

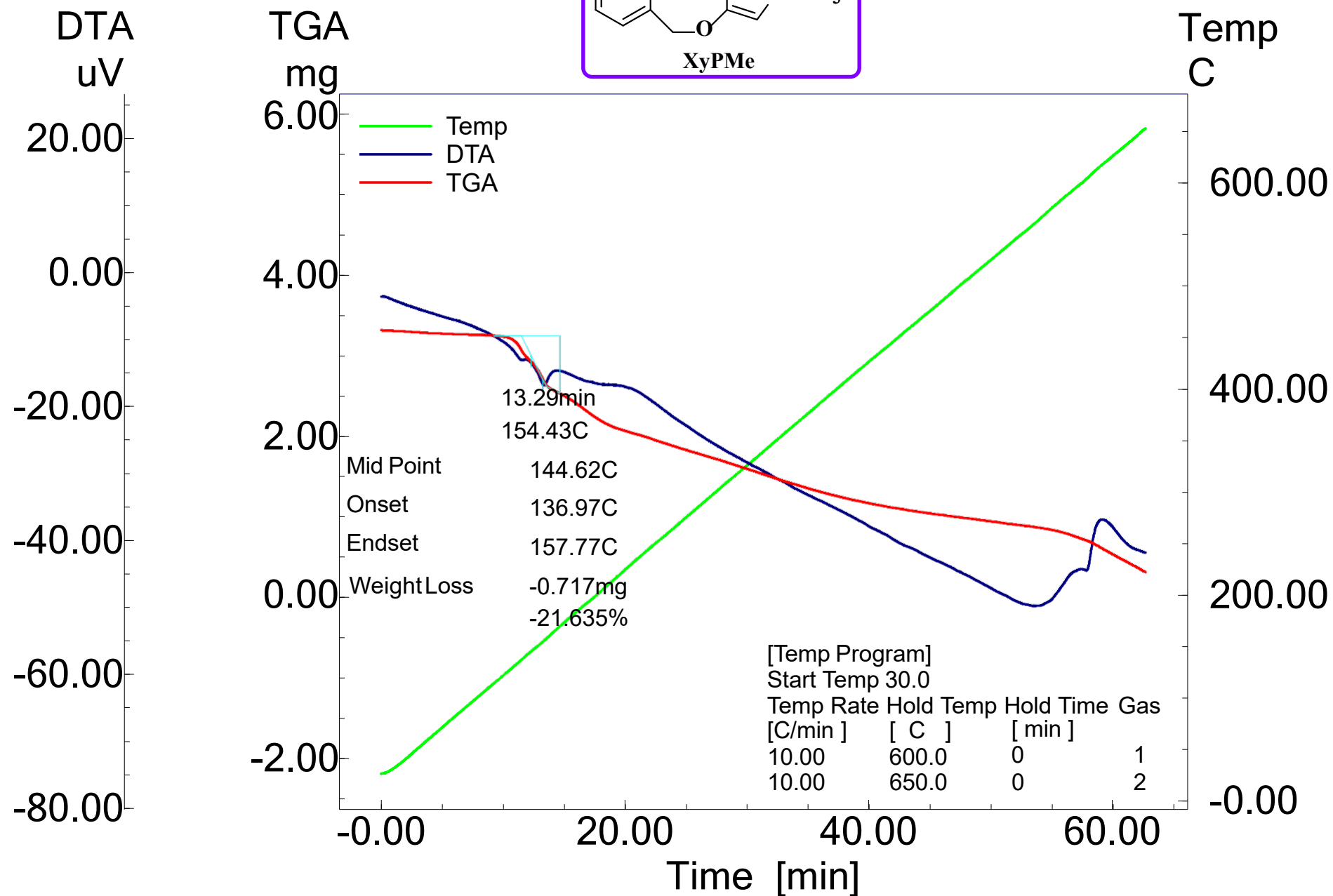
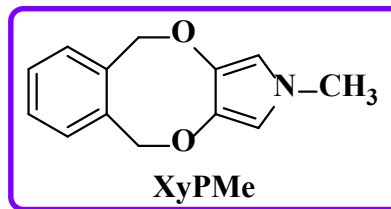


Figure S2. TGA Analysis of XyPBu

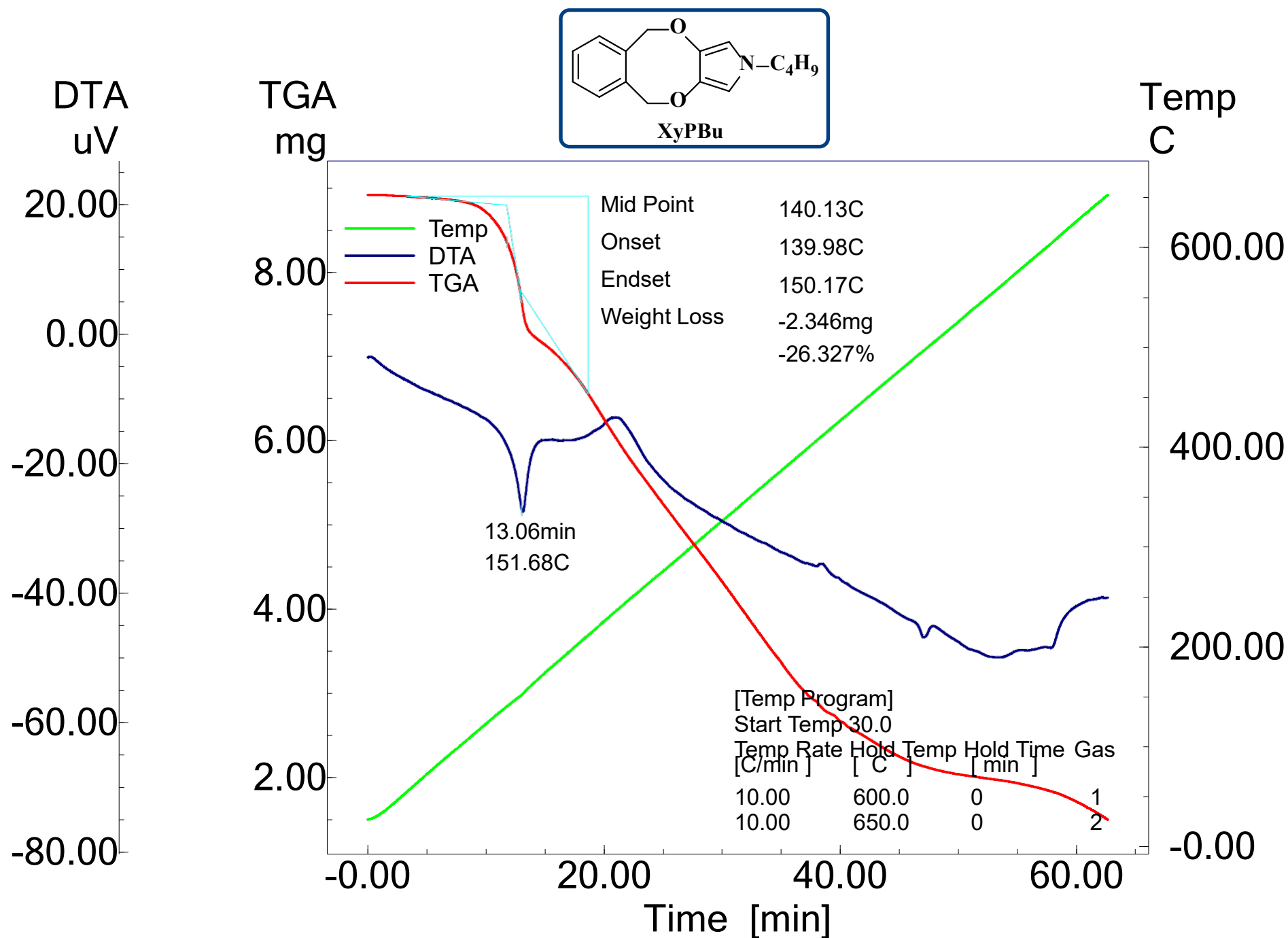


Figure S3. TGA Analysis of XyS

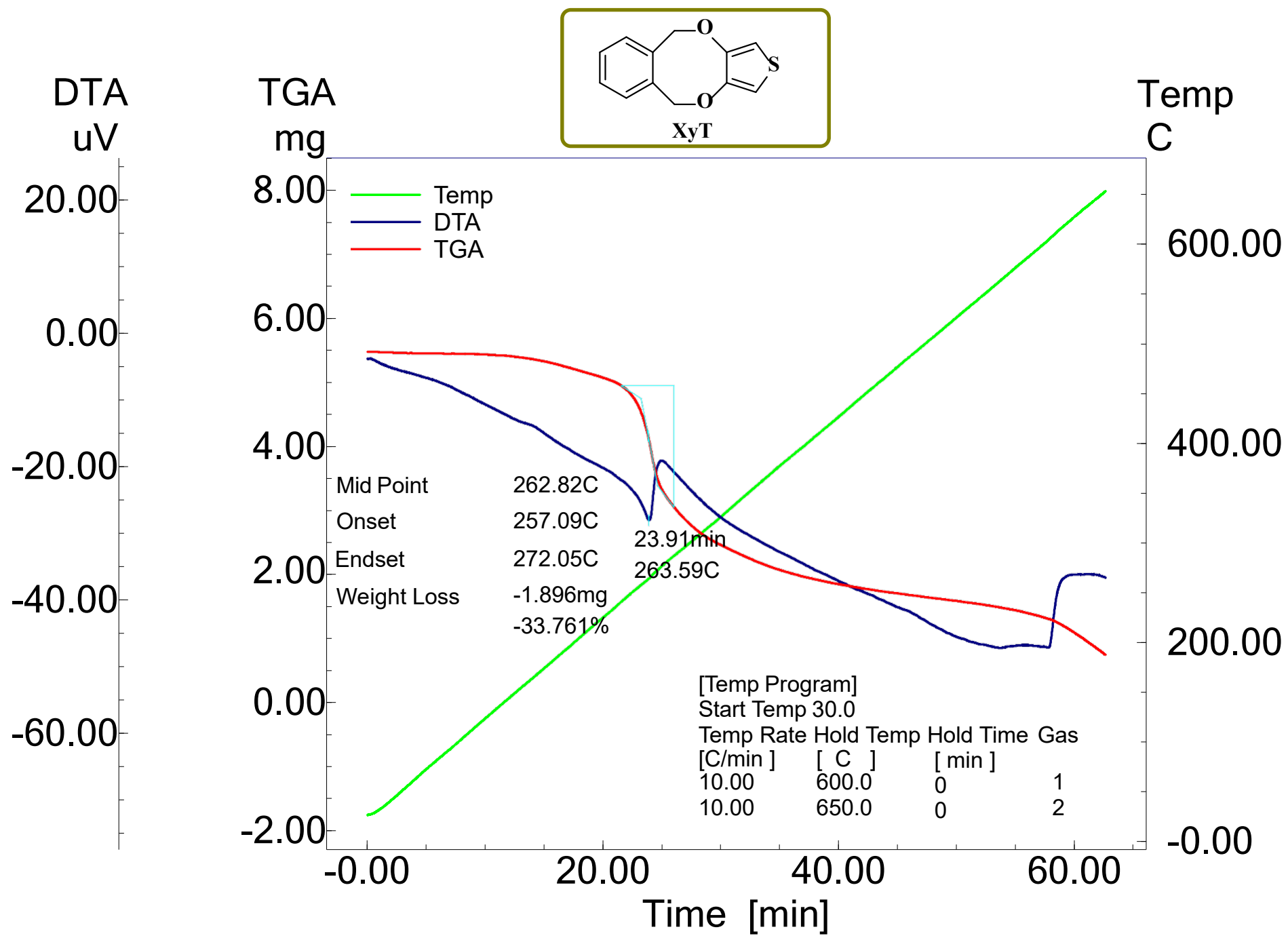


Figure S4. FT-IR spectrum of dimethyl iminodiacetate (1)

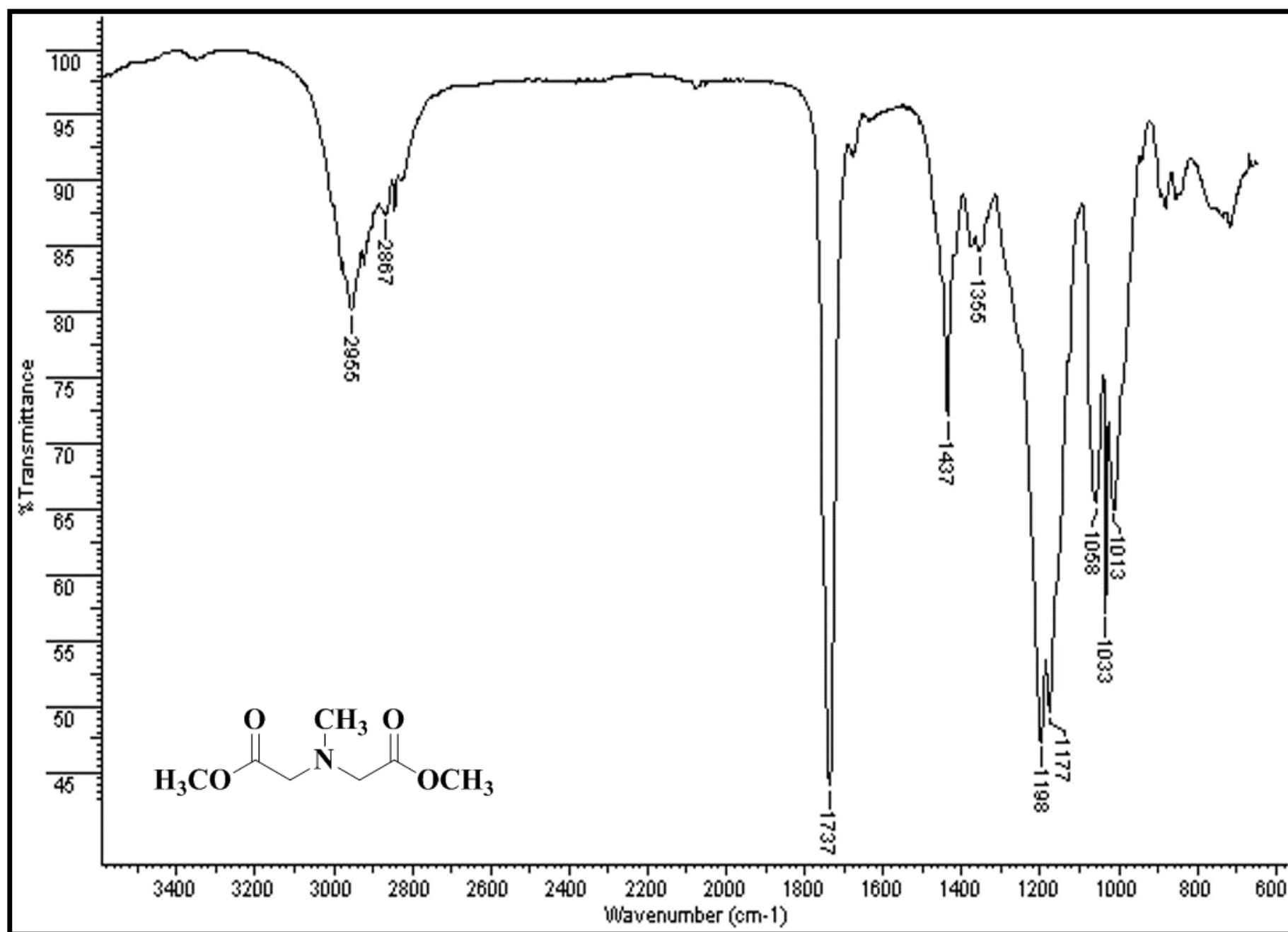


Figure S5. GC-MS spectrum of dimethyl iminodiacetate (1)

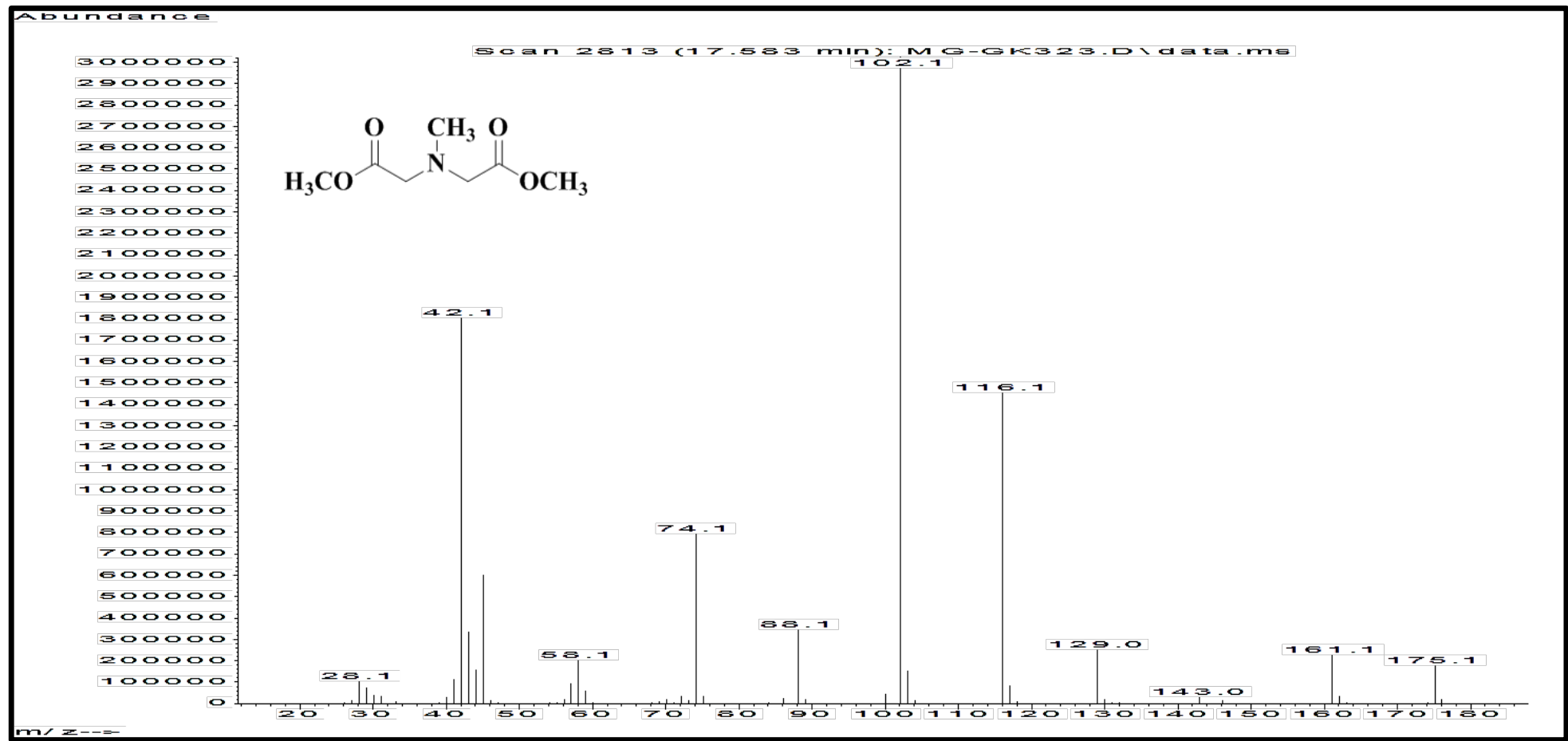


Figure S6. FT-IR spectrum of diethyl 3,4-dihydroxy-1-methyl-1H-pyrrole-2,5-dicarboxylate (2)

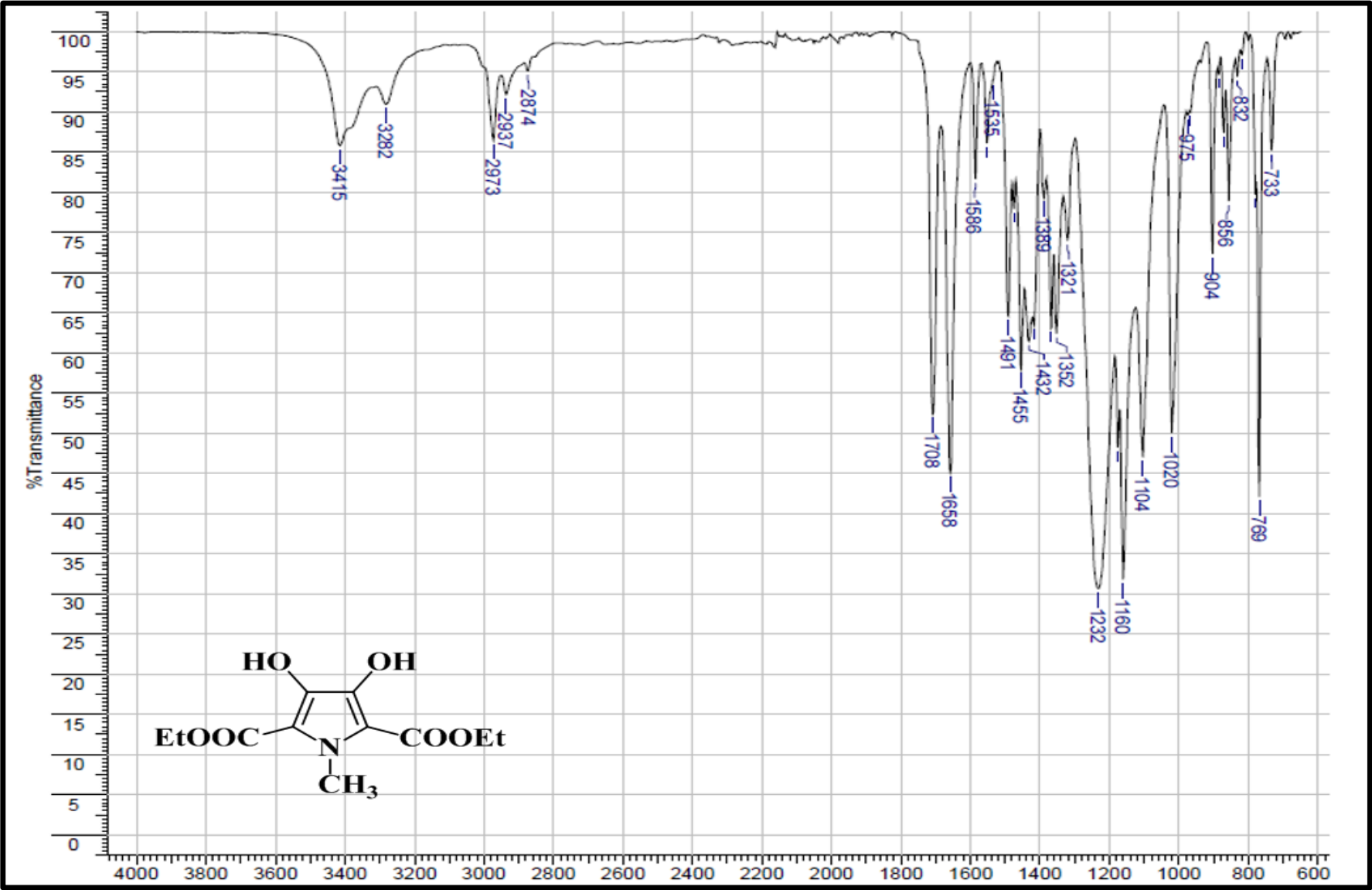


Figure S7. GC-MS spectrum of diethyl 3,4-dihydroxy-1-methyl-1H-pyrrole-2,5-dicarboxylate (2)

