.5 | 6.50 | 2260 | 0.757 | 2.48 | 521 | 2906 | 458 | 8.68 | 2016 | 0.884 | 3.31 | 525 | 2786 |
| THF | 453.5 | 7.15 | 2204 | 0.818 | 2.70 | 523 | 2930 | 459 | 8.95 | 2384 | 0.946 | 3.42 | 526 | 2775 |
| MeAc | 456.5 | 6.79 | 2299 | 0.803 | 2.59 | 531 | 3073 | 461.5 | 7.72 | 2123 | 0.842 | 2.95 | 532 | 2871 |
| MeCN | 458 | 6.66 | 2304 | 0.802 | 2.56 | 535 | 3142 | 464.5 | 8.43 | 2170 | 0.943 | 3.22 | 539 | 2976 |
| DMF | 463.5 | 7.17 | 2271 | 0.841 | 2.71 | 543 | 3159 | 469 | 7.93 | 2102 | 0.861 | 3.03 | 542 | 2872 |
| DMSO | 468.5 | 6.50 | 2687 | 0.776 | 2.48 | 547 | 3063 | 472.5 | 7.11 | 2107 | 0.782 | 2.72 | 548 | 2916 |
| Compound 3 | | | | | | | Compound 4 | | | | | | | |
| 1,4-Dx | 452.5 | 7.46 | 2179 | 0.819 | 2.82 | 520 | 2869 | 462.5 | 5.61 | 2388 | 0.688 | 2.14 | 537 | 3000 |
| Toluene | 454.5 | 7.89 | 2011 | 0.793 | 3.00 | 522 | 2845 | 464 | 5.99 | 2214 | 0.672 | 2.29 | 539 | 2999 |
| Et ₂ O | 448.5 | 8.14 | 2083 | 0.860 | 3.11 | 518 | 2992 | 458.5 | 5.52 | 2268 | 0.632 | 2.08 | 530 | 2942 |
| EtOAc | 455 | 7.75 | 2165 | 0.864 | 2.96 | 527 | 3003 | 465.5 | 5.85 | 2323 | 0.701 | 2.23 | 539 | 2929 |
| THF | 455 | 7.58 | 2142 | 0.839 | 2.89 | 529 | 3074 | 466.5 | 5.87 | 2295 | 0.697 | 2.24 | 541 | 2952 |
| MeAc | 459 | 7.93 | 2218 | 0.904 | 3.03 | 538 | 3199 | 469.5 | 5.96 | 2383 | 0.733 | 2.27 | 543 | 2883 |
| MeCN | 462 | 8.06 | 2212 | 0.927 | 3.08 | 541 | 3161 | 472.5 | 6.04 | 2408 | 0.757 | 2.31 | 547 | 2882 |
| DMF | 465 | 7.03 | 2187 | 0.796 | 2.69 | 545 | 3157 | 477.5 | 5.69 | 2326 | 0.680 | 2.16 | 554 | 2892 |
| DMSO | 470.5 | 6.87 | 2198 | 0.789 | 2.62 | 553 | 3171 | 482 | 5.72 | 2356 | 0.692 | 2.19 | 560 | 2890 |
| Compound 5 | | | | | | | Compound 6 | | | | | | | |
| 1,4-Dx | 458 | 8.55 | 2051 | 0.886 | 3.26 | 524 | 2750 | 455.5 | 8.02 | 2096 | 0.852 | 3.06 | 524 | 2870 |

| | | | | | | | | | | | | | | |
|-------------------|-------|------|------|-------|------|-----|------|-------------|------|------|-------|------|-----|------|
| Toluene | 459 | 8.10 | 1909 | 0.773 | 3.09 | 524 | 2703 | 459 | 7.83 | 1936 | 0.749 | 2.99 | 528 | 2847 |
| Et ₂ O | 454 | 8.56 | 1960 | 0.841 | 3.27 | 523 | 2906 | 452 | 6.85 | 2037 | 0.688 | 2.61 | 520 | 2893 |
| EtOAc | 460.5 | 8.32 | 2044 | 0.870 | 3.18 | 532 | 2919 | 458.5 | 7.62 | 2125 | 0.819 | 2.91 | 529 | 2907 |
| THF | 461.5 | 8.43 | 2005 | 0.873 | 3.22 | 534 | 2942 | 460 | 7.68 | 2039 | 0.804 | 2.87 | 531 | 2907 |
| MeAc | 464.5 | 8.52 | 2095 | 0.921 | 3.25 | 539 | 2976 | 462.5 | 7.78 | 2142 | 0.858 | 2.96 | 535 | 2930 |
| MeCN | 467 | 8.11 | 2102 | 0.881 | 3.10 | 544 | 3031 | 465 | 7.63 | 2146 | 0.848 | 2.91 | 538 | 2918 |
| DMF | 471 | 7.44 | 2082 | 0.794 | 2.81 | 548 | 2983 | 468.5 | 7.36 | 2126 | 0.805 | 2.81 | 544 | 2962 |
| DMSO | 475 | 7.60 | 2101 | 0.824 | 2.90 | 554 | 3002 | 471 | 7.40 | 2143 | 0.817 | 2.83 | 547 | 2950 |
| Compound 7 | | | | | | | | Compound 8 | | | | | | |
| 1,4-Dx | 453.5 | 5.73 | 2480 | 0.736 | 2.19 | 530 | 3183 | 439 | 5.02 | 2904 | 0.786 | 1.92 | 515 | 3388 |
| Toluene | 456.5 | 5.87 | 2301 | 0.683 | 2.24 | 532 | 3109 | 441 | 5.15 | 2682 | 0.737 | 1.97 | 518 | 3345 |
| Et ₂ O | 450.5 | 6.32 | 2404 | 0.781 | 2.41 | 533 | 3436 | 436 | - | 2815 | - | - | 516 | 3582 |
| EtOAc | 457 | 6.18 | 2500 | 0.794 | 2.33 | 545 | 3533 | 442 | 5.06 | 2912 | 0.809 | 1.93 | 524 | 3540 |
| THF | 458 | 6.42 | 2896 | 0.824 | 2.45 | 545 | 3485 | 443 | 4.82 | 2822 | 0.734 | 1.84 | 527 | 3573 |
| MeAc | 460.5 | 5.91 | 2481 | 0.761 | 2.25 | 543 | 3299 | 447 | 5.42 | 2979 | 0.858 | 2.05 | 535 | 3705 |
| MeCN | 464 | 6.48 | 2484 | 0.838 | 2.47 | 543 | 3136 | 447 | 5.06 | 2987 | 0.802 | 1.93 | 537 | 3774 |
| DMF | 468 | 5.66 | 2434 | 0.714 | 2.16 | 548 | 3119 | 453 | 4.96 | 2928 | 0.782 | 1.90 | 543 | 3635 |
| DMSO | 472.5 | 5.53 | 2414 | 0.686 | 2.10 | 553 | 3081 | 458 | 4.51 | 2932 | 0.701 | 1.72 | 551 | 3685 |
| Compound 9 | | | | | | | | Compound 10 | | | | | | |
| 1,4-Dx | 464.5 | 6.72 | 2678 | 0.776 | 2.57 | 531 | 2696 | 462.5 | 7.59 | 2046 | 0.777 | 2.87 | 524 | 2538 |
| Toluene | 468 | 6.93 | 2123 | 0.752 | 2.65 | 535 | 2676 | 464.5 | 7.81 | 1900 | 0.736 | 2.99 | 525 | 2481 |
| Et ₂ O | 460 | - | 2204 | - | - | 524 | 2655 | 458 | 6.90 | 2002 | 0.700 | 2.64 | 521 | 2640 |
| EtOAc | 469 | 6.12 | 2226 | 0.711 | 2.34 | 534 | 2630 | 465 | 7.87 | 2073 | 0.835 | 3.01 | 532 | 2708 |
| THF | 469.5 | 6.42 | 2190 | 0.733 | 2.45 | 535 | 2608 | 466.5 | 7.72 | 2023 | 0.805 | 2.95 | 533 | 2675 |
| MeAc | 473.5 | 6.72 | 2237 | 0.810 | 2.66 | 538 | 2532 | 470 | 7.55 | 2088 | 0.811 | 2.87 | 542 | 2826 |

