Supporting Information

for

Engineering Frontier Energy Levels in Donor-Acceptor Fluoren-9-ylidene Malononitriles versus Fluorenones

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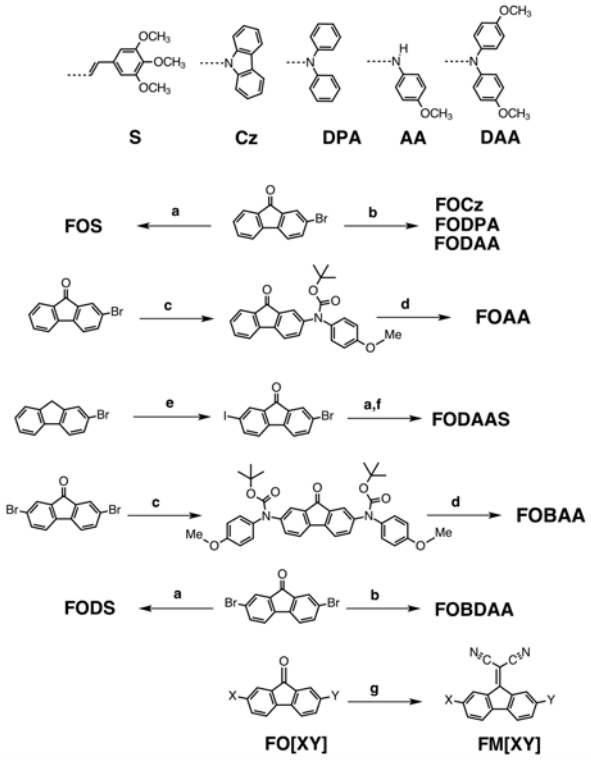
General Methods

All solvents and commercial reagents were used as received unless otherwise stated. All new compounds were identified by ^{1}H-NMR and high resolution mass spectrometry (FAB). ^{1}H-NMR spectra were recorded on a Bruker Avance 400 MHz FT-NMR spectrometer, and the chemical shifts recorded in ppm. Mass spectral data were obtained at the University of Massachusetts Mass Spectrometry Facility, which is supported in part by the National Science Foundation. UV-Vis, photoluminescence, and FT-IR spectra were obtained at room temperature using a Shimadzu UV-3600 UV-VIS-NIR spectrophotometer, a Photon Technology International QuantaMaster 30 Phosphorescence/Fluorescence spectro-photometer, and a Bruker Alpha FT-IR spectrophotometer fitted with a Platinum ATR QuickSnap sampling module, respectively. Purities were established by HPLC using a Buck Scientific BLC-10-11 instrument with a C18 reverse-phase column, using acetonitrile as solvent eluting at a rate of 0.25 mL/min. Cyclic voltammograms were obtained using a BASi Epsilon Electrochemical Workstation equipped with platinum auxiliary and working electrodes, and an Ag/AgCl in acetonitrile reference electrode, with tetrabutylammonium hexafluorophosphate as conducting electrolyte. Ferrocene in acetonitrile was used as external oxidation standard.



Scheme S1. General synthetic routes for substituted fluorenones and fluorenylidenemalononitriles in this study; x and y denote the substituents S, DPA, DAA, and Cz. (a) $Pd(OAc)_2$, P(*o*-tolyl)$_3$, DMF, "S", heat; (b) $Pd_3(dba)_2$, 1,1'- bis(diphenylphosphino)-ferrocene = DPPF, NaO-^{t}Bu, PhMe, heat with "Cz", "DPA", or "DAA"; (c) CuI, DMEDA, K_2CO_3, PhMe, anisidine-BOC = AA-boc (pg S6), heat; (d) HCl, EtOAc, room temp (e) I_2, KIO_3, H_2SO_4, HOAc / then CrO_3/Ac_2O/room temp; (f) $Pd_3(dba)_2$, DPPF, NaO-^{t}Bu, PhMe, heat with DAA; (g) $CH_2(CN)_2$, DMSO, heat.

General Procedure for Knoevenagel Condensation Reactions between Fluorenone Derivatives and Malononitrile:

One (1) eq of the fluorenone derivative and 6 eq of malononitrile were combined under a dry nitrogen atmosphere. Enough dry DMSO was added to make a 0.1 M solution, and the reaction mixture heated at 110 ^{o}C until complete by TLC. The reaction was then cooled to room temperature, and worked up and purified as described.

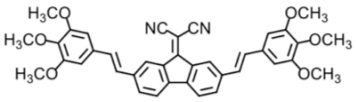
General Procedure for Buchwald-Hartwig Amination Reactions:

To a three-necked round-bottom flask under nitrogen atmosphere were added aryl halide (ArX), aryl amine, 0.1 eq of 1,1'- bis(diphenylphosphino) ferrocene (DPPF), 0.025 eq of Pd_2dba_3 (dba = dibenzylideneacetone) and 1.4 eq of *t*-BuONa. Toluene (5 mL, freshly distilled from potassium) per 1 mmol ArX was added and the reaction mixture was heated to 110 ^{o}C until complete by TLC. The reaction mixture was allowed to cool to

room temperature, filtered through Celite, concentrated in vacuo, and purified as described.

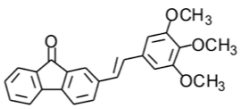
General Procedure for Buchwald/Ullmann-Goldberg Amidation:

Aryl halide (ArX), aryl amide, 0.2 eq *N,N'*-dimethylethylenediamine (DMEDA), 0.1 eq CuI, and 1.5 eq K_2CO_3 were combined under N_2. 5 mL toluene (freshly distilled over potassium) per 1 mmol ArX was added and the reaction mixture heated at 110 ^oC until complete by TLC. The reaction mixture was allowed to cool to room temperature, filtered through Celite, and concentrated in vacuo. The resulting solids were purified as described individually, below. See Klapars, A.; Antilla, J. C.; Huang, X.; Buchwald, S. L. *J. Am. Chem. Soc.* **2001**, *123*, 7727-7729; Klapars, A.; Antilla, J.; Huang, X.; Buchwald, S. L. *J. Am. Chem. Soc.* **2002**, *124*, 7421-7428.



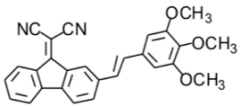
2,7-Bis(1-(3,4,5-trimethoxyphenyl-2-ethenyl)-fluoren-9-ylidene malononitrile (FMDS):

Prepared using the general procedure for Knoevenagel condensation using 1.00 g (1.77 mmol) of FODS (prepared per H. Rathnayake, *et al. Chem. Mater*., **2007**, 19(13), 3265–3270) and 0.700 g (10.6 mmol) of malononitrile overnight, during which time the solution turned from bright red to dark greenish-blue. The reaction mixture was then cooled to room temperature and poured into 300 mL water. The precipitate was collected *via* suction filtration, dissolved in chloroform, dried over $MgSO_4$, and concentrated *in vacuo*. The resulting blue solid was purified by crystallization from hot ethanol to yield 0.900 g (83 %) pure product. Mp 267-269 ^oC (d); ATR-IR (neat, cm^{-1}) 2225 (s, C≡N str); ^{1}H-NMR (400 MHz, $CDCl_3$): 3.89 (s, 6H), 3.94 (s, 12H), 6.75 (s, 4H), 6.97-7.01 (d, 2H, J = 16 Hz), 7.07-7.11 (d, 2H, J = 16 Hz), 7.49-7.51 (d, 2H, J = 8 Hz), 7.61-7.63 (d, 2H, J = 8 Hz), 8.48 (s, 2H); MS (FAB, *m/z*): found *m/z* = 612.2260, calculated for $C_{38}H_{32}N_2O_6$ *m/z* = 612.2260.



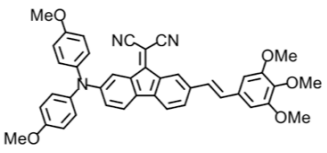
(*E*)-2-(3,4,5-trimethoxystyryl)-*9H*-fluoren-9-one (FOS):

To a three-necked round-bottom flask under nitrogen atmosphere were added 0.500 g (1.93 mmol) of 2-bromofluorenone, 0.375 g (1.93 mmol) of 3,4,5-trimethoxystyrene, 0.118 g (0.366 mmol) of P(*o*-tolyl), 0.030 mmol (0.135 mmol) of $Pd(OAc)_2$, and 10 mL of dry DMF. The reaction mixture was heated to 80 ºC, then stirred for 30 min. Then, 2 mL of triethylamine was added and the reaction stirred with continued heating for three days. The reaction mixture was poured into acidified water, stirred for 10 min, extracted with dichloromethane, and filtered through Celite to give an orange-red solution. The filtrate was washed with H_2O, dried over $MgSO_4$, and conc. *in vacuo* to give an orangey-red pasty solid. The crude material was recrystallized from 100% EtOH and further purified by flash chromatography on silica eluted with 1:3 ethyl acetate/hexanes to give 0.121 g of FOS as a pure orange solid (17 % yield). Mp 147-149 ºC; ATR-IR (neat, cm^{-1}) 1703 (s, C=O str); ^{1}H-NMR (400 MHz, $CDCl_3$): 3.88 (s, 3H), 3.93 (s, 6H), 6.75 (s, 2H), 6.99-7.03 (d, 1H, J = 16 Hz), 7.10-7.14 (d, 1H, J = 16 Hz), 7.30-7.31 (td, 1H, J = 16 Hz, J' = 8 Hz, J'' = 1.6 Hz), 7.48-7.53 (m, 3H), 7.56-7.57 (dd, 1H, J = 16 Hz, J' = 8 Hz), 7.66-7.68 (d, 1H, J = 8 Hz), 7.87 (s, 1H); MS (FAB, *m/z*): found *m/z* = 372.1362, calculated for $C_{24}H_{20}O_4$ *m/z* = 372.1362.



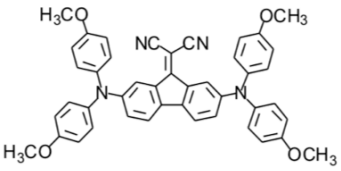
2-(1-(3,4,5-Trimethoxyphenyl-2-ethenyl)-fluoren-9-ylidene malononitrile (**FMS**):

Prepared using the general procedure for Knoevenagel condensation using 0.100 g (0.269 mmol) of FOS and 0.106 g (1.61 mmol) of malononitrile after a 22 h reaction time. The reaction mixture was poured into water, stirred for 10 min, and extracted with dichloromethane. The organic layers were combined, dried over $MgSO_4$, and conc. *in vacuo* to give a dark purple pasty solid. The crude material was recrystallized from 100 % EtOH to furnish 0.0810 g (72 % yield) pure product as a dark purple crystalline solid. Crystallization from dichloromethane by slow evaporation yielded dark purple needles. Mp 203-204 ºC; ATR-IR (neat, cm^{-1}) 2220 (s, C≡N str); ^{1}H-NMR (400 MHz, DMSO-d_6): 3.68 (s, 3 H), 3.85 (s, 6H), 6.96 (s, 2H), 7.16-7.20 (d, 1H, J = 16 Hz), 7.29-7.33 (d, 1H, J = 16 Hz), 7.43-7.47 (t, 1H, J = 16 Hz, J' = 8 Hz), 7.61-7.65 (t, 1H, J = 16 Hz, J' = 8 Hz), 7.86-7.89 (m, 3H), 8.22-8.24 (d, 1H, J = 8 Hz), 8.36 (s, 1H); ^{1}H-NMR (400 MHz, $CDCl_3$): 3.89 (s, 3 H), 3.94 (s, 6H), 6.76 (s, 2H), 6.99-7.03 (d, 1H, J = 16 Hz), 7.08-7.12 (d, 1H, J = 16 Hz), 7.29-7.33 (t, 1H, J = 16 Hz, J' = 8 Hz), 7.48-7.54 (m, 3H), 7.62-7.64 (d, 1H, J = 8 Hz), 8.36-8.38 (d, 1H, J = 8 Hz), 8.50 (s, 1H); MS (FAB, *m/z*): found *m/z* = 420.14606, calculated for $C_{27}H_{20}N_2O_3$ *m/z* = 420.14740.



2-(*N,N*-Dianisylamino)-7-(3,4,5-trimethoxyphenyl-2-ethenyl)-fluoren-9-ylidene malononitrile (FMDAAS):

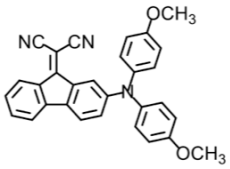
Prepared using the general procedure for Knoevenagel condensation using 0.0670 g (0.112 mmol) of FODAAS (prepared per P. J. Homnick, P. M. Lahti, *Phys. Chem. Chem. Phys*., **2012**, 14, 11961-11968) and 0.0444 g (0.672 mmol) of malononitrile after an 18 hour reaction time. The reaction mixture was poured into water, stirred for 10 min, and extracted with EtOAc. The organic layers were combined, dried over $MgSO_4$, and conc. *in vacuo* to give a pasty green solid. The crude material was purified by a quick recrystallization from 100 % EtOH to remove malononitrile, then by flash chromatography on silica eluted with 40 % EtOAc/hexanes to furnish 0.060 g (83 % yield) pure product as a greasy dark green film. Mp N/A (greasy film); ATR-IR (neat, cm^{-1}) 2222 (s, C≡N str); ^{1}H-NMR (400 MHz, DMSO-d_6): 3.67 (s, 3 H), 3.75 (s, 6 H), 3.83 (s, 6 H), 6.85-6.87 (dd, 1 H, J = 8 Hz, J' = 2 Hz), 6.92-6.96 (m, 6 H), 7.08-7.11 (m, 5 H), 7.22-7.26 (d, 1 H, J = 16 Hz), 7.55-7.57 (d, 1 H, J = 8 Hz), 7.62-7.64 (d, 1 H, J = 8 Hz), 7.75-7.77 (dd, 2 H, J = 8 Hz, J' = 1.6 Hz), 8.24 (s, 1 H); MS (FAB, *m/z*): found *m/z* = 647.2413, calculated for $C_{41}H_{33}N_3O_5$ *m/z* = 647.24202.



2,7-Bis(*N,N*-Dianisylamino)-fluoren-9-ylidene malononitrile (FMBDAA):

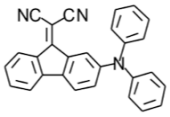
Prepared using the general procedure for Knoevenagel condensation using 0.250 g (0.394 mmol) of FOBDAA (prepared per P. J. Homnick, P. M. Lahti, *Phys. Chem. Chem. Phys*., **2012**, 14, 11961-11968) and 0.156 g (2.36 mmol) of malononitrile after a 4 day reaction time. The reaction mixture was poured into water, stirred for 10 min, and extracted with EtOAc. The organic layers were combined, dried over $MgSO_4$, and conc. *in vacuo* to give a pasty black solid. The crude material was recrystallized from a gradient of hot acetone and 95 % EtOH to furnish 0.198 g (73 % yield) pure black crystalline solid. Mp 106-108 ºC; ATR-IR (neat, cm^{-1}) 2221 (s, C≡N str); ^{1}H-NMR (400

MHz, DMSO-d_6): 3.73 (s, 12 H), 6.81-6.83 (dd, 2H, J = 8 Hz, J' = 2 Hz), 6.91-6.93 (d, 8H), 7.03-7.05 (d, 8H, J = 8 Hz), 7.34-7.36 (d, 2H, J = 8 Hz), 7.68-7.69 (d, 2H, J = 2 Hz); MS (FAB, *m/z*): found *m/z* = 682.2580, calculated for $C_{44}H_{34}N_4O_4$ *m/z* = 682.2580.



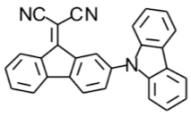
2-(*N,N*-Dianisylamino)-fluoren-9-ylidene malononitrile (FMDAA):

Prepared using the general procedure for Knoevenagel condensation using 0.250 g (0.614 mmol) of FODAA (prepared per P. J. Homnick, P. M. Lahti, *Phys. Chem. Chem. Phys*., **2012**, 14, 11961-11968) and 0.243 g (3.68 mmol) of malononitrile after a 2 day reaction time. The reaction mixture was poured into water, stirred for 10 min, and extracted with EtOAc. The organic layers were combined, dried over $MgSO_4$, and conc. *in vacuo* to give a dark green pasty solid. The crude material was recrystallized from 95% EtOH to furnish 0.176 g (63 % yield) pure product as fine green needles. Mp 182-184 ºC; ATR-IR (neat, cm^{-1}) 2224 (s, C≡N str); ^{1}H-NMR (400 MHz, DMSO-d_6): 3.75 (s, 6 H), 6.85-6.88 (dd, 1H, J = 8 Hz, J' = 2 Hz), 6.94-6.96 (d, 4H, J = 8 Hz), 7.09-7.11 (d, 4H, J = 8 Hz), 7.26-7.30 (t, 1H, J = 16 Hz, J' = 8 Hz), 7.50-7.54 (t, 1H, J = 16 Hz, J' = 8 Hz), 7.56-7.58 (d, 1H, J = 8 Hz), 7.62-7.63 (d, 1H, J = 2 Hz), 7.77 (d, 1H, J = 8 Hz), 8.09-8.11 (d, 1H, J = 8 Hz); MS (FAB, *m/z*): found *m/z* = 455.1634, calculated for $C_{30}H_{21}N_3O_2$ *m/z* = 455.1634.



2-(*N,N*-Diphenylamino)-fluoren-9-ylidene malononitrile (FMDPA):

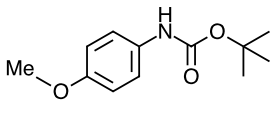
Prepared using the general procedure for Knoevenagel condensation using 0.250 g (0.720 mmol) of FODPA (prepared per P. J. Homnick, P. M. Lahti, *Phys. Chem. Chem. Phys*., **2012**, 14, 11961-11968) and 0.285 g (4.31 mmol) of malononitrile after a 22 hour reaction time. The reaction mixture was poured into water, stirred for 10 min, and extracted with dichloromethane. The organic layers were combined, dried over $MgSO_4$, and conc. *in vacuo* to give a dark blue pasty solid. The crude material was recrystallized from 100 % EtOH to furnish 0.203 g (71 % yield) pure product as a dark blue crystalline solid. Crystallization from 1:1 EtOAc/dichloromethane by slow evaporation yielded dark blue needles. Mp 199-200 ºC; ATR-IR (neat, cm^{-1}) 2219 (s, C≡N str); ^{1}H-NMR (400 MHz, DMSO-d_6): 7.09-7.15 (m, 7 H), 7.32-7.38 (m, 5H), 7.54-7.58 (t, 1H, J = 16 Hz, J' = 8 Hz), 7.68-7.72 (t, 2H, J = 16 Hz, J' = 8 Hz), 7.92 (s, 1H), 8.13-8.15 (d, 1H, J = 8 Hz); ^{1}H-NMR (400 MHz, $CDCl_3$): 7.09-7.16 (m, 7 H), 7.18-7.22 (td, 1H, J = 16 Hz, J' = 8 Hz, J'' = 1.2 Hz), 7.29-7.35 (m, 5H), 7.40-7.45 (m, 2H), 8.06 (d, 1H, J = 1.6 Hz), 8.28-8.29 (d, 1H, J = 8 Hz); MS (FAB, *m/z*): found *m/z* = 395.14180, calculated for $C_{28}H_{17}N_3$ *m/z* = 395.14225.



2-(1-Carbazolyl)-fluoren-9-ylidene malononitrile (FMCz):

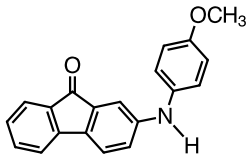
Prepared using the general procedure for Knoevenagel condensation using 0.100 g (0.290 mmol) of FOCz (prepared per P. J. Homnick, P. M. Lahti, *Phys. Chem. Chem. Phys*., **2012**, 14, 11961-11968) and 0.115 g (1.74 mmol) of malononitrile after a 5 hour reaction time. The reaction mixture was poured into water, stirred for 10 min, and filtered to give an orangey-red powdery solid. The filter cake was dissolved in dichloromethane, washed with H_2O, dried over $MgSO_4$, and conc. *in vacuo* to give an orangey-red pasty solid. The crude material was recrystallized from 100 % EtOH to furnish 0.0830 g (73 % yield) pure product as a orangey-red solid. Mp >260 ºC; ATR-IR (neat, cm^{-1}) 2224 (s, C≡N str); ^{1}H-NMR (400 MHz, DMSO-d_6): 7.32-7.36 (t, 2H, J = 16 Hz, J' = 8 Hz), 7.46-7.55 (m, 5H), 7.70-7.74 (t, 1H, J = 16 Hz, J' = 8 Hz), 7.94-7.96 (dd, 1H, J = 8 Hz, J' = 1.2 Hz), 8.02-8.04 (dd, 1H, J = 8 Hz, J' = 0.4 Hz), 8.18-8.20 (d,

1H, J = 8 Hz), 8.28-8.31 (t, 3H, J = 12 Hz, J' = 8 Hz), 8.45 (s, 1H); ^{1}H-NMR (400 MHz, $CDCl_3$): 7.32 (m, 2 H), 7.39-7.45 (m, 5H), 7.58-7.60 (t, 1H, J = 16 Hz, J' = 8 Hz), 7.64-7.66 (d, 1H, J = 8 Hz), 7.71-7.73 (d, 1H, J = 8 Hz), 7.78-7.80 (d, 1H, J = 8 Hz), 8.14-8.16 (d, 2H, J = 8 Hz), 8.44-8.46 (d, 1H, J = 8 Hz), 8.64 (s, 1H); MS (FAB, *m/z*): found *m/z* = 393.12562, calculated for $C_{28}H_{15}N_3$ *m/z* = 393.12660.



