Electronic Supplementary Material (ESI) for RSC Advances.


**ELECTRONIC SUPPORTING INFORMATION (ESI)**

# The Non-Innocent Nature of Graphene Oxide as Theranostic Platform for Biomedical Applications and its Reactivity towards Metal-Based Anticancer Drugs

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## Theoretical calculations (geometry optimization Fe-Pz$_2$Py)

Input File (Spartan 14) for the calculation of the geometry optimized structure of Fe-Pz$_2$Py (charge = +2, multiplicity = 5)

MEM_TOTAL 2000 # MB [ 4 processes ]
Processing $rem in C:/Program Files/Wavefunction/Spartan14v100/P4e//../auxdir/config/preferences.
(Site specific preferences)
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... SCF_CONVERGENCE 7
... SMALL_PROD_XCMAT 9
... BASIS_LIN_DEP_THRESH 5
... SCF_ALGORITHM DIIS_GDM
... MAXSCF 100
... MAXDIIS 50
... THRESHDIIS -1 (i.e. don't switch on delta-E)
... ONEEXE_SPAR TRUE
... GUI GUI_SPARTAN
... TERSE_OUTPUT TRUE
Processing $rem in input file
... JOBTYPE OPT
... TIDY_SYM TRUE
... EXCHANGE M06
... CORRELATION none (built-in)
... INCDFT FALSE (N/A in MetaGGA)
... IGRDTY 70000302 (70,302) M06* default
... PSEUDOPOTENTIAL LACVP
... IGRDTY 70000302 (70,302)
... MAXSCF 1000
... UNRESTRICTED TRUE (setting default UHF)
... VARTHRESH 2 (default DFT)
... BASIS LACVP*
... GEOM_OPT_HESSIAN READ
... EXTERNAL_HESSIAN 1
... GUI GUI_SPARTAN
... TERSE_OUTPUT TRUE

### Coordinate (xyz) of the Fe-Pz$_2$Py complex from optimized geometry

| | | Coordinates (Angstroms) | | |
|---|---|---|---|---|
| | ATOM | X | Y | Z |
| 1 | H | 0.000000 | 0.000000 | 4.752645 |
| 2 | C | 0.000000 | 0.000000 | 3.665240 |
| 3 | N | 0.000000 | 0.000000 | 0.929633 |
| 4 | C | -1.213099 | 0.001082 | 2.982360 |
| 5 | C | 1.213099 | -0.001082 | 2.982360 |
| 6 | C | 1.155745 | -0.001370 | 1.596865 |
| 7 | C | -1.155745 | 0.001370 | 1.596865 |
| 8 | H | -2.154863 | 0.001366 | 3.522046 |
| 9 | H | 2.154863 | -0.001366 | 3.522046 |
| 10 | N | -2.284786 | 0.002812 | 0.763129 |
| 11 | N | -2.102030 | -0.002947 | -0.589849 |
| 12 | C | -3.324671 | 0.001178 | -1.109418 |
| 13 | C | -4.310481 | 0.009849 | -0.106597 |
| 14 | C | -3.613793 | 0.010761 | 1.073677 |
| 15 | H | -3.453156 | -0.001888 | -2.186249 |
| 16 | H | -5.384785 | 0.015066 | -0.232088 |
| 17 | H | -3.961376 | 0.016654 | 2.099078 |
| 18 | N | 2.284786 | -0.002812 | 0.763129 |
| 19 | C | 3.613793 | -0.010761 | 1.073677 |
| 20 | C | 4.310481 | -0.009849 | -0.106597 |
| 21 | C | 3.324671 | -0.001178 | -1.109418 |
| 22 | N | 2.102030 | 0.002947 | -0.589849 |

```
23  H            3.961376   -0.016654    2.099078
24  H            5.384785   -0.015066   -0.232088
25  H            3.453156    0.001888   -2.186249
26  Fe           0.000000    0.000000   -1.208249
27  O           -0.013334    2.152433   -1.526782
28  H            0.759561    2.711368   -1.352350
29  H           -0.795144    2.698706   -1.351748
30  O            0.000000    0.000000   -3.291293
31  H            0.007136   -0.789511   -3.854483
32  H           -0.007136    0.789511   -3.854483
33  O            0.013334   -2.152433   -1.526782
34  H            0.795144   -2.698706   -1.351748
35  H           -0.759561   -2.711368   -1.352350
Point Group: c2    Number of degrees of freedom:  48
Energy = -1050.057740208 au
```

**Figure S1.** The optimized structure of Fe-Pz$_2$Py with the relevant Fe-N/O distances, spin density isosurface and Mulliken atomic charges as calculated by DFT UM06/6-31G*/LanL2DZ.

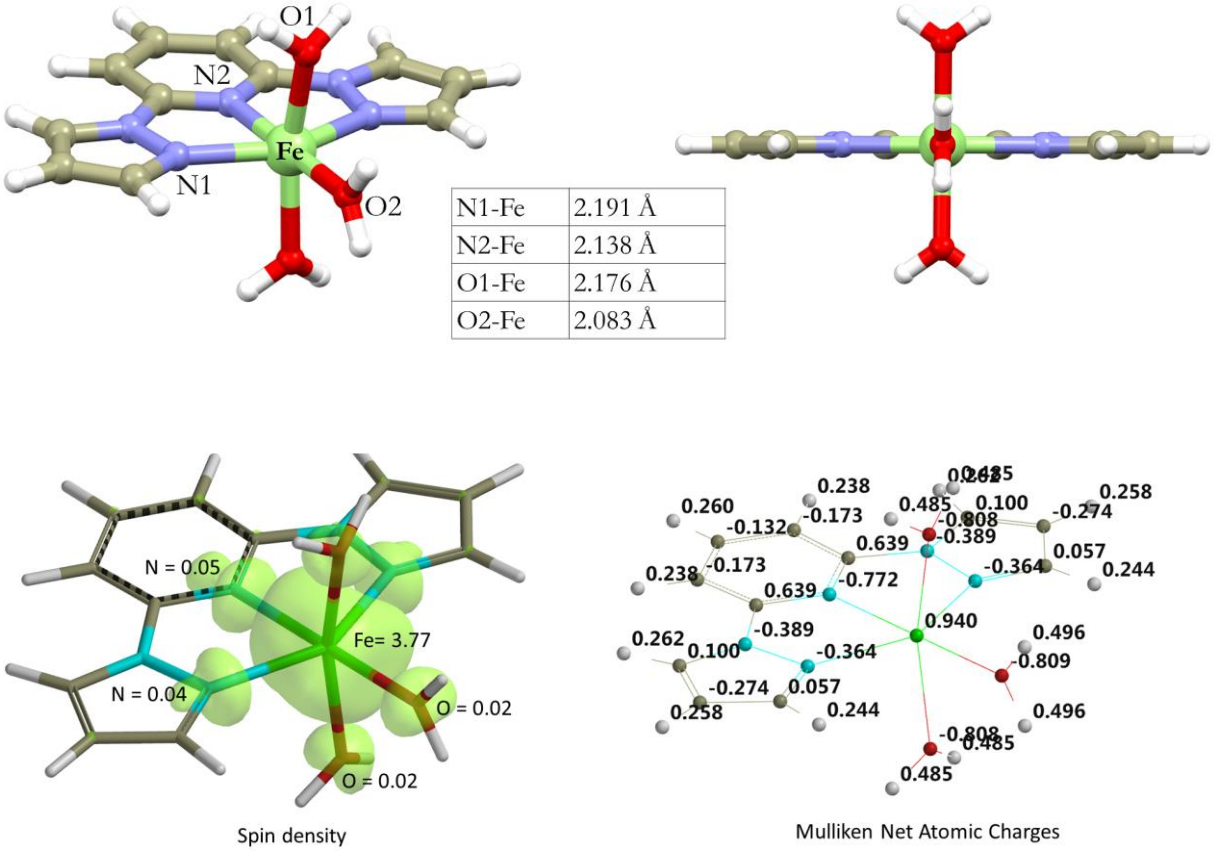


**Figure S2.** Mossbauer spectra of Fe-Pz$_2$Py (powder) recorded at $T$ = 300 K (a) and $T$ =5 K (b) validating the presence in the complex of only Fe(II) cation in high spin ($S$ = 2) state.