| | | | | | | | | | | | | | | |
|--------------------|-------|------|------|-------|------|-----|------|--------------------|------|------|-------|------|-----|------|
| MeCN | 477.5 | 6.92 | 2224 | 0.799 | 2.67 | 543 | 2526 | 473.5 | 7.79 | 2078 | 0.839 | 2.98 | 547 | 2838 |
| DMF | 482 | 6.82 | 2169 | 0.767 | 2.61 | 550 | 2565 | 477 | 7.65 | 2064 | 0.817 | 2.92 | 552 | 2848 |
| DMSO | 487 | 6.76 | 2151 | 0.752 | 2.58 | 555 | 2516 | 482 | 6.23 | 2054 | 0.649 | 2.38 | 558 | 2826 |
| Compound 11 | | | | | | | | Compound 12 | | | | | | |
| 1,4-Dx | 474 | 8.31 | 1838 | 0.765 | 3.17 | 535 | 2405 | 459 | 3.18 | 2832 | 0.481 | 3.18 | 594 | 4951 |
| Toluene | 476 | 9.33 | 1730 | 0.793 | 3.57 | 537 | 2386 | 463.5 | 3.67 | 2644 | 0.517 | 1.40 | 583 | 4422 |
| Et ₂ O | 470.5 | 8.78 | 1770 | 0.776 | 3.35 | 532 | 2457 | 456.5 | 4.42 | 2701 | 0.637 | 1.69 | 597 | 5155 |
| EtOAc | 477 | 9.33 | 1852 | 0.873 | 3.56 | 541 | 2480 | 456 | 4.06 | 2853 | 0.645 | 1.55 | 642 | 6354 |
| THF | 479 | 8.88 | 1772 | 0.809 | 3.37 | 544 | 2494 | 458 | 2.59 | 2818 | 0.392 | 0.98 | 644 | 6306 |
| MeAc | 482.5 | 8.58 | 1895 | 0.833 | 3.28 | 549 | 2510 | 456 | 3.69 | 2959 | 0.580 | 1.41 | 685 | 7331 |
| MeCN | 486 | 9.01 | 1873 | 0.872 | 3.50 | 554 | 2526 | 458 | 3.66 | 2970 | 0.577 | 1.40 | 686 | 7257 |
| DMF | 489.5 | 8.60 | 1859 | 0.819 | 3.28 | 558 | 2508 | 460 | 3.05 | 2977 | 0.480 | 1.16 | 680 | 7033 |
| DMSO | 494 | 8.35 | 1856 | 0.799 | 3.19 | 563 | 2481 | 462.5 | 3.49 | 3021 | 0.558 | 1.32 | 684 | 7002 |
| Compound 13 | | | | | | | | | | | | | | |
| 1,4-Dx | 469 | 2.15 | 3225 | 0.371 | 0.82 | 526 | 2311 | | | | | | | |
| Toluene | 476 | 2.27 | 2877 | 0.345 | 0.87 | 531 | 2176 | | | | | | | |
| Et ₂ O | 469.5 | 2.21 | 2995 | 0.354 | 0.84 | 534 | 2573 | | | | | | | |
| EtOAc | 471 | 2.06 | 3230 | 0.357 | 0.79 | 542 | 2781 | | | | | | | |
| THF | 473 | 1.94 | 3744 | 0.326 | 0.73 | 544 | 2759 | | | | | | | |
| MeAc | 473 | 1.95 | 3371 | 0.351 | 1.94 | 546 | 2827 | | | | | | | |
| MeCN | 477 | 1.73 | 3427 | 0.318 | 0.66 | 557 | 3011 | | | | | | | |
| DMF | 481 | 1.73 | 3450 | 0.321 | 0.66 | 560 | 2933 | | | | | | | |
| DMSO | 484 | 1.86 | 3402 | 0.327 | 0.71 | 567 | 3024 | | | | | | | |

^aAbsorption ($\lambda_{\max}^{ab}; nm$), fluorescence maxima ($\lambda_{\max}^{fl}; nm$), shift ($\Delta\nu; cm^{-1}$), maximum extinction coefficient ($\epsilon_{max}; 10^4 M^{-1}cm^{-1}$), full width at half maximum (FWHM; cm^{-1}), one-photon absorption cross-section ($\delta_{IPA}; \text{\AA}^2$) and oscillator strength (f_{os}).

Table S2. Estimated from eq. (13), coefficients (y_0 , a_{SP} , b_{SDP} , c_{SA} , and d_{SB}), their standard errors and correlation coefficients (R^2) for the multiple linear regression analysis of v_{Ab} , v_{Fl} and Δv^{SS} of **1-13** in 9 solvents as a function of the Catalán four-parameter solvent scale