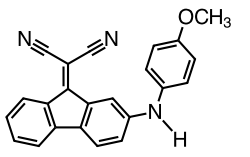
***Tert*-butyl (4-methoxyphenyl)carbamate (AA-boc):**

To 0.035 g (0.100 mmol) of indium(III) bromide was added to 2.18 g (10.0 mmol) of di-*tert*-butylcarbonate with stirring, then 1.24 g (10.0 mmol) of 4-anisylamine was added in one portion and the reaction mixture was stirred 30 min. Hexane was added during the reaction as needed to prevent clumping. The reaction mixture was then diluted with ethyl acetate and washed with water. The organic layer was dried over anhydrous $MgSO_4$ and concentrated in vacuo to give a gray-brown solid. Recrystallization twice from hot heptane yielded 2.14 g (96 %) of large, gun-metal gray needles. Mp 94-96 ºC (lit mp 92-94 °C [Chankeshwara, S. V.; Chakraborti. A. K. *Synthesis*. **2006**, *16*, 2784-2788]); ^{1}H-NMR (400 MHz, acetone-d_6): 1.47 (s, 9H), 3.75 (s, 3 H), 6.84-6.86 (d, 2H, J = 8 Hz), 7.44-7.46 (d, 2H, J = 8 Hz), 8.18 (s, 1H).



2-(*N*-Anisylamino)-fluoren-9-one (**FOAA**): Prepared using the general procedure for Buchwald/Ullmann-Goldberg amidation using 0.250 g (0.965 mmol) of 2-bromofluorenone and 0.259 g (1.16 mmol) of AA-boc after a 3 day reaction time. The dark orange-brown reaction mixture was worked up using the general method, and crudely purified on silica gel eluted with 20% ethyl acetate (EtOAc) in hexanes to give a yellow-orange solid. The solid was dissolved in EtOAc at room temperature and a few mL of conc HCl was added. The reaction was allowed to stir for about 2 h and then quenched with saturated aq Na_2CO_3. The organic layer was separated, washed again with saturated aq Na_2CO_3, dried over anhydrous Na_2SO_4, and concentrated in vacuo to give a dark red-purple solid. Recrystallization from hot heptane yielded a combined 0.261 g (67 %) of purified product as dark red-purple crystalline solid after two steps. Mp 152-154 ºC; ATR-IR (neat, cm^{-1}) 3355 (N-H str), 1704 (s, C=O str); ^{1}H-NMR (400 MHz, DMSO-d_6): 3.74 (s, 3 H), 6.92-6.96 (d, 2H, J = 8 Hz), 7.00-7.02 (dd, 1H, J = 8 Hz, J' = 1.6 Hz), 7.06-7.10 (m, 3H), 7.17-7.21 (t, 1H, J = 8 Hz), 7.47-7.56 (m, 4H), 8.31 (s, 1H); MS (FAB) found m/z = 301.3, calculated for $C_{20}H_{15}NO_2$ m/z = 301.1; HR-MS (ESI) found m/z = 302.1171 (M+H), calculated for $C_{20}H_{15}NO_2$ m/z = 301.11028.

2(*N*-Anisylamino)-fluoren-9-ylidene malononitrile (**FMAA**): Prepared using the general procedure for Knoevenagel condensation using 0.100 g (0.332 mmol) FOAA and 0.132 g (1.99 mmol) malononitrile after a 16 h reaction time. The dark aqua-blue reaction mixture was cooled to room temperature, poured into water, stirred for 10 min, and filtered to get a purple solid. The solid was dissolved in DCM to give an aqua-blue solution, washed sequentially with water and brine, dried over $MgSO_4$, and conc. *in vacuo* to give a dark purple pasty solid. The crude material was crystallized from hot EtOH to yield 0.0790 g (68 %) of black/green crystalline solid. Mp 187-188 ºC; ATR-IR (neat, cm^{-1}) 3337 (N-H str), 2222 (sh, C≡N str); ^{1}H-NMR (400 MHz, DMSO-d_6): 3.73 (s, 3 H), 6.89-6.91 (d, 2H, J = 8 Hz), 7.01-7.03 (dd, 1H, J = 8 Hz, J' = 2 Hz), 7.09-7.11 (d, 2H, J = 8 Hz), 7.22-7.26 (t, 1H, J = 8 Hz), 7.47-7.51 (t, 1H, J = 8 Hz), 7.55-7.59 (t, 2H, J

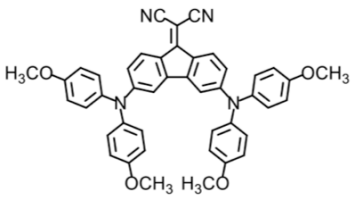


= 8 Hz), 7.89 (dd, 1H, J = 2 Hz), 8.08-8.10 (d, 1H, J = 8 Hz), 8.49 (s, 1H); MS (FAB) found m/z = 349.4, calculated for $C_{23}H_{15}N_3O$ m/z = 349.1; HR-MS (ESI) found m/z = 372.1087 (M+Na), calculated for $C_{23}H_{15}N_3O$ m/z = 349.12151.

2,7-Bis(*N*-Anisylamino)-fluoren-9-one (**FOBAA**): Prepared using the general procedure for Buchwald/Ullmann-Goldberg amidation using 0.250 g (0.740 mmol) of 2,7-dibromofluorenone and 0.397 g (1.78 mmol) of AA-boc after a 3 day reaction time. The dark red-brown reaction mixture was worked up using the general method, and crudely purified on silica gel eluted with 20 % EtOAc in hexanes to give a red solid. The solid was dissolved in EtOAc at room temperature and a few mL of conc HCl was added. The reaction was allowed to stir for about 2 h and then quenched with saturated aq Na_2CO_3. The dark blue organic layer was separated, washed with saturated aq Na_2CO_3, dried over anhydrous Na_2SO_4, and concentrated in vacuo to give a shiny gold-colored solid. Recrystallization from hot heptane yielded 0.149 g (48%) of purified product as shiny gold-colored crystalline solid. Mp 214-216 ºC; ATR-IR (neat, cm^{-1}) 3329-3394 (N-H str), 1714 (s, C=O str); ^{1}H-NMR (400 MHz, DMSO-d_6): 3.74 (s, 3 H), 6.92-6.96 (d, 2H, J = 8 Hz), 7.00-7.02 (dd, 1H, J = 8 Hz, J' = 1.6 Hz), 7.06-7.10 (m, 3H), 7.17-7.21 (t, 1H, J = 8 Hz), 7.47-7.56 (m, 4H), 8.31 (s, 1H); HR-MS (ESI) found m/z = 422.1596, calculated for $C_{27}H_{22}N_2O_3$ m/z = 422.16304.

2,7-Bis(*N*-Anisylamino)-fluoren-9-one (**FMBAA**): Prepared using the general procedure for Knoevenagel condensation with 0.0500 g (0.119 mmol) FOBAA and 0.0469 g (0.710 mmol) malononitrile after a 16 h reaction time. The reaction mixture was cooled to room temperature, poured into water, stirred for 10 min, and extracted with Et_2O. The organic layers were combined, dried over anhydrous $MgSO_4$, and conc. *in vacuo* to give a pasty reddish solid. The crude material was purified on silica gel eluted with 20 % EtOAc in hexanes to give a dark green/gray solution which when concentrated yielded 0.039 g (70 %) of dark green/black solid. Slow crystallization from the elution solvent yielded fine, long, green/gray needles. Mp 204-205 ºC; ATR-IR (neat, cm^{-1}) 3344 (N-H str), 2225 (sh, C≡N str); ^{1}H-NMR (400 MHz, DMSO-d_6): 3.72 (s, 6 H), 6.86-6.88 (d, 4H, J = 8 Hz), 6.94-6.96 (dd, 2H, J = 8 Hz, J' = 1.6 Hz), 7.04-7.06 (d, 4H, J = 8 Hz), 7.30-7.32 (d, 2H, J = 8 Hz), 7.80-7.81 (d, 2H, J = 1.6 Hz), 8.26 (s, 2H); MS (FAB) found m/z = 470.2, calculated for $C_{30}H_{22}N_4O_2$ m/z = 470.2; HR-MS (ESI) found m/z = 471.1793 (M+H), calculated for $C_{30}H_{22}N_4O_2$ m/z = 470.17428.

3,6-Bis(bis(4-methoxyphenyl)amino)-9*H*-fluoren-9-one (FOBDAA36): Prepared using the general procedure for Buchwald-Hartwig amination using 0.250 g (0.740 mmol) of 3,6-dibromofluorenone [Kobin, B. et al. *J. Mater. Chem.*, 2012, *22*, 4383-4390] and 0.442 g (1.85 mmol) of dianisylamine. After reacting for 2 days the red reaction mixture was worked up using the general method. The crude mixture was purified on silica eluted with 30:70 EtOAc/hexanes to yield 0.306 g (65 %) dark red crystalline solid. Mp 119-120 ºC; ATR-IR (neat, cm^{-1}) 1684 (s, C=O str); ^{1}H-NMR (400 MHz, DMSO-d_6): 3.75 (s, 12 H), 6.42-6.44 (dd, 2H, J = 8 Hz, J' = 2 Hz), 6.58-6.59 (d, 2H, J = 1.6 Hz), 6.94-6.96 (d, 8H, J = 8 Hz), 7.12-7.14 (d, 8H, J = 8 Hz), 7.30-7.32 (d, 2H, J = 8 Hz); MS (FAB, *m/z*): found *m/z* = 634.2455, calculated for $C_{41}H_{34}N_2O_5$ *m/z* = 634.24677.



2-(3,6-Bis(bis(4-methoxyphenyl)amino)-9*H*-fluoren-9-ylidene)malononitrile (FMBDAA36): Prepared using the general procedure for Knoevenagel condensation using 0.0183 g (0.0288 mmol) of FOBDAA36 and 0.0114 g (0.173 mmol) of malononitrile after a 2 day reaction time. The reaction mixture was poured into water, stirred for 10 min, and extracted with Et_2O. The organic layers were combined, dried over $MgSO_4$, and conc. *in vacuo* to give a pasty purple solid. The crude material was recrystallized from hot EtOH to yield 0.013 g (66 %) pure purple powdery solid. Mp 178-180 ºC; ATR-IR (neat, cm^{-1}) 2212 (s, C≡N str); ^{1}H-NMR (400 MHz, DMSO-d_6): 3.76 (s, 12 H), 6.48-6.51 (dd, 2H, J = 8 Hz, J' = 2 Hz), 6.54-6.55 (d, 2H, J = 1.6 Hz), 6.96-6.98 (d, 8H, J = 8 Hz), 7.16-7.18 (d, 8H, J = 8 Hz), 7.90-7.92 (d, 2H, J = 8 Hz); MS (FAB, *m/z*): found *m/z* = 682.2580, calculated for $C_{44}H_{34}N_4O_4$ *m/z* = 682.25801.

Figure S1. Cyclic voltammograms compared for structural building blocks and for FO and FM based push-pull compounds. See Scheme S1 for structural abbreviations. All potentials in volts were calibrated against the ferrocene-ferrocenium redox system in acetonitrile; oxidation is positive for all the plots.

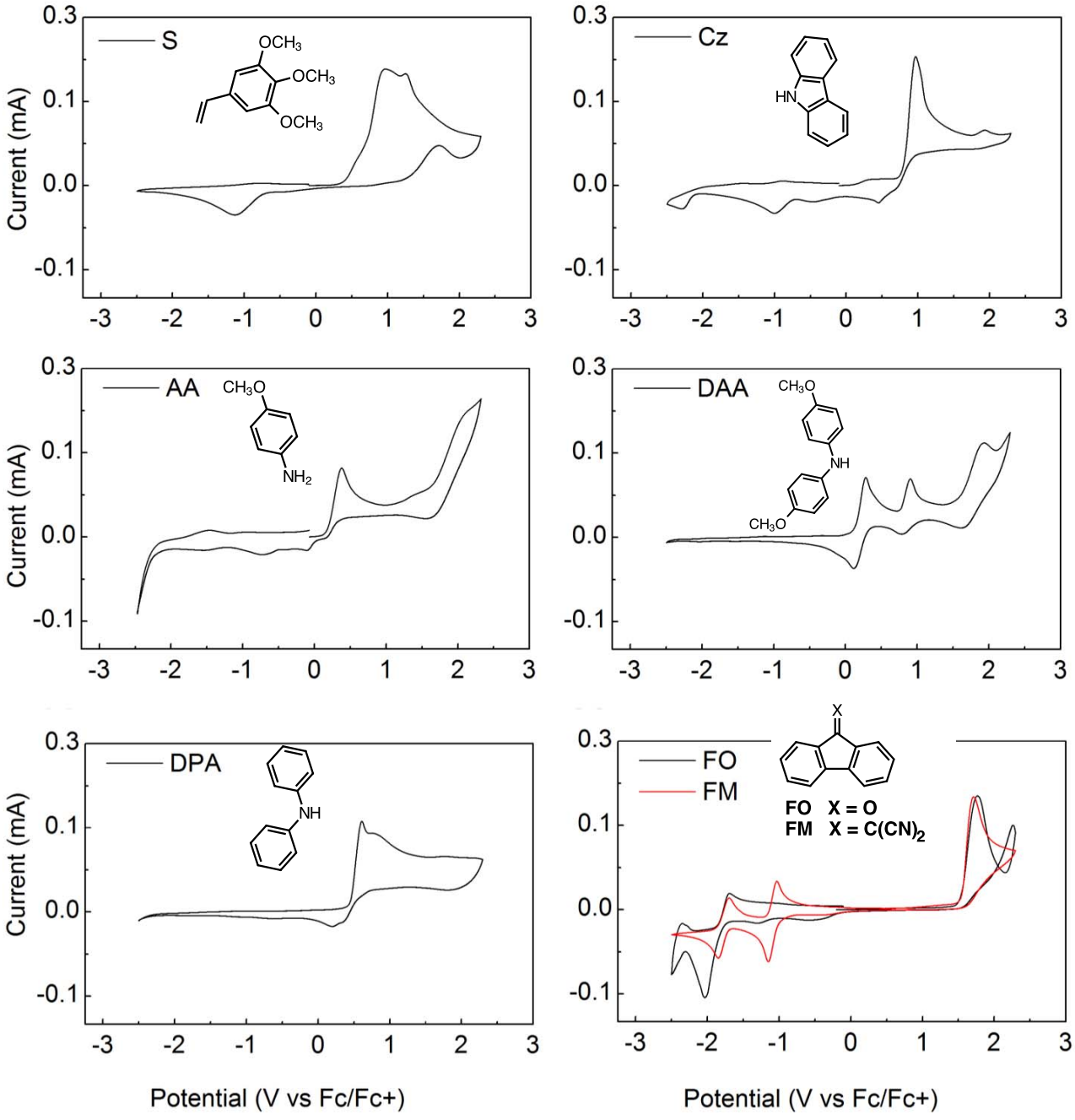


Figure S1 continued. Cyclic voltammograms compared for structural building blocks and for FO and FM based push-pull compounds. See Scheme S1 for structural abbreviations. All potentials in volts were calibrated against the ferrocene-ferrocenium redox system in acetonitrile; oxidation is positive for all the plots.

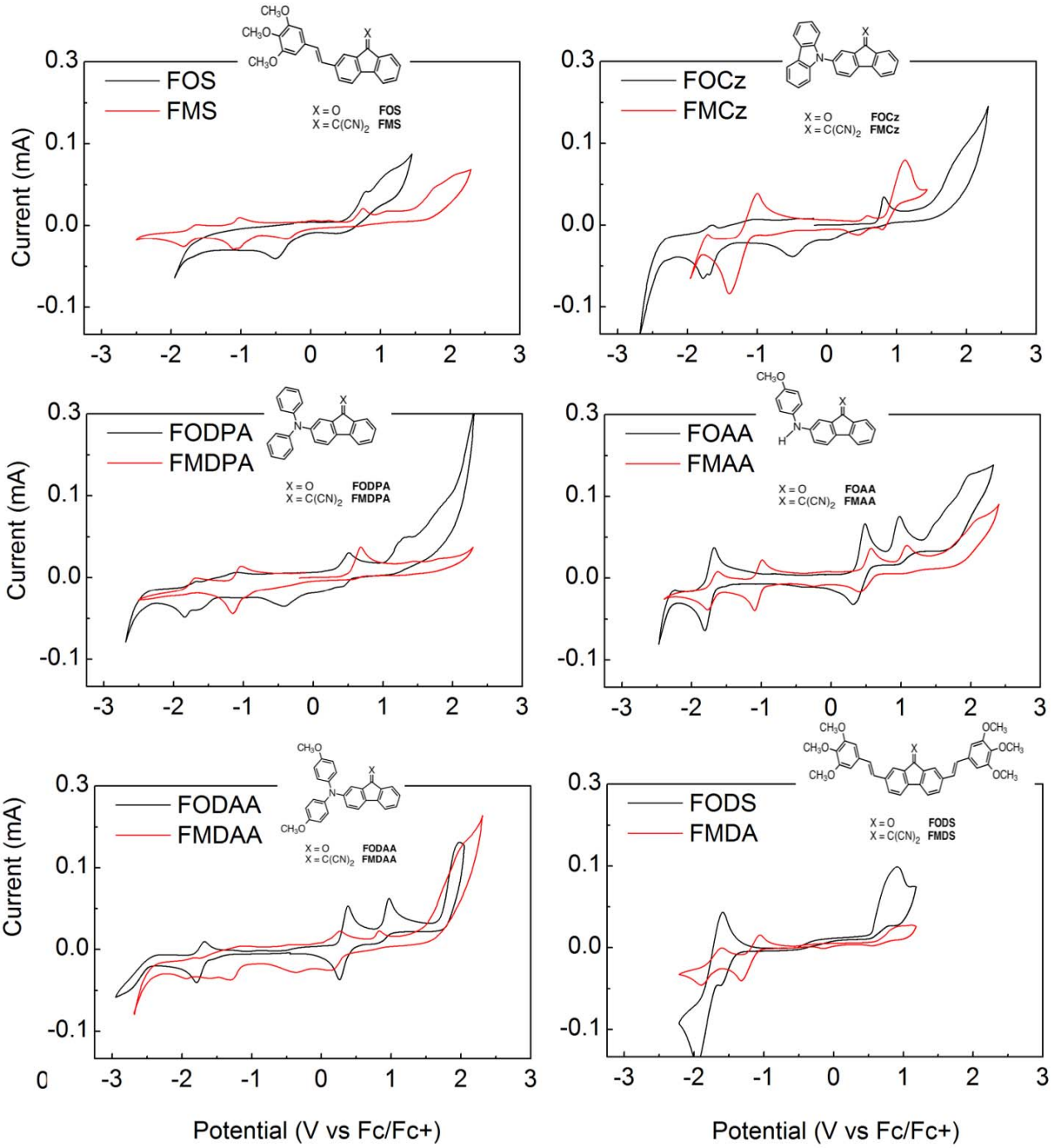
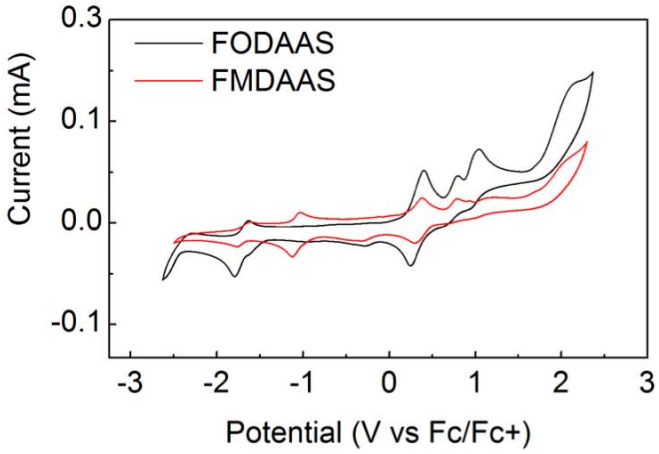
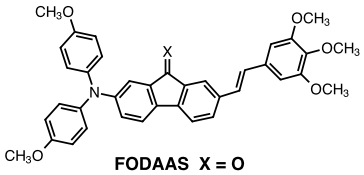
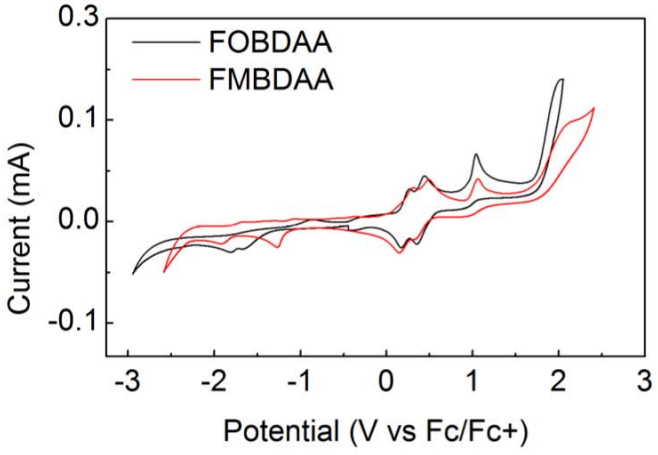


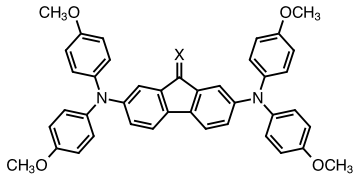
Figure S1 continued. Cyclic voltammograms compared for structural building blocks and for FO and FM based push-pull compounds. See Scheme S1 for structural abbreviations. All potentials in volts were calibrated against the ferrocene-ferrocenium redox system in acetonitrile; oxidation is positive for all the plots.



