# Supplementary materials

## Indane based molecular motors. UV-switching increases number of isomers.

Valeriy P. Shendrikov 1,2, Anna S. Alekseeva 1, Erik F. Kot 1, Konstantin S. Mineev 1, Daria S. Tretiakova 1, Abdulilah Ece 3 and Ivan A. Boldyrev 1,*

1 Shemyakin-Ovchinnikov Institute of Bioorganic, Chemistry of the Russian Academy of Sciences, GSP-7, Ulitsa Miklukho-Maklaya, 16/10, 117997 Moscow, Russia
2 Higher Chemical College, Mendeleev University of Chemical Technology of Russia, Miusskaya sq. 9, 125047 Moscow, Russia
3 Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Biruni University, Istanbul 34010, Turkey
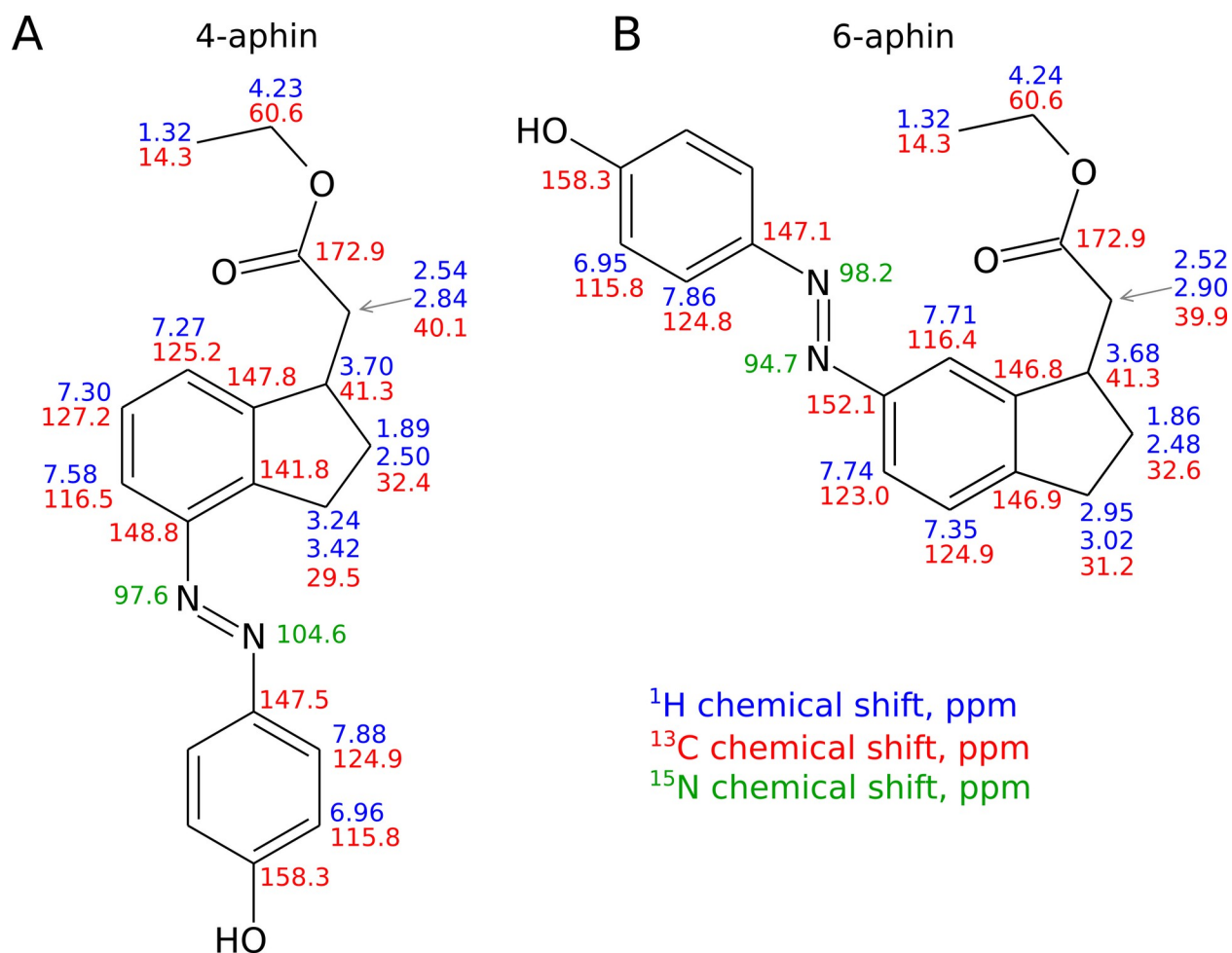* Correspondence: ivan@lipids.ibch.ru; Tel.: +7-495-330-66-10