| y | y_0 | a_{SP} | b_{SDP} | c_{SA} | d_{SB} | R^2 |
|-----------------|-----------|--------------------|--------------------|--------------|------------|-------|
| Compound 1 | | | | | | |
| v_{ab} | 24068±155 | -(2181±200) | -(798±69) | -(1491±779) | -(9±78) | 0.989 |
| v_{fl} | 21269±201 | -(1943±258) | -(1295±89) | -(1497±1006) | -(2±100) | 0.991 |
| Δv^{SS} | 2801±194 | -(238±250) | 497±86 | 6±974 | -(7±97) | 0.920 |
| Compound 2 | | | | | | |
| v_{ab} | 23568±169 | -(1862±218) | -(815±75) | -(1297±850) | 56±85 | 0.986 |
| v_{fl} | 20584±211 | -(1150±271) | -(1170±93) | -(2693±1058) | -(39±105) | 0.988 |
| Δv^{SS} | 2984±121 | -(711±156) | 354±54 | 1396±609 | 94±61 | 0.966 |
| Compound 3 | | | | | | |
| v_{ab} | 23584±164 | -(1767±211) | -(753±72) | -(2577±822) | 121±82 | 0.988 |
| v_{fl} | 20681±130 | -(1505±167) | -(1192±57) | -(2142±650) | 25±65 | 0.996 |
| Δv^{SS} | 2903±163 | -(262±210) | 439±72 | -(435±818) | 96±82 | 0.928 |
| Compound 4 | | | | | | |
| v_{ab} | 23315±154 | -(1949±189) | -(841±68) | -(1741±773) | 6±77 | 0.990 |
| v_{fl} | 20439±162 | -(2164±209) | -(715±72) | -(1397±814) | 27±81 | 0.987 |
| Δv^{SS} | 2877±53 | 215±68 | -(125±23) | -(344±264) | -(21±26) | 0.940 |
| Compound 5 | | | | | | |
| v_{ab} | 23373±133 | -(1751±171) | -(799±59) | -(1329±666) | 31±66 | 0.991 |
| v_{fl} | 20314±154 | -(1159±198) | -(1067±68) | -(1989±771) | -(142±77) | 0.993 |
| Δv^{SS} | 3059±150 | -(592±193) | 268±66 | 661±751 | 173±75 | 0.916 |
| Compound 6 | | | | | | |
| v_{ab} | 23469±148 | -(1866±190) | -(852±65) | 106±741 | 229±74 | 0.987 |
| v_{fl} | 20668±166 | -(1874±214) | -(946±74) | 111±834 | 147±83 | 0.987 |
| Δv^{SS} | 2801±40 | 7±52 | 95±18 | -(4±201) | 83±20 | 0.942 |
| Compound 7 | | | | | | |
| v_{ab} | 23634±184 | -(1906±237) | -(821±81) | -(1814±922) | 91±92 | 0.985 |
| v_{fl} | 19812±631 | -(881±811) | -(794±279) | 1167±3162 | -(419±315) | 0.738 |
| Δv^{SS} | 3822±503 | -(1025±647) | -(26±222) | -(3482±2522) | 511±251 | 0.617 |
| Compound 8 | | | | | | |
| v_{ab} | 24892±233 | -(2480±300) | -(921±130) | -(419±1169) | -(59±117) | 0.979 |
| v_{fl} | 20913±247 | -(1533±317) | -(1244±109) | -(1936±1236) | -(127±123) | 0.986 |
| Δv^{SS} | 3979±187 | -(947±241) | 323±83 | 1517±939 | 68±94 | 0.917 |

| Compound 9 | | | | | | |
|------------------|-----------|--------------------|--------------------|--------------|------------|-------|
| ν_{ab} | 23359±232 | -(2194±298) | -(1014±103) | -(1569±1163) | 181±116 | 0.982 |
| ν_{fl} | 20670±294 | -(2258±378) | -(800±130) | -(1344±1472) | 150±147 | 0.961 |
| $\Delta\nu^{SS}$ | 2689±96 | 63±123 | -(215±42) | -(225±481) | 32±48 | 0.905 |
| Compound 10 | | | | | | |
| ν_{ab} | 23278±106 | -(1943±137) | -(887±47) | -(1708±533) | 136±53 | 0.995 |
| ν_{fl} | 20600±129 | -(1521±166) | -(1288±57) | -(2124±648) | 22±65 | 0.996 |
| $\Delta\nu^{SS}$ | 2677±65 | -(422±84) | 401±29 | 417±328 | 114±33 | 0.989 |
| Compound 11 | | | | | | |
| ν_{ab} | 22593±72 | -(1720±92) | -(888±32) | -(1453±359) | 103±36 | 0.998 |
| ν_{fl} | 20081±111 | -(1495±143) | -(1049±49) | -(1070±558) | -(66±56) | 0.995 |
| $\Delta\nu^{SS}$ | 2512±56 | -(225±72) | 161±25 | -(384±279) | 37±28 | 0.935 |
| Compound 12 | | | | | | |
| ν_{ab} | 22663±180 | -(1434±232) | 88±80 | -(1333±903) | 235±90 | 0.907 |
| ν_{fl} | 17969±779 | 318±1002 | -(3906±344) | 6256±3903 | -(130±389) | 0.974 |
| $\Delta\nu^{SS}$ | 4695±929 | -(1752±1196) | 3994±411 | -(7589±4659) | 365±464 | 0.965 |
| Compound 13 | | | | | | |
| ν_{ab} | 22414±429 | -(1607±551) | -(392±189) | -(2239±2149) | 186±214 | 0.829 |
| ν_{fl} | 19738±661 | -(617±850) | -(1134±292) | -(4083±3313) | -(249±330) | 0.903 |
| $\Delta\nu^{SS}$ | 2676±395 | -(990±508) | 742±174 | 1845±1978 | 435±197 | 0.917 |

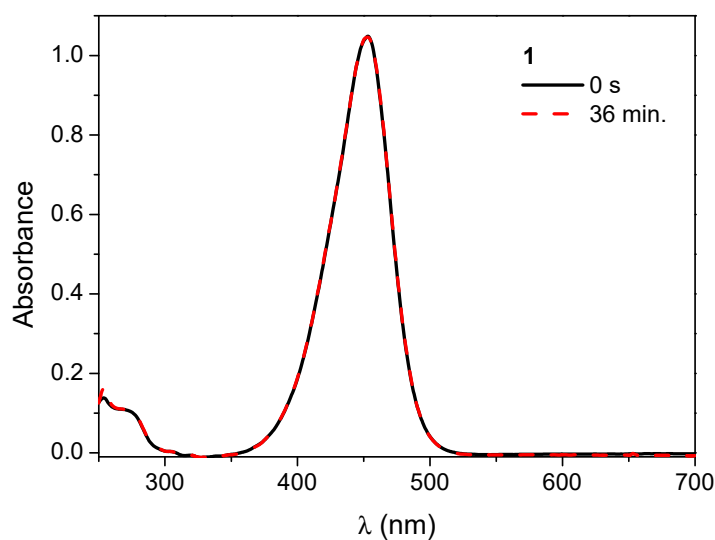


Figure S1. Changes of the electronic absorption spectra of **1** during an argon-ion laser irradiation ($I_0 = 50$ mW) in ethyl acetate. Time of irradiation marked in Figure.