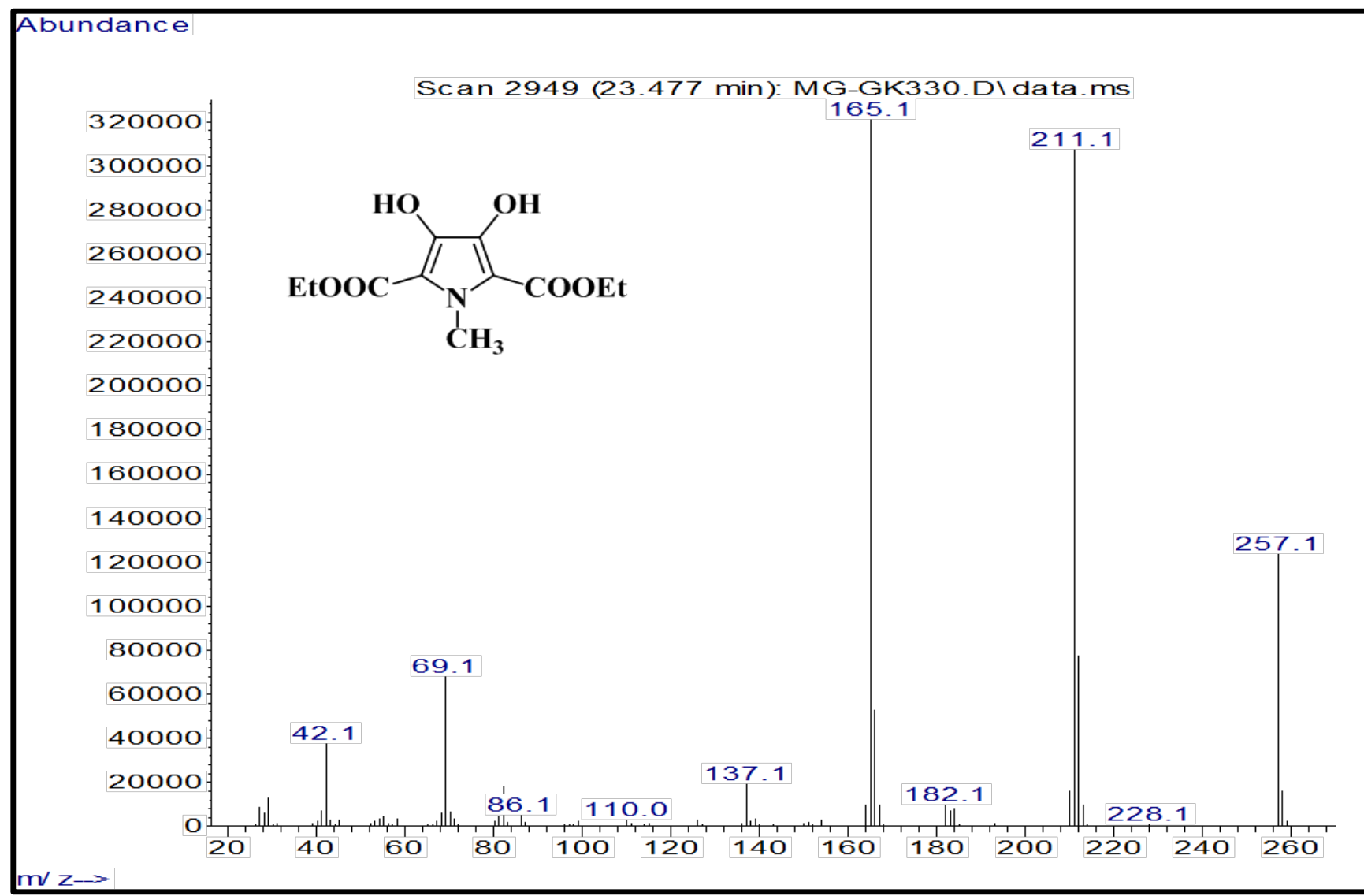


Figure S8. ^1H -NMR spectrum of diethyl 3,4-dihydroxy-1-methyl-1H-pyrrole-2,5-dicarboxylate (2)

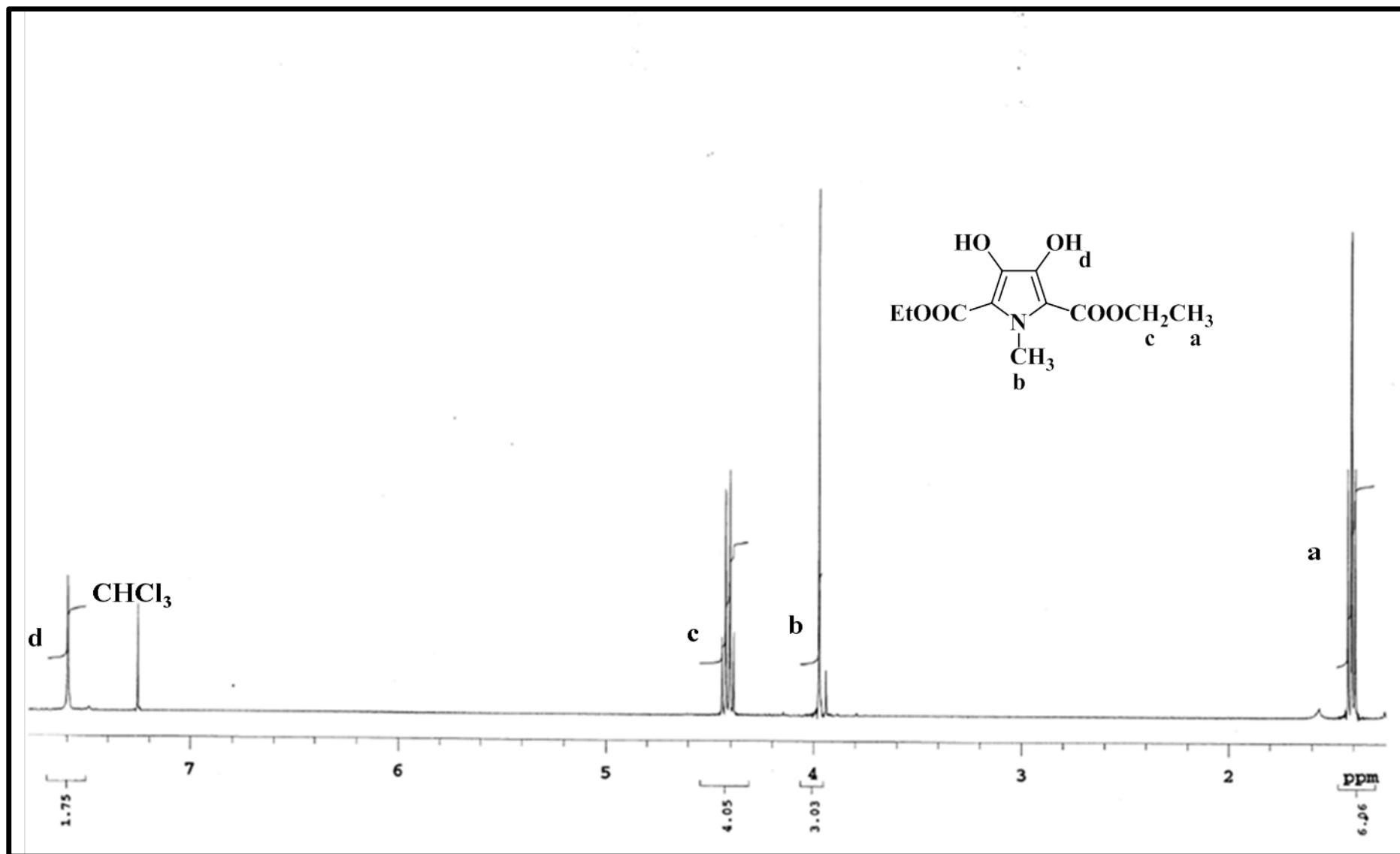


Figure S9. FT-IR spectrum of 1,2-bis(bromomethyl)benzene (3)

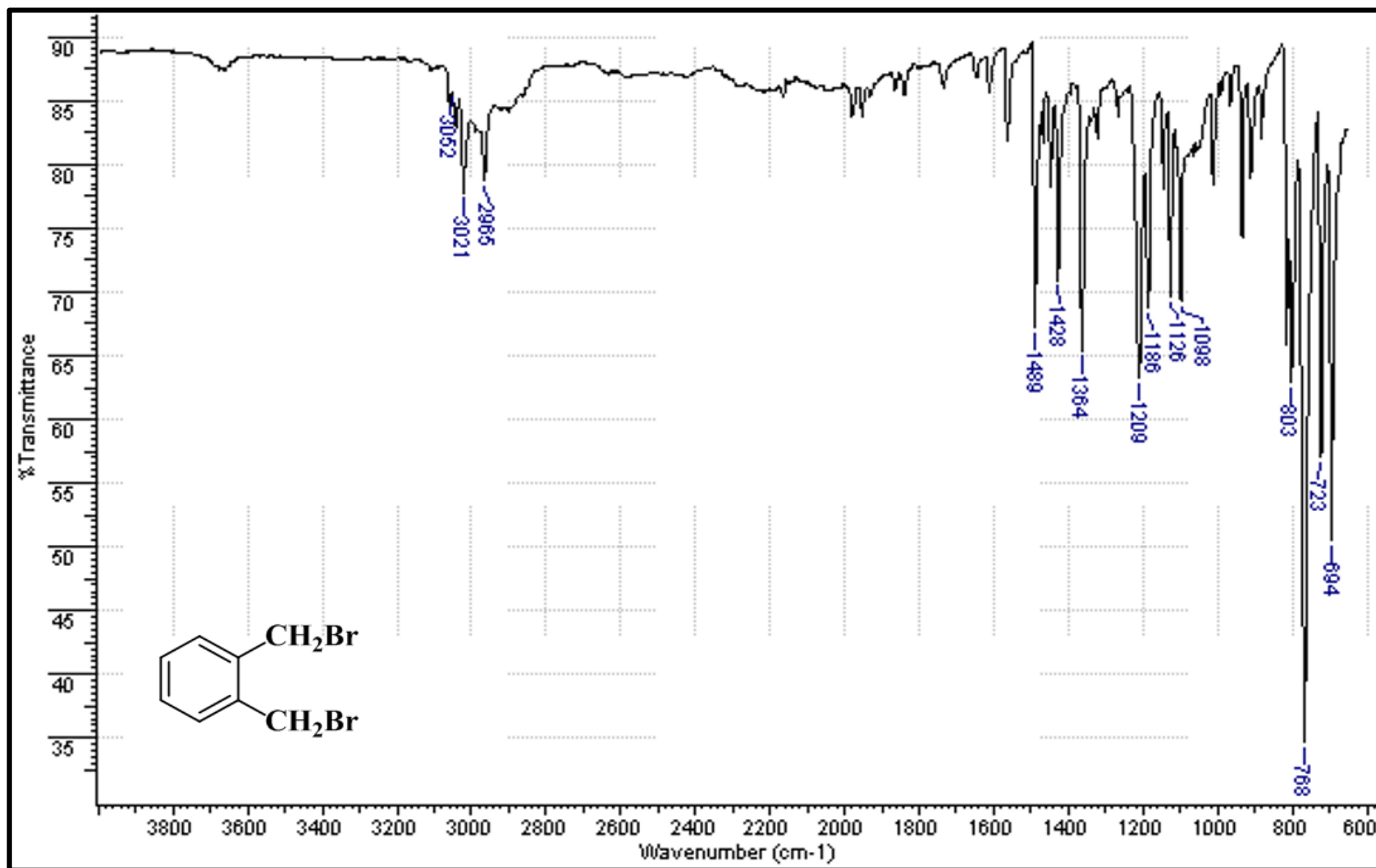


Figure S10. GC-MS spectrum of 1,2-bis(bromomethyl)benzene (3)

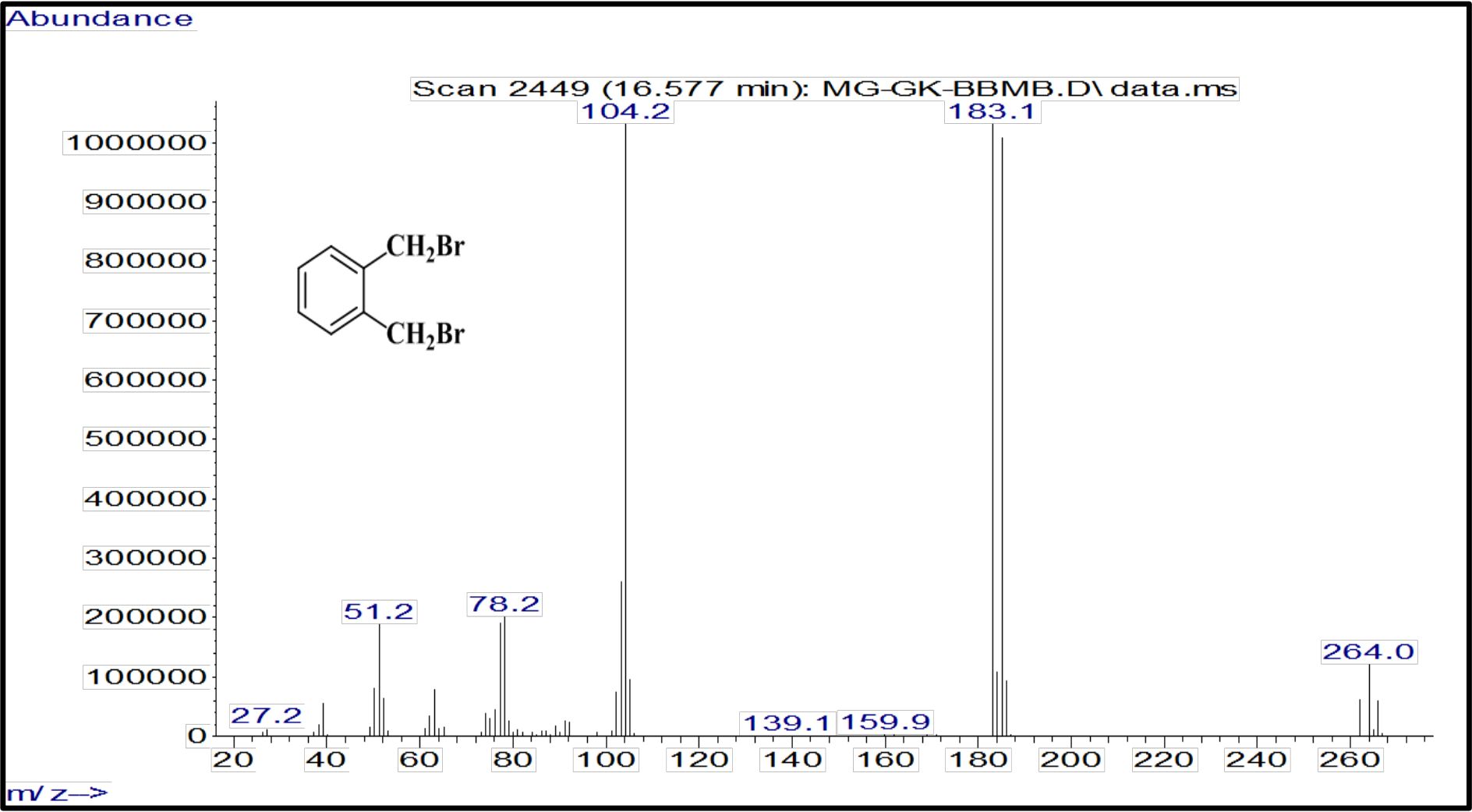


Figure S11. FT-IR spectrum of diethyl 2-methyl-5,10-dihydro-2H-benzo[6,7][1,4]dioxocino[2,3-c]pyrrole-1,3-dicarboxylate (4)

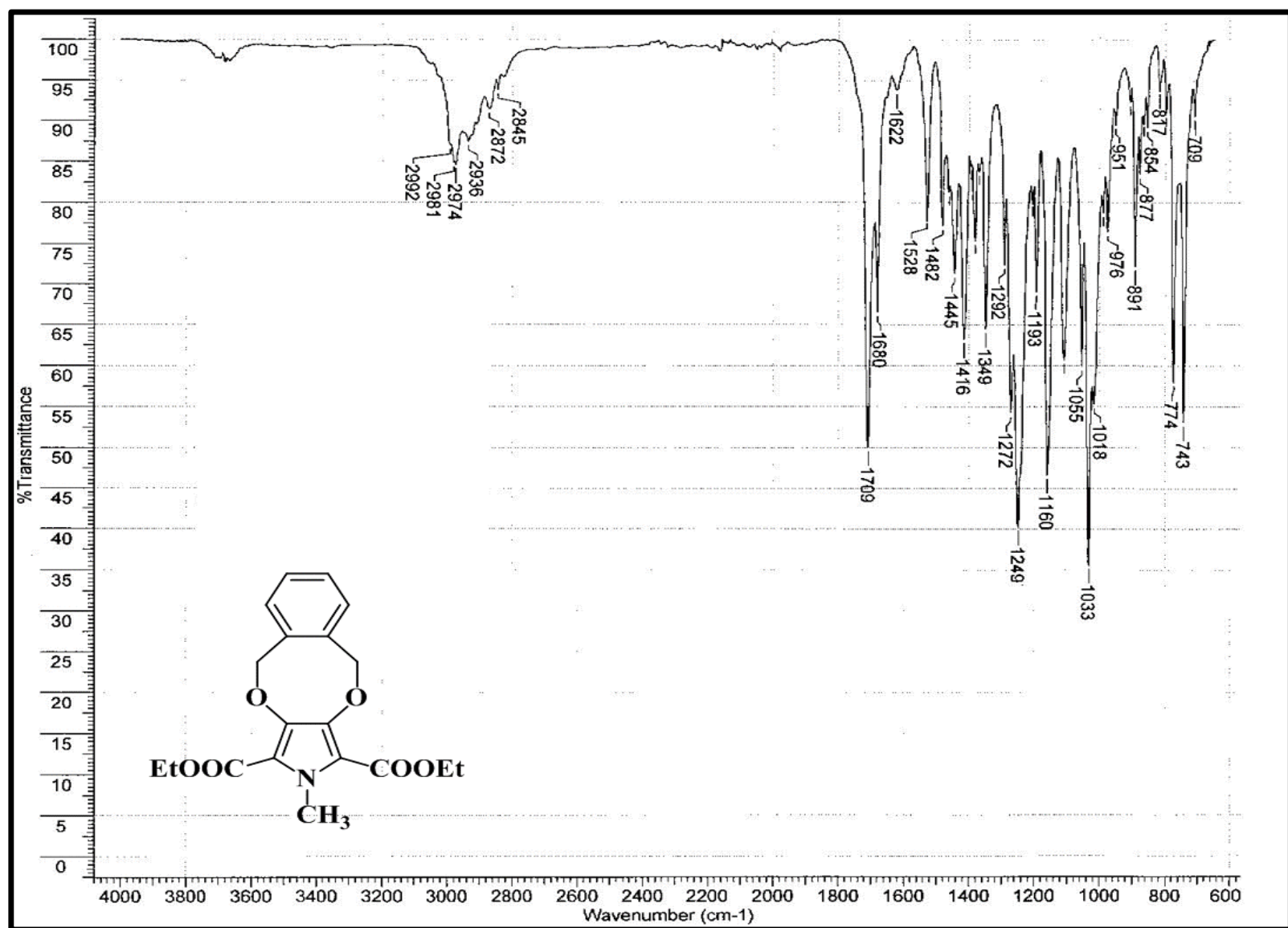


Figure S12. GC-MS spectrum of diethyl 2-methyl-5,10-dihydro-2H-benzo[6,7][1,4]dioxocino[2,3-c]pyrrole-1,3-dicarboxylate (4)

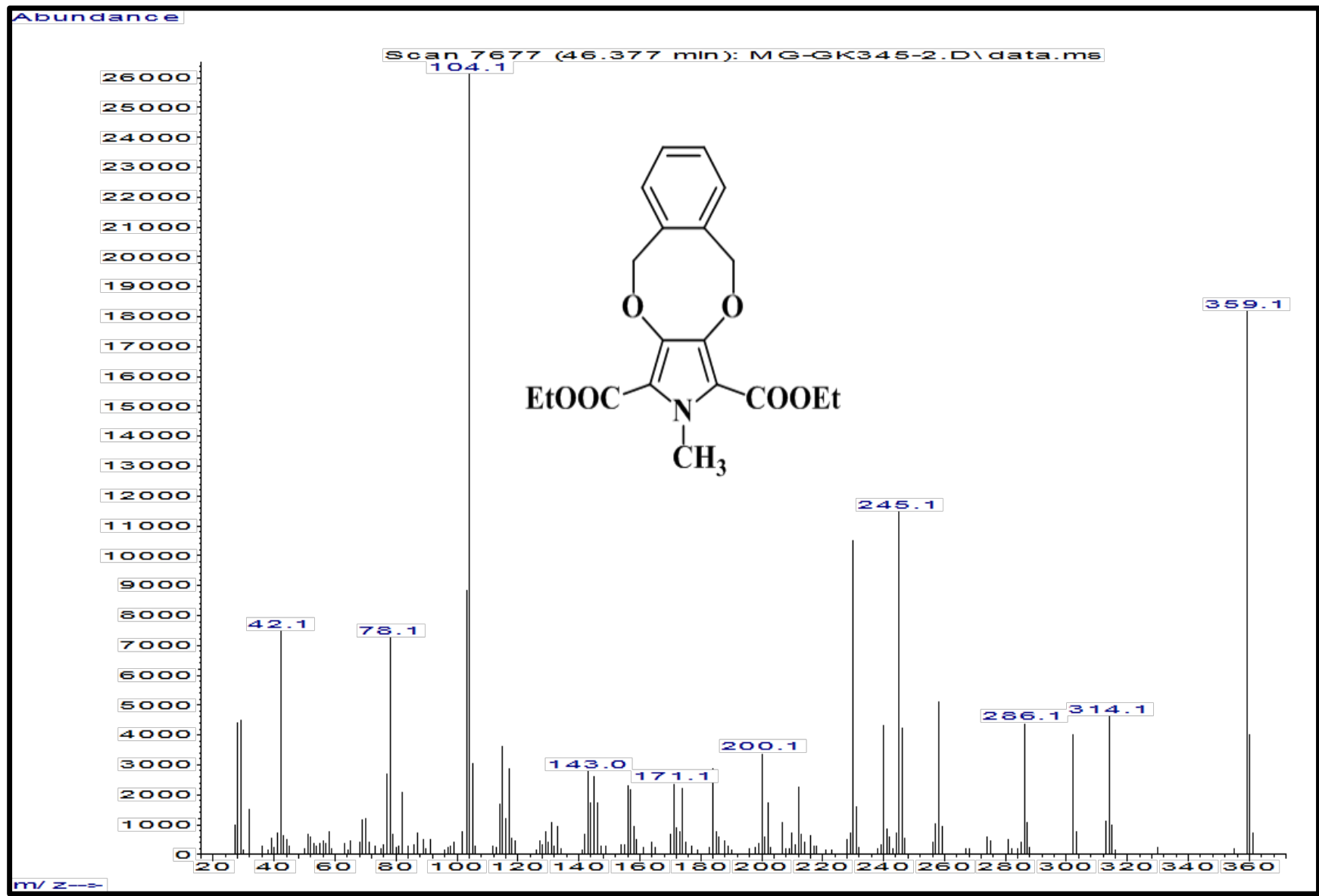


Figure S13. FT-IR spectrum of 2-methyl-5,10-dihydro-2H-benzo[6,7][1,4]dioxocino[2,3-c]pyrrole-1,3-dicarboxylic acid (5).

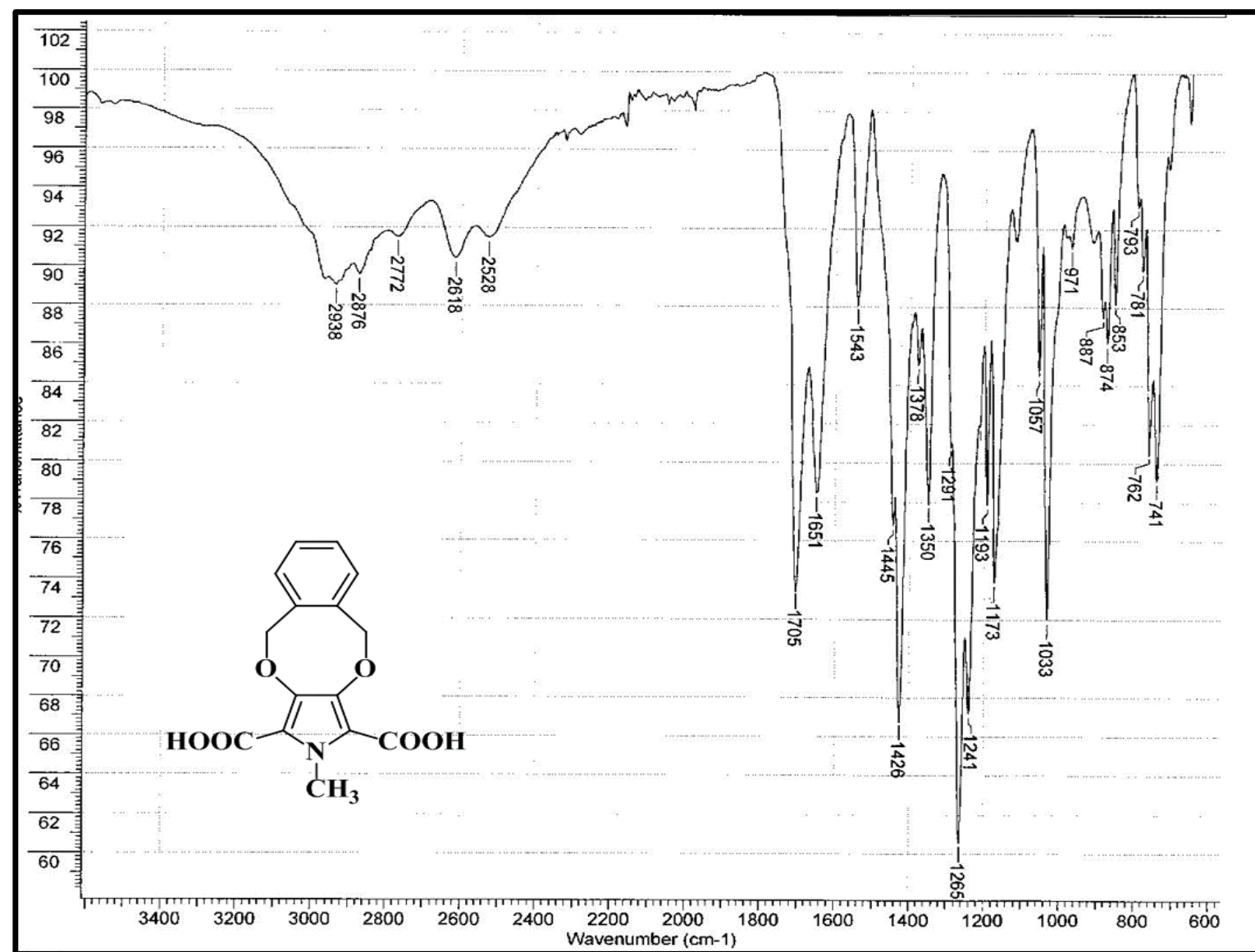


Figure S14. FT-IR spectrum of 2-methyl-5,10-dihydro-2H-benzo[6,7][1,4]dioxocino[2,3-c]pyrrole (XyPMe) (6).