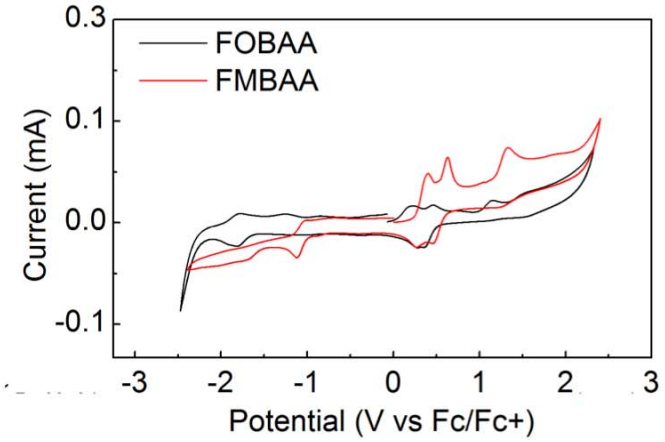


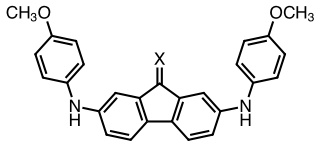
FODAAS X = O
FMDAAS X = C(CN)$_2$





FOBDAA X = O
FMBDAA X=C(CN)$_2$





FOBAA X = O
FMBAA X = C(CN)$_2$

Figure S2. Absorption spectra of trimethoxystyrene incorporating systems in acetonitrile for **FOS** (black), **FODS** (red), and **FODAAS** (blue), left chart; compared to those of **FMS** (black), **FMDS** (red), and **FMDAAS** (blue), right chart.

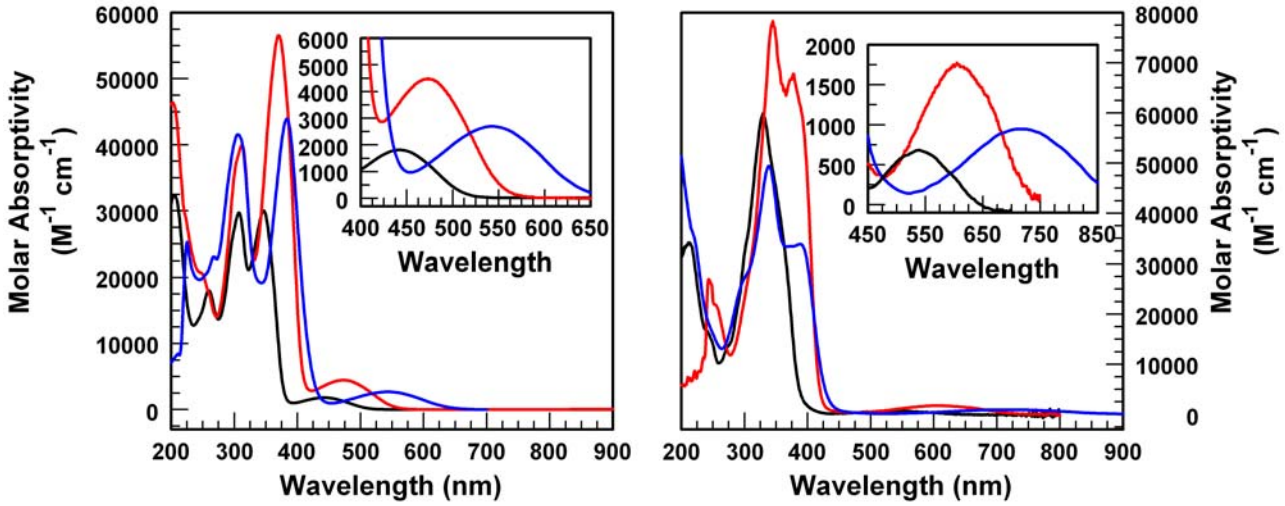


Figure S3. Absorption spectra of diarylamine incorporating systems in acetonitrile for **FOCz** (black), **FODPA** (red), and **FODAA** (blue), left chart; compared to those of **FMCz** (black), **FMDPA** (red), and **FMDAA** (blue), right chart.

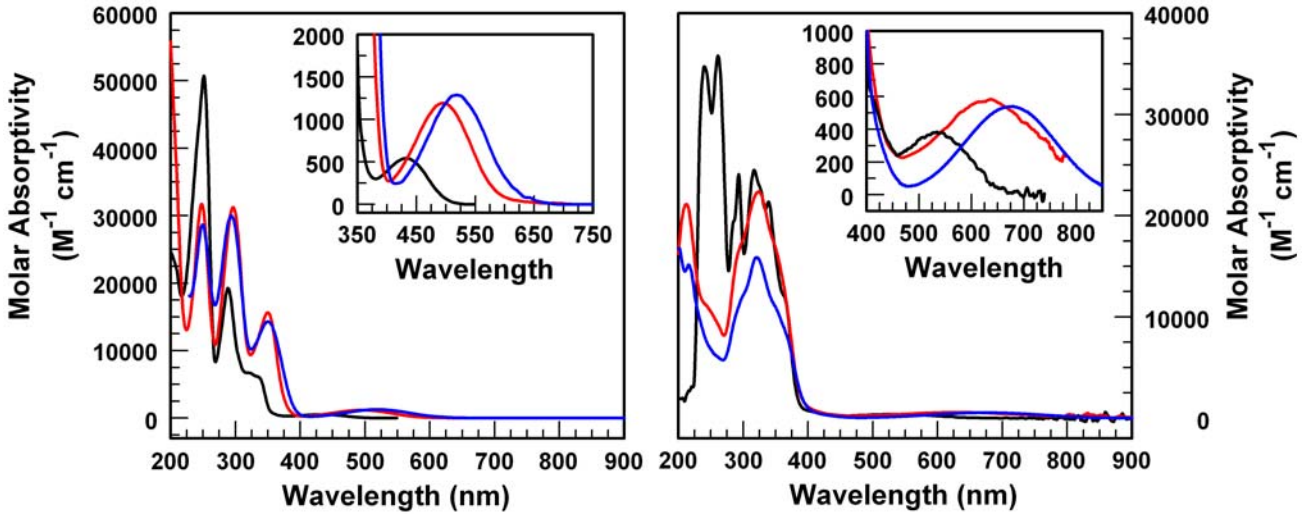


Figure S4. Absorption spectra of anisylamine incorporating systems in acetonitrile for **FOAA** and **FOBAA (**black); compared to **FMAA (**black) and **FMBAA** (red), right chart.

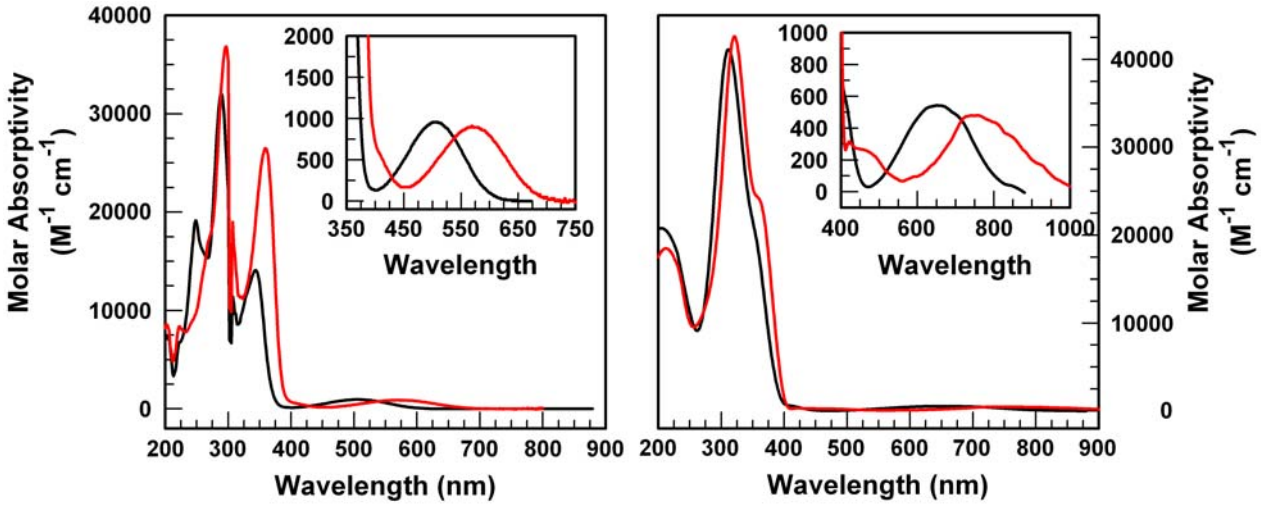


Figure S5. Full scale absorption spectra in diethyl ether and in acetonitrile for **FODAA** and **FMDAA**.

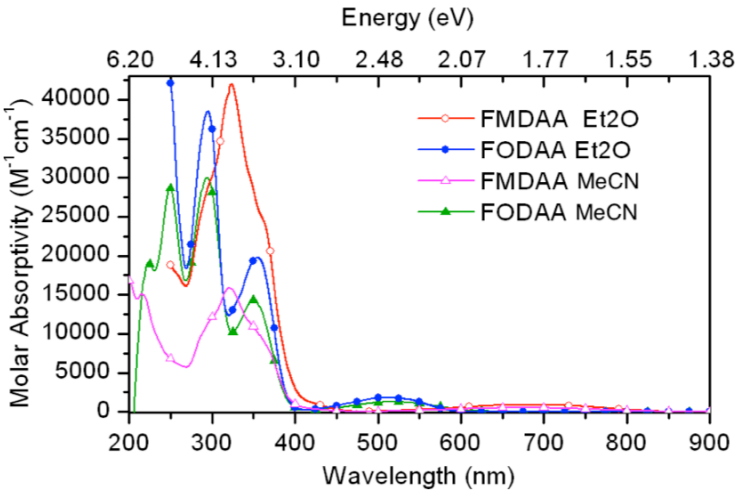


Figure S6. Absorption spectra in acetonitrile showing effects of connectivity changes in **FOBDAA (**black) versus **FOBDAA36** (red), left chart; comparison of **FMBDAA (**black) versus **FMBDAA36** (red), right chart.

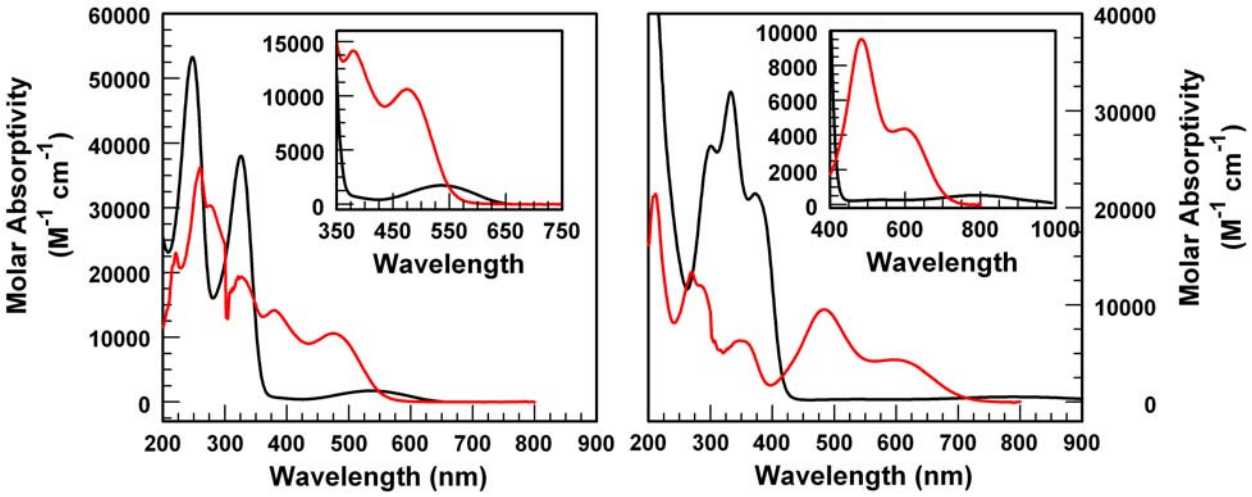


Figure S7. Cyclic voltammograms compared for FOBDAA36 (red trace) and FMBDAA36 (black trace). Potentials in volts were calibrated against the ferrocene-ferrocenium redox system in acetonitrile; oxidation is positive

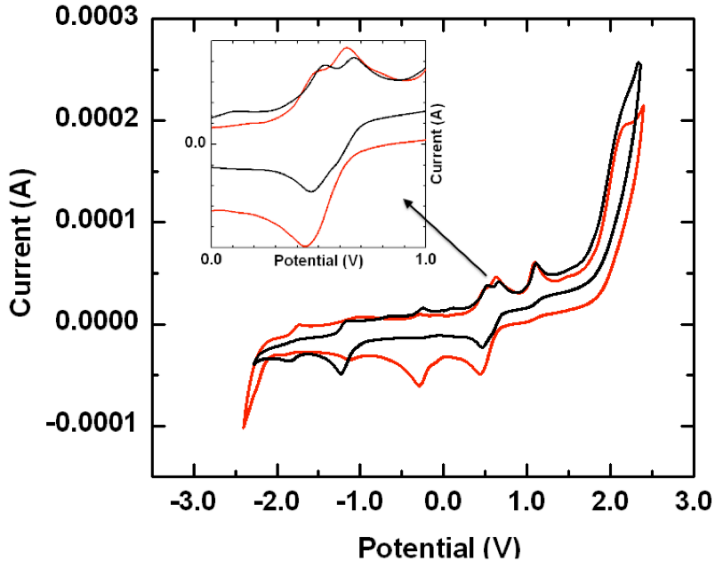


Table S1: Absorption wavelengths, energies, and solvatochromic shift comparisons

Compound	Absorption (nm)			Absorption (eV)			Solvatochromic Shift from Hex to MeCN (meV)	Solvatochromic Shift from Et_2O to MeCN (meV)
Name	Hex	Et_2O	MeCN	Hex	Et_2O	MeCN		
FODS	454	468	474	2.73	2.65	2.62	115	34
FOS	433	439	441	2.86	2.82	2.81	52	13
FODAAS	524	534	543	2.37	2.32	2.28	83	38
FOBDAA	554	564	586	2.24	2.20	2.12	122	83
FODAA	502	510	518	2.47	2.43	2.39	76	38
FODPA	479	485	496	2.59	2.56	2.50	89	57
FOCz	430	428	432	2.88	2.90	2.87	20	27
FOAA	N/A	498	505	N/A	2.49	2.46	N/A	80
FOBAA	N/A	560	568	N/A	2.21	2.18	N/A	38
FOBDAA36	N/A	463	474	N/A	2.68	2.62	N/A	62
FMDS	N/A	586	589	N/A	2.12	2.11	N/A	11
FMS	N/A	544	539	N/A	2.28	2.30	N/A	-21
FMDAAS	N/A	722	710	N/A	1.72	1.75	N/A	-29
FMBDAA	N/A	788	785	N/A	1.57	1.58	N/A	-6
FMDAA	677	684	672	1.83	1.81	1.85	-14	-32
FMDPA	627	634	635	1.98	1.96	1.95	25	3
FMCz	N/A	537	520	N/A	2.31	2.38	N/A	-75
FMAA	N/A	N/A	649	N/A	N/A	1.91	N/A	N/A
FMBAA	N/A	N/A	762	N/A	N/A	1.63	N/A	N/A
FMBDAA36	N/A	585	597	N/A	2.12	2.08	N/A	43

* Limited solubility

Table S2: TDDFT computational predictions of absorption bands for 2,7- versus 3,6- connectivity systems.

Name	Long Wavelength Band Position*
FOBDAA	1.98 eV (f = 0.090)
FMBDAA	1.19 eV (f = 0.035)
FOBDAA36	2.53 eV (f = 0.228)
FMBDAA36	2.01 eV (f = 0.244)

*B3LYP 6-31G(d,p) computations *in vacuo*, using Gaussian 09 (Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.)

Summary S1. Computational modeling summaries and frontier orbital plots

FOS B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p)

Orbital energies and kinetic energies (alpha):

		1	2
94	O	-0.269032	1.188251
95	O	-0.261376	2.264456
96	O	-0.241170	1.452447
97	O	-0.227404	1.580256
98	O	-0.205331	1.391744
99	V	-0.094828	1.544851
100	V	-0.070293	1.280347
101	V	-0.031157	1.331882
102	V	-0.015585	1.328796
103	V	-0.006759	0.382844

Total kinetic energy from orbitals= 2.049240095254D+03

1\1\GINC-SKYNET\SP\RB3LYP\6-31+G(d,p)\C24H20O4\GUEST\12-Dec-2012\0\\#p
B3LYP/6-31+G(d,p) SP guess=read geom=AllCheck Pop=Regular gfinput\\FO
PV\\0,1\C,0,2.5811946575,-0.9407333072,-0.4442674472\C,0,1.7789932076,
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9766004\PG=C01 [X(C24H20O4)]\\@

FMS B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p)

Orbital energies and kinetic energies (alpha):

		1	2
106	O	-0.278365	1.357804
107	O	-0.262828	1.317197
108	O	-0.246605	1.469021
109	O	-0.228729	1.582163
110	O	-0.209481	1.416970
111	V	-0.126824	1.405323
112	V	-0.078419	1.283328
113	V	-0.037778	1.328693
114	V	-0.028411	1.349128
115	V	-0.025018	1.615365

Total kinetic energy from orbitals= 1.363227350059D+03

1\1\GINC-SKYNET\SP\RB3LYP\6-31+G(d,p)\C27H20N2O3\GUEST\13-Dec-2012\0\\
#p B3LYP/6-31+G(d,p) SP guess=read geom=AllCheck Pop=Regular gfinput\\
BCN-FOPV\\0,1\C,0,2.5818892878,-0.929957541,-0.4524746926\C,0,1.792318
7856,0.1683872692,-0.0387493681\C,0,0.4065200881,0.0910426974,-0.10354
96585\C,0,-0.2282559659,-1.0844943848,-0.581075786\C,0,0.5331325503,-2
.1711733356,-0.987155666\C,0,1.9255151302,-2.0850473668,-0.9190642664\
C,0,-1.6791624712,-0.8834580861,-0.5385929018\C,0,-2.7205422155,-1.729
9389031,-0.898355713\C,0,-4.0372550414,-1.2773887547,-0.7544290144\C,0
,-4.3015059893,0.0009607771,-0.2584710759\C,0,-3.2583118492,0.85919661
61,0.1060759246\C,0,-1.9407601036,0.4166248853,-0.033924797\C,0,-0.646
2457037,1.0702246155,0.2561127167\C,0,-0.4563109359,2.3354421892,0.759
6166111\H,0,2.2782811767,1.0609175356,0.328529039\H,0,0.0618519831,-3.
0782346936,-1.3536849275\H,0,2.5251724496,-2.9336551371,-1.2370145225\
H,0,-2.5212110281,-2.724862919,-1.2847918885\H,0,-4.8613528627,-1.9278
938407,-1.031804175\H,0,-3.4882966699,1.8453236811,0.4878187337\C,0,4.
0443157452,-0.9130563707,-0.4136329238\C,0,4.8318481644,0.1169043234,-
0.0372518101\C,0,6.2944188476,0.1422345117,0.0003795906\H,0,4.51067780
14,-1.843626785,-0.7312972491\H,0,4.3657720794,1.0488720173,0.27658116
97\C,0,6.9247361477,1.3102125837,0.4357387333\C,0,7.0941272357,-0.9572
373069,-0.3776104136\C,0,8.479209132,-0.8647009442,-0.3232390445\C,0,9
.1184006139,0.3183564603,0.1307159471\C,0,8.3208710716,1.4107074177,0.
5089509646\H,0,6.3445543881,2.1757934749,0.7377107812\H,0,6.6289393832
,-1.8684114816,-0.7283044642\O,0,8.7877260838,2.6309733709,0.900759098
3\C,0,10.0073161414,2.7515501523,1.6317083379\H,0,10.062359823,2.01181
46001,2.4396524484\H,0,9.9840185469,3.7518933489,2.0697496413\H,0,10.8
811519474,2.6483593523,0.9861796371\O,0,10.486371215,0.4397681356,0.08
97892256\C,0,11.2375013082,-0.4073198842,0.9674528046\H,0,10.968467581
3,-0.2237278071,2.0156366616\H,0,12.2857539671,-0.1432727628,0.8140593
964\H,0,11.0856258223,-1.4622683763,0.7304482999\O,0,9.3295136016,-1.8
617600408,-0.7151887896\C,0,8.7705305305,-3.0511598749,-1.250398494\H,
0,8.1484043292,-3.5752611461,-0.5136479731\H,0,9.6168321988,-3.6841564
699,-1.5207475858\H,0,8.1713646758,-2.8461515901,-2.1461598029\C,0,0.8
371221097,2.8930859964,1.0120710144\C,0,-1.5325363547,3.2213657537,1.0
82441504\N,0,1.8770978336,3.370648867,1.2270154866\N,0,-2.3863642082,3
.9646390193,1.3548305552\H,0,-5.3276883779,0.3378161511,-0.152677319\\
Version=EM64L-G09RevB.01\State=1-A\HF=-1376.0804422\RMSD=6.783e-09\Dip
ole=0.4257473,-3.2516472,-0.5506226\Quadrupole=15.8495942,-8.0417716,-
7.8078226,10.6067289,15.0296887,2.6686984\PG=C01 [X(C27H20N2O3)]\\@

FODS B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p)

Orbital energies and kinetic energies (alpha):

		1	2
145	O	-0.240806	1.544313
146	O	-0.229636	1.529886
147	O	-0.227627	1.578369
148	O	-0.213344	1.479027
149	O	-0.197718	1.394769
150	V	-0.095438	1.535714
151	V	-0.076517	1.283523
152	V	-0.054169	1.348705
153	V	-0.019587	1.341351
154	V	-0.015072	1.317808

Total kinetic energy from orbitals= 1.862218134843D+03

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Wed Dec 12 14:10:30 2012, MaxMem= 268435456 cpu: 15.1

(Enter /usr/exe/g09/l9999.exe)

