

## Supporting Information

for

### **The first examples of multiply bonded dirhenium(III,II) paramagnetic complexes that contain nitrobenzoate ligands: spectroscopic, structural, cytotoxicity and computational studies†**

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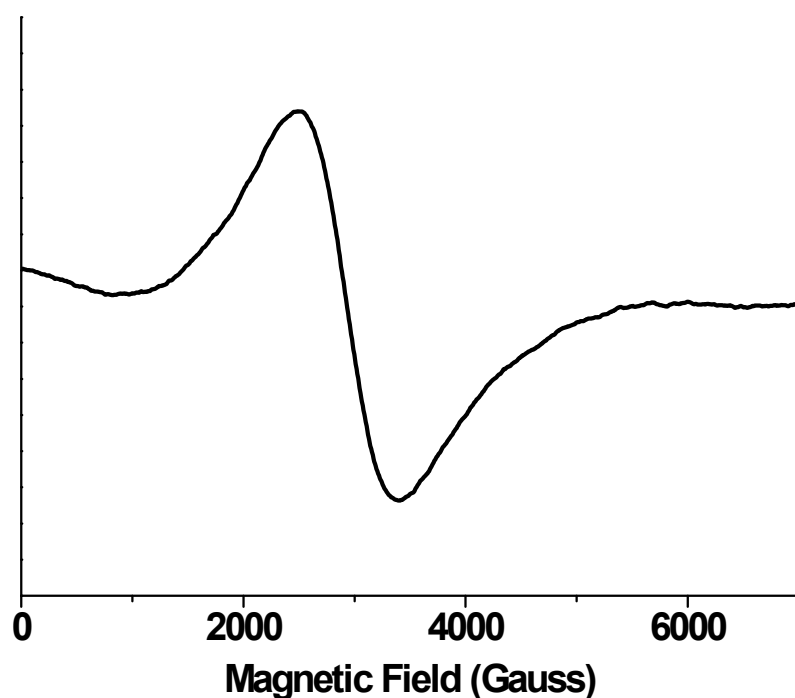
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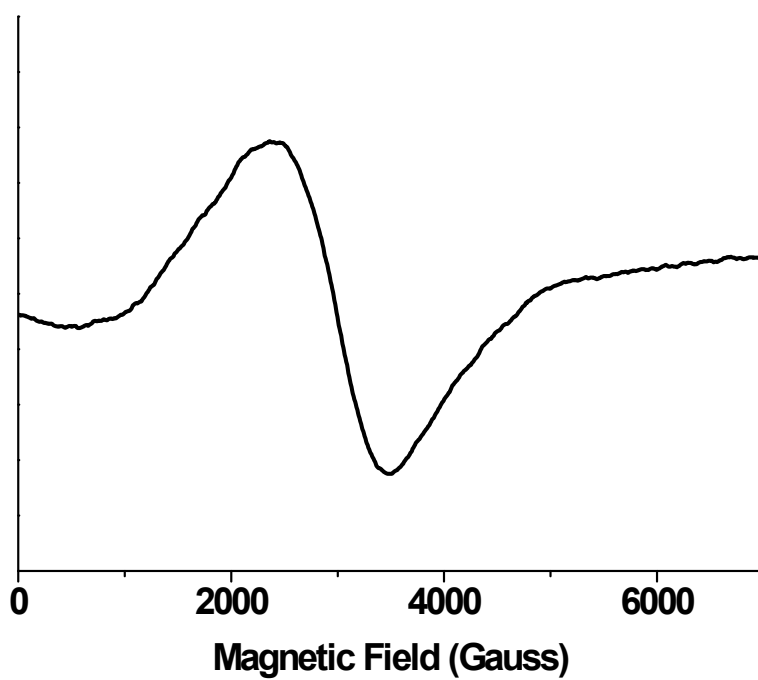
**Table S6** Cartesian coordinates (Å) for DFT energy-minimized model of **2**.

**Table S7** Cartesian coordinates (Å) for DFT energy-minimized model of **3**.

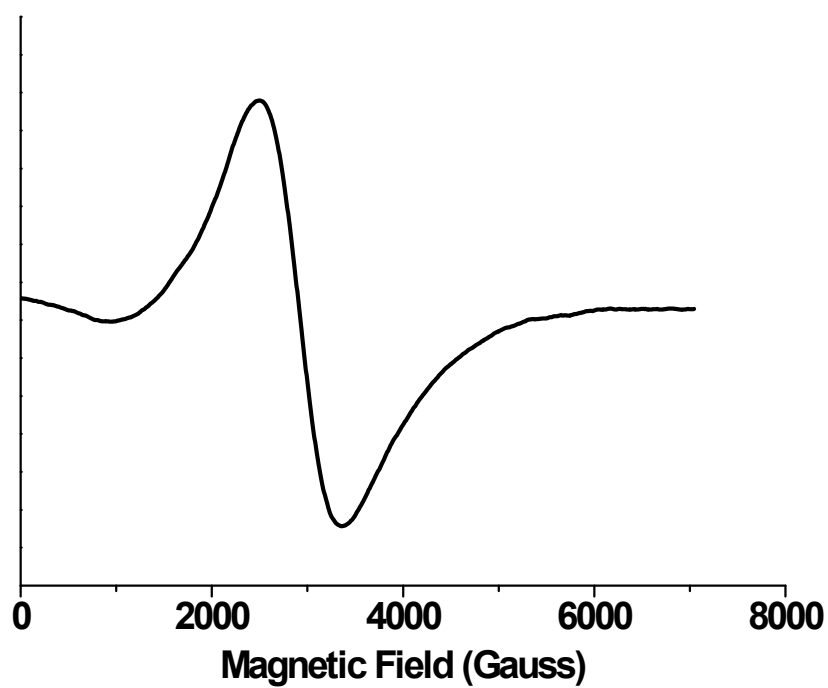
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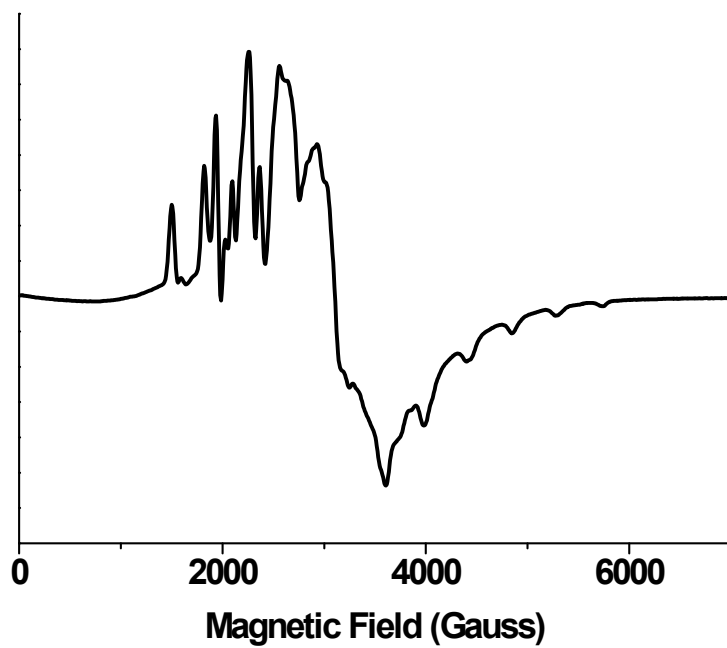
**Fig. S1** Solid state powder X-band EPR spectrum of **2** at 298 K