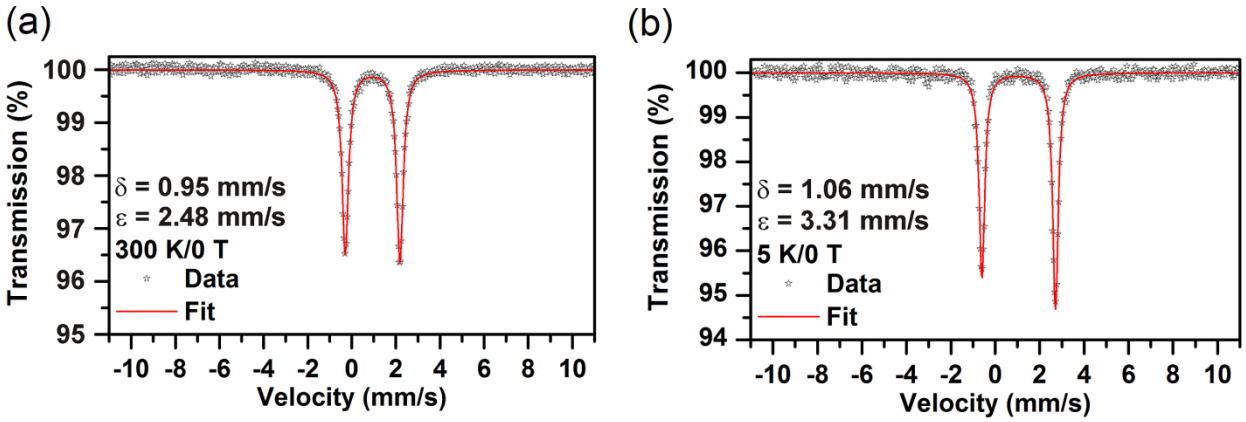



**Figure S3.** FT-IR spectra of GO (a), Fe-Pz$_2$Py/GO (b) and Fe-Pz$_2$Py (c).

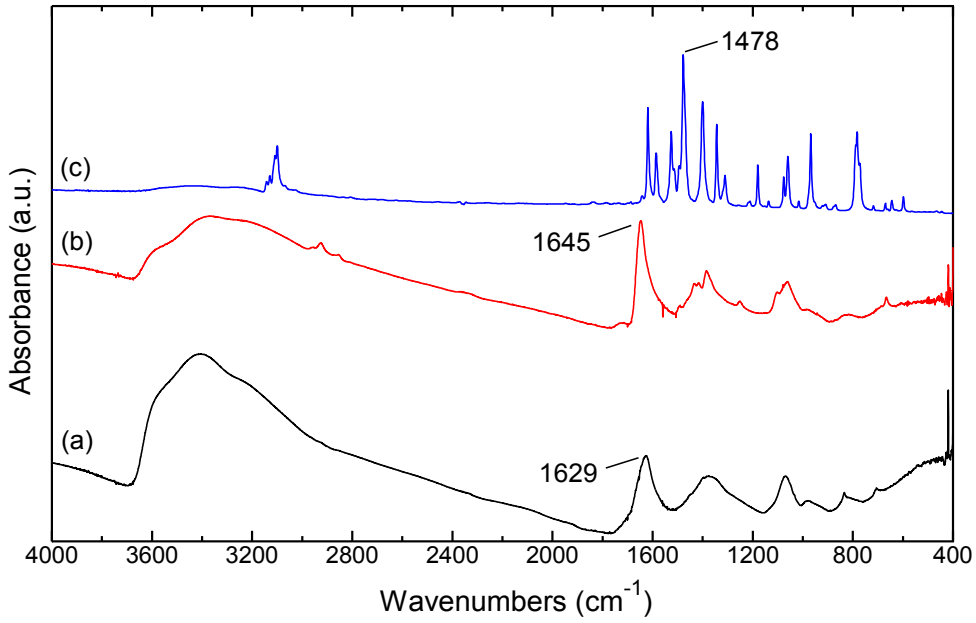


**Figure S4.** Raman spectra of GO (a), and Fe-Pz$_2$Py/GO (b)

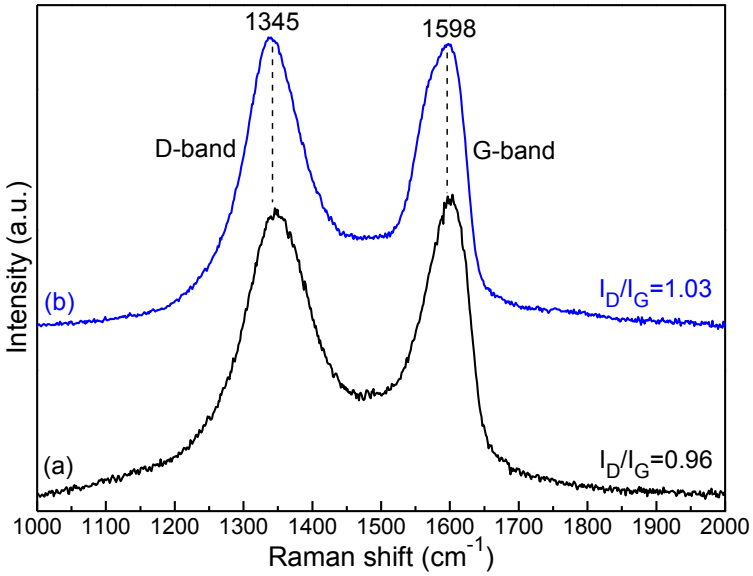
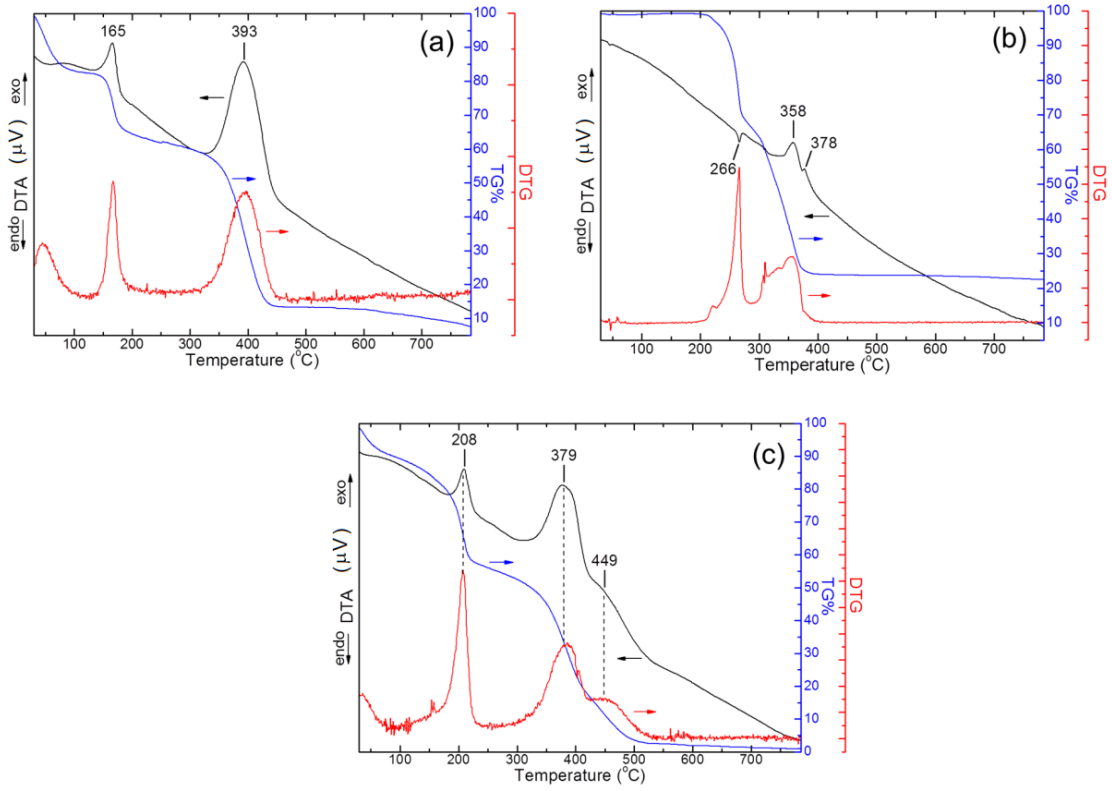