1\1\GINC-SKYNET\SP\RB3LYP\6-31+G(d,p)\C35H32O7\GUEST\12-Dec-2012\0\\#p
B3LYP/6-31+G(d,p) SP guess=read geom=AllCheck Pop=Regular gfinput\\OF
OPV\\0,1\C,0,2.5905785327,-0.8867359938,-0.3923263374\C,0,1.8104457349
,0.2276159537,-0.0002035435\C,0,0.4342582712,0.1339294353,-0.035084416
1\C,0,-0.2344291211,-1.0393179366,-0.4513337315\C,0,0.5162531724,-2.14
3187919,-0.8406709719\C,0,1.9113310726,-2.0517906359,-0.8058824241\C,0
,-1.689307317,-0.8061189635,-0.3732291496\C,0,-2.7834429972,-1.6143361
196,-0.6621429048\C,0,-4.0687229589,-1.0930251646,-0.4828912612\C,0,-4
.3034402125,0.2191394198,-0.0212553944\C,0,-3.1778308501,1.0273889103,
0.2683156514\C,0,-1.911266527,0.5100212811,0.0905286354\C,0,-0.5862192
37,1.1712633199,0.3282602854\O,0,-0.3836940448,2.3038188511,0.72922290

08\H,0,2.268504457,1.1559917128,0.3257487063\H,0,0.0415799286,-3.06381
31559,-1.1676889784\H,0,2.5014387979,-2.9127217208,-1.1096660275\H,0,-
2.6567406167,-2.6318416162,-1.0205255481\H,0,-4.9263423374,-1.72197411
2,-0.7078032558\H,0,-3.2860658313,2.0459267073,0.6271945117\C,0,4.0530
345977,-0.8874663039,-0.3913830489\C,0,4.8620118534,0.1237397458,-0.01
09242254\C,0,6.3255560144,0.1360331958,-0.0141475672\H,0,4.5014531221,
-1.8176422296,-0.7355198886\H,0,4.4113224737,1.0466145541,0.34813639\C
,0,6.9810831411,1.253711301,0.5076877381\C,0,7.1036220646,-0.928705667
2,-0.5161464834\C,0,8.4909420941,-0.8535616643,-0.4918874603\C,0,9.154
9297693,0.2757428696,0.0531089764\C,0,8.3794128569,1.3344265819,0.5524
850246\H,0,6.4192276089,2.0926182056,0.9046830723\H,0,6.6180823281,-1.
7949501254,-0.9449493451\O,0,8.8724323432,2.509268073,1.0422590505\C,0
,10.1029483585,2.5419135609,1.7637638278\H,0,10.1563079318,1.728127984
3,2.4972771193\H,0,10.1025660998,3.49655823,2.294852716\H,0,10.9668358
798,2.4869105774,1.0991725763\O,0,10.5229298909,0.3908815394,-0.015065
2035\C,0,11.2879850477,-0.5417106359,0.757223562\H,0,11.0454339894,-0.
4601197983,1.8246682581\H,0,12.3345131711,-0.2700831706,0.6048413891\H
,0,11.1221182638,-1.5677601135,0.4225194722\O,0,9.319392615,-1.8150179
83,-1.0021093509\C,0,8.7331633861,-2.9427015546,-1.6331565334\H,0,8.12
59075709,-3.530418869,-0.9329568795\H,0,9.5648678171,-3.553429447,-1.9
871600046\H,0,8.1116772853,-2.6473161942,-2.487422823\C,0,-5.684372661
7,0.6746281176,0.1331695862\C,0,-6.0919292482,1.8885135198,0.560336410
5\C,0,-7.4689944998,2.3597765571,0.7185049829\H,0,-6.434372427,-0.0684
948971,-0.1307675703\H,0,-5.3366088055,2.6242150056,0.8295557052\C,0,-
7.6648081667,3.6555202812,1.2260351881\C,0,-8.589011579,1.5768033454,0
.3837478223\C,0,-9.8769767704,2.0821642049,0.5622799615\H,0,-8.4498432
034,0.5822398124,-0.0184228224\C,0,-10.0726122585,3.3760668624,1.08453
10948\C,0,-8.9549364129,4.1652955443,1.4030701114\H,0,-6.7986652423,4.
2561004741,1.4762304649\O,0,-11.3365130807,3.8439080971,1.3282878987\C
,0,-11.9722218964,4.4583378652,0.205549571\H,0,-11.4058432268,5.331974
1288,-0.1388255595\H,0,-12.9573558022,4.7806792797,0.5491986295\H,0,-1
2.0914915131,3.747057652,-0.6197788473\O,0,-9.237759405,5.4121559243,1
.8760715584\C,0,-8.1527733374,6.2473546915,2.2483564101\H,0,-7.5553433
145,5.8006737242,3.0530979845\H,0,-8.5998034902,7.1756544399,2.6067395
488\H,0,-7.4974158962,6.468281467,1.395979382\O,0,-11.0234920118,1.406
3776354,0.2603328752\C,0,-10.909316827,0.082957149,-0.2364914629\H,0,-
10.370455244,0.0518437147,-1.1924212649\H,0,-11.9306768007,-0.26866922
82,-0.3890977804\H,0,-10.4043723698,-0.576060284,0.4811130162\\Version
=EM64L-G09RevB.01\State=1-A\HF=-1879.5775345\RMSD=9.877e-09\Dipole=0.6
663158,-2.0612989,-0.6398952\Quadrupole=5.9542771,10.0790867,-16.03336
37,-11.8935151,22.2753635,9.3331154\PG=C01 [X(C35H32O7)]\\@

FMDS B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p)

Orbital energies and kinetic energies (alpha):

		1	2
157	O	-0.244229	1.548995
158	O	-0.230182	1.531244
159	O	-0.228437	1.580482
160	O	-0.215588	1.495518
161	O	-0.201313	1.415026
162	V	-0.126052	1.407402
163	V	-0.084737	1.280479
164	V	-0.057608	1.348489
165	V	-0.026733	1.340654
166	V	-0.025807	1.410134

Total kinetic energy from orbitals= 2.009332346831D+03

Leave Link 601 at Thu Dec 13 16:02:00 2012, MaxMem= 268435456 cpu: 8.3
(Enter /usr/exe/g09/l9999.exe)
1\1\GINC-SKYNET\SP\RB3LYP\6-31+G(d,p)\C38H32N2O6\GUEST\13-Dec-2012\0\\
#p B3LYP/6-31+G(d,p) SP guess=read geom=AllCheck Pop=Regular gfinput\\
BCN-OFOPV\\0,1\C,0,2.583907083,-0.8676921573,-0.414172359\C,0,1.824476
5942,0.2484802723,0.0073776429\C,0,0.4362393374,0.1970887347,-0.025385
1882\C,0,-0.2333754864,-0.9704842713,-0.4796752086\C,0,0.5001630658,-2
.0742235344,-0.8949562087\C,0,1.8944649237,-2.0131462817,-0.8580303461
\C,0,-1.6749724379,-0.7417280796,-0.4057475912\C,0,-2.7520859535,-1.55
6929336,-0.7288527928\C,0,-4.0482375787,-1.0681032394,-0.5534204954\C,

0,-4.3009933582,0.2265128561,-0.0589989097\C,0,-3.1947013426,1.0456588
959,0.2653159905\C,0,-1.9014578016,0.5680587283,0.0946378514\C,0,-0.58
67997688,1.1995960669,0.3503095113\C,0,-0.3616216114,2.4649348373,0.84
01033149\H,0,2.3347329279,1.1355596548,0.3546332699\H,0,0.0039600326,-
2.9747149107,-1.2444104796\H,0,2.4711099212,-2.8751834814,-1.182624714
1\H,0,-2.5967442906,-2.560845032,-1.112596524\H,0,-4.8927836969,-1.703
999199,-0.8051215174\H,0,-3.367091276,2.0421975765,0.6454547164\C,0,4.
0465547837,-0.8806578376,-0.4070922478\C,0,4.8642626925,0.1281527979,-
0.0376998728\C,0,6.3275261325,0.1223961315,-0.0318384443\H,0,4.4861268
242,-1.8184269012,-0.7411190099\H,0,4.4255211395,1.0649268074,0.299878
6482\C,0,6.9911492315,1.2592783308,0.435648867\C,0,7.0963290266,-0.976
7753649,-0.4702530704\C,0,8.4840295513,-0.9153863733,-0.4402013892\C,0
,9.1567364562,0.2344880823,0.0486560045\C,0,8.3900938683,1.3270236254,
0.4855649196\H,0,6.4354176402,2.1238221014,0.7831641566\H,0,6.60455460
6,-1.8616601584,-0.8512159449\O,0,8.8934651928,2.5201235138,0.91491577
56\C,0,10.1180379439,2.5781681891,1.6451458736\H,0,10.1552115008,1.804
9037058,2.4221649343\H,0,10.1237742969,3.5601383457,2.1235737882\H,0,1
0.9868770172,2.4775834065,0.9924569443\O,0,10.5258441466,0.3310604331,
-0.0143526361\C,0,11.276508393,-0.5689356253,0.8093970185\H,0,11.02432
43353,-0.434210751,1.8691036722\H,0,12.3263076235,-0.3120433381,0.6543
805303\H,0,11.1061067347,-1.6086318773,0.5226727515\O,0,9.3051134905,-
1.9122403497,-0.8909736967\C,0,8.7106373556,-3.0658074326,-1.464603956
4\H,0,8.0923923695,-3.6084213605,-0.7380448532\H,0,9.5377513441,-3.703
6202179,-1.7793927325\H,0,8.0980135622,-2.8100201854,-2.3378950366\C,0
,-5.6861343719,0.6689962496,0.0988109782\C,0,-6.1019278183,1.868194278
,0.559523281\C,0,-7.4811546484,2.3285437063,0.7247200657\H,0,-6.429248
0467,-0.070638124,-0.1923284061\H,0,-5.3542142846,2.6018154804,0.85450
35956\C,0,-7.6801602729,3.6137739799,1.2570231442\C,0,-8.5976212236,1.
5470908819,0.3746096591\C,0,-9.8871569679,2.0450437346,0.5618262934\H,
0,-8.4547590697,0.5602302993,-0.0449905084\C,0,-10.086596201,3.3281256
864,1.1093632068\C,0,-8.9719473011,4.1157163832,1.4435019139\H,0,-6.81
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617981719\C,0,-11.9811608986,4.4419533807,0.259348961\H,0,-11.41356499
97,5.3287458128,-0.0468195739\H,0,-12.9690288138,4.7494868386,0.608517
2944\H,0,-12.0938114783,3.7628465481,-0.5936506422\O,0,-9.2590258022,5
.3514989028,1.9399580556\C,0,-8.1758699451,6.183592713,2.3286576771\H,
0,-7.5777926176,5.7234048988,3.1249179899\H,0,-8.6264462556,7.10332897
31,2.7040014357\H,0,-7.5210539706,6.4218227452,1.480901927\O,0,-11.031
6011952,1.3722247995,0.2463796883\C,0,-10.913434876,0.0597050927,-0.27
72596468\H,0,-10.3732481542,0.0495949419,-1.2329505017\H,0,-11.9336615
308,-0.2913543422,-0.4384534062\H,0,-10.407785747,-0.6127610945,0.4273
415686\C,0,0.9470296129,2.9996398928,1.061156767\C,0,-1.4138625035,3.3
736490975,1.1790442434\N,0,1.9997643378,3.4595168553,1.2512207991\N,0,
-2.2504991693,4.1324230012,1.4624428008\\Version=EM64L-G09RevB.01\Stat
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124953\Quadrupole=6.4648275,7.6866018,-14.1514293,-13.1863291,22.92292
31,7.1023542\PG=C01 [X(C38H32N2O6)]\\@

FODPA, B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p)

Orbital energies and kinetic energies (alpha):

		1	2
87	O	-0.263639	1.162808
88	O	-0.261121	1.336088
89	O	-0.260068	2.034858
90	O	-0.245994	1.226376
91	O	-0.196497	1.509265
92	V	-0.093098	1.551524
93	V	-0.052237	1.257001
94	V	-0.031444	1.222428
95	V	-0.030243	1.233096
96	V	-0.012501	1.284106

Total kinetic energy from orbitals= 1.082573789074D+03

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Wed Dec 12 08:09:27 2012, MaxMem= 268435456 cpu: 3.4

(Enter /usr/exe/g09/l9999.exe)

1\1\GINC-SKYNET\SP\RB3LYP\6-31+G(d,p)\C25H17N1O1\GUEST\12-Dec-2012\0\\

#p B3LYP/6-31+G(d,p) SP guess=read geom=AllCheck Pop=Regular gfinput\\
DPAFO\\0,1\C,0,3.426564805,-0.3725660332,0.0379290093\C,0,2.4688797634
,0.650064228,0.043094769\C,0,1.1297188247,0.2969128913,-0.0205033092\C
,0,0.717807621,-1.0511184245,-0.0877422768\C,0,1.6703110834,-2.0646421
924,-0.0911218569\C,0,3.0261988103,-1.7101564162,-0.0282393342\C,0,-0.
7608824718,-1.0887943755,-0.1408836308\C,0,-1.6686790378,-2.1396900835
,-0.2100817771\C,0,-3.0377118989,-1.8561844125,-0.251511175\C,0,-3.521
5952787,-0.5345626764,-0.2048190263\C,0,-2.5968472906,0.5295331948,-0.
12920326\C,0,-1.2470435983,0.2335776805,-0.1069285445\C,0,-0.082011001
2,1.1778537875,-0.0278830832\O,0,-0.1167962045,2.3948081841,0.01837995
09\N,0,-4.9122701002,-0.2763388177,-0.2315777809\C,0,-5.8193486744,-1.
1427123003,0.4425409606\C,0,-7.0128920394,-1.5410362732,-0.1789466325\
C,0,-7.9076839565,-2.3747556384,0.4889579141\C,0,-7.6214136735,-2.8387
509,1.7742039189\C,0,-6.430268254,-2.4507613355,2.3911078162\C,0,-5.53
7954773,-1.6024613105,1.7388356505\C,0,-5.4179196194,0.8487112711,-0.9
44286231\C,0,-4.9305637097,1.1620954462,-2.2225345028\C,0,-5.426668460
5,2.2677363489,-2.9105401398\C,0,-6.4262911134,3.063438006,-2.34810055
58\C,0,-6.9201047445,2.7467747048,-1.08099542\C,0,-6.4167751842,1.6549
270234,-0.3771091507\H,0,2.7540960227,1.6965979145,0.0950197917\H,0,1.
3813163296,-3.1104685368,-0.1406896269\H,0,3.7797665939,-2.492629381,-
0.0309717338\H,0,-1.3361663589,-3.1731790801,-0.2477069684\H,0,-3.7497
559269,-2.6713131388,-0.3199578079\H,0,-2.9319229295,1.5602876329,-0.0
864397921\H,0,-7.2327966043,-1.1916075593,-1.182095425\H,0,-8.82762585
43,-2.6729912642,-0.0056060253\H,0,-6.1985495023,-2.7966925115,3.39435
86284\H,0,-4.6213087592,-1.2903201794,2.2281038296\H,0,-4.1649970744,0
.5374426,-2.6706967874\H,0,-5.0374157379,2.4984043599,-3.8979196848\H,
0,-7.6925212075,3.3615660905,-0.6280670116\H,0,-6.7924728835,1.4199044
927,0.6130442055\H,0,-6.8148911934,3.9200812769,-2.8898630482\H,0,-8.3
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O1)]\\@

FMDPA, B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p)

Orbital energies and kinetic energies (alpha):

		1	2
99	O	-0.268928	1.143285
100	O	-0.263959	1.137534
101	O	-0.259981	1.296703
102	O	-0.253455	1.218225
103	O	-0.201949	1.512940
104	V	-0.125138	1.407491
105	V	-0.060737	1.279106
106	V	-0.037295	1.203050
107	V	-0.033118	1.279461
108	V	-0.022986	1.618536

Total kinetic energy from orbitals= 1.229687230536D+03
No NMR shielding tensors so no spin-rotation constants.
Leave Link 601 at Thu Dec 13 14:03:19 2012, MaxMem= 268435456 cpu: 3.7
(Enter /usr/exe/g09/l9999.exe)
1\1\GINC-SKYNET\SP\RB3LYP\6-31+G(d,p)\C28H17N3\GUEST\13-Dec-2012\0\\#p
 B3LYP/6-31+G(d,p) SP guess=read geom=AllCheck Pop=Regular gfinput\\BC
N-DPAFO\\0,1\C,0,3.4250359603,-0.4162702575,0.0164890923\C,0,2.5001556
779,0.6337329702,0.0250625871\C,0,1.1368724529,0.3329382394,-0.0236412
507\C,0,0.7098174365,-1.0190850886,-0.0792506454\C,0,1.6342032394,-2.0
563485916,-0.0856805148\C,0,2.9982054608,-1.7445371597,-0.0379516643\C
,0,-0.754437059,-1.0440498927,-0.1199754224\C,0,-1.6509777742,-2.10305
69732,-0.1752533052\C,0,-3.0213257808,-1.8422886939,-0.2155685036\C,0,
-3.5112126867,-0.5237630624,-0.1837155393\C,0,-2.5997686297,0.55294506
41,-0.116431002\C,0,-1.2332976297,0.2889882756,-0.0927882694\C,0,-0.06
30714425,1.1974545155,-0.025942918\C,0,-0.0877374421,2.570941582,0.025
4258754\N,0,-4.8993918861,-0.2716506546,-0.2166058194\C,0,-5.809809173
3,-1.1476397329,0.4413441441\C,0,-6.9941922253,-1.5467386539,-0.196461
5379\C,0,-7.8918559032,-2.3895319741,0.4561553413\C,0,-7.6176452244,-2
.8603581212,1.741465896\C,0,-6.4363915583,-2.4693718223,2.3753686015\C

,0,-5.541471344,-1.6121980218,1.7385460441\C,0,-5.4084986546,0.8527128
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1.6800519592,-0.3502773667\H,0,2.8548460405,1.6551571718,0.0682700585\
H,0,1.3090675734,-3.0915526145,-0.1268588598\H,0,3.7315641281,-2.54551
97868,-0.0432722477\H,0,-1.2996038506,-3.1302435231,-0.2045851794\H,0,
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61,-0.0802269623\H,0,-7.2047745701,-1.1910488376,-1.1994010816\H,0,-8.
8048653134,-2.6889264012,-0.0503055155\H,0,-6.2153956722,-2.819020738,
3.3796845525\H,0,-4.6342507155,-1.2951808771,2.2421347807\H,0,-4.20957
1681,0.49097951,-2.6876493821\H,0,-5.0858348583,2.4498374726,-3.921733
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0843516129\N,0,2.0372866404,4.0568440402,0.1325267627\H,0,-6.809128168
2,3.9138777787,-2.8840186298\H,0,-8.3165554388,-3.521637906,2.24403785
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419,-0.1582454\Quadrupole=7.292569,-9.6234107,2.3308417,-14.2718065,-0
.6962745,-4.5240456\PG=C01 [X(C28H17N3)]\\@

FOCz B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p)

Orbital energies and kinetic energies (alpha):

		1	2
86	O	-0.269505	2.266406
87	O	-0.262679	1.134234
88	O	-0.249457	1.227599
89	O	-0.224486	1.206464
90	O	-0.209926	1.430888
91	V	-0.102695	1.558516
92	V	-0.061230	1.278618
93	V	-0.042801	1.249863
94	V	-0.025005	1.348357
95	V	-0.010077	1.297767

Total kinetic energy from orbitals= 1.081463020289D+03
No NMR shielding tensors so no spin-rotation constants.
Leave Link 601 at Tue Dec 11 18:52:09 2012, MaxMem= 268435456 cpu: 4.0
(Enter /usr/exe/g09/l9999.exe)
1\1\GINC-SKYNET\SP\RB3LYP\6-31+G(d,p)\C25H15N1O1\GUEST\11-Dec-2012\0\\
#p B3LYP/6-31+G(d,p) SP guess=read geom=AllCheck Pop=Regular gfinput\\
CzFO\\0,1\C,0,3.578628911,-0.3457310158,0.129088789\C,0,2.6154727514,0
.6678863615,0.2156158006\C,0,1.2789943521,0.3140571234,0.1082017191\C,
0,0.8784359196,-1.0245915779,-0.0818273141\C,0,1.8353508194,-2.0293543
799,-0.1667352953\C,0,3.1884342202,-1.6745572529,-0.0597308698\C,0,-0.
6014397601,-1.0676920455,-0.1532236903\C,0,-1.4927416331,-2.1210237819
,-0.3235826983\C,0,-2.865061065,-1.8455907218,-0.3575321401\C,0,-3.351
4235704,-0.5385691066,-0.1998344966\C,0,-2.4506569632,0.5264954206,-0.
0184152425\C,0,-1.096060182,0.2435901361,-0.0088790966\C,0,0.061567135
2,1.1849036939,0.1645301044\O,0,0.0148013263,2.3922057929,0.3153713715
\N,0,-4.747512418,-0.2957049451,-0.2232527391\C,0,-5.707565423,-0.9398
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.1155460282,-0.9065986605,0.9245604864\C,0,-7.9530529214,-1.8798941129
,1.9058534243\C,0,-6.6743316313,-2.3678822861,2.2228633828\C,0,-5.5363
837035,-1.906020465,1.5648424344\C,0,-5.4044465589,0.6280234578,-1.048
6334731\C,0,-4.8793562522,1.4748802684,-2.0283153709\C,0,-5.7697241633
,2.2870744712,-2.7272690155\C,0,-7.1498948691,2.2562994412,-2.46631414
35\C,0,-7.668371585,1.3999350215,-1.4997652142\C,0,-6.7958087908,0.573
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,-0.1247724673\H,0,-1.1456022357,-3.1427107808,-0.445580832\H,0,-3.574
5891627,-2.6502749272,-0.518461128\H,0,-2.8060797601,1.5418244486,0.12
27129719\H,0,-9.1032974609,-0.5213019481,0.6884458886\H,0,-6.566327615
4,-3.1194431199,2.9993185599\H,0,-4.5526396989,-2.280851419,1.82462414
5\H,0,-3.8172083131,1.5002491479,-2.2445902081\H,0,-5.3847524298,2.956
0733787,-3.4910962087\H,0,-8.7367104567,1.3692069114,-1.3058986614\H,0