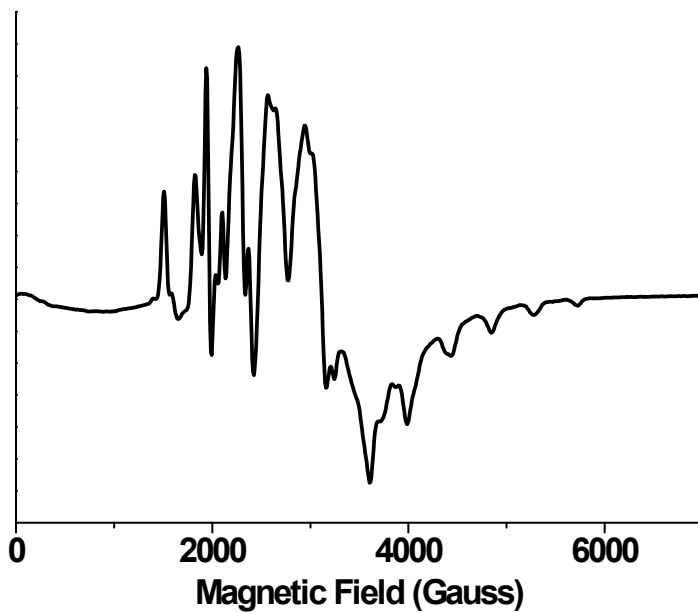
**Fig. S2** Solid state powder X-band EPR spectrum of **3** at 298 K



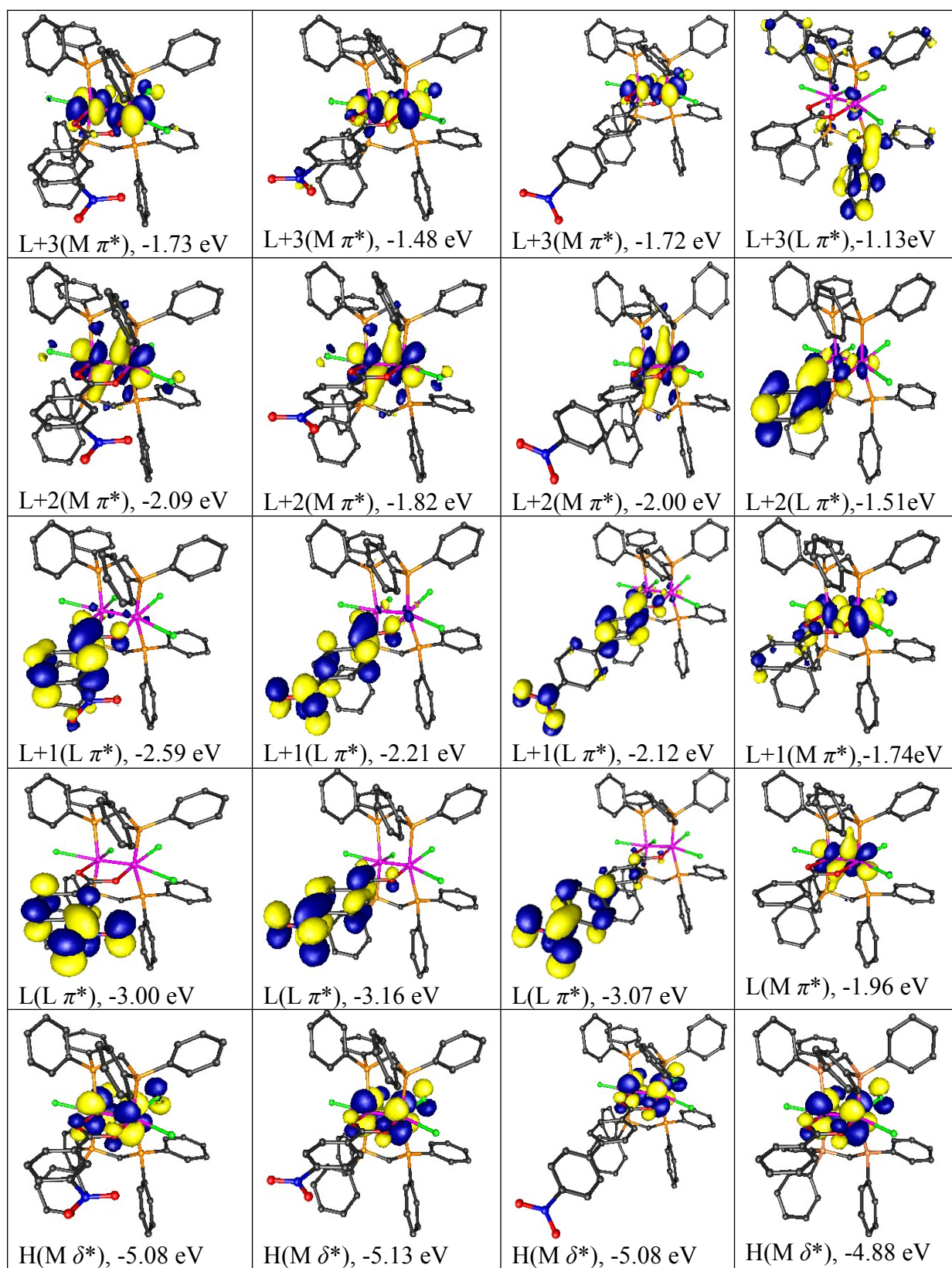
**Fig. S3** Solid state powder X-band EPR spectrum of **4** at 298 K

