Supporting Information

Dual fluorescent phenanthridinones and crinasiadine derivatives by consecutive palladium-catalyzed three-component syntheses

Regina Kohlbecher, and Thomas J. J. Müller*

Heinrich Heine University Duesseldorf, Faculty of Mathematics and Natural Sciences, Institute of Organic Chemistry and Macromolecular Chemistry, Universitätstrasse 1, Düsseldorf D-40225, Germany

E-mail: ThomasJJ.Mueller@hhu.de

Table of contents

1 General considerations 3
2 Synthesis and spectroscopic data of 6-bromobenzo[*d*][1,3]dioxolo-5-carbaldehyde[1] 5
3 Synthesis and spectroscopic data of methyl 6-bromobenzo[*d*][1,3]-dioxol-5-carboxylate[3] 5
4 Synthesis and spectroscopic data of Piperonal boronic acid pinacol ester **3b**[4] 6
5 Synthesis of *N*-arylphenanthridinones 4 and *N*-arylcrinasiadines **5** 7
5.1 Optimization of *N*-arylphenanthridinones 4 and *N*-arylcrinasiadines **5** 7
5.2 General procedure (**GP1**) for the synthesis of *N*-arylphenanthridinones **4** and *N*-arylcrinasiadines **5** 15
5.3 Spectroscopic data of *N*-arylphenanthridinones 4 and *N*-arylcrinasiadines **5** 17
6 Synthesis of *N*-alkylphenanthridinones 6 and *N*-alkylcrinasiadines **7** 21
6.1 Optimization of *N*-alkylphenanthridinones 6 and *N*-alkylcrinasiadines **7** 21
6.2 General procedure (**GP2**) for the synthesis of *N*-alkylphenanthridinones **6** and *N*-alkylcrinasiadines **7** 22
6.3 Spectroscopic data of *N*-alkylphenanthridinones **6** and *N*-alkylcrinasiadines **7** 24
7 Synthesis of 6(*5H*)-phenanthridinone **8** 27
8 ^{1}H and ^{13}C spectra of *N*-arylphenanthridinones 4 and *N*-arylcrinasiadines **5** 28
9 ^{1}H and ^{13}C spectra of *N*-alkylphenanthridinones 6 and *N*-alkylcrinasiadines **7** 35
10 High-Performance Liquid Chromatography (HPLC) Data of *N*-arylphenanthridinones 4 and *N*-arylcrinasiadines **5** 40
10.1 HPLC Data of 5-(4-(*tert*-Butyl)phenyl)-2-fluorophenanthridin-6(5*H*)-one (**4b**) 40
10.2 HPLC Data of 2-Fluoro-5-phenylphenanthridin-6(5*H*)-one (**4c**) 40
10.3 HPLC Data of 5-(4-(*tert*-Butyl)phenyl)-2-fluoro-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (**5b**) 41
10.4 HPLC Data of 2-Fluoro-5-Phenyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (**5c**) ... 41

11 Absorption and emission spectra 42
11.1 Absorption and emission spectra of 6(5*H*)-phenanthridinone (**8**) 42
11.2 Absorption and emission spectra of *N*-arylphenanthridinones **4** and *N*-arylcrinasiadines **5** 42
11.3 Absorption and emission spectra of *N*-alkylphenanthridinones **6** and *N*-alkylcrinasiadines **7** 46
11.4 Degassed and non-degassed emission spectra of *N*-arylphenanthridinone **4b** and *N*-arylcrinasiadine **5b** 48
11.5 Jacobian[10] energy-corrected emission spectra and corresponding integrated emission intensities of *N*-arylphenanthridinone **4b** and *N*-arylcrinasiadine **5b** 50
12 Data of quantum chemical calculations 52
12.1 Comparison of the potential scans of 5-(4-(*tert*-butyl)phenyl)-2-fluorophenanthridin-6(5*H*)-one (**4b**) and 5-(4-(*tert*-Butyl)phenyl)-2-fluoro-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (**5b**) 52
12.2 Quantum chemical calculation data of 5-(4-(*tert*-butyl)phenyl)-2-fluorophenanthridin-6(5*H*)-one (**4b**) 53
12.2.1 Computed xyz-coordinates of compound **4b** (B3LYP/6-31G* PCM CH_2Cl_2) 53
12.2.2 Computed excitations energies of compound **4b** (B3LYP/6-31G* PCM CH_2Cl_2) 54
12.2.3 Computed LE emission energies of compound **4b** (B3LYP/6-31G* PCM CH_2Cl_2) 56
12.2.4 Potential scan of compound **4b** ground state (B3LYP/6-31G* PCM CH_2Cl_2) 58
12.2.5 Potential scan of compound **4b** excited state (B3LYP/6-31G* PCM CH_2Cl_2) 100
12.2.6 Computed CT emission energies of compound **4b** (B3LYP/6-31G* PCM CH_2Cl_2) 146
12.2.7 Computed excitations energies of the triplet state of compound **4b** (B3LYP/6-31G* PCM CH_2Cl_2) 146
12.2.8 Computed emission energies of the triplet state of compound **4b** (B3LYP/6-31G* PCM CH_2Cl_2) 149
12.3 Quantum chemical calculation data of 5-(4-(*tert*-Butyl)phenyl)-2-fluoro-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (**5b**) 153
12.3.1 Computed xyz-coordinates of compound **5b** (B3LYP/6-31G* PCM CH_2Cl_2) 153
12.3.2 Computed excitations energies of compound **5b** (B3LYP/6-31G* PCM CH_2Cl_2) 154
12.3.3 Computed emission energies of compound **5b** (B3LYP/6-31G* PCM CH_2Cl_2) 156
12.3.4 Potential scan of compound **5b** ground state (B3LYP/6-31G* PCM CH_2Cl_2) 157
12.3.5 Potential scan of compound **5b** excited state (B3LYP/6-31G* PCM CH_2Cl_2) 202
12.3.6 Computed CT emission energies of compound **5b** (B3LYP/6-31G* PCM CH_2Cl_2) 249
12.3.7 Computed excitations energies of the triplet state of compound **5b** (B3LYP/6-31G* PCM CH_2Cl_2) 250
12.3.8 Computed emission energies of the triplet state of compound **5b** (B3LYP/6-31G* PCM CH_2Cl_2) 252
13 References 256

1 General considerations

All reactions were carried out in oven dried Schlenk glassware using septa and syringes under nitrogen atmosphere. The reagents and catalyst were purchased reagent-grade and used without purification. Dry solvents were dried by a solvent purification system.

The reaction progress was monitored qualitatively using TLC Silica gel 60 F234 aluminum sheets obtained from Macherey Nagel GmbH & Co. KG. The spots were detected with UV light at 254 and 366 nm. The purification of the products was performed on silica gel 60 M (0.04-0.063 mm) from Macherey-Nagel GmbH & Co. KG using flash technique under pressure of 2 bar. The crude mixtures were absorbed on Celite® 545 form Carl Roth GmbH & Co. KG before chromatographic purification. Ethyl acetate and mixtures of *n*-hexane/ethyl acetate were used as eluent.

^{1}H, ^{19}F, ^{13}C and 135-DEPT ^{13}C NMR spectra were recorded on Bruker AVIII-300 and AVIII-600. DMSO-d_6 and chloroform-d_1 were used as deuterated solvents. The resonances of the solvents were locked as internal standard (DMSO-d_6: ^{1}H δ 2.50 (water in DMSO-d_6 ^{1}H δ 3.33)*, ^{13}C δ 39.52; $CDCl_3$: ^{1}H δ 7.26, ^{13}C δ 77.00). For recording ^{19}F NMR spectra, trichlorofluoromethane (^{19}F δ 0.0) was added to the solvent chloroform-d_1, which served as an internal standard. A relaxation delay time d_1 of 10 s was selected for the spectrum recording. The multiplicities of the signals were abbreviated as follows: s: singlet; d: doublet; t: triplet; q: quartet; dd: doublet of doublet; dt: doublet of triplet; tt: triplet of triplets; ddd: doublet of doublet of doublets; m: multiplet. The type of carbon nucleus was determined based on 135-DEPT ^{13}C NMR spectra. For the description of the ^{13}C NMR spectra primary carbon nuclei are abbreviated with CH_3, secondary carbon nuclei with CH_2, tertiary carbon nuclei with CH and quaternary carbon nuclei with C_{quat}. The program Mestrenova 11.0 was used to evaluate the NMR spectra.

EI mass spectra were measured on Finnigan MAT TSQ 7000.

IR spectra were obtained on Shimadzu IR Affinity-1 which works with the attenuated total reflection (ATR) method. The intensity of signals is abbreviated as follows: s (strong), m (medium), w (weak).

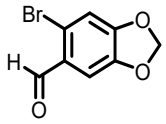
The melting points (uncorrected) were measured on Büchi Melting Point B-540.

* Due to the water content in DMSO-d_6, the water peaks in the ^{1}H NMR spectra are also labeled with "DMSO-d_6".

Absorption spectra were recorded in dichloromethane and acetonitrile (high performance liquid chromatography (HPLC) grade) at 293 K on a Perkin–Elmer UV/Vis/NIR Lambda 19 spectrometer. For the determination of the molar extinction coefficients ε absorption measurements at five different concentrations were carried out. Emission spectra were recorded in ethyl acetate HPLC grade at 293 K on a Hitachi F-7000 spectrometer.

Quantum chemical calculations were carried out utilizing the HPC-Cluster Hilbert of the Center for Information and Media Technology at the Heinrich Heine University Düsseldorf.

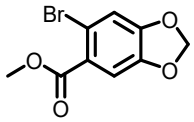
2 Synthesis and spectroscopic data of 6-bromobenzo[*d*][1,3]dioxolo-5-carbaldehyde[1]



In a 100 mL three-neck flask with magnetic stir bar, piperonal (1.95 g, 13.0 mmol, 1.00 equiv) was placed and dissolved in dry methanol (10 mL) at 0 °C. Subsequently, elemental bromine (3.20 g, 20.0 mmol, 1.50 equiv) was dissolved in dry methanol (10 mL) and slowly added dropwise. After stirring at room temperature for 16 h, the reaction mixture was treated with a saturated sodium sulfite solution, dichloromethane, and deionized water, and the organic phase was separated. The aqueous phase was extracted three times with dichloromethane. The combined organic phases were then dried with anhydrous magnesium sulfate, and the solvent was removed under reduced pressure. After subsequent recrystallization from *n*-hexane, the product was obtained as colorless crystals in a yield of 83% (2.49 g, 10.9 mmol).

Mp 130 °C (Lit.: 132 – 134 °C[2]). R_f 0.47 (*n*-hexane/ethyl acetate 5:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.08 (s, 2 H), 7.06 (s, 1 H), 7.36 (s, 1 H), 10.18 (s, 1 H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 102.9 (CH_2), 108.3 (CH), 113.4 (CH), 121.8 (C_{quat}), 128.2 (C_{quat}), 148.3 (C_{quat}), 153.5 (C_{quat}), 190.5 (C_{quat}). EI MS (70 eV, m/z (%)) 230 ($[C_8H_5{}^{81}BrO_3]^+$, 86), 229 ($C_8H_5{}^{79}BrO_3]^+$, 100), 228 ($[C_8H_3{}^{81}BrO_3]^+$, 21), 227 ($[C_8H_3{}^{79}BrO_3]^+$, 15), 201 ($[C_7H_4{}^{81}BrO_2]^+$, 27), 199 ($[C_7H_4{}^{79}BrO_2]^+$, 30), 145 ($[C_4H^{81}BrO]^+$, 7) 143 ($[C_4H^{79}BrO]^+$, 11), 63 ($[C_5H_3]^+$, 18), 62 (($[C_5H_2]^+$, 23).

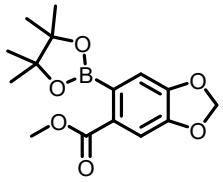
3 Synthesis and spectroscopic data of methyl 6-bromobenzo[*d*][1,3]-dioxol-5-carboxylate[3]



In a 250 mL two-neck flask, potassium hydroxide (813 mg, 14.5 mmol, 8.00 equiv) was placed and dissolved in methanol (50 mL) at 0 °C. Subsequently, 6-bromobenzo[d][1,3]dioxole-5-carbaldehyde (415 mg, 1.81 mmol, 1.00 equiv) was dissolved in methanol (80 mL) and added dropwise. This was followed by the addition of elemental iodine (1.84 g, 7.24 mmol, 4.00 equiv). The reaction mixture was stirred for 2 h at 0 °C and then for 14 h at 20 °C. The solution was then decolorized by the addition of sodium thiosulfate. Most of the solvent was subsequently removed under reduced pressure using a rotary evaporator. The residue was treated with a saturated sodium thiosulfate solution, dichloromethane, and deionized water, and the organic phase was separated. The aqueous phase was extracted three times with dichloromethane. The combined organic phases were then dried with anhydrous magnesium sulfate, and the solvent was removed under reduced pressure. After purification by column chromatography (*n*-hexane/ethyl acetate 20:1) and subsequent recrystallization from *n*-hexane, the product was obtained as colorless crystals in a yield of 94% (440 mg, 1.70 mmol).

Mp 88 °C (Lit.: 83 – 85 °C[3]). R_f 0.46 (*n*-hexane/ethyl acetate 15:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.89 (s, 3 H), 6.04 (s, 1H), 7.09 (s, 1 H), 7.32 (s, 1 H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 52.5 (CH_3), 102.6 (CH_2), 111.2 (CH), 114.5 (CH), 115.1 (C_{quat}), 124.7 (C_{quat}), 147.3 (C_{quat}), 151.1 (C_{quat}), 165.9 (C_{quat}). EI MS (70 eV, m/z (%)) 260 ([$C_9H_7{}^{81}BrO_4$]$^+$, 69), 258 ([$C_9H_7{}^{79}BrO_4$]$^+$, 74), 229 ([$C_8H_4{}^{81}BrO_3$]$^+$, 100), 227 ([$C_8H_4{}^{79}BrO_3$]$^+$, 100), 201 ([$C_7H_4{}^{81}BrO_2$]$^+$, 25), 199 ([$C_7H_4{}^{79}BrO_2$]$^+$, 27), 143 (14), 62 (18).

4 Synthesis and spectroscopic data of Piperonal boronic acid pinacol ester 3b[4]



In a sealed Schlenk tube, methyl 6-bromobenzo[d][1,3]dioxole-5-carboxylate (130 mg, 0.500 mmol, 1.00 equiv), palladium(II) acetate (6 mg, 25.0 μmol, 5.00 mol%), 2-dicyclohexylphosphino-2′,4′,6′-triisopropylbiphenyl (48 mg, 100 μmol, 20.0 mol%), and triethylamine (202 mg, 2.00 mmol, 4.00 equiv) were placed and dissolved in dry 1,4-dioxane (1.3 mL). After the slow dropwise addition of pinacolborane (192 mg, 1.50 mmol, 3.00 equiv), the mixture was stirred for 15 h at 80 °C. The reaction mixture was then treated with deionized water and dichloromethane, and the organic phase was separated. The aqueous phase was extracted three times with dichloromethane. The combined organic phases were then dried with anhydrous magnesium sulfate, and the solvent was removed under reduced pressure. After purification by column chromatography (*n*-hexane/ethyl acetate 5:1), the product **3b** was obtained as a pale-yellow resin in a yield of 49% (75 mg, 0.245 mmol).

R_f 0.41 (*n*-hexane/ethyl acetate 5:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 1.40 (s, 12 H), 3.87 (s, 3 H), 6.01 (s, 2 H), 6.87 (s, 1 H), 7.38 (s, 1 H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 25.0 (CH_3), 52.4 (CH_3), 84.1 (C_{quat}), 101.8 (CH_2), 109.3 (CH), 111.5 (CH), 127.7 (C_{quat}), 148.4 (C_{quat}), 151.2 (C_{quat}), 167.9 (C_{quat}). EI MS (70 eV, m/z (%)) 306 ([$C_{15}H_{19}{}^{11}BO_6$]$^+$, 11), 305 ([$C_{15}H_{19}{}^{10}BO_6$]$^+$, 3), 248 ([$C_{13}H_{17}{}^{11}BO_4$]$^+$, 100), 247 ([$C_{13}H_{17}{}^{12}BO_4$]$^+$, 28), 233 ([$C_{12}H_{14}{}^{11}BO_4$]$^+$, 53), 232 ([$C_{12}H_{14}{}^{10}BO_4$]$^+$, 13), 193 ([$C_9H_{10}{}^{11}BO_4$]$^+$, 32), 192 ([$C_9H_{10}{}^{10}BO_4$]$^+$, 22), 191 ([$C_8H_4{}^{11}BO_5$]$^+$, 88), 190 ([$C_8H_4{}^{10}BO_5$]$^+$, 28), 175 ([$C_8H_4{}^{11}BO_4$]$^+$, 66), 174 ([$C_8H_4{}^{10}BO_4$]$^+$, 16), 148 ([$C_7H_5{}^{11}BO_3$]$^+$, 11), 147 ([$C_7H_5{}^{10}BO_3$]$^+$, 24), 91 ([$C_{15}H_{10}NO$]$^+$, 18).

5 Synthesis of *N*-arylphenanthridinones 4 and *N*-arylcrinasiadines 5

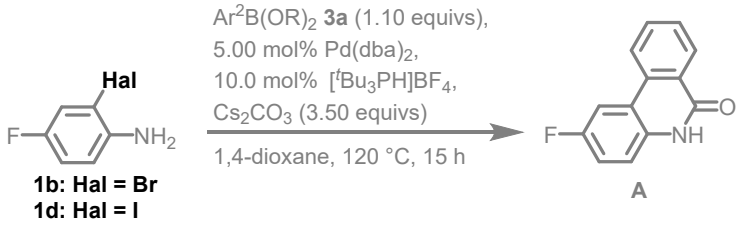
5.1 Optimization of *N*-arylphenanthridinones 4 and *N*-arylcrinasiadines 5

Table S 1. Chemical shifts of the relevant compounds in the ^{19}F NMR spectrum

compound	chemical shift δ
trichlorofluoromethane[a]	0.0
2-bromo-4-fluoroaniline (**1b**)	-126.77
4-fluoro-2-iodoaniline (**1d**)	-126.81
phenanthridinone **A**	-120.69
diarylamine **B**	-121.59
N-arylphenanthridinone **4b**	-121.01
N-arylphenanthridinone **4c**	-120.85
dihydrophenazine **C**	-122.50
dihydrophenazine **D**	-123.71

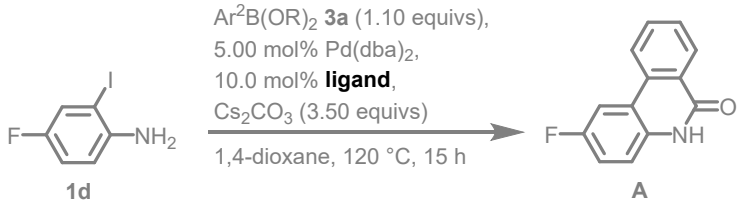
[a] Reference

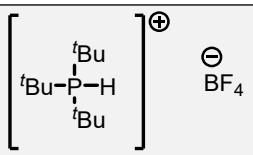
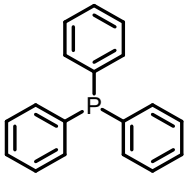
Table S2. Experimental details on the optimization of the 4-fluoro-2-haloaniline **1b** and **1d** used for the preparation of phenanthridinone **A**.

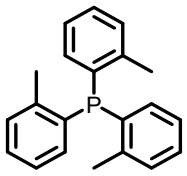
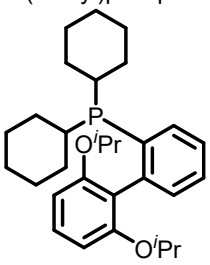
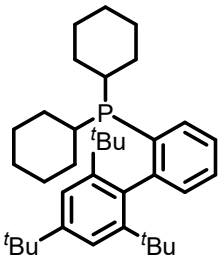
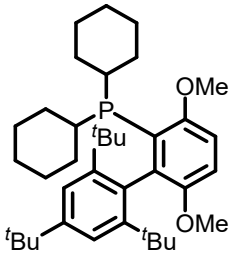
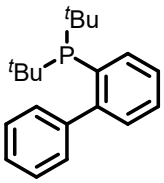
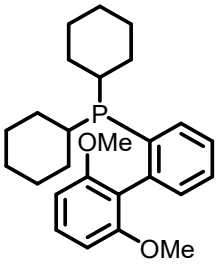


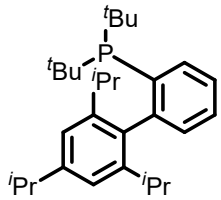
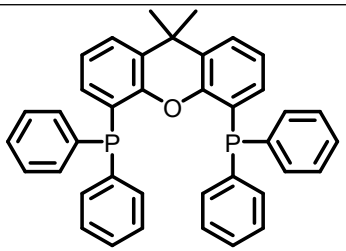
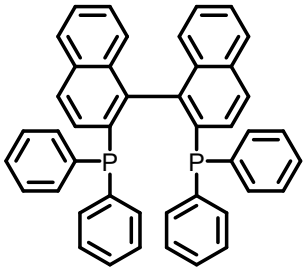
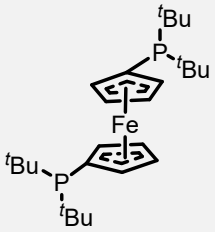
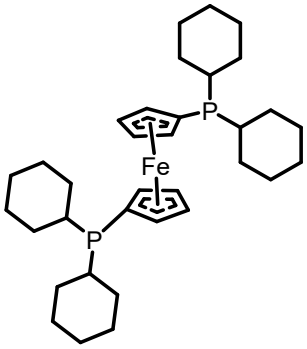
entry	aniline	yield (%)
1	2-bromo-4-fluoroaniline (**1b**)	30
2	4-fluoro-2-iodaniline (**1d**)	41

Table S3. Experimental details on the optimization of the ligand used for the preparation of phenanthridinone **A**.



entry	ligand	yield of compound A (%)
1	 [^{t}Bu$_3$PH]BF$_4$	41
2	 Triphenylphosphan	-

3	 Tri(*o*-tolyl)phosphan	-
4	 RuPhos	10
5	 XPhos	16
6	 BrettPhos	10
7	 JohnPhos	7
8	 SPhos	16

9	 *t*BuXPhos	-
10	 Xantphos	6
11	 BINAP	-
12	 DTBPF	43
13	 DCPF	12

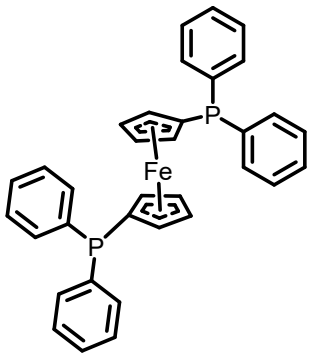
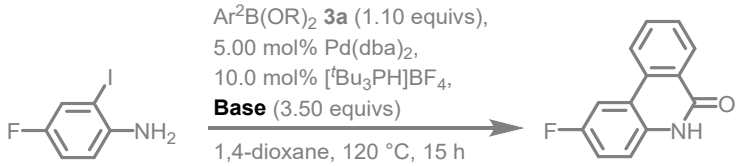
14		10
	DPPF	

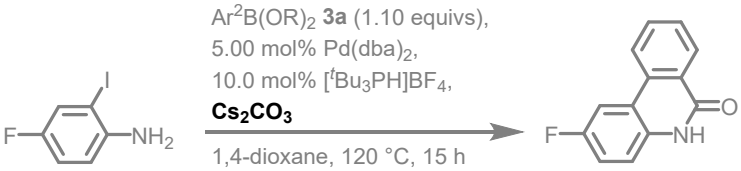
Table S4. Experimental details on the optimization of the base used for the synthesis of phenanthridinone **A**.



1d **A**

entry	base	yield of compound A (%)
1	$NaHCO_3$	-
2	Na_2CO_3	6
3	NaO^tBu	1
4	K_2CO_3	36
5	CsF	40
6	Cs_2CO_3	41

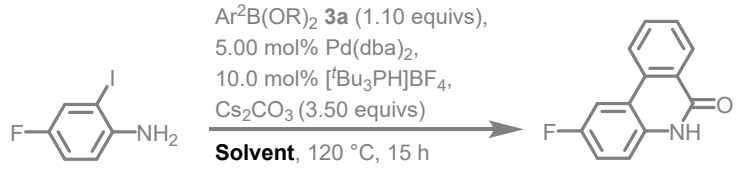
Table S5. Experimental details on the optimization of the amount of cesium carbonate base used for the synthesis of phenanthridinone **A**.



1d **A**

entry	equivs of Cs_2CO_3	yield of compound A (%)
1	2.50	10
2	3.50	41
3	4.50	-

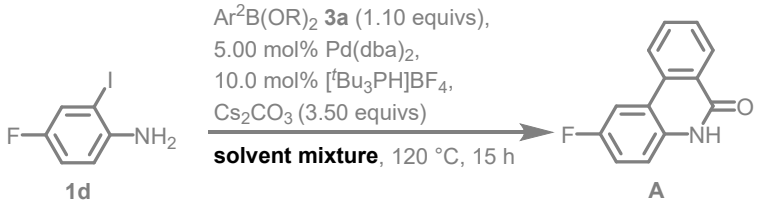
Table S6. Experimental details on the optimization of the solvent used for the preparation of phenanthridinone **A**.



1d **A**

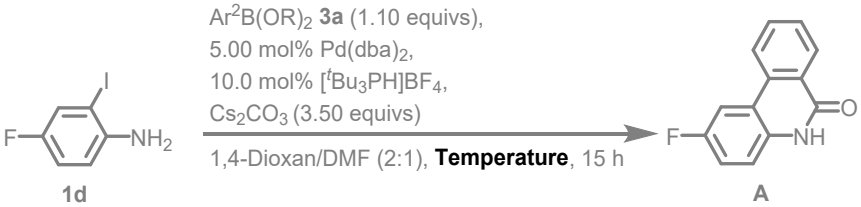
entry	solvent	yield of compound A (%)
1	1,4-dioxane	41
2	DMSO	3
3	DMF	9

Table S7. Experimental details on the optimization of the solvent mixture used for the preparation of phenanthridinone **A**.



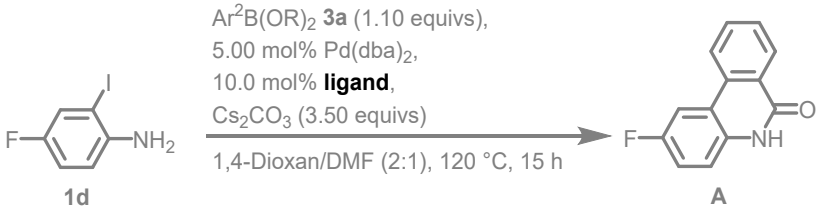
entry	Solvent mixture (ratio)	yield of compound A (%)
1	1,4-dioxane/DMF (1:1)	30
2	1,4-dioxane/DMF (2:1)	45
3	1,4-dioxane/DMF (3:1)	31

Table S8. Experimental details on the optimization of the solvent mixture for the preparation of phenanthridinone **A**.



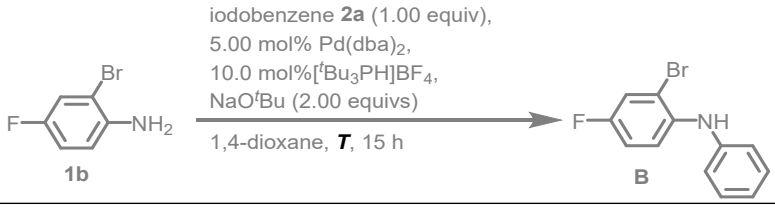
entry	temperature (°C)	yield of compound A (%)
1	80	14
2	100	3
3	120	45
4	140	15

Table S9. Experimental details on the optimization of the ligand used for the preparation of phenanthridinone **A**.



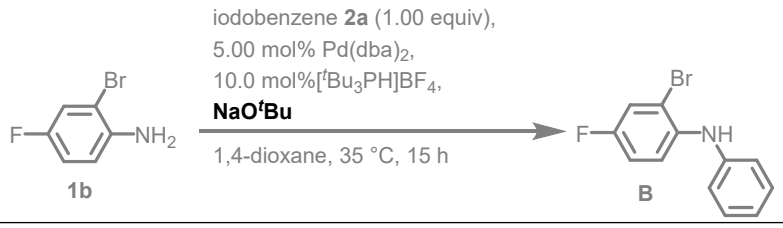
entry	ligand	yield of compound A (%)
1	[^{t}Bu$_3$PH]BF$_4$	45
2	DTBPF	9

Table S10. Experimental details on the optimization of the reaction temperature for the presentation of diarylamine **B**.



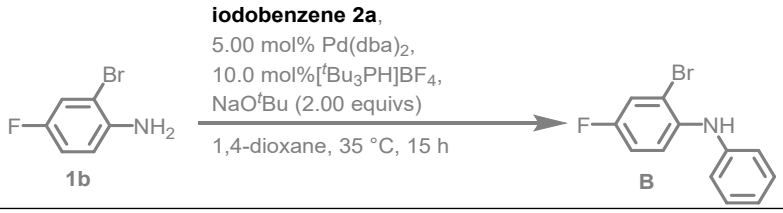
entry	*T* (°C)	yield of compound B (%)
1	20	55
2	30	67
3	35	86
4	40	72
5	50	56
6	60	30

Table S11. Experimental details for optimizing the amount of sodium tert-butoxide used for the preparation of diarylamine **B**.



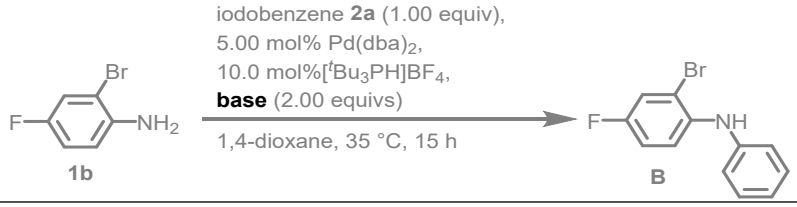
entry	NaO^tBu equivs	yield of compound B (%)
1	1.50	62
2	2.00	86
3	2.50	58

Table S12. Experimental details for optimizing the amount of aryl halide (**2a**) used for the preparation of diarylamine **B**.

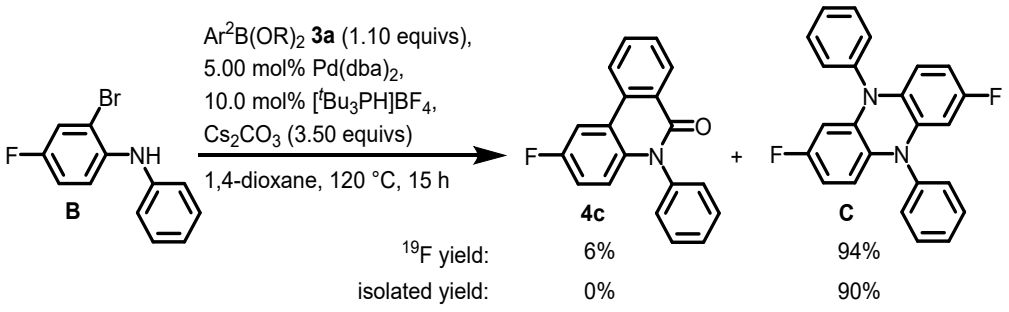


entry	aryl halide 2a equivs	yield of compound B (%)
1	1.10	74
2	1.00	86
3	0.90	64

Table S13. Experimental details on the optimization of the base used for the presentation of diarylamine **B**.

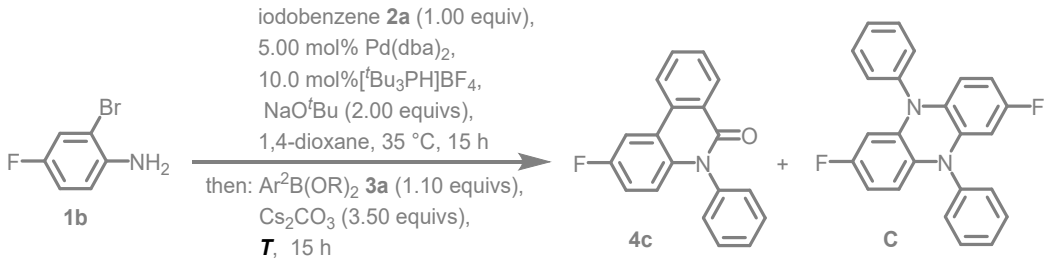


entry	base	yield of compound B (%)
1	Na_2CO_3	1
2	NaO^tBu	86
3	K_2CO_3	1
4	KO^tBu	5
5	Cs_2CO_3	10



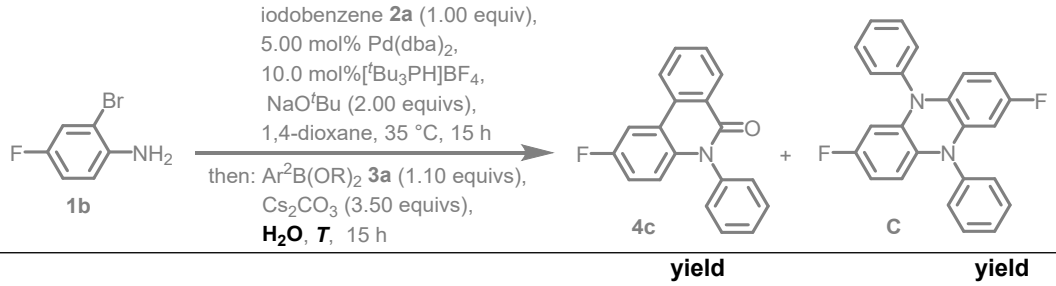
Scheme S1. *Suzuki* coupling and homocoupling of the diarylamine **B**.

Table S14. Experimental details on the optimization of the reaction temperature for the preparation of *N*-arylphenanthridinone **4c**.



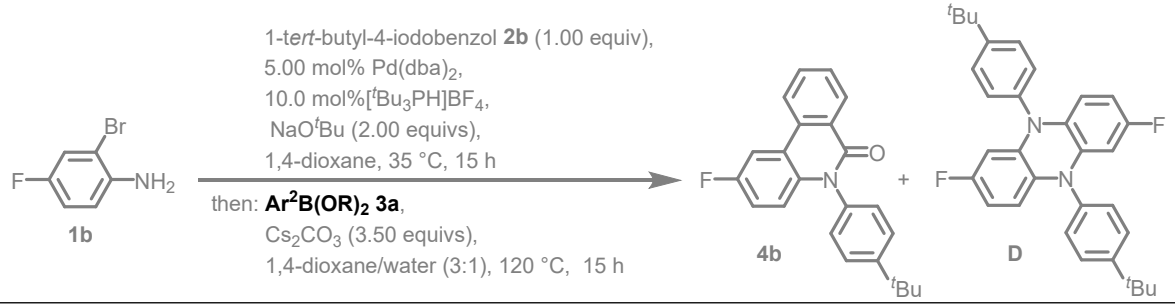
entry	temperature (°C)	yield *N*-arylphenanthridinone 4c (%)	yield dihydrophenazine C (%)
1	20	-	-
2	35	-	-
3	60	-	6
4	80	6	67
5	120	6	94

Table S15. Experimental details on the optimization of the amount of water and the reaction temperature in the *Suzuki* coupling for the preparation of the *N*-arylphenanthridinone **4c**.



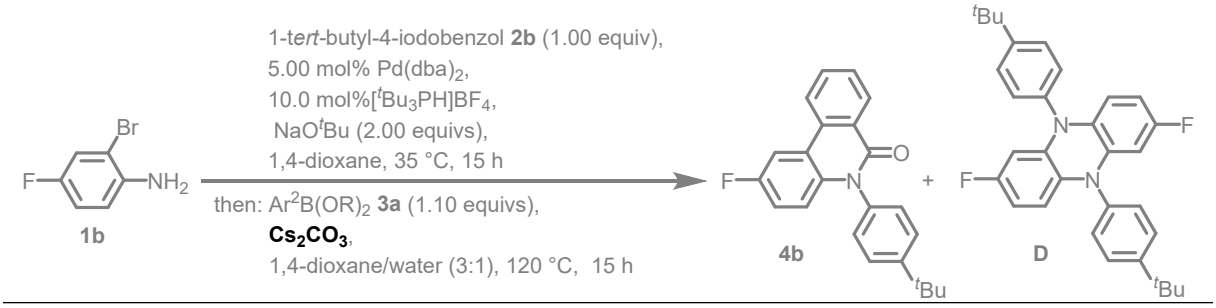
entry	ratio 1,4-dioxane:water	temperature	yield *N*-arylphenanthridinone 4c (%)	yield dihydrophenazine C (%)
1	3:1	80 °C	15	52
2	3:1	100 °C	6	30
3	2:1	120 °C	38	33
4	3:1	120 °C	40	30
5	4:1	120 °C	1	67
6	5:1	120 °C	3	32
7	1:1	120 °C	25	43

Table S16. Experimental details to optimize the amount of boronic acid for the preparation of *N*-arylphenanthridinone **4b**.

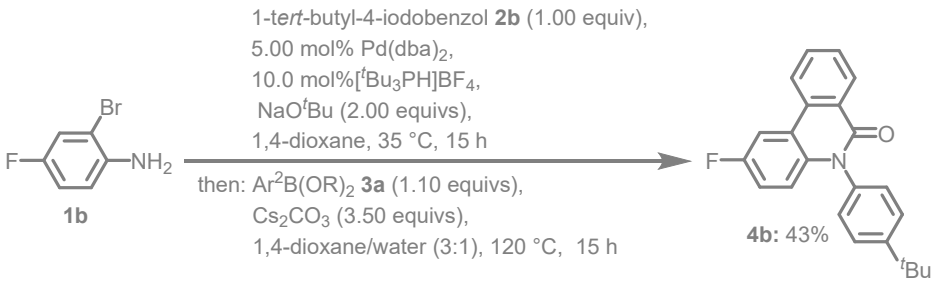


entry	boronic acid 2n equivs	yield *N*-arylphenanthridinone 4b (%)	yield dihydrophenazine D (%)
1	1.10	47	31
2	2.00	20	29
3	2.50	20	30
4	3.00	8	14

Table S17. Experimental details to optimize the amount of boronic acid for the preparation of *N*-arylphenanthridinone **4b**.

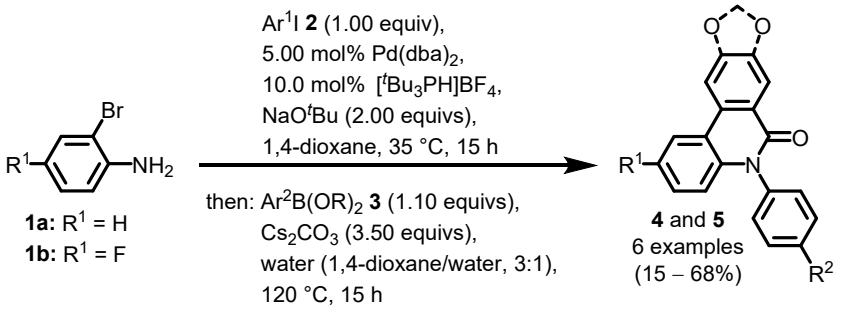


entry	Cs_2CO_3 equivs	yield *N*-arylphenanthridinon 4b (%)	yield dihydrophenazin D (%)
1	0	1	66
2	2.5	37	33
3	3.5	47	31
4	4.5	13	35



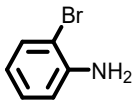
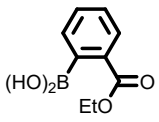
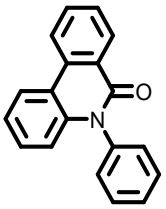
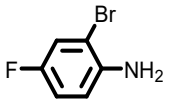
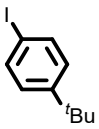
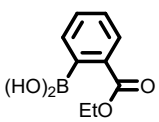
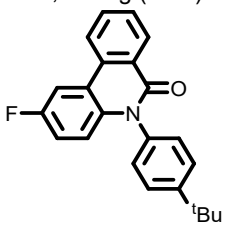
Scheme S2. Optimized reaction conditions for the three-component synthesis of *N*-arylphenanthridinone **4b**.

5.2 General procedure (GP1) for the synthesis of *N*-arylphenanthridinones 4 and *N*-arylcrinasiadines 5



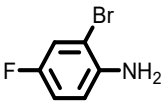
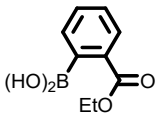
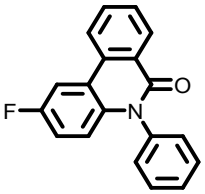
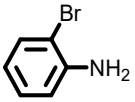
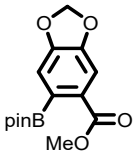
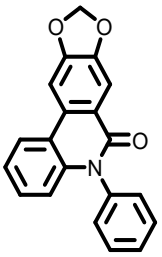
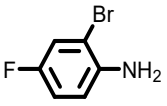
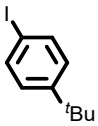
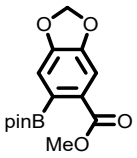
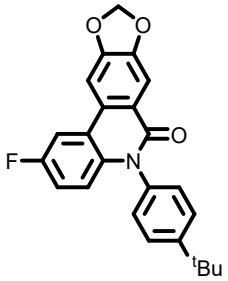
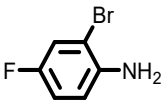
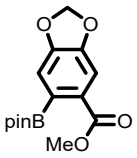
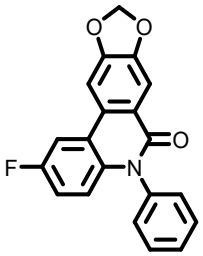
In a sealed Schlenk tube, bromoaniline **1** (0.500 mmol, 1.00 equiv), aryl iodide **2** (0.500 mmol, 1.00 equiv), bis(dibenzylideneacetone)palladium(0) (14.0 mg, 25.0 μmol, 5.00 mol%), tri-*tert*-butylphosphonium tetrafluoroborate (15.0 mg, 50.0 μmol, 10.0 mol%), and sodium *tert*-butoxide (96 mg, 1.00 mmol, 2.00 equiv) were placed and dissolved in dry 1,4-dioxane (3.5 mL). The reaction mixture was then stirred for 15 h at 35 °C. After cooling to room temperature, (hetero)arylboronic acid **3** (0.550 mmol, 1.10 equiv), cesium carbonate (570 mg, 1.75 mmol, 3.50 equiv), and water (1.2 mL) were added under a nitrogen atmosphere. The suspension was then stirred for 15 h at 120 °C. After cooling to room temperature, the reaction mixture was treated with dichloromethane and deionized water, and the organic phase was separated. The aqueous phase was then extracted three times with dichloromethane. The combined organic phases were dried with anhydrous magnesium sulfate, and the solvent was removed under reduced pressure. The crude product was purified by column chromatography and subsequently recrystallized.

Table S18. Experimental details for the synthesis of *N*-arylphenanthridinones **4** and *N*-arylcrinasiadines **5**.

entry	bromoaniline **1**	aryl iodide **2**	arylboronic acid or ester **3**	yield of product **4** or **5**[a]
1	 **1a**, 86 mg	 **2a**, 120 mg	 **3a**, 107 mg	 **4a**, 21 mg (15%)
2	 **1b**, 95 mg	 **2b**, 130 mg	 **3a**, 107 mg	 **4b**,75 mg (43%)

[a] Yields after flash chromatography on silica gel.

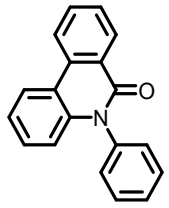
Table S19. Experimental details for the synthesis of *N*-arylphenanthridinones **4** and *N*-arylcrinasiadines **5**.

entry	bromoaniline **1**	aryl iodide **2**	arylboronic acid or ester **3**	yield of product **4** or **5**[a]
3	 **1b**, 95 mg	 **2a**, 120 mg	 **3a**, 107 mg	 **4c**, 41 mg (28%)
4	 **1a**, 86 mg	 **2a**, 120 mg	 **3b**, 168 mg	 **5a**, 61 mg (39%)
5	 **1b**, 95 mg	 **2b**, 130 mg	 **3b**, 168 mg	 **5b**, 87 mg (47%)
6	 **1b**, 95 mg	 **2a**, 120 mg	 **3b**, 168 mg	 **5c**, 113 mg (68%)

[a] Yields after flash chromatography on silica gel.

5.3 Spectroscopic data of *N*-arylphenanthridinones 4 and *N*-arylcrinasiadines 5

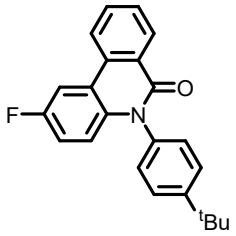
5-Phenylphenanthridin-6(5*H*)-one (4a)



The synthesis was performed by GP1. After chromatography on silica gel (*n*-hexane/ethyl acetate 2:1) and recrystallization from *n*-hexane, compound **4a** (21 mg, 77.0 μmol, 15%) was isolated as colorless crystals.

Mp 219 °C (Lit.: 220 – 222 °C[5]). R_f 0.23 (*n*-hexane/ethyl acetate 5:1). ^{1}H NMR (600 MHz, DMSO-d$_6$) δ 6.55 (dd, ^3J = 8.4 Hz, ^4J = 1.2 Hz, 1 H), 7.33 (td, ^3J = 7.6 Hz, ^4J = 1.2 Hz, 1 H), 7.38-7.42 (m, 3H), 7.56-7.59 (m, 1 H), 7.65 (dd, ^3J = 8.4 Hz, 7.0 Hz, 2 H), 7.70 (ddd, ^3J = 8.0 Hz, 7.1 Hz, ^4J = 1.0 Hz, 1 H), 7.92 (ddd, ^3J = 8.4 Hz, 7.2 Hz, ^4J = 1.5 Hz, 1 H), 8.35 (dd, ^3J = 8.0 Hz, ^4J = 1.4 Hz, 1 H), 8.55 (dd, ^3J = 8.0 Hz, ^4J = 1.6 Hz, 1 H), 8.62 (d, ^3J = 8.2 Hz, 1 H). ^{13}C NMR (150 MHz, DMSO-d$_6$) δ 116.4 (CH), 118.3 (C$_{quat}$), 122.6 (CH), 122.7 (CH), 123.6 (C$_{quat}$), 125.3 (CH), 128.0 (CH), 128.4 (CH), 128.7 (CH), 129.3 (CH), 129.5 (CH), 130.1 (CH), 133.2 (CH), 133.7 (C$_{quat}$), 138.2 (C$_{quat}$), 138.8 (C$_{quat}$), 160.4 (C$_{quat}$). EI MS (70 eV, m/z (%)) 271 (49), 270 ([M]$^+$, 100), 241 ([C$_{17}$H$_7$NO]$^+$, 28), 121 ([C$_7$H$_7$NO]$^+$, 28).

5-(4-(*tert*-Butyl)phenyl)-2-fluorophenanthridin-6(5*H*)-one (4b)

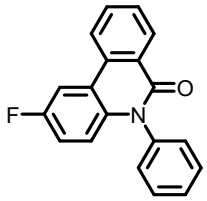


The synthesis was performed by GP1. After chromatography on silica gel (*n*-hexane/ethyl acetate 10:1) and recrystallization from *n*-hexane, compound **4b** (75 mg, 0.217 mmol, 43%) was isolated as colorless crystals.

Mp 208 °C. R_f 0.21 (*n*-hexane/ethyl acetate 10:1). ^{1}H NMR (600 MHz, DMSO-d$_6$) δ 1.39 (s, 9 H), 6.55 (dd, ^3J = 9.3 Hz, ^4J = 4.9 Hz, 1 H), 7.21-7.33 (m, 3 H), 7.59-7.68 (m, 2 H), 7.73 (ddd, ^3J = 8.2 Hz, 7.2 Hz, ^{4}J = 1.1 Hz, 1 H), 7.93 (ddd, ^3J = 8.4 Hz, 7.1 Hz, ^4J = 1.5 Hz, 1 H), 8.35 (dd, ^3J = 8.0 Hz, ^4J = 1.4 Hz, 1 H), 8.42 (dd, ^3J = 10.2 Hz, ^4J = 2.9 Hz, 1 H), 8.62 (d, ^3J = 8.2 Hz, 1 H). ^{13}C NMR (150 MHz, DMSO-d$_6$) δ 31.2 (CH$_3$), 34.6 (C$_{quat}$), 109.6 (d, CH, ^2J = 24.2 Hz), 116.9 (d, CH, ^2J = 23.5 Hz), 118.3 (d, CH, ^3J = 8.8 Hz), 119.8 (d, C$_{quat}$, ^3J = 8.6 Hz), 123.2 (CH), 125.5 (C$_{quat}$), 126.9 (CH), 128.1 (CH), 128.7 (CH), 129.0 (CH), 132.9 (d, C$_{quat}$, ^4J = 2.8 Hz), 133.2 (CH), 135.4 (C$_{quat}$), 135.6 (C$_{quat}$), 151.2 (C$_{quat}$), 158.0 (d, C$_{quat}$, ^2J = 239.4 Hz), 160.2 (C$_{quat}$). EI MS (70 eV, m/z (%)) 346 (19), 345 ([M]$^+$, 69), 331 (26), 330 ([C$_{23}$H$_{21}$FN]$^+$, 100), 196 ([C$_{13}$H$_5$FO]$^+$, 33), 151 (35). IR ($\tilde{\nu}$ [cm^{-1}]) 1647 (s), 1607 (w), 1589 (m), 1570 (w), 1497 (m), 1460 (w), 1447 (w), 1423 (m), 1408 (w), 1393 (w), 1341 (m), 1331 (m), 1308 (m), 1290 (w), 1265 (w), 1231 (w), 1184 (m), 1136 (m), 1105 (w), 1042 (w), 1022 (w), 970 (w), 899 (m),

889 (m), 839 (m), 824 (m), 802 (s), 772 (s), 716 (m), 692 (m), 665 (m), 617 (s). HRMS (ESI) calcd. for $[C_{23}H_{20}FNO]^+$ 346.1602, found 346.1605. HPLC (ethyl acetate): 95% (6.8 min).

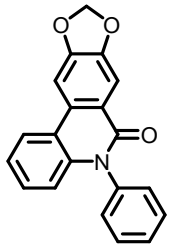
2-Fluoro-5-phenylphenanthridin-6(5*H*)-one (4c)



The synthesis was performed by GP1. After chromatography on silica gel (*n*-hexane/ethyl acetate 2:1) and recrystallization from *n*-hexane, compound **4c** (41 mg, 0.142 mmol, 28%) was isolated as colorless crystals.

Mp 286 °C. R_f 0.07 (*n*-hexane/ethyl acetate 10:1). ^{1}H NMR (600 MHz, DMSO-d_6) δ 6.55 (dd, ^3J = 9.2 Hz, ^4J = 4.9 Hz, 1H), 7.28 (ddd, ^3J = 9.3 Hz, 8.0 Hz, ^4J = 2.9 Hz, 1 H), 7.37-7.44 (m, 2 H), 7.50-7.62 (m, 1 H), 7.63-7.69 (m, 2 H), 7.74 (ddd, ^3J = 8.1 Hz, 7.2 Hz, ^4J = 1.1 Hz, 1 H), 7.93 (ddd, ^3J = 8.3 Hz, 7.2 Hz, ^4J = 1.5 Hz, 1 H), 8.35 (dd, ^3J = 7.9 Hz, ^4J = 1.0 Hz, 1 H), 8.44 (dd, ^3J = 10.3 Hz, ^4J = 2.9 Hz, 1 H), 8.63 (d, ^3J = 8.6 Hz, 1 H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 109.7 (d, CH, ^2J = 24.3 Hz), 116.8 (d, CH, ^2J = 23.5 Hz), 118.2 (d, CH, ^3J = 8.6 Hz), 119.8 (d, C_{quat}, ^3J = 8.4 Hz), 123.3 (CH), 125.5 (CH), 128.1 (CH), 128.8 (CH), 129.1 (CH), 129.3 (CH), 130.2 (CH), 132.9 (d, C_{quat}, ^4J = 2.5 Hz), 133.3 (C_{quat}), 135.6 (C_{quat}), 138.1 (C_{quat}), 158.0 (d, C_{quat}, ^1J = 239.2 Hz), 160.1 (C_{quat}). EI MS (70 eV, m/z (%)) 290 (18), 289 ([M]$^+$, 89), 288 ($[C_{19}H_{11}FNO]^+$, 100), 259 ($[C_{19}H_{17}N]^+$, 17). IR ($\tilde{\nu}$ [cm^{-1}]) 1651 (s), 1609 (w), 1587 (w), 1564 (w), 1539 (w), 1491 (m), 1445 (w), 1422 (w), 1335 (m), 1310 (w), 1285 (w), 1269 (w), 1227 (w), 1213 (w), 1184 (m), 1173 (w), 1152 (w), 1136 (m), 1123 (w), 1030 (w), 962 (w), 916 (w), 897 (w), 866 (m), 827 (m), 766 (m), 756 (m), 727 (m), 716 (m), 691 (s), 667 (w), 650 (m), 610 (m). HRMS (ESI) calcd. for $[C_{19}H_{12}FNO+H]^+$ 290.0976, found 290.0967. HPLC (acetonitrile): 99% (5.2 min).

5-Phenyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (5a)

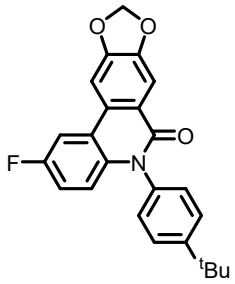


The synthesis was performed by GP1. After chromatography on silica gel (*n*-hexane/ethyl acetate 2:1) and recrystallization from *n*-hexane, compound **5a** (61 mg, 0.193 mmol, 39%) was isolated as colorless crystals.

Mp 232 °C. R_f 0.10 (*n*-hexane/ethyl acetate 5:1). ^{1}H NMR (600 MHz, DMSO-d_6) δ 6.26 (s, 2 H), 6.51 (dd, ^3J = 8.4 Hz, ^4J = 1.2 Hz, 1 H), 7.28 (ddd, ^3J = 8.2 Hz, 7.1 Hz, ^4J = 1.2 Hz, 1 H), 7.32-7.34 (m, 1 H), 7.35-7.37 (m, 2 H), 7.56 (tt, , ^3J = 6.8 Hz, ^4J = 1.2 Hz, 1 H), 7.62-7.65 (m, 2 H), 7.66 (s, 1 H), 8.15 (s, 1 H), 8.44 (dd, ^3J = 8.1 Hz, ^3J = 1.5 Hz, 1 H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 101.5 (CH), 102.4 (CH_2), 105.5 (CH), 116.2 (CH), 118.4 (C_{quat}), 120.6 (C_{quat}), 122.5

(CH), 123.6 (CH), 128.6 (CH), 128.8 (CH), 129.3 (CH), 130.0 (CH), 130.7 (C_{quart}), 138.1 (C_{quat}), 138.2 (C_{quat}), 148.4 (C_{quat}), 152.5 (C_{quat}), 159.7 (C_{quat}). EI MS (70 eV, m/z (%)) 316 (22), 315 (95), 314 ([M]$^+$, 100), 256 ([$C_{19}H_{14}N$]$^+$, 18), 228 ([$C_{14}H_{14}NO_2$]$^+$, 22), 114 (31), 77 ([C_6H_5]$^+$, 13). IR ($\tilde{\nu}$ [cm^{-1}]) 1649 (m), 1636 (m), 1622 (m), 1599 (m), 1574 (w), 1499 (m), 1479 (m), 1456 (s), 1393 (m), 1341 (m), 1310 (m), 1269 (m), 1252 (m), 1238 (m), 1196 (m), 1165 (w), 1144 (w), 1119 (w), 1069 (m), 1030 (s), 1005 (w), 974 (w), 928 (m), 903 (w), 881 (w), 833 (w), 814 (w), 781 (w), 758 (m), 739 (s), 694 (s), 675 (m), 635 (m), 611 (w). Anal. calcd. for $C_{20}H_{13}NO_3$ [315.1] C 76.18, H 4.16, N 4.44; Found C 76.27, H 4.18, N 4.26.

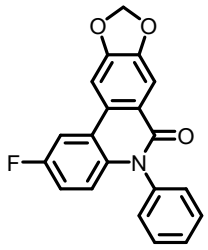
5-(4-(*tert*-Butyl)phenyl)-2-fluoro-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (5b)



The synthesis was performed by GP1. After chromatography on silica gel (*n*-hexane/ethyl acetate 5:1) and recrystallization from *n*-hexane, compound **5b** (87 mg, 0.223 mmol, 45%) was isolated as colorless crystals.

Mp 296 °C. R_f 0.23 (*n*-hexane/ethyl acetate 5:1). ^{1}H NMR (600 MHz, DMSO-d$_6$) δ 1.38 (s, 9 H), 6.27 (s, 2 H), 6.51 (dd, ^3J = 9.2 Hz, ^4J = 5.0 Hz, 1 H), 7.24 (ddd, ^3J = 9.2 Hz, 7.9 Hz, ^4J = 2.8 Hz, 1 H), 7.26-7.29 (m, 2 H), 7.59-7.67 (m, 3 H), 8.16 (s, 1 H), 8.32 (dd, ^3J = 10.5 Hz, ^3J = 2.9 Hz, 1 H). ^{13}C NMR (150 MHz, DMSO-d$_6$) δ 30.9 (CH_3), 101.8 (CH), 102.3 (CH_2), 105.3 (CH), 109.2 (d, CH, ^2J = 23.8 Hz), 115.8 (d, CH, ^2J = 23.9 Hz), 117.8 (d, CH, ^3J = 8.6 Hz), 119.5 (d, C_{quat}, ^3J = 8.4 Hz), 120.8 (C_{quat}), 126.6 (CH), 128.4 (CH), 129.6 (d, C_{quat}, ^4J = 2.7 Hz), 134.7 (C_{quat}), 135.2 (C_{quat}), 148.6 (C_{quat}), 150.8 (C_{quat}), 152.2 (C_{quat}), 157.7 (d, C_{quat}, ^1J = 238.2 Hz), 159.3 (C_{quat}). EI MS (70 eV, m/z (%)) 390 (22), 389 ([M]$^+$, 75), 388 (11), 375 ([$C_{24}H_{22}FNO_2$]$^+$, 29), 374 ([$C_{23}H_{18}FNO_3$]$^+$, 100), 332 ([$C_{20}H_{11}FNO_3$]$^+$, 13), 240 ([$C_{16}H_{15}FN$]$^+$, 23), 182 (21), 173 ([$C_{11}H_{11}NO$]$^+$, 36). IR ($\tilde{\nu}$ [cm^{-1}]) 1649 (s), 1622 (m), 1584 (w), 1501 (s), 1485 (s), 1456 (s), 1429 (w), 1406 (w), 1383 (m), 1362 (w), 1341 (w), 1315 (m), 1298 (m), 1277 (w), 1256 (s), 1204 (s), 1177 (m), 1146 (w), 1113 (w), 1059 (w), 1036 (s), 1007 (m), 968 (w), 924 (m), 899 (m), 860 (s), 839 (w), 810 (s), 779 (w), 725 (w), 716 (w), 687 (w), 656 (m), 638 (w), 617 (s). HRMS (ESI) calcd. for [$C_{24}H_{20}FNO_3$+H]$^+$ 390.1500, found 390.1505. HPLC (acetone): 99% (6.8 min).

2-Fluoro-5-Phenyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (5c)

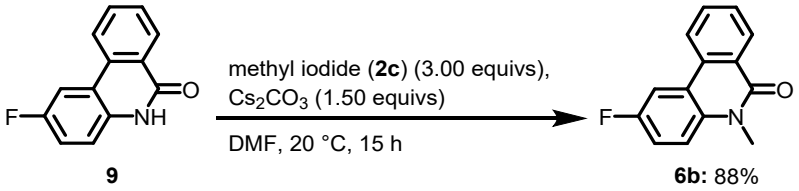


The synthesis was performed by GP1. After chromatography on silica gel (*n*-hexane/ethyl acetate 2:1) and recrystallization from *n*-hexane, compound **5c** (113 mg, 0.339 mmol, 68%) was isolated as colorless crystals.

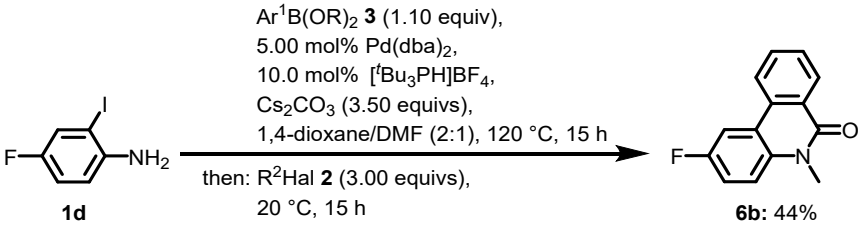
Mp 320 °C. R_f 0.09 (*n*-hexane/ethyl acetate 5:1). ^{1}H NMR (600 MHz, DMSO-d_6) δ 6.28 (s, 2 H), 6.51 (dd, ^3J = 9.2 Hz, ^4J = 5.0 Hz, 1 H), 7.22 (ddd, ^3J = 9.3 Hz, 7.9 Hz, ^4J = 2.9 Hz, 1 H), 7.35-7.41 (m, 2 H), 7.54-7.60 (m, 1 H), 7.61-7.69 (m, 3 H), 8.18 (s, 1 H), 8.34 (dd, ^3J = 10.5 Hz, ^4J = 2.9 Hz, 1 H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 102.1 (CH), 102.6 (CH_2), 105.6 (CH), 108.9 (d, C_{quart}, ^3J = 7.6 Hz), 109.5 (d, CH, ^2J = 24.3 Hz), 117.6 (d, CH, ^3J = 7.0 Hz), 121.1 (C_{quart}), 128.8 (CH), 129.3 (CH), 129.8 (d, CH, ^2J = 27.7 Hz), 130.1 (CH), 131.1 (d, C_{quart}, ^4J = 3.7 Hz), 138.2 (C_{quart}), 140.7 (C_{quart}), 140.8 (C_{quart}), 148.9 (C_{quart}), 152.5 (C_{quart}), 159.5 (d, C_{quart}, ^1J = 238.2 Hz). EI MS (70 eV, m/z (%)) 334 (15), 333 (69), 332 ([M]$^+$, 100), 274 ([$C_{18}H_{12}NO_2$]$^+$, 23), 246 ([$C_{14}H_{13}FNO_2$]$^+$, 26), 245 ([$C_{14}H_{12}FNO_2$]$^+$, 11), 182 ([$C_{12}H_5FN$]$^+$, 14), 138 (13), 123 ([$C_7H_7O_2$]$^+$, 21). IR ($\tilde{\nu}$ [cm^{-1}]) 1647 (s), 1626 (w), 1611 (w), 1582 (w), 1562 (w), 1504 (m), 1485 (s), 1452 (m), 1423 (m), 1381 (m), 1342 (w), 1315 (m), 1302 (m), 1287 (w), 1269 (w), 1254 (m), 1240 (m), 1196 (m), 1177 (m), 1140 (w), 1119 (w), 1105 (w), 1076 (w), 1061 (w), 1038 (s), 1003 (m), 991 (w), 968 (w), 937 (s), 887 (w), 852 (s), 812 (m), 793 (w), 779 (w), 758 (s), 727 (w), 712 (w), 696 (s), 654 (s), 625 (s), 602 (s). HRMS (ESI) calcd. for [$C_{20}H_{12}FNO_3$+H]$^+$ 334.0874, found 334.0855. HPLC (acetonitrile): 99% (5.2 min).

6 Synthesis of *N*-alkylphenanthridinones 6 and *N*-alkylcrinasiadines 7

6.1 Optimization of *N*-alkylphenanthridinones 6 and *N*-alkylcrinasiadines 7

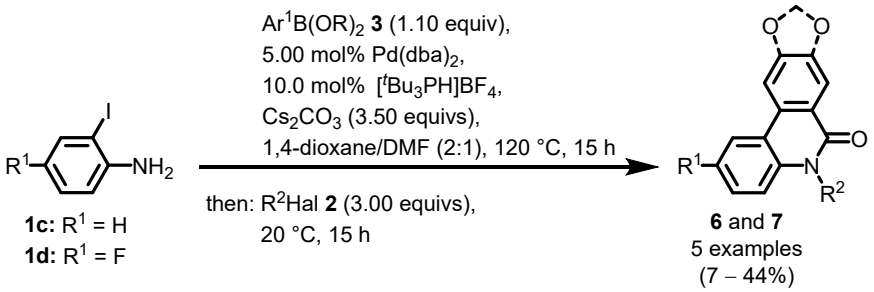


Scheme S3. Preparation of the *N*-alkylphenanthridinone **6b** via nucleophilic substitution with methyl iodide (**2c**).



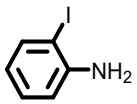
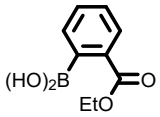
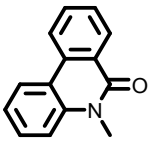
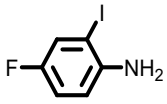
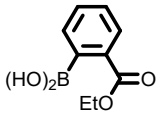
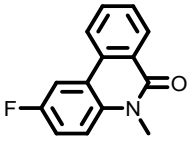
Scheme S4. Optimized reaction conditions for the three-component synthesis of *N*-alkylphenanthridinone **6b**.

6.2 General procedure (GP2) for the synthesis of *N*-alkylphenanthridinones 6 and *N*-alkylcrinasiadines 7



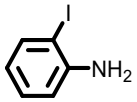
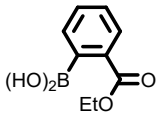
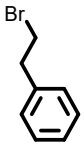
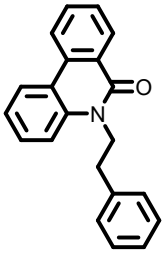
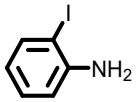
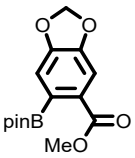
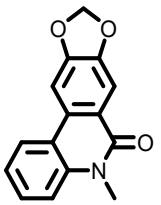
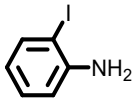
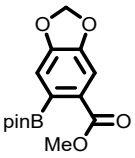
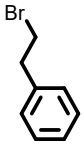
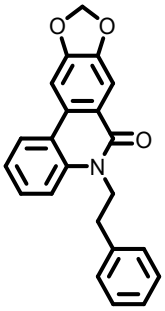
In a sealed Schlenk tube, 2-iodoaniline **1** (0.500 mmol, 1.00 equiv), (hetero)arylboronic acid **3** (0.550 mmol, 1.10 equiv), bis(dibenzylideneacetone)palladium(0) (14.0 mg, 25.0 μmol, 5.00 mol%), tri-*tert*-butylphosphonium tetrafluoroborate (15.0 mg, 50.0 μmol, 10.0 mol%), and cesium carbonate (570 mg, 1.75 mmol, 3.50 equiv) were placed and dissolved in dry 1,4-dioxane (2.3 mL) and dry DMF (1.2 mL). The reaction mixture was then stirred for 15 h at 120 °C. After cooling to room temperature, alkyl halide **2** (1.50 mmol, 3.00 equiv) was added under a nitrogen atmosphere, and the suspension was stirred for 15 h at 20 °C. After cooling to room temperature, the reaction mixture was treated with dichloromethane and deionized water, and the organic phase was separated. The aqueous phase was then extracted three times with dichloromethane. The combined organic phases were dried with anhydrous magnesium sulfate, and the solvent was removed under reduced pressure. The crude product was purified by column chromatography and subsequently recrystallized.

Table S20. Experimental details for the synthesis of *N*-alkylphenanthridinones **6** and *N*-alkylcrinasiadines **7**.

entry	iodoaniline **1**	arylboronic acid or ester **3**	aryl halide **2**	yield of product **6** or **7**[a]
1	 **1c**, 110 mg	 **3a**, 107 mg	 **2c**, 213 mg	 **6a**, 42 mg (40%)
2	 **1d**, 119 mg	 **3a**, 107 mg	 **2c**, 213 mg	 **6b**, 51 mg (44%)

[a] Yields after flash chromatography on silica gel.

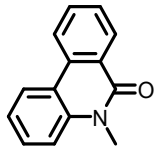
Table 20. Experimental details for the synthesis of *N*-alkylphenanthridinones **6** and *N*-alkylcrinasiadines **7**.

entry	iodoaniline **1**	arylboronic acid or ester **3**	aryl halide **2**	yield of product **6** or **7**[a]
3	 **1c**, 110 mg	 **3a**, 107 mg	 **2d**, 278 mg	 **6c**, 27 mg (17%)
4	 **1c**, 110 mg	 **3b**, 168 mg	 **2c**, 213 mg	 **7a**, 47 mg (37%)
5	 **1c**, 110 mg	 **3b**, 168 mg	 **2d**, 278 mg	 **7b**, 12 mg (7%)

[a] Yields after flash chromatography on silica gel.

6.3 Spectroscopic data of *N*-alkylphenanthridinones 6 and *N*-alkylcrinasiadines 7

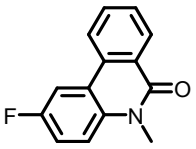
5-Methylphenanthridin-6(5*H*)-one (6a)



The synthesis was performed by GP2. After chromatography on silica gel (*n*-hexane/ethyl acetate 2:1) and recrystallization from *n*-hexane, compound **6a** (42 mg, 0.201 mmol, 40%) was isolated as colorless crystals.

Mp 111 °C (Lit.: 108 – 110 °C[6]). R_f 0.52 (*n*-hexane/ethyl acetate 2:1). ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.82 (s, 3 H), 7.33 (ddd, ^3J = 8.2 Hz, 7.1 Hz, ^4J = 1.2 Hz, 1 H), 7.42 (dd, ^3J = 8.5 Hz, ^4J = 1.2 Hz, 1 H), 7.57 (dddd, ^3J = 9.9 Hz, 8.6 Hz, 7.1 Hz, ^4J = 1.3 Hz, 2 H), 7.76 (ddd, ^3J = 8.4 Hz, 7.2 Hz, ^4J = 1.5 Hz, 1 H), 8.25-8.33 (m, 2 H), 8.56 (ddd, ^3J = 8.0 Hz, ^4J = 1.5 Hz, 0.6 Hz, 1 H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 30.1 (CH_3), 115.2 (CH), 119.5 (CH), 121.8 (C_{quat}), 122.6 (CH), 123.4 (C_{quat}), 125.8 (C_{quat}), 128.1 (CH), 129.1 (CH), 129.7 (CH), 132.6 (CH), 133.7 (CH), 138.2 (C_{quat}), 161.8 (C_{quat}). EI MS (70 eV, m/z (%)) 209 ([M]$^+$, 100), 180 ([$C_{13}H_{10}N$]$^+$, 35), 178 ([$C_{13}H_8N$]$^+$, 33), 152 ([$C_{12}H_8$]$^+$, 19).

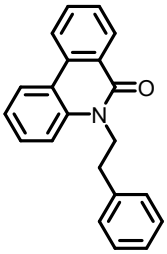
2-Fluoro-5-methylphenanthridin-6(5*H*)-one (6b)



The synthesis was performed by GP2. After chromatography on silica gel (*n*-hexane/ethyl acetate 1:1) and recrystallization from *n*-hexane, compound **6b** (51 mg, 0.224 mmol, 44%) was isolated as colorless crystals.

Mp 170 – 171 °C (Lit.: 126 – 128 °C[7]). R_f 0.20 (*n*-hexane/ethyl acetate 5:1). ^{1}H NMR (600 MHz, DMSO-d_6) δ 3.72 (s, 3 H), 7.47 (ddd, ^3J = 9.2 Hz, 8.0 Hz, ^4J = 2.9 Hz, 1 H), 7.60 (dd, ^3J = 9.2 Hz, 4.8 Hz, 1 H), 7.68 (ddd, ^3J = 8.0 Hz, 7.1 Hz, ^4J = 1.1 z, 1 H), 7.85 (ddd, ^3J = 8.3 Hz, 7.1 Hz, ^4J = 1.5 Hz, 1 H), 8.33 8.38 (m, 2 H), 8.53 (d, ^3J = 8.1 Hz, 1 H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 30.0 (CH_3), 109.6 (d, CH, ^2J = 23.9 Hz), 117.0 (d, CH, ^2J = 23.4 Hz), 117.6 (d, CH , ^3J = 8.3 Hz), 120.0 (d, C_{quat}, ^3J = 8.1 Hz), 123.0 (CH), 125.2 (C_{quat}), 128.1 (CH), 128.8 (CH), 132.4 (d, C_{quat}, ^4J = 2.9 Hz), 132.8 (CH), 134.3 (C_{quat}), 158.0 (d, C_{quat}, ^1J = 238.8 Hz), 160.1 (C_{quat}). EI MS (70 eV, m/z (%)) 227 ([M]$^+$, 100), 226 ([$C_{14}H_9FNO$]$^+$, 24), 198 ([$C_{13}H_9FN$]$^+$, 31), 196 ([$C_{13}H_7FN$]$^+$, 31), 170 ([$C_{11}H_8NO$]$^+$, 20).