,-7.8160430079,2.9040286829,-3.0276901967\H,0,-8.8195620921,-2.2626965
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47051,-1.4271126,-0.1758708\Quadrupole=11.5762435,-4.6351084,-6.941135
1,-8.9488464,-1.0070062,-4.6463785\PG=C01 [X(C25H15N1O1)]\\@

FMCz B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p)

Orbital energies and kinetic energies (alpha):

		1	2
98	O	-0.269994	1.308517
99	O	-0.264833	1.146145
100	O	-0.257716	1.229223
101	O	-0.226696	1.207220
102	O	-0.213612	1.428634
103	V	-0.134145	1.409208
104	V	-0.070511	1.295309
105	V	-0.045017	1.251855
106	V	-0.037496	1.366273
107	V	-0.029909	1.626043

Total kinetic energy from orbitals= 1.228574408875D+03
No NMR shielding tensors so no spin-rotation constants.
Leave Link 601 at Thu Dec 13 12:18:22 2012, MaxMem= 268435456 cpu: 3.5
(Enter /usr/exe/g09/l9999.exe)
1\1\GINC-SKYNET\SP\RB3LYP\6-31+G(d,p)\C28H15N3\GUEST\13-Dec-2012\0\\#p
 B3LYP/6-31+G(d,p) SP guess=read geom=AllCheck Pop=Regular gfinput\\BC
N-CzFO\\0,1\C,0,3.5565370663,-0.4180727567,0.0829852242\C,0,2.63076216
07,0.6292115294,0.1468334671\C,0,1.2691495591,0.3313851604,0.052434188
\C,0,0.8477318708,-1.013175968,-0.1038907072\C,0,1.7717953529,-2.04775
34863,-0.1666741211\C,0,3.1344085407,-1.7397182594,-0.0720665117\C,0,-
0.617982187,-1.0378226627,-0.1690363587\C,0,-1.5029867428,-2.098577310
4,-0.3096885704\C,0,-2.8753323723,-1.8398046803,-0.3452987715\C,0,-3.3
615655715,-0.5310409596,-0.2151768092\C,0,-2.4696656224,0.5453685209,-
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1826,1.1934488927,0.0820052273\C,0,0.037931886,2.5620102636,0.19931230
61\N,0,-4.756384144,-0.292126867,-0.2329252655\C,0,-5.7083335283,-0.93
83923188,0.5701646703\C,0,-6.9956782153,-0.4441485177,0.2424557179\C,0
,-8.1154598493,-0.928381083,0.927764963\C,0,-7.9400848648,-1.883205511
6,1.9249884045\C,0,-6.6555697173,-2.3504123659,2.2484010752\C,0,-5.524
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725195276\C,0,-4.9151294583,1.4515796303,-2.0644099691\C,0,-5.81776108
46,2.2402069706,-2.7744839177\C,0,-7.1969708627,2.1916833427,-2.512988
1668\C,0,-7.7020565928,1.3422946018,-1.5334622263\C,0,-6.8165789339,0.
540095692,-0.8049579387\H,0,2.9832209807,1.6450828948,0.268045849\H,0,
1.4490170588,-3.0774893637,-0.2863409447\H,0,3.8693288198,-2.537609632
9,-0.1195112015\H,0,-1.1423470066,-3.1179265048,-0.4073409829\H,0,-3.5
805024668,-2.6521239042,-0.4830323543\H,0,-2.8709028586,1.5425073474,0
.0599534591\H,0,-9.107870392,-0.5581951092,0.6874130116\H,0,-6.5372965
801,-3.0870125797,3.037516363\H,0,-4.5359097485,-2.2431076029,1.847924
8324\H,0,-3.8536730905,1.4941535905,-2.2802029746\H,0,-5.4425310281,2.
9060231129,-3.5456495595\H,0,-8.7695916729,1.2986867121,-1.337987948\H
,0,-7.8727882842,2.8218388651,-3.0826012419\H,0,-8.8012972064,-2.26704
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=9.6668459,-8.6397409,-1.027105,-15.5148239,-1.5275768,-5.8400055\PG=C
01 [X(C28H15N3)]\\@

FODAA B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p)

Orbital energies and kinetic energies (alpha):

		1	2
103	O	-0.261949	1.141951
104	O	-0.255955	2.254966
105	O	-0.238184	1.577148

```
 106         O                -0.234238          1.358653
 107         O                -0.185005          1.620181
 108         V                -0.088231          1.555205
 109         V                -0.046648          1.256095
 110         V                -0.028853          1.199823
 111         V                -0.018207          1.367279
 112         V                -0.012544          1.338129
 Total kinetic energy from orbitals= 1.309628045907D+03
 No NMR shielding tensors so no spin-rotation constants.
 Leave Link  601 at Tue Dec 11 19:57:35 2012, MaxMem=  268435456 cpu:       4.9
 (Enter /usr/exe/g09/l9999.exe)
 1\1\GINC-SKYNET\SP\RB3LYP\6-31+G(d,p)\C27H21N1O3\GUEST\11-Dec-2012\0\\
 #p B3LYP/6-31+G(d,p) SP guess=read geom=AllCheck Pop=Regular gfinput\\
 DAAFO-neutral\\0,1\C,0,5.6367323131,-1.3857181084,-1.9647691054\C,0,6.
 5679394482,-2.2015382415,-2.5908246847\C,0,7.7200417384,-2.6199634589,
 -1.9071899505\O,0,8.5777061038,-3.4110865301,-2.6172839352\C,0,9.75975
 06282,-3.8603018681,-1.9754221527\C,0,7.9170773925,-2.2134423612,-0.58
 2964594\C,0,6.9637644212,-1.410037406,0.0472151348\C,0,5.8176775446,-0
 .9826560636,-0.629903458\N,0,4.8650193322,-0.1356764932,0.011604096\C,
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 5,1.300046916,2.0100879614\C,0,5.3600926047,2.4314476049,2.6904389249\
 C,0,6.286076855,3.2853838066,2.0811099895\O,0,6.8052646363,4.411149425
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 ,-3.0129190409,-1.8762211257,-0.1945458327\C,0,-3.4670139759,-0.555184
 7618,-0.1372734028\C,0,-2.54941179,0.5017704656,-0.068245851\C,0,-1.19
63899718,0.1993535,-0.0571264094\C,0,-0.0203969666,1.1248771037,0.0100
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 ,0,10.2911597145,-4.4636137883,-2.7137355068\H,0,9.532770516,-4.479782
 5111,-1.0973834755\H,0,10.3969062735,-3.020403253,-1.6675415213\H,0,8.
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 0775936296\H,0,6.6073274065,1.6755627559,-0.9018703532\H,0,7.452120458
 8,3.6696686721,0.3215817061\H,0,4.1963361067,0.6354678726,2.4958999465
 \H,0,4.9958294395,2.6245694542,3.6929013275\H,0,6.8830932502,5.6916405
 827,4.2055946382\H,0,6.6150376526,3.9953125381,4.6932554529\H,0,5.2778
 967033,4.9436178694,3.9756652278\H,0,2.8071159142,1.6212623244,0.05858
 41869\H,0,1.4136656542,-3.1718038299,-0.175422275\H,0,3.8018424781,-2.
 5795318929,-0.0958627141\H,0,-1.3125178595,-3.213618129,-0.2313486527\
 H,0,-3.735104997,-2.6869171237,-0.2482520376\H,0,-2.876716478,1.536958
 7461,-0.0237815504\H,0,-4.5338457943,-0.3503835495,-0.1465716421\\Vers
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```

FMDAA B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p)