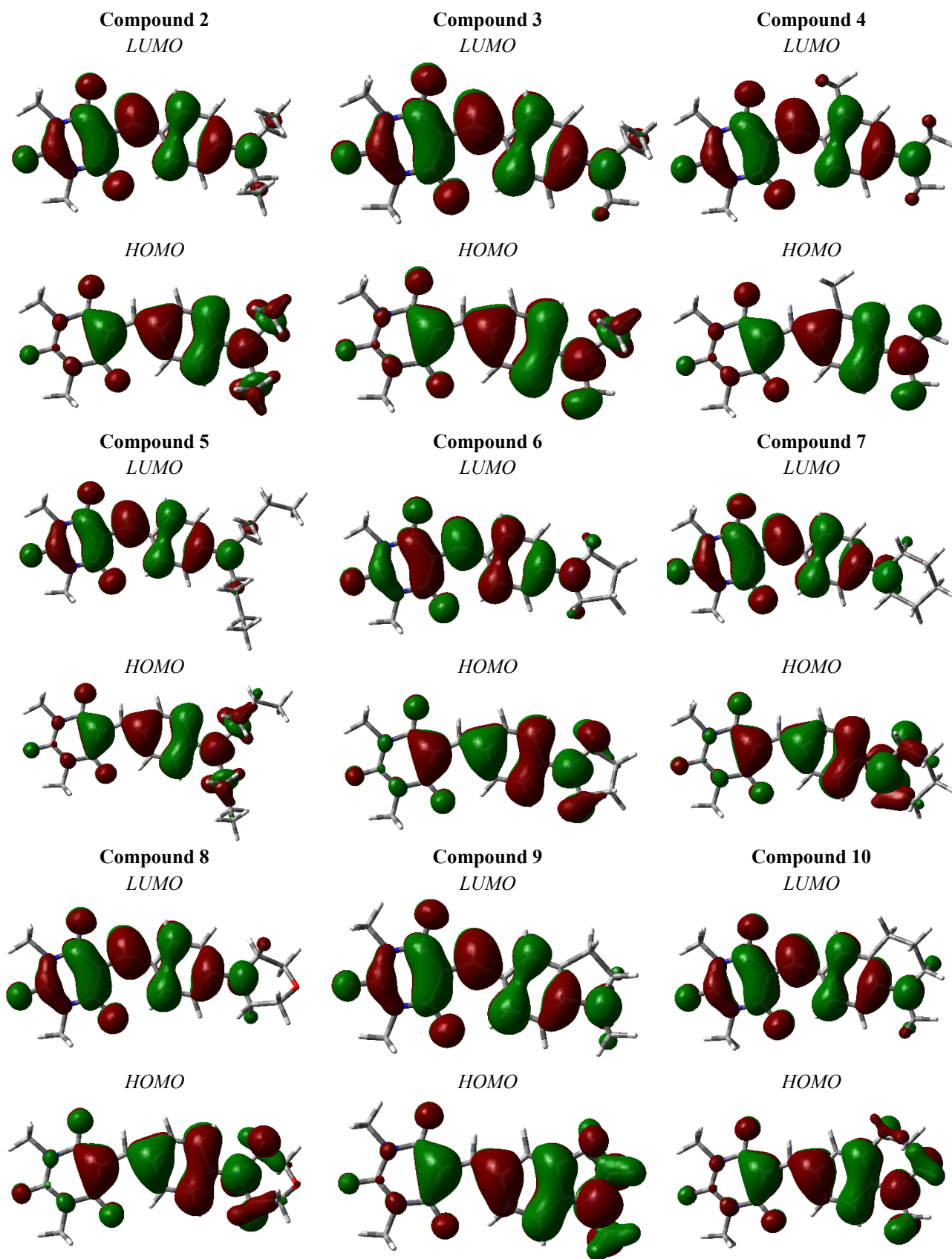


Figure S2. The HOMO – LUMO orbitals of selected merocyanine-type dyes.

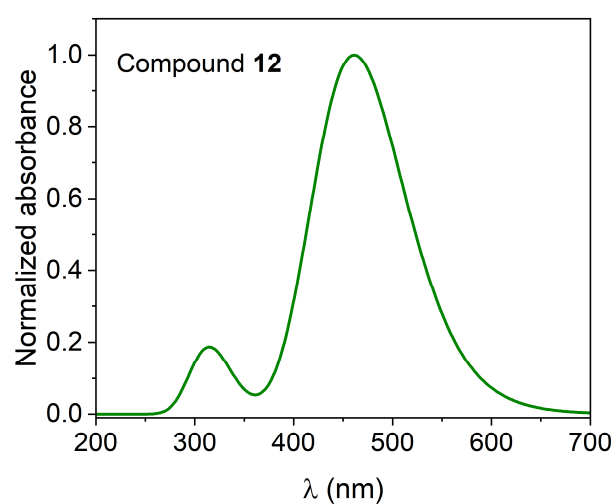
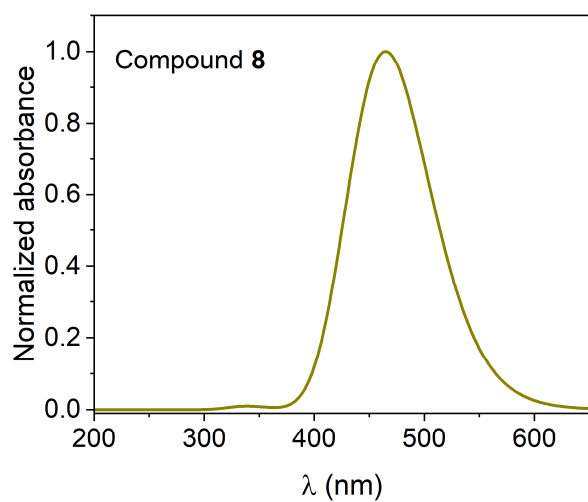
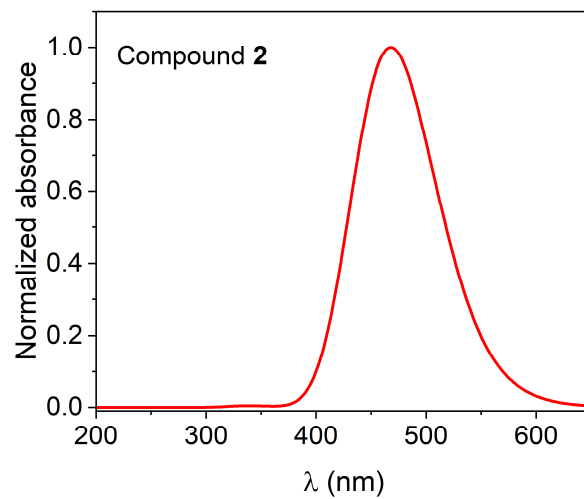
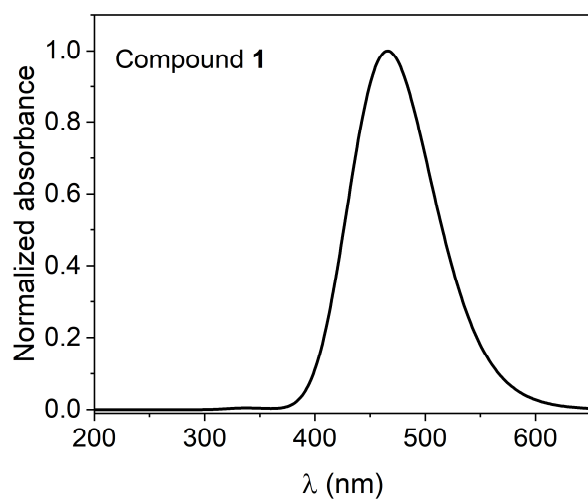
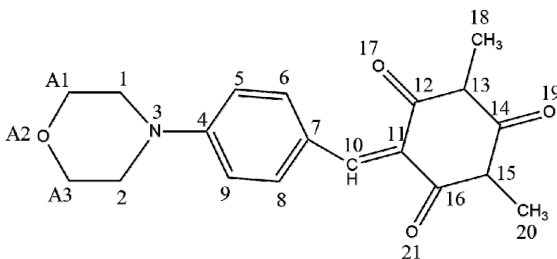
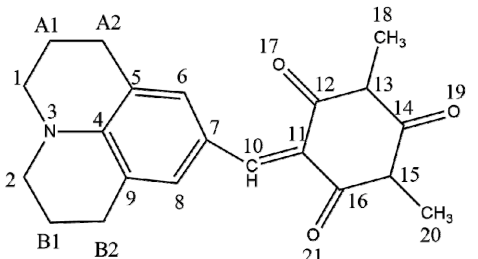


Figure S5. Graphical representation of the calculated absorption spectra for selected derivatives.