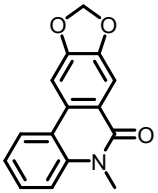
5-Phenethylphenanthridin-6(5*H*)-one (6c)



The synthesis was performed by GP2. After chromatography on silica gel (*n*-hexane/ethyl acetate 10:1) and recrystallization from *n*-hexane, compound **6c** (27 mg, 0.085 mmol, 17%) was isolated as colorless crystals.

Mp 91 °C (Lit.: 81.2 – 82.2 °C[8]). R_f 0.29 (*n*-hexane/ethyl acetate 10:1). ^{1}H NMR (600 MHz, DMSO-d_6) δ 2.91-3.05 (m, 2 H), 4.46-4.65 (m, 2 H), 7.22-7.27 (m, 1 H), 7.34 (dd, ^3J = 8.4 Hz, 6.8 Hz, 2 H), 7.36-7.41 (m, 3 H), 7.63-7.69 (m, 2 H), 7.72 (dd, ^3J = 8.6 Hz, ^4J = 1.1 Hz, 1 H), 7.87 (ddd, ^3J = 8.3 Hz, 7.1 Hz, ^4J = 1.5 Hz, 1 H), 8.38 (ddd, ^3J = 7.9 Hz, ^4J =1.5, 0.5 Hz, 1 H), 8.54 (dd, ^3J = 8.1 Hz, ^4J = 1.5 Hz, 1 H), 8.56 (dd, ^3J = 8.1 Hz, ^4J = 0.9 Hz, 1 H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 33.1 (CH_2), 43.4 (CH_2), 115.5 (CH), 118.6 (CH), 122.5 (CH), 123.9 (CH), 124.8 (C_{quat}), 126.5 (CH), 128.0 (CH), 128.2 (CH), 128.5 (CH), 128.8 (CH), 130.2 (CH), 132.9 (CH), 133.3 (C_{quat}), 136.5 (C_{quat}), 138.4 (C_{quat}),138.5 (C_{quat}), 160.1 (C_{quat}). EI MS (70 eV, m/z (%)) 299 ([M]$^+$, 100), 208 ([$C_{14}H_{10}NO$]$^+$, 14), 196 (16), 195 ([$C_{13}H_9NO$]$^+$, 100), 178 ([$C_{13}H_8N$]$^+$, 75), 152 ([$C_{11}H_6N$]$^+$, 20), 151 (12), 91 ([C_7H_7]$^+$, 16), 77 ([C_6H_5]$^+$, 12).

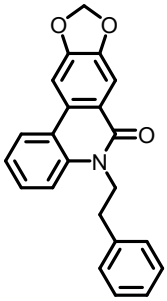
5-Methyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (7a)



The synthesis was performed by GP2. After chromatography on silica gel (*n*-hexane/ethyl acetate 2:1) and recrystallization from *n*-hexane, compound **7a** (47 mg, 0.186 mmol, 37%) was isolated as colorless crystals.

Mp 244 °C (Lit.: 243 – 245 °C[9]). R_f 0.12 (*n*-hexane/ethyl acetate 5:1). ^{1}H NMR (300 MHz, DMSO-d_6) δ 3.71 (s, 3 H), 6.23 (s, 2 H), 7.32 (ddd, ^3J = 8.2 Hz, 6.4 Hz, ^4J = 1.8 Hz, 1 H), 7.53-7.59 (m, 2 H), 7.69 (s, 1 H), 8.07 (s, 1 H), 8.40 (dd, ^3J = 8.0 Hz, ^3J = 1.3 Hz, 1 H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 29.7 (CH_3), 101.3 (CH), 102.3 (CH_2), 105.6 (CH), 115.4 (CH), 118.5 (C_{quat}), 120.4 (C_{quat}), 122.3 (CH), 123.6 (CH), 129.2 (CH), 130.1 (C_{quat}), 137.0 (C_{quat}), 148.2 (C_{quat}), 152.1 (C_{quat}), 159.7 (C_{quat}). EI MS (70 eV, m/z (%)) 254 (17), 253 ([M]$^+$, 100), 252 (14).

5-Phenethyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (7b)

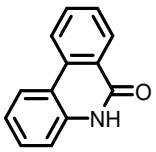


The synthesis was performed by GP2. After chromatography on silica gel (*n*-hexane/ethyl acetate 5:1) and recrystallization

from *n*-hexane, compound **7b** (12 mg, 0.035 mmol, 7%) was isolated as colorless crystals.

Mp 154 °C (Lit.: 154 – 157 °C[9]). R_f 0.21 (*n*-hexane/ethyl acetate 5:1). ^{1}H NMR (600 MHz, DMSO-d_6) δ 2.90-3.07 (m, 2 H), 4.47-4.60 (m, 2 H), 6.24 (s, 2 H), 7.23-7.27 (m, 1 H), 7.30-7.35 (m, 3 H), 7.36-7.40 (m, 2H), 7.59 (ddd, ^3J = 8.5 Hz, 7.0 Hz, ^4J = 1.4 Hz, 1 H), 7.68 (dd, ^3J = 8.6 Hz, ^4J = 1.1 Hz, 1 H), 7.69 (s, 1 H), 8.08 (s, 1 H), 8.43 (dd, ^3J = 8.3 Hz, ^4J = 1.4 Hz, 1 H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 33.2 (CH_2), 43.4 (CH_2), 101.3 (CH), 102.3 (CH_2), 105.5 (CH), 115.3 (CH), 118.7 (C_{quat}), 120.3 (C_{quat}), 122.3 (CH), 123.9 (CH), 126.5 (CH), 128.5 (CH), 128.8 (CH), 129.4 (CH), 130.2 (C_{quat}), 135.9 (C_{quat}), 138.5 (C_{quat}), 148.2 (C_{quat}), 152.3 (C_{quat}), 159.4 (C_{quat}). EI MS (70 eV, m/z (%)) 344 (18), 343 ($[M]^+$, 47), 252 ($[C_{15}H_{10}NO_3]^+$, 24), 240 (17), 239 ($[C_{14}H_8NO_3]^+$, 100), 223 (17), 222 ($[C_{14}H_8NO_2]^+$, 62), 91 ($[C_7H_7]^+$, 14).

7 Synthesis of 6(*5H*)-phenanthridinone 8



In a sealed Schlenk tube were placed 2-iodoaniline (219 mg, 1.00 mmol, 1.00 equiv), 2-(ethoxycarbonyl)phenylboronic acid **3a** (233 mg, 1.20 mmol, 1.20 equiv), bis(dibenzylideneacetone)palladium(0) (29.0 mg, 50.0 µmol, 5.00 mol%), tri tert-butylphosphonium tetrafluoroborate (29.0 mg, 100 µmol, 10.0 mol%) and cesium carbonate (1.14 g, 3.50 mmol, 3.50 equiv) and the mixture was dissolved in dry 1,4-dioxane (4 mL). The reaction mixture was degassed with nitrogen for 5 min and then stirred for 15 h at 120 °C. After cooling to room temperature, deionized water and dichloromethane were added to the resulting suspension and the organic layer was separated. The aqueous phase was extracted three times with dichloromethane. The combined organic phases were dried over anhydrous magnesium sulfate and the solvent was removed under reduced pressure. The crude product was purified by column chromatography (*n*-hexane/ethyl acetate, 1:1). After final recrystallization from acetone, product **8** was obtained as a colorless solid in 71% yield (138 mg, 0.707 mmol).

Mp 295°C (Lit.: 295 – 296 °C[11]). R_f 0.46 (*n*-hexane/ethyl acetate 1:1). ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.24-7.29 (m, 1 H), 7.37 (dd, ^3J = 8.2 Hz, ^4J = 1.2 Hz, 1 H), 7.46-7.52 (m, 1 H), 7.64 (t, ^3J = 7.5 Hz, 1 H), 7.83-7.88 (m, 1 H), 8.32 (dd, ^3J = 8.0 Hz, ^4J = 1.5 Hz, 1 H), 8.39 (d, ^3J = 8.0 Hz, 1 H), 8.51 (d, ^3J = 8.1 Hz, 1 H), 11.68 (s, 1 H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 116.1 (CH), 117.5 (C_{quart}), 122.3 (CH), 122.6 (CH), 123.3 (CH), 125.7 (C_{quart}), 127.5 (CH), 127.9 (CH), 129.6 (CH), 132.8 (CH), 134.3 (C_{quart}), 136.6 (C_{quart}), 160.8 (C_{quart}). EI MS (70 eV, m/z (%)) 195 ([M]$^+$, 100), 167 ([$C_{13}H_{11}$]$^+$, 40), 166 ([$C_{13}H_{10}$]$^+$, 21), 139 (15). Anal. calcd. for $C_{13}H_9NO$ [195.2] C 79.98, H 4.65, N 7.17; Found C 80.12, H 4.46, N 7.15.

8 ^{1}H and ^{13}C spectra of *N*-arylphenanthridinones 4 and *N*-arylcrinasiadines 5

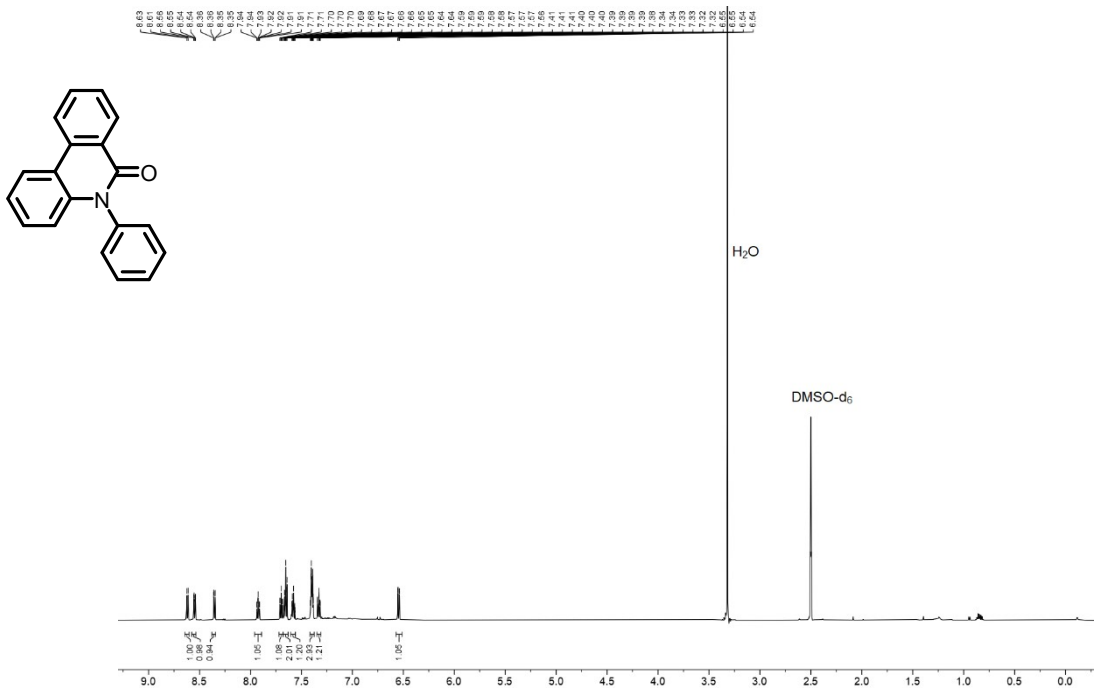


Figure S1. ^{1}H NMR spectrum of 5-Phenylphenanthridin-6(5*H*)-one (**4a**) (DMSO-d_6, 600 MHz, 293 K)

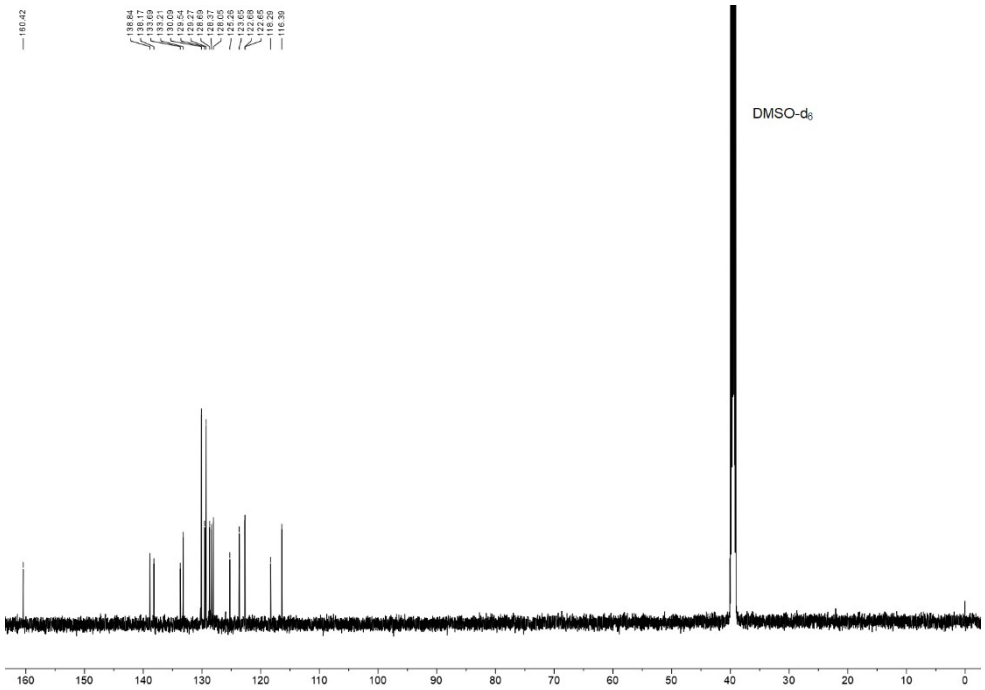


Figure S2. ^{13}C NMR spectrum of 5-Phenylphenanthridin-6(5*H*)-one (**4a**) (DMSO-d_6, 150 MHz, 293 K)

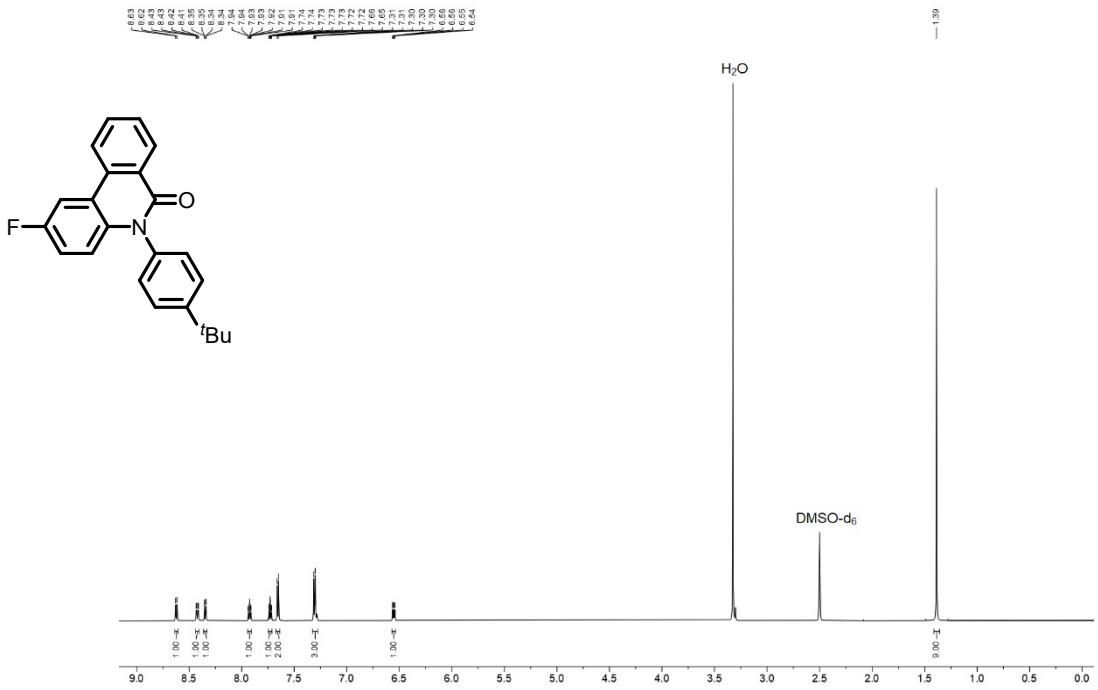


Figure S3. ^{1}H NMR spectrum of 5-(4-(*tert*-butyl)phenyl)-2-fluorophenanthridin-6(5*H*)-one (**4b**) (DMSO-d_6, 600 MHz, 293 K)

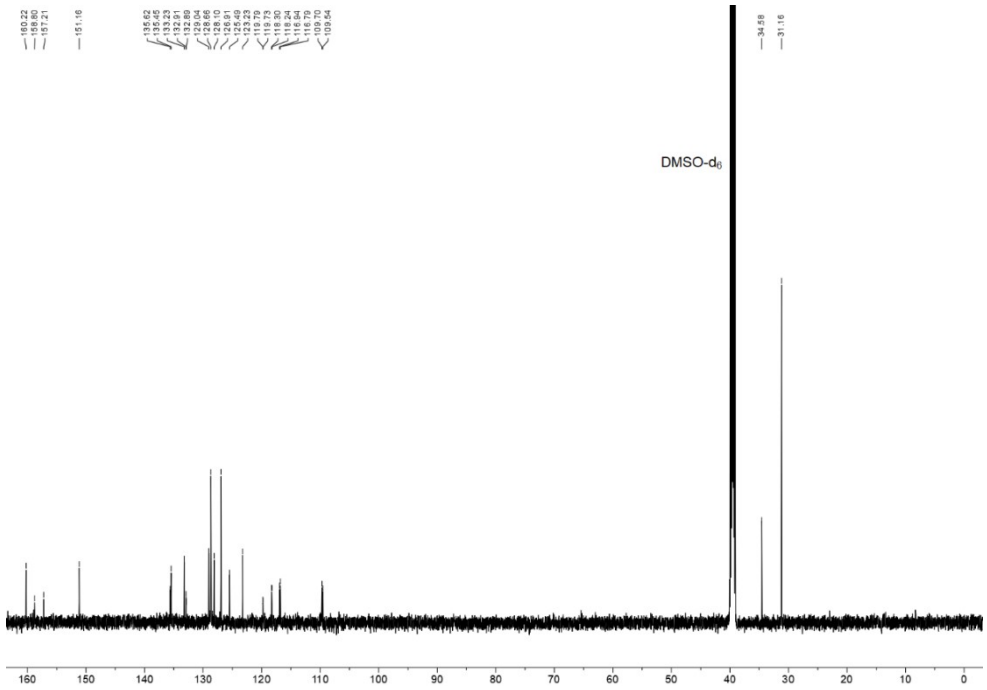


Figure S4. ^{13}C NMR spectrum of 5-(4-(*tert*-butyl)phenyl)-2-fluorophenanthridin-6(5*H*)-one (**4b**) (DMSO-d_6, 150 MHz, 293 K)

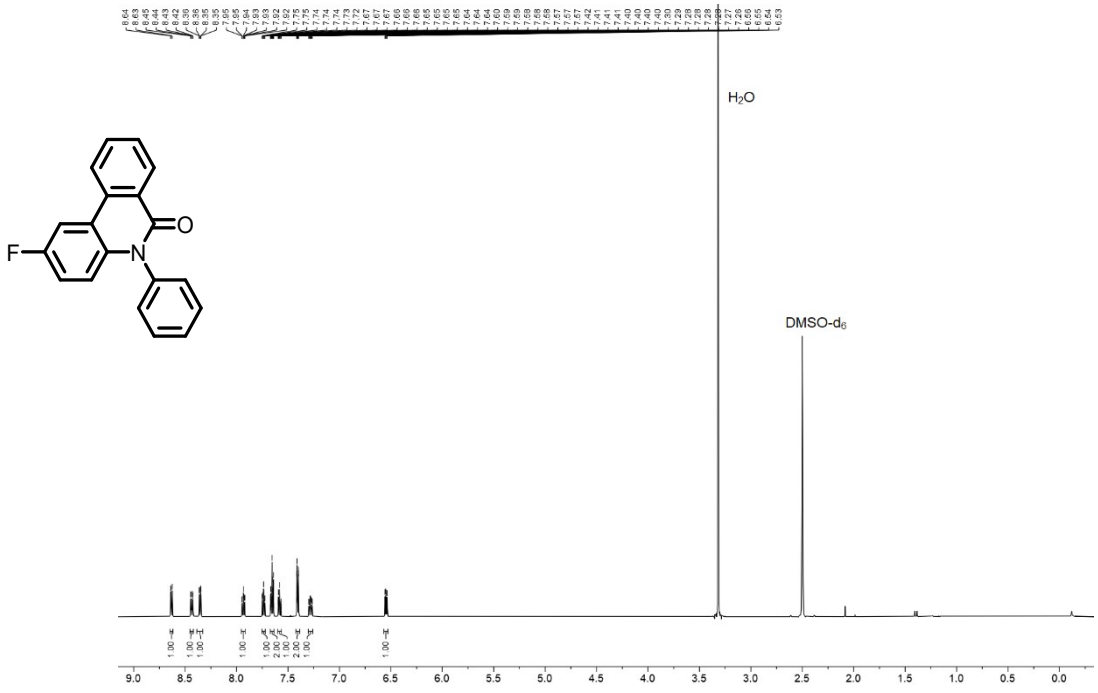


Figure S5. ^{1}H NMR spectrum of 2-fluoro-5-phenylphenanthridin-6(5*H*)-one (**4c**) (DMSO-d_6, 600 MHz, 293 K)

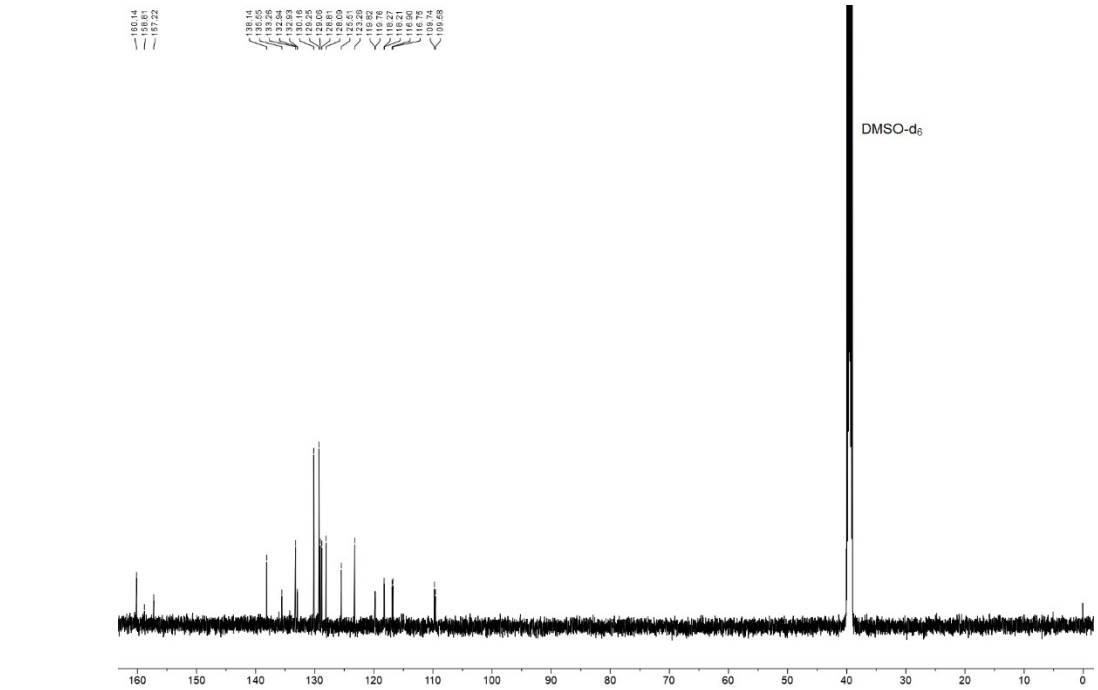


Figure S6. ^{13}C NMR spectrum of 2-fluoro-5-phenylphenanthridin-6(5*H*)-one (**4c**) (DMSO-d_6, 150 MHz, 293 K)

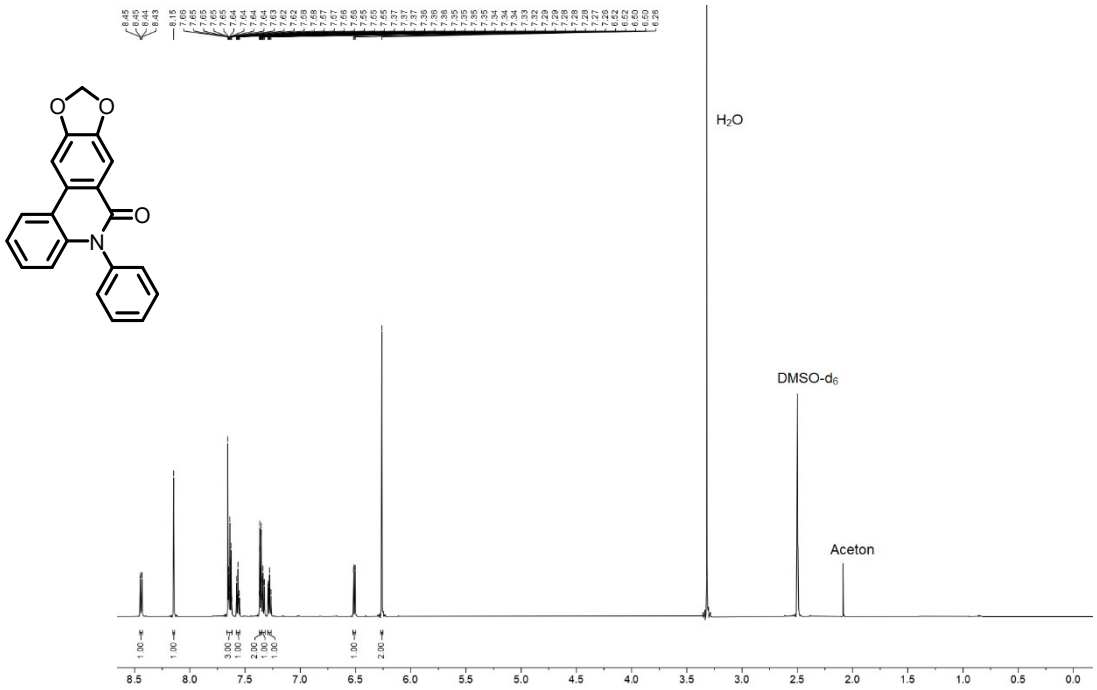


Figure S7. ^{1}H NMR spectrum of 5-phenyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (**5a**) (DMSO-d_6, 600 MHz, 293 K)

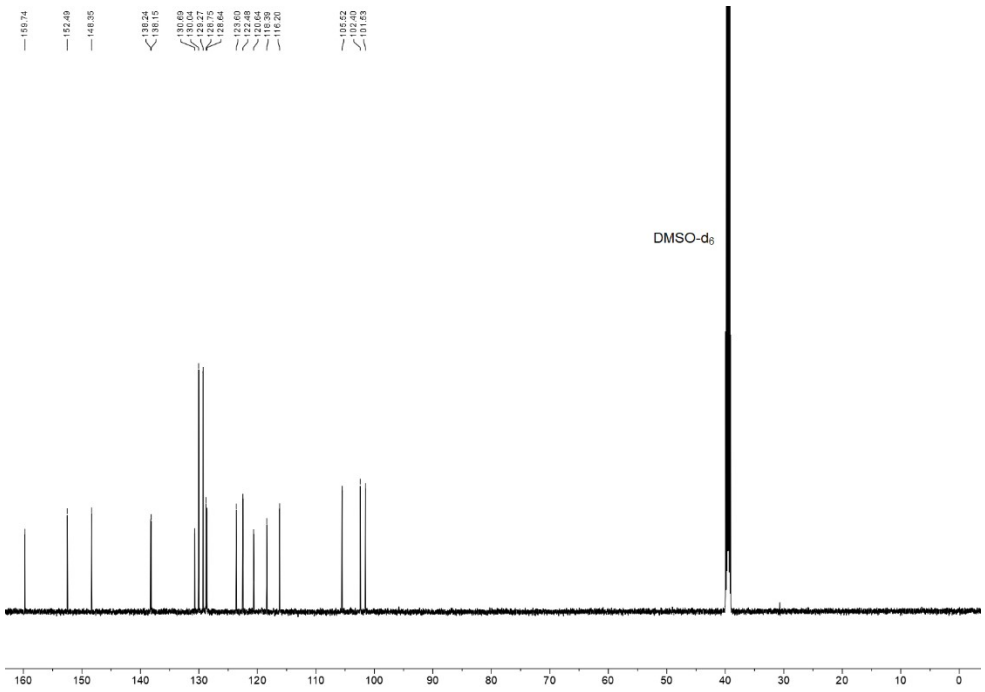


Figure S8. ^{13}C NMR spectrum of 5-phenyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (**5a**) (DMSO-d_6, 150 MHz, 293 K)

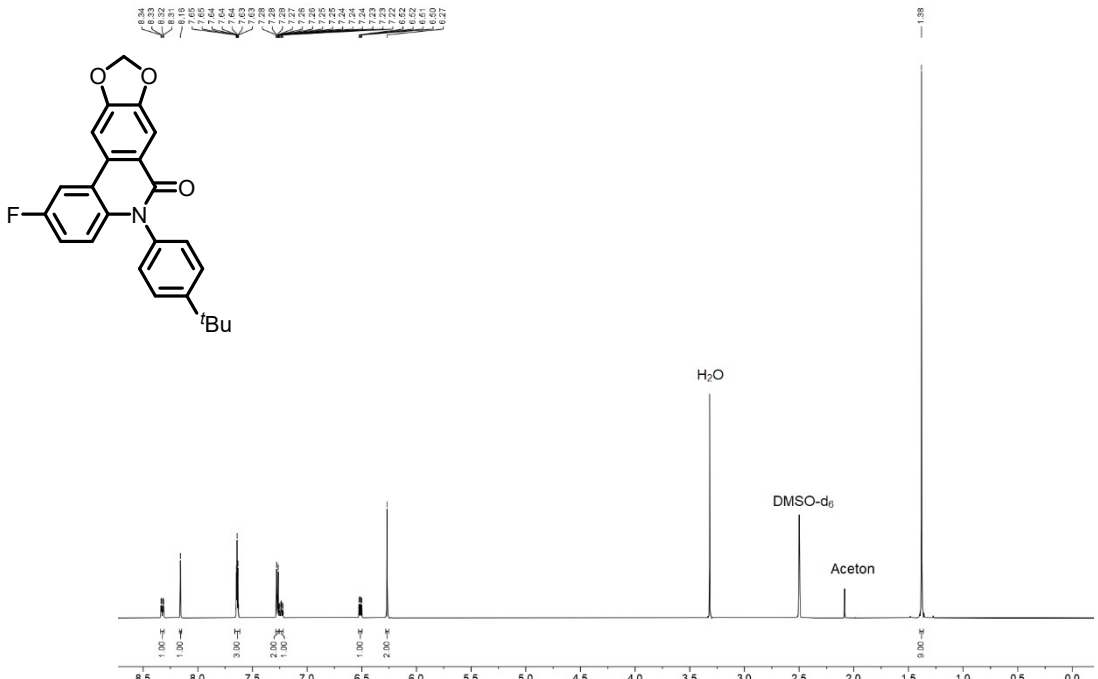


Figure S9. ^{1}H NMR spectrum of 5-(4-(*tert*-butyl)phenyl)-2-fluoro-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (**5b**) (DMSO-d_6, 600 MHz, 293 K)

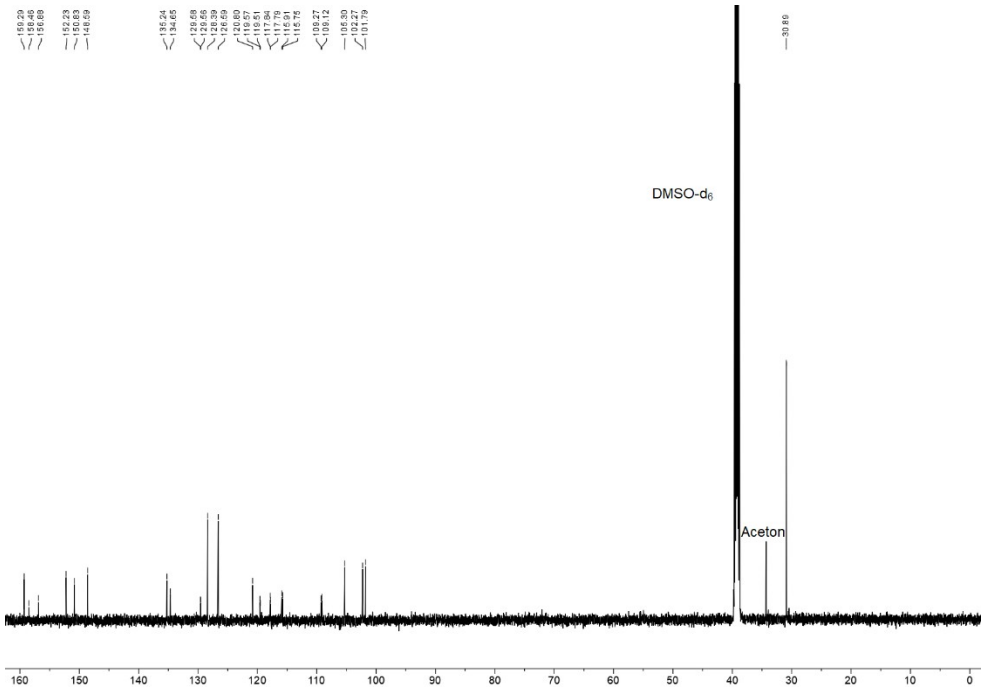


Figure S10. ^{13}C NMR spectrum of 5-(4-(*tert*-butyl)phenyl)-2-fluoro-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (**5b**) (DMSO-d_6, 150 MHz, 293 K)

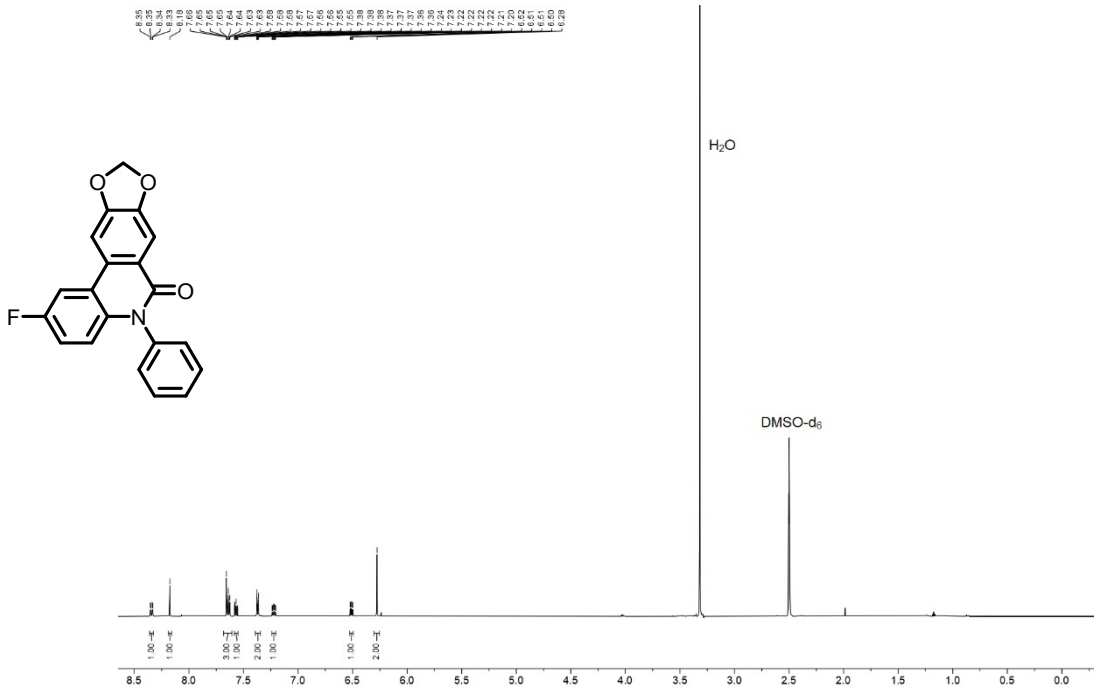


Figure S11. ^{1}H NMR spectrum of 2-fluoro-5-phenyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (**5c**) (DMSO-d_6, 600 MHz, 293 K)

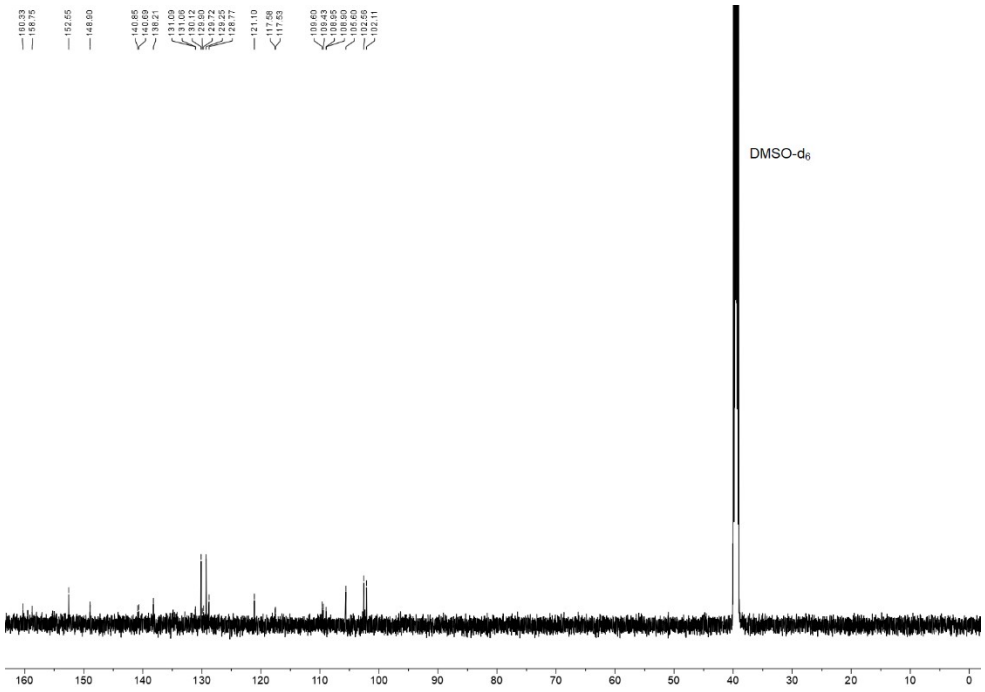


Figure S12. ^{13}C NMR spectrum of 2-fluoro-5-phenyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (**5c**) (DMSO-d_6, 150 MHz, 293 K)

9 ^{1}H and ^{13}C spectra of *N*-alkylphenanthridinones 6 and *N*-alkylcrinasiadines 7

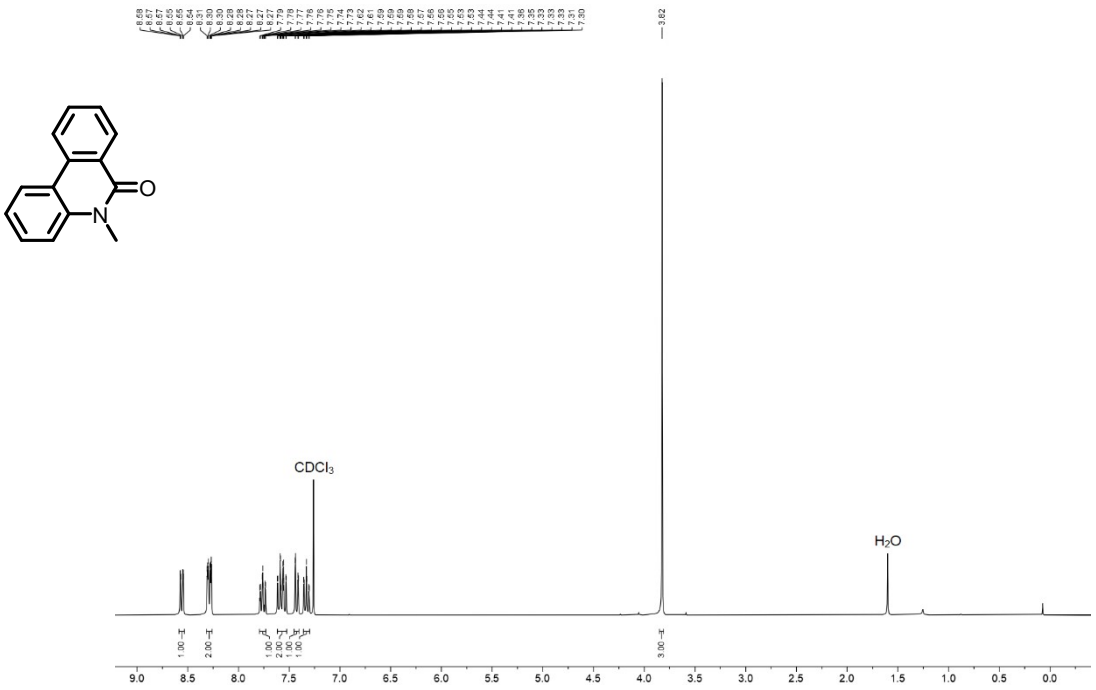


Figure S13. ^{1}H NMR spectrum of 5-methylphenanthridin-6(5*H*)-one (**6a**) ($CDCl_3$, 300 MHz, 293 K)

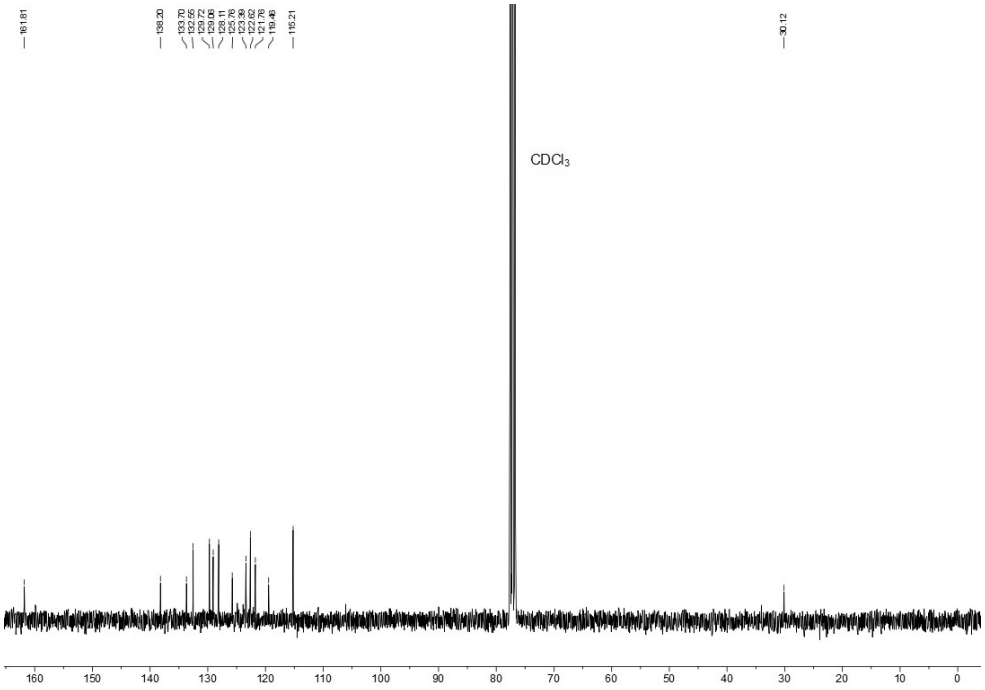


Figure S14. ^{13}C NMR spectrum of 5-methylphenanthridin-6(5*H*)-one (**6a**) ($CDCl_3$, 75 MHz, 293 K)

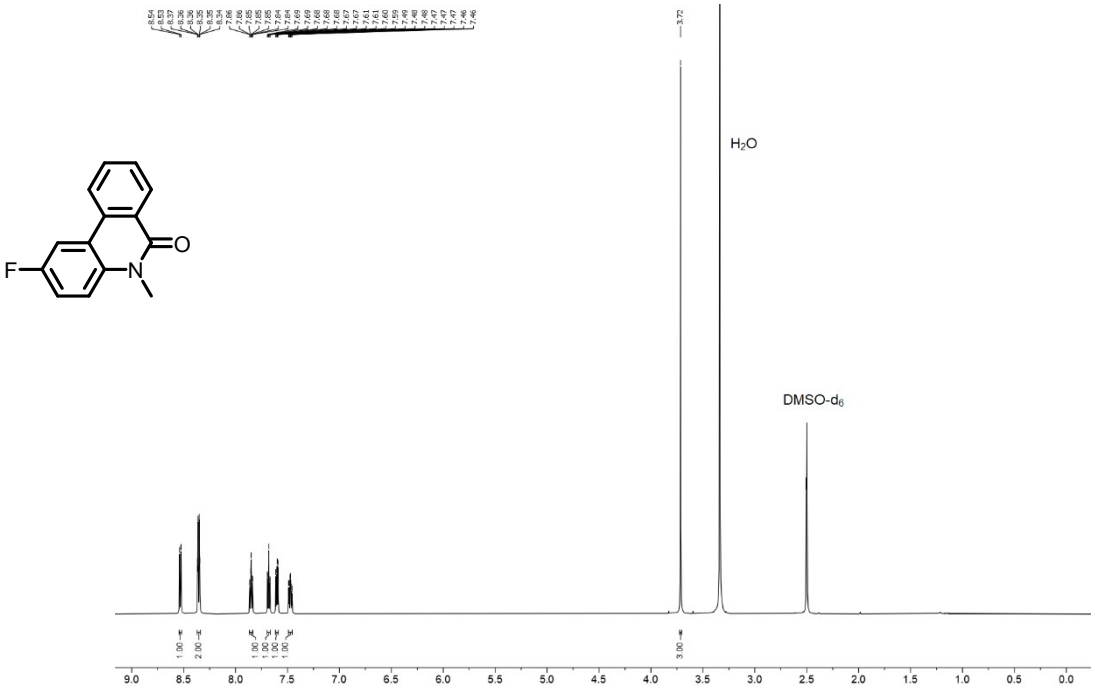


Figure S15. ^{1}H NMR spectrum of 2-fluoro-5-methylphenanthridin-6(5*H*)-one (**6b**) (DMSO-d_6, 600 MHz, 293 K)

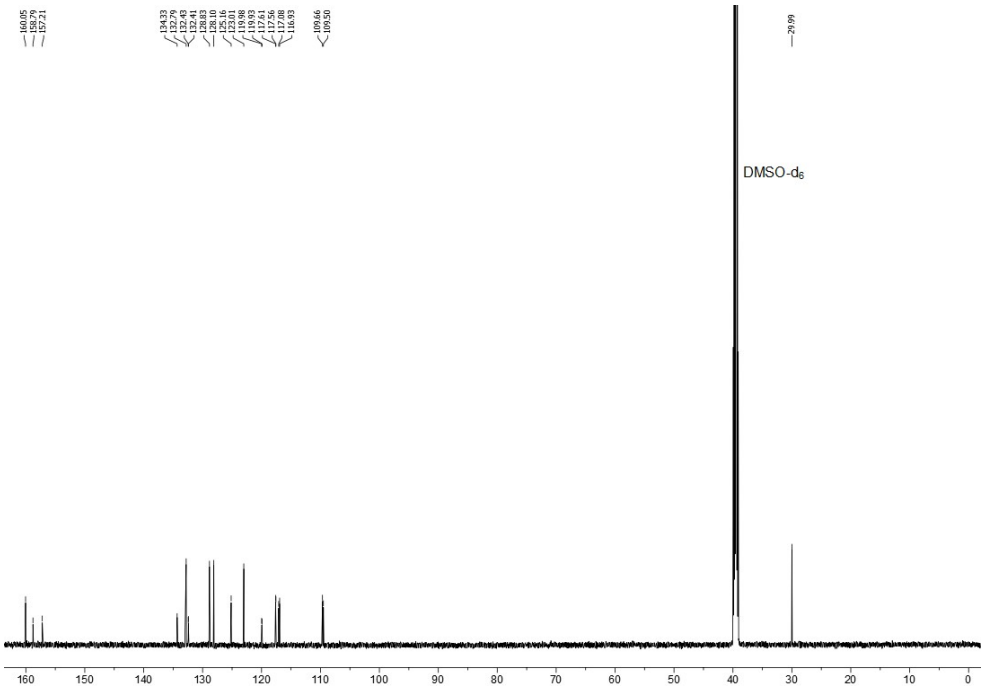


Figure S16. ^{13}C NMR spectrum of 2-fluoro-5-methylphenanthridin-6(5*H*)-one (**6b**) (DMSO-d_6, 150 MHz, 293 K)

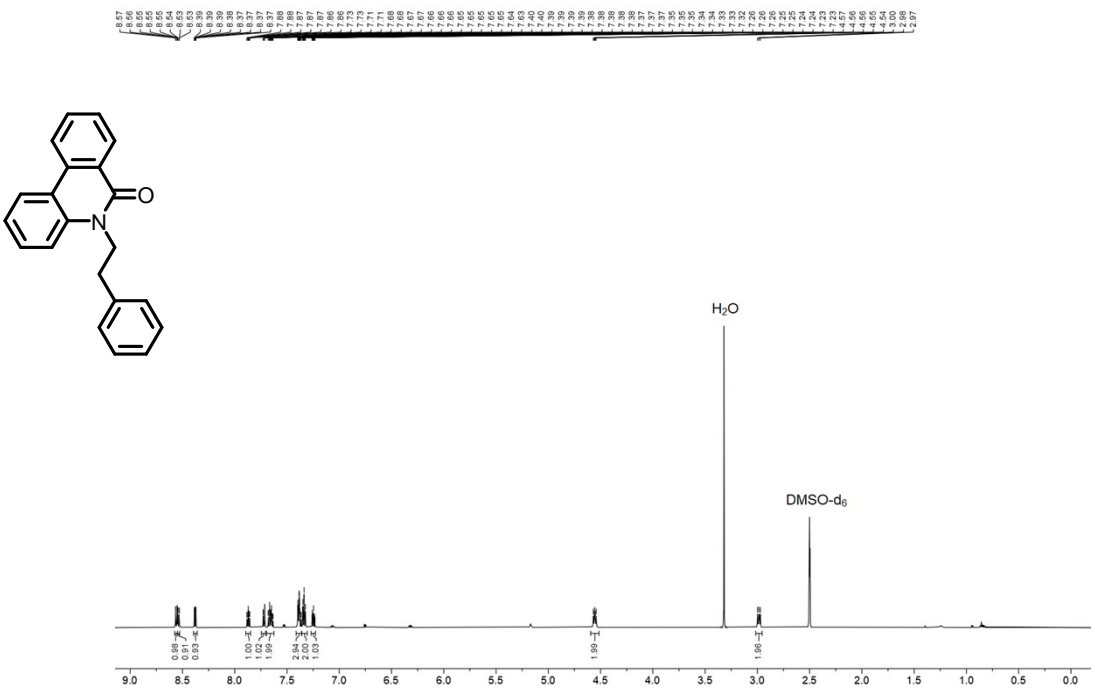


Figure S17. ^{1}H NMR spectrum of 5-phenethylphenanthridin-6(5*H*)-one (**6c**) (DMSO-d_6, 600 MHz, 293 K)

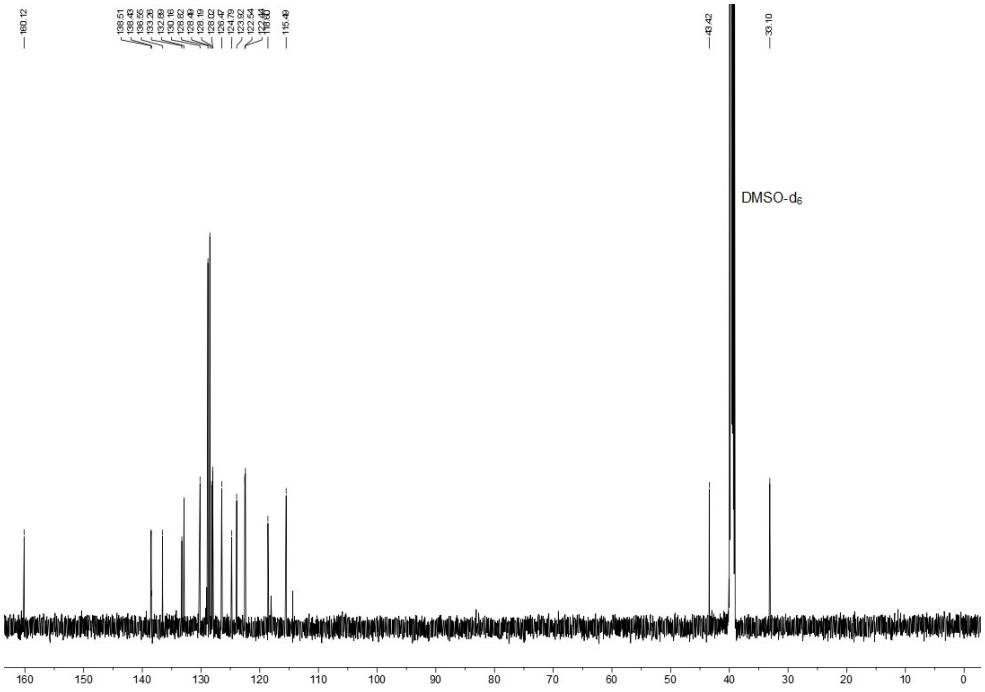


Figure S18. ^{13}C NMR spectrum of 5-phenethylphenanthridin-6(5*H*)-one I(**6c**) (DMSO-d_6, 150 MHz, 293 K)

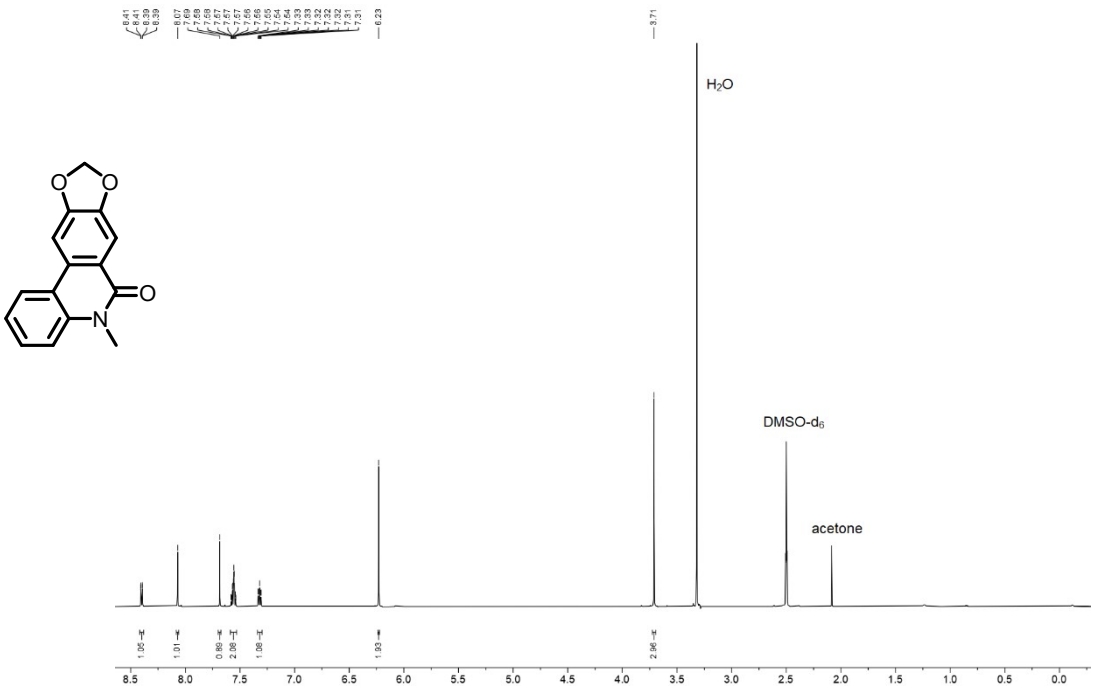


Figure S19. ^{1}H NMR spectrum of 5-methyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (**7a**) (DMSO-d_6, 600 MHz, 293 K)

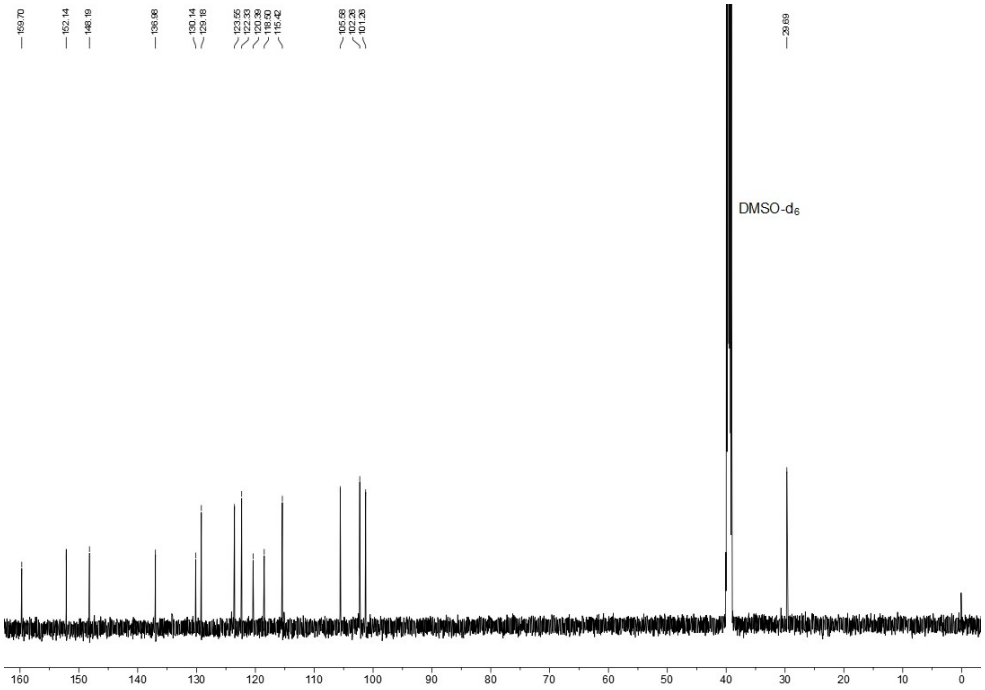


Figure S20. ^{13}C NMR spectrum of 5-methyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (**7a**) (DMSO-d_6, 150 MHz, 293 K)

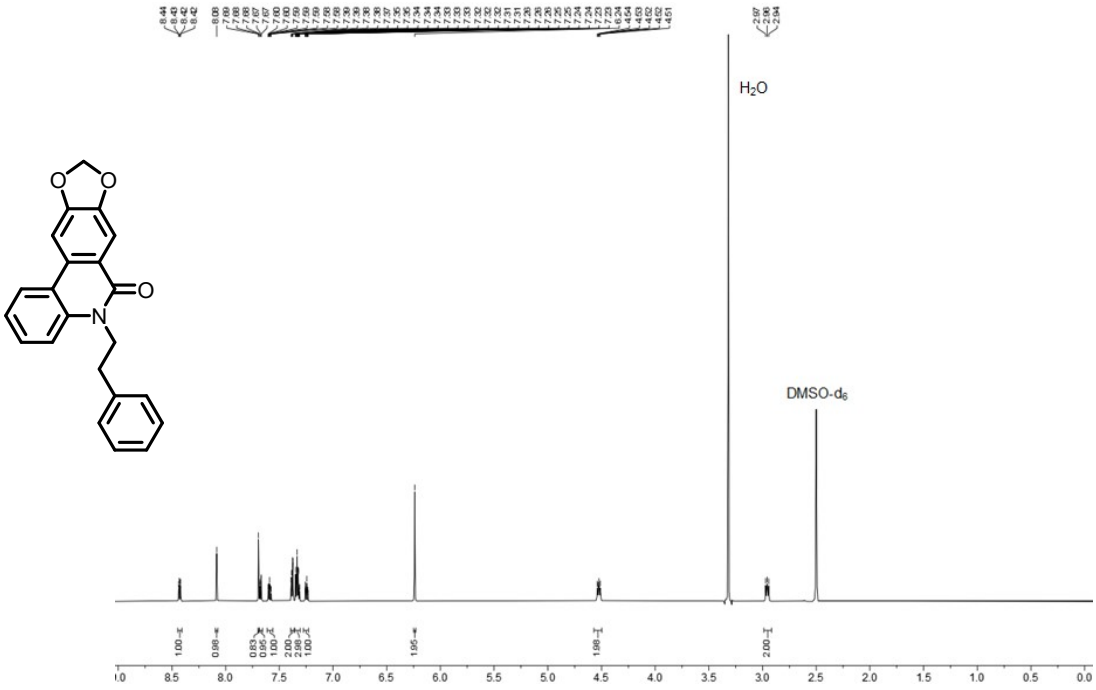


Figure S21. ^{1}H NMR spectrum of 5-phenethyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (**7b**) (DMSO-d_6, 600 MHz, 293 K)

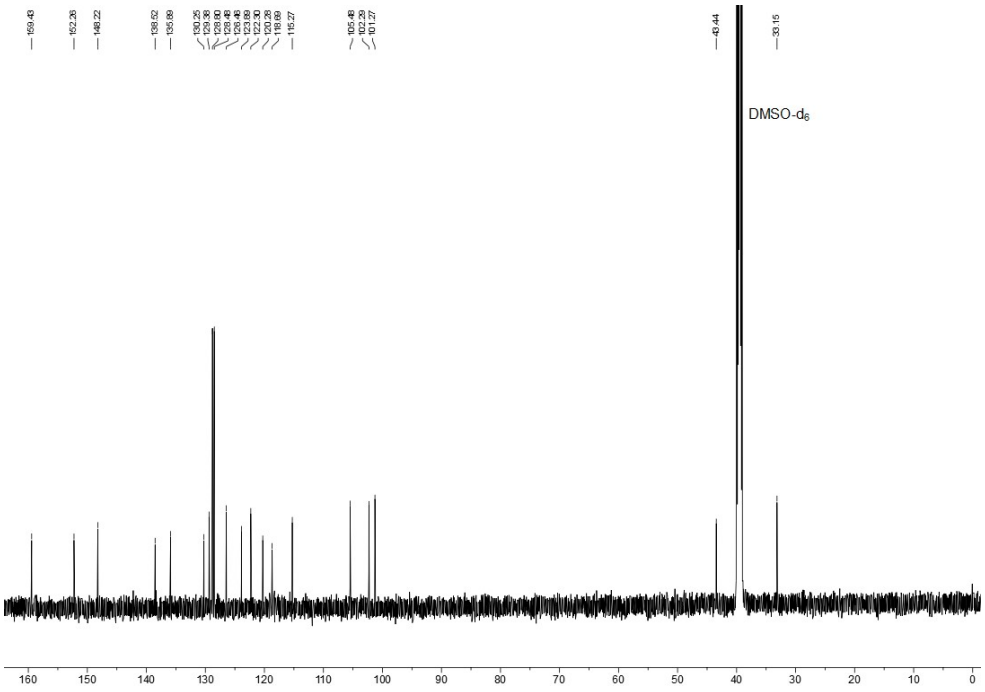
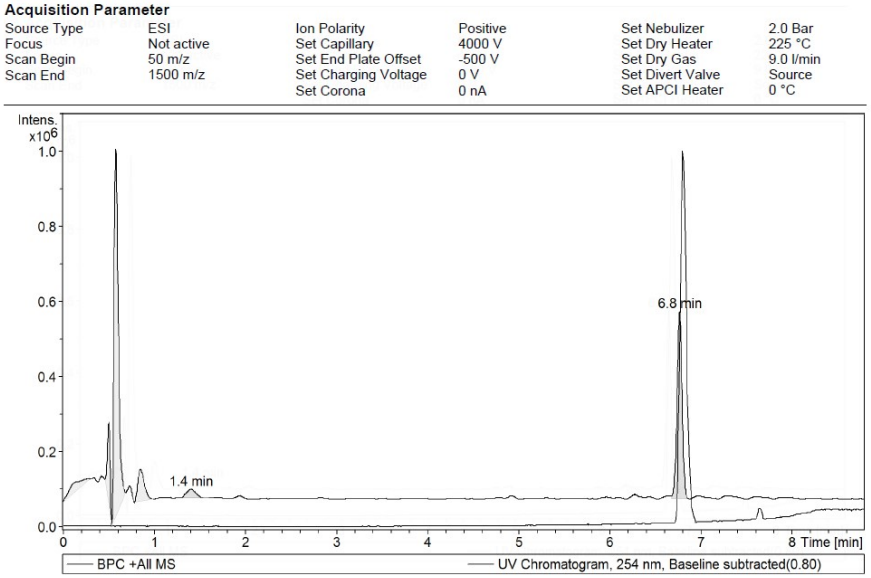


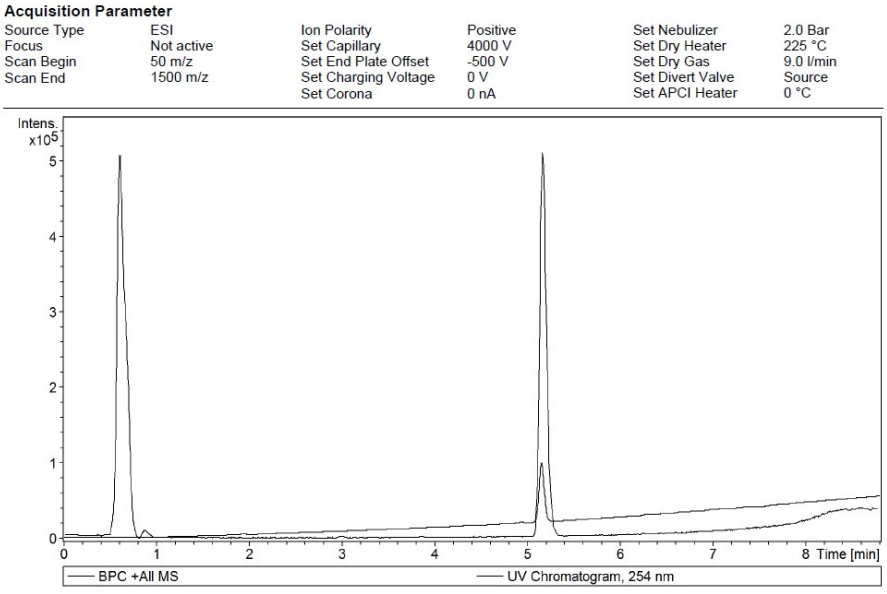
Figure S22. ^{13}C NMR spectrum of 5-phenethyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (**7b**) (DMSO-d_6, 150 MHz, 293 K)

10 High-Performance Liquid Chromatography (HPLC) Data of *N*-arylphenanthridinones 4 and *N*-arylcrinasiadines 5

10.1 HPLC Data of 5-(4-(*tert*-Butyl)phenyl)-2-fluorophenanthridin-6(5*H*)-one (4b)



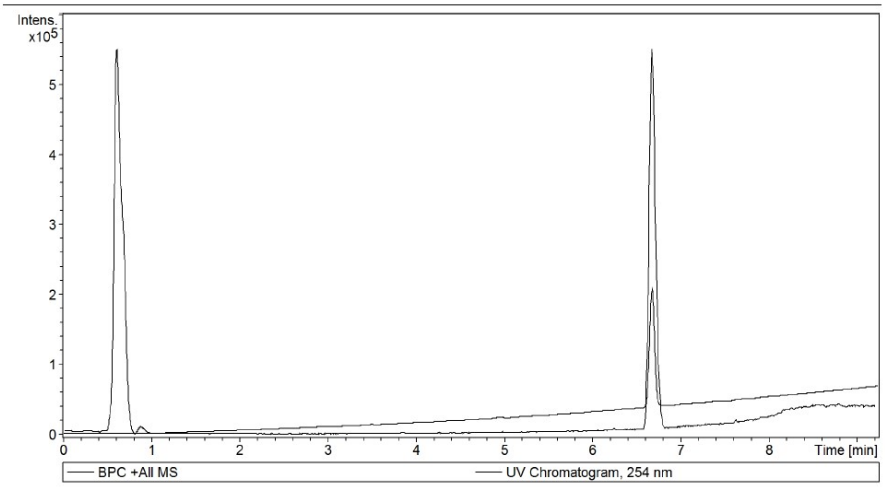
10.2 HPLC Data of 2-Fluoro-5-phenylphenanthridin-6(5*H*)-one (4c)



10.3 HPLC Data of 5-(4-(*tert*-Butyl)phenyl)-2-fluoro-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (5b)

Acquisition Parameter

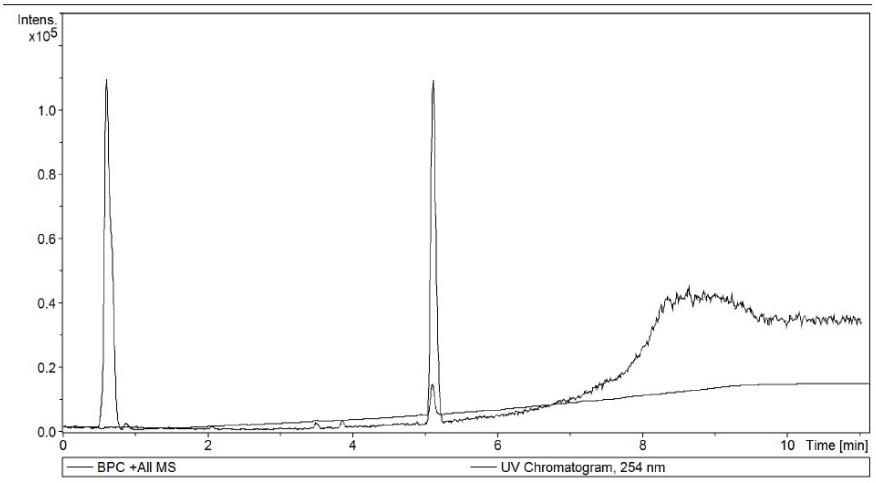
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	225 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	9.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



10.4 HPLC Data of 2-Fluoro-5-Phenyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (5c)

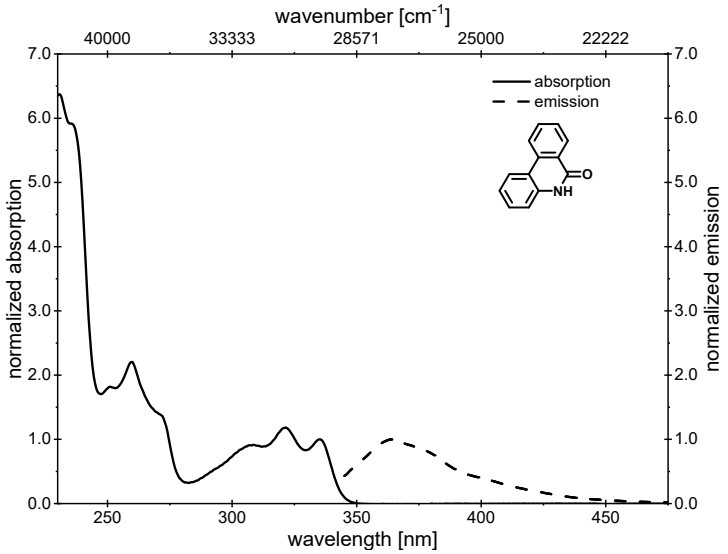
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	225 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	9.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



11 Absorption and emission spectra

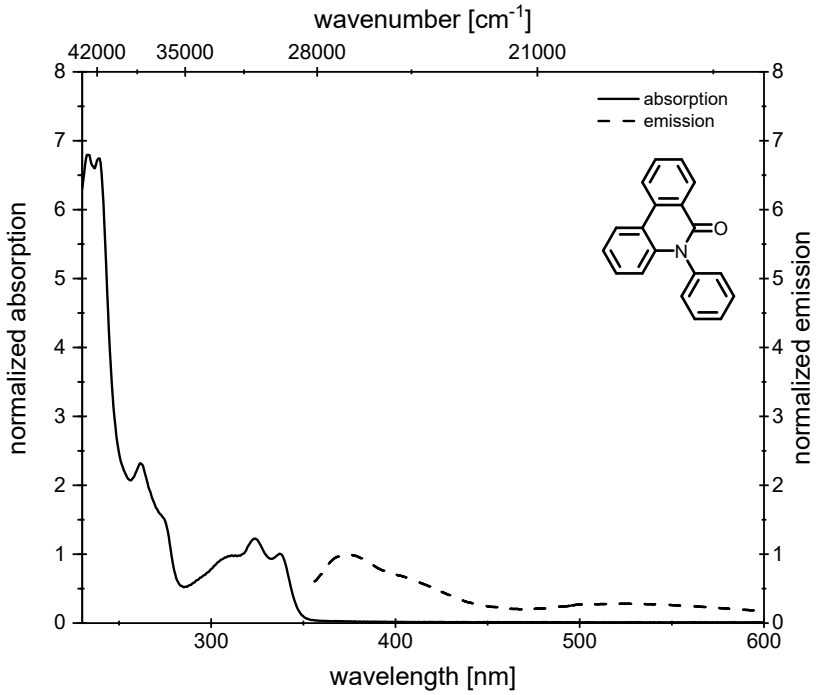
11.1 Absorption and emission spectra of 6(5*H*)-phenanthridinone (8)



Recorded in dichloromethane, T = 293 K, c_{abs}(**8**) = 10–5 M, c_{em}(**8**) = 10–7 M, $\lambda_{ex} = \lambda_{max,\ abs}$.