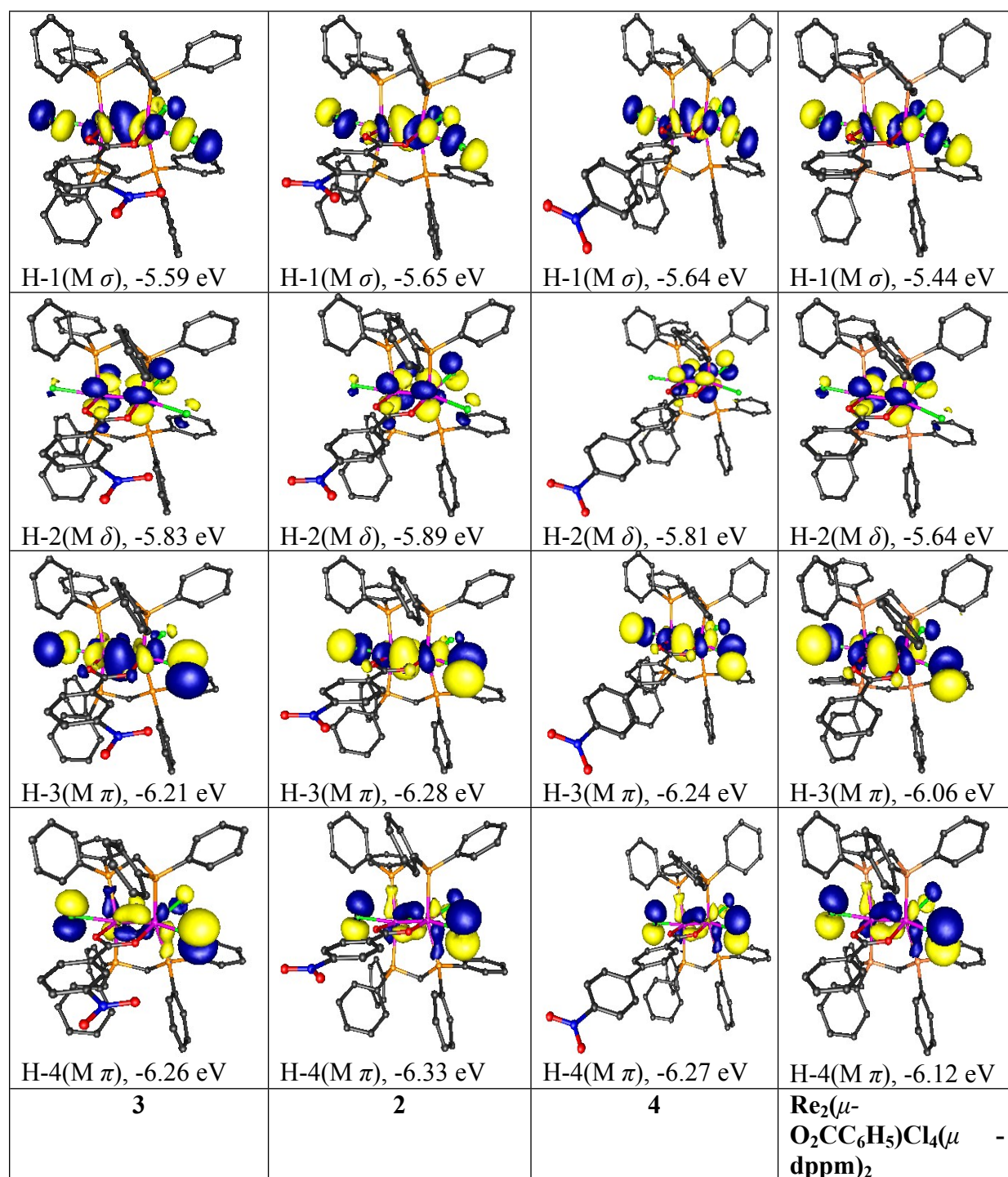


**Fig. S4** X-Band EPR spectrum of dichloromethane glass of **2** recorded at 126 K



**Fig. S5** X-Band EPR spectrum of dichloromethane glass of **3** recorded at 126 K





**Fig. S6** Isodensity plot of spin-up frontier molecular orbitals of **2**, **3**, **4** and the model Re<sub>2</sub>( $\mu$ -O<sub>2</sub>CC<sub>6</sub>H<sub>5</sub>)Cl<sub>4</sub>( $\mu$ -dppm)<sub>2</sub> complex

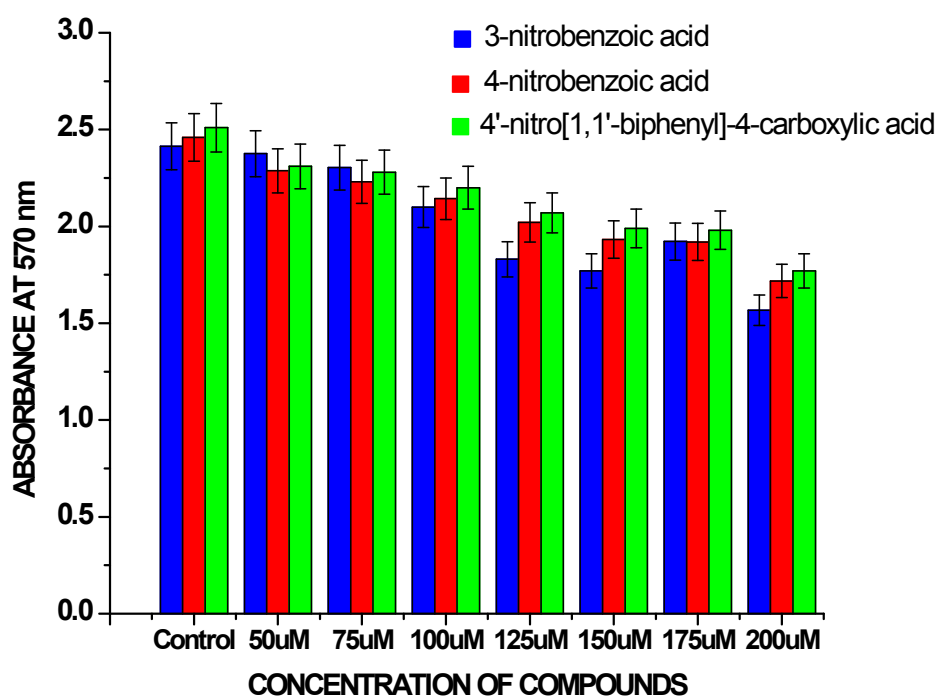


Fig. S7 Growth inhibitory effect of the nitrobenzoic acid ligands on MCF-7 cells.