**Figure S5.** DTA/TG%/DTG curves of GO (a), Fe-$Pz_2Py$ (b) and Fe-$Pz_2Py$/GO (c)




Comparison of all DTA/TG%/DTG curves of GO, Fe-$Pz_2Py$ and Fe-$Pz_2Py$/GO clearly confirms the formation of the hybrids system (Fe-$Pz_2Py$/GO). GO materials exhibit two exothermic peaks; one at around 160-210 °C and one at ~400 °C (Panel a), that are ascribed to their decomposition and combustion respectively. The hybrid material demonstrates additional exothermic peaks which are associated with the Fe-$Pz_2Py$ content and its combustion (Panel c). All exothermic peaks are accompanied by corresponding weight losses which are better displayed by the DTG signals. Moreover, in the temperature region ~130-550 °C which includes all decomposing and combustion of organic/inorganic carbon-based content of the materials, Fe-$Pz_2Py$/GO losses 85% of its weight, and GO just 69%. This difference is associated with the Fe-$Pz_2Py$ presence (Panel b). Thus, while combustion peaks of pristine GO and Fe-$Pz_2Py$ are overlapping and the exact Fe-$Pz_2Py$ content cannot be exactly calculated, an estimation from the TG% signal leads to ~16 wt% Fe-$Pz_2Py$ content for Fe-$Pz_2Py$/GO. This amount of loaded Fe-$Pz_2Py$ has been further validated by atomic absorption spectroscopy following analysis of the Fe cation (16.3±0.3 wt% of Fe-$Pz_2Py$ in the hybrid). After drying the sample Fe-$Pz_2Py$/GO being kept in water for weeks no significant signal shifts or changes in the DTA/TG%/DTG relative intensity were observed, indicating a highly stable material, both as dry powder and in solution, even after prolonged storage.