```
Orbital energies and kinetic energies (alpha):
                             1                2
 115         O                -0.264170          1.126946
 116         O                -0.256688          1.315579
 117         O                -0.242278          1.449771
 118         O                -0.238289          1.510856
 119         O                -0.190190          1.626810
 120         V                -0.120922          1.408180
 121         V                -0.054385          1.293632
 122         V                -0.034940          1.192778
 123         V                -0.020720          1.498284
 124         V                -0.019397          1.454117
 Total kinetic energy from orbitals= 1.456765386101D+03
 No NMR shielding tensors so no spin-rotation constants.
 Leave Link  601 at Thu Dec 13 13:20:07 2012, MaxMem=  268435456 cpu:       4.8
```

(Enter /usr/exe/g09/l9999.exe)
1\1\GINC-SKYNET\SP\RB3LYP\6-31+G(d,p)\C30H21N3O2\GUEST\13-Dec-2012\0\\
#p B3LYP/6-31+G(d,p) SP guess=read geom=AllCheck Pop=Regular gfinput\\
BCN-DAAFO\\0,1\C,0,3.4421935307,-0.383295348,0.0026463179\C,0,2.510541
2374,0.6592576612,-0.0527656047\C,0,1.1486911026,0.348486993,-0.066344
675\C,0,0.7284171361,-1.0067624756,-0.0226924761\C,0,1.6602175793,-2.0
363643214,0.0343057123\C,0,3.0225309121,-1.7143185538,0.0459483218\C,0
,-0.7350883537,-1.0420039334,-0.0485225539\C,0,-1.6294346518,-2.104321
9832,-0.0218059564\C,0,-3.0008725128,-1.8541499945,-0.0702090796\C,0,-
3.4999676125,-0.5378439935,-0.1338969663\C,0,-2.5883241289,0.543658595
,-0.1489238246\C,0,-1.2215758277,0.2868438246,-0.1118799572\C,0,-0.056
2723431,1.2042020117,-0.1163109118\C,0,-0.0883666415,2.5784564175,-0.1
534864148\N,0,-4.8822331017,-0.290635967,-0.18508782\C,0,-5.8136633325
,-1.1738966467,0.4376118193\C,0,-6.9556493405,-1.6064625558,-0.2574834
417\C,0,-7.8809166949,-2.4417781648,0.3511746698\C,0,-7.6812579169,-2.
8844011346,1.6672955515\O,0,-8.645473737,-3.7112168751,2.1689713496\C,
0,-8.5010770716,-4.1784794216,3.5006699957\C,0,-6.543211698,-2.4662845
022,2.3665116027\C,0,-5.6280777033,-1.6072678824,1.7546308615\C,0,-5.3
861611987,0.8509872528,-0.8837027963\C,0,-5.0082983655,1.1006099289,-2
.2136438498\C,0,-5.4984609756,2.2070899564,-2.8909937369\C,0,-6.396941
6807,3.082424131,-2.2620773195\O,0,-6.8255465866,4.1339391854,-3.01724
44198\C,0,-7.6901920604,5.0846984351,-2.4146933166\C,0,-6.7929897743,2
.8318732162,-0.9430761138\C,0,-6.2790887957,1.727428686,-0.261997533\H
,0,2.8591921267,1.6832020673,-0.0852854739\H,0,1.3415579185,-3.0738719
193,0.0686389332\H,0,3.760656075,-2.5098851496,0.0889345883\H,0,-1.274
536262,-3.1300284422,0.0197696736\H,0,-3.6987539031,-2.6833962804,-0.0
645574907\H,0,-2.9770573735,1.5518840213,-0.1827945046\H,0,-7.11400468
22,-1.2747172778,-1.2782377881\H,0,-8.765812854,-2.7769244238,-0.17956
07712\H,0,-9.3687585716,-4.8106316375,3.694181945\H,0,-8.490030231,-3.
3510940718,4.2218289125\H,0,-7.5870446598,-4.7735366612,3.6251501142\H
,0,-6.3662402691,-2.7841080845,3.3870104368\H,0,-4.7575138572,-1.27218
08972,2.309226918\H,0,-4.3226266372,0.4215077427,-2.7103279923\H,0,-5.
2074465096,2.411484568,-3.9158039478\H,0,-7.8835837333,5.8406503913,-3
.1768983785\H,0,-7.222046748,5.5607177255,-1.5440749869\H,0,-8.6417161
566,4.6309680435,-2.1084932514\H,0,-7.4824636516,3.4926314077,-0.43204
71151\H,0,-6.5777542385,1.542988065,0.7648316806\C,0,-1.2984480005,3.3
415039183,-0.1822569164\N,0,-2.2578376675,4.0011518828,-0.2013040534\C
,0,1.0901189125,3.39030862,-0.1588144699\N,0,2.0280311883,4.0803825491
,-0.1646201731\H,0,4.5018803928,-0.1494986985,0.011566677\\Version=EM6
4L-G09RevB.01\State=1-A\HF=-1470.5633039\RMSD=3.698e-09\Dipole=-1.1912
314,-2.2888115,0.793832\Quadrupole=2.957423,-5.1761576,2.2187346,-22.5
696135,-4.8409444,-7.2317896\PG=C01 [X(C30H21N3O2)]\\@

FOAA B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p) [anti anisyl vs C=O]

Orbital energies and kinetic energies (alpha):

		1	2
75	O	-0.268035	1.130714
76	O	-0.265366	1.141196
77	O	-0.258229	2.259737
78	O	-0.236255	1.403352
79	O	-0.194902	1.537763
80	V	-0.089511	1.558648
81	V	-0.045066	1.267800
82	V	-0.025695	1.217503
83	V	-0.014749	1.252592
84	V	-0.009219	0.954676

1\1\GINC-SKYNET\SP\RB3LYP\6-31G(d,p)\C20H15N1O2\GUEST\03-Jul-2013\0\\#
p B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p) Pop=Regular gfinput\\FOAA-anti g
roundstate geom opt/energy\\0,1\C,-0.8918766774,3.3735383748,-0.043684
8317\C,0.2660077816,4.3224553671,-0.0259684864\C,1.4667150079,3.580666
2075,0.0182752647\C,1.1301269166,2.1401569618,0.0313801649\C,-0.272222
6947,2.0058315858,-0.007615297\C,1.9106712187,0.9911080901,0.076521919
\C,1.294369473,-0.2652698302,0.0782829041\C,-0.1082461389,-0.396155891
8,0.0218513404\C,-0.8982697335,0.7766841243,-0.018746054\C,0.261827222
6,5.7086672122,-0.0486817161\C,1.4924276114,6.3780713256,-0.02603253\C
,2.6853238659,5.6510178692,0.0177997042\C,2.6869368559,4.2482295099,0.

0401992894\N,-0.757550207,-1.6256108888,0.034488145\C,1.2571207897,-4.
4788311236,-1.2686085261\C,0.777093357,-3.1881290194,-1.0979228315\C,-
0.2138231021,-2.9136888183,-0.1375794338\C,-0.7187582369,-3.9780871023
,0.6169860343\C,0.7439892333,-5.5401193449,-0.5090681086\C,-0.25944374
88,-5.2835330211,0.4304567346\C,0.7959277166,-7.8771772106,-0.02196393
43\O,1.281586416,-6.7709837547,-0.7642353051\O,-2.0793741195,3.6460697
78,-0.0787832524\H,2.9947152043,1.0475148526,0.1232871599\H,1.90836632
39,-1.1555393807,0.1432518096\H,-1.9830935442,0.7178754909,-0.06277225
14\H,-0.6794027853,6.2493198077,-0.0834381284\H,1.5225488785,7.4631518
716,-0.0426423624\H,3.632838842,6.1823165879,0.0346561084\H,3.62664770
2,3.7045184889,0.0732917609\H,-1.730413992,-1.5955361526,0.2995168011\
H,2.0221208556,-4.693737728,-2.0074002343\H,1.1570787778,-2.3884485647
,-1.7238914599\H,-1.4822253638,-3.7854910392,1.3662149684\H,-0.6809697
153,-6.0803142469,1.0313489468\H,1.3524569681,-8.746268485,-0.37557257
85\H,-0.275908158,-8.0420773196,-0.1933337799\H,0.9702511989,-7.751434
5837,1.0546120458\\Version=EM64L-G09RevB.01\State=1-A\HF=-976.4205451\
RMSD=6.332e-09\Dipole=0.744507,-1.3803952,0.4268174\Quadrupole=-4.0526
902,12.3345334,-8.2818432,14.5407975,-2.3069924,-5.3335581\PG=C01 [X(C
20H15N1O2)]\\@

FOAA B3LYP B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p) [syn anisyl vs C=O]

Orbital energies and kinetic energies (alpha):

		1	2
75	O	-0.265940	1.132229
76	O	-0.264080	1.149220
77	O	-0.257108	2.257875
78	O	-0.234842	1.400878
79	O	-0.193439	1.544881
80	V	-0.089071	1.553128
81	V	-0.044348	1.282192
82	V	-0.023347	1.200496
83	V	-0.012719	0.848895
84	V	-0.011345	1.166437

1\1\GINC-SKYNET\SP\RB3LYP\6-31G(d,p)\C20H15N1O2\GUEST\03-Jul-2013\0\\#
p B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p) Pop=Regular gfinput\\FOAA-syn gr
oundstate geom opt/energy\\0,1\C,-0.6967513597,2.5553325424,0.49198734
48\C,-0.0567873459,3.8811746629,0.217104268\C,1.3032960153,3.675948399
,-0.1006883096\C,1.5864455312,2.2252906185,-0.040416131\C,0.4027338768
,1.5474231981,0.3088263275\C,2.7455363008,1.4844887335,-0.247972381\C,
2.6962694438,0.0951907665,-0.1191712473\C,1.5083547202,-0.583212062,0.
2298675943\C,0.3365569993,0.1742948599,0.4549417131\C,-0.6190627916,5.
1478722475,0.2457157697\C,0.1989061917,6.245823451,-0.0527389663\C,1.5
462515393,6.0509008576,-0.368701589\C,2.1130794748,4.7676692473,-0.395
9635921\N,1.5520432386,-1.9654228002,0.3687994239\C,-1.7134820101,-3.6
840331016,-0.1648643214\C,-0.6992948015,-2.7432294657,-0.2729193712\C,
0.4819299882,-2.8755607959,0.4794235613\C,0.6166248622,-3.990767251,1.
3131986191\C,-1.5695559113,-4.8000111407,0.6717845727\C,-0.3885583112,
-4.9555717565,1.4043312905\C,-2.5342351369,-6.8066546166,1.5350079986\
O,-2.6252526533,-5.6681696815,0.6950543141\O,-1.8566670622,2.337319518
,0.7953254551\H,3.6835110969,1.9631497848,-0.5150226326\H,3.5968203962
,-0.4882197851,-0.2956876467\H,-0.5938324726,-0.2939349622,0.754068337
6\H,-1.6689161856,5.2714339236,0.4946322193\H,-0.212055953,7.250583321
2,-0.0396171079\H,2.1696351478,6.9105599245,-0.5983810496\H,3.16303126
13,4.6408050966,-0.6438138098\H,2.4722994164,-2.3602448008,0.489562651
7\H,-2.6277352445,-3.582567331,-0.7400681626\H,-0.8152349931,-1.908986
6453,-0.9555565643\H,1.520479598,-4.107602391,1.9056089862\H,-0.242437
2211,-5.8074507806,2.0575324482\H,-3.4710746942,-7.351116876,1.4084589
473\H,-2.4213034245,-6.524996867,2.5900917001\H,-1.6982675266,-7.45805
80422,1.2479293394\\Version=EM64L-G09RevB.01\State=1-A\HF=-976.4201354
\RMSD=4.295e-09\Dipole=1.5588997,-0.9373354,0.0946321\Quadrupole=-4.57
27144,15.0337885,-10.461074,4.6900652,-0.8722312,-9.4754935\PG=C01 [X(
C20H15N1O2)]\\@

FMAA B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p) [anti anisyl vs CC(CN)2]

Orbital energies and kinetic energies (alpha):

		1	2
87	O	-0.277894	1.140376
88	O	-0.272763	1.116381
89	O	-0.260096	1.313681
90	O	-0.243338	1.418195
91	O	-0.202338	1.547140
92	V	-0.123706	1.410273
93	V	-0.054547	1.285014
94	V	-0.030292	1.229600
95	V	-0.026347	1.347130
96	V	-0.024419	1.523549

1\GINC-SKYNET\SP\RB3LYP\6-31G(d,p)\C23H15N3O1\LAHTI\02-Jul-2013\0\\#
p B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p) Pop=Regular Prop=EPR gfinput\\FM
AA-anti groundstate geom opt/energy\\0,1\C,12.8894412758,11.0280286613
,2.6187952033\C,14.1320749821,11.6541593419,2.1216854638\C,13.99120177
83,11.8729100245,0.7257448327\C,12.6721945976,11.3918722674,0.30845463
68\C,11.9994913677,10.8731209317,1.442161304\C,12.0449943713,11.378154
176,-0.9297793683\C,10.7584721436,10.8496994672,-1.0556360045\C,10.087
1623506,10.3134361921,0.0602353262\C,10.7256847252,10.3324455288,1.322
9539118\C,15.3102834187,12.0254100816,2.7739786771\C,16.3392359236,12.
6130293726,2.0300187569\C,16.1946715425,12.8265002251,0.6577301534\C,1
5.0181864214,12.4572570365,-0.0055407071\N,8.8061858197,9.784770981,-0
.0062982421\C,7.7786075141,8.5562359561,-3.3736258612\C,8.5790728425,8
.8644429733,-2.2829042127\C,8.0325936241,9.4928746671,-1.1495131956\C,
6.6617361128,9.7696141593,-1.1384761792\C,6.404661621,8.8373146258,-3.
3547726656\C,5.8455744482,9.4361479958,-2.2210973295\C,4.3167632897,8.
7538422035,-4.5111670721\O,5.7096588912,8.4867153531,-4.4770943927\C,1
2.6066139632,10.6695750262,3.9162622774\C,13.520638285,10.8570951623,5
.000856531\C,11.3658232185,10.077557494,4.3121117657\N,14.2411392971,1
0.9954502133,5.9050523365\N,10.3631069848,9.5974293467,4.6587440131\H,
12.538729934,11.7862547718,-1.8069782299\H,10.2649456467,10.8685481556
,-2.0194489957\H,10.2038246432,9.9163128296,2.1757773124\H,15.44371649
95,11.8689157436,3.8365319273\H,17.2576406873,12.9041011838,2.52937470
81\H,17.0042167541,13.284031376,0.0965896858\H,14.914879697,12.6258402
242,-1.073220532\H,8.3308363992,9.6898868016,0.8788899009\H,8.19602443
1,8.0731675883,-4.2508350493\H,9.6308080043,8.60049073,-2.2991982962\H
,6.2227077075,10.2561307728,-0.2715488102\H,4.7870909457,9.661112929,-
2.1710592761\H,3.9667761739,8.4068970518,-5.484297678\H,4.1076453094,9
.8270519089,-4.4143786854\H,3.780176287,8.2121014388,-3.7215014705\\Ve
rsion=EM64L-G09RevB.01\State=1-A\HF=-1124.9795129\RMSD=4.075e-09\Dipol
e=-0.8695564,0.5489629,-2.6604161\Quadrupole=24.222322,-2.2162769,-22.
0060451,5.3089852,-2.1021499,0.762119\PG=C01 [X(C23H15N3O1)]\\@

FMAA B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p) [syn anisyl vs CC(CN)2]

Orbital energies and kinetic energies (alpha):

		1	2
87	O	-0.277232	1.140351
88	O	-0.265401	1.121433
89	O	-0.258917	1.315012
90	O	-0.239628	1.417442
91	O	-0.199024	1.557819
92	V	-0.122601	1.405412
93	V	-0.053014	1.299777
94	V	-0.025918	1.291792
95	V	-0.024113	1.351843
96	V	-0.020758	1.423379

Total kinetic energy from orbitals= 1.114369788652D+03

1\1\GINC-SKYNET\SP\RB3LYP\6-31G(d,p)\C23H15N3O1\LAHTI\02-Jul-2013\0\\#
p B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p) Pop=Regular Prop=EPR gfinput geo
m=check\\FMAA-syn groundstate geom opt/energy start nonplanar\\0,1\C,2
.25092,0.786145,-0.069386\C,3.661669,0.34366,-0.077336\C,3.680839,-1.0
73077,0.009307\C,2.298841,-1.555785,0.050198\C,1.424468,-0.445122,-0.0
11921\C,1.775437,-2.841421,0.118354\C,0.394565,-3.018722,0.131587\C,-0

.49048,-1.92209,0.055219\C,0.042329,-0.615263,-0.026095\C,4.860329,1.0
57589,-0.142057\C,6.069551,0.353441,-0.118513\C,6.081992,-1.039694,-0.
030113\C,4.885645,-1.764654,0.0344\N,-1.852776,-2.180195,0.037655\C,-4
.065099,0.677739,0.968013\C,-2.961018,-0.161719,0.935035\C,-2.936384,-
1.274893,0.076742\C,-4.060446,-1.530671,-0.715134\C,-5.189853,0.41264,
0.174113\C,-5.186735,-0.707768,-0.663359\C,-7.378041,1.085675,-0.50486
5\O,-6.225972,1.294191,0.294941\C,1.795675,2.083439,-0.075081\C,2.6646
62,3.219255,-0.128929\C,0.41059,2.434988,-0.002568\N,3.3428,4.164661,-
0.174693\N,-0.704364,2.76327,0.069607\H,2.428011,-3.708185,0.16607\H,-
0.016665,-4.022825,0.198215\H,-0.628121,0.225679,-0.123499\H,4.874458,
2.137456,-0.211404\H,7.005033,0.901027,-0.169591\H,7.030226,-1.568961,
-0.0118\H,4.904398,-2.848267,0.102196\H,-2.102207,-3.134591,-0.173962\
H,-4.080467,1.546054,1.617475\H,-2.119247,0.043766,1.585997\H,-4.05717
2,-2.384796,-1.387627\H,-6.039863,-0.943,-1.288154\H,-8.06394,1.898904
,-0.263705\H,-7.862871,0.127086,-0.277431\H,-7.14015,1.120831,-1.57595
3\\Version=EM64L-G09RevB.01\State=1-A\HF=-1124.9777152\RMSD=9.735e-09\
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617,-7.5684535,-6.0744244,6.7085886,1.6117787\PG=C01 [X(C23H15N3O1)]\\

FODAAS B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p)

Orbital energies and kinetic energies (alpha):

		1	2
154	O	-0.238506	1.559777
155	O	-0.235865	1.514794
156	O	-0.223888	1.577144
157	O	-0.205187	1.455641
158	O	-0.181905	1.586964
159	V	-0.087977	1.554259
160	V	-0.064263	1.294928
161	V	-0.030926	1.195899
162	V	-0.026053	1.341628
163	V	-0.017375	1.374395

Total kinetic energy from orbitals= 1.955709264741D+03
No NMR shielding tensors so no spin-rotation constants.
Leave Link 601 at Wed Dec 12 07:27:48 2012, MaxMem= 268435456 cpu: 13.0
(Enter /usr/exe/g09/l9999.exe)
1\1\GINC-SKYNET\SP\RB3LYP\6-31+G(d,p)\C38H33N1O6\GUEST\12-Dec-2012\0\\
#p B3LYP/6-31+G(d,p) SP guess=read geom=AllCheck Pop=Regular gfinput\\
DAAFOPV\\0,1\C,0,3.6560561244,0.3249117743,0.141829776\C,0,2.598318809
,1.2579911354,0.0170573695\C,0,1.2959798711,0.8031943888,-0.015693981\
C,0,0.9701417141,-0.5694936647,0.0735379577\C,0,1.9962807667,-1.499063
2944,0.2024114692\C,0,3.317834388,-1.0408733403,0.2351921548\C,0,-0.49
66146364,-0.7105535386,0.0103024468\C,0,-1.3367971917,-1.8192206815,0.
0541037922\C,0,-2.7190944772,-1.634456288,-0.0333207844\C,0,-3.2929168
979,-0.3504102327,-0.1486269906\C,0,-2.4357956711,0.7731748108,-0.1888
141094\C,0,-1.0705050107,0.5716467483,-0.1159644872\C,0,0.027577055,1.
5948959708,-0.1359439633\O,0,-0.0859812482,2.804429256,-0.2295923313\N
,0,-4.6909027191,-0.1929670617,-0.221335758\C,0,-5.5613917307,-1.10231
15244,0.4504151163\C,0,-6.6478344867,-1.6815751294,-0.2271587945\C,0,-
7.5081348945,-2.5522608052,0.4265123899\C,0,-7.2956405208,-2.884072543
6,1.7731868554\O,0,-8.1924520536,-3.7578743734,2.3193187767\C,0,-8.027
8019984,-4.1224131768,3.6797720058\C,0,-6.2124403063,-2.3186877187,2.4
558857901\C,0,-5.3642351098,-1.4261807133,1.7968292238\C,0,-5.26576500
67,0.8849933941,-0.9585061174\C,0,-4.8349795143,1.1759306334,-2.264813
2238\C,0,-5.4011489435,2.2204392151,-2.9812492277\C,0,-6.432156403,2.9
901279886,-2.4214166145\O,0,-6.930078002,3.9844019302,-3.2142972856\C,
0,-7.9613072801,4.8043586926,-2.6899399125\C,0,-6.8782478053,2.6999496
13,-1.1271460369\C,0,-6.2877032365,1.6616612845,-0.403903015\H,0,2.788
5008844,2.3250673228,-0.0508100785\H,0,1.790146045,-2.5636184781,0.277
2377491\H,0,4.1221972922,-1.7665047348,0.3343219525\H,0,-0.9386140226,
-2.827108791,0.1400750088\H,0,-3.3730702842,-2.499705643,-0.0143284873
\H,0,-2.8347470129,1.7788003081,-0.2705266745\H,0,-6.8137933981,-1.438
8913915,-1.2722378716\H,0,-8.3493727025,-3.0016348462,-0.0919879397\H,
0,-8.837546192,-4.8193604303,3.9035921767\H,0,-8.1057761812,-3.2514944
599,4.3443330286\H,0,-7.0638777769,-4.6200544759,3.8514971393\H,0,-6.0
263160331,-2.5483200362,3.4988599772\H,0,-4.534463483,-0.9798523102,2.

3365317753\H,0,-4.0482660265,0.5777820256,-2.7142709942\H,0,-5.0690950
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81593\H,0,-7.6299998666,5.3470998408,-1.7945298745\H,0,-8.8578913413,4
.219266277,-2.4444292386\H,0,-7.6703684201,3.2783830325,-0.6655197739\
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19,0.1786591267\C,0,5.5788001458,1.9474206693,0.0492437036\C,0,6.99122
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,4.4247149844,-0.2337585865\H,0,7.8115104792,0.3547704901,0.3979466739
\O,0,8.8050490255,5.463254189,-0.2932986221\C,0,9.8783042086,6.1889185
529,0.3019538123\H,0,9.9883080453,5.936501367,1.3644027189\H,0,9.59773
84501,7.2418513738,0.2147089308\H,0,10.8246788581,6.0124354535,-0.2132
995525\O,0,10.9995539888,3.6110107175,0.0433136055\C,0,11.7926566262,3
.4724248873,1.2265775669\H,0,11.3616131706,4.0470874405,2.057554675\H,
0,12.7749907463,3.8806099995,0.9770198034\H,0,11.8925503801,2.42454409
02,1.5191625868\O,0,10.4351967857,0.9985310476,0.4175198139\C,0,10.195
9431649,-0.3968124962,0.5022556986\H,0,9.6138498983,-0.6550759423,1.39
68968989\H,0,11.1804613951,-0.8641744838,0.5653726876\H,0,9.6730079807
,-0.7690256202,-0.3881305144\\Version=EM64L-G09RevB.01\State=1-A\HF=-1
974.0568894\RMSD=6.644e-09\Dipole=-0.4662646,-1.5658604,1.5906284\Quad
rupole=25.0100328,-6.9851754,-18.0248574,-9.355268,6.0726597,-4.020829
6\PG=C01 [X(C38H33N1O6)]\\@

FMDAAS B3LYP/6-31+G(d,p) electronic computations at 6-31G* optimized geometry

Orbital energies and kinetic energies (alpha):

		1	2
166	O	-0.243872	1.473221
167	O	-0.236193	1.616333
168	O	-0.231793	1.502965
169	O	-0.208345	1.604319
170	O	-0.194466	1.594492
171	V	-0.128652	1.441271
172	V	-0.068791	1.324121
173	V	-0.048932	1.721037
174	V	-0.036716	1.346377
175	V	-0.030296	1.295392

1\1\GINC-SKYNET\SP\RB3LYP\6-31+G(d,p)\C41H33N3O5\GUEST\17-Jan-2013\0\\
#p B3LYP/6-31+G(d,p) Pop=Regular gfinput guess=read geom=AllCheck\\BCN
-DAAFOPV-neutral\\0,1\C,0,14.06296,10.92345,-0.56611\C,0,15.25656,10.1
7702,-0.51155\C,0,16.43818,10.83965,-0.25967\C,0,16.42902,12.24495,-0.
17969\C,0,13.99497,12.30625,-0.26748\C,0,15.23822,12.96041,-0.25257\C,
0,17.85089,12.66797,-0.03077\C,0,18.68053,11.42103,0.01864\C,0,17.7991
4,10.33575,-0.12741\C,0,18.29534,9.03765,-0.11522\C,0,19.68793,8.8351,
-0.03011\C,0,20.57868,9.91813,0.07101\C,0,20.04152,11.20747,0.17435\C,
0,22.0481,9.72133,0.11322\C,0,22.91624,10.68924,-0.24466\C,0,24.38948,
10.70022,-0.1428\C,0,26.4212,12.06922,-0.14318\C,0,25.03509,11.9438,-0
.29213\C,0,25.16586,9.57391,0.14431\C,0,27.19655,10.93119,0.14697\C,0,
26.5567,9.69045,0.30507\C,0,26.3574,14.46024,-0.19701\C,0,29.43808,10.
1314,-0.0028\C,0,27.41321,7.55832,-0.11374\N,0,12.73401,13.03405,0.006
72\C,0,12.08713,16.70898,-0.71202\C,0,12.0092,15.30846,-0.77004\C,0,12
.76956,14.49604,0.08742\C,0,13.62262,15.16022,0.99329\C,0,13.01896,17.
33484,0.11196\C,0,13.7902,16.55612,0.9666\C,0,10.25057,10.20629,0.5413
8\C,0,11.41391,10.98506,0.64118\C,0,11.46546,12.33292,0.24244\C,0,10.2
0561,12.93467,0.09274\C,0,9.05239,10.79669,0.17742\C,0,9.02164,12.1783
6,0.03984\C,0,18.32989,13.9307,0.\C,0,17.50726,15.0942,-0.04577\C,0,19
.60191,14.20107,0.\C,0,7.93532,8.73865,-0.17805\C,0,14.35674,19.27911,
0.17102\O,0,7.86547,10.15202,-0.01767\O,0,13.05988,18.69998,0.04043\O,
0,27.10623,13.25434,-0.27067\O,0,28.53639,11.1729,0.33543\O,0,27.24379
,8.62029,0.82105\N,0,16.90542,16.07937,-0.07937\N,0,20.87394,14.47145,
0.\H,0,13.17517,10.37196,-0.8604\H,0,15.23183,9.10324,-0.66704\H,0,15.
27425,14.03542,-0.29421\H,0,17.62967,8.18265,-0.18367\H,0,20.07141,7.8
1682,-0.05262\H,0,20.71316,12.02877,0.37533\H,0,22.39012,8.75623,0.471
\H,0,22.52507,11.63312,-0.62366\H,0,24.43329,12.82405,-0.50348\H,0,24.

69691,8.60845,0.303\H,0,27.06864,15.29087,-0.14333\H,0,25.738,14.49636
,0.70555\H,0,25.7533,14.60014,-1.09874\H,0,30.41968,10.58249,-0.17668\
H,0,29.15196,9.6163,-0.92575\H,0,29.54868,9.43422,0.83234\H,0,26.67715
,6.77369,0.07883\H,0,28.41045,7.13751,0.0557\H,0,27.35938,7.88699,-1.1
5738\H,0,11.44192,17.31327,-1.34477\H,0,11.34388,14.8669,-1.50645\H,0,
14.22683,14.58805,1.69391\H,0,14.53332,17.00218,1.62009\H,0,10.32727,9
.1457,0.75421\H,0,12.29504,10.48544,1.03194\H,0,10.08134,14.00453,-0.0
0961\H,0,8.07497,12.68115,-0.14277\H,0,6.93185,8.37844,-0.42452\H,0,8.
24089,8.25436,0.75454\H,0,8.60132,8.45968,-1.00294\H,0,14.25979,20.353
54,-0.01995\H,0,15.05001,18.87071,-0.57233\H,0,14.75332,19.16535,1.184
07\\Version=EM64L-G09RevB.01\State=1-A\HF=-2122.5142636\RMSD=7.557e-10
\Dipole=-0.7194263,-2.5015405,-0.556997\Quadrupole=-5.6367995,18.11106
2,-12.4742625,2.1840924,-4.4055347,3.8096327\PG=C01 [X(C41H33N3O5)]\\@

FOBAA B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p) [syn, anti]

Orbital energies and kinetic energies (alpha):

		1	2
107	O	-0.259217	1.471172
108	O	-0.254863	2.202944
109	O	-0.232859	1.463745
110	O	-0.202217	1.585318
111	O	-0.179715	1.567869
112	V	-0.085465	1.557655
113	V	-0.038984	1.306296
114	V	-0.022260	1.214129
115	V	-0.019152	1.215631
116	V	-0.012017	1.146248

1\1\GINC-SKYNET\SP\RB3LYP\6-31G(d,p)\C27H22N2O3\GUEST\03-Jul-2013\0\\#
p B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p) Pop=Regular gfinput\\FOBAA-syn g
roundstate geom opt/energy\\0,1\C,-0.1763536931,0.2688456752,-0.106646
0788\C,1.0759538933,-0.4712305692,-0.4740276311\C,0.7518418847,-1.8207
701473,-0.726347387\C,-0.7024047873,-1.9990568545,-0.5357680376\C,-1.2
662061016,-0.7607680311,-0.1670685677\C,2.3632567119,0.0148278027,-0.5
7892763\C,3.404421577,-0.8710885607,-0.9395901337\C,3.0882280216,-2.22
36188408,-1.1740817926\C,1.7734025818,-2.6957214202,-1.0769714041\C,-1
.5398053624,-3.1049280324,-0.6451783355\C,-2.9071023921,-2.9506602014,
-0.4035233305\C,-3.4689734314,-1.7105390769,-0.033667361\C,-2.61423892
81,-0.5929430712,0.0922777715\O,-0.2838926026,1.449710343,0.1761303207
\C,-6.3737557157,1.7124403311,-0.3007365366\C,-5.4990335572,0.63017392
13,-0.4255978645\C,-5.6714009812,-0.527778937,0.3422804892\C,-6.767628
8721,-0.5848595873,1.2220818584\C,-7.4600332018,1.6421899105,0.5764407
521\C,-7.6546910034,0.4756728841,1.3293298219\N,-4.8349763365,-1.65321
28025,0.2291183642\C,-8.2214370183,3.8399148316,0.0351299884\O,-8.3782
42716,2.6376337255,0.7700476808\N,4.7017243826,-0.3674772053,-1.014735
3534\C,8.2672932522,-1.278565365,-1.5010805942\C,7.0915936145,-0.76147
58031,-0.9528434496\C,5.8496992027,-0.9661693286,-1.5647580757\C,5.811
0917482,-1.7128962357,-2.7571176674\C,8.2125266231,-2.0407207216,-2.67
18936526\C,6.9727225928,-2.2518148868,-3.291746515\C,10.5682397629,-2.
4299250444,-2.6959898888\O,9.2928272341,-2.6114417834,-3.2872683802\H,
2.5654636076,1.0662078808,-0.3892498759\H,3.8824665865,-2.9194911719,-
1.4168714607\H,1.5749433908,-3.7472850405,-1.2650268295\H,-1.153985355
,-4.0816489585,-0.9232571656\H,-3.5646710362,-3.8109533814,-0.50490784
07\H,-2.988604083,0.3750929401,0.4034332046\H,-6.2020296822,2.59348269
65,-0.9073784023\H,-4.686773393,0.6895853533,-1.1409651136\H,-6.917224
2148,-1.4730289491,1.8307833379\H,-8.5012643692,0.429196066,2.00628515
93\H,-5.2767584,-2.5400509562,0.4176697252\H,-9.0401656163,4.491738170
4,0.3436302662\H,-8.2880477738,3.6669507148,-1.0470920626\H,-7.2657006
409,4.3313955228,0.2592909257\H,4.8597432021,0.4889390431,-0.505773039
8\H,9.2084065995,-1.0912315933,-0.9980405297\H,7.1430260306,-0.1901020
651,-0.029541386\H,4.8685856415,-1.8546671135,-3.274062526\H,6.9450239
994,-2.8291737445,-4.2100344609\H,11.2761304674,-2.9599298244,-3.33494
03758\H,10.6107118648,-2.8528953469,-1.6836445155\H,10.8488867917,-1.3
693271609,-2.6511084138\\Version=EM64L-G09RevB.01\State=1-A\HF=-1377.3
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e=22.9598949,-3.963733,-18.996162,0.5624368,5.264266,-3.2758952\PG=C01
[X(C27H22N2O3)]\\@

FMBAA B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p) [syn,anti]

Orbital energies and kinetic energies (alpha):

		1	2
119	O	-0.260018	1.246251
120	O	-0.255712	1.314992
121	O	-0.236614	1.475686
122	O	-0.207043	1.585263
123	O	-0.185157	1.578736
124	V	-0.118626	1.408559
125	V	-0.045525	1.324014
126	V	-0.025671	1.229156
127	V	-0.022481	1.343573
128	V	-0.021000	1.401265

1\1\GINC-SKYNET\SP\RB3LYP\6-31G(d,p)\C30H22N4O2\GUEST\02-Jul-2013\0\\#
p B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p) Pop=Regular gfinput\\FMBAA-anti
groundstate geom opt/energy\\0,1\C,0.4351093175,0.7798290087,0.5171100
104\C,-0.9617122733,0.2965630751,0.4073650408\C,-0.9416880869,-1.12036
90794,0.4504660251\C,0.4490797711,-1.5646434684,0.5489437431\C,1.29265
01149,-0.4272050399,0.5696017093\C,1.0115918501,-2.8346736878,0.601918
0322\C,2.3961716674,-2.9686539775,0.6796296526\C,3.2495382833,-1.84556
14526,0.6810606498\C,2.6798617587,-0.5552771957,0.6168036086\C,-2.1620
732191,0.9854984334,0.2802778025\C,-3.3787862107,0.2684412439,0.214418
6225\C,-3.3487304933,-1.1367358009,0.2834780578\C,-2.1366503787,-1.824
2703584,0.3917204745\N,4.6215870923,-2.0657450185,0.7200749917\C,6.700
9475688,0.8301249757,1.8224897169\C,5.6239526377,-0.0381706521,1.71518
78656\C,5.6738420111,-1.1328984023,0.8340048695\C,6.8446011075,-1.3390
360297,0.0963536536\C,7.8718276656,0.6140608011,1.0827900315\C,7.94302
90479,-0.4869393589,0.2233172243\C,10.0713131969,1.36069506,0.53067340
55\O,8.8757055361,1.5216793096,1.2746012272\C,0.8463382963,2.089159875
9,0.6075028388\N,-4.5570632169,1.0006800971,0.1139038685\C,-7.39717936
11,-0.8303582828,-1.4609921112\C,-6.100165787,-0.4348798304,-1.1661831
926\C,-5.8551529389,0.542627171,-0.1843015358\C,-6.9520982468,1.121987
2052,0.4627661453\C,-8.4907701737,-0.2438835352,-0.8078883357\C,-8.260
6518018,0.7480602778,0.1505522619\C,-10.8621477878,-0.1446051732,-0.54
48066331\O,-9.7236307592,-0.7033691499,-1.1791779298\C,-0.0577011648,3
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7715171118,4.1172466591,0.5345832888\N,3.3071221023,2.8399256265,0.945
1358932\H,0.3867873914,-3.7228253447,0.5874790353\H,2.8352458396,-3.96
18035409,0.7348007152\H,3.325829219,0.3093326432,0.5783968876\H,-2.191
939685,2.0665117076,0.2220124242\H,-4.2779662749,-1.6931395545,0.26890
73631\H,-2.1451645688,-2.9092988709,0.4416499972\H,4.9077135139,-2.997
4654508,0.4598134943\H,6.6574949177,1.6841052877,2.489509602\H,4.74498
3999,0.1313268002,2.3259160036\H,6.9008018366,-2.1777960535,-0.5931324
037\H,8.8329656294,-0.6851245393,-0.3618531687\H,10.7223810427,2.18588
56759,0.8227942388\H,9.8870929368,1.4128891905,-0.5503270724\H,10.5701
256482,0.410185748,0.7622851565\H,-4.4876685904,1.9702824771,0.3844036
058\H,-7.5896442555,-1.5849517163,-2.2164972978\H,-5.2707901904,-0.871
0742727,-1.7118321997\H,-6.7829791134,1.8771252662,1.2258882748\H,-9.0
822512807,1.2260540407,0.6702888437\H,-11.7271577641,-0.6497282119,-0.
9768959977\H,-10.9442002254,0.9338367443,-0.7333206675\H,-10.848332544
7,-0.3174972119,0.5392241873\\Version=EM64L-G09RevB.01\State=1-A\HF=-1
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rupole=36.9938446,-18.6282417,-18.3656029,-15.5885994,-13.0225031,1.57
87182\PG=C01 [X(C30H22N4O2)]\\@

FOBDAA B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p)

Orbital energies and kinetic energies (alpha):

		1	2
163	O	-0.235121	1.552638
164	O	-0.234553	1.582192
165	O	-0.231571	1.440345
166	O	-0.189836	1.640970
167	O	-0.172883	1.641960
168	V	-0.083516	1.554428
169	V	-0.042470	1.290057
170	V	-0.029229	1.146183

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 171         V                -0.022220          1.228532
 172         V                -0.014592          1.370133

 1\1\GINC-SKYNET\SP\RB3LYP\6-31+G(d,p)\C41H34N2O5\GUEST\11-Dec-2012\0\\
 #p B3LYP/6-31+G(d,p) SP guess=read geom=AllCheck Pop=Regular gfinput\\
 BDAAFO\\0,1\C,0,-0.0010704039,-1.2554179105,-0.9265624405\C,0,-0.20617
 97449,-1.873227018,0.2984847696\C,0,0.6783613938,-1.6497951374,1.36479
 14219\O,0,0.3926757866,-2.3158538662,2.5234635898\C,0,1.2538814769,-2.
 1259682406,3.6334634429\C,0,1.7661887296,-0.7889548385,1.1835465266\C,
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 322,-1.1163604602\N,0,1.2952556651,0.2522465775,-2.3774003455\C,0,2.60
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FMBDAA B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p)