# Section S1.
# NMR of target and intermediate compounds

Chemical shifts of 4-aphin, 6-aphin

**A**  4-aphin
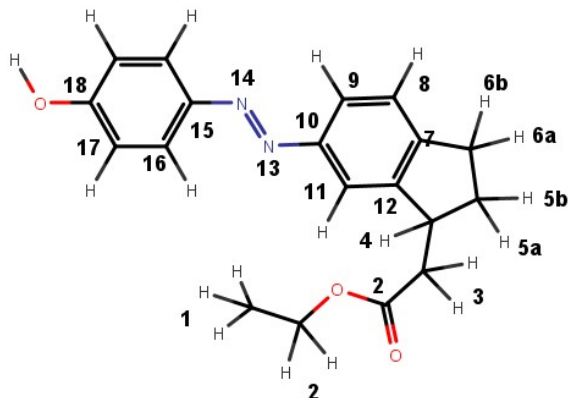


**B**  6-aphin



¹H chemical shift, ppm
¹³C chemical shift, ppm
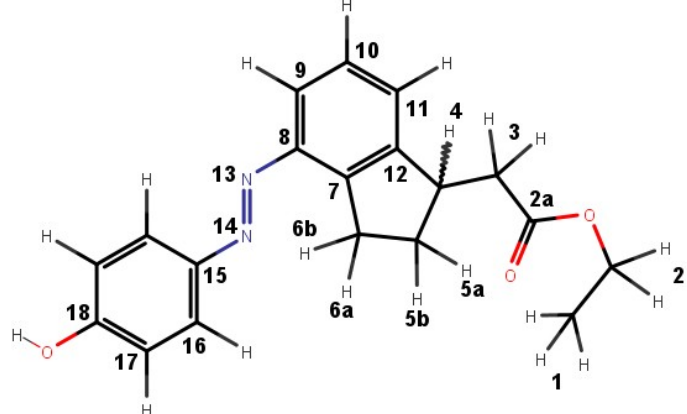¹⁵N chemical shift, ppm

# Chemical shifts of 4-aphin, 6-aphin

## 6-aphin
ethyl 2-{6-[(1E)-2-(4-hydroxyphenyl)diazen-1-yl]-2,3-dihydro-1H-inden-1-yl}acetate

## 4-aphin
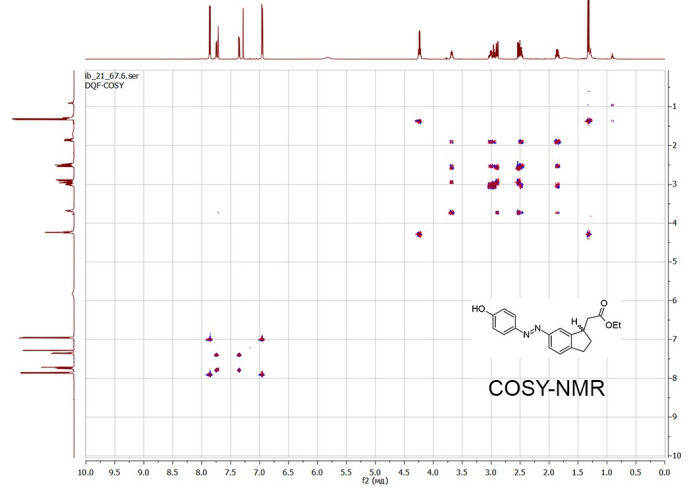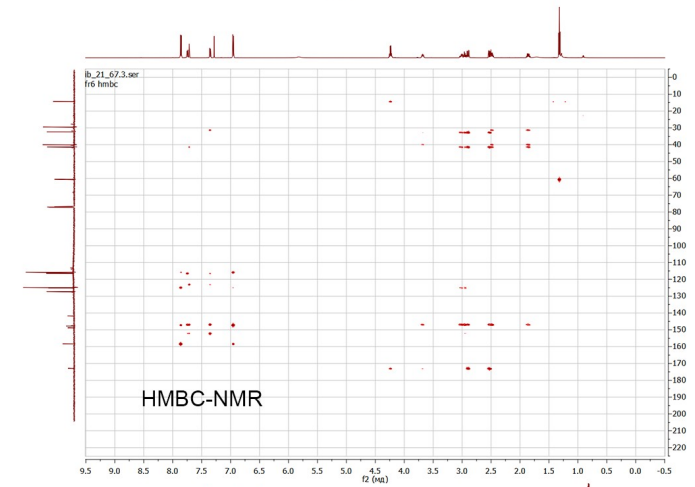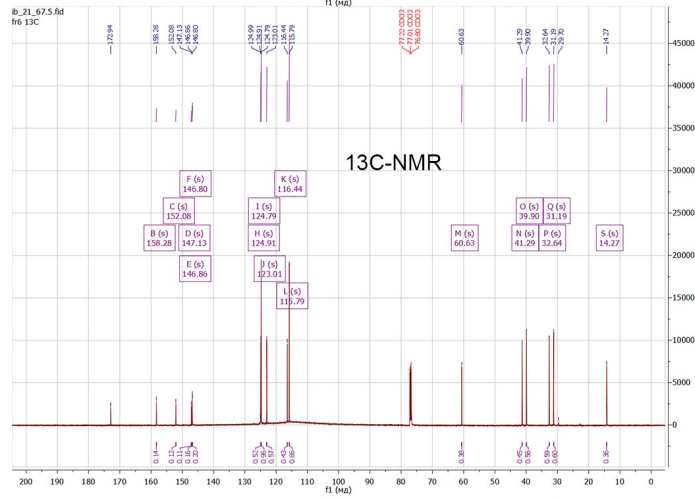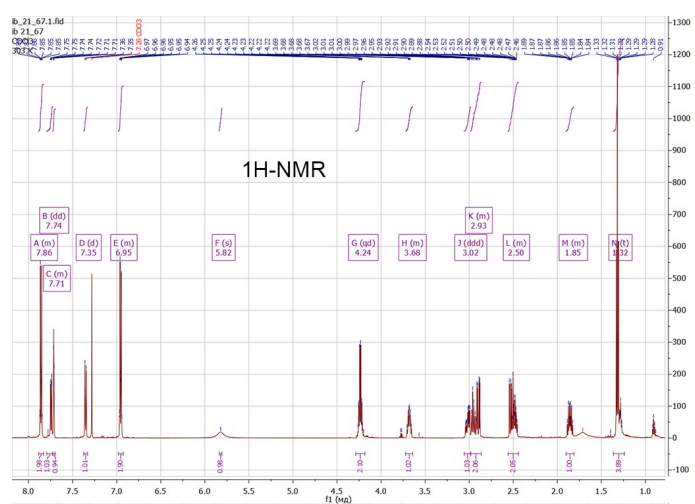ethyl 2-{4-[(1E)-2-(4-hydroxyphenyl)diazen-1-yl]-2,3-dihydro-1H-inden-1-yl}acetate