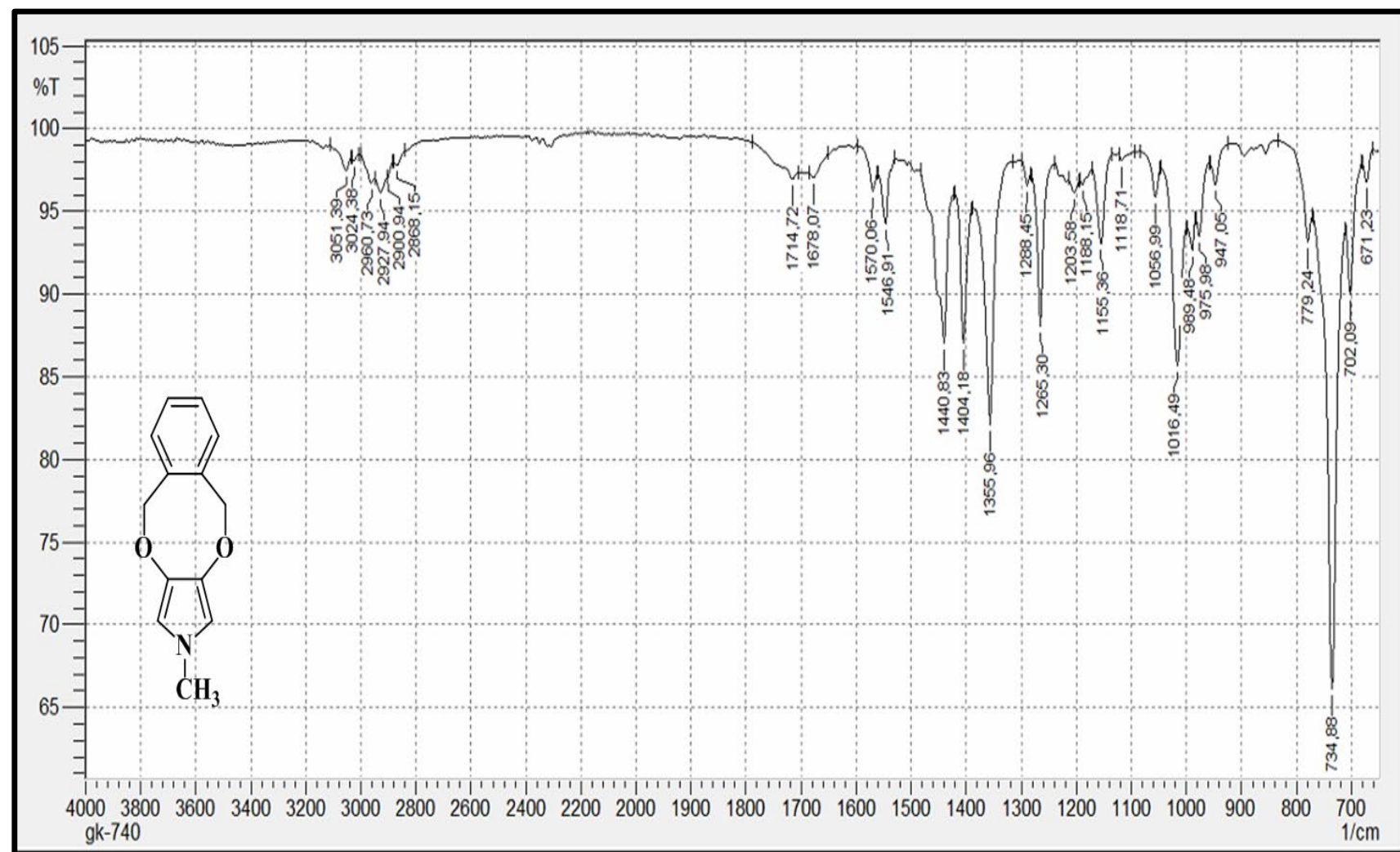


Figure S15 GC-MS spectrum of 2-methyl-5,10-dihydro-2H-benzo[6,7][1,4]dioxocino[2,3-c]pyrrole (XyPMe) (6).

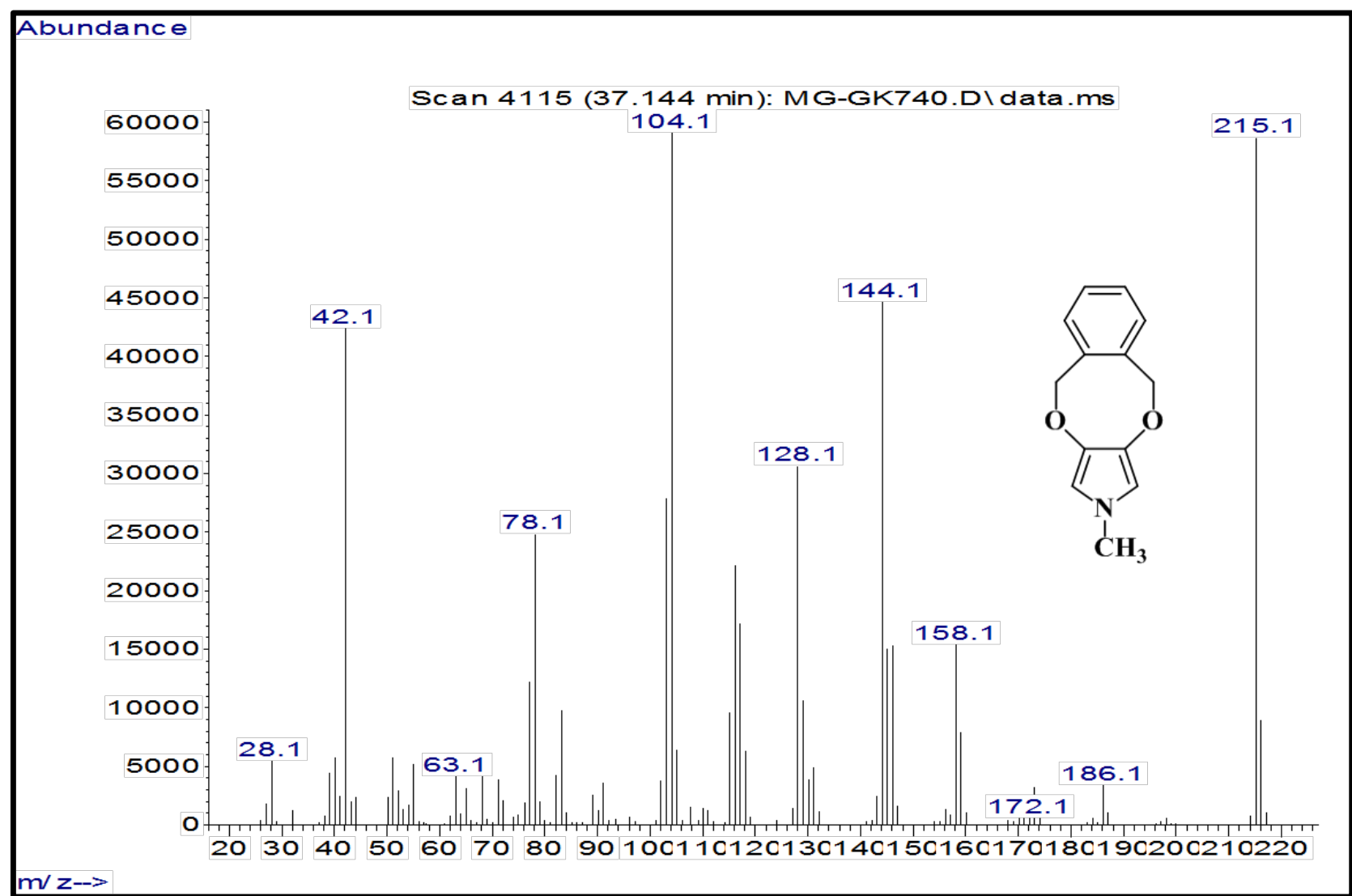


Figure S16 ^1H -NMR spectrum of 2-methyl-5,10-dihydro-2H-benzo[6,7][1,4]dioxocino[2,3-c]pyrrole (XyPMe) (6).

GK-740

Sample Name:

GK-740

Data Collected on:

mercury400-mercury400

Archive directory:

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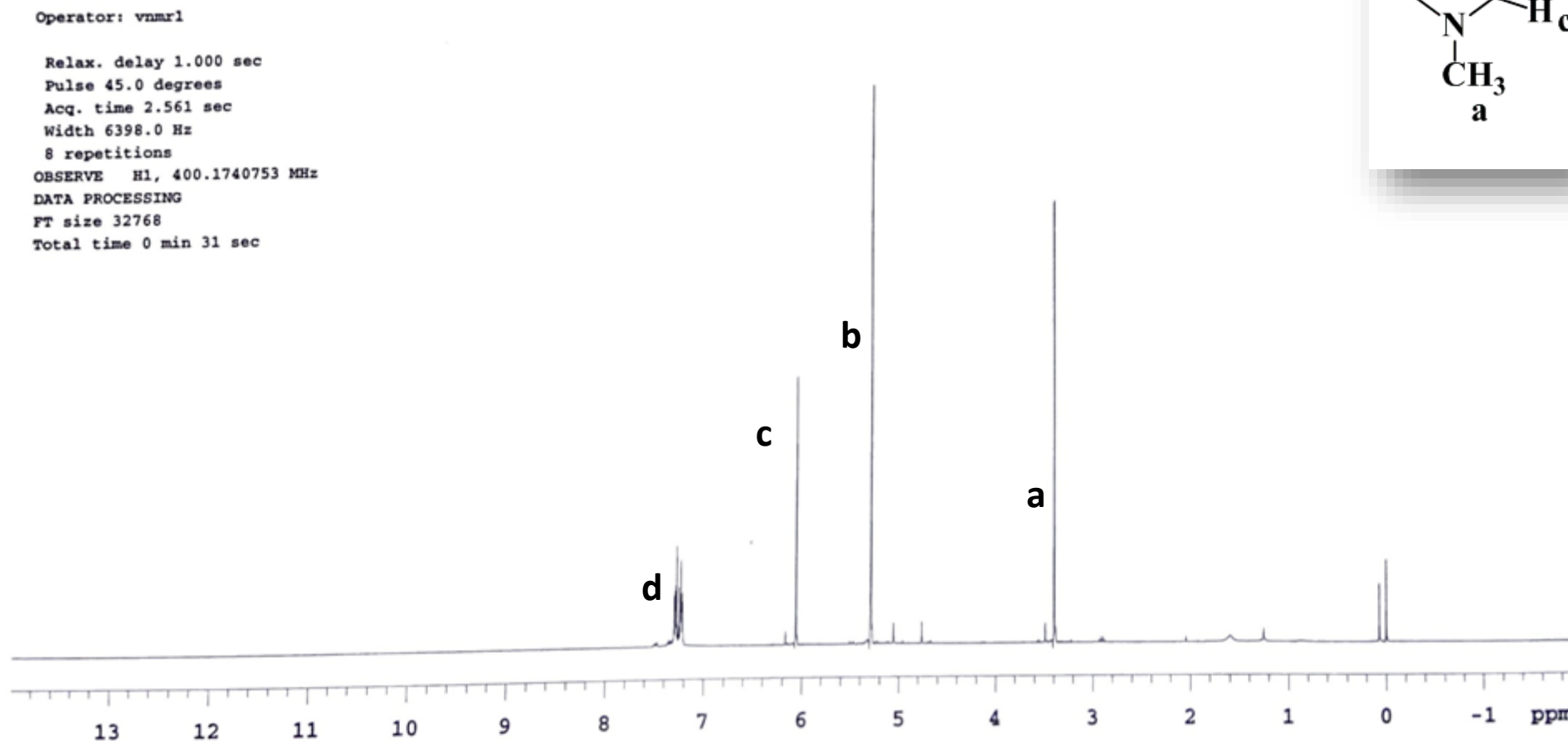
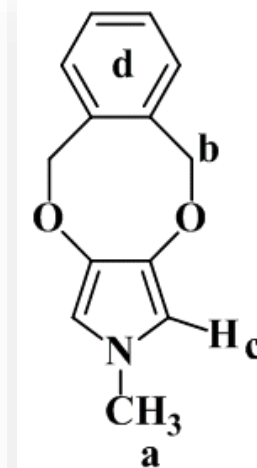


Figure S16 ¹H-NMR spectrum of 2-methyl-5,10-dihydro-2H-benzo[6,7][1,4]dioxocino[2,3-c]pyrrole (XyPMe) (6).

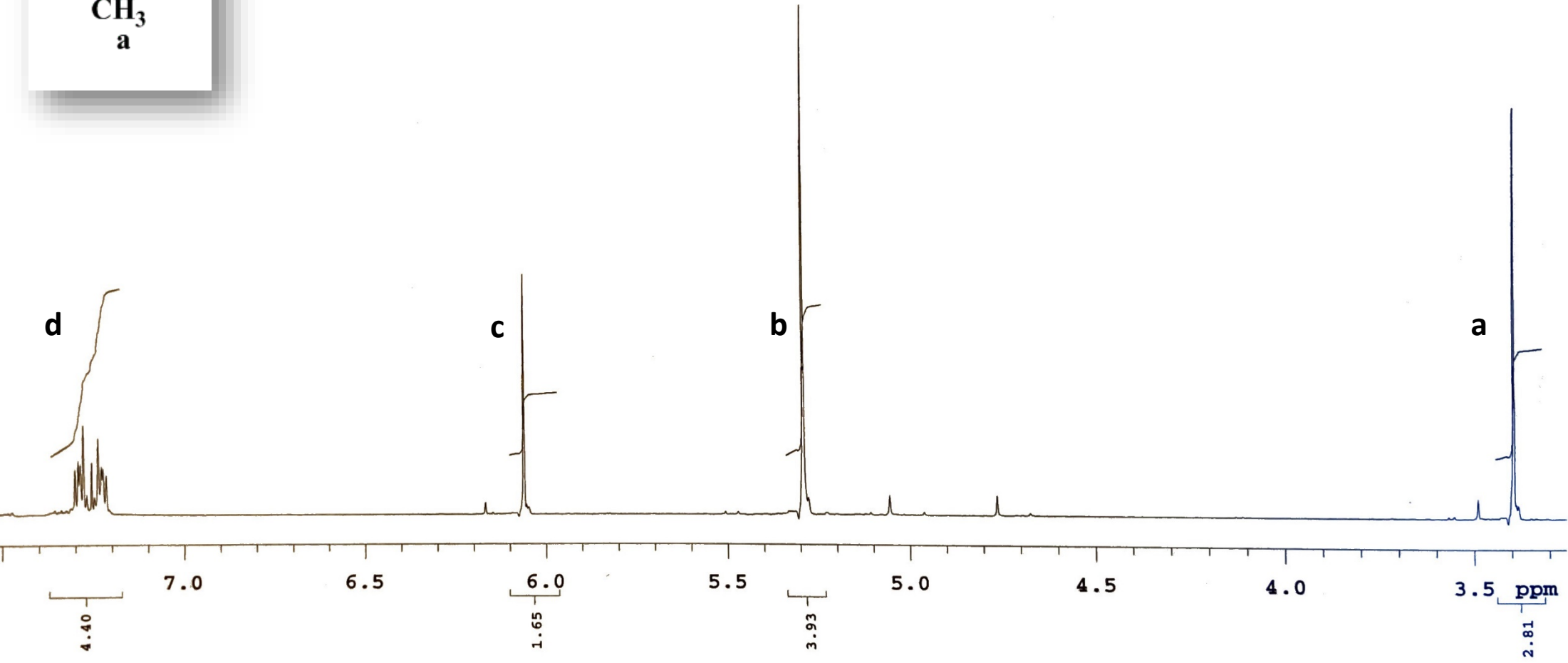
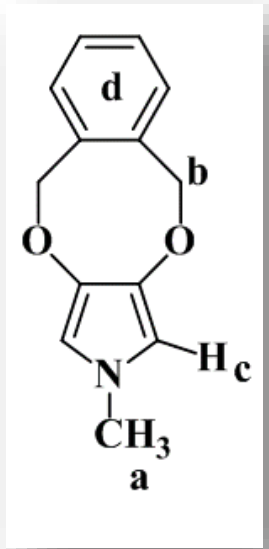


Figure S16 ^1H -NMR spectrum of 2-methyl-5,10-dihydro-2H-benzo[6,7][1,4]dioxocino[2,3-c]pyrrole (XyPMe) (6).

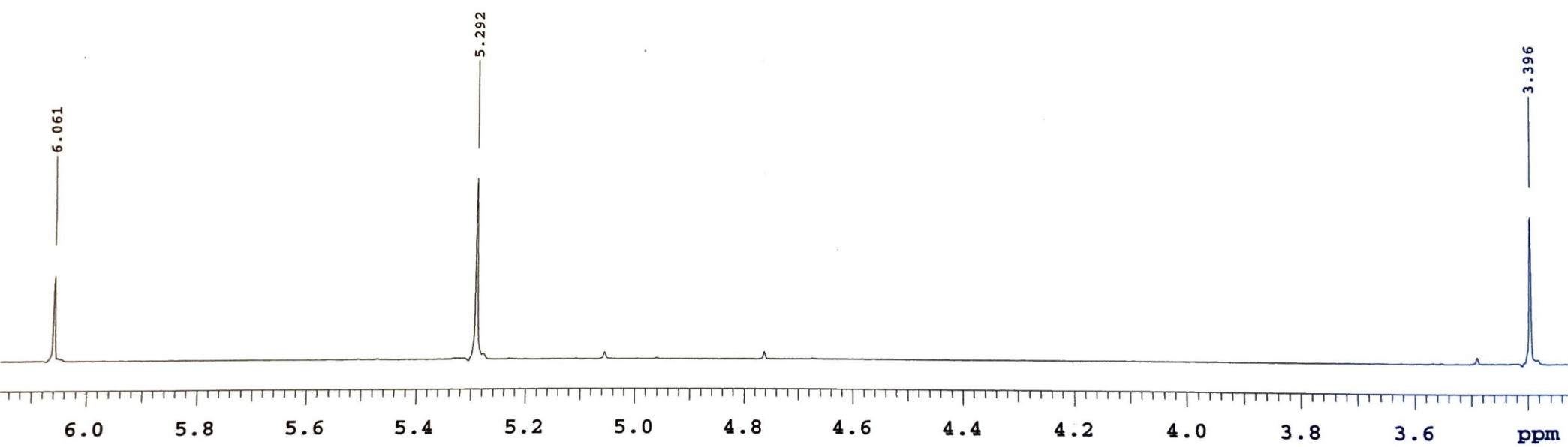


Figure S16 ^1H -NMR spectrum of 2-methyl-5,10-dihydro-2H-benzo[6,7][1,4]dioxocino[2,3-c]pyrrole (XyPMe) (6).