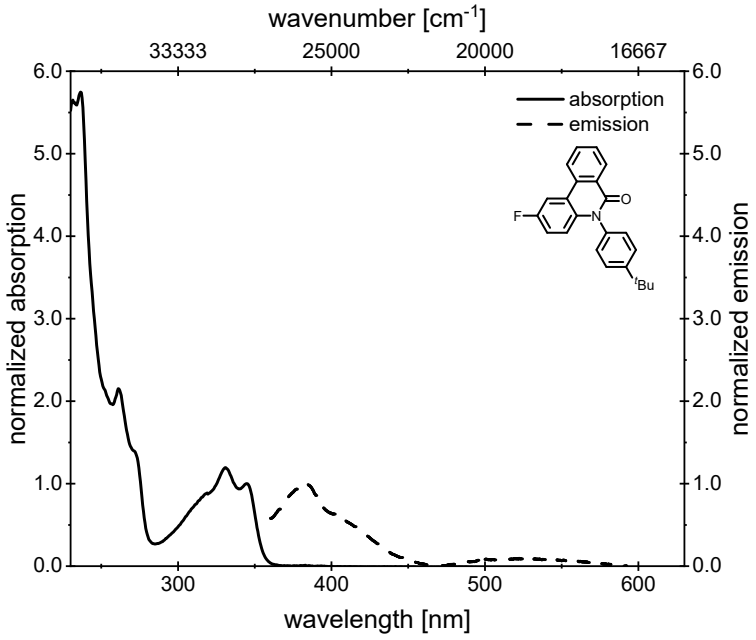
11.2 Absorption and emission spectra of *N*-arylphenanthridinones 4 and *N*-arylcrinasiadines 5

Absorption and emission spectra of 5-phenylphenanthridin-6(5*H*)-one (4a)



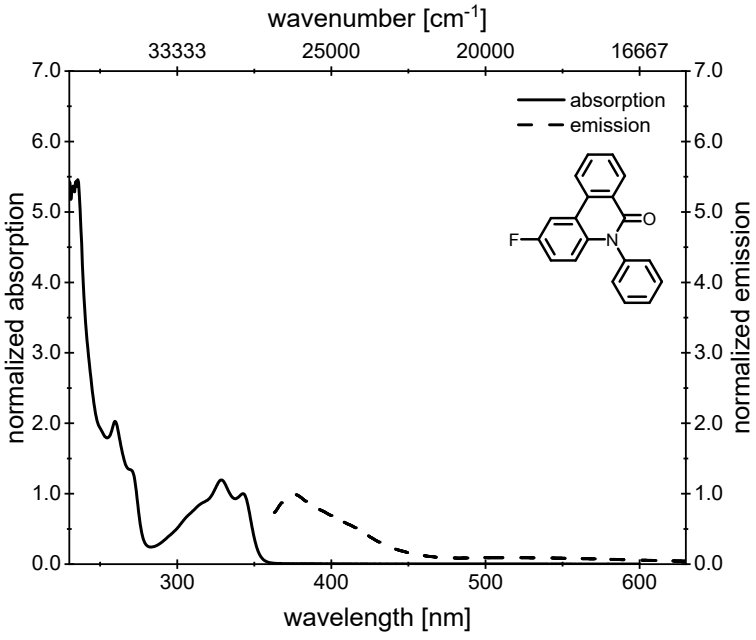
Recorded in dichloromethane, T = 293 K, c_{abs}(**4a**) = 10–5 M, c_{em}(**4a**) = 10–7 M, $\lambda_{ex} = \lambda_{max,\ abs}$.

Absorption and emission spectra of 5-(4-(*tert*-butyl)phenyl)-2-fluorophenanthridin-6(5*H*)-one (4b)



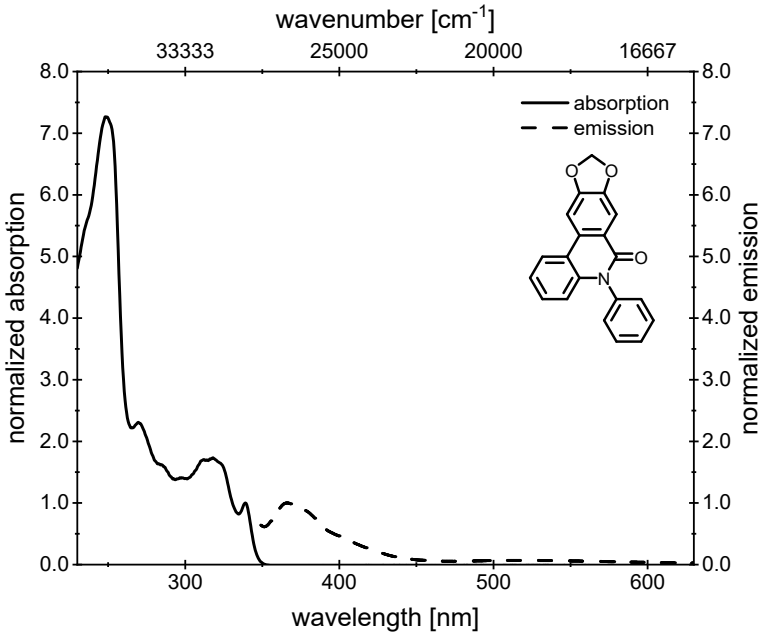
Recorded in dichloromethane, T = 293 K, c_{abs}(**4b**) = 10–5 M, c_{em}(**4b**) = 10–7 M, $\lambda_{ex} = \lambda_{max,\ abs}$.

Absorption and emission spectra of 2-fluoro-5-phenylphenanthridin-6(5*H*)-one (4c)



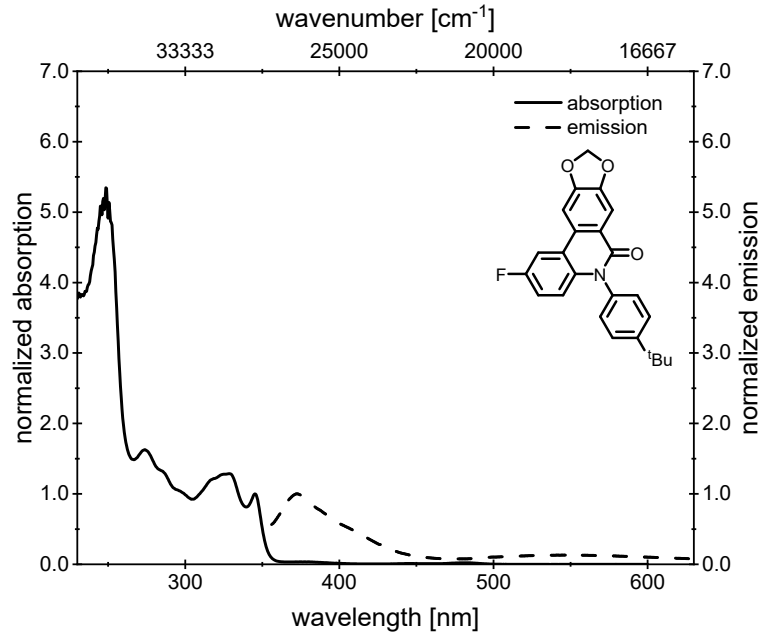
Recorded in dichloromethane, T = 293 K, c_{abs}(**4c**) = 10–5 M, c_{em}(**4c**) = 10–7 M, $\lambda_{ex} = \lambda_{max,\ abs}$.

Absorption and emission spectra of 5-phenyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (5a)



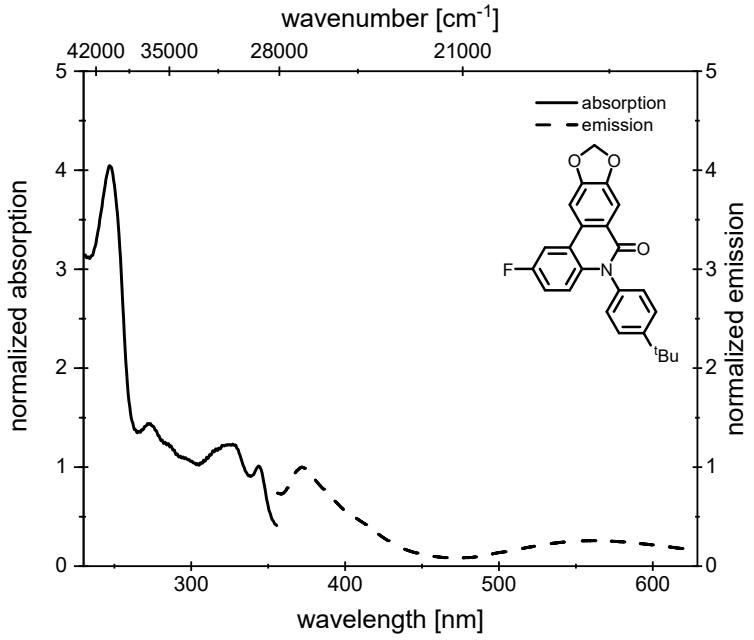
Recorded in dichloromethane, T = 293 K, c_{abs}(**5a**) = 10^{-5} M, c_{em}(**5a**) = 10^{-7} M, $\lambda_{ex} = \lambda_{max,\ abs}$.

Absorption and emission spectra of 5-(4-(*tert*-butyl)phenyl)-2-fluoro-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (5b)



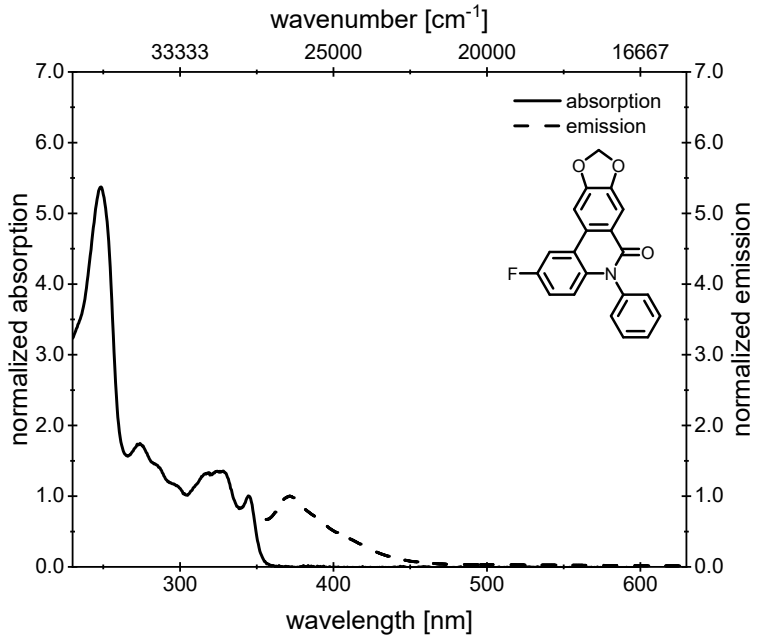
Recorded in dichloromethane, T = 293 K, c_{abs}(**5b**) = 10^{-5} M, c_{em}(**5b**) = 10^{-7} M, $\lambda_{ex} = \lambda_{max,\ abs}$.

Absorption and emission spectra of 5-(4-(*tert*-butyl)phenyl)-2-fluoro-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (5b)



Recorded in acetonitrile, T = 293 K, c_{abs}(**5b**) = 10^{-5} M, c_{em}(**5b**) = 10^{-7} M, $\lambda_{ex} = \lambda_{max,\ abs}$.

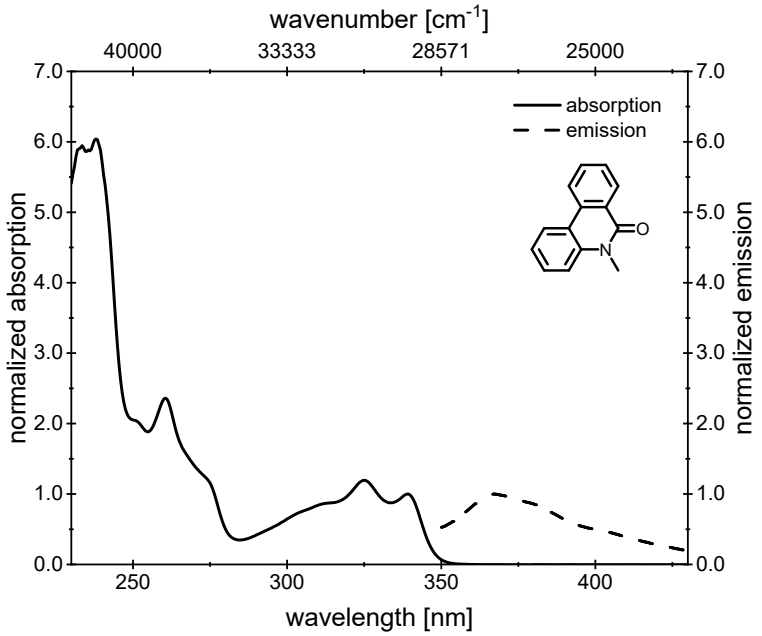
Absorption and emission spectra of 2-fluoro-5-phenyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (5c)



Recorded in dichloromethane, T = 293 K, c_{abs}(**5c**) = 10^{-5} M, c_{em}(**5c**) = 10^{-7} M, $\lambda_{ex} = \lambda_{max,\ abs}$.

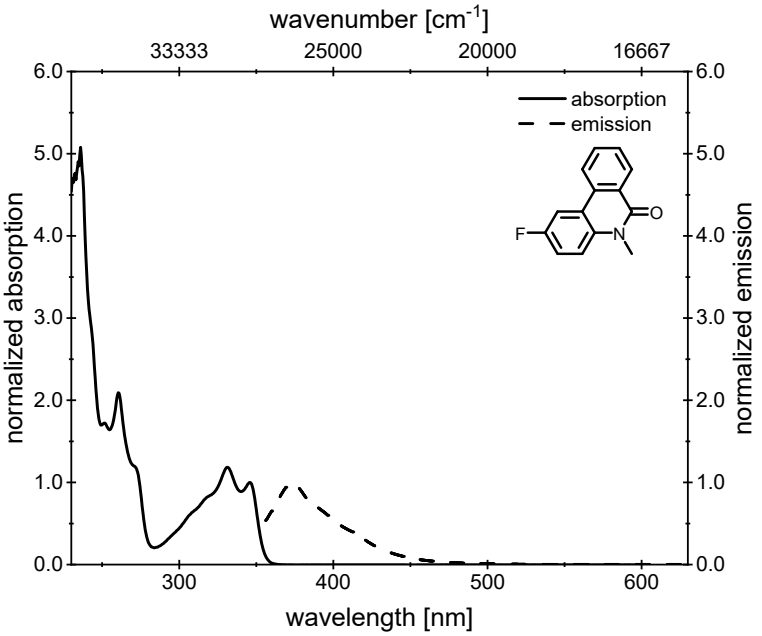
11.3 Absorption and emission spectra of *N*-alkylphenanthridinones 6 and *N*-alkylcrinasiadines 7

Absorption and emission spectra of 5-methylphenanthridin-6(5*H*)-one (6a)



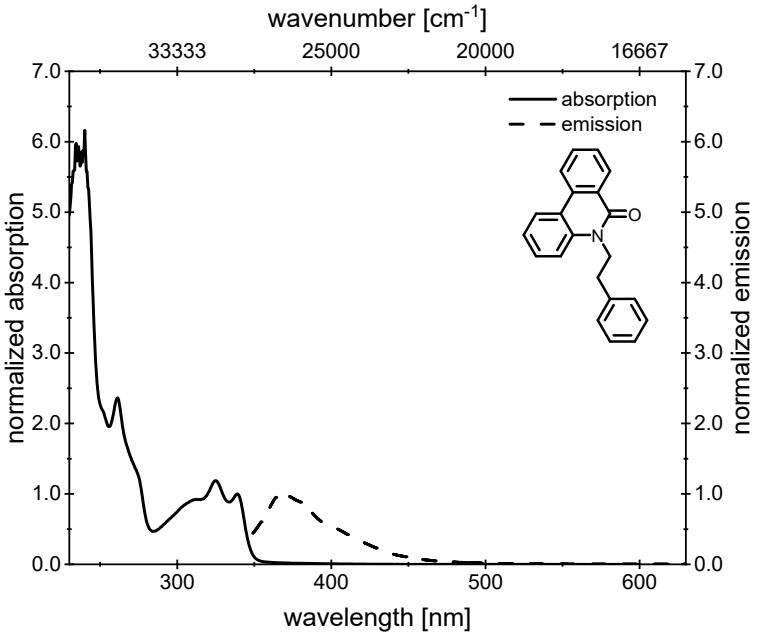
Recorded in dichloromethane, T = 293 K, c_{abs}(**6a**) = 10–5 M, c_{em}(**6a**) = 10–7 M, $\lambda_{ex} = \lambda_{max,\ abs}$.

Absorption and emission spectra of 2-fluoro-5-methylphenanthridin-6(5*H*)-one (6b)



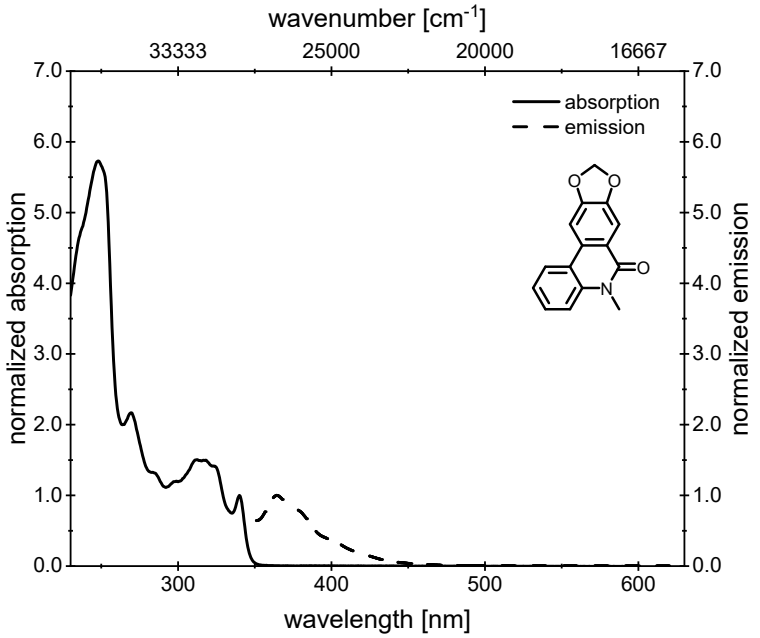
Recorded in dichloromethane, T = 293 K, c_{abs}(**6b**) = 10–5 M, c_{em}(**6b**) = 10–7 M, $\lambda_{ex} = \lambda_{max,\ abs}$.

Absorption and emission spectra of 5-phenethylphenanthridin-6(5*H*)-one (6c)



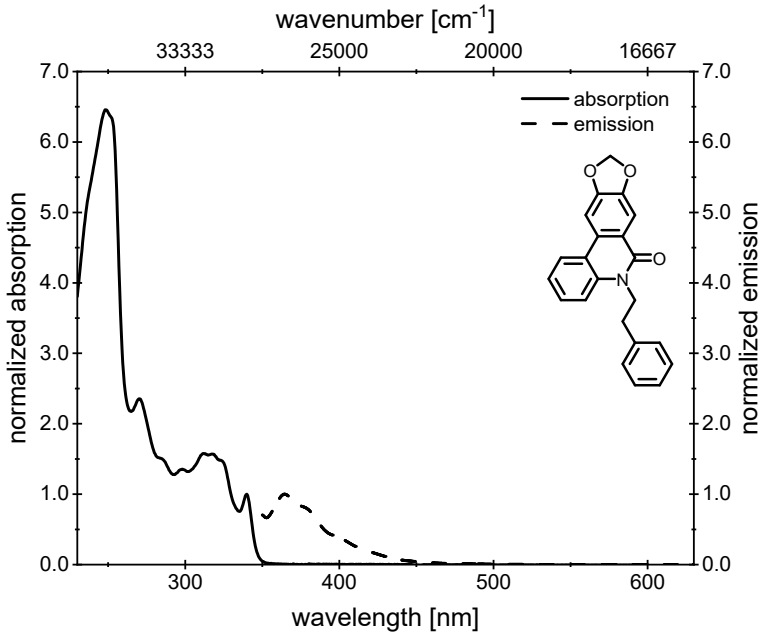
Recorded in dichloromethane, T = 293 K, c_{abs}(**6c**) = 10–5 M, c_{em}(**6c**) = 10–7 M, $\lambda_{ex} = \lambda_{max,\ abs}$.

Absorption and emission spectra of 5-methyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (7a)



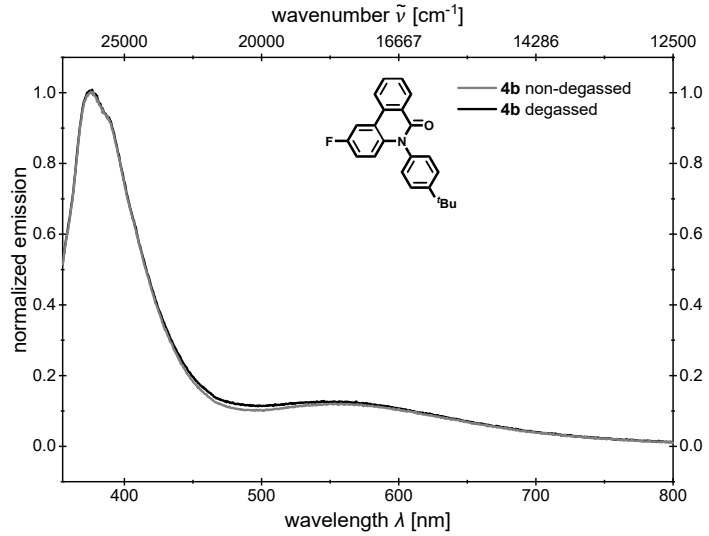
Recorded in dichloromethane, T = 293 K, c_{abs}(**7a**) = 10–5 M, c_{em}(**7a**) = 10–7 M, $\lambda_{ex} = \lambda_{max,\ abs}$.

Absorption and emission spectra of 5-methyl-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (7b)

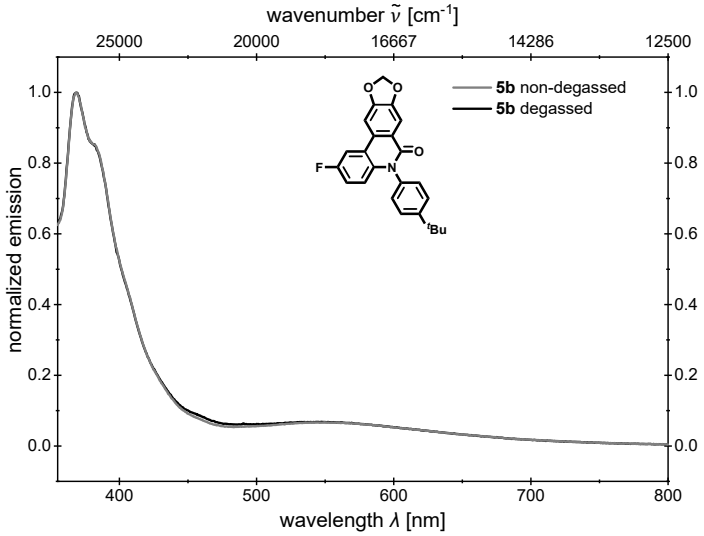


Recorded in dichloromethane, T = 293 K, c_{abs}(**7b**) = 10–5 M, c_{em}(**7b**) = 10–7 M, $\lambda_{ex} = \lambda_{max,\ abs}$.

11.4 Degassed and non-degassed emission spectra of *N*-arylphenanthridinone 4b and *N*-arylcrinasiadine 5b

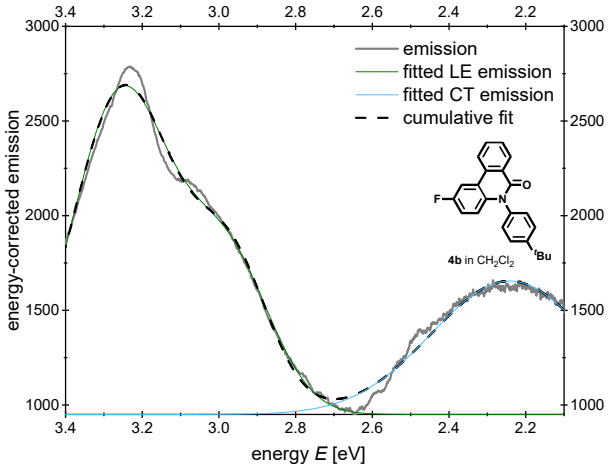


Recorded in acetonitrile, T = 298 K, c_{em}(**4b**) = 10–7 M, $\lambda_{ex} = \lambda_{max,\ abs}$.

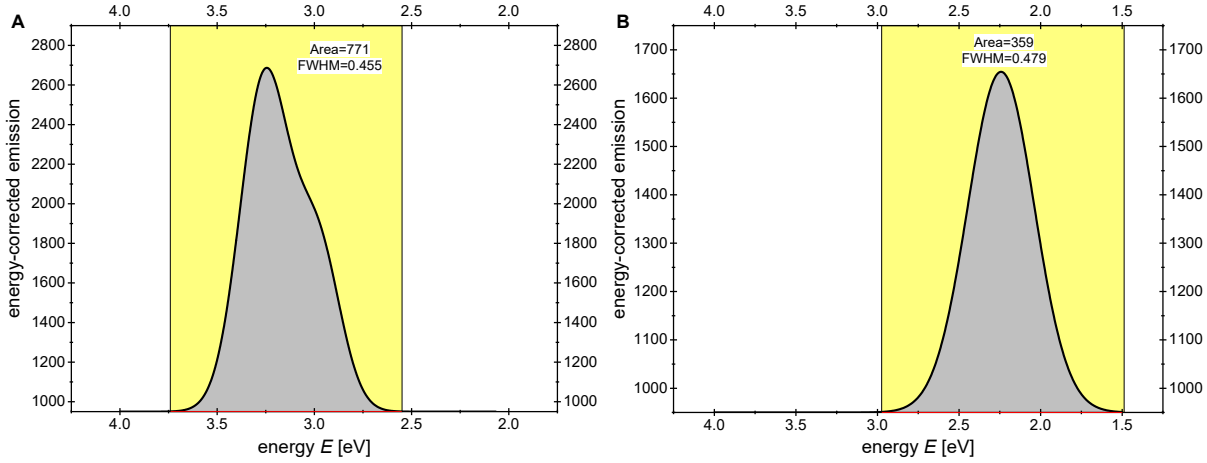


Recorded in acetonitrile, T = 298 K, c_{em}(**5b**) = 10^{-7} M, $\lambda_{ex} = \lambda_{max,\ abs}$.

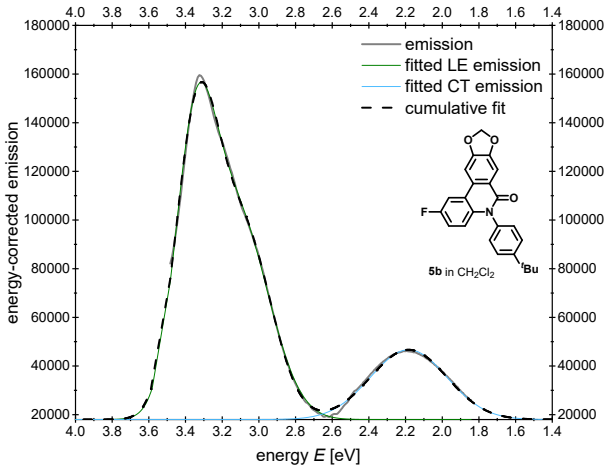
11.5 Jacobian[10] energy-corrected emission spectra and corresponding integrated emission intensities of *N*-arylphenanthridinone 4b and *N*-arylcrinasiadine 5b



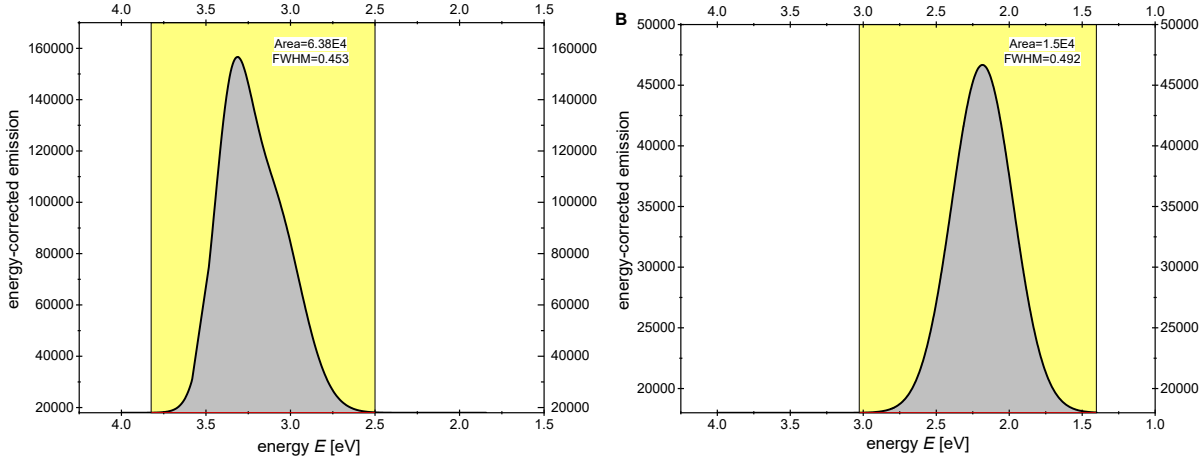
Jacobian energy-corrected simulated emission spectra of *N*-arylphenanthridinone **4b** in dichloromethane, generated from superimposed Gaussian functions, compared to the corresponding Jacobian energy-corrected experimental emission spectra (recorded in CH_2Cl_2, T = 293 K, c = 10^{-5} M, gray solid line).



Integrated emission intensity of the fitted LE emission (**A**) and the fitted CT emission (**B**) of *N*-arylphenanthridinone **4b**.



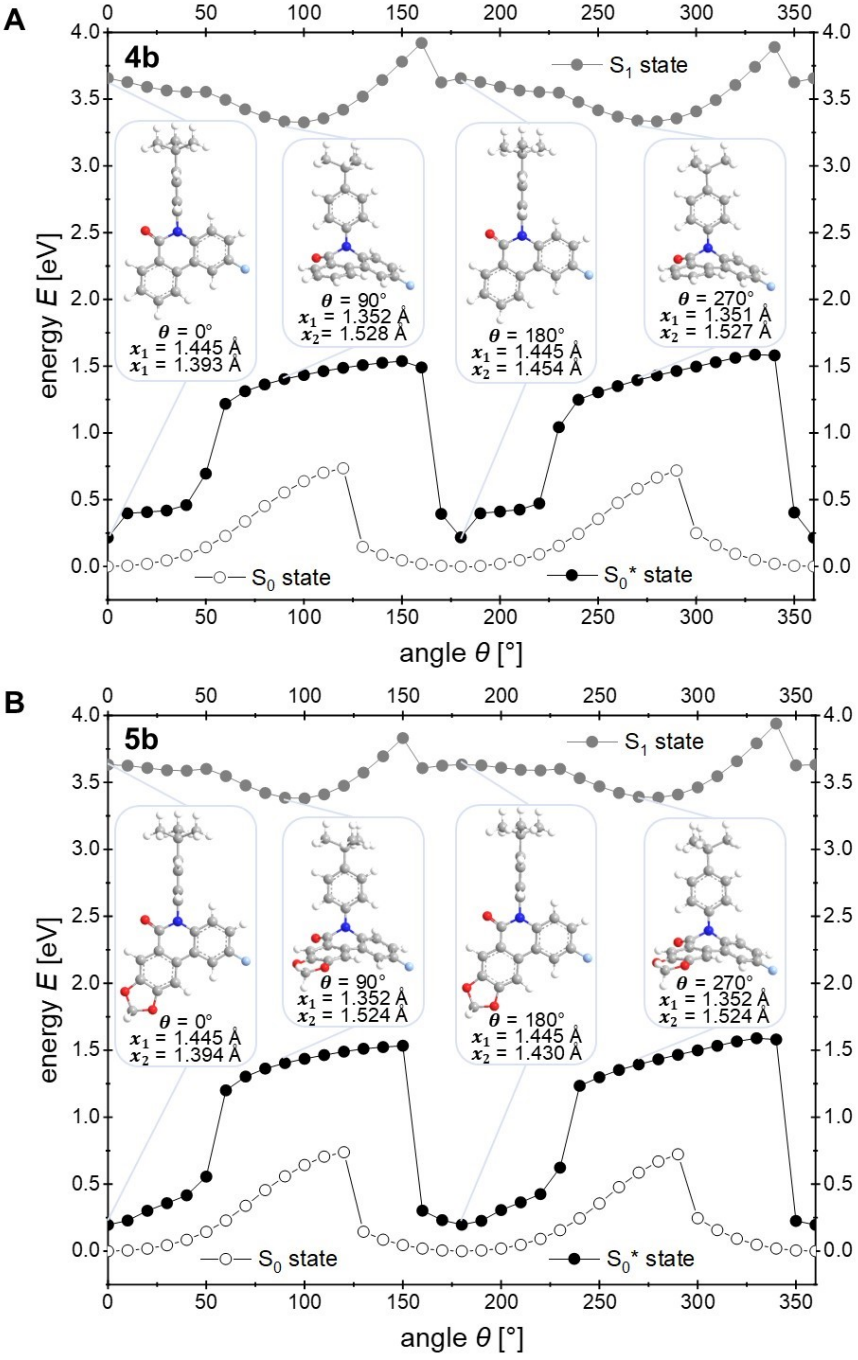
Jacobian energy-corrected simulated emission spectra of *N*-arylcrinasiadine **5b** in dichloromethane, generated from superimposed Gaussian functions, compared to the corresponding Jacobian energy-corrected experimental emission spectra (recorded in CH_2Cl_2, T = 293 K, c = 10^{-5} M, gray solid line).



Integrated emission intensity of the fitted LE emission (**A**) and the fitted CT emission (**B**) of *N*-arylcrinasiadine **5b**.

12 Data of quantum chemical calculations

12.1 Comparison of the potential scans of 5-(4-(*tert*-butyl)phenyl)-2-fluorophenanthridin-6(5*H*)-one (4b) and 5-(4-(*tert*-Butyl)phenyl)-2-fluoro-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (5b)



Potential energy scan of rotation of the *N*-aryl substituent along the torsional angle θ, starting from the geometry of compounds **4b** (**A**) and **5b** (**B**) at $\theta = 0°$, in the S_0 (open dots), S_0* (filled dots), and S_1 state (grey dots) in dichloromethane. Shown are the respective geometries after 90° rotation and x_1, the *N*-aryl bond length and x_2, the *N*-*CO* amide bond length (Gaussian 16, B3LYP/6-31G*, PCM CH_2Cl_2).

12.2 Quantum chemical calculation data of 5-(4-(*tert*-butyl)phenyl)-2-fluorophenanthridin-6(5*H*)-one (4b)

12.2.1 Computed xyz-coordinates of compound 4b (B3LYP/6-31G* PCM CH_2Cl_2)

C	-2.746525	3.18432	-0.002734
C	-1.356662	3.256873	0.003212
C	-0.628506	2.075155	0.007489
C	-1.276129	0.825937	0.005774
C	-2.692608	0.76706	-0.000664
C	-3.413465	1.976299	-0.004729
N	-0.519074	-0.362816	0.010394
C	-1.080226	-1.638008	0.007529
C	-2.55563	-1.704276	0.000985
C	-3.352843	-0.53928	-0.002968
C	-3.14871	-2.977518	-0.001206
C	-4.528507	-3.110176	-0.007185
C	-5.330818	-1.959202	-0.011158
C	-4.754266	-0.696784	-0.009117
O	-0.365114	-2.640792	0.010468
C	0.925375	-0.296467	0.016973
C	1.618512	-0.257589	1.223674
C	3.013746	-0.186494	1.224704
C	3.747602	-0.152279	0.030221
C	3.020566	-0.19403	-1.173495
C	1.62995	-0.264979	-1.187606
F	-3.465145	4.331815	-0.006734
C	5.284609	-0.072364	-0.003898
C	5.900519	-0.035141	1.407567
C	5.846351	-1.309912	-0.74398
C	5.715309	1.211529	-0.752976
H	-0.860898	4.221567	0.004494
H	0.452717	2.119924	0.012352
H	-4.496389	1.986337	-0.009474
H	-2.497348	-3.844489	0.001936
H	-4.984857	-4.095531	-0.008786
H	-6.413207	-2.05189	-0.015903
H	-5.402348	0.172306	-0.012371
H	1.070489	-0.2841	2.160975
H	3.523135	-0.158904	2.180997
H	3.544783	-0.171763	-2.12429
H	1.089302	-0.29729	-2.128972
H	6.991821	0.021912	1.329265
H	5.563994	0.838462	1.977456
H	5.657073	-0.935277	1.983315
H	6.941323	-1.262844	-0.781431
H	5.479962	-1.37129	-1.774059
H	5.563026	-2.235747	-0.23033

H	5.338367	2.107007	-0.245367
H	6.809242	1.277784	-0.7909
H	5.344695	1.227493	-1.783289

SCF Done: E(RB3LYP) = -1118.36221818 A.U. after 14 cycles

Zero-point correction = 0.372888 (Hartree/Particle)

Thermal correction to Energy = 0.394492

Thermal correction to Enthalpy = 0.395436

Thermal correction to Gibbs Free Energy = 0.321657

Sum of electronic and zero-point Energies = -1117.989330

Sum of electronic and thermal Energies = -1117.967726

Sum of electronic and thermal Enthalpies = -1117.966782

Sum of electronic and thermal Free Energies = -1118.040562

12.2.2 Computed excitations energies of compound 4b (B3LYP/6-31G* PCM CH_2Cl_2)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.9214 eV 316.17 nm f=0.2320 <S**2>=0.000
90 -> 93 -0.11391
91 -> 92 0.68202
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1118.21810996
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 4.2527 eV 291.54 nm f=0.0311 <S**2>=0.000
87 -> 92 -0.16898
91 -> 93 0.67190

Excited State 3: Singlet-A 4.5472 eV 272.66 nm f=0.0005 <S**2>=0.000
86 -> 92 0.36817
86 -> 93 0.27948
89 -> 92 0.48641
89 -> 93 0.18169

Excited State 4: Singlet-A 4.6162 eV 268.58 nm f=0.0506 <S**2>=0.000
87 -> 92 0.16784
87 -> 93 -0.12878
90 -> 92 0.59398
90 -> 93 0.24329
91 -> 96 0.15004

Excited State 5: Singlet-A 4.7795 eV 259.41 nm f=0.0005 <S**2>=0.000
86 -> 92 -0.36467
86 -> 93 -0.27793
89 -> 92 0.50348

89 -> 93 -0.13312

Excited State 6: Singlet-A 4.8504 eV 255.62 nm f=0.1342 <S**2>=0.000
87 -> 92 0.27119
88 -> 92 0.14729
90 -> 92 -0.23159
90 -> 93 0.48203
91 -> 92 0.11833
91 -> 94 0.18918
91 -> 96 -0.21484

Excited State 7: Singlet-A 4.8568 eV 255.28 nm f=0.0135 <S**2>=0.000
90 -> 93 -0.13448
91 -> 94 0.65936
91 -> 95 -0.12151

Excited State 8: Singlet-A 5.0078 eV 247.58 nm f=0.0256 <S**2>=0.000
87 -> 92 -0.14872
88 -> 92 0.66342
89 -> 93 -0.11195
90 -> 93 -0.11747

Excited State 9: Singlet-A 5.0388 eV 246.06 nm f=0.0010 <S**2>=0.000
89 -> 93 -0.12852
91 -> 94 0.12500
91 -> 95 0.66872

Excited State 10: Singlet-A 5.0435 eV 245.83 nm f=0.0013 <S**2>=0.000
86 -> 92 -0.37639
86 -> 93 0.15670
88 -> 92 0.10526
89 -> 93 0.53651
91 -> 95 0.15971

Excited State 11: Singlet-A 5.2383 eV 236.69 nm f=0.0018 <S**2>=0.000
86 -> 92 -0.26473
86 -> 93 0.52561
89 -> 93 -0.33360

Excited State 12: Singlet-A 5.2810 eV 234.77 nm f=0.2417 <S**2>=0.000
85 -> 92 0.10547
87 -> 92 0.45267
90 -> 93 -0.37603
91 -> 96 -0.29877

Excited State 13: Singlet-A 5.3573 eV 231.43 nm f=0.3859 <S**2>=0.000
85 -> 93 0.12627
87 -> 92 0.27699

87 -> 93 -0.12348
88 -> 93 0.10595
90 -> 92 -0.21149
90 -> 96 -0.13999
90 -> 97 0.10572
91 -> 93 0.12557
91 -> 96 0.49566
91 -> 97 0.14375

Excited State 14: Singlet-A 5.3998 eV 229.61 nm f=0.0123 <S**2>=0.000
88 -> 93 -0.33549
88 -> 94 0.36091
88 -> 95 -0.11403
89 -> 94 0.15887
89 -> 95 0.41195

Excited State 15: Singlet-A 5.4189 eV 228.80 nm f=0.0247 <S**2>=0.000
86 -> 93 -0.12126
88 -> 93 0.58969
88 -> 94 0.19791
89 -> 95 0.22308

12.2.3 Computed LE emission energies of compound 4b (B3LYP/6-31G* PCM CH_2Cl_2)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.1103 eV 398.62 nm f=0.2521 <S**2>=0.000
91 -> 92 0.69985
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1118.22986912
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.6893 eV 336.07 nm f=0.0121 <S**2>=0.000
90 -> 92 -0.20799
91 -> 93 0.66591

Excited State 3: Singlet-A 3.9714 eV 312.19 nm f=0.0974 <S**2>=0.000
86 -> 92 0.11959
88 -> 92 0.11666
89 -> 92 -0.10689
90 -> 92 0.61609
91 -> 93 0.17222
91 -> 94 -0.16228

Excited State 4: Singlet-A 4.1772 eV 296.81 nm f=0.0218 <S**2>=0.000
86 -> 92 -0.31606
88 -> 92 -0.38342
89 -> 92 0.42146
90 -> 92 0.13704

Excited State 5: Singlet-A 4.3199 eV 287.01 nm f=0.0208 <S**2>=0.000
88 -> 92 0.47577
89 -> 92 0.48999
90 -> 93 -0.10270

Excited State 6: Singlet-A 4.3562 eV 284.62 nm f=0.2089 <S**2>=0.000
87 -> 92 -0.17232
90 -> 92 0.10524
90 -> 93 0.19935
91 -> 94 0.62497

Excited State 7: Singlet-A 4.6058 eV 269.19 nm f=0.0088 <S**2>=0.000
86 -> 92 0.52313
87 -> 92 0.12853
88 -> 92 -0.28957
88 -> 93 0.10093
89 -> 92 0.17842
90 -> 93 -0.15531
91 -> 95 0.16596

Excited State 8: Singlet-A 4.6563 eV 266.27 nm f=0.1856 <S**2>=0.000
86 -> 92 0.19291
87 -> 92 -0.33882
89 -> 92 0.11978
90 -> 92 -0.16667
90 -> 93 0.45933
91 -> 94 -0.22635
91 -> 96 0.11102

Excited State 9: Singlet-A 4.8364 eV 256.36 nm f=0.1075 <S**2>=0.000
86 -> 92 -0.10529
89 -> 92 -0.11680
89 -> 94 -0.18499
91 -> 95 0.61916
91 -> 96 0.11643

Excited State 10: Singlet-A 4.9626 eV 249.84 nm f=0.2433 <S**2>=0.000
87 -> 92 0.36198
88 -> 93 0.36961
90 -> 93 0.35544
90 -> 94 -0.13017
91 -> 96 -0.22732

Excited State 11: Singlet-A 5.0763 eV 244.24 nm f=0.0304 <S**2>=0.000
86 -> 92 0.12753
86 -> 93 -0.12981
88 -> 93 -0.15130

89 -> 93 0.64901

Excited State 12: Singlet-A 5.1349 eV 241.45 nm f=0.1978 <S**2>=0.000
88 -> 93 0.35062
89 -> 93 0.13736
90 -> 93 -0.10775
90 -> 94 -0.27923
91 -> 95 -0.11234
91 -> 96 0.45750

Excited State 13: Singlet-A 5.1751 eV 239.58 nm f=0.1728 <S**2>=0.000
85 -> 92 -0.14235
87 -> 92 -0.32646
88 -> 93 0.38691
90 -> 93 -0.21625
90 -> 94 0.14900
91 -> 96 -0.31687

Excited State 14: Singlet-A 5.3599 eV 231.32 nm f=0.0261 <S**2>=0.000
86 -> 93 0.13706
87 -> 92 0.10299
88 -> 93 0.10357
89 -> 93 0.13816
90 -> 94 0.45203
91 -> 96 0.15359
91 -> 97 0.40092

Excited State 15: Singlet-A 5.4865 eV 225.98 nm f=0.2097 <S**2>=0.000
85 -> 92 -0.38739
86 -> 93 -0.18495
87 -> 92 0.15397
87 -> 93 0.48183
91 -> 97 0.11572

12.2.4 Potential scan of compound 4b ground state (B3LYP/6-31G* PCM CH_2Cl_2)

D(4,7,16,17)
0 -1118.36221818 89.7321
8 -1118.36203573 99.7321
13 -1118.36151163 109.7321
17 -1118.36056026 119.7321
22 -1118.35912163 129.732
27 -1118.35692421 139.732
32 -1118.35381294 149.732
37 -1118.34981414 159.732
43 -1118.34559512 169.732
48 -1118.34185493 179.732
53 -1118.33873715 -170.268

59 -1118.3364122 -160.268
65 -1118.33518676 -150.2679
79 -1118.35679542 -140.2678
84 -1118.35903127 -130.2678
88 -1118.36053027 -120.2678
92 -1118.36148199 -110.2678
96 -1118.36202852 -100.2678
101 -1118.36222523 -90.2678
105 -1118.36206125 -80.2678
109 -1118.36149877 -70.2679
114 -1118.36048434 -60.268
118 -1118.35886609 -50.2679
122 -1118.35649963 -40.2679
127 -1118.35323519 -30.268
133 -1118.34914562 -20.268
140 -1118.34471913 -10.268
146 -1118.34082082 -0.268
152 -1118.33776926 9.732
158 -1118.3358048 19.732
175 -1118.35303058 29.7322
180 -1118.35630923 39.7323
184 -1118.35874732 49.7322
188 -1118.36041406 59.7323
193 -1118.36146025 69.7322
198 -1118.36201614 79.7322
202 -1118.36220704 89.7322

Progress of structural optimization and emission calculation

-1118.362218
-1118.361918
-1118.362018
-1118.362024
-1118.362033
-1118.362035
-1118.362036
-1118.362036
-1118.362036
-1118.361392
-1118.361507
-1118.361509
-1118.361512
-1118.361512
-1118.360451
-1118.360559
-1118.36056
-1118.36056
-1118.358964
-1118.359119

-1118.359121
-1118.359122
-1118.359122
-1118.356756
-1118.356916
-1118.356923
-1118.356924
-1118.356924
-1118.353553
-1118.353802
-1118.353812
-1118.353813
-1118.353813
-1118.349361
-1118.34978
-1118.349811
-1118.349814
-1118.349814
-1118.344719
-1118.345453
-1118.345583
-1118.345593
-1118.345595
-1118.345595
-1118.340985
-1118.341798
-1118.341852
-1118.341855
-1118.341855
-1118.337883
-1118.338691
-1118.338735
-1118.338737
-1118.338737
-1118.335499
-1118.336362
-1118.336408
-1118.336412
-1118.336412
-1118.336412
-1118.334155
-1118.335079
-1118.335171
-1118.335185
-1118.335187
-1118.335187
-1118.334321
-1118.335809

-1118.337218
-1118.331216
-1118.344828
-1118.319631
-1118.35213
-1118.355111
-1118.356051
-1118.356641
-1118.356778
-1118.356793
-1118.356795
-1118.356795
-1118.358856
-1118.359025
-1118.359031
-1118.359031
-1118.359031
-1118.360399
-1118.360529
-1118.36053
-1118.36053
-1118.361358
-1118.361481
-1118.361482
-1118.361482
-1118.361911
-1118.362027
-1118.362028
-1118.362029
-1118.362093
-1118.362222
-1118.362225
-1118.362225
-1118.362225
-1118.36192
-1118.36206
-1118.362061
-1118.362061
-1118.361322
-1118.361497
-1118.361499
-1118.361499
-1118.360251
-1118.360477
-1118.360484
-1118.360484
-1118.360484
-1118.358581

-1118.358853
-1118.358866
-1118.358866
-1118.356149
-1118.356473
-1118.356499
-1118.3565
-1118.352781
-1118.353202
-1118.353234
-1118.353235
-1118.353235
-1118.348532
-1118.34908
-1118.34914
-1118.349145
-1118.349146
-1118.349146
-1118.343788
-1118.344573
-1118.344688
-1118.344718
-1118.344719
-1118.344719
-1118.344719
-1118.339681
-1118.3407
-1118.340807
-1118.34082
-1118.340821
-1118.340821
-1118.336703
-1118.337661
-1118.337745
-1118.337768
-1118.337769
-1118.337769
-1118.334762
-1118.335672
-1118.335778
-1118.335804
-1118.335805
-1118.335805
-1118.334312
-1118.335229
-1118.335426
-1118.335653
-1118.335733

-1118.335901
-1118.337361
-1118.340849
-1118.344827
-1118.348816
-1118.350737
-1118.352391
-1118.352807
-1118.35302
-1118.353029
-1118.35303
-1118.353031
-1118.35591
-1118.356276
-1118.356308
-1118.356309
-1118.356309
-1118.35844
-1118.358737
-1118.358747
-1118.358747
-1118.360175
-1118.360407
-1118.360414
-1118.360414
-1118.361251
-1118.361455
-1118.36146
-1118.36146
-1118.36146
-1118.361831
-1118.362012
-1118.362016
-1118.362016
-1118.362016
-1118.362058
-1118.362206
-1118.362207

Geometries of structural optimization

1 Energy:-1118.36221818
C -2.746525 3.184320 -0.002734
C -1.356662 3.256873 0.003212
C -0.628506 2.075155 0.007489
C -1.276129 0.825937 0.005774
C -2.692608 0.767060 -0.000664
C -3.413465 1.976299 -0.004729

N -0.519074 -0.362816 0.010394
C -1.080226 -1.638008 0.007529
C -2.555630 -1.704276 0.000985
C -3.352843 -0.539280 -0.002968
C -3.148710 -2.977518 -0.001206
C -4.528507 -3.110176 -0.007185
C -5.330818 -1.959202 -0.011158
C -4.754266 -0.696784 -0.009117
O -0.365114 -2.640792 0.010468
C 0.925375 -0.296467 0.016973
C 1.618512 -0.257589 1.223674
C 3.013746 -0.186494 1.224704
C 3.747602 -0.152279 0.030221
C 3.020566 -0.194030 -1.173495
C 1.629950 -0.264979 -1.187606
F -3.465145 4.331815 -0.006734
C 5.284609 -0.072364 -0.003898
C 5.900519 -0.035141 1.407567
C 5.846351 -1.309912 -0.743980
C 5.715309 1.211529 -0.752976
H -0.860898 4.221567 0.004494
H 0.452717 2.119924 0.012352
H -4.496389 1.986337 -0.009474
H -2.497348 -3.844489 0.001936
H -4.984857 -4.095531 -0.008786
H -6.413207 -2.051890 -0.015903
H -5.402348 0.172306 -0.012371
H 1.070489 -0.284100 2.160975
H 3.523135 -0.158904 2.180997
H 3.544783 -0.171763 -2.124290
H 1.089302 -0.297290 -2.128972
H 6.991821 0.021912 1.329265
H 5.563994 0.838462 1.977456
H 5.657073 -0.935277 1.983315
H 6.941323 -1.262844 -0.781431
H 5.479962 -1.371290 -1.774059
H 5.563026 -2.235747 -0.230330
H 5.338367 2.107007 -0.245367
H 6.809242 1.277784 -0.790900
H 5.344695 1.227493 -1.783289

2 Energy:-1118.36203573
C -2.763585 3.183421 -0.160651
C -1.375345 3.265575 -0.105272
C -0.641804 2.089916 -0.026058
C -1.281790 0.836820 -0.005410
C -2.697048 0.768842 -0.051968
C -3.423607 1.971966 -0.133187

N -0.518515 -0.345432 0.076818
C -1.073850 -1.623328 0.116877
C -2.548525 -1.697973 0.081066
C -3.350758 -0.539893 -0.007553
C -3.135453 -2.973205 0.129146
C -4.513903 -3.114436 0.091732
C -5.321114 -1.970304 0.003284
C -4.750679 -0.706077 -0.045726
O -0.355180 -2.621815 0.174359
C 0.925344 -0.272394 0.067074
C 1.639109 -0.354916 1.259314
C 3.034532 -0.294336 1.242842
C 3.749065 -0.152097 0.044525
C 3.001956 -0.075349 -1.144954
C 1.610761 -0.137379 -1.141717
F -3.487551 4.324734 -0.240111
C 5.286007 -0.081450 -0.008533
C 5.925157 -0.173832 1.390029
C 5.823668 -1.253460 -0.864210
C 5.717069 1.259815 -0.648845
H -0.885045 4.232908 -0.122171
H 0.438004 2.142652 0.021462
H -4.505820 1.974566 -0.173346
H -2.480475 -3.834869 0.195603
H -4.965431 -4.101257 0.130107
H -6.402467 -2.069769 -0.027391
H -5.402388 0.157609 -0.113987
H 1.106615 -0.466766 2.199057
H 3.559875 -0.361683 2.188460
H 3.510352 0.030656 -2.098667
H 1.055270 -0.082179 -2.073417
H 7.015450 -0.117065 1.298518
H 5.604800 0.647850 2.040743
H 5.684280 -1.119967 1.887794
H 6.918309 -1.212409 -0.916000
H 5.439880 -1.220368 -1.889237
H 5.539724 -2.218639 -0.429400
H 5.356432 2.110204 -0.058594
H 6.810850 1.320406 -0.698496
H 5.331018 1.369257 -1.667753

3 Energy:-1118.36151163
C -2.782339 3.175963 -0.317066
C -1.398354 3.273854 -0.207699
C -0.659363 2.109541 -0.051450
C -1.287939 0.850876 -0.010611
C -2.700202 0.768760 -0.102910
C -3.432731 1.960401 -0.263124

N -0.517736 -0.319444 0.153727
C -1.068919 -1.598446 0.242917
C -2.541416 -1.685218 0.167641
C -3.347090 -0.540955 -0.014855
C -3.121696 -2.960847 0.264577
C -4.496833 -3.115463 0.184457
C -5.307380 -1.984916 0.001876
C -4.743474 -0.720659 -0.096404
O -0.349136 -2.589857 0.366384
C 0.925434 -0.242428 0.126711
C 1.660975 -0.440791 1.291872
C 3.056296 -0.393683 1.253715
C 3.751045 -0.152694 0.059593
C 2.983164 0.035243 -1.103853
C 1.591810 -0.015051 -1.079671
F -3.511781 4.305714 -0.473085
C 5.287400 -0.093046 -0.016710
C 5.951321 -0.317932 1.354979
C 5.795548 -1.188023 -0.985107
C 5.721857 1.296361 -0.541730
H -0.915659 4.244586 -0.240599
H 0.416486 2.176387 0.042858
H -4.512763 1.950832 -0.341544
H -2.464239 -3.812163 0.401748
H -4.943189 -4.102400 0.261162
H -6.386126 -2.095067 -0.063850
H -5.397583 0.132275 -0.237667
H 1.145513 -0.631372 2.228039
H 3.597737 -0.551460 2.179300
H 3.474891 0.217705 -2.054739
H 1.021688 0.122511 -1.993864
H 7.040343 -0.264580 1.247506
H 5.653240 0.444955 2.083214
H 5.708053 -1.302534 1.770091
H 6.889401 -1.152853 -1.054818
H 5.392844 -1.058964 -1.995225
H 5.509094 -2.185764 -0.633385
H 5.381756 2.093346 0.129676
H 6.815159 1.350821 -0.607039
H 5.318084 1.501031 -1.538879

4 Energy:-1118.36056026
C -2.803233 3.161677 -0.470584
C -1.427367 3.282659 -0.299501
C -0.683102 2.135247 -0.064758
C -1.295492 0.868690 -0.009857
C -2.701994 0.766260 -0.154004
C -3.440540 1.940635 -0.395236

N -0.517111 -0.283407 0.237492
C -1.064167 -1.563537 0.366806
C -2.532945 -1.666962 0.250647
C -3.340830 -0.543683 -0.025193
C -3.105722 -2.941632 0.395595
C -4.475357 -3.115027 0.272215
C -5.287844 -2.005154 -0.004301
C -4.731309 -0.742347 -0.150871
O -0.344928 -2.545319 0.551962
C 0.925281 -0.202342 0.193124
C 1.681788 -0.512422 1.320288
C 3.076492 -0.481465 1.257457
C 3.752858 -0.151163 0.074417
C 2.965294 0.143255 -1.053166
C 1.574300 0.109129 -1.004983
F -3.537976 4.274065 -0.705318
C 5.288128 -0.107610 -0.027503
C 5.973621 -0.461541 1.305846
C 5.760860 -1.121009 -1.097346
C 5.735164 1.316000 -0.437787
H -0.955271 4.258135 -0.343718
H 0.385261 2.222638 0.082026
H -4.516130 1.913378 -0.517684
H -2.446859 -3.777302 0.603471
H -4.915902 -4.100878 0.386969
H -6.362212 -2.130282 -0.105339
H -5.386765 0.094381 -0.364221
H 1.183621 -0.775311 2.247598
H 3.632324 -0.725350 2.155444
H 3.440449 0.395041 -1.996677
H 0.991400 0.325144 -1.895526
H 7.061243 -0.416001 1.181651
H 5.702314 0.239400 2.103488
H 5.720981 -1.474658 1.638612
H 6.853804 -1.096737 -1.183961
H 5.343434 -0.897844 -2.084809
H 5.463629 -2.141267 -0.828990
H 5.421981 2.055628 0.308196
H 6.827687 1.359928 -0.521823
H 5.314330 1.613510 -1.403989

5 Energy:-1118.35912163
C -2.809158 3.141630 -0.611056
C -1.447619 3.288883 -0.362881
C -0.704688 2.161088 -0.045253
C -1.300158 0.886075 0.012636
C -2.695847 0.761019 -0.199470
C -3.434111 1.915292 -0.525253

N -0.518207 -0.243722 0.348871
C -1.068862 -1.519719 0.526839
C -2.529615 -1.642644 0.344382
C -3.329809 -0.547723 -0.042353
C -3.099036 -2.913929 0.529053
C -4.457261 -3.110790 0.335230
C -5.261412 -2.029098 -0.054096
C -4.708176 -0.770054 -0.240154
O -0.359966 -2.488431 0.798140
C 0.924028 -0.164949 0.281359
C 1.706131 -0.576837 1.358418
C 3.099176 -0.561487 1.260608
C 3.752220 -0.153417 0.089378
C 2.940649 0.233541 -0.992151
C 1.551441 0.216622 -0.909710
F -3.542811 4.233846 -0.928319
C 5.284774 -0.121097 -0.048268
C 5.997660 -0.584383 1.236275
C 5.717552 -1.054200 -1.204491
C 5.740950 1.324539 -0.359746
H -0.986573 4.269499 -0.409537
H 0.350613 2.271286 0.166181
H -4.501402 1.868331 -0.701931
H -2.446587 -3.728734 0.822068
H -4.895047 -4.093773 0.480954
H -6.326393 -2.173371 -0.212576
H -5.356611 0.044715 -0.541623
H 1.230932 -0.900862 2.277169
H 3.672209 -0.881136 2.123399
H 3.395018 0.544201 -1.928350
H 0.953489 0.501518 -1.770043
H 7.082507 -0.542520 1.088607
H 5.755400 0.056566 2.091637
H 5.739007 -1.616887 1.497052
H 6.808203 -1.035199 -1.317443
H 5.278397 -0.750935 -2.160706
H 5.414071 -2.088823 -1.007621
H 5.456096 2.008318 0.448302
H 6.831608 1.362194 -0.468022
H 5.300414 1.700107 -1.289349

6 Energy:-1118.35692421
C -2.817556 3.119673 -0.735630
C -1.478314 3.302719 -0.403280
C -0.737466 2.199711 -0.005562
C -1.307674 0.912379 0.045453
C -2.685956 0.755540 -0.241359
C -3.423592 1.884281 -0.649099

N -0.521012 -0.187037 0.470946
C -1.072190 -1.461760 0.680937
C -2.520287 -1.613300 0.428095
C -3.310167 -0.554776 -0.064375
C -3.083093 -2.882786 0.644453
C -4.423757 -3.112298 0.377856
C -5.216507 -2.066793 -0.118729
C -4.669815 -0.809993 -0.336627
O -0.374313 -2.413138 1.029407
C 0.921414 -0.108839 0.381560
C 1.726132 -0.617089 1.400779
C 3.116401 -0.621864 1.264380
C 3.748331 -0.148899 0.107068
C 2.915579 0.326070 -0.921929
C 1.529772 0.332977 -0.800939
F -3.549551 4.186357 -1.132473
C 5.276610 -0.140428 -0.072099
C 6.013372 -0.696242 1.161181
C 5.655806 -1.010220 -1.294602
C 5.757388 1.311349 -0.308884
H -1.034648 4.291524 -0.444791
H 0.297995 2.339086 0.275744
H -4.477713 1.810532 -0.885364
H -2.439562 -3.670737 1.018928
H -4.856285 -4.093537 0.548791
H -6.267142 -2.237463 -0.335820
H -5.308507 -0.023097 -0.721408
H 1.274047 -0.992562 2.309974
H 3.703661 -1.012367 2.087638
H 3.349756 0.686045 -1.850118
H 0.920088 0.681357 -1.628402
H 7.094614 -0.666203 0.986529
H 5.806860 -0.105155 2.060696
H 5.740194 -1.737783 1.364972
H 6.743008 -1.007325 -1.438453
H 5.196573 -0.640097 -2.217269
H 5.334538 -2.048326 -1.151543
H 5.510721 1.950588 0.546780
H 6.845244 1.332325 -0.446192
H 5.300196 1.752149 -1.201061

7 Energy:-1118.35381294
C -2.812308 3.093028 -0.856104
C -1.506904 3.318852 -0.427926
C -0.774619 2.244834 0.054568
C -1.313965 0.943442 0.092753
C -2.664565 0.747825 -0.282269
C -3.395451 1.846500 -0.776357

N -0.527453 -0.119283 0.612193
C -1.088141 -1.384375 0.872227
C -2.513151 -1.574467 0.525631
C -3.277518 -0.565402 -0.092812
C -3.071802 -2.840358 0.772646
C -4.381369 -3.114071 0.409914
C -5.146278 -2.118492 -0.215842
C -4.604024 -0.865171 -0.463422
O -0.415295 -2.307207 1.328376
C 0.916181 -0.049806 0.498734
C 1.744314 -0.646166 1.451960
C 3.129588 -0.673150 1.268275
C 3.738709 -0.145217 0.124042
C 2.884189 0.411912 -0.843955
C 1.504479 0.444841 -0.676152
F -3.536410 4.129981 -1.336352
C 5.259827 -0.162323 -0.105305
C 6.020232 -0.812804 1.065778
C 5.577457 -0.961815 -1.391728
C 5.770739 1.289458 -0.266850
H -1.085538 4.317705 -0.459371
H 0.231880 2.416857 0.413440
H -4.429295 1.740993 -1.080380
H -2.449444 -3.591498 1.245365
H -4.810347 -4.092451 0.604514
H -6.171192 -2.325315 -0.510523
H -5.219489 -0.116552 -0.949293
H 1.319405 -1.063607 2.353684
H 3.730484 -1.128403 2.047357
H 3.295246 0.815639 -1.764715
H 0.884242 0.851286 -1.467464
H 7.095852 -0.798961 0.857471
H 5.858294 -0.274503 2.006617
H 5.725398 -1.857872 1.213737
H 6.659259 -0.975738 -1.571433
H 5.098865 -0.523403 -2.273785
H 5.234201 -1.998973 -1.303071
H 5.568239 1.878999 0.634864
H 6.853856 1.293055 -0.439002
H 5.296819 1.796724 -1.113876

8 Energy:-1118.34981414
C -2.798124 3.065913 -0.963437
C -1.537241 3.340845 -0.439859
C -0.816919 2.299512 0.124632
C -1.318716 0.982889 0.148314
C -2.630155 0.740493 -0.320413
C -3.351830 1.805352 -0.896043

N -0.538062 -0.038821 0.760190
C -1.127753 -1.271823 1.108990
C -2.509819 -1.519876 0.639358
C -3.225516 -0.579571 -0.126758
C -3.066370 -2.780207 0.917354
C -4.321220 -3.116986 0.433275
C -5.032302 -2.192319 -0.345628
C -4.493832 -0.942845 -0.620971
O -0.508783 -2.137221 1.724906
C 0.907367 0.005940 0.620790
C 1.755868 -0.677454 1.498703
C 3.133175 -0.728774 1.262129
C 3.721920 -0.145581 0.135995
C 2.849297 0.494551 -0.761413
C 1.478540 0.555068 -0.542056
F -3.511721 4.070215 -1.521514
C 5.232970 -0.188275 -0.147136
C 6.012146 -0.933415 0.953040
C 5.484879 -0.910796 -1.492309
C 5.779605 1.256841 -0.233533
H -1.144668 4.351622 -0.459437
H 0.152525 2.507424 0.559894
H -4.359382 1.663306 -1.266527
H -2.485100 -3.478475 1.508384
H -4.747592 -4.091773 0.650383
H -6.011679 -2.451144 -0.737859
H -5.064623 -0.248180 -1.226962
H 1.357736 -1.138450 2.388622
H 3.744009 -1.250036 1.990687
H 3.237080 0.943124 -1.671633
H 0.852137 1.021418 -1.292889
H 7.080423 -0.935127 0.709334
H 5.896454 -0.453097 1.931335
H 5.691851 -1.977524 1.044045
H 6.559263 -0.941576 -1.710504
H 4.989931 -0.403699 -2.327299
H 5.115360 -1.942168 -1.458125
H 5.625128 1.791481 0.710904
H 6.855807 1.243418 -0.444360
H 5.291128 1.830348 -1.028446

9 Energy:-1118.34559512
C -2.810852 3.042672 -1.061382
C -1.595308 3.377382 -0.469517
C -0.873644 2.376529 0.163661
C -1.328012 1.043918 0.186640
C -2.596890 0.741077 -0.354605
C -3.322931 1.763805 -0.996095

N -0.549956 0.063932 0.871397
C -1.185924 -1.100884 1.353787
C -2.499663 -1.443845 0.759342
C -3.156303 -0.593423 -0.151082
C -3.041029 -2.702433 1.070602
C -4.216655 -3.128736 0.470043
C -4.862624 -2.296578 -0.455612
C -4.341688 -1.045793 -0.760764
O -0.650409 -1.848975 2.168231
C 0.894465 0.060969 0.706112
C 1.741667 -0.725350 1.499533
C 3.109557 -0.809189 1.221490
C 3.699642 -0.153604 0.137575
C 2.830676 0.590859 -0.677662
C 1.468504 0.684615 -0.419591
F -3.526500 4.007436 -1.682288
C 5.201225 -0.226474 -0.185120
C 5.975119 -1.085405 0.832704
C 5.396698 -0.846299 -1.589604
C 5.799861 1.200331 -0.169404
H -1.241508 4.402373 -0.487988
H 0.058547 2.628371 0.654762
H -4.304354 1.575517 -1.413733
H -2.510513 -3.330397 1.777159
H -4.629736 -4.103978 0.709640
H -5.777063 -2.628300 -0.939056
H -4.858031 -0.421245 -1.481623
H 1.347646 -1.246105 2.356381
H 3.712751 -1.415268 1.888494
H 3.212507 1.100582 -1.557891
H 0.852954 1.230872 -1.122127
H 7.037499 -1.104451 0.565012
H 5.896500 -0.682789 1.849021
H 5.618888 -2.121729 0.846463
H 6.464043 -0.896796 -1.836891
H 4.901899 -0.256263 -2.368335
H 4.990274 -1.863539 -1.628799
H 5.685649 1.662423 0.818053
H 6.870083 1.165845 -0.406775
H 5.316132 1.852890 -0.904000

10 Energy:-1118.34185493
C -2.846602 3.004312 -1.179787
C -1.669011 3.401411 -0.551872
C -0.935572 2.445971 0.137797
C -1.340496 1.099206 0.178591
C -2.577563 0.734553 -0.396978
C -3.316529 1.709564 -1.093701

N -0.555978 0.159923 0.914005
C -1.219554 -0.943509 1.498124
C -2.483674 -1.373082 0.853289
C -3.102626 -0.608497 -0.154884
C -3.007997 -2.623968 1.217307
C -4.125777 -3.130479 0.568858
C -4.729462 -2.386802 -0.455000
C -4.227277 -1.140857 -0.810755
O -0.736617 -1.578485 2.431465
C 0.885604 0.113007 0.732331
C 1.703421 -0.786880 1.434145
C 3.064763 -0.901816 1.140856
C 3.684983 -0.161128 0.130504
C 2.847227 0.699325 -0.595701
C 1.489489 0.825501 -0.322665
F -3.572983 3.923708 -1.854265
C 5.182689 -0.260833 -0.202210
C 5.916310 -1.261858 0.710142
C 5.356301 -0.725086 -1.668194
C 5.841367 1.128293 -0.026199
H -1.354715 4.438832 -0.584546
H -0.037013 2.747011 0.663062
H -4.277595 1.473830 -1.534605
H -2.510190 -3.184080 2.000774
H -4.525044 -4.101128 0.847334
H -5.596784 -2.783109 -0.975205
H -4.709590 -0.583312 -1.606518
H 1.291559 -1.374746 2.238098
H 3.639617 -1.602002 1.737165
H 3.248758 1.283633 -1.419003
H 0.904905 1.465141 -0.968832
H 6.977587 -1.296515 0.439605
H 5.852577 -0.973761 1.765644
H 5.515337 -2.276675 0.607525
H 6.421360 -0.792601 -1.921286
H 4.889738 -0.029992 -2.374312
H 4.907098 -1.713059 -1.822033
H 5.744330 1.479857 1.007547
H 6.909784 1.075989 -0.268625
H 5.387037 1.879742 -0.680833

11 Energy:-1118.33873715
C -2.887062 2.951184 -1.306836
C -1.741303 3.406386 -0.661722
C -0.993685 2.496614 0.075561
C -1.352333 1.138992 0.142624
C -2.567971 0.718516 -0.442800
C -3.320485 1.645317 -1.186851