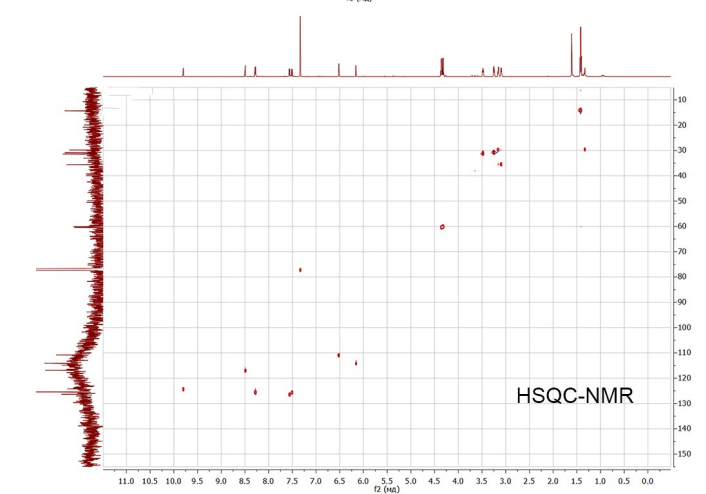| Atom # | $^1$H | $^{13}$C | $^{15}$N | $^1$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|---|---|
| 1 | 1.32 t | 14.3 | - | 1.32 | 14.3 | - |
| 2 | 4.24 m | 60.6 | - | 4.23 | 60.6 | - |
| 2a | - | 172.9 | - | - | 172.9 | - |
| 3 | a: 2.52 m <br> b: 2.90 m | 39.9 | - | 2.54 <br> 2.84 | 40.1 | - |
| 4 | 3.68 | 41.3 | - | 3.70 | 41.3 | - |
| 5 | a: 1.86 <br> b: 2.48 | 32.6 | - | 1.89 <br> 2.50 | 32.4 | - |
| 6 | a: 2.95 <br> b: 3.02 | 31.2 | - | 3.24 <br> 3.42 | 29.5 | - |
| 7 | - | 146.9 | - | - | 141.8 | - |
| 8 | 7.35 | 124.9 | - | - | 148.8 | - |
| 9 | 7.74 | 123.0 | - | 7.58 | 116.5 | - |
| 10 | - | 152.1 | - | 7.30 | 127.2 | - |
| 11 | 7.71 | 116.4 | - | 7.27 | 125.2 | - |
| 12 | - | 146.8 | - | - | 147.8 | - |
| 13 | - | - | 94.7 | - | - | 97.6 |
| 14 | - | - | 98.2 | - | - | 104.6 |
| 15 | - | 147.1 | - | - | 147.5 | - |
| 16 | 7.86 | 124.8 | - | 7.88 | 124.9 | - |
| 17 | 6.95 | 115.8 | - | 6.96 | 115.8 | - |
| 18 | - | 158.3 | - | - | 158.3 | - |