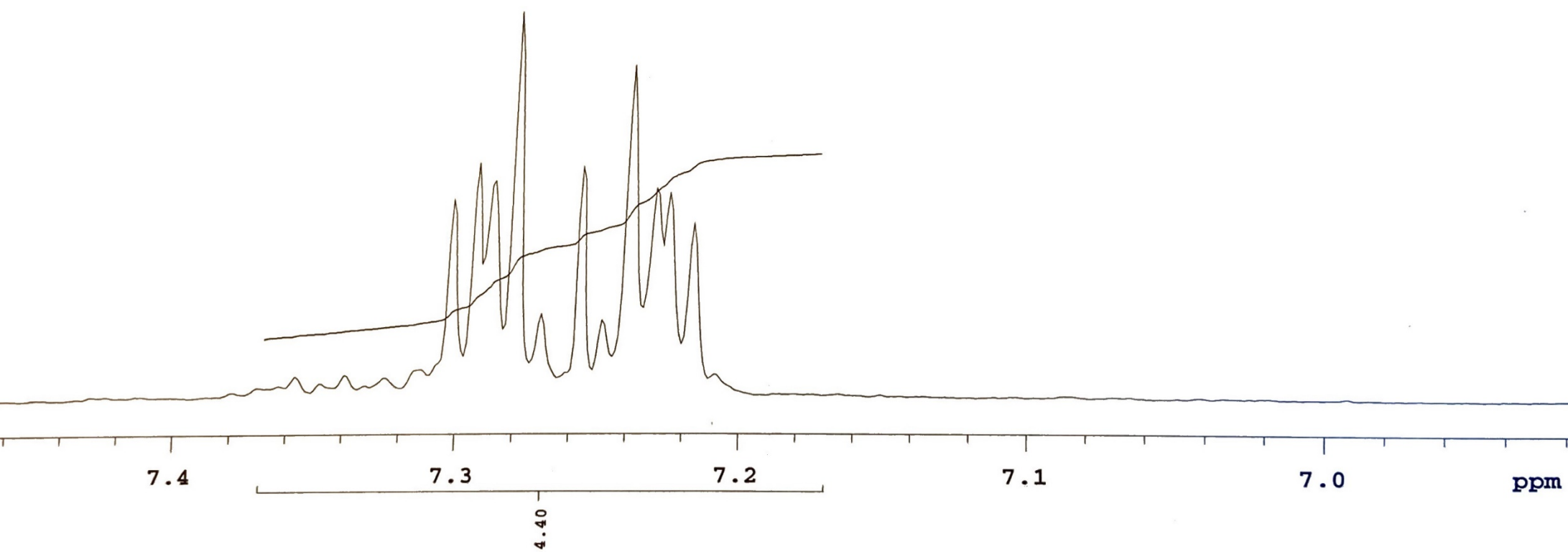


Figure S17-1 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPMe-monomer

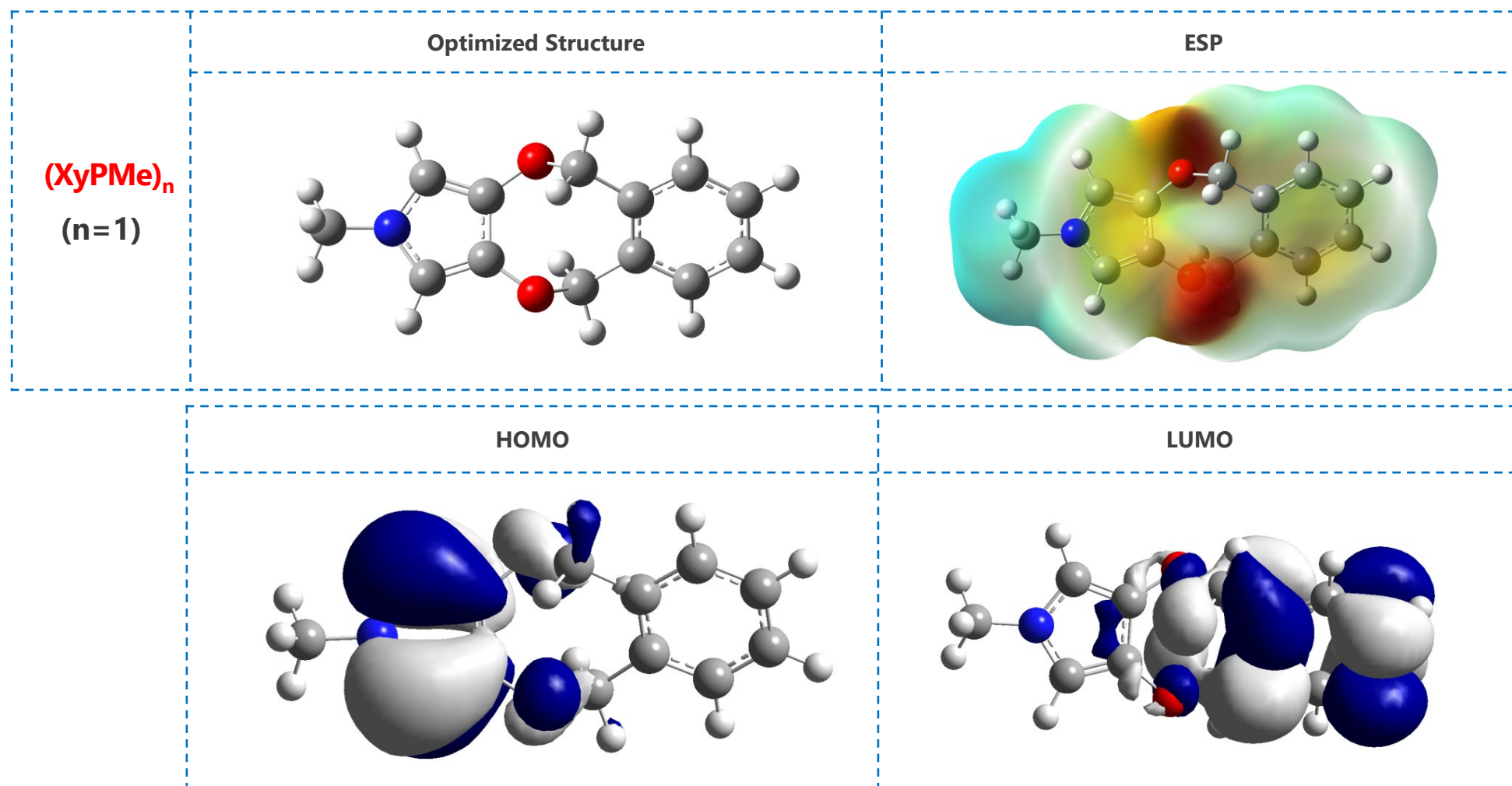


Figure S17-2 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPMe-dimer

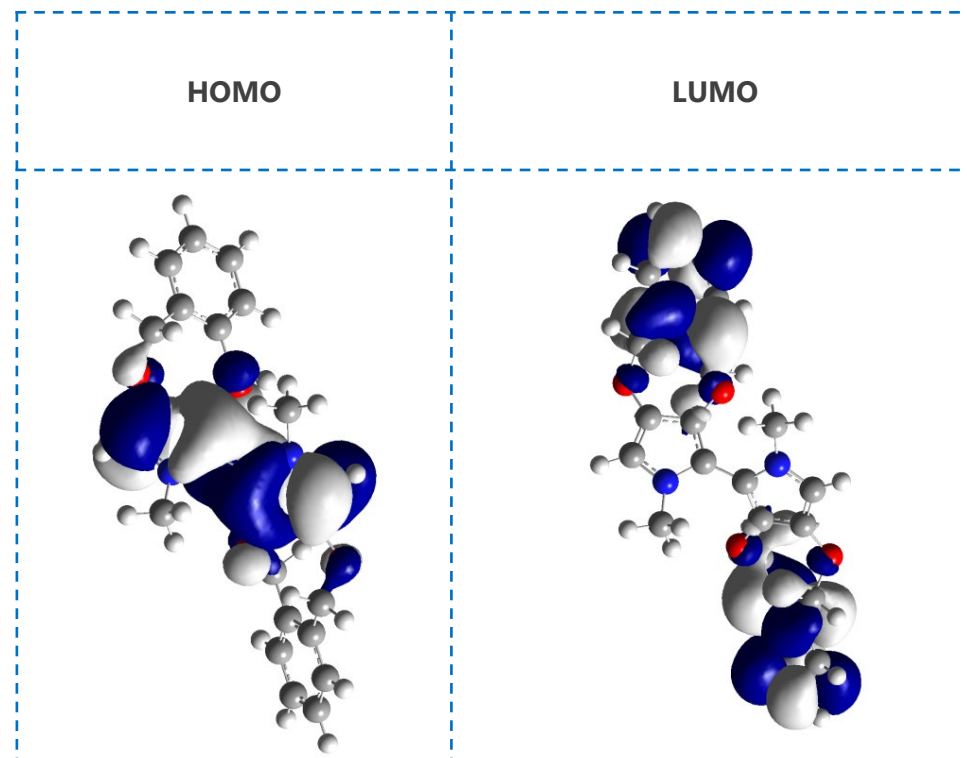
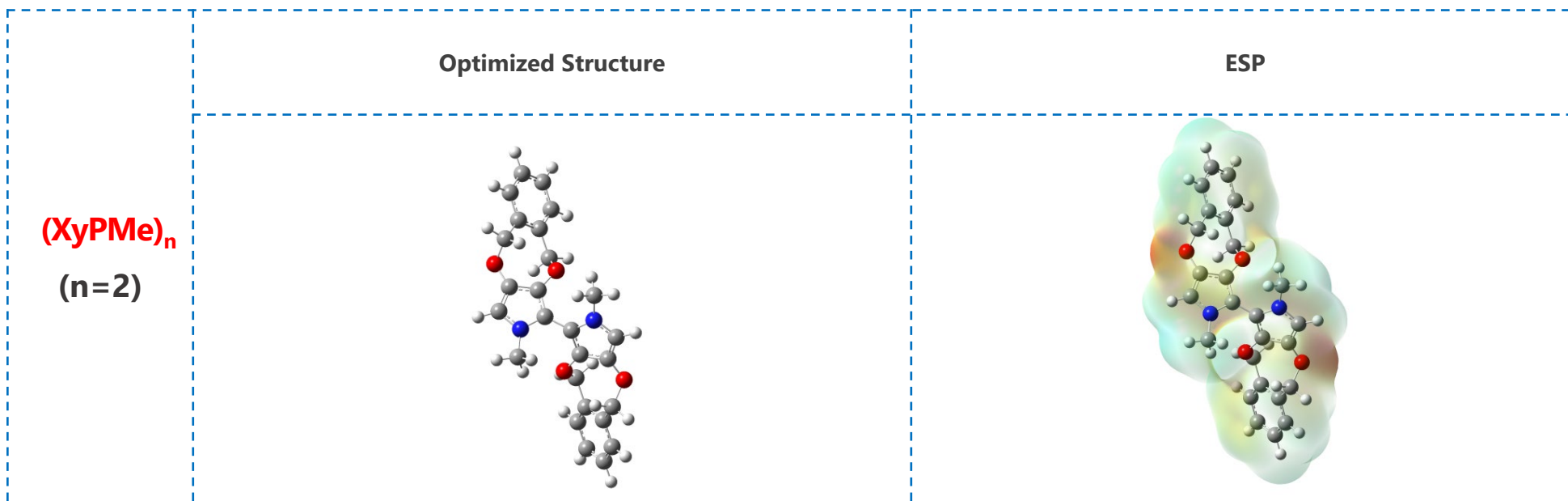
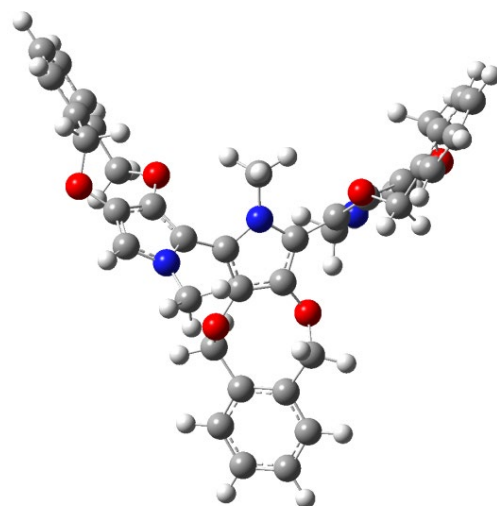


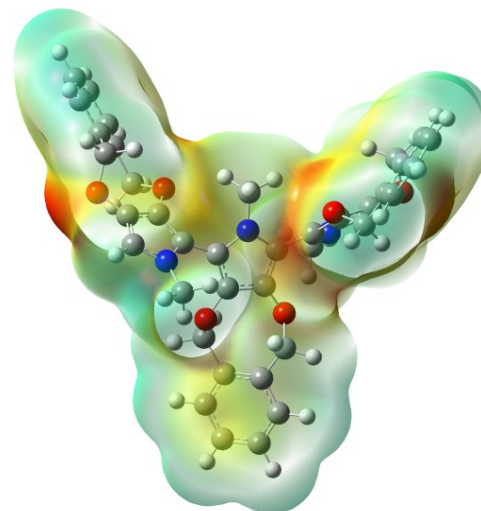
Figure S17-3 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPMe-trimer

(XyPMe)_n
(n=3)

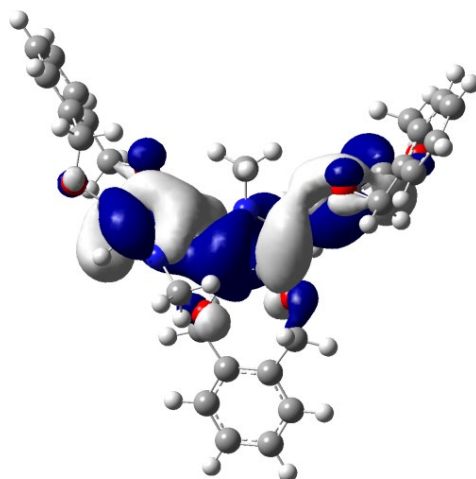
Optimized Structure



ESP



HOMO



LUMO

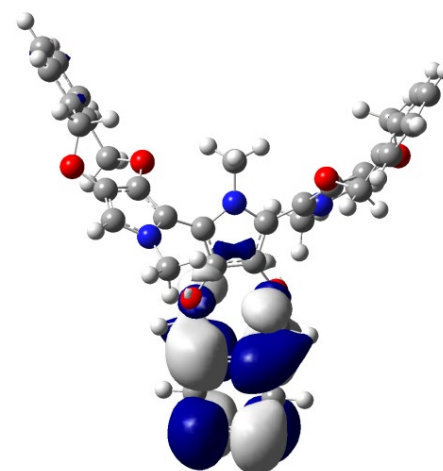
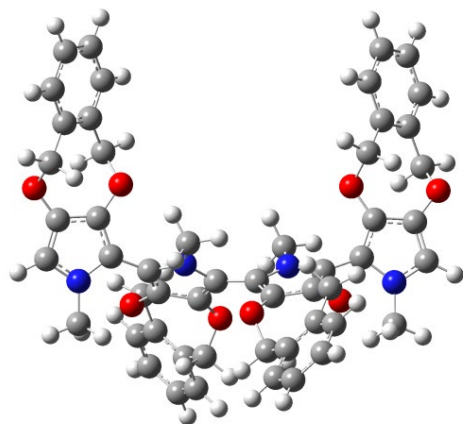


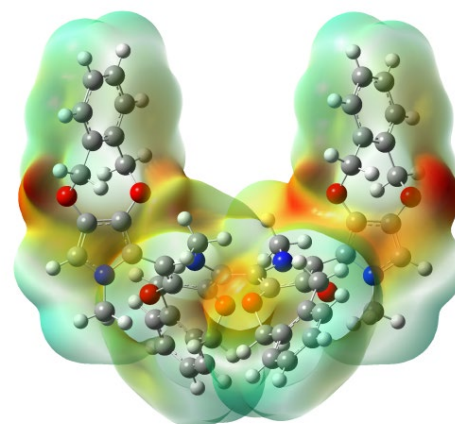
Figure S17-4 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPMe-tetramer

(XyPMe)_n
(n=4)

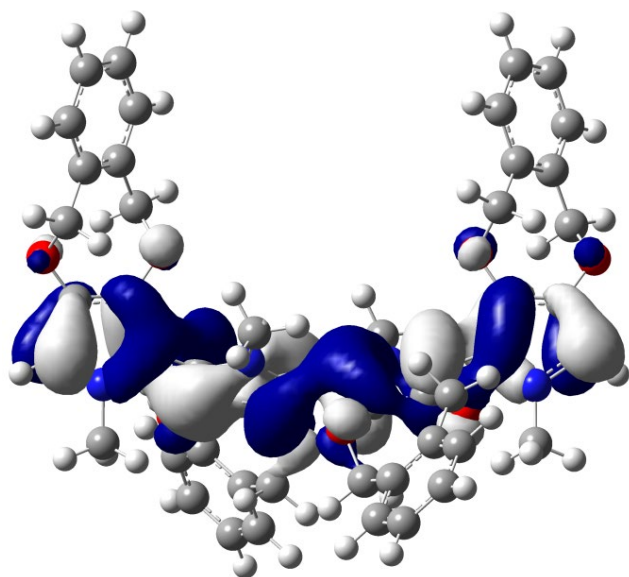
Optimized Structure



ESP



HOMO



LUMO

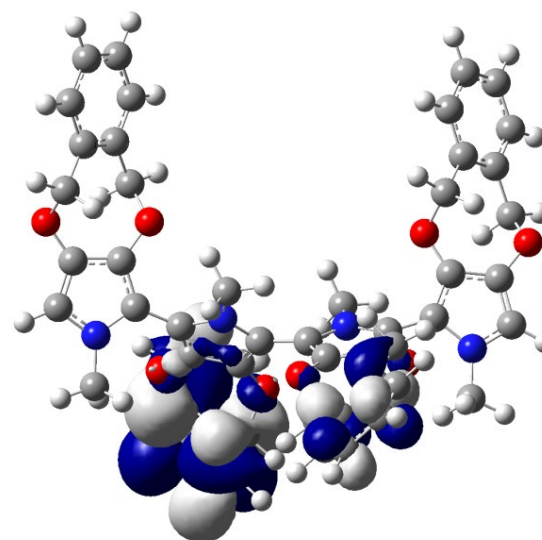
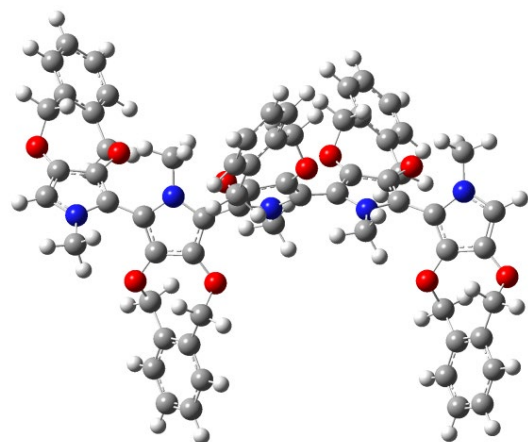


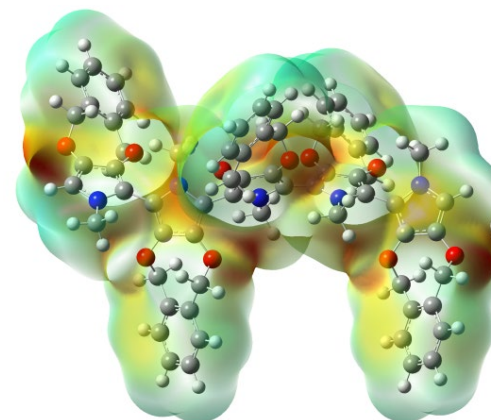
Figure S17-5 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPMe-pentamer

(XyPMe)_n
(n=5)

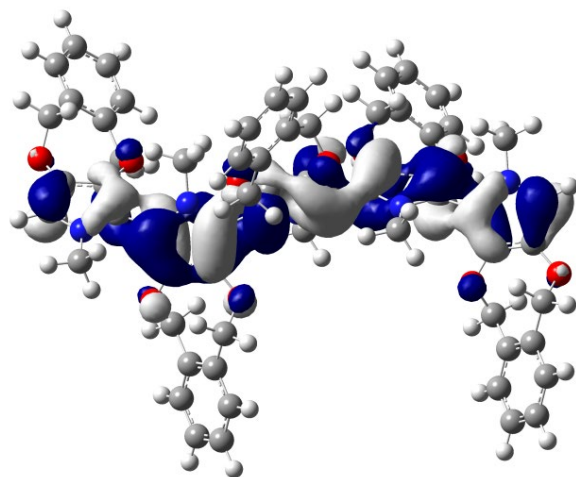
Optimized Structure



ESP



HOMO



LUMO

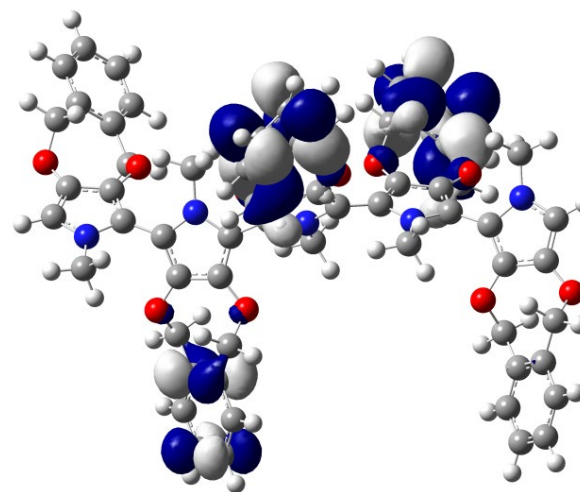
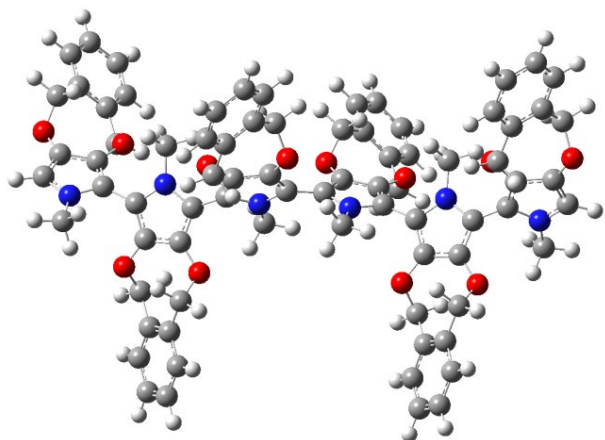


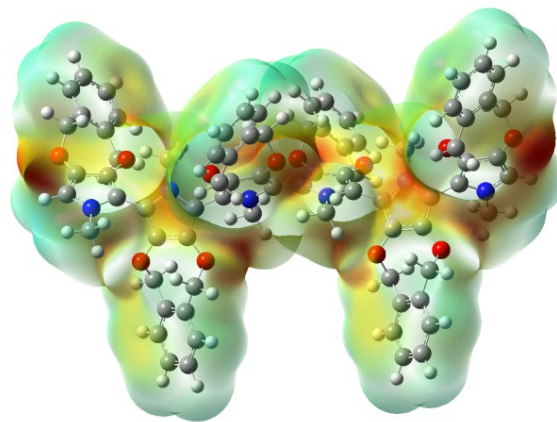
Figure S17-6 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPMe-hexamer

(XyPMe)_n
(n=6)

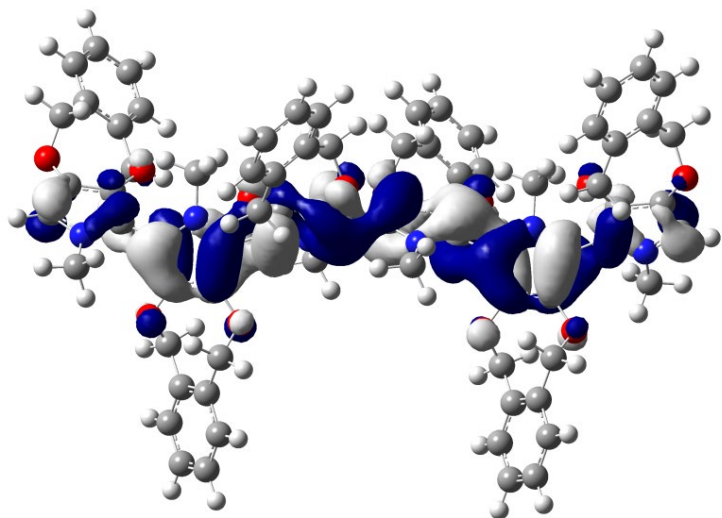
Optimized Structure



ESP



HOMO



LUMO

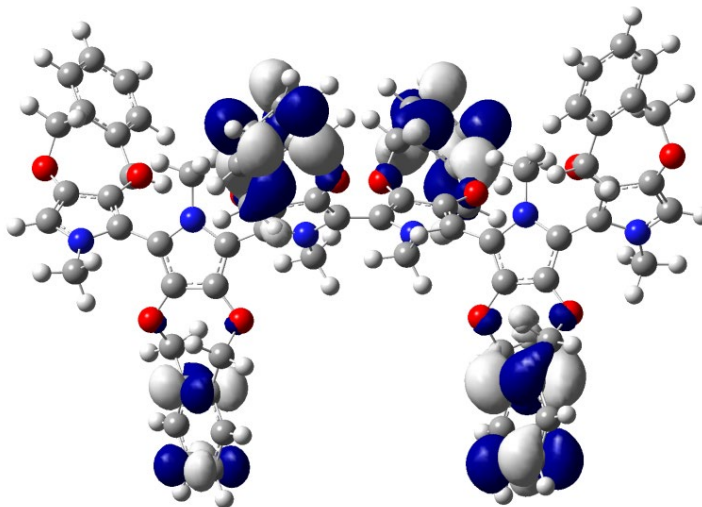
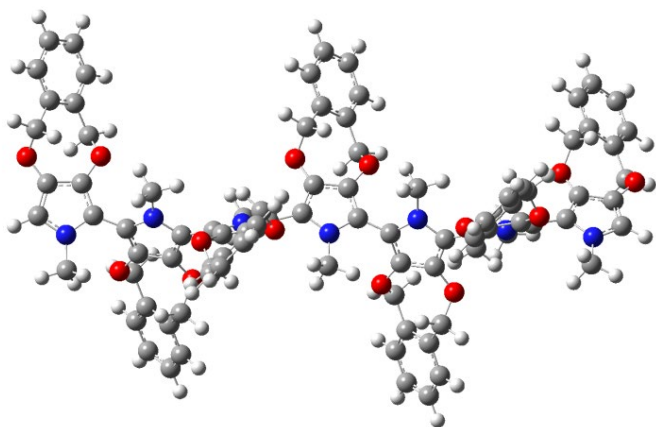


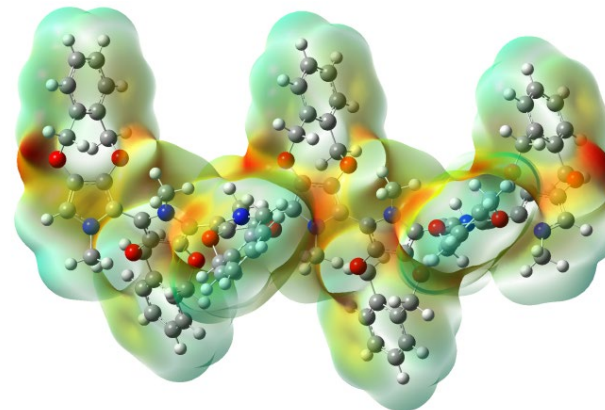
Figure S17-7 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPMe-heptamer

(XyPMe)_n
(n=7)

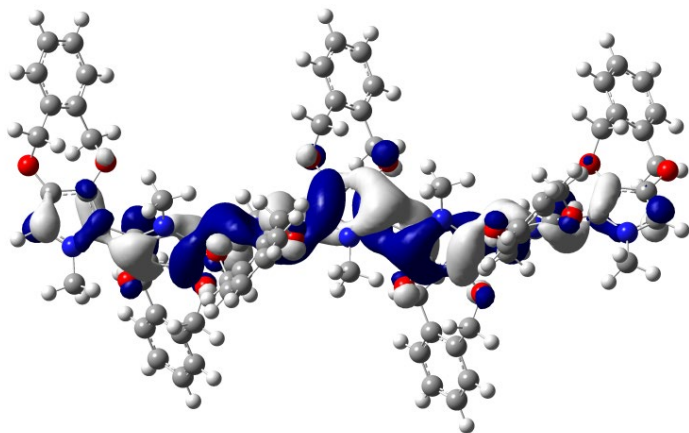
Optimized Structure



ESP



HOMO



LUMO

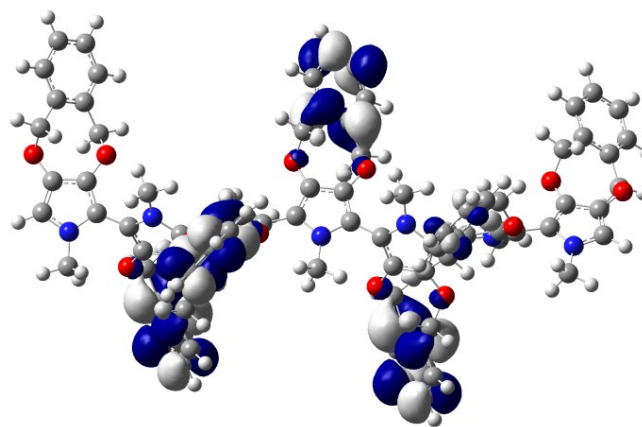
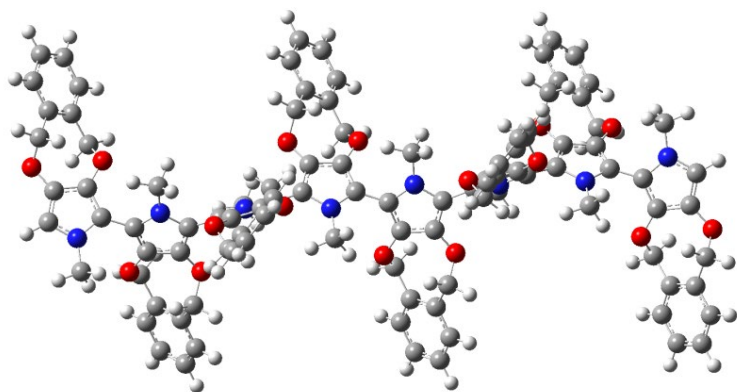


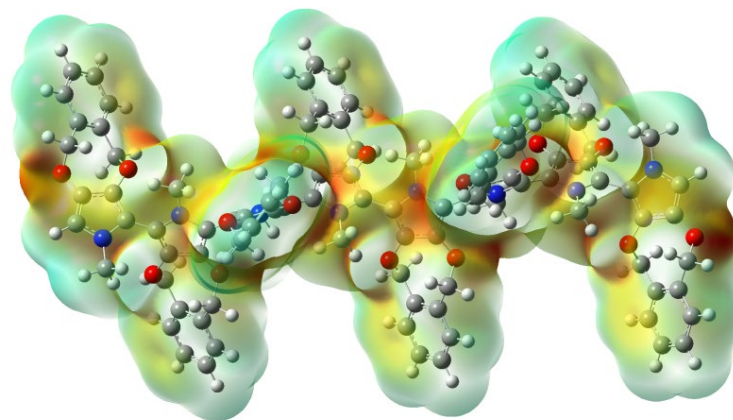
Figure S17-8 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPMe-octamer