N -0.556895 0.235385 0.911496
C -1.230912 -0.816612 1.575590
C -2.469046 -1.312322 0.927948
C -3.067893 -0.624604 -0.146288
C -2.981512 -2.547606 1.354237
C -4.066290 -3.117667 0.701216
C -4.646991 -2.453242 -0.387894
C -4.157470 -1.220493 -0.804853
O -0.767030 -1.360096 2.573042
C 0.881524 0.154529 0.721748
C 1.654118 -0.858013 1.315690
C 3.012645 -0.995105 1.025174
C 3.679804 -0.162366 0.120855
C 2.888702 0.813653 -0.501292
C 1.532211 0.965125 -0.227804
F -3.625563 3.824071 -2.028092
C 5.177261 -0.284452 -0.205236
C 5.854603 -1.418771 0.586744
C 5.354747 -0.575168 -1.714758
C 5.889718 1.043738 0.144966
H -1.462795 4.453110 -0.715241
H -0.128846 2.847566 0.625354
H -4.265815 1.366083 -1.636558
H -2.500461 -3.046950 2.187899
H -4.456505 -4.077217 1.026899
H -5.487394 -2.900207 -0.911192
H -4.623322 -0.723157 -1.649052
H 1.211917 -1.525459 2.038160
H 3.547572 -1.789194 1.534795
H 3.325776 1.478868 -1.240968
H 0.990353 1.703375 -0.800143
H 6.917822 -1.465648 0.325794
H 5.785561 -1.258021 1.668676
H 5.414229 -2.395776 0.357106
H 6.419958 -0.655823 -1.963423
H 4.926890 0.218972 -2.335843
H 4.868732 -1.517796 -1.991928
H 5.791434 1.271539 1.212706
H 6.958667 0.975833 -0.091271
H 5.476528 1.887457 -0.418078

12 Energy:-1118.3364122
C -2.934416 2.880772 -1.445599
C -1.809941 3.389860 -0.805612
C -1.045167 2.528154 -0.026901
C -1.364364 1.164234 0.081996
C -2.570314 0.693781 -0.488986
C -3.339003 1.570493 -1.274028

N -0.553411 0.292651 0.871728
C -1.221506 -0.713054 1.610430
C -2.455231 -1.257107 0.994575
C -3.051671 -0.640644 -0.124010
C -2.959301 -2.468650 1.491654
C -4.032984 -3.088375 0.865389
C -4.609378 -2.497625 -0.267335
C -4.128452 -1.286979 -0.754511
O -0.746916 -1.183733 2.638531
C 0.881637 0.188416 0.677670
C 1.598768 -0.927129 1.145044
C 2.957646 -1.081668 0.872052
C 3.682661 -0.160744 0.106953
C 2.948368 0.923121 -0.391436
C 1.590773 1.095689 -0.129146
F -3.687398 3.704898 -2.207909
C 5.183227 -0.299890 -0.197500
C 5.793025 -1.560023 0.445195
C 5.393604 -0.386973 -1.728141
C 5.935609 0.936075 0.350743
H -1.561250 4.441950 -0.891114
H -0.211211 2.930577 0.533712
H -4.275984 1.251727 -1.714985
H -2.479773 -2.912226 2.357236
H -4.417022 -4.030221 1.245485
H -5.440330 -2.984369 -0.769810
H -4.592365 -0.845992 -1.630546
H 1.113435 -1.675735 1.752245
H 3.445456 -1.961881 1.276537
H 3.432738 1.667130 -1.017887
H 1.100956 1.932141 -0.602521
H 6.860949 -1.614944 0.205901
H 5.698236 -1.547243 1.536999
H 5.322861 -2.476858 0.071580
H 6.461698 -0.477824 -1.960379
H 5.015282 0.502681 -2.242802
H 4.879617 -1.260753 -2.145194
H 5.814061 1.018785 1.437008
H 7.007768 0.856148 0.133574
H 5.572202 1.865907 -0.099729

13 Energy:-1118.33518676
C -3.002886 2.782608 -1.607896
C -1.873578 3.335228 -1.017386
C -1.083226 2.524707 -0.208057
C -1.380518 1.164793 -0.021449
C -2.599470 0.656623 -0.536507
C -3.392492 1.481250 -1.351508

N -0.545187 0.319443 0.771043
C -1.184946 -0.639968 1.591388
C -2.443273 -1.208468 1.053789
C -3.069630 -0.654947 -0.081454
C -2.937614 -2.384525 1.637710
C -4.032168 -3.034086 1.081690
C -4.637996 -2.509168 -0.067920
C -4.166501 -1.332755 -0.640743
O -0.664986 -1.058068 2.619853
C 0.889413 0.214001 0.581846
C 1.545577 -0.990493 0.892915
C 2.908605 -1.157438 0.659312
C 3.700527 -0.152451 0.088626
C 3.031183 1.029932 -0.248374
C 1.668573 1.217173 -0.015258
F -3.779101 3.555572 -2.400083
C 5.208255 -0.303756 -0.172624
C 5.738721 -1.682870 0.262667
C 5.490763 -0.131760 -1.684274
C 5.977601 0.782558 0.616318
H -1.639397 4.384509 -1.159607
H -0.263109 2.979254 0.328778
H -4.336763 1.131714 -1.751439
H -2.433559 -2.778740 2.513325
H -4.409190 -3.949036 1.528639
H -5.485007 -3.020342 -0.516461
H -4.654797 -0.943132 -1.527803
H 1.002948 -1.813880 1.334202
H 3.345381 -2.112788 0.928834
H 3.573407 1.849437 -0.711835
H 1.242344 2.150980 -0.341381
H 6.813960 -1.743715 0.060607
H 5.592999 -1.855981 1.335024
H 5.252494 -2.498285 -0.285005
H 6.564796 -0.230764 -1.883345
H 5.173670 0.851029 -2.048992
H 4.964789 -0.894129 -2.270559
H 5.805877 0.679735 1.694034
H 7.055446 0.693518 0.433565
H 5.671258 1.792028 0.321955

14 Energy:-1118.35679542
C -2.857767 2.376571 -2.114348
C -1.511656 2.261770 -2.449459
C -0.752698 1.286863 -1.819277
C -1.311921 0.438007 -0.843697
C -2.696304 0.531336 -0.558751
C -3.452475 1.530357 -1.202665

N -0.505692 -0.554611 -0.232252
C -1.041932 -1.518879 0.637186
C -2.495816 -1.452989 0.893204
C -3.306647 -0.433537 0.354654
C -3.043623 -2.422572 1.750426
C -4.390003 -2.391321 2.078119
C -5.203792 -1.376669 1.552438
C -4.672018 -0.414152 0.705823
O -0.327931 -2.359258 1.182656
C 0.932989 -0.396620 -0.219487
C 1.771076 -1.491552 -0.428522
C 3.156508 -1.349186 -0.320084
C 3.750665 -0.128088 0.023803
C 2.884602 0.953528 0.264301
C 1.503172 0.824808 0.163739
F -3.607427 3.328944 -2.716049
C 5.272648 0.059970 0.150496
C 6.049056 -1.236686 -0.147227
C 5.740390 1.144281 -0.849705
C 5.617548 0.509959 1.590511
H -1.076325 2.915990 -3.196978
H 0.288862 1.177953 -2.091350
H -4.511868 1.644128 -1.009961
H -2.383919 -3.186099 2.146672
H -4.810896 -3.143753 2.738293
H -6.259241 -1.340064 1.806954
H -5.327268 0.356605 0.316237
H 1.349053 -2.452180 -0.694970
H 3.770341 -2.223210 -0.505601
H 3.288476 1.919239 0.553783
H 0.867172 1.675689 0.385568
H 7.124248 -1.051695 -0.045992
H 5.784610 -2.039962 0.549755
H 5.869661 -1.594870 -1.167364
H 6.823412 1.295063 -0.765791
H 5.254223 2.107803 -0.663730
H 5.517708 0.848269 -1.881424
H 5.304139 -0.243670 2.322076
H 6.699929 0.653835 1.692835
H 5.129922 1.455199 1.851310

15 Energy:-1118.35903127
C -2.847602 2.286881 -2.215895
C -1.480815 2.217869 -2.469269
C -0.721205 1.293240 -1.767345
C -1.305406 0.447394 -0.804583
C -2.705515 0.500454 -0.591657
C -3.460922 1.448065 -1.309215

N -0.505963 -0.492779 -0.113097
C -1.042075 -1.431709 0.778220
C -2.506600 -1.403375 0.969215
C -3.325397 -0.446244 0.335043
C -3.061322 -2.347120 1.850118
C -4.423150 -2.352736 2.107970
C -5.245910 -1.401868 1.485710
C -4.707303 -0.464949 0.615061
O -0.318824 -2.221148 1.385158
C 0.932959 -0.350897 -0.114449
C 1.749463 -1.433574 -0.434338
C 3.138827 -1.309329 -0.365826
C 3.754012 -0.116245 0.037599
C 2.907992 0.953708 0.380562
C 1.522083 0.841051 0.321861
F -3.597708 3.189489 -2.889990
C 5.281437 0.052969 0.121610
C 6.035663 -1.223506 -0.296331
C 5.722570 1.203434 -0.814711
C 5.681197 0.396153 1.576743
H -1.028324 2.870013 -3.208393
H 0.338683 1.222166 -1.972529
H -4.532321 1.530143 -1.175529
H -2.394613 -3.061896 2.319148
H -4.849499 -3.084842 2.787229
H -6.314002 -1.394944 1.683795
H -5.370148 0.256319 0.150682
H 1.304131 -2.371192 -0.746421
H 3.739218 -2.171692 -0.631867
H 3.332080 1.895982 0.714809
H 0.897027 1.679519 0.613666
H 7.115264 -1.051696 -0.222828
H 5.791375 -2.072951 0.351537
H 5.815537 -1.507255 -1.331794
H 6.809213 1.340570 -0.759673
H 5.252484 2.154313 -0.542489
H 5.460348 0.983962 -1.856204
H 5.387920 -0.406308 2.263311
H 6.767674 0.526307 1.649741
H 5.210661 1.322804 1.921801

16 Energy:-1118.36053027
C -2.829495 2.193773 -2.311996
C -1.450335 2.165979 -2.496595
C -0.694465 1.290176 -1.730368
C -1.298620 0.450636 -0.775147
C -2.707810 0.468011 -0.622233
C -3.458363 1.365551 -1.405760

N -0.507956 -0.437496 -0.012936
C -1.046176 -1.349284 0.900201
C -2.516709 -1.353394 1.038276
C -3.336595 -0.457298 0.320590
C -3.079075 -2.269353 1.943010
C -4.450016 -2.308006 2.143361
C -5.274445 -1.419276 1.437031
C -4.728336 -0.509992 0.542102
O -0.318954 -2.091461 1.560453
C 0.932014 -0.312443 -0.026170
C 1.726494 -1.370489 -0.460210
C 3.118264 -1.261245 -0.424711
C 3.753961 -0.104841 0.049304
C 2.928629 0.942642 0.496377
C 1.540197 0.842962 0.472945
F -3.575617 3.048049 -3.050782
C 5.284763 0.048651 0.098280
C 6.015733 -1.200793 -0.428389
C 5.706586 1.257807 -0.770537
C 5.730887 0.288900 1.560536
H -0.984542 2.813849 -3.231223
H 0.376780 1.253420 -1.877534
H -4.536626 1.419334 -1.321710
H -2.410827 -2.936851 2.475437
H -4.882451 -3.018214 2.841762
H -6.349966 -1.439250 1.588628
H -5.392874 0.163192 0.012478
H 1.260234 -2.278049 -0.828861
H 3.704335 -2.103446 -0.774133
H 3.371780 1.855775 0.882601
H 0.927627 1.661515 0.839276
H 7.098384 -1.041745 -0.373883
H 5.782092 -2.091459 0.165845
H 5.764646 -1.410401 -1.474405
H 6.795377 1.384765 -0.739179
H 5.251897 2.190381 -0.420107
H 5.411776 1.111277 -1.816123
H 5.450711 -0.556271 2.199653
H 6.820242 0.405556 1.608853
H 5.280040 1.193403 1.982152

17 Energy:-1118.36148199
C -2.809260 2.084828 -2.415823
C -1.423395 2.094694 -2.543267
C -0.673305 1.271157 -1.715454
C -1.292711 0.445136 -0.758853
C -2.706508 0.430411 -0.655299
C -3.450476 1.274232 -1.501924

N -0.510841 -0.387521 0.069217
C -1.052014 -1.263041 1.011901
C -2.525573 -1.296174 1.106875
C -3.342957 -0.465813 0.310672
C -3.095077 -2.177156 2.041099
C -4.470963 -2.246186 2.194244
C -5.293176 -1.424332 1.408785
C -4.740012 -0.549725 0.484071
O -0.324016 -1.954496 1.724784
C 0.930404 -0.278495 0.045395
C 1.702869 -1.300154 -0.500079
C 3.096054 -1.202371 -0.493163
C 3.752175 -0.092068 0.057658
C 2.947557 0.921062 0.609676
C 1.557910 0.832372 0.614063
F -3.549550 2.887289 -3.216327
C 5.285126 0.047025 0.080131
C 5.992177 -1.157106 -0.570301
C 5.696215 1.323566 -0.692028
C 5.768878 0.157266 1.545993
H -0.947626 2.732763 -3.280091
H 0.404307 1.265890 -1.813171
H -4.532202 1.302096 -1.459243
H -2.428412 -2.794280 2.633072
H -4.909026 -2.929115 2.915964
H -6.372677 -1.469340 1.521892
H -5.403130 0.071750 -0.107020
H 1.217823 -2.170919 -0.930091
H 3.666726 -2.015256 -0.927101
H 3.408420 1.797879 1.054820
H 0.959063 1.623121 1.056550
H 7.077082 -1.009643 -0.530366
H 5.766639 -2.094073 -0.048572
H 5.713084 -1.274806 -1.623583
H 6.786610 1.439269 -0.677749
H 5.259645 2.225976 -0.251326
H 5.374117 1.269880 -1.738449
H 5.498075 -0.738598 2.116415
H 6.859927 0.263384 1.576707
H 5.335220 1.024171 2.055452

18 Energy:-1118.36202852
C -2.788165 1.967923 -2.517983
C -1.399466 2.012501 -2.599050
C -0.656172 1.242858 -1.714930
C -1.286977 0.434587 -0.751077
C -2.702549 0.390346 -0.687614
C -3.439094 1.178916 -1.591834

N -0.513808 -0.339713 0.137708
C -1.059601 -1.174373 1.111663
C -2.534107 -1.234727 1.171093
C -3.346218 -0.472527 0.303958
C -3.110720 -2.077783 2.135270
C -4.488674 -2.175961 2.249329
C -5.305746 -1.422885 1.392760
C -4.745539 -0.586216 0.437643
O -0.333489 -1.814349 1.873258
C 0.928671 -0.247364 0.105866
C 1.678729 -1.221604 -0.546913
C 3.072711 -1.133669 -0.564551
C 3.749799 -0.079573 0.065658
C 2.966588 0.887897 0.720914
C 1.576482 0.809877 0.747585
F -3.521596 2.717261 -3.374471
C 5.284067 0.046700 0.066052
C 5.966195 -1.097944 -0.706822
C 5.690128 1.385419 -0.595654
C 5.799529 0.019850 1.525000
H -0.916254 2.637505 -3.342213
H 0.424199 1.267360 -1.771945
H -4.522008 1.182938 -1.582652
H -2.447871 -2.643299 2.780742
H -4.932307 -2.829353 2.994610
H -6.386840 -1.492093 1.473951
H -5.404887 -0.018230 -0.208914
H 1.175680 -2.047904 -1.040187
H 3.626894 -1.908650 -1.081305
H 3.445476 1.720406 1.227684
H 0.992796 1.565453 1.265390
H 7.052913 -0.961600 -0.678890
H 5.744614 -2.076911 -0.266982
H 5.662452 -1.117878 -1.759700
H 6.781669 1.490605 -0.596167
H 5.272927 2.247364 -0.064433
H 5.344219 1.430291 -1.634863
H 5.532915 -0.922237 2.017609
H 6.891842 0.115482 1.541682
H 5.383787 0.839850 2.119885

19 Energy:-1118.36222523
C -2.769329 1.844383 -2.617210
C -1.380394 1.921955 -2.661585
C -0.643731 1.207301 -1.727150
C -1.281927 0.418831 -0.751938
C -2.697468 0.348286 -0.719136
C -3.427068 1.080305 -1.675031

N -0.516246 -0.298311 0.189115
C -1.067773 -1.092951 1.191862
C -2.542085 -1.173582 1.226617
C -3.347640 -0.476757 0.300162
C -3.125350 -1.975277 2.221534
C -4.503508 -2.095712 2.308836
C -5.314055 -1.408252 1.392937
C -4.747268 -0.613233 0.406634
O -0.345686 -1.687629 1.993161
C 0.927103 -0.221608 0.151637
C 1.657041 -1.132582 -0.607071
C 3.051375 -1.052218 -0.642020
C 3.747801 -0.068224 0.074407
C 2.984124 0.837752 0.832848
C 1.594042 0.768162 0.875436
F -3.496240 2.538686 -3.524195
C 5.282788 0.048194 0.057786
C 5.942238 -1.026126 -0.827559
C 5.686192 1.438764 -0.488585
C 5.824927 -0.113045 1.498213
H -0.892010 2.531303 -3.414306
H 0.436838 1.260504 -1.752307
H -4.509738 1.061570 -1.692245
H -2.467483 -2.491808 2.911651
H -4.952305 -2.716493 3.078499
H -6.395219 -1.496108 1.452203
H -5.401677 -0.095901 -0.285836
H 1.138440 -1.904235 -1.168458
H 3.589990 -1.777013 -1.241460
H 3.478755 1.616160 1.406192
H 1.024763 1.477138 1.469370
H 7.030394 -0.900453 -0.806107
H 5.719578 -2.039413 -0.474532
H 5.621116 -0.948168 -1.872549
H 6.778209 1.538245 -0.499321
H 5.283714 2.251544 0.125054
H 5.322487 1.578212 -1.513229
H 5.560743 -1.094296 1.908858
H 6.918024 -0.025500 1.502241
H 5.426714 0.652148 2.172732

20 Energy:-1118.36206125
C -2.761369 1.710667 -2.716213
C -1.374650 1.827798 -2.730558
C -0.641414 1.174834 -1.749457
C -1.280131 0.405439 -0.759335
C -2.694250 0.303831 -0.750777
C -3.420345 0.972107 -1.754852

N -0.518045 -0.248705 0.229894
C -1.073455 -1.010801 1.256076
C -2.546770 -1.110666 1.274657
C -3.347755 -0.480530 0.297998
C -3.133378 -1.869507 2.300815
C -4.510493 -2.010886 2.371117
C -5.316535 -1.389561 1.405341
C -4.746368 -0.638244 0.387268
O -0.354887 -1.566650 2.087911
C 0.925807 -0.188186 0.185667
C 1.635888 -1.027008 -0.669458
C 3.030435 -0.956063 -0.717625
C 3.747151 -0.053105 0.080574
C 3.003162 0.783616 0.932560
C 1.613205 0.724546 0.987306
F -3.485000 2.342378 -3.670323
C 5.283063 0.048311 0.054602
C 5.919138 -0.944975 -0.936262
C 5.696353 1.479728 -0.363810
C 5.840504 -0.253826 1.466323
H -0.885158 2.421033 -3.495325
H 0.437084 1.262611 -1.749562
H -4.501552 0.924652 -1.793986
H -2.478986 -2.336587 3.028441
H -4.961911 -2.597338 3.165762
H -6.396837 -1.494617 1.450683
H -5.397392 -0.171288 -0.343113
H 1.102187 -1.736876 -1.294733
H 3.552738 -1.624342 -1.392414
H 3.513397 1.500061 1.569448
H 1.059563 1.381026 1.651838
H 7.008933 -0.833940 -0.916792
H 5.688221 -1.984578 -0.677548
H 5.587131 -0.765293 -1.965181
H 6.789261 1.567963 -0.379881
H 5.311409 2.235360 0.328966
H 5.321638 1.719143 -1.365749
H 5.569699 -1.266581 1.786105
H 6.934549 -0.178663 1.464530
H 5.459359 0.448263 2.215231

21 Energy:-1118.36149877
C -2.757788 1.575310 -2.808384
C -1.375896 1.739561 -2.795683
C -0.645216 1.151913 -1.772487
C -1.279846 0.397228 -0.768067
C -2.690853 0.258201 -0.781495
C -3.414579 0.858949 -1.829223

N -0.519682 -0.188925 0.265944
C -1.079737 -0.914820 1.317467
C -2.550945 -1.040966 1.319309
C -3.346781 -0.486285 0.294312
C -3.139824 -1.756234 2.375166
C -4.514395 -1.926593 2.428135
C -5.315361 -1.380276 1.414022
C -4.742766 -0.673371 0.365952
O -0.366021 -1.424398 2.182299
C 0.924599 -0.149377 0.215383
C 1.614895 -0.911712 -0.724027
C 3.009671 -0.853970 -0.782596
C 3.747601 -0.039998 0.088303
C 3.023847 0.721930 1.023903
C 1.634064 0.677216 1.088485
F -3.478800 2.141007 -3.804819
C 5.284211 0.044645 0.052802
C 5.895680 -0.859757 -1.034004
C 5.711589 1.503748 -0.235866
C 5.853754 -0.393989 1.423212
H -0.888220 2.320067 -3.571303
H 0.428669 1.281332 -1.750591
H -4.492891 0.777779 -1.887219
H -2.489301 -2.167198 3.139168
H -4.967668 -2.478367 3.246211
H -6.393598 -1.509009 1.445098
H -5.390006 -0.263914 -0.401292
H 1.066329 -1.553842 -1.407033
H 3.514672 -1.462204 -1.524055
H 3.550546 1.369453 1.718628
H 1.097475 1.277570 1.816472
H 6.987031 -0.764615 -1.017949
H 5.653515 -1.915956 -0.870173
H 5.554544 -0.580930 -2.037534
H 6.805327 1.579967 -0.257380
H 5.344488 2.196030 0.529076
H 5.328610 1.840012 -1.206368
H 5.573324 -1.428735 1.651158
H 6.948611 -0.332147 1.414698
H 5.490314 0.240220 2.238507

22 Energy:-1118.36048434
C -2.755875 1.445882 -2.888496
C -1.382806 1.668942 -2.848269
C -0.655401 1.149887 -1.786700
C -1.281197 0.401063 -0.771746
C -2.686163 0.213472 -0.808762
C -3.407200 0.743800 -1.895901

N -0.522040 -0.111015 0.304134
C -1.089629 -0.792771 1.383991
C -2.556357 -0.960547 1.363099
C -3.343807 -0.497397 0.288158
C -3.147279 -1.634343 2.445014
C -4.515706 -1.852673 2.474131
C -5.308125 -1.398706 1.409041
C -4.733344 -0.733573 0.335163
O -0.385367 -1.240661 2.289402
C 0.922595 -0.100083 0.245664
C 1.591960 -0.787667 -0.764950
C 2.986791 -0.749353 -0.834097
C 3.748499 -0.027658 0.095311
C 3.047015 0.661927 1.101190
C 1.657555 0.637270 1.176772
F -3.473855 1.942689 -3.922887
C 5.285738 0.034259 0.049234
C 5.869886 -0.781952 -1.119307
C 5.735718 1.505673 -0.116590
C 5.861842 -0.531183 1.369482
H -0.899765 2.243850 -3.630918
H 0.410127 1.330957 -1.742603
H -4.480472 0.621713 -1.971942
H -2.503144 -1.976392 3.247348
H -4.970599 -2.371806 3.312418
H -6.381282 -1.567022 1.420409
H -5.373870 -0.396071 -0.471671
H 1.028023 -1.359972 -1.495609
H 3.472380 -1.299438 -1.631849
H 3.591657 1.238426 1.843100
H 1.141094 1.183513 1.959028
H 6.962872 -0.706807 -1.108087
H 5.610773 -1.844220 -1.045219
H 5.523177 -0.410892 -2.090556
H 6.830376 1.565459 -0.144158
H 5.388444 2.134797 0.709732
H 5.348833 1.931228 -1.049786
H 5.566221 -1.577214 1.510014
H 6.957448 -0.486337 1.353577
H 5.517452 0.035494 2.240845

23 Energy:-1118.35886609
C -2.754848 1.322639 -2.957768
C -1.395962 1.615650 -2.890715
C -0.673015 1.167263 -1.794944
C -1.284540 0.415265 -0.772902
C -2.679399 0.169431 -0.832937
C -3.396979 0.626969 -1.955265

N -0.525524 -0.018275 0.340224
C -1.101932 -0.659150 1.444334
C -2.561620 -0.876981 1.401234
C -3.337115 -0.513322 0.281135
C -3.154258 -1.511344 2.506054
C -4.512386 -1.787937 2.512382
C -5.292201 -1.435137 1.400732
C -4.715607 -0.809444 0.304349
O -0.410084 -1.042209 2.387887
C 0.919207 -0.043626 0.273242
C 1.569477 -0.658203 -0.796507
C 2.964137 -0.644433 -0.874381
C 3.748986 -0.014933 0.101193
C 3.068594 0.607860 1.163132
C 1.679730 0.606887 1.249331
F -3.468757 1.748292 -4.025848
C 5.286639 0.018792 0.045960
C 5.843788 -0.713347 -1.189553
C 5.767116 1.488991 -0.006231
C 5.860622 -0.662171 1.311508
H -0.921612 2.191887 -3.677668
H 0.379351 1.408292 -1.728979
H -4.462242 0.456667 -2.048509
H -2.519578 -1.778100 3.343610
H -4.968623 -2.275862 3.368489
H -6.356749 -1.651477 1.393392
H -5.346028 -0.550516 -0.538645
H 0.992554 -1.162339 -1.565708
H 3.430554 -1.140106 -1.718014
H 3.629868 1.115481 1.942065
H 1.183881 1.104251 2.074890
H 6.938181 -0.661714 -1.183657
H 5.562760 -1.772604 -1.197676
H 5.496560 -0.259020 -2.124564
H 6.862610 1.527905 -0.038254
H 5.439117 2.057511 0.870345
H 5.383116 1.995612 -0.899269
H 5.543555 -1.709693 1.370915
H 6.956828 -0.639245 1.289268
H 5.535021 -0.159908 2.228478

24 Energy:-1118.35649963
C -2.756186 1.205754 -3.017620
C -1.417445 1.575911 -2.927458
C -0.699727 1.198112 -1.802536
C -1.290833 0.435992 -0.775315
C -2.671251 0.126263 -0.854414
C -3.384893 0.510493 -2.006832

N -0.529899 0.082495 0.368192
C -1.113743 -0.529002 1.489941
C -2.564707 -0.797730 1.430685
C -3.326615 -0.532175 0.275086
C -3.157852 -1.394881 2.556002
C -4.502691 -1.730219 2.546680
C -5.267863 -1.477119 1.398375
C -4.690623 -0.888921 0.281696
O -0.434073 -0.855197 2.462811
C 0.914560 0.015802 0.293278
C 1.550866 -0.524066 -0.825570
C 2.945006 -0.538023 -0.908461
C 3.749061 -0.000827 0.105313
C 3.085442 0.559871 1.210966
C 1.697333 0.584181 1.304988
F -3.465217 1.559454 -4.114465
C 5.286653 0.000027 0.045103
C 5.821772 -0.654671 -1.242490
C 5.802824 1.458108 0.096396
C 5.847782 -0.783912 1.255591
H -0.956409 2.158502 -3.717604
H 0.334578 1.503166 -1.717111
H -4.438795 0.286865 -2.114732
H -2.534108 -1.587417 3.421550
H -4.959449 -2.188235 3.418875
H -6.321287 -1.741663 1.378303
H -5.309212 -0.706928 -0.589697
H 0.965543 -0.961896 -1.627522
H 3.395094 -0.981058 -1.789497
H 3.659758 1.001720 2.020070
H 1.220102 1.038391 2.164156
H 6.917166 -0.631458 -1.237850
H 5.513603 -1.703092 -1.325795
H 5.483712 -0.125368 -2.140711
H 6.898870 1.472991 0.062268
H 5.491096 1.969926 1.012941
H 5.428674 2.036599 -0.756244
H 5.506207 -1.825319 1.240513
H 6.944204 -0.785055 1.230572
H 5.536167 -0.341843 2.207729

25 Energy:-1118.35323519
C -2.752150 1.105511 -3.064414
C -1.440538 1.558349 -2.951579
C -0.731476 1.248799 -1.801104
C -1.298005 0.469724 -0.772258
C -2.657724 0.087955 -0.871556
C -3.364485 0.401884 -2.049680

N -0.536408 0.197839 0.397231
C -1.133495 -0.374912 1.537640
C -2.570152 -0.711722 1.456963
C -3.309250 -0.556200 0.267840
C -3.165398 -1.276688 2.597853
C -4.488436 -1.689266 2.568979
C -5.228593 -1.549219 1.385617
C -4.649442 -0.992576 0.253695
O -0.474905 -0.626225 2.545963
C 0.906966 0.080885 0.315846
C 1.531166 -0.388781 -0.842792
C 2.923859 -0.436598 -0.931900
C 3.746941 0.010240 0.109511
C 3.099906 0.516767 1.249665
C 1.713157 0.571376 1.352890
F -3.453406 1.390987 -4.185417
C 5.283480 -0.026014 0.041782
C 5.796271 -0.617022 -1.285108
C 5.838467 1.412257 0.177082
C 5.827951 -0.894969 1.200709
H -0.996663 2.153372 -3.742253
H 0.279020 1.620903 -1.695341
H -4.403144 0.121547 -2.171795
H -2.560382 -1.384906 3.490801
H -4.946744 -2.121876 3.453243
H -6.263585 -1.877219 1.350032
H -5.247524 -0.898167 -0.645498
H 0.939028 -0.762705 -1.670657
H 3.357098 -0.832384 -1.843428
H 3.686445 0.896501 2.081395
H 1.256179 0.989954 2.238756
H 6.891923 -0.624576 -1.284334
H 5.458355 -1.649554 -1.429439
H 5.470481 -0.025726 -2.148505
H 6.934461 1.400559 0.139234
H 5.542569 1.876386 1.123751
H 5.477265 2.050043 -0.638044
H 5.457795 -1.924010 1.126395
H 6.923837 -0.924535 1.169452
H 5.532479 -0.501437 2.178934

26 Energy:-1118.34914562
C -2.751115 1.011780 -3.107608
C -1.477795 1.560248 -2.977335
C -0.777523 1.327232 -1.803927
C -1.309209 0.529015 -0.771191
C -2.636316 0.055189 -0.888788
C -3.336996 0.291978 -2.088629

N -0.547577 0.349162 0.420467
C -1.168264 -0.148821 1.588268
C -2.573626 -0.599114 1.480663
C -3.273403 -0.587737 0.258800
C -3.167837 -1.136630 2.635311
C -4.447341 -1.668322 2.584809
C -5.143526 -1.677571 1.367230
C -4.566511 -1.145669 0.222043
O -0.550853 -0.264293 2.645269
C 0.893159 0.175911 0.337403
C 1.506724 -0.234455 -0.851925
C 2.896033 -0.329291 -0.947487
C 3.738195 0.021370 0.114741
C 3.108575 0.481506 1.282490
C 1.724504 0.581779 1.394787
F -3.445020 1.223294 -4.248973
C 5.271961 -0.067447 0.039833
C 5.760645 -0.590914 -1.324021
C 5.881337 1.337040 0.265375
C 5.784075 -1.028588 1.139121
H -1.060366 2.170714 -3.770591
H 0.200635 1.774316 -1.680936
H -4.353777 -0.055948 -2.221036
H -2.595946 -1.131630 3.556079
H -4.904174 -2.080697 3.479440
H -6.141929 -2.102416 1.315157
H -5.127859 -1.167624 -0.705270
H 0.908885 -0.542874 -1.701165
H 3.311094 -0.684222 -1.884074
H 3.707405 0.794161 2.133376
H 1.290676 0.971145 2.302802
H 6.855292 -0.638930 -1.328204
H 5.384375 -1.598904 -1.532706
H 5.455475 0.065966 -2.146610
H 6.976062 1.286570 0.222125
H 5.605064 1.749560 1.241414
H 5.542971 2.039512 -0.505124
H 5.376908 -2.036640 0.999218
H 6.878228 -1.095882 1.104560
H 5.501881 -0.688281 2.140978

27 Energy:-1118.34471913
C -2.781729 0.925536 -3.156369
C -1.562619 1.587041 -3.030239
C -0.858770 1.447372 -1.843582
C -1.331750 0.632756 -0.796693
C -2.607322 0.038239 -0.914376
C -3.315247 0.183119 -2.123991

N -0.566588 0.555893 0.407283
C -1.222882 0.189105 1.607806
C -2.554849 -0.449680 1.490428
C -3.197060 -0.620954 0.249148
C -3.125302 -0.974930 2.662162
C -4.317325 -1.682293 2.606594
C -4.949178 -1.877429 1.370037
C -4.398482 -1.353109 0.207721
O -0.685393 0.316388 2.705080
C 0.869180 0.330403 0.333331
C 1.481824 -0.024036 -0.877502
C 2.864444 -0.189354 -0.967366
C 3.713450 0.029957 0.123628
C 3.091771 0.431392 1.315489
C 1.714045 0.604806 1.424650
F -3.480217 1.049468 -4.307378
C 5.240679 -0.136894 0.054654
C 5.715887 -0.586326 -1.340007
C 5.922161 1.212230 0.386726
C 5.687933 -1.201296 1.084851
H -1.193009 2.212333 -3.835545
H 0.075404 1.981287 -1.719174
H -4.299940 -0.249559 -2.251325
H -2.603987 -0.824265 3.600484
H -4.753866 -2.089035 3.513842
H -5.876165 -2.441130 1.316328
H -4.905335 -1.518934 -0.736557
H 0.887179 -0.244888 -1.754286
H 3.268570 -0.496934 -1.925409
H 3.693255 0.642563 2.195497
H 1.294954 0.948604 2.355818
H 6.806251 -0.694655 -1.339604
H 5.287082 -1.553995 -1.624652
H 5.456608 0.144374 -2.114685
H 7.013148 1.105565 0.349839
H 5.655520 1.567855 1.387557
H 5.631856 1.985779 -0.333682
H 5.229039 -2.173068 0.868804
H 6.777263 -1.325270 1.054168
H 5.412707 -0.919483 2.106654

28 Energy:-1118.34082082
C -2.843685 0.810381 -3.211338
C -1.674285 1.560511 -3.120766
C -0.951398 1.511902 -1.936758
C -1.357095 0.700718 -0.861471
C -2.587406 0.012872 -0.945286
C -3.316375 0.067607 -2.148424

N -0.579790 0.707844 0.338786
C -1.260061 0.467125 1.560129
C -2.518993 -0.312287 1.484196
C -3.120108 -0.636055 0.252315
C -3.052567 -0.806762 2.685435
C -4.162520 -1.640116 2.668099
C -4.748321 -1.988520 1.443014
C -4.236552 -1.491143 0.250366
O -0.790860 0.804712 2.642648
C 0.851539 0.453912 0.281755
C 1.493008 0.193558 -0.939192
C 2.870125 -0.025592 -1.003973
C 3.690622 0.034199 0.127182
C 3.042104 0.327222 1.336050
C 1.671015 0.554021 1.422404
F -3.560553 0.847778 -4.356860
C 5.211042 -0.191601 0.086720
C 5.715708 -0.505199 -1.334470
C 5.934617 1.081318 0.587645
C 5.579072 -1.381559 1.004743
H -1.358929 2.184535 -3.949774
H -0.060558 2.120134 -1.835798
H -4.272351 -0.432397 -2.246567
H -2.567679 -0.534928 3.616242
H -4.569278 -2.026600 3.597756
H -5.609267 -2.650508 1.421435
H -4.705626 -1.774470 -0.685815
H 0.926710 0.085893 -1.853702
H 3.291863 -0.248422 -1.977912
H 3.618005 0.405718 2.254249
H 1.239422 0.813201 2.375344
H 6.800235 -0.660328 -1.313965
H 5.258477 -1.416046 -1.737747
H 5.512274 0.316904 -2.030196
H 7.021083 0.931511 0.572948
H 5.646879 1.336185 1.613147
H 5.701474 1.941381 -0.050779
H 5.089651 -2.302662 0.667542
H 6.663012 -1.548803 0.993993
H 5.279513 -1.202599 2.042809

29 Energy:-1118.33776926
C -2.901010 0.656380 -3.260264
C -1.773656 1.470418 -3.216535
C -1.031108 1.506235 -2.042417
C -1.375694 0.713306 -0.934399
C -2.574788 -0.033590 -0.969159
C -3.323130 -0.063876 -2.159627

N -0.583568 0.781906 0.254583
C -1.269288 0.646630 1.489029
C -2.488499 -0.196951 1.476144
C -3.067111 -0.638781 0.269682
C -2.998825 -0.631434 2.709398
C -4.060983 -1.525105 2.750823
C -4.620473 -1.992573 1.553760
C -4.133126 -1.552752 0.327877
O -0.824972 1.116353 2.530971
C 0.846686 0.527665 0.214121
C 1.536832 0.406285 -1.001665
C 2.911038 0.158069 -1.037457
C 3.681142 0.039933 0.122786
C 2.982525 0.177302 1.331990
C 1.614982 0.427388 1.390495
F -3.634915 0.610857 -4.394492
C 5.196592 -0.218734 0.116262
C 5.759288 -0.345149 -1.312061
C 5.921865 0.952775 0.820686
C 5.498331 -1.533845 0.873706
H -1.506225 2.080796 -4.072100
H -0.183860 2.177507 -1.974640
H -4.257199 -0.609546 -2.220088
H -2.533609 -0.267791 3.618854
H -4.449561 -1.866887 3.705415
H -5.442635 -2.701998 1.579571
H -4.582252 -1.926182 -0.586406
H 1.015526 0.434055 -1.946973
H 3.370162 0.057052 -2.014804
H 3.514469 0.101585 2.276582
H 1.152594 0.553807 2.356577
H 6.838568 -0.529247 -1.267568
H 5.303351 -1.179399 -1.857491
H 5.603504 0.570327 -1.894220
H 7.004605 0.777733 0.832446
H 5.591535 1.070648 1.858183
H 5.736111 1.898908 0.299181
H 5.006206 -2.386020 0.390724
H 6.578023 -1.726614 0.885547
H 5.155748 -1.492898 1.913130

30 Energy:-1118.3358048
C -2.957670 0.448335 -3.301102
C -1.854041 1.292908 -3.319726
C -1.090163 1.409792 -2.162954
C -1.388620 0.662516 -1.011711
C -2.578961 -0.103011 -0.981101
C -3.346554 -0.215700 -2.152704

N -0.577549 0.772473 0.160164
C -1.247622 0.748140 1.408092
C -2.467487 -0.091532 1.470969
C -3.050223 -0.626466 0.303977
C -2.967830 -0.432735 2.736611
C -4.023726 -1.327766 2.852626
C -4.585152 -1.889827 1.698181
C -4.108146 -1.541290 0.438907
O -0.781678 1.295609 2.400990
C 0.857118 0.556462 0.132110
C 1.609793 0.625405 -1.048159
C 2.985178 0.372668 -1.050782
C 3.690157 0.050315 0.110611
C 2.924526 -0.024582 1.285638
C 1.556666 0.220333 1.308589
F -3.709043 0.321463 -4.417569
C 5.203618 -0.216966 0.141873
C 5.847543 -0.079234 -1.250637
C 5.885883 0.795217 1.092949
C 5.462780 -1.653424 0.655621
H -1.620982 1.869180 -4.208354
H -0.280829 2.127382 -2.143989
H -4.271544 -0.779881 -2.164608
H -2.499071 0.001345 3.612913
H -4.404822 -1.598137 3.832786
H -5.401587 -2.601272 1.782834
H -4.560773 -1.986050 -0.441095
H 1.148435 0.824348 -2.002164
H 3.497096 0.437145 -2.004648
H 3.400483 -0.283019 2.227662
H 1.042264 0.154992 2.255379
H 6.923469 -0.274208 -1.179543
H 5.428155 -0.795361 -1.966575
H 5.720101 0.929262 -1.660493
H 6.966480 0.611208 1.131752
H 5.497731 0.719540 2.114216
H 5.728276 1.823930 0.748717
H 5.000061 -2.395406 -0.005437
H 6.540236 -1.855375 0.692024
H 5.061217 -1.804180 1.663321

31 Energy:-1118.35303058
C -2.747787 -0.106245 -3.292182
C -1.402793 -0.453794 -3.384473
C -0.682125 -0.622123 -2.212105
C -1.272015 -0.421093 -0.948008
C -2.658539 -0.145093 -0.874995
C -3.377921 0.030573 -2.074028

N -0.495401 -0.629358 0.224895
C -1.099826 -0.679793 1.496881
C -2.558065 -0.449688 1.567215
C -3.318836 -0.117659 0.429092
C -3.157287 -0.491692 2.837817
C -4.505212 -0.205620 2.988923
C -5.267567 0.138644 1.862826
C -4.684806 0.182450 0.603844
O -0.433194 -0.860524 2.514811
C 0.929494 -0.358350 0.212064
C 1.470733 0.624285 -0.621601
C 2.850027 0.835208 -0.672198
C 3.744533 0.058848 0.075360
C 3.183459 -0.950394 0.876190
C 1.811029 -1.173641 0.936437
F -3.461870 0.070192 -4.427468
C 5.268822 0.264341 0.041219
C 5.682551 1.414394 -0.896368
C 5.773484 0.596285 1.465913
C 5.952698 -1.032759 -0.453532
H -0.941423 -0.604565 -4.354346
H 0.356427 -0.919032 -2.276078
H -4.438265 0.249615 -2.064482
H -2.535975 -0.745029 3.689234
H -4.966025 -0.242216 3.971478
H -6.322561 0.373500 1.971906
H -5.299811 0.453034 -0.246900
H 0.820453 1.264831 -1.206877
H 3.215268 1.626423 -1.317041
H 3.829088 -1.597427 1.463089
H 1.424056 -1.976512 1.547990
H 6.772776 1.522879 -0.885113
H 5.379776 1.225513 -1.932656
H 5.251552 2.371880 -0.582368
H 6.861180 0.736629 1.459354
H 5.544434 -0.205013 2.176277
H 5.313899 1.518587 1.839595
H 5.620213 -1.289617 -1.466012
H 7.041342 -0.901904 -0.476326
H 5.733200 -1.884420 0.198907

32 Energy:-1118.35630923
C -2.743245 -0.215120 -3.293854
C -1.377320 -0.472008 -3.369232
C -0.654224 -0.563667 -2.189404
C -1.268346 -0.379565 -0.934658
C -2.670729 -0.185957 -0.876025
C -3.390286 -0.087609 -2.083303

N -0.499174 -0.497884 0.251253
C -1.091840 -0.489614 1.525053
C -2.560817 -0.348545 1.583179
C -3.337817 -0.146516 0.424859
C -3.161232 -0.357114 2.853720
C -4.528011 -0.168639 2.986274
C -5.308996 0.041007 1.839857
C -4.724806 0.052518 0.580974
O -0.407959 -0.562710 2.545657
C 0.931501 -0.276706 0.220447
C 1.484085 0.746678 -0.551366
C 2.868822 0.919144 -0.610931
C 3.747575 0.071183 0.075782
C 3.169264 -0.968913 0.824728
C 1.791837 -1.154670 0.890200
F -3.458749 -0.113236 -4.437730
C 5.277034 0.234327 0.032682
C 5.713554 1.427681 -0.838045
C 5.809091 0.462667 1.467793
C 5.915335 -1.049066 -0.550735
H -0.898763 -0.609624 -4.332738
H 0.403048 -0.786395 -2.241731
H -4.461526 0.069966 -2.086753
H -2.525999 -0.509435 3.718939
H -4.990009 -0.179445 3.968902
H -6.380184 0.195828 1.933058
H -5.355909 0.216957 -0.284908
H 0.838745 1.434142 -1.088304
H 3.251383 1.737358 -1.210336
H 3.804247 -1.664220 1.366024
H 1.382622 -1.976015 1.464600
H 6.806619 1.502801 -0.835812
H 5.392317 1.312548 -1.879559
H 5.316008 2.376176 -0.459336
H 6.900101 0.573493 1.453866
H 5.567103 -0.374865 2.130416
H 5.380449 1.371957 1.904693
H 5.562975 -1.232743 -1.572373
H 7.007007 -0.948810 -0.580672
H 5.678409 -1.932791 0.051009

33 Energy:-1118.35874732
C -2.731848 -0.342492 -3.291833
C -1.352659 -0.517894 -3.354528
C -0.630563 -0.533096 -2.170113
C -1.264271 -0.357996 -0.924431
C -2.675560 -0.233159 -0.876144
C -3.392461 -0.213410 -2.088393

N -0.504107 -0.389549 0.269103
C -1.091239 -0.337651 1.540028
C -2.564580 -0.257589 1.591204
C -3.347242 -0.167653 0.421801
C -3.167617 -0.224581 2.859925
C -4.543206 -0.105894 2.981134
C -5.330888 -0.011110 1.823995
C -4.744155 -0.040820 0.566670
O -0.399259 -0.334170 2.558232
C 0.930726 -0.210891 0.227134
C 1.494400 0.856909 -0.470600
C 2.882349 1.000372 -0.536677
C 3.746589 0.084856 0.078756
C 3.153342 -0.991368 0.763300
C 1.772520 -1.148901 0.832243
F -3.445829 -0.317107 -4.441281
C 5.279257 0.214072 0.026403
C 5.735261 1.455555 -0.763372
C 5.834497 0.326629 1.466475
C 5.877497 -1.039566 -0.655857
H -0.861304 -0.649252 -4.312467
H 0.439181 -0.687464 -2.212183
H -4.470321 -0.110898 -2.102010
H -2.527341 -0.291231 3.732346
H -5.007333 -0.083918 3.962582
H -6.409597 0.086323 1.907746
H -5.381117 0.034304 -0.307245
H 0.854303 1.589946 -0.951829
H 3.279620 1.849064 -1.081468
H 3.778565 -1.733717 1.250695
H 1.345415 -1.994128 1.359601
H 6.829821 1.503471 -0.770672
H 5.399030 1.422964 -1.806009
H 5.366631 2.384133 -0.312869
H 6.927595 0.412271 1.444674
H 5.580637 -0.550002 2.071509
H 5.433929 1.212289 1.972935
H 5.508694 -1.140506 -1.683199
H 6.970941 -0.964442 -0.693305
H 5.624889 -1.958150 -0.115848

34 Energy:-1118.36041406
C -2.720985 -0.484907 -3.283781
C -1.334157 -0.586516 -3.339864
C -0.614221 -0.523715 -2.155328
C -1.261922 -0.348860 -0.917408
C -2.677625 -0.283488 -0.874072
C -3.391258 -0.344438 -2.086552

N -0.509150 -0.297547 0.277106
C -1.091877 -0.209008 1.544536
C -2.567058 -0.173013 1.593277
C -3.351494 -0.182332 0.420803
C -3.172215 -0.093319 2.858686
C -4.551698 -0.024957 2.974854
C -5.341444 -0.030755 1.815232
C -4.752769 -0.107640 0.560827
O -0.394923 -0.145624 2.557768
C 0.928626 -0.153947 0.226142
C 1.505143 0.958579 -0.383888
C 2.895382 1.078266 -0.453314
C 3.744412 0.097506 0.077839
C 3.135819 -1.018736 0.680372
C 1.752378 -1.152792 0.750119
F -3.432392 -0.539030 -4.434080
C 5.279180 0.200301 0.022834
C 5.755073 1.489778 -0.672656
C 5.845529 0.190739 1.463015
C 5.847727 -1.008339 -0.758787
H -0.834444 -0.719379 -4.293287
H 0.463009 -0.615643 -2.190681
H -4.472698 -0.292505 -2.105661
H -2.530402 -0.084864 3.732567
H -5.017366 0.034470 3.954023
H -6.423418 0.025345 1.894769
H -5.391563 -0.109768 -0.315027
H 0.872238 1.737752 -0.798285
H 3.307266 1.959716 -0.931040
H 3.750321 -1.808282 1.102728
H 1.308687 -2.026651 1.215289
H 6.850297 1.516209 -0.685447
H 5.411133 1.544464 -1.711849
H 5.408822 2.387987 -0.148821
H 6.939964 0.256212 1.439237
H 5.577771 -0.724508 2.001311
H 5.466342 1.042789 2.038836
H 5.470712 -1.022249 -1.788011
H 6.942174 -0.951838 -0.798631
H 5.580268 -1.960915 -0.289542

35 Energy:-1118.36146025
C -2.704526 -0.634310 -3.268224
C -1.314324 -0.671102 -3.320698
C -0.599816 -0.530711 -2.139224
C -1.259199 -0.346924 -0.909333
C -2.676473 -0.334714 -0.868800
C -3.383853 -0.475739 -2.077991

N -0.514544 -0.211003 0.281450
C -1.096509 -0.076332 1.542405
C -2.572319 -0.084784 1.590225
C -3.354344 -0.193656 0.420575
C -3.181624 0.042470 2.849537
C -4.562928 0.061432 2.963230
C -5.350385 -0.044325 1.806861
C -4.757682 -0.169301 0.558215
O -0.398508 0.054253 2.548654
C 0.925648 -0.096501 0.226317
C 1.518456 1.054838 -0.286900
C 2.910414 1.152582 -0.357793
C 3.742248 0.112196 0.079459
C 3.116144 -1.039659 0.590164
C 1.730448 -1.151577 0.660061
F -3.410365 -0.766242 -4.415864
C 5.278497 0.188660 0.019075
C 5.775757 1.522240 -0.570177
C 5.855240 0.046785 1.448064
C 5.815880 -0.961042 -0.866544
H -0.807487 -0.811553 -4.269270
H 0.481029 -0.566534 -2.170010
H -4.466502 -0.468828 -2.100681
H -2.541501 0.125882 3.720786
H -5.031803 0.158426 3.937866
H -6.433847 -0.028648 1.884436
H -5.394859 -0.248648 -0.315265
H 0.895927 1.877049 -0.627742
H 3.337986 2.063411 -0.760744
H 3.717897 -1.873299 0.939862
H 1.270593 -2.052522 1.053918
H 6.871150 1.527268 -0.591345
H 5.424791 1.671265 -1.597704
H 5.452817 2.379889 0.030779
H 6.950580 0.091828 1.419685
H 5.572365 -0.904840 1.910039
H 5.498303 0.854940 2.096751
H 5.429537 -0.881787 -1.889326
H 6.910798 -0.921982 -0.913105
H 5.534084 -1.944302 -0.475516

36 Energy:-1118.36201614
C -2.688365 -0.800729 -3.243370
C -1.297810 -0.781159 -3.297252
C -0.589354 -0.560732 -2.124214
C -1.256838 -0.356696 -0.902276
C -2.673616 -0.390208 -0.860500
C -3.374443 -0.613888 -2.060867

N -0.519354 -0.136964 0.278947
C -1.102165 0.048215 1.531291
C -2.577517 0.004357 1.580850
C -3.355251 -0.200421 0.420806
C -3.191052 0.185969 2.831270
C -4.572311 0.166253 2.945946
C -5.355468 -0.035328 1.799443
C -4.758626 -0.215306 0.559493
O -0.405067 0.242862 2.527900
C 0.922435 -0.044249 0.222555
C 1.532393 1.139842 -0.183606
C 2.925621 1.219763 -0.251566
C 3.740189 0.128178 0.081637
C 3.096235 -1.055292 0.487028
C 1.708780 -1.148294 0.555714
F -3.388094 -1.013283 -4.382753
C 5.277343 0.182263 0.017368
C 5.796611 1.558485 -0.440061
C 5.860388 -0.112199 1.420257
C 5.786412 -0.883343 -0.982819
H -0.786209 -0.938262 -4.240645
H 0.492195 -0.547856 -2.154672
H -4.456649 -0.647316 -2.083254
H -2.554136 0.341331 3.695027
H -5.044464 0.306223 3.913755
H -6.438861 -0.051399 1.877903
H -5.392509 -0.368312 -0.306587
H 0.921703 1.999473 -0.444107
H 3.368419 2.156414 -0.569919
H 3.684676 -1.927772 0.755096
H 1.233390 -2.072747 0.869517
H 6.891784 1.545515 -0.467833
H 5.443757 1.815155 -1.445434
H 5.492738 2.358010 0.245080
H 6.956119 -0.082630 1.387696
H 5.564445 -1.100739 1.786588
H 5.521559 0.632336 2.149736
H 5.396281 -0.694297 -1.989632
H 6.881638 -0.861738 -1.033365
H 5.486244 -1.894937 -0.690012

37 Energy:-1118.36220704
C -2.688892 -0.958994 -3.214500
C -1.300298 -0.891702 -3.280458
C -0.592564 -0.597366 -2.123258
C -1.259284 -0.370599 -0.905063
C -2.674150 -0.442554 -0.852440
C -3.374188 -0.742237 -2.036544

N -0.522818 -0.073359 0.259038
C -1.102669 0.159346 1.504268
C -2.576655 0.086901 1.563635
C -3.353954 -0.204982 0.421875
C -3.189062 0.320719 2.805853
C -4.568668 0.268824 2.930279
C -5.351265 -0.020082 1.802217
C -4.755548 -0.252823 0.570529
O -0.404086 0.410589 2.487129
C 0.919867 -0.000289 0.199734
C 1.548090 1.207835 -0.089960
C 2.942428 1.272602 -0.148111
C 3.739563 0.141561 0.079571
C 3.077196 -1.065218 0.369809
C 1.688168 -1.142471 0.430689
F -3.387706 -1.245671 -4.338147
C 5.277585 0.178470 0.023268
C 5.818111 1.583246 -0.304474
C 5.851871 -0.252323 1.394177
C 5.774554 -0.797671 -1.069922
H -0.789843 -1.067314 -4.221210
H 0.487478 -0.542574 -2.163076
H -4.454994 -0.809439 -2.050224
H -2.552545 0.541269 3.655630
H -5.039998 0.450114 3.891610
H -6.433322 -0.062974 1.888611
H -5.388815 -0.473109 -0.281395
H 0.950329 2.097056 -0.267542
H 3.400453 2.228536 -0.374284
H 3.651920 -1.967821 0.554989
H 1.198087 -2.084437 0.658722
H 6.913007 1.556531 -0.333000
H 5.470807 1.937269 -1.281837
H 5.525057 2.320366 0.451689
H 6.948009 -0.236212 1.366296
H 5.540449 -1.265846 1.667783
H 5.521789 0.427127 2.188303
H 5.390788 -0.510746 -2.055838
H 6.870145 -0.787541 -1.115767
H 5.458768 -1.827458 -0.872496

12.2.5 Potential scan of compound 4b excited state (B3LYP/6-31G* PCM CH_2Cl_2)

D(4,7,16,17)
8 -1118.35426335 89.7321
25 -1118.34757909 99.732
30 -1118.34724539 109.7322

35 -1118.34684541 119.7323
41 -1118.34530216 129.7321
74 -1118.33667721 139.7323
83 -1118.31746675 149.732
89 -1118.31399405 159.7323
94 -1118.31213834 169.7322
98 -1118.31063726 179.7322
103 -1118.30952388 -170.2679
107 -1118.30847019 -160.268
112 -1118.30756353 -150.268
117 -1118.30680329 -140.268
123 -1118.30616419 -130.268
128 -1118.30569227 -120.268
135 -1118.30742515 -110.268
167 -1118.34773491 -100.2679
185 -1118.35420583 -90.268
195 -1118.34759786 -80.2678
200 -1118.3470889 -70.2677
205 -1118.3465484 -60.2678
210 -1118.34487532 -50.2679
231 -1118.32387 -40.2678
238 -1118.31632964 -30.2677
244 -1118.31425907 -20.2677
248 -1118.31256204 -10.2679
253 -1118.31093582 -0.2678
258 -1118.30962756 9.7322
262 -1118.3084268 19.7321
266 -1118.30721663 29.732
270 -1118.30599352 39.732
276 -1118.3047836 49.732
282 -1118.30392108 59.732
288 -1118.30411319 69.732
319 -1118.3473684 79.7321
342 -1118.35426345 89.7321

Progress of structural optimization and emission calculation

-1118.362218 -1118.219854 320.05 nm
-1118.357476 -1118.226864 348.84 nm
-1118.354813 -1118.227664 358.35 nm
-1118.354388 -1118.227768 359.84 nm
-1118.354288 -1118.227816 360.26 nm
-1118.354287 -1118.227833 360.32 nm
-1118.35436 -1118.227844 360.14 nm
-1118.354291 -1118.227847 360.34 nm
-1118.354263 -1118.227847 360.42 nm
-1118.353923 -1118.227712 361.01 nm
-1118.354146 -1118.227975 361.12 nm

-1118.353851 -1118.228109 362.36 nm
-1118.353133 -1118.228283 364.94 nm
-1118.352215 -1118.228428 368.08 nm
-1118.34756 -1118.228538 382.82 nm
-1118.352327 -1118.228593 368.24 nm
-1118.350104 -1118.228835 375.72 nm
-1118.349672 -1118.228858 377.14 nm
-1118.345093 -1118.228783 391.74 nm
-1118.348413 -1118.228906 381.26 nm
-1118.348895 -1118.228901 379.72 nm
-1118.347703 -1118.228919 383.58 nm
-1118.347806 -1118.228919 383.25 nm
-1118.347987 -1118.228918 382.66 nm
-1118.347608 -1118.22892 383.89 nm
-1118.347579 -1118.22892 383.99 nm
-1118.347662 -1118.229995 387.22 nm
-1118.347313 -1118.230206 389.08 nm
-1118.34727 -1118.230222 389.27 nm
-1118.347195 -1118.230224 389.53 nm
-1118.347245 -1118.230224 389.36 nm
-1118.346852 -1118.23101 393.32 nm
-1118.347304 -1118.231217 392.49 nm
-1118.346342 -1118.231222 395.79 nm
-1118.346873 -1118.231231 394 nm
-1118.346845 -1118.231231 394.1 nm
-1118.345831 -1118.231393 398.15 nm
-1118.345796 -1118.231649 399.16 nm
-1118.345451 -1118.231665 400.43 nm
-1118.345321 -1118.231668 400.9 nm
-1118.345303 -1118.231668 400.96 nm
-1118.345302 -1118.231668 400.97 nm
-1118.343636 -1118.231033 404.64 nm
-1118.342557 -1118.23144 410.05 nm
-1118.341384 -1118.231499 414.65 nm
-1118.339494 -1118.231548 422.1 nm
-1118.339018 -1118.23156 424.01 nm
-1118.338595 -1118.231567 425.71 nm
-1118.338304 -1118.231569 426.88 nm
-1118.337866 -1118.23157 428.65 nm
-1118.172965 -1118.076905 474.32 nm
-1118.331679 -1118.231265 453.76 nm
-1118.337672 -1118.23157 429.43 nm
-1118.335728 -1118.231544 437.34 nm
-1118.337699 -1118.231569 429.32 nm
-1118.335178 -1118.231554 439.7 nm
-1118.336554 -1118.231572 434.01 nm
-1118.337901 -1118.23157 428.5 nm
-1118.33601 -1118.231545 436.16 nm

-1118.336975 -1118.231571 432.27 nm
-1118.336989 -1118.231573 432.22 nm
-1118.337513 -1118.231571 430.08 nm
-1118.334438 -1118.231513 442.69 nm
-1118.336586 -1118.231569 433.87 nm
-1118.336744 -1118.231573 433.23 nm
-1118.33782 -1118.23157 428.83 nm
-1118.336037 -1118.231559 436.1 nm
-1118.337123 -1118.231572 431.67 nm
-1118.336918 -1118.231573 432.52 nm
-1118.337714 -1118.231571 429.26 nm
-1118.331465 -1118.23136 455.15 nm
-1118.335784 -1118.231563 437.18 nm
-1118.336555 -1118.231573 434.01 nm
-1118.336729 -1118.231573 433.3 nm
-1118.336677 -1118.231573 433.51 nm
-1118.335689 -1118.231632 437.87 nm
-1118.324257 -1118.233132 500.01 nm
-1118.320654 -1118.233598 523.38 nm
-1118.318214 -1118.233755 539.47 nm
-1118.319188 -1118.233735 533.2 nm
-1118.314716 -1118.233741 562.69 nm
-1118.317344 -1118.233786 545.29 nm
-1118.317474 -1118.233794 544.49 nm
-1118.317467 -1118.233794 544.54 nm
-1118.318083 -1118.235942 554.7 nm
-1118.313536 -1118.236368 590.45 nm
-1118.314254 -1118.236391 585.17 nm
-1118.313943 -1118.236394 587.55 nm
-1118.313998 -1118.236395 587.13 nm
-1118.313994 -1118.236395 587.16 nm
-1118.314676 -1118.238096 594.97 nm
-1118.312163 -1118.238478 618.35 nm
-1118.3123 -1118.238487 617.28 nm
-1118.312089 -1118.238488 619.06 nm
-1118.312138 -1118.238488 618.65 nm
-1118.312695 -1118.239424 621.84 nm
-1118.310439 -1118.239767 644.71 nm
-1118.310659 -1118.239772 642.76 nm
-1118.310637 -1118.239772 642.96 nm
-1118.310896 -1118.239675 639.75 nm
-1118.309336 -1118.239971 656.87 nm
-1118.309521 -1118.239974 655.15 nm
-1118.309532 -1118.239974 655.04 nm
-1118.309524 -1118.239974 655.12 nm
-1118.309334 -1118.238619 644.32 nm
-1118.308368 -1118.238895 655.85 nm
-1118.308452 -1118.238896 655.07 nm

-1118.30847 -1118.238896 654.89 nm
-1118.307737 -1118.236201 636.93 nm
-1118.30744 -1118.236494 642.22 nm
-1118.307551 -1118.236497 641.25 nm
-1118.307553 -1118.236498 641.24 nm
-1118.307564 -1118.236498 641.14 nm
-1118.3063 -1118.232542 617.74 nm
-1118.306666 -1118.232883 617.53 nm
-1118.306776 -1118.232885 616.62 nm
-1118.306811 -1118.232885 616.34 nm
-1118.306803 -1118.232885 616.4 nm
-1118.305104 -1118.227904 590.2 nm
-1118.306111 -1118.228341 585.87 nm
-1118.306223 -1118.228347 585.07 nm
-1118.306202 -1118.228347 585.24 nm
-1118.306184 -1118.228347 585.37 nm
-1118.306164 -1118.228347 585.52 nm
-1118.304227 -1118.222762 559.3 nm
-1118.305336 -1118.223273 555.22 nm
-1118.305555 -1118.223282 553.8 nm
-1118.305686 -1118.223283 552.93 nm
-1118.305692 -1118.223283 552.89 nm
-1118.303691 -1118.217437 528.24 nm
-1118.305373 -1118.218077 521.94 nm
-1118.306197 -1118.21812 517.32 nm
-1118.306933 -1118.218138 513.13 nm
-1118.307164 -1118.21814 511.81 nm
-1118.30738 -1118.218141 510.58 nm
-1118.307425 -1118.218141 510.32 nm
-1118.305599 -1118.212836 491.18 nm
-1118.31015 -1118.214368 475.7 nm
-1118.316866 -1118.214603 445.55 nm
-1118.324902 -1118.218407 427.84 nm
-1118.336168 -1118.222073 399.35 nm
-1118.346105 -1118.225327 377.25 nm
-1118.348166 -1118.226381 374.13 nm
-1118.348352 -1118.226736 374.65 nm
-1118.349815 -1118.22689 370.66 nm
-1118.350409 -1118.227014 369.25 nm
-1118.352691 -1118.227283 363.32 nm
-1118.353425 -1118.227464 361.72 nm
-1118.354501 -1118.227747 359.46 nm
-1118.353802 -1118.227743 361.45 nm
-1118.352727 -1118.228048 365.45 nm
-1118.35263 -1118.227774 364.93 nm
-1118.352671 -1118.228435 366.75 nm
-1118.351415 -1118.228204 369.8 nm
-1118.348069 -1118.228786 381.98 nm

-1118.35186 -1118.228321 368.82 nm
-1118.350352 -1118.228893 375.13 nm
-1118.351059 -1118.228664 372.27 nm
-1118.347545 -1118.228942 384.17 nm
-1118.351966 -1118.228395 368.72 nm
-1118.349306 -1118.228953 378.58 nm
-1118.349468 -1118.22894 378.03 nm
-1118.34723 -1118.228975 385.3 nm
-1118.348981 -1118.228958 379.62 nm
-1118.347846 -1118.228979 383.31 nm
-1118.34817 -1118.228977 382.26 nm
-1118.347741 -1118.228979 383.65 nm
-1118.347735 -1118.228979 383.67 nm
-1118.34691 -1118.227377 381.18 nm
-1118.348901 -1118.227677 375.86 nm
-1118.349931 -1118.227719 372.82 nm
-1118.350924 -1118.22774 369.88 nm
-1118.352671 -1118.227777 364.82 nm
-1118.353788 -1118.227754 361.52 nm
-1118.353391 -1118.227803 362.8 nm
-1118.35227 -1118.227769 365.97 nm
-1118.354533 -1118.227752 359.39 nm
-1118.35411 -1118.227824 360.8 nm
-1118.352251 -1118.227768 366.02 nm
-1118.354372 -1118.227818 360.03 nm
-1118.35425 -1118.227826 360.4 nm
-1118.354248 -1118.227819 360.39 nm
-1118.354113 -1118.227834 360.81 nm
-1118.354299 -1118.227832 360.28 nm
-1118.354175 -1118.227834 360.64 nm
-1118.354206 -1118.227834 360.55 nm
-1118.353815 -1118.227544 360.84 nm
-1118.352802 -1118.228365 366.16 nm
-1118.351838 -1118.228618 369.77 nm
-1118.349742 -1118.228778 376.67 nm
-1118.349026 -1118.228827 379.06 nm
-1118.348165 -1118.228872 381.95 nm
-1118.347638 -1118.228889 383.7 nm
-1118.347536 -1118.22889 384.03 nm
-1118.347609 -1118.22889 383.79 nm
-1118.347598 -1118.22889 383.83 nm
-1118.347786 -1118.229965 386.72 nm
-1118.345929 -1118.23016 393.57 nm
-1118.347809 -1118.230186 387.37 nm
-1118.347134 -1118.230199 389.65 nm
-1118.347089 -1118.230199 389.8 nm
-1118.346769 -1118.230977 393.49 nm
-1118.346393 -1118.231191 395.51 nm

-1118.3466 -1118.231198 394.82 nm
-1118.346572 -1118.231202 394.93 nm
-1118.346548 -1118.231202 395.01 nm
-1118.345501 -1118.231335 399.1 nm
-1118.345106 -1118.231607 401.44 nm
-1118.344892 -1118.231615 402.23 nm
-1118.344907 -1118.231615 402.18 nm
-1118.344875 -1118.231615 402.29 nm
-1118.343031 -1118.230965 406.58 nm
-1118.341711 -1118.231436 413.18 nm
-1118.340036 -1118.231533 419.92 nm
-1118.338172 -1118.231597 427.52 nm
-1118.336092 -1118.231649 436.25 nm
-1118.33358 -1118.231691 447.19 nm
-1118.333041 -1118.231721 449.7 nm
-1118.332166 -1118.231734 453.68 nm
-1118.32342 -1118.231701 496.77 nm
-1118.329164 -1118.231785 467.9 nm
-1118.328085 -1118.231803 473.23 nm
-1118.320392 -1118.23174 513.96 nm
-1118.324519 -1118.23181 491.46 nm
-1118.326505 -1118.231819 481.21 nm
-1118.327127 -1118.231807 478.01 nm
-1118.320919 -1118.231807 511.3 nm
-1118.324157 -1118.231836 493.53 nm
-1118.325539 -1118.23183 486.22 nm
-1118.323785 -1118.231837 495.54 nm
-1118.324859 -1118.231834 489.8 nm
-1118.32387 -1118.231837 495.08 nm
-1118.324 -1118.233572 503.86 nm
-1118.314894 -1118.234245 564.96 nm
-1118.317708 -1118.234345 546.56 nm
-1118.316287 -1118.234388 556.33 nm
-1118.316349 -1118.23439 555.93 nm
-1118.316321 -1118.23439 556.12 nm
-1118.31633 -1118.23439 556.06 nm
-1118.316781 -1118.236158 565.14 nm
-1118.312913 -1118.236598 597.04 nm
-1118.314694 -1118.236639 583.74 nm
-1118.31428 -1118.236645 586.89 nm
-1118.314276 -1118.236645 586.92 nm
-1118.314259 -1118.236645 587.05 nm
-1118.314694 -1118.237965 593.83 nm
-1118.312536 -1118.238382 614.44 nm
-1118.312676 -1118.238393 613.38 nm
-1118.312562 -1118.238394 614.32 nm
-1118.312936 -1118.239142 617.43 nm
-1118.311024 -1118.239488 636.93 nm

-1118.310951 -1118.239495 637.64 nm
-1118.310957 -1118.239496 637.6 nm
-1118.310936 -1118.239496 637.79 nm
-1118.311131 -1118.239443 635.58 nm
-1118.309353 -1118.239713 654.26 nm
-1118.309663 -1118.239716 651.4 nm
-1118.309641 -1118.239716 651.6 nm
-1118.309628 -1118.239716 651.73 nm
-1118.309467 -1118.238647 643.38 nm
-1118.308318 -1118.238888 656.25 nm
-1118.308404 -1118.238891 655.46 nm
-1118.308427 -1118.238891 655.25 nm
-1118.307805 -1118.23669 640.69 nm
-1118.307172 -1118.23694 648.75 nm
-1118.307199 -1118.236942 648.52 nm
-1118.307217 -1118.236942 648.36 nm
-1118.306125 -1118.233565 627.93 nm
-1118.305893 -1118.233845 632.4 nm
-1118.305979 -1118.233847 631.67 nm
-1118.305994 -1118.233847 631.54 nm
-1118.304388 -1118.229318 606.95 nm
-1118.304602 -1118.229684 608.18 nm
-1118.304768 -1118.229689 606.87 nm
-1118.304786 -1118.229689 606.73 nm
-1118.304789 -1118.229689 606.7 nm
-1118.304784 -1118.229689 606.75 nm
-1118.302774 -1118.224254 580.28 nm
-1118.303717 -1118.22471 576.7 nm
-1118.303858 -1118.22472 575.75 nm
-1118.303909 -1118.224721 575.38 nm
-1118.303913 -1118.224721 575.36 nm
-1118.303921 -1118.224722 575.3 nm
-1118.301652 -1118.218654 548.97 nm
-1118.303018 -1118.219247 543.9 nm
-1118.303598 -1118.219275 540.34 nm
-1118.303967 -1118.21928 538.02 nm
-1118.304091 -1118.219281 537.24 nm
-1118.304113 -1118.219282 537.1 nm
-1118.301803 -1118.213161 514.01 nm
-1118.304958 -1118.21413 501.64 nm
-1118.30845 -1118.214658 485.79 nm
-1118.313921 -1118.21565 463.65 nm
-1118.318723 -1118.216847 447.24 nm
-1118.331948 -1118.218536 401.75 nm
-1118.336597 -1118.221948 397.42 nm
-1118.340247 -1118.2241 392.29 nm
-1118.345822 -1118.226075 380.5 nm
-1118.348732 -1118.226435 372.56 nm

-1118.349708 -1118.226843 370.84 nm
-1118.350834 -1118.227034 368.04 nm
-1118.352304 -1118.227162 364.09 nm
-1118.352856 -1118.22731 362.92 nm
-1118.35421 -1118.227753 360.31 nm
-1118.353813 -1118.227785 361.53 nm
-1118.35368 -1118.22817 363.03 nm
-1118.352431 -1118.228503 367.66 nm
-1118.34168 -1118.22783 400.21 nm
-1118.350632 -1118.228832 374.08 nm
-1118.351391 -1118.228288 370.12 nm
-1118.347934 -1118.228882 382.72 nm
-1118.347798 -1118.228897 383.2 nm
-1118.348303 -1118.228924 381.67 nm
-1118.347943 -1118.228926 382.83 nm
-1118.347439 -1118.228932 384.48 nm
-1118.34798 -1118.228942 382.76 nm
-1118.34771 -1118.228944 383.64 nm
-1118.347271 -1118.228947 385.07 nm
-1118.347354 -1118.228947 384.8 nm
-1118.347368 -1118.228947 384.76 nm
-1118.346469 -1118.227382 382.61 nm
-1118.348016 -1118.227663 378.58 nm
-1118.349035 -1118.227698 375.51 nm
-1118.350253 -1118.227718 371.84 nm
-1118.351571 -1118.227738 367.94 nm
-1118.297625 -1118.174197 369.15 nm
-1118.352039 -1118.224414 357.01 nm
-1118.351977 -1118.227746 366.76 nm
-1118.341549 -1118.219574 373.55 nm
-1118.354281 -1118.227453 359.25 nm
-1118.353409 -1118.227774 362.67 nm
-1118.353832 -1118.227755 361.39 nm
-1118.353737 -1118.227689 361.48 nm
-1118.354197 -1118.227787 360.44 nm
-1118.353441 -1118.227803 362.65 nm
-1118.354029 -1118.227829 361.04 nm
-1118.354402 -1118.227825 359.97 nm
-1118.354217 -1118.22784 360.54 nm
-1118.354172 -1118.227839 360.66 nm
-1118.354293 -1118.227841 360.32 nm
-1118.354249 -1118.227841 360.45 nm
-1118.354267 -1118.227841 360.4 nm
-1118.354263 -1118.227841 360.41 nm