**Figure S6.** The N1*s* core level X-ray photoemission spectra of sample Fe-Pz$_2$Py/GO.

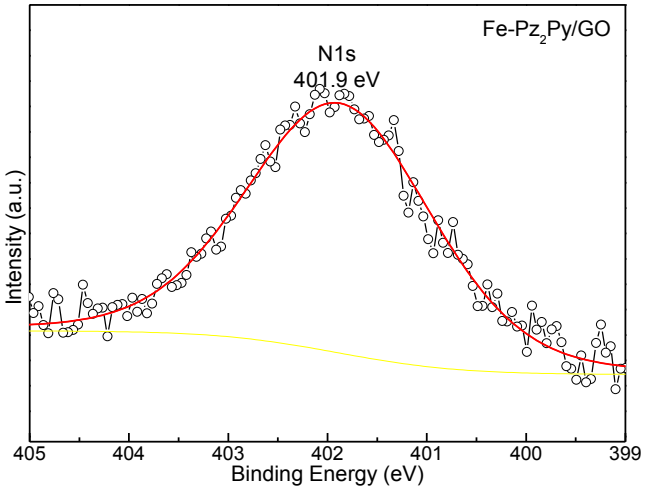


**Figure S7.** The SEM and TEM micrographs of the drug loaded GO composite (Fe-$Pz_2Py$/GO).

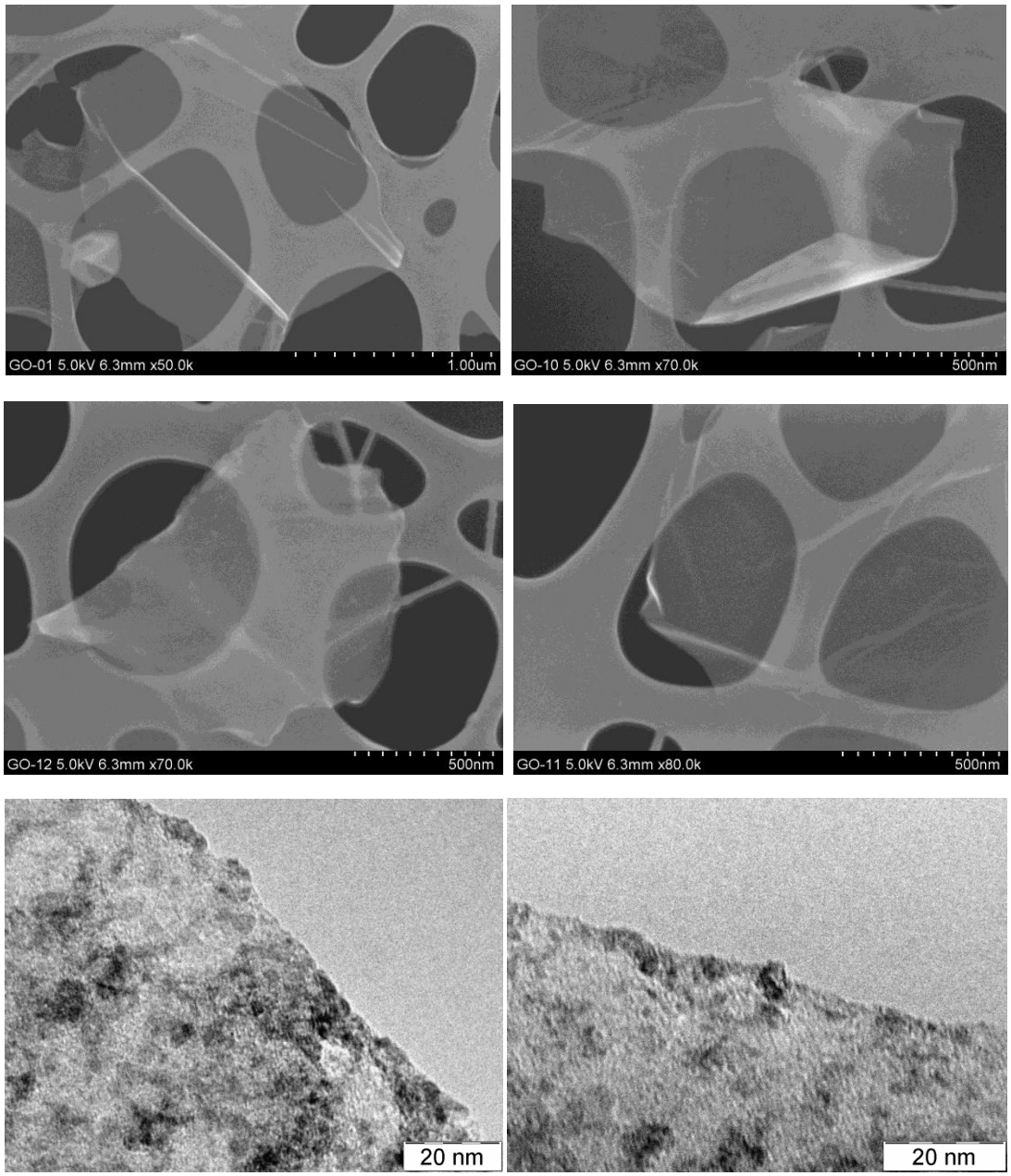


**Figure S8.** The UV-Vis spectrum of Fe-Pz$_2$Py in water (0.03 mM) (b) and the calculated absorption envelope (a) by TDDFT-UEDF2/6-31G** in vacuum (excited states = 30, frozen cores = 28).

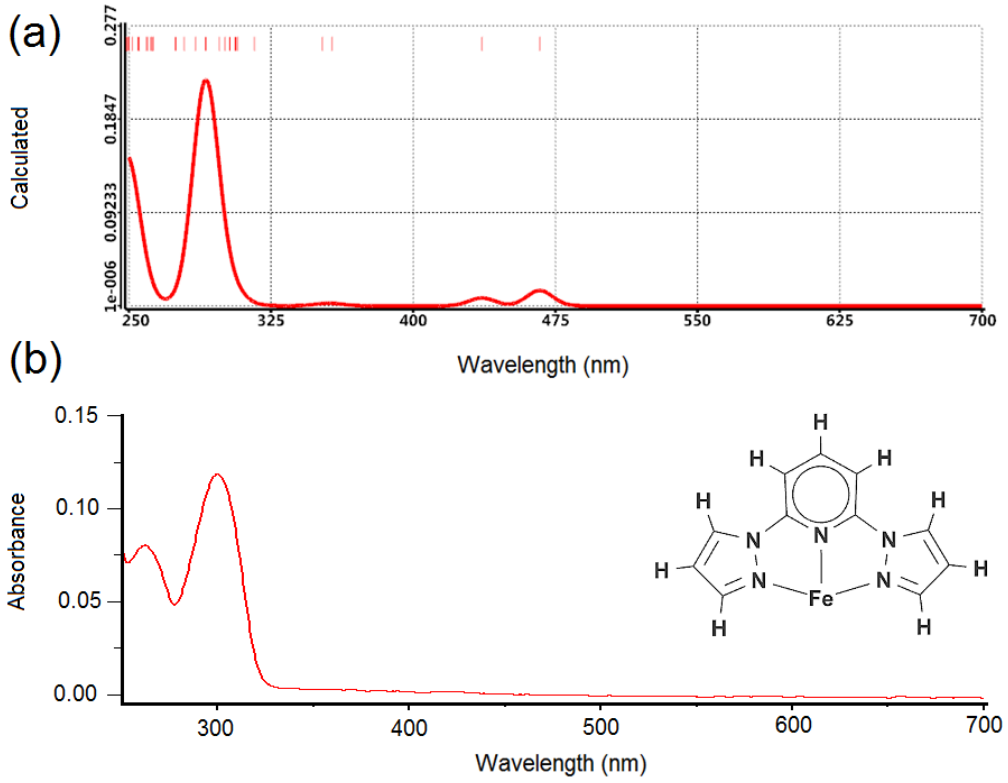
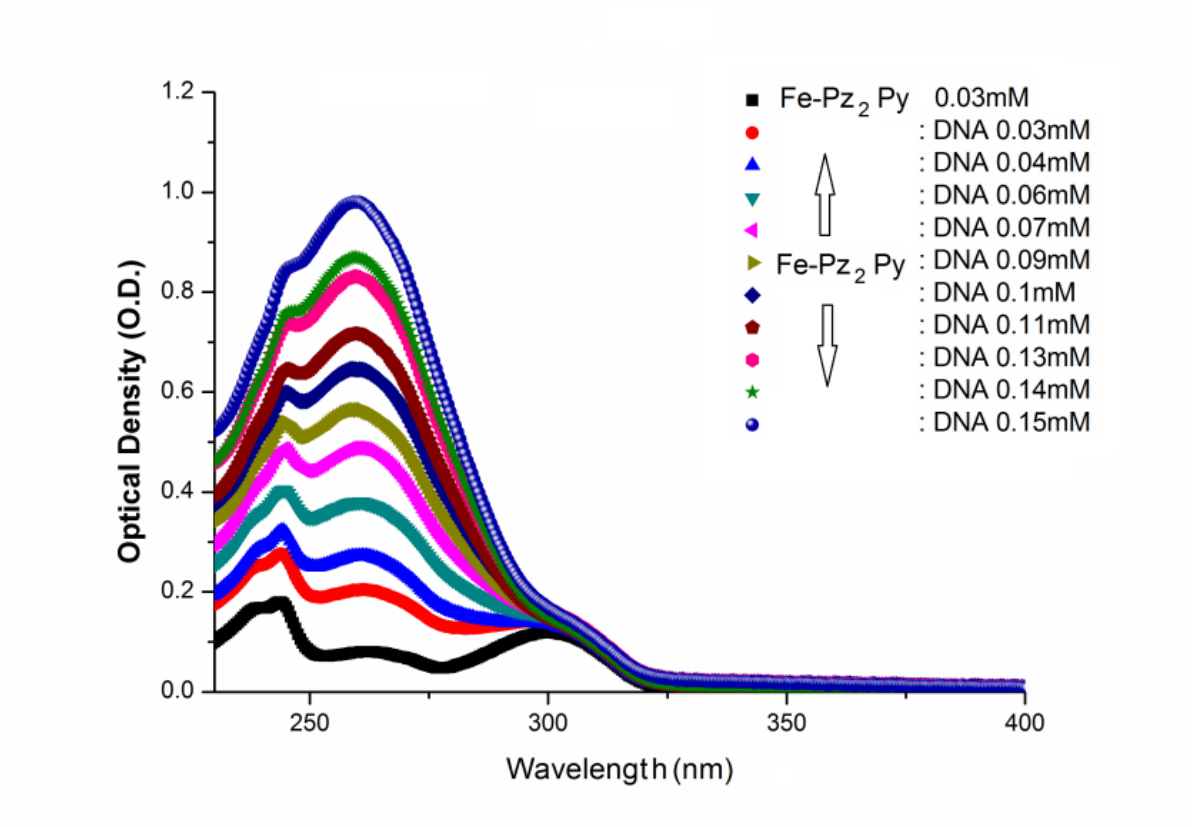
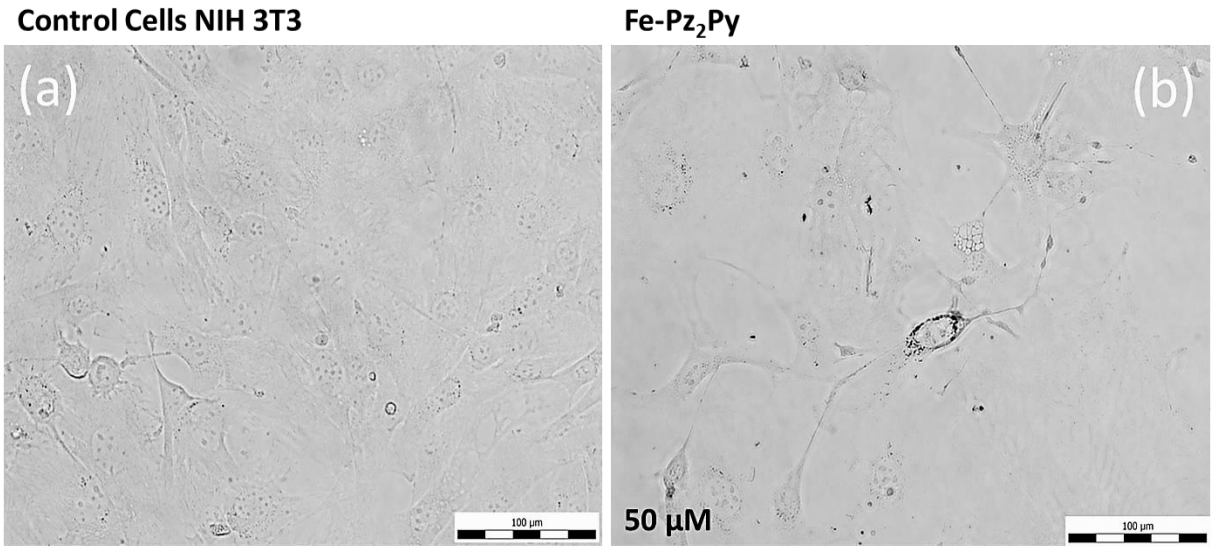