(XyPMe)_n
(n=8)

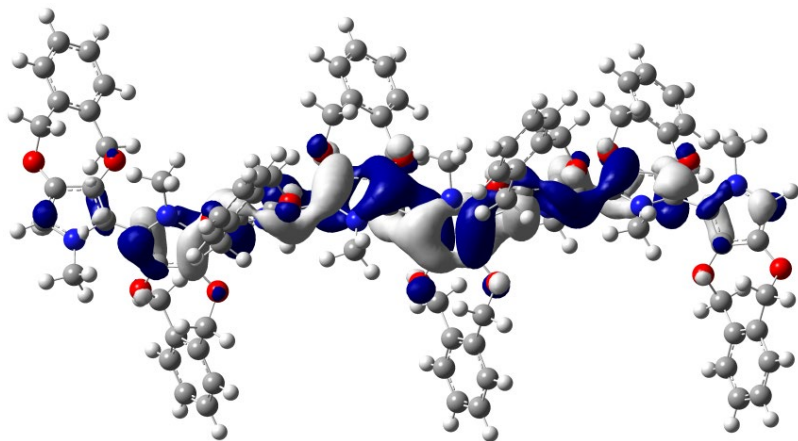
Optimized Structure



ESP



HOMO



LUMO

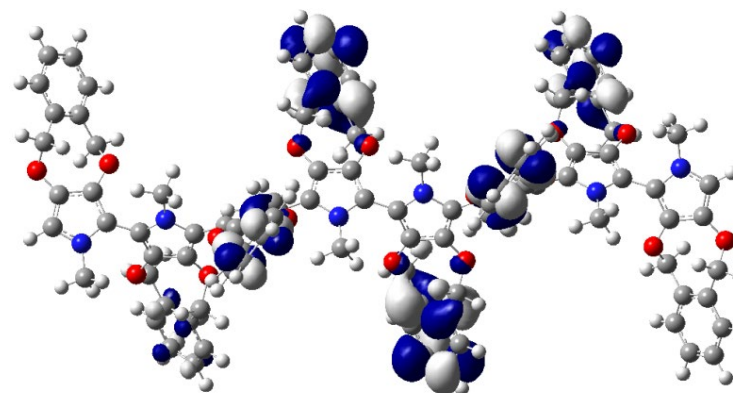
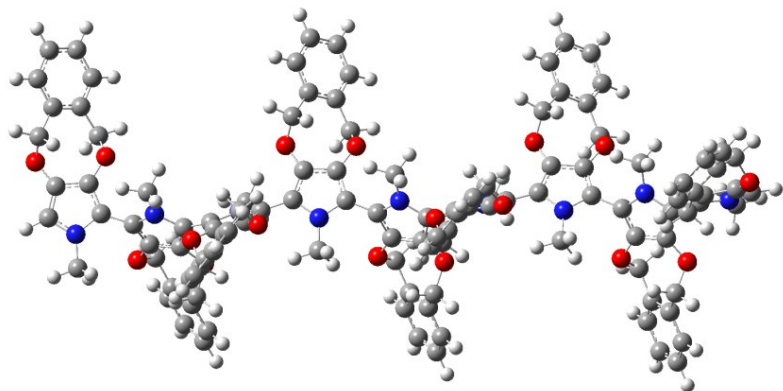


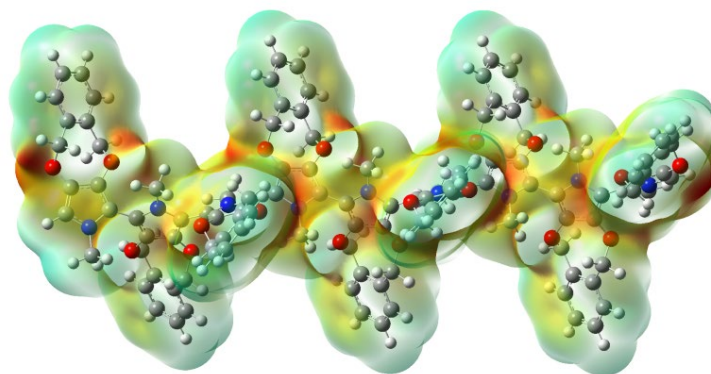
Figure S17-9 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPMe-nonamer

(XyPMe)_n
(n=9)

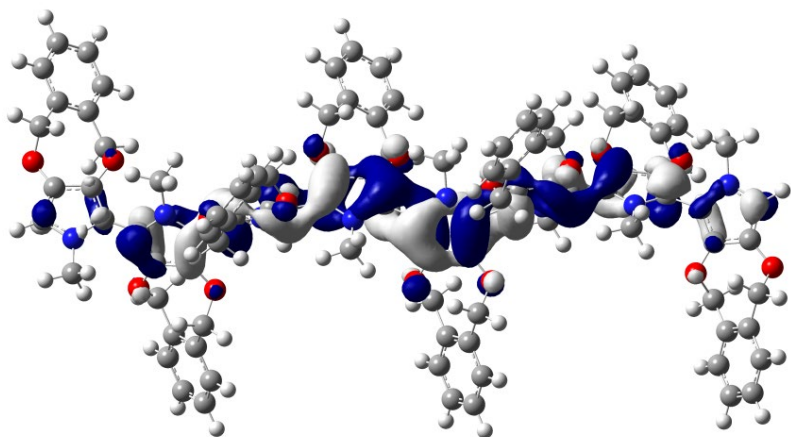
Optimized Structure



ESP



HOMO



LUMO

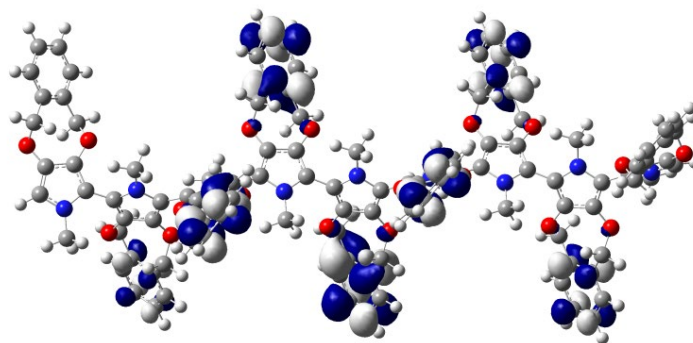


Figure S17-10 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPMe-decamer

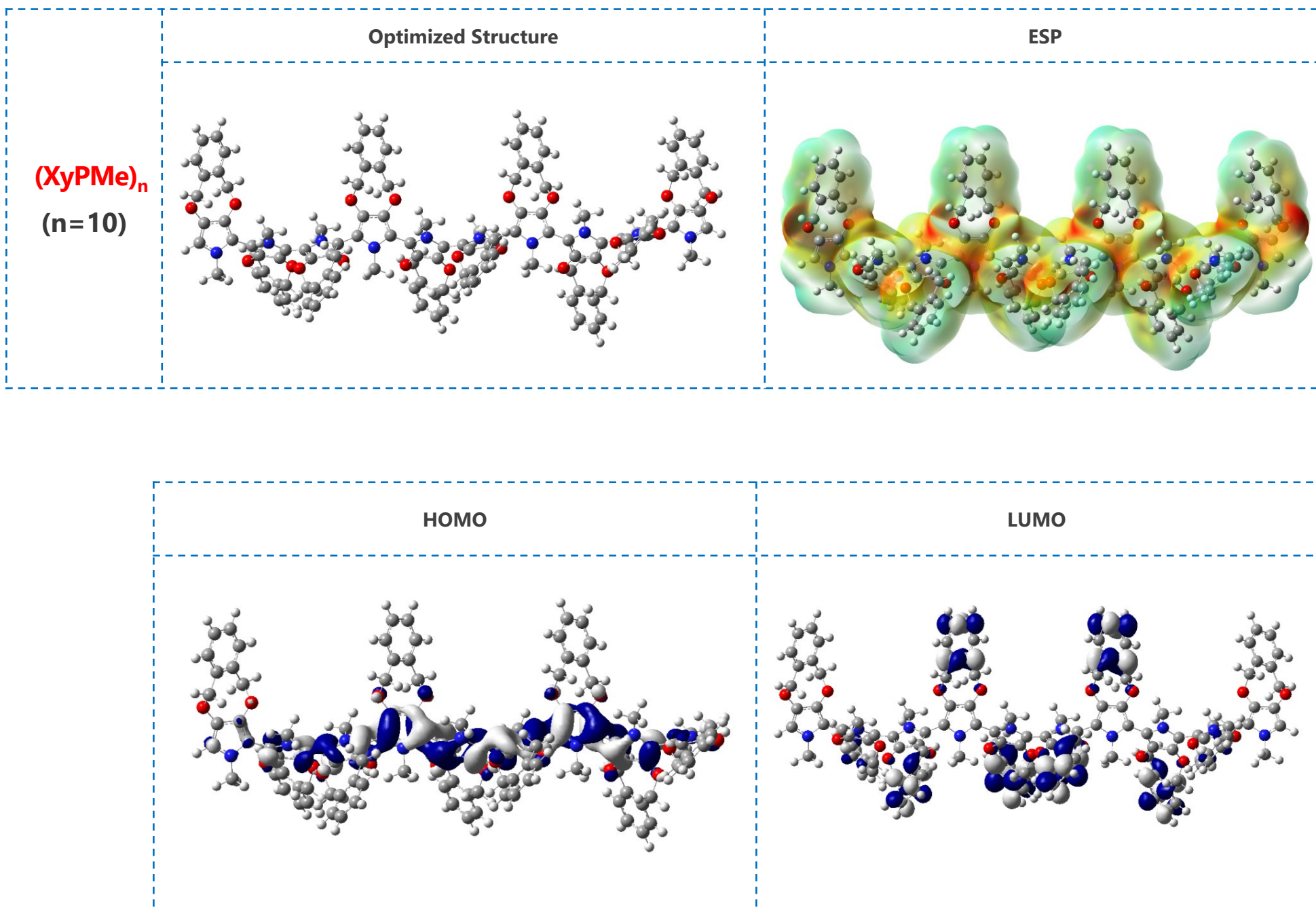


Figure S17-11 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPMe-undecamer

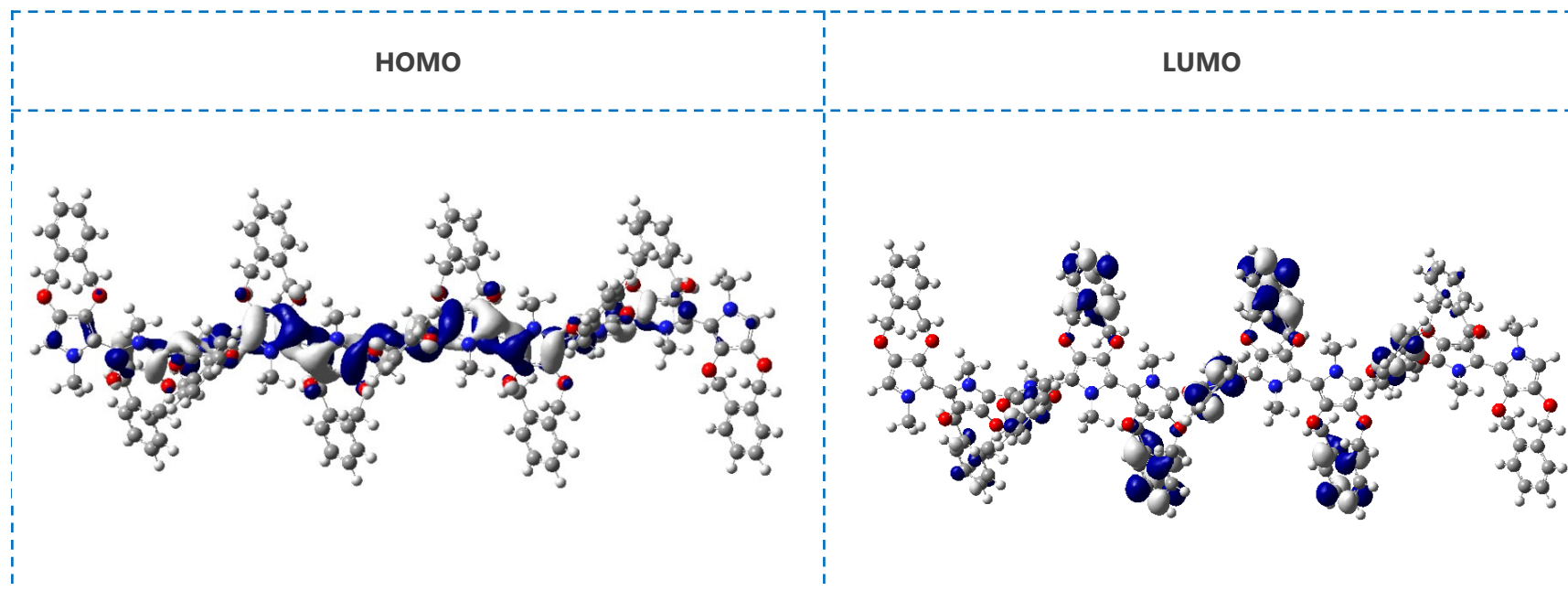
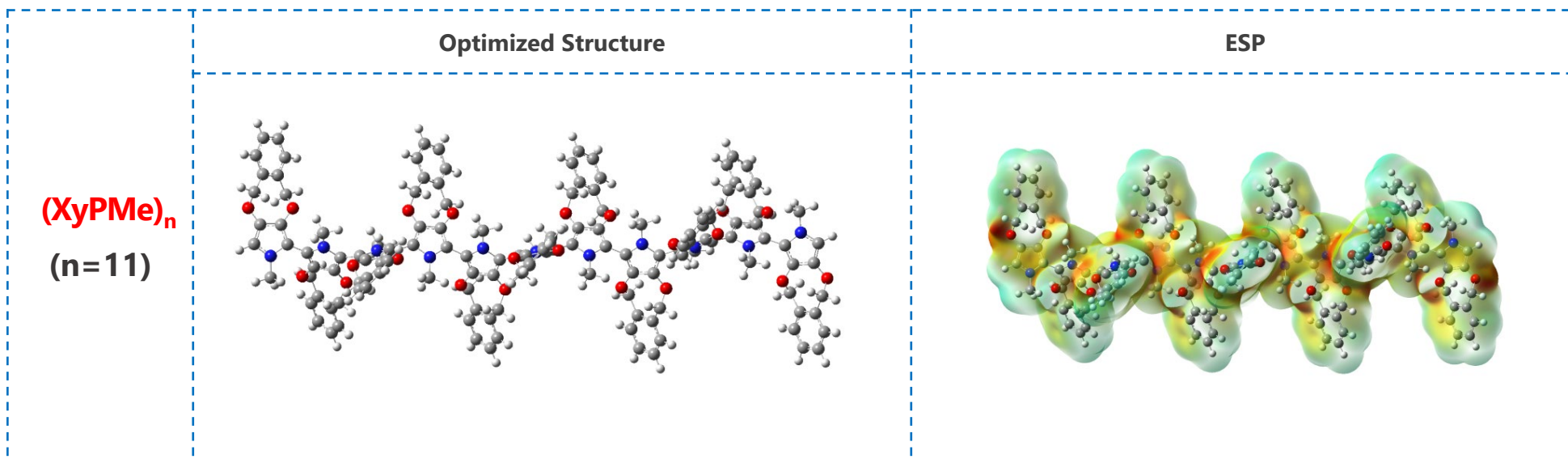