1H-NMR

13C-NMR

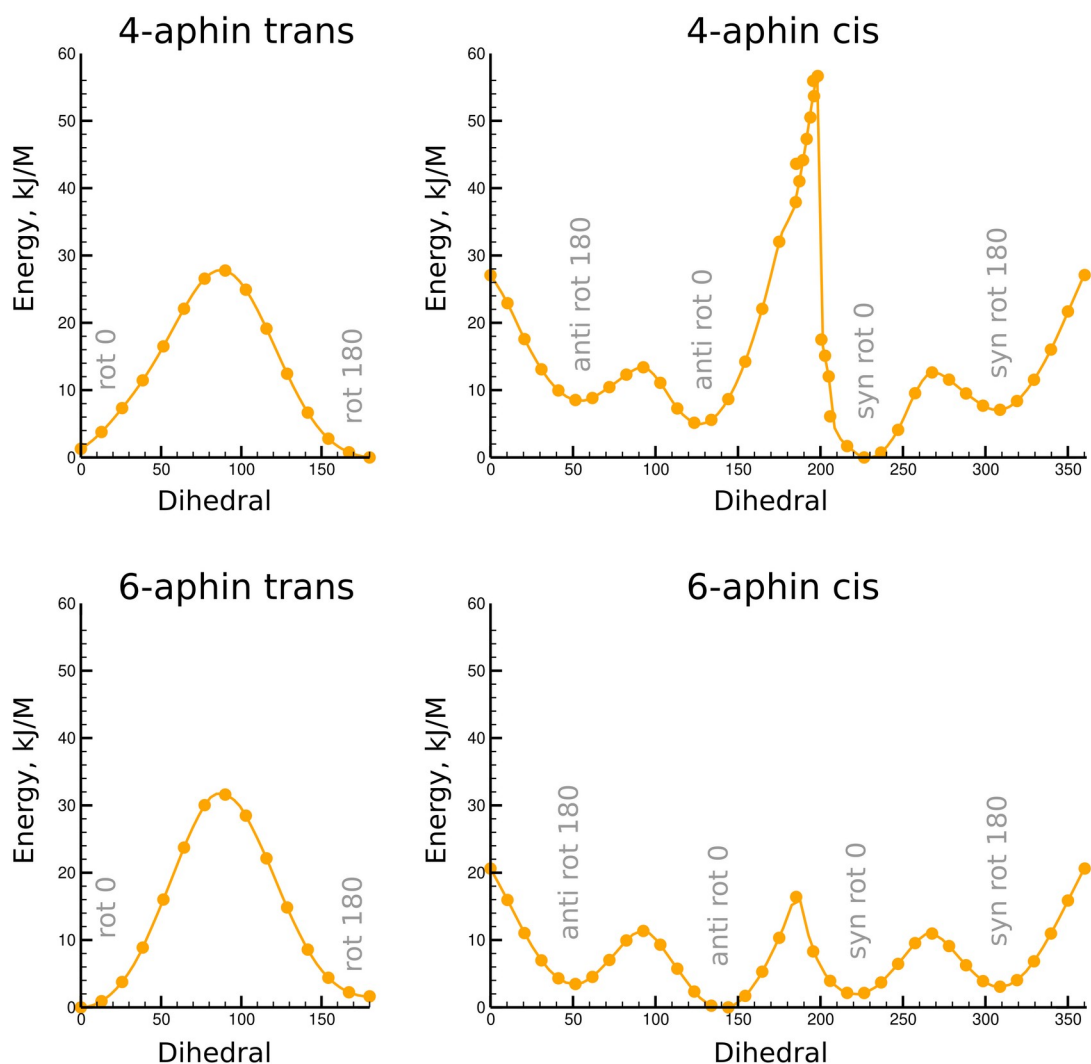HMBC-NMR

COSY-NMR

1H-NMR

13C-NMR

HMBC-NMR

COSY-NMR

4
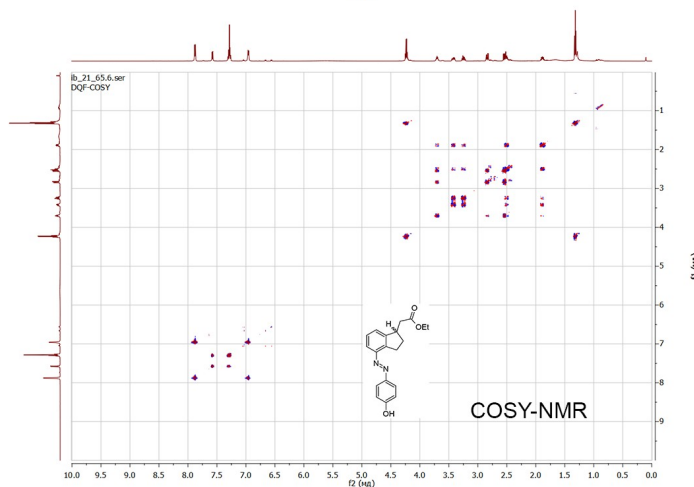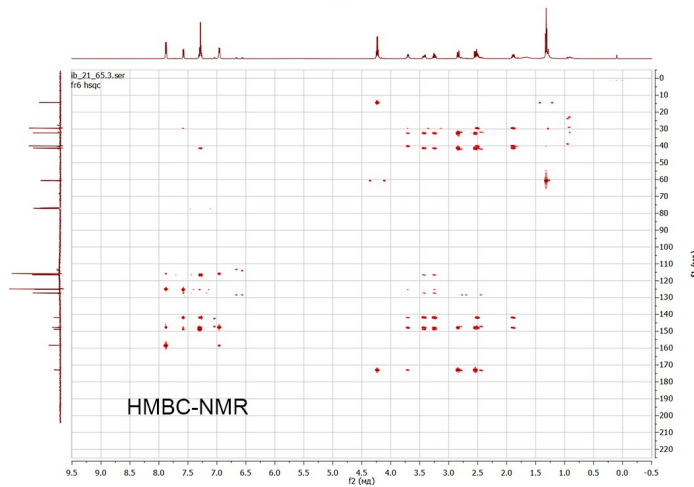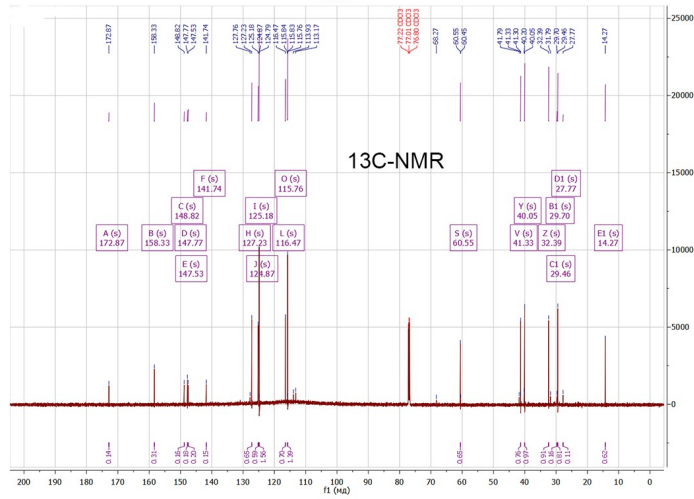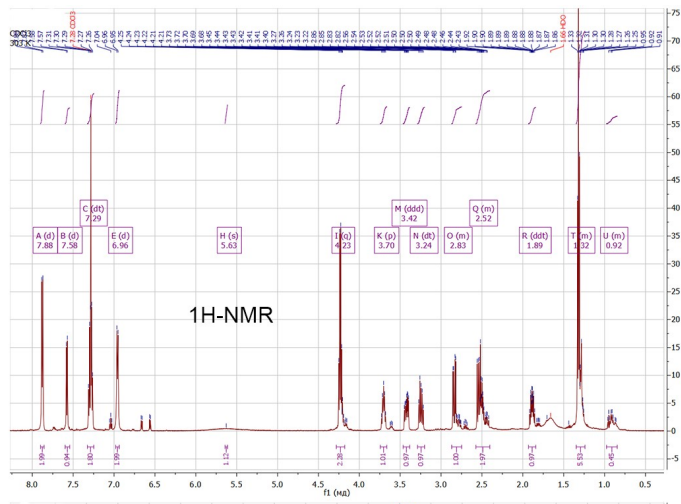