**Figure S9**. Steady-state optical absorption spectra of Fe-$Pz_2Py$ in water in presence of increasing amounts of DNA showing the absorbance changes with the increase of DNA concentration.




The optical spectrum of the Fe-$Pz_2Py$ complex (black line) displays transitions centered at ~ 238nm, 243nm, 262nm, 300nm and between 350-400 nm. The 475 nm band likely arises from a charge transfer transition between the iron and the nitrogen-ligands of the $Pz_2Py$ backbone.

**Figure S10.** Confocal microscopy images of the mouse fibroblast NIH 3T3 cells culture without (a) and with 50μM ($IC_{50}$) of Fe-$Pz_2Py$ (b). Cells were maintained at 37°C with 5% humidified $CO_2$ in an incubation chamber for 24 hours. Images were collected using an optical microscope (Olympus IX 70) with an objective of 40×.




**NOTE:**

It is interesting to report also that when the cell line NIH 3T3 (mouse fibroblasts) was used in the cytotoxicity screening for Fe-$Pz_2Py$, the calculated $IC_{50}$ decreased considerably, down to 50 μM, showing that the L929 cells are less affected to the drug exposure. Kamatchi et al. demonstrated that the $IC_{50}$ for NIH 3T3 cells equals to 177μM for cisplatin and 109μM to 248μM for different types or ruthenium complexes containing bidentate carboxylates ligands, hence Fe-$Pz_2Py$ is more toxic than cis-Pt and Ru-based drugs against the NIH 3T3 cell's line.

**Reference**

T. S. Kamatchi, N. Chitrapriya, H. Lee, C. F. Fronczek, F. R. Fronczek, K. Natarajan, *Dalton Trans.*, 2012, **41**, 2066-2077.

**Figure S11**. Fluorescence quenching spectra of Fe-$Pz_2Py$ at different concentrations of base pairs at 298 K; Fe-$Pz_2Py$ = 0.03 mM, Base pairs from 0.015 mM to 0.15 mM ($E_{ex}$= 295 nm) with (a) Adenine, (b) Thymine, (c) Guanine and (d) Cytosine. The arrows in (b) and (d) indicate the fluorescence quenching process.

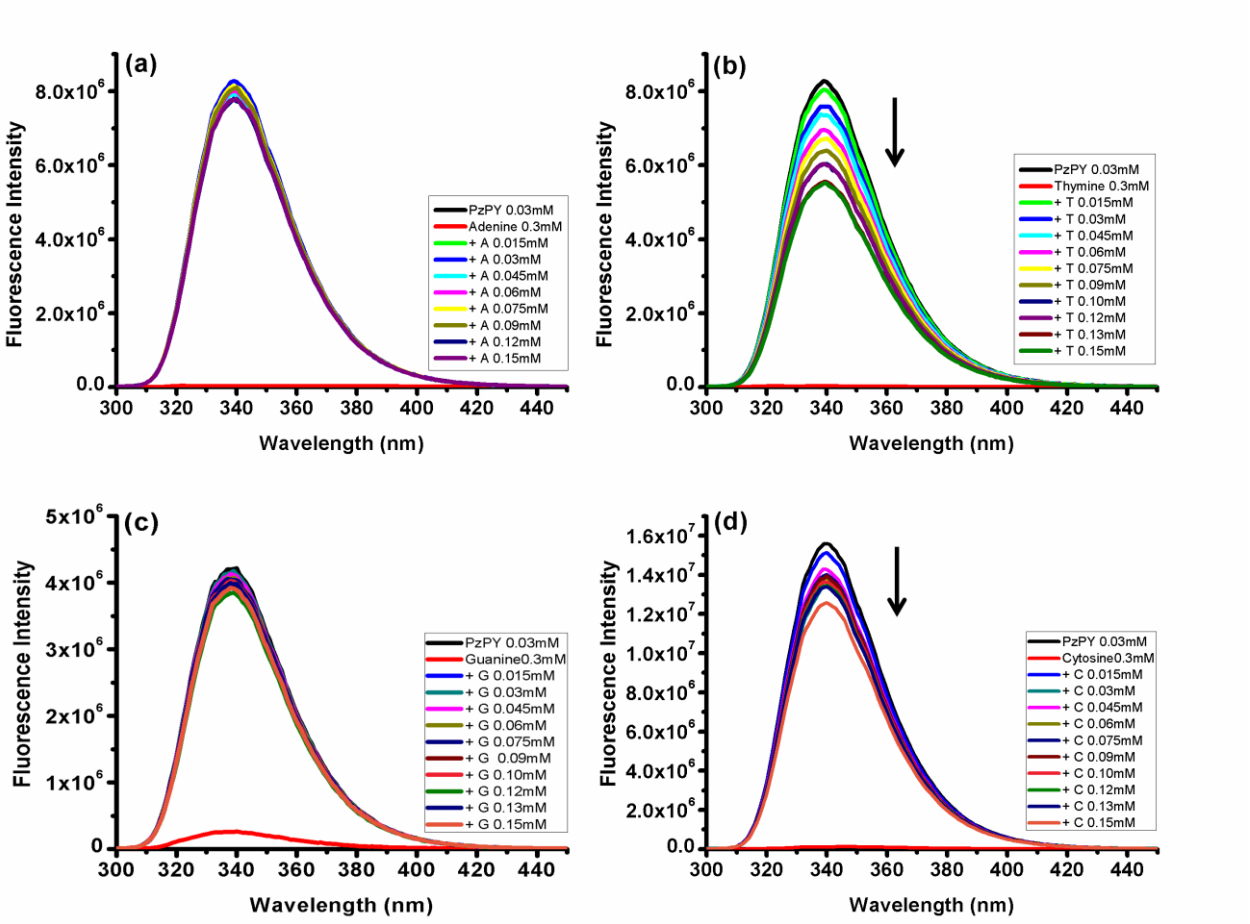


**Figure S12**. Stern-Volmer plot of the binding of Fe-Pz$_2$Py to DNA (a), thymine (b) and cytosine (c) recorded at room temperature. Plot of log[($F_0$-F)/F] *vs* log [Substrate] for the binding of Fe-Pz$_2$Py to DNA (d), thymine (e) and cytosine (f). The Table in the bottom shows a summary of the constant *K*q, *K*sv, *K* and *n* for DNA, thymine and cytosine.