Table S3. Calculated geometries of the selected merocyanine dyes in THF

| Compound 1 | | | Compound 12 | | |
|-----------------|-----------|-----------|-----------------|-----------|-----------|
| | | | | | |
| Bond | GS | ES | Bond | GS | ES |
| C1-N3 | 1.45072 | 1.45477 | C1-N3 | 1.42372 | 1.38923 |
| C2-N3 | 1.45043 | 1.45454 | C2-N3 | 1.42335 | 1.38995 |
| N3-C4 | 1.35132 | 1.34409 | N3-C4 | 1.38025 | 1.43871 |
| C4-C5 | 1.42013 | 1.42613 | C4-C5 | 1.41078 | 1.39516 |
| C5-C6 | 1.37268 | 1.36687 | C5-C6 | 1.37524 | 1.38078 |
| C6-C7 | 1.41612 | 1.41637 | C6-C7 | 1.41370 | 1.42194 |
| C7-C8 | 1.41897 | 1.41634 | C7-C8 | 1.41662 | 1.42483 |
| C8-C9 | 1.37123 | 1.36684 | C8-C9 | 1.37399 | 1.37800 |
| C4-C9 | 1.41907 | 1.42620 | C4-C9 | 1.40957 | 1.39685 |
| C7-C10 | 1.42371 | 1.46555 | C7-C10 | 1.43002 | 1.42223 |
| C10=C11 | 1.38027 | 1.40161 | C10=C11 | 1.37580 | 1.41007 |
| C11-C12 | 1.45413 | 1.42870 | C11-C12 | 1.45717 | 1.43645 |
| C12-N13 | 1.39469 | 1.40271 | C12-N13 | 1.39294 | 1.40727 |
| N13-C14 | 1.38360 | 1.37817 | N13-C14 | 1.38437 | 1.37647 |
| C14-N15 | 1.38403 | 1.37848 | C14-N15 | 1.38469 | 1.37870 |
| N15-C16 | 1.38776 | 1.40315 | N15-C16 | 1.38640 | 1.39889 |
| C11-C16 | 1.47169 | 1.43672 | C11-C16 | 1.47522 | 1.45006 |
| C12=O17 | 1.22312 | 1.24076 | C12=O17 | 1.22181 | 1.23348 |
| N13-C18 | 1.45846 | 1.45434 | N13-C18 | 1.45887 | 1.45537 |
| C14=O19 | 1.21661 | 1.22788 | C14=O19 | 1.21563 | 1.22482 |
| N15-C20 | 1.45814 | 1.45462 | N15-C20 | 1.45852 | 1.45523 |
| C16=O21 | 1.22290 | 1.23500 | C16=O21 | 1.22160 | 1.23203 |
| Dihedral angles | | | Dihedral angles | | |
| C1-N3-C4-C5 | 0.22361 | 7.77369 | C1-N3-C4-C5 | 23.12534 | 78.98517 |
| C1-N3-C4-C9 | 179.77579 | 172.21194 | C1-N3-C4-C9 | 156.83584 | 101.03481 |
| C2-N3-C4-C9 | 0.25148 | 8.01540 | C2-N3-C4-C9 | 21.70378 | 78.91148 |
| C2-N3-C4-C5 | 179.74792 | 172.04897 | C2-N3-C4-C5 | 158.33504 | 101.66854 |
| C7-C10=C11 | 138.95236 | 124.68649 | C7-C10=C11 | 138.85884 | 135.69855 |

| | Compound 5 | | | Compound 13 | |
|---|-------------------|-----------|--|--------------------|-----------|
| Bond | GS | ES | Bond | GS | ES |
| C1-N3 | 1.45772 | 1.46384 | C1-N3 | 1.44821 | 1.45582 |
| C2-N3 | 1.45788 | 1.46218 | C2-N3 | 1.44732 | 1.45587 |
| N3-C4 | 1.35483 | 1.34730 | N3-C4 | 1.36205 | 1.34459 |
| C4-C5 | 1.42204 | 1.42772 | C4-C5 | 1.42618 | 1.42308 |
| C5-C6 | 1.37210 | 1.36694 | C5-C6 | 1.38563 | 1.37061 |
| C6-C7 | 1.41608 | 1.41540 | C6-C7 | 1.42064 | 1.42866 |
| C7-C8 | 1.41880 | 1.41528 | C7-C8 | 1.49899 | 1.42863 |
| C8-C9 | 1.37065 | 1.36715 | C8-C9 | 1.47743 | 1.37063 |
| C4-C9 | 1.42094 | 1.42762 | C4-C9 | 1.38883 | 1.42308 |
| C6-X1 | | | C6-X1 | 1.50419 | 1.49536 |
| C8-X2 | | | C8-X2 | 1.55092 | 1.49537 |
| C7-C10 | 1.42258 | 1.46531 | C7-C10 | 1.39882 | 1.46541 |
| C10=C11 | 1.38105 | 1.40138 | C10=C11 | 1.40122 | 1.40238 |
| C11-C12 | 1.45349 | 1.42881 | C11-C12 | 1.46073 | 1.43683 |
| C12-N13 | 1.35502 | 1.40320 | C12-N13 | 1.39616 | 1.40759 |
| N13-C14 | 1.38345 | 1.37818 | N13-C14 | 1.37953 | 1.37567 |
| C14-N15 | 1.38395 | 1.37851 | C14-N15 | 1.38053 | 1.37754 |
| N15-C16 | 1.38827 | 1.40304 | N15-C16 | 1.39800 | 1.40125 |
| C11-C16 | 1.47104 | 1.43692 | C11-C16 | 1.44632 | 1.42847 |
| C12=O17 | 1.22322 | 1.24065 | C12=O17 | 1.22624 | 1.23476 |
| N13-C18 | 1.45837 | 1.45437 | N13-C18 | 1.45705 | 1.45451 |
| C14=O19 | 1.21674 | 1.22796 | C14=O19 | 1.21940 | 1.22772 |
| N15-C20 | 1.45813 | 1.45475 | N15-C20 | 1.45675 | 1.45382 |
| C16=O21 | 1.22307 | 1.23517 | C16=O21 | 1.22826 | 1.24134 |
| Dihedral angles | | | Dihedral angles | | |
| C1-N3-C4-C5 | 0.81029 | 6.14506 | C1-N3-C4-C5 | 2.13469 | 1.92009 |
| C1-N3-C4-C9 | 179.89408 | 173.75373 | C1-N3-C4-C9 | 177.34801 | 178.14492 |
| C2-N3-C4-C9 | 2.59585 | 3.45524 | C2-N3-C4-C9 | 1.80189 | 2.21464 |
| C2-N3-C4-C5 | 178.10851 | 176.64597 | C2-N3-C4-C5 | 177.68081 | 177.72034 |
| C7-C10=C11 | 138.95586 | 125.01537 | C7-C10=C11 | 135.53757 | 124.85573 |
| | | | | | |
| Compound 8 | | | Compound 11 | | |
|  | | |  | | |