# NMR spectra of intermediate compounds
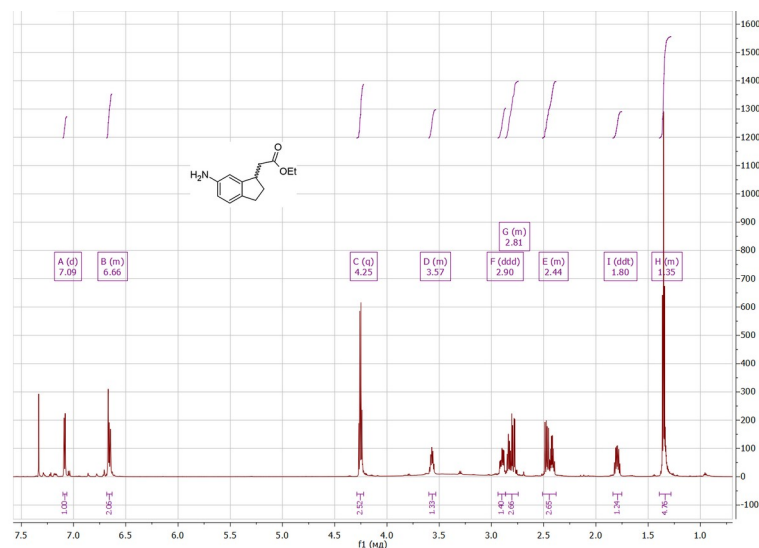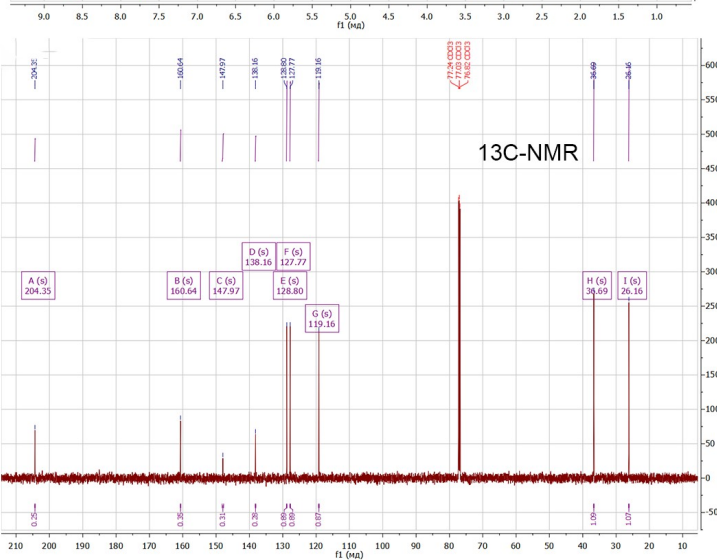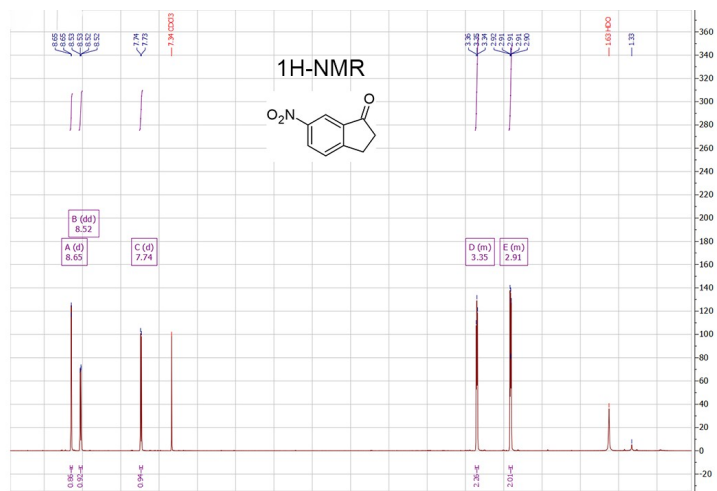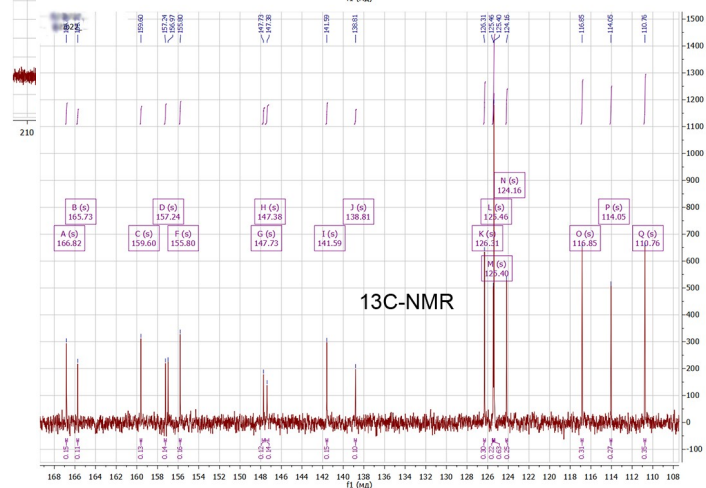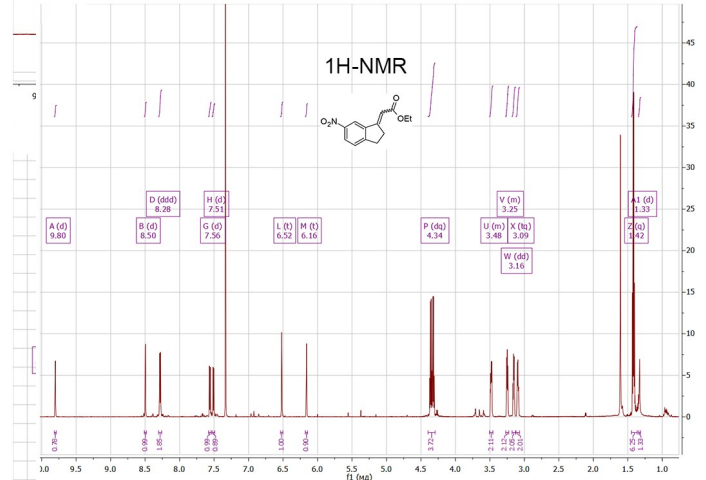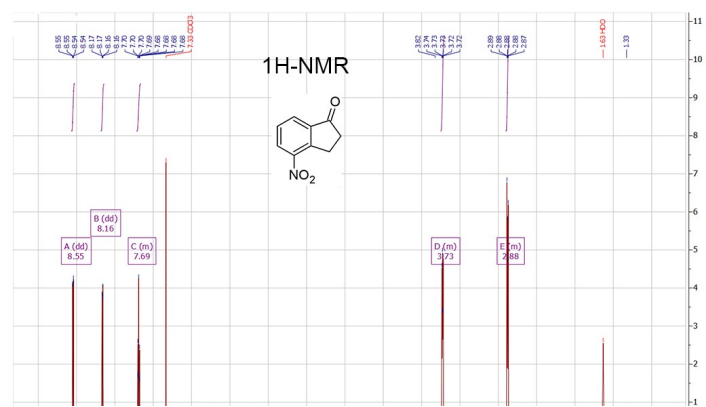
# Section S2. Energy barriers of rotation.

