# Supporting Information

## Synthesis, Physical and Electroluminescence Properties of 3,6-Dipyrenylcarbazole End Capped Oligofluorenes

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**Content:**

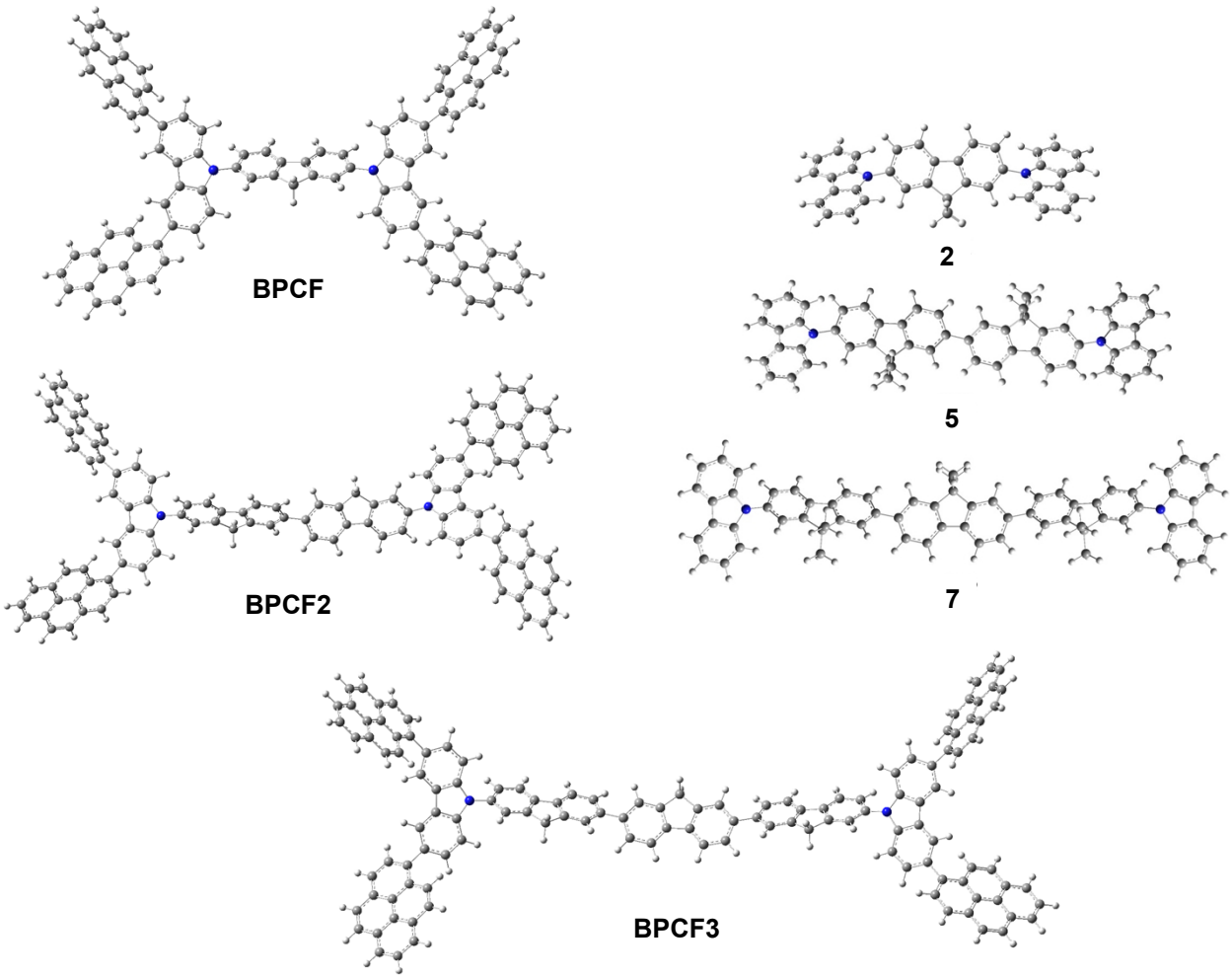



**Figure S1** The optimized structures of **BPCF*n***, **2**, **5** and **7** calculated by B3LYP/6-31G(d,p) in $CH_2Cl_2$ solvent.

Coordinate of the compounds optimized using B3LYP/6-31G(d,p) level of theory.

**Compound 2**

| | | | |
|---|---|---|---|
| C | 3.016120 | -1.150947 | -1.441838 |
| C | 3.460371 | -0.317323 | -0.404243 |
| C | 2.537425 | 0.347558 | 0.419402 |
| C | 1.179540 | 0.175510 | 0.185193 |
| C | 0.733395 | -0.670861 | -0.850115 |
| C | 1.651971 | -1.339366 | -1.662776 |
| H | 3.745599 | -1.641978 | -2.077028 |
| H | 2.897698 | 0.975239 | 1.228513 |
| H | 1.320319 | -1.989349 | -2.466840 |
| C | 0.000000 | 0.791758 | 0.937468 |
| C | -1.179540 | 0.175510 | 0.185193 |
| C | -2.537425 | 0.347558 | 0.419401 |
| C | -3.460371 | -0.317323 | -0.404243 |
| C | -3.016120 | -1.150947 | -1.441839 |
| C | -1.651971 | -1.339366 | -1.662776 |
| C | -0.733395 | -0.670861 | -0.850115 |
| H | -2.897699 | 0.975239 | 1.228512 |
| H | -3.745599 | -1.641979 | -2.077028 |
| H | -1.320319 | -1.989349 | -2.466840 |
| C | 5.539871 | 1.074709 | -0.177064 |
| C | 5.776603 | -1.167712 | 0.073062 |

| | | | |
|---|---|---|---|
| C | 5.055140 | 2.365305 | -0.412471 |
| C | 6.913959 | 0.834070 | 0.085159 |
| C | 5.563779 | -2.544750 | 0.193299 |
| C | 7.064643 | -0.597235 | 0.247164 |
| C | 5.966222 | 3.418740 | -0.364593 |
| H | 4.007285 | 2.543330 | -0.626766 |
| C | 7.808605 | 1.911134 | 0.128068 |
| C | 6.666602 | -3.348633 | 0.475421 |
| H | 4.575612 | -2.974399 | 0.073338 |
| C | 8.156372 | -1.428204 | 0.529761 |
| C | 7.329057 | 3.199273 | -0.094327 |
| H | 5.613085 | 4.430170 | -0.542523 |
| H | 8.862772 | 1.741853 | 0.328171 |
| C | 7.951803 | -2.801057 | 0.639746 |
| H | 6.526778 | -4.421255 | 0.571736 |
| H | 9.147962 | -1.005763 | 0.664807 |
| N | 4.856271 | -0.145787 | -0.183760 |
| C | -5.776603 | -1.167712 | 0.073063 |
| C | -5.539871 | 1.074709 | -0.177065 |
| C | -5.563778 | -2.544750 | 0.193300 |
| C | -7.064643 | -0.597235 | 0.247165 |
| C | -5.055141 | 2.365304 | -0.412475 |
| C | -6.913959 | 0.834070 | 0.085158 |
| C | -6.666601 | -3.348633 | 0.475424 |
| H | -4.575612 | -2.974399 | 0.073339 |
| C | -8.156372 | -1.428204 | 0.529763 |
| C | -5.966223 | 3.418740 | -0.364597 |
| H | -4.007286 | 2.543330 | -0.626770 |
| C | -7.808606 | 1.911133 | 0.128066 |
| C | -7.951802 | -2.801057 | 0.639749 |
| H | -6.526776 | -4.421255 | 0.571740 |
| H | -9.147961 | -1.005763 | 0.664809 |
| C | -7.329057 | 3.199272 | -0.094330 |
| H | -5.613086 | 4.430169 | -0.542527 |
| H | -8.862772 | 1.741853 | 0.328171 |
| N | -4.856272 | -0.145787 | -0.183760 |
| H | 8.789606 | -3.456327 | 0.857097 |
| H | 8.011697 | 4.042784 | -0.062612 |
| H | -8.011698 | 4.042783 | -0.062615 |
| H | -8.789604 | -3.456327 | 0.857101 |
| C | 0.000000 | 0.379892 | 2.426829 |
| H | 0.000000 | -0.708340 | 2.535805 |
| H | 0.884758 | 0.776318 | 2.934906 |
| H | -0.884759 | 0.776318 | 2.934906 |
| C | 0.000000 | 2.332833 | 0.815210 |
| H | 0.884901 | 2.756617 | 1.300507 |
| H | 0.000000 | 2.645467 | -0.232954 |
| H | -0.884901 | 2.756617 | 1.300507 |

**Compound 5**

| | | | |
|---|---|---|---|
| C | 1.162264 | 1.456762 | -0.911301 |
| C | 0.722929 | 0.168359 | -0.544996 |
| C | 1.687113 | -0.793453 | -0.177471 |
| C | 3.035388 | -0.465480 | -0.182336 |
| C | 3.455447 | 0.829280 | -0.547624 |
| C | 2.514547 | 1.794600 | -0.913565 |
| H | 0.432258 | 2.197468 | -1.222111 |
| H | 1.364531 | -1.783498 | 0.131631 |
| H | 2.823001 | 2.793900 | -1.207074 |
| C | 4.231465 | -1.346838 | 0.180604 |
| C | 5.389198 | -0.371864 | -0.033449 |
| C | 6.748176 | -0.591014 | 0.148647 |
| C | 7.647935 | 0.456089 | -0.109388 |
| C | 7.179426 | 1.707696 | -0.536213 |
| C | 5.812696 | 1.932219 | -0.701577 |
| C | 4.917288 | 0.888686 | -0.454338 |
| H | 7.126470 | -1.548403 | 0.493494 |
| H | 7.893008 | 2.497656 | -0.745168 |
| H | 5.461264 | 2.905592 | -1.030465 |
| C | -9.813154 | 0.730209 | -0.577744 |
| C | -9.884550 | -0.980841 | 0.909136 |
| C | -9.425958 | 1.678486 | -1.530007 |
| C | -11.159949 | 0.621514 | -0.142412 |
| C | -9.571506 | -2.036273 | 1.771729 |
| C | -11.205003 | -0.469461 | 0.809150 |
| C | -10.407486 | 2.531043 | -2.031836 |
| H | -8.398585 | 1.748900 | -1.869431 |
| C | -12.126775 | 1.491690 | -0.662607 |
| C | -10.606761 | -2.585673 | 2.525641 |
| H | -8.558853 | -2.415150 | 1.853646 |
| C | -12.227312 | -1.040719 | 1.577962 |
| C | -11.744531 | 2.444277 | -1.603473 |

| | | | |
|---|---|---|---|
| H | -10.130918 | 3.276693 | -2.771365 |
| H | -13.161190 | 1.420258 | -0.338776 |
| C | -11.922931 | -2.098341 | 2.430891 |
| H | -10.388871 | -3.407311 | 3.201527 |
| H | -13.242606 | -0.660264 | 1.511499 |
| N | -9.045790 | -0.246615 | 0.064615 |
| C | 9.884546 | 0.980873 | 0.909110 |
| C | 9.813159 | -0.730237 | -0.577700 |
| C | 9.571496 | 2.036347 | 1.771651 |
| C | 11.205003 | 0.469499 | 0.809139 |
| C | 9.425963 | -1.678558 | -1.529920 |
| C | 11.159955 | -0.621514 | -0.142375 |
| C | 10.606744 | 2.585782 | 2.525543 |
| H | 8.558839 | 2.415222 | 1.853537 |
| C | 12.227306 | 1.040794 | 1.577934 |
| C | 10.407491 | -2.531129 | -2.031720 |
| H | 8.398586 | -1.748988 | -1.869328 |
| C | 12.126783 | -1.491705 | -0.662544 |
| C | 11.922915 | 2.098445 | 2.430821 |
| H | 10.388855 | 3.407455 | 3.201386 |
| H | 13.242604 | 0.660346 | 1.511491 |
| C | 11.744537 | -2.444341 | -1.603359 |
| H | 10.130927 | -3.276818 | -2.771211 |
| H | 13.161202 | -1.420256 | -0.338730 |
| N | 9.045790 | 0.246608 | 0.064617 |
| C | -4.231466 | 1.346822 | 0.180640 |
| C | -3.035389 | 0.465472 | -0.182315 |
| C | -5.389196 | 0.371847 | -0.033421 |
| C | -1.687116 | 0.793451 | -0.177456 |
| C | -3.455443 | -0.829290 | -0.547605 |
| C | -6.748173 | 0.590996 | 0.148675 |
| C | -4.917283 | -0.888701 | -0.454318 |
| C | -0.722928 | -0.168353 | -0.544996 |
| H | -1.364538 | 1.783495 | 0.131656 |
| C | -2.514539 | -1.794603 | -0.913551 |
| C | -7.647936 | -0.456100 | -0.109378 |
| H | -7.126463 | 1.548380 | 0.493540 |
| C | -5.812693 | -1.932230 | -0.701563 |
| C | -1.162258 | -1.456757 | -0.911297 |
| H | -2.822988 | -2.793908 | -1.207055 |
| C | -7.179425 | -1.707702 | -0.536214 |
| H | -5.461267 | -2.905606 | -1.030447 |
| H | -0.432250 | -2.197463 | -1.222106 |
| H | -7.893004 | -2.497659 | -0.745192 |
| H | 12.706209 | 2.550822 | 3.031142 |
| H | 12.483814 | -3.125373 | -2.013533 |
| H | -12.483803 | 3.125299 | -2.013675 |
| H | -12.706230 | -2.550703 | 3.031216 |
| C | 4.340879 | -2.565012 | -0.764325 |
| H | 4.393985 | -2.249876 | -1.810432 |
| H | 5.237172 | -3.150620 | -0.535578 |
| H | 3.471796 | -3.220184 | -0.647319 |
| C | 4.159278 | -1.824149 | 1.648716 |
| H | 4.082026 | -0.976999 | 2.336285 |
| H | 3.287936 | -2.469288 | 1.799914 |
| H | 5.052824 | -2.399533 | 1.911318 |
| C | -4.159270 | 1.824106 | 1.648763 |
| H | -4.082014 | 0.976943 | 2.336314 |
| H | -3.287926 | 2.469241 | 1.799966 |
| H | -5.052813 | 2.399487 | 1.911382 |
| C | -4.340890 | 2.565012 | -0.764263 |
| H | -4.393997 | 2.249898 | -1.810377 |
| H | -5.237187 | 3.150609 | -0.535501 |
| H | -3.471812 | 3.220189 | -0.647247 |