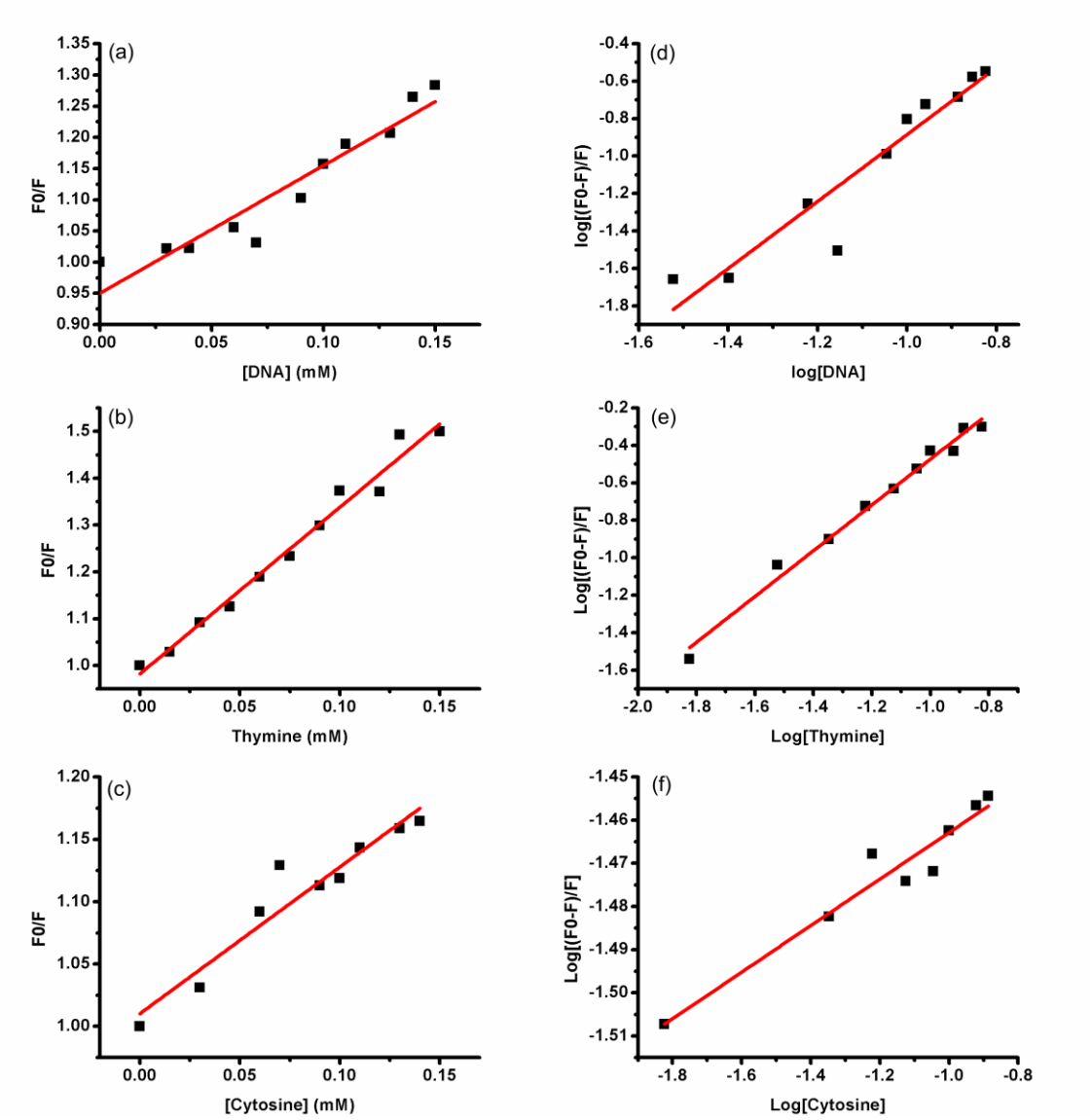



**Table S1**

| | Kq ($M^{-1}s^{-1}$) | $K_{sv}$ ($M^{-1}$) | K ($M^{-1}$) | n |
|---|---|---|---|---|
| **DNA** | 2.0 x $10^{11}$ | 2.0x $10^{3}$ | 7.9 ± 1.6 | 1.8 |
| **Thymine** | 7.2 x $10^{12}$ | 3.6 x $10^{3}$ | 5.0 ± 1.1 | 1.2 |
| **Cytosine** | 2.4 x $10^{12}$ | 1.2 x $10^{3}$ | 0.04 ± 1 | 0.05 |

**Note:** Using the following equation, the formation of complex between Fe-Pz$_2$Py and DNA, thymine or cytosine can be confirmed from the values of quenching rate constant $K_q$:

$$K_q = K_{sv}/\tau_0$$

where $\tau_0$ is the average lifetime of the molecule without the quencher. For various quenchers, the maximum scatter collision quenching constant, $K_q$, with biopolymer is 2 x $10^{10}$ $M^{-1}s^{-1}$. If we assume the lifetime ($\tau_0$) ($10^{-12}$ $s^{-1}$) of the calf thymus, which is equal to 10 ps, is similar to the salmon sperm DNA, then we can extract $K_q$.

## Theoretical calculations (UV-Vis of Fe-$Pz_2Py$)

Input File (Spartan 14) for the calculation of the UV-Vis spectrum of Fe-$Pz_2Py$ (charge = +2, multiplicity = 5) as shown in Figure S7.

Job type: Single point.
Excited States: 30
Method: UEDF2(FC)
Basis set: 6-31G**
Number of shells: 128
Number of basis functions: 389
Charge : +2
Multiplicity: 5

Processing $rem in C:/Program Files/Wavefunction/Spartan14v100/P4e//../auxdir/config/preferences.
(Site specific preferences)
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... SCF_CONVERGENCE 7
... SMALL_PROD_XCMAT 9
... BASIS_LIN_DEP_THRESH 5
... SCF_ALGORITHM DIIS_GDM
... MAXSCF 100
... MAXDIIS 50
... THRESHDIIS -1 (i.e. don't switch on delta-E)
... ONEEXE_SPAR TRUE
... GUI GUI_SPARTAN
... TERSE_OUTPUT TRUE
Processing $rem in input file
... EXCHANGE EDF2
... CORRELATION None (default)
... BASIS 6-31G**
... CIS_N_ROOTS 6
... CIS_STATE_DERIV 1
... IGRDTY 70000302 (70,302)
... MAXSCF 1000
... CIS_N_ROOTS 30
... N_FROZEN_CORE 28
... UNRESTRICTED TRUE (setting default UHF)
... VARTHRESH 2 (default DFT)
... INCDFT TRUE (default DFT)
... GUI GUI_SPARTAN
... TERSE_OUTPUT TRUE