Energy barriers of rotation calculated at BP86 level of theory



4-aphin trans



4-aphin cis



6-aphin trans



6-aphin cis

Extremum points of the above calculated at B3LYP level of theory

**4-aphin**

| Dihedral | 51,47 | 92,65 | 123,53 | 195,59 | 226,47 | 267,65 | 308,82 |
|---|---|---|---|---|---|---|---|
| E, H | -1071,09712 | -1071,08504 | -1071,08758 | -1071,06496 | -1071,08847 | -1071,08538 | -1071,08749 |
| E, kJ/mol | 3,54 | 9,01 | 2,31 | 61,72 | 0 | 8,1 | 2,57 |

**6-aphin**

| Dihedral | 51,47 | 92,65 | 144,12 | 185,29 | 226,47 | 267,65 | 308,82 |
|---|---|---|---|---|---|---|---|
| E, H | -1071,08660 | -1071,08359 | -1071,08694 | -1071,08053 | -1071,08677 | -1071,08336 | -1071,08650 |
| E, kJ/mol | 0,9 | 8,81 | 0 | 16,85 | 0,46 | 9,4 | 1,16 |

# B3LYP vs BP86 at stationary point

## 4-aphin

|  | trans_rot180 | trans_rot0 | cis_anti_rot180 | cis_anti_rot0 | cis_syn_rot180 | cis_syn_rot0 |
|---|---|---|---|---|---|---|
| E, H (B3LYP) | -1071,112446 | -1071,112043 | -1071,095227 | -1071,095513 | -1071,095531 | -1071,096916 |
| E, kJ/mol (B3LYP) | 0,0 | 1,1 | 45,2 | 44,5 | 44,4 | 40,8 |
| E, H (BP86) | -1070,552879 | -1070,552389 | -1070,523108 | -1070,524394 | -1070,523660 | -1070,526357 |
| E, kJ/mol (BP86) | 0,0 | 1,3 | 78,2 | 74,8 | 76,7 | 69,6 |

## 6-aphin

|  | trans_rot180 | trans_rot0 | cis_anti_rot180 | cis_anti_rot0 | cis_syn_rot180 | cis_syn_rot0 |
|---|---|---|---|---|---|---|
| E, H (B3LYP) | -1071,113069 | -1071,113641 | -1071,094469 | -1071,094707 | -1071,094533 | -1071,095148 |
| E, kJ/mol (B3LYP) | 1,5 | 0,0 | 50,3 | 49,7 | 50,2 | 48,6 |
| E, H (BP86) | -1070,552181 | -1070,552803 | -1070,521928 | -1070,522286 | -1070,521776 | -1070,523098 |
| E, kJ/mol (BP86) | 1,6 | 0,0 | 81,1 | 80,1 | 81,5 | 78,0 |

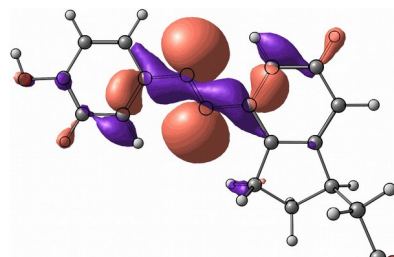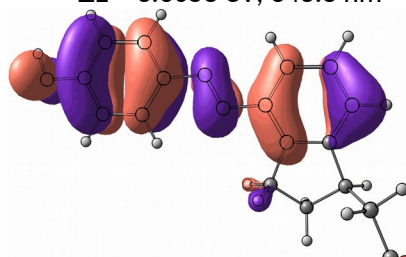# Section S3.
## Frontier molecular orbitals calculated at B3LYP level of theory.
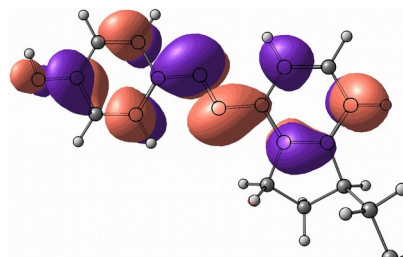
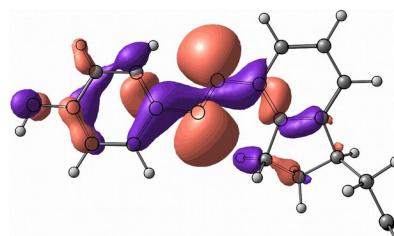### 4-aphin R trans rot 180
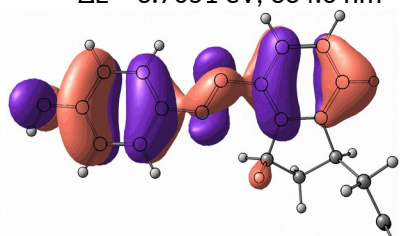ΔE = 3.6058 eV, 343.8 nm