**Compound 7**

| | | | |
|---|---|---|---|
| C | -5.448520 | -0.969768 | -1.654329 |
| C | -4.939749 | 0.024797 | -0.794550 |
| C | -5.843056 | 0.737852 | 0.021090 |
| C | -7.201176 | 0.457837 | -0.033633 |
| C | -7.691123 | -0.540781 | -0.899100 |
| C | -6.810930 | -1.258383 | -1.712228 |
| H | -4.766320 | -1.506854 | -2.305711 |
| H | -5.464136 | 1.489051 | 0.708084 |
| H | -7.174656 | -2.025251 | -2.390135 |
| C | -8.339360 | 1.098073 | 0.762481 |
| C | -9.544716 | 0.329232 | 0.220669 |
| C | -10.881618 | 0.458905 | 0.572676 |
| C | -11.835083 | -0.356033 | -0.059535 |
| C | -11.440316 | -1.293331 | -1.026040 |
| C | -10.094748 | -1.436687 | -1.364222 |
| C | -9.146558 | -0.620151 | -0.743033 |

| | | | |
|---|---|---|---|
| H | -11.201607 | 1.167779 | 1.330197 |
| H | -12.194501 | -1.901007 | -1.514671 |
| H | -9.800798 | -2.167641 | -2.111539 |
| C | 14.032599 | -1.259562 | 0.758610 |
| C | 13.971398 | 0.940391 | 0.209716 |
| C | 13.716962 | -2.595454 | 1.026586 |
| C | 15.333783 | -0.742466 | 0.992201 |
| C | 13.598223 | 2.214002 | -0.231543 |
| C | 15.295186 | 0.661743 | 0.639776 |
| C | 14.731016 | -3.414787 | 1.518851 |
| H | 12.718082 | -2.982537 | 0.859464 |
| C | 16.335165 | -1.588151 | 1.486773 |
| C | 14.568844 | 3.213899 | -0.220680 |
| H | 12.589448 | 2.418629 | -0.572249 |
| C | 16.251444 | 1.685414 | 0.641299 |
| C | 16.028795 | -2.921643 | 1.745169 |
| H | 14.510586 | -4.456354 | 1.733172 |
| H | 17.335604 | -1.206480 | 1.669730 |
| C | 15.882161 | 2.957848 | 0.213280 |
| H | 14.302544 | 4.211506 | -0.557214 |
| H | 17.268027 | 1.486865 | 0.968539 |
| N | 13.211458 | -0.231515 | 0.283744 |
| C | -14.032528 | -1.259532 | 0.758744 |
| C | -13.971460 | 0.940310 | 0.209411 |
| C | -13.716831 | -2.595383 | 1.026850 |
| C | -15.333653 | -0.742386 | 0.992569 |
| C | -13.598365 | 2.213838 | -0.232156 |
| C | -15.295142 | 0.661754 | 0.639860 |
| C | -14.730764 | -3.414628 | 1.519506 |
| H | -12.717994 | -2.982492 | 0.859527 |
| C | -16.334916 | -1.587989 | 1.487523 |
| C | -14.568967 | 3.213752 | -0.221230 |
| H | -12.589664 | 2.418379 | -0.573132 |
| C | -16.251384 | 1.685441 | 0.641428 |
| C | -16.028485 | -2.921439 | 1.746066 |
| H | -14.510290 | -4.456162 | 1.733940 |
| H | -17.335310 | -1.206289 | 1.670663 |
| C | -15.882183 | 2.957792 | 0.213091 |
| H | -14.302738 | 4.211300 | -0.557997 |
| H | -17.267890 | 1.486971 | 0.968955 |
| N | -13.211524 | -0.231590 | 0.283422 |
| C | -0.000002 | -1.400227 | -0.974569 |
| C | -1.180836 | -0.435957 | -0.852550 |
| C | 1.180819 | -0.435942 | -0.852540 |
| C | -2.538102 | -0.721512 | -0.890944 |
| C | -0.732728 | 0.888491 | -0.671139 |
| C | 2.538090 | -0.721477 | -0.890919 |
| C | 0.732693 | 0.888501 | -0.671134 |
| C | -3.484625 | 0.315148 | -0.750542 |
| H | -2.880475 | -1.746183 | -1.005011 |
| C | -1.656389 | 1.926887 | -0.527927 |
| C | 3.484594 | 0.315198 | -0.750503 |
| H | 2.880483 | -1.746141 | -1.004987 |
| C | 1.656336 | 1.926911 | -0.527908 |
| C | -3.018477 | 1.632958 | -0.569468 |
| H | -1.327605 | 2.953821 | -0.396147 |
| C | 3.018428 | 1.633001 | -0.569431 |
| H | 1.327531 | 2.953839 | -0.396131 |
| H | -3.736730 | 2.442626 | -0.486142 |
| H | 3.736674 | 2.442675 | -0.486091 |
| C | 8.339287 | 1.098119 | 0.762665 |
| C | 7.201124 | 0.457899 | -0.033495 |
| C | 9.544659 | 0.329293 | 0.220864 |
| C | 5.843000 | 0.737903 | 0.021199 |
| C | 7.691097 | -0.540689 | -0.898981 |
| C | 10.881549 | 0.458954 | 0.572922 |
| C | 9.146528 | -0.620065 | -0.742871 |
| C | 4.939724 | 0.024864 | -0.794489 |
| H | 5.464048 | 1.489078 | 0.708202 |
| C | 6.810935 | -1.258270 | -1.712160 |
| C | 11.835041 | -0.355968 | -0.059271 |
| H | 11.201501 | 1.167795 | 1.330488 |
| C | 10.094743 | -1.436590 | -1.364038 |
| C | 5.448521 | -0.969667 | -1.654289 |
| H | 7.174691 | -2.025112 | -2.390080 |
| C | 11.440297 | -1.293248 | -1.025808 |
| H | 9.800822 | -2.167529 | -2.111382 |
| H | 4.766337 | -1.506734 | -2.305704 |
| H | 12.194485 | -1.900921 | -1.514434 |
| H | 16.795937 | -3.587783 | 2.127693 |
| H | 16.613369 | 3.760274 | 0.210678 |
| H | -16.795536 | -3.587514 | 2.128885 |

| | | | |
|---|---|---|---|
| H | -16.613385 | 3.760225 | 0.210514 |
| C | 8.163477 | 0.873019 | 2.281584 |
| H | 7.261114 | 1.377134 | 2.641890 |
| H | 8.078476 | -0.191955 | 2.515999 |
| H | 9.018045 | 1.279080 | 2.832292 |
| C | 8.456649 | 2.610197 | 0.465394 |
| H | 9.315490 | 3.040395 | 0.990624 |
| H | 8.581559 | 2.793900 | -0.605635 |
| H | 7.558217 | 3.137425 | 0.801665 |
| C | 0.000004 | -2.438199 | 0.170674 |
| H | 0.000002 | -1.947173 | 1.148143 |
| H | -0.884980 | -3.079839 | 0.109381 |
| H | 0.884997 | -3.079827 | 0.109380 |
| C | 0.000008 | -2.123415 | -2.339973 |
| H | 0.000010 | -1.406625 | -3.166283 |
| H | 0.885233 | -2.760013 | -2.438234 |
| H | -0.885214 | -2.760017 | -2.438243 |
| C | -8.163589 | 0.873012 | 2.281410 |
| H | -8.078608 | -0.191956 | 2.515856 |
| H | -7.261229 | 1.377124 | 2.641726 |
| H | -9.018165 | 1.279099 | 2.832088 |
| C | -8.456721 | 2.610144 | 0.465169 |
| H | -8.581619 | 2.793817 | -0.605867 |
| H | -9.315568 | 3.040354 | 0.990377 |
| H | -7.558294 | 3.137382 | 0.801435 |

**Compound BPCF**

| | | | |
|---|---|---|---|
| H | -0.000090 | -2.017292 | 1.032237 |
| C | -3.018960 | 0.894256 | -1.415033 |
| C | -3.461310 | 0.110195 | -0.338173 |
| C | -2.538657 | -0.516638 | 0.514125 |
| C | -1.182088 | -0.354826 | 0.268254 |
| C | -0.733936 | 0.442066 | -0.807110 |
| C | -1.655227 | 1.071705 | -1.648271 |
| H | -3.749886 | 1.355183 | -2.071751 |
| H | -2.892931 | -1.106377 | 1.354387 |
| H | -1.325953 | 1.683857 | -2.483106 |
| C | -0.000093 | -0.919110 | 1.029053 |
| H | -0.000177 | -0.607888 | 2.082185 |
| C | 1.182020 | -0.354816 | 0.268445 |
| C | 2.538555 | -0.516616 | 0.514525 |
| C | 3.461319 | 0.110245 | -0.337621 |
| C | 3.019150 | 0.894310 | -1.414544 |
| C | 1.655449 | 1.071735 | -1.647995 |
| C | 0.734032 | 0.442066 | -0.806995 |
| H | 2.892700 | -1.106356 | 1.354838 |
| H | 3.750165 | 1.355261 | -2.071144 |
| H | 1.326294 | 1.683901 | -2.482867 |
| C | -5.537678 | -1.265674 | -0.011877 |
| C | -5.771123 | 0.982647 | 0.130551 |
| C | -5.063493 | -2.569022 | -0.185073 |
| C | -6.903207 | -1.015175 | 0.278259 |
| C | -5.565239 | 2.364295 | 0.178210 |
| C | -7.051513 | 0.423326 | 0.373664 |
| C | -5.970066 | -3.614925 | -0.044906 |
| H | -4.024257 | -2.766097 | -0.425761 |
| C | -7.793591 | -2.084587 | 0.414852 |
| C | -6.661390 | 3.177536 | 0.448901 |
| H | -4.582236 | 2.795345 | 0.021527 |
| C | -8.136057 | 1.262886 | 0.645211 |
| C | -7.337212 | -3.400013 | 0.254656 |
| H | -5.619897 | -4.633811 | -0.183181 |
| H | -8.833693 | -1.897322 | 0.665844 |
| C | -7.956447 | 2.651794 | 0.676790 |
| H | -6.512173 | 4.251427 | 0.509259 |
| H | -9.122173 | 0.842245 | 0.822721 |
| N | -4.857217 | -0.048664 | -0.104003 |
| C | 5.771130 | 0.982650 | 0.131220 |
| C | 5.537656 | -1.265665 | -0.011278 |
| C | 5.565280 | 2.364304 | 0.178959 |
| C | 7.051541 | 0.423303 | 0.374182 |
| C | 5.063446 | -2.569001 | -0.184483 |
| C | 6.903218 | -1.015182 | 0.278718 |
| C | 6.661479 | 3.177515 | 0.449523 |
| H | 4.582265 | 2.795379 | 0.022421 |
| C | 8.136134 | 1.262837 | 0.645616 |
| C | 5.970035 | -3.614915 | -0.044499 |
| H | 4.024184 | -2.766058 | -0.425078 |
| C | 7.793612 | -2.084608 | 0.415167 |
| C | 7.956560 | 2.651748 | 0.677256 |
| H | 6.512285 | 4.251406 | 0.509939 |
| H | 9.122262 | 0.842172 | 0.823004 |

| | | | |
|---|---|---|---|
| C | 7.337215 | -3.400018 | 0.254901 |
| H | 5.619849 | -4.633792 | -0.182792 |
| H | 8.833733 | -1.897364 | 0.666089 |
| N | 4.857187 | -0.048647 | -0.103224 |
| C | -9.100886 | 3.543959 | 1.014938 |
| C | -9.486003 | 4.645777 | 0.204355 |
| C | -9.825796 | 3.282590 | 2.189170 |
| C | -10.569016 | 5.484373 | 0.627062 |
| C | -8.859026 | 4.945718 | -1.057385 |
| C | -10.884083 | 4.085729 | 2.596951 |
| H | -9.527457 | 2.441284 | 2.808307 |
| C | -10.963526 | 6.608231 | -0.164670 |
| C | -11.269247 | 5.202671 | 1.840451 |
| C | -9.240119 | 6.013189 | -1.813460 |
| H | -8.070697 | 4.293011 | -1.414654 |
| H | -11.411662 | 3.859827 | 3.520222 |
| C | -10.293724 | 6.892806 | -1.393591 |
| C | -12.034342 | 7.453228 | 0.266313 |
| C | -12.342797 | 6.066905 | 2.247524 |
| H | -8.750105 | 6.210418 | -2.763821 |
| C | -10.693604 | 8.004563 | -2.154377 |
| C | -12.398130 | 8.555145 | -0.525900 |
| C | -12.706833 | 7.144296 | 1.498617 |
| H | -12.861891 | 5.839978 | 3.175455 |
| C | -11.733172 | 8.826242 | -1.721411 |
| H | -10.182286 | 8.217379 | -3.089829 |
| H | -13.210326 | 9.198035 | -0.195931 |
| H | -13.519701 | 7.790489 | 1.820344 |
| H | -12.029510 | 9.682607 | -2.320878 |
| C | -8.236518 | -4.569767 | 0.460843 |
| C | -9.485213 | -4.716477 | -0.202195 |
| C | -7.828369 | -5.568072 | 1.361122 |
| C | -10.312087 | -5.848140 | 0.100492 |
| C | -9.953551 | -3.794473 | -1.204958 |
| C | -8.620393 | -6.672908 | 1.647576 |
| H | -6.874503 | -5.452863 | 1.868029 |
| C | -11.581363 | -6.007239 | -0.539491 |
| C | -9.875291 | -6.831496 | 1.040728 |
| C | -11.160076 | -3.950989 | -1.818309 |
| H | -9.317142 | -2.962438 | -1.483375 |
| H | -8.276369 | -7.416828 | 2.361775 |
| C | -12.027005 | -5.050045 | -1.501210 |
| C | -12.412465 | -7.128106 | -0.223979 |
| C | -10.728853 | -7.949230 | 1.335326 |
| H | -11.482781 | -3.239881 | -2.574891 |
| C | -13.279828 | -5.221344 | -2.114259 |
| C | -13.658442 | -7.257109 | -0.860437 |
| C | -11.942772 | -8.090355 | 0.734904 |
| H | -10.381007 | -8.685517 | 2.055712 |
| C | -14.085558 | -6.312760 | -1.793403 |
| H | -13.614857 | -4.490723 | -2.846215 |
| H | -14.289973 | -8.107996 | -0.617555 |
| H | -12.579160 | -8.940145 | 0.968945 |
| H | -15.052141 | -6.430166 | -2.275546 |
| C | 9.101061 | 3.543870 | 1.015259 |
| C | 9.486030 | 4.645757 | 0.204697 |
| C | 9.826205 | 3.282412 | 2.189331 |
| C | 10.569126 | 5.484319 | 0.627261 |
| C | 8.858820 | 4.945796 | -1.056902 |
| C | 10.884572 | 4.085514 | 2.596972 |
| H | 9.527985 | 2.441066 | 2.808471 |
| C | 10.963487 | 6.608240 | -0.164456 |
| C | 11.269592 | 5.202521 | 1.840491 |
| C | 9.239779 | 6.013320 | -1.812971 |
| H | 8.070422 | 4.293123 | -1.414083 |
| H | 11.412335 | 3.859523 | 3.520116 |
| C | 10.293459 | 6.892908 | -1.393233 |
| C | 12.034380 | 7.453206 | 0.266396 |
| C | 12.343211 | 6.066726 | 2.247436 |
| H | 8.749596 | 6.210605 | -2.763234 |
| C | 10.693196 | 8.004726 | -2.154006 |
| C | 12.398019 | 8.555185 | -0.525800 |
| C | 12.707100 | 7.144182 | 1.498550 |
| H | 12.862480 | 5.839724 | 3.175251 |
| C | 11.732841 | 8.826373 | -1.721168 |
| H | 10.181705 | 8.217614 | -3.089348 |
| H | 13.210276 | 9.198052 | -0.195934 |
| H | 13.520020 | 7.790356 | 1.820187 |
| H | 12.029066 | 9.682788 | -2.320620 |
| C | 8.236569 | -4.569784 | 0.460894 |
| C | 9.485141 | -4.716475 | -0.202385 |
| C | 7.828562 | -5.568121 | 1.361195 |