Geometries of structural optimization

1 Energy:-1118.35426335

C -2.749096 3.181287 0.001204
C -1.351786 3.291935 0.004979
C -0.617686 2.107198 0.006949
C -1.262847 0.846144 0.005632
C -2.725727 0.746312 0.000975
C -3.433451 1.969534 -0.001021
N -0.517494 -0.311358 0.009071
C -1.095448 -1.645374 0.003967
C -2.529687 -1.733890 -0.001544
C -3.348799 -0.537700 -0.001790
C -3.135825 -3.004425 -0.006367
C -4.513593 -3.142451 -0.010776
C -5.332273 -1.975791 -0.010269
C -4.763581 -0.719387 -0.005959
O -0.302751 -2.587753 0.004908
C 0.925884 -0.249074 0.015642
C 1.614712 -0.213422 1.224714
C 3.011033 -0.161187 1.224534
C 3.745113 -0.140477 0.029919
C 3.018766 -0.173968 -1.174522
C 1.627084 -0.226397 -1.190833
F -3.474137 4.310858 -0.000776
C 5.283059 -0.084651 -0.003442
C 5.898518 -0.053639 1.408340
C 5.825177 -1.332959 -0.740195
C 5.733739 1.190570 -0.755579
H -0.876329 4.265063 0.006201
H 0.463010 2.147092 0.009727
H -4.515089 1.996589 -0.004548
H -2.490996 -3.878048 -0.006251
H -4.967165 -4.128708 -0.014306
H -6.413997 -2.075217 -0.013294
H -5.416562 0.147424 -0.005681
H 1.065233 -0.232861 2.160990
H 3.520233 -0.139001 2.180925
H 3.543515 -0.161312 -2.125041
H 1.085741 -0.255704 -2.131552
H 6.990546 -0.013680 1.330385
H 5.575394 0.826481 1.975929
H 5.641029 -0.948615 1.985989
H 6.920721 -1.303217 -0.776750
H 5.458780 -1.391039 -1.770435
H 5.526866 -2.252861 -0.224447
H 5.370921 2.093073 -0.250203
H 6.828537 1.239263 -0.793150
H 5.363901 1.209892 -1.786088

2 Energy:-1118.34757909

C -2.670928 3.154314 -0.262658
C -1.302286 3.252808 0.012232
C -0.603614 2.067943 0.202082
C -1.247567 0.809125 0.080509
C -2.686563 0.728281 -0.135569
C -3.360603 1.943101 -0.323830
N -0.516275 -0.355089 0.102167
C -1.148078 -1.652645 0.447697
C -2.558648 -1.723729 0.281988
C -3.333667 -0.562280 -0.112084
C -3.218174 -2.970609 0.453928
C -4.569059 -3.100501 0.212534
C -5.327502 -1.974833 -0.219182
C -4.710264 -0.741592 -0.366169
O -0.378379 -2.540699 0.825265
C 0.915992 -0.315666 0.090722
C 1.661549 -0.469496 1.263117
C 3.054039 -0.391026 1.215111
C 3.739983 -0.149015 0.015248
C 2.963045 0.019718 -1.148272
C 1.575375 -0.049882 -1.117192
F -3.368004 4.283615 -0.453297
C 5.273207 -0.060561 -0.067534
C 5.947414 -0.266644 1.302019
C 5.797164 -1.150644 -1.033741
C 5.678736 1.334525 -0.601741
H -0.824012 4.222271 0.082499
H 0.453908 2.096514 0.430209
H -4.427275 1.975934 -0.506484
H -2.624531 -3.825244 0.764006
H -5.054834 -4.063372 0.343517
H -6.387221 -2.079213 -0.430026
H -5.311326 0.103899 -0.687963
H 1.153965 -0.652258 2.203824
H 3.602526 -0.516536 2.141501
H 3.447621 0.205740 -2.101935
H 0.995907 0.078221 -2.026606
H 7.034766 -0.196149 1.188480
H 5.640997 0.495703 2.027321
H 5.722208 -1.252635 1.723895
H 6.889746 -1.094443 -1.108116
H 5.387826 -1.033769 -2.042621
H 5.531556 -2.151951 -0.676004
H 5.327367 2.128166 0.067735
H 6.770489 1.408300 -0.672539
H 5.266618 1.526851 -1.597882

3 Energy:-1118.34724539

C -2.668536 3.139734 -0.417762
C -1.316080 3.258878 -0.083836
C -0.621814 2.085873 0.184659
C -1.251597 0.820205 0.080962
C -2.677563 0.721199 -0.185776
C -3.348243 1.922161 -0.457245
N -0.512501 -0.338705 0.185357
C -1.151871 -1.625075 0.563697
C -2.556715 -1.705601 0.359439
C -3.321437 -0.570504 -0.120307
C -3.219284 -2.945192 0.575180
C -4.560621 -3.093195 0.296674
C -5.306832 -1.995106 -0.218429
C -4.687753 -0.768706 -0.409964
O -0.393509 -2.500935 0.990707
C 0.911324 -0.297587 0.153241
C 1.683126 -0.561767 1.292408
C 3.073799 -0.490349 1.220359
C 3.738817 -0.149651 0.031985
C 2.938839 0.128065 -1.096630
C 1.553789 0.068479 -1.042476
F -3.363279 4.255473 -0.686858
C 5.269810 -0.067962 -0.075330
C 5.970136 -0.397204 1.256498
C 5.761309 -1.076041 -1.142979
C 5.679432 1.364252 -0.497075
H -0.847009 4.233535 -0.024736
H 0.422336 2.131083 0.466952
H -4.406259 1.939586 -0.686913
H -2.633987 -3.780036 0.948428
H -5.047954 -4.050145 0.461268
H -6.358804 -2.114616 -0.458262
H -5.280087 0.056637 -0.794334
H 1.193890 -0.816023 2.224980
H 3.639759 -0.697128 2.121261
H 3.405776 0.389389 -2.041337
H 0.958502 0.274782 -1.926839
H 7.055516 -0.326692 1.125730
H 5.687066 0.302594 2.051004
H 5.743415 -1.413861 1.596795
H 6.852683 -1.023644 -1.234967
H 5.333206 -0.868858 -2.129263
H 5.491911 -2.101824 -0.866864
H 5.353371 2.100322 0.246737
H 6.770099 1.432419 -0.587279
H 5.247016 1.646286 -1.462699

4 Energy:-1118.34684541

C -2.677625 3.123907 -0.559040
C -1.344990 3.273563 -0.168846
C -0.651621 2.118943 0.176080
C -1.259738 0.843266 0.091928
C -2.669278 0.716212 -0.226769
C -3.340064 1.896764 -0.578583
N -0.508774 -0.301876 0.285750
C -1.151630 -1.586035 0.676286
C -2.548249 -1.683097 0.427476
C -3.304872 -0.577842 -0.126997
C -3.208565 -2.919199 0.673912
C -4.537857 -3.091830 0.357377
C -5.274474 -2.023776 -0.229749
C -4.658611 -0.801394 -0.453715
O -0.404440 -2.450794 1.143657
C 0.906418 -0.258045 0.230950
C 1.703832 -0.621693 1.328642
C 3.092028 -0.566727 1.227454
C 3.737267 -0.149054 0.051805
C 2.915682 0.225078 -1.034518
C 1.533654 0.183713 -0.952474
F -3.373527 4.218934 -0.904634
C 5.265376 -0.083448 -0.085518
C 5.990297 -0.526808 1.199204
C 5.714374 -1.012614 -1.240484
C 5.689777 1.370964 -0.405512
H -0.889764 4.255417 -0.122755
H 0.376515 2.190025 0.508437
H -4.386914 1.890744 -0.855481
H -2.629297 -3.731546 1.102005
H -5.022776 -4.045620 0.545839
H -6.316882 -2.163000 -0.499121
H -5.244172 0.001307 -0.892531
H 1.233125 -0.930446 2.253017
H 3.674535 -0.845618 2.097796
H 3.365884 0.543904 -1.969524
H 0.924004 0.456222 -1.808452
H 7.073375 -0.465134 1.047112
H 5.739640 0.114215 2.051999
H 5.752132 -1.562687 1.465614
H 6.804048 -0.969158 -1.354027
H 5.267597 -0.722258 -2.197002
H 5.434248 -2.052635 -1.038499
H 5.393487 2.052275 0.400263
H 6.779164 1.428172 -0.516040
H 5.240857 1.733254 -1.336173

5 Energy:-1118.34530216

C -2.680780 3.110148 -0.665084
C -1.376186 3.294584 -0.206686
C -0.686707 2.161840 0.213311
C -1.267730 0.874885 0.135556
C -2.651126 0.714310 -0.254854
C -3.320224 1.870947 -0.681247
N -0.507463 -0.249463 0.426132
C -1.162205 -1.530090 0.835556
C -2.538359 -1.654178 0.501793
C -3.273415 -0.587375 -0.146763
C -3.199622 -2.887961 0.764897
C -4.502685 -3.095393 0.371453
C -5.212805 -2.067440 -0.310987
C -4.598867 -0.846000 -0.549246
O -0.441680 -2.368313 1.384673
C 0.898621 -0.208865 0.338665
C 1.727699 -0.659320 1.384423
C 3.111084 -0.624745 1.240254
C 3.730152 -0.147703 0.071630
C 2.882040 0.306599 -0.963562
C 1.504615 0.287016 -0.840068
F -3.375063 4.181348 -1.084321
C 5.253068 -0.102982 -0.110221
C 6.008572 -0.627703 1.125189
C 5.645851 -0.977541 -1.327206
C 5.696724 1.358422 -0.367430
H -0.939078 4.284809 -0.164294
H 0.318563 2.261568 0.604442
H -4.350037 1.836787 -1.014628
H -2.639060 -3.670637 1.266650
H -4.986258 -4.047603 0.571429
H -6.233186 -2.235119 -0.641565
H -5.164961 -0.072273 -1.059942
H 1.281623 -1.007668 2.305545
H 3.714596 -0.964331 2.073915
H 3.309161 0.667355 -1.894141
H 0.877086 0.612454 -1.663538
H 7.087327 -0.576080 0.942206
H 5.796062 -0.029690 2.018595
H 5.759743 -1.672391 1.342856
H 6.732016 -0.947937 -1.473581
H 5.174734 -0.627827 -2.251578
H 5.351338 -2.021438 -1.171232
H 5.439875 2.001630 0.481923
H 6.783096 1.400099 -0.509598
H 5.227047 1.777811 -1.263166

6 Energy:-1118.33667721

C -2.677429 3.107911 -0.721262
C -1.430537 3.350349 -0.148875
C -0.741561 2.255755 0.363119
C -1.271550 0.951368 0.268460
C -2.585131 0.726329 -0.270080
C -3.262327 1.841611 -0.774751
N -0.515337 -0.148802 0.664921
C -1.246009 -1.348411 1.240537
C -2.517970 -1.583003 0.653948
C -3.149587 -0.616415 -0.217754
C -3.204242 -2.799654 0.939886
C -4.397002 -3.102687 0.319224
C -4.973841 -2.193010 -0.605211
C -4.356045 -0.968384 -0.842601
O -0.680771 -1.992236 2.129333
C 0.871225 -0.163895 0.502681
C 1.751482 -0.691966 1.475565
C 3.122382 -0.684934 1.253706
C 3.694675 -0.160728 0.078712
C 2.803526 0.367591 -0.882545
C 1.436385 0.374996 -0.685567
F -3.370809 4.143707 -1.225220
C 5.204783 -0.147841 -0.184400
C 6.010500 -0.750102 0.982039
C 5.505476 -0.973622 -1.460874
C 5.675268 1.312456 -0.398978
H -1.034673 4.357461 -0.094503
H 0.221281 2.398423 0.840907
H -4.253021 1.754630 -1.204770
H -2.742670 -3.498066 1.631149
H -4.890107 -4.048687 0.526763
H -5.898758 -2.443058 -1.115508
H -4.829093 -0.269088 -1.527012
H 1.344882 -1.079195 2.398014
H 3.760274 -1.082321 2.034588
H 3.188895 0.763153 -1.817178
H 0.778422 0.750003 -1.462112
H 7.078772 -0.716979 0.742471
H 5.862912 -0.190307 1.912499
H 5.745041 -1.797430 1.164408
H 6.582563 -0.964607 -1.665292
H 4.995068 -0.568423 -2.340675
H 5.190833 -2.015890 -1.336881
H 5.482843 1.921584 0.491441
H 6.753214 1.331578 -0.598227
H 5.170960 1.785387 -1.247937

7 Energy:-1118.31746675

C -2.854561 3.121428 -0.753270
C -1.656686 3.480025 -0.140725
C -0.878307 2.461570 0.404904
C -1.299959 1.127337 0.314870
C -2.547216 0.772458 -0.285348
C -3.315177 1.806443 -0.826318
N -0.514144 0.047256 0.734396
C -1.278922 -1.017879 1.533648
C -2.406509 -1.477460 0.789136
C -2.970528 -0.638791 -0.241471
C -3.051832 -2.700484 1.106369
C -4.109451 -3.157366 0.340839
C -4.587604 -2.391320 -0.745243
C -4.034391 -1.138005 -1.004292
O -0.946992 -1.236056 2.707935
C 0.831416 -0.061316 0.501743
C 1.683591 -0.754011 1.406331
C 3.048946 -0.809877 1.175165
C 3.649607 -0.197215 0.058359
C 2.790697 0.495054 -0.832163
C 1.430707 0.576364 -0.625341
F -3.621409 4.091248 -1.288533
C 5.153977 -0.258162 -0.222146
C 5.922506 -1.045884 0.855470
C 5.389348 -0.947842 -1.590151
C 5.722023 1.182771 -0.271881
H -1.356438 4.520411 -0.093750
H 0.060454 2.692730 0.897529
H -4.273362 1.617736 -1.297104
H -2.665995 -3.290881 1.932505
H -4.564022 -4.118426 0.566546
H -5.399580 -2.764110 -1.362145
H -4.451599 -0.532090 -1.804983
H 1.249366 -1.205965 2.287832
H 3.662144 -1.334992 1.897973
H 3.203272 0.966269 -1.718656
H 0.800479 1.088238 -1.343695
H 6.988791 -1.058790 0.605741
H 5.820814 -0.589012 1.846253
H 5.585470 -2.086523 0.919248
H 6.463487 -0.988070 -1.805428
H 4.904576 -0.409223 -2.410783
H 5.004393 -1.973687 -1.583666
H 5.577964 1.694574 0.686244
H 6.797248 1.150963 -0.483069
H 5.246598 1.785113 -1.052719

8 Energy:-1118.31399405

C -2.918116 3.115531 -0.837147
C -1.779550 3.548623 -0.164010
C -0.979665 2.582344 0.445772
C -1.327503 1.230971 0.358273
C -2.514779 0.796801 -0.300063
C -3.303567 1.778207 -0.909640
N -0.514657 0.191385 0.848984
C -1.267505 -0.880341 1.641405
C -2.324805 -1.418886 0.844896
C -2.870219 -0.633561 -0.236857
C -2.928393 -2.662881 1.159891
C -3.919836 -3.189662 0.351879
C -4.372482 -2.474929 -0.778682
C -3.865372 -1.204071 -1.042625
O -0.995401 -1.036196 2.842255
C 0.808505 0.046699 0.569200
C 1.641096 -0.745184 1.416434
C 2.996833 -0.854504 1.158795
C 3.609804 -0.204156 0.069935
C 2.772371 0.585129 -0.762740
C 1.423239 0.722849 -0.530040
F -3.702314 4.034897 -1.436734
C 5.103411 -0.321658 -0.242294
C 5.849952 -1.205947 0.773993
C 5.279614 -0.942568 -1.651877
C 5.741460 1.090650 -0.222766
H -1.535976 4.604039 -0.123869
H -0.081330 2.870842 0.982107
H -4.221978 1.529433 -1.429351
H -2.560631 -3.212861 2.021424
H -4.339935 -4.166065 0.578535
H -5.130968 -2.901995 -1.427759
H -4.265174 -0.639974 -1.881796
H 1.199932 -1.222396 2.281129
H 3.593876 -1.453733 1.835720
H 3.197325 1.088888 -1.624897
H 0.811651 1.311869 -1.203086
H 6.910005 -1.254807 0.503454
H 5.786592 -0.802497 1.790802
H 5.464193 -2.231407 0.784696
H 6.346568 -1.022107 -1.890129
H 4.808119 -0.334629 -2.430675
H 4.844542 -1.947190 -1.695356
H 5.637897 1.554630 0.764419
H 6.810276 1.016572 -0.454280
H 5.286090 1.758395 -0.961167

9 Energy:-1118.31213834

C -2.945073 3.099080 -0.934439
C -1.882118 3.602034 -0.190264
C -1.078924 2.687729 0.493247
C -1.351573 1.322096 0.406505
C -2.466030 0.814298 -0.317708
C -3.256557 1.744263 -1.005729
N -0.517338 0.330163 0.976959
C -1.263290 -0.758968 1.745648
C -2.247261 -1.360178 0.901916
C -2.763379 -0.626569 -0.230792
C -2.816575 -2.621112 1.217060
C -3.737698 -3.210467 0.371251
C -4.155135 -2.544992 -0.802809
C -3.686832 -1.261913 -1.074167
O -1.030821 -0.898937 2.957119
C 0.785515 0.150462 0.653032
C 1.596888 -0.728498 1.439248
C 2.938721 -0.890292 1.146310
C 3.561044 -0.211079 0.080141
C 2.746367 0.662885 -0.691968
C 1.411774 0.853487 -0.425248
F -3.729096 3.967718 -1.608426
C 5.041052 -0.377656 -0.267694
C 5.762741 -1.354489 0.679395
C 5.164236 -0.919351 -1.715268
C 5.742996 1.001447 -0.176082
H -1.694071 4.668951 -0.155884
H -0.233732 3.029839 1.082145
H -4.123306 1.439321 -1.581256
H -2.475478 -3.132096 2.112872
H -4.128798 -4.198050 0.601449
H -4.857658 -3.020842 -1.480343
H -4.060905 -0.738186 -1.950508
H 1.152318 -1.226401 2.290208
H 3.518577 -1.554717 1.775295
H 3.181131 1.193010 -1.532919
H 0.819301 1.509883 -1.050470
H 6.814527 -1.434620 0.385459
H 5.735661 -1.010534 1.719352
H 5.330183 -2.360224 0.636557
H 6.222394 -1.033195 -1.977093
H 4.710163 -0.244398 -2.447768
H 4.681970 -1.898465 -1.810375
H 5.678339 1.408266 0.839172
H 6.802826 0.893021 -0.433388
H 5.306117 1.732826 -0.863582

10 Energy:-1118.31063726

C -2.956341 3.070156 -1.039063
C -1.975967 3.639561 -0.231611
C -1.177114 2.778135 0.522961
C -1.373700 1.400860 0.442525
C -2.411393 0.823578 -0.338743
C -3.195162 1.701882 -1.102434
N -0.521959 0.460582 1.088093
C -1.263442 -0.643740 1.838182
C -2.176084 -1.301853 0.959433
C -2.657577 -0.622260 -0.222309
C -2.713293 -2.576379 1.281536
C -3.563109 -3.225734 0.407062
C -3.941878 -2.610956 -0.808181
C -3.508814 -1.319724 -1.093692
O -1.060033 -0.772854 3.055922
C 0.767194 0.254433 0.738305
C 1.547138 -0.712981 1.454472
C 2.872557 -0.924670 1.125819
C 3.511482 -0.210712 0.092195
C 2.730606 0.752649 -0.607699
C 1.412374 0.991652 -0.307383
F -3.732378 3.887243 -1.785132
C 4.974897 -0.426948 -0.292917
C 5.659471 -1.502359 0.571249
C 5.047695 -0.871962 -1.776604
C 5.746836 0.906434 -0.119454
H -1.843345 4.715002 -0.206083
H -0.390344 3.171839 1.158888
H -4.005839 1.343494 -1.726897
H -2.401391 -3.047503 2.209203
H -3.927596 -4.221411 0.646031
H -4.588009 -3.133828 -1.506860
H -3.853477 -0.837253 -2.005008
H 1.094708 -1.239604 2.283328
H 3.426976 -1.657877 1.698469
H 3.181263 1.315538 -1.418206
H 0.846778 1.717771 -0.877095
H 6.700682 -1.615410 0.251845
H 5.667306 -1.230203 1.632538
H 5.174380 -2.479347 0.468179
H 6.094668 -1.020644 -2.064229
H 4.618817 -0.125743 -2.452953
H 4.514257 -1.816472 -1.929924
H 5.718311 1.244040 0.922410
H 6.795640 0.763449 -0.403254
H 5.337401 1.704678 -0.746755

11 Energy:-1118.30952388

C -2.957174 3.028873 -1.147250
C -2.050372 3.656854 -0.297746
C -1.259450 2.845561 0.518390
C -1.390341 1.460364 0.455986
C -2.361606 0.822453 -0.361502
C -3.135325 1.652027 -1.190389
N -0.526301 0.571363 1.168015
C -1.264371 -0.541116 1.910151
C -2.119888 -1.249032 1.015467
C -2.570366 -0.623033 -0.208119
C -2.631058 -2.530778 1.356036
C -3.422462 -3.233527 0.469656
C -3.768799 -2.669039 -0.780394
C -3.362879 -1.375553 -1.090316
O -1.074335 -0.658297 3.130749
C 0.756414 0.345372 0.810525
C 1.493609 -0.711978 1.443356
C 2.802499 -0.965377 1.082631
C 3.469143 -0.206307 0.099423
C 2.732888 0.846940 -0.515859
C 1.430434 1.125325 -0.186272
F -3.722553 3.797044 -1.955237
C 4.917290 -0.463085 -0.315078
C 5.550477 -1.639563 0.450913
C 4.960245 -0.785936 -1.831274
C 5.755574 0.811698 -0.038194
H -1.964954 4.737314 -0.288506
H -0.526469 3.285874 1.187262
H -3.896646 1.245852 -1.846890
H -2.343587 -2.962145 2.310513
H -3.766302 -4.232331 0.725641
H -4.369423 -3.233789 -1.487027
H -3.682140 -0.933931 -2.031081
H 1.025826 -1.277814 2.236591
H 3.322216 -1.769715 1.588155
H 3.207293 1.449701 -1.282753
H 0.899313 1.921258 -0.691695
H 6.582267 -1.779004 0.112165
H 5.579415 -1.456467 1.530745
H 5.014544 -2.578462 0.273062
H 5.997187 -0.961913 -2.138756
H 4.566739 0.034327 -2.439967
H 4.379586 -1.686894 -2.057509
H 5.747585 1.063092 1.028075
H 6.794723 0.640071 -0.340759
H 5.384726 1.678268 -0.594779

12 Energy:-1118.30847019

C -2.941520 2.979321 -1.255978
C -2.104931 3.660656 -0.375521
C -1.328030 2.897667 0.498493
C -1.401911 1.507606 0.462040
C -2.309968 0.814722 -0.382561
C -3.067751 1.597285 -1.272104
N -0.532998 0.670472 1.238533
C -1.271438 -0.446318 1.974806
C -2.073575 -1.200428 1.070651
C -2.489258 -0.627383 -0.190969
C -2.562649 -2.486190 1.432093
C -3.297819 -3.238460 0.539150
C -3.608788 -2.723542 -0.742321
C -3.225093 -1.430580 -1.078596
O -1.095948 -0.548483 3.198393
C 0.749065 0.427571 0.886692
C 1.436940 -0.712638 1.425599
C 2.728538 -1.000755 1.032033
C 3.427850 -0.196678 0.108530
C 2.742805 0.939841 -0.411116
C 1.456233 1.250567 -0.051506
F -3.690969 3.699827 -2.121757
C 4.859169 -0.489877 -0.337578
C 5.434663 -1.757732 0.320429
C 4.878692 -0.683423 -1.876197
C 5.762388 0.712837 0.039718
H -2.060074 4.743511 -0.387288
H -0.647410 3.380328 1.193055
H -3.781731 1.147678 -1.953030
H -2.301808 -2.878589 2.410708
H -3.624716 -4.238011 0.813780
H -4.165461 -3.327088 -1.452862
H -3.516321 -1.029085 -2.046048
H 0.949048 -1.320449 2.173983
H 3.208247 -1.871220 1.461629
H 3.244675 1.581911 -1.126839
H 0.962755 2.110119 -0.485434
H 6.456489 -1.919565 -0.037845
H 5.477759 -1.668598 1.411537
H 4.850913 -2.649938 0.068378
H 5.903961 -0.885239 -2.205909
H 4.525899 0.205220 -2.408995
H 4.251219 -1.530645 -2.173747
H 5.773473 0.870910 1.123707
H 6.789479 0.515606 -0.287127
H 5.433100 1.641810 -0.436454

13 Energy:-1118.30756353

C -2.910144 2.921762 -1.362587
C -2.127194 3.646946 -0.467527
C -1.368414 2.925713 0.456258
C -1.405357 1.533799 0.454360
C -2.266962 0.796539 -0.401555
C -3.004363 1.538107 -1.343703
N -0.538137 0.741810 1.286350
C -1.280001 -0.370217 2.025324
C -2.049990 -1.160931 1.126390
C -2.435082 -0.637931 -0.166580
C -2.530659 -2.442176 1.517263
C -3.228630 -3.234941 0.630579
C -3.509559 -2.768057 -0.676935
C -3.133710 -1.482542 -1.046649
O -1.109734 -0.453267 3.250484
C 0.745676 0.479990 0.944663
C 1.379192 -0.736348 1.371259
C 2.657271 -1.044443 0.950475
C 3.397428 -0.187000 0.109846
C 2.765682 1.022111 -0.301508
C 1.490959 1.350967 0.082745
F -3.640146 3.600547 -2.278052
C 4.817822 -0.498443 -0.357294
C 5.337613 -1.841989 0.187057
C 4.836264 -0.556082 -1.907182
C 5.767677 0.628211 0.125886
H -2.107822 4.729910 -0.506051
H -0.728993 3.443402 1.164670
H -3.682057 1.053180 -2.037360
H -2.292355 -2.797083 2.515737
H -3.549661 -4.229326 0.929780
H -4.037244 -3.403568 -1.381707
H -3.400998 -1.119190 -2.035816
H 0.863005 -1.395123 2.054481
H 3.093272 -1.975321 1.290537
H 3.299597 1.707660 -0.950381
H 1.037041 2.268064 -0.268589
H 6.354635 -2.012178 -0.180802
H 5.376450 -1.852050 1.281912
H 4.720999 -2.684243 -0.145659
H 5.854104 -0.769682 -2.252063
H 4.522040 0.389690 -2.359763
H 4.176488 -1.347647 -2.278891
H 5.778199 0.691394 1.219493
H 6.787637 0.416427 -0.213753
H 5.481353 1.608095 -0.268985

14 Energy:-1118.30680329

C -2.870676 2.851452 -1.473412
C -2.126851 3.616901 -0.578269
C -1.387937 2.936102 0.391120
C -1.404179 1.544445 0.434471
C -2.234089 0.767615 -0.418744
C -2.948787 1.468798 -1.409459
N -0.541722 0.794713 1.315392
C -1.288018 -0.304510 2.066393
C -2.043293 -1.127382 1.185568
C -2.403821 -0.655450 -0.133988
C -2.524813 -2.396557 1.614997
C -3.201780 -3.225480 0.746039
C -3.459477 -2.808770 -0.583860
C -3.081687 -1.536865 -0.994782
O -1.119046 -0.359082 3.292687
C 0.745758 0.513049 0.986543
C 1.323200 -0.765470 1.287578
C 2.591322 -1.082546 0.844456
C 3.377020 -0.173574 0.104518
C 2.799481 1.095274 -0.186711
C 1.532194 1.431416 0.216730
F -3.579407 3.489255 -2.434372
C 4.790954 -0.493427 -0.375852
C 5.248719 -1.906200 0.031797
C 4.831258 -0.390931 -1.922984
C 5.776427 0.537660 0.232977
H -2.120890 4.698226 -0.650974
H -0.779901 3.486389 1.102543
H -3.599698 0.951850 -2.105617
H -2.303609 -2.712391 2.630400
H -3.524484 -4.209528 1.075965
H -3.970860 -3.472919 -1.274114
H -3.330356 -1.213271 -2.002420
H 0.770771 -1.475738 1.885672
H 2.982042 -2.063638 1.083152
H 3.368899 1.822809 -0.754666
H 1.118257 2.396907 -0.042377
H 6.264027 -2.078418 -0.339813
H 5.269877 -2.031326 1.120055
H 4.605069 -2.683621 -0.394456
H 5.845067 -0.609676 -2.276320
H 4.562489 0.608865 -2.277998
H 4.146262 -1.111633 -2.382635
H 5.772851 0.486072 1.327218
H 6.792332 0.321211 -0.115729
H 5.534298 1.563938 -0.060561

15 Energy:-1118.30616419

C -2.826618 2.766439 -1.586846
C -2.107012 3.569179 -0.704433
C -1.388315 2.928526 0.306602
C -1.399992 1.539586 0.404344
C -2.213490 0.727299 -0.433461
C -2.903863 1.387676 -1.469397
N -0.543278 0.827036 1.324866
C -1.296885 -0.247165 2.099491
C -2.053735 -1.099293 1.249548
C -2.395749 -0.680310 -0.092751
C -2.546784 -2.346898 1.726830
C -3.219680 -3.207606 0.886419
C -3.459942 -2.844850 -0.462985
C -3.069467 -1.594197 -0.923271
O -1.134846 -0.254449 3.327451
C 0.748745 0.525159 1.006493
C 1.270369 -0.798863 1.166622
C 2.533729 -1.114009 0.708374
C 3.368834 -0.157232 0.091928
C 2.843999 1.155950 -0.064757
C 1.578795 1.489472 0.350783
F -3.513040 3.363505 -2.589482
C 4.781686 -0.474988 -0.393611
C 5.175304 -1.943406 -0.147515
C 4.866669 -0.191568 -1.916155
C 5.788577 0.436442 0.355108
H -2.103078 4.646951 -0.818015
H -0.801311 3.509447 1.011075
H -3.537297 0.841845 -2.159600
H -2.337658 -2.621194 2.756799
H -3.552589 -4.174909 1.253473
H -3.967956 -3.534441 -1.130452
H -3.304767 -1.313016 -1.946693
H 0.673113 -1.555704 1.655531
H 2.879512 -2.132499 0.832137
H 3.451801 1.922077 -0.533342
H 1.204601 2.493268 0.197722
H 6.192914 -2.111366 -0.514672
H 5.162890 -2.197257 0.918178
H 4.514455 -2.638347 -0.677371
H 5.880293 -0.408776 -2.270908
H 4.646361 0.853531 -2.155333
H 4.166887 -0.823807 -2.473377
H 5.754384 0.255964 1.435027
H 6.804504 0.222356 0.004943
H 5.592121 1.498991 0.180838

16 Energy:-1118.30569227

C -2.787009 2.677676 -1.690532
C -2.072089 3.511528 -0.833270
C -1.371190 2.907910 0.212194
C -1.396197 1.524474 0.370108
C -2.209331 0.683877 -0.442109
C -2.877888 1.305905 -1.515757
N -0.544778 0.843947 1.320098
C -1.305411 -0.200819 2.122174
C -2.073323 -1.078170 1.309856
C -2.408054 -0.706901 -0.048187
C -2.578776 -2.301293 1.834588
C -3.259883 -3.186782 1.026926
C -3.494231 -2.873175 -0.335882
C -3.089887 -1.645658 -0.843994
O -1.154035 -0.149198 3.350602
C 0.753688 0.523801 1.010888
C 1.220723 -0.825977 1.016818
C 2.484396 -1.131776 0.551241
C 3.369561 -0.138743 0.077728
C 2.894295 1.200472 0.066143
C 1.627486 1.525679 0.489233
F -3.454157 3.236829 -2.727164
C 4.784895 -0.449142 -0.406947
C 5.125028 -1.948585 -0.319268
C 4.919964 -0.000405 -1.885386
C 5.800008 0.336237 0.463410
H -2.057931 4.583526 -0.991611
H -0.789458 3.514338 0.899083
H -3.504668 0.736592 -2.192937
H -2.372547 -2.538695 2.874305
H -3.603423 -4.135760 1.430080
H -4.008361 -3.582662 -0.977345
H -3.320973 -1.402825 -1.878053
H 0.577175 -1.614256 1.383862
H 2.788016 -2.171145 0.550552
H 3.539901 1.995319 -0.291006
H 1.290477 2.553699 0.453038
H 6.147570 -2.108539 -0.676274
H 5.072474 -2.320407 0.709927
H 4.459566 -2.556451 -0.942153
H 5.935678 -0.210395 -2.238670
H 4.737834 1.071539 -2.010296
H 4.216498 -0.542697 -2.526540
H 5.728931 0.038369 1.515204
H 6.817845 0.125208 0.116929
H 5.644783 1.418080 0.404553

17 Energy:-1118.30742515

C -2.804243 2.562187 -1.805078
C -2.027410 3.416190 -1.024495
C -1.323284 2.849159 0.037550
C -1.403130 1.479917 0.291200
C -2.276506 0.625833 -0.447740
C -2.946787 1.208375 -1.540511
N -0.543173 0.829819 1.242570
C -1.282136 -0.184874 2.096336
C -2.110865 -1.072634 1.364061
C -2.500067 -0.742017 0.010916
C -2.620835 -2.260359 1.959919
C -3.365004 -3.155056 1.220066
C -3.657005 -2.885239 -0.140476
C -3.244554 -1.688919 -0.714771
O -1.081672 -0.070215 3.314361
C 0.774899 0.512538 0.952315
C 1.192791 -0.836178 0.787359
C 2.469289 -1.124124 0.337995
C 3.407214 -0.109612 0.053778
C 2.977474 1.231718 0.215577
C 1.697997 1.541582 0.625582
F -3.476195 3.081776 -2.856484
C 4.836865 -0.403412 -0.405068
C 5.115076 -1.912179 -0.540183
C 5.074174 0.263902 -1.784097
C 5.829560 0.187704 0.628685
H -1.972596 4.474255 -1.252144
H -0.698810 3.473426 0.667560
H -3.609432 0.625338 -2.169870
H -2.369041 -2.466283 2.996235
H -3.714227 -4.077943 1.675386
H -4.220303 -3.602886 -0.729296
H -3.519098 -1.480238 -1.745472
H 0.500927 -1.640982 1.003131
H 2.736685 -2.164280 0.197990
H 3.665939 2.044769 0.011442
H 1.398960 2.576919 0.733507
H 6.148475 -2.061999 -0.869633
H 4.993130 -2.437697 0.413403
H 4.460605 -2.383913 -1.281620
H 6.098607 0.062609 -2.117157
H 4.943766 1.350030 -1.745439
H 4.385941 -0.134996 -2.537390
H 5.690528 -0.271158 1.613745
H 6.857920 -0.006774 0.303591
H 5.712741 1.270471 0.738822

18 Energy:-1118.34773491

C -2.851473 2.223066 -1.999150
C -1.489959 2.153543 -2.315142
C -0.723952 1.219208 -1.630435
C -1.295200 0.398727 -0.623432
C -2.728216 0.433875 -0.360139
C -3.471045 1.390490 -1.066904
N -0.498013 -0.399159 0.163451
C -1.051901 -1.576525 0.875513
C -2.457539 -1.571013 1.092772
C -3.300498 -0.514430 0.565534
C -3.042904 -2.592762 1.887828
C -4.386254 -2.573071 2.196249
C -5.211614 -1.515069 1.718391
C -4.667219 -0.521675 0.918622
O -0.230033 -2.429615 1.222389
C 0.929348 -0.301234 0.090125
C 1.688315 -1.219768 -0.640894
C 3.074021 -1.072220 -0.714205
C 3.739401 -0.012906 -0.078641
C 2.948326 0.908245 0.636769
C 1.566806 0.779511 0.714936
F -3.612373 3.119925 -2.642971
C 5.265157 0.171211 -0.138339
C 5.956521 -0.926877 -0.968362
C 5.592871 1.541294 -0.779799
C 5.841636 0.127548 1.297711
H -1.067826 2.801351 -3.073867
H 0.330982 1.121255 -1.851270
H -4.538236 1.499413 -0.920381
H -2.398557 -3.382628 2.261847
H -4.815019 -3.360015 2.810335
H -6.265706 -1.486388 1.976192
H -5.318562 0.269641 0.559258
H 1.196346 -2.044282 -1.144890
H 3.633321 -1.802348 -1.287694
H 3.417189 1.742894 1.149025
H 0.976552 1.497654 1.276283
H 7.037771 -0.750843 -0.978838
H 5.787989 -1.924385 -0.547151
H 5.612413 -0.930532 -2.008907
H 6.678786 1.687937 -0.820850
H 5.165807 2.372819 -0.209494
H 5.203514 1.598596 -1.802845
H 5.630888 -0.836025 1.775478
H 6.929377 0.263733 1.271368
H 5.421957 0.916379 1.930683

19 Energy:-1118.35420583

C -2.920875 2.059233 -2.191231
C -1.531859 2.170745 -2.343192
C -0.734422 1.360382 -1.537392
C -1.309720 0.464173 -0.603396
C -2.764760 0.352283 -0.461627
C -3.537905 1.192605 -1.294038
N -0.502385 -0.313854 0.195301
C -1.006708 -1.285857 1.151611
C -2.433554 -1.394410 1.279130
C -3.316905 -0.569730 0.477813
C -2.969575 -2.313093 2.201496
C -4.337493 -2.449731 2.365995
C -5.218577 -1.644181 1.587481
C -4.719261 -0.737198 0.676277
O -0.163132 -1.932483 1.773921
C 0.935448 -0.213609 0.096919
C 1.633025 -1.030654 -0.788347
C 3.023982 -0.929053 -0.874278
C 3.743947 -0.016688 -0.089713
C 3.008702 0.798140 0.790639
C 1.622175 0.709066 0.887481
F -3.706174 2.832704 -2.957068
C 5.275721 0.117980 -0.160659
C 5.903316 -0.858334 -1.173530
C 5.643921 1.559550 -0.586544
C 5.881598 -0.175570 1.232801
H -1.110403 2.862915 -3.061739
H 0.342373 1.414882 -1.621902
H -4.619240 1.183928 -1.257599
H -2.278051 -2.914096 2.784285
H -4.736547 -3.162500 3.080958
H -6.293105 -1.744055 1.711601
H -5.418683 -0.139970 0.100107
H 1.095361 -1.746828 -1.402222
H 3.540400 -1.581160 -1.568948
H 3.522095 1.519272 1.419400
H 1.074263 1.344888 1.576298
H 6.990546 -0.724087 -1.185139
H 5.702127 -1.903445 -0.912269
H 5.538059 -0.682160 -2.191712
H 6.733579 1.672011 -0.635127
H 5.263281 2.304477 0.120063
H 5.234021 1.793090 -1.575989
H 5.642354 -1.194624 1.557607
H 6.973130 -0.077029 1.197502
H 5.509100 0.516621 1.995132

20 Energy:-1118.34759786

C -2.933744 1.854366 -2.382927
C -1.578517 2.199773 -2.337611
C -0.787392 1.551772 -1.398300
C -1.327019 0.550232 -0.549572
C -2.753536 0.254362 -0.563442
C -3.523063 0.926709 -1.523000
N -0.501805 -0.200081 0.254098
C -1.026557 -0.902388 1.453878
C -2.426360 -1.153942 1.464745
C -3.293143 -0.668748 0.407272
C -2.982429 -1.943617 2.507476
C -4.317392 -2.286795 2.506203
C -5.164516 -1.851655 1.447149
C -4.649469 -1.056816 0.433712
O -0.190361 -1.210733 2.307226
C 0.921650 -0.095261 0.131231
C 1.564464 -0.790803 -0.897832
C 2.953323 -0.747566 -1.009688
C 3.740760 -0.019678 -0.102521
C 3.069369 0.661864 0.930029
C 1.684882 0.624121 1.059920
F -3.719489 2.463468 -3.282445
C 5.274228 0.052345 -0.199012
C 5.825722 -0.760763 -1.385450
C 5.706674 1.527558 -0.380969
C 5.898083 -0.506746 1.102534
H -1.180554 2.953529 -3.006196
H 0.263802 1.796819 -1.316762
H -4.588291 0.756116 -1.614851
H -2.321749 -2.285433 3.298376
H -4.722828 -2.896283 3.308979
H -6.211571 -2.137649 1.432919
H -5.316763 -0.729816 -0.358406
H 0.974967 -1.372653 -1.600130
H 3.418214 -1.304790 -1.814575
H 3.636516 1.236815 1.655956
H 1.191685 1.153212 1.867658
H 6.917709 -0.676264 -1.410338
H 5.578552 -1.825103 -1.301355
H 5.444037 -0.394000 -2.345097
H 6.799318 1.594836 -0.444375
H 5.382045 2.154851 0.455815
H 5.286443 1.948849 -1.301520
H 5.614962 -1.554545 1.254503
H 6.992067 -0.454043 1.048483
H 5.580271 0.059121 1.984371

21 Energy:-1118.3470889

C -2.917394 1.728827 -2.482557
C -1.579711 2.127324 -2.407281
C -0.798050 1.545389 -1.417141
C -1.327198 0.556064 -0.550370
C -2.738602 0.212016 -0.592771
C -3.500067 0.815644 -1.602849
N -0.499459 -0.128107 0.313617
C -1.039699 -0.791289 1.531623
C -2.431467 -1.080892 1.513592
C -3.278991 -0.682125 0.406304
C -2.997062 -1.831158 2.581719
C -4.319117 -2.218384 2.557666
C -5.144036 -1.870591 1.450341
C -4.621254 -1.113993 0.411343
O -0.221155 -1.046279 2.419722
C 0.915871 -0.039241 0.181076
C 1.533543 -0.653863 -0.918966
C 2.918809 -0.631250 -1.048371
C 3.736545 -0.002360 -0.092786
C 3.093969 0.602260 1.004954
C 1.712192 0.584393 1.154742
F -3.696472 2.271958 -3.430121
C 5.268760 0.043447 -0.206323
C 5.784556 -0.670483 -1.470104
C 5.734862 1.519027 -0.259678
C 5.895300 -0.646266 1.030103
H -1.187991 2.873568 -3.087846
H 0.238032 1.839650 -1.306391
H -4.555595 0.603741 -1.718672
H -2.352119 -2.107992 3.410084
H -4.730868 -2.797711 3.379414
H -6.180222 -2.192602 1.418737
H -5.272300 -0.852337 -0.417835
H 0.922512 -1.164061 -1.657432
H 3.359892 -1.128365 -1.904390
H 3.684042 1.105045 1.765225
H 1.243817 1.059716 2.007929
H 6.877687 -0.607911 -1.504841
H 5.514116 -1.732431 -1.478608
H 5.397922 -0.209859 -2.386318
H 6.827893 1.565331 -0.333712
H 5.437657 2.074725 0.635774
H 5.313202 2.032537 -1.131387
H 5.589152 -1.696857 1.090075
H 6.989401 -0.613560 0.964522
H 5.602289 -0.156149 1.964344

22 Energy:-1118.3465484

C -2.892226 1.616307 -2.564352
C -1.575844 2.069760 -2.459397
C -0.807196 1.551164 -1.423532
C -1.325451 0.571712 -0.542057
C -2.718906 0.177293 -0.613233
C -3.467869 0.712933 -1.670581
N -0.498284 -0.041930 0.380883
C -1.056257 -0.686706 1.603898
C -2.437914 -1.017772 1.553171
C -3.262451 -0.692834 0.405942
C -3.014010 -1.740091 2.636025
C -4.321792 -2.169543 2.589707
C -5.121978 -1.894425 1.444507
C -4.590230 -1.166179 0.389973
O -0.259844 -0.900725 2.522352
C 0.909504 0.017276 0.237875
C 1.501767 -0.523205 -0.919669
C 2.882974 -0.523595 -1.068616
C 3.730721 0.012643 -0.081417
C 3.117152 0.549928 1.068234
C 1.739265 0.554523 1.239740
F -3.660542 2.094089 -3.556362
C 5.260506 0.032567 -0.216315
C 5.741489 -0.600100 -1.535848
C 5.759258 1.498222 -0.171715
C 5.888608 -0.756984 0.958338
H -1.189830 2.809897 -3.149765
H 0.210973 1.894079 -1.287196
H -4.510093 0.455395 -1.812152
H -2.386536 -1.961792 3.493824
H -4.740752 -2.727572 3.422505
H -6.146607 -2.249761 1.395881
H -5.223405 -0.959337 -0.468061
H 0.869836 -0.967370 -1.682581
H 3.299635 -0.966750 -1.965474
H 3.729760 0.987765 1.850456
H 1.295907 0.986228 2.127418
H 6.835194 -0.560558 -1.582569
H 5.445410 -1.652124 -1.616329
H 5.353801 -0.065633 -2.410520
H 6.851858 1.524955 -0.259712
H 5.488068 1.994841 0.765653
H 5.337231 2.081568 -0.998040
H 5.560180 -1.802454 0.948215
H 6.982039 -0.742529 0.877577
H 5.620073 -0.328629 1.929480

23 Energy:-1118.34487532

C -2.867406 1.525601 -2.626510
C -1.577925 2.039749 -2.492604
C -0.823094 1.583519 -1.417122
C -1.325095 0.606507 -0.526131
C -2.693346 0.151060 -0.629000
C -3.430169 0.622307 -1.724780
N -0.499791 0.069674 0.452395
C -1.081161 -0.552528 1.684326
C -2.442232 -0.950282 1.589116
C -3.234996 -0.711372 0.400254
C -3.030682 -1.650651 2.681596
C -4.313757 -2.143669 2.602694
C -5.077474 -1.956898 1.416162
C -4.536574 -1.247407 0.352622
O -0.319070 -0.695579 2.644285
C 0.900411 0.083742 0.297082
C 1.466862 -0.394501 -0.905670
C 2.843444 -0.424159 -1.075810
C 3.721553 0.025278 -0.071107
C 3.137810 0.508893 1.119155
C 1.765157 0.542718 1.313754
F -3.624580 1.940403 -3.655955
C 5.247811 0.012114 -0.228914
C 5.692717 -0.558977 -1.588557
C 5.785953 1.460152 -0.111262
C 5.871153 -0.857007 0.891219
H -1.201379 2.778693 -3.189460
H 0.172652 1.978702 -1.256099
H -4.455039 0.314032 -1.890429
H -2.429724 -1.805155 3.572410
H -4.740242 -2.686117 3.442045
H -6.081375 -2.363423 1.342492
H -5.143191 -1.105539 -0.537282
H 0.814814 -0.779939 -1.682897
H 3.234023 -0.823417 -2.004445
H 3.773405 0.887931 1.913560
H 1.348522 0.940644 2.228408
H 6.786333 -0.547084 -1.649194
H 5.365751 -1.596297 -1.722576
H 5.308980 0.034009 -2.426424
H 6.877410 1.462504 -0.215310
H 5.542130 1.910429 0.856455
H 5.367826 2.099290 -0.897244
H 5.515577 -1.891655 0.828534
H 6.963238 -0.865376 0.793866
H 5.627962 -0.476372 1.888507

24 Energy:-1118.32387

C -3.019564 1.502947 -2.658683
C -1.826184 2.208535 -2.522955
C -1.006243 1.886114 -1.445731
C -1.373221 0.865561 -0.549686
C -2.621106 0.172823 -0.679520
C -3.433142 0.515246 -1.762166
N -0.521854 0.415868 0.458229
C -1.207186 0.143459 1.807031
C -2.351719 -0.686589 1.643483
C -2.990912 -0.803757 0.353603
C -2.929842 -1.353551 2.757618
C -3.995836 -2.215877 2.586165
C -4.551856 -2.419295 1.301465
C -4.062613 -1.695272 0.214965
O -0.780490 0.716380 2.816465
C 0.849986 0.354233 0.298909
C 1.390238 -0.090458 -0.940083
C 2.755770 -0.243596 -1.105675
C 3.663766 0.008172 -0.057295
C 3.111735 0.410943 1.179552
C 1.750809 0.566733 1.375189
F -3.830288 1.797610 -3.691368
C 5.180587 -0.150262 -0.208383
C 5.585823 -0.609999 -1.621516
C 5.863746 1.211616 0.074998
C 5.691176 -1.199486 0.810778
H -1.565201 2.985303 -3.232192
H -0.073692 2.418178 -1.290351
H -4.391960 0.037081 -1.926598
H -2.484378 -1.205459 3.736973
H -4.399466 -2.752087 3.441025
H -5.371172 -3.118154 1.163909
H -4.535493 -1.818502 -0.756325
H 0.715726 -0.339686 -1.751984
H 3.115827 -0.597407 -2.064631
H 3.770580 0.613777 2.018362
H 1.358097 0.884275 2.330808
H 6.675941 -0.700711 -1.676974
H 5.160181 -1.588577 -1.870765
H 5.274348 0.107056 -2.389436
H 6.951314 1.109213 -0.018533
H 5.647927 1.575855 1.084591
H 5.530774 1.973775 -0.638517
H 5.229568 -2.177039 0.631769
H 6.777514 -1.312928 0.716107
H 5.475180 -0.907510 1.843531

25 Energy:-1118.31632964

C -3.124516 1.432799 -2.707766
C -1.980422 2.219578 -2.607000
C -1.118255 1.975505 -1.539843
C -1.406311 0.956696 -0.621346
C -2.600032 0.177611 -0.712948
C -3.453753 0.436980 -1.787763
N -0.528341 0.571793 0.400164
C -1.206842 0.363820 1.765061
C -2.269545 -0.581529 1.643149
C -2.886391 -0.796437 0.356399
C -2.801286 -1.246169 2.777708
C -3.791941 -2.200927 2.633466
C -4.315236 -2.498679 1.356053
C -3.878824 -1.779026 0.244570
O -0.888403 1.104704 2.706115
C 0.825444 0.455645 0.247055
C 1.389172 0.092502 -1.011972
C 2.749092 -0.112209 -1.143201
C 3.632253 0.003882 -0.046641
C 3.057112 0.321661 1.204647
C 1.700339 0.524138 1.370442
F -3.970955 1.652399 -3.732996
C 5.143920 -0.212270 -0.166198
C 5.577163 -0.564184 -1.601799
C 5.875755 1.086292 0.259063
C 5.572544 -1.370031 0.770258
H -1.783493 2.994749 -3.338533
H -0.217271 2.567536 -1.416041
H -4.379807 -0.110024 -1.923914
H -2.380227 -1.023322 3.753923
H -4.157820 -2.735722 3.505989
H -5.072914 -3.267834 1.241184
H -4.332910 -1.975654 -0.723669
H 0.735668 -0.049188 -1.865109
H 3.128685 -0.399611 -2.116554
H 3.694635 0.414010 2.078316
H 1.291073 0.786930 2.336265
H 6.663434 -0.700625 -1.630981
H 5.118179 -1.496130 -1.950559
H 5.324926 0.231589 -2.311694
H 6.960086 0.941369 0.188041
H 5.643054 1.368936 1.290743
H 5.600360 1.923358 -0.392232
H 5.074410 -2.305279 0.491306
H 6.655238 -1.525244 0.696737
H 5.336147 -1.159839 1.818260

26 Energy:-1118.31425907

C -3.155527 1.363317 -2.756566
C -2.072076 2.231034 -2.657528
C -1.203727 2.063737 -1.578749
C -1.430392 1.042740 -0.650827
C -2.563014 0.181772 -0.736171
C -3.422130 0.361155 -1.825416
N -0.537812 0.736181 0.394106
C -1.208572 0.511035 1.753547
C -2.204005 -0.507185 1.641004
C -2.795616 -0.784472 0.353643
C -2.703856 -1.181418 2.784295
C -3.631982 -2.198367 2.652425
C -4.124425 -2.552883 1.377235
C -3.723732 -1.830316 0.255085
O -0.938968 1.285413 2.684132
C 0.800073 0.553491 0.238246
C 1.371675 0.237536 -1.032385
C 2.723035 -0.014584 -1.150585
C 3.592864 0.009907 -0.034876
C 3.011562 0.290863 1.223029
C 1.662981 0.540099 1.378195
F -4.005031 1.506846 -3.794584
C 5.095453 -0.262139 -0.144004
C 5.537893 -0.560194 -1.588976
C 5.872166 0.982478 0.357039
C 5.459967 -1.481973 0.739704
H -1.921620 3.005727 -3.400536
H -0.344967 2.716426 -1.457978
H -4.305762 -0.252355 -1.960481
H -2.305464 -0.913245 3.758650
H -3.971055 -2.738276 3.532598
H -4.831952 -3.369795 1.272250
H -4.155857 -2.074673 -0.712289
H 0.730184 0.170599 -1.902884
H 3.109720 -0.264722 -2.131243
H 3.638721 0.316730 2.108374
H 1.250815 0.781305 2.348447
H 6.617724 -0.741503 -1.608343
H 5.046385 -1.453130 -1.991259
H 5.332051 0.280193 -2.261366
H 6.950472 0.796664 0.291316
H 5.636939 1.220973 1.399189
H 5.639920 1.862267 -0.253381
H 4.930756 -2.381101 0.405007
H 6.536867 -1.676355 0.676186
H 5.212509 -1.315251 1.792879

27 Energy:-1118.31256204

C -3.162495 1.290283 -2.803707
C -2.153451 2.242589 -2.697337
C -1.290766 2.153754 -1.603576
C -1.452611 1.128142 -0.671241
C -2.513125 0.183383 -0.758106
C -3.364913 0.281323 -1.866173
N -0.548997 0.903137 0.395058
C -1.215123 0.649919 1.747492
C -2.139212 -0.433608 1.638120
C -2.696909 -0.771747 0.349026
C -2.610999 -1.117132 2.788694
C -3.471984 -2.191790 2.666944
C -3.925405 -2.600795 1.392962
C -3.556203 -1.876995 0.261973
O -0.983945 1.435765 2.679494
C 0.772173 0.651343 0.236785
C 1.350736 0.375721 -1.041880
C 2.691581 0.076128 -1.151900
C 3.546542 0.016662 -0.023885
C 2.961116 0.270613 1.238618
C 1.623184 0.568327 1.386983
F -4.003044 1.355570 -3.858507
C 5.037414 -0.312017 -0.127000
C 5.488849 -0.560758 -1.578544
C 5.857181 0.874243 0.442826
C 5.336297 -1.586227 0.703470
H -2.050865 3.018044 -3.447643
H -0.484406 2.869697 -1.478974
H -4.196571 -0.399936 -2.006603
H -2.241818 -0.805845 3.761658
H -3.787232 -2.735486 3.553647
H -4.579327 -3.462213 1.296283
H -3.959122 -2.167741 -0.705110
H 0.721988 0.378836 -1.923554
H 3.084976 -0.141390 -2.137454
H 3.577944 0.237726 2.130711
H 1.209824 0.794429 2.360302
H 6.560452 -0.785676 -1.591780
H 4.967650 -1.412913 -2.028926
H 5.328145 0.317883 -2.213240
H 6.927446 0.646250 0.380663
H 5.618010 1.072427 1.492415
H 5.670082 1.790927 -0.127367
H 4.775450 -2.445547 0.319503
H 6.404978 -1.822581 0.645212
H 5.079700 -1.458174 1.759823

28 Energy:-1118.31093582

C -3.158580 1.216875 -2.845240
C -2.226824 2.244534 -2.731995
C -1.374335 2.227269 -1.626213
C -1.471861 1.198890 -0.690803
C -2.460178 0.180900 -0.777901
C -3.299091 0.204566 -1.902359
N -0.559846 1.050242 0.391635
C -1.225646 0.774827 1.738332
C -2.081999 -0.362598 1.634644
C -2.602862 -0.758539 0.345411
C -2.527960 -1.051772 2.793344
C -3.322888 -2.176292 2.683594
C -3.736498 -2.635772 1.412316
C -3.395378 -1.914742 0.272049
O -1.022810 1.566209 2.672442
C 0.745407 0.736440 0.235240
C 1.338359 0.516206 -1.048990
C 2.668263 0.173956 -1.152877
C 3.501094 0.022921 -0.015375
C 2.906371 0.240099 1.250500
C 1.579621 0.581433 1.393284
F -3.985582 1.210757 -3.914108
C 4.979237 -0.357631 -0.113256
C 5.443164 -0.560125 -1.568050
C 5.834079 0.770377 0.520245
C 5.215740 -1.677701 0.664432
H -2.171258 3.019760 -3.487472
H -0.622659 2.999895 -1.498081
H -4.077660 -0.536163 -2.046316
H -2.188699 -0.700961 3.763700
H -3.616430 -2.720723 3.577306
H -4.338493 -3.535304 1.325863
H -3.767336 -2.248204 -0.693619
H 0.727996 0.595564 -1.939448
H 3.073373 0.000176 -2.142168
H 3.508396 0.144649 2.147913
H 1.162431 0.782921 2.370221
H 6.504898 -0.827645 -1.575811
H 4.895542 -1.369624 -2.063499
H 5.328514 0.351445 -2.165115
H 6.895440 0.503305 0.462965
H 5.586246 0.931741 1.574064
H 5.691422 1.717553 -0.011602
H 4.627669 -2.496813 0.236027
H 6.275147 -1.952697 0.608792
H 4.949658 -1.585652 1.722136

29 Energy:-1118.30962756

C -3.149807 1.137227 -2.881386
C -2.279490 2.218275 -2.770793
C -1.437478 2.260120 -1.657614
C -1.484992 1.237856 -0.712968
C -2.417938 0.169216 -0.791686
C -3.243834 0.131792 -1.927512
N -0.566651 1.154396 0.379443
C -1.235940 0.873936 1.723385
C -2.045375 -0.297308 1.635084
C -2.535719 -0.746300 0.350532
C -2.474411 -0.978002 2.806417
C -3.220922 -2.135964 2.716705
C -3.603303 -2.642417 1.452475
C -3.279930 -1.936300 0.298870
O -1.043843 1.671425 2.654426
C 0.724796 0.787021 0.229325
C 1.342917 0.644676 -1.054947
C 2.664987 0.275158 -1.154624
C 3.468799 0.026895 -0.012591
C 2.855046 0.184790 1.253778
C 1.536654 0.555281 1.392246
F -3.963766 1.072203 -3.959338
C 4.937213 -0.388279 -0.106333
C 5.423899 -0.519468 -1.561848
C 5.809363 0.676857 0.607654
C 5.121498 -1.757511 0.597169
H -2.259753 2.987010 -3.534632
H -0.729414 3.073500 -1.532997
H -3.981136 -0.650859 -2.066986
H -2.158751 -0.590849 3.770891
H -3.500584 -2.670995 3.620514
H -4.167705 -3.567410 1.382715
H -3.626926 -2.308385 -0.661958
H 0.756506 0.805509 -1.950147
H 3.089702 0.163791 -2.144538
H 3.437158 0.021527 2.154373
H 1.110038 0.715181 2.372570
H 6.476602 -0.820353 -1.565497
H 4.861466 -1.280229 -2.114599
H 5.350458 0.428939 -2.105604
H 6.863683 0.382763 0.554419
H 5.544994 0.784399 1.664272
H 5.703798 1.656657 0.128917
H 4.519654 -2.533185 0.111005
H 6.173815 -2.058567 0.543999
H 4.837816 -1.719467 1.653576

30 Energy:-1118.3084268

C -3.144042 1.050056 -2.913084
C -2.321385 2.169483 -2.815118
C -1.487571 2.263296 -1.699081
C -1.495428 1.254672 -0.739265
C -2.387132 0.150598 -0.800557
C -3.202685 0.059612 -1.942525
N -0.570201 1.228937 0.357277
C -1.241775 0.955259 1.701656
C -2.021303 -0.236273 1.637879
C -2.489646 -0.735075 0.363144
C -2.438339 -0.897481 2.825722
C -3.152008 -2.076902 2.763959
C -3.513016 -2.628436 1.511366
C -3.201175 -1.946619 0.340965
O -1.046429 1.760573 2.624935
C 0.709802 0.816854 0.214931
C 1.363095 0.770128 -1.059576
C 2.680381 0.384372 -1.154807
C 3.447939 0.031106 -0.015395
C 2.805619 0.111400 1.244862
C 1.493124 0.501701 1.378511
F -3.947848 0.933095 -3.995069
C 4.909033 -0.408398 -0.103674
C 5.430193 -0.445104 -1.552614
C 5.784228 0.582308 0.707359
C 5.045508 -1.828750 0.503062
H -2.329640 2.926482 -3.590782
H -0.814454 3.107332 -1.584734
H -3.908928 -0.753181 -2.069872
H -2.139000 -0.475621 3.780785
H -3.422550 -2.594606 3.680560
H -4.052104 -3.569823 1.464405
H -3.530533 -2.355150 -0.611221
H 0.805783 1.017948 -1.953382
H 3.132107 0.349917 -2.138293
H 3.362085 -0.126720 2.144859
H 1.050112 0.604425 2.358919
H 6.475235 -0.771473 -1.552744
H 4.864581 -1.148844 -2.173380
H 5.393441 0.542128 -2.026425
H 6.833116 0.269104 0.657230
H 5.495938 0.618191 1.762538
H 5.711008 1.596461 0.299561
H 4.439699 -2.553200 -0.052169
H 6.092139 -2.149244 0.453009
H 4.736217 -1.859988 1.552431

31 Energy:-1118.30721663

C -3.139977 0.954037 -2.941412
C -2.352234 2.100304 -2.865222
C -1.524754 2.241874 -1.749604
C -1.503795 1.254338 -0.768511
C -2.366862 0.126448 -0.804251
C -3.173819 -0.014111 -1.948679
N -0.570821 1.280084 0.327793
C -1.243434 1.025193 1.674910
C -2.007842 -0.176167 1.643951
C -2.462125 -0.723216 0.383812
C -2.417612 -0.807245 2.851406
C -3.112330 -1.998547 2.824863
C -3.460800 -2.594841 1.588450
C -3.155007 -1.946315 0.398378
O -1.037305 1.843214 2.584068
C 0.699158 0.827827 0.193014
C 1.393992 0.887592 -1.059088
C 2.709591 0.495612 -1.149339
C 3.436859 0.034489 -0.022519
C 2.758028 0.020635 1.221671
C 1.448843 0.422302 1.350282
F -3.935805 0.789025 -4.023662
C 4.893634 -0.418923 -0.104827
C 5.459927 -0.335192 -1.534775
C 5.756385 0.480468 0.818255
C 4.989409 -1.890027 0.376206
H -2.380707 2.840306 -3.656620
H -0.877954 3.108337 -1.651988
H -3.857821 -0.848294 -2.057927
H -2.127689 -0.350801 3.793393
H -3.377992 -2.491565 3.756384
H -3.985573 -3.545267 1.569805
H -3.473668 -2.390590 -0.541337
H 0.867971 1.224394 -1.942745
H 3.193499 0.548842 -2.116428
H 3.284753 -0.298589 2.114223
H 0.982649 0.450521 2.324624
H 6.499669 -0.677947 -1.532416
H 4.904368 -0.971206 -2.232848
H 5.452382 0.690834 -1.919084
H 6.802003 0.156467 0.769743
H 5.437491 0.425088 1.863725
H 5.708665 1.528337 0.502408
H 4.392169 -2.551523 -0.260847
H 6.032539 -2.222302 0.330686
H 4.645137 -2.009350 1.408238

32 Energy:-1118.30599352

C -3.139878 0.861577 -2.963718
C -2.377474 2.026531 -2.913023
C -1.554235 2.210108 -1.800559
C -1.512026 1.246360 -0.796779
C -2.355275 0.102645 -0.804183
C -3.155842 -0.081888 -1.948026
N -0.569565 1.316696 0.295183
C -1.240721 1.084105 1.645831
C -1.999425 -0.120398 1.650150
C -2.446826 -0.710479 0.407012
C -2.403134 -0.718622 2.876812
C -3.087841 -1.915474 2.886816
C -3.431428 -2.552026 1.668498
C -3.129999 -1.938547 0.459424
O -1.021254 1.916565 2.538003
C 0.691185 0.826594 0.165159
C 1.431572 1.000448 -1.049606
C 2.747077 0.606507 -1.134464
C 3.430907 0.034044 -0.032827
C 2.710681 -0.084000 1.183190
C 1.402929 0.323498 1.306539
F -3.930033 0.654112 -4.043323
C 4.885987 -0.425111 -0.107662
C 5.498496 -0.225403 -1.506691
C 5.724413 0.383726 0.916202
C 4.956232 -1.932785 0.248554
H -2.421106 2.748000 -3.720652
H -0.927560 3.093102 -1.722132
H -3.823754 -0.931405 -2.037026
H -2.116879 -0.231167 3.804288
H -3.349858 -2.382114 3.832834
H -3.948875 -3.506605 1.678983
H -3.443796 -2.414654 -0.466195
H 0.938891 1.430592 -1.911957
H 3.265774 0.753181 -2.073397
H 3.204843 -0.488829 2.059469
H 0.906985 0.264188 2.264664
H 6.534029 -0.580525 -1.501692
H 4.958880 -0.791524 -2.274038
H 5.514080 0.829925 -1.800713
H 6.768524 0.054160 0.873425
H 5.370978 0.242518 1.942297
H 5.694791 1.455144 0.689945
H 4.374498 -2.532081 -0.460320
H 5.998043 -2.269402 0.205935
H 4.580181 -2.136741 1.255929

33 Energy:-1118.3047836

C -3.146048 0.756185 -2.981849
C -2.400431 1.933168 -2.966812
C -1.578504 2.160610 -1.861543
C -1.521252 1.228751 -0.828828
C -2.352456 0.075732 -0.798710
C -3.149412 -0.154879 -1.937547
N -0.566929 1.339899 0.254052
C -1.233322 1.141694 1.610323
C -1.994004 -0.060016 1.659628
C -2.441190 -0.694651 0.438508
C -2.392714 -0.616066 2.907832
C -3.074618 -1.813096 2.961614
C -3.419261 -2.492625 1.766453
C -3.121375 -1.922155 0.536021
O -1.005011 2.000844 2.473984
C 0.687547 0.818478 0.125618
C 1.476774 1.112580 -1.033141
C 2.794734 0.722474 -1.109129
C 3.431286 0.034149 -0.048018
C 2.662472 -0.203401 1.120905
C 1.354246 0.204779 1.236707
F -3.933309 0.504688 -4.054542
C 4.886394 -0.425943 -0.111577
C 5.557147 -0.083686 -1.455081
C 5.685007 0.262302 1.026038
C 4.935188 -1.963605 0.084647
H -2.455006 2.629879 -3.795210
H -0.966062 3.055541 -1.810551
H -3.806326 -1.015336 -1.999435
H -2.104741 -0.096171 3.816990
H -3.333673 -2.246981 3.923862
H -3.934588 -3.447370 1.811653
H -3.435316 -2.432040 -0.371354
H 1.019537 1.638235 -1.861730
H 3.351684 0.968995 -2.004226
H 3.119242 -0.703490 1.967718
H 0.819153 0.040819 2.161288
H 6.590168 -0.445993 -1.445625
H 5.047644 -0.560261 -2.299889
H 5.588960 0.996800 -1.633674
H 6.729025 -0.068112 0.988855
H 5.291011 0.013794 2.016346
H 5.667485 1.351969 0.915431
H 4.382954 -2.479216 -0.708572
H 5.976631 -2.302330 0.051434
H 4.514447 -2.270397 1.047291

34 Energy:-1118.30392108

C -3.157155 0.640022 -2.995569
C -2.415891 1.819519 -3.026253
C -1.593492 2.090789 -1.931356
C -1.532043 1.200648 -0.862726
C -2.360986 0.046968 -0.787140
C -3.156509 -0.230001 -1.917134
N -0.564897 1.349963 0.207005
C -1.220531 1.190777 1.570852
C -1.990863 -0.000691 1.671901
C -2.447894 -0.676845 0.477079
C -2.383219 -0.508315 2.942605
C -3.071388 -1.698604 3.044610
C -3.427139 -2.419087 1.876692
C -3.133780 -1.896512 0.624199
O -0.984789 2.083909 2.396991
C 0.689694 0.810135 0.077461
C 1.529709 1.232260 -1.001089
C 2.851120 0.846832 -1.065523
C 3.437093 0.036344 -0.065885
C 2.615379 -0.331340 1.032338
C 1.305005 0.073850 1.138392
F -3.943925 0.344361 -4.057372
C 4.893130 -0.422407 -0.116398
C 5.625844 0.072967 -1.377193
C 5.638429 0.119737 1.131050
C 4.930530 -1.972863 -0.103382
H -2.473666 2.484318 -3.880230
H -0.984978 2.989523 -1.915826
H -3.809228 -1.095344 -1.946408
H -2.085595 0.042521 3.830261
H -3.326734 -2.095827 4.023489
H -3.947191 -3.368728 1.959954
H -3.455951 -2.438585 -0.261324
H 1.110549 1.860326 -1.777344
H 3.448624 1.197666 -1.897430
H 3.031776 -0.933670 1.832207
H 0.725068 -0.199662 2.009157
H 6.657130 -0.294162 -1.363561
H 5.155673 -0.296641 -2.295197
H 5.666348 1.166814 -1.424270
H 6.682281 -0.212263 1.104156
H 5.197070 -0.241181 2.065213
H 5.628621 1.214957 1.150042
H 4.414710 -2.385991 -0.977018
H 5.971874 -2.312453 -0.129315
H 4.465376 -2.389487 0.795447

35 Energy:-1118.30411319

C -3.174569 0.497772 -3.005182
C -2.418749 1.664790 -3.097754
C -1.594499 1.982762 -2.017398
C -1.546072 1.152676 -0.900247
C -2.389729 0.013043 -0.765679
C -3.184723 -0.314318 -1.882178
N -0.565813 1.338193 0.149387
C -1.198689 1.223353 1.525322
C -1.992784 0.056991 1.689393
C -2.477691 -0.656396 0.528307
C -2.377755 -0.389349 2.984828
C -3.089009 -1.559949 3.143750
C -3.473746 -2.319217 2.010264
C -3.185789 -1.854570 0.733457
O -0.945688 2.156511 2.301237
C 0.703205 0.806761 0.019096
C 1.593430 1.367211 -0.944351
C 2.919966 0.987738 -0.994099
C 3.452835 0.046465 -0.087066
C 2.575072 -0.464320 0.905532
C 1.260376 -0.065947 0.999545
F -3.962374 0.154435 -4.050827
C 4.910473 -0.410939 -0.123528
C 5.712409 0.260044 -1.254238
C 5.585573 -0.066147 1.229197
C 4.947534 -1.946237 -0.339368
H -2.467493 2.283863 -3.985936
H -0.975201 2.873350 -2.049476
H -3.843040 -1.175738 -1.870162
H -2.056303 0.190600 3.845257
H -3.340246 -1.911746 4.140840
H -4.011509 -3.253905 2.138181
H -3.530802 -2.426278 -0.124261
H 1.214201 2.103800 -1.642501
H 3.559205 1.448959 -1.736397
H 2.948099 -1.178022 1.632073
H 0.632748 -0.453505 1.791369
H 6.742122 -0.111502 -1.236767
H 5.295873 0.032528 -2.241775
H 5.752784 1.348688 -1.137167
H 6.629524 -0.398585 1.210844
H 5.093568 -0.557937 2.074122
H 5.574237 1.014206 1.410050
H 4.483750 -2.220428 -1.293218
H 5.988554 -2.287785 -0.355193
H 4.429929 -2.487373 0.458875