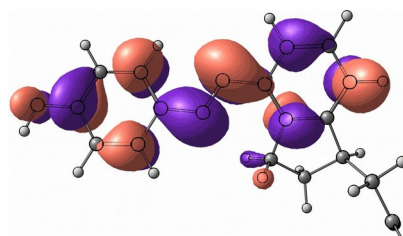HOMO-1                     HOMO                      LUMO

### 4-aphin R trans rot 0
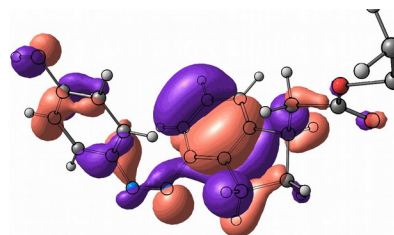ΔE = 3.7051 eV, 334.6 nm
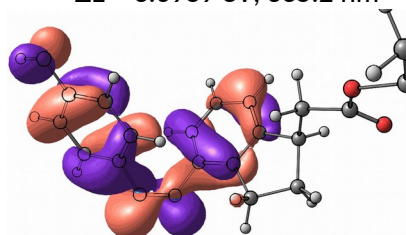
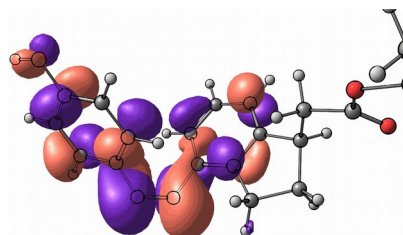HOMO-1                     HOMO                      LUMO

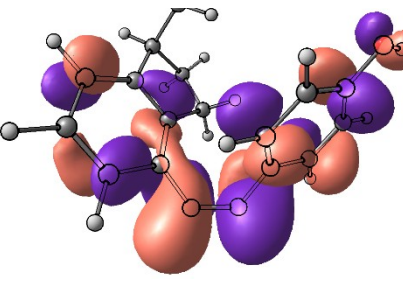### 4-aphin cis syn rot 180
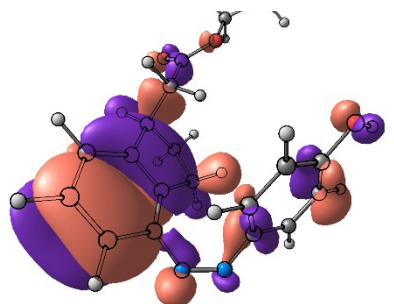ΔE = 3.6989 eV, 335.2 nm