| | | | |
|---|---|---|---|
| C | 10.312073 | -5.848144 | 0.100138 |
| C | 9.953296 | -3.794478 | -1.205247 |
| C | 8.620634 | -6.672966 | 1.647478 |
| H | 6.874779 | -5.452922 | 1.868261 |
| C | 11.581248 | -6.007227 | -0.540052 |
| C | 9.875431 | -6.831527 | 1.040420 |
| C | 11.159724 | -3.950977 | -1.818790 |
| H | 9.316820 | -2.962471 | -1.483584 |
| H | 8.276737 | -7.416913 | 2.361712 |
| C | 12.026727 | -5.050013 | -1.501825 |
| C | 12.412410 | -7.128093 | -0.224697 |
| C | 10.729043 | -7.949271 | 1.334843 |
| H | 11.482297 | -3.239877 | -2.575435 |
| C | 13.279458 | -5.221282 | -2.115069 |
| C | 13.658291 | -7.257067 | -0.861346 |
| C | 11.942869 | -8.090371 | 0.734229 |
| H | 10.381313 | -8.685586 | 2.055256 |
| C | 14.085254 | -6.312692 | -1.794355 |
| H | 13.614363 | -4.490645 | -2.847067 |
| H | 14.289867 | -8.107952 | -0.618573 |
| H | 12.579291 | -8.940172 | 0.968140 |
| H | 15.051763 | -6.430074 | -2.276652 |

**Compound BPCF2**

| | | | |
|---|---|---|---|
| H | -4.243050 | -2.067540 | -1.584576 |
| C | -1.218304 | -0.255147 | 1.751659 |
| C | -0.733107 | -0.691710 | 0.501418 |
| C | -1.661492 | -0.969893 | -0.522857 |
| C | -3.020148 | -0.807996 | -0.290484 |
| C | -3.488031 | -0.363255 | 0.964119 |
| C | -2.580984 | -0.087770 | 1.990540 |
| H | -0.514136 | -0.065239 | 2.556212 |
| H | -1.307848 | -1.284447 | -1.501126 |
| H | -2.923453 | 0.245814 | 2.966543 |
| C | -4.187595 | -1.028686 | -1.232325 |
| H | -4.117459 | -0.402409 | -2.131805 |
| C | -5.380924 | -0.658397 | -0.374596 |
| C | -6.729425 | -0.645811 | -0.705223 |
| C | -7.662143 | -0.256123 | 0.269044 |
| C | -7.238271 | 0.120092 | 1.552964 |
| C | -5.882107 | 0.123704 | 1.877773 |
| C | -4.950757 | -0.270036 | 0.913043 |
| H | -7.070020 | -0.918225 | -1.699934 |
| H | -7.978905 | 0.401235 | 2.294958 |
| H | -5.566010 | 0.420583 | 2.873845 |
| C | 9.624878 | 1.112209 | -0.214795 |
| C | 10.039607 | -0.976332 | 0.556269 |
| C | 9.044676 | 2.273232 | -0.733703 |
| C | 11.014542 | 1.048393 | 0.062058 |
| C | 9.946200 | -2.296978 | 1.004792 |
| C | 11.278574 | -0.285896 | 0.561662 |
| C | 9.871282 | 3.369916 | -0.956474 |
| H | 7.985655 | 2.322655 | -0.963640 |
| C | 11.823013 | 2.165300 | -0.170283 |
| C | 11.111379 | -2.921651 | 1.438984 |
| H | 8.996592 | -2.820864 | 1.026144 |
| C | 12.433578 | -0.934981 | 1.008386 |
| C | 11.260726 | 3.341187 | -0.685180 |
| H | 9.438399 | 4.277104 | -1.368211 |
| H | 12.883036 | 2.127619 | 0.064150 |
| C | 12.365459 | -2.264269 | 1.444363 |
| H | 11.051899 | -3.941490 | 1.807353 |
| H | 13.387727 | -0.414837 | 1.009904 |
| N | 9.039988 | -0.120760 | 0.085100 |
| C | -9.894369 | 0.872744 | 0.039535 |
| C | -9.805499 | -1.325988 | -0.493702 |
| C | -9.600335 | 2.188358 | 0.409226 |
| C | -11.203283 | 0.496857 | -0.356588 |
| C | -9.417931 | -2.650426 | -0.715475 |
| C | -11.147926 | -0.912018 | -0.691659 |
| C | -10.637955 | 3.115122 | 0.399025 |
| H | -8.595006 | 2.486205 | 0.687425 |
| C | -12.227541 | 1.448926 | -0.361124 |
| C | -10.388701 | -3.548764 | -1.147641 |
| H | -8.396242 | -2.976310 | -0.551397 |
| C | -12.103792 | -1.835078 | -1.126423 |
| C | -11.959424 | 2.767915 | 0.026733 |
| H | -10.421329 | 4.145196 | 0.665954 |
| H | -13.235413 | 1.167300 | -0.654072 |
| C | -11.736153 | -3.167662 | -1.356593 |
| H | -10.106793 | -4.584343 | -1.315296 |
| H | -13.127837 | -1.516932 | -1.299869 |

| | | | |
|---|---|---|---|
| N | -9.051321 | -0.237923 | -0.047657 |
| C | 13.585960 | -2.940190 | 1.968261 |
| C | 14.053450 | -4.183970 | 1.465484 |
| C | 14.300600 | -2.317536 | 3.004365 |
| C | 15.212196 | -4.788749 | 2.053673 |
| C | 13.435563 | -4.859364 | 0.353358 |
| C | 15.429542 | -2.895893 | 3.572407 |
| H | 13.939352 | -1.367271 | 3.387364 |
| C | 15.694758 | -6.045221 | 1.570216 |
| C | 15.900889 | -4.138791 | 3.123811 |
| C | 13.900416 | -6.053308 | -0.110155 |
| H | 12.584906 | -4.393084 | -0.130806 |
| H | 15.948188 | -2.390645 | 4.383300 |
| C | 15.036380 | -6.698806 | 0.484255 |
| C | 16.843237 | -6.654210 | 2.167289 |
| C | 17.052340 | -4.773405 | 3.704091 |
| H | 13.415041 | -6.535992 | -0.954943 |
| C | 15.525259 | -7.933842 | 0.025547 |
| C | 17.294686 | -7.891127 | 1.677058 |
| C | 17.501445 | -5.976246 | 3.250616 |
| H | 17.561676 | -4.267242 | 4.520440 |
| C | 16.641238 | -8.521974 | 0.618798 |
| H | 15.022146 | -8.427785 | -0.801917 |
| H | 18.166296 | -8.353921 | 2.133047 |
| H | 18.373275 | -6.444715 | 3.700458 |
| H | 17.006158 | -9.477724 | 0.252867 |
| C | 12.075468 | 4.571130 | -0.893085 |
| C | 13.276422 | 4.585874 | -1.653154 |
| C | 11.633214 | 5.767823 | -0.305094 |
| C | 14.024952 | 5.804150 | -1.759938 |
| C | 13.767761 | 3.433719 | -2.364634 |
| C | 12.348968 | 6.953486 | -0.416005 |
| H | 10.715878 | 5.753384 | 0.276670 |
| C | 15.245255 | 5.838966 | -2.505205 |
| C | 13.557044 | 6.997284 | -1.127945 |
| C | 14.927568 | 3.469998 | -3.078556 |
| H | 13.186348 | 2.519453 | -2.337184 |
| H | 11.981681 | 7.856097 | 0.065867 |
| C | 15.718619 | 4.664419 | -3.165729 |
| C | 15.998694 | 7.051539 | -2.598410 |
| C | 14.332525 | 8.201739 | -1.241001 |
| H | 15.268972 | 2.584044 | -3.608403 |
| C | 16.922542 | 4.718314 | -3.888363 |
| C | 17.197808 | 7.057824 | -3.330733 |
| C | 15.500859 | 8.228225 | -1.939801 |
| H | 13.962924 | 9.099116 | -0.750946 |
| C | 17.653035 | 5.903051 | -3.966358 |
| H | 17.278863 | 3.822251 | -4.390242 |
| H | 17.770391 | 7.979440 | -3.398773 |
| H | 16.078170 | 9.146341 | -2.015025 |
| H | 18.582427 | 5.927947 | -4.528623 |
| C | -13.038982 | 3.794028 | -0.018838 |
| C | -13.371908 | 4.610263 | 1.095712 |
| C | -13.752976 | 3.960687 | -1.216577 |
| C | -14.391529 | 5.608049 | 0.956137 |
| C | -12.754166 | 4.458998 | 2.388155 |
| C | -14.749839 | 4.919470 | -1.353449 |
| H | -13.494399 | 3.336266 | -2.067096 |
| C | -14.732940 | 6.450666 | 2.060157 |
| C | -15.081116 | 5.766667 | -0.285388 |
| C | -13.084987 | 5.258384 | 3.440661 |
| H | -12.014844 | 3.677712 | 2.522684 |
| H | -15.270702 | 5.029015 | -2.301360 |
| C | -14.073608 | 6.291610 | 3.317118 |
| C | -15.740099 | 7.456177 | 1.914963 |
| C | -16.089925 | 6.783560 | -0.401937 |
| H | -12.604035 | 5.116094 | 4.405367 |
| C | -14.420850 | 7.132342 | 4.388197 |
| C | -16.052540 | 8.275414 | 3.012855 |
| C | -16.403181 | 7.593434 | 0.646908 |
| H | -16.601581 | 6.893272 | -1.354935 |
| C | -15.398344 | 8.114171 | 4.233914 |
| H | -13.917472 | 7.007410 | 5.343616 |
| H | -16.816286 | 9.040869 | 2.900506 |
| H | -17.167498 | 8.359589 | 0.543268 |
| H | -15.654458 | 8.756966 | 5.071613 |
| C | -12.714262 | -4.169001 | -1.866979 |
| C | -13.961211 | -4.423144 | -1.233974 |
| C | -12.386425 | -4.888858 | -3.027696 |
| C | -14.866654 | -5.367970 | -1.819721 |
| C | -14.352628 | -3.799997 | 0.004450 |
| C | -13.255831 | -5.814122 | -3.592306 |

| | | | |
|---|---|---|---|
| H | -11.433164 | -4.691906 | -3.510124 |
| C | -16.134339 | -5.627227 | -1.210036 |
| C | -14.510056 | -6.064284 | -3.015474 |
| C | -15.558098 | -4.052332 | 0.586923 |
| H | -13.658185 | -3.122142 | 0.487132 |
| H | -12.972472 | -6.340942 | -4.500066 |
| C | -16.500902 | -4.960771 | -0.001199 |
| C | -17.043146 | -6.558719 | -1.804143 |
| C | -15.441181 | -6.996964 | -3.588354 |
| H | -15.821879 | -3.569169 | 1.524572 |
| C | -17.753176 | -5.225427 | 0.578768 |
| C | -18.285372 | -6.790309 | -1.189730 |
| C | -16.652839 | -7.231360 | -3.012997 |
| H | -15.154418 | -7.515100 | -4.500145 |
| C | -18.634585 | -6.129129 | -0.012616 |
| H | -18.028097 | -4.716580 | 1.499275 |
| H | -18.975812 | -7.496495 | -1.644070 |
| H | -17.348043 | -7.938242 | -3.458994 |
| H | -19.599522 | -6.321856 | 0.448109 |
| C | 4.161578 | 0.722459 | 1.148194 |
| C | 3.004518 | -0.109718 | 0.632532 |
| H | 4.083991 | 1.773877 | 0.840262 |
| C | 5.363218 | 0.039296 | 0.528036 |
| C | 1.644731 | 0.043067 | 0.861602 |
| C | 3.484189 | -1.148994 | -0.192557 |
| C | 6.709926 | 0.350470 | 0.654673 |
| C | 4.947290 | -1.059461 | -0.255386 |
| C | 0.725017 | -0.846375 | 0.268907 |
| H | 1.283240 | 0.863069 | 1.476350 |
| C | 2.585442 | -2.039175 | -0.786394 |
| C | 7.654531 | -0.433830 | -0.026366 |
| H | 7.042143 | 1.178608 | 1.273810 |
| C | 5.891527 | -1.843667 | -0.923881 |
| C | 1.220581 | -1.881009 | -0.551254 |
| H | 2.935996 | -2.851793 | -1.417223 |
| C | 7.244205 | -1.520622 | -0.813720 |
| H | 5.586602 | -2.688823 | -1.534612 |
| H | 0.523546 | -2.587506 | -0.992155 |
| H | 7.990038 | -2.102954 | -1.345507 |
| H | 4.211331 | 0.726321 | 2.245368 |