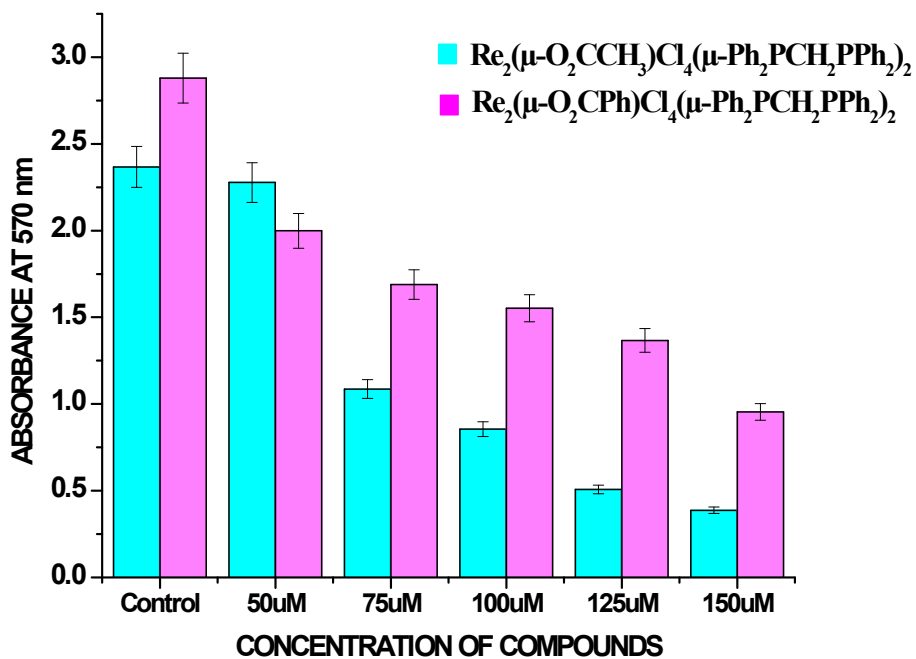


Fig. S8 Growth inhibitory effect of the acetate and benzoate complexes on MCF-7 cells.

**Table S1** Spin-up frontier molecular orbital composition (%) in the ground state for **2**.

| Orbital | Energy (eV) | Contribution (%) |                 |      |      |
|---------|-------------|------------------|-----------------|------|------|
|         |             | Re               | 4-nitrobenzoate | dppm | Cl   |
| H-5     | -6.5260     | 2.0              | 0.3             | 21.3 | 76.4 |
| H-4     | -6.3271     | 22.3             | 0.7             | 15.1 | 61.9 |
| H-3     | -6.2775     | 40.2             | 2.1             | 7.1  | 50.6 |
| H-2     | -5.8866     | 52.4             | 7.2             | 10.1 | 30.2 |
| H-1     | -5.6516     | 49.2             | 1.1             | 5.2  | 44.5 |
| H       | -5.1266     | 68.4             | 7.8             | 5.9  | 17.9 |
| L       | -3.1647     | 0.6              | 91.7            | 7.2  | 0.5  |
| L+1     | -2.2119     | 5.8              | 90.1            | 3.9  | 0.2  |
| L+2     | -1.8222     | 75.3             | 0.0             | 20.1 | 4.6  |
| L+3     | -1.4843     | 81.2             | 6.9             | 2.9  | 9.0  |
| L+4     | -1.3189     | 4.2              | 13.0            | 81.9 | 0.9  |
| L+5     | -1.3038     | 1.4              | 83.1            | 15.5 | 0.0  |

**Table S2** Spin-up frontier molecular orbital composition (%) in the ground state for **3**.

| Orbital | Energy (eV) | Contribution (%) |                 |      |      |
|---------|-------------|------------------|-----------------|------|------|
|         |             | Re               | 3-nitrobenzoate | dppm | Cl   |
| H-5     | -6.4393     | 1.8              | 0.2             | 22.1 | 75.9 |
| H-4     | -6.2571     | 24.5             | 0.6             | 14.2 | 60.7 |
| H-3     | -6.2091     | 41.3             | 1.9             | 6.8  | 50.0 |
| H-2     | -5.8321     | 52.1             | 7.5             | 9.8  | 30.6 |
| H-1     | -5.5892     | 50.2             | 1.6             | 5.4  | 42.8 |
| H       | -5.0836     | 69.4             | 6.8             | 5.2  | 18.6 |
| L       | -3.0003     | 0.5              | 92.1            | 6.5  | 0.9  |
| L+1     | -2.1594     | 4.8              | 91.2            | 4.0  | 0.0  |
| L+2     | -2.0962     | 74.2             | 0.0             | 20.6 | 5.2  |
| L+3     | -1.7255     | 81.3             | 7.1             | 3.5  | 8.1  |
| L+4     | -1.2629     | 3.7              | 2.9             | 92.6 | 0.8  |
| L+5     | -1.2195     | 2.8              | 5.4             | 91.4 | 0.4  |

**Table S3** Spin-up frontier molecular orbital composition (%) in the ground state for **4**.

| Orbital | Energy (eV) | Contribution (%) |                                       |      |      |
|---------|-------------|------------------|---------------------------------------|------|------|
|         |             | Re               | 4'-nitro[1,1'-biphenyl]-4-carboxylate | dppm | Cl   |
| H-5     | -6.4971     | 2.2              | 0.5                                   | 20.7 | 76.6 |
| H-4     | -6.2730     | 20.2             | 0.5                                   | 14.3 | 65.0 |
| H-3     | -6.2387     | 41.1             | 2.2                                   | 6.8  | 49.9 |
| H-2     | -5.8063     | 51.3             | 7.0                                   | 9.5  | 32.2 |
| H-1     | -5.6376     | 48.2             | 1.0                                   | 5.0  | 45.8 |
| H       | -5.0778     | 67.9             | 7.4                                   | 6.1  | 18.6 |

|     |         |      |      |      |     |
|-----|---------|------|------|------|-----|
| L   | -3.0673 | 0.4  | 91.3 | 8.3  | 0.0 |
| L+1 | -2.1192 | 5.7  | 89.4 | 4.5  | 0.4 |
| L+2 | -2.0035 | 74.2 | 0.0  | 19.6 | 6.2 |
| L+3 | -1.7206 | 80.6 | 6.8  | 3.2  | 9.4 |
| L+4 | -1.2782 | 4.1  | 12.1 | 82.9 | 0.9 |
| L+5 | -1.2729 | 1.1  | 82.4 | 16.5 | 0.0 |