36 Energy:-1118.3473684

C -3.034141 -0.079622 -2.943213
C -1.673812 -0.298454 -3.186696
C -0.840128 -0.415597 -2.082630
C -1.344838 -0.275065 -0.763404
C -2.773209 -0.114755 -0.528159
C -3.586607 -0.003560 -1.663917
N -0.486359 -0.226824 0.309182
C -0.954317 -0.551343 1.683076
C -2.353705 -0.434155 1.906106
C -3.269983 -0.111490 0.828561
C -2.862772 -0.583512 3.225083
C -4.198839 -0.384616 3.499128
C -5.095256 -0.021095 2.453956
C -4.625812 0.101182 1.154064
O -0.077262 -0.869843 2.490520
C 0.928559 -0.149913 0.102480
C 1.499456 1.087664 -0.212698
C 2.879866 1.201419 -0.369130
C 3.730504 0.094724 -0.211796
C 3.131196 -1.136404 0.114908
C 1.756186 -1.266300 0.280412
F -3.861244 0.037958 -3.991800
C 5.256917 0.184870 -0.378885
C 5.724794 1.609433 -0.731932
C 5.943861 -0.236587 0.942656
C 5.704905 -0.766702 -1.514715
H -1.303815 -0.384715 -4.201192
H 0.217124 -0.601693 -2.221880
H -4.657877 0.130373 -1.581735
H -2.165658 -0.840663 4.016764
H -4.567800 -0.496775 4.514837
H -6.143772 0.157165 2.671026
H -5.329457 0.370700 0.371756
H 0.860970 1.959265 -0.322062
H 3.288210 2.177158 -0.605148
H 3.748664 -2.019891 0.246715
H 1.319120 -2.224717 0.536967
H 6.814797 1.619532 -0.841324
H 5.294461 1.958471 -1.677512
H 5.464728 2.330761 0.051037
H 7.033770 -0.182977 0.834282
H 5.687237 -1.261997 1.228248
H 5.650694 0.425578 1.765288
H 5.240174 -0.486882 -2.467203
H 6.793118 -0.717405 -1.640178
H 5.440546 -1.808154 -1.303688

37 Energy:-1118.35426345

C -3.015167 -0.320321 -2.944000
C -1.633732 -0.270270 -3.176447
C -0.800716 -0.200753 -2.061355
C -1.333997 -0.181133 -0.749281
C -2.781368 -0.238008 -0.521572
C -3.591590 -0.306387 -1.677469
N -0.492374 -0.105095 0.337616
C -0.951747 -0.097141 1.716893
C -2.371312 -0.156913 1.930966
C -3.290467 -0.223560 0.811626
C -2.864258 -0.148016 3.249434
C -4.223500 -0.200267 3.508073
C -5.139681 -0.264187 2.418185
C -4.682786 -0.275280 1.116982
O -0.081322 -0.038348 2.586243
C 0.938492 -0.041471 0.148239
C 1.567683 1.192899 0.012718
C 2.953051 1.248505 -0.160961
C 3.734956 0.085273 -0.205483
C 3.068199 -1.146008 -0.068666
C 1.688276 -1.217889 0.105427
F -3.834250 -0.386617 -4.005260
C 5.262728 0.113257 -0.391787
C 5.809691 1.546566 -0.530729
C 5.939715 -0.546353 0.833640
C 5.638786 -0.673645 -1.670175
H -1.244513 -0.285718 -4.187021
H 0.271594 -0.159907 -2.195720
H -4.670572 -0.350112 -1.609313
H -2.146151 -0.098392 4.062320
H -4.589267 -0.192557 4.530128
H -6.207713 -0.304677 2.612309
H -5.408013 -0.324902 0.311135
H 0.981249 2.105984 0.049054
H 3.415503 2.223681 -0.259298
H 3.631540 -2.073854 -0.094843
H 1.194156 -2.178629 0.213492
H 6.896840 1.511827 -0.661575
H 5.388415 2.062217 -1.401246
H 5.603400 2.150970 0.359810
H 7.029444 -0.539193 0.711668
H 5.625483 -1.587296 0.963009
H 5.696848 -0.004299 1.754737
H 5.177869 -0.224386 -2.557462
H 6.726138 -0.665890 -1.811471
H 5.317632 -1.719158 -1.616412

12.2.6 Computed CT emission energies of compound 4b (B3LYP/6-31G* PCM CH_2Cl_2)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.9127 eV 648.22 nm f=0.0470 <S**2>=0.000
91 -> 92 0.70478
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1118.23951628
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1824 eV 389.60 nm f=0.0109 <S**2>=0.000
90 -> 92 -0.25490
91 -> 93 0.65333

Excited State 3: Singlet-A 3.2414 eV 382.50 nm f=0.0390 <S**2>=0.000
86 -> 92 -0.12675
88 -> 92 -0.14186
90 -> 92 0.61658
91 -> 93 0.26056

Excited State 4: Singlet-A 3.6103 eV 343.41 nm f=0.0164 <S**2>=0.000
88 -> 92 -0.12574
89 -> 92 0.67128
90 -> 92 -0.12053

Excited State 5: Singlet-A 3.7648 eV 329.32 nm f=0.0615 <S**2>=0.000
86 -> 92 0.19694
88 -> 92 0.61264
89 -> 92 0.18531
90 -> 92 0.14326

Excited State 6: Singlet-A 4.0368 eV 307.13 nm f=0.0867 <S**2>=0.000
91 -> 94 0.68666

12.2.7 Computed excitations energies of the triplet state of compound 4b (B3LYP/6-31G* PCM CH_2Cl_2)

Excitation energies and oscillator strengths:

Excited State 1: Triplet-A 3.0101 eV 411.89 nm f=0.0000 <S**2>=2.000
85 -> 97 0.10588
87 -> 93 0.16727
90 -> 92 -0.30618
90 -> 93 0.10126
91 -> 92 0.54174
91 -> 93 -0.17152
91 -> 96 -0.10978
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1118.25159796
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A 3.3244 eV 372.96 nm f=0.0000 <S**2>=2.000
90 -> 92 0.34424
90 -> 93 -0.12593
90 -> 96 0.12796
91 -> 92 0.41257
91 -> 93 0.34429
91 -> 96 0.17954

Excited State 3: Triplet-A 3.6419 eV 340.43 nm f=0.0000 <S**2>=2.000
87 -> 92 0.11976
90 -> 92 -0.38699
91 -> 93 0.53484

Excited State 4: Triplet-A 3.7162 eV 333.63 nm f=0.0000 <S**2>=2.000
88 -> 94 -0.15064
88 -> 95 -0.37838
89 -> 94 0.50678
89 -> 95 -0.14426

Excited State 5: Triplet-A 3.7925 eV 326.92 nm f=0.0000 <S**2>=2.000
85 -> 92 -0.17018
87 -> 92 0.20686
87 -> 93 0.45692
88 -> 93 0.15014
90 -> 96 0.15852
90 -> 97 0.11589
91 -> 92 -0.11493
91 -> 96 0.26925
91 -> 97 -0.14285

Excited State 6: Triplet-A 4.1868 eV 296.13 nm f=0.0000 <S**2>=2.000
87 -> 92 -0.26373
87 -> 93 -0.20543
88 -> 92 -0.10769
90 -> 92 -0.26679
90 -> 93 0.16290
90 -> 96 0.12045
91 -> 96 0.47424

Excited State 7: Triplet-A 4.2503 eV 291.71 nm f=0.0000 <S**2>=2.000
86 -> 92 0.43003
86 -> 93 0.40480
86 -> 98 -0.12791
89 -> 92 0.27763
89 -> 93 0.19799

Excited State 8: Triplet-A 4.3134 eV 287.44 nm f=0.0000 <S**2>=2.000

84 -> 92 0.10730
85 -> 92 0.10157
85 -> 93 0.10470
87 -> 92 -0.29051
87 -> 93 0.11311
88 -> 93 0.10127
90 -> 92 0.16063
90 -> 93 0.48461
90 -> 96 -0.12845
91 -> 93 0.14713
91 -> 96 -0.12897

Excited State 9: Triplet-A 4.4802 eV 276.74 nm f=0.0000 <S**2>=2.000
85 -> 92 0.26727
87 -> 92 0.41218
87 -> 93 -0.15043
88 -> 92 0.19432
90 -> 93 0.29055
90 -> 96 -0.10981
90 -> 97 -0.14745
91 -> 96 0.19142
91 -> 97 0.10545

Excited State 10: Triplet-A 4.5941 eV 269.87 nm f=0.0000 <S**2>=2.000
86 -> 92 -0.12861
88 -> 94 -0.23123
88 -> 95 0.11180
89 -> 92 0.41837
89 -> 93 -0.11936
89 -> 94 0.11674
89 -> 95 0.42202

Excited State 11: Triplet-A 4.6513 eV 266.56 nm f=0.0000 <S**2>=2.000
87 -> 95 -0.10184
88 -> 92 0.19652
88 -> 94 0.21348
88 -> 95 0.41499
89 -> 94 0.40269
89 -> 95 -0.14951

Excited State 12: Triplet-A 4.6753 eV 265.19 nm f=0.0000 <S**2>=2.000
85 -> 92 0.31921
85 -> 93 -0.14746
87 -> 92 -0.20030
87 -> 93 0.31902
90 -> 93 -0.23199
90 -> 96 -0.22013
90 -> 97 -0.15790

91 -> 95 0.11461
91 -> 96 0.19776
91 -> 97 0.15316

Excited State 13: Triplet-A 4.7898 eV 258.85 nm f=0.0000 <S**2>=2.000
86 -> 92 -0.14471
86 -> 93 -0.15536
88 -> 94 0.26511
88 -> 95 -0.15036
89 -> 92 0.45980
89 -> 94 -0.11786
89 -> 95 -0.24099
91 -> 94 -0.21200

Excited State 14: Triplet-A 4.8417 eV 256.08 nm f=0.0000 <S**2>=2.000
89 -> 92 0.13334
89 -> 95 -0.14126
91 -> 94 0.64517
91 -> 95 -0.12366

Excited State 15: Triplet-A 5.0099 eV 247.48 nm f=0.0000 <S**2>=2.000
86 -> 92 0.17722
88 -> 92 0.21605
88 -> 94 0.12382
89 -> 93 -0.26066
91 -> 94 0.10570
91 -> 95 0.51079
91 -> 96 -0.13520

12.2.8 Computed emission energies of the triplet state of compound 4b (B3LYP/6-31G* PCM CH_2Cl_2)

Excitation energies and oscillator strengths:
Excited State 1: Triplet-A 2.3456 eV 528.58 nm f=0.0000 <S**2>=2.000
85 -> 97 0.10152
86 -> 93 -0.10479
90 -> 92 0.21212
91 -> 92 0.64939
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1118.26327667
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A 3.1828 eV 389.55 nm f=0.0000 <S**2>=2.000
90 -> 92 0.51628
90 -> 96 0.10895
91 -> 92 -0.24662
91 -> 93 -0.37147

Excited State 3: Triplet-A 3.4247 eV 362.02 nm f=0.0000 <S**2>=2.000
86 -> 92 -0.10597
90 -> 92 0.38090
91 -> 93 0.56566

Excited State 4: Triplet-A 3.7138 eV 333.84 nm f=0.0000 <S**2>=2.000
87 -> 94 -0.10541
88 -> 94 -0.15823
88 -> 95 -0.39476
89 -> 94 0.51011
89 -> 95 -0.14091

Excited State 5: Triplet-A 3.8304 eV 323.68 nm f=0.0000 <S**2>=2.000
85 -> 92 -0.29762
86 -> 93 0.42297
88 -> 93 0.10492
90 -> 93 0.17288
90 -> 96 0.19446
90 -> 97 -0.11426
91 -> 96 -0.19399
91 -> 97 -0.26091

Excited State 6: Triplet-A 4.1438 eV 299.20 nm f=0.0000 <S**2>=2.000
86 -> 92 0.56717
86 -> 93 0.22538
88 -> 92 0.12676
90 -> 92 0.10113
90 -> 93 -0.13560
91 -> 96 0.21941

Excited State 7: Triplet-A 4.2011 eV 295.12 nm f=0.0000 <S**2>=2.000
87 -> 92 0.33901
87 -> 93 0.33818
89 -> 92 0.46325
89 -> 93 0.18248

Excited State 8: Triplet-A 4.2538 eV 291.46 nm f=0.0000 <S**2>=2.000
85 -> 92 -0.14720
86 -> 92 -0.29560
86 -> 93 0.13705
88 -> 92 -0.10011
90 -> 93 -0.11847
90 -> 96 -0.15604
91 -> 95 0.10710
91 -> 96 0.51774

Excited State 9: Triplet-A 4.3538 eV 284.77 nm f=0.0000 <S**2>=2.000
84 -> 92 0.14885

85 -> 92 0.33692
86 -> 93 0.29478
88 -> 93 0.10826
90 -> 93 0.34765
90 -> 96 -0.21878
90 -> 97 0.12630
91 -> 97 0.13236
91 -> 98 -0.13384

Excited State 10: Triplet-A 4.4017 eV 281.67 nm f=0.0000 <S**2>=2.000
87 -> 92 -0.29994
87 -> 93 -0.30306
89 -> 92 0.50040
89 -> 93 -0.13691
89 -> 95 0.16320

Excited State 11: Triplet-A 4.4843 eV 276.49 nm f=0.0000 <S**2>=2.000
85 -> 92 -0.17709
86 -> 92 0.16285
86 -> 93 -0.30684
90 -> 93 0.48243
91 -> 95 0.10124
91 -> 96 0.20630
91 -> 97 -0.14723

Excited State 12: Triplet-A 4.5892 eV 270.16 nm f=0.0000 <S**2>=2.000
86 -> 92 -0.12169
88 -> 92 0.47837
88 -> 94 0.16095
88 -> 95 0.28637
89 -> 94 0.32158
89 -> 95 -0.13908

Excited State 13: Triplet-A 4.6967 eV 263.98 nm f=0.0000 <S**2>=2.000
87 -> 93 0.11525
88 -> 94 -0.31357
88 -> 95 0.13418
89 -> 92 -0.14496
89 -> 94 0.13570
89 -> 95 0.40627
90 -> 94 0.11614
91 -> 94 -0.34937

Excited State 14: Triplet-A 4.7226 eV 262.54 nm f=0.0000 <S**2>=2.000
87 -> 92 -0.14369
87 -> 93 0.14233
88 -> 94 -0.16691
89 -> 95 0.23726

91 -> 94 0.56854

Excited State 15: Triplet-A 4.7427 eV 261.42 nm f=0.0000 <S**2>=2.000
87 -> 92 0.49202
87 -> 93 -0.30361
88 -> 92 0.10807
88 -> 94 -0.13271
89 -> 93 -0.27570
89 -> 95 0.14119
91 -> 94 0.14229

12.3 Quantum chemical calculation data of 5-(4-(*tert*-Butyl)phenyl)-2-fluoro-[1,3]dioxolo[4,5-j]phenanthridin-6(5*H*)-one (5b)

12.3.1 Computed xyz-coordinates of compound 5b (B3LYP/6-31G* PCM CH_2Cl_2)

C	-1.410243	3.870927	-0.002967
C	-0.029083	3.698394	0.003153
C	0.478388	2.40664	0.008594
C	-0.379107	1.290882	0.007812
C	-1.784442	1.480918	0.001308
C	-2.279586	2.799637	-0.003903
N	0.154431	-0.011324	0.013327
C	-0.625167	-1.166645	0.01141
C	-2.085284	-0.973382	0.00545
C	-2.665169	0.313913	0.000234
C	-2.875991	-2.148834	0.004769
C	-4.236665	-1.989939	-0.001143
C	-4.823517	-0.717121	-0.006537
C	-4.080093	0.437503	-0.006033
C	1.587173	-0.203402	0.018873
O	-0.097695	-2.281387	0.014677
F	-1.916235	5.127129	-0.008149
C	2.27709	-0.291909	1.224838
C	3.662209	-0.474283	1.224679
C	4.389239	-0.571697	0.029501
C	3.665906	-0.4779	-1.173505
C	2.285361	-0.296491	-1.186251
O	-5.214474	-2.947407	-0.002845
C	-6.468379	-2.248079	-0.011378
O	-6.182641	-0.837545	-0.011859
C	5.915207	-0.771921	-0.006473
C	6.528125	-0.858736	1.404111
C	6.571037	0.418683	-0.74629
C	6.243478	-2.084716	-0.757222
H	0.628777	4.560687	0.003635
H	1.550457	2.259064	0.013614
H	-3.343232	3.002552	-0.008706
H	-2.395247	-3.118822	0.008846
H	-4.576908	1.399053	-0.010459
H	1.733904	-0.221408	2.162679
H	4.168785	-0.541354	2.180523
H	4.184896	-0.548838	-2.124762
H	1.747109	-0.229425	-2.127155
H	-7.024485	-2.504791	-0.917888
H	-7.035145	-2.501992	0.889246
H	6.124142	-1.703409	1.973611
H	7.611381	-1.001927	1.324139
H	6.357714	0.057329	1.981112

H	6.207523	0.51043	-1.775204
H	7.658757	0.285529	-0.787197
H	6.3637	1.363336	-0.230277
H	7.328842	-2.236831	-0.794728
H	5.796271	-2.947994	-0.251227
H	5.87341	-2.070011	-1.787718
C	-1.410243	3.870927	-0.002967
C	-0.029083	3.698394	0.003153
C	0.478388	2.40664	0.008594
C	-0.379107	1.290882	0.007812
C	-1.784442	1.480918	0.001308
C	-2.279586	2.799637	-0.003903
N	0.154431	-0.011324	0.013327
C	-0.625167	-1.166645	0.01141
C	-2.085284	-0.973382	0.00545
C	-2.665169	0.313913	0.000234
C	-2.875991	-2.148834	0.004769
C	-4.236665	-1.989939	-0.001143
C	-4.823517	-0.717121	-0.006537
C	-4.080093	0.437503	-0.006033
C	1.587173	-0.203402	0.018873

SCF Done: E(RB3LYP) = -1306.89399943 A.U. after 15 cycles

Zero-point correction = 0.388088 (Hartree/Particle)

Thermal correction to Energy = 0.412225

Thermal correction to Enthalpy = 0.413170

Thermal correction to Gibbs Free Energy = 0.332730

Sum of electronic and zero-point Energies = -1306.505912

Sum of electronic and thermal Energies = -1306.481774

Sum of electronic and thermal Enthalpies = -1306.480830

Sum of electronic and thermal Free Energies = -1306.561270

12.3.2 Computed excitations energies of compound 5b (B3LYP/6-31G* PCM CH_2Cl_2)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.8837 eV 319.24 nm f=0.2547 <S**2>=0.000
101 ->103 -0.12483
101 ->104 0.15190
102 ->103 0.66866
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1306.75127474
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 4.1247 eV 300.59 nm f=0.0114 <S**2>=0.000
99 ->103 -0.15872

101 ->103 -0.45287
102 ->104 0.50483

Excited State 3: Singlet-A 4.3309 eV 286.28 nm f=0.1849 <S**2>=0.000
99 ->103 -0.17901
101 ->103 0.49478
102 ->103 0.10048
102 ->104 0.40324
102 ->107 -0.14422

Excited State 4: Singlet-A 4.6111 eV 268.88 nm f=0.0021 <S**2>=0.000
97 ->103 0.36078
97 ->104 0.24410
100 ->103 0.51405
100 ->104 0.16493

Excited State 5: Singlet-A 4.6194 eV 268.40 nm f=0.1603 <S**2>=0.000
99 ->103 -0.23227
101 ->104 0.62038
102 ->103 -0.15040
102 ->104 -0.13756

Excited State 6: Singlet-A 4.7659 eV 260.15 nm f=0.0006 <S**2>=0.000
101 ->105 -0.22574
102 ->105 0.65652

Excited State 7: Singlet-A 4.8598 eV 255.12 nm f=0.0003 <S**2>=0.000
97 ->103 -0.41837
97 ->104 -0.26062
100 ->103 0.47480
100 ->104 -0.12388

Excited State 8: Singlet-A 4.9348 eV 251.25 nm f=0.0154 <S**2>=0.000
99 ->103 -0.15076
101 ->106 -0.17984
102 ->105 0.10066
102 ->106 0.64876

Excited State 9: Singlet-A 5.0155 eV 247.20 nm f=0.5248 <S**2>=0.000
98 ->103 0.12215
99 ->103 0.46831
101 ->104 0.19946
102 ->104 0.17832
102 ->106 0.15592
102 ->107 0.35771

Excited State 10: Singlet-A 5.0728 eV 244.41 nm f=0.0712 <S**2>=0.000
98 ->103 0.68581

Excited State 11: Singlet-A 5.1538 eV 240.57 nm f=0.1814 <S**2>=0.000
99 ->103 -0.34566
99 ->104 -0.10225
100 ->104 0.12441
101 ->104 -0.15840
102 ->107 0.51241
102 ->108 -0.11447

Excited State 12: Singlet-A 5.1572 eV 240.41 nm f=0.0075 <S**2>=0.000
97 ->103 -0.35225
97 ->104 0.20599
100 ->104 0.54349
102 ->107 -0.11830

Excited State 13: Singlet-A 5.2368 eV 236.76 nm f=0.0033 <S**2>=0.000
101 ->105 0.64714
102 ->105 0.22651

Excited State 14: Singlet-A 5.3579 eV 231.41 nm f=0.0010 <S**2>=0.000
97 ->103 -0.19109
97 ->104 0.45115
98 ->105 0.26729
100 ->104 -0.25175
100 ->105 0.10049
100 ->106 0.27447
101 ->106 0.10500

Excited State 15: Singlet-A 5.3863 eV 230.19 nm f=0.0008 <S**2>=0.000
97 ->104 -0.11751
99 ->104 -0.17382
101 ->106 0.62518
102 ->106 0.17850

12.3.3 Computed emission energies of compound 5b (B3LYP/6-31G* PCM CH_2Cl_2)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.2457 eV 382.00 nm f=0.2638 <S**2>=0.000
102 ->103 0.68944
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1306.76038558
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.6822 eV 336.72 nm f=0.0717 <S**2>=0.000
101 ->103 0.59994
102 ->104 -0.34893

Excited State 3: Singlet-A 3.9264 eV 315.77 nm f=0.1130 <S**2>=0.000

99 ->103 0.12522
101 ->103 0.31813
102 ->104 0.58161
102 ->105 -0.11697

Excited State 4: Singlet-A 4.2050 eV 294.85 nm f=0.0489 <S**2>=0.000
97 ->103 0.18363
98 ->103 0.35434
100 ->103 0.32774
101 ->104 0.44586

Excited State 5: Singlet-A 4.2749 eV 290.03 nm f=0.0824 <S**2>=0.000
97 ->103 -0.22253
99 ->103 0.38299
100 ->103 -0.36175
101 ->104 0.34877
102 ->105 0.11137

Excited State 6: Singlet-A 4.4028 eV 281.61 nm f=0.0172 <S**2>=0.000
97 ->103 -0.15144
98 ->103 -0.29262
99 ->103 0.37202
100 ->103 0.47391

12.3.4 Potential scan of compound 5b ground state (B3LYP/6-31G* PCM CH_2Cl_2)

D(4,7,15,18)
0 -1306.89399943 89.9445
8 -1306.89382614 99.9444
13 -1306.89331088 109.9445
18 -1306.89238581 119.9444
23 -1306.89090604 129.9444
27 -1306.88870497 139.9443
32 -1306.8855944 149.9443
38 -1306.88154428 159.9444
49 -1306.87726563 169.9444
54 -1306.87347219 179.9443
59 -1306.87035239 -170.0556
65 -1306.86805809 -160.0557
71 -1306.86685238 -150.0555
86 -1306.88867426 -140.0554
90 -1306.89087476 -130.0554
95 -1306.89234323 -120.0554
99 -1306.89327627 -110.0555
103 -1306.89380241 -100.0554
108 -1306.8940003 -90.0555
114 -1306.89382569 -80.0556
119 -1306.89326886 -70.0556

125 -1306.89226914 -60.0556
131 -1306.89063978 -50.0556
137 -1306.88825423 -40.0556
142 -1306.88500122 -30.0557
150 -1306.8809055 -20.0557
156 -1306.87643617 -10.0556
163 -1306.87246673 -0.0556
169 -1306.86940084 9.9444
176 -1306.86743765 19.9444
201 -1306.88495076 29.9445
206 -1306.88821583 39.9446
210 -1306.89061252 49.9446
215 -1306.89224062 59.9446
219 -1306.89327076 69.9446
223 -1306.89381672 79.9446
228 -1306.89399056 89.9445

Progress of structural optimization and emission calculation

-1306.893999
-1306.893695
-1306.893805
-1306.893815
-1306.893822
-1306.893825
-1306.893826
-1306.893826
-1306.893826
-1306.893195
-1306.89331
-1306.893311
-1306.893311
-1306.893311
-1306.892268
-1306.892384
-1306.892386
-1306.892386
-1306.892386
-1306.890777
-1306.890902
-1306.890905
-1306.890906
-1306.890906
-1306.888526
-1306.888699
-1306.888704
-1306.888705
-1306.885289
-1306.885578

-1306.885593
-1306.885594
-1306.885594
-1306.881091
-1306.881485
-1306.881537
-1306.881544
-1306.881544
-1306.881544
-1306.876368
-1306.877125
-1306.877246
-1306.877259
-1306.877262
-1306.877262
-1306.877264
-1306.877265
-1306.877265
-1306.877266
-1306.877266
-1306.872586
-1306.87337
-1306.873468
-1306.873472
-1306.873472
-1306.869456
-1306.870315
-1306.870351
-1306.870352
-1306.870352
-1306.867138
-1306.86801
-1306.868055
-1306.868058
-1306.868058
-1306.868058
-1306.86582
-1306.866739
-1306.866839
-1306.86685
-1306.866852
-1306.866852
-1306.865988
-1306.867385
-1306.86871
-1306.868561
-1306.877175
-1306.882306

-1306.8748
-1306.887042
-1306.888008
-1306.888569
-1306.888652
-1306.888671
-1306.888674
-1306.888674
-1306.888674
-1306.890707
-1306.890868
-1306.890874
-1306.890875
-1306.892212
-1306.89234
-1306.892343
-1306.892343
-1306.892343
-1306.893161
-1306.893273
-1306.893276
-1306.893276
-1306.893686
-1306.8938
-1306.893802
-1306.893802
-1306.893863
-1306.893995
-1306.893999
-1306.894
-1306.894
-1306.893688
-1306.893823
-1306.893825
-1306.893826
-1306.893826
-1306.893826
-1306.893082
-1306.893266
-1306.893269
-1306.893269
-1306.893269
-1306.892038
-1306.892261
-1306.892269
-1306.892269
-1306.892269
-1306.892269

-1306.890355
-1306.890627
-1306.890639
-1306.89064
-1306.89064
-1306.89064
-1306.887889
-1306.888231
-1306.888254
-1306.888254
-1306.888254
-1306.888254
-1306.884569
-1306.884957
-1306.885
-1306.885001
-1306.885001
-1306.880299
-1306.880825
-1306.880887
-1306.880902
-1306.880905
-1306.880905
-1306.880905
-1306.880906
-1306.875555
-1306.876308
-1306.876419
-1306.876435
-1306.876436
-1306.876436
-1306.871282
-1306.872339
-1306.872438
-1306.872463
-1306.872466
-1306.872467
-1306.872467
-1306.868333
-1306.869287
-1306.86938
-1306.869399
-1306.869401
-1306.869401
-1306.866424
-1306.867317
-1306.867411
-1306.867435

-1306.867437
-1306.867438
-1306.867438
-1306.865984
-1306.866887
-1306.867093
-1306.867387
-1306.867604
-1306.662881
-1306.866165
-1306.86775
-1306.866168
-1306.772278
-1306.78212
-1306.868047
-1306.803526
-1306.871795
-1306.873924
-1306.873067
-1306.880097
-1306.878796
-1306.883171
-1306.884256
-1306.884863
-1306.884927
-1306.884948
-1306.884951
-1306.884951
-1306.887853
-1306.888191
-1306.888215
-1306.888216
-1306.888216
-1306.890305
-1306.8906
-1306.890612
-1306.890613
-1306.891983
-1306.892229
-1306.89224
-1306.892241
-1306.892241
-1306.893071
-1306.893267
-1306.893271
-1306.893271
-1306.893646
-1306.893815

-1306.893817
-1306.893817
-1306.893828
-1306.893988
-1306.89399
-1306.893991

Geometries of structural optimization

1 Energy:-1306.89399943
C -1.410243 3.870927 -0.002967
C -0.029083 3.698394 0.003153
C 0.478388 2.406640 0.008594
C -0.379107 1.290882 0.007812
C -1.784442 1.480918 0.001308
C -2.279586 2.799637 -0.003903
N 0.154431 -0.011324 0.013327
C -0.625167 -1.166645 0.011410
C -2.085284 -0.973382 0.005450
C -2.665169 0.313913 0.000234
C -2.875991 -2.148834 0.004769
C -4.236665 -1.989939 -0.001143
C -4.823517 -0.717121 -0.006537
C -4.080093 0.437503 -0.006033
C 1.587173 -0.203402 0.018873
O -0.097695 -2.281387 0.014677
F -1.916235 5.127129 -0.008149
C 2.277090 -0.291909 1.224838
C 3.662209 -0.474283 1.224679
C 4.389239 -0.571697 0.029501
C 3.665906 -0.477900 -1.173505
C 2.285361 -0.296491 -1.186251
O -5.214474 -2.947407 -0.002845
C -6.468379 -2.248079 -0.011378
O -6.182641 -0.837545 -0.011859
C 5.915207 -0.771921 -0.006473
C 6.528125 -0.858736 1.404111
C 6.571037 0.418683 -0.746290
C 6.243478 -2.084716 -0.757222
H 0.628777 4.560687 0.003635
H 1.550457 2.259064 0.013614
H -3.343232 3.002552 -0.008706
H -2.395247 -3.118822 0.008846
H -4.576908 1.399053 -0.010459
H 1.733904 -0.221408 2.162679
H 4.168785 -0.541354 2.180523
H 4.184896 -0.548838 -2.124762

H 1.747109 -0.229425 -2.127155
H -7.024485 -2.504791 -0.917888
H -7.035145 -2.501992 0.889246
H 6.124142 -1.703409 1.973611
H 7.611381 -1.001927 1.324139
H 6.357714 0.057329 1.981112
H 6.207523 0.510430 -1.775204
H 7.658757 0.285529 -0.787197
H 6.363700 1.363336 -0.230277
H 7.328842 -2.236831 -0.794728
H 5.796271 -2.947994 -0.251227
H 5.873410 -2.070011 -1.787718

2 Energy:-1306.89382614
C -1.421371 3.874030 -0.156736
C -0.040566 3.708718 -0.097978
C 0.470864 2.420975 -0.019118
C -0.381776 1.301513 -0.002020
C -1.787122 1.484898 -0.052408
C -2.286450 2.799608 -0.133296
N 0.156563 0.003565 0.081861
C -0.620553 -1.153332 0.127784
C -2.080794 -0.966116 0.083466
C -2.664171 0.315956 -0.012427
C -2.867765 -2.143159 0.130264
C -4.228284 -1.990982 0.079598
C -4.818536 -0.723377 -0.016028
C -4.078752 0.432652 -0.063314
C 1.589661 -0.184673 0.070193
O -0.091471 -2.265114 0.195526
F -1.931307 5.126109 -0.235381
C 2.278697 -0.396380 1.260986
C 3.662234 -0.587850 1.242468
C 4.389361 -0.573415 0.043389
C 3.666890 -0.360211 -1.144661
C 2.287135 -0.171654 -1.139328
O -5.202839 -2.951352 0.108041
C -6.458085 -2.259499 0.023922
O -6.176644 -0.850044 -0.050196
C 5.913888 -0.779937 -0.012065
C 6.526247 -1.000903 1.384047
C 6.578388 0.469045 -0.639193
C 6.232408 -2.020073 -0.881233
H 0.613910 4.573473 -0.111577
H 1.542578 2.279672 0.031673
H -3.350289 2.997058 -0.175896
H -2.384455 -3.109178 0.202249
H -4.578038 1.390066 -0.137171

H 1.735938 -0.413405 2.201346
H 4.167933 -0.751335 2.187084
H 4.185152 -0.344183 -2.098853
H 1.749515 -0.015004 -2.070001
H -6.987682 -2.570639 -0.881441
H -7.049276 -2.463634 0.921488
H 6.117183 -1.892294 1.873001
H 7.608651 -1.142543 1.290685
H 6.361201 -0.141237 2.043529
H 6.216233 0.657604 -1.655291
H 7.665174 0.332517 -0.692219
H 6.377453 1.363609 -0.038366
H 7.316636 -2.175609 -0.934434
H 5.779569 -2.923256 -0.456420
H 5.861287 -1.907596 -1.905282

3 Energy:-1306.89331088
C -1.437291 3.872870 -0.314796
C -0.058201 3.721444 -0.203136
C 0.458762 2.442612 -0.051350
C -0.385168 1.316615 -0.017148
C -1.789868 1.488062 -0.110534
C -2.295195 2.793743 -0.267082
N 0.160228 0.027585 0.142268
C -0.614737 -1.130592 0.225910
C -2.074757 -0.952963 0.149634
C -2.662241 0.318054 -0.028518
C -2.856899 -2.130498 0.244410
C -4.216805 -1.989292 0.159125
C -4.811108 -0.732351 -0.017782
C -4.076007 0.423620 -0.113966
C 1.593286 -0.158159 0.117918
O -0.085004 -2.237237 0.347455
F -1.952688 5.115781 -0.467202
C 2.277003 -0.496248 1.282458
C 3.658167 -0.700324 1.247685
C 4.389483 -0.576891 0.057470
C 3.672243 -0.243726 -1.105742
C 2.294333 -0.043504 -1.084800
O -5.187141 -2.952293 0.221749
C -6.443816 -2.273358 0.076173
O -6.167590 -0.868618 -0.071200
C 5.912151 -0.791459 -0.014349
C 6.518015 -1.151444 1.355438
C 6.589861 0.505970 -0.516610
C 6.222476 -1.944901 -0.998252
H 0.590697 4.590044 -0.230913
H 1.528890 2.314221 0.044674

H -3.358713 2.980530 -0.348087
H -2.370512 -3.088377 0.377711
H -4.578333 1.372602 -0.249612
H 1.732086 -0.599831 2.215569
H 4.159018 -0.961095 2.172865
H 4.192413 -0.143927 -2.053822
H 1.761571 0.202795 -1.998692
H -6.954966 -2.637391 -0.820003
H -7.050741 -2.430583 0.972695
H 6.100036 -2.082341 1.755087
H 7.599529 -1.292566 1.251619
H 6.357666 -0.358081 2.094385
H 6.232395 0.795072 -1.510533
H 7.675550 0.365225 -0.580323
H 6.395169 1.340254 0.167274
H 7.305461 -2.104407 -1.063965
H 5.760457 -2.880713 -0.663441
H 5.855359 -1.730844 -2.007447

4 Energy:-1306.89238581
C -1.455599 3.868520 -0.460631
C -0.081146 3.739064 -0.283615
C 0.441639 2.474646 -0.053228
C -0.389348 1.338903 -0.008728
C -1.791276 1.491459 -0.158322
C -2.303214 2.782533 -0.395471
N 0.165035 0.065008 0.234225
C -0.608390 -1.093727 0.357327
C -2.066840 -0.931500 0.232505
C -2.657551 0.320181 -0.042100
C -2.843035 -2.108873 0.371029
C -4.200126 -1.986141 0.231138
C -4.797416 -0.748146 -0.042713
C -4.068076 0.406951 -0.183231
C 1.597867 -0.118770 0.191054
O -0.080211 -2.191376 0.545789
F -1.976879 5.096580 -0.691702
C 2.284230 -0.570231 1.315467
C 3.661745 -0.790991 1.253091
C 4.388816 -0.577270 0.073334
C 3.669223 -0.136438 -1.051834
C 2.294751 0.080138 -1.004225
O -5.164667 -2.953010 0.318502
C -6.420686 -2.296251 0.089502
O -6.149903 -0.900734 -0.135637
C 5.907367 -0.807895 -0.027673
C 6.515865 -1.291352 1.302302
C 6.602099 0.517052 -0.423818

C 6.193827 -1.878654 -1.107671
H 0.559407 4.613514 -0.319875
H 1.507423 2.366053 0.098293
H -3.364881 2.952724 -0.523253
H -2.354437 -3.052578 0.576971
H -4.572497 1.340944 -0.394068
H 1.745399 -0.746317 2.240507
H 4.163005 -1.138747 2.149013
H 4.183973 0.033794 -1.992801
H 1.761978 0.405470 -1.892935
H -6.898632 -2.719785 -0.798791
H -7.056338 -2.403286 0.973428
H 6.086087 -2.246527 1.624668
H 7.594508 -1.438964 1.179282
H 6.371737 -0.561235 2.106858
H 6.243127 0.894154 -1.387240
H 7.685137 0.366251 -0.507031
H 6.424300 1.293587 0.329206
H 7.273790 -2.048129 -1.194822
H 5.719654 -2.832433 -0.849248
H 5.823684 -1.575085 -2.092566

5 Energy:-1306.89090604
C -1.472286 3.860135 -0.596362
C -0.106470 3.759603 -0.347896
C 0.420793 2.514072 -0.039692
C -0.393601 1.365937 0.008434
C -1.789808 1.493751 -0.202472
C -2.307259 2.765527 -0.519797
N 0.170263 0.112724 0.335246
C -0.602583 -1.045835 0.493517
C -2.057809 -0.903749 0.316221
C -2.649311 0.321332 -0.056281
C -2.828152 -2.079561 0.496585
C -4.179886 -1.981081 0.298418
C -4.777495 -0.769315 -0.074191
C -4.053790 0.383426 -0.257029
C 1.602750 -0.071099 0.271920
O -0.077976 -2.131150 0.749069
F -1.998287 5.068616 -0.905571
C 2.290800 -0.631571 1.346005
C 3.663573 -0.870377 1.252608
C 4.386294 -0.575931 0.088206
C 3.664919 -0.034396 -0.990856
C 2.295634 0.202653 -0.912516
O -5.138055 -2.951955 0.408068
C -6.390110 -2.325386 0.090137
O -6.123645 -0.943099 -0.209837

C 5.898988 -0.826571 -0.045239
C 6.509598 -1.419428 1.238754
C 6.616222 0.510711 -0.348557
C 6.154987 -1.818890 -1.204873
H 0.523159 4.641795 -0.387341
H 1.478525 2.430574 0.171907
H -3.364811 2.914348 -0.697994
H -2.339358 -3.003773 0.776695
H -4.558026 1.296796 -0.544581
H 1.759275 -0.874077 2.259008
H 4.164024 -1.299586 2.112973
H 4.173031 0.198169 -1.922135
H 1.764305 0.601691 -1.771204
H -6.828376 -2.808080 -0.788367
H -7.059232 -2.385487 0.953534
H 6.065401 -2.388568 1.492538
H 7.584396 -1.576061 1.094717
H 6.385010 -0.749582 2.097216
H 6.256418 0.965148 -1.277640
H 7.695360 0.346125 -0.453593
H 6.460073 1.232097 0.461914
H 7.230570 -2.002276 -1.315378
H 5.664072 -2.780004 -1.013566
H 5.782413 -1.435258 -2.160459

6 Energy:-1306.88870497
C -1.479697 3.845344 -0.725921
C -0.129535 3.781238 -0.393257
C 0.397546 2.559548 -0.002183
C -0.396626 1.396589 0.041887
C -1.781486 1.493216 -0.242737
C -2.300128 2.740462 -0.645380
N 0.174984 0.171109 0.459623
C -0.600283 -0.985017 0.652625
C -2.048678 -0.868750 0.409056
C -2.634474 0.319918 -0.072214
C -2.815042 -2.040677 0.629363
C -4.156285 -1.973837 0.359813
C -4.747322 -0.798122 -0.122553
C -4.027358 0.349796 -0.346219
C 1.607232 -0.015917 0.372941
O -0.085171 -2.053289 0.985601
F -2.006051 5.029097 -1.117888
C 2.300273 -0.674087 1.388452
C 3.666331 -0.933694 1.255460
C 4.379675 -0.573808 0.104667
C 3.653335 0.057554 -0.920768
C 2.291892 0.318475 -0.803004

O -5.108538 -2.948294 0.487652
C -6.349923 -2.361358 0.068476
O -6.082985 -0.999029 -0.311976
C 5.883729 -0.847152 -0.071291
C 6.499891 -1.541269 1.158102
C 6.626628 0.492110 -0.293079
C 6.099379 -1.761112 -1.301438
H 0.486454 4.673102 -0.429805
H 1.440963 2.506179 0.279246
H -3.349285 2.862769 -0.883131
H -2.331382 -2.938246 0.992365
H -4.525802 1.235167 -0.718840
H 1.782161 -0.969468 2.291985
H 4.167975 -1.434410 2.075645
H 4.150435 0.341071 -1.843883
H 1.760477 0.781393 -1.628268
H -6.740286 -2.907959 -0.794993
H -7.059442 -2.371760 0.901118
H 6.037640 -2.515934 1.351275
H 7.568660 -1.710604 0.986128
H 6.402933 -0.930368 2.062849
H 6.262618 1.018365 -1.181806
H 7.699955 0.311917 -0.428068
H 6.499867 1.158189 0.568275
H 7.168727 -1.958971 -1.443253
H 5.590296 -2.722698 -1.169021
H 5.720248 -1.303690 -2.221362

7 Energy:-1306.8855944
C -1.473086 3.828046 -0.839732
C -0.147630 3.808411 -0.413891
C 0.373077 2.616006 0.064838
C -0.397229 1.436424 0.101232
C -1.762378 1.493735 -0.269767
C -2.276653 2.711015 -0.761312
N 0.178161 0.246653 0.616750
C -0.608261 -0.894777 0.867929
C -2.041459 -0.816535 0.530677
C -2.607985 0.318214 -0.083440
C -2.806931 -1.981289 0.789917
C -4.125574 -1.961628 0.419790
C -4.695171 -0.840698 -0.199252
C -3.976231 0.299941 -0.460991
C 1.609046 0.045741 0.499925
O -0.115617 -1.930944 1.315162
F -1.994115 4.981997 -1.317304
C 2.312282 -0.699892 1.448483
C 3.668126 -0.983463 1.262414

C 4.364176 -0.572406 0.119709
C 3.627644 0.138751 -0.844193
C 2.278336 0.427452 -0.673657
O -5.070994 -2.941632 0.555964
C -6.284675 -2.416485 -0.003019
O -6.009456 -1.083128 -0.470594
C 5.855182 -0.871841 -0.112654
C 6.483681 -1.652736 1.056936
C 6.627097 0.459444 -0.275598
C 6.015729 -1.716226 -1.399656
H 0.451261 4.712043 -0.444263
H 1.394555 2.597168 0.422213
H -3.311884 2.801519 -1.065077
H -2.339779 -2.838829 1.256265
H -4.456317 1.142869 -0.940809
H 1.817370 -1.035665 2.348666
H 4.174356 -1.546641 2.038253
H 4.105836 0.462989 -1.763976
H 1.744065 0.946210 -1.461989
H -6.598113 -3.037997 -0.846984
H -7.056753 -2.375897 0.770952
H 6.000870 -2.625413 1.204468
H 7.543077 -1.837975 0.847318
H 6.424999 -1.094673 1.998377
H 6.253791 1.046685 -1.121269
H 7.691470 0.261357 -0.450666
H 6.540302 1.075893 0.626687
H 7.075690 -1.930799 -1.582058
H 5.485974 -2.671586 -1.309911
H 5.624660 -1.196322 -2.280598

8 Energy:-1306.88154428
C -1.460873 3.810455 -0.948778
C -0.167524 3.844553 -0.433329
C 0.345178 2.687187 0.131610
C -0.395727 1.488812 0.163181
C -1.733430 1.496329 -0.295509
C -2.242518 2.677870 -0.872796
N 0.179933 0.341219 0.774771
C -0.630444 -0.761770 1.119503
C -2.035543 -0.742827 0.667472
C -2.567032 0.315103 -0.095640
C -2.802413 -1.896041 0.970747
C -4.082811 -1.944236 0.485915
C -4.613516 -0.902426 -0.286686
C -3.893746 0.227439 -0.590895
C 1.606800 0.110382 0.627671
O -0.179297 -1.733639 1.725391

F -1.975552 4.929397 -1.508449
C 2.314085 -0.722158 1.502040
C 3.655484 -1.034327 1.259498
C 4.338998 -0.573976 0.129895
C 3.599699 0.219968 -0.764228
C 2.266482 0.540067 -0.538584
O -5.018925 -2.931970 0.630654
C -6.184658 -2.495619 -0.084715
O -5.892414 -1.204485 -0.650506
C 5.813024 -0.902940 -0.160625
C 6.442139 -1.781942 0.936726
C 6.623719 0.412052 -0.251924
C 5.916361 -1.660665 -1.506051
H 0.409103 4.762651 -0.459341
H 1.338920 2.708750 0.561184
H -3.260230 2.729941 -1.238620
H -2.364983 -2.695236 1.554632
H -4.340429 1.009087 -1.191756
H 1.839093 -1.099115 2.393854
H 4.159484 -1.662139 1.985817
H 4.061394 0.585833 -1.676950
H 1.736601 1.116609 -1.287177
H -6.405531 -3.201637 -0.890679
H -7.026603 -2.404473 0.607707
H 5.930360 -2.746500 1.030124
H 7.489673 -1.985918 0.688372
H 6.423708 -1.288310 1.915066
H 6.248662 1.067583 -1.045048
H 7.676650 0.194452 -0.468366
H 6.578688 0.966758 0.692500
H 6.964270 -1.894624 -1.729693
H 5.358149 -2.603240 -1.468569
H 5.522066 -1.069198 -2.339153

9 Energy:-1306.87726563
C -1.470361 3.805542 -1.046902
C -0.208810 3.902358 -0.464587
C 0.308452 2.783523 0.170786
C -0.394799 1.563999 0.205092
C -1.703367 1.509063 -0.324846
C -2.220196 2.650923 -0.969981
N 0.182238 0.456922 0.891235
C -0.664400 -0.566224 1.374235
C -2.023565 -0.645976 0.799909
C -2.510210 0.311406 -0.111315
C -2.785226 -1.789041 1.149338
C -4.009520 -1.933555 0.550354
C -4.489986 -0.996259 -0.374031

C -3.776138 0.125523 -0.721802
C 1.597224 0.171815 0.714808
O -0.274159 -1.409231 2.180744
F -1.990425 4.887099 -1.670715
C 2.281888 -0.762437 1.504960
C 3.605556 -1.110522 1.218142
C 4.303705 -0.584208 0.127949
C 3.589459 0.312414 -0.684218
C 2.273122 0.668911 -0.417370
O -4.922315 -2.942581 0.697921
C -6.043274 -2.600293 -0.131155
O -5.712532 -1.387951 -0.833554
C 5.760959 -0.945758 -0.203586
C 6.358883 -1.941929 0.807684
C 6.624371 0.338295 -0.187428
C 5.826443 -1.586482 -1.610709
H 0.336834 4.839143 -0.491709
H 1.275116 2.851737 0.655089
H -3.222200 2.657041 -1.380925
H -2.387006 -2.509876 1.851567
H -4.178558 0.826621 -1.441907
H 1.800443 -1.194807 2.366213
H 4.084676 -1.820610 1.883233
H 4.056408 0.736283 -1.568933
H 1.770091 1.322162 -1.118077
H -6.220541 -3.400190 -0.854983
H -6.923674 -2.426293 0.495602
H 5.808090 -2.889306 0.821247
H 7.395919 -2.166001 0.533758
H 6.365404 -1.535162 1.825353
H 6.271257 1.075128 -0.916743
H 7.666316 0.098687 -0.432128
H 6.607522 0.809530 0.802180
H 6.862771 -1.841616 -1.863429
H 5.230696 -2.505717 -1.650675
H 5.451941 -0.909014 -2.385420

10 Energy:-1306.87347219
C -1.502302 3.795683 -1.159349
C -0.266560 3.953750 -0.537500
C 0.264787 2.872803 0.151928
C -0.398406 1.632831 0.198653
C -1.687705 1.519093 -0.367676
C -2.219479 2.620570 -1.066526
N 0.187524 0.559122 0.931684
C -0.678375 -0.398098 1.510979
C -2.006503 -0.563077 0.883374
C -2.469177 0.309863 -0.120731

C -2.757477 -1.696127 1.282681
C -3.943978 -1.920710 0.633087
C -4.397401 -1.070424 -0.384284
C -3.694887 0.043676 -0.779318
C 1.590324 0.226924 0.739868
O -0.321449 -1.126033 2.435162
F -2.035409 4.838718 -1.835116
C 2.218941 -0.818428 1.435184
C 3.529396 -1.198628 1.133863
C 4.277984 -0.592374 0.120958
C 3.621831 0.417360 -0.599757
C 2.317079 0.807811 -0.318518
O -4.836270 -2.943451 0.808526
C -5.921692 -2.694676 -0.097560
O -5.582034 -1.532383 -0.876314
C 5.724670 -0.984649 -0.220913
C 6.253464 -2.109352 0.689083
C 6.644725 0.248012 -0.052304
C 5.793727 -1.475480 -1.686899
H 0.247265 4.908008 -0.574565
H 1.207581 2.990016 0.672850
H -3.209623 2.581291 -1.503949
H -2.380604 -2.350354 2.058347
H -4.075254 0.679333 -1.569120
H 1.703300 -1.315628 2.240295
H 3.958105 -2.000023 1.725809
H 4.125705 0.912482 -1.425327
H 1.866417 1.550956 -0.961129
H -6.045822 -3.552246 -0.763995
H -6.835654 -2.494514 0.470775
H 5.660436 -3.025825 0.591352
H 7.285519 -2.352007 0.412123
H 6.254263 -1.813233 1.744298
H 6.342581 1.073523 -0.705626
H 7.680378 -0.013489 -0.301485
H 6.625639 0.612768 0.981249
H 6.823124 -1.750401 -1.947207
H 5.158816 -2.356640 -1.835253
H 5.467004 -0.703258 -2.391439

11 Energy:-1306.87035239
C -1.547031 3.771360 -1.284387
C -0.331916 3.986869 -0.641485
C 0.218665 2.943151 0.091618
C -0.404337 1.684600 0.156814
C -1.682406 1.517348 -0.423806
C -2.233456 2.579088 -1.165559
N 0.194382 0.638339 0.919851

C -0.675996 -0.265978 1.575233
C -1.989132 -0.496473 0.937196
C -2.441590 0.302308 -0.131881
C -2.729747 -1.614692 1.391606
C -3.894780 -1.903755 0.727700
C -4.335727 -1.130250 -0.354184
C -3.643267 -0.029422 -0.802865
C 1.586182 0.269439 0.721930
O -0.324672 -0.902581 2.565510
F -2.097432 4.775834 -2.003074
C 2.141986 -0.881668 1.306050
C 3.445045 -1.285927 1.010090
C 4.264019 -0.597442 0.109313
C 3.682674 0.521244 -0.504008
C 2.384501 0.939173 -0.225033
O -4.772087 -2.931285 0.945420
C -5.840579 -2.758438 0.002250
O -5.497445 -1.646834 -0.846099
C 5.706633 -1.013549 -0.221334
C 6.143628 -2.268075 0.558411
C 6.670321 0.141804 0.140272
C 5.822469 -1.318989 -1.733922
H 0.150647 4.956625 -0.693249
H 1.137219 3.111504 0.640555
H -3.216236 2.498687 -1.614261
H -2.361842 -2.210724 2.217046
H -4.013733 0.547838 -1.640883
H 1.576398 -1.452304 2.025267
H 3.810833 -2.174744 1.512751
H 4.242234 1.090929 -1.240914
H 2.000508 1.774656 -0.791248
H -5.940171 -3.660335 -0.607131
H -6.768930 -2.532181 0.536593
H 5.516307 -3.134921 0.321193
H 7.175761 -2.524440 0.294322
H 6.109041 -2.106999 1.641934
H 6.433993 1.056596 -0.413739
H 7.704158 -0.136063 -0.098624
H 6.619480 0.374074 1.210368
H 6.849719 -1.609883 -1.985263
H 5.156688 -2.141615 -2.019612
H 5.563544 -0.448811 -2.346465

12 Energy:-1306.86805809
C -1.599182 3.732169 -1.421144
C -0.396569 3.998198 -0.776088
C 0.175601 2.991490 -0.006139
C -0.412399 1.719059 0.088989

C -1.688249 1.506466 -0.485603
C -2.260484 2.529186 -1.263089
N 0.202133 0.694821 0.869351
C -0.658240 -0.169657 1.589450
C -1.973249 -0.442836 0.973201
C -2.429841 0.293267 -0.138948
C -2.704498 -1.540833 1.486913
C -3.864386 -1.877512 0.835955
C -4.307301 -1.170016 -0.289270
C -3.624348 -0.087825 -0.795418
C 1.586026 0.302381 0.671115
O -0.287915 -0.744564 2.609242
F -2.169264 4.698464 -2.175771
C 2.061931 -0.941352 1.122769
C 3.362327 -1.363724 0.847508
C 4.260846 -0.598358 0.095300
C 3.761792 0.617870 -0.388538
C 2.466384 1.057680 -0.123789
O -4.733251 -2.899062 1.107846
C -5.792793 -2.797731 0.144126
O -5.461709 -1.724291 -0.756473
C 5.703864 -1.032976 -0.209143
C 6.040990 -2.403551 0.407842
C 6.687470 0.013206 0.367443
C 5.902972 -1.129610 -1.740648
H 0.059578 4.979196 -0.850467
H 1.071964 3.211028 0.559656
H -3.241498 2.413468 -1.708056
H -2.333236 -2.087770 2.344332
H -3.997338 0.438858 -1.665128
H 1.433437 -1.584135 1.719718
H 3.660874 -2.329841 1.239824
H 4.387978 1.256772 -1.005269
H 2.157090 1.981878 -0.586169
H -5.865735 -3.731950 -0.418865
H -6.732289 -2.564264 0.654994
H 5.395606 -3.197511 0.014911
H 7.076563 -2.670152 0.168541
H 5.945267 -2.393717 1.499583
H 6.521632 1.006825 -0.062471
H 7.722653 -0.276914 0.149787
H 6.578997 0.095215 1.455159
H 6.931952 -1.431026 -1.971727
H 5.225128 -1.871927 -2.177794
H 5.717241 -0.171302 -2.237282

13 Energy:-1306.86685238
C -1.669364 3.672687 -1.577265

C -0.460557 3.974691 -0.963236
C 0.138910 3.003108 -0.167574
C -0.427324 1.726674 -0.017691
C -1.716856 1.484061 -0.555267
C -2.315378 2.470540 -1.357783
N 0.208917 0.714838 0.761200
C -0.623006 -0.123586 1.542248
C -1.959292 -0.412168 0.983093
C -2.445605 0.282448 -0.143266
C -2.676529 -1.487647 1.559773
C -3.854749 -1.847030 0.955550
C -4.327403 -1.183393 -0.184056
C -3.658009 -0.123018 -0.750877
C 1.593893 0.323605 0.575746
O -0.209098 -0.668995 2.561073
F -2.264560 4.603159 -2.357225
C 1.990949 -0.995539 0.859583
C 3.294116 -1.429053 0.626205
C 4.277503 -0.592172 0.082975
C 3.863643 0.708720 -0.226942
C 2.565114 1.161964 0.006147
O -4.717306 -2.854771 1.291592
C -5.797101 -2.796794 0.347077
O -5.494991 -1.752692 -0.597330
C 5.725392 -1.039359 -0.178114
C 5.964098 -2.505494 0.229710
C 6.693226 -0.146615 0.634699
C 6.045626 -0.897526 -1.685338
H -0.018918 4.958597 -1.076729
H 1.025844 3.270439 0.388722
H -3.304486 2.329570 -1.776727
H -2.280281 -2.002473 2.425901
H -4.055513 0.369017 -1.629888
H 1.289856 -1.701863 1.279690
H 3.526652 -2.458996 0.873839
H 4.564056 1.412154 -0.668627
H 2.339029 2.169888 -0.298937
H -5.872546 -3.750937 -0.181448
H -6.728123 -2.554069 0.868709
H 5.327600 -3.195210 -0.336357
H 7.006471 -2.777884 0.029761
H 5.778595 -2.666927 1.297739
H 6.598548 0.909625 0.360999
H 7.732110 -0.447455 0.452223
H 6.497732 -0.234315 1.709693
H 7.079240 -1.205513 -1.884886
H 5.381028 -1.527175 -2.288232
H 5.933372 0.135971 -2.029885

14 Energy:-1306.88867426
C -1.580183 3.336777 -1.955197
C -0.247201 3.058120 -2.243714
C 0.302709 1.882175 -1.755865
C -0.450550 0.990216 -0.967045
C -1.821706 1.261485 -0.733684
C -2.363497 2.464255 -1.230344
N 0.142810 -0.206726 -0.499676
C -0.599172 -1.192181 0.173596
C -2.036262 -0.932560 0.368673
C -2.639419 0.278558 -0.027652
C -2.769733 -1.947680 1.032681
C -4.096979 -1.708700 1.272354
C -4.704931 -0.506654 0.885398
C -4.016665 0.493099 0.242882
C 1.583408 -0.297744 -0.397993
O -0.063883 -2.215021 0.603327
F -2.128070 4.484994 -2.417203
C 2.248368 -1.469504 -0.758022
C 3.627520 -1.583953 -0.567885
C 4.383519 -0.554309 0.007297
C 3.686785 0.604336 0.394513
C 2.312985 0.729776 0.214768
O -5.018227 -2.513165 1.886288
C -6.258835 -1.790655 1.877843
O -6.020755 -0.520364 1.244149
C 5.902961 -0.651338 0.230432
C 6.481861 -1.991768 -0.260409
C 6.210377 -0.516213 1.741162
C 6.608927 0.490835 -0.538864
H 0.337545 3.743990 -2.846932
H 1.331820 1.647865 -1.994228
H -3.402758 2.721657 -1.069483
H -2.273124 -2.862223 1.330015
H -4.527478 1.404699 -0.038446
H 1.697531 -2.287814 -1.204054
H 4.105242 -2.507049 -0.875723
H 4.218378 1.426965 0.863902
H 1.806953 1.628004 0.553696
H -7.003511 -2.348069 1.301810
H -6.592736 -1.624727 2.906189
H 6.320010 -2.137425 -1.334552
H 7.562929 -2.011086 -0.083121
H 6.044403 -2.844501 0.271037
H 5.862018 0.440299 2.144869
H 7.291585 -0.577515 1.914351
H 5.728559 -1.318163 2.312198

H 7.693219 0.438887 -0.382829
H 6.416817 0.415734 -1.615477
H 6.270960 1.477468 -0.204769

15 Energy:-1306.89087476
C -1.575967 3.264647 -2.055307
C -0.222150 3.013405 -2.258491
C 0.331514 1.872753 -1.695735
C -0.443810 0.988463 -0.920758
C -1.830937 1.235246 -0.762086
C -2.375185 2.401720 -1.335653
N 0.146052 -0.170649 -0.369395
C -0.593593 -1.137692 0.325253
C -2.041599 -0.901036 0.454882
C -2.655408 0.267867 -0.041540
C -2.778431 -1.893712 1.147883
C -4.120419 -1.676647 1.315685
C -4.740016 -0.518045 0.827791
C -4.048788 0.459279 0.154707
C 1.585561 -0.274930 -0.285148
O -0.046202 -2.125372 0.818445
F -2.127148 4.378220 -2.592775
C 2.240671 -1.410940 -0.755877
C 3.623858 -1.535303 -0.608696
C 4.390734 -0.546062 0.022317
C 3.703245 0.579256 0.511144
C 2.324350 0.712146 0.376479
O -5.048444 -2.467850 1.936693
C -6.302042 -1.774580 1.842621
O -6.070470 -0.547062 1.127460
C 5.916191 -0.652059 0.197235
C 6.484203 -1.955266 -0.396037
C 6.265112 -0.615141 1.704487
C 6.598047 0.540793 -0.514873
H 0.377550 3.694451 -2.852476
H 1.379240 1.661331 -1.863507
H -3.426536 2.640417 -1.235779
H -2.272901 -2.775303 1.520496
H -4.569339 1.337174 -0.205079
H 1.674833 -2.195449 -1.245066
H 4.097122 -2.430339 -0.995803
H 4.246950 1.368533 1.021863
H 1.821132 1.583615 0.784097
H -7.018262 -2.387029 1.287176
H -6.669408 -1.544077 2.847104
H 6.295539 -2.029927 -1.473058
H 7.569443 -1.982747 -0.247811
H 6.061769 -2.842781 0.088587

H 5.928055 0.312198 2.179423
H 7.350726 -0.685334 1.843058
H 5.799624 -1.453667 2.235055
H 7.686330 0.483113 -0.392345
H 6.376508 0.535290 -1.588441
H 6.267221 1.502169 -0.107936

16 Energy:-1306.89234323
C -1.567685 3.180948 -2.162931
C -0.199963 2.957249 -2.291314
C 0.354538 1.856269 -1.654509
C -0.437551 0.983926 -0.883752
C -1.835115 1.206146 -0.790577
C -2.379211 2.331988 -1.439918
N 0.148349 -0.132140 -0.250999
C -0.589173 -1.072332 0.475688
C -2.044948 -0.860616 0.545007
C -2.665181 0.258783 -0.049331
C -2.785551 -1.827213 1.269657
C -4.138222 -1.635908 1.369733
C -4.764759 -0.527631 0.783631
C -4.070031 0.423827 0.077919
C 1.587129 -0.251726 -0.184082
O -0.032440 -2.018130 1.036608
F -2.119446 4.255593 -2.774463
C 2.230206 -1.344270 -0.760505
C 3.616132 -1.477471 -0.653251
C 4.395082 -0.536301 0.034995
C 3.719072 0.547998 0.622652
C 2.337094 0.688339 0.528357
O -5.071936 -2.411047 2.002305
C -6.337437 -1.760485 1.811125
O -6.105707 -0.573761 1.030452
C 5.924320 -0.651749 0.167498
C 6.480145 -1.903290 -0.537939
C 6.306149 -0.731563 1.665054
C 6.589488 0.594658 -0.464208
H 0.410880 3.630220 -2.883165
H 1.414754 1.667449 -1.758954
H -3.438461 2.551729 -1.393855
H -2.274741 -2.670687 1.716179
H -4.596470 1.262558 -0.358612
H 1.650906 -2.089070 -1.295973
H 4.082558 -2.338380 -1.118175
H 4.275084 1.298387 1.176811
H 1.839635 1.527880 1.004984
H -7.012520 -2.426259 1.265516
H -6.754725 -1.478648 2.782455

H 6.267676 -1.894503 -1.613087
H 7.568408 -1.939248 -0.416369
H 6.069496 -2.826887 -0.114500
H 5.977568 0.154473 2.218333
H 7.394700 -0.808138 1.773979
H 5.854345 -1.610835 2.138410
H 7.680206 0.529698 -0.370625
H 6.344176 0.672517 -1.529753
H 6.267704 1.520737 0.023764

17 Energy:-1306.89327627
C -1.558301 3.087373 -2.276657
C -0.182015 2.890685 -2.343143
C 0.371548 1.830637 -1.639180
C -0.432789 0.971978 -0.866464
C -1.836398 1.171013 -0.826210
C -2.378954 2.254701 -1.544566
N 0.149327 -0.100316 -0.162242
C -0.587272 -1.014416 0.593352
C -2.047288 -0.822686 0.618821
C -2.670102 0.247260 -0.059171
C -2.790916 -1.759748 1.377956
C -4.149328 -1.590162 1.428021
C -4.778670 -0.532204 0.757955
C -4.081173 0.389808 0.016805
C 1.587505 -0.232688 -0.108082
O -0.025354 -1.923403 1.208168
F -2.108940 4.121397 -2.955835
C 2.223311 -1.265917 -0.791009
C 3.610786 -1.404913 -0.713657
C 4.396360 -0.524725 0.044551
C 3.727311 0.504522 0.731190
C 2.343839 0.649701 0.666765
O -5.086880 -2.344748 2.079522
C -6.358146 -1.733217 1.812527
O -6.125476 -0.591312 0.968012
C 5.927254 -0.648348 0.148609
C 6.476392 -1.832387 -0.669586
C 6.326047 -0.857926 1.629147
C 6.583881 0.649706 -0.379283
H 0.436547 3.554101 -2.937780
H 1.439490 1.663960 -1.690205
H -3.442934 2.455873 -1.543139
H -2.277938 -2.565597 1.887188
H -4.610069 1.189629 -0.484973
H 1.636036 -1.961055 -1.382814
H 4.073207 -2.219814 -1.258499
H 4.290753 1.207686 1.337386

H 1.849597 1.446534 1.214955
H -7.003765 -2.444580 1.289235
H -6.809763 -1.402001 2.752413
H 6.251323 -1.730635 -1.737372
H 7.566073 -1.875808 -0.564271
H 6.072474 -2.790496 -0.323380
H 6.003665 -0.023885 2.261265
H 7.415761 -0.942503 1.718517
H 5.879734 -1.775601 2.029094
H 7.675609 0.578991 -0.303735
H 6.326613 0.819745 -1.431202
H 6.266553 1.528878 0.191266

18 Energy:-1306.89380241
C -1.547844 2.987612 -2.388413
C -0.166594 2.816716 -2.403538
C 0.384799 1.799869 -1.636664
C -0.428359 0.957830 -0.855471
C -1.835508 1.134723 -0.859789
C -2.375471 2.174168 -1.642341
N 0.150295 -0.067322 -0.083461
C -0.586428 -0.944344 0.711965
C -2.049378 -0.774844 0.695814
C -2.672865 0.238102 -0.064686
C -2.796367 -1.679391 1.490030
C -4.158820 -1.536609 1.490700
C -4.788966 -0.536295 0.737945
C -4.088221 0.353813 -0.038315
C 1.587783 -0.214084 -0.041506
O -0.021838 -1.808524 1.386422
F -2.096270 3.979257 -3.129932
C 2.216255 -1.178416 -0.824478
C 3.604747 -1.322470 -0.773744
C 4.396934 -0.513558 0.053763
C 3.734894 0.450114 0.836039
C 2.351026 0.600609 0.796970
O -5.100100 -2.269791 2.161029
C -6.375484 -1.710688 1.811830
O -6.140058 -0.612063 0.912337
C 5.928797 -0.644919 0.131891
C 6.470163 -1.749360 -0.795496
C 6.341056 -0.987801 1.583584
C 6.580716 0.696099 -0.282224
H 0.457666 3.468166 -3.005408
H 1.457261 1.655374 -1.642476
H -3.442031 2.357977 -1.677658
H -2.282941 -2.442186 2.061387
H -4.617729 1.108871 -0.604703

H 1.622584 -1.816695 -1.472045
H 4.062402 -2.083457 -1.395209
H 4.304910 1.097912 1.495425
H 1.861084 1.347567 1.414801
H -6.981445 -2.468516 1.306345
H -6.871830 -1.339938 2.713456
H 6.235680 -1.550923 -1.847551
H 7.560713 -1.801683 -0.704252
H 6.069023 -2.735185 -0.534354
H 6.023737 -0.215282 2.291836
H 7.431583 -1.078516 1.655076
H 5.898925 -1.938678 1.902355
H 7.673089 0.619014 -0.224584
H 6.312905 0.961155 -1.311623
H 6.270045 1.519680 0.369187

19 Energy:-1306.8940003
C -1.549282 2.874518 -2.515742
C -0.164903 2.731819 -2.491387
C 0.387881 1.760586 -1.668387
C -0.427767 0.934418 -0.873234
C -1.837004 1.089408 -0.908583
C -2.378357 2.081325 -1.749614
N 0.151370 -0.043816 -0.043780
C -0.584771 -0.895783 0.777491
C -2.048776 -0.739870 0.741668
C -2.674010 0.224313 -0.078704
C -2.795256 -1.609978 1.573772
C -4.159039 -1.481612 1.552931
C -4.790834 -0.529316 0.741581
C -4.090659 0.325776 -0.073634
C 1.587968 -0.200131 -0.006430
O -0.017514 -1.729577 1.487279
F -2.099138 3.819867 -3.314449
C 2.220237 -1.075426 -0.885148
C 3.609299 -1.220122 -0.847112
C 4.397224 -0.500494 0.062697
C 3.731097 0.375719 0.938911
C 2.347341 0.528712 0.910354
O -5.100250 -2.188792 2.250660
C -6.376894 -1.656572 1.865458
O -6.142967 -0.610286 0.905370
C 5.929058 -0.637174 0.132025
C 6.475681 -1.635676 -0.905830
C 6.335929 -1.132630 1.540552
C 6.580715 0.740995 -0.134043
H 0.460649 3.370639 -3.105333
H 1.462961 1.639870 -1.640041

H -3.446897 2.244771 -1.813678
H -2.280488 -2.336502 2.189505
H -4.621476 1.044426 -0.684485
H 1.629388 -1.644547 -1.596885
H 4.070398 -1.910588 -1.543834
H 4.298436 0.952861 1.663011
H 1.854021 1.209608 1.597760
H -6.977322 -2.444997 1.402203
H -6.878411 -1.237077 2.742692
H 6.244374 -1.326642 -1.931601
H 7.566015 -1.695716 -0.816794
H 6.075602 -2.644338 -0.752587
H 6.013846 -0.440615 2.325706
H 7.426314 -1.228823 1.606908
H 5.894408 -2.112834 1.753961
H 7.672936 0.658847 -0.080978
H 6.316292 1.114201 -1.130246
H 6.267096 1.490340 0.600309

20 Energy:-1306.89382569
C -1.550483 2.763284 -2.629173
C -0.164278 2.655800 -2.564266
C 0.389720 1.734947 -1.686080
C -0.426120 0.921536 -0.877855
C -1.836969 1.049378 -0.945969
C -2.379722 1.988366 -1.844887
N 0.154242 -0.005024 0.008888
C -0.583971 -0.829800 0.856479
C -2.048922 -0.692163 0.796164
C -2.674781 0.216239 -0.084919
C -2.796118 -1.528525 1.661678
C -4.161073 -1.422547 1.612864
C -4.793450 -0.524673 0.742043
C -4.092636 0.296787 -0.106486
C 1.589287 -0.176897 0.037038
O -0.017952 -1.629470 1.605518
F -2.101802 3.657065 -3.484215
C 2.219402 -0.961429 -0.925507
C 3.608249 -1.112540 -0.903458
C 4.398519 -0.489142 0.072707
C 3.735017 0.299206 1.030736
C 2.352117 0.459904 1.017289
O -5.103043 -2.103269 2.335468
C -6.381350 -1.627043 1.887656
O -6.146610 -0.615301 0.891379
C 5.930028 -0.635569 0.126763
C 6.472454 -1.537295 -0.998223
C 6.338517 -1.257314 1.483719

C 6.584089 0.759854 -0.014550
H 0.461914 3.283667 -3.188769
H 1.466283 1.644965 -1.624102
H -3.449720 2.125198 -1.939341
H -2.280901 -2.213421 2.323046
H -4.623760 0.975401 -0.761296
H 1.627347 -1.456456 -1.689839
H 4.066837 -1.731652 -1.665794
H 4.304442 0.802601 1.806399
H 1.861555 1.074467 1.766149
H -6.943275 -2.452333 1.439818
H -6.923117 -1.186694 2.729621
H 6.242629 -1.134964 -1.991456
H 7.562534 -1.609808 -0.915509
H 6.067965 -2.554017 -0.937526
H 6.020157 -0.638410 2.329080
H 7.428776 -1.361747 1.538381
H 5.894861 -2.251710 1.608683
H 7.676245 0.671636 0.029757
H 6.319360 1.221906 -0.972695
H 6.272026 1.440092 0.784856

21 Energy:-1306.89326886
C -1.563428 2.641513 -2.751209
C -0.176730 2.576774 -2.651439
C 0.382177 1.711344 -1.721703
C -0.427816 0.907313 -0.897815
C -1.839892 1.002800 -0.992791
C -2.387929 1.883540 -1.946039
N 0.158314 0.035747 0.041286
C -0.580693 -0.761303 0.916632
C -2.046246 -0.643487 0.838900
C -2.675612 0.203873 -0.098143
C -2.790410 -1.442296 1.741877
C -4.156081 -1.359674 1.673914
C -4.792070 -0.521371 0.748052
C -4.094172 0.262064 -0.138019
C 1.591512 -0.151090 0.062714
O -0.014947 -1.525269 1.702039
F -2.119793 3.477954 -3.659215
C 2.226158 -0.835284 -0.971360
C 3.614408 -0.993005 -0.957198
C 4.400949 -0.476642 0.082130
C 3.733548 0.211882 1.111812
C 2.351891 0.380641 1.105894
O -5.095698 -2.012118 2.425075
C -6.375883 -1.583025 1.936935
O -6.145225 -0.623031 0.889718

C 5.931476 -0.634142 0.130006
C 6.478247 -1.412766 -1.081501
C 6.328433 -1.399231 1.415315
C 6.591715 0.765450 0.142691
H 0.446269 3.195420 -3.288208
H 1.459036 1.658868 -1.631505
H -3.458913 1.988839 -2.065971
H -2.272439 -2.081929 2.445049
H -4.628249 0.896447 -0.833420
H 1.638599 -1.248436 -1.786115
H 4.074912 -1.532405 -1.776856
H 4.299614 0.631354 1.938214
H 1.859951 0.919525 1.909622
H -6.918437 -2.440965 1.528169
H -6.935420 -1.106899 2.747136
H 6.255439 -0.906004 -2.027421
H 7.567599 -1.497608 -1.000859
H 6.070450 -2.428728 -1.131985
H 6.006064 -0.873170 2.319986
H 7.417938 -1.513447 1.465763
H 5.880526 -2.399456 1.430105
H 7.683198 0.668164 0.184395
H 6.335336 1.328242 -0.762392
H 6.276853 1.358111 1.008000