**Compound BPCF3**

| | | | |
|---|---|---|---|
| H | 8.175705 | -2.292714 | 0.459972 |
| C | 5.422942 | 0.316426 | -2.573270 |
| C | 4.837370 | -0.448249 | -1.543010 |
| C | 5.672986 | -0.980506 | -0.539708 |
| C | 7.040305 | -0.747159 | -0.579297 |
| C | 7.610381 | 0.020134 | -1.617198 |
| C | 6.795642 | 0.554049 | -2.619015 |
| H | 4.791939 | 0.710590 | -3.364544 |
| H | 5.238630 | -1.550928 | 0.277062 |
| H | 7.217474 | 1.141011 | -3.430687 |
| C | 8.118019 | -1.198351 | 0.386616 |
| H | 7.939183 | -0.830881 | 1.406057 |
| C | 9.374850 | -0.605998 | -0.218099 |
| C | 10.683789 | -0.673249 | 0.239414 |
| C | 11.694753 | -0.040528 | -0.501783 |
| C | 11.384775 | 0.655087 | -1.680842 |
| C | 10.066002 | 0.740081 | -2.126785 |
| C | 9.058007 | 0.104903 | -1.396307 |
| H | 10.933871 | -1.194016 | 1.159080 |
| H | 12.184049 | 1.120448 | -2.248839 |
| H | 9.838414 | 1.285459 | -3.038389 |
| C | -14.086802 | 1.730563 | -0.869034 |
| C | -14.124852 | -0.524011 | -1.073387 |
| C | -13.721126 | 3.078277 | -0.811092 |
| C | -15.413521 | 1.317514 | -0.583298 |
| C | -13.816200 | -1.866767 | -1.309546 |
| C | -15.438753 | -0.125157 | -0.718038 |
| C | -14.704239 | 4.005170 | -0.478548 |
| H | -12.704148 | 3.397404 | -1.013463 |
| C | -16.382423 | 2.269544 | -0.252576 |
| C | -14.833346 | -2.804787 | -1.163127 |
| H | -12.819832 | -2.173276 | -1.610006 |
| C | -16.442091 | -1.088241 | -0.575748 |
| C | -16.038789 | 3.626945 | -0.194639 |
| H | -14.435654 | 5.056127 | -0.420949 |
| H | -17.405512 | 1.959984 | -0.059147 |
| C | -16.150144 | -2.442233 | -0.787399 |
| H | -14.613555 | -3.848568 | -1.366052 |
| H | -17.448048 | -0.791577 | -0.291409 |
| N | -13.310339 | 0.607114 | -1.163007 |

| | | | |
|---|---|---|---|
| C | 13.870981 | 0.992601 | 0.213671 |
| C | 13.765977 | -1.269817 | 0.216752 |
| C | 13.596185 | 2.360567 | 0.127144 |
| C | 15.134444 | 0.526369 | 0.658067 |
| C | 13.382963 | -2.607754 | 0.085670 |
| C | 15.068877 | -0.921047 | 0.655938 |
| C | 14.608852 | 3.252007 | 0.467562 |
| H | 12.622532 | 2.723164 | -0.184522 |
| C | 16.134253 | 1.443281 | 0.996063 |
| C | 14.314647 | -3.586911 | 0.416277 |
| H | 12.394324 | -2.881599 | -0.266855 |
| C | 15.986359 | -1.924511 | 0.981323 |
| C | 15.887464 | 2.818469 | 0.895083 |
| H | 14.403071 | 4.317325 | 0.424064 |
| H | 17.108062 | 1.092640 | 1.327092 |
| C | 15.620205 | -3.271994 | 0.864220 |
| H | 14.035999 | -4.631751 | 0.313361 |
| H | 16.976609 | -1.660497 | 1.341431 |
| N | 13.045086 | -0.103152 | -0.052492 |
| C | -17.231926 | -3.461461 | -0.686354 |
| C | -17.111557 | -4.643348 | 0.094396 |
| C | -18.421223 | -3.243116 | -1.401491 |
| C | -18.179920 | -5.599304 | 0.091427 |
| C | -15.970364 | -4.917745 | 0.929599 |
| C | -19.465904 | -4.159125 | -1.394382 |
| H | -18.509822 | -2.341145 | -2.000322 |
| C | -18.071494 | -6.806303 | 0.851282 |
| C | -19.366215 | -5.354463 | -0.666759 |
| C | -15.871085 | -6.065283 | 1.657386 |
| H | -15.177310 | -4.180923 | 0.984715 |
| H | -20.364992 | -3.960803 | -1.972446 |
| C | -16.905448 | -7.060008 | 1.636035 |
| C | -19.131132 | -7.767163 | 0.833334 |
| C | -20.416754 | -6.334861 | -0.662248 |
| H | -14.998138 | -6.240764 | 2.281401 |
| C | -16.815173 | -8.255405 | 2.369318 |
| C | -18.996126 | -8.949246 | 1.580732 |
| C | -20.304242 | -7.489614 | 0.050446 |
| H | -21.310488 | -6.133107 | -1.247537 |
| C | -17.849808 | -9.189055 | 2.337865 |
| H | -15.926225 | -8.444406 | 2.965880 |
| H | -19.801188 | -9.679649 | 1.563863 |
| H | -21.105990 | -8.223776 | 0.042388 |
| H | -17.764151 | -10.108919 | 2.909739 |
| C | -17.057874 | 4.674832 | 0.093529 |
| C | -17.899762 | 4.640727 | 1.237945 |
| C | -17.196789 | 5.736290 | -0.815995 |
| C | -18.897724 | 5.656113 | 1.406778 |
| C | -17.776265 | 3.644980 | 2.271562 |
| C | -18.153440 | 6.730245 | -0.649436 |
| H | -16.553080 | 5.760052 | -1.690828 |
| C | -19.770385 | 5.630007 | 2.539677 |
| C | -19.028308 | 6.706801 | 0.447146 |
| C | -18.603706 | 3.625546 | 3.353772 |
| H | -16.992569 | 2.901073 | 2.186108 |
| H | -18.240505 | 7.527272 | -1.383611 |
| C | -19.640592 | 4.603263 | 3.524024 |
| C | -20.777635 | 6.633539 | 2.697276 |
| C | -20.046252 | 7.703943 | 0.632963 |
| H | -18.481204 | 2.863281 | 4.119366 |
| C | -20.511728 | 4.592077 | 4.626556 |
| C | -21.627827 | 6.580825 | 3.814692 |
| C | -20.885184 | 7.667893 | 1.704927 |
| H | -20.133586 | 8.493998 | -0.108813 |
| C | -21.495211 | 5.570119 | 4.766345 |
| H | -20.409366 | 3.809492 | 5.374149 |
| H | -22.394534 | 7.342589 | 3.931633 |
| H | -21.652340 | 8.427881 | 1.830647 |
| H | -22.161562 | 5.546566 | 5.624210 |
| C | 16.937224 | 3.795237 | 1.299867 |
| C | 17.369830 | 4.856189 | 0.458952 |
| C | 17.520685 | 3.658618 | 2.570154 |
| C | 18.352011 | 5.780879 | 0.943869 |
| C | 16.893196 | 5.030473 | -0.889215 |
| C | 18.481868 | 4.545507 | 3.039846 |
| H | 17.186229 | 2.848156 | 3.211571 |
| C | 18.790823 | 6.865488 | 0.121214 |
| C | 18.907312 | 5.625002 | 2.251283 |
| C | 17.316545 | 6.060919 | -1.673664 |
| H | 16.187169 | 4.311032 | -1.287988 |
| H | 18.899815 | 4.415544 | 4.034942 |
| C | 18.267659 | 7.024901 | -1.198148 |

| | | | |
|---|---|---|---|
| C | 19.760019 | 7.796097 | 0.612121 |
| C | 19.881464 | 6.573083 | 2.717259 |
| H | 16.941285 | 6.162786 | -2.689063 |
| C | 18.708304 | 8.099983 | -1.988562 |
| C | 20.169340 | 8.857111 | -0.213058 |
| C | 20.287043 | 7.612606 | 1.936871 |
| H | 20.290334 | 6.441078 | 3.715976 |
| C | 19.647154 | 9.005935 | -1.497614 |
| H | 18.308536 | 8.217088 | -2.992682 |
| H | 20.903970 | 9.565174 | 0.162226 |
| H | 21.023566 | 8.323343 | 2.303297 |
| H | 19.976763 | 9.832504 | -2.121062 |
| C | 16.548545 | -4.369087 | 1.257355 |
| C | 17.867294 | -4.488852 | 0.741324 |
| C | 16.096310 | -5.322573 | 2.184411 |
| C | 18.713075 | -5.546067 | 1.213274 |
| C | 18.393418 | -3.613833 | -0.274898 |
| C | 16.908599 | -6.355390 | 2.636314 |
| H | 15.088039 | -5.228519 | 2.577795 |
| C | 20.049498 | -5.676560 | 0.720725 |
| C | 18.227872 | -6.483407 | 2.176516 |
| C | 19.664680 | -3.743226 | -0.747462 |
| H | 17.750009 | -2.841332 | -0.680074 |
| H | 16.527829 | -7.065335 | 3.366264 |
| C | 20.546530 | -4.765758 | -0.260757 |
| C | 20.897284 | -6.722686 | 1.203954 |
| C | 19.100566 | -7.525845 | 2.642216 |
| H | 20.030234 | -3.069678 | -1.518768 |
| C | 21.864050 | -4.908110 | -0.728142 |
| C | 22.208312 | -6.825180 | 0.709124 |
| C | 20.376807 | -7.639249 | 2.181318 |
| H | 18.715961 | -8.227767 | 3.378059 |
| C | 22.684379 | -5.926378 | -0.244954 |
| H | 22.238069 | -4.213204 | -1.475806 |
| H | 22.851905 | -7.619249 | 1.079307 |
| H | 21.026058 | -8.432027 | 2.544525 |
| H | 23.701037 | -6.022236 | -0.616047 |
| C | -0.038863 | 1.011699 | -2.248836 |
| C | 1.104659 | 0.086651 | -1.880829 |
| H | -0.036611 | 1.929393 | -1.645078 |
| C | -1.260354 | 0.155354 | -1.977714 |
| C | 2.471562 | 0.321801 | -1.918535 |
| C | 0.599091 | -1.155659 | -1.440558 |
| C | -2.603535 | 0.470211 | -2.125143 |
| C | -0.865206 | -1.113734 | -1.502555 |
| C | 3.372167 | -0.684793 | -1.513294 |
| H | 2.852208 | 1.289432 | -2.234756 |
| C | 1.479431 | -2.163073 | -1.036353 |
| C | -3.592057 | -0.482795 | -1.802546 |
| H | -2.898091 | 1.459909 | -2.464096 |
| C | -1.832846 | -2.069231 | -1.180352 |
| C | 2.851414 | -1.920037 | -1.075961 |
| H | 1.109355 | -3.128636 | -0.701619 |
| C | -3.180367 | -1.747699 | -1.334068 |
| H | -1.548521 | -3.055440 | -0.822753 |
| H | 3.537174 | -2.710566 | -0.785380 |
| H | -3.930912 | -2.499706 | -1.109046 |
| H | 0.013283 | 1.334519 | -3.297507 |
| C | -8.509265 | -0.786358 | -0.341399 |
| C | -7.326587 | -0.362138 | -1.189667 |
| H | -8.631627 | -1.877622 | -0.319733 |
| C | -9.673034 | -0.100443 | -1.027999 |
| C | -5.982812 | -0.674599 | -1.040950 |
| C | -7.759517 | 0.473441 | -2.240863 |
| C | -11.020059 | -0.111166 | -0.692106 |
| C | -9.213705 | 0.637209 | -2.141086 |
| C | -5.033889 | -0.160737 | -1.948858 |
| H | -5.654839 | -1.294523 | -0.210872 |
| C | -6.831984 | 0.990436 | -3.149031 |
| C | -11.922650 | 0.612003 | -1.487817 |
| H | -11.382182 | -0.656476 | 0.174675 |
| C | -10.114574 | 1.362868 | -2.925387 |
| C | -5.484525 | 0.668635 | -2.996967 |
| H | -7.148102 | 1.627895 | -3.970549 |
| C | -11.470499 | 1.339885 | -2.599018 |
| H | -9.775785 | 1.931378 | -3.786978 |
| H | -4.766762 | 1.047944 | -3.718174 |
| H | -12.189329 | 1.878540 | -3.208395 |
| H | -8.403667 | -0.468042 | 0.704465 |

**Table S1**. The excitation energies ($E_{ex}$), oscillator strength (f), transition compositions of the two lowest excitations of the compounds calculated by TD-B3LYP/6-31G(d,p) in $CH_2Cl_2$ solvent.

| Compounds | | $E_{ex}$ (eV/nm) | *f* | Transition composition |
|---|---|---|---|---|
| **2** | $S_0 \rightarrow S_1$ | 3.52 (352) | 1.2856 | 0.63 (H→L)+0.20 (H-4→L) |
| | $S_0 \rightarrow S_2$ | 4.36 (284) | 0.0053 | 0.47 (H→L+2)+0.44 (H-1→L+1) |
| **5** | $S_0 \rightarrow S_1$ | 3.30 (376) | 1.6888 | 0.69 (H→L) |
| | $S_0 \rightarrow S_2$ | 3.53 (351) | 0.0026 | 0.69 (H-1→L) |
| **7** | $S_0 \rightarrow S_1$ | 3.19 (388) | 2.7264 | 0.69 (H→L) |
| | $S_0 \rightarrow S_2$ | 3.44 (360) | 0.0137 | 0.69 (H-1→L) |
| **BPCF** | $S_0 \rightarrow S_1$ | 3.13 (397) | 0.0259 | 0.57 (H→L) |
| | $S_0 \rightarrow S_2$ | 3.11 (399) | 0.9592 | 0.57 (H→L+1) |
| **BPCF2** | $S_0 \rightarrow S_1$ | 3.11 (399) | 0.3871 | 0.51 (H→L)+ 0.44 (H-1→L) |
| | $S_0 \rightarrow S_2$ | 3.11 (399) | 0.5617 | 0.50 (H→L+1) |
| **BPCF3** | $S_0 \rightarrow S_1$ | 3.10 (400) | 0.4836 | 0.51 (H→L)+0.44 (H-1→L) |
| | $S_0 \rightarrow S_2$ | 3.10 (401) | 0.4730 | 0.48 (H→L+1) |