Figure S18-1 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPBu-monomer

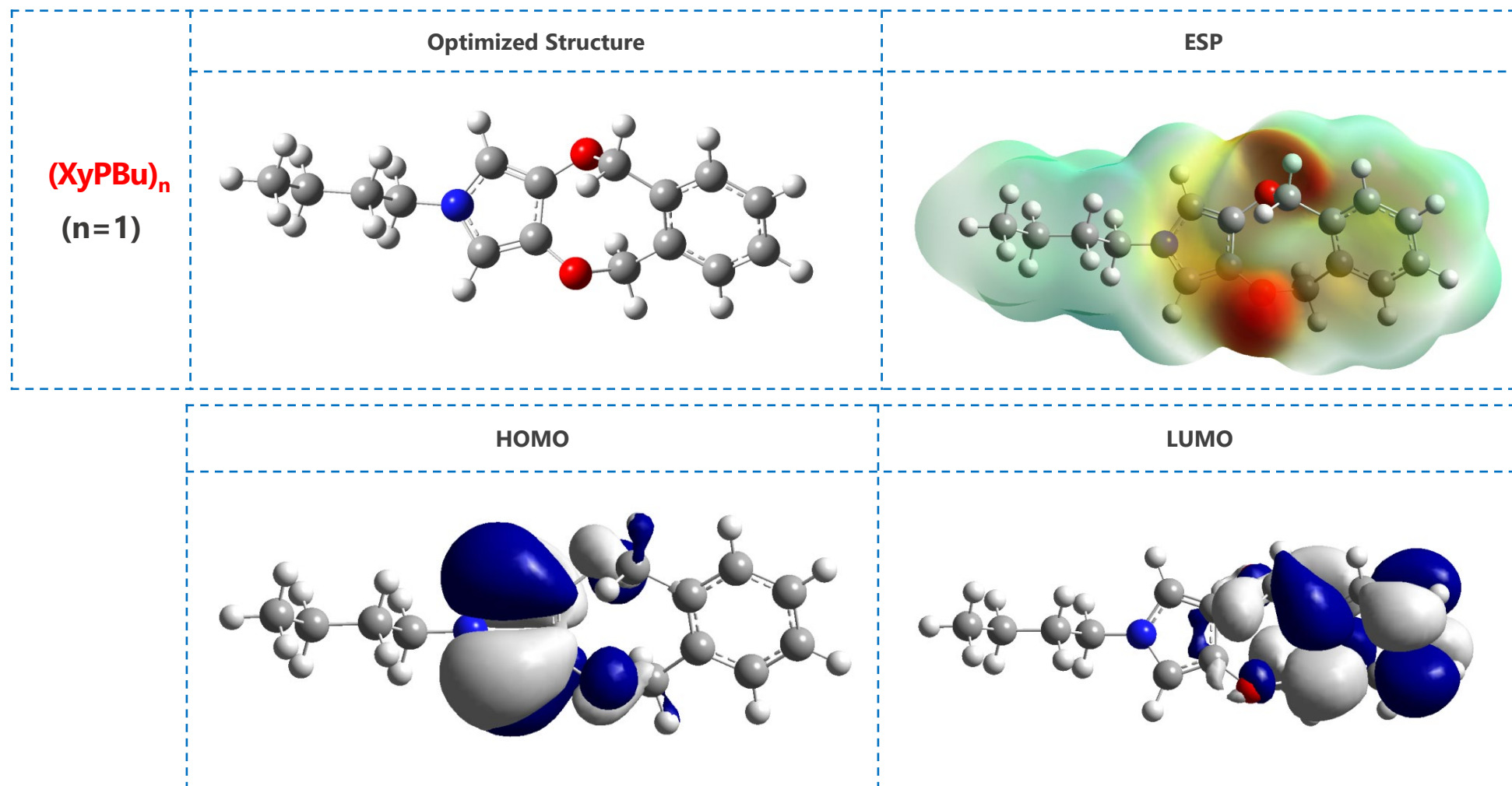


Figure S18-2 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPBu-dimer

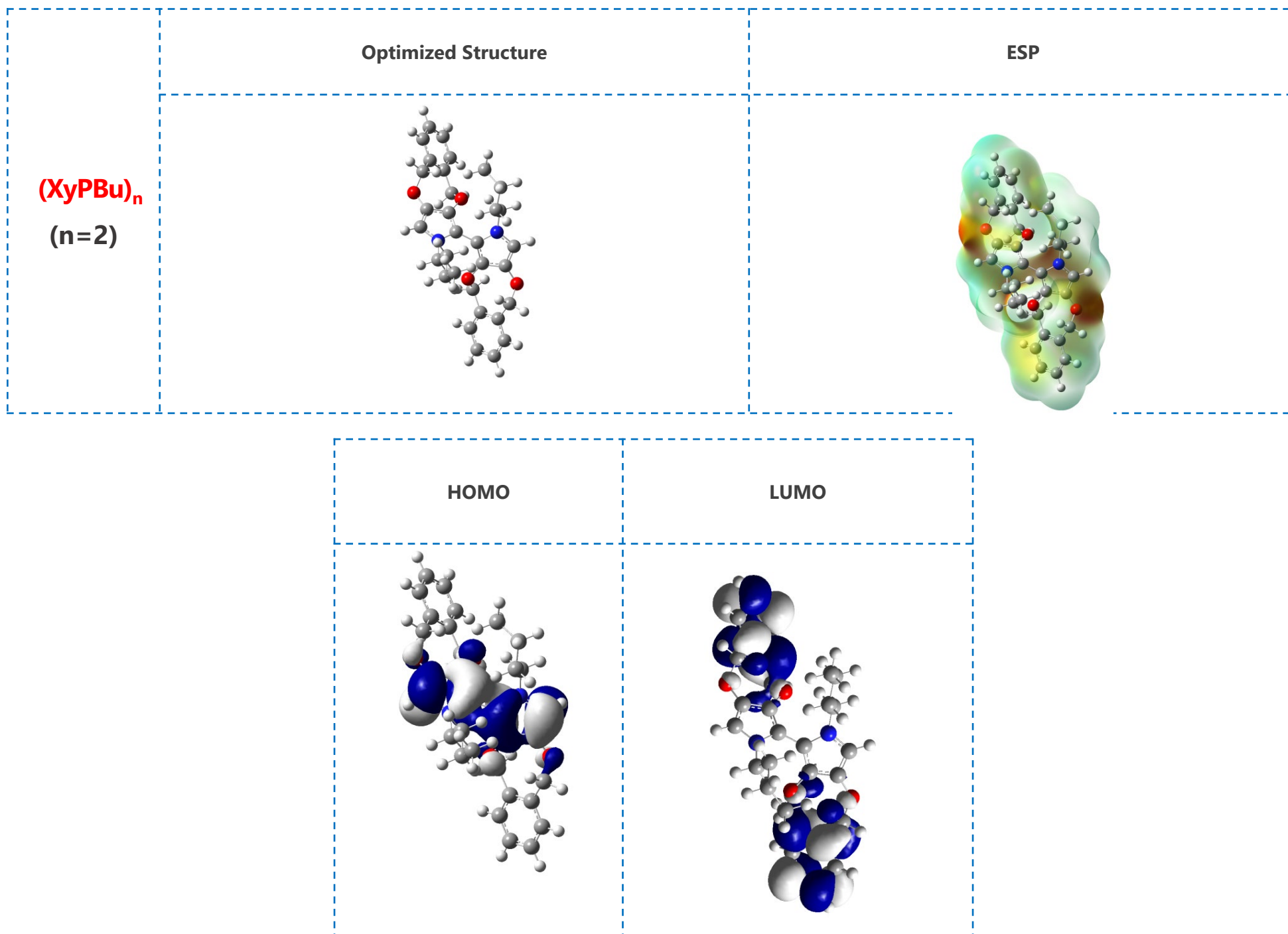


Figure S18-3 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPBu-trimer

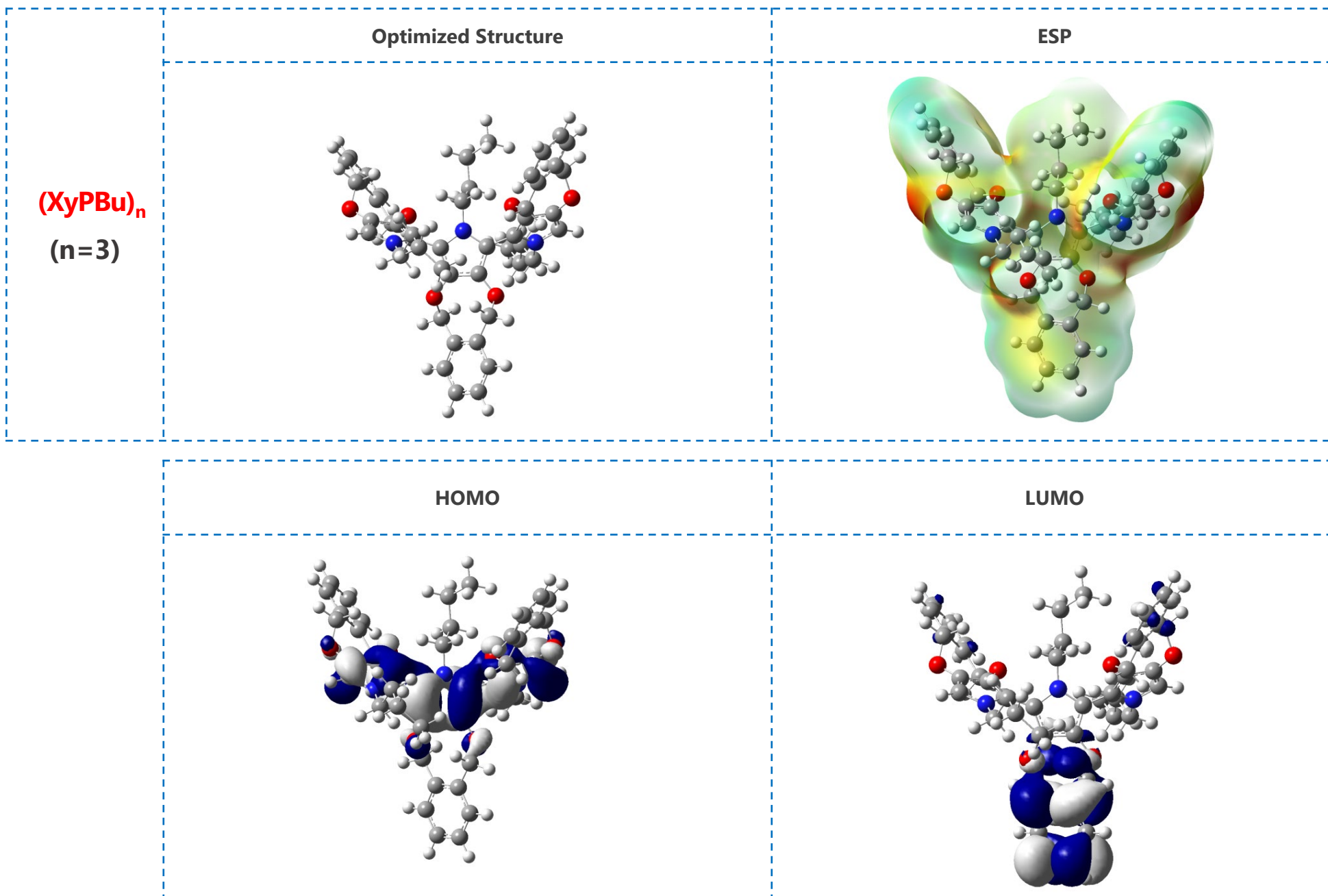


Figure S18-4 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPBu-tetramer

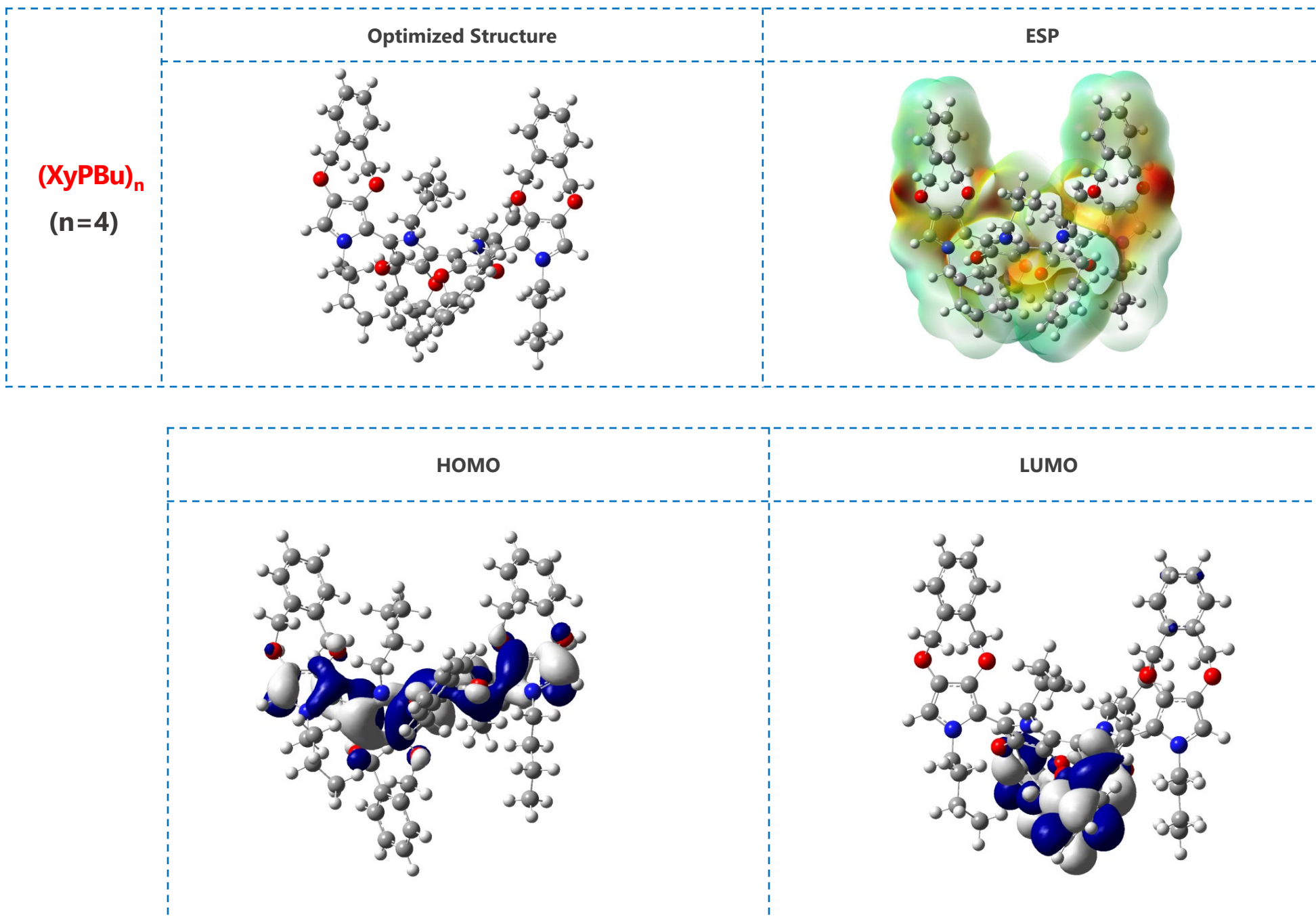


Figure S18-5 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPBu-pentamer

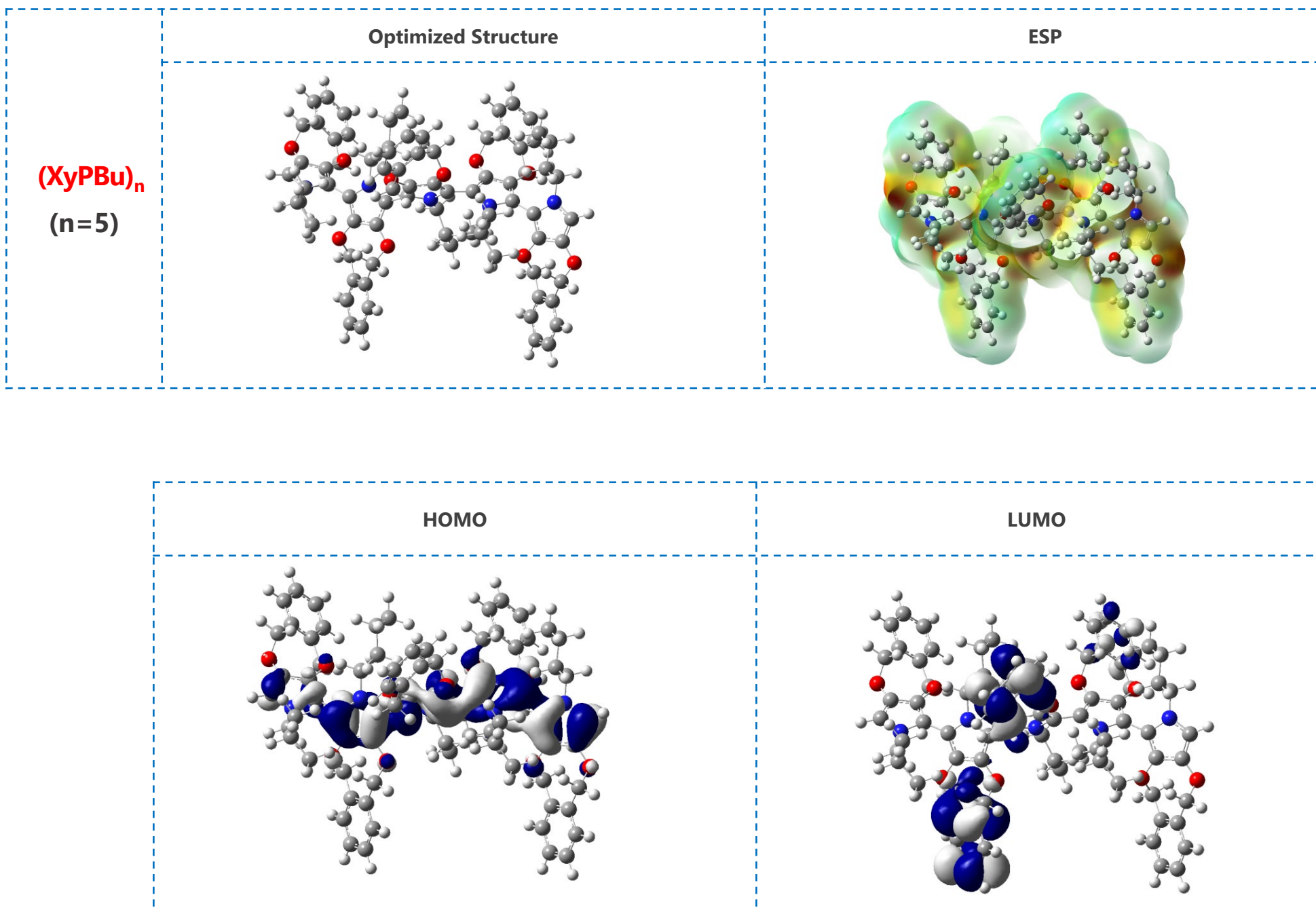


Figure S18-6 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPBu-hexamer

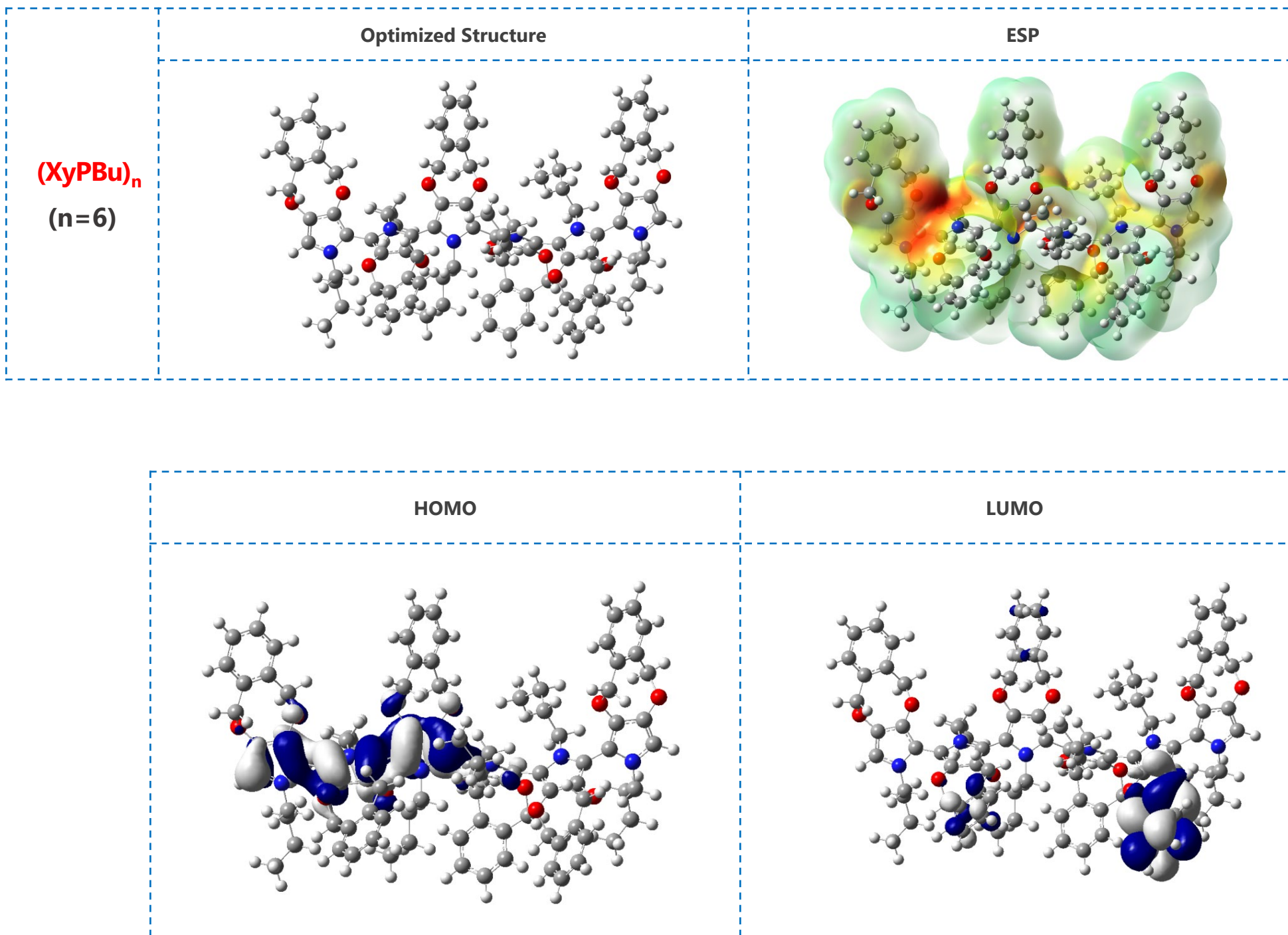


Figure S18-7 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPBu-heptamer

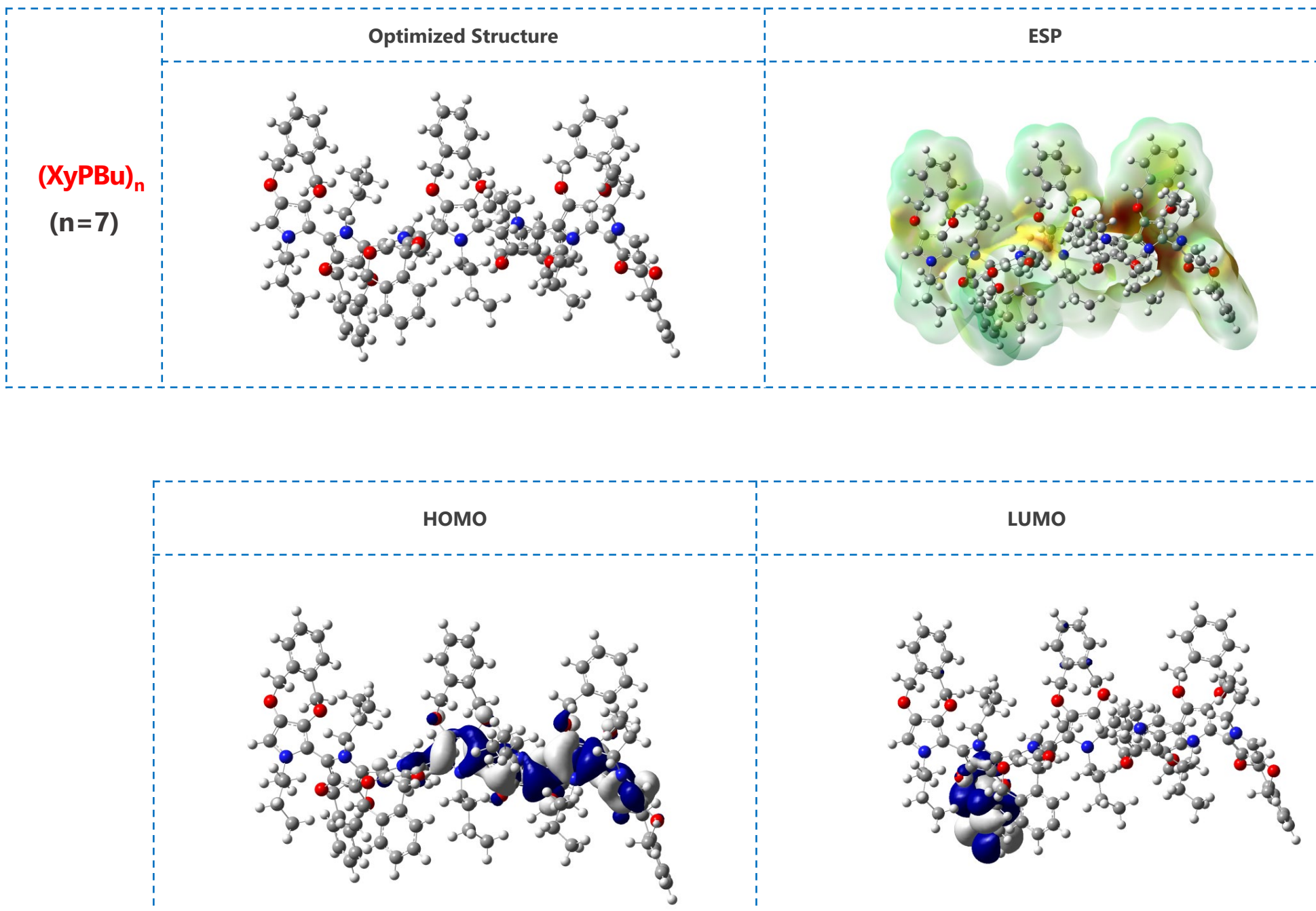


Figure S18-8 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPBu-octamer

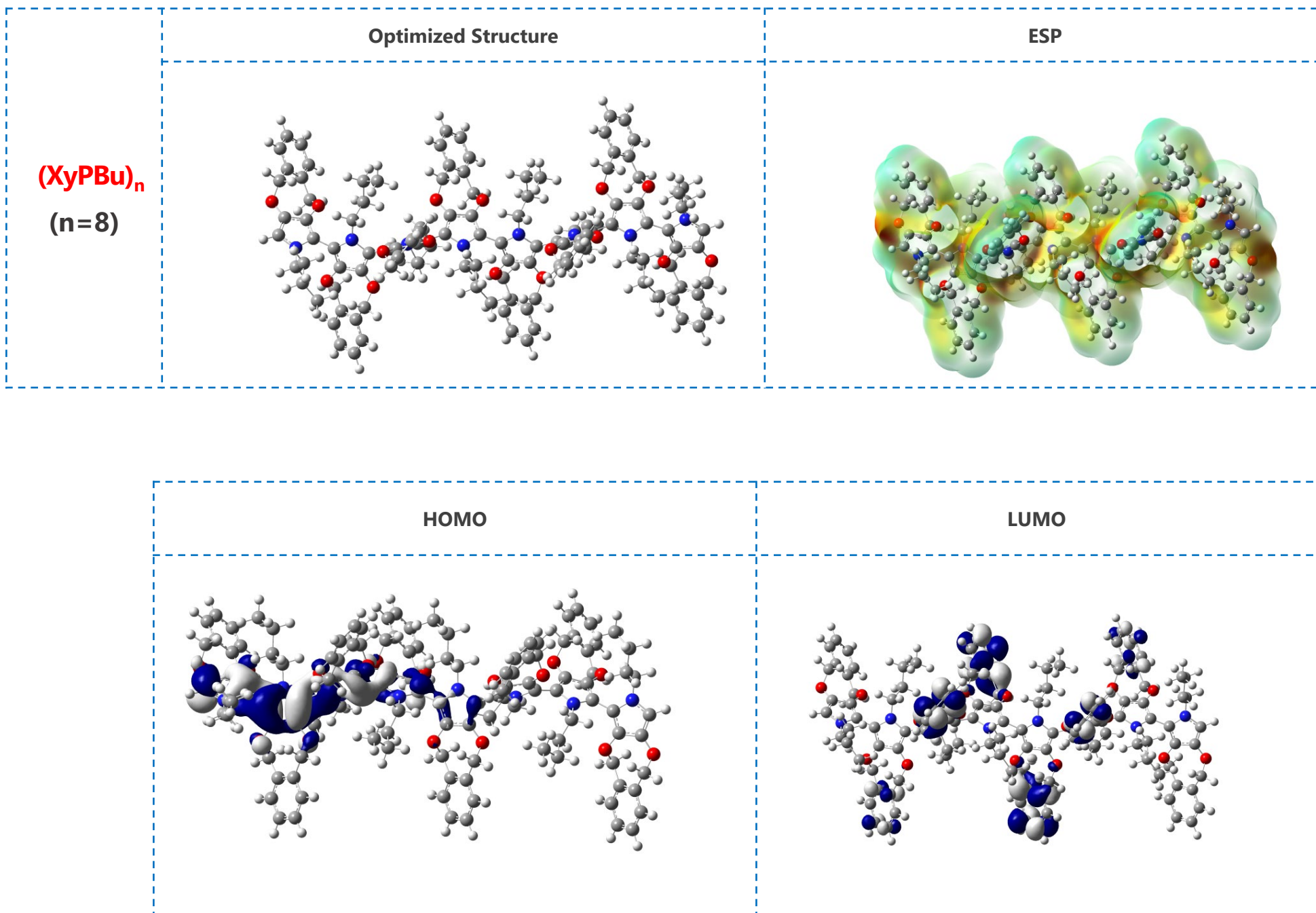


Figure S18-9 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPBu-nonamer

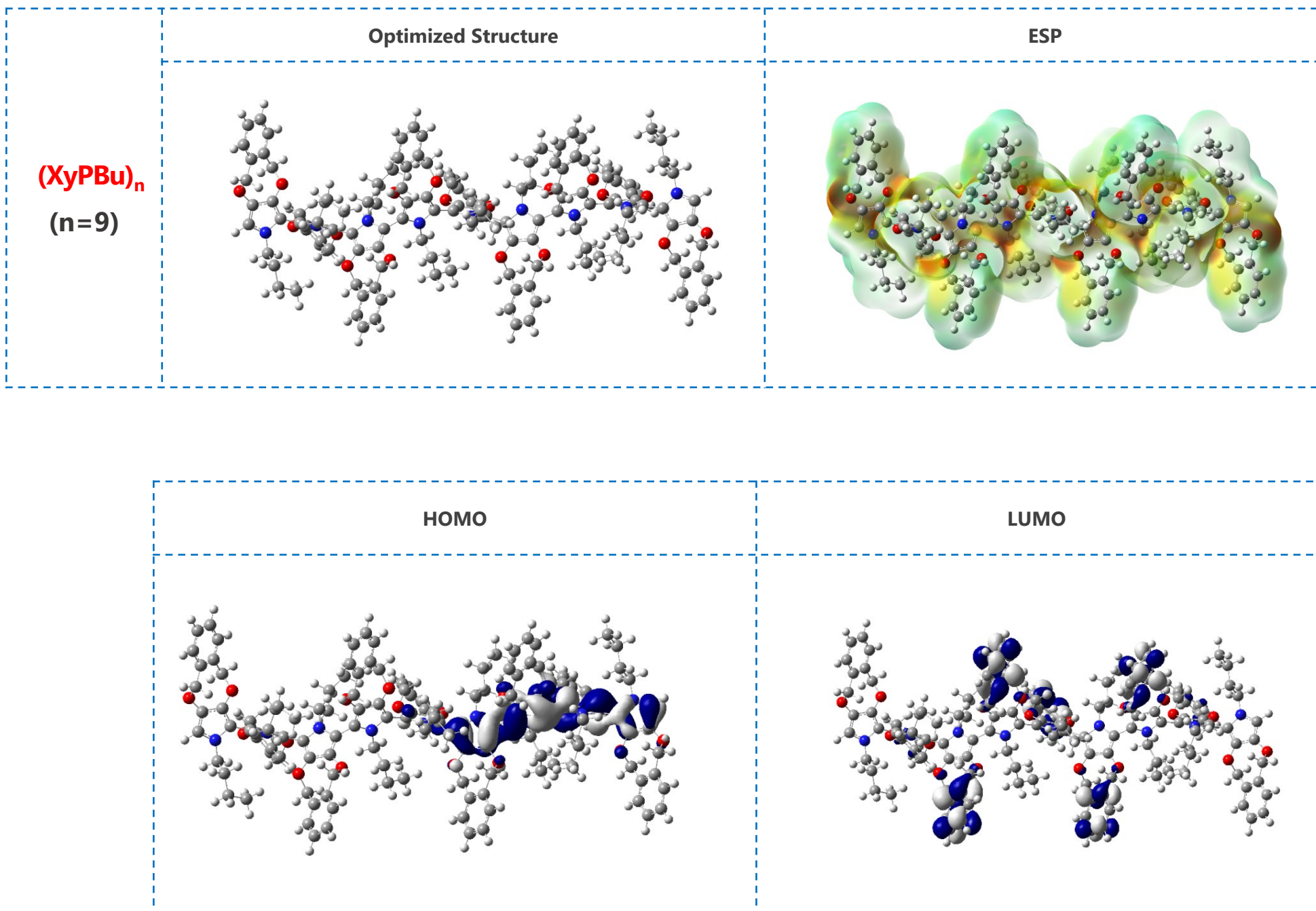


Figure S18-10 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPBu-decamer

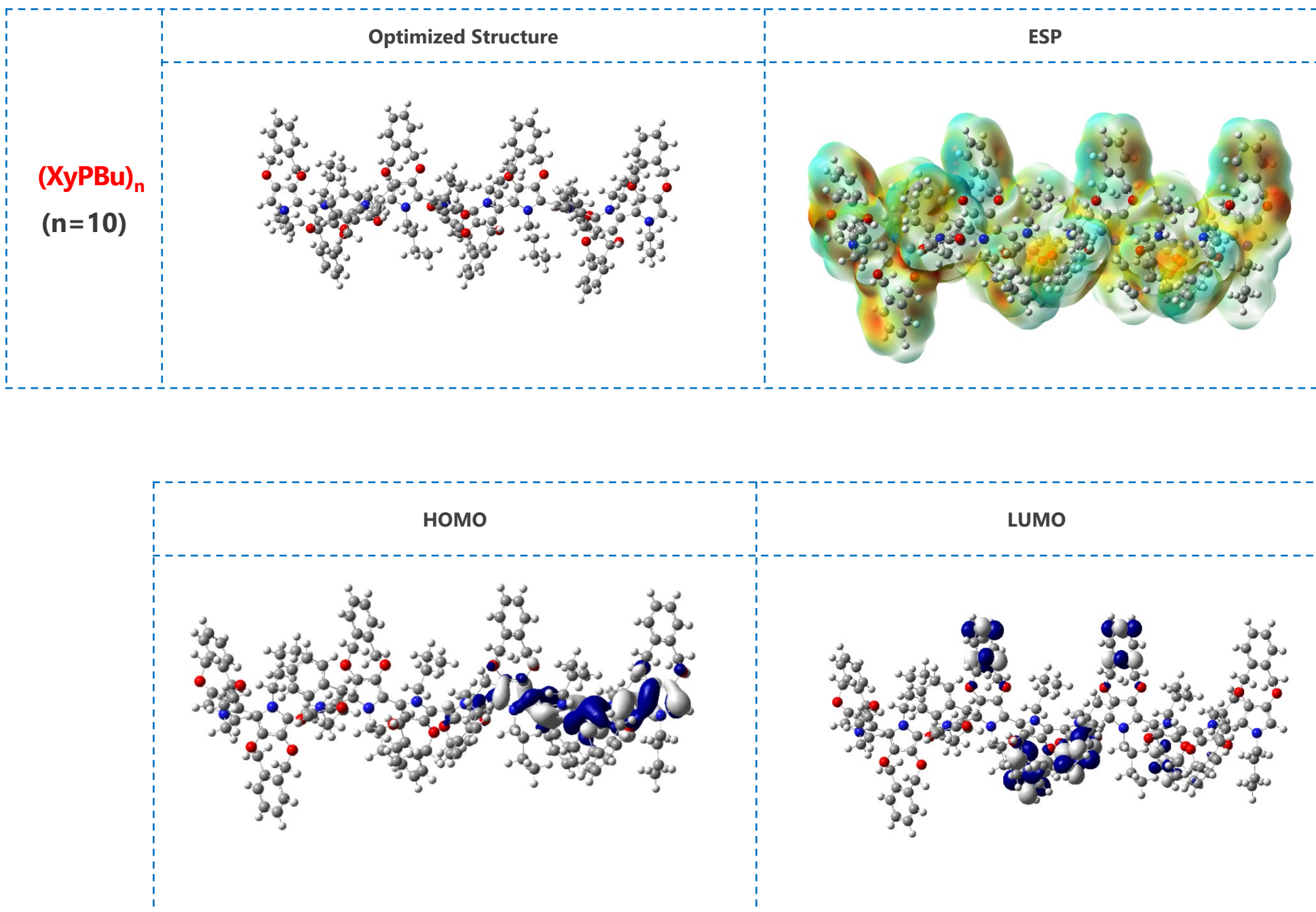


Figure S18-11 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyPBu-undecamer