```
Orbital energies and kinetic energies (alpha):
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 175         O                -0.237912          1.497422
 176         O                -0.235866          1.578657
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 177         O                -0.233915          1.519494
 178         O                -0.193680          1.636876
 179         O                -0.176775          1.651078
 180         V                -0.115091          1.410989
 181         V                -0.048621          1.313984
 182         V                -0.032907          1.163396
 183         V                -0.025693          1.216632
 184         V                -0.017582          1.409282
 Total kinetic energy from orbitals= 2.196395837662D+03
 No NMR shielding tensors so no spin-rotation constants.
 Leave Link  601 at Thu Dec 13 21:30:14 2012, MaxMem=  268435456 cpu:      10.4
 (Enter /usr/exe/g09/l9999.exe)
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 291,-3.9521096174,-1.9197415436\C,7.8725359014,-2.2471403754,-0.553806
 3405\C,6.935359289,-1.4150184614,0.0624860709\C,5.7898606284,-0.989906
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FOBDAA36 B3LYP/6-31+G(d,p)

Orbital energies and kinetic energies (alpha):

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164	O	-0.237789	1.848994
165	O	-0.227487	1.292472
166	O	-0.191369	1.663107
167	O	-0.182639	1.619873
168	V	-0.073758	1.604161
169	V	-0.044065	1.174992
170	V	-0.029934	1.144939
171	V	-0.020840	1.280657
172	V	-0.018489	1.356690

Leave Link 602 at Thu Aug 23 15:30:52 2012, MaxMem= 268435456 cpu: 4.2
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FMBDAA36 B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p)

Orbital energies and kinetic energies (alpha):

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175	O	-0.244915	1.583633
176	O	-0.241254	1.448969
177	O	-0.235451	1.302347
178	O	-0.197895	1.612740
179	O	-0.191834	1.617518
180	V	-0.102164	1.486178
181	V	-0.052098	1.187711
182	V	-0.036031	1.159095
183	V	-0.027477	1.276851
184	V	-0.026137	1.330650

Leave Link 602 at Mon Aug 27 12:21:38 2012, MaxMem= 268435456 cpu: 4.1
 (Enter /usr/exe/g09/l9999.exe)
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4H34N4O4)]\\@

TDDFT summaries for bis-DAA isomers

FOBDAA

1\1\GINC-SKYNET\SP\RB3LYP TD-FC\6-31G(d,p)\C41H34N2O5\GUEST\14-Nov-201
2\0\\#p B3LYP/6-31G(d,p) TD=(NStates=3)

Orbital energies and kinetic energies (alpha):

		1	2
163	O	-0.224512	1.566299
164	O	-0.223946	1.599114
165	O	-0.221060	1.448130
166	O	-0.179468	1.649279
167	O	-0.162621	1.646382
168	V	-0.069513	1.612704
169	V	-0.027239	1.396755
170	V	-0.011297	1.300137
171	V	-0.005617	1.358826
172	V	0.001570	1.517563

Excited State 1: Singlet-A 1.9848 eV 624.66 nm f=0.0900 <S**2>=0.000
167 ->168 0.70333
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -2068.39891984
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.5209 eV 491.83 nm f=0.0070
<S**2>=0.000
166 ->168 0.70211
Excited State 3: Singlet-A 3.1699 eV 391.13 nm f=0.0008 <S**2>=0.000
162 ->168 0.67975
164 ->168 0.10314

FMBDAA

1\1\GINC-SKYNET\SP\RB3LYP TD-FC\6-31G(d,p)\C44H34N4O4\GUEST\14-Nov-201
2\0\\#p B3LYP/6-31G(d,p) TD=(NStates=3) guess=read

Orbital energies and kinetic energies (alpha):

		1	2
175	O	-0.227559	1.505231
176	O	-0.225443	1.591689
177	O	-0.223642	1.534681
178	O	-0.183493	1.645642

```
 179         O                -0.166777          1.656066
 180         V                -0.103553          1.430708
 181         V                -0.034109          1.421383
 182         V                -0.015503          1.311166
 183         V                -0.009079          1.345241
 184         V                -0.001588          1.591020

Excited State   1:      Singlet-A      1.1898 eV 1042.09 nm  f=0.0346  <S**2>=0.000
     179 ->180         0.70486
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -2216.98373378
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State     2:          Singlet-A          1.7208 eV   720.49 nm   f=0.0013
   <S**2>=0.000
     178 ->180         0.70579

 Excited State     3:          Singlet-A          2.7032 eV   458.66 nm   f=0.0130
   <S**2>=0.000
     175 ->180         0.30182
     176 ->180        -0.10494
     177 ->180         0.62042
```

FOBDAA36

```
1\1\GINC-SKYNET\SP\RB3LYP TD-FC\6-31G(d,p)\C41H34N2O5\GUEST\16-Jan-201
 3\0\\#p B3LYP/6-31G(d,p) TD=(Read,NStates=3) Density=Current guess=rea
 d geom=AllCheck Pop=Regular gfinput\\36BDAAFO neutral geom

Orbital energies and kinetic energies (alpha):
                             1                2
 163         O               -0.228366          1.616851
 164         O               -0.224933          2.163654
 165         O               -0.216602          1.301444
 166         O               -0.180423          1.673810
 167         O               -0.172009          1.626322
 168         V               -0.060317          1.649983
 169         V               -0.027187          1.298102
 170         V               -0.011967          1.311510
 171         V               -0.005138          1.376710
 172         V               -0.002082          1.495417

Excited State     1:          Singlet-?Sym       2.5286 eV   490.33 nm   f=0.2280
   <S**2>=0.000
     167 ->168         0.70039
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -2068.38335174
 Copying the excited state density for this state as the 1-particle RhoCI density.
 Excited state symmetry could not be determined.
 Excited State     2:          Singlet-?Sym       2.9893 eV   414.75 nm   f=0.1712
   <S**2>=0.000
     166 ->168         0.69772
 Excited state symmetry could not be determined.
 Excited State     3:          Singlet-?Sym       3.1821 eV   389.64 nm   f=0.0000
   <S**2>=0.000
     162 ->168        -0.25409
     163 ->168         0.12573
     164 ->168         0.63751
```

FMBDAA36

```
1\1\GINC-SKYNET\SP\RB3LYP TD-FC\6-31G(d,p)\C44H34N4O4\GUEST\11-Dec-201
 2\0\\#p B3LYP/6-31G(d,p) TD=(NStates=3) guess=read

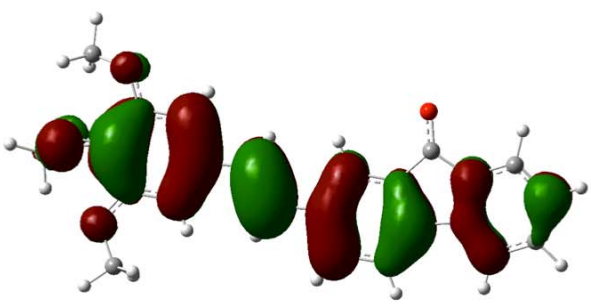
Orbital energies and kinetic energies (alpha):
                             1                2
 175         O               -0.234253          1.597969
 176         O               -0.230458          1.459223
 177         O               -0.224892          1.311327
```

```
 178         O                -0.187293          1.621793
 179         O                -0.181458          1.624273
 180         V                -0.090911          1.499438
 181         V                -0.036047          1.297090
 182         V                -0.018642          1.319040
 183         V                -0.012235          1.376026
 184         V                -0.010813          1.457036

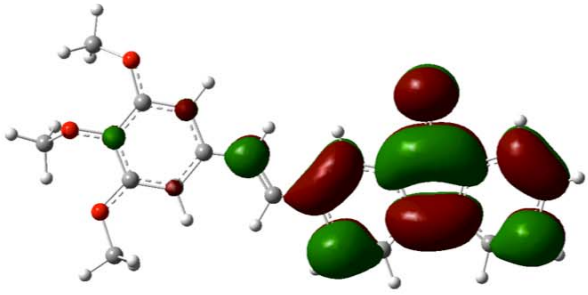
Excited state symmetry could not be determined.
 Excited  State     1:          Singlet-?Sym      2.0115  eV   616.38  nm   f=0.2438
  <S**2>=0.000
     177 ->180         0.10423
     179 ->180         0.69702
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -2216.96320311
 Copying the excited state density for this state as the 1-particle RhoCI density.
 Excited state symmetry could not be determined.
 Excited  State     2:          Singlet-?Sym      2.4723  eV   501.50  nm   f=0.4010
  <S**2>=0.000
     178 ->180         0.69989
 Excited state symmetry could not be determined.
 Excited  State     3:          Singlet-?Sym      2.9628  eV   418.47  nm   f=0.0692
  <S**2>=0.000
     177 ->180         0.68260
     179 ->181        -0.11727
```

Molecular orbital diagrams, default Gaussview settings,
B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p)

FOS

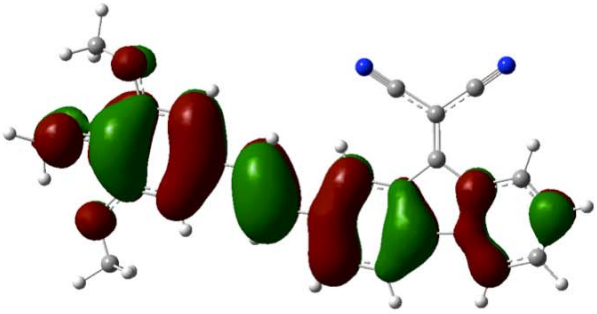


E(HOMO) = -0.205 a.u.

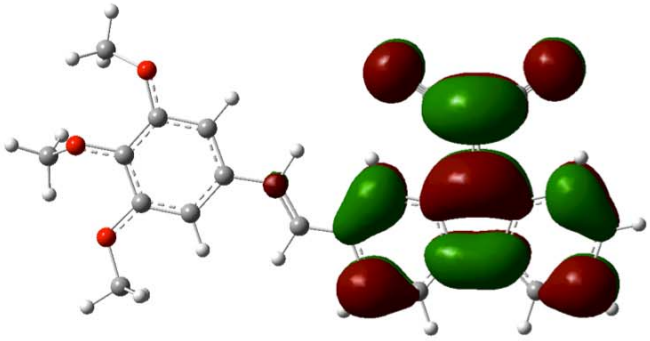


E(LUMO) = -0.095 a.u.

FMS

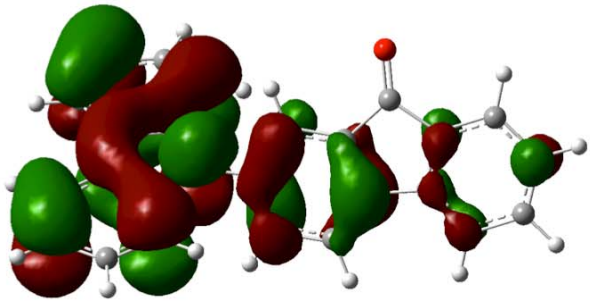


E(HOMO) = -0.209 a.u.

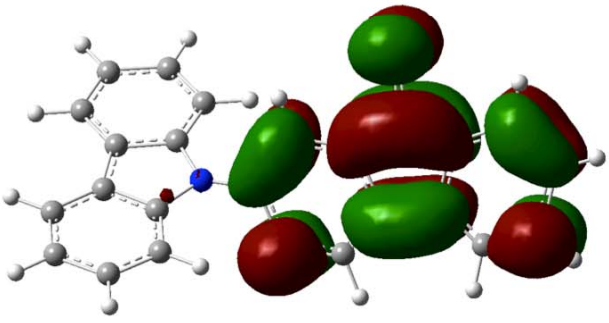


E(LUMO) = -0.127 a.u.

FOCz

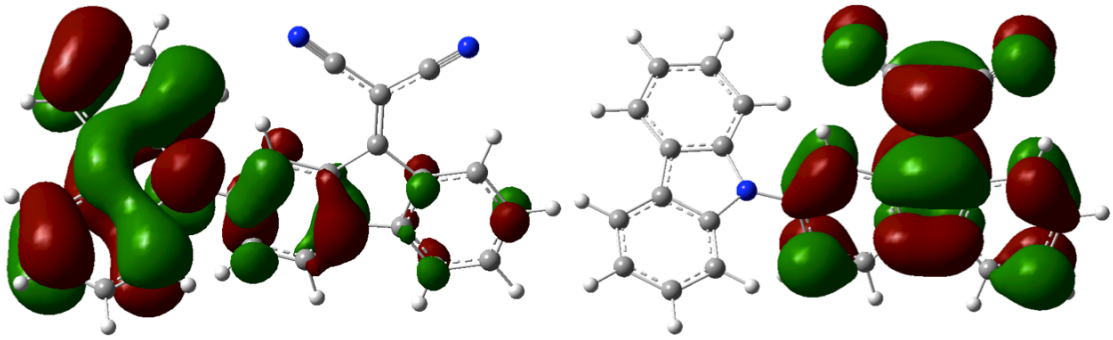


E(HOMO) = -0.210 a.u.



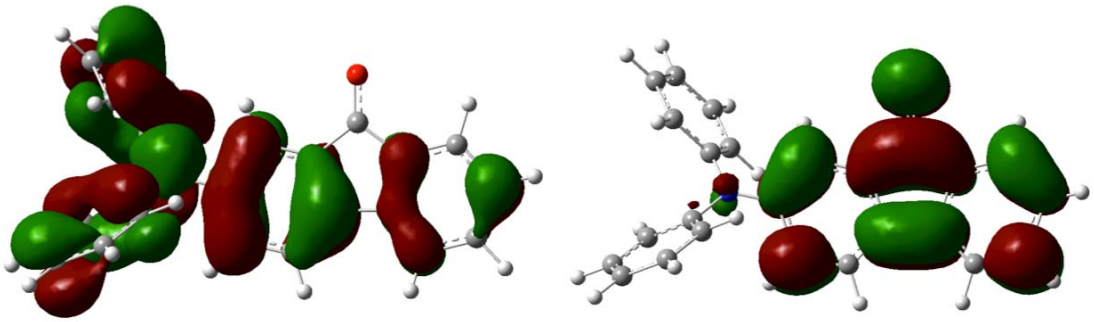
E(LUMO) = -0.103 a.u.

FMCz



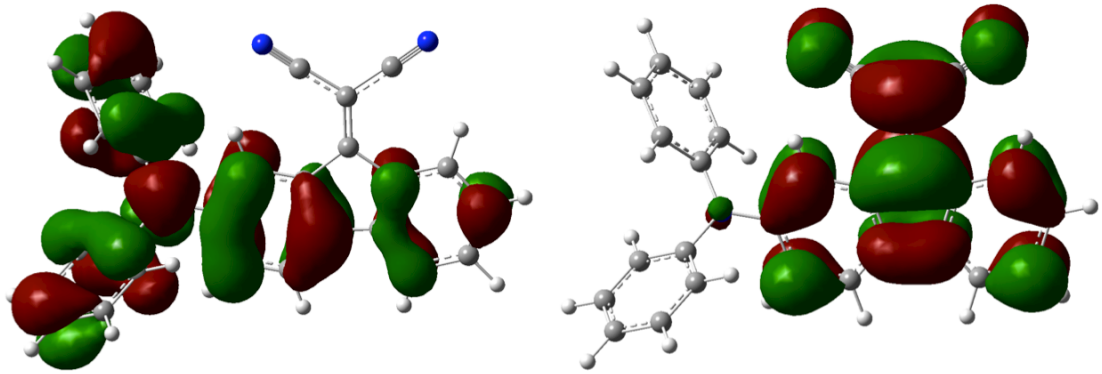
E(HOMO) = -0.214 a.u. E(LUMO) = -0.134 a.u.

FODPA



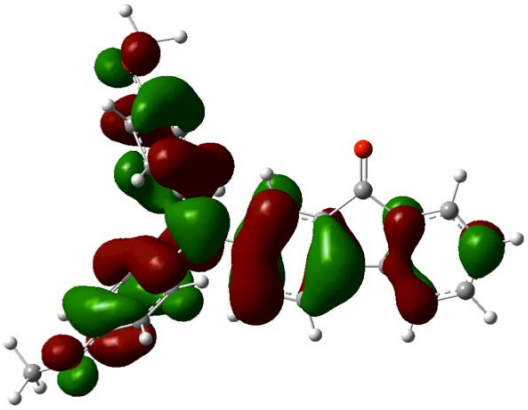
E(HOMO) = -0.196 a.u. E(LUMO) = -0.093 a.u.

FMDPA

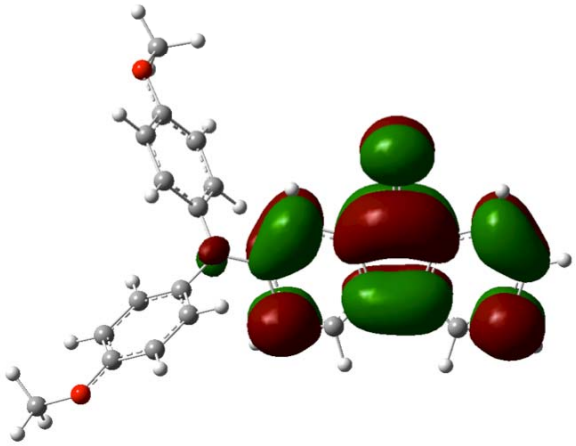


E(HOMO) = -0.202 a.u. E(LUMO) = -0.125 a.u.

FODAA

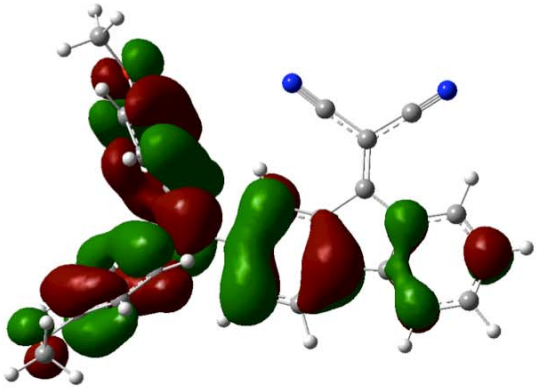


E(HOMO) = -0.185 a.u.