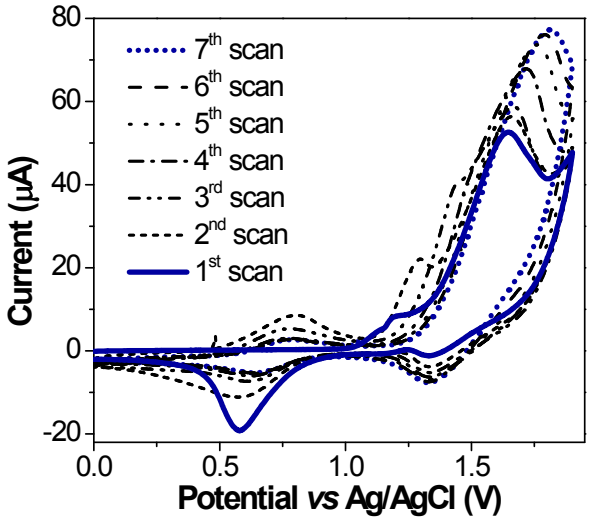



**Figure S2.** CV traces of **BPCF2** measured in $CH_2Cl_2$/*n*-$Bu_4NPF_6$ at scan rate of 50 mV $s^{-1}$

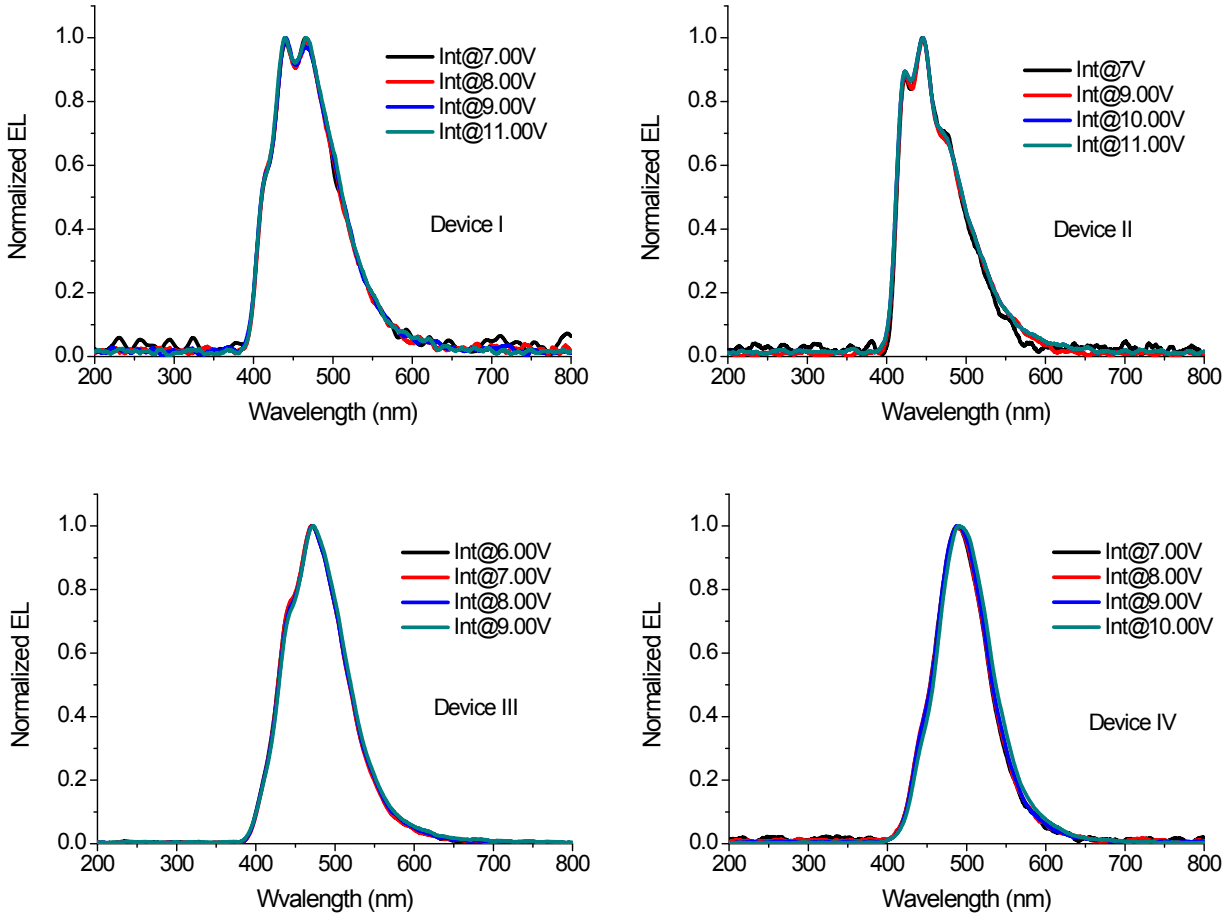
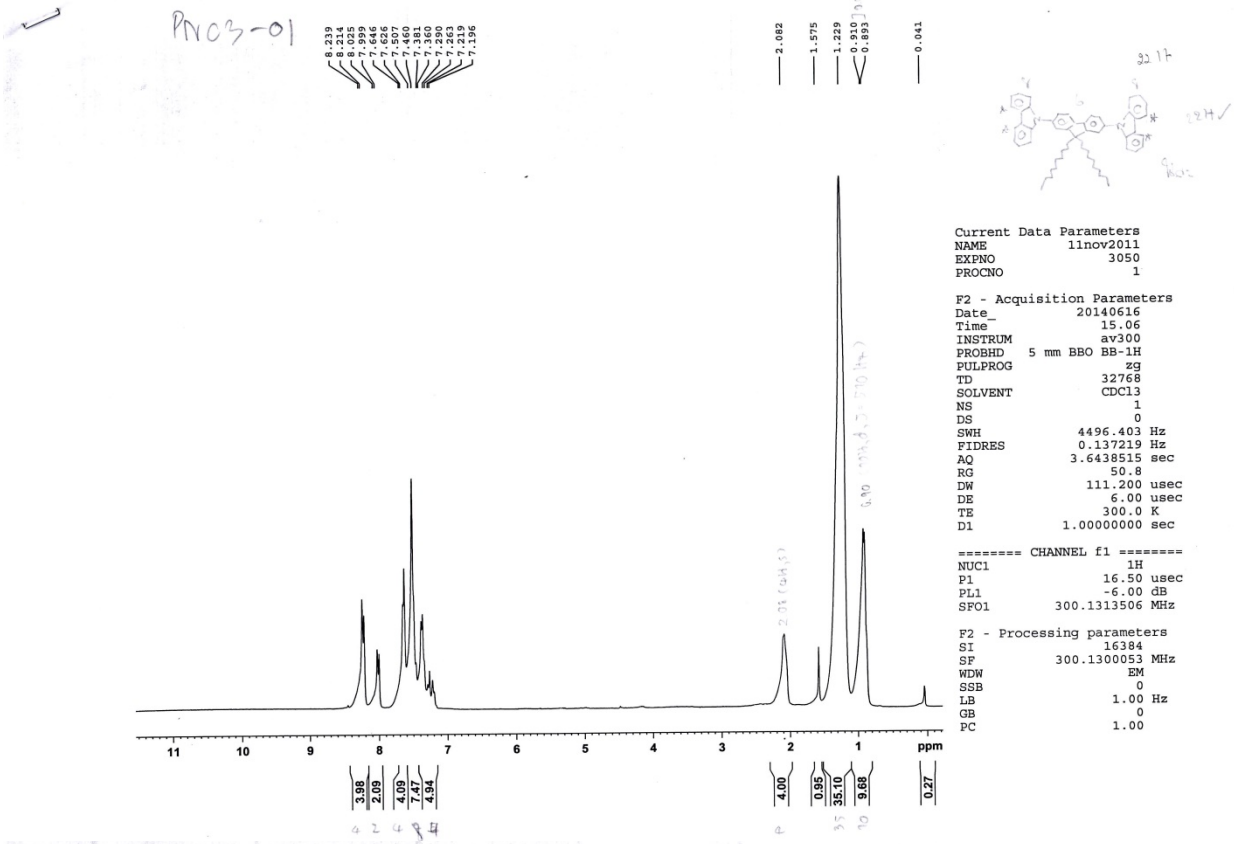
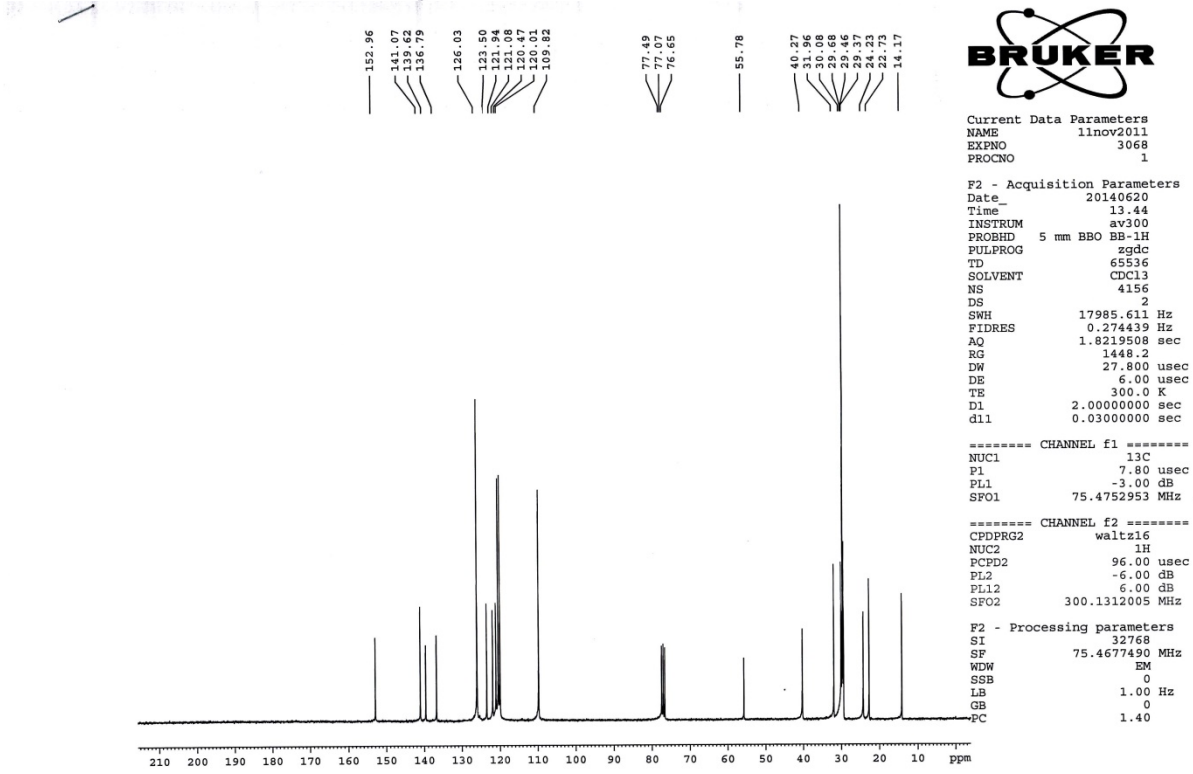