| Bond | GS | ES | Bond | GS | ES |
|------------------------|-----------|-----------|------------------------|-----------|-----------|
| C1-N3 | 1.45735 | 1.46273 | C1-N3 | 1.45599 | 1.46157 |
| C2-N3 | 1.45685 | 1.46355 | C2-N3 | 1.45583 | 1.46119 |
| C1-CA1 | 1.51628 | 1.51670 | C1-CA1 | 1.51481 | 1.51257 |
| CA1-OA2 | 1.41823 | 1.41645 | CA1-CA2 | 1.51870 | 1.51726 |
| OA2-CA3 | 1.41870 | 1.41550 | CA2-C5 | 1.50552 | 1.49839 |
| CA3-C2 | 1.51625 | 1.51671 | C2-CB1 | 1.51505 | 1.51236 |
| N3-C4 | 1.35338 | 1.34390 | CB1-CB2 | 1.51895 | 1.51761 |
| C4-C5 | 1.41906 | 1.42653 | CB2-C9 | 1.50526 | 1.49898 |
| C5-C6 | 1.37302 | 1.36652 | N3-C4 | 1.35663 | 1.34644 |
| C6-C7 | 1.41563 | 1.41688 | C4-C5 | 1.42754 | 1.43674 |
| C7-C8 | 1.41838 | 1.41702 | C5-C6 | 1.37355 | 1.37061 |
| C8-C9 | 1.37148 | 1.36654 | C6-C7 | 1.41505 | 1.41062 |
| C4-C9 | 1.41797 | 1.42647 | C7-C8 | 1.41897 | 1.41047 |
| C7-C10 | 1.42459 | 1.46497 | C8-C9 | 1.37181 | 1.37089 |
| C10=C11 | 1.37945 | 1.40130 | C4-C9 | 1.42649 | 1.43688 |
| C11-C12 | 1.45471 | 1.43657 | C7-C10 | 1.42012 | 1.46780 |
| C12-N13 | 1.39431 | 1.40308 | C10=C11 | 1.38485 | 1.40273 |
| N13-C14 | 1.38369 | 1.37870 | C11-C12 | 1.45250 | 1.43800 |
| C14-N15 | 1.38407 | 1.37849 | C12-N13 | 1.39527 | 1.440737 |
| N15-C16 | 1.38769 | 1.40196 | N13-C14 | 1.38151 | 1.37521 |
| C11-C16 | 1.47235 | 1.42829 | C14-N15 | 1.38086 | 1.37638 |
| C12=O17 | 1.22295 | 1.23495 | N15-C16 | 1.39245 | 1.40368 |
| N13-C18 | 1.45848 | 1.45470 | C11-C16 | 1.47097 | 1.43055 |
| C14=O19 | 1.21635 | 1.22769 | C12=O17 | 1.22397 | 1.23536 |
| N15-C20 | 1.45830 | 1.45454 | N13-C18 | 1.45756 | 1.45435 |
| C16=O21 | 1.22262 | 1.24105 | C14=O19 | 1.21758 | 1.22841 |
| | | | N15-C20 | 1.45801 | 1.45362 |
| | | | C16=O21 | 1.22346 | 1.23955 |
| Dihedral angles | | | Dihedral angles | | |
| C1-N3-C4-C5 | 9.34885 | 8.91062 | C1-N3-C4-C5 | 5.20762 | 2.12992 |
| C1-N3-C4-C9 | 170.69096 | 171.18084 | C1-N3-C4-C9 | 175.32794 | 177.60016 |
| C2-N3-C4-C9 | 9.49233 | 7.86765 | C2-N3-C4-C9 | 5.56457 | 3.49860 |
| C2-N3-C4-C5 | 170.46786 | 172.04088 | C2-N3-C4-C5 | 174.97100 | 176.23148 |
| C7-C10=C11 | 138.92993 | 124.62726 | C7-C10=C11 | 139.13035 | 125.43461 |

Table S4. The frontier orbital energies in selected solvents. All values are given in eV

| | GP | Toluene | THF | DMF | | GP | Toluene | THF | DMF |
|-------------------|---------|---------|---------|---------|-------------------|---------|---------|---------|---------|
| Compound 1 | | | | | Compound 2 | | | | |
| E _{HOMO} | -6.0412 | -6.0145 | -6.0140 | -6.0181 | E _{HOMO} | -5.9903 | -5.9786 | -5.9884 | -5.9979 |
| E _{LUMO} | -2.3254 | -2.4054 | -2.4792 | -2.5167 | E _{LUMO} | -2.2998 | -2.3875 | -2.4661 | -2.5069 |
| E _{GAP} | 3.7158 | 3.6091 | 3.5348 | 3.5013 | E _{GAP} | 3.6905 | 3.5911 | 3.5223 | 3.4910 |
| η | 1.8579 | 1.8046 | 1.7674 | 1.7507 | η | 1.8452 | 1.7956 | 1.7611 | 1.7455 |
| μ | -4.1833 | -4.2100 | -4.2466 | -4.2674 | μ | -4.1451 | -4.1830 | -4.2273 | -4.2524 |
| χ | 4.1833 | 4.2100 | 4.2466 | 4.2674 | χ | 4.1451 | 4.1830 | 4.2273 | 4.2524 |
| Compound 3 | | | | | Compound 4 | | | | |
| E _{HOMO} | -6.0026 | -5.9824 | -5.9868 | -5.9938 | E _{HOMO} | -5.9696 | -5.9604 | -5.9718 | -5.9819 |
| E _{LUMO} | -2.3045 | -2.3886 | -2.4650 | -2.5045 | E _{LUMO} | -2.3292 | -2.4117 | -2.4882 | -2.5282 |
| E _{GAP} | 3.6981 | 3.5939 | 3.5217 | 3.4894 | E _{GAP} | 3.6404 | 3.5487 | 3.4836 | 3.4537 |
| η | 1.8490 | 1.7969 | 1.7609 | 1.7447 | η | 1.8202 | 1.7743 | 1.7418 | 1.7269 |
| μ | -4.1535 | -4.1855 | -4.2259 | -4.2492 | μ | -4.1494 | -4.1860 | -4.2300 | -4.2550 |
| χ | 4.1535 | 4.1855 | 4.2259 | 4.2492 | χ | 4.1494 | 4.1860 | 4.2300 | 4.2550 |
| Compound 5 | | | | | Compound 6 | | | | |
| E _{HOMO} | -5.9370 | -5.9457 | -5.9623 | -5.9729 | E _{HOMO} | -5.9522 | -5.9438 | -5.9541 | -5.9626 |
| E _{LUMO} | -2.2710 | -2.3758 | -2.4599 | -2.5012 | E _{LUMO} | -2.2713 | -2.3668 | -2.4490 | -2.4901 |
| E _{GAP} | 3.6660 | 3.5699 | 3.5024 | 3.4717 | E _{GAP} | 3.6809 | 3.5770 | 3.5051 | 3.4725 |
| η | 1.8330 | 1.7850 | 1.7512 | 1.7358 | η | 1.8405 | 1.7885 | 1.7526 | 1.7362 |
| μ | -4.1040 | -4.1607 | -4.2111 | -4.2371 | μ | -4.1117 | -4.1553 | -4.2015 | -4.2263 |
| χ | 4.1040 | 4.1607 | 4.2111 | 4.2371 | χ | 4.1117 | 4.1553 | 4.2015 | 4.2263 |
| Compound 7 | | | | | Compound 8 | | | | |
| E _{HOMO} | -6.0466 | -6.0028 | -5.9381 | -5.9274 | E _{HOMO} | -6.1190 | -6.0801 | -6.0630 | -6.0567 |
| E _{LUMO} | -2.3736 | -2.4400 | -2.4593 | -2.4805 | E _{LUMO} | -2.3932 | -2.4544 | -2.5094 | -2.5369 |
| E _{GAP} | 3.6731 | 3.5628 | 3.4787 | 3.4469 | E _{GAP} | 3.7258 | 3.6257 | 3.5536 | 3.5198 |
| η | 1.8365 | 1.7814 | 1.7394 | 1.7235 | η | 1.8629 | 1.8129 | 1.7768 | 1.7599 |
| μ | -4.2101 | -4.2214 | -4.1987 | -4.2040 | μ | -4.2561 | -4.2673 | -4.2862 | -4.2968 |
| χ | 4.2101 | 4.2214 | 4.1987 | 4.2040 | χ | 4.2561 | 4.2673 | 4.2862 | 4.2968 |
| Compound 9 | | | | | Compound 10 | | | | |
| E _{HOMO} | -5.9536 | -5.8923 | -5.8605 | -5.8491 | E _{HOMO} | -5.8932 | -5.8657 | -5.8678 | -5.8747 |
| E _{LUMO} | -2.3249 | -2.3853 | -2.4419 | -2.4716 | E _{LUMO} | -2.2666 | -2.3483 | -2.4258 | -2.4667 |
| E _{GAP} | 3.6287 | 3.5070 | 3.4186 | 3.3775 | E _{GAP} | 3.6265 | 3.5174 | 3.4420 | 3.4080 |
| η | 1.8143 | 1.7535 | 1.7093 | 1.6888 | η | 1.8133 | 1.7587 | 1.7210 | 1.7040 |
| μ | -4.1392 | -4.1388 | -4.1512 | -4.1603 | μ | -4.0799 | -4.1070 | -4.1468 | -4.1707 |
| χ | 4.1392 | 4.1388 | 4.1512 | 4.1603 | χ | 4.0799 | 4.1070 | 4.1468 | 4.1707 |