---

**TDDFT/TDA Excitation Energies**

---

Excited state 1: excitation energy (eV) = 0.0391
Total energy for state 1: -2190.442481939248
<S**2> : 6.0110
Trans. Mom.: 0.1355 X 0.0013 Y 0.0000 Z
Strength : 0.0000
D( 52) --> S( 1) amplitude = 0.8220 beta
D( 52) --> S( 4) amplitude = 0.5426 beta

Excited state 2: excitation energy (eV) = 0.1262
Total energy for state 2: -2190.439281151341
<S**2> : 6.0072
Trans. Mom.: 0.0000 X 0.0000 Y 0.0035 Z
Strength : 0.0000
D( 52) --> S( 3) amplitude = 0.9883 beta

Excited state 3: excitation energy (eV) = 0.9847
Total energy for state 3: -2190.407733138254
<S**2> : 6.0061
Trans. Mom.: -0.0024 X 0.0104 Y 0.0000 Z
Strength : 0.0000
D( 52) --> V( 1) amplitude = 0.9631 beta
D( 52) --> V( 4) amplitude = 0.2099 beta

Excited state 4: excitation energy (eV) = 1.4444
Total energy for state 4: -2190.390838883862
<S**2> : 6.0077
Trans. Mom.: 0.0021 X 0.0059 Y 0.0000 Z
Strength : 0.0000
D( 52) --> V( 1) amplitude = -0.2189 beta
D( 52) --> V( 2) amplitude = -0.5845 beta
D( 52) --> V( 4) amplitude = 0.7228 beta
D( 52) --> V( 7) amplitude = 0.2655 beta

Excited state 5: excitation energy (eV) = 2.6563
Total energy for state 5: -2190.346301921167
<S**2> : 7.1826
Trans. Mom.: 0.0000 X 0.0000 Y 0.4812 Z
Strength : 0.0151
D( 52) --> S( 2) amplitude = 0.9733 beta

Excited state 6: excitation energy (eV) = 2.8418
Total energy for state 6: -2190.339484954966
<S**2> : 7.0280
Trans. Mom.: -0.3322 X -0.0006 Y 0.0000 Z
Strength : 0.0077
D( 52) --> S( 1) amplitude = -0.5546 beta
D( 52) --> S( 4) amplitude = 0.8213 beta

Excited state 7: excitation energy (eV) = 3.4719
Total energy for state 7: -2190.316328029332
<S**2> : 7.7851
Trans. Mom.: 0.0000 X 0.0000 Y -0.1419 Z
Strength : 0.0017
S( 4) --> V( 2) amplitude = -0.6091 alpha
D( 51) --> S( 1) amplitude = 0.6531 beta
D( 51) --> S( 4) amplitude = -0.3240 beta

Excited state 8: excitation energy (eV) = 3.5206

Total energy for state 8: -2190.314538389789
<S**2> : 7.9817
Trans. Mom.: -0.1036 X -0.0001 Y 0.0000 Z
Strength : 0.0009
S( 4) --> V( 1) amplitude = 0.7053 alpha
D( 51) --> S( 2) amplitude = 0.6670 beta

Excited state 9: excitation energy (eV) = 3.9212
Total energy for state 9: -2190.299818806492
<S**2> : 6.2670
Trans. Mom.: 0.0005 X -0.0689 Y 0.0000 Z
Strength : 0.0005
S( 3) --> V( 1) amplitude = 0.9925 alpha

Excited state 10: excitation energy (eV) = 4.0335
Total energy for state 10: -2190.295692020174
<S**2> : 7.7892
Trans. Mom.: 0.0000 X 0.0000 Y -0.0793 Z
Strength : 0.0006
S( 1) --> V( 2) amplitude = 0.3795 alpha
S( 2) --> V( 1) amplitude = -0.4473 alpha
D( 49) --> S( 1) amplitude = 0.3934 beta
D( 49) --> S( 4) amplitude = -0.1720 beta
D( 50) --> S( 2) amplitude = 0.4524 beta
D( 52) --> V( 3) amplitude = -0.2941 beta

Excited state 11: excitation energy (eV) = 4.0457
Total energy for state 11: -2190.295241064957
<S**2> : 7.7855
Trans. Mom.: 0.0372 X -0.0030 Y 0.0000 Z
Strength : 0.0001
D( 52) --> V( 2) amplitude = 0.1641 alpha
S( 1) --> V( 1) amplitude = -0.4798 alpha
S( 1) --> V( 3) amplitude = 0.1624 alpha
S( 2) --> V( 2) amplitude = 0.3586 alpha
D( 48) --> S( 1) amplitude = 0.1730 beta
D( 49) --> S( 2) amplitude = 0.3885 beta
D( 49) --> V( 3) amplitude = -0.1603 beta
D( 50) --> S( 1) amplitude = 0.5170 beta
D( 50) --> S( 4) amplitude = -0.1833 beta

Excited state 12: excitation energy (eV) = 4.0517
Total energy for state 12: -2190.295021136484
<S**2> : 7.0286
Trans. Mom.: -0.0009 X -0.0898 Y 0.0000 Z
Strength : 0.0008
D( 52) --> V( 2) amplitude = 0.7963 beta
D( 52) --> V( 4) amplitude = 0.5883 beta

Excited state 13: excitation energy (eV) = 4.0878
Total energy for state 13: -2190.293695368173
<S**2> : 6.3860
Trans. Mom.: 0.0000 X 0.0000 Y -0.3844 Z
Strength : 0.0148
S( 4) --> V( 2) amplitude = 0.3528 alpha
D( 51) --> S( 1) amplitude = 0.6725 beta
D( 51) --> S( 4) amplitude = 0.5922 beta

Excited state 14: excitation energy (eV) = 4.1230
Total energy for state 14: -2190.292400956618
<S**2> : 6.0463
Trans. Mom.: 0.0781 X 0.0056 Y 0.0000 Z

Strength : 0.0006
D( 51) --> S( 3) amplitude = 0.9925 beta

Excited state 15: excitation energy (eV) = 4.1639
Total energy for state 15: -2190.290898737517
<S**2> : 7.1130
Trans. Mom.: 0.0000 X 0.0000 Y 0.0623 Z
Strength : 0.0004
S( 2) --> V( 1) amplitude = -0.1513 alpha
D( 52) --> V( 3) amplitude = 0.9317 beta

Excited state 16: excitation energy (eV) = 4.2679
Total energy for state 16: -2190.287075471239
<S**2> : 6.0446
Trans. Mom.: 1.4522 X 0.0022 Y 0.0000 Z
Strength : 0.2205
S( 4) --> V( 1) amplitude = -0.6557 alpha
D( 51) --> S( 2) amplitude = 0.6731 beta

Excited state 17: excitation energy (eV) = 4.3489
Total energy for state 17: -2190.284101578425
<S**2> : 6.2351
Trans. Mom.: 0.0000 X 0.0000 Y -0.0030 Z
Strength : 0.0000
S( 3) --> V( 2) amplitude = 0.9946 alpha