**Table S4** Spin-up frontier molecular orbital composition (%) in the ground state for the model  $\text{Re}_2(\mu\text{-O}_2\text{CC}_6\text{H}_4)\text{Cl}_4(\mu\text{-dppm})_2$  complex

| Orbital | Energy (eV) | Contribution (%) |          |      |      |
|---------|-------------|------------------|----------|------|------|
|         |             | Re               | benzoate | dppm | Cl   |
| H-5     | -6.3063     | 1.9              | 0.2      | 19.5 | 78.4 |
| H-4     | -6.1192     | 21.5             | 0.6      | 14.8 | 63.1 |
| H-3     | -6.0612     | 42.4             | 1.9      | 7.2  | 48.5 |
| H-2     | -5.6360     | 52.4             | 7.2      | 8.5  | 31.9 |
| H-1     | -5.4359     | 49.5             | 1.1      | 5.4  | 44.0 |
| H       | -4.8823     | 69.1             | 6.2      | 6.5  | 18.2 |
| L       | -1.9638     | 91.5             | 0.4      | 7.2  | 0.9  |
| L+1     | -1.7364     | 88.5             | 7.2      | 1.2  | 3.1  |
| L+2     | -1.5163     | 9.2              | 80.2     | 8.1  | 2.5  |
| L+3     | -1.1338     | 4.2              | 6.5      | 88.1 | 1.2  |
| L+4     | -1.0999     | 3.9              | 2.1      | 92.5 | 1.5  |
| L+5     | -1.0180     | 1.4              | 5.2      | 93.4 | 0.0  |

**Table S5** Summary of X-ray crystallography for **4**

|                   |                         |
|-------------------|-------------------------|
| Empirical Formula | C63 H52 Cl4 N O4 P4 Re2 |
| Formula weight    | 1525.13                 |
| Crystal system    | Monoclinic              |
| Space group       | P2 <sub>1</sub> /c      |
| <i>a</i> (Å)      | 18.327(3)               |
| <i>b</i> (Å)      | 12.580(2)               |
| <i>c</i> (Å)      | 25.840(5)               |
| $\alpha$ (°)      | 90                      |
| $\beta$ (°)       | 90.809(4)               |
| $\gamma$ (°)      | 90                      |

|                                                                    |                |
|--------------------------------------------------------------------|----------------|
| $V(\text{\AA}^3)$                                                  | 5956.9(18)     |
| $Z$                                                                | 4              |
| $\mu$ (Mo $K\alpha$ ) ( $\text{mm}^{-1}$ )                         | 4.396          |
| Total reflections                                                  | 88298          |
| Independent reflections                                            | 23237          |
| $R_1, wR_2$ [ $I > 2\sigma(I)$ ]                                   | 0.0483, 0.1032 |
| GOF on $F^2$                                                       | 1.125          |
| Largest difference in peak and hole<br>( $\text{e}/\text{\AA}^3$ ) | 2.964, -2.055  |

**Table S6** Cartesian coordinates ( $\text{\AA}$ ) for DFT energy-minimized model of **2**.

| Atoms | x         | y        | z         |
|-------|-----------|----------|-----------|
| Re    | 3.402953  | 9.341656 | 5.177664  |
| Re    | 5.030105  | 7.685887 | 5.161251  |
| C     | 0.238342  | 7.461147 | 4.264053  |
| C     | 0.346634  | 8.027859 | 2.979278  |
| H     | 1.183155  | 8.698317 | 2.753866  |
| C     | -0.623631 | 7.748268 | 1.999355  |
| H     | -0.528478 | 8.195546 | 1.001090  |
| C     | -1.710632 | 6.907938 | 2.293583  |
| H     | -2.468591 | 6.695474 | 1.526940  |
| C     | -1.830595 | 6.346843 | 3.578941  |
| H     | -2.684024 | 5.699620 | 3.823526  |
| C     | -0.862770 | 6.622403 | 4.559298  |
| H     | -0.978363 | 6.194322 | 5.564354  |
| C     | 0.524653  | 8.077863 | 7.074433  |
| C     | -0.635721 | 8.874197 | 6.951969  |
| H     | -0.939158 | 9.254606 | 5.969356  |
| C     | -1.393951 | 9.197073 | 8.089314  |
| H     | -2.294115 | 9.816775 | 7.979586  |
| C     | -1.000788 | 8.736999 | 9.358203  |
| H     | -1.595734 | 8.990666 | 10.246054 |
| C     | 0.165254  | 7.963421 | 9.487652  |
| H     | 0.492020  | 7.615455 | 10.476534 |
| C     | 0.931502  | 7.642260 | 8.354308  |