22 Energy:-1306.89226914
C -1.577802 2.531329 -2.854642
C -0.192811 2.520932 -2.718015
C 0.371215 1.715827 -1.738867
C -0.429351 0.913403 -0.903452
C -1.841272 0.964438 -1.029625
C -2.395172 1.783200 -2.033724
N 0.164751 0.107102 0.090300
C -0.576161 -0.654038 0.999426
C -2.042228 -0.573493 0.892463
C -2.674492 0.193379 -0.109018
C -2.783385 -1.336497 1.828594
C -4.148915 -1.299600 1.727204
C -4.787712 -0.541577 0.736337
C -4.092755 0.205430 -0.182888
C 1.594584 -0.105575 0.098143
O -0.012373 -1.365067 1.834171
F -2.139474 3.307116 -3.811636
C 2.225731 -0.701308 -0.992233
C 3.611877 -0.876542 -0.990523
C 4.402910 -0.464064 0.090633
C 3.740851 0.139855 1.175280
C 2.361804 0.326430 1.182441

O -5.086071 -1.931755 2.498486
C -6.366571 -1.575705 1.955542
O -6.140119 -0.675601 0.855510
C 5.930995 -0.644932 0.126678
C 6.471511 -1.316430 -1.149958
C 6.313994 -1.529337 1.337455
C 6.609394 0.738737 0.268762
H 0.424776 3.136732 -3.362750
H 1.446175 1.711641 -1.618101
H -3.466104 1.850559 -2.178389
H -2.263400 -1.916091 2.580557
H -4.629117 0.777103 -0.928976
H 1.637670 -1.036407 -1.841533
H 4.066710 -1.346891 -1.854716
H 4.309706 0.479908 2.035625
H 1.876863 0.800759 2.029096
H -6.871988 -2.474582 1.589288
H -6.960395 -1.068655 2.721292
H 6.257442 -0.722562 -2.045901
H 7.559518 -1.421964 -1.075705
H 6.051407 -2.318369 -1.293771
H 5.994291 -1.084131 2.285421
H 7.401846 -1.661296 1.380322
H 5.853903 -2.521084 1.259485
H 7.699446 0.623658 0.302221
H 6.362205 1.385844 -0.580818
H 6.300618 1.253256 1.184771

23 Energy:-1306.89063978
C -1.592487 2.430779 -2.944466
C -0.212681 2.485397 -2.770257
C 0.355659 1.742664 -1.745858
C -0.431585 0.933034 -0.903874
C -1.840912 0.930417 -1.061927
C -2.400308 1.685076 -2.112584
N 0.172117 0.196176 0.140198
C -0.572128 -0.533161 1.077290
C -2.037534 -0.496786 0.941480
C -2.670754 0.182076 -0.120261
C -2.775434 -1.225783 1.907168
C -4.138415 -1.244030 1.772618
C -4.777829 -0.574701 0.720190
C -4.086001 0.137651 -0.228487
C 1.597132 -0.050287 0.133140
O -0.012059 -1.190149 1.957155
F -2.158860 3.143592 -3.946293
C 2.225160 -0.561364 -1.002259
C 3.607775 -0.760989 -1.012446

C 4.403686 -0.451919 0.098798
C 3.748027 0.075124 1.226223
C 2.372579 0.284629 1.247072
O -5.072279 -1.860193 2.560646
C -6.350125 -1.586567 1.966113
O -6.127116 -0.750953 0.815600
C 5.927980 -0.662730 0.122491
C 6.459159 -1.243977 -1.201509
C 6.291909 -1.644569 1.261951
C 6.631158 0.693126 0.371495
H 0.396665 3.104996 -3.419158
H 1.425308 1.794701 -1.593631
H -3.469436 1.707630 -2.282019
H -2.255050 -1.739784 2.705068
H -4.622597 0.640251 -1.022532
H 1.637642 -0.820366 -1.877711
H 4.055455 -1.167791 -1.911927
H 4.319810 0.338266 2.111325
H 1.897260 0.700913 2.127805
H -6.814367 -2.524792 1.647158
H -6.980733 -1.053586 2.683309
H 6.258914 -0.578825 -2.049282
H 7.544779 -1.375861 -1.134390
H 6.020188 -2.223500 -1.422673
H 5.977183 -1.268041 2.240842
H 7.377143 -1.798874 1.296303
H 5.814582 -2.619007 1.106984
H 7.718887 0.555995 0.397468
H 6.397962 1.408095 -0.426043
H 6.329095 1.141085 1.323963

24 Energy:-1306.88825423
C -1.601796 2.339283 -3.020850
C -0.232066 2.467409 -2.808280
C 0.337482 1.788834 -1.741483
C -0.433496 0.965692 -0.896779
C -1.836428 0.901169 -1.088283
C -2.398694 1.589907 -2.182303
N 0.179834 0.302486 0.194051
C -0.571104 -0.390618 1.158698
C -2.033802 -0.409072 0.990004
C -2.662932 0.170639 -0.130432
C -2.770080 -1.104305 1.981828
C -4.126474 -1.189921 1.811577
C -4.760908 -0.621471 0.698579
C -4.070630 0.056728 -0.276023
C 1.597863 0.012156 0.170882
O -0.019157 -0.983359 2.087411

F -2.170178 2.987539 -4.064134
C 2.222511 -0.422090 -0.999401
C 3.599817 -0.652870 -1.022797
C 4.401753 -0.442425 0.106551
C 3.754644 0.019494 1.266367
C 2.384077 0.257066 1.302858
O -5.057455 -1.792109 2.613699
C -6.326096 -1.619462 1.964209
O -6.103603 -0.850769 0.767727
C 5.920766 -0.687861 0.115056
C 6.439430 -1.192537 -1.244809
C 6.262683 -1.749974 1.187333
C 6.653591 0.632914 0.451913
H 0.366672 3.095992 -3.458378
H 1.397328 1.902330 -1.556738
H -3.463334 1.562157 -2.377143
H -2.253557 -1.543801 2.825361
H -4.602603 0.480737 -1.117584
H 1.636158 -0.609837 -1.892921
H 4.038264 -1.004049 -1.949893
H 4.330111 0.211774 2.167290
H 1.921851 0.626508 2.209459
H -6.736032 -2.597648 1.694532
H -7.003853 -1.071692 2.624922
H 6.255598 -0.468211 -2.046552
H 7.521592 -1.354162 -1.187428
H 5.977396 -2.144505 -1.530114
H 5.955559 -1.431758 2.189111
H 7.344281 -1.929891 1.210663
H 5.764292 -2.701545 0.969262
H 7.738051 0.470471 0.468774
H 6.437179 1.403478 -0.297114
H 6.360019 1.024263 1.431584

25 Energy:-1306.88500122
C -1.608379 2.243448 -3.092862
C -0.253698 2.448470 -2.845505
C 0.314687 1.833547 -1.740680
C -0.436552 0.993595 -0.894044
C -1.829510 0.864695 -1.115675
C -2.392506 1.487536 -2.248632
N 0.186878 0.403533 0.237100
C -0.573655 -0.255764 1.224124
C -2.031977 -0.328172 1.027478
C -2.652877 0.151559 -0.142754
C -2.768168 -0.986955 2.044201
C -4.115134 -1.137644 1.846202
C -4.740089 -0.670784 0.681873

C -4.049677 -0.030061 -0.317870
C 1.596878 0.065891 0.200406
O -0.034178 -0.786723 2.195867
F -2.176497 2.827056 -4.173363
C 2.226164 -0.289801 -0.995459
C 3.598012 -0.548670 -1.029114
C 4.400390 -0.432496 0.112842
C 3.755600 -0.035075 1.296764
C 2.389868 0.227401 1.345648
O -5.043266 -1.725429 2.662124
C -6.301901 -1.635187 1.977470
O -6.073516 -0.951997 0.731091
C 5.913700 -0.709536 0.109410
C 6.428952 -1.124154 -1.281798
C 6.227147 -1.854168 1.102532
C 6.672597 0.566850 0.545189
H 0.331817 3.088365 -3.496561
H 1.360539 2.009703 -1.526375
H -3.449998 1.407313 -2.466350
H -2.258988 -1.351883 2.926746
H -4.573289 0.314980 -1.199796
H 1.646840 -0.411199 -1.903993
H 4.031786 -0.844180 -1.977661
H 4.329898 0.090753 2.210216
H 1.937793 0.552726 2.272228
H -6.681367 -2.641012 1.774054
H -7.007062 -1.057700 2.582166
H 6.262910 -0.339872 -2.029199
H 7.507443 -1.311193 -1.232906
H 5.949519 -2.043357 -1.637219
H 5.919334 -1.603493 2.123097
H 7.304726 -2.057751 1.118515
H 5.711049 -2.776747 0.812729
H 7.753308 0.380397 0.553845
H 6.476326 1.394838 -0.145875
H 6.382648 0.891436 1.550043

26 Energy:-1306.8809055
C -1.615914 2.178103 -3.152021
C -0.284419 2.475566 -2.872818
C 0.283928 1.933141 -1.730868
C -0.438888 1.072282 -0.880636
C -1.812912 0.853624 -1.136002
C -2.378965 1.404598 -2.304341
N 0.195362 0.570446 0.291118
C -0.581169 -0.009111 1.321039
C -2.023853 -0.194338 1.075642
C -2.623303 0.138224 -0.154591

C -2.758205 -0.822037 2.113293
C -4.078497 -1.095672 1.870808
C -4.678277 -0.781715 0.643727
C -3.989779 -0.171577 -0.376671
C 1.592034 0.171250 0.242266
O -0.066967 -0.401639 2.368389
F -2.185572 2.692784 -4.265767
C 2.218234 -0.129410 -0.973059
C 3.577745 -0.442040 -1.022690
C 4.384593 -0.426511 0.121485
C 3.752235 -0.071568 1.323975
C 2.397659 0.242901 1.391215
O -4.996569 -1.692437 2.691636
C -6.229553 -1.737689 1.957675
O -5.984449 -1.172282 0.656541
C 5.885717 -0.761450 0.099911
C 6.383664 -1.120826 -1.312802
C 6.155208 -1.968609 1.029792
C 6.693572 0.459544 0.601373
H 0.279454 3.132477 -3.525975
H 1.309092 2.181878 -1.487818
H -3.425365 1.260866 -2.542515
H -2.267530 -1.073736 3.044460
H -4.490260 0.052161 -1.309797
H 1.642972 -0.182316 -1.889560
H 3.998414 -0.697968 -1.988621
H 4.328920 -0.015587 2.243036
H 1.965754 0.539460 2.334496
H -6.550651 -2.777056 1.845185
H -6.986263 -1.139857 2.474729
H 6.248773 -0.291467 -2.016527
H 7.453861 -1.353142 -1.276979
H 5.867526 -1.999633 -1.715886
H 5.858023 -1.760815 2.063081
H 7.224061 -2.214569 1.032161
H 5.603485 -2.853773 0.692721
H 7.766323 0.231357 0.598710
H 6.529854 1.329919 -0.044615
H 6.415422 0.741336 1.622362

27 Energy:-1306.87643617
C -1.644872 2.124388 -3.228136
C -0.344262 2.527802 -2.935725
C 0.234779 2.072039 -1.761131
C -0.444400 1.194513 -0.893805
C -1.790574 0.865295 -1.167947
C -2.370841 1.330772 -2.365577
N 0.203680 0.788675 0.310882

C -0.593248 0.337200 1.392937
C -2.000040 -0.014411 1.110877
C -2.568442 0.139194 -0.168260
C -2.721811 -0.612422 2.174193
C -3.992286 -1.048633 1.902372
C -4.555351 -0.919181 0.625651
C -3.880509 -0.334845 -0.419522
C 1.583120 0.326263 0.263193
O -0.121126 0.167312 2.516002
F -2.225993 2.557532 -4.369907
C 2.218067 0.074168 -0.961654
C 3.557872 -0.312162 -1.016436
C 4.348406 -0.424098 0.133120
C 3.714480 -0.119663 1.347135
C 2.379294 0.269749 1.422218
O -4.884595 -1.664227 2.737655
C -6.065269 -1.912633 1.959661
O -5.811237 -1.449128 0.620356
C 5.828729 -0.839943 0.105464
C 6.326077 -1.132057 -1.322879
C 6.018818 -2.118992 0.955322
C 6.694897 0.298233 0.696260
H 0.184227 3.200073 -3.602658
H 1.233627 2.402579 -1.503649
H -3.402073 1.109687 -2.611377
H -2.259650 -0.721429 3.146661
H -4.347416 -0.254720 -1.392943
H 1.661918 0.106285 -1.889447
H 3.975873 -0.524788 -1.994128
H 4.276039 -0.161116 2.276519
H 1.954581 0.525799 2.378773
H -6.269869 -2.986692 1.937365
H -6.906606 -1.354533 2.381594
H 6.247558 -0.251375 -1.970573
H 7.381073 -1.426453 -1.291810
H 5.767327 -1.951354 -1.789588
H 5.718161 -1.963838 1.996839
H 7.072583 -2.423264 0.953275
H 5.424860 -2.948195 0.553787
H 7.753565 0.011548 0.690914
H 6.588800 1.217101 0.107985
H 6.416581 0.527031 1.730405

28 Energy:-1306.87246673
C -1.709360 2.051014 -3.326709
C -0.441410 2.554608 -3.049087
C 0.164383 2.185289 -1.856085
C -0.456912 1.296992 -0.959620

C -1.776123 0.865359 -1.221269
C -2.384607 1.243919 -2.433945
N 0.210712 0.969094 0.259707
C -0.596740 0.648693 1.382364
C -1.958445 0.141607 1.111951
C -2.506103 0.137393 -0.185724
C -2.651241 -0.426478 2.209466
C -3.868833 -1.001612 1.950593
C -4.407224 -1.031610 0.657253
C -3.761449 -0.474378 -0.421633
C 1.577676 0.470962 0.229081
O -0.161614 0.704424 2.530186
F -2.315770 2.400359 -4.483682
C 2.260535 0.303107 -0.985746
C 3.581478 -0.146920 -1.021080
C 4.308583 -0.422909 0.141433
C 3.625390 -0.221098 1.349803
C 2.310061 0.232178 1.407874
O -4.720081 -1.631993 2.817117
C -5.864182 -2.028234 2.045705
O -5.606288 -1.679740 0.672694
C 5.767265 -0.909142 0.135906
C 6.323607 -1.065761 -1.291972
C 5.854493 -2.282680 0.843056
C 6.653323 0.110092 0.891402
H 0.040173 3.237588 -3.740195
H 1.134152 2.598231 -1.605445
H -3.399904 0.947718 -2.668059
H -2.208651 -0.409783 3.197115
H -4.206665 -0.515921 -1.407802
H 1.758317 0.450840 -1.931536
H 4.034808 -0.278670 -1.997434
H 4.131686 -0.400491 2.294520
H 1.853980 0.403620 2.369131
H -6.001435 -3.109930 2.123886
H -6.748599 -1.486684 2.396049
H 6.317253 -0.115782 -1.838609
H 7.361497 -1.414219 -1.246430
H 5.753361 -1.799167 -1.873583
H 5.508183 -2.228817 1.880631
H 6.891806 -2.638899 0.855058
H 5.244372 -3.030527 0.323302
H 7.696489 -0.228652 0.903583
H 6.620747 1.092682 0.406520
H 6.331829 0.237415 1.930530

29 Energy:-1306.86940084
C -1.779364 1.945200 -3.421209

C -0.537859 2.521497 -3.172269
C 0.096492 2.224195 -1.972140
C -0.470516 1.333834 -1.044349
C -1.772948 0.835047 -1.275162
C -2.409943 1.140897 -2.492073
N 0.215937 1.056958 0.177415
C -0.586411 0.835036 1.327181
C -1.924407 0.250236 1.099122
C -2.465100 0.129750 -0.196635
C -2.594162 -0.270466 2.232950
C -3.780169 -0.923575 2.012198
C -4.308038 -1.072706 0.722969
C -3.685637 -0.559820 -0.391941
C 1.579776 0.554255 0.168272
O -0.155487 1.026551 2.460897
F -2.411926 2.223390 -4.583328
C 2.340666 0.516779 -1.010339
C 3.650803 0.032179 -1.017095
C 4.287984 -0.420169 0.141539
C 3.521626 -0.366886 1.315794
C 2.216497 0.114778 1.345507
O -4.603078 -1.534367 2.919073
C -5.720560 -2.042736 2.174718
O -5.472036 -1.779538 0.781099
C 5.732834 -0.944707 0.169534
C 6.386923 -0.923435 -1.224904
C 5.741737 -2.403148 0.686414
C 6.582270 -0.063499 1.116436
H -0.098874 3.207079 -3.888685
H 1.036653 2.708629 -1.738699
H -3.414521 0.793952 -2.701985
H -2.158773 -0.162095 3.218190
H -4.122735 -0.691977 -1.373981
H 1.914511 0.799494 -1.961388
H 4.167632 0.017204 -1.970474
H 3.950019 -0.699129 2.257668
H 1.700645 0.155566 2.291658
H -5.802672 -3.121777 2.329268
H -6.633695 -1.523906 2.483249
H 6.439141 0.091545 -1.635257
H 7.411515 -1.305971 -1.156865
H 5.844845 -1.553898 -1.939038
H 5.322002 -2.480092 1.695033
H 6.768283 -2.787880 0.721785
H 5.156724 -3.055776 0.028004
H 7.614940 -0.431354 1.154267
H 6.604289 0.976081 0.769396
H 6.188691 -0.068138 2.138448

30 Energy:-1306.86743765
C -1.853587 1.780299 -3.515016
C -0.629619 2.404814 -3.306651
C 0.033173 2.174429 -2.105496
C -0.487182 1.298543 -1.138654
C -1.785490 0.764336 -1.324276
C -2.449255 1.001574 -2.540729
N 0.218822 1.050666 0.077152
C -0.558485 0.910787 1.254264
C -1.898306 0.311871 1.083240
C -2.451660 0.108315 -0.197412
C -2.550939 -0.141912 2.254585
C -3.733702 -0.817096 2.088079
C -4.272618 -1.051654 0.816405
C -3.666834 -0.603788 -0.335378
C 1.594223 0.587410 0.091246
O -0.098356 1.169886 2.362339
F -2.511095 1.990347 -4.677629
C 2.452250 0.732485 -1.007634
C 3.761184 0.241146 -0.980352
C 4.294620 -0.408779 0.134431
C 3.423326 -0.557716 1.225700
C 2.118581 -0.078806 1.217235
O -4.541078 -1.378058 3.039940
C -5.665604 -1.933449 2.341116
O -5.428930 -1.764343 0.930948
C 5.734033 -0.944248 0.200854
C 6.515111 -0.676148 -1.099397
C 5.705007 -2.472418 0.442312
C 6.484759 -0.258213 1.367185
H -0.225137 3.080115 -4.052537
H 0.943735 2.721387 -1.900492
H -3.448929 0.623422 -2.717883
H -2.105246 0.029716 3.226231
H -4.114031 -0.800094 -1.302018
H 2.118876 1.181204 -1.929584
H 4.361185 0.384803 -1.872289
H 3.762227 -1.065093 2.124889
H 1.516318 -0.221904 2.101490
H -5.747135 -2.999503 2.568183
H -6.575668 -1.393759 2.622198
H 6.594229 0.395866 -1.313406
H 7.532917 -1.071135 -1.005671
H 6.048995 -1.164130 -1.963065
H 5.193762 -2.727384 1.376674
H 6.726520 -2.867350 0.502244
H 5.188528 -2.988469 -0.375371

H 7.511746 -0.637620 1.433936
H 6.532175 0.826768 1.218293
H 5.997108 -0.444034 2.330035

31 Energy:-1306.88495076
C -1.735557 1.052196 -3.620579
C -0.421472 0.600575 -3.707397
C 0.169734 0.071728 -2.570478
C -0.515484 0.012415 -1.340188
C -1.876306 0.402184 -1.293138
C -2.462393 0.946070 -2.454608
N 0.126298 -0.560130 -0.210344
C -0.594506 -0.845220 0.967215
C -2.026489 -0.499007 0.991943
C -2.651029 0.175312 -0.075998
C -2.723119 -0.804416 2.188213
C -4.035695 -0.420528 2.265581
C -4.662754 0.258376 1.211927
C -4.009895 0.567735 0.043671
C 1.564835 -0.456435 -0.058021
O -0.038173 -1.328327 1.954307
F -2.324557 1.580457 -4.718254
C 2.271142 0.633538 -0.573645
C 3.663143 0.690235 -0.478180
C 4.407088 -0.345282 0.101195
C 3.681436 -1.450771 0.577212
C 2.294470 -1.522171 0.488165
O -4.921493 -0.590434 3.294732
C -6.163894 -0.016866 2.860628
O -5.955332 0.534573 1.547327
C 5.940661 -0.314704 0.220223
C 6.546265 0.978124 -0.358357
C 6.541016 -1.516153 -0.548596
C 6.341210 -0.411180 1.711762
H 0.113905 0.648924 -4.649310
H 1.181198 -0.306870 -2.636619
H -3.496329 1.266872 -2.464296
H -2.211119 -1.313929 2.994129
H -4.533096 1.094177 -0.743915
H 1.740921 1.469598 -1.015972
H 4.159722 1.569428 -0.872697
H 4.205942 -2.293395 1.018737
H 1.777496 -2.401542 0.846126
H -6.929220 -0.797292 2.807620
H -6.456915 0.783290 3.546076
H 6.180487 1.869420 0.164113
H 7.636143 0.954059 -0.248207
H 6.324344 1.091138 -1.425698

H 6.181886 -2.472989 -0.155293
H 7.634587 -1.510694 -0.465660
H 6.280872 -1.470343 -1.612493
H 7.433260 -0.399505 1.812492
H 5.938200 0.434177 2.281338
H 5.973091 -1.333333 2.173478

32 Energy:-1306.88821583
C -1.739663 0.942087 -3.647304
C -0.401093 0.563313 -3.696923
C 0.198743 0.102497 -2.534724
C -0.508582 0.035746 -1.317850
C -1.887614 0.362752 -1.301926
C -2.480535 0.836648 -2.489850
N 0.132131 -0.459039 -0.155641
C -0.574496 -0.702906 1.034477
C -2.018803 -0.415481 1.032918
C -2.664478 0.156839 -0.081942
C -2.711681 -0.680591 2.240711
C -4.043107 -0.361865 2.283270
C -4.692920 0.212826 1.182425
C -4.044222 0.481326 0.001985
C 1.573197 -0.397101 -0.032066
O 0.003278 -1.109834 2.043965
F -2.336279 1.402608 -4.771468
C 2.283476 0.721571 -0.470838
C 3.677667 0.750341 -0.392457
C 4.410539 -0.335338 0.104545
C 3.675416 -1.461031 0.516420
C 2.286657 -1.504766 0.440787
O -4.931059 -0.514353 3.313299
C -6.193613 -0.023201 2.837963
O -6.002899 0.438236 1.487876
C 5.946035 -0.336152 0.204574
C 6.565278 0.983476 -0.293364
C 6.516777 -1.491647 -0.652146
C 6.364139 -0.539651 1.680556
H 0.149267 0.617224 -4.629885
H 1.232017 -0.215773 -2.571600
H -3.527924 1.108177 -2.525625
H -2.182750 -1.112364 3.080495
H -4.586524 0.926376 -0.822039
H 1.753765 1.588984 -0.850895
H 4.185111 1.646536 -0.730734
H 4.193530 -2.336284 0.897553
H 1.754606 -2.394444 0.752957
H -6.927440 -0.834719 2.842381
H -6.519910 0.813015 3.463061

H 6.221328 1.842640 0.293707
H 7.655928 0.934801 -0.200586
H 6.331394 1.172481 -1.347311
H 6.146689 -2.467298 -0.320042
H 7.611197 -1.508938 -0.583645
H 6.244349 -1.369312 -1.706876
H 7.457450 -0.550299 1.766232
H 5.981509 0.270769 2.311615
H 5.988646 -1.485793 2.084231

33 Energy:-1306.89061252
C -1.744056 0.825242 -3.671612
C -0.386104 0.520534 -3.689458
C 0.221362 0.132601 -2.504346
C -0.503212 0.061470 -1.298466
C -1.896447 0.325692 -1.308510
C -2.495584 0.724450 -2.520227
N 0.137882 -0.350480 -0.108264
C -0.557147 -0.554365 1.091551
C -2.011013 -0.323574 1.069353
C -2.673581 0.144860 -0.084287
C -2.700759 -0.547756 2.286961
C -4.046948 -0.295327 2.301151
C -4.714623 0.173768 1.161576
C -4.069275 0.401354 -0.029147
C 1.580473 -0.329692 -0.009344
O 0.037501 -0.888601 2.118289
F -2.347511 1.213011 -4.819664
C 2.301428 0.809257 -0.367005
C 3.696986 0.807749 -0.304061
C 4.413500 -0.324326 0.106913
C 3.663708 -1.464328 0.448815
C 2.273777 -1.477911 0.384600
O -4.935753 -0.427329 3.333286
C -6.218910 -0.043129 2.816444
O -6.037508 0.349886 1.443732
C 5.949852 -0.358715 0.190626
C 6.588699 0.979171 -0.227562
C 6.491571 -1.466037 -0.744916
C 6.377446 -0.664494 1.646153
H 0.175458 0.577549 -4.615560
H 1.272192 -0.123729 -2.515006
H -3.553829 0.945446 -2.578420
H -2.158502 -0.900537 3.154785
H -4.626239 0.764433 -0.883069
H 1.777976 1.706902 -0.681488
H 4.218869 1.716012 -0.582773
H 4.170733 -2.370606 0.766787

H 1.724062 -2.374842 0.645594
H -6.902310 -0.896559 2.860970
H -6.604039 0.806279 3.387736
H 6.268173 1.804229 0.418649
H 7.679131 0.904229 -0.151529
H 6.346847 1.241148 -1.263953
H 6.108387 -2.454949 -0.472221
H 7.586124 -1.505735 -0.689860
H 6.210794 -1.271475 -1.786523
H 7.471105 -0.699409 1.719782
H 6.014998 0.109865 2.332002
H 5.988842 -1.628149 1.991779

34 Energy:-1306.89224062
C -1.743067 0.684394 -3.695630
C -0.370976 0.451452 -3.685937
C 0.240406 0.139850 -2.480073
C -0.498727 0.070261 -1.283579
C -1.901962 0.274701 -1.316023
C -2.504086 0.594408 -2.549139
N 0.141829 -0.258262 -0.070259
C -0.545485 -0.418930 1.136663
C -2.006230 -0.239391 1.097455
C -2.679767 0.125444 -0.087550
C -2.694548 -0.417496 2.323196
C -4.050700 -0.224914 2.314961
C -4.729854 0.139373 1.144296
C -4.086263 0.320320 -0.055312
C 1.584992 -0.269529 0.012581
O 0.060713 -0.682000 2.177568
F -2.350155 0.995257 -4.865240
C 2.315900 0.887495 -0.250536
C 3.711856 0.862260 -0.198794
C 4.414112 -0.310208 0.112465
C 3.651855 -1.465140 0.366720
C 2.261295 -1.454445 0.311808
O -4.941110 -0.334205 3.348356
C -6.233890 -0.025217 2.805659
O -6.062106 0.269675 1.407424
C 5.950568 -0.372365 0.179920
C 6.605835 0.987474 -0.127440
C 6.468622 -1.402525 -0.852269
C 6.384638 -0.807883 1.600049
H 0.199592 0.507136 -4.606618
H 1.304184 -0.055960 -2.466374
H -3.570208 0.766123 -2.627356
H -2.143777 -0.692475 3.213599
H -4.652628 0.602038 -0.933469

H 1.798617 1.812198 -0.488811
H 4.245769 1.782637 -0.405421
H 4.149117 -2.399898 0.608401
H 1.697898 -2.361061 0.505672
H -6.893073 -0.891554 2.914156
H -6.643392 0.853328 3.312922
H 6.301983 1.758638 0.589526
H 7.695510 0.890795 -0.066813
H 6.360998 1.340586 -1.135690
H 6.072554 -2.405671 -0.662569
H 7.562812 -1.462432 -0.810398
H 6.183091 -1.114703 -1.870735
H 7.478206 -0.863353 1.660831
H 6.038111 -0.090665 2.352951
H 5.985467 -1.792476 1.865120

35 Energy:-1306.89327076
C -1.744818 0.532083 -3.717209
C -0.364070 0.359311 -3.689308
C 0.250507 0.121933 -2.467980
C -0.497284 0.063224 -1.276856
C -1.906325 0.219091 -1.323445
C -2.511133 0.461736 -2.572469
N 0.144401 -0.185266 -0.047434
C -0.536327 -0.305195 1.165020
C -2.001151 -0.163402 1.116374
C -2.682385 0.109439 -0.089399
C -2.687209 -0.292440 2.349289
C -4.048838 -0.144140 2.328204
C -4.735773 0.128377 1.137307
C -4.094656 0.259626 -0.070069
C 1.587681 -0.220872 0.023503
O 0.078505 -0.508268 2.214471
F -2.354913 0.767836 -4.902904
C 2.326737 0.949714 -0.131175
C 3.722549 0.906960 -0.084873
C 4.413477 -0.296270 0.116060
C 3.641623 -1.463111 0.265733
C 2.250881 -1.434245 0.215659
O -4.938337 -0.220477 3.365370
C -6.239130 0.010509 2.803300
O -6.072363 0.231292 1.390914
C 5.949505 -0.378833 0.174543
C 6.617311 0.997412 -0.006952
C 6.456396 -1.314052 -0.949451
C 6.380982 -0.948029 1.547377
H 0.211115 0.406094 -4.607620
H 1.322306 -0.022355 -2.436667

H -3.582146 0.591663 -2.664189
H -2.130673 -0.498378 3.254692
H -4.666958 0.470887 -0.964058
H 1.814834 1.895449 -0.283851
H 4.265825 1.836899 -0.206797
H 4.131145 -2.419845 0.421670
H 1.677075 -2.348580 0.329822
H -6.867430 -0.871370 2.959879
H -6.681737 0.901223 3.258848
H 6.320950 1.701876 0.778498
H 7.706036 0.885461 0.043120
H 6.375482 1.444242 -0.978062
H 6.050314 -2.326436 -0.852656
H 7.549948 -1.388528 -0.915000
H 6.173144 -0.930345 -1.936447
H 7.474116 -1.017176 1.601052
H 6.040571 -0.301477 2.364318
H 5.974769 -1.950159 1.720112

36 Energy:-1306.89381672
C -1.751920 0.376934 -3.734899
C -0.365840 0.255913 -3.697181
C 0.252705 0.089805 -2.465960
C -0.498410 0.047246 -1.276623
C -1.911035 0.161587 -1.330509
C -2.519655 0.330635 -2.589609
N 0.146626 -0.124957 -0.037353
C -0.528081 -0.205881 1.179965
C -1.995630 -0.094474 1.127174
C -2.683732 0.093978 -0.091177
C -2.678266 -0.174216 2.365987
C -4.043306 -0.061940 2.338704
C -4.737012 0.126330 1.135530
C -4.099487 0.207543 -0.078123
C 1.589808 -0.179205 0.024588
O 0.093540 -0.355907 2.234434
F -2.365767 0.540766 -4.930853
C 2.335865 0.996058 -0.010307
C 3.731125 0.939181 0.035729
C 4.413108 -0.283147 0.118514
C 3.633614 -1.454025 0.150949
C 2.242888 -1.410387 0.101722
O -4.930471 -0.103049 3.379857
C -6.237036 0.059867 2.807425
O -6.075918 0.208733 1.385022
C 5.948463 -0.380999 0.173900
C 6.625640 1.001759 0.124737
C 6.454286 -1.209735 -1.031163

C 6.370507 -1.079272 1.488873
H 0.210484 0.289353 -4.615366
H 1.329426 -0.009715 -2.424418
H -3.593875 0.424177 -2.688474
H -2.116767 -0.317109 3.280468
H -4.676752 0.354088 -0.981840
H 1.829004 1.954802 -0.070953
H 4.281501 1.872484 0.008089
H 4.116349 -2.424732 0.214875
H 1.661668 -2.327242 0.126454
H -6.839880 -0.829966 3.012047
H -6.705319 0.960747 3.214665
H 6.331378 1.631046 0.972322
H 7.713432 0.878245 0.166962
H 6.389855 1.539785 -0.800546
H 6.043049 -2.224613 -1.030692
H 7.547319 -1.292821 -1.000625
H 6.176323 -0.733939 -1.978773
H 7.462859 -1.162140 1.538900
H 6.032352 -0.508893 2.361570
H 5.955510 -2.089614 1.566248

37 Energy:-1306.89399056
C -1.766259 0.213222 -3.749236
C -0.376588 0.145395 -3.708927
C 0.247840 0.052084 -2.472980
C -0.501733 0.026000 -1.282330
C -1.917043 0.097080 -1.337587
C -2.531655 0.190997 -2.601564
N 0.149321 -0.071679 -0.038608
C -0.519379 -0.110713 1.183610
C -1.989099 -0.030705 1.130832
C -2.684825 0.071630 -0.093596
C -2.666550 -0.059810 2.374656
C -4.034064 0.016557 2.346425
C -4.735377 0.118306 1.137229
C -4.103092 0.147730 -0.081512
C 1.592206 -0.138689 0.017063
O 0.108426 -0.205445 2.240870
F -2.385842 0.303600 -4.950071
C 2.343760 1.029632 0.109294
C 3.738147 0.960154 0.160506
C 4.413477 -0.268158 0.120591
C 3.628462 -1.431755 0.025489
C 2.238035 -1.375414 -0.025915
O -4.917614 0.007875 3.391489
C -6.227747 0.129882 2.817081
O -6.075557 0.176559 1.386706

C 5.947804 -0.380170 0.178203
C 6.632300 0.996273 0.277588
C 6.460293 -1.083186 -1.101575
C 6.354289 -1.212765 1.417763
H 0.197949 0.165168 -4.628627
H 1.327779 -0.001772 -2.428209
H -3.608343 0.246799 -2.702179
H -2.099321 -0.138959 3.293342
H -4.686078 0.227873 -0.989888
H 1.841457 1.991953 0.144121
H 4.293643 1.887914 0.234294
H 4.106210 -2.406429 -0.007524
H 1.651791 -2.286933 -0.096391
H -6.828810 -0.742647 3.088520
H -6.693961 1.057968 3.161804
H 6.334353 1.536337 1.183432
H 7.719075 0.862613 0.315064
H 6.406791 1.628358 -0.588908
H 6.043609 -2.090076 -1.209567
H 7.552521 -1.175841 -1.070197
H 6.193781 -0.510313 -1.997355
H 7.445693 -1.306946 1.468398
H 6.011009 -0.733226 2.341589
H 5.933438 -2.223242 1.387055

12.3.5 Potential scan of compound 5b excited state (B3LYP/6-31G* PCM CH_2Cl_2)

D(4,7,15,18)
7 -1306.88679547 89.9445
23 -1306.88558948 99.9445
32 -1306.88292221 109.9446
38 -1306.88085697 119.9445
44 -1306.87868586 129.9444
52 -1306.87355915 139.9444
62 -1306.84986482 149.9446
68 -1306.84608602 159.9446
73 -1306.84388801 169.9445
78 -1306.84238895 179.9446
83 -1306.84122216 -170.0555
87 -1306.84020717 -160.0556
91 -1306.83925325 -150.0556
96 -1306.83846514 -140.0557
100 -1306.83799436 -130.0557
105 -1306.83763537 -120.0556
147 -1306.88289445 -110.0555
157 -1306.88547947 -100.0555
164 -1306.88675061 -90.0555

175 -1306.88568317 -80.0555
183 -1306.88273569 -70.0555
189 -1306.88062702 -60.0554
195 -1306.87833346 -50.0555
204 -1306.87107662 -40.0555
215 -1306.84864298 -30.0554
220 -1306.84627099 -20.0554
225 -1306.84428315 -10.0555
230 -1306.84277725 -0.0554
235 -1306.8413697 9.9445
240 -1306.84013661 19.9444
245 -1306.83890187 29.9444
249 -1306.83766887 39.9443
253 -1306.83647347 49.9443
259 -1306.83558386 59.9444
265 -1306.83592743 69.9444
295 -1306.8857163 79.9444
303 -1306.88677465 89.9445

Progress of structural optimization and emission calculation

-1306.893999 -1306.753157 323.51 nm
-1306.889711 -1306.759729 350.54 nm
-1306.886844 -1306.760427 360.42 nm
-1306.886672 -1306.760473 361.04 nm
-1306.886715 -1306.760485 360.96 nm
-1306.886765 -1306.760489 360.82 nm
-1306.886805 -1306.760491 360.72 nm
-1306.886795 -1306.760492 360.74 nm
-1306.886453 -1306.760321 361.24 nm
-1306.886548 -1306.760512 361.51 nm
-1306.886497 -1306.760589 361.88 nm
-1306.886105 -1306.760662 363.22 nm
-1306.885959 -1306.760714 363.79 nm
-1306.885533 -1306.760757 365.16 nm
-1306.885625 -1306.760761 364.9 nm
-1306.885607 -1306.760761 364.96 nm
-1306.885599 -1306.760761 364.98 nm
-1306.8856 -1306.760761 364.98 nm
-1306.885606 -1306.760761 364.96 nm
-1306.885612 -1306.760761 364.94 nm
-1306.885613 -1306.760762 364.94 nm
-1306.885606 -1306.760762 364.96 nm
-1306.885597 -1306.760763 364.99 nm
-1306.885589 -1306.760763 365.01 nm
-1306.885282 -1306.76104 366.73 nm
-1306.883568 -1306.761347 372.8 nm
-1306.883429 -1306.761384 373.33 nm

-1306.882949 -1306.7614 374.86 nm
-1306.88296 -1306.761404 374.83 nm
-1306.882903 -1306.761405 375.01 nm
-1306.882915 -1306.761406 374.98 nm
-1306.882921 -1306.761406 374.96 nm
-1306.882922 -1306.761406 374.96 nm
-1306.88241 -1306.761791 377.75 nm
-1306.880492 -1306.762006 384.55 nm
-1306.881254 -1306.762024 382.15 nm
-1306.880894 -1306.762031 383.33 nm
-1306.880865 -1306.762031 383.42 nm
-1306.880857 -1306.762031 383.45 nm
-1306.879772 -1306.761919 386.61 nm
-1306.878918 -1306.762159 390.23 nm
-1306.878677 -1306.76217 391.08 nm
-1306.878689 -1306.762172 391.04 nm
-1306.878689 -1306.762173 391.05 nm
-1306.878686 -1306.762173 391.06 nm
-1306.876899 -1306.761272 394.06 nm
-1306.875849 -1306.761606 398.83 nm
-1306.875091 -1306.761644 401.63 nm
-1306.874194 -1306.761668 404.91 nm
-1306.873897 -1306.761673 406 nm
-1306.873608 -1306.761677 407.07 nm
-1306.87356 -1306.761677 407.24 nm
-1306.873559 -1306.761677 407.24 nm
-1306.871642 -1306.760537 410.1 nm
-1306.864341 -1306.761936 444.93 nm
-1306.857266 -1306.762668 481.65 nm
-1306.854283 -1306.763257 500.55 nm
-1306.850841 -1306.763503 521.69 nm
-1306.850972 -1306.763588 521.42 nm
-1306.849865 -1306.763621 528.3 nm
-1306.849957 -1306.763628 527.79 nm
-1306.849829 -1306.763629 528.58 nm
-1306.849865 -1306.76363 528.36 nm
-1306.85055 -1306.765758 537.36 nm
-1306.844298 -1306.766145 583 nm
-1306.846608 -1306.766205 566.68 nm
-1306.846173 -1306.766211 569.82 nm
-1306.846097 -1306.766212 570.36 nm
-1306.846086 -1306.766212 570.44 nm
-1306.84679 -1306.767902 577.57 nm
-1306.844041 -1306.768279 601.39 nm
-1306.844044 -1306.76829 601.46 nm
-1306.843838 -1306.768292 603.12 nm
-1306.843888 -1306.768292 602.72 nm
-1306.844476 -1306.769228 605.51 nm

-1306.842096 -1306.769556 628.12 nm
-1306.842442 -1306.769562 625.19 nm
-1306.84238 -1306.769562 625.72 nm
-1306.842389 -1306.769563 625.64 nm
-1306.842655 -1306.769458 622.47 nm
-1306.840917 -1306.769746 640.19 nm
-1306.841235 -1306.769749 637.38 nm
-1306.841222 -1306.76975 637.5 nm
-1306.841222 -1306.76975 637.49 nm
-1306.841035 -1306.76839 627.21 nm
-1306.840037 -1306.768669 638.43 nm
-1306.840181 -1306.768672 637.17 nm
-1306.840207 -1306.768672 636.94 nm
-1306.8395 -1306.766004 619.95 nm
-1306.839083 -1306.766299 626.01 nm
-1306.839229 -1306.766301 624.78 nm
-1306.839253 -1306.766302 624.57 nm
-1306.838025 -1306.762369 602.25 nm
-1306.83841 -1306.762706 601.86 nm
-1306.83841 -1306.76271 601.89 nm
-1306.838476 -1306.76271 601.38 nm
-1306.838465 -1306.76271 601.46 nm
-1306.836798 -1306.757773 576.57 nm
-1306.837949 -1306.758203 571.35 nm
-1306.837985 -1306.758208 571.13 nm
-1306.837994 -1306.758208 571.07 nm
-1306.836106 -1306.752666 546.06 nm
-1306.837351 -1306.753171 541.26 nm
-1306.83752 -1306.753187 540.28 nm
-1306.837617 -1306.753189 539.67 nm
-1306.837635 -1306.753189 539.55 nm
-1306.835712 -1306.747444 516.19 nm
-1306.837314 -1306.748066 510.53 nm
-1306.83808 -1306.748108 506.41 nm
-1306.839027 -1306.748133 501.28 nm
-1306.839868 -1306.748148 496.76 nm
-1306.840835 -1306.748158 491.64 nm
-1306.841442 -1306.748161 488.46 nm
-1306.841812 -1306.748163 486.53 nm
-1306.841958 -1306.748163 485.77 nm
-1306.84267 -1306.748164 482.12 nm
-1306.847713 -1306.748069 457.26 nm
-1306.833597 -1306.741338 493.87 nm
-1306.828791 -1306.741202 520.2 nm
-1306.836716 -1306.745107 497.36 nm
-1306.836931 -1306.745082 496.07 nm
-1306.837698 -1306.746524 499.74 nm
-1306.842667 -1306.748164 482.14 nm

-1306.854382 -1306.74842 429.99 nm
-1306.857547 -1306.749191 420.5 nm
-1306.866487 -1306.750308 392.18 nm
-1306.87247 -1306.752669 380.33 nm
-1306.871245 -1306.752267 382.95 nm
-1306.879206 -1306.756433 371.12 nm
-1306.881673 -1306.757871 368.03 nm
-1306.882992 -1306.758327 365.49 nm
-1306.884398 -1306.758651 362.34 nm
-1306.884978 -1306.75916 362.14 nm
-1306.885364 -1306.759564 362.19 nm
-1306.885502 -1306.759895 362.74 nm
-1306.885364 -1306.760072 363.66 nm
-1306.884745 -1306.760432 366.52 nm
-1306.883665 -1306.760733 370.64 nm
-1306.883626 -1306.761179 372.11 nm
-1306.883739 -1306.761379 372.37 nm
-1306.882704 -1306.7614 375.61 nm
-1306.882819 -1306.761403 375.27 nm
-1306.883417 -1306.761406 373.44 nm
-1306.882692 -1306.761425 375.73 nm
-1306.882875 -1306.761429 375.17 nm
-1306.882877 -1306.76143 375.17 nm
-1306.882883 -1306.76143 375.15 nm
-1306.882894 -1306.76143 375.12 nm
-1306.88264 -1306.760424 372.81 nm
-1306.884272 -1306.760699 368.72 nm
-1306.885141 -1306.760752 366.3 nm
-1306.885457 -1306.760762 365.4 nm
-1306.885543 -1306.760765 365.15 nm
-1306.88557 -1306.760767 365.08 nm
-1306.88555 -1306.760768 365.14 nm
-1306.885479 -1306.760769 365.35 nm
-1306.885478 -1306.760769 365.36 nm
-1306.885479 -1306.760769 365.35 nm
-1306.885083 -1306.760012 364.3 nm
-1306.886409 -1306.760378 361.53 nm
-1306.886667 -1306.760438 360.96 nm
-1306.886753 -1306.760461 360.78 nm
-1306.886756 -1306.760467 360.79 nm
-1306.886749 -1306.76047 360.82 nm
-1306.886751 -1306.76047 360.81 nm
-1306.886445 -1306.760278 361.13 nm
-1306.886035 -1306.760631 363.33 nm
-1306.885905 -1306.760671 363.83 nm
-1306.885699 -1306.760679 364.45 nm
-1306.885706 -1306.76068 364.43 nm
-1306.885705 -1306.76068 364.44 nm

-1306.8857 -1306.76068 364.45 nm
-1306.885696 -1306.760681 364.46 nm
-1306.885672 -1306.76068 364.53 nm
-1306.885688 -1306.760681 364.49 nm
-1306.885683 -1306.760681 364.5 nm
-1306.885332 -1306.76085 366.02 nm
-1306.883212 -1306.761261 373.62 nm
-1306.882963 -1306.761318 374.56 nm
-1306.882705 -1306.76133 375.39 nm
-1306.882714 -1306.761331 375.37 nm
-1306.882758 -1306.761331 375.23 nm
-1306.882735 -1306.761331 375.31 nm
-1306.882736 -1306.761331 375.3 nm
-1306.882235 -1306.761669 377.91 nm
-1306.879931 -1306.761919 386.09 nm
-1306.880908 -1306.761942 383 nm
-1306.880652 -1306.761951 383.85 nm
-1306.880635 -1306.761951 383.91 nm
-1306.880627 -1306.761951 383.93 nm
-1306.87948 -1306.761788 387.14 nm
-1306.878387 -1306.762059 391.68 nm
-1306.878346 -1306.762068 391.85 nm
-1306.87837 -1306.762069 391.77 nm
-1306.878334 -1306.762069 391.89 nm
-1306.878333 -1306.762069 391.89 nm
-1306.876339 -1306.761122 395.46 nm
-1306.875116 -1306.761539 401.17 nm
-1306.87393 -1306.761606 405.64 nm
-1306.872977 -1306.761643 409.25 nm
-1306.872266 -1306.761655 411.93 nm
-1306.871489 -1306.761662 414.87 nm
-1306.871094 -1306.761663 416.37 nm
-1306.871054 -1306.761663 416.52 nm
-1306.871077 -1306.761664 416.43 nm
-1306.869146 -1306.760918 420.99 nm
-1306.860582 -1306.762748 465.72 nm
-1306.853861 -1306.763451 503.96 nm
-1306.851495 -1306.763603 518.4 nm
-1306.847605 -1306.763981 544.86 nm
-1306.849738 -1306.764171 532.49 nm
-1306.849064 -1306.764212 536.98 nm
-1306.848082 -1306.764218 543.3 nm
-1306.848867 -1306.764221 538.29 nm
-1306.848622 -1306.764222 539.85 nm
-1306.848643 -1306.764222 539.72 nm
-1306.849096 -1306.766016 548.43 nm
-1306.845248 -1306.766457 578.28 nm
-1306.846599 -1306.766485 568.74 nm

-1306.846289 -1306.76649 570.98 nm
-1306.846271 -1306.76649 571.1 nm
-1306.846723 -1306.767827 577.51 nm
-1306.844543 -1306.768236 597.11 nm
-1306.844444 -1306.768249 597.98 nm
-1306.844271 -1306.76825 599.35 nm
-1306.844283 -1306.768251 599.26 nm
-1306.844643 -1306.768996 602.32 nm
-1306.842605 -1306.769328 621.79 nm
-1306.842807 -1306.769332 620.12 nm
-1306.842741 -1306.769333 620.68 nm
-1306.842777 -1306.769333 620.38 nm
-1306.842926 -1306.769251 618.44 nm
-1306.841158 -1306.769523 636.05 nm
-1306.84139 -1306.769526 634.02 nm
-1306.841365 -1306.769526 634.25 nm
-1306.84137 -1306.769526 634.2 nm
-1306.841193 -1306.768446 626.33 nm
-1306.839951 -1306.768687 639.36 nm
-1306.840127 -1306.768689 637.8 nm
-1306.840136 -1306.76869 637.72 nm
-1306.840137 -1306.76869 637.72 nm
-1306.839512 -1306.766497 624.02 nm
-1306.838796 -1306.766742 632.34 nm
-1306.838862 -1306.766743 631.78 nm
-1306.838888 -1306.766744 631.56 nm
-1306.838902 -1306.766744 631.44 nm
-1306.837793 -1306.763377 612.27 nm
-1306.837643 -1306.763668 615.93 nm
-1306.837668 -1306.763671 615.74 nm
-1306.837669 -1306.763672 615.75 nm
-1306.836083 -1306.759188 592.54 nm
-1306.836394 -1306.759546 592.9 nm
-1306.836511 -1306.759553 592.05 nm
-1306.836473 -1306.759553 592.34 nm
-1306.834508 -1306.754174 567.18 nm
-1306.835312 -1306.754628 564.71 nm
-1306.835389 -1306.754641 564.26 nm
-1306.83553 -1306.754643 563.29 nm
-1306.835569 -1306.754643 563.03 nm
-1306.835584 -1306.754643 562.92 nm
-1306.833346 -1306.74862 537.77 nm
-1306.83486 -1306.749186 531.83 nm
-1306.835521 -1306.749217 527.94 nm
-1306.835809 -1306.749222 526.22 nm
-1306.835914 -1306.749222 525.58 nm
-1306.835927 -1306.749222 525.5 nm
-1306.833641 -1306.74315 503.51 nm

-1306.836984 -1306.744266 491.42 nm
-1306.841871 -1306.745306 471.84 nm
-1306.847289 -1306.743635 439.57 nm
-1306.854826 -1306.748108 426.95 nm
-1306.86407 -1306.749794 398.71 nm
-1306.86776 -1306.750538 388.69 nm
-1306.87108 -1306.751173 379.99 nm
-1306.87728 -1306.752263 364.46 nm
-1306.878376 -1306.753178 363.93 nm
-1306.879678 -1306.753876 362.18 nm
-1306.88218 -1306.755966 361 nm
-1306.884145 -1306.757843 360.75 nm
-1306.883619 -1306.758907 365.35 nm
-1306.881636 -1306.759815 374.02 nm
-1306.881631 -1306.760146 375.05 nm
-1306.881847 -1306.760328 374.95 nm
-1306.882615 -1306.760435 372.92 nm
-1306.883203 -1306.760479 371.27 nm
-1306.884243 -1306.760546 368.35 nm
-1306.88532 -1306.760632 365.42 nm
-1306.886105 -1306.76068 363.27 nm
-1306.885723 -1306.760695 364.43 nm
-1306.885649 -1306.760697 364.65 nm
-1306.885751 -1306.760703 364.37 nm
-1306.885736 -1306.760706 364.42 nm
-1306.885699 -1306.760707 364.53 nm
-1306.885707 -1306.760707 364.51 nm
-1306.885714 -1306.760707 364.49 nm
-1306.885716 -1306.760707 364.48 nm
-1306.885348 -1306.760048 363.63 nm
-1306.886626 -1306.760447 361.1 nm
-1306.886812 -1306.760496 360.71 nm
-1306.886802 -1306.760497 360.74 nm
-1306.886774 -1306.760502 360.84 nm
-1306.886777 -1306.760502 360.83 nm
-1306.886776 -1306.760502 360.83 nm
-1306.886775 -1306.760502 360.83 nm

Geometries of structural optimization

1 Energy:-1306.88679547
C -1.418417 3.866247 -0.005166
C -0.023001 3.712946 0.005844
C 0.490722 2.413341 0.013326
C -0.365072 1.294183 0.009803
C -1.820106 1.463272 0.000109
C -2.305512 2.811119 -0.008211
N 0.163541 0.013036 0.014192

C -0.636622 -1.171591 0.015397
C -2.070065 -1.003728 0.008215
C -2.663454 0.331216 -0.000387
C -2.869116 -2.163834 0.008353
C -4.235318 -1.997701 0.000250
C -4.832424 -0.707766 -0.008229
C -4.103966 0.440941 -0.008794
C 1.594866 -0.182002 0.019367
O -0.050832 -2.261268 0.022182
F -1.914093 5.122380 -0.013010
C 2.281904 -0.272521 1.226538
C 3.666083 -0.465116 1.224922
C 4.391517 -0.566236 0.029104
C 3.669394 -0.465318 -1.174168
C 2.289832 -0.273581 -1.187385
O -5.210066 -2.950849 -0.000998
C -6.466253 -2.256474 -0.012223
O -6.192382 -0.850812 -0.014884
C 5.915817 -0.778606 -0.007305
C 6.528456 -0.871049 1.403039
C 6.580678 0.407311 -0.746610
C 6.233309 -2.093537 -0.758968
H 0.622763 4.583108 0.008303
H 1.561746 2.262875 0.021692
H -3.365331 3.027031 -0.017023
H -2.404901 -3.142880 0.014682
H -4.601352 1.402056 -0.015196
H 1.738625 -0.200022 2.163968
H 4.172254 -0.537894 2.180483
H 4.187666 -0.539531 -2.125471
H 1.751187 -0.201721 -2.127519
H -7.017373 -2.524317 -0.918793
H -7.030177 -2.518364 0.888140
H 6.118152 -1.712914 1.972174
H 7.610518 -1.022633 1.322534
H 6.365441 0.046006 1.980581
H 6.217863 0.502423 -1.775447
H 7.667300 0.265616 -0.787580
H 6.380720 1.353249 -0.230083
H 7.317411 -2.254212 -0.796760
H 5.779414 -2.953544 -0.253345
H 5.863177 -2.075248 -1.789379

2 Energy:-1306.88558948
C -1.389443 3.842180 -0.235976
C -0.007091 3.692568 -0.038951
C 0.493234 2.396611 0.095995
C -0.361261 1.277143 0.030264

C -1.809721 1.446986 -0.110302
C -2.277924 2.787234 -0.275450
N 0.162590 -0.003742 0.075535
C -0.651760 -1.178918 0.216046
C -2.079353 -1.004476 0.144124
C -2.660388 0.318907 -0.060337
C -2.891070 -2.155414 0.244213
C -4.250992 -1.987986 0.140206
C -4.834490 -0.708807 -0.068894
C -4.094841 0.428633 -0.171139
C 1.589522 -0.205929 0.067604
O -0.070616 -2.259803 0.370534
F -1.872541 5.093030 -0.385549
C 2.275943 -0.463232 1.252783
C 3.661010 -0.644711 1.226907
C 4.390848 -0.569460 0.032090
C 3.670756 -0.300928 -1.147950
C 2.291581 -0.114929 -1.137273
O -5.234190 -2.932246 0.198275
C -6.482363 -2.236720 0.061595
O -6.193467 -0.848946 -0.144089
C 5.915979 -0.765957 -0.028688
C 6.525897 -1.050511 1.356902
C 6.576219 0.514698 -0.593791
C 6.242424 -1.961641 -0.955514
H 0.636983 4.562825 0.003656
H 1.554281 2.245347 0.242740
H -3.327618 3.002593 -0.424319
H -2.437138 -3.128215 0.391656
H -4.581669 1.382837 -0.326866
H 1.731403 -0.525759 2.189598
H 4.166096 -0.846220 2.164458
H 4.191304 -0.237719 -2.098798
H 1.754955 0.088158 -2.059267
H -7.021117 -2.630569 -0.804903
H -7.064850 -2.357995 0.980618
H 6.119530 -1.965803 1.801961
H 7.609095 -1.182934 1.259645
H 6.355651 -0.223745 2.055920
H 6.216243 0.749675 -1.600897
H 7.663734 0.385555 -0.649766
H 6.369360 1.378729 0.048259
H 7.327559 -2.108616 -1.013844
H 5.793778 -2.886418 -0.575031
H 5.872454 -1.802270 -1.973723

3 Energy:-1306.88292221
C -1.365010 3.811771 -0.425583

C -0.007779 3.687341 -0.089389
C 0.477866 2.405038 0.155712
C -0.362086 1.275147 0.052575
C -1.795996 1.428213 -0.196389
C -2.245485 2.746017 -0.482393
N 0.165744 0.000776 0.151114
C -0.666779 -1.163952 0.401998
C -2.082237 -0.992970 0.257878
C -2.649154 0.295923 -0.115996
C -2.909319 -2.132613 0.436369
C -4.255615 -1.980660 0.235596
C -4.820296 -0.735057 -0.149873
C -4.068539 0.387024 -0.327891
C 1.583331 -0.202565 0.127458
O -0.085849 -2.216193 0.691641
F -1.839705 5.044488 -0.689519
C 2.275947 -0.607184 1.272024
C 3.659072 -0.787416 1.218703
C 4.388309 -0.568790 0.040638
C 3.665722 -0.152393 -1.096621
C 2.290245 0.036915 -1.059580
O -5.247097 -2.918848 0.322992
C -6.484463 -2.220564 0.121122
O -6.172535 -0.890227 -0.310668
C 5.911232 -0.762569 -0.048391
C 6.524618 -1.212547 1.291004
C 6.575911 0.573340 -0.460593
C 6.228479 -1.841218 -1.112606
H 0.624188 4.564769 -0.023906
H 1.519553 2.265560 0.414274
H -3.279094 2.948342 -0.731329
H -2.468384 -3.084107 0.709362
H -4.540990 1.317182 -0.618501
H 1.735767 -0.777725 2.196460
H 4.166160 -1.099772 2.124295
H 4.184041 0.021835 -2.034614
H 1.753075 0.350136 -1.949782
H -7.063036 -2.728486 -0.653963
H -7.035933 -2.179908 1.067596
H 6.116128 -2.172974 1.625101
H 7.606908 -1.336273 1.174526
H 6.359888 -0.474499 2.084280
H 6.214092 0.928080 -1.431344
H 7.662513 0.446369 -0.535789
H 6.375794 1.355972 0.280304
H 7.312753 -1.983910 -1.192872
H 5.777768 -2.802953 -0.842207
H 5.854803 -1.560778 -2.102959

4 Energy:-1306.88085697
C -1.359619 3.794280 -0.567096
C -0.023380 3.704019 -0.153474
C 0.455961 2.439809 0.178394
C -0.365208 1.295552 0.077383
C -1.783437 1.420596 -0.243273
C -2.226840 2.713356 -0.614571
N 0.172429 0.032118 0.255346
C -0.673308 -1.125827 0.564987
C -2.077232 -0.968849 0.355375
C -2.633254 0.280673 -0.139745
C -2.912513 -2.100507 0.584890
C -4.244778 -1.974697 0.308259
C -4.793829 -0.768690 -0.202456
C -4.036368 0.343015 -0.428602
C 1.580053 -0.170665 0.208589
O -0.097240 -2.150022 0.948385
F -1.836082 5.004273 -0.914897
C 2.284368 -0.689078 1.304589
C 3.662516 -0.881012 1.216892
C 4.384073 -0.567892 0.054481
C 3.654038 -0.040585 -1.033108
C 2.284685 0.163461 -0.963106
O -5.238114 -2.913032 0.413284
C -6.465843 -2.231564 0.119848
O -6.135534 -0.948073 -0.426223
C 5.901644 -0.773632 -0.069015
C 6.523185 -1.347008 1.218463
C 6.581277 0.583966 -0.372582
C 6.190554 -1.760231 -1.227156
H 0.595271 4.590897 -0.090736
H 1.481014 2.323983 0.507411
H -3.249323 2.893738 -0.920869
H -2.481281 -3.025060 0.950225
H -4.497344 1.243811 -0.815380
H 1.755156 -0.927983 2.218624
H 4.175506 -1.275684 2.086252
H 4.163618 0.206005 -1.959573
H 1.743144 0.554727 -1.818868
H -7.030202 -2.805514 -0.618351
H -7.039300 -2.100279 1.045412
H 6.104546 -2.327289 1.472657
H 7.602101 -1.474724 1.077889
H 6.378342 -0.678732 2.074911
H 6.214050 1.026212 -1.304508
H 7.664820 0.448292 -0.472005
H 6.401379 1.301932 0.435821

H 7.271671 -1.910438 -1.332042
H 5.728365 -2.735311 -1.035683
H 5.810791 -1.389252 -2.184783

5 Energy:-1306.87868586
C -1.355147 3.779405 -0.686961
C -0.042430 3.729082 -0.205667
C 0.431170 2.487537 0.210826
C -0.367983 1.327767 0.119817
C -1.765678 1.417005 -0.272156
C -2.205594 2.681889 -0.722422
N 0.179890 0.081741 0.393836
C -0.680041 -1.069831 0.744469
C -2.068393 -0.936593 0.452957
C -2.608565 0.267456 -0.154179
C -2.910721 -2.060389 0.719634
C -4.224120 -1.969616 0.361801
C -4.752169 -0.810385 -0.264319
C -3.989969 0.292444 -0.524996
C 1.577054 -0.123828 0.315781
O -0.118984 -2.061101 1.223152
F -1.833446 4.962644 -1.114683
C 2.298488 -0.734809 1.357352
C 3.668310 -0.946367 1.224877
C 4.374599 -0.568610 0.070833
C 3.632055 0.045845 -0.962625
C 2.271361 0.271045 -0.849746
O -5.216136 -2.911753 0.472664
C -6.430447 -2.257283 0.081187
O -6.077050 -1.022481 -0.555785
C 5.883932 -0.791470 -0.097599
C 6.518461 -1.469734 1.131165
C 6.582633 0.573454 -0.314441
C 6.132176 -1.694073 -1.331787
H 0.561829 4.626276 -0.151309
H 1.437199 2.402347 0.603338
H -3.215545 2.834015 -1.081753
H -2.493191 -2.951982 1.172200
H -4.435059 1.158146 -1.000845
H 1.787748 -1.016455 2.268097
H 4.191283 -1.405366 2.055779
H 4.126347 0.340338 -1.883277
H 1.721417 0.719276 -1.670984
H -6.969591 -2.889021 -0.627771
H -7.037121 -2.050145 0.971519
H 6.084518 -2.457728 1.321776
H 7.591444 -1.607528 0.958789
H 6.404600 -0.863306 2.036838

H 6.205698 1.089553 -1.203517
H 7.661188 0.426165 -0.445995
H 6.432129 1.232437 0.548293
H 7.208242 -1.854665 -1.467842
H 5.655209 -2.672411 -1.204274
H 5.742925 -1.245849 -2.251781

6 Energy:-1306.87355915
C -1.334287 3.775159 -0.755526
C -0.060696 3.778349 -0.185507
C 0.402737 2.568991 0.328266
C -0.365572 1.390506 0.239594
C -1.720232 1.424293 -0.264412
C -2.157101 2.652764 -0.795080
N 0.186427 0.170004 0.624650
C -0.712521 -0.938446 1.084887
C -2.051805 -0.873411 0.615226
C -2.540695 0.245545 -0.168168
C -2.915215 -1.977692 0.921379
C -4.176129 -1.958849 0.405261
C -4.638710 -0.894189 -0.408347
C -3.862145 0.195080 -0.698266
C 1.562981 -0.063971 0.483582
O -0.212492 -1.817361 1.794147
F -1.811159 4.923111 -1.272009
C 2.321618 -0.750602 1.457010
C 3.674762 -0.988846 1.247737
C 4.342252 -0.569451 0.082162
C 3.569436 0.115577 -0.882817
C 2.224014 0.368279 -0.696409
O -5.162469 -2.911371 0.500087
C -6.329892 -2.328805 -0.093767
O -5.913690 -1.176051 -0.837601
C 5.833836 -0.822714 -0.166806
C 6.506235 -1.570497 0.999884
C 6.558701 0.532613 -0.359371
C 5.997999 -1.676212 -1.449787
H 0.522923 4.689458 -0.136164
H 1.378442 2.523825 0.798534
H -3.144801 2.763648 -1.225320
H -2.543715 -2.802789 1.517325
H -4.256975 0.992739 -1.317039
H 1.847278 -1.061176 2.376017
H 4.222644 -1.499762 2.030925
H 4.027544 0.439878 -1.812081
H 1.651250 0.859592 -1.475507
H -6.789642 -3.050350 -0.772059
H -7.028534 -2.023037 0.695522

H 6.055873 -2.555259 1.167386
H 7.565953 -1.726487 0.770841
H 6.450491 -1.002615 1.935473
H 6.154459 1.097118 -1.205951
H 7.624881 0.362384 -0.550127
H 6.468678 1.156356 0.537204
H 7.061844 -1.856831 -1.643882
H 5.501751 -2.647119 -1.341067
H 5.577989 -1.178286 -2.329764

7 Energy:-1306.84986482
C -1.478715 3.881113 -0.737518
C -0.235229 4.003516 -0.124152
C 0.322838 2.853813 0.435152
C -0.354619 1.631245 0.357411
C -1.652202 1.522389 -0.235679
C -2.193577 2.684686 -0.796569
N 0.208923 0.418126 0.777126
C -0.736984 -0.476583 1.581455
C -1.945255 -0.698765 0.861895
C -2.344682 0.230395 -0.172035
C -2.811927 -1.773025 1.240361
C -3.943405 -1.958681 0.496277
C -4.280267 -1.115475 -0.581884
C -3.520452 -0.020952 -0.920055
C 1.504654 0.049742 0.525905
O -0.427769 -0.786948 2.742054
F -2.036509 4.977175 -1.290226
C 2.221620 -0.794271 1.419642
C 3.547876 -1.108993 1.170239
C 4.239417 -0.621585 0.044054
C 3.515416 0.220510 -0.837150
C 2.199261 0.560127 -0.611737
O -4.876403 -2.964103 0.591104
C -5.925316 -2.610149 -0.320679
O -5.423069 -1.585781 -1.188309
C 5.701666 -0.964565 -0.254515
C 6.319596 -1.887891 0.812183
C 6.530461 0.343926 -0.307552
C 5.788068 -1.679767 -1.626914
H 0.267762 4.962775 -0.089265
H 1.290170 2.896919 0.925053
H -3.168820 2.689117 -1.269847
H -2.536214 -2.435278 2.053143
H -3.830680 0.634520 -1.727167
H 1.720612 -1.156634 2.306930
H 4.059508 -1.741537 1.886050
H 3.997773 0.603834 -1.730678

H 1.668690 1.183074 -1.322590
H -6.200500 -3.484938 -0.913307
H -6.785110 -2.224589 0.242654
H 5.792975 -2.846544 0.877169
H 7.361564 -2.100350 0.550218
H 6.316484 -1.424631 1.805199
H 6.167556 1.028767 -1.080823
H 7.577849 0.111133 -0.532332
H 6.496718 0.869046 0.653591
H 6.832960 -1.921315 -1.853898
H 5.216055 -2.614268 -1.618960
H 5.405756 -1.055244 -2.440759

8 Energy:-1306.84608602
C -1.537365 3.914363 -0.816228
C -0.331706 4.113264 -0.150571
C 0.254196 3.007065 0.468146
C -0.363508 1.757028 0.396351
C -1.623652 1.567438 -0.246231
C -2.191998 2.685509 -0.870821
N 0.228578 0.574173 0.883152
C -0.711076 -0.317032 1.692480
C -1.873649 -0.624557 0.926922
C -2.263856 0.248253 -0.158428
C -2.712639 -1.718048 1.309856
C -3.802287 -1.978494 0.526482
C -4.124326 -1.191551 -0.596953
C -3.394167 -0.080806 -0.946070
C 1.492388 0.166851 0.585979
O -0.441974 -0.547460 2.882642
F -2.117959 4.968026 -1.428466
C 2.162595 -0.777923 1.420777
C 3.466905 -1.151091 1.146072
C 4.183345 -0.630639 0.050338
C 3.507009 0.309077 -0.772255
C 2.214656 0.709590 -0.522124
O -4.697887 -3.017712 0.621370
C -5.720750 -2.739124 -0.344431
O -5.220913 -1.730471 -1.231567
C 5.622855 -1.034239 -0.276603
C 6.190495 -2.055734 0.726581
C 6.522702 0.227586 -0.251477
C 5.666370 -1.664388 -1.692304
H 0.125833 5.095371 -0.125072
H 1.197609 3.108242 0.995212
H -3.143917 2.628971 -1.386490
H -2.447137 -2.337300 2.159155
H -3.694587 0.530571 -1.790579

H 1.646328 -1.162623 2.289879
H 3.942057 -1.858591 1.814998
H 4.011944 0.721745 -1.639656
H 1.723332 1.409748 -1.186949
H -5.939413 -3.645840 -0.912049
H -6.616379 -2.365054 0.168707
H 5.612624 -2.986617 0.733162
H 7.218853 -2.307368 0.446544
H 6.214138 -1.656731 1.746808
H 6.198591 0.978285 -0.979414
H 7.554977 -0.049458 -0.494707
H 6.519189 0.692596 0.740632
H 6.695970 -1.948403 -1.938786
H 5.043403 -2.564383 -1.740692
H 5.318725 -0.969031 -2.463060

9 Energy:-1306.84388801
C -1.566312 3.935819 -0.901848
C -0.418432 4.215924 -0.166753
C 0.179385 3.159232 0.524761
C -0.372215 1.881475 0.454794
C -1.578106 1.607738 -0.252980
C -2.156286 2.676481 -0.954919
N 0.247191 0.739182 1.020335
C -0.693122 -0.164326 1.809383
C -1.798558 -0.547530 0.994800
C -2.167514 0.267973 -0.142454
C -2.611546 -1.661568 1.376354
C -3.647366 -1.996694 0.550394
C -3.942340 -1.266193 -0.618024
C -3.240844 -0.139916 -0.973300
C 1.481100 0.294903 0.679820
O -0.462405 -0.362239 3.013869
F -2.154330 4.940735 -1.587477
C 2.105814 -0.733725 1.454990
C 3.380811 -1.168057 1.142017
C 4.113446 -0.630625 0.064880
C 3.485402 0.394346 -0.695239
C 2.223252 0.856149 -0.408106
O -4.503339 -3.069693 0.639882
C -5.485146 -2.870500 -0.385942
O -4.981615 -1.875049 -1.285641
C 5.520711 -1.100140 -0.307004
C 6.039773 -2.206469 0.630265
C 6.494844 0.103329 -0.230498
C 5.504497 -1.654303 -1.755072
H -0.009813 5.219521 -0.147562
H 1.083486 3.321732 1.103224

H -3.070254 2.556317 -1.525482
H -2.364501 -2.237383 2.260994
H -3.520786 0.425451 -1.855972
H 1.580349 -1.131977 2.312264
H 3.820522 -1.939163 1.762857
H 4.007630 0.825332 -1.543038
H 1.770343 1.622672 -1.024385
H -5.637401 -3.806021 -0.928006
H -6.420714 -2.516235 0.066518
H 5.406601 -3.100043 0.597648
H 7.046536 -2.503626 0.318515
H 6.102951 -1.865260 1.669567
H 6.207673 0.910019 -0.912540
H 7.504842 -0.222077 -0.504829
H 6.532712 0.513867 0.784605
H 6.511929 -1.983000 -2.034818
H 4.829706 -2.513322 -1.838942
H 5.185965 -0.899978 -2.481642

10 Energy:-1306.84238895
C -1.581041 3.936711 -0.998687
C -0.493126 4.291643 -0.206288
C 0.109241 3.283719 0.551523
C -0.379296 1.981800 0.489141
C -1.531212 1.631826 -0.270360
C -2.111206 2.652495 -1.042954
N 0.263715 0.883049 1.127477
C -0.679396 -0.030451 1.900647
C -1.733529 -0.478162 1.053311
C -2.080273 0.280390 -0.130389
C -2.524270 -1.606649 1.442729
C -3.510914 -2.009007 0.588306
C -3.780348 -1.333104 -0.619229
C -3.102791 -0.197854 -0.988890
C 1.475631 0.408369 0.761609
O -0.472878 -0.209974 3.112225
F -2.170023 4.893574 -1.751082
C 2.042890 -0.703920 1.467169
C 3.288201 -1.191133 1.119104
C 4.048465 -0.628057 0.074215
C 3.479915 0.480481 -0.614793
C 2.247433 0.993948 -0.294247
O -4.333082 -3.108165 0.682928
C -5.278163 -2.979314 -0.387570
O -4.769175 -2.003616 -1.305132
C 5.425771 -1.151380 -0.333378
C 5.876733 -2.351839 0.519498
C 6.468033 -0.015175 -0.170715