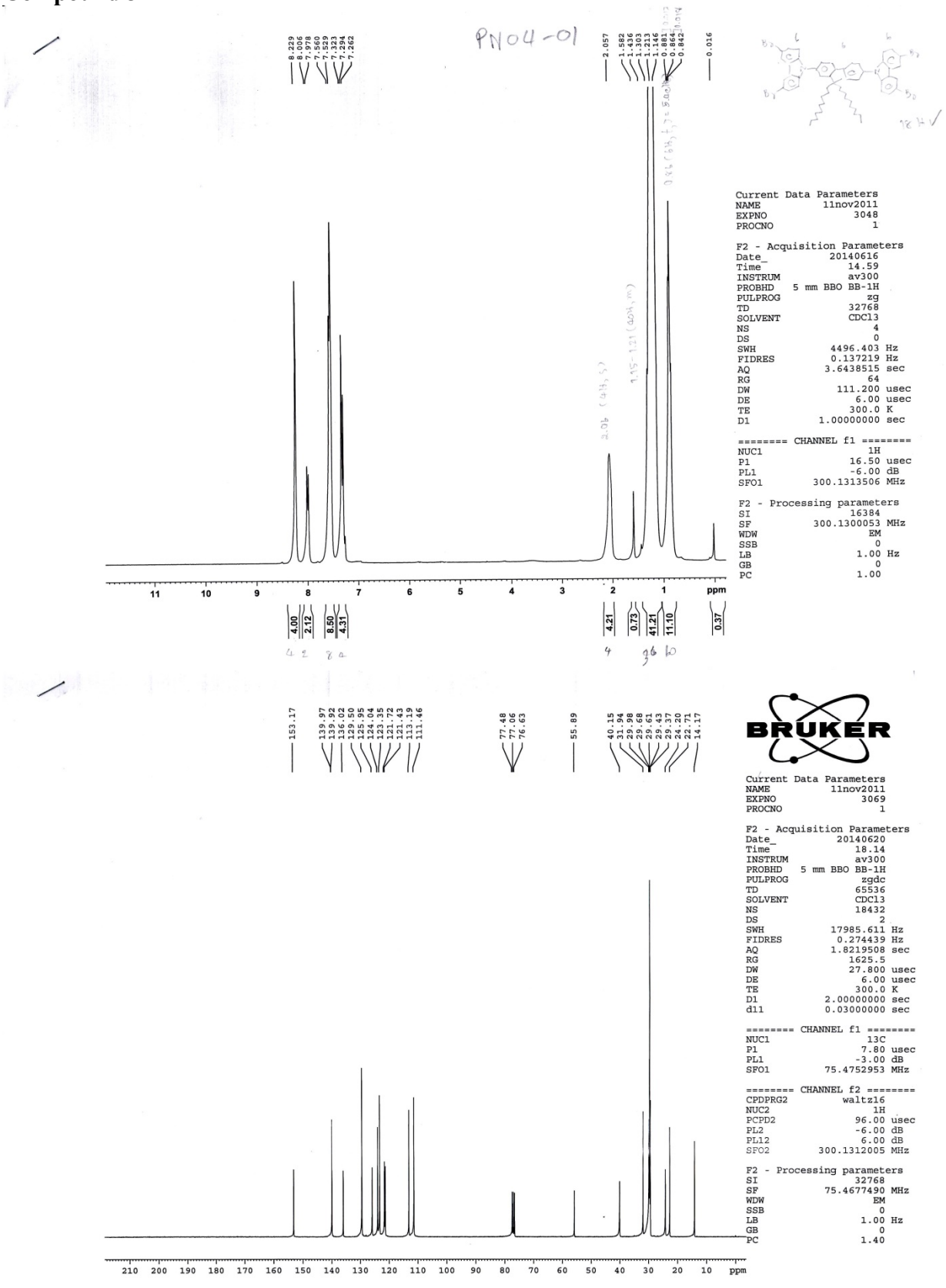

**Figure S3.** EL spectra of the OELDs at different applied voltages

**$^{1}$H-NMR and $^{13}$C-NMR spectra**
**Compound 2**

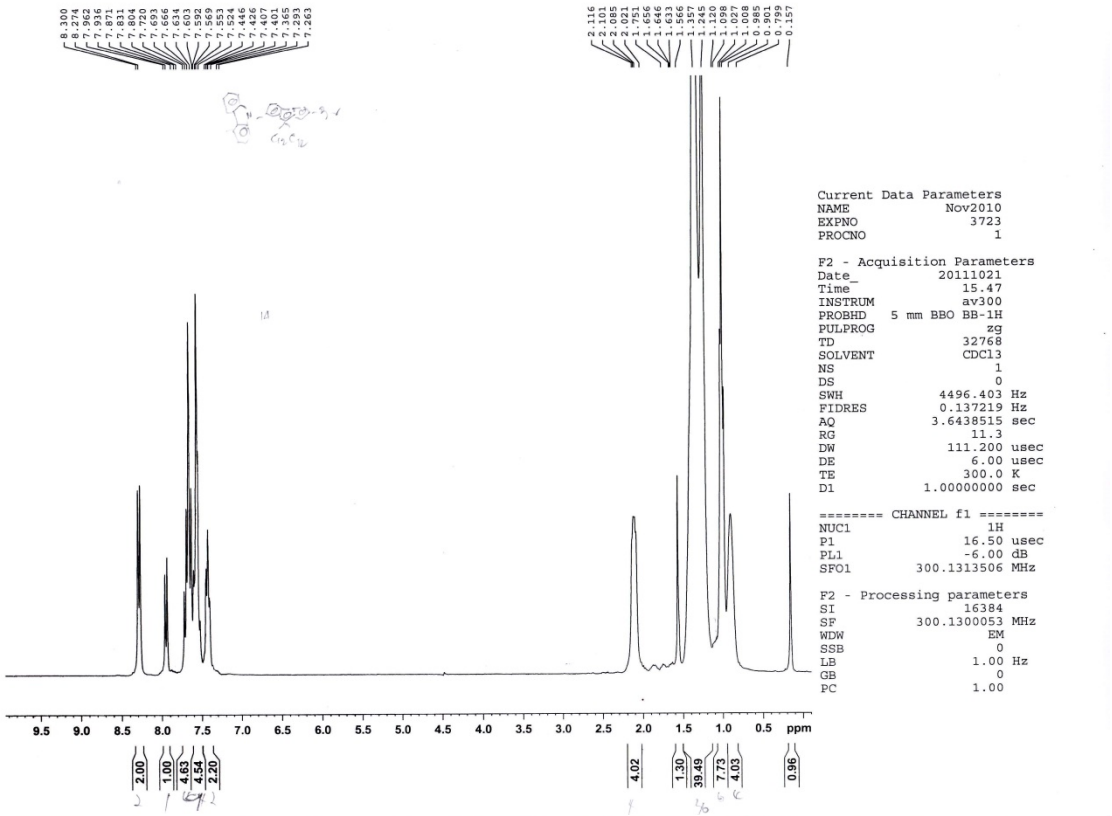


**Compound 3**


PN04-01
8.229
8.006
7.578
7.560
7.529
7.323
7.294
7.262
2.057
1.502
1.436
1.303
1.213
1.146
0.864
0.842
0.016
Current Data Parameters
NAME 11nov2011
EXPNO 3048
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140616
Time 14.59
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 64
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 16.50 usec
PL1 -6.00 dB
SFO1 300.1313506 MHz
F2 - Processing parameters
SI 16384
SF 300.1300053 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
11 10 9 8 7 6 5 4 3 2 1 ppm
4.00 2.12 8.50 4.31 4.21 0.73 41.21 11.10 0.37
153.17
139.97
139.92
136.02
135.56
125.95
124.04
123.35
121.72
121.43
113.19
111.46
77.48
77.06
76.63
55.89
40.15
31.94
29.98
29.68
29.61
29.43
29.37
24.20
22.71
14.17
BRUKER
Current Data Parameters
NAME 11nov2011
EXPNO 3069
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140620
Time 18.14
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 18432
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1625.5
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.80 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 96.00 usec
PL2 -6.00 dB
PL12 6.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

## Compound 4



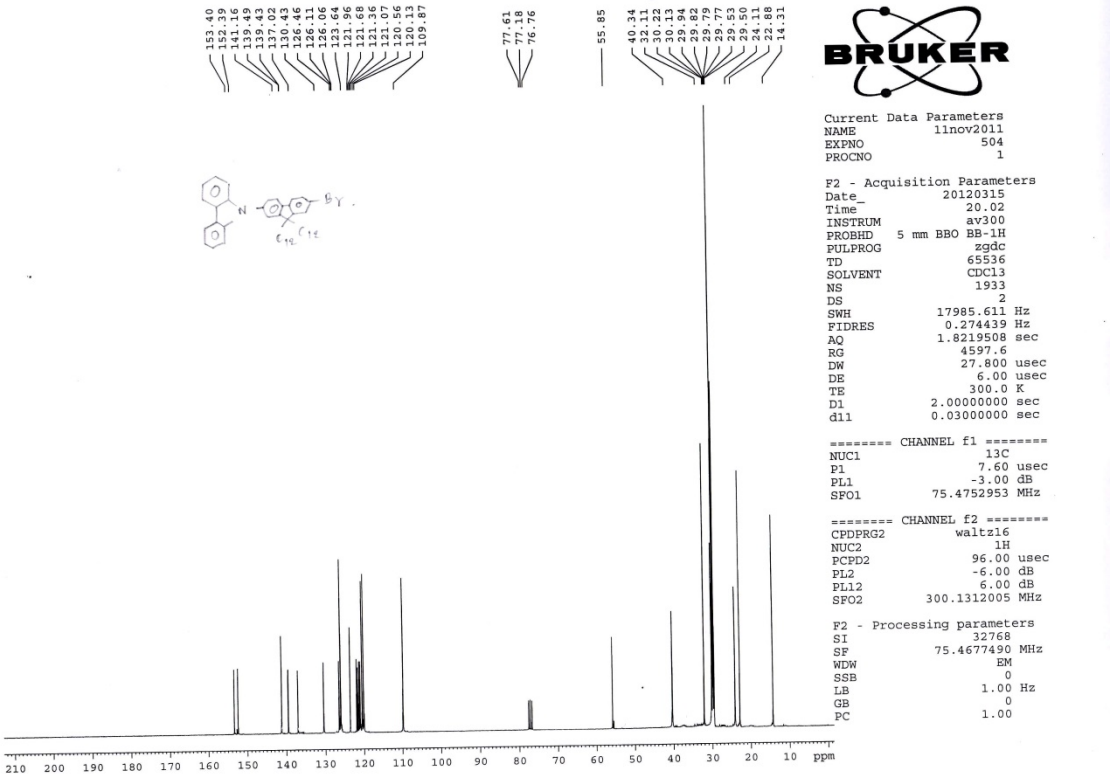

Current Data Parameters
NAME Nov2010
EXPNO 3723
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111021
Time 15.47
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 11.3
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 16.50 usec
PL1 -6.00 dB
SFO1 300.1313506 MHz

F2 - Processing parameters
SI 16384
SF 300.1300053 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

AV 01-5




Current Data Parameters
NAME 11nov2011
EXPNO 504
PROCNO 1

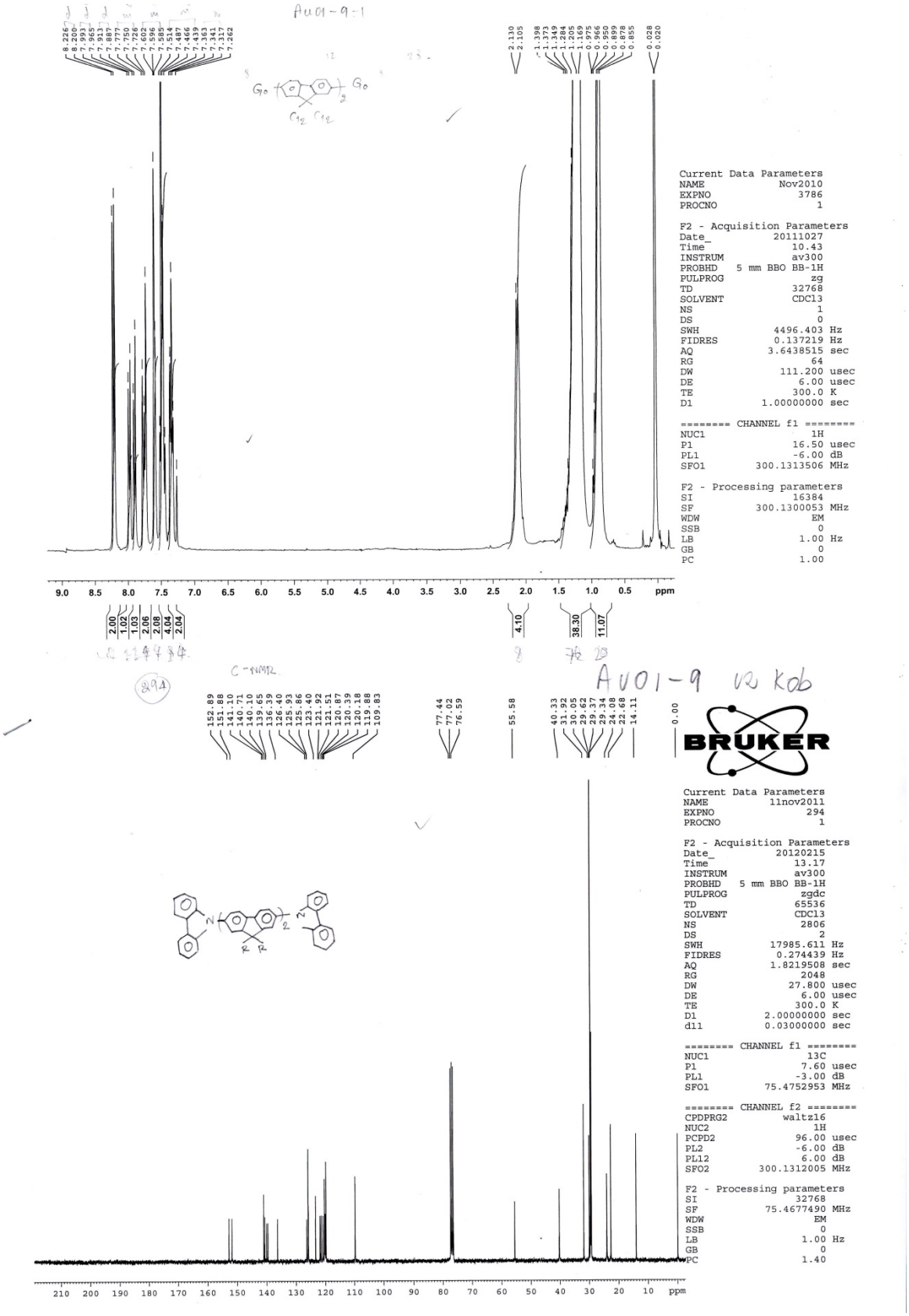
F2 - Acquisition Parameters
Date_ 20120315
Time 20.02
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 1933
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4597.6
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 7.60 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz

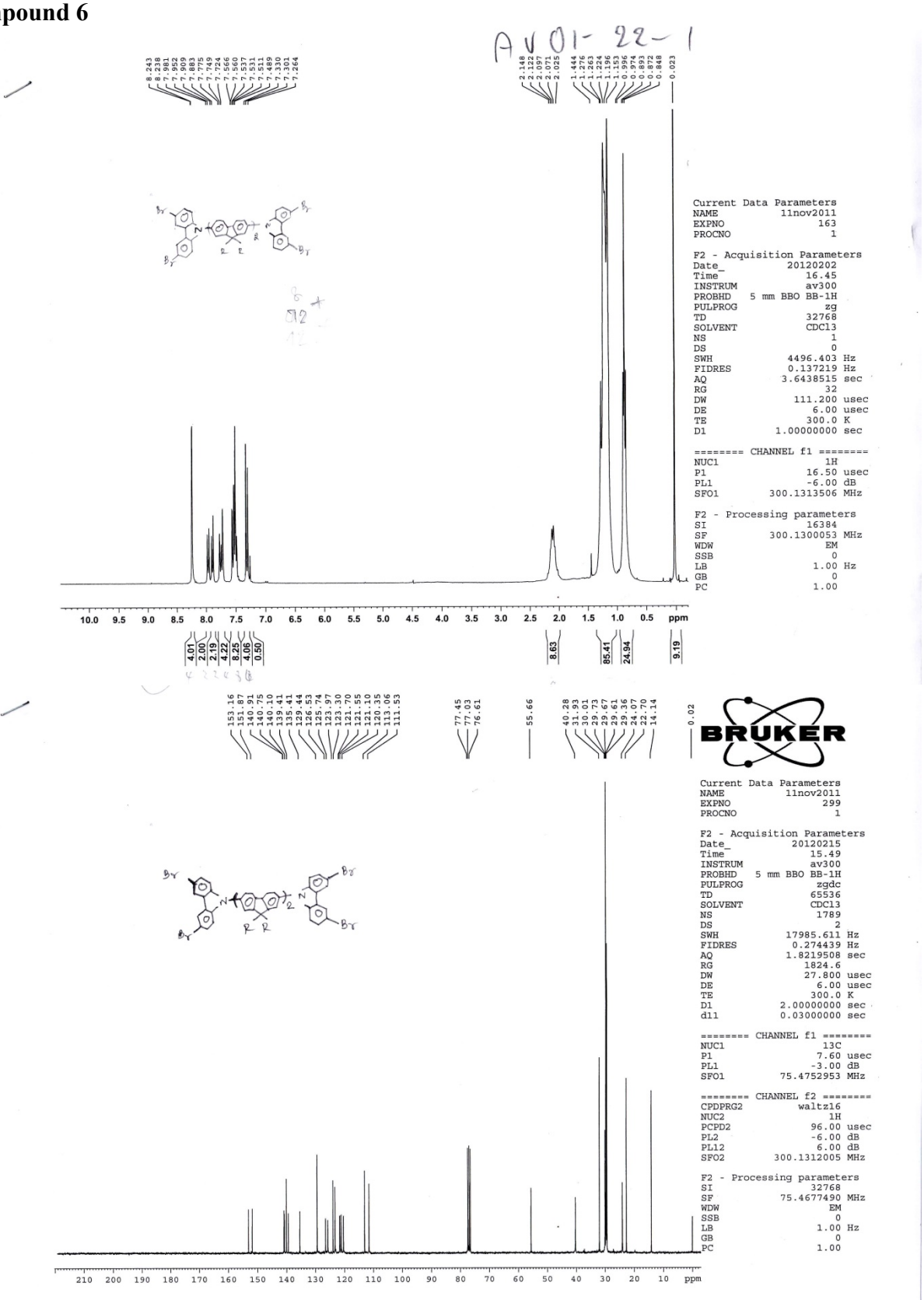
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 96.00 usec
PL2 -6.00 dB
PL12 6.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