|   |          |           |           |
|---|----------|-----------|-----------|
| H | 1.861825 | 7.076346  | 8.488443  |
| C | 2.114172 | 5.957580  | 5.871022  |
| H | 2.432684 | 5.898945  | 6.928203  |
| H | 1.311482 | 5.214503  | 5.710200  |
| C | 3.282550 | 5.018038  | 3.248607  |
| C | 1.972547 | 4.822480  | 2.764899  |
| H | 1.101019 | 5.074243  | 3.381106  |
| C | 1.768879 | 4.308337  | 1.470410  |
| H | 0.744253 | 4.162586  | 1.103127  |
| C | 2.866175 | 3.984204  | 0.656349  |
| H | 2.703708 | 3.579568  | -0.351480 |
| C | 4.175211 | 4.181735  | 1.135835  |
| H | 5.037169 | 3.927935  | 0.504568  |
| C | 4.387014 | 4.700252  | 2.422494  |
| H | 5.409261 | 4.858004  | 2.795411  |
| C | 4.228681 | 3.997842  | 5.750877  |
| C | 5.452460 | 3.863222  | 6.436948  |
| H | 6.145785 | 4.709405  | 6.491463  |
| C | 5.787640 | 2.633053  | 7.032153  |
| H | 6.745759 | 2.536840  | 7.559966  |
| C | 4.911815 | 1.537656  | 6.951261  |
| H | 5.179237 | 0.580732  | 7.419657  |
| C | 3.693525 | 1.666784  | 6.259321  |
| H | 3.007115 | 0.812354  | 6.180372  |
| C | 3.355409 | 2.888775  | 5.656482  |
| H | 2.413460 | 2.967558  | 5.096022  |
| C | 4.111550 | 12.941283 | 5.989368  |
| C | 4.604297 | 13.378785 | 7.237628  |
| H | 5.395245 | 12.825738 | 7.757733  |
| C | 4.084576 | 14.537918 | 7.840034  |
| H | 4.478635 | 14.865096 | 8.811049  |
| C | 3.065185 | 15.267797 | 7.206624  |
| H | 2.659036 | 16.172194 | 7.678716  |
| C | 2.565997 | 14.832550 | 5.966553  |
| H | 1.762542 | 15.390041 | 5.467018  |
| C | 3.083494 | 13.677345 | 5.359412  |
| H | 2.673763 | 13.344008 | 4.399876  |
| C | 5.313504 | 12.119344 | 3.507249  |
| C | 4.358814 | 12.170546 | 2.465955  |
| H | 3.362320 | 11.735336 | 2.619533  |
| C | 4.684399 | 12.776834 | 1.240049  |
| H | 3.935094 | 12.816726 | 0.437819  |
| C | 5.962707 | 13.325529 | 1.038188  |
| H | 6.216289 | 13.793368 | 0.077430  |
| C | 6.916444 | 13.272114 | 2.070057  |
| H | 7.918278 | 13.695637 | 1.920408  |
| C | 6.593395 | 12.677582 | 3.301314  |
| H | 7.351379 | 12.648859 | 4.093708  |
| C | 6.282390 | 10.982895 | 6.114375  |
| H | 7.080893 | 11.747914 | 6.128488  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 5.886250  | 10.862820 | 7.139266  |
| C  | 8.135203  | 9.688010  | 4.295560  |
| C  | 8.005565  | 9.200692  | 2.980791  |
| H  | 7.183518  | 8.519273  | 2.735253  |
| C  | 8.939803  | 9.569767  | 1.995480  |
| H  | 8.828087  | 9.184503  | 0.973367  |
| C  | 10.013133 | 10.417914 | 2.315185  |
| H  | 10.743161 | 10.699829 | 1.544101  |
| C  | 10.156071 | 10.897141 | 3.630974  |
| H  | 11.000541 | 11.548658 | 3.894873  |
| C  | 9.223290  | 10.533901 | 4.616021  |
| H  | 9.358696  | 10.897233 | 5.644369  |
| C  | 7.971753  | 8.829221  | 7.053878  |
| C  | 7.592224  | 9.133490  | 8.379755  |
| H  | 6.645403  | 9.644493  | 8.591583  |
| C  | 8.410816  | 8.752519  | 9.456813  |
| H  | 8.103386  | 8.998434  | 10.482126 |
| C  | 9.606057  | 8.050724  | 9.224212  |
| H  | 10.243384 | 7.751730  | 10.067358 |
| C  | 9.975498  | 7.722949  | 7.907907  |
| H  | 10.900144 | 7.162439  | 7.715732  |
| C  | 9.163648  | 8.105458  | 6.827317  |
| H  | 9.452426  | 7.830812  | 5.805965  |
| C  | 4.215135  | 8.525106  | 2.453607  |
| C  | 4.209136  | 8.522837  | 0.975669  |
| C  | 5.161844  | 7.755616  | 0.260501  |
| H  | 5.893436  | 7.159766  | 0.818838  |
| C  | 5.167602  | 7.754704  | -1.137982 |
| H  | 5.899072  | 7.171658  | -1.708509 |
| C  | 4.206643  | 8.519051  | -1.823718 |
| C  | 3.245198  | 9.283697  | -1.138568 |
| H  | 2.510890  | 9.862450  | -1.709903 |
| C  | 3.253321  | 9.285667  | 0.259883  |
| H  | 2.516458  | 9.877226  | 0.816262  |
| N  | 4.205674  | 8.517647  | -3.304557 |
| O  | 3.363584  | 9.252245  | 3.093630  |
| O  | 5.074180  | 7.799538  | 3.083581  |
| O  | 5.079245  | 7.852554  | -3.882637 |
| O  | 3.331176  | 9.181759  | -3.882678 |
| P  | 1.541398  | 7.717815  | 5.566067  |
| P  | 3.688411  | 5.589532  | 4.955994  |
| P  | 4.776016  | 11.433178 | 5.136998  |
| P  | 6.891802  | 9.285670  | 5.615487  |
| Cl | 1.320530  | 10.793105 | 4.661948  |
| Cl | 3.268424  | 9.909317  | 7.472346  |
| Cl | 5.112606  | 7.087914  | 7.456014  |
| Cl | 7.159159  | 6.279985  | 4.609167  |

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**Table S7** Cartesian coordinates (Å) for DFT energy-minimized model of **3**.