C 5.379913 -1.596265 -1.818155
H -0.130318 5.312821 -0.196293
H 0.971590 3.503630 1.173274
H -2.986093 2.473942 -1.657812
H -2.295151 -2.139669 2.358432
H -3.362835 0.322731 -1.904488
H 1.500614 -1.125206 2.302337
H 3.682676 -2.026645 1.684143
H 4.027328 0.936482 -1.432933
H 1.840990 1.825320 -0.855596
H -5.380082 -3.939198 -0.897875
H -6.241567 -2.638084 0.013806
H 5.191402 -3.201333 0.423972
H 6.864267 -2.684738 0.183510
H 5.959402 -2.091659 1.580584
H 6.229624 0.855204 -0.790327
H 7.457334 -0.378378 -0.471333
H 6.528330 0.315880 0.871901
H 6.366772 -1.963491 -2.121839
H 4.655212 -2.404898 -1.963451
H 5.109812 -0.773565 -2.487760

11 Energy:-1306.84122216
C -1.583282 3.924184 -1.094919
C -0.551629 4.344585 -0.259688
C 0.049458 3.382338 0.556300
C -0.384151 2.061274 0.508149
C -1.486625 1.645385 -0.289442
C -2.062718 2.621243 -1.123615
N 0.276432 1.005528 1.210978
C -0.671205 0.086613 1.972774
C -1.681001 -0.416221 1.104858
C -2.004832 0.288304 -0.118760
C -2.452457 -1.555259 1.505871
C -3.394488 -2.016777 0.632421
C -3.639463 -1.391801 -0.608186
C -2.981586 -0.251580 -0.995056
C 1.474551 0.505871 0.836261
O -0.479869 -0.079178 3.188455
F -2.168175 4.835910 -1.905746
C 1.972803 -0.688685 1.457703
C 3.189473 -1.219784 1.077000
C 3.989999 -0.622263 0.082043
C 3.491514 0.567203 -0.522641
C 2.286852 1.122709 -0.171532
O -4.187384 -3.136822 0.736775
C -5.097341 -3.072421 -0.369053
O -4.582995 -2.116125 -1.303663

C 5.339556 -1.189237 -0.356599
C 5.717043 -2.472295 0.406969
C 6.440651 -0.126782 -0.105832
C 5.280875 -1.519206 -1.870742
H -0.228234 5.378949 -0.262639
H 0.871845 3.652886 1.211417
H -2.901114 2.391503 -1.771467
H -2.240860 -2.048686 2.447570
H -3.221732 0.227206 -1.938419
H 1.404580 -1.142056 2.257660
H 3.529111 -2.119460 1.574821
H 4.073187 1.053699 -1.298270
H 1.934451 2.016913 -0.668557
H -5.155677 -4.052229 -0.847325
H -6.083137 -2.744438 -0.013428
H 4.988018 -3.273974 0.245040
H 6.688101 -2.832624 0.051972
H 5.804177 -2.295997 1.484806
H 6.256713 0.797581 -0.662549
H 7.411180 -0.521975 -0.426290
H 6.508969 0.124560 0.958287
H 6.248127 -1.918314 -2.196262
H 4.513205 -2.272399 -2.079250
H 5.063603 -0.634771 -2.477935

12 Energy:-1306.84020717
C -1.574997 3.893170 -1.200214
C -0.593945 4.372546 -0.335575
C 0.001192 3.454772 0.534006
C -0.386660 2.119153 0.509086
C -1.445771 1.644752 -0.313989
C -2.013520 2.576818 -1.204570
N 0.285444 1.106598 1.272036
C -0.667033 0.187403 2.027980
C -1.642105 -0.362932 1.151532
C -1.943023 0.287567 -0.107841
C -2.400058 -1.505329 1.571726
C -3.304371 -2.019909 0.689195
C -3.525639 -1.446448 -0.581224
C -2.881330 -0.307301 -0.991505
C 1.477354 0.586022 0.903071
O -0.483205 0.035985 3.246211
F -2.151983 4.760589 -2.064546
C 1.900617 -0.682605 1.427087
C 3.091586 -1.246860 1.015869
C 3.941853 -0.611032 0.087622
C 3.520119 0.652346 -0.417998
C 2.338777 1.238343 -0.039990

O -4.075631 -3.153585 0.811452
C -4.954851 -3.148120 -0.320464
O -4.431859 -2.217769 -1.276110
C 5.267168 -1.211610 -0.377956
C 5.557328 -2.577534 0.271568
C 6.418745 -0.239527 -0.012756
C 5.222719 -1.399867 -1.916816
H -0.302936 5.416227 -0.357399
H 0.786080 3.771519 1.214001
H -2.819268 2.301065 -1.875492
H -2.205683 -1.958964 2.536826
H -3.102209 0.129557 -1.959554
H 1.297468 -1.173755 2.177161
H 3.370511 -2.205672 1.434496
H 4.143703 1.172946 -1.136683
H 2.044109 2.189599 -0.462769
H -4.981847 -4.146008 -0.762740
H -5.956223 -2.826141 -0.004954
H 4.788273 -3.318444 0.026646
H 6.513635 -2.959375 -0.100486
H 5.633003 -2.504134 1.362114
H 6.297133 0.740733 -0.484391
H 7.372536 -0.657977 -0.353133
H 6.478537 -0.091075 1.070990
H 6.173535 -1.822129 -2.260793
H 4.419690 -2.086764 -2.205562
H 5.067556 -0.453758 -2.444901

13 Energy:-1306.83925325
C -1.550221 3.847380 -1.305642
C -0.615046 4.377736 -0.419818
C -0.032597 3.501179 0.499461
C -0.386092 2.155982 0.502667
C -1.407251 1.631864 -0.338501
C -1.959196 2.522669 -1.281659
N 0.290419 1.184150 1.320987
C -0.668477 0.268309 2.071949
C -1.617690 -0.320207 1.193815
C -1.894410 0.279712 -0.096154
C -2.369480 -1.459646 1.635612
C -3.243605 -2.018404 0.750454
C -3.440854 -1.493235 -0.545346
C -2.802230 -0.360774 -0.980684
C 1.480154 0.643449 0.965008
O -0.490081 0.131245 3.292124
F -2.112749 4.672876 -2.219873
C 1.827279 -0.688243 1.375559
C 2.998697 -1.272126 0.937534

C 3.904554 -0.595869 0.093483
C 3.559019 0.728993 -0.299506
C 2.395099 1.333171 0.102821
O -4.002355 -3.158340 0.893610
C -4.853669 -3.204384 -0.258393
O -4.318840 -2.302089 -1.233979
C 5.210140 -1.218335 -0.397454
C 5.419698 -2.648392 0.134292
C 6.398676 -0.340295 0.072597
C 5.190548 -1.268985 -1.947563
H -0.347682 5.427021 -0.463168
H 0.716993 3.858833 1.198787
H -2.734741 2.207299 -1.970482
H -2.192582 -1.875768 2.620751
H -3.003944 0.036967 -1.969519
H 1.181400 -1.220822 2.058563
H 3.216362 -2.280975 1.264763
H 4.227753 1.283842 -0.948492
H 2.157308 2.332930 -0.235202
H -4.857988 -4.217623 -0.665157
H -5.866265 -2.884281 0.021230
H 4.624064 -3.327009 -0.192455
H 6.366735 -3.041629 -0.249243
H 5.470036 -2.674646 1.228431
H 6.336770 0.681403 -0.315117
H 7.338325 -0.776427 -0.284352
H 6.440301 -0.288038 1.166034
H 6.127854 -1.705552 -2.310108
H 4.362656 -1.888027 -2.310048
H 5.091727 -0.273802 -2.392352

14 Energy:-1306.83846514
C -1.519726 3.783011 -1.414760
C -0.616551 4.355071 -0.521388
C -0.048953 3.516005 0.441134
C -0.384048 2.166645 0.479958
C -1.381564 1.603485 -0.365508
C -1.914954 2.455991 -1.355196
N 0.293251 1.230108 1.343721
C -0.670935 0.325648 2.099052
C -1.611957 -0.290058 1.232385
C -1.871600 0.262709 -0.082196
C -2.365783 -1.416907 1.704003
C -3.226929 -2.008624 0.828337
C -3.408536 -1.529304 -0.488094
C -2.766673 -0.411827 -0.955162
C 1.481997 0.668556 1.000274
O -0.491719 0.210229 3.320750

F -2.065395 4.569958 -2.372680
C 1.755806 -0.712016 1.277925
C 2.916997 -1.300999 0.820152
C 3.884419 -0.582189 0.085889
C 3.608348 0.788598 -0.181817
C 2.452271 1.396938 0.237653
O -3.985452 -3.144819 1.001103
C -4.822489 -3.231982 -0.158675
O -4.276386 -2.363583 -1.158621
C 5.185181 -1.207423 -0.413930
C 5.316107 -2.691506 -0.024027
C 6.384367 -0.432710 0.191463
C 5.232170 -1.099667 -1.960564
H -0.361166 5.405848 -0.591517
H 0.674754 3.907721 1.149399
H -2.668956 2.108388 -2.052370
H -2.200086 -1.797885 2.705177
H -2.956048 -0.050729 -1.960324
H 1.058298 -1.288307 1.868614
H 3.075982 -2.348897 1.041113
H 4.325447 1.377574 -0.743006
H 2.267496 2.435410 -0.002919
H -4.821036 -4.258735 -0.530012
H -5.838710 -2.903427 0.096934
H 4.510899 -3.299368 -0.451172
H 6.263790 -3.083599 -0.407109
H 5.316247 -2.830222 1.062735
H 6.378957 0.624554 -0.091648
H 7.321376 -0.870446 -0.170275
H 6.379268 -0.492907 1.285241
H 6.167886 -1.535706 -2.327777
H 4.398931 -1.644191 -2.417862
H 5.189934 -0.061329 -2.304138

15 Energy:-1306.83799436
C -1.494402 3.700506 -1.528311
C -0.604186 4.305786 -0.643722
C -0.049404 3.501547 0.355419
C -0.383802 2.154164 0.439878
C -1.375039 1.561348 -0.394553
C -1.891527 2.377169 -1.424394
N 0.293918 1.247730 1.338330
C -0.671554 0.361111 2.108804
C -1.622065 -0.272792 1.267526
C -1.876726 0.237024 -0.065461
C -2.383041 -1.378391 1.777508
C -3.249362 -1.992717 0.923237
C -3.427667 -1.556465 -0.409088

C -2.777433 -0.460956 -0.914587
C 1.484320 0.668916 1.004950
O -0.485733 0.278916 3.331754
F -2.025659 4.450967 -2.523102
C 1.692771 -0.742006 1.130951
C 2.854041 -1.322908 0.662874
C 3.884928 -0.564677 0.066348
C 3.668655 0.835459 -0.060979
C 2.509992 1.435799 0.366442
O -4.017074 -3.116265 1.134169
C -4.855873 -3.234942 -0.021371
O -4.302934 -2.405301 -1.050255
C 5.192741 -1.181188 -0.426447
C 5.245183 -2.705586 -0.213573
C 6.374361 -0.536496 0.344013
C 5.348556 -0.890945 -1.941938
H -0.348260 5.353579 -0.747704
H 0.662904 3.920362 1.059536
H -2.635384 2.004146 -2.119297
H -2.218994 -1.726821 2.790767
H -2.965024 -0.133895 -1.931608
H 0.937700 -1.355797 1.601926
H 2.960770 -2.395814 0.761513
H 4.433450 1.455694 -0.515294
H 2.371481 2.501058 0.236784
H -4.863730 -4.273479 -0.358204
H -5.868925 -2.888895 0.223368
H 4.447823 -3.222774 -0.758704
H 6.200882 -3.089692 -0.584603
H 5.170880 -2.973293 0.846171
H 6.422284 0.546776 0.195078
H 7.318351 -0.965019 -0.010678
H 6.294226 -0.729537 1.419316
H 6.288645 -1.324510 -2.300793
H 4.527031 -1.335631 -2.514046
H 5.372429 0.181820 -2.157685

16 Energy:-1306.83763537
C -1.467876 3.610168 -1.638617
C -0.580127 4.242815 -0.770698
C -0.038989 3.472926 0.262208
C -0.384931 2.132461 0.398121
C -1.377609 1.515958 -0.419953
C -1.876354 2.295006 -1.486700
N 0.290581 1.252476 1.324359
C -0.676530 0.386892 2.111356
C -1.639871 -0.262648 1.298933
C -1.892428 0.208581 -0.048531

C -2.410512 -1.343230 1.846477
C -3.286381 -1.974656 1.014654
C -3.463179 -1.578603 -0.330622
C -2.802878 -0.506747 -0.872717
C 1.487522 0.659792 1.004871
O -0.490460 0.353214 3.336715
F -1.984123 4.324676 -2.666864
C 1.638982 -0.759577 0.967442
C 2.806143 -1.327227 0.495517
C 3.896201 -0.544160 0.056671
C 3.733861 0.866822 0.087512
C 2.568215 1.455418 0.518175
O -4.066109 -3.082027 1.262752
C -4.908401 -3.228735 0.112995
O -4.349544 -2.436746 -0.942336
C 5.210256 -1.149473 -0.435078
C 5.202914 -2.689007 -0.397003
C 6.367536 -0.641419 0.463402
C 5.458141 -0.695075 -1.897025
H -0.315830 5.284073 -0.912293
H 0.669594 3.914821 0.955454
H -2.614778 1.900396 -2.175375
H -2.246720 -1.661502 2.869691
H -2.991004 -0.210762 -1.899049
H 0.829488 -1.393254 1.304645
H 2.868090 -2.407701 0.460306
H 4.545141 1.506919 -0.241403
H 2.471844 2.533481 0.515905
H -4.926731 -4.277106 -0.191377
H -5.917526 -2.865392 0.348359
H 4.423682 -3.110667 -1.041511
H 6.166526 -3.064184 -0.756607
H 5.057496 -3.072213 0.619022
H 6.459097 0.449040 0.441347
H 7.315387 -1.063698 0.111395
H 6.221773 -0.950251 1.504266
H 6.403444 -1.118100 -2.254883
H 4.656651 -1.042499 -2.558008
H 5.524852 0.393811 -1.985637

17 Energy:-1306.88289445
C -1.591292 3.215713 -1.863015
C -0.253003 2.930106 -2.176025
C 0.300776 1.773867 -1.631501
C -0.453054 0.933437 -0.783982
C -1.874918 1.187594 -0.549264
C -2.392684 2.397060 -1.087179
N 0.151565 -0.126415 -0.133298

C -0.615861 -1.212533 0.454121
C -2.027121 -1.007855 0.594390
C -2.653405 0.232760 0.157166
C -2.786422 -2.029353 1.223092
C -4.123837 -1.803600 1.413284
C -4.743838 -0.589513 1.012644
C -4.058581 0.416498 0.400845
C 1.578043 -0.253421 -0.119863
O 0.014406 -2.214246 0.811669
F -2.130093 4.343886 -2.364454
C 2.221320 -1.266758 -0.836175
C 3.613751 -1.359607 -0.808463
C 4.400772 -0.455747 -0.079752
C 3.726546 0.562466 0.625738
C 2.342139 0.672764 0.604474
O -5.054204 -2.612244 2.006077
C -6.319344 -1.951521 1.856734
O -6.069214 -0.631058 1.359446
C 5.935373 -0.537860 -0.026108
C 6.490356 -1.703961 -0.865705
C 6.385274 -0.741070 1.441220
C 6.540459 0.779662 -0.568316
H 0.313026 3.591404 -2.820883
H 1.330757 1.519368 -1.845607
H -3.419761 2.694885 -0.920806
H -2.302344 -2.943591 1.545905
H -4.571939 1.324192 0.108652
H 1.635575 -1.975603 -1.410542
H 4.081260 -2.155897 -1.375986
H 4.290975 1.281921 1.211173
H 1.843676 1.459758 1.162446
H -6.934142 -2.504751 1.137344
H -6.809706 -1.886689 2.830818
H 6.228980 -1.604981 -1.925436
H 7.583539 -1.717644 -0.794844
H 6.124006 -2.673767 -0.510545
H 6.058925 0.081362 2.086328
H 7.479179 -0.794721 1.495912
H 5.978000 -1.672644 1.850460
H 7.635382 0.736681 -0.526605
H 6.246425 0.946490 -1.610993
H 6.218799 1.648265 0.015674

18 Energy:-1306.88547947
C -1.626069 3.127951 -2.021015
C -0.252726 2.906610 -2.213597
C 0.322054 1.803358 -1.580940
C -0.450647 0.945279 -0.772024

C -1.895012 1.146962 -0.630939
C -2.438605 2.304380 -1.268906
N 0.152636 -0.089330 -0.077550
C -0.590456 -1.122149 0.591020
C -2.018452 -0.957858 0.673896
C -2.670590 0.210788 0.091024
C -2.757769 -1.942834 1.364972
C -4.115473 -1.761893 1.473826
C -4.766622 -0.625351 0.922054
C -4.098266 0.348836 0.247032
C 1.587315 -0.223715 -0.075088
O 0.049678 -2.068653 1.064557
F -2.180052 4.204554 -2.616239
C 2.215783 -1.141716 -0.914378
C 3.608605 -1.250879 -0.904068
C 4.403275 -0.451246 -0.070390
C 3.740447 0.473622 0.759386
C 2.354113 0.595212 0.758320
O -5.037025 -2.562688 2.083164
C -6.309626 -1.916308 1.932493
O -6.106342 -0.710217 1.186785
C 5.938693 -0.549477 -0.035186
C 6.480326 -1.615107 -1.006744
C 6.396257 -0.922853 1.395406
C 6.549189 0.817549 -0.427565
H 0.328153 3.578428 -2.834258
H 1.378934 1.607108 -1.702707
H -3.488288 2.552723 -1.185705
H -2.252296 -2.800482 1.792971
H -4.635439 1.195835 -0.160139
H 1.620590 -1.771099 -1.568286
H 4.067703 -1.976816 -1.565128
H 4.312666 1.112530 1.425283
H 1.862633 1.312592 1.408760
H -6.986347 -2.577120 1.382641
H -6.709412 -1.672513 2.921740
H 6.215828 -1.392340 -2.046721
H 7.573644 -1.645906 -0.943453
H 6.106751 -2.616407 -0.764257
H 6.080095 -0.178167 2.133314
H 7.490045 -0.989670 1.436294
H 5.984669 -1.892564 1.697936
H 7.644132 0.764260 -0.399464
H 6.249075 1.104387 -1.442076
H 6.236750 1.615478 0.254213

19 Energy:-1306.88675061
C -1.672790 2.998748 -2.223807

C -0.273253 2.894683 -2.259503
C 0.324397 1.873238 -1.516205
C -0.453811 0.977114 -0.757218
C -1.913916 1.092587 -0.725543
C -2.486331 2.153394 -1.499891
N 0.157244 -0.031820 -0.029702
C -0.560255 -0.972114 0.773187
C -1.998671 -0.857768 0.803529
C -2.678436 0.186317 0.040581
C -2.716537 -1.781521 1.588200
C -4.087967 -1.668752 1.611238
C -4.768979 -0.662311 0.873843
C -4.120449 0.251971 0.103303
C 1.595230 -0.170095 -0.044964
O 0.096148 -1.821322 1.388234
F -2.249491 3.986409 -2.941633
C 2.207811 -0.972722 -1.003112
C 3.598842 -1.107170 -1.009881
C 4.404418 -0.446942 -0.070974
C 3.755883 0.359842 0.881874
C 2.370482 0.502931 0.900265
O -4.994879 -2.432186 2.284832
C -6.292190 -1.904708 1.971224
O -6.113607 -0.794358 1.084324
C 5.938352 -0.575363 -0.049898
C 6.464604 -1.497374 -1.166097
C 6.385147 -1.160503 1.311306
C 6.573083 0.823285 -0.239162
H 0.312106 3.590721 -2.848610
H 1.400744 1.767229 -1.523562
H -3.555681 2.312897 -1.532096
H -2.189229 -2.546606 2.145622
H -4.680309 1.000406 -0.442166
H 1.601956 -1.495158 -1.737387
H 4.046485 -1.743105 -1.764737
H 4.337800 0.888869 1.630603
H 1.889755 1.128133 1.646649
H -6.885107 -2.678719 1.474541
H -6.774629 -1.564033 2.892347
H 6.205557 -1.121769 -2.162587
H 7.557184 -1.554634 -1.108424
H 6.074800 -2.517209 -1.071340
H 6.079212 -0.525402 2.149223
H 7.477509 -1.251577 1.342841
H 5.956074 -2.156541 1.469659
H 7.666851 0.747329 -0.219536
H 6.280161 1.260079 -1.200912
H 6.273207 1.518687 0.551784

20 Energy:-1306.88568317
C -1.689301 2.856036 -2.400265
C -0.288855 2.875820 -2.299592
C 0.315037 1.938695 -1.459495
C -0.456384 1.001268 -0.742954
C -1.919816 1.027495 -0.808432
C -2.497510 1.984123 -1.699729
N 0.163986 0.025918 0.019304
C -0.548095 -0.835297 0.922295
C -1.986551 -0.766265 0.902249
C -2.677689 0.147575 -0.002351
C -2.700840 -1.630779 1.759918
C -4.073556 -1.586043 1.711870
C -4.764223 -0.712275 0.828819
C -4.120709 0.139448 -0.014784
C 1.598132 -0.114995 -0.009198
O 0.121081 -1.588031 1.640002
F -2.274253 3.750244 -3.224207
C 2.202602 -0.792721 -1.066538
C 3.589728 -0.950140 -1.090142
C 4.403749 -0.438095 -0.067922
C 3.764866 0.240099 0.985985
C 2.382305 0.402147 1.024636
O -4.977000 -2.316540 2.427580
C -6.280036 -1.871591 2.022666
O -6.110804 -0.895438 0.987990
C 5.935080 -0.593223 -0.063695
C 6.449091 -1.365644 -1.293411
C 6.369850 -1.362799 1.206721
C 6.592131 0.808056 -0.063727
H 0.290127 3.599555 -2.860817
H 1.392400 1.922853 -1.362173
H -3.568611 2.052206 -1.835990
H -2.166601 -2.303234 2.420686
H -4.687175 0.788883 -0.669737
H 1.589909 -1.203086 -1.863744
H 4.028287 -1.488690 -1.922106
H 4.353311 0.652294 1.800247
H 1.910624 0.925591 1.850215
H -6.846439 -2.722477 1.633647
H -6.786946 -1.414583 2.878742
H 6.198471 -0.855767 -2.230614
H 7.540465 -1.447924 -1.243843
H 6.042689 -2.382512 -1.336290
H 6.073444 -0.840927 2.122577
H 7.460505 -1.475452 1.224870
H 5.924055 -2.363778 1.230417

H 7.684528 0.712937 -0.053227
H 6.309086 1.373925 -0.958848
H 6.300377 1.396222 0.812658

21 Energy:-1306.88273569
C -1.687667 2.713703 -2.546740
C -0.306133 2.852915 -2.342564
C 0.293446 2.004476 -1.414798
C -0.459413 1.030880 -0.723028
C -1.913250 0.963071 -0.871980
C -2.483003 1.817980 -1.853217
N 0.173752 0.100611 0.080565
C -0.547107 -0.677330 1.078107
C -1.977012 -0.670076 0.993818
C -2.666250 0.094294 -0.037273
C -2.699679 -1.475651 1.913497
C -4.062611 -1.518844 1.788726
C -4.745949 -0.798774 0.772141
C -4.097274 -0.007801 -0.127818
C 1.597469 -0.044484 0.038291
O 0.131981 -1.304082 1.899077
F -2.275635 3.513646 -3.457019
C 2.195005 -0.600770 -1.098303
C 3.575162 -0.785161 -1.143212
C 4.400600 -0.423677 -0.064496
C 3.773920 0.131221 1.066770
C 2.396718 0.317412 1.130507
O -4.969485 -2.229193 2.526764
C -6.267924 -1.841026 2.054884
O -6.088105 -1.061686 0.865859
C 5.926862 -0.612665 -0.081450
C 6.426080 -1.234030 -1.399632
C 6.341174 -1.546587 1.081409
C 6.615795 0.762134 0.096498
H 0.257288 3.599491 -2.889115
H 1.357194 2.077972 -1.228104
H -3.543881 1.804209 -2.067051
H -2.170009 -2.040313 2.671764
H -4.657851 0.525140 -0.885834
H 1.574622 -0.900942 -1.937466
H 4.002054 -1.229775 -2.034617
H 4.371032 0.428775 1.923585
H 1.938689 0.746205 2.014523
H -6.848526 -2.735813 1.818986
H -6.765013 -1.234016 2.820516
H 6.188624 -0.603764 -2.264197
H 7.515234 -1.346076 -1.361698
H 5.997586 -2.228060 -1.570842

H 6.053253 -1.138462 2.055804
H 7.429136 -1.683989 1.085019
H 5.874023 -2.532593 0.977814
H 7.705620 0.640772 0.092764
H 6.347112 1.444066 -0.718505
H 6.336874 1.239755 1.041534

22 Energy:-1306.88062702
C -1.671752 2.607530 -2.641733
C -0.309045 2.816057 -2.390967
C 0.282109 2.034293 -1.402221
C -0.456615 1.054186 -0.703705
C -1.896486 0.924671 -0.898916
C -2.457660 1.709166 -1.934750
N 0.183889 0.181661 0.159736
C -0.553886 -0.553129 1.196595
C -1.974326 -0.595288 1.060950
C -2.649849 0.065574 -0.044771
C -2.709247 -1.361967 2.012522
C -4.059769 -1.469421 1.836496
C -4.724741 -0.855463 0.742149
C -4.066127 -0.103132 -0.186124
C 1.594946 0.012982 0.102539
O 0.118449 -1.100374 2.077364
F -2.259368 3.338769 -3.606991
C 2.182834 -0.449728 -1.086707
C 3.555624 -0.658542 -1.156291
C 4.395256 -0.411718 -0.054486
C 3.784228 0.055367 1.125382
C 2.413429 0.264299 1.216830
O -4.972563 -2.168412 2.583127
C -6.261861 -1.841404 2.046133
O -6.058684 -1.173817 0.794106
C 5.916102 -0.626913 -0.099265
C 6.394728 -1.148593 -1.467381
C 6.320277 -1.658989 0.981687
C 6.631759 0.716734 0.184115
H 0.244830 3.565551 -2.942971
H 1.331295 2.166478 -1.168985
H -3.508879 1.646180 -2.185510
H -2.191190 -1.850414 2.829437
H -4.613278 0.349110 -1.004467
H 1.552945 -0.667695 -1.943663
H 3.968135 -1.033952 -2.085447
H 4.392814 0.271011 1.998454
H 1.972809 0.633292 2.134360
H -6.827690 -2.760453 1.879454
H -6.785268 -1.171275 2.738960

H 6.165712 -0.445241 -2.276008
H 7.481478 -1.285176 -1.446573
H 5.944745 -2.116490 -1.715776
H 6.047289 -1.325294 1.988132
H 7.405432 -1.815738 0.964587
H 5.833973 -2.624736 0.803068
H 7.718934 0.575376 0.162255
H 6.371202 1.467009 -0.571197
H 6.367585 1.121145 1.166732

23 Energy:-1306.87833346
C -1.654108 2.516218 -2.717629
C -0.311836 2.786252 -2.432477
C 0.270529 2.065557 -1.392943
C -0.452873 1.082894 -0.683467
C -1.875536 0.894823 -0.916292
C -2.428975 1.615737 -1.996979
N 0.194423 0.275132 0.242333
C -0.563242 -0.426720 1.304473
C -1.971706 -0.525231 1.116920
C -2.628992 0.042623 -0.047436
C -2.719070 -1.259752 2.090349
C -4.054695 -1.429029 1.871118
C -4.697093 -0.909596 0.716958
C -4.028071 -0.188652 -0.230978
C 1.590980 0.068665 0.166910
O 0.092453 -0.898199 2.239344
F -2.239979 3.184492 -3.728354
C 2.169466 -0.315715 -1.060675
C 3.534465 -0.549465 -1.154959
C 4.387846 -0.400828 -0.044998
C 3.792814 -0.003672 1.170023
C 2.429914 0.229072 1.288584
O -4.972262 -2.120843 2.622416
C -6.249701 -1.856933 2.027145
O -6.019627 -1.279510 0.735323
C 5.902031 -0.643125 -0.117083
C 6.360300 -1.081857 -1.520735
C 6.292483 -1.752583 0.890225
C 6.646686 0.664863 0.249311
H 0.233220 3.536043 -2.992642
H 1.303788 2.251224 -1.125756
H -3.469245 1.505664 -2.276296
H -2.215823 -1.678328 2.953882
H -4.558545 0.192267 -1.095602
H 1.531427 -0.466370 -1.925522
H 3.931940 -0.868524 -2.111311
H 4.412601 0.144692 2.049138

H 2.007506 0.553382 2.229706
H -6.796222 -2.795144 1.912231
H -6.804492 -1.146548 2.652859
H 6.142032 -0.320931 -2.278553
H 7.443792 -1.243019 -1.517336
H 5.887466 -2.020940 -1.829759
H 6.032725 -1.481868 1.918774
H 7.374284 -1.927716 0.853863
H 5.786708 -2.694944 0.651225
H 7.730367 0.502471 0.209889
H 6.397187 1.468153 -0.453270
H 6.397185 1.008902 1.258319

24 Energy:-1306.87107662
C -1.642995 2.479910 -2.771040
C -0.342490 2.860153 -2.442134
C 0.238994 2.233937 -1.341613
C -0.445710 1.235832 -0.620591
C -1.820581 0.914704 -0.919470
C -2.380497 1.549451 -2.041610
N 0.210833 0.519645 0.379550
C -0.591108 -0.029393 1.529733
C -1.941761 -0.339143 1.221330
C -2.539612 0.011316 -0.052849
C -2.714868 -1.019908 2.221610
C -3.988331 -1.382267 1.899487
C -4.551921 -1.100620 0.630712
C -3.866821 -0.414232 -0.337107
C 1.577272 0.235004 0.272555
O -0.011005 -0.182529 2.609681
F -2.234943 3.057885 -3.832842
C 2.112860 -0.135974 -0.987718
C 3.456456 -0.444885 -1.127024
C 4.343980 -0.398802 -0.034703
C 3.797683 -0.024315 1.213350
C 2.458351 0.285938 1.379952
O -4.897951 -2.093480 2.645597
C -6.122987 -2.064556 1.901506
O -5.814048 -1.642914 0.566774
C 5.836405 -0.728060 -0.154015
C 6.239494 -1.117388 -1.588681
C 6.176201 -1.911497 0.786066
C 6.667152 0.511488 0.264416
H 0.174498 3.620509 -3.014774
H 1.241913 2.507762 -1.033713
H -3.397511 1.349368 -2.356342
H -2.266918 -1.259780 3.178586
H -4.338155 -0.205226 -1.290843

H 1.448165 -0.223942 -1.840226
H 3.810019 -0.748230 -2.105523
H 4.445699 0.047876 2.081491
H 2.078691 0.592797 2.342944
H -6.553553 -3.067442 1.873698
H -6.814284 -1.346982 2.362004
H 6.051253 -0.305749 -2.300507
H 7.311349 -1.340937 -1.618559
H 5.706325 -2.009976 -1.934836
H 5.951662 -1.681366 1.832578
H 7.244691 -2.147566 0.717461
H 5.610587 -2.807950 0.508128
H 7.737279 0.284691 0.190762
H 6.454211 1.365194 -0.388852
H 6.460549 0.814735 1.295870

25 Energy:-1306.84864298
C -1.874193 2.576088 -2.851443
C -0.622663 3.117842 -2.573459
C 0.078712 2.595741 -1.486139
C -0.470339 1.555985 -0.727420
C -1.775622 1.034542 -0.991966
C -2.462181 1.566697 -2.089151
N 0.233995 0.889517 0.286278
C -0.576490 0.654965 1.566285
C -1.787493 -0.030811 1.264233
C -2.326332 0.027979 -0.076151
C -2.519551 -0.679067 2.308601
C -3.657431 -1.349149 1.954644
C -4.127423 -1.381712 0.626433
C -3.501331 -0.697700 -0.388504
C 1.548747 0.524968 0.190672
O -0.187672 1.172505 2.624255
F -2.569206 3.061104 -3.900306
C 2.126550 0.207754 -1.074805
C 3.428382 -0.245625 -1.162464
C 4.232901 -0.436193 -0.016947
C 3.636194 -0.160249 1.234472
C 2.334065 0.285182 1.356371
O -4.475777 -2.124107 2.741984
C -5.595937 -2.471296 1.916362
O -5.241101 -2.187737 0.556881
C 5.680556 -0.931153 -0.087241
C 6.144721 -1.191825 -1.532644
C 5.810860 -2.251820 0.712796
C 6.611602 0.138789 0.538215
H -0.221394 3.915864 -3.187156
H 1.058304 2.985007 -1.227891

H -3.454513 1.225524 -2.361296
H -2.140717 -0.674386 3.324300
H -3.913517 -0.705594 -1.392133
H 1.524457 0.300327 -1.971222
H 3.818215 -0.486070 -2.144403
H 4.212402 -0.299286 2.143865
H 1.909555 0.506179 2.326056
H -5.806752 -3.537401 2.021612
H -6.464083 -1.863561 2.203135
H 6.101956 -0.284557 -2.145687
H 7.184367 -1.536040 -1.524500
H 5.544358 -1.967312 -2.021590
H 5.540785 -2.122679 1.765740
H 6.846991 -2.607852 0.674972
H 5.166923 -3.031463 0.290760
H 7.650976 -0.208154 0.503984
H 6.549391 1.083922 -0.012748
H 6.360277 0.339403 1.584623

26 Energy:-1306.84627099
C -1.910508 2.543304 -2.919704
C -0.698250 3.165525 -2.638504
C 0.019514 2.709751 -1.530608
C -0.478504 1.658542 -0.758572
C -1.744822 1.055460 -1.022128
C -2.447140 1.518677 -2.142584
N 0.247528 1.057307 0.289626
C -0.561580 0.818968 1.564316
C -1.727703 0.055726 1.267596
C -2.251892 0.048789 -0.080349
C -2.438486 -0.600565 2.321461
C -3.535147 -1.339181 1.974553
C -3.985201 -1.434305 0.642689
C -3.382505 -0.748321 -0.384487
C 1.532668 0.625622 0.186549
O -0.208302 1.385565 2.610616
F -2.618434 2.962537 -3.989901
C 2.132507 0.354474 -1.081731
C 3.414429 -0.149762 -1.158499
C 4.180774 -0.434231 -0.003770
C 3.565450 -0.195114 1.246798
C 2.282340 0.300020 1.360040
O -4.321622 -2.134253 2.774660
C -5.411325 -2.562886 1.946782
O -5.054532 -2.299264 0.583812
C 5.607254 -0.986003 -0.065954
C 6.096903 -1.194455 -1.511399
C 5.661675 -2.349092 0.669596

C 6.565510 0.011550 0.634220
H -0.335540 3.970540 -3.266924
H 0.973022 3.159036 -1.271439
H -3.414185 1.113313 -2.417857
H -2.073097 -0.547108 3.340686
H -3.780329 -0.807803 -1.392130
H 1.562385 0.523904 -1.987114
H 3.822596 -0.353909 -2.141087
H 4.112906 -0.403206 2.160517
H 1.847195 0.499671 2.329675
H -5.567476 -3.635247 2.080225
H -6.313789 -1.993992 2.206083
H 6.108512 -0.256828 -2.078374
H 7.120516 -1.583312 -1.495800
H 5.477358 -1.918056 -2.053003
H 5.371679 -2.260931 1.721449
H 6.682690 -2.746533 0.636649
H 4.996295 -3.078356 0.194228
H 7.589610 -0.378463 0.607179
H 6.557418 0.983893 0.129184
H 6.296159 0.172089 1.682992

27 Energy:-1306.84428315
C -1.927331 2.503089 -2.987009
C -0.768073 3.214886 -2.694784
C -0.043806 2.832381 -1.562678
C -0.485856 1.767221 -0.780360
C -1.701855 1.074970 -1.049852
C -2.408797 1.462054 -2.198477
N 0.260787 1.238746 0.301730
C -0.552341 0.984038 1.566605
C -1.665295 0.144828 1.270460
C -2.166398 0.070818 -0.085245
C -2.355536 -0.522705 2.331541
C -3.402459 -1.331637 1.989837
C -3.824370 -1.489254 0.654473
C -3.244551 -0.799644 -0.382486
C 1.514307 0.737738 0.191055
O -0.234829 1.578688 2.609416
F -2.638018 2.849114 -4.082803
C 2.132632 0.501010 -1.076946
C 3.391086 -0.056730 -1.147632
C 4.118957 -0.425534 0.010157
C 3.491270 -0.206210 1.258971
C 2.231548 0.343028 1.367524
O -4.155379 -2.148884 2.800441
C -5.205440 -2.660987 1.969134
O -4.841842 -2.415733 0.604658

C 5.518063 -1.042111 -0.048663
C 6.029744 -1.209283 -1.491882
C 5.488579 -2.438073 0.624438
C 6.507094 -0.126011 0.717175
H -0.446782 4.028329 -3.334793
H 0.873531 3.348285 -1.296544
H -3.340236 0.985705 -2.482749
H -2.009880 -0.420793 3.353954
H -3.621056 -0.911163 -1.393860
H 1.594443 0.740293 -1.985522
H 3.814888 -0.232997 -2.128837
H 4.011643 -0.472307 2.173166
H 1.790341 0.531660 2.336585
H -5.303553 -3.736346 2.130961
H -6.142629 -2.137108 2.198652
H 6.100519 -0.248917 -2.014711
H 7.032323 -1.649193 -1.472754
H 5.388216 -1.876137 -2.078755
H 5.177389 -2.383024 1.672427
H 6.490175 -2.882244 0.595912
H 4.801417 -3.112014 0.100998
H 7.511780 -0.563198 0.688625
H 6.554927 0.868926 0.260855
H 6.225174 -0.004485 1.767855

28 Energy:-1306.84277725
C -1.930675 2.450226 -3.046374
C -0.824196 3.238684 -2.744608
C -0.100373 2.920423 -1.592169
C -0.491768 1.844203 -0.800835
C -1.660087 1.078041 -1.074022
C -2.364006 1.398315 -2.247300
N 0.272324 1.380978 0.307609
C -0.546992 1.112503 1.564234
C -1.615881 0.217591 1.271871
C -2.094199 0.084139 -0.088401
C -2.291460 -0.452271 2.342084
C -3.296609 -1.315090 2.009689
C -3.692895 -1.527186 0.673390
C -3.129126 -0.842251 -0.374382
C 1.496715 0.819079 0.193075
O -0.250249 1.717535 2.607246
F -2.637511 2.731737 -4.164205
C 2.145076 0.634941 -1.069870
C 3.384204 0.037361 -1.136939
C 4.067232 -0.418240 0.018591
C 3.417534 -0.235704 1.262878
C 2.177652 0.354656 1.368493

O -4.024364 -2.143406 2.832650
C -5.041601 -2.719504 2.002700
O -4.668501 -2.498831 0.636853
C 5.443450 -1.082954 -0.038254
C 5.986318 -1.197371 -1.475229
C 5.343403 -2.508717 0.562208
C 6.444852 -0.244517 0.797556
H -0.539557 4.058217 -3.394118
H 0.780694 3.493339 -1.319988
H -3.260511 0.862415 -2.537831
H -1.964389 -0.307412 3.365413
H -3.485577 -0.998633 -1.387037
H 1.644449 0.946790 -1.977413
H 3.832100 -0.097022 -2.113868
H 3.906592 -0.562012 2.174612
H 1.724232 0.519026 2.336170
H -5.100161 -3.792860 2.194145
H -6.001737 -2.226633 2.204824
H 6.108200 -0.215591 -1.946279
H 6.970332 -1.677132 -1.453645
H 5.335730 -1.808074 -2.111143
H 5.008176 -2.493984 1.604064
H 6.327960 -2.989282 0.534232
H 4.644880 -3.128275 -0.010956
H 7.432862 -0.718003 0.770377
H 6.541170 0.769519 0.394105
H 6.140811 -0.165676 1.846060

29 Energy:-1306.8413697
C -1.932555 2.393916 -3.098172
C -0.872044 3.243013 -2.793429
C -0.149546 2.978543 -1.626696
C -0.497110 1.896278 -0.824621
C -1.625507 1.072885 -1.095440
C -2.325309 1.337212 -2.287059
N 0.282022 1.488619 0.302838
C -0.544202 1.216647 1.554195
C -1.579324 0.281138 1.271869
C -2.037815 0.094057 -0.089570
C -2.242858 -0.384896 2.353163
C -3.213601 -1.290099 2.034141
C -3.588716 -1.550889 0.699644
C -3.037693 -0.875684 -0.360163
C 1.480229 0.873826 0.188599
O -0.256193 1.828931 2.595364
F -2.635199 2.621497 -4.231834
C 2.172741 0.760629 -1.060043
C 3.396849 0.134123 -1.124012

C 4.025637 -0.415235 0.022126
C 3.340991 -0.287757 1.255285
C 2.116998 0.333282 1.357875
O -3.921034 -2.122120 2.871583
C -4.910832 -2.751736 2.047649
O -4.530089 -2.556699 0.680257
C 5.384551 -1.113638 -0.031441
C 5.966906 -1.167134 -1.456446
C 5.229324 -2.565792 0.488908
C 6.380945 -0.347367 0.876826
H -0.619045 4.065415 -3.452325
H 0.699387 3.597500 -1.353121
H -3.192185 0.754751 -2.578001
H -1.931305 -0.202134 3.375244
H -3.376891 -1.071616 -1.371830
H 1.716633 1.150624 -1.960477
H 3.879581 0.056879 -2.090318
H 3.792043 -0.680048 2.160426
H 1.641837 0.457167 2.320855
H -4.938371 -3.820818 2.267827
H -5.887958 -2.283800 2.226657
H 6.132659 -0.165849 -1.869387
H 6.935024 -1.677977 -1.432874
H 5.317804 -1.721944 -2.143071
H 4.863894 -2.597413 1.520114
H 6.201767 -3.070350 0.463211
H 4.532840 -3.135062 -0.136457
H 7.356584 -0.845830 0.852899
H 6.515624 0.683379 0.530834
H 6.047038 -0.315336 1.918664

30 Energy:-1306.84013661
C -1.939135 2.322812 -3.150452
C -0.916787 3.220459 -2.852303
C -0.194707 3.005760 -1.675311
C -0.504462 1.924949 -0.856488
C -1.600885 1.056377 -1.116470
C -2.297767 1.269218 -2.321727
N 0.289564 1.569763 0.284986
C -0.540821 1.301411 1.534349
C -1.551723 0.336122 1.270233
C -1.996749 0.098189 -0.088097
C -2.203091 -0.318584 2.366837
C -3.148069 -1.256578 2.068540
C -3.509998 -1.563259 0.739459
C -2.970669 -0.904503 -0.335845
C 1.467051 0.913157 0.174531
O -0.251715 1.920556 2.570912

F -2.639140 2.500410 -4.295395
C 2.216242 0.885114 -1.046455
C 3.431229 0.241494 -1.105641
C 3.998626 -0.404757 0.021978
C 3.267468 -0.345674 1.234161
C 2.054609 0.296106 1.332272
O -3.838509 -2.083903 2.925123
C -4.809973 -2.757335 2.114481
O -4.425766 -2.592953 0.744191
C 5.341629 -1.132663 -0.027044
C 5.985236 -1.094481 -1.425875
C 5.126202 -2.615016 0.373497
C 6.315403 -0.466040 0.979137
H -0.690849 4.040310 -3.524068
H 0.626705 3.663035 -1.406923
H -3.140595 0.649380 -2.606084
H -1.901162 -0.099944 3.384706
H -3.298705 -1.137668 -1.343267
H 1.809415 1.355157 -1.932032
H 3.958562 0.233549 -2.051380
H 3.674835 -0.807221 2.127041
H 1.549128 0.367548 2.284839
H -4.816191 -3.820112 2.364698
H -5.797848 -2.305477 2.275242
H 6.194910 -0.069870 -1.752499
H 6.937915 -1.633389 -1.400468
H 5.353567 -1.576457 -2.180328
H 4.714088 -2.713493 1.382632
H 6.085965 -3.143286 0.350996
H 4.444592 -3.115548 -0.322955
H 7.278618 -0.988015 0.955989
H 6.489932 0.584161 0.720684
H 5.938352 -0.505726 2.005856

31 Energy:-1306.83890187
C -1.945503 2.249043 -3.195393
C -0.950461 3.180879 -2.908382
C -0.228864 3.006494 -1.724568
C -0.511593 1.932487 -0.887489
C -1.586743 1.033386 -1.132863
C -2.280665 1.203879 -2.347918
N 0.296319 1.619010 0.262353
C -0.535401 1.359640 1.512248
C -1.535724 0.379187 1.269772
C -1.974313 0.099074 -0.082834
C -2.178675 -0.257802 2.382578
C -3.110173 -1.215418 2.107588
C -3.466831 -1.560441 0.785843

C -2.934939 -0.922951 -0.305281
C 1.455228 0.924853 0.153253
O -0.234934 1.982763 2.542823
F -2.643230 2.385534 -4.347943
C 2.268449 0.994500 -1.024626
C 3.479975 0.344361 -1.079052
C 3.983583 -0.401517 0.016422
C 3.195928 -0.428809 1.194716
C 1.988410 0.222921 1.288398
O -3.790772 -2.030478 2.984053
C -4.754463 -2.733638 2.189871
O -4.369306 -2.601502 0.816427
C 5.319964 -1.141064 -0.027385
C 6.028119 -1.004943 -1.388382
C 5.070987 -2.646573 0.247957
C 6.251898 -0.565760 1.070721
H -0.743560 3.994680 -3.593476
H 0.572265 3.691536 -1.464390
H -3.106743 0.557748 -2.622866
H -1.880465 -0.009295 3.394633
H -3.258059 -1.186844 -1.306640
H 1.912369 1.547299 -1.883927
H 4.057924 0.416413 -1.991816
H 3.556457 -0.964605 2.065934
H 1.442613 0.224326 2.220949
H -4.751379 -3.789545 2.467597
H -5.746815 -2.286923 2.337162
H 6.266530 0.038193 -1.623852
H 6.971382 -1.560043 -1.361895
H 5.425855 -1.416220 -2.206105
H 4.610231 -2.816042 1.226112
H 6.025612 -3.184087 0.229997
H 4.418734 -3.083418 -0.516122
H 7.210631 -1.095939 1.050271
H 6.446952 0.499041 0.902697
H 5.827719 -0.680302 2.073093

32 Energy:-1306.83766887
C -1.956377 2.166719 -3.239632
C -0.981858 3.125536 -2.970480
C -0.259201 2.990174 -1.782286
C -0.520359 1.928778 -0.922528
C -1.580395 1.006091 -1.147558
C -2.273023 1.135417 -2.369567
N 0.302136 1.653354 0.232055
C -0.527399 1.408629 1.485094
C -1.524472 0.419578 1.269839
C -1.961796 0.099052 -0.074248

C -2.159179 -0.194126 2.400948
C -3.083417 -1.165665 2.153585
C -3.440133 -1.548029 0.841646
C -2.915208 -0.936253 -0.267060
C 1.445975 0.927046 0.122997
O -0.213510 2.041765 2.505086
F -2.653419 2.263356 -4.397093
C 2.327737 1.099352 -0.993281
C 3.539391 0.448578 -1.040275
C 3.976414 -0.398237 0.008254
C 3.124438 -0.522191 1.135509
C 1.919166 0.134347 1.222843
O -3.756174 -1.962946 3.052453
C -4.716478 -2.693086 2.278986
O -4.334961 -2.594298 0.901739
C 5.309430 -1.143632 -0.028547
C 6.092931 -0.891704 -1.330495
C 5.037205 -2.665368 0.093919
C 6.181284 -0.679403 1.167173
H -0.790432 3.929173 -3.671847
H 0.525719 3.698425 -1.535220
H -3.086571 0.467957 -2.630723
H -1.860292 0.083182 3.405296
H -3.237758 -1.229887 -1.260233
H 2.023515 1.735815 -1.813929
H 4.171489 0.605415 -1.905165
H 3.433259 -1.137659 1.973278
H 1.323436 0.052372 2.120573
H -4.705577 -3.741353 2.584115
H -5.711668 -2.249593 2.416573
H 6.350292 0.165872 -1.455947
H 7.029938 -1.457214 -1.303328
H 5.534522 -1.220134 -2.214140
H 4.519817 -2.918411 1.024529
H 5.988643 -3.208585 0.081380
H 4.428134 -3.024235 -0.742925
H 7.137218 -1.214681 1.150738
H 6.390041 0.394330 1.107893
H 5.702049 -0.880534 2.130270

33 Energy:-1306.83647347
C -1.975951 2.079210 -3.280924
C -1.012409 3.056030 -3.037232
C -0.285461 2.956741 -1.848119
C -0.531957 1.914055 -0.961598
C -1.584942 0.976214 -1.159681
C -2.279706 1.067152 -2.384785
N 0.306766 1.670119 0.192507

C -0.514911 1.446058 1.452366
C -1.515999 0.455220 1.270743
C -1.960500 0.098712 -0.061909
C -2.140967 -0.130532 2.422363
C -3.065610 -1.108901 2.206828
C -3.430721 -1.525283 0.907124
C -2.914051 -0.942725 -0.220776
C 1.439992 0.917743 0.079285
O -0.187670 2.099191 2.454953
F -2.675838 2.138952 -4.439489
C 2.391718 1.197558 -0.953716
C 3.607544 0.552313 -0.989398
C 3.977486 -0.396071 -0.005729
C 3.054552 -0.628300 1.047064
C 1.847442 0.026072 1.125175
O -3.731369 -1.883890 3.130196
C -4.696209 -2.634075 2.382239
O -4.324082 -2.570101 1.000300
C 5.311263 -1.140341 -0.029742
C 6.179477 -0.759254 -1.243467
C 5.033386 -2.665217 -0.083285
C 6.100385 -0.807391 1.263243
H -0.832096 3.845086 -3.757796
H 0.490405 3.681118 -1.619870
H -3.086336 0.384526 -2.627604
H -1.834727 0.172787 3.416960
H -3.242771 -1.263401 -1.203458
H 2.139131 1.918774 -1.720419
H 4.295465 0.798582 -1.788357
H 3.308934 -1.328549 1.834948
H 1.192071 -0.151268 1.966144
H -4.682352 -3.674251 2.713796
H -5.690873 -2.187989 2.515072
H 6.442805 0.304261 -1.240898
H 7.113510 -1.329494 -1.212919
H 5.681681 -0.991234 -2.191516
H 4.458840 -3.010560 0.781890
H 5.984564 -3.208916 -0.091892
H 4.479079 -2.932695 -0.989521
H 7.055527 -1.344242 1.255286
H 6.312042 0.265346 1.329589
H 5.557965 -1.104054 2.166295

34 Energy:-1306.83558386
C -2.001010 1.978541 -3.321786
C -1.042216 2.967593 -3.110861
C -0.309685 2.906126 -1.922578
C -0.546717 1.889789 -1.003560

C -1.597733 0.941972 -1.168719
C -2.295986 0.992394 -2.394664
N 0.309394 1.675784 0.146431
C -0.498787 1.472940 1.415823
C -1.509135 0.486376 1.273463
C -1.967152 0.096395 -0.045137
C -2.124314 -0.065634 2.447056
C -3.055585 -1.044712 2.267127
C -3.434712 -1.494134 0.982206
C -2.926352 -0.945194 -0.166184
C 1.441712 0.909514 0.027992
O -0.158031 2.153987 2.394891
F -2.705135 1.999380 -4.479220
C 2.462623 1.299850 -0.894714
C 3.683458 0.660445 -0.916200
C 3.985171 -0.392494 -0.022472
C 2.988589 -0.739516 0.927889
C 1.778129 -0.089374 0.994752
O -3.716115 -1.791546 3.217033
C -4.690581 -2.557768 2.498628
O -4.332038 -2.531110 1.111644
C 5.321016 -1.133436 -0.031771
C 6.277325 -0.614884 -1.121962
C 5.055553 -2.640084 -0.286474
C 6.007207 -0.958960 1.348020
H -0.869245 3.736499 -3.854596
H 0.461791 3.642365 -1.719375
H -3.098680 0.297650 -2.615046
H -1.806020 0.262186 3.430051
H -3.266282 -1.291715 -1.136148
H 2.263323 2.108902 -1.586254
H 4.427126 0.997770 -1.627048
H 3.186463 -1.529167 1.644373
H 1.060156 -0.362852 1.755813
H -4.676545 -3.589013 2.856983
H -5.682545 -2.105190 2.629265
H 6.532741 0.440301 -0.974430
H 7.209944 -1.187205 -1.086787
H 5.855146 -0.732640 -2.126103
H 4.415524 -3.081996 0.483530
H 6.006867 -3.183616 -0.283399
H 4.576317 -2.796048 -1.259114
H 6.962878 -1.494878 1.349614
H 6.207676 0.097548 1.556595
H 5.398995 -1.358052 2.165687

35 Energy:-1306.83592743
C -2.034438 1.863269 -3.361921

C -1.059483 2.845208 -3.197233
C -0.320497 2.819014 -2.012059
C -0.567103 1.846489 -1.048485
C -1.632854 0.906097 -1.170999
C -2.336213 0.918025 -2.394752
N 0.305597 1.657645 0.090908
C -0.478275 1.469551 1.374814
C -1.509072 0.501508 1.278827
C -1.998233 0.092907 -0.022326
C -2.111016 -0.013161 2.475984
C -3.063761 -0.978017 2.334652
C -3.474372 -1.447809 1.066743
C -2.977589 -0.933423 -0.102948
C 1.458215 0.903441 -0.028231
O -0.112999 2.180591 2.323812
F -2.745410 1.847235 -4.514348
C 2.544671 1.413655 -0.798089
C 3.771892 0.780478 -0.805125
C 4.006988 -0.382142 -0.040290
C 2.938300 -0.851714 0.768213
C 1.720824 -0.210579 0.821853
O -3.720063 -1.691488 3.312147
C -4.719320 -2.457853 2.628556
O -4.387341 -2.464687 1.234499
C 5.346471 -1.118206 -0.035896
C 6.383109 -0.463960 -0.968180
C 5.117974 -2.578876 -0.503808
C 5.916782 -1.124536 1.406105
H -0.880196 3.581359 -3.971908
H 0.463269 3.550760 -1.844421
H -3.145819 0.222949 -2.586408
H -1.767466 0.328393 3.445721
H -3.342275 -1.295670 -1.057971
H 2.396823 2.314215 -1.381856
H 4.569173 1.211537 -1.397503
H 3.081192 -1.734001 1.382701
H 0.941518 -0.581631 1.474768
H -4.713017 -3.481720 3.007662
H -5.701862 -1.988109 2.768603
H 6.617722 0.562092 -0.663794
H 7.314408 -1.038556 -0.933488
H 6.043424 -0.447577 -2.009741
H 4.422548 -3.116643 0.148207
H 6.071275 -3.119021 -0.494107
H 4.719900 -2.607450 -1.524018
H 6.874031 -1.657723 1.417719
H 6.089805 -0.104063 1.764866
H 5.247285 -1.624715 2.112809

36 Energy:-1306.8857163
C -2.002447 1.131594 -3.364123
C -0.629450 0.876717 -3.511281
C 0.072032 0.430605 -2.389836
C -0.576736 0.248564 -1.151575
C -2.021020 0.458642 -1.023742
C -2.696950 0.941685 -2.186980
N 0.150663 -0.113609 -0.030374
C -0.460907 -0.499930 1.210976
C -1.889593 -0.350734 1.316361
C -2.670472 0.169536 0.198044
C -2.500497 -0.693163 2.542215
C -3.859235 -0.516636 2.649204
C -4.634658 -0.001810 1.575033
C -4.092338 0.340974 0.375216
C 1.588731 -0.189335 -0.090766
O 0.282009 -0.916078 2.107897
F -2.679161 1.579526 -4.442154
C 2.344669 0.978217 -0.000815
C 3.738674 0.909438 -0.038550
C 4.409601 -0.316524 -0.167315
C 3.619919 -1.477336 -0.254956
C 2.228894 -1.424588 -0.215713
O -4.671512 -0.770035 3.715911
C -6.002097 -0.409683 3.316362
O -5.943164 0.070593 1.968106
C 5.944118 -0.427199 -0.212949
C 6.633964 0.945649 -0.101349
C 6.371774 -1.075580 -1.551601
C 6.430422 -1.309564 0.961799
H -0.144434 1.025994 -4.468620
H 1.132284 0.229571 -2.466789
H -3.756790 1.158399 -2.173211
H -1.900307 -1.074282 3.359979
H -4.721492 0.726234 -0.416866
H 1.845237 1.936508 0.106791
H 4.297860 1.834349 0.041270
H 4.094634 -2.448924 -0.354293
H 1.639785 -2.333826 -0.280799
H -6.644144 -1.294620 3.362171
H -6.372507 0.384191 3.972050
H 6.395506 1.447139 0.843455
H 7.720823 0.813170 -0.139793
H 6.353032 1.612363 -0.924585
H 5.948592 -2.078143 -1.673582
H 7.463700 -1.166696 -1.595199
H 6.047572 -0.466819 -2.403566

H 7.522881 -1.401943 0.937471
H 6.147651 -0.870168 1.925231
H 6.009404 -2.319346 0.916107

37 Energy:-1306.88677465
C -2.017488 0.910657 -3.419460
C -0.618644 0.835701 -3.511000
C 0.095029 0.515659 -2.352835
C -0.569241 0.276285 -1.133740
C -2.029326 0.358170 -1.046486
C -2.722784 0.687841 -2.256072
N 0.155976 -0.041194 0.003721
C -0.442729 -0.297271 1.276311
C -1.881080 -0.214199 1.361797
C -2.678637 0.117919 0.183696
C -2.482369 -0.463263 2.611129
C -3.854216 -0.382291 2.686235
C -4.648413 -0.060111 1.552219
C -4.114696 0.187965 0.325926
C 1.596487 -0.132448 -0.054780
O 0.308545 -0.573048 2.219719
F -2.706438 1.219241 -4.539059
C 2.376625 0.994344 0.188246
C 3.769877 0.898870 0.134810
C 4.411591 -0.311896 -0.163106
C 3.595489 -1.431460 -0.408092
C 2.205823 -1.350556 -0.358939
O -4.662069 -0.579394 3.766750
C -6.008107 -0.356368 3.321520
O -5.964799 -0.054960 1.922083
C 5.943468 -0.451472 -0.225850
C 6.665170 0.879114 0.059660
C 6.358387 -0.932823 -1.636907
C 6.406505 -1.488169 0.825759
H -0.121436 1.022388 -4.455530
H 1.173929 0.450261 -2.391679
H -3.801171 0.767863 -2.282563
H -1.868967 -0.708151 3.470150
H -4.758096 0.429730 -0.509952
H 1.899586 1.940895 0.424092
H 4.350607 1.792050 0.333815
H 4.046981 -2.391277 -0.640406
H 1.594380 -2.227691 -0.548396
H -6.595647 -1.264963 3.482482
H -6.431472 0.493101 3.866617
H 6.438459 1.260107 1.061857
H 7.748647 0.727497 0.001309
H 6.399832 1.652607 -0.670062

H 5.913668 -1.902054 -1.885834
H 7.448077 -1.041763 -1.693385
H 6.048952 -0.213114 -2.403617
H 7.496412 -1.603319 0.788203
H 6.132961 -1.168710 1.837883
H 5.960888 -2.473213 0.652029

12.3.6 Computed CT emission energies of compound 5b (B3LYP/6-31G* PCM CH_2Cl_2)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.9690 eV 629.67 nm f=0.0554 <S**2>=0.000

102 ->103 0.70488

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -1306.76929579

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.0485 eV 406.71 nm f=0.0681 <S**2>=0.000

99 ->103 0.15282

101 ->103 0.66918

102 ->104 0.10914

Excited State 3: Singlet-A 3.2743 eV 378.65 nm f=0.0078 <S**2>=0.000

102 ->104 0.69383

Excited State 4: Singlet-A 3.5890 eV 345.46 nm f=0.0464 <S**2>=0.000

96 ->103 0.17227

97 ->103 0.11841

99 ->103 0.36932

100 ->103 0.51428

101 ->103 -0.16394

Excited State 5: Singlet-A 3.7203 eV 333.26 nm f=0.0136 <S**2>=0.000

99 ->103 0.51184

100 ->103 -0.45644

Excited State 6: Singlet-A 3.9564 eV 313.38 nm f=0.0036 <S**2>=0.000

98 ->103 0.56397

101 ->104 0.41023

12.3.7 Computed excitations energies of the triplet state of compound 5b (B3LYP/6-31G* PCM CH_2Cl_2)

Excitation energies and oscillator strengths:
Excited State 1: Triplet-A 2.8748 eV 431.28 nm f=0.0000 <S**2>=2.000
99 ->104 0.14994
101 ->103 0.14427
102 ->103 0.63410
102 ->107 -0.10706
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1306.78835260
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A 3.3121 eV 374.34 nm f=0.0000 <S**2>=2.000
99 ->103 0.17312
101 ->103 -0.38329
101 ->107 -0.15397
102 ->103 0.19149
102 ->104 0.46768
102 ->107 0.10703

Excited State 3: Triplet-A 3.4561 eV 358.74 nm f=0.0000 <S**2>=2.000
101 ->103 0.49241
101 ->104 0.12155
102 ->103 -0.12390
102 ->104 0.45442

Excited State 4: Triplet-A 3.7144 eV 333.80 nm f=0.0000 <S**2>=2.000
97 ->105 -0.10771
98 ->105 -0.15338
98 ->106 -0.39864
100 ->105 0.51303
100 ->106 -0.13252

Excited State 5: Triplet-A 3.8256 eV 324.09 nm f=0.0000 <S**2>=2.000
96 ->103 -0.15342
96 ->104 0.16597
99 ->103 -0.30579
101 ->103 -0.19342
101 ->104 0.18551
101 ->107 0.33230
102 ->104 0.15549
102 ->107 -0.23261

102 ->108 -0.19488

Excited State 6: Triplet-A 3.8597 eV 321.23 nm f=0.0000 <S**2>=2.000
99 ->104 0.36368
99 ->108 -0.10846
101 ->103 -0.10787
101 ->104 0.51543
102 ->103 -0.11992

Excited State 7: Triplet-A 4.1843 eV 296.31 nm f=0.0000 <S**2>=2.000
96 ->103 -0.10625
96 ->104 -0.12403
99 ->103 -0.35586
99 ->104 0.40757
101 ->103 -0.10857
101 ->104 -0.23176
101 ->108 -0.11184
102 ->104 0.10196
102 ->107 0.20461

Excited State 8: Triplet-A 4.2759 eV 289.96 nm f=0.0000 <S**2>=2.000
96 ->104 0.15830
99 ->103 -0.33192
99 ->104 -0.17798
101 ->104 0.22615
101 ->107 -0.26201
102 ->107 0.37937
102 ->108 -0.11604

Excited State 9: Triplet-A 4.3307 eV 286.29 nm f=0.0000 <S**2>=2.000
97 ->103 0.43844
97 ->104 0.36966
97 ->109 -0.11466
100 ->103 0.31606
100 ->104 0.19079

Excited State 10: Triplet-A 4.5351 eV 273.39 nm f=0.0000 <S**2>=2.000
96 ->103 0.42727
98 ->103 0.14611
99 ->103 -0.29425
99 ->107 0.11494
99 ->108 -0.13978
102 ->107 -0.28532
102 ->108 0.20094

Excited State 11: Triplet-A 4.6124 eV 268.81 nm f=0.0000 <S**2>=2.000
97 ->103 -0.13972
97 ->106 -0.10555

98 ->105 -0.28153
98 ->106 0.10865
100 ->103 0.33411
100 ->104 -0.11777
100 ->105 0.11394
100 ->106 0.46984

Excited State 12: Triplet-A 4.6536 eV 266.43 nm f=0.0000 <S**2>=2.000
98 ->103 0.19209
98 ->105 0.19791
98 ->106 0.44766
100 ->105 0.40988
100 ->106 -0.12368

Excited State 13: Triplet-A 4.7495 eV 261.05 nm f=0.0000 <S**2>=2.000
101 ->105 -0.23359
102 ->105 0.64363
102 ->106 -0.10105

Excited State 14: Triplet-A 4.8493 eV 255.68 nm f=0.0000 <S**2>=2.000
97 ->103 -0.19459
97 ->104 -0.16307
98 ->105 0.29582
98 ->106 -0.13847
100 ->103 0.50671
100 ->105 -0.10485
100 ->106 -0.19787

Excited State 15: Triplet-A 4.8793 eV 254.10 nm f=0.0000 <S**2>=2.000
96 ->104 0.10898
96 ->107 0.12555
99 ->104 0.13359
99 ->107 0.13218
101 ->104 -0.17000
101 ->107 -0.33492
102 ->106 0.36368
102 ->107 -0.30732
102 ->108 -0.17983

12.3.8 Computed emission energies of the triplet state of compound 5b (B3LYP/6-31G* PCM CH_2Cl_2)

Excited State 1: Triplet-A 2.2453 eV 552.19 nm f=0.0000 <S**2>=2.000
102 ->103 0.67851
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1306.79944341
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A 3.1369 eV 395.25 nm f=0.0000 <S**2>=2.000
99 ->103 -0.14501
101 ->103 0.53884
102 ->103 -0.10843
102 ->104 -0.38781

Excited State 3: Triplet-A 3.2755 eV 378.53 nm f=0.0000 <S**2>=2.000
101 ->103 0.41372
102 ->104 0.55414

Excited State 4: Triplet-A 3.6742 eV 337.44 nm f=0.0000 <S**2>=2.000
96 ->103 0.19101
96 ->104 -0.10044
99 ->103 0.50782
101 ->103 0.10958
101 ->104 -0.14693
101 ->107 -0.21653
102 ->104 -0.14118
102 ->108 0.20421

Excited State 5: Triplet-A 3.7112 eV 334.08 nm f=0.0000 <S**2>=2.000
97 ->105 -0.12091
98 ->105 -0.15199
98 ->106 -0.39617
100 ->105 0.50849
100 ->106 -0.12577

Excited State 6: Triplet-A 3.9561 eV 313.40 nm f=0.0000 <S**2>=2.000
96 ->104 -0.10561
99 ->104 0.35312
101 ->104 0.50464
102 ->107 -0.18594

Excited State 7: Triplet-A 4.1064 eV 301.93 nm f=0.0000 <S**2>=2.000
96 ->103 0.14601
96 ->104 -0.13968
99 ->103 -0.33004
99 ->104 0.25573
101 ->104 -0.11355
101 ->107 -0.26294
102 ->107 0.35586
102 ->108 0.18730

Excited State 8: Triplet-A 4.1730 eV 297.11 nm f=0.0000 <S**2>=2.000
97 ->103 0.41574
97 ->104 0.28149
100 ->103 0.44921
100 ->104 0.15627

Excited State 9: Triplet-A 4.2918 eV 288.89 nm f=0.0000 <S**2>=2.000

95 ->103	0.11790
96 ->103	-0.28724
99 ->103	0.16372
101 ->104	0.21431
101 ->107	-0.18058
102 ->106	0.16165
102 ->107	0.42267
102 ->108	-0.22493

Excited State 10: Triplet-A 4.3502 eV 285.01 nm f=0.0000 <S**2>=2.000

96 ->103	-0.34793
96 ->104	-0.20643
98 ->103	-0.15128
99 ->103	0.15503
99 ->104	0.35354
99 ->107	-0.10530
101 ->104	-0.23937
101 ->107	0.17509

Excited State 11: Triplet-A 4.4603 eV 277.97 nm f=0.0000 <S**2>=2.000

97 ->103	-0.37023
97 ->104	-0.19032
100 ->103	0.49685
100 ->106	0.21062

Excited State 12: Triplet-A 4.5743 eV 271.04 nm f=0.0000 <S**2>=2.000

101 ->105	-0.14913
102 ->105	0.67556
102 ->106	-0.10096

Excited State 13: Triplet-A 4.6115 eV 268.86 nm f=0.0000 <S**2>=2.000

98 ->103	0.39968
98 ->105	0.18197
98 ->106	0.34516
100 ->105	0.34901
100 ->106	-0.15038

Excited State 14: Triplet-A 4.7107 eV 263.20 nm f=0.0000 <S**2>=2.000

97 ->103	0.11550
97 ->106	-0.12282
98 ->105	-0.35524
98 ->106	0.15577
100 ->103	-0.19658
100 ->105	0.16448
100 ->106	0.44717
102 ->106	0.12167

Excited State 15: Triplet-A 4.7159 eV 262.91 nm f=0.0000 <S**2>=2.000

99 ->104	0.12670
99 ->107	0.13844
100 ->106	-0.11784
101 ->104	-0.17620
101 ->107	-0.29970
102 ->106	0.38691
102 ->107	-0.32130
102 ->108	-0.12976

13 References

1 L. Liang, J. Li, B. Shen, Y. Zhang, J. Liu, J. Chen, D. Liu, *The effect of carbonyl on the isomerization of a galanthan ring system and total synthesis of (±)-β-lycorane*, *Org. Biomol. Chem.* **2021**, *19*, 2767-2772, DOI: 10.1039/D0OB02398A.

2 M. Yang, Z. Xing, B. Fang, X. Xie, X. She, *Visible light photoredox catalyzed deprotection of 1,3-oxathiolanes*, *Org. Biomol. Chem.* **2020**, *18*, 288-291, DOI: 10.1039/c9ob02517k.

3 C. A. Moore, B. F. Ohman, M. J. Garman, M. E. Liquori, D. M. Degan, K. B. Voellinger, M. J. DePersis, E. T. Pelkey, *Investigating the stereochemical outcome of a tandem cyclization-coupling reaction leading to a 3-arylmethylideneisobenzofuran-1-one*, *Arkivoc* **2018**, 50-69, DOI: 10.24820/ark.5550190.p010.480.

4 U. V. Mentzel, D. Tanner, J. E. Tønder, *Comparative study of the Kumada, Negishi, Stille, and Suzuki-Miyaura reactions in the synthesis of the indole alkaloids hippadine and pratosine*, *J. Org. Chem.* **2006**, *71*, 5807-5810, DOI: 10.1021/jo060729b.

5 S. K. Bera, P. Mal, *Mechanochemical-Cascaded C–N Cross-Coupling and Halogenation Using N-Bromo- and N-Chlorosuccinimide as Bifunctional Reagents*, *J. Org. Chem.* **2021**, *86*, 14144-14159, DOI: 10.1021/acs.joc.1c01742.

6 J. V. Suárez-Meneses, A. Oukhrib, M. Gouygou, M. Urrutigoïty, J.-C. Daran, A. Cordero-Vargas, M. C. Ortega-Alfaro, J. G. López-Cortés, *[N,P]-pyrrole $PdCl_2$ complexes catalyzed the formation of dibenzo-α-pyrone and lactam analogues*, *Dalton Trans.* **2016**, *45*, 9621-9630, DOI: 10.1039/C6DT01022A.

7 D. Nageswar Rao, S. Rasheed, P. Das, *Palladium/Silver synergistic catalysis in direct aerobic carbonylation of C(sp^2)−H bonds using DMF as a carbon source: Synthesis of pyrido-fused quinazolinones and phenanthridinones*, *Org. Lett.* **2016**, *18*, 3142-3145, DOI: 10.1021/acs.orglett.6b01292.

8 Y. Yang, H. Huang, L. Wu, *Palladium-catalyzed annulation of benzynes with N-substituted-N-(2-halophenyl)formamides: synthesis of phenanthridinones*, *Org. Biomol. Chem.* **2014**, *12*, 5351-5355, DOI: 10.1039/C4OB00997E.

9 Y. Kuwata, M. Sonoda, S. Tanimori, *Facile Synthesis of Phenanthridinone Alkaloids via Suzuki–Miyaura Cross-coupling*, *J. Heterocycl. Chem.* **2017**, *54*, 1645-1651, DOI: 10.1002/jhet.2725.

10 J. Mooney, P. Kambhampati, *Get the basics right: Jacobian conversion of wavelength and energy scales for quantitative analysis of emission spectra*, *J. Phys. Chem. Lett.* **2013**, *4*, 3316-3318, DOI: 10.1021/jz401508t.

11 J. S. Swenton, T. J. Ikeler, G. L. Smyser, *Effect of biphenyl geometry and substituents on the multiplicity and efficiency of the photocyclization reactions of 2-substituted biphenyls*, *J. Org. Chem* **1973**, *38*, 1157-1166, DOI: 10.1021/jo00946a021.