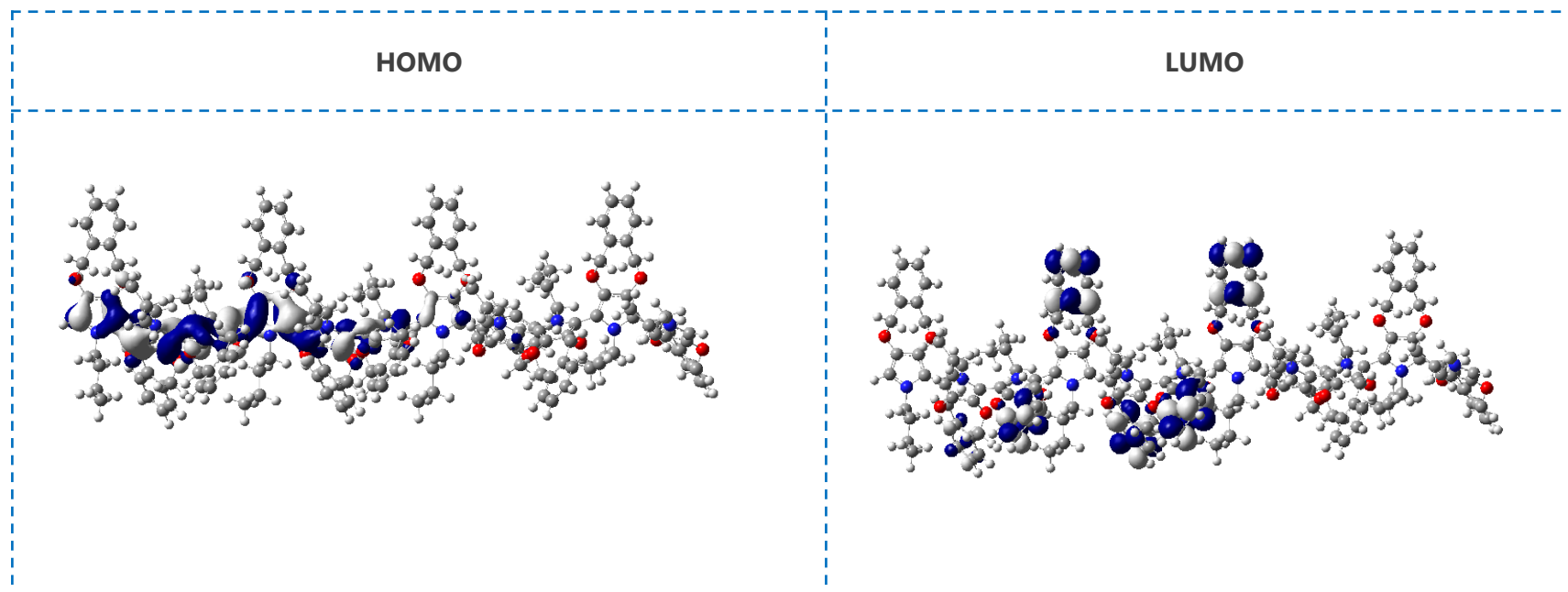
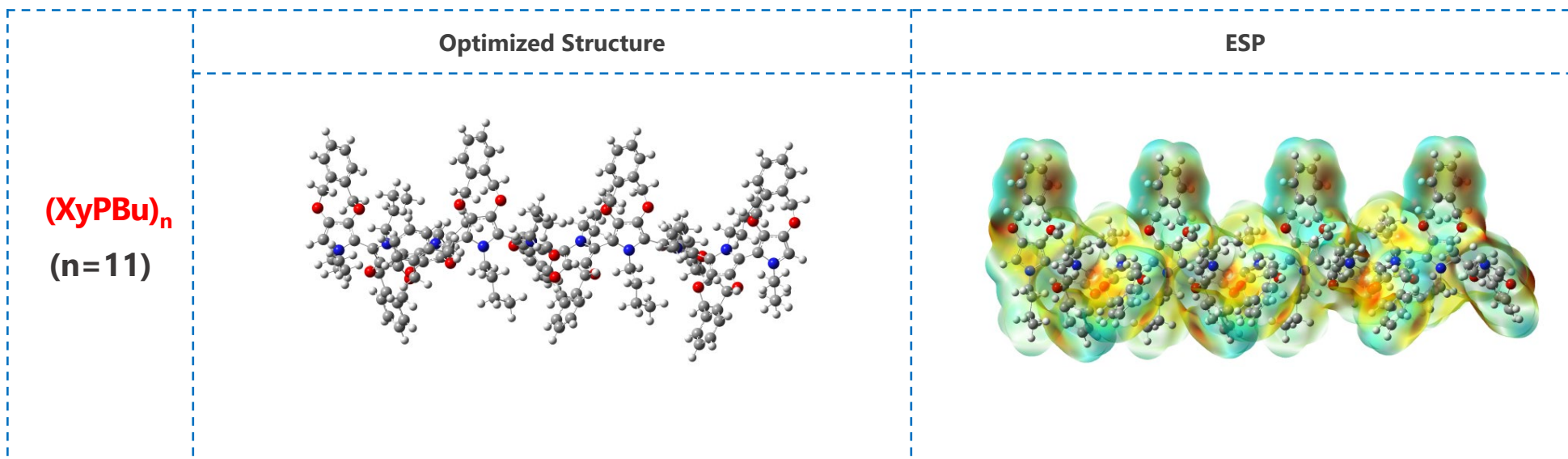


Figure S19-1 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyT-monomer

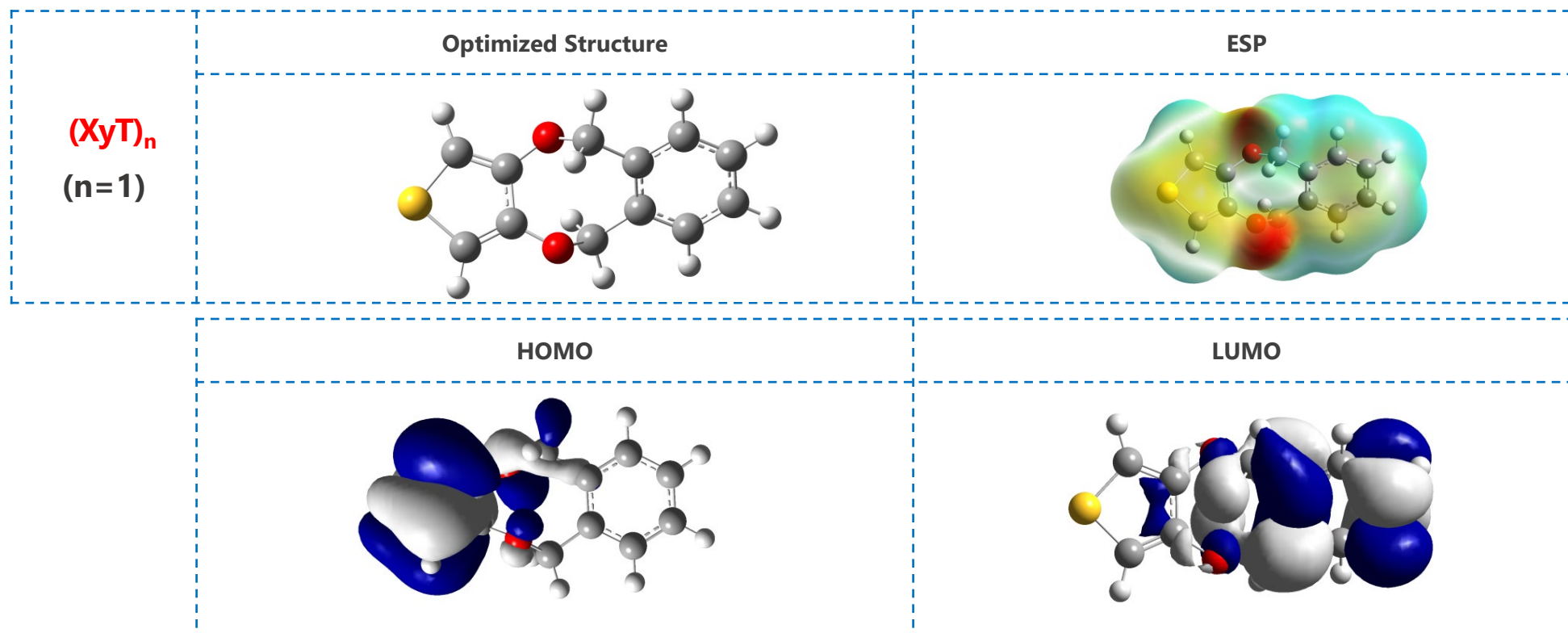


Figure S19-2 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyT-dimer

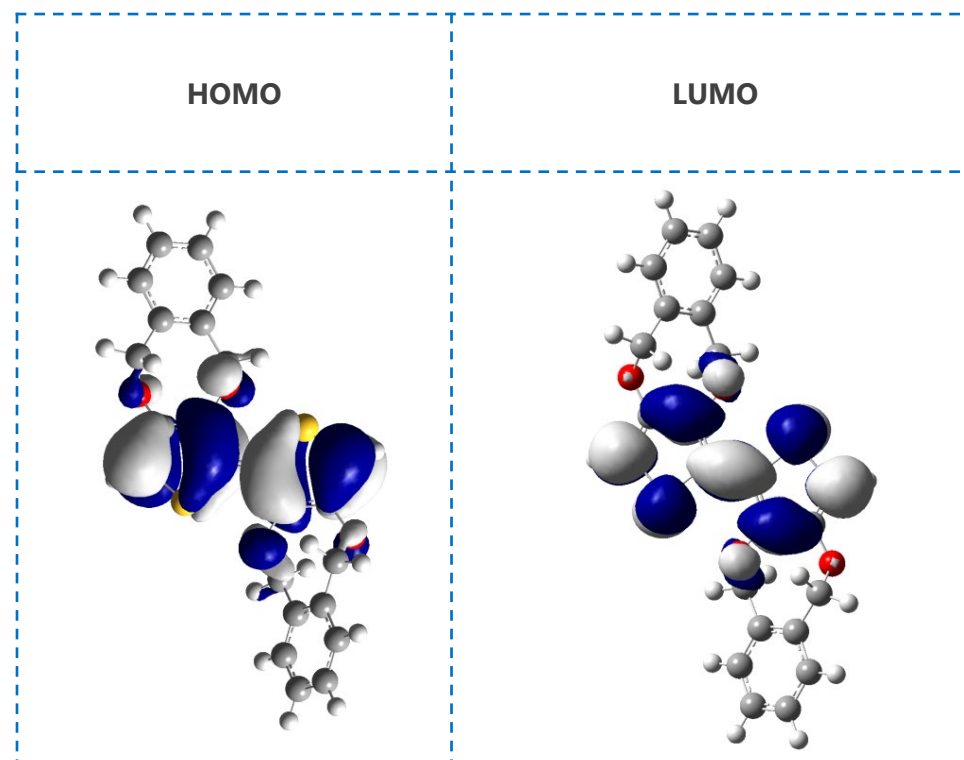
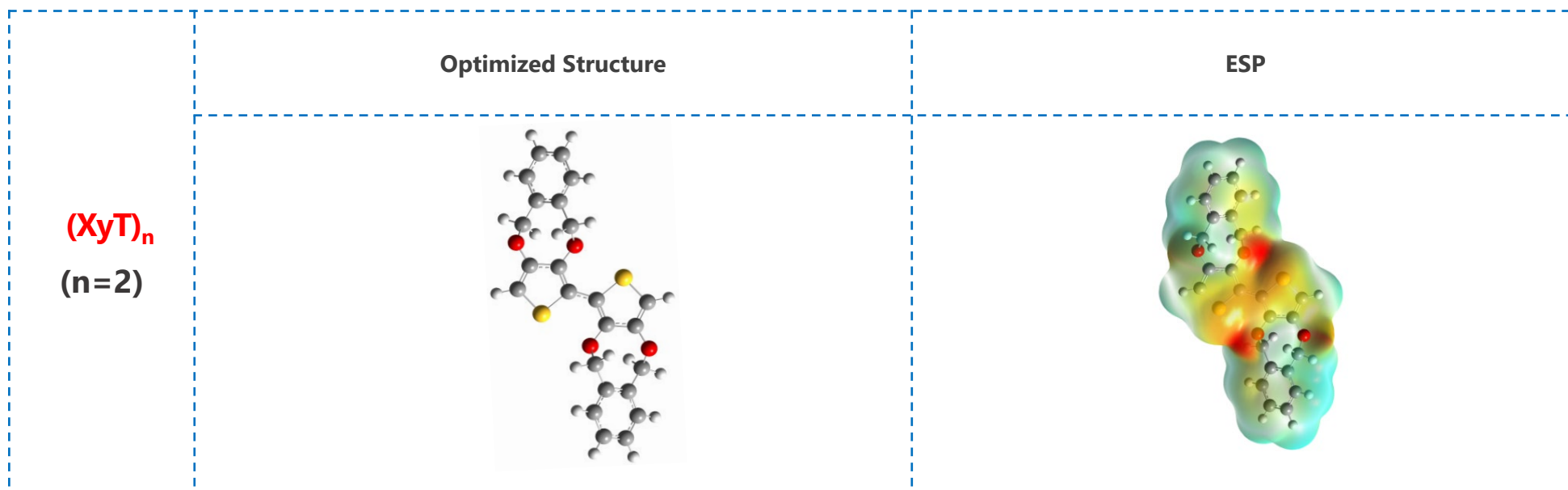


Figure S19-3 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyT-trimer

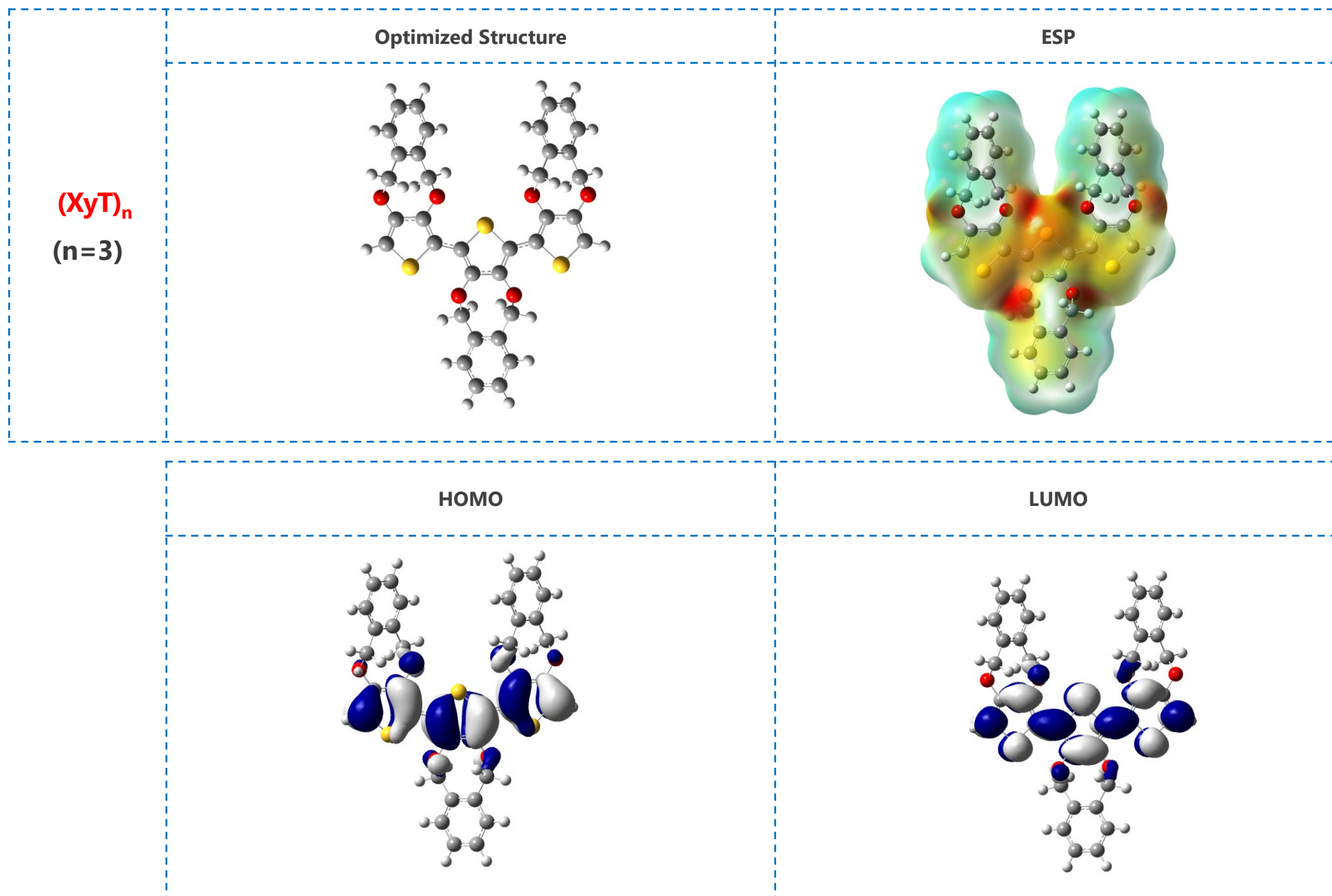


Figure S19-4 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyT-tetramer

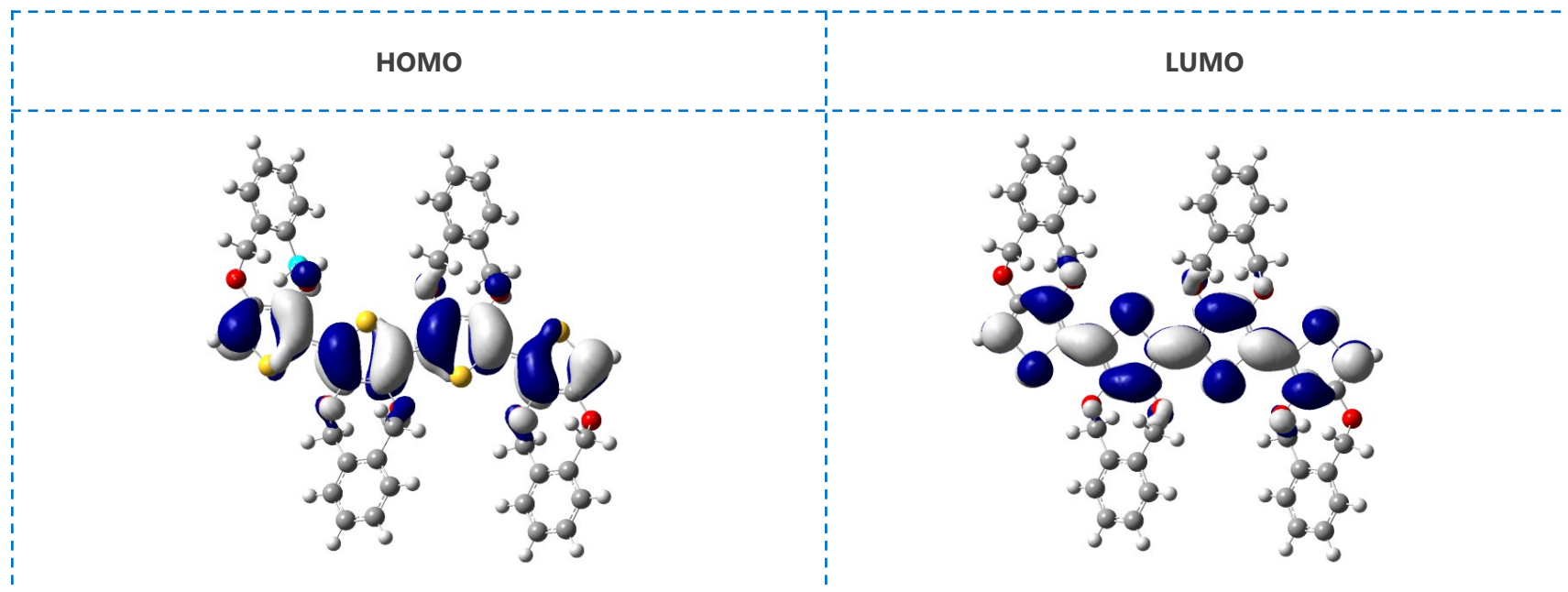
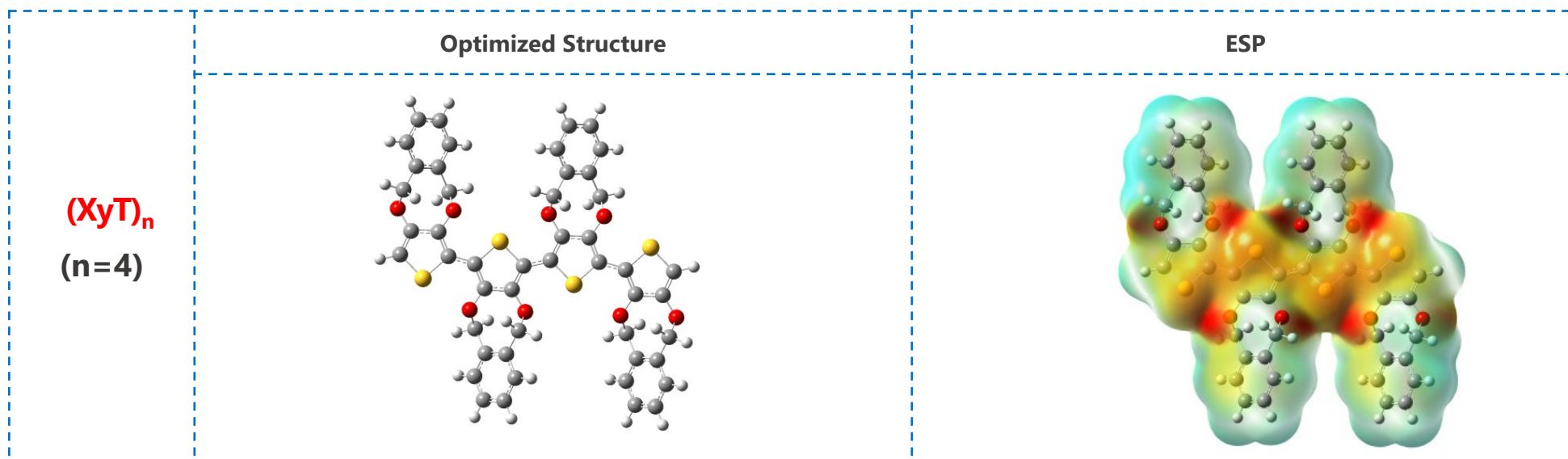