| Atoms | x         | y         | z         |
|-------|-----------|-----------|-----------|
| Re    | 1.589915  | 0.538872  | -0.835565 |
| Re    | -0.356274 | -0.078926 | 0.258756  |
| C     | 2.410226  | -2.460699 | -3.004950 |
| C     | 3.451486  | -2.752923 | -2.102143 |
| C     | 4.282035  | -3.868616 | -2.317754 |
| C     | 4.082813  | -4.698551 | -3.434235 |
| C     | 3.050061  | -4.407125 | -4.345635 |
| C     | 2.220060  | -3.293345 | -4.134194 |
| C     | 1.203600  | -0.234713 | -4.401012 |
| C     | 2.394294  | -0.157251 | -5.156796 |
| C     | 2.399849  | 0.494137  | -6.401441 |
| C     | 1.223279  | 1.078948  | -6.901530 |
| C     | 0.041968  | 1.025376  | -6.141609 |
| C     | 0.032328  | 0.381784  | -4.892461 |
| C     | -0.419737 | -1.926307 | -2.677410 |
| C     | -0.307735 | -3.752300 | -0.275219 |
| C     | 0.514334  | -4.627760 | -1.013760 |
| C     | 0.935024  | -5.846151 | -0.447460 |
| C     | 0.536546  | -6.197973 | 0.852284  |
| C     | -0.280735 | -5.323601 | 1.593917  |
| C     | -0.698962 | -4.104268 | 1.039015  |
| C     | -2.782629 | -2.650009 | -1.189008 |
| C     | -3.857198 | -1.896312 | -0.675210 |
| C     | -5.179821 | -2.305433 | -0.926806 |
| C     | -5.439176 | -3.458227 | -1.686710 |
| C     | -4.368199 | -4.217555 | -2.192919 |
| C     | -3.045809 | -3.819210 | -1.941068 |
| C     | 3.286797  | 3.848946  | -0.323958 |
| C     | 2.662498  | 5.070946  | -0.654101 |
| C     | 3.388436  | 6.090124  | -1.294742 |
| C     | 4.741365  | 5.898610  | -1.619475 |
| C     | 5.366574  | 4.680889  | -1.299581 |
| C     | 4.646878  | 3.661691  | -0.655785 |
| C     | 3.460539  | 2.136229  | 1.987690  |
| C     | 4.530700  | 1.229046  | 1.811774  |
| C     | 5.447686  | 1.007925  | 2.854023  |
| C     | 5.297528  | 1.675540  | 4.082267  |
| C     | 4.229982  | 2.572528  | 4.263728  |
| C     | 3.318217  | 2.808204  | 3.220737  |
| C     | 0.810045  | 3.271280  | 1.114613  |
| C     | -0.071870 | 1.877066  | 3.500209  |
| C     | 0.317888  | 0.675547  | 4.122775  |
| C     | 0.616632  | 0.657266  | 5.497453  |
| C     | 0.520334  | 1.831401  | 6.262739  |
| C     | 0.116688  | 3.032505  | 5.649607  |
| C     | -0.178536 | 3.055476  | 4.276734  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -2.015852 | 2.906177  | 1.619926  |
| C  | -2.308809 | 3.788264  | 0.556556  |
| C  | -3.543628 | 4.457900  | 0.509829  |
| C  | -4.504916 | 4.241116  | 1.511998  |
| C  | -4.228481 | 3.344395  | 2.559264  |
| C  | -2.993333 | 2.677031  | 2.613680  |
| C  | 2.039784  | -1.414958 | 1.344661  |
| C  | 2.804494  | -2.320053 | 2.236718  |
| C  | 2.153339  | -2.989603 | 3.300882  |
| C  | 2.872070  | -3.840601 | 4.155430  |
| C  | 4.248029  | -4.044797 | 3.964282  |
| C  | 4.879111  | -3.376603 | 2.901234  |
| N  | 6.337095  | -3.587697 | 2.685691  |
| C  | 4.186614  | -2.520285 | 2.036450  |
| O  | 2.640139  | -0.810927 | 0.379368  |
| O  | 0.781028  | -1.250171 | 1.558166  |
| O  | 6.875859  | -2.982492 | 1.749130  |
| O  | 6.926642  | -4.356960 | 3.456823  |
| P  | 1.234469  | -1.043895 | -2.733158 |
| P  | -1.003817 | -2.172538 | -0.930952 |
| P  | 2.376089  | 2.476285  | 0.530275  |
| P  | -0.413430 | 1.972347  | 1.675791  |
| Cl | 3.914807  | 0.581074  | -1.987913 |
| Cl | 0.847104  | 2.287762  | -2.248193 |
| Cl | -2.009495 | 0.918303  | -1.122138 |
| Cl | -2.129848 | -0.681666 | 2.097589  |
| H  | 3.622212  | -2.095197 | -1.243901 |
| H  | 5.095107  | -4.080113 | -1.610370 |
| H  | 4.736797  | -5.565520 | -3.601142 |
| H  | 2.896294  | -5.041087 | -5.229725 |
| H  | 1.433552  | -3.062504 | -4.865966 |
| H  | 3.320844  | -0.594250 | -4.766562 |
| H  | 3.332997  | 0.547164  | -6.978483 |
| H  | 1.229207  | 1.584747  | -7.876289 |
| H  | -0.877515 | 1.497581  | -6.512491 |
| H  | -0.890735 | 0.394263  | -4.298345 |
| H  | -1.172545 | -1.225202 | -3.084216 |
| H  | -0.437089 | -2.842414 | -3.295458 |
| H  | 0.842305  | -4.371573 | -2.027924 |
| H  | 1.576433  | -6.519335 | -1.032137 |
| H  | 0.862178  | -7.151951 | 1.288100  |
| H  | -0.598347 | -5.594046 | 2.609627  |
| H  | -1.334156 | -3.419213 | 1.619449  |
| H  | -3.661738 | -1.003308 | -0.071782 |
| H  | -6.010073 | -1.713375 | -0.520002 |
| H  | -6.474507 | -3.771010 | -1.880078 |
| H  | -4.561361 | -5.127670 | -2.776974 |
| H  | -2.218353 | -4.435370 | -2.318810 |
| H  | 1.606392  | 5.247706  | -0.420172 |
| H  | 2.887580  | 7.035533  | -1.543672 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 5.306330  | 6.695247  | -2.122493 |
| H | 6.420918  | 4.515220  | -1.557112 |
| H | 5.147799  | 2.715026  | -0.424890 |
| H | 4.644347  | 0.699061  | 0.856406  |
| H | 6.281167  | 0.308369  | 2.701796  |
| H | 6.011679  | 1.496261  | 4.897974  |
| H | 4.102944  | 3.094488  | 5.221594  |
| H | 2.493670  | 3.513043  | 3.383633  |
| H | 0.943669  | 4.095702  | 1.838968  |
| H | 0.383731  | 3.682962  | 0.181803  |
| H | 0.368935  | -0.245777 | 3.532666  |
| H | 0.921818  | -0.285234 | 5.971319  |
| H | 0.750701  | 1.811519  | 7.336763  |
| H | 0.022434  | 3.952914  | 6.242283  |
| H | -0.514584 | 3.994277  | 3.815016  |
| H | -1.593793 | 3.942686  | -0.261561 |
| H | -3.756656 | 5.140592  | -0.324105 |
| H | -5.471577 | 4.761329  | 1.470922  |
| H | -4.979591 | 3.154774  | 3.338412  |
| H | -2.793538 | 1.966108  | 3.424029  |
| H | 1.076840  | -2.834820 | 3.441964  |
| H | 2.355600  | -4.352777 | 4.977509  |
| H | 4.834083  | -4.703363 | 4.614755  |
| H | 4.713507  | -2.017554 | 1.219595  |

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**Table S8** Cartesian coordinates (Å) for DFT energy-minimized model of **4**.