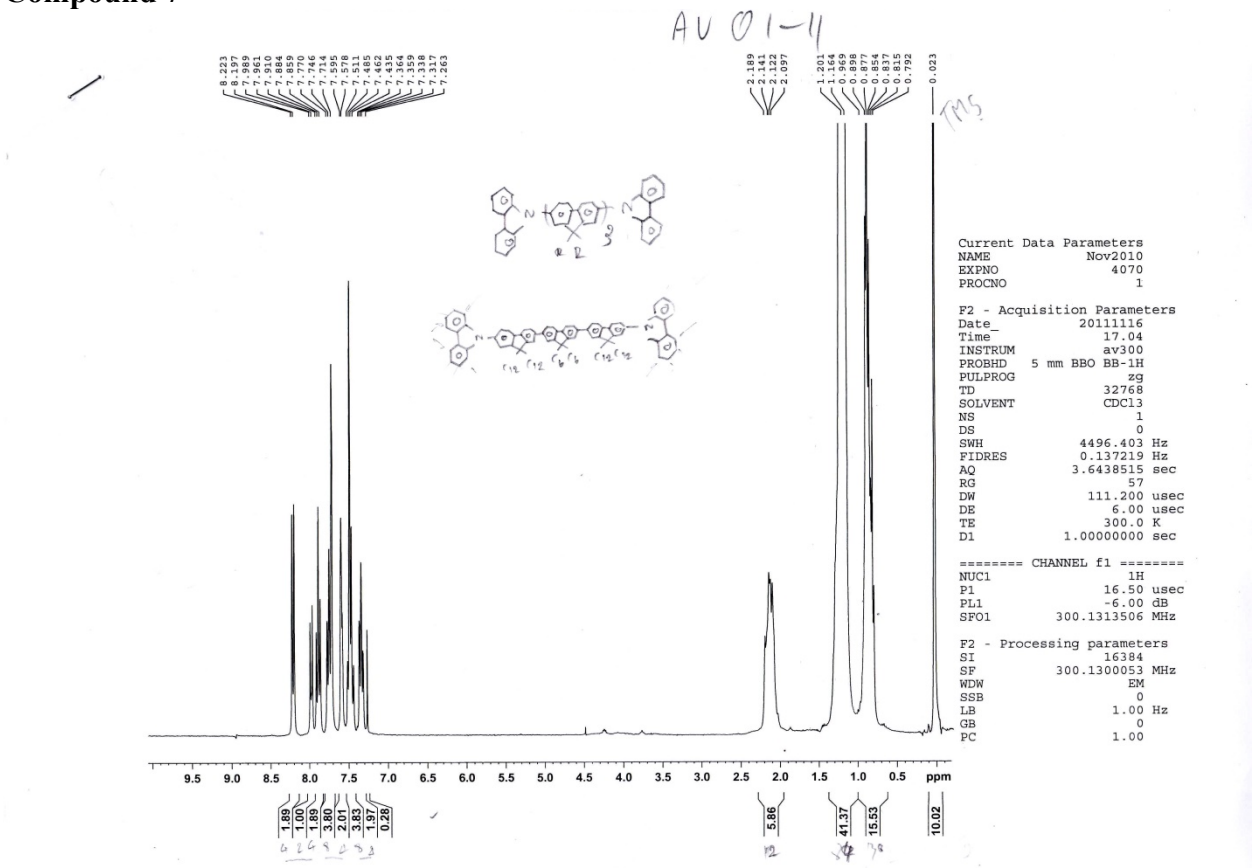
**Compound 5**

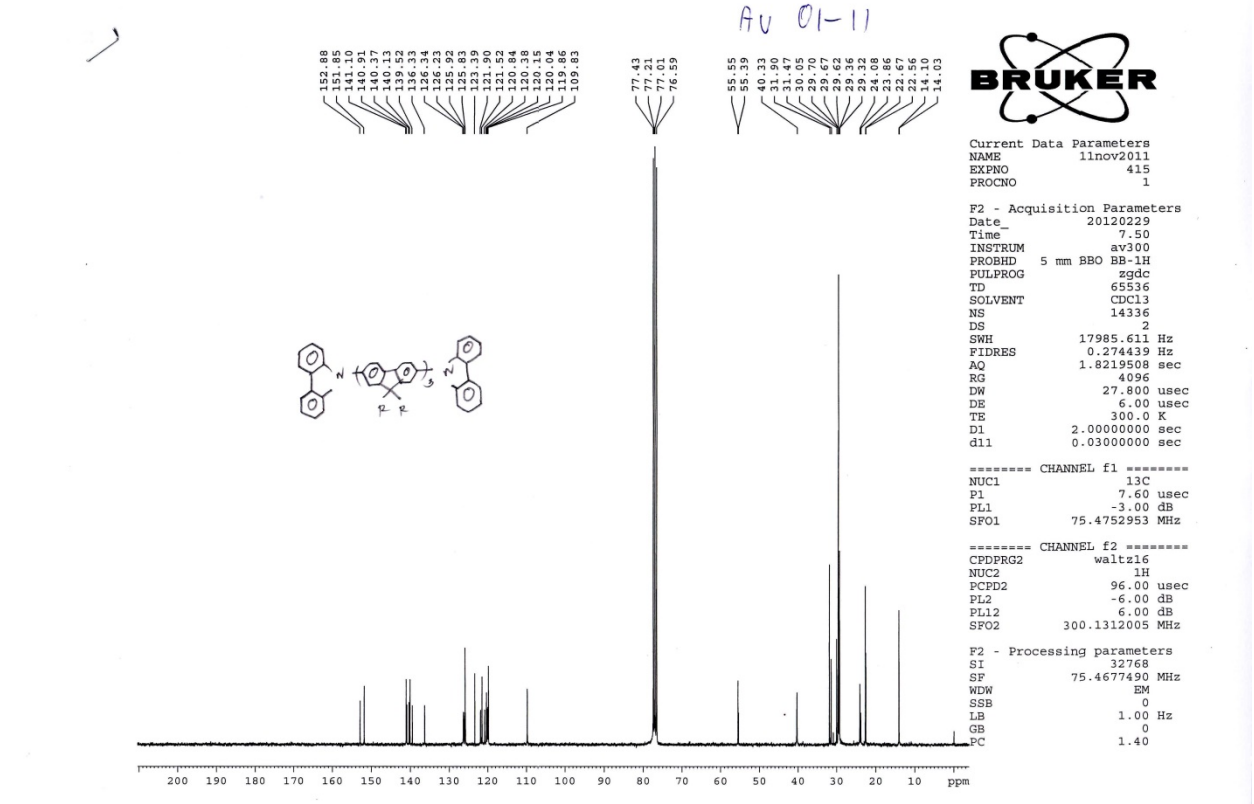

AV01-9-1
8.226
8.200
7.993
7.965
7.913
7.887
7.777
7.750
7.726
7.602
7.585
7.514
7.487
7.466
7.363
7.341
7.317
7.262
2.130
2.105
1.398
1.373
1.349
1.284
1.205
1.168
0.975
0.966
0.950
0.899
0.878
0.855
0.028
0.020
Current Data Parameters
NAME Nov2010
EXPNO 3786
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111027
Time 10.43
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 64
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 16.50 usec
PL1 -6.00 dB
SFO1 300.1313506 MHz
F2 - Processing parameters
SI 16384
SF 300.1300053 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.00 1.02 1.03 2.06 2.08 4.04 2.04
4.10 38.30 11.07
C-NMR
AV01-9 12 Kdb
152.89
151.88
141.10
140.71
140.10
139.65
136.39
126.40
125.93
125.86
123.40
121.92
121.51
120.87
120.39
120.18
119.88
109.83
77.44
77.02
76.59
55.58
40.33
31.92
30.05
29.62
29.37
29.34
29.10
22.68
14.11
0.00
BRUKER
Current Data Parameters
NAME 11nov2011
EXPNO 294
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120215
Time 13.17
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 2806
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.60 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 96.00 usec
PL2 -6.00 dB
PL12 6.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**Compound 6**

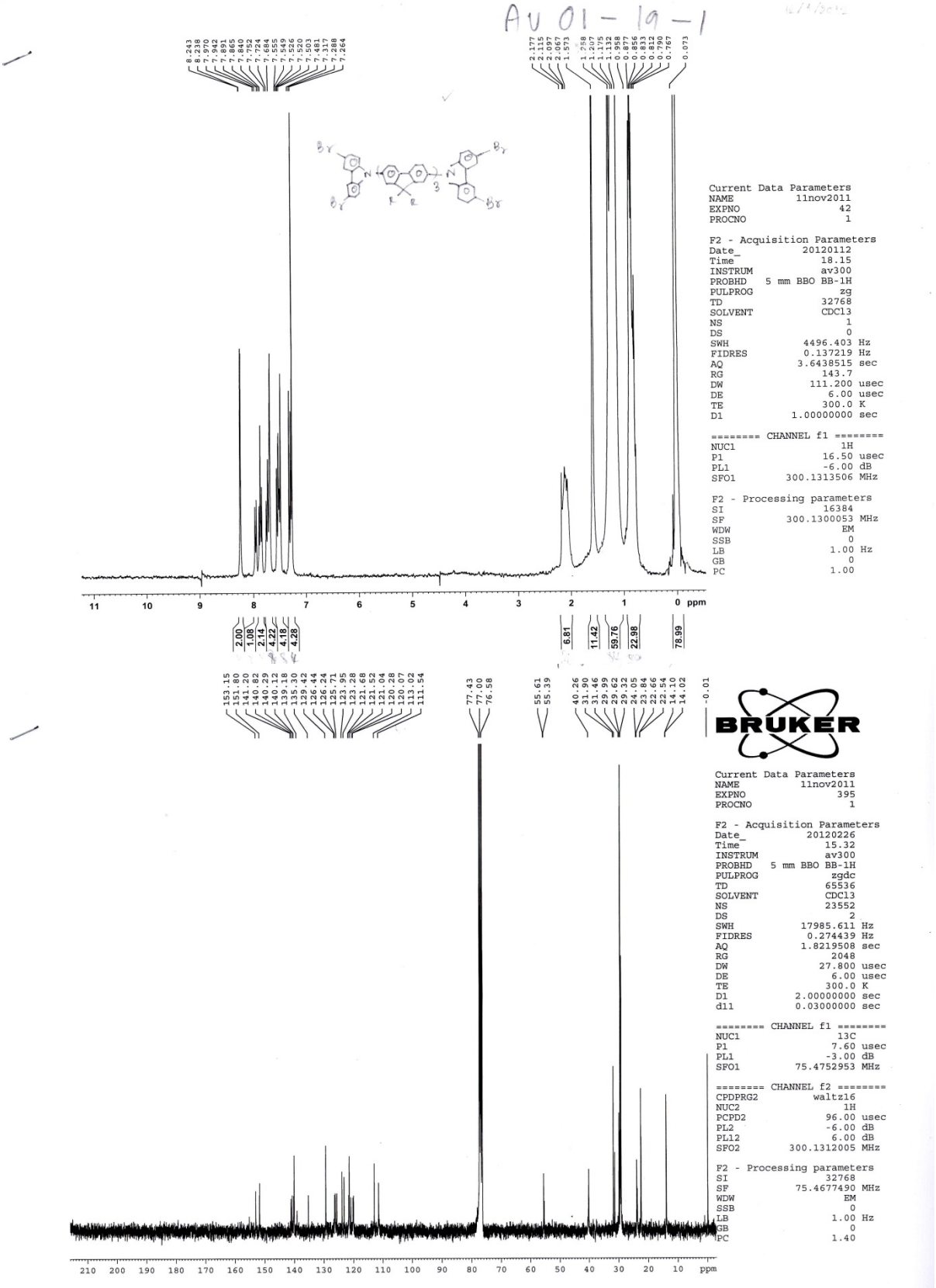

AV01-22-1
Current Data Parameters
NAME 11nov2011
EXPNO 163
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120202
Time 16.45
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 32
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 16.50 usec
PL1 -6.00 dB
SFO1 300.1313506 MHz
F2 - Processing parameters
SI 16384
SF 300.1300053 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
BRUKER
Current Data Parameters
NAME 11nov2011
EXPNO 299
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120215
Time 15.49
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 1789
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1824.6
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.60 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 96.00 usec
PL2 -6.00 dB
PL12 6.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