Figure S19-5 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyT-pentamer

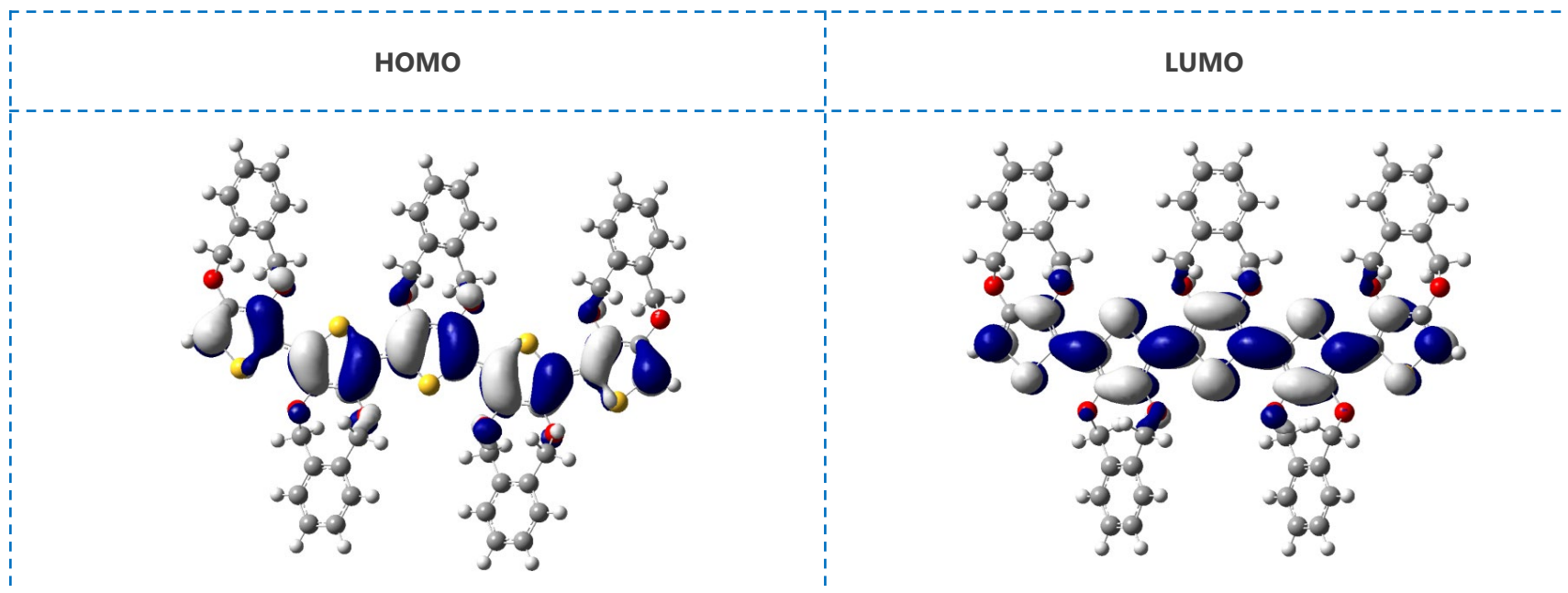
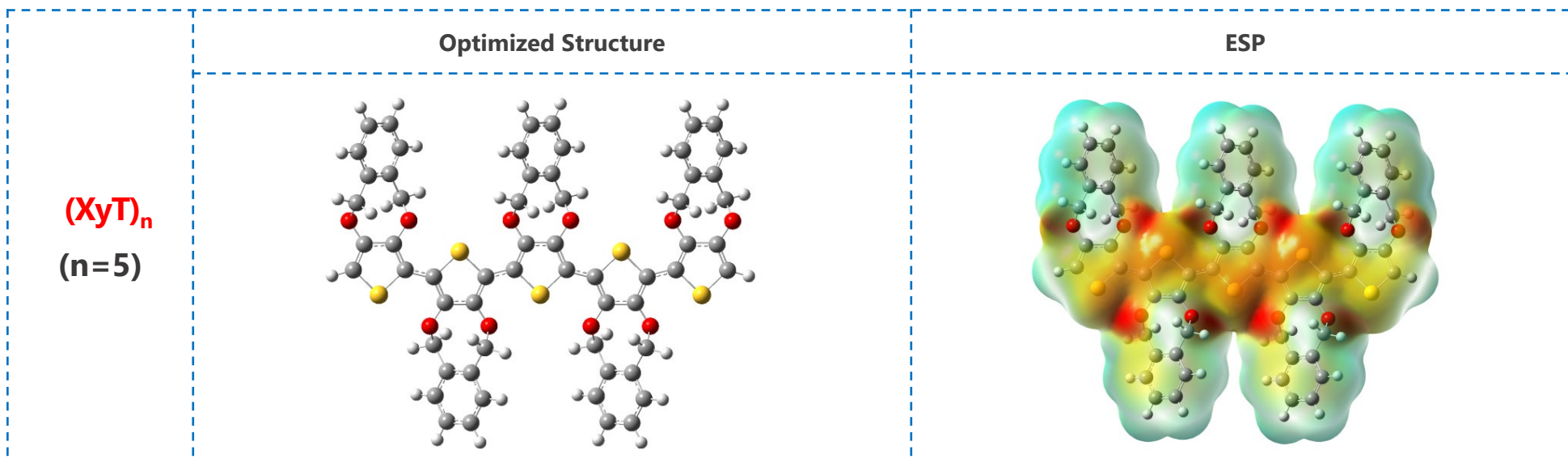


Figure S19-6 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyT-hexamer

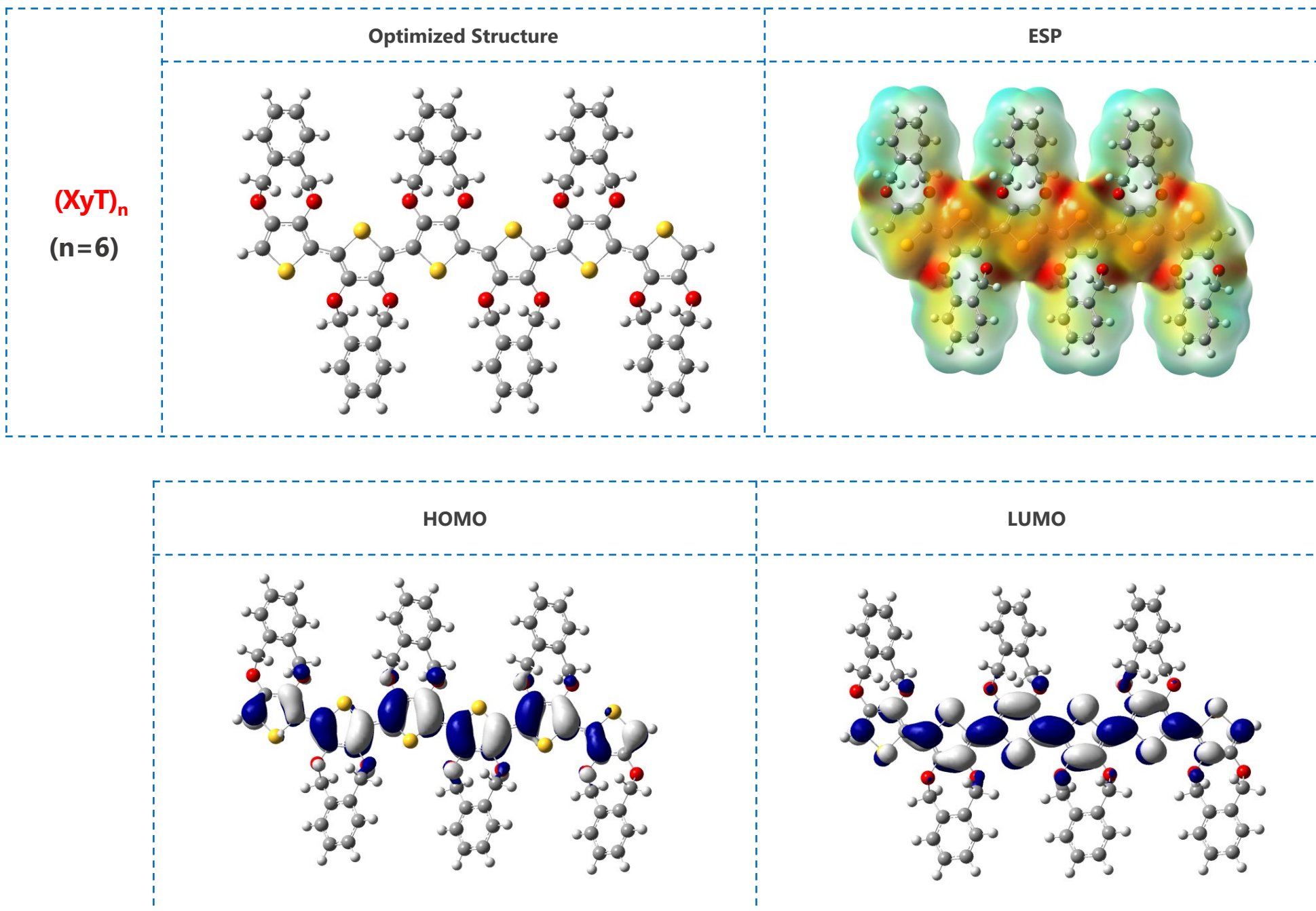


Figure S19-7 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyT-heptamer

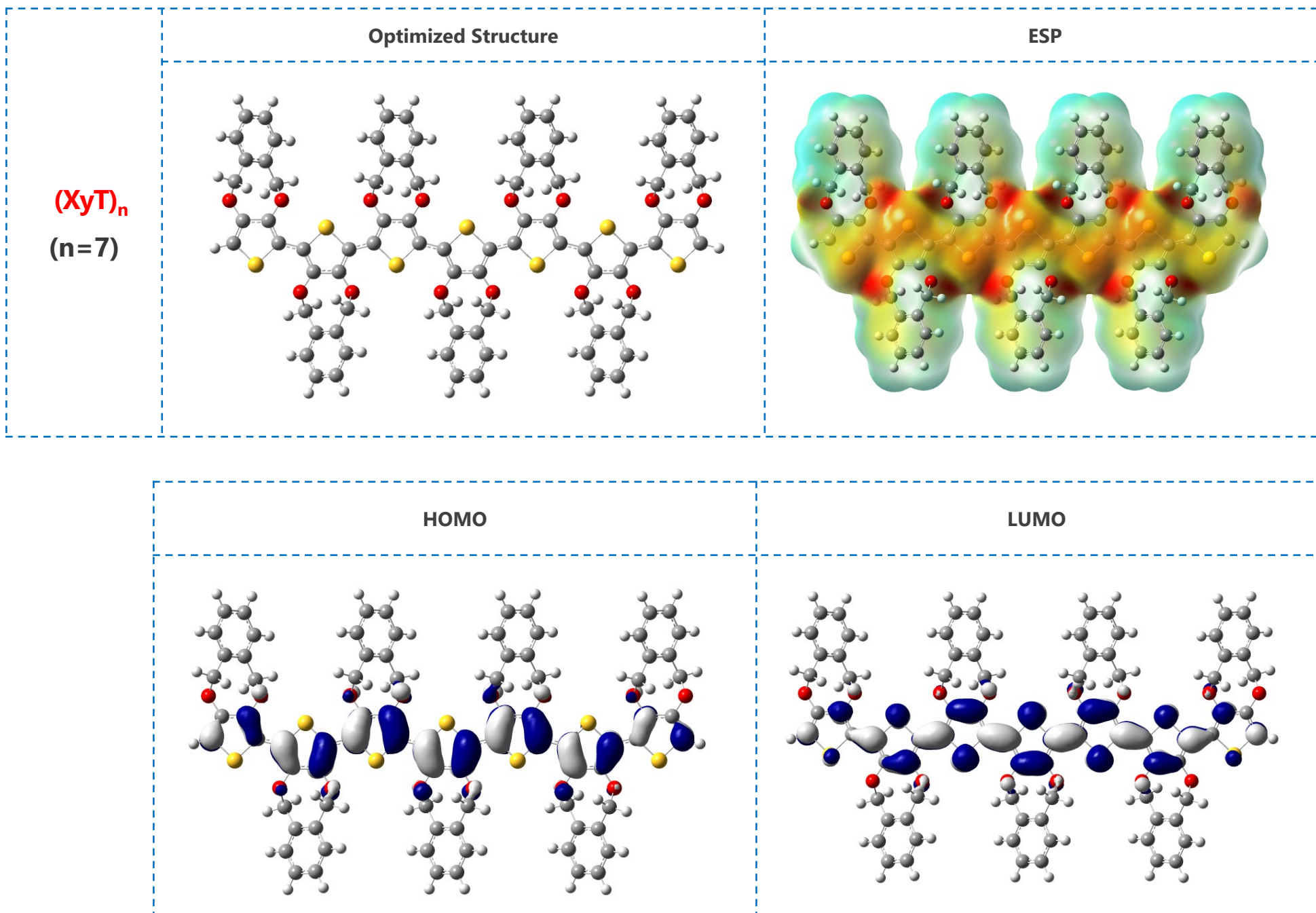


Figure S19-8 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyT-octamer

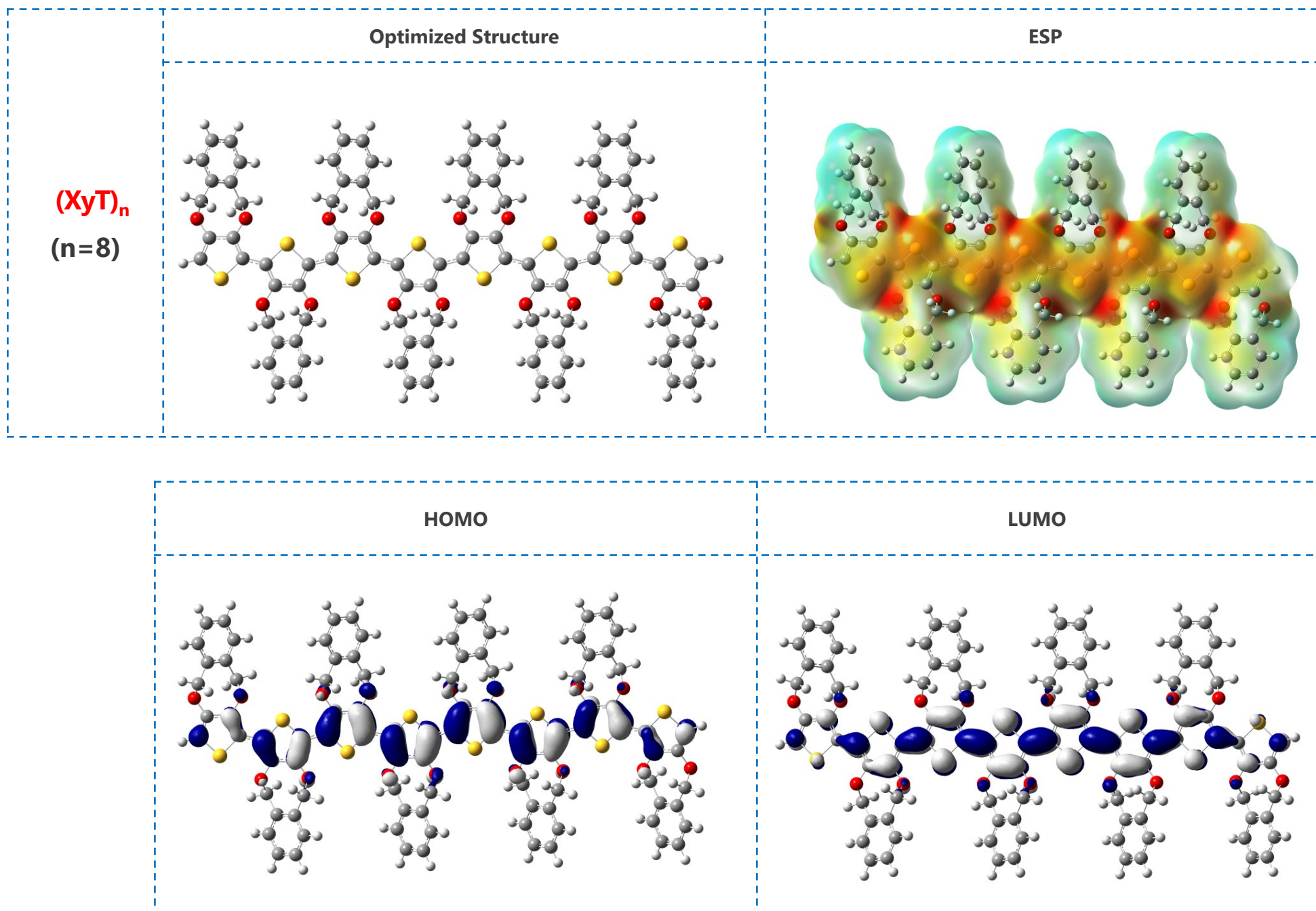


Figure S19-9 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyT-nonamer

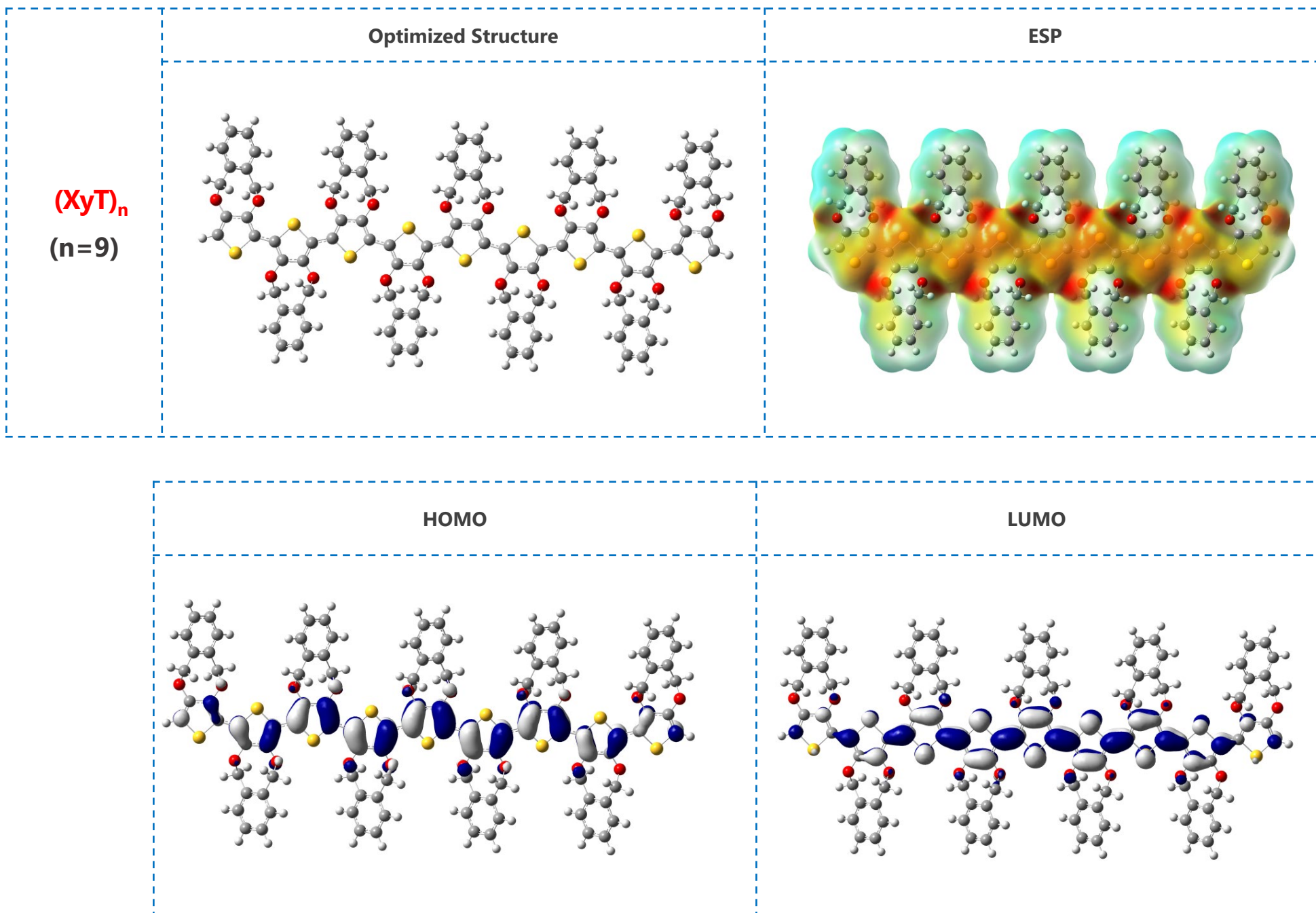


Figure S19-10 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyT-decamer

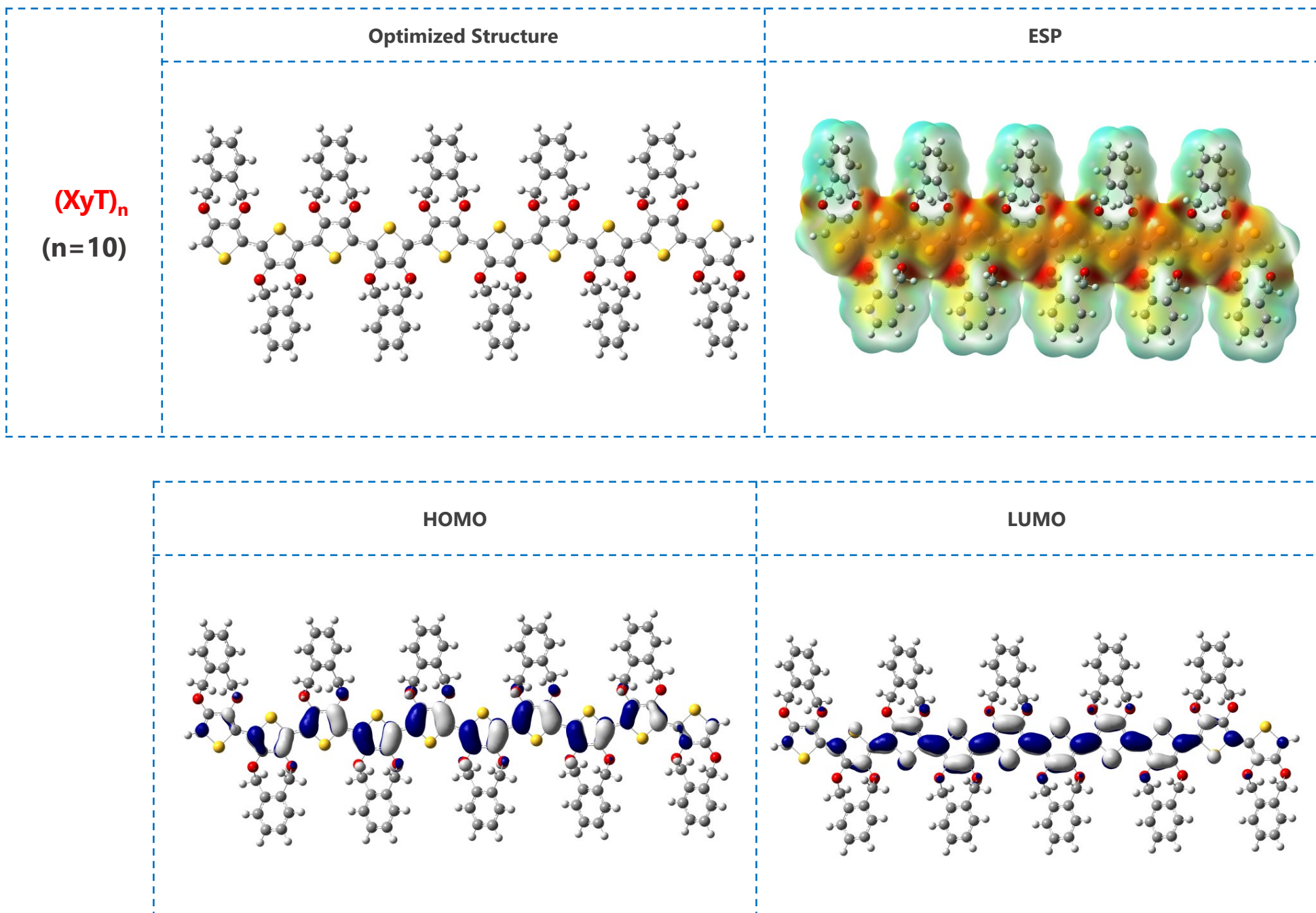


Figure S19-11 Optimized Structure, HOMO-LUMO contour plots and ESP map of the XyT-undecamer