| Compound 11 | | | | | Compound 12 | | | | |
|-------------------|---------|---------|---------|---------|-------------------|---------|---------|---------|---------|
| E_{HOMO} | -5.7805 | -5.7612 | -5.7696 | -5.7794 | E_{HOMO} | -5.9136 | -5.9182 | -5.9375 | -5.9522 |
| E_{LUMO} | -2.2283 | -2.3132 | -2.3943 | -2.4373 | E_{LUMO} | -2.5467 | -2.6065 | -2.6653 | -2.6931 |
| E_{GAP} | 3.5522 | 3.4480 | 3.3753 | 3.3421 | E_{GAP} | 3.3669 | 3.3117 | 3.2722 | 3.2591 |
| η | 1.7761 | 1.7240 | 1.6877 | 1.6711 | η | 1.6834 | 1.6558 | 1.6361 | 1.6296 |
| μ | -4.0044 | -4.0372 | -4.0819 | -4.1083 | μ | -4.2301 | -4.2624 | -4.3014 | -4.3226 |
| χ | 4.0044 | 4.0372 | 4.0819 | 4.1083 | χ | 4.2301 | 4.2624 | 4.3014 | 4.3226 |

| Compound 13 | | | | |
|-------------------|---------|---------|---------|---------|
| E_{HOMO} | -5.7993 | -5.7936 | -5.8112 | -5.8273 |
| E_{LUMO} | -2.2827 | -2.3774 | -2.4634 | -2.5094 |
| E_{GAP} | 3.5166 | 3.4162 | 3.3478 | 3.3179 |
| η | 1.7583 | 1.7081 | 1.6739 | 1.6590 |
| μ | -4.0410 | -4.0855 | -4.1373 | -4.1683 |
| χ | 4.0410 | 4.0855 | 4.1373 | 4.1683 |

Table S5. CT parameters for the bright low-lying excited state

| Compound | GP | | Toluene | | THF | | DMF | |
|-----------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| | q_{CT} | D_{CT} | q_{CT} | D_{CT} | q_{CT} | D_{CT} | q_{CT} | D_{CT} |
| 1 | 0.443 | 2.134 | 0.451 | 2.499 | 0.458 | 2.371 | 0.449 | 2.550 |
| 2 | 0.451 | 2.074 | 0.466 | 2.300 | 0.458 | 2.415 | 0.457 | 2.477 |
| 3 | 0.445 | 2.132 | 0.458 | 2.351 | 0.451 | 2.471 | 0.449 | 2.525 |
| 4 | 0.425 | 1.912 | 0.437 | 2.135 | 0.429 | 2.230 | 0.428 | 2.272 |
| 5 | 0.466 | 2.187 | 0.479 | 2.379 | 0.472 | 2.500 | 0.470 | 2.567 |
| 6 | 0.445 | 2.096 | 0.458 | 2.330 | 0.449 | 2.433 | 0.447 | 2.489 |
| 7 | 0.475 | 2.267 | 0.481 | 2.485 | 0.454 | 2.512 | 0.449 | 2.516 |
| 8 | 0.458 | 2.224 | 0.471 | 2.456 | 0.464 | 2.579 | 0.465 | 2.622 |
| 9 | 0.444 | 2.175 | 0.450 | 2.413 | 0.437 | 2.522 | 0.432 | 2.565 |
| 10 | 0.443 | 2.104 | 0.451 | 2.317 | 0.440 | 2.425 | 0.437 | 2.468 |
| 11 | 0.444 | 1.974 | 0.447 | 2.182 | 0.432 | 2.284 | 0.427 | 2.315 |
| 12 | 0.577 | 3.142 | 0.588 | 3.484 | 0.590 | 3.741 | 0.593 | 3.844 |
| 13 | 0.558 | 2.212 | 0.546 | 2.498 | 0.525 | 2.636 | 0.517 | 2.710 |

Table S6. The values of free energies (ΔG_{solv}) of solvation in kcal/mol obtained using SMD solvation model

| Compound | ΔG_{solv} | | |
|----------|-------------------|--------|--------|
| | Toluene | THF | DMF |
| 1 | -17.21 | -19.19 | -19.13 |
| 2 | -18.68 | -20.00 | -20.92 |
| 3 | -17.32 | -20.24 | -21.52 |
| 4 | -16.34 | -17.80 | -18.88 |
| 5 | -19.38 | -22.20 | -24.80 |
| 6 | -17.74 | -20.23 | -21.24 |
| 7 | -18.37 | -20.67 | -20.61 |
| 8 | -19.78 | -20.48 | -22.75 |
| 9 | -18.08 | -21.26 | -23.39 |
| 10 | -18.45 | -21.40 | -22.43 |
| 11 | -19.70 | -22.46 | -22.00 |
| 12 | -22.33 | -24.06 | -24.14 |
| 13 | -16.74 | -19.48 | -20.21 |