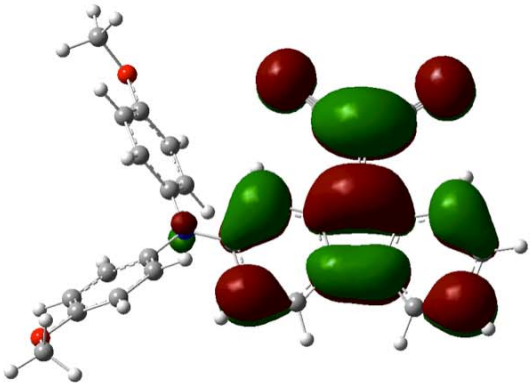


E(LUMO) = -0.088 a.u.

FMDAA

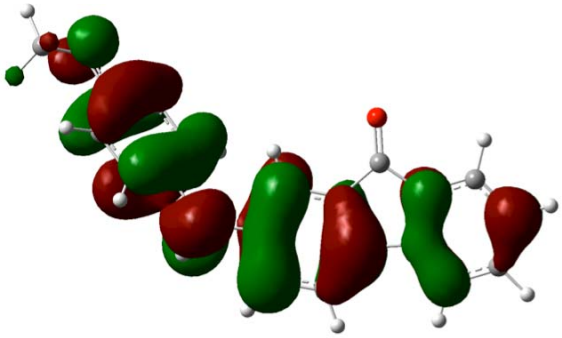


E(HOMO) = -0.190 a.u.

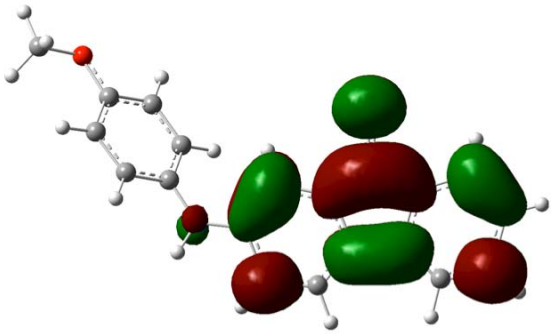


E(LUMO) = -0.121 a.u.

FOAA [syn]

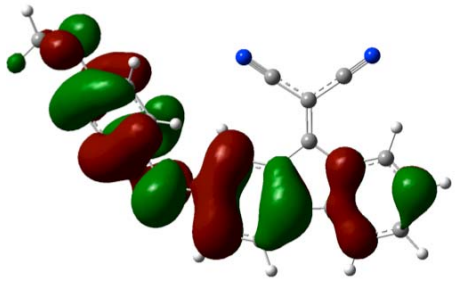


E(HOMO) = -0.193 a.u.

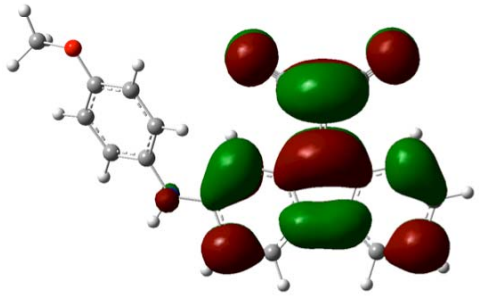


E(LUMO) = -0.089 a.u.

FMAA [syn]

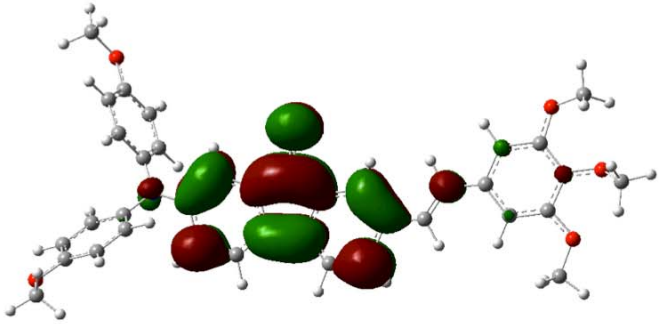


E(HOMO) = -0.199 a.u.

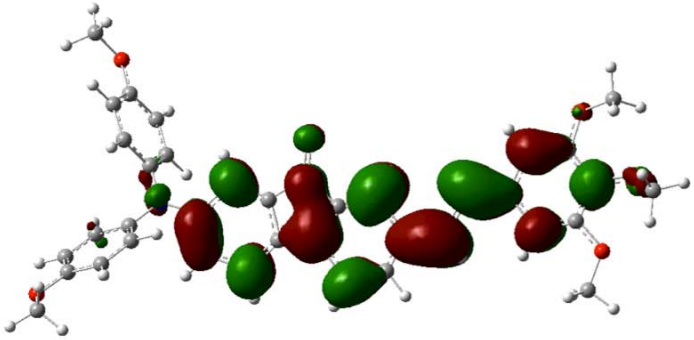


E(LUMO) = -0.123 a.u.

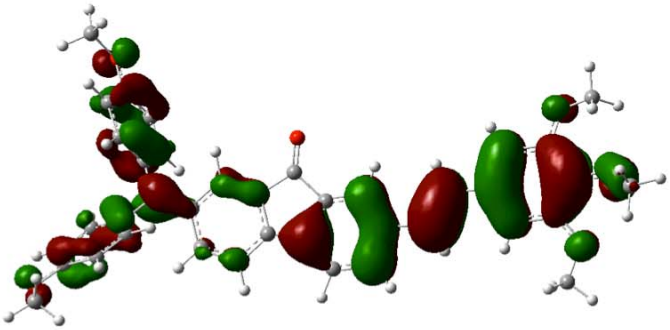
FODAAS



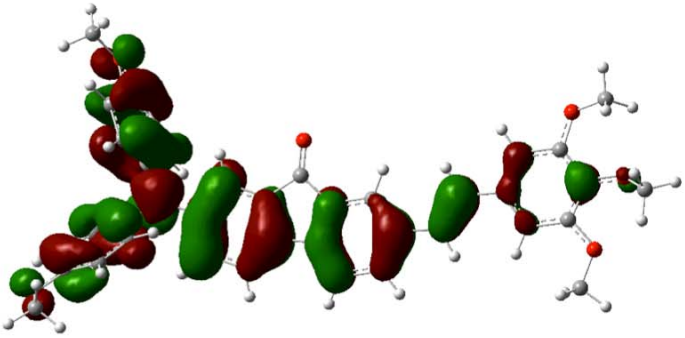
E(LUMO) = -0.088 a.u.



E(LUMO+1) = -0.064 a.u.

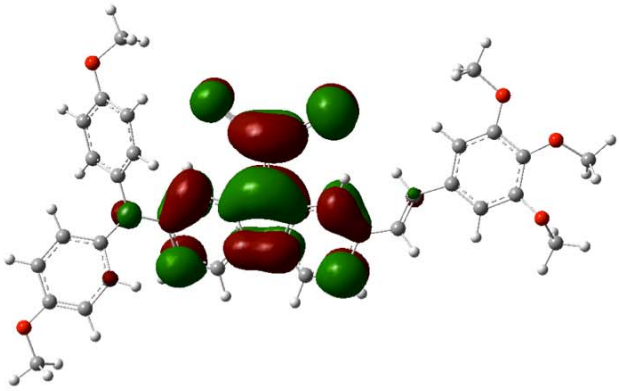


E(HOMO-1) = -0.205 a.u.

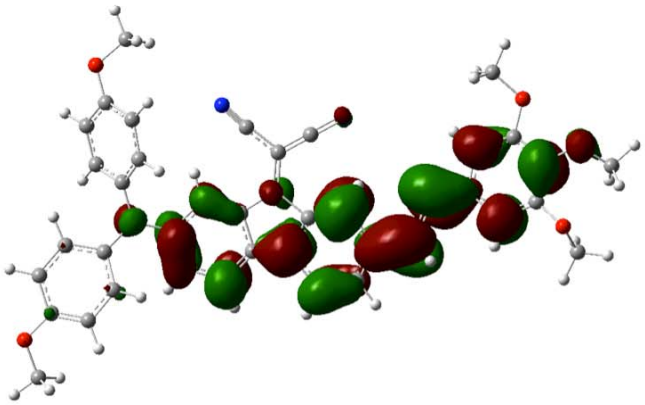


E(HOMO) = -0.182 a.u.

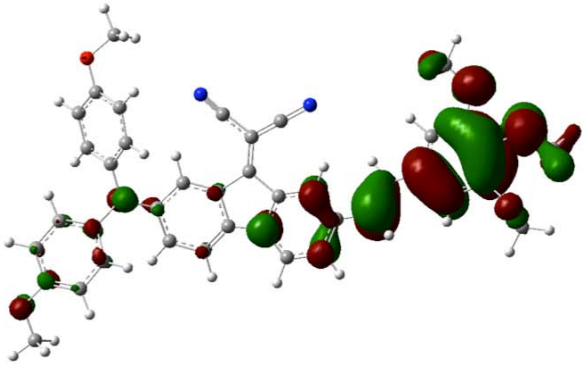
FMDAAS



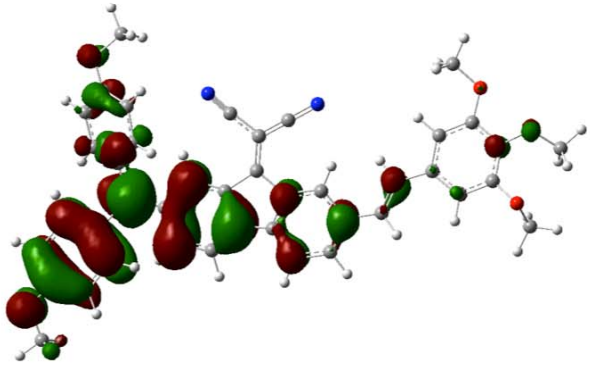
E(LUMO) = -0.129 a.u.



E(LUMO+1) = -0.069 a.u.

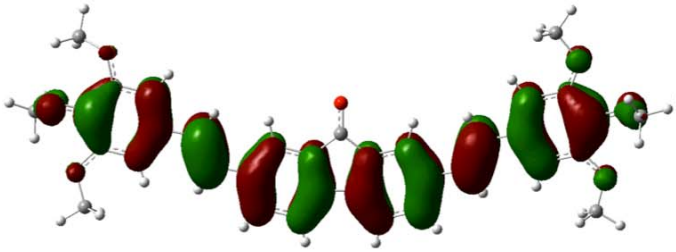


E(HOMO-1) = -0.208 a.u.

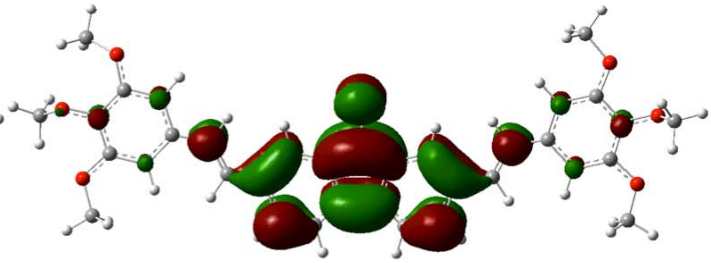


E(HOMO) = -0.195 a.u.

FODS

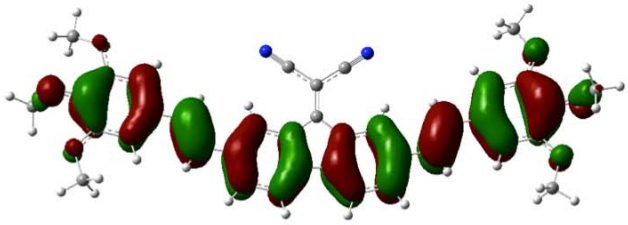


E(HOMO) = -0.198 a.u.

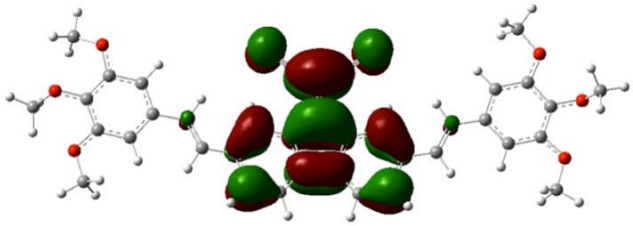


E(LUMO) = -0.095 a.u.

FMDS

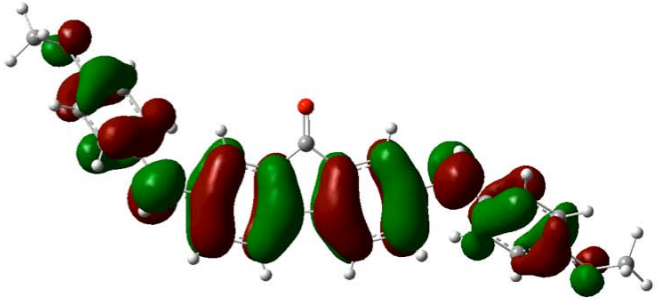


E(HOMO) = -0.201 a.u.

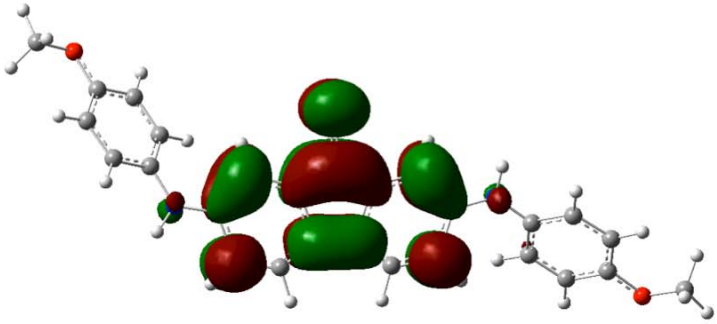


E(LUMO) = -0.126 a.u.

FOBAA (syn,anti)

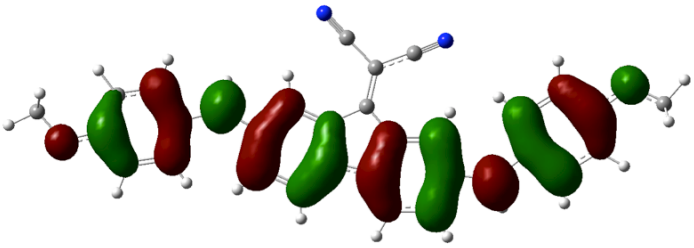


E(HOMO) = -0.180 a.u.

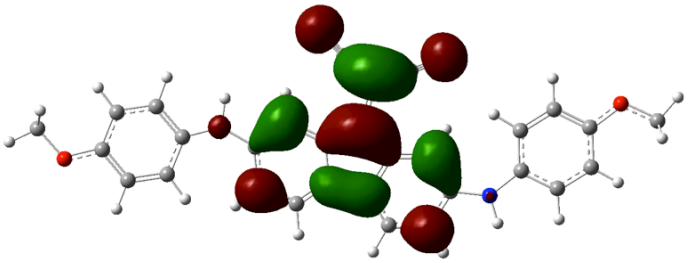


E(LUMO) = -0.085 a.u.

FMBAA (syn,anti)

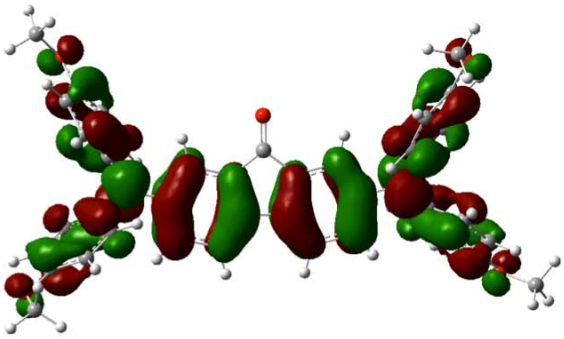


E(HOMO) = -0.185 a.u.

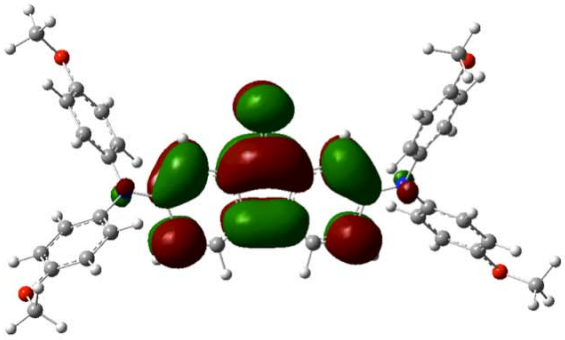


E(LUMO) = -0.119 a.u.

FOBDAA

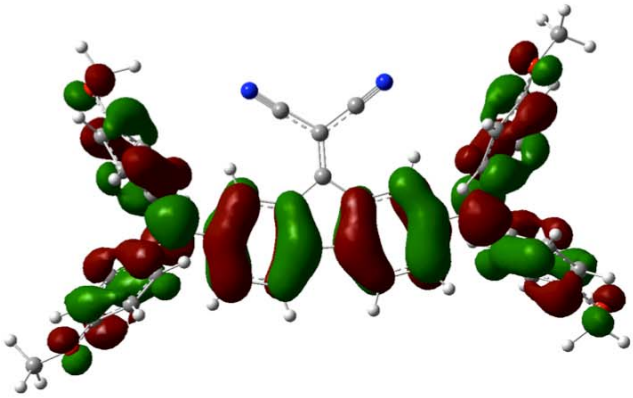


E(HOMO) = -0.173 a.u.

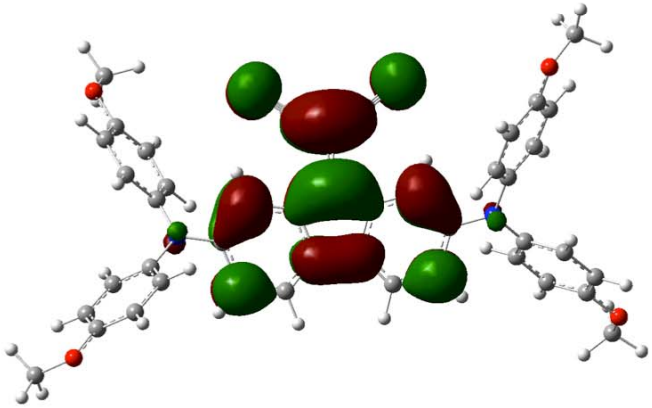


E(LUMO) = -0.084 a.u.

FMBDAA

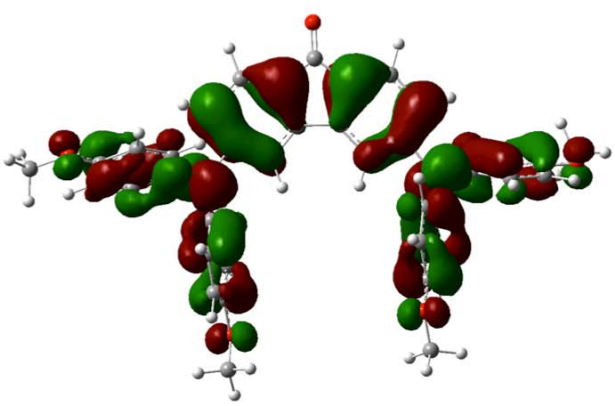


E(HOMO) = -0.177 a.u.

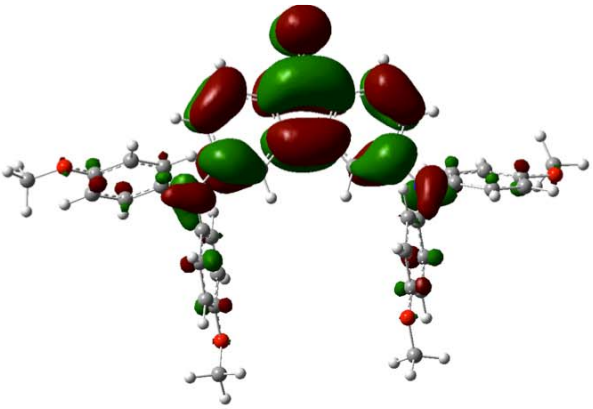


E(LUMO) = -0.115 a.u.

FOBDAA36

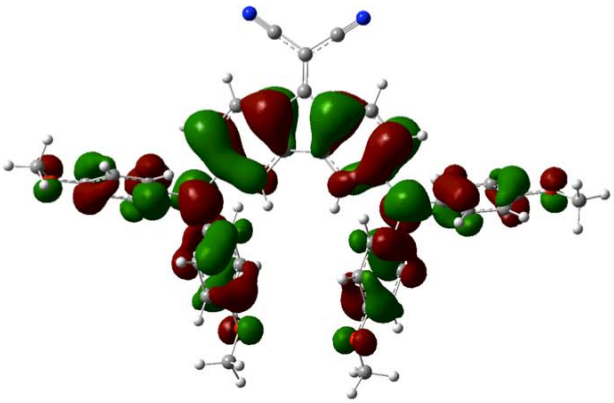


E(HOMO) = -0.183 a.u.

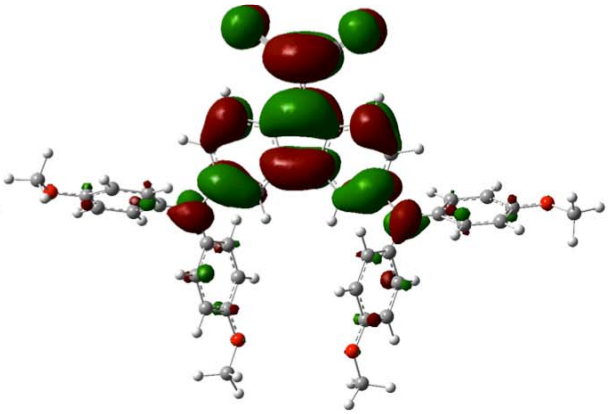


E(LUMO) = -0.074 a.u.

FMBDAA36



E(HOMO) = -0.192 a.u.



E(LUMO) = -0.102 a.u.