**Compound 7**

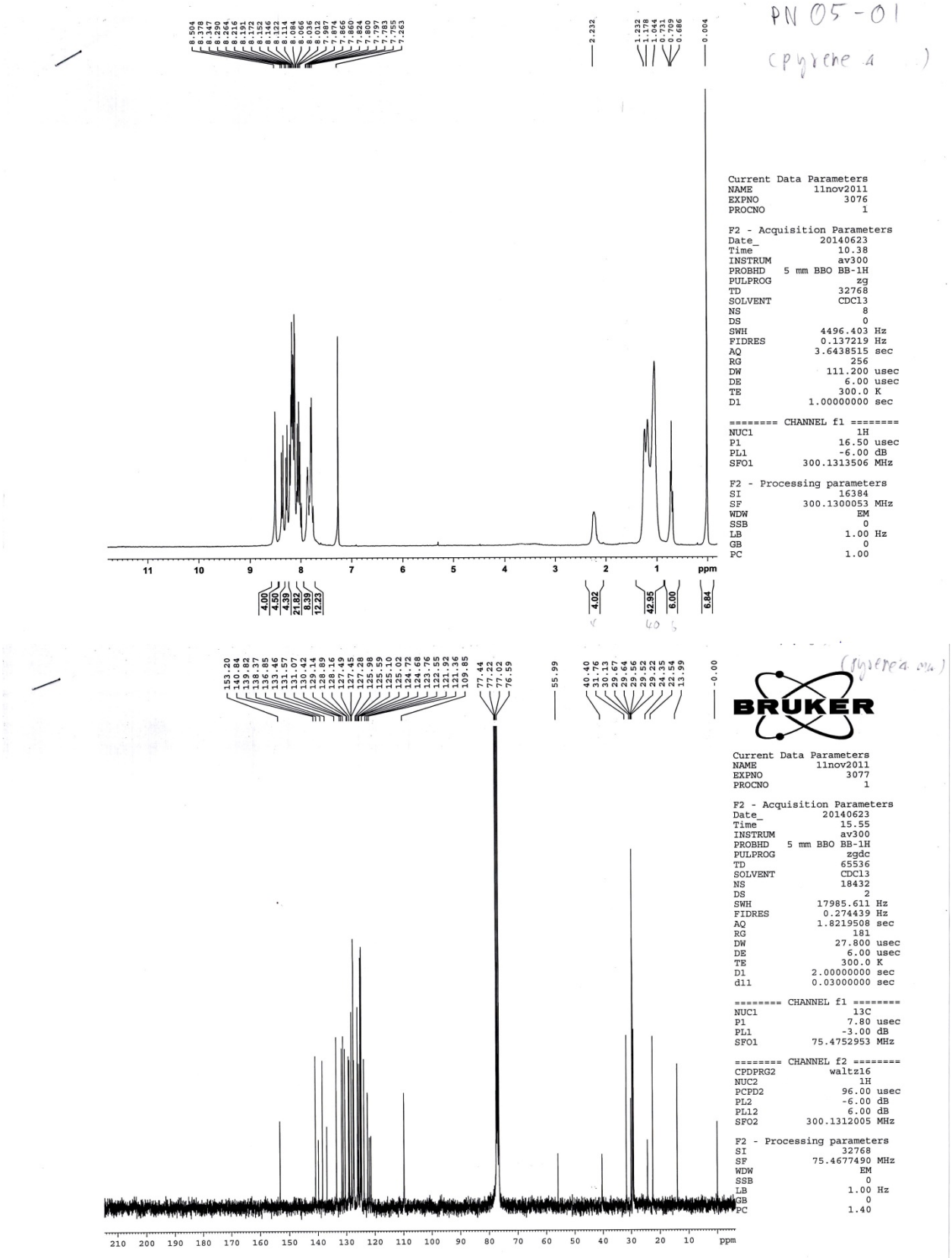

AU 01-1
TMS
Current Data Parameters
NAME Nov2010
EXPNO 4070
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111116
Time 17.04
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 57
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 16.50 usec
PL1 -6.00 dB
SFO1 300.1313506 MHz
F2 - Processing parameters
SI 16384
SF 300.1300053 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
ppm


AU 01-11
BRUKER
Current Data Parameters
NAME 11nov2011
EXPNO 415
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120229
Time 7.50
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 14336
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4096
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.60 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 96.00 usec
PL2 -6.00 dB
PL12 6.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm

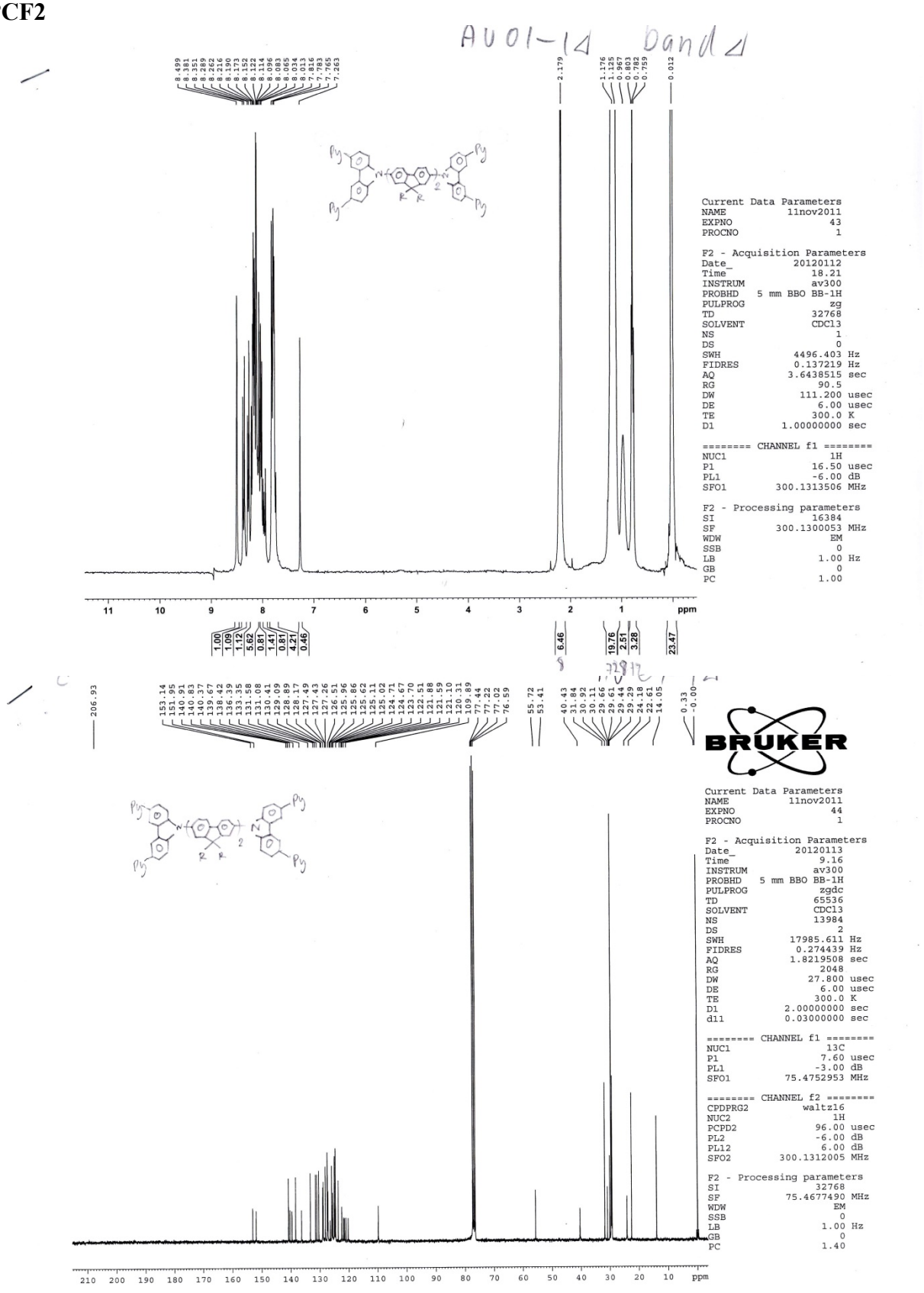
**Compound 8**


Av 01 - 19 - 1
Current Data Parameters
NAME 11nov2011
EXPNO 42
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120112
Time 18.15
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 143.7
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 16.50 usec
PL1 -6.00 dB
SFO1 300.1313506 MHz
F2 - Processing parameters
SI 16384
SF 300.1300053 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
BRUKER
Current Data Parameters
NAME 11nov2011
EXPNO 395
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120226
Time 15.32
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 23552
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.60 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 96.00 usec
PL2 -6.00 dB
PL12 6.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

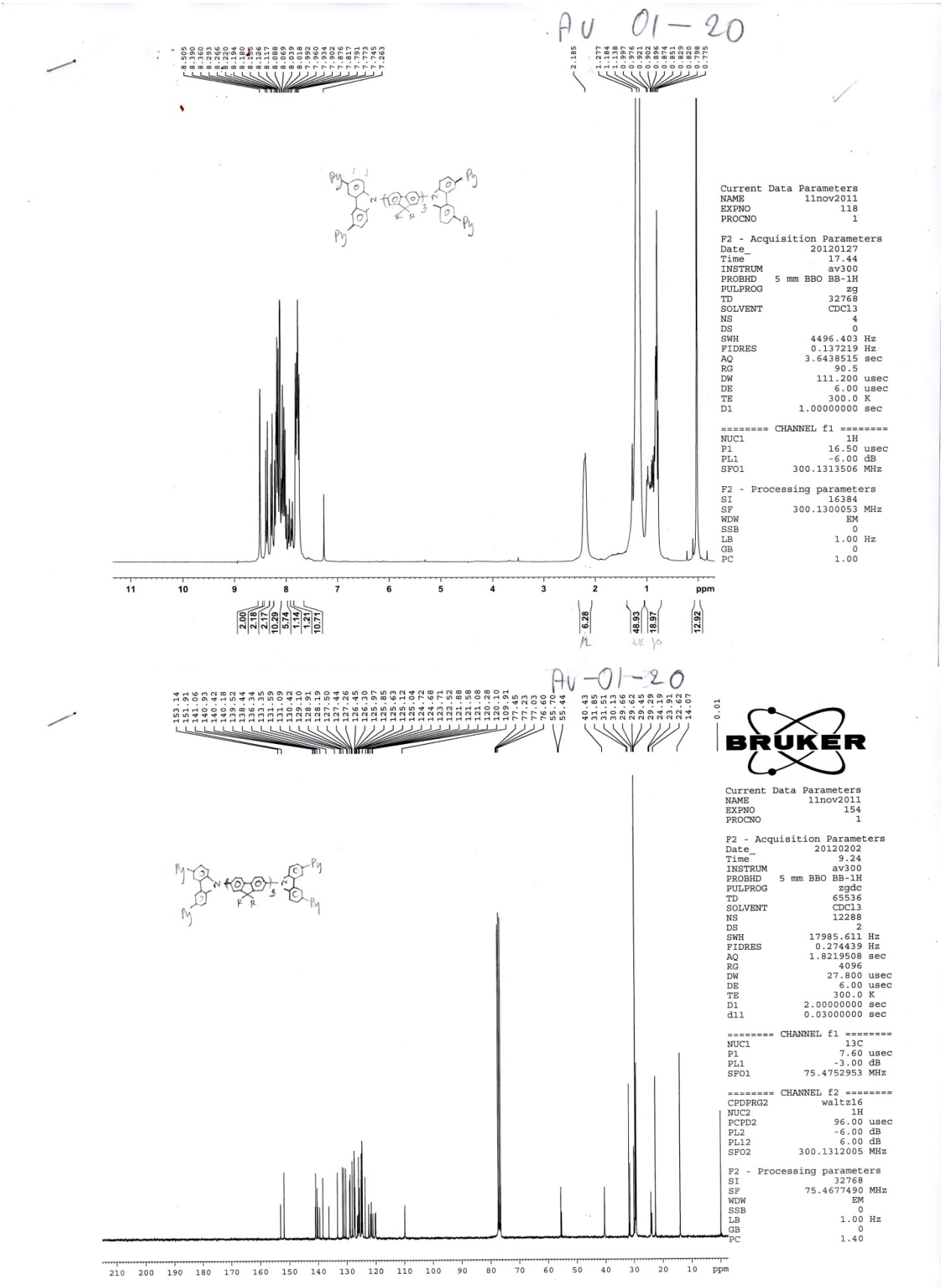
**BPCF**


PN 05-01
(pyrene a ...)
8.504
8.378
8.347
8.290
8.264
8.216
8.191
8.172
8.152
8.146
8.122
8.114
8.084
8.066
8.036
8.012
7.897
7.874
7.866
7.860
7.824
7.800
7.797
7.783
7.755
7.263
2.232
1.232
1.178
1.044
0.731
0.709
0.686
0.004
4.00
4.50
4.39
21.82
8.39
12.23
4.02
42.95
6.00
6.84
11
10
9
8
7
6
5
4
3
2
1
ppm
Current Data Parameters
NAME 11nov2011
EXPNO 3076
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140623
Time 10.38
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 256
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 16.50 usec
PL1 -6.00 dB
SFO1 300.1313506 MHz
F2 - Processing parameters
SI 16384
SF 300.1300053 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
153.20
140.84
139.82
138.37
136.85
133.46
131.57
131.07
130.42
129.14
128.89
128.16
127.49
127.45
127.28
125.98
125.59
125.10
125.02
124.72
124.68
123.76
122.55
121.92
121.36
109.85
77.44
77.22
77.02
76.59
55.99
40.40
31.76
30.13
29.67
29.64
29.55
29.22
24.35
22.54
13.99
-0.00
(pyrene a ...)
BRUKER
Current Data Parameters
NAME 11nov2011
EXPNO 3077
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140623
Time 15.55
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 18432
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 181
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.80 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 96.00 usec
PL2 -6.00 dB
PL12 6.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

**BPCF2**


AU01-14 Band 4
8.499
8.381
8.351
8.289
8.262
8.216
8.190
8.173
8.152
8.122
8.114
8.096
8.083
8.065
8.034
8.011
7.816
7.783
7.765
7.263
2.179
1.176
1.125
0.967
0.803
0.782
0.759
0.012
Current Data Parameters
NAME 11nov2011
EXPNO 43
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120112
Time 18.21
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 90.5
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 16.50 usec
PL1 -6.00 dB
SFO1 300.1313506 MHz
F2 - Processing parameters
SI 16384
SF 300.1300053 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
11 10 9 8 7 6 5 4 3 2 1 ppm
1.00 1.09 1.12 5.62 0.81 1.41 0.81 4.21 0.46
6.46
19.76 2.51 3.28
23.47
206.93
153.14 151.95 140.91 140.83 140.37 139.67 138.42 138.19 133.35 131.58 131.08 130.41 129.09 128.89 128.17 127.49 127.33 127.26 126.51 125.96 125.86 125.62 125.11 125.02 124.71 124.57 123.70 122.51 121.88 121.59 121.10 120.31 109.89
77.44 77.22 77.01 76.59
55.72 53.41
40.43 31.84 30.12 30.02 29.66 29.61 29.44 29.29 24.18 22.61 14.05
0.33 -0.00
BRUKER
Current Data Parameters
NAME 11nov2011
EXPNO 44
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120113
Time 9.16
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 13984
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.60 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 96.00 usec
PL2 -6.00 dB
PL12 6.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**BPCF3**


AV 01-20
Current Data Parameters
NAME 11nov2011
EXPNO 118
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120127
Time 17.44
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 90.5
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 16.50 usec
PL1 -6.00 dB
SFO1 300.1313506 MHz
F2 - Processing parameters
SI 16384
SF 300.1300053 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
AV-01-20
BRUKER
Current Data Parameters
NAME 11nov2011
EXPNO 154
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120202
Time 9.24
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 12288
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4096
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.60 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 96.00 usec
PL2 -6.00 dB
PL12 6.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40