HOMO-1                     HOMO                      LUMO

### 4-aphin cis syn rot 0
ΔE = 3.7187 eV; 333.4 nm
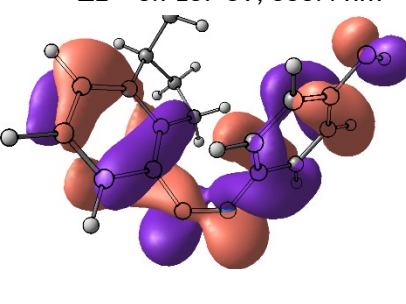
## 4-aphin cis anti rot 180
ΔE = 3.6934 eV; 335.7 nm
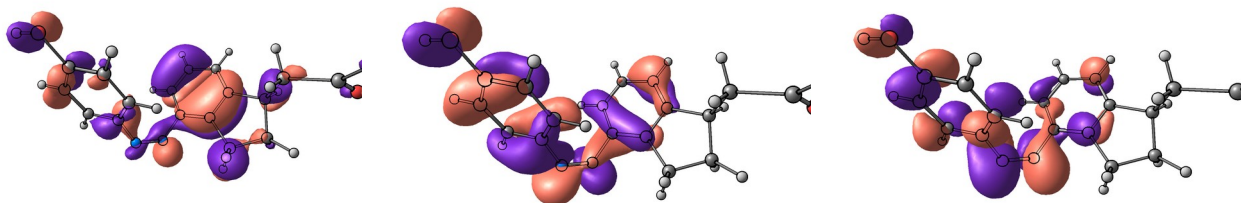
## 4-aphin cis anti rot 0
ΔE = 3.7655 eV; 329.3 nm
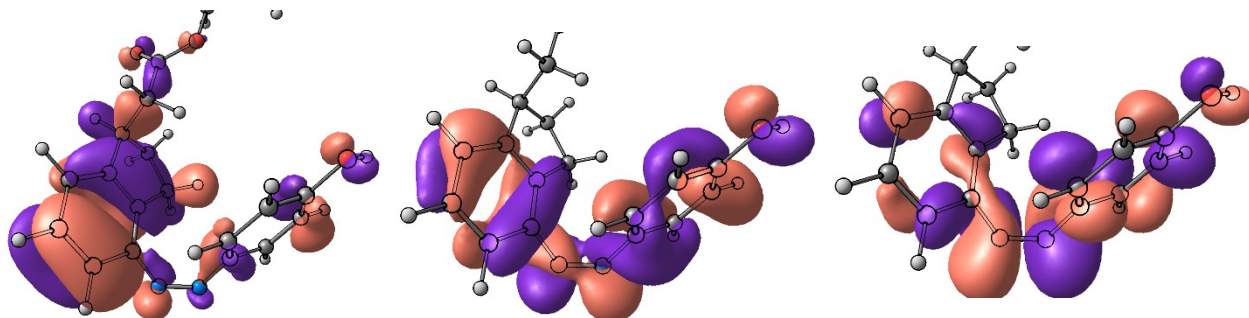
## 6-aphin trans rot 180
ΔE = 3.5987 eV; 344.5 nm
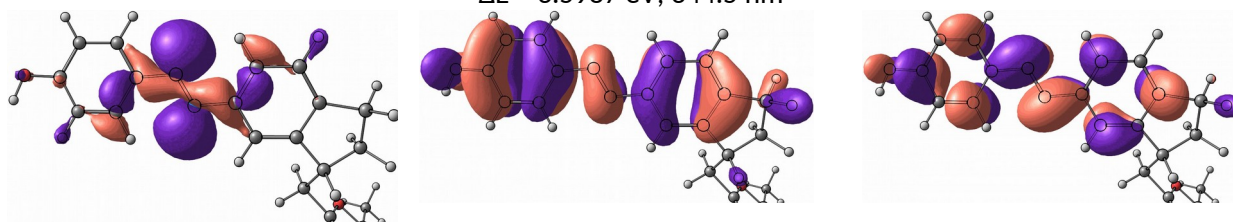
## 6-aphin trans rot 0
ΔE = 3.5903 eV; 345.3 nm
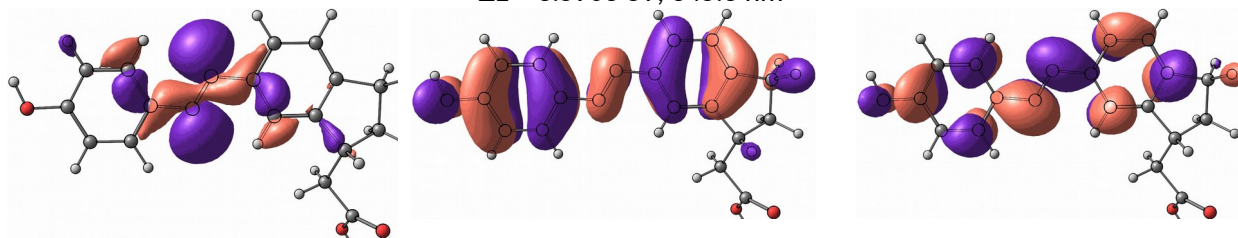
## 6-aphin cis syn rot 180
ΔE = 3.6270 eV; 341.8 nm
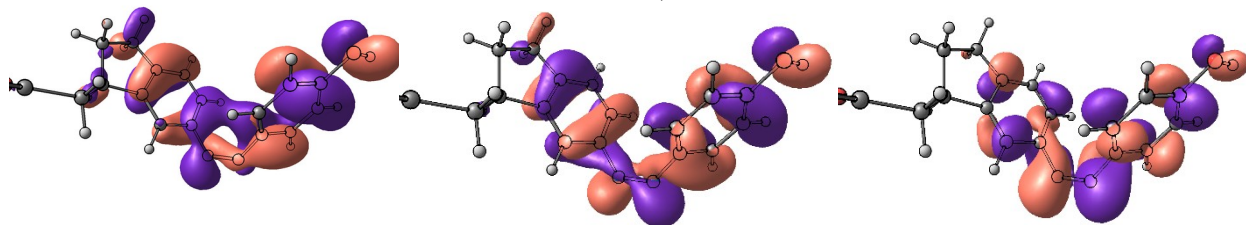
## 6-aphin cis syn rot 0
ΔE = 3.6115 eV; 343.3 nm
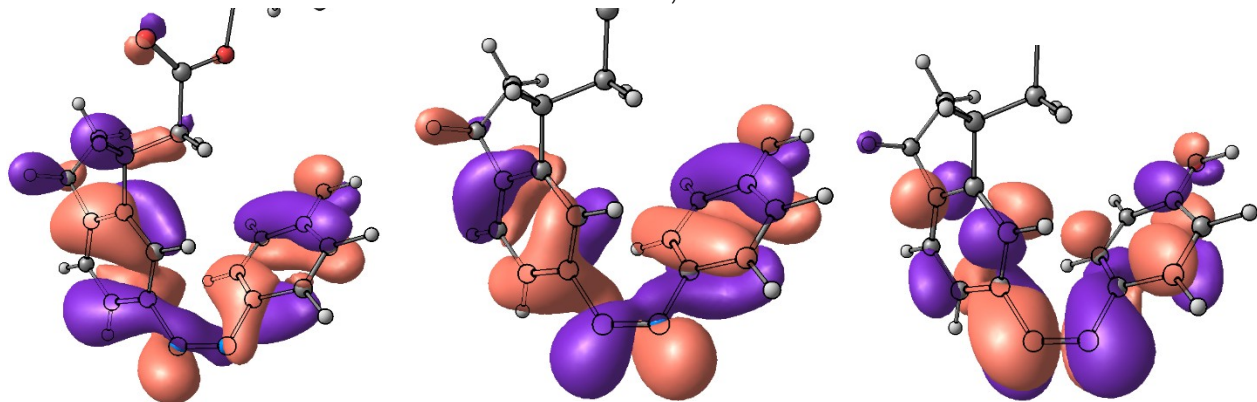
## 6-aphin cis anti rot 180
ΔE = 3.6153 eV; 342.9 nm

## 6-aphin cis anti rot 0
ΔE = 3.6034 eV; 344.1 nm