Excited state 18: excitation energy (eV) = 4.4406
Total energy for state 18: -2190.280728831889
<S**2> : 7.6551
Trans. Mom.: 0.0000 X 0.0000 Y 0.0213 Z
Strength : 0.0000
D( 49) --> V( 1) amplitude = 0.1803 alpha
D( 50) --> V( 1) amplitude = -0.1554 alpha
D( 52) --> V( 1) amplitude = 0.4713 alpha
S( 1) --> V( 2) amplitude = -0.1734 alpha
S( 2) --> V( 1) amplitude = -0.4502 alpha
D( 47) --> S( 2) amplitude = -0.2081 beta
D( 48) --> S( 2) amplitude = -0.3051 beta
D( 49) --> S( 1) amplitude = -0.3271 beta
D( 50) --> S( 2) amplitude = 0.3286 beta
D( 51) --> S( 4) amplitude = -0.1840 beta

Excited state 19: excitation energy (eV) = 4.5145
Total energy for state 19: -2190.278014781491
<S**2> : 7.0745
Trans. Mom.: 0.1570 X 0.0002 Y 0.0000 Z
Strength : 0.0027
D( 50) --> V( 2) amplitude = 0.1841 alpha
S( 1) --> V( 1) amplitude = 0.2508 alpha
S( 4) --> V( 3) amplitude = 0.2337 alpha
D( 48) --> S( 1) amplitude = -0.3506 beta
D( 49) --> S( 2) amplitude = -0.2277 beta
D( 50) --> S( 1) amplitude = 0.6822 beta
D( 51) --> V( 3) amplitude = 0.2072 beta

Excited state 20: excitation energy (eV) = 4.7168
Total energy for state 20: -2190.270581125494
<S**2> : 6.0450
Trans. Mom.: 0.0000 X 0.0000 Y -0.0005 Z
Strength : 0.0000
D( 50) --> S( 3) amplitude = 0.7568 beta
D( 51) --> V( 1) amplitude = -0.6430 beta

Excited state 21: excitation energy (eV) = 4.7272
Total energy for state 21: -2190.270198399535
<S**2> : 6.0453
Trans. Mom.: 0.0000 X 0.0000 Y 0.0266 Z
Strength : 0.0001
D( 50) --> S( 3) amplitude = 0.6373 beta
D( 51) --> V( 1) amplitude = 0.7637 beta

Excited state 22: excitation energy (eV) = 4.7402
Total energy for state 22: -2190.269721830728
<S**2> : 6.9799
Trans. Mom.: -0.0102 X -0.0018 Y 0.0000 Z
Strength : 0.0000
D( 50) --> V( 2) amplitude = -0.1784 alpha
S( 2) --> V( 2) amplitude = -0.4565 alpha
S( 4) --> V( 3) amplitude = -0.2975 alpha
D( 48) --> S( 1) amplitude = 0.3305 beta
D( 49) --> S( 2) amplitude = -0.1682 beta
D( 50) --> S( 1) amplitude = 0.4614 beta
D( 50) --> S( 4) amplitude = 0.3009 beta
D( 51) --> V( 3) amplitude = -0.2815 beta
D( 52) --> V( 6) amplitude = -0.2135 beta

Excited state 23: excitation energy (eV) = 4.7693
Total energy for state 23: -2190.268649819271
<S**2> : 7.0363
Trans. Mom.: 0.0000 X 0.0000 Y -0.0447 Z
Strength : 0.0002
D( 52) --> V( 5) amplitude = 0.9709 beta

Excited state 24: excitation energy (eV) = 4.7831
Total energy for state 24: -2190.268143813801
<S**2> : 6.1772
Trans. Mom.: 0.0032 X 0.1695 Y 0.0000 Z
Strength : 0.0034
D( 51) --> V( 1) amplitude = 0.9911 alpha

Excited state 25: excitation energy (eV) = 4.8565
Total energy for state 25: -2190.265447970550
<S**2> : 6.5812
Trans. Mom.: 0.0000 X 0.0000 Y 0.0645 Z
Strength : 0.0005
D( 49) --> V( 1) amplitude = 0.1518 alpha
D( 50) --> V( 1) amplitude = 0.2585 alpha
D( 52) --> V( 1) amplitude = 0.4164 alpha
S( 1) --> V( 2) amplitude = 0.2857 alpha
S( 2) --> V( 1) amplitude = 0.5313 alpha
S( 4) --> V( 2) amplitude = 0.1630 alpha
D( 48) --> S( 2) amplitude = 0.2358 beta
D( 50) --> S( 2) amplitude = 0.3401 beta
D( 51) --> S( 4) amplitude = -0.2163 beta
D( 52) --> V( 5) amplitude = 0.1563 beta

Excited state 26: excitation energy (eV) = 4.8664
Total energy for state 26: -2190.265083234634
<S**2> : 6.9060
Trans. Mom.: 0.0000 X 0.0000 Y -0.0542 Z
Strength : 0.0004
D( 50) --> V( 1) amplitude = -0.3212 alpha
D( 52) --> V( 1) amplitude = -0.3518 alpha
S( 2) --> V( 1) amplitude = 0.2945 alpha

S( 4) --> V( 6) amplitude = -0.1500 alpha
D( 47) --> S( 2) amplitude = 0.3149 beta
D( 49) --> S( 1) amplitude = -0.2279 beta
D( 50) --> S( 2) amplitude = 0.5930 beta

Excited state 27: excitation energy (eV) = 4.9245
Total energy for state 27: -2190.262949246336
<S**2> : 7.1325
Trans. Mom.: -0.2780 X 0.0001 Y 0.0000 Z
Strength : 0.0093
S( 1) --> V( 1) amplitude = -0.2203 alpha
S( 2) --> V( 2) amplitude = -0.2649 alpha
D( 50) --> S( 4) amplitude = 0.2323 beta
D( 52) --> V( 6) amplitude = 0.8696 beta

Excited state 28: excitation energy (eV) = 4.9592
Total energy for state 28: -2190.261672027625
<S**2> : 6.0473
Trans. Mom.: 0.0285 X 0.0339 Y 0.0000 Z
Strength : 0.0002
D( 49) --> S( 3) amplitude = 0.9805 beta

Excited state 29: excitation energy (eV) = 4.9651
Total energy for state 29: -2190.261457242253
<S**2> : 7.0578
Trans. Mom.: 0.0000 X 0.0000 Y -0.0568 Z
Strength : 0.0004
D( 52) --> V( 1) amplitude = 0.4462 alpha
S( 2) --> V( 1) amplitude = 0.1816 alpha
S( 4) --> V( 2) amplitude = 0.1838 alpha
S( 4) --> V( 6) amplitude = -0.1596 alpha
D( 47) --> S( 2) amplitude = 0.1853 beta
D( 48) --> S( 2) amplitude = -0.3610 beta
D( 49) --> S( 1) amplitude = 0.5864 beta

Excited state 30: excitation energy (eV) = 4.9857
Total energy for state 30: -2190.260697917812
<S**2> : 6.6327
Trans. Mom.: 0.0000 X 0.0000 Y 1.0615 Z
Strength : 0.1376
D( 49) --> V( 1) amplitude = 0.2710 alpha
D( 50) --> V( 1) amplitude = -0.1608 alpha
S( 1) --> V( 2) amplitude = -0.2231 alpha
S( 2) --> V( 1) amplitude = 0.2421 alpha
S( 4) --> V( 2) amplitude = -0.3683 alpha
D( 47) --> S( 2) amplitude = -0.3365 beta
D( 49) --> S( 1) amplitude = 0.4039 beta
D( 49) --> S( 4) amplitude = 0.3221 beta
D( 50) --> S( 2) amplitude = 0.2576 beta
D( 51) --> S( 4) amplitude = 0.2642 beta