Table S7. The values of vertical excitation energies (in nm)

| Compound | GAZ | | Toluene | | THF | | DMF | |
|----------|----------------------|--------|----------------------|--------|----------------------|--------|----------------------|--------|
| | λ_{max}^{Ab} | f | λ_{max}^{Ab} | f | λ_{max}^{Ab} | f | λ_{max}^{Ab} | f |
| 1 | 424.22 | 1.0137 | 453.35 | 1.2007 | 457.13 | 1.1973 | 465.89 | 1.2122 |
| 2 | 427.74 | 1.0664 | 455.81 | 1.2524 | 459.33 | 1.2506 | 467.89 | 1.2657 |
| 3 | 426.21 | 1.0482 | 454.97 | 1.2371 | 458.66 | 1.2363 | 467.30 | 1.2518 |
| 4 | 433.29 | 0.9694 | 461.71 | 1.1576 | 464.59 | 1.1553 | 473.02 | 1.1710 |
| 5 | 430.87 | 1.1121 | 458.27 | 1.2879 | 461.92 | 1.2891 | 470.53 | 1.3051 |
| 6 | 428.06 | 1.1010 | 457.27 | 1.2885 | 460.83 | 1.2882 | 469.56 | 1.3035 |
| 7 | 430.32 | 1.0931 | 459.18 | 1.2938 | 463.07 | 1.3428 | 471.26 | 1.3618 |
| 8 | 424.40 | 1.0861 | 452.22 | 1.2699 | 456.06 | 1.2707 | 464.79 | 1.2856 |
| 9 | 434.40 | 0.9212 | 465.41 | 1.1183 | 470.73 | 1.1196 | 480.30 | 1.1389 |
| 10 | 433.49 | 0.9755 | 463.09 | 1.1765 | 467.03 | 1.1759 | 475.92 | 1.1929 |
| 11 | 440.84 | 0.9695 | 470.39 | 1.1804 | 473.89 | 1.1852 | 482.58 | 1.2056 |
| 12 | 436.54 | 0.9716 | 459.77 | 1.1809 | 458.83 | 1.1823 | 460.74 | 1.2011 |
| 13 | 446.92 | 0.9649 | 471.16 | 0.9497 | 470.90 | 0.9694 | 479.50 | 0.9928 |

Table S8. The values of cLR corrected excitation energies (in nm)

| Compound | λ_{cLR}^{Ab} | | |
|----------|----------------------|--------|--------|
| | Toluene | THF | DMF |
| 1 | 443.19 | 444.55 | 455.24 |
| 2 | 446.06 | 447.12 | 457.65 |
| 3 | 444.93 | 446.13 | 456.70 |
| 4 | 450.44 | 451.02 | 461.30 |
| 5 | 449.22 | 450.43 | 461.08 |
| 6 | 446.56 | 447.68 | 458.28 |
| 7 | 449.73 | 450.11 | 460.02 |
| 8 | 433.19 | 434.56 | 445.29 |
| 9 | 455.23 | 457.85 | 469.08 |
| 10 | 452.47 | 453.86 | 464.55 |
| 11 | 458.98 | 459.91 | 470.27 |
| 12 | 450.12 | 447.94 | 450.02 |
| 13 | 465.00 | 462.30 | 470.69 |

Table S9. Calculated values of dipole moments (in D) for the ground and CT excited state

| Compound | GP | | Toluene | | THF | | DMF | |
|----------|---------|------------|---------|------------|---------|------------|---------|------------|
| | μ_g | μ_{CT} | μ_g | μ_{CT} | μ_g | μ_{CT} | μ_g | μ_{CT} |
| 1 | 7.93 | 12.46 | 9.63 | 14.80 | 10.94 | 16.31 | 11.57 | 17.03 |
| 2 | 8.16 | 12.66 | 9.89 | 15.04 | 11.22 | 16.56 | 11.87 | 17.30 |
| 3 | 8.14 | 12.66 | 9.90 | 15.04 | 11.26 | 16.56 | 11.90 | 17.29 |
| 4 | 7.95 | 11.81 | 9.69 | 14.10 | 11.06 | 15.60 | 11.73 | 16.34 |
| 5 | 8.47 | 13.34 | 10.13 | 15.60 | 11.42 | 17.08 | 12.05 | 17.82 |
| 6 | 8.74 | 13.21 | 10.54 | 15.61 | 11.92 | 17.14 | 12.59 | 17.87 |
| 7 | 7.72 | 12.87 | 9.53 | 15.25 | 11.66 | 17.08 | 12.62 | 18.03 |
| 8 | 6.16 | 11.03 | 7.61 | 13.15 | 8.73 | 14.49 | 9.27 | 15.14 |
| 9 | 7.73 | 12.36 | 9.70 | 14.89 | 11.40 | 16.67 | 12.29 | 17.57 |
| 10 | 8.42 | 12.87 | 10.42 | 15.41 | 11.98 | 17.08 | 12.75 | 17.90 |
| 11 | 8.51 | 12.67 | 10.60 | 15.28 | 12.31 | 17.02 | 13.19 | 17.90 |
| 12 | 6.36 | 15.05 | 8.25 | 17.57 | 8.71 | 18.77 | 9.14 | 20.05 |
| 13 | 6.41 | 12.38 | 7.95 | 14.50 | 9.12 | 15.77 | 9.68 | 16.40 |

Table S10. The values of vertical and cLR corrected de-excitation energies (in nm)

| Compound | GP | Toluene | | THF | | DMF | |
|----------|----------------------|----------------------|-----------------------|----------------------|-----------------------|----------------------|-----------------------|
| | λ_{max}^{Fl} | λ_{max}^{Fl} | $\lambda_{cl.R}^{Fl}$ | λ_{max}^{Fl} | $\lambda_{cl.R}^{Fl}$ | λ_{max}^{Fl} | $\lambda_{cl.R}^{Fl}$ |
| 1 | 500.68 | 517.30 | 530.00 | 525.57 | 535.90 | 537.13 | 545.34 |
| 2 | 507.31 | 525.37 | 537.29 | 531.55 | 541.13 | 538.08 | 553.27 |
| 3 | 500.06 | 521.20 | 534.38 | 533.71 | 541.14 | 536.09 | 552.86 |
| 4 | 528.45 | 538.48 | 527.12 | 539.81 | 526.73 | 556.53 | 566.03 |
| 5 | 506.52 | 522.99 | 532.21 | 535.90 | 549.72 | 542.12 | 555.70 |
| 6 | 504.58 | 526.96 | 541.89 | 539.68 | 547.34 | 540.37 | 549.17 |
| 7 | 503.84 | 532.11 | 546.79 | 555.03 | 568.69 | 544.87 | 551.76 |
| 8 | 496.02 | 507.15 | 518.37 | 514.19 | 524.08 | 523.66 | 536.60 |
| 9 | 516.86 | 526.77 | 539.38 | 538.19 | 551.92 | 526.04 | 535.08 |
| 10 | 514.15 | 524.76 | 538.80 | 540.98 | 552.96 | 550.27 | 564.57 |
| 11 | 507.57 | 528.75 | 541.23 | 545.60 | 555.72 | 553.53 | 564.12 |
| 12 | 563.34 | 576.70 | 587.45 | 631.42 | 648.79 | 651.90 | 664.04 |
| 13 | 506.56 | 514.73 | 525.59 | 549.45 | 563.13 | 558.83 | 572.02 |