| Atoms | x        | y        | z         |
|-------|----------|----------|-----------|
| C     | 4.528389 | 8.611363 | 18.489884 |
| C     | 4.569437 | 7.735785 | 19.680791 |
| C     | 5.746086 | 7.636992 | 20.459816 |
| H     | 6.620121 | 8.237487 | 20.182937 |
| C     | 5.787748 | 6.797706 | 21.577546 |
| H     | 6.703100 | 6.760645 | 22.182966 |
| C     | 4.658271 | 6.032102 | 21.965878 |
| C     | 3.481734 | 6.145939 | 21.181844 |
| H     | 2.600611 | 5.541574 | 21.434081 |
| C     | 3.436296 | 6.977751 | 20.058429 |
| H     | 2.526969 | 7.037598 | 19.448014 |
| C     | 4.707673 | 5.138711 | 23.148953 |
| C     | 5.962538 | 3.626069 | 24.625923 |
| H     | 6.884630 | 3.103624 | 24.903357 |
| C     | 4.801213 | 3.434144 | 25.392375 |
| C     | 3.594584 | 4.074429 | 25.065061 |
| H     | 2.709787 | 3.910346 | 25.690390 |
| C     | 3.556826 | 4.919543 | 23.950600 |
| H     | 2.623315 | 5.445039 | 23.713353 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.244448  | 12.830938 | 15.929823 |
| C | 1.761436  | 13.752532 | 14.993584 |
| H | 2.840405  | 13.940898 | 14.924619 |
| C | 0.899288  | 14.420279 | 14.107312 |
| H | 1.315840  | 15.137393 | 13.386549 |
| C | -0.481833 | 14.160682 | 14.131833 |
| H | -1.153153 | 14.682002 | 13.435645 |
| C | -0.997524 | 13.221507 | 15.042357 |
| H | -2.073017 | 12.997349 | 15.057286 |
| C | -0.141144 | 12.556585 | 15.935394 |
| H | -0.549938 | 11.812580 | 16.629906 |
| C | 1.331615  | 11.750455 | 18.614431 |
| C | 1.231944  | 10.544351 | 19.335032 |
| H | 1.715560  | 9.641661  | 18.948373 |
| C | 0.500024  | 10.498381 | 20.535592 |
| H | 0.430654  | 9.552129  | 21.088525 |
| C | -0.141637 | 11.648991 | 21.024050 |
| H | -0.714554 | 11.607295 | 21.960389 |
| C | -0.055006 | 12.854805 | 20.302990 |
| H | -0.563134 | 13.757357 | 20.668871 |
| C | 0.675845  | 12.905124 | 19.104298 |
| H | 0.719331  | 13.847563 | 18.540542 |
| C | 3.602856  | 13.210994 | 17.583373 |
| H | 3.883779  | 13.765996 | 16.669137 |
| H | 3.183342  | 13.932902 | 18.308412 |
| C | 5.144708  | 12.043224 | 19.901001 |
| C | 6.309082  | 11.456284 | 20.451785 |
| H | 7.161593  | 11.221684 | 19.797937 |
| C | 6.374125  | 11.180725 | 21.826405 |
| H | 7.285521  | 10.734558 | 22.247385 |
| C | 5.280606  | 11.476334 | 22.662656 |
| H | 5.333752  | 11.257111 | 23.737921 |
| C | 4.120367  | 12.049835 | 22.116938 |
| H | 3.260028  | 12.279843 | 22.759459 |
| C | 4.050011  | 12.335623 | 20.740386 |
| H | 3.131620  | 12.777759 | 20.335218 |
| C | 6.334876  | 13.941834 | 18.119693 |
| C | 7.497704  | 14.033621 | 17.328198 |
| H | 7.793447  | 13.193953 | 16.689312 |
| C | 8.285949  | 15.198538 | 17.376961 |
| H | 9.192997  | 15.257863 | 16.760824 |
| C | 7.921386  | 16.274271 | 18.203733 |
| H | 8.539371  | 17.182382 | 18.233913 |
| C | 6.765416  | 16.182260 | 19.000917 |
| H | 6.477107  | 17.014487 | 19.657756 |
| C | 5.979485  | 15.019247 | 18.964834 |
| H | 5.093937  | 14.950800 | 19.612296 |
| C | 7.593892  | 9.813030  | 13.561679 |
| C | 8.988660  | 9.921617  | 13.756281 |
| H | 9.450860  | 9.498490  | 14.655812 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 9.784930  | 10.584922 | 12.807580 |
| H  | 10.868825 | 10.661324 | 12.970769 |
| C  | 9.199766  | 11.152065 | 11.661808 |
| H  | 9.824782  | 11.667531 | 10.919561 |
| C  | 7.809087  | 11.068003 | 11.476225 |
| H  | 7.338757  | 11.525646 | 10.595456 |
| C  | 7.007005  | 10.411175 | 12.424914 |
| H  | 5.918542  | 10.398277 | 12.279230 |
| C  | 7.648333  | 7.598905  | 15.428427 |
| C  | 7.803340  | 7.290248  | 16.794090 |
| H  | 7.323263  | 7.920696  | 17.549401 |
| C  | 8.584370  | 6.186409  | 17.183016 |
| H  | 8.698129  | 5.955814  | 18.250938 |
| C  | 5.297054  | 8.052566  | 13.811517 |
| H  | 4.969645  | 8.737302  | 13.006566 |
| H  | 5.722751  | 7.147198  | 13.340326 |
| C  | 4.996481  | 5.335356  | 15.674375 |
| H  | 5.893642  | 5.611338  | 15.107596 |
| C  | 4.982507  | 4.117937  | 16.381490 |
| H  | 5.865583  | 3.465621  | 16.348502 |
| C  | 3.849169  | 3.741224  | 17.120668 |
| H  | 3.839025  | 2.788203  | 17.666373 |
| C  | 2.726449  | 4.590157  | 17.159767 |
| H  | 1.835962  | 4.300950  | 17.734076 |
| C  | 2.735509  | 5.808565  | 16.463664 |
| H  | 1.859752  | 6.473264  | 16.497729 |
| C  | 3.872073  | 6.185583  | 15.708898 |
| C  | 2.563743  | 7.239864  | 13.394741 |
| C  | 2.889142  | 6.069708  | 12.669646 |
| H  | 3.773571  | 5.475500  | 12.938952 |
| C  | 2.073164  | 5.641457  | 11.610740 |
| H  | 2.335288  | 4.730948  | 11.054888 |
| C  | 0.919115  | 6.371823  | 11.273411 |
| H  | 0.277223  | 6.036568  | 10.446995 |
| C  | 0.586259  | 7.525374  | 12.002107 |
| H  | -0.318961 | 8.094830  | 11.752368 |
| C  | 1.402514  | 7.964653  | 13.060204 |
| H  | 1.130701  | 8.858797  | 13.631440 |
| Cl | 8.088626  | 10.623147 | 17.125847 |
| Cl | 5.834322  | 12.298052 | 14.927861 |
| Cl | 3.020588  | 10.816528 | 13.925655 |
| Cl | 0.874268  | 9.182791  | 16.260384 |
| N  | 4.850208  | 2.537106  | 26.571379 |
| O  | 3.437216  | 8.714863  | 17.811221 |
| O  | 5.590146  | 9.256942  | 18.143383 |
| O  | 5.934350  | 2.000573  | 26.842755 |
| O  | 3.805049  | 2.377527  | 27.218922 |
| P  | 6.549312  | 8.984570  | 14.851576 |
| P  | 3.723283  | 7.758663  | 14.753055 |
| P  | 5.217777  | 12.454260 | 18.102103 |

|    |          |           |           |
|----|----------|-----------|-----------|
| P  | 2.365828 | 11.896799 | 17.074602 |
| Re | 5.550377 | 10.557229 | 16.512679 |
| Re | 3.387762 | 9.857361  | 16.063969 |
| C  | 5.907463 | 4.473403  | 23.513916 |
| H  | 6.805910 | 4.598873  | 22.896186 |
| C  | 8.295309 | 6.795691  | 14.459442 |
| H  | 8.206873 | 7.038584  | 13.391410 |
| C  | 9.219435 | 5.386886  | 16.218022 |
| H  | 9.831881 | 4.528590  | 16.527598 |
| C  | 9.075543 | 5.695218  | 14.852276 |
| H  | 9.577635 | 5.083818  | 14.